Full wwPDB EM Validation Report (i)

Nov 23, 2022 – 10:36 AM JST

PDB ID	:	7VD5
EMDB ID	:	EMD-31905
Title	:	Structure of C2S2M2-type PSII-FCPII supercomplex from diatom
Authors	:	Nagao, R.; Kato, K.; Akita, F.; Miyazaki, N.; Shen, J.R.
Deposited on	:	2021-09-06
Resolution	:	2.50 Å(reported)
Based on initial model	:	6J40

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

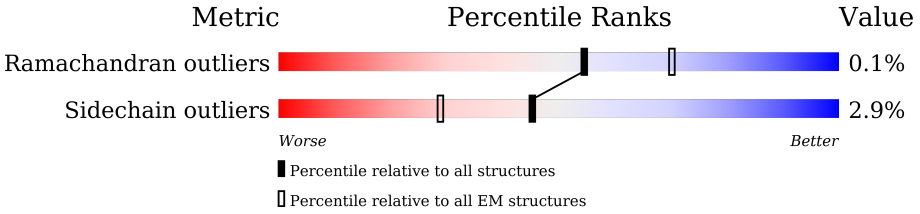
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	99%
1	a	334	99%
2	B	484	99%
2	b	484	99%
3	C	451	99%
3	c	451	99%
4	D	341	100%
4	d	341	100%
5	E	75	99%

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Mol	Chain	Length	Quality of chain
5	e	75	99%
6	F	28	100%
6	f	28	100%
7	H	66	100%
7	h	66	100%
8	I	35	100%
8	i	35	100%
9	J	34	100%
9	j	34	100%
10	K	37	95% 5%
10	k	37	95% 5%
11	L	38	100%
11	l	38	100%
12	M	42	5% 100%
12	m	42	5% 100%
13	O	245	96%
13	o	245	96%
14	T	30	100%
14	t	30	100%
15	U	93	99%
15	u	93	99%
16	V	136	99%
16	v	136	99%
17	Y	34	100%
17	y	34	100%

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Mol	Chain	Length	Quality of chain
18	X	37	5% 97%
18	x	37	5% 97%
19	Z	59	100%
19	z	59	100%
20	Q	151	98%
20	q	151	98%
21	W	52	100%
21	w	52	100%
22	0	31	97%
22	5	31	97%
23	1	30	100%
23	6	30	100%
24	11	176	98%
24	31	176	99%
25	12	169	98%
25	32	169	100%
26	13	169	6% 97%
26	33	169	5% 96%
27	14	172	97%
27	34	172	97%
28	15	170	75% 90% 7%
28	35	170	75% 90% 8%
29	16	179	12% 95%
29	36	179	12% 95%
30	17	176	21% 94% 5%

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Mol	Chain	Length	Quality of chain
30	37	176	21% 95%
31	18	168	78% 94%
31	38	168	80% 92% 5%
32	19	227	8% 96%
32	39	227	8% 96%
33	20	155	41% 89% 8%
33	40	155	47% 89% 8%
34	21	162	94% 85% 10%
34	41	162	94% 85% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CLA	11	303	X	-	-	-
37	CLA	11	305	X	-	-	-
37	CLA	11	308	X	-	-	-
37	CLA	11	310	X	-	-	-
37	CLA	12	203	X	-	-	-
37	CLA	12	204	X	-	-	-
37	CLA	12	205	X	-	-	-
37	CLA	12	207	X	-	-	-
37	CLA	12	209	X	-	-	-
37	CLA	12	212	X	-	-	-
37	CLA	13	303	X	-	-	-
37	CLA	13	305	X	-	-	-
37	CLA	13	307	X	-	-	-
37	CLA	14	302	X	-	-	-
37	CLA	14	305	X	-	-	-
37	CLA	14	307	X	-	-	-
37	CLA	14	308	X	-	-	-
37	CLA	14	310	X	-	-	-
37	CLA	15	305	X	-	-	-
37	CLA	15	307	X	-	-	-
37	CLA	15	308	X	-	-	-
37	CLA	15	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CLA	16	303	X	-	-	-
37	CLA	16	306	X	-	-	-
37	CLA	16	307	X	-	-	-
37	CLA	16	309	X	-	-	-
37	CLA	17	304	X	-	-	-
37	CLA	17	307	X	-	-	-
37	CLA	17	309	X	-	-	-
37	CLA	18	201	X	-	-	-
37	CLA	18	203	X	-	-	-
37	CLA	18	204	X	-	-	-
37	CLA	18	206	X	-	-	-
37	CLA	18	208	X	-	-	-
37	CLA	18	209	X	-	-	-
37	CLA	19	301	X	-	-	-
37	CLA	19	302	X	-	-	-
37	CLA	19	303	X	-	-	-
37	CLA	19	304	X	-	-	-
37	CLA	19	305	X	-	-	-
37	CLA	19	306	X	-	-	-
37	CLA	19	307	X	-	-	-
37	CLA	19	309	X	-	-	-
37	CLA	19	310	X	-	-	-
37	CLA	20	303	X	-	-	-
37	CLA	20	306	X	-	-	-
37	CLA	20	307	X	-	-	-
37	CLA	20	308	X	-	-	-
37	CLA	21	202	X	-	-	-
37	CLA	21	205	X	-	-	-
37	CLA	21	206	X	-	-	-
37	CLA	21	208	X	-	-	-
37	CLA	21	209	X	-	-	-
37	CLA	31	301	X	-	-	-
37	CLA	31	304	X	-	-	-
37	CLA	31	306	X	-	-	-
37	CLA	31	310	X	-	-	-
37	CLA	32	202	X	-	-	-
37	CLA	32	204	X	-	-	-
37	CLA	32	205	X	-	-	-
37	CLA	32	206	X	-	-	-
37	CLA	32	208	X	-	-	-
37	CLA	32	210	X	-	-	-
37	CLA	32	213	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CLA	33	303	X	-	-	-
37	CLA	33	305	X	-	-	-
37	CLA	33	307	X	-	-	-
37	CLA	34	302	X	-	-	-
37	CLA	34	305	X	-	-	-
37	CLA	34	307	X	-	-	-
37	CLA	34	308	X	-	-	-
37	CLA	34	310	X	-	-	-
37	CLA	35	305	X	-	-	-
37	CLA	35	307	X	-	-	-
37	CLA	35	310	X	-	-	-
37	CLA	36	303	X	-	-	-
37	CLA	36	306	X	-	-	-
37	CLA	36	307	X	-	-	-
37	CLA	36	309	X	-	-	-
37	CLA	37	303	X	-	-	-
37	CLA	37	306	X	-	-	-
37	CLA	37	308	X	-	-	-
37	CLA	38	201	X	-	-	-
37	CLA	38	203	X	-	-	-
37	CLA	38	204	X	-	-	-
37	CLA	38	208	X	-	-	-
37	CLA	38	209	X	-	-	-
37	CLA	39	301	X	-	-	-
37	CLA	39	302	X	-	-	-
37	CLA	39	303	X	-	-	-
37	CLA	39	304	X	-	-	-
37	CLA	39	305	X	-	-	-
37	CLA	39	307	X	-	-	-
37	CLA	39	309	X	-	-	-
37	CLA	39	310	X	-	-	-
37	CLA	40	205	X	-	-	-
37	CLA	40	208	X	-	-	-
37	CLA	40	209	X	-	-	-
37	CLA	40	210	X	-	-	-
37	CLA	41	202	X	-	-	-
37	CLA	41	205	X	-	-	-
37	CLA	41	206	X	-	-	-
37	CLA	41	208	X	-	-	-
37	CLA	41	209	X	-	-	-
37	CLA	A	403	X	-	-	-
37	CLA	B	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CLA	B	502	X	-	-	-
37	CLA	B	503	X	-	-	-
37	CLA	B	504	X	-	-	-
37	CLA	B	505	X	-	-	-
37	CLA	B	506	X	-	-	-
37	CLA	B	507	X	-	-	-
37	CLA	B	509	X	-	-	-
37	CLA	B	510	X	-	-	-
37	CLA	B	511	X	-	-	-
37	CLA	B	512	X	-	-	-
37	CLA	B	513	X	-	-	-
37	CLA	B	514	X	-	-	-
37	CLA	B	515	X	-	-	-
37	CLA	B	516	X	-	-	-
37	CLA	B	524	X	-	-	-
37	CLA	C	501	X	-	-	-
37	CLA	C	502	X	-	-	-
37	CLA	C	503	X	-	-	-
37	CLA	C	504	X	-	-	-
37	CLA	C	505	X	-	-	-
37	CLA	C	506	X	-	-	-
37	CLA	C	507	X	-	-	-
37	CLA	C	508	X	-	-	-
37	CLA	C	509	X	-	-	-
37	CLA	C	510	X	-	-	-
37	CLA	C	511	X	-	-	-
37	CLA	C	512	X	-	-	-
37	CLA	C	513	X	-	-	-
37	CLA	D	401	X	-	-	-
37	CLA	D	405	X	-	-	-
37	CLA	D	406	X	-	-	-
37	CLA	W	101	X	-	-	-
37	CLA	W	102	X	-	-	-
37	CLA	Z	101	X	-	-	-
37	CLA	Z	102	X	-	-	-
37	CLA	a	403	X	-	-	-
37	CLA	a	404	X	-	-	-
37	CLA	b	501	X	-	-	-
37	CLA	b	502	X	-	-	-
37	CLA	b	503	X	-	-	-
37	CLA	b	504	X	-	-	-
37	CLA	b	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CLA	b	506	X	-	-	-
37	CLA	b	507	X	-	-	-
37	CLA	b	509	X	-	-	-
37	CLA	b	510	X	-	-	-
37	CLA	b	511	X	-	-	-
37	CLA	b	512	X	-	-	-
37	CLA	b	513	X	-	-	-
37	CLA	b	514	X	-	-	-
37	CLA	b	515	X	-	-	-
37	CLA	b	516	X	-	-	-
37	CLA	b	523	X	-	-	-
37	CLA	c	501	X	-	-	-
37	CLA	c	502	X	-	-	-
37	CLA	c	503	X	-	-	-
37	CLA	c	504	X	-	-	-
37	CLA	c	505	X	-	-	-
37	CLA	c	506	X	-	-	-
37	CLA	c	507	X	-	-	-
37	CLA	c	508	X	-	-	-
37	CLA	c	509	X	-	-	-
37	CLA	c	510	X	-	-	-
37	CLA	c	511	X	-	-	-
37	CLA	c	512	X	-	-	-
37	CLA	c	513	X	-	-	-
37	CLA	d	403	X	-	-	-
37	CLA	d	404	X	-	-	-
37	CLA	w	101	X	-	-	-
37	CLA	z	101	X	-	-	-
37	CLA	z	102	X	-	-	-

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 100884 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	334	2619	1712	429	463	15	0	0
1	a	334	2619	1712	429	463	15	0	0

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	484	3812	2494	645	660	13	0	0
2	b	484	3812	2494	645	660	13	0	0

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	451	3504	2289	589	612	14	0	0
3	c	451	3504	2289	589	612	14	0	0

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	341	2697	1781	441	465	10	0	0
4	d	341	2697	1781	441	465	10	0	0

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	75	616	401	102	113	0	0
5	e	75	616	401	102	113	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	28	228	155	39	33	1	0	0
6	f	28	228	155	39	33	1	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	66	513	340	83	88	2	0	0
7	h	66	513	340	83	88	2	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	35	287	194	45	47	1	0	0
8	i	35	287	194	45	47	1	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	34	254	172	38	43	1	0	0
9	j	34	254	172	38	43	1	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	K	37	302	212	45	45	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	k	37	302	212	45	45	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	38	310	208	48	53	1	0	0
			Total	C	N	O	S		
11	l	38	310	208	48	53	1	0	0

- Molecule 12 is a protein called Photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	M	42	316	207	51	58	0	0
			Total	C	N	O		
12	m	42	316	207	51	58	0	0

- Molecule 13 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	245	1845	1166	306	365	8	0	0
			Total	C	N	O	S		
13	o	245	1845	1166	306	365	8	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	T	30	250	174	36	38	2	0	0
			Total	C	N	O	S		
14	t	30	250	174	36	38	2	0	0

- Molecule 15 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	U	93	713	455	119	137	2	0	0
			Total	C	N	O	S		
15	u	93	713	455	119	137	2	0	0

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	V	136	1037	647	180	206	4	0	0
16	v	136	1037	647	180	206	4	0	0

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Y	34	250	166	41	40	3	0	0
17	y	34	250	166	41	40	3	0	0

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	X	37	263	171	45	46	1	0	0
18	x	37	263	171	45	46	1	0	0

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	59	447	305	68	73	1	0	0
19	z	59	447	305	68	73	1	0	0

- Molecule 20 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Q	151	1180	749	196	234	1	0	0
20	q	151	1180	749	196	234	1	0	0

- Molecule 21 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	W	52	422	273	65	84	0	0
21	w	52	422	273	65	84	0	0

- Molecule 22 is a protein called Unknown protein 0.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	0	31	155	93	31	31	0	0
22	5	31	155	93	31	31	0	0

- Molecule 23 is a protein called Unknown protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	1	30	150	90	30	30	0	0
23	6	30	150	90	30	30	0	0

- Molecule 24 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	11	176	1343	852	228	256	7	0	0
24	31	176	1343	852	228	256	7	0	0

- Molecule 25 is a protein called Fcpb2, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	12	169	1302	828	222	244	8	0	0
25	32	169	1302	828	222	244	8	0	0

- Molecule 26 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	13	169	1296	823	220	246	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	33	169	1296	823	220	246	7	0	0

- Molecule 27 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	14	172	1319	838	223	251	7	0	0
			Total	C	N	O	S		
27	34	172	1319	838	223	251	7	0	0

- Molecule 28 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	15	170	1307	832	221	247	7	0	0
			Total	C	N	O	S		
28	35	170	1307	832	221	247	7	0	0

- Molecule 29 is a protein called Fcpb3, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	16	179	1386	891	233	256	6	0	0
			Total	C	N	O	S		
29	36	179	1386	891	233	256	6	0	0

- Molecule 30 is a protein called Fcpb4, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	17	176	1353	862	227	258	6	0	0
			Total	C	N	O	S		
30	37	176	1353	862	227	258	6	0	0

- Molecule 31 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	18	168	1289	818	219	245	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	38	168	1289	818	219	245	7	0	0

- Molecule 32 is a protein called Fcpb5, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	19	227	1746	1128	291	322	5	0	0
			Total	C	N	O	S		
32	39	227	1746	1128	291	322	5	0	0

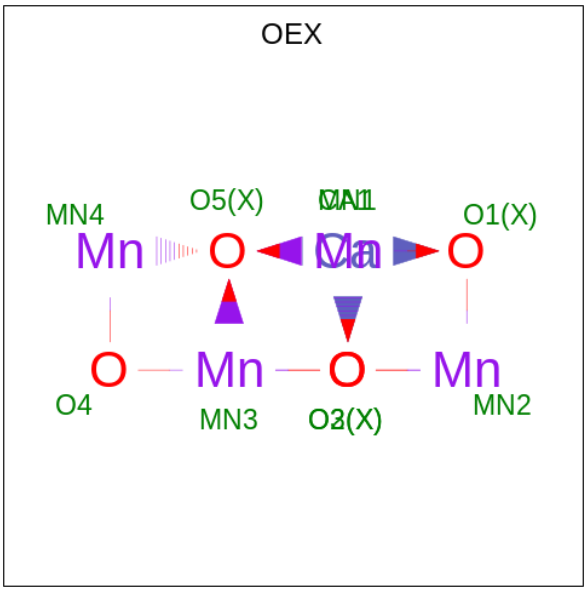
- Molecule 33 is a protein called Fcpb6, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	20	155	1193	769	201	215	8	0	0
			Total	C	N	O	S		
33	40	155	1193	769	201	215	8	0	0

- Molecule 34 is a protein called Fcpb7, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	21	162	1262	822	206	229	5	0	0
			Total	C	N	O	S		
34	41	162	1262	822	206	229	5	0	0

- Molecule 35 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).

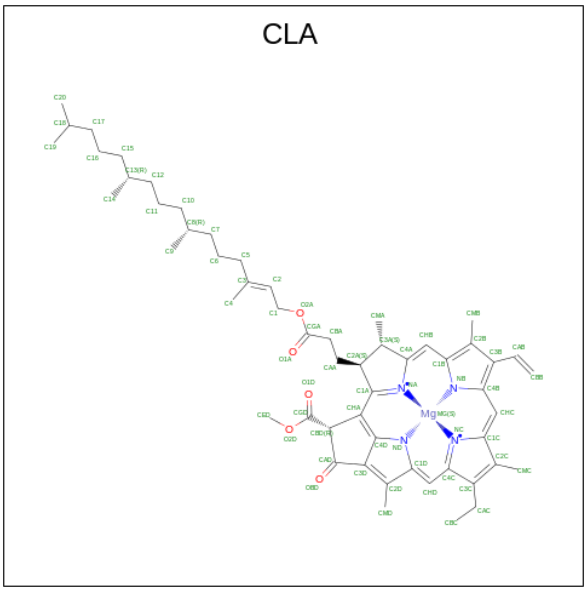


Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
35	A	1	10	1	4	5	0
35	a	1	10	1	4	5	0

- Molecule 36 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
36	A	1	1	1	0
36	a	1	1	1	0

- Molecule 37 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	A	1	130	110	2	8	10	0
			Total	C	Mg	N	O	
37	A	1	130	110	2	8	10	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	B	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	C	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	D	1	260	220	4	16	20	0
			Total	C	Mg	N	O	
37	D	1	260	220	4	16	20	0
			Total	C	Mg	N	O	
37	D	1	260	220	4	16	20	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	D	1	260	220	4	16	20	0
			Total	C	Mg	N	O	
37	Z	1	110	90	2	8	10	0
			Total	C	Mg	N	O	
37	Z	1	110	90	2	8	10	0
			Total	C	Mg	N	O	
37	W	1	130	110	2	8	10	0
			Total	C	Mg	N	O	
37	W	1	130	110	2	8	10	0
			Total	C	Mg	N	O	
37	a	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
37	a	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
37	a	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	b	1	1102	932	17	68	85	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	c	1	845	715	13	52	65	0
			Total	C	Mg	N	O	
37	d	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
37	d	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
37	d	1	195	165	3	12	15	0
			Total	C	Mg	N	O	
37	z	1	110	90	2	8	10	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	z	1	110	90	2	8	10	0
			Total	C	Mg	N	O	
37	w	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
37	11	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	11	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	11	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	11	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	11	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	11	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	12	1	407	337	7	28	35	0
			Total	C	Mg	N	O	
37	12	1	407	337	7	28	35	0
			Total	C	Mg	N	O	
37	12	1	407	337	7	28	35	0
			Total	C	Mg	N	O	
37	12	1	407	337	7	28	35	0
			Total	C	Mg	N	O	
37	12	1	407	337	7	28	35	0
			Total	C	Mg	N	O	
37	12	1	407	337	7	28	35	0
			Total	C	Mg	N	O	
37	12	1	407	337	7	28	35	0
			Total	C	Mg	N	O	
37	13	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	13	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	13	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	13	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	13	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	13	1	329	269	6	24	30	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	14	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	14	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	14	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	14	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	14	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	14	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	14	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	15	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	15	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	15	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	15	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	15	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	15	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	16	1	293	243	5	20	25	0
			Total	C	Mg	N	O	
37	16	1	293	243	5	20	25	0
			Total	C	Mg	N	O	
37	16	1	293	243	5	20	25	0
			Total	C	Mg	N	O	
37	16	1	293	243	5	20	25	0
			Total	C	Mg	N	O	
37	16	1	293	243	5	20	25	0
			Total	C	Mg	N	O	
37	17	1	238	198	4	16	20	0
			Total	C	Mg	N	O	
37	17	1	238	198	4	16	20	0
			Total	C	Mg	N	O	
37	17	1	238	198	4	16	20	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	17	1	238	198	4	16	20	0
			Total	C	Mg	N	O	
37	18	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	18	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	18	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	18	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	18	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	18	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	18	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	18	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	19	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	19	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	19	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	19	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	19	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	19	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	19	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	19	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	19	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	20	1	254	204	5	20	25	0
			Total	C	Mg	N	O	
37	20	1	254	204	5	20	25	0
			Total	C	Mg	N	O	
37	20	1	254	204	5	20	25	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	20	1	254	204	5	20	25	0
			Total	C	Mg	N	O	
37	20	1	254	204	5	20	25	0
			Total	C	Mg	N	O	
37	21	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	21	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	21	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	21	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	21	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	21	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	21	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	31	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	31	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	31	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	31	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	31	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	31	1	343	283	6	24	30	0
			Total	C	Mg	N	O	
37	32	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
37	32	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
37	32	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
37	32	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
37	32	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
37	32	1	472	392	8	32	40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	32	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
37	32	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
37	33	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	33	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	33	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	33	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	33	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	33	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	34	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	34	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	34	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	34	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	34	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	34	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	34	1	394	324	7	28	35	0
			Total	C	Mg	N	O	
37	35	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	35	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	35	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	35	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	35	1	329	269	6	24	30	0
			Total	C	Mg	N	O	
37	35	1	329	269	6	24	30	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	36	1	293	243	5	20	25	0
			Total	C	Mg	N	O	
37	36	1	293	243	5	20	25	0
			Total	C	Mg	N	O	
37	36	1	293	243	5	20	25	0
			Total	C	Mg	N	O	
37	36	1	293	243	5	20	25	0
			Total	C	Mg	N	O	
37	36	1	293	243	5	20	25	0
			Total	C	Mg	N	O	
37	37	1	238	198	4	16	20	0
			Total	C	Mg	N	O	
37	37	1	238	198	4	16	20	0
			Total	C	Mg	N	O	
37	37	1	238	198	4	16	20	0
			Total	C	Mg	N	O	
37	37	1	238	198	4	16	20	0
			Total	C	Mg	N	O	
37	38	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	38	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	38	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	38	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	38	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	38	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	38	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	38	1	459	379	8	32	40	0
			Total	C	Mg	N	O	
37	39	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	39	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	39	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	39	1	531	441	9	36	45	0

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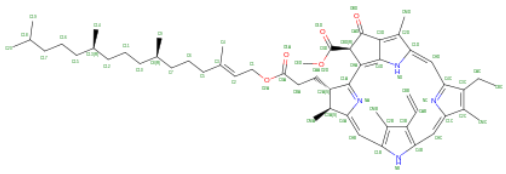
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	39	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	39	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	39	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	39	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	39	1	531	441	9	36	45	0
			Total	C	Mg	N	O	
37	40	1	254	204	5	20	25	0
			Total	C	Mg	N	O	
37	40	1	254	204	5	20	25	0
			Total	C	Mg	N	O	
37	40	1	254	204	5	20	25	0
			Total	C	Mg	N	O	
37	40	1	254	204	5	20	25	0
			Total	C	Mg	N	O	
37	40	1	254	204	5	20	25	0
			Total	C	Mg	N	O	
37	41	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	41	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	41	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	41	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	41	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	41	1	380	310	7	28	35	0
			Total	C	Mg	N	O	
37	41	1	380	310	7	28	35	0

- Molecule 38 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).

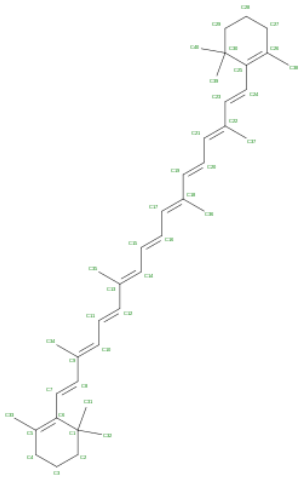
PHO



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
38	A	1	64	55	4	5	0
			Total	C	N	O	
38	D	1	64	55	4	5	0
			Total	C	N	O	
38	a	1	128	110	8	10	0
			Total	C	N	O	
38	a	1	128	110	8	10	0

- Molecule 39 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

BCR



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
39	A	1	80	80	0
			Total	C	
39	A	1	80	80	0
			Total	C	
39	B	1	120	120	0
			Total	C	
39	B	1	120	120	0
			Total	C	
39	B	1	120	120	0
			Total	C	
39	C	1	120	120	0
			Total	C	
39	C	1	120	120	0
			Total	C	
39	C	1	120	120	0
			Total	C	
39	D	1	40	40	0
			Total	C	
39	H	1	40	40	0
			Total	C	
39	K	1	40	40	0
			Total	C	
39	0	1	40	40	0
			Total	C	
39	a	1	80	80	0
			Total	C	
39	a	1	80	80	0
			Total	C	
39	b	1	120	120	0
			Total	C	
39	b	1	120	120	0
			Total	C	
39	b	1	120	120	0
			Total	C	
39	c	1	120	120	0
			Total	C	
39	c	1	120	120	0
			Total	C	
39	c	1	120	120	0
			Total	C	
39	d	1	40	40	0
			Total	C	
39	h	1	40	40	0

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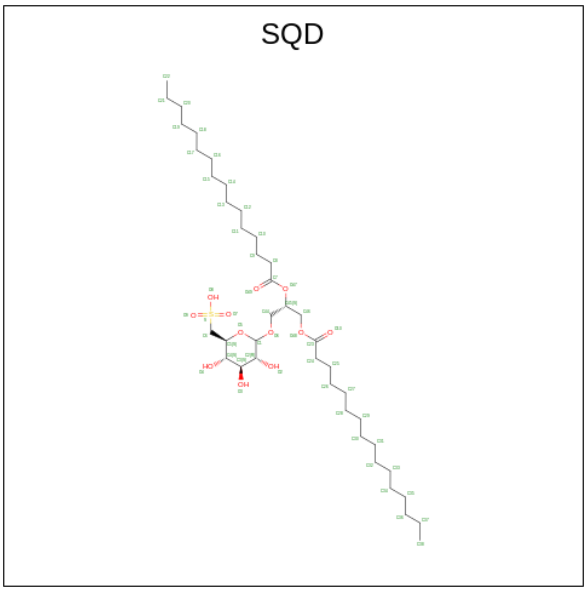
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
39	y	1	40	40	0
			Total	C	
39	5	1	40	40	0

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
40	A	1	54	41	12	1	0
			Total	C	O	S	
40	B	1	91	65	24	2	0
			Total	C	O	S	
40	B	1	91	65	24	2	0
			Total	C	O	S	
40	L	1	54	41	12	1	0
			Total	C	O	S	
40	a	1	54	41	12	1	0
			Total	C	O	S	
40	b	1	37	24	12	1	0
			Total	C	O	S	
40	16	1	54	41	12	1	0
			Total	C	O	S	
40	17	1	49	36	12	1	0
			Total	C	O	S	
40	36	1	49	36	12	1	0

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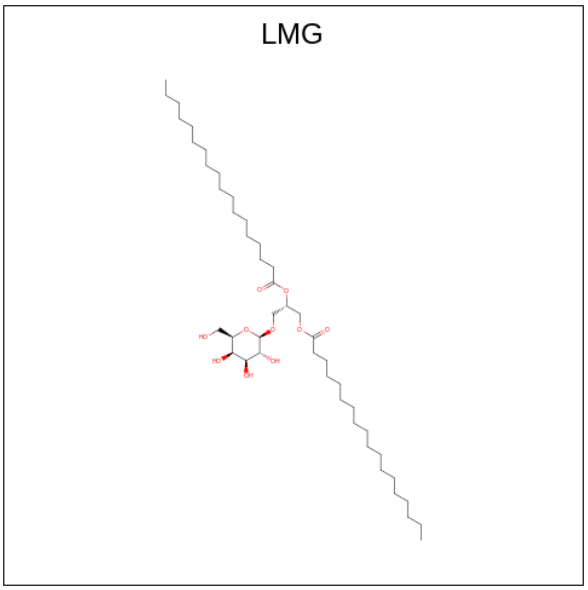
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
40	40	1	54	41	12	1	0

- Molecule 41 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
41	A	1	51	41	10	0
41	B	1	102	82	20	0
41	B	1	102	82	20	0
41	C	1	51	41	10	0
41	D	1	51	41	10	0
41	L	1	40	30	10	0
41	a	1	51	41	10	0
41	b	1	102	82	20	0
41	b	1	102	82	20	0
41	c	1	51	41	10	0

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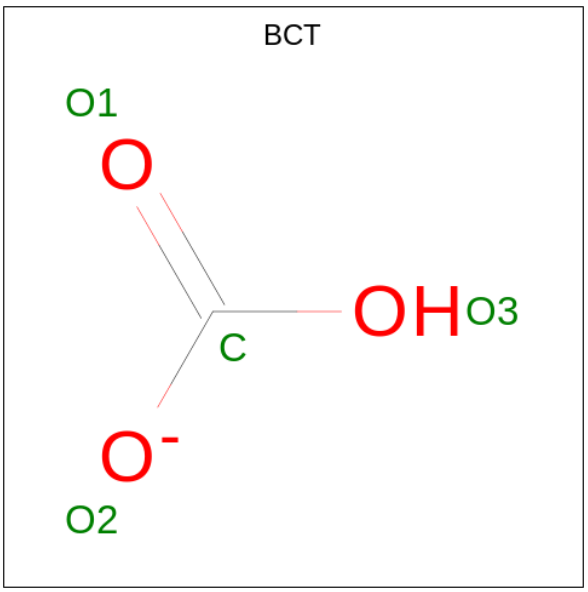
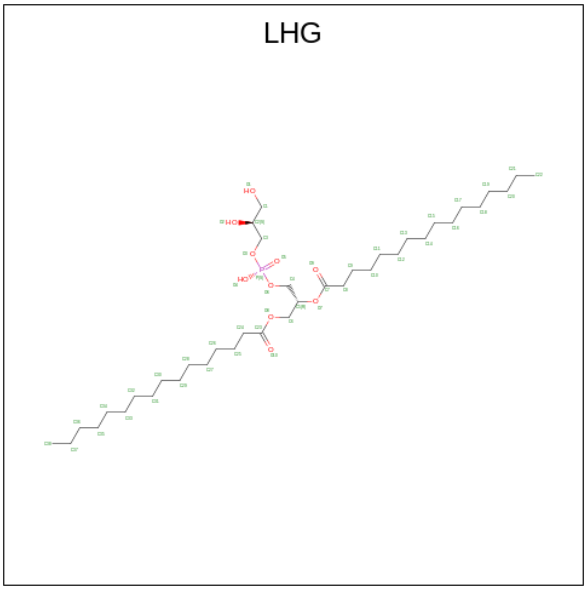
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
41	d	1	51	41	10	0
			Total	C	O	
41	l	1	40	30	10	0
			Total	C	O	
41	11	1	74	54	20	0
			Total	C	O	
41	11	1	74	54	20	0
			Total	C	O	
41	12	1	39	29	10	0
			Total	C	O	
41	16	1	36	26	10	0
			Total	C	O	
41	17	1	37	27	10	0
			Total	C	O	
41	31	1	74	54	20	0
			Total	C	O	
41	31	1	74	54	20	0
			Total	C	O	
41	32	1	39	29	10	0
			Total	C	O	
41	36	1	36	26	10	0
			Total	C	O	
41	37	1	37	27	10	0

- Molecule 42 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	A	1	4	1	3	0
			Total	C	O	
42	a	1	4	1	3	0

- Molecule 43 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
43	B	1	49	38	10	1	0
			Total	C	O	P	
43	D	1	144	111	30	3	0
			Total	C	O	P	
43	D	1	144	111	30	3	0
			Total	C	O	P	
43	D	1	144	111	30	3	0
			Total	C	O	P	
43	a	1	46	35	10	1	0
			Total	C	O	P	
43	b	1	49	38	10	1	0
			Total	C	O	P	
43	d	1	98	76	20	2	0
			Total	C	O	P	
43	d	1	98	76	20	2	0
			Total	C	O	P	
43	17	1	44	33	10	1	0

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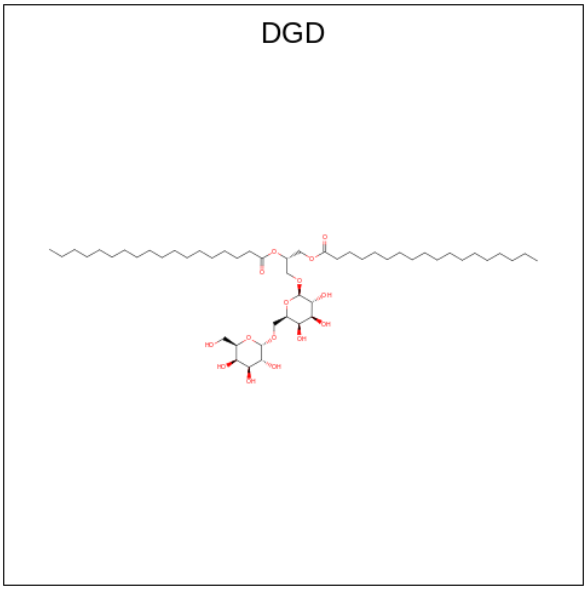
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
43	19	1	49	38	10	1	0
			Total	C	O	P	
43	21	1	80	59	19	2	0
			Total	C	O	P	
43	21	1	80	59	19	2	0
			Total	C	O	P	
43	37	1	89	67	20	2	0
			Total	C	O	P	
43	37	1	89	67	20	2	0
			Total	C	O	P	
43	39	1	49	38	10	1	0
			Total	C	O	P	
43	41	1	35	25	9	1	0

- Molecule 44 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
44	C	1	124	94	30	0
			Total	C	O	
44	C	1	124	94	30	0
			Total	C	O	
44	H	1	62	47	15	0
			Total	C	O	
44	J	1	62	47	15	0

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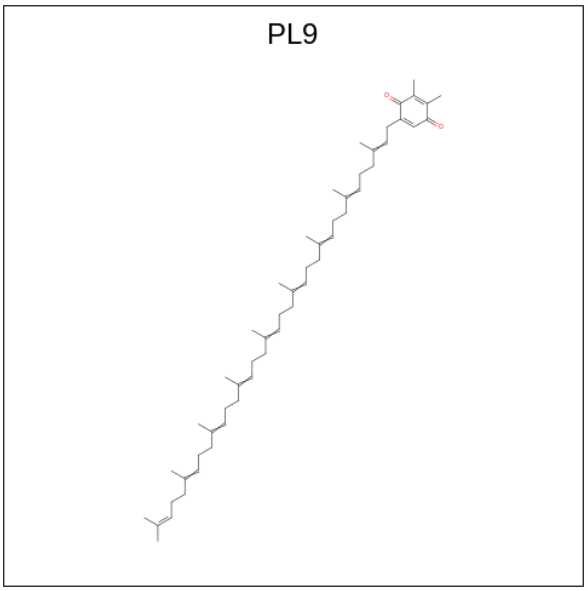
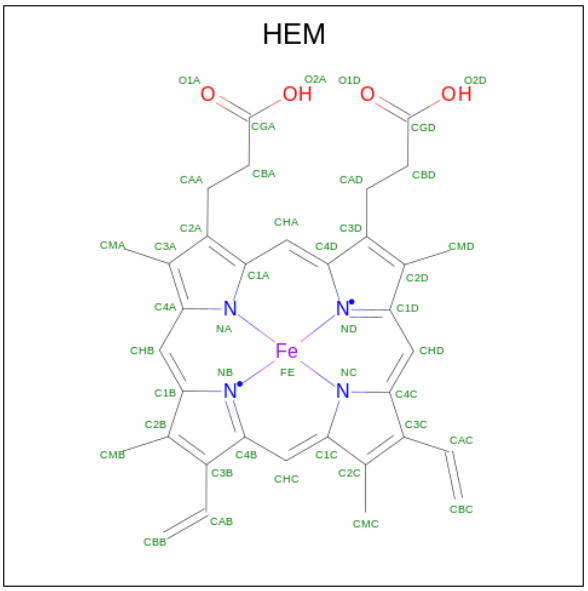
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
44	c	1	124	94	30	0
44	c	1	124	94	30	0
44	h	1	62	47	15	0
44	j	1	62	47	15	0

- Molecule 45 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



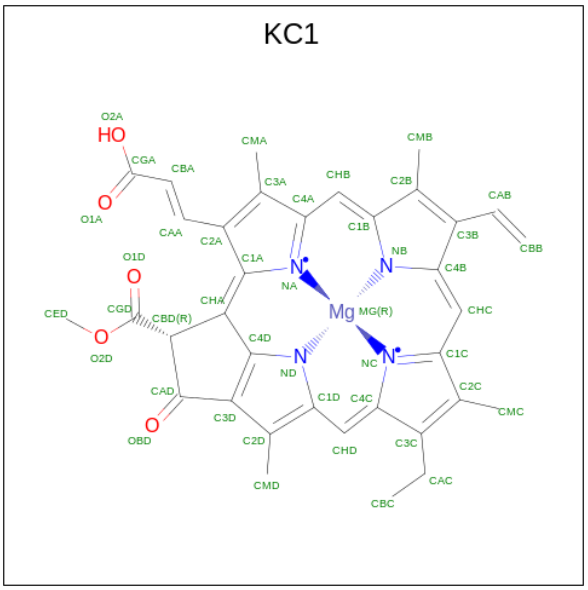
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	D	1	110	106	4	0
45	D	1	110	106	4	0
45	d	1	110	106	4	0
45	d	1	110	106	4	0

- Molecule 46 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
46	F	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
46	V	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
46	f	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
46	v	1	43	34	1	4	4	0

- Molecule 47 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
47	11	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	11	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	11	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	11	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	12	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	12	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	12	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	13	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	13	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	13	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	13	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	14	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	14	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	14	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	15	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	15	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	15	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	15	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	16	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	16	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	16	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	16	1	180	140	4	16	20	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
47	17	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	17	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	17	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	17	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	18	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	18	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	18	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	19	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
47	20	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	20	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	20	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	21	1	90	70	2	8	10	0
			Total	C	Mg	N	O	
47	21	1	90	70	2	8	10	0
			Total	C	Mg	N	O	
47	31	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	31	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	31	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	31	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	32	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	32	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	32	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	33	1	180	140	4	16	20	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
47	33	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	33	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	33	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	34	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	34	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	34	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	35	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	35	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	35	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	35	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	36	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	36	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	36	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	36	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	37	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	37	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	37	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	37	1	180	140	4	16	20	0
			Total	C	Mg	N	O	
47	38	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	38	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	38	1	135	105	3	12	15	0

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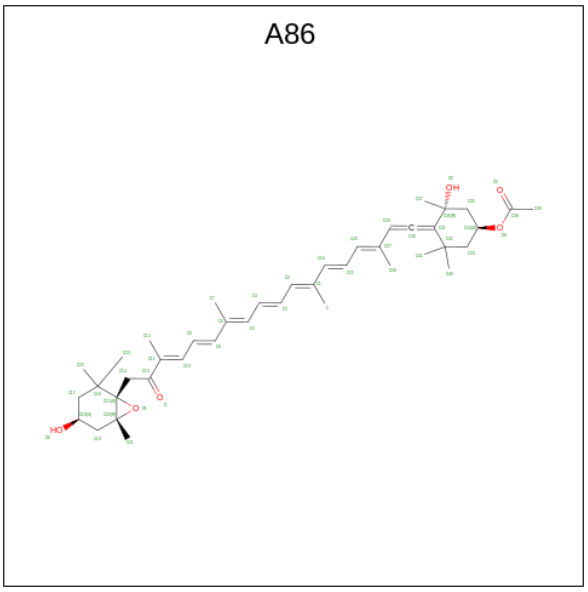
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
47	39	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
47	40	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	40	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	40	1	135	105	3	12	15	0
			Total	C	Mg	N	O	
47	41	1	90	70	2	8	10	0
			Total	C	Mg	N	O	
47	41	1	90	70	2	8	10	0

- Molecule 48 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (three-letter code: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	11	1	288	252	36	0
			Total	C	O	
48	11	1	288	252	36	0
			Total	C	O	
48	11	1	288	252	36	0
			Total	C	O	
48	11	1	288	252	36	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	11	1	288	252	36	0
			Total	C	O	
48	11	1	288	252	36	0
			Total	C	O	
48	12	1	336	294	42	0
			Total	C	O	
48	12	1	336	294	42	0
			Total	C	O	
48	12	1	336	294	42	0
			Total	C	O	
48	12	1	336	294	42	0
			Total	C	O	
48	12	1	336	294	42	0
			Total	C	O	
48	12	1	336	294	42	0
			Total	C	O	
48	12	1	336	294	42	0
			Total	C	O	
48	13	1	240	210	30	0
			Total	C	O	
48	13	1	240	210	30	0
			Total	C	O	
48	13	1	240	210	30	0
			Total	C	O	
48	13	1	240	210	30	0
			Total	C	O	
48	13	1	240	210	30	0
			Total	C	O	
48	14	1	288	252	36	0
			Total	C	O	
48	14	1	288	252	36	0
			Total	C	O	
48	14	1	288	252	36	0
			Total	C	O	
48	14	1	288	252	36	0
			Total	C	O	
48	14	1	288	252	36	0
			Total	C	O	
48	14	1	288	252	36	0
			Total	C	O	
48	15	1	336	294	42	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	15	1	336	294	42	0
			Total	C	O	
48	15	1	336	294	42	0
			Total	C	O	
48	15	1	336	294	42	0
			Total	C	O	
48	15	1	336	294	42	0
			Total	C	O	
48	15	1	336	294	42	0
			Total	C	O	
48	15	1	336	294	42	0
			Total	C	O	
48	16	1	192	168	24	0
			Total	C	O	
48	16	1	192	168	24	0
			Total	C	O	
48	16	1	192	168	24	0
			Total	C	O	
48	16	1	192	168	24	0
			Total	C	O	
48	17	1	336	294	42	0
			Total	C	O	
48	17	1	336	294	42	0
			Total	C	O	
48	17	1	336	294	42	0
			Total	C	O	
48	17	1	336	294	42	0
			Total	C	O	
48	17	1	336	294	42	0
			Total	C	O	
48	17	1	336	294	42	0
			Total	C	O	
48	17	1	336	294	42	0
			Total	C	O	
48	18	1	192	168	24	0
			Total	C	O	
48	18	1	192	168	24	0
			Total	C	O	
48	18	1	192	168	24	0
			Total	C	O	
48	18	1	192	168	24	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	19	1	96	84	12	0
			Total	C	O	
48	19	1	96	84	12	0
			Total	C	O	
48	20	1	96	84	12	0
			Total	C	O	
48	20	1	96	84	12	0
			Total	C	O	
48	21	1	192	168	24	0
			Total	C	O	
48	21	1	192	168	24	0
			Total	C	O	
48	21	1	192	168	24	0
			Total	C	O	
48	21	1	192	168	24	0
			Total	C	O	
48	31	1	288	252	36	0
			Total	C	O	
48	31	1	288	252	36	0
			Total	C	O	
48	31	1	288	252	36	0
			Total	C	O	
48	31	1	288	252	36	0
			Total	C	O	
48	31	1	288	252	36	0
			Total	C	O	
48	31	1	288	252	36	0
			Total	C	O	
48	32	1	336	294	42	0
			Total	C	O	
48	32	1	336	294	42	0
			Total	C	O	
48	32	1	336	294	42	0
			Total	C	O	
48	32	1	336	294	42	0
			Total	C	O	
48	32	1	336	294	42	0
			Total	C	O	
48	32	1	336	294	42	0
			Total	C	O	
48	32	1	336	294	42	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	33	1	240	210	30	0
			Total	C	O	
48	33	1	240	210	30	0
			Total	C	O	
48	33	1	240	210	30	0
			Total	C	O	
48	33	1	240	210	30	0
			Total	C	O	
48	33	1	240	210	30	0
			Total	C	O	
48	34	1	288	252	36	0
			Total	C	O	
48	34	1	288	252	36	0
			Total	C	O	
48	34	1	288	252	36	0
			Total	C	O	
48	34	1	288	252	36	0
			Total	C	O	
48	34	1	288	252	36	0
			Total	C	O	
48	34	1	288	252	36	0
			Total	C	O	
48	35	1	336	294	42	0
			Total	C	O	
48	35	1	336	294	42	0
			Total	C	O	
48	35	1	336	294	42	0
			Total	C	O	
48	35	1	336	294	42	0
			Total	C	O	
48	35	1	336	294	42	0
			Total	C	O	
48	35	1	336	294	42	0
			Total	C	O	
48	35	1	336	294	42	0
			Total	C	O	
48	36	1	144	126	18	0
			Total	C	O	
48	36	1	144	126	18	0
			Total	C	O	
48	36	1	144	126	18	0

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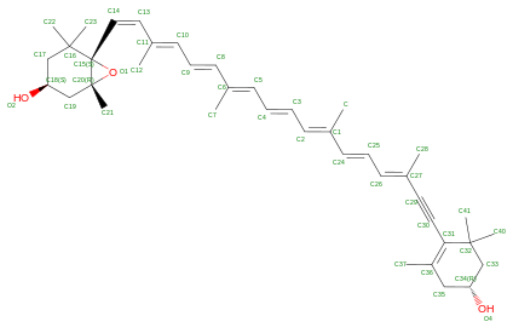
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	37	1	336	294	42	0
48	37	1	336	294	42	0
48	37	1	336	294	42	0
48	37	1	336	294	42	0
48	37	1	336	294	42	0
48	37	1	336	294	42	0
48	37	1	336	294	42	0
48	38	1	192	168	24	0
48	38	1	192	168	24	0
48	38	1	192	168	24	0
48	38	1	192	168	24	0
48	39	1	96	84	12	0
48	39	1	96	84	12	0
48	40	1	144	126	18	0
48	40	1	144	126	18	0
48	40	1	144	126	18	0
48	41	1	192	168	24	0
48	41	1	192	168	24	0
48	41	1	192	168	24	0
48	41	1	192	168	24	0

- Molecule 49 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	AltConf
49	11	1	Total C O 19 17 2	0
49	12	2	Total C O 34 32 2	0
49	13	3	Total C O 49 47 2	0
49	14	1	Total C 16 16	0
49	15	2	Total C 28 28	0
49	16	2	Total C 24 24	0
49	17	3	Total C O 54 48 6	0
49	18	4	Total C 58 58	0
49	19	1	Total C 12 12	0
49	31	1	Total C O 19 17 2	0
49	32	2	Total C O 34 32 2	0
49	33	3	Total C O 49 47 2	0
49	34	1	Total C 16 16	0
49	35	2	Total C 28 28	0
49	36	2	Total C 24 24	0
49	37	3	Total C O 54 48 6	0
49	38	4	Total C 58 58	0
49	39	1	Total C 12 12	0

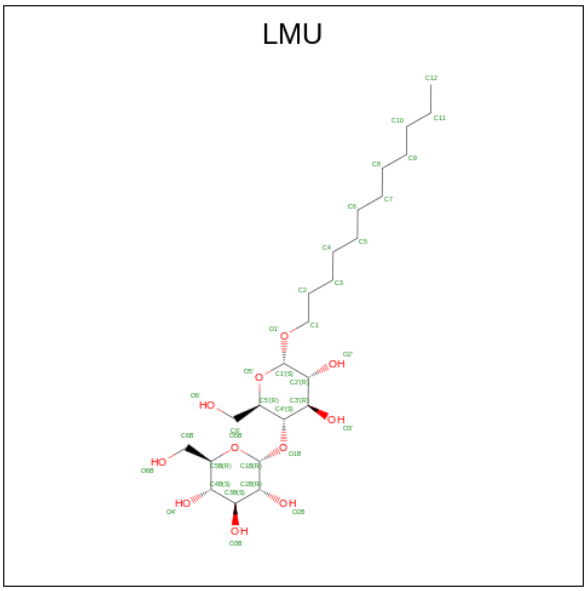
- Molecule 50 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: $C_{40}H_{54}O_3$).

DD6



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	16	1	43	40	3	0
			Total	C	O	
50	19	1	43	40	3	0
			Total	C	O	
50	20	1	86	80	6	0
			Total	C	O	
50	20	1	86	80	6	0
			Total	C	O	
50	21	1	86	80	6	0
			Total	C	O	
50	21	1	86	80	6	0
			Total	C	O	
50	36	1	43	40	3	0
			Total	C	O	
50	39	1	43	40	3	0
			Total	C	O	
50	40	1	86	80	6	0
			Total	C	O	
50	40	1	86	80	6	0
			Total	C	O	
50	41	1	86	80	6	0
			Total	C	O	
50	41	1	86	80	6	0

- Molecule 51 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
51	19	1	Total	C	O	0
			35	24	11	
51	39	1	Total	C	O	0
			35	24	11	

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	B	5	Total	O	0
			5	5	
52	C	3	Total	O	0
			3	3	
52	D	4	Total	O	0
			4	4	
52	Z	1	Total	O	0
			1	1	
52	a	2	Total	O	0
			2	2	
52	b	5	Total	O	0
			5	5	
52	c	3	Total	O	0
			3	3	
52	d	2	Total	O	0
			2	2	
52	z	1	Total	O	0
			1	1	
52	11	3	Total	O	0
			3	3	

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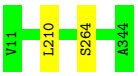
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
52	12	2	2	2	0
52	13	1	1	1	0
52	14	1	1	1	0
52	15	1	1	1	0
52	16	1	1	1	0
52	17	2	2	2	0
52	18	1	1	1	0
52	19	1	1	1	0
52	31	3	3	3	0
52	32	2	2	2	0
52	33	1	1	1	0
52	34	1	1	1	0
52	35	1	1	1	0
52	36	1	1	1	0
52	37	2	2	2	0
52	38	1	1	1	0
52	39	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

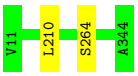
• Molecule 1: Photosystem II protein D1

Chain A: 99%



• Molecule 1: Photosystem II protein D1

Chain a: 99%



• Molecule 2: Photosystem II CP47 reaction center protein

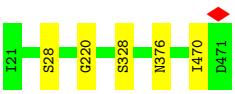
Chain B: 99%

• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 99%

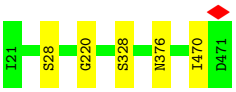
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 99%



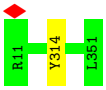
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 99%



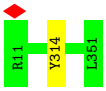
• Molecule 4: Photosystem II D2 protein

Chain D: 100%



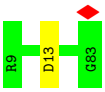
• Molecule 4: Photosystem II D2 protein

Chain d: 100%



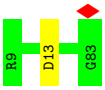
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 99%



• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 99%



• Molecule 6: Cytochrome b559 subunit beta

Chain F: 100%

There are no outlier residues recorded for this chain.

• Molecule 6: Cytochrome b559 subunit beta

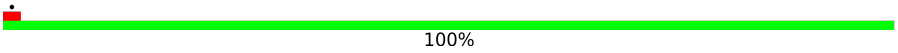
Chain f: 100%

There are no outlier residues recorded for this chain.

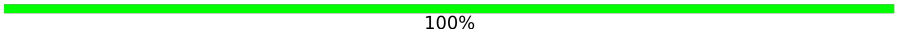
• Molecule 7: Photosystem II reaction center protein H

Chain H: 100%

• Molecule 7: Photosystem II reaction center protein H

Chain h: 

• Molecule 8: Photosystem II reaction center protein I

Chain I: 

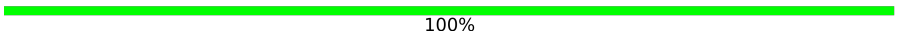
There are no outlier residues recorded for this chain.

• Molecule 8: Photosystem II reaction center protein I

Chain i:

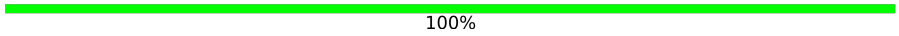
There are no outlier residues recorded for this chain.

• Molecule 9: Photosystem II reaction center protein J

Chain J: 

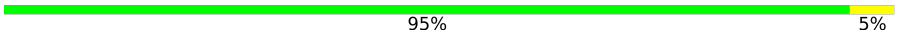
There are no outlier residues recorded for this chain.

• Molecule 9: Photosystem II reaction center protein J

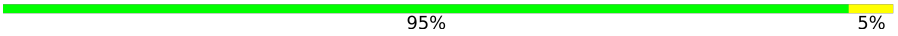
Chain j: 

There are no outlier residues recorded for this chain.

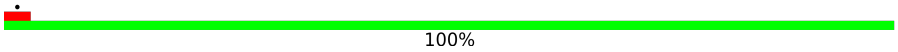
• Molecule 10: Photosystem II reaction center protein K

Chain K: 

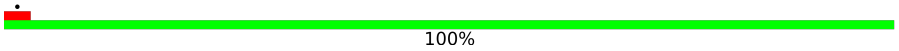
• Molecule 10: Photosystem II reaction center protein K

Chain k: 

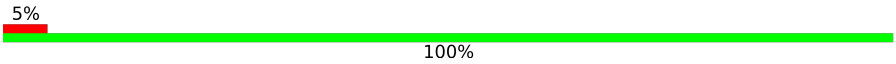
• Molecule 11: Photosystem II reaction center protein L

Chain L: 

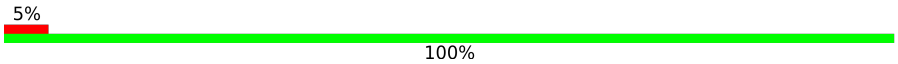
• Molecule 11: Photosystem II reaction center protein L

Chain l: 

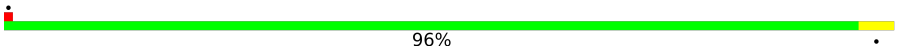
• Molecule 12: Photosystem II subunit

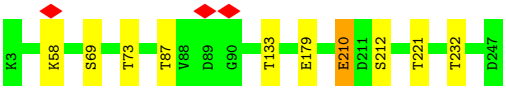
Chain M: 

• Molecule 12: Photosystem II subunit

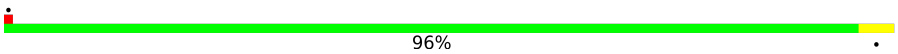
Chain m: 

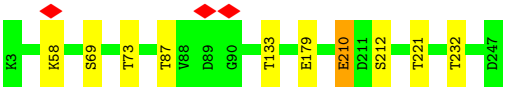
• Molecule 13: Extrinsic protein in photosystem II

Chain O: 

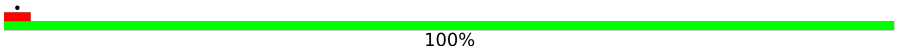


• Molecule 13: Extrinsic protein in photosystem II

Chain o: 



• Molecule 14: Photosystem II reaction center protein T

Chain T: 

• Molecule 14: Photosystem II reaction center protein T

Chain t: 100%

• Molecule 15: Extrinsic protein in photosystem II

Chain U: 99%

• Molecule 15: Extrinsic protein in photosystem II

Chain u: 99%

• Molecule 16: Cytochrome c-550

Chain V: 99%

• Molecule 16: Cytochrome c-550

Chain v: 99%

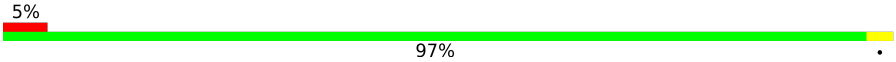
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 100%

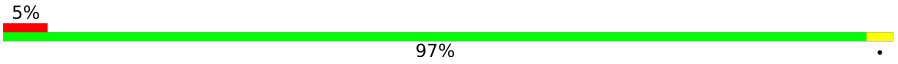
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 100%

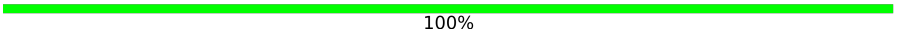
• Molecule 18: Photosystem II reaction center X protein

Chain X: 

• Molecule 18: Photosystem II reaction center X protein

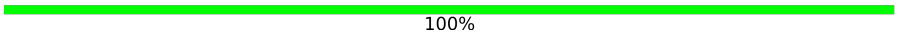
Chain x: 

• Molecule 19: Photosystem II reaction center protein Z

Chain Z: 

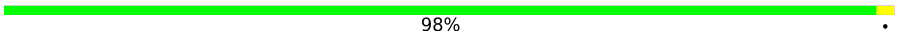
There are no outlier residues recorded for this chain.

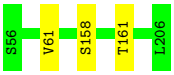
• Molecule 19: Photosystem II reaction center protein Z

Chain z: 

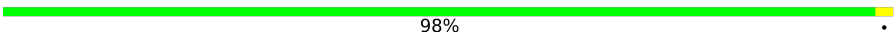
There are no outlier residues recorded for this chain.

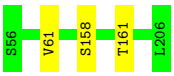
• Molecule 20: Extrinsic protein in photosystem II

Chain Q: 

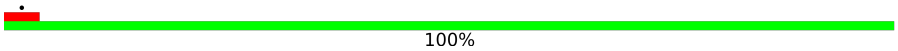


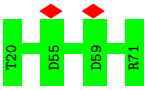
• Molecule 20: Extrinsic protein in photosystem II

Chain q: 

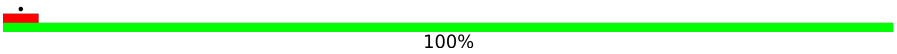


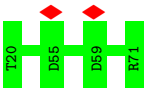
• Molecule 21: Photosystem II reaction center protein W

Chain W: 

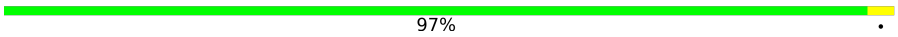


• Molecule 21: Photosystem II reaction center protein W

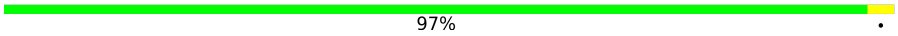
Chain w: 



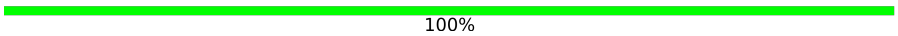
• Molecule 22: Unknown protein 0

Chain 0: 

• Molecule 22: Unknown protein 0

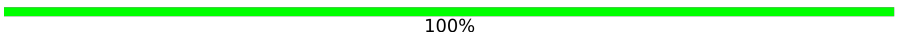
Chain 5: 

• Molecule 23: Unknown protein 1

Chain 1: 

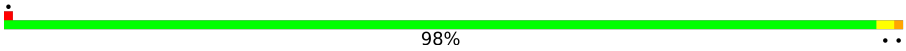
There are no outlier residues recorded for this chain.

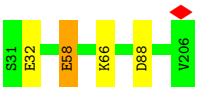
• Molecule 23: Unknown protein 1

Chain 6: 

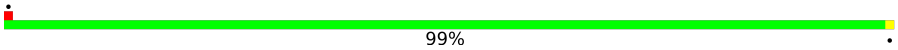
There are no outlier residues recorded for this chain.

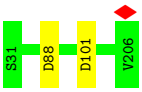
• Molecule 24: Chlorophyll a/b-binding protein

Chain 11: 

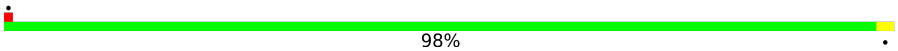


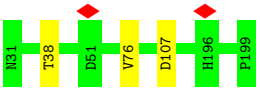
• Molecule 24: Chlorophyll a/b-binding protein

Chain 31: 



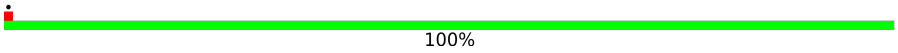
• Molecule 25: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein

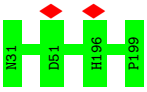
Chain 12: 



• Molecule 25: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein

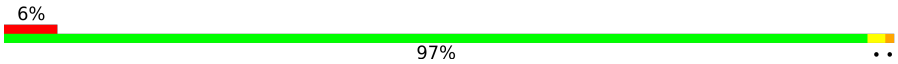
Chain 32:

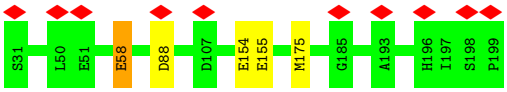




• Molecule 26: Chlorophyll a/b-binding protein

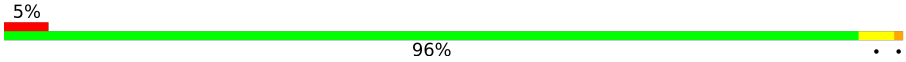
Chain 13:

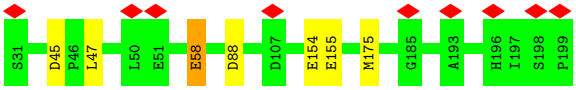




• Molecule 26: Chlorophyll a/b-binding protein

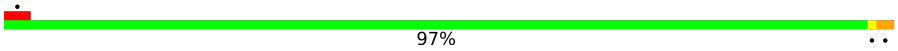
Chain 33:

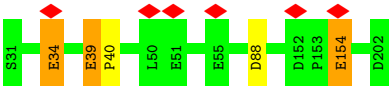




• Molecule 27: Chlorophyll a/b-binding protein

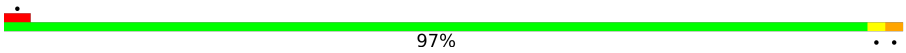
Chain 14:

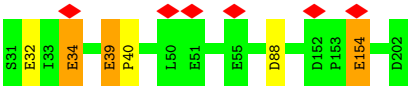




• Molecule 27: Chlorophyll a/b-binding protein

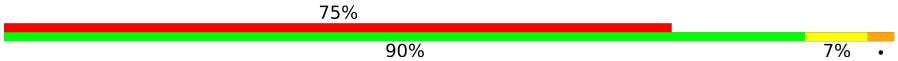
Chain 34:

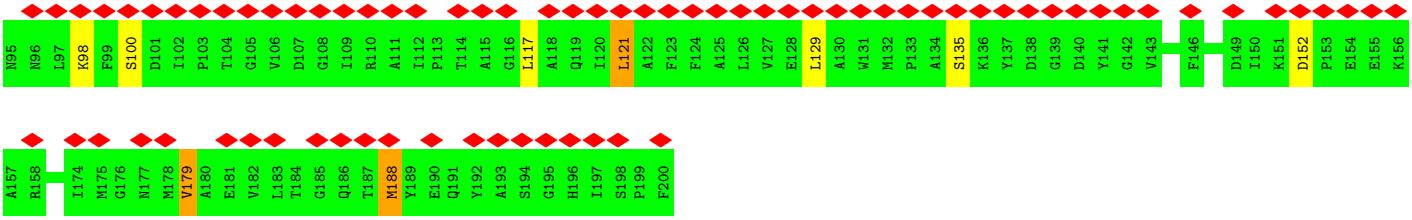




• Molecule 28: Chlorophyll a/b-binding protein

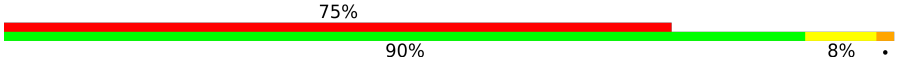
Chain 15:

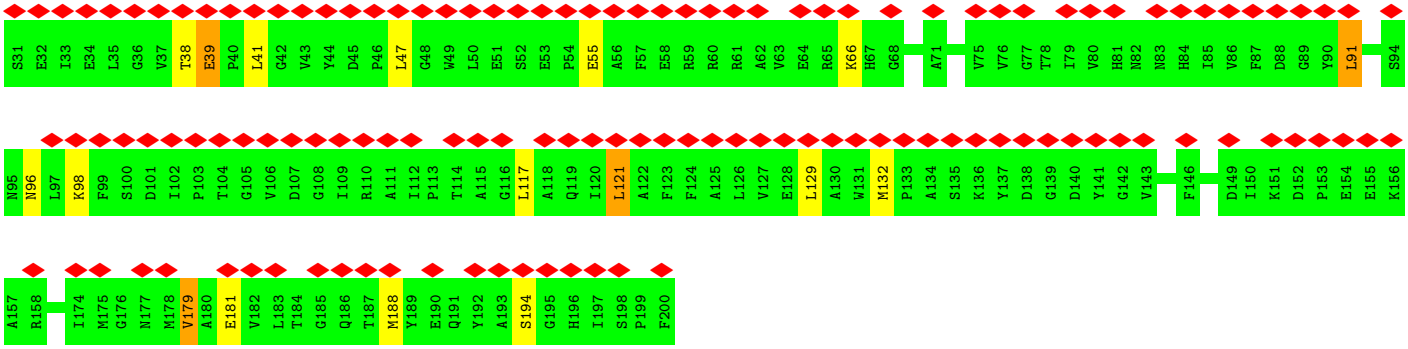




- Molecule 28: Chlorophyll a/b-binding protein

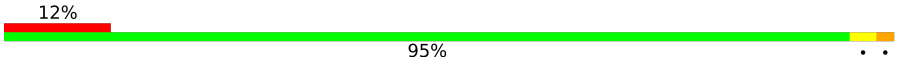
Chain 35:

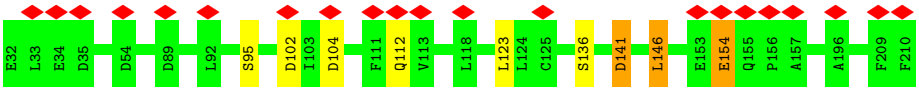




- Molecule 29: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein

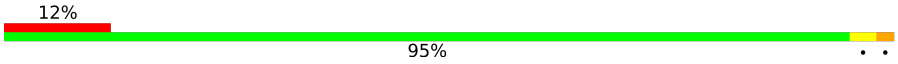
Chain 16:

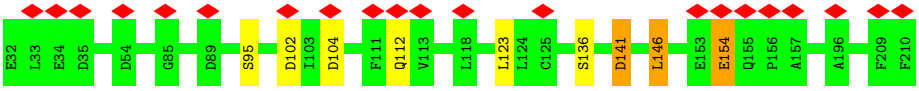




- Molecule 29: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein

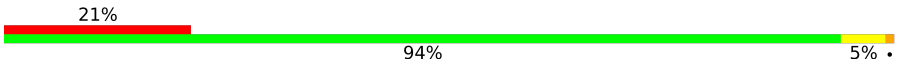
Chain 36:

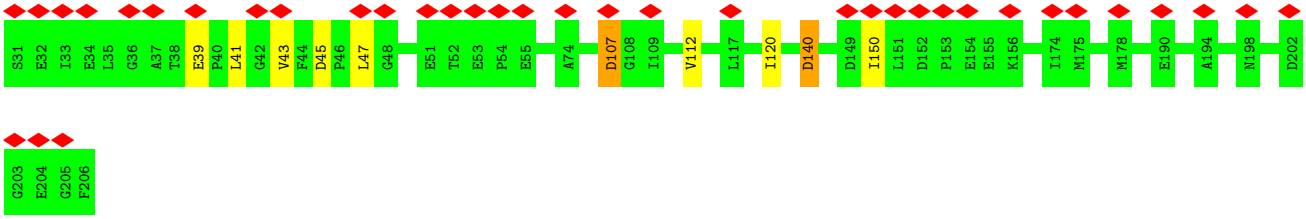




- Molecule 30: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein

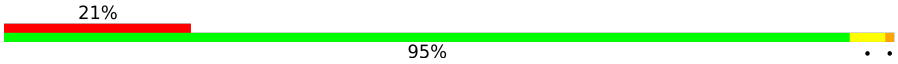
Chain 17:

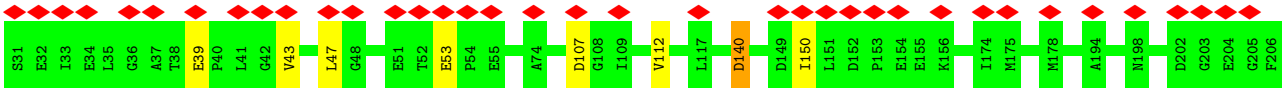




- Molecule 30: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein

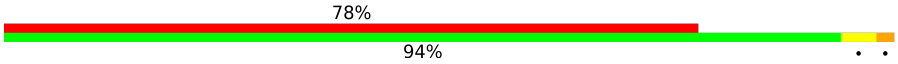
Chain 37:

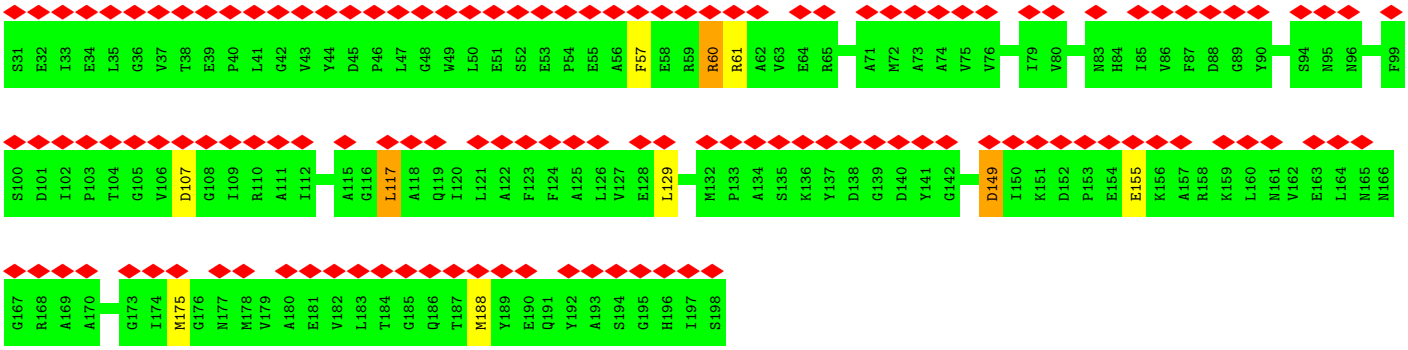




• Molecule 31: Chlorophyll a/b-binding protein

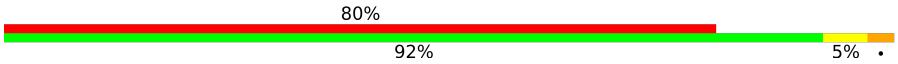
Chain 18:

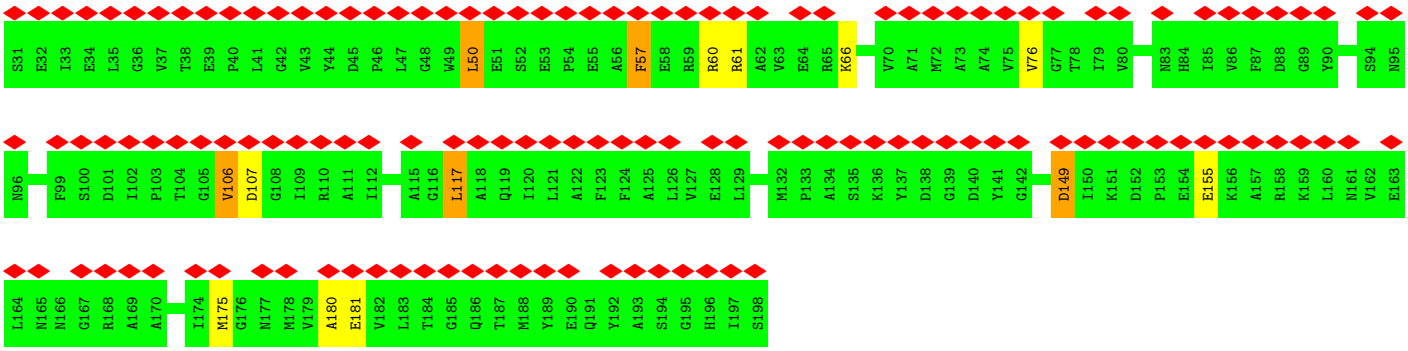




• Molecule 31: Chlorophyll a/b-binding protein

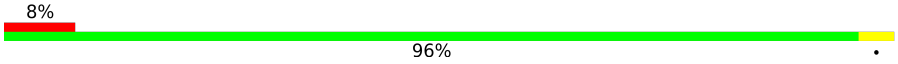
Chain 38:

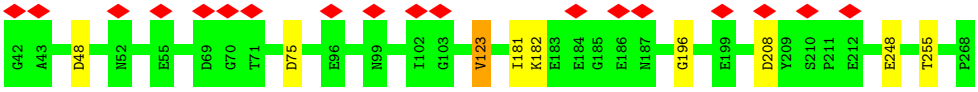




• Molecule 32: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein

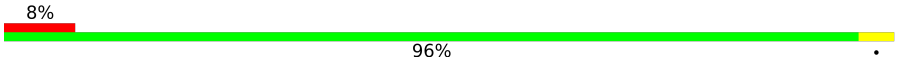
Chain 19:





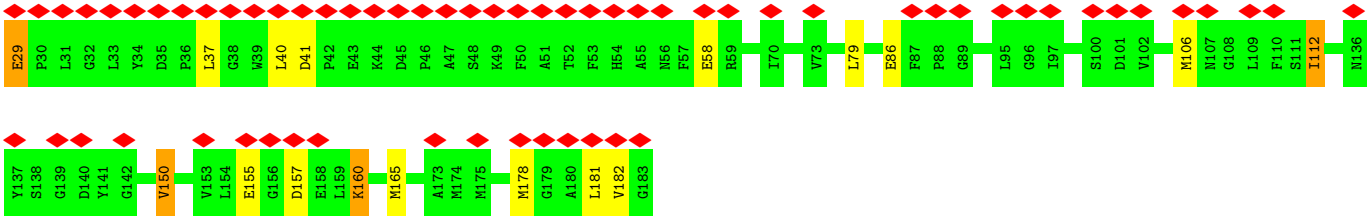
• Molecule 32: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein

Chain 39:



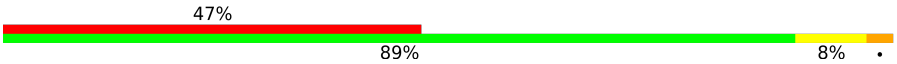
• Molecule 33: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein

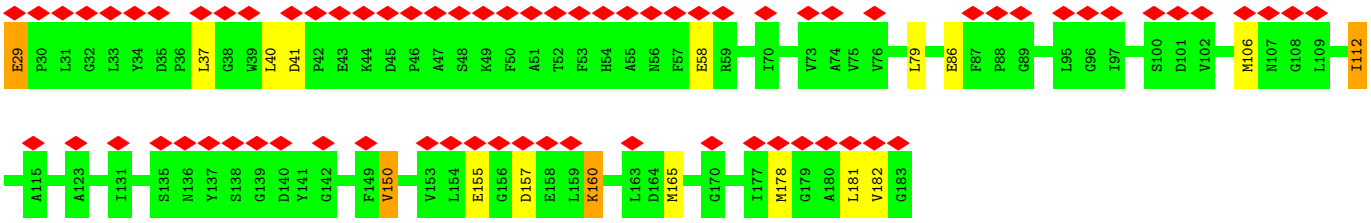
Chain 20:



• Molecule 33: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein

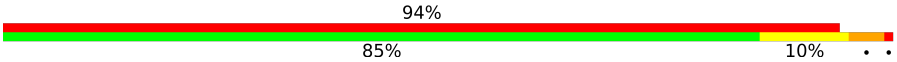
Chain 40:

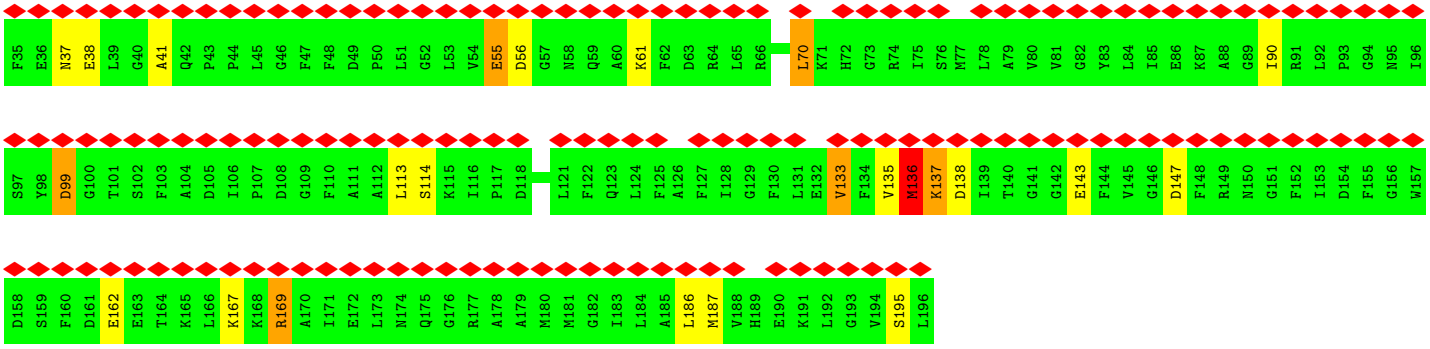




• Molecule 34: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein

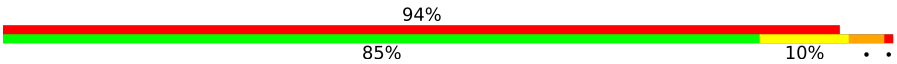
Chain 21:

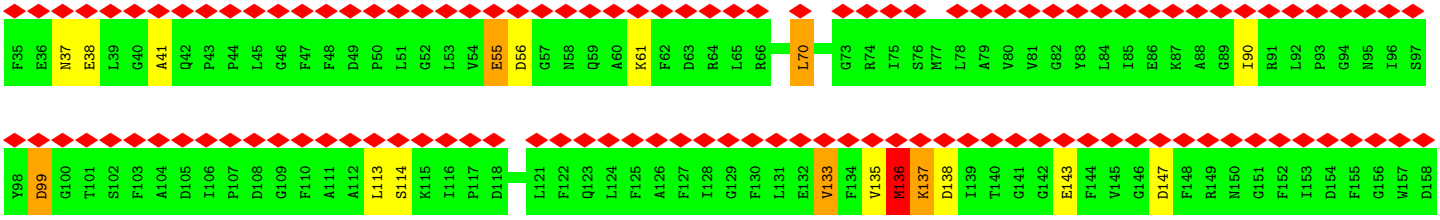


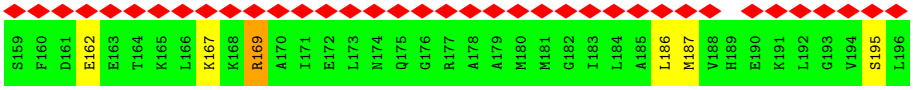


• Molecule 34: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein

Chain 41:






S159
F160
D161
E162
E163
T164
K165
L166
K167
K168
R169
A170
I171
E172
L173
N174
Q175
G176
R177
A178
A179
M180
M181
G182
I183
L184
A185
L186
M187
V188
H189
E190
K191
L192
G193
V194
S195
L196

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	210825	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.369	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	569.856, 569.856, 569.856	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, SQD, HEM, BCT, UNL, PHO, OEX, LMU, PL9, A86, KC1, DGD, LMG, CLA, DD6, FE2, LHG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.44	0/2702	0.52	1/3682 (0.0%)
1	a	0.44	0/2702	0.52	1/3682 (0.0%)
2	B	0.46	0/3942	0.52	0/5362
2	b	0.46	0/3942	0.52	0/5362
3	C	0.48	0/3620	0.52	0/4933
3	c	0.48	0/3620	0.52	0/4933
4	D	0.48	1/2789 (0.0%)	0.53	0/3803
4	d	0.48	1/2789 (0.0%)	0.53	0/3803
5	E	0.38	0/634	0.48	0/864
5	e	0.38	0/634	0.48	0/864
6	F	0.38	0/235	0.56	0/316
6	f	0.38	0/235	0.56	0/316
7	H	0.39	0/523	0.56	0/714
7	h	0.39	0/523	0.56	0/714
8	I	0.42	0/294	0.58	0/397
8	i	0.42	0/294	0.58	0/397
9	J	0.36	0/260	0.47	0/351
9	j	0.36	0/260	0.46	0/351
10	K	0.45	0/313	0.61	0/429
10	k	0.45	0/313	0.61	0/429
11	L	0.50	0/319	0.49	0/433
11	l	0.50	0/319	0.49	0/433
12	M	0.37	0/321	0.56	0/433
12	m	0.37	0/321	0.56	0/433
13	O	0.40	0/1875	0.58	1/2528 (0.0%)
13	o	0.40	0/1875	0.58	1/2528 (0.0%)
14	T	0.41	0/256	0.44	0/346
14	t	0.41	0/256	0.45	0/346
15	U	0.37	0/728	0.54	0/989
15	u	0.37	0/728	0.54	0/989
16	V	0.41	0/1056	0.56	1/1435 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.41	0/1056	0.56	1/1435 (0.1%)
17	Y	0.28	0/252	0.55	0/341
17	y	0.28	0/252	0.55	0/341
18	X	0.29	0/263	0.45	0/355
18	x	0.29	0/263	0.45	0/355
19	Z	0.36	0/456	0.56	0/624
19	z	0.36	0/456	0.56	0/624
20	Q	0.36	0/1203	0.55	0/1623
20	q	0.36	0/1203	0.55	0/1623
21	W	0.40	0/434	0.57	0/590
21	w	0.40	0/434	0.57	0/590
24	11	0.53	2/1373 (0.1%)	0.61	3/1861 (0.2%)
24	31	0.46	0/1373	0.57	1/1861 (0.1%)
25	12	0.44	0/1334	0.61	2/1810 (0.1%)
25	32	0.43	0/1334	0.56	0/1810
26	13	0.48	1/1325 (0.1%)	0.75	4/1797 (0.2%)
26	33	0.49	1/1325 (0.1%)	0.75	4/1797 (0.2%)
27	14	0.50	2/1349 (0.1%)	0.73	3/1829 (0.2%)
27	34	0.51	2/1349 (0.1%)	0.76	5/1829 (0.3%)
28	15	0.40	0/1337	0.90	9/1813 (0.5%)
28	35	0.43	0/1337	0.86	6/1813 (0.3%)
29	16	0.40	1/1425 (0.1%)	0.69	2/1930 (0.1%)
29	36	0.40	1/1425 (0.1%)	0.69	2/1930 (0.1%)
30	17	0.42	0/1386	0.77	4/1879 (0.2%)
30	37	0.48	2/1386 (0.1%)	0.76	4/1879 (0.2%)
31	18	0.53	0/1317	1.07	12/1785 (0.7%)
31	38	0.60	3/1317 (0.2%)	1.07	12/1785 (0.7%)
32	19	0.44	0/1796	0.66	4/2445 (0.2%)
32	39	0.46	1/1796 (0.1%)	0.66	2/2445 (0.1%)
33	20	0.45	1/1224 (0.1%)	0.85	7/1656 (0.4%)
33	40	0.45	1/1224 (0.1%)	0.85	7/1656 (0.4%)
34	21	0.53	0/1290	1.33	17/1735 (1.0%)
34	41	0.53	0/1290	1.33	17/1735 (1.0%)
All	All	0.45	20/75262 (0.0%)	0.67	133/102176 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	c	0	1
13	O	0	2
13	o	0	2
20	Q	0	1
20	q	0	1
22	0	0	1
22	5	0	1
27	14	0	1
27	34	0	1
28	35	0	2
29	16	0	1
29	36	0	1
32	19	0	1
32	39	0	1
33	20	0	3
33	40	0	3
34	21	0	3
34	41	0	3
All	All	0	30

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	34	154	GLU	CB-CG	-8.12	1.36	1.52
27	14	154	GLU	CB-CG	-8.09	1.36	1.52
31	38	106	VAL	CB-CG1	-7.57	1.36	1.52
24	11	58	GLU	CD-OE1	-7.35	1.17	1.25
32	39	248	GLU	CG-CD	-7.11	1.41	1.51
24	11	32	GLU	CD-OE1	-6.72	1.18	1.25
31	38	181	GLU	CB-CG	-6.54	1.39	1.52
29	36	154	GLU	CD-OE1	-6.41	1.18	1.25
29	16	154	GLU	CD-OE1	-6.41	1.18	1.25
4	d	314	TYR	CD1-CE1	-6.12	1.30	1.39
4	D	314	TYR	CD1-CE1	-6.08	1.30	1.39
30	37	39	GLU	CD-OE2	-5.99	1.19	1.25
31	38	60	ARG	CZ-NH1	-5.93	1.25	1.33
26	13	58	GLU	CD-OE1	-5.72	1.19	1.25
26	33	58	GLU	CD-OE1	-5.71	1.19	1.25
33	40	29	GLU	CB-CG	5.41	1.62	1.52
33	20	29	GLU	CB-CG	5.40	1.62	1.52
30	37	39	GLU	CD-OE1	-5.26	1.19	1.25
27	34	34	GLU	CD-OE2	-5.26	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	14	34	GLU	CD-OE2	-5.23	1.20	1.25

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	21	70	LEU	CA-CB-CG	21.70	165.22	115.30
34	41	70	LEU	CA-CB-CG	21.69	165.18	115.30
34	21	136	MET	CB-CG-SD	13.12	151.75	112.40
34	41	136	MET	CB-CG-SD	13.12	151.75	112.40
34	41	136	MET	CA-CB-CG	-12.95	91.28	113.30
34	21	136	MET	CA-CB-CG	-12.94	91.30	113.30
26	33	175	MET	CG-SD-CE	-12.51	80.19	100.20
26	13	175	MET	CG-SD-CE	-12.27	80.56	100.20
34	41	70	LEU	CB-CG-CD1	-12.19	90.28	111.00
34	21	70	LEU	CB-CG-CD1	-12.17	90.31	111.00
31	38	60	ARG	NE-CZ-NH2	12.08	126.34	120.30
31	18	149	ASP	CB-CG-OD1	11.90	129.01	118.30
31	38	149	ASP	CB-CG-OD1	11.59	128.73	118.30
27	34	154	GLU	CA-CB-CG	11.18	137.99	113.40
34	41	70	LEU	CB-CG-CD2	10.61	129.04	111.00
34	21	70	LEU	CB-CG-CD2	10.59	129.00	111.00
34	21	133	VAL	CG1-CB-CG2	-10.15	94.66	110.90
34	41	133	VAL	CG1-CB-CG2	-10.15	94.66	110.90
28	15	50	LEU	CA-CB-CG	10.03	138.38	115.30
34	21	135	VAL	CG1-CB-CG2	-9.94	95.00	110.90
34	41	135	VAL	CG1-CB-CG2	-9.93	95.02	110.90
27	14	154	GLU	CA-CB-CG	9.70	134.75	113.40
34	21	169	ARG	CA-CB-CG	9.46	134.22	113.40
34	41	169	ARG	CA-CB-CG	9.46	134.20	113.40
26	13	88	ASP	CB-CG-OD1	9.20	126.58	118.30
33	20	112	ILE	CG1-CB-CG2	-9.09	91.41	111.40
33	40	112	ILE	CG1-CB-CG2	-9.09	91.41	111.40
34	41	38	GLU	CA-CB-CG	8.89	132.96	113.40
34	21	147	ASP	CB-CG-OD1	8.89	126.30	118.30
34	41	147	ASP	CB-CG-OD1	8.88	126.30	118.30
34	21	38	GLU	CA-CB-CG	8.86	132.88	113.40
34	41	56	ASP	CB-CG-OD2	-8.77	110.41	118.30
34	21	56	ASP	CB-CG-OD2	-8.73	110.44	118.30
34	21	169	ARG	CB-CG-CD	8.62	134.01	111.60
34	41	169	ARG	CB-CG-CD	8.62	134.01	111.60
31	38	117	LEU	CB-CG-CD1	8.49	125.44	111.00
31	18	117	LEU	CB-CG-CD1	8.44	125.35	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	41	56	ASP	CB-CG-OD1	8.26	125.73	118.30
34	21	56	ASP	CB-CG-OD1	8.25	125.72	118.30
28	35	179	VAL	CG1-CB-CG2	-8.10	97.94	110.90
30	37	39	GLU	OE1-CD-OE2	-8.04	113.66	123.30
34	21	55	GLU	CA-CB-CG	7.86	130.69	113.40
34	41	55	GLU	CA-CB-CG	7.85	130.67	113.40
28	15	91	LEU	CB-CG-CD1	-7.63	98.03	111.00
16	V	86	GLU	CA-CB-CG	7.61	130.15	113.40
31	18	60	ARG	CG-CD-NE	7.59	127.73	111.80
16	v	86	GLU	CA-CB-CG	7.58	130.08	113.40
27	34	154	GLU	N-CA-CB	7.46	124.02	110.60
31	18	129	LEU	CA-CB-CG	7.37	132.25	115.30
13	o	210	GLU	CA-CB-CG	7.33	129.53	113.40
13	O	210	GLU	CA-CB-CG	7.31	129.47	113.40
33	40	178	MET	CG-SD-CE	7.25	111.79	100.20
33	20	178	MET	CG-SD-CE	7.24	111.78	100.20
28	15	179	VAL	CG1-CB-CG2	-7.23	99.33	110.90
30	37	140	ASP	CB-CG-OD2	6.98	124.58	118.30
30	17	140	ASP	CB-CG-OD2	6.95	124.55	118.30
31	38	117	LEU	CA-CB-CG	6.92	131.22	115.30
31	18	60	ARG	NE-CZ-NH1	6.81	123.71	120.30
33	20	29	GLU	CA-CB-CG	6.79	128.34	113.40
31	18	188	MET	CG-SD-CE	6.79	111.06	100.20
33	40	29	GLU	CA-CB-CG	6.77	128.29	113.40
27	14	154	GLU	N-CA-CB	6.75	122.74	110.60
28	15	53	GLU	CA-CB-CG	6.70	128.14	113.40
31	18	117	LEU	CA-CB-CG	6.69	130.68	115.30
25	12	76	VAL	CG1-CB-CG2	-6.56	100.40	110.90
24	11	58	GLU	CA-CB-CG	6.55	127.81	113.40
31	38	149	ASP	CB-CG-OD2	-6.52	112.43	118.30
32	39	123	VAL	CG1-CB-CG2	-6.48	100.54	110.90
32	19	123	VAL	CG1-CB-CG2	-6.46	100.57	110.90
28	15	129	LEU	CA-CB-CG	6.43	130.08	115.30
28	35	121	LEU	CB-CG-CD2	6.42	121.92	111.00
31	38	61	ARG	CG-CD-NE	6.37	125.19	111.80
28	15	121	LEU	CB-CG-CD2	6.32	121.75	111.00
26	13	88	ASP	CB-CG-OD2	-6.27	112.66	118.30
31	38	50	LEU	CB-CG-CD1	6.25	121.62	111.00
24	11	32	GLU	OE1-CD-OE2	-6.22	115.84	123.30
28	35	91	LEU	CB-CG-CD1	-6.18	100.50	111.00
26	33	175	MET	CA-CB-CG	-6.17	102.81	113.30
27	34	154	GLU	CB-CA-C	-6.13	98.13	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	18	61	ARG	NE-CZ-NH1	6.11	123.35	120.30
24	11	58	GLU	OE1-CD-OE2	-6.10	115.98	123.30
26	13	175	MET	CA-CB-CG	-6.09	102.95	113.30
28	15	121	LEU	CA-CB-CG	6.09	129.30	115.30
34	41	169	ARG	CG-CD-NE	-6.03	99.15	111.80
34	21	169	ARG	CG-CD-NE	-6.02	99.15	111.80
28	15	188	MET	CB-CG-SD	6.01	130.42	112.40
28	35	121	LEU	CA-CB-CG	6.00	129.11	115.30
31	38	61	ARG	CB-CG-CD	5.99	127.17	111.60
34	21	187	MET	CG-SD-CE	-5.98	90.63	100.20
30	17	107	ASP	CB-CG-OD1	5.97	123.68	118.30
34	41	187	MET	CG-SD-CE	-5.96	90.67	100.20
32	19	248	GLU	CA-CB-CG	-5.90	100.42	113.40
31	38	117	LEU	CB-CG-CD2	-5.87	101.02	111.00
31	18	117	LEU	CB-CG-CD2	-5.81	101.12	111.00
30	37	107	ASP	CB-CG-OD1	5.79	123.52	118.30
31	18	61	ARG	CB-CG-CD	5.75	126.54	111.60
31	38	57	PHE	CB-CG-CD2	5.69	124.78	120.80
33	20	150	VAL	CG1-CB-CG2	-5.68	101.81	110.90
33	40	150	VAL	CG1-CB-CG2	-5.68	101.81	110.90
30	17	45	ASP	CB-CG-OD1	5.68	123.41	118.30
28	35	129	LEU	CA-CB-CG	5.67	128.34	115.30
28	15	45	ASP	CB-CG-OD1	5.64	123.38	118.30
31	18	60	ARG	CD-NE-CZ	5.57	131.40	123.60
33	20	181	LEU	CB-CG-CD2	-5.57	101.54	111.00
28	35	132	MET	CA-CB-CG	5.56	122.75	113.30
26	33	45	ASP	CB-CG-OD2	5.54	123.29	118.30
33	40	181	LEU	CB-CG-CD2	-5.53	101.60	111.00
32	39	248	GLU	CA-CB-CG	-5.50	101.31	113.40
32	19	182	LYS	CG-CD-CE	-5.45	95.56	111.90
26	33	47	LEU	CA-CB-CG	5.44	127.82	115.30
33	40	160	LYS	CA-CB-CG	5.41	125.31	113.40
33	20	160	LYS	CA-CB-CG	5.39	125.27	113.40
32	19	182	LYS	CD-CE-NZ	5.39	124.10	111.70
27	34	88	ASP	CB-CG-OD1	5.37	123.13	118.30
30	37	107	ASP	CB-CG-OD2	-5.34	113.50	118.30
24	31	101	ASP	CB-CG-OD1	5.29	123.06	118.30
29	16	141	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	210	LEU	CA-CB-CG	5.20	127.26	115.30
29	36	141	ASP	CB-CG-OD1	5.20	122.98	118.30
34	41	99	ASP	N-CA-CB	-5.20	101.24	110.60
1	a	210	LEU	CA-CB-CG	5.19	127.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	21	99	ASP	N-CA-CB	-5.19	101.26	110.60
31	38	61	ARG	NE-CZ-NH2	-5.19	117.71	120.30
27	14	88	ASP	CB-CG-OD1	5.18	122.96	118.30
31	38	180	ALA	C-N-CA	-5.18	108.74	121.70
31	18	60	ARG	CA-CB-CG	5.18	124.79	113.40
33	20	157	ASP	CB-CG-OD1	5.16	122.95	118.30
25	12	107	ASP	CB-CG-OD1	5.14	122.92	118.30
33	40	157	ASP	CB-CG-OD1	5.13	122.92	118.30
30	17	107	ASP	CB-CG-OD2	-5.09	113.72	118.30
27	34	154	GLU	CB-CG-CD	-5.05	100.57	114.20
29	36	112	GLN	CA-CB-CG	5.05	124.50	113.40
29	16	112	GLN	CA-CB-CG	5.02	124.44	113.40

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	0	7	UNK	Peptide
27	14	39	GLU	Peptide
29	16	146	LEU	Peptide
32	19	196	GLY	Peptide
33	20	40	LEU	Peptide
33	20	41	ASP	Peptide
33	20	86	GLU	Peptide
34	21	136	MET	Peptide
34	21	137	LYS	Peptide
34	21	41	ALA	Peptide
27	34	39	GLU	Peptide
28	35	38	THR	Peptide
28	35	39	GLU	Peptide
29	36	146	LEU	Peptide
32	39	196	GLY	Peptide
33	40	40	LEU	Peptide
33	40	41	ASP	Peptide
33	40	86	GLU	Peptide
34	41	136	MET	Peptide
34	41	137	LYS	Peptide
34	41	41	ALA	Peptide
22	5	7	UNK	Peptide
3	C	220	GLY	Peptide
13	O	58	LYS	Peptide
13	O	73	THR	Peptide

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Mol	Chain	Res	Type	Group
20	Q	61	VAL	Peptide
3	c	220	GLY	Peptide
13	o	58	LYS	Peptide
13	o	73	THR	Peptide
20	q	61	VAL	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	324 (98%)	8 (2%)	0	100	100
1	a	332/334 (99%)	324 (98%)	8 (2%)	0	100	100
2	B	482/484 (100%)	467 (97%)	15 (3%)	0	100	100
2	b	482/484 (100%)	467 (97%)	15 (3%)	0	100	100
3	C	449/451 (100%)	431 (96%)	18 (4%)	0	100	100
3	c	449/451 (100%)	431 (96%)	18 (4%)	0	100	100
4	D	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
4	d	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
5	E	73/75 (97%)	73 (100%)	0	0	100	100
5	e	73/75 (97%)	73 (100%)	0	0	100	100
6	F	26/28 (93%)	26 (100%)	0	0	100	100
6	f	26/28 (93%)	26 (100%)	0	0	100	100
7	H	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
7	h	64/66 (97%)	63 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
8	i	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
9	J	32/34 (94%)	32 (100%)	0	0	100	100
9	j	32/34 (94%)	32 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	M	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
12	m	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
13	O	243/245 (99%)	232 (96%)	11 (4%)	0	100	100
13	o	243/245 (99%)	231 (95%)	12 (5%)	0	100	100
14	T	28/30 (93%)	28 (100%)	0	0	100	100
14	t	28/30 (93%)	28 (100%)	0	0	100	100
15	U	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
15	u	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
16	V	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
16	v	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
17	Y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
17	y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
18	X	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
18	x	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
19	Z	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
19	z	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
20	Q	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
20	q	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
21	W	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
21	w	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
24	11	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
24	31	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
25	12	167/169 (99%)	160 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	32	167/169 (99%)	159 (95%)	8 (5%)	0	100	100
26	13	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
26	33	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
27	14	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	13	24
27	34	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	13	24
28	15	168/170 (99%)	147 (88%)	20 (12%)	1 (1%)	25	43
28	35	168/170 (99%)	147 (88%)	20 (12%)	1 (1%)	25	43
29	16	177/179 (99%)	171 (97%)	6 (3%)	0	100	100
29	36	177/179 (99%)	171 (97%)	6 (3%)	0	100	100
30	17	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
30	37	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
31	18	166/168 (99%)	156 (94%)	10 (6%)	0	100	100
31	38	166/168 (99%)	156 (94%)	10 (6%)	0	100	100
32	19	225/227 (99%)	211 (94%)	14 (6%)	0	100	100
32	39	225/227 (99%)	214 (95%)	11 (5%)	0	100	100
33	20	153/155 (99%)	133 (87%)	20 (13%)	0	100	100
33	40	153/155 (99%)	133 (87%)	20 (13%)	0	100	100
34	21	160/162 (99%)	142 (89%)	18 (11%)	0	100	100
34	41	160/162 (99%)	142 (89%)	18 (11%)	0	100	100
All	All	9322/9450 (99%)	8876 (95%)	440 (5%)	6 (0%)	54	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	14	39	GLU
27	34	39	GLU
27	14	40	PRO
28	15	39	GLU
27	34	40	PRO
28	35	39	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/272 (100%)	271 (100%)	1 (0%)	91	97
1	a	272/272 (100%)	271 (100%)	1 (0%)	91	97
2	B	385/385 (100%)	379 (98%)	6 (2%)	62	84
2	b	385/385 (100%)	379 (98%)	6 (2%)	62	84
3	C	356/356 (100%)	352 (99%)	4 (1%)	73	89
3	c	356/356 (100%)	352 (99%)	4 (1%)	73	89
4	D	273/273 (100%)	273 (100%)	0	100	100
4	d	273/273 (100%)	273 (100%)	0	100	100
5	E	69/69 (100%)	68 (99%)	1 (1%)	67	86
5	e	69/69 (100%)	68 (99%)	1 (1%)	67	86
6	F	22/22 (100%)	22 (100%)	0	100	100
6	f	22/22 (100%)	22 (100%)	0	100	100
7	H	55/55 (100%)	55 (100%)	0	100	100
7	h	55/55 (100%)	55 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	27/27 (100%)	27 (100%)	0	100	100
9	j	27/27 (100%)	27 (100%)	0	100	100
10	K	32/32 (100%)	30 (94%)	2 (6%)	18	34
10	k	32/32 (100%)	30 (94%)	2 (6%)	18	34
11	L	34/34 (100%)	34 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	31/31 (100%)	31 (100%)	0	100	100
12	m	31/31 (100%)	31 (100%)	0	100	100
13	O	196/198 (99%)	188 (96%)	8 (4%)	30	55
13	o	196/198 (99%)	188 (96%)	8 (4%)	30	55
14	T	27/27 (100%)	27 (100%)	0	100	100
14	t	27/27 (100%)	27 (100%)	0	100	100
15	U	77/77 (100%)	76 (99%)	1 (1%)	69	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	u	77/77 (100%)	76 (99%)	1 (1%)	69	87
16	V	114/114 (100%)	113 (99%)	1 (1%)	78	92
16	v	114/114 (100%)	113 (99%)	1 (1%)	78	92
17	Y	27/27 (100%)	27 (100%)	0	100	100
17	y	27/27 (100%)	27 (100%)	0	100	100
18	X	29/29 (100%)	28 (97%)	1 (3%)	37	63
18	x	29/29 (100%)	28 (97%)	1 (3%)	37	63
19	Z	48/48 (100%)	48 (100%)	0	100	100
19	z	48/48 (100%)	48 (100%)	0	100	100
20	Q	122/122 (100%)	120 (98%)	2 (2%)	62	84
20	q	122/122 (100%)	120 (98%)	2 (2%)	62	84
21	W	43/43 (100%)	43 (100%)	0	100	100
21	w	43/43 (100%)	43 (100%)	0	100	100
24	11	138/138 (100%)	135 (98%)	3 (2%)	52	77
24	31	138/138 (100%)	137 (99%)	1 (1%)	84	94
25	12	133/133 (100%)	132 (99%)	1 (1%)	81	93
25	32	133/133 (100%)	133 (100%)	0	100	100
26	13	134/134 (100%)	131 (98%)	3 (2%)	52	77
26	33	134/134 (100%)	130 (97%)	4 (3%)	41	68
27	14	136/136 (100%)	134 (98%)	2 (2%)	65	85
27	34	136/136 (100%)	133 (98%)	3 (2%)	52	77
28	15	135/135 (100%)	122 (90%)	13 (10%)	8	16
28	35	135/135 (100%)	122 (90%)	13 (10%)	8	16
29	16	137/137 (100%)	129 (94%)	8 (6%)	20	38
29	36	137/137 (100%)	129 (94%)	8 (6%)	20	38
30	17	137/137 (100%)	128 (93%)	9 (7%)	16	32
30	37	137/137 (100%)	131 (96%)	6 (4%)	28	52
31	18	133/133 (100%)	126 (95%)	7 (5%)	22	43
31	38	133/133 (100%)	123 (92%)	10 (8%)	13	26
32	19	174/174 (100%)	168 (97%)	6 (3%)	37	63
32	39	174/174 (100%)	166 (95%)	8 (5%)	27	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	20	121/121 (100%)	110 (91%)	11 (9%)	9 18
33	40	121/121 (100%)	110 (91%)	11 (9%)	9 18
34	21	129/129 (100%)	111 (86%)	18 (14%)	3 6
34	41	129/129 (100%)	111 (86%)	18 (14%)	3 6
All	All	7560/7564 (100%)	7343 (97%)	217 (3%)	45 69

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	SER
2	B	22	VAL
2	B	348	ASP
2	B	388	SER
2	B	391	SER
2	B	435	THR
2	B	446	SER
3	C	28	SER
3	C	328	SER
3	C	376	ASN
3	C	470	ILE
5	E	13	ASP
10	K	17	SER
10	K	22	VAL
13	O	69	SER
13	O	87	THR
13	O	133	THR
13	O	179	GLU
13	O	210	GLU
13	O	212	SER
13	O	221	THR
13	O	232	THR
15	U	22	SER
16	V	86	GLU
18	X	36	LEU
20	Q	158	SER
20	Q	161	THR
1	a	264	SER
2	b	22	VAL
2	b	348	ASP
2	b	388	SER
2	b	391	SER

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Mol	Chain	Res	Type
2	b	435	THR
2	b	446	SER
3	c	28	SER
3	c	328	SER
3	c	376	ASN
3	c	470	ILE
5	e	13	ASP
10	k	17	SER
10	k	22	VAL
13	o	69	SER
13	o	87	THR
13	o	133	THR
13	o	179	GLU
13	o	210	GLU
13	o	212	SER
13	o	221	THR
13	o	232	THR
15	u	22	SER
16	v	86	GLU
18	x	36	LEU
20	q	158	SER
20	q	161	THR
24	11	58	GLU
24	11	66	LYS
24	11	88	ASP
25	12	38	THR
26	13	58	GLU
26	13	154	GLU
26	13	155	GLU
27	14	34	GLU
27	14	154	GLU
28	15	41	LEU
28	15	47	LEU
28	15	53	GLU
28	15	66	LYS
28	15	91	LEU
28	15	98	LYS
28	15	100	SER
28	15	117	LEU
28	15	121	LEU
28	15	135	SER
28	15	152	ASP

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Mol	Chain	Res	Type
28	15	179	VAL
28	15	188	MET
29	16	95	SER
29	16	102	ASP
29	16	104	ASP
29	16	123	LEU
29	16	136	SER
29	16	141	ASP
29	16	146	LEU
29	16	154	GLU
30	17	39	GLU
30	17	41	LEU
30	17	43	VAL
30	17	47	LEU
30	17	107	ASP
30	17	112	VAL
30	17	120	ILE
30	17	140	ASP
30	17	150	ILE
31	18	57	PHE
31	18	60	ARG
31	18	107	ASP
31	18	117	LEU
31	18	149	ASP
31	18	155	GLU
31	18	175	MET
32	19	48	ASP
32	19	75	ASP
32	19	123	VAL
32	19	181	ILE
32	19	208	ASP
32	19	255	THR
33	20	29	GLU
33	20	37	LEU
33	20	58	GLU
33	20	79	LEU
33	20	106	MET
33	20	112	ILE
33	20	150	VAL
33	20	155	GLU
33	20	160	LYS
33	20	165	MET

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Mol	Chain	Res	Type
33	20	182	VAL
34	21	37	ASN
34	21	55	GLU
34	21	61	LYS
34	21	70	LEU
34	21	90	ILE
34	21	99	ASP
34	21	113	LEU
34	21	114	SER
34	21	133	VAL
34	21	136	MET
34	21	137	LYS
34	21	138	ASP
34	21	143	GLU
34	21	162	GLU
34	21	167	LYS
34	21	169	ARG
34	21	186	LEU
34	21	195	SER
24	31	88	ASP
26	33	58	GLU
26	33	88	ASP
26	33	154	GLU
26	33	155	GLU
27	34	32	GLU
27	34	34	GLU
27	34	154	GLU
28	35	41	LEU
28	35	47	LEU
28	35	55	GLU
28	35	66	LYS
28	35	91	LEU
28	35	96	ASN
28	35	98	LYS
28	35	117	LEU
28	35	121	LEU
28	35	179	VAL
28	35	181	GLU
28	35	188	MET
28	35	194	SER
29	36	95	SER
29	36	102	ASP

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Mol	Chain	Res	Type
29	36	104	ASP
29	36	123	LEU
29	36	136	SER
29	36	141	ASP
29	36	146	LEU
29	36	154	GLU
30	37	43	VAL
30	37	47	LEU
30	37	53	GLU
30	37	112	VAL
30	37	140	ASP
30	37	150	ILE
31	38	50	LEU
31	38	57	PHE
31	38	66	LYS
31	38	76	VAL
31	38	106	VAL
31	38	107	ASP
31	38	117	LEU
31	38	149	ASP
31	38	155	GLU
31	38	175	MET
32	39	75	ASP
32	39	114	ILE
32	39	123	VAL
32	39	139	GLU
32	39	149	LEU
32	39	181	ILE
32	39	208	ASP
32	39	255	THR
33	40	29	GLU
33	40	37	LEU
33	40	58	GLU
33	40	79	LEU
33	40	106	MET
33	40	112	ILE
33	40	150	VAL
33	40	155	GLU
33	40	160	LYS
33	40	165	MET
33	40	182	VAL
34	41	37	ASN

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Mol	Chain	Res	Type
34	41	55	GLU
34	41	61	LYS
34	41	70	LEU
34	41	90	ILE
34	41	99	ASP
34	41	113	LEU
34	41	114	SER
34	41	133	VAL
34	41	136	MET
34	41	137	LYS
34	41	138	ASP
34	41	143	GLU
34	41	162	GLU
34	41	167	LYS
34	41	169	ARG
34	41	186	LEU
34	41	195	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
2	B	179	GLN
2	B	331	ASN
2	B	457	ASN
3	C	203	ASN
3	C	227	ASN
3	C	311	GLN
3	C	413	ASN
3	C	416	ASN
4	D	229	ASN
5	E	59	GLN
5	E	62	GLN
7	H	50	ASN
11	L	5	ASN
13	O	13	GLN
15	U	28	ASN
15	U	31	ASN
20	Q	121	ASN
20	Q	162	GLN
20	Q	192	ASN
1	a	26	ASN

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Mol	Chain	Res	Type
2	b	179	GLN
2	b	331	ASN
2	b	457	ASN
3	c	203	ASN
3	c	227	ASN
3	c	311	GLN
3	c	413	ASN
3	c	416	ASN
4	d	229	ASN
5	e	59	GLN
5	e	62	GLN
7	h	50	ASN
11	l	5	ASN
13	o	13	GLN
15	u	28	ASN
15	u	31	ASN
20	q	121	ASN
20	q	162	GLN
20	q	192	ASN
24	11	161	ASN
25	12	161	ASN
26	13	161	ASN
27	14	177	ASN
28	15	161	ASN
30	17	83	ASN
31	18	83	ASN
31	18	191	GLN
32	19	120	GLN
24	31	161	ASN
25	32	161	ASN
26	33	161	ASN
27	34	177	ASN
28	35	161	ASN
30	37	83	ASN
31	38	83	ASN
32	39	120	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 548 ligands modelled in this entry, 2 are monoatomic and 38 are unknown - leaving 508 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	CLA	B	502	-	65,73,73	1.97	15 (23%)	76,113,113	2.82	27 (35%)
48	A86	31	315	-	44,50,50	3.86	23 (52%)	51,76,76	7.78	17 (33%)
46	HEM	F	101	6,5	41,50,50	1.46	5 (12%)	45,82,82	1.39	6 (13%)
43	LHG	37	321	-	44,44,48	0.65	1 (2%)	47,50,54	1.18	3 (6%)
50	DD6	36	312	-	39,45,45	6.71	23 (58%)	52,67,67	6.77	28 (53%)
48	A86	15	316	-	44,50,50	4.11	22 (50%)	51,76,76	7.78	23 (45%)
51	LMU	39	315	-	36,36,36	1.12	2 (5%)	47,47,47	1.03	2 (4%)
37	CLA	B	508	-	65,73,73	1.93	15 (23%)	76,113,113	2.68	27 (35%)
43	LHG	21	201	-	34,34,48	0.74	1 (2%)	37,39,54	1.39	5 (13%)
48	A86	39	311	-	44,50,50	3.96	23 (52%)	51,76,76	7.78	19 (37%)
37	CLA	41	206	34	65,73,73	2.01	16 (24%)	76,113,113	2.72	27 (35%)
39	BCR	5	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	5 (8%)
48	A86	14	311	-	44,50,50	3.89	22 (50%)	51,76,76	8.34	21 (41%)
43	LHG	B	523	-	48,48,48	0.73	1 (2%)	51,54,54	1.27	6 (11%)
47	KC1	36	308	29	48,53,53	3.46	25 (52%)	55,89,89	3.65	31 (56%)
50	DD6	20	310	-	39,45,45	6.70	23 (58%)	52,67,67	7.34	27 (51%)
37	CLA	18	209	52	65,73,73	2.03	17 (26%)	76,113,113	2.66	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	CLA	D	402	52	65,73,73	1.99	16 (24%)	76,113,113	2.72	26 (34%)
37	CLA	21	210	-	45,53,73	2.48	16 (35%)	52,89,113	3.26	24 (46%)
41	LMG	31	317	-	32,32,55	0.97	1 (3%)	40,40,63	1.24	5 (12%)
46	HEM	f	101	6,5	41,50,50	1.46	4 (9%)	45,82,82	1.39	6 (13%)
48	A86	21	214	-	44,50,50	4.15	23 (52%)	51,76,76	8.33	16 (31%)
46	HEM	v	201	16	41,50,50	1.52	3 (7%)	45,82,82	1.38	5 (11%)
48	A86	37	313	-	44,50,50	3.98	23 (52%)	51,76,76	8.68	18 (35%)
37	CLA	16	301	29	65,73,73	1.97	17 (26%)	76,113,113	2.78	26 (34%)
39	BCR	K	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.28	8 (14%)
43	LHG	17	316	-	43,43,48	0.63	0	46,49,54	1.28	6 (13%)
47	KC1	18	207	31	48,53,53	3.47	26 (54%)	55,89,89	3.79	33 (60%)
37	CLA	36	301	29	65,73,73	1.97	16 (24%)	76,113,113	2.77	26 (34%)
37	CLA	40	208	33	50,58,73	2.29	17 (34%)	58,95,113	3.00	26 (44%)
37	CLA	15	307	28	52,60,73	2.27	15 (28%)	60,97,113	2.92	28 (46%)
48	A86	17	312	-	44,50,50	4.09	22 (50%)	51,76,76	7.42	19 (37%)
47	KC1	17	306	30	48,53,53	3.46	25 (52%)	55,89,89	3.72	31 (56%)
37	CLA	33	301	26	65,73,73	2.02	16 (24%)	76,113,113	2.65	24 (31%)
48	A86	32	221	-	44,50,50	3.83	22 (50%)	51,76,76	7.97	21 (41%)
50	DD6	21	216	-	39,45,45	6.79	21 (53%)	52,67,67	7.22	29 (55%)
37	CLA	b	510	52	65,73,73	1.93	16 (24%)	76,113,113	2.74	27 (35%)
37	CLA	b	512	-	65,73,73	1.93	18 (27%)	76,113,113	2.66	30 (39%)
47	KC1	35	304	28	48,53,53	3.51	26 (54%)	55,89,89	3.88	32 (58%)
47	KC1	35	306	28	48,53,53	3.48	26 (54%)	55,89,89	3.75	31 (56%)
39	BCR	C	519	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
37	CLA	20	308	-	47,55,73	2.40	17 (36%)	54,91,113	3.08	26 (48%)
47	KC1	11	309	24	48,53,53	3.34	23 (47%)	55,89,89	3.70	32 (58%)
37	CLA	12	203	25	65,73,73	1.95	17 (26%)	76,113,113	2.64	27 (35%)
37	CLA	C	506	-	65,73,73	1.97	16 (24%)	76,113,113	2.72	28 (36%)
37	CLA	c	513	-	65,73,73	1.94	16 (24%)	76,113,113	2.76	27 (35%)
47	KC1	11	306	24	48,53,53	3.38	23 (47%)	55,89,89	3.72	27 (49%)
37	CLA	A	405	-	65,73,73	1.94	17 (26%)	76,113,113	2.77	26 (34%)
37	CLA	c	507	52	65,73,73	1.95	15 (23%)	76,113,113	2.70	27 (35%)
37	CLA	b	509	-	65,73,73	1.90	14 (21%)	76,113,113	2.74	29 (38%)
44	DGD	H	102	-	63,63,67	1.03	5 (7%)	77,77,81	1.36	8 (10%)
48	A86	33	312	-	44,50,50	4.13	23 (52%)	51,76,76	7.94	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	CLA	d	404	-	65,73,73	1.95	16 (24%)	76,113,113	2.78	28 (36%)
48	A86	15	312	-	44,50,50	4.10	23 (52%)	51,76,76	7.85	19 (37%)
37	CLA	32	213	-	45,53,73	2.43	15 (33%)	52,89,113	3.21	24 (46%)
47	KC1	21	207	34	48,53,53	3.48	27 (56%)	55,89,89	3.94	32 (58%)
47	KC1	15	306	28	48,53,53	3.48	26 (54%)	55,89,89	3.76	31 (56%)
41	LMG	A	408	-	51,51,55	0.87	3 (5%)	59,59,63	1.37	7 (11%)
37	CLA	13	305	-	45,53,73	2.48	17 (37%)	52,89,113	3.17	24 (46%)
37	CLA	W	101	-	65,73,73	1.96	16 (24%)	76,113,113	2.90	29 (38%)
48	A86	15	311	-	44,50,50	4.05	22 (50%)	51,76,76	7.92	15 (29%)
50	DD6	41	212	-	39,45,45	6.75	22 (56%)	52,67,67	7.12	34 (65%)
37	CLA	18	211	-	45,53,73	2.51	16 (35%)	52,89,113	3.17	23 (44%)
37	CLA	41	208	-	65,73,73	2.07	17 (26%)	76,113,113	2.71	27 (35%)
37	CLA	39	305	32	51,59,73	2.23	15 (29%)	59,96,113	3.11	27 (45%)
48	A86	12	202	-	44,50,50	3.88	21 (47%)	51,76,76	7.73	20 (39%)
37	CLA	40	209	33	45,53,73	2.48	16 (35%)	52,89,113	3.14	25 (48%)
48	A86	33	313	-	44,50,50	4.17	24 (54%)	51,76,76	8.69	20 (39%)
39	BCR	a	413	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	6 (10%)
37	CLA	14	305	-	45,53,73	2.46	16 (35%)	52,89,113	3.16	25 (48%)
44	DGD	C	516	-	63,63,67	1.05	7 (11%)	77,77,81	1.49	14 (18%)
48	A86	20	309	-	44,50,50	4.14	23 (52%)	51,76,76	8.56	14 (27%)
48	A86	35	313	-	44,50,50	4.12	22 (50%)	51,76,76	7.52	16 (31%)
48	A86	38	215	-	44,50,50	4.04	23 (52%)	51,76,76	7.90	17 (33%)
41	LMG	c	518	-	51,51,55	0.95	4 (7%)	59,59,63	1.46	7 (11%)
47	KC1	17	305	30	48,53,53	3.44	26 (54%)	55,89,89	3.66	28 (50%)
47	KC1	38	210	31	48,53,53	3.48	25 (52%)	55,89,89	3.78	32 (58%)
37	CLA	C	507	52	65,73,73	1.95	15 (23%)	76,113,113	2.69	25 (32%)
43	LHG	D	409	-	48,48,48	0.70	1 (2%)	51,54,54	1.30	7 (13%)
37	CLA	16	303	-	57,65,73	2.17	16 (28%)	66,103,113	2.95	28 (42%)
43	LHG	b	522	-	48,48,48	0.72	1 (2%)	51,54,54	1.27	6 (11%)
37	CLA	B	506	-	65,73,73	1.89	15 (23%)	76,113,113	2.87	27 (35%)
37	CLA	b	505	-	65,73,73	1.90	15 (23%)	76,113,113	2.79	26 (34%)
42	BCT	a	411	36	2,3,3	1.34	0	2,3,3	4.09	2 (100%)
37	CLA	21	205	34	45,53,73	2.46	17 (37%)	52,89,113	3.13	24 (46%)
43	LHG	39	314	37	48,48,48	0.29	0	51,54,54	0.32	0
37	CLA	36	309	-	45,53,73	2.44	17 (37%)	52,89,113	3.33	25 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
47	KC1	34	306	27	48,53,53	3.41	23 (47%)	55,89,89	3.75	31 (56%)
47	KC1	37	307	30	48,53,53	3.47	24 (50%)	55,89,89	3.69	31 (56%)
48	A86	37	312	-	44,50,50	4.07	23 (52%)	51,76,76	8.42	20 (39%)
37	CLA	a	403	-	65,73,73	1.98	15 (23%)	76,113,113	2.74	30 (39%)
47	KC1	20	305	33	48,53,53	3.46	25 (52%)	55,89,89	3.82	28 (50%)
37	CLA	35	303	-	57,65,73	2.21	17 (29%)	66,103,113	2.99	29 (43%)
48	A86	19	311	-	44,50,50	3.96	24 (54%)	51,76,76	7.78	19 (37%)
48	A86	11	319	-	44,50,50	3.84	23 (52%)	51,76,76	7.58	18 (35%)
37	CLA	36	307	52	61,69,73	2.08	17 (27%)	71,108,113	2.77	25 (35%)
48	A86	41	213	-	44,50,50	4.22	23 (52%)	51,76,76	8.17	17 (33%)
47	KC1	37	304	30	48,53,53	3.46	26 (54%)	55,89,89	3.78	31 (56%)
37	CLA	38	206	-	45,53,73	2.49	17 (37%)	52,89,113	3.22	25 (48%)
47	KC1	31	305	24	48,53,53	3.40	24 (50%)	55,89,89	3.73	28 (50%)
48	A86	15	319	-	44,50,50	4.03	23 (52%)	51,76,76	7.39	21 (41%)
37	CLA	21	209	34	45,53,73	2.50	16 (35%)	52,89,113	3.19	24 (46%)
48	A86	13	315	-	44,50,50	4.07	23 (52%)	51,76,76	7.69	20 (39%)
37	CLA	31	308	24	52,60,73	2.21	17 (32%)	60,97,113	3.10	27 (45%)
47	KC1	14	306	27	48,53,53	3.41	23 (47%)	55,89,89	3.75	31 (56%)
47	KC1	20	302	-	48,53,53	3.43	24 (50%)	55,89,89	4.04	31 (56%)
37	CLA	35	301	28	65,73,73	2.05	15 (23%)	76,113,113	2.74	24 (31%)
37	CLA	B	513	-	65,73,73	1.95	16 (24%)	76,113,113	2.76	27 (35%)
43	LHG	D	411	-	45,45,48	0.85	2 (4%)	48,51,54	1.23	7 (14%)
47	KC1	13	309	26	48,53,53	3.39	25 (52%)	55,89,89	3.72	32 (58%)
48	A86	21	213	-	44,50,50	4.23	23 (52%)	51,76,76	8.18	17 (33%)
41	LMG	36	314	-	36,36,55	0.96	1 (2%)	44,44,63	1.20	4 (9%)
50	DD6	19	312	-	39,45,45	6.59	22 (56%)	52,67,67	6.51	31 (59%)
48	A86	14	312	-	44,50,50	3.95	23 (52%)	51,76,76	7.92	22 (43%)
37	CLA	d	401	52	65,73,73	1.99	16 (24%)	76,113,113	2.72	26 (34%)
35	OEX	a	401	1,3	0,15,15	-	-	-		
44	DGD	c	516	-	63,63,67	1.05	7 (11%)	77,77,81	1.49	14 (18%)
48	A86	31	314	-	44,50,50	3.95	23 (52%)	51,76,76	8.35	22 (43%)
37	CLA	32	210	25	52,60,73	2.22	16 (30%)	60,97,113	3.03	30 (50%)
37	CLA	19	302	-	65,73,73	1.99	18 (27%)	76,113,113	2.80	27 (35%)
48	A86	11	312	-	44,50,50	3.85	22 (50%)	51,76,76	7.79	22 (43%)
37	CLA	21	208	-	65,73,73	2.07	17 (26%)	76,113,113	2.70	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	A86	41	214	-	44,50,50	4.15	23 (52%)	51,76,76	8.32	17 (33%)
37	CLA	W	102	-	65,73,73	2.05	16 (24%)	76,113,113	2.57	28 (36%)
47	KC1	16	304	29	48,53,53	3.48	26 (54%)	55,89,89	3.84	29 (52%)
39	BCR	b	517	-	41,41,41	1.23	2 (4%)	56,56,56	1.30	7 (12%)
37	CLA	b	503	-	65,73,73	1.90	15 (23%)	76,113,113	2.75	28 (36%)
37	CLA	15	301	28	65,73,73	2.05	15 (23%)	76,113,113	2.74	24 (31%)
48	A86	32	203	-	44,50,50	3.89	20 (45%)	51,76,76	7.72	21 (41%)
47	KC1	34	304	27	48,53,53	3.44	24 (50%)	55,89,89	3.91	26 (47%)
37	CLA	b	514	-	62,70,73	1.96	15 (24%)	72,109,113	2.82	29 (40%)
48	A86	32	216	-	44,50,50	4.12	22 (50%)	51,76,76	8.16	14 (27%)
48	A86	40	201	-	44,50,50	4.10	21 (47%)	51,76,76	8.50	22 (43%)
37	CLA	B	515	-	65,73,73	1.95	16 (24%)	76,113,113	2.71	29 (38%)
37	CLA	15	308	52	65,73,73	2.03	17 (26%)	76,113,113	2.72	27 (35%)
39	BCR	b	518	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	7 (12%)
47	KC1	41	203	-	48,53,53	3.50	26 (54%)	55,89,89	3.85	27 (49%)
37	CLA	41	210	-	45,53,73	2.49	16 (35%)	52,89,113	3.26	24 (46%)
48	A86	31	313	-	44,50,50	3.85	22 (50%)	51,76,76	7.12	18 (35%)
37	CLA	14	303	-	57,65,73	2.17	16 (28%)	66,103,113	3.08	32 (48%)
37	CLA	34	308	52	65,73,73	2.01	17 (26%)	76,113,113	2.70	30 (39%)
39	BCR	c	514	-	41,41,41	1.23	2 (4%)	56,56,56	1.40	10 (17%)
40	SQD	B	519	-	53,54,54	0.94	5 (9%)	62,65,65	1.69	9 (14%)
47	KC1	40	204	-	48,53,53	3.43	25 (52%)	55,89,89	4.03	31 (56%)
48	A86	11	314	-	44,50,50	3.95	22 (50%)	51,76,76	8.34	22 (43%)
47	KC1	39	308	-	48,53,53	3.39	24 (50%)	55,89,89	3.83	32 (58%)
37	CLA	37	308	52	65,73,73	2.11	17 (26%)	76,113,113	2.88	31 (40%)
47	KC1	38	205	31	48,53,53	3.51	26 (54%)	55,89,89	3.74	29 (52%)
47	KC1	17	303	-	48,53,53	3.46	25 (52%)	55,89,89	3.70	30 (54%)
37	CLA	41	209	34	45,53,73	2.50	16 (35%)	52,89,113	3.19	24 (46%)
39	BCR	c	519	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
37	CLA	c	509	-	65,73,73	2.01	15 (23%)	76,113,113	2.78	28 (36%)
37	CLA	21	206	34	65,73,73	2.01	16 (24%)	76,113,113	2.73	27 (35%)
48	A86	14	313	-	44,50,50	4.12	25 (56%)	51,76,76	7.58	19 (37%)
41	LMG	B	521	-	51,51,55	0.88	4 (7%)	59,59,63	1.31	6 (10%)
47	KC1	19	308	-	48,53,53	3.40	24 (50%)	55,89,89	3.84	32 (58%)
37	CLA	C	505	-	65,73,73	1.91	15 (23%)	76,113,113	2.74	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
47	KC1	18	210	31	48,53,53	3.48	26 (54%)	55,89,89	3.79	32 (58%)
48	A86	16	311	-	44,50,50	3.90	22 (50%)	51,76,76	7.68	22 (43%)
48	A86	36	311	-	44,50,50	3.90	22 (50%)	51,76,76	7.69	22 (43%)
37	CLA	c	501	-	65,73,73	1.91	16 (24%)	76,113,113	2.80	28 (36%)
41	LMG	b	519	-	51,51,55	0.81	1 (1%)	59,59,63	1.30	5 (8%)
37	CLA	c	504	52	65,73,73	1.92	16 (24%)	76,113,113	2.74	27 (35%)
37	CLA	19	310	32	65,73,73	1.99	16 (24%)	76,113,113	2.62	27 (35%)
43	LHG	d	408	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	7 (13%)
39	BCR	d	405	-	41,41,41	1.13	3 (7%)	56,56,56	1.27	7 (12%)
48	A86	15	314	-	44,50,50	4.19	23 (52%)	51,76,76	8.38	20 (39%)
37	CLA	36	306	29	65,73,73	2.02	16 (24%)	76,113,113	2.65	28 (36%)
37	CLA	15	305	-	45,53,73	2.49	16 (35%)	52,89,113	3.15	25 (48%)
40	SQD	A	407	-	53,54,54	0.94	6 (11%)	62,65,65	1.69	11 (17%)
48	A86	38	213	-	44,50,50	4.09	23 (52%)	51,76,76	8.05	22 (43%)
47	KC1	14	309	27	48,53,53	3.37	22 (45%)	55,89,89	3.76	31 (56%)
37	CLA	B	524	-	65,73,73	1.93	18 (27%)	76,113,113	2.70	29 (38%)
48	A86	39	313	-	44,50,50	4.17	25 (56%)	51,76,76	8.80	20 (39%)
37	CLA	b	504	-	65,73,73	1.84	16 (24%)	76,113,113	2.63	30 (39%)
43	LHG	37	315	-	43,43,48	0.63	0	46,49,54	1.29	7 (15%)
37	CLA	b	508	-	65,73,73	1.93	15 (23%)	76,113,113	2.68	27 (35%)
37	CLA	16	307	52	61,69,73	2.08	17 (27%)	71,108,113	2.76	25 (35%)
37	CLA	15	303	-	57,65,73	2.21	17 (29%)	66,103,113	2.97	30 (45%)
41	LMG	L	102	-	40,40,55	0.96	3 (7%)	48,48,63	1.32	4 (8%)
38	PHO	A	404	-	51,69,69	1.02	6 (11%)	47,99,99	1.28	6 (12%)
39	BCR	a	408	-	41,41,41	1.22	2 (4%)	56,56,56	1.30	6 (10%)
39	BCR	B	517	-	41,41,41	1.22	2 (4%)	56,56,56	1.30	8 (14%)
37	CLA	33	307	26	52,60,73	2.27	16 (30%)	60,97,113	2.84	30 (50%)
37	CLA	D	406	-	65,73,73	1.95	15 (23%)	76,113,113	2.79	27 (35%)
37	CLA	34	305	-	45,53,73	2.46	17 (37%)	52,89,113	3.16	25 (48%)
37	CLA	11	310	52	51,59,73	2.22	17 (33%)	59,96,113	2.99	27 (45%)
48	A86	18	214	-	44,50,50	4.15	23 (52%)	51,76,76	8.13	19 (37%)
37	CLA	21	202	34	57,65,73	2.21	18 (31%)	66,103,113	2.90	26 (39%)
39	BCR	A	410	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	6 (10%)
37	CLA	C	501	-	65,73,73	1.92	16 (24%)	76,113,113	2.80	27 (35%)
40	SQD	B	522	-	36,37,54	1.18	6 (16%)	45,48,65	1.67	11 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	CLA	17	304	-	56,64,73	2.20	17 (30%)	65,102,113	3.05	30 (46%)
47	KC1	17	308	30	48,53,53	3.48	24 (50%)	55,89,89	3.70	31 (56%)
37	CLA	37	301	30	65,73,73	2.06	17 (26%)	76,113,113	2.66	24 (31%)
45	PL9	d	402	-	55,55,55	1.22	4 (7%)	68,69,69	1.52	15 (22%)
37	CLA	39	306	32	65,73,73	1.95	15 (23%)	76,113,113	2.69	27 (35%)
39	BCR	0	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	5 (8%)
37	CLA	14	308	52	65,73,73	2.01	16 (24%)	76,113,113	2.72	30 (39%)
48	A86	31	311	-	44,50,50	3.83	22 (50%)	51,76,76	7.52	20 (39%)
37	CLA	B	510	52	65,73,73	1.93	16 (24%)	76,113,113	2.74	27 (35%)
37	CLA	39	310	32	65,73,73	1.99	15 (23%)	76,113,113	2.62	27 (35%)
37	CLA	11	308	52	65,73,73	1.96	16 (24%)	76,113,113	2.66	28 (36%)
39	BCR	C	514	-	41,41,41	1.23	2 (4%)	56,56,56	1.40	10 (17%)
47	KC1	13	304	26	48,53,53	3.40	23 (47%)	55,89,89	3.73	28 (50%)
37	CLA	18	203	-	65,73,73	2.06	16 (24%)	76,113,113	2.68	29 (38%)
41	LMG	D	412	-	51,51,55	0.88	4 (7%)	59,59,63	1.41	7 (11%)
47	KC1	37	302	-	48,53,53	3.47	24 (50%)	55,89,89	3.69	30 (54%)
37	CLA	13	310	-	45,53,73	2.52	16 (35%)	52,89,113	3.16	23 (44%)
48	A86	17	310	-	44,50,50	4.06	22 (50%)	51,76,76	8.41	17 (33%)
48	A86	14	316	-	44,50,50	3.99	24 (54%)	51,76,76	7.53	21 (41%)
39	BCR	B	525	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	7 (12%)
37	CLA	c	512	-	65,73,73	1.94	15 (23%)	76,113,113	2.74	29 (38%)
37	CLA	C	503	-	65,73,73	1.94	15 (23%)	76,113,113	2.83	30 (39%)
48	A86	13	314	-	44,50,50	4.17	23 (52%)	51,76,76	8.64	19 (37%)
47	KC1	40	206	33	48,53,53	3.48	24 (50%)	55,89,89	3.60	29 (52%)
48	A86	32	214	-	44,50,50	3.92	23 (52%)	51,76,76	8.09	21 (41%)
41	LMG	11	317	-	32,32,55	0.97	1 (3%)	40,40,63	1.24	5 (12%)
44	DGD	J	101	-	63,63,67	1.08	9 (14%)	77,77,81	1.50	12 (15%)
46	HEM	V	201	16	41,50,50	1.52	3 (7%)	45,82,82	1.39	5 (11%)
48	A86	21	211	-	44,50,50	4.16	23 (52%)	51,76,76	8.17	13 (25%)
37	CLA	a	404	52	65,73,73	2.01	15 (23%)	76,113,113	2.81	26 (34%)
41	LMG	C	518	-	51,51,55	0.95	4 (7%)	59,59,63	1.45	7 (11%)
37	CLA	B	516	-	65,73,73	1.91	15 (23%)	76,113,113	2.79	30 (39%)
37	CLA	35	307	28	52,60,73	2.27	15 (28%)	60,97,113	2.92	27 (45%)
48	A86	15	313	-	44,50,50	4.12	22 (50%)	51,76,76	7.52	15 (29%)
37	CLA	15	310	-	45,53,73	2.50	17 (37%)	52,89,113	3.20	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	CLA	B	501	52	65,73,73	1.97	17 (26%)	76,113,113	2.66	26 (34%)
39	BCR	h	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	5 (8%)
40	SQD	b	521	-	36,37,54	1.17	6 (16%)	45,48,65	1.67	10 (22%)
48	A86	37	311	-	44,50,50	4.09	22 (50%)	51,76,76	7.40	20 (39%)
37	CLA	38	204	-	56,64,73	2.22	16 (28%)	65,102,113	3.11	32 (49%)
37	CLA	B	504	-	65,73,73	1.84	16 (24%)	76,113,113	2.62	30 (39%)
37	CLA	39	304	32	45,53,73	2.42	17 (37%)	52,89,113	3.27	22 (42%)
48	A86	13	312	-	44,50,50	4.13	23 (52%)	51,76,76	7.95	19 (37%)
45	PL9	D	408	-	55,55,55	1.80	8 (14%)	68,69,69	1.44	12 (17%)
39	BCR	y	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.27	7 (12%)
44	DGD	h	102	-	63,63,67	1.03	5 (7%)	77,77,81	1.36	8 (10%)
37	CLA	w	101	-	65,73,73	1.95	16 (24%)	76,113,113	2.89	29 (38%)
41	LMG	b	520	-	51,51,55	0.88	4 (7%)	59,59,63	1.31	6 (10%)
48	A86	19	313	-	44,50,50	4.12	24 (54%)	51,76,76	8.79	23 (45%)
37	CLA	37	306	30	52,60,73	2.27	16 (30%)	60,97,113	2.96	29 (48%)
37	CLA	31	301	-	65,73,73	2.06	16 (24%)	76,113,113	2.58	28 (36%)
47	KC1	31	303	-	48,53,53	3.39	22 (45%)	55,89,89	3.75	28 (50%)
48	A86	16	314	-	44,50,50	3.79	23 (52%)	51,76,76	7.71	18 (35%)
37	CLA	B	512	-	65,73,73	1.93	17 (26%)	76,113,113	2.67	30 (39%)
37	CLA	19	301	32	65,73,73	1.99	16 (24%)	76,113,113	2.70	29 (38%)
48	A86	12	213	-	44,50,50	3.91	23 (52%)	51,76,76	8.08	20 (39%)
38	PHO	a	405	-	51,69,69	1.04	5 (9%)	47,99,99	1.29	7 (14%)
48	A86	34	314	-	44,50,50	4.14	23 (52%)	51,76,76	8.43	18 (35%)
47	KC1	40	207	33	48,53,53	3.46	25 (52%)	55,89,89	3.80	29 (52%)
37	CLA	12	205	-	65,73,73	1.99	15 (23%)	76,113,113	2.80	32 (42%)
37	CLA	13	307	26	52,60,73	2.27	16 (30%)	60,97,113	2.84	30 (50%)
37	CLA	33	305	-	45,53,73	2.48	17 (37%)	52,89,113	3.18	24 (46%)
48	A86	38	214	-	44,50,50	4.15	23 (52%)	51,76,76	8.19	19 (37%)
47	KC1	32	209	25	48,53,53	3.33	23 (47%)	55,89,89	3.70	31 (56%)
47	KC1	16	308	29	48,53,53	3.46	25 (52%)	55,89,89	3.65	31 (56%)
41	LMG	32	201	-	39,39,55	1.04	3 (7%)	47,47,63	1.14	2 (4%)
37	CLA	B	505	-	65,73,73	1.90	15 (23%)	76,113,113	2.79	26 (34%)
48	A86	17	315	-	44,50,50	4.04	24 (54%)	51,76,76	7.86	19 (37%)
37	CLA	20	306	33	50,58,73	2.29	16 (32%)	58,95,113	3.01	26 (44%)
37	CLA	33	303	-	57,65,73	2.18	16 (28%)	66,103,113	2.96	30 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
37	CLA	d	403	-	65,73,73	1.88	16 (24%)	76,113,113	2.91	29 (38%)
40	SQD	40	202	-	53,54,54	0.96	6 (11%)	62,65,65	1.61	10 (16%)
47	KC1	11	304	24	48,53,53	3.42	24 (50%)	55,89,89	3.73	28 (50%)
40	SQD	16	315	-	53,54,54	0.96	6 (11%)	62,65,65	1.61	10 (16%)
41	LMG	12	201	-	39,39,55	1.04	3 (7%)	47,47,63	1.14	2 (4%)
47	KC1	33	304	26	48,53,53	3.41	23 (47%)	55,89,89	3.74	28 (50%)
37	CLA	c	503	-	65,73,73	1.94	16 (24%)	76,113,113	2.83	30 (39%)
47	KC1	33	306	26	48,53,53	3.39	24 (50%)	55,89,89	3.73	30 (54%)
41	LMG	17	317	-	37,37,55	0.97	2 (5%)	45,45,63	1.28	5 (11%)
37	CLA	C	511	3	65,73,73	1.96	17 (26%)	76,113,113	2.68	29 (38%)
37	CLA	C	504	52	65,73,73	1.92	16 (24%)	76,113,113	2.74	27 (35%)
48	A86	35	315	-	44,50,50	4.05	24 (54%)	51,76,76	7.81	21 (41%)
37	CLA	13	301	26	65,73,73	2.02	16 (24%)	76,113,113	2.65	24 (31%)
44	DGD	c	517	-	63,63,67	1.21	8 (12%)	77,77,81	1.50	13 (16%)
47	KC1	20	304	33	48,53,53	3.47	24 (50%)	55,89,89	3.59	29 (52%)
37	CLA	38	209	52	65,73,73	2.04	16 (24%)	76,113,113	2.68	27 (35%)
37	CLA	12	210	52	65,73,73	2.01	18 (27%)	76,113,113	2.64	27 (35%)
37	CLA	38	201	52	65,73,73	2.04	16 (24%)	76,113,113	2.66	28 (36%)
50	DD6	16	312	-	39,45,45	6.73	23 (58%)	52,67,67	6.79	28 (53%)
48	A86	12	220	-	44,50,50	3.83	22 (50%)	51,76,76	7.96	21 (41%)
48	A86	37	319	-	44,50,50	4.01	23 (52%)	51,76,76	7.77	21 (41%)
37	CLA	12	204	-	65,73,73	1.93	17 (26%)	76,113,113	2.46	27 (35%)
37	CLA	32	208	52	50,58,73	2.29	17 (34%)	58,95,113	3.16	30 (51%)
37	CLA	36	303	-	57,65,73	2.17	17 (29%)	66,103,113	2.94	29 (43%)
43	LHG	D	410	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	7 (13%)
41	LMG	a	410	-	51,51,55	0.87	3 (5%)	59,59,63	1.37	7 (11%)
47	KC1	13	302	-	48,53,53	3.42	27 (56%)	55,89,89	3.91	30 (54%)
37	CLA	38	202	31	65,73,73	2.04	15 (23%)	76,113,113	2.76	28 (36%)
37	CLA	b	502	-	65,73,73	1.97	15 (23%)	76,113,113	2.82	28 (36%)
37	CLA	38	211	-	45,53,73	2.54	16 (35%)	52,89,113	3.13	23 (44%)
47	KC1	34	309	27	48,53,53	3.36	22 (45%)	55,89,89	3.76	30 (54%)
37	CLA	20	301	33	56,64,73	2.19	17 (30%)	65,102,113	3.05	28 (43%)
37	CLA	z	102	33	45,53,73	2.51	16 (35%)	52,89,113	3.19	27 (51%)
37	CLA	35	305	-	45,53,73	2.49	16 (35%)	52,89,113	3.12	25 (48%)
47	KC1	16	305	29	48,53,53	3.48	25 (52%)	55,89,89	3.69	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
41	LMG	B	520	-	51,51,55	0.82	1 (1%)	59,59,63	1.30	5 (8%)
48	A86	11	313	-	44,50,50	3.82	22 (50%)	51,76,76	7.06	18 (35%)
43	LHG	41	201	-	34,34,48	0.74	1 (2%)	37,39,54	1.39	5 (13%)
41	LMG	37	316	-	37,37,55	0.97	2 (5%)	45,45,63	1.27	5 (11%)
48	A86	38	212	-	44,50,50	4.10	23 (52%)	51,76,76	8.13	18 (35%)
47	KC1	11	302	-	48,53,53	3.39	22 (45%)	55,89,89	3.75	28 (50%)
48	A86	33	311	-	44,50,50	3.95	23 (52%)	51,76,76	8.00	20 (39%)
48	A86	37	309	-	44,50,50	4.06	22 (50%)	51,76,76	8.40	17 (33%)
48	A86	34	313	-	44,50,50	4.12	23 (52%)	51,76,76	7.57	19 (37%)
47	KC1	15	302	-	48,53,53	3.47	26 (54%)	55,89,89	3.85	31 (56%)
37	CLA	19	309	32	45,53,73	2.41	16 (35%)	52,89,113	3.12	24 (46%)
47	KC1	15	304	28	48,53,53	3.49	26 (54%)	55,89,89	3.87	31 (56%)
39	BCR	C	515	-	41,41,41	1.20	2 (4%)	56,56,56	1.24	6 (10%)
50	DD6	39	312	-	39,45,45	6.59	22 (56%)	52,67,67	6.51	31 (59%)
48	A86	13	311	-	44,50,50	3.96	23 (52%)	51,76,76	8.00	21 (41%)
37	CLA	C	508	-	65,73,73	1.95	15 (23%)	76,113,113	2.75	25 (32%)
48	A86	34	311	-	44,50,50	3.90	22 (50%)	51,76,76	8.35	21 (41%)
37	CLA	39	303	52	65,73,73	2.00	17 (26%)	76,113,113	2.79	26 (34%)
42	BCT	A	409	36	2,3,3	1.34	0	2,3,3	4.09	2 (100%)
37	CLA	41	204	-	58,66,73	2.20	17 (29%)	67,104,113	3.01	31 (46%)
37	CLA	b	515	-	65,73,73	1.95	16 (24%)	76,113,113	2.72	29 (38%)
48	A86	37	314	-	44,50,50	4.04	24 (54%)	51,76,76	7.85	19 (37%)
37	CLA	D	401	52	65,73,73	2.01	15 (23%)	76,113,113	2.80	26 (34%)
39	BCR	H	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.24	6 (10%)
48	A86	17	313	-	44,50,50	4.07	23 (52%)	51,76,76	8.39	20 (39%)
37	CLA	Z	102	33	45,53,73	2.50	17 (37%)	52,89,113	3.18	27 (51%)
37	CLA	38	208	31	53,61,73	2.24	17 (32%)	61,98,113	2.89	26 (42%)
48	A86	35	311	-	44,50,50	4.04	22 (50%)	51,76,76	7.93	15 (29%)
37	CLA	B	503	-	65,73,73	1.90	15 (23%)	76,113,113	2.75	28 (36%)
47	KC1	32	207	25	48,53,53	3.34	22 (45%)	55,89,89	3.63	26 (47%)
47	KC1	33	309	26	48,53,53	3.40	24 (50%)	55,89,89	3.72	32 (58%)
39	BCR	B	518	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	7 (12%)
37	CLA	20	307	33	45,53,73	2.49	16 (35%)	52,89,113	3.14	25 (48%)
51	LMU	19	315	-	36,36,36	1.13	2 (5%)	47,47,47	1.04	3 (6%)
47	KC1	35	309	28	48,53,53	3.48	24 (50%)	55,89,89	3.63	31 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	A86	35	312	-	44,50,50	4.11	23 (52%)	51,76,76	7.85	20 (39%)
48	A86	14	315	-	44,50,50	3.99	23 (52%)	51,76,76	8.04	18 (35%)
48	A86	41	211	-	44,50,50	4.17	23 (52%)	51,76,76	8.18	13 (25%)
43	LHG	d	407	-	48,48,48	0.70	1 (2%)	51,54,54	1.30	7 (13%)
50	DD6	20	312	-	39,45,45	6.85	22 (56%)	52,67,67	6.89	31 (59%)
37	CLA	11	301	24	65,73,73	1.92	15 (23%)	76,113,113	2.71	27 (35%)
37	CLA	19	306	32	65,73,73	1.95	15 (23%)	76,113,113	2.69	27 (35%)
47	KC1	41	207	34	48,53,53	3.49	27 (56%)	55,89,89	3.94	31 (56%)
37	CLA	12	212	-	45,53,73	2.43	15 (33%)	52,89,113	3.22	24 (46%)
37	CLA	37	303	-	56,64,73	2.20	15 (26%)	65,102,113	3.05	30 (46%)
48	A86	41	215	-	44,50,50	4.00	23 (52%)	51,76,76	8.34	18 (35%)
37	CLA	32	211	52	65,73,73	2.00	17 (26%)	76,113,113	2.64	27 (35%)
48	A86	21	215	-	44,50,50	4.00	23 (52%)	51,76,76	8.33	18 (35%)
50	DD6	41	216	-	39,45,45	6.80	21 (53%)	52,67,67	7.21	29 (55%)
37	CLA	b	523	-	65,73,73	1.92	19 (29%)	76,113,113	2.70	29 (38%)
37	CLA	b	511	-	65,73,73	1.97	15 (23%)	76,113,113	2.76	28 (36%)
37	CLA	14	310	-	45,53,73	2.44	17 (37%)	52,89,113	3.17	24 (46%)
45	PL9	D	404	-	55,55,55	1.22	4 (7%)	68,69,69	1.52	14 (20%)
39	BCR	c	515	-	41,41,41	1.20	2 (4%)	56,56,56	1.24	6 (10%)
37	CLA	c	508	-	65,73,73	1.96	15 (23%)	76,113,113	2.76	25 (32%)
37	CLA	19	304	32	45,53,73	2.42	17 (37%)	52,89,113	3.27	22 (42%)
50	DD6	21	212	-	39,45,45	6.74	22 (56%)	52,67,67	7.11	34 (65%)
47	KC1	21	203	-	48,53,53	3.49	26 (54%)	55,89,89	3.84	27 (49%)
48	A86	40	213	-	44,50,50	4.22	23 (52%)	51,76,76	8.69	16 (31%)
37	CLA	z	101	52	65,73,73	2.05	16 (24%)	76,113,113	2.73	26 (34%)
37	CLA	17	307	30	52,60,73	2.27	16 (30%)	60,97,113	2.97	29 (48%)
48	A86	17	314	-	44,50,50	3.96	23 (52%)	51,76,76	8.68	17 (33%)
35	OEX	A	401	1,3	0,15,15	-	-	-		
37	CLA	32	205	-	65,73,73	1.93	17 (26%)	76,113,113	2.46	26 (34%)
48	A86	31	312	-	44,50,50	3.84	22 (50%)	51,76,76	7.79	22 (43%)
37	CLA	18	202	31	65,73,73	1.99	16 (24%)	76,113,113	2.85	28 (36%)
47	KC1	36	305	29	48,53,53	3.48	25 (52%)	55,89,89	3.69	28 (50%)
48	A86	35	316	-	44,50,50	4.09	23 (52%)	51,76,76	7.79	23 (45%)
40	SQD	a	409	-	53,54,54	0.95	6 (11%)	62,65,65	1.69	11 (17%)
37	CLA	C	512	-	65,73,73	1.94	15 (23%)	76,113,113	2.76	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
41	LMG	31	316	-	42,42,55	1.05	3 (7%)	50,50,63	1.22	3 (6%)
48	A86	18	212	-	44,50,50	4.09	23 (52%)	51,76,76	8.13	18 (35%)
48	A86	11	311	-	44,50,50	3.83	22 (50%)	51,76,76	7.53	19 (37%)
37	CLA	33	308	52	65,73,73	2.05	17 (26%)	76,113,113	2.69	25 (32%)
48	A86	20	311	-	44,50,50	4.21	23 (52%)	51,76,76	8.69	16 (31%)
48	A86	12	217	-	44,50,50	3.99	24 (54%)	51,76,76	7.59	20 (39%)
37	CLA	C	513	-	65,73,73	1.95	16 (24%)	76,113,113	2.77	26 (34%)
47	KC1	16	302	-	48,53,53	3.51	26 (54%)	55,89,89	3.54	29 (52%)
47	KC1	36	302	-	48,53,53	3.50	26 (54%)	55,89,89	3.54	29 (52%)
37	CLA	41	205	34	45,53,73	2.46	17 (37%)	52,89,113	3.13	24 (46%)
37	CLA	a	407	-	65,73,73	1.94	17 (26%)	76,113,113	2.77	27 (35%)
47	KC1	33	302	-	48,53,53	3.42	27 (56%)	55,89,89	3.92	30 (54%)
37	CLA	31	306	52	45,53,73	2.38	17 (37%)	52,89,113	3.15	25 (48%)
48	A86	32	218	-	44,50,50	3.98	24 (54%)	51,76,76	7.60	21 (41%)
50	DD6	40	212	-	39,45,45	6.69	23 (58%)	52,67,67	7.33	27 (51%)
48	A86	33	314	-	44,50,50	4.17	23 (52%)	51,76,76	8.63	19 (37%)
37	CLA	34	301	27	65,73,73	1.97	16 (24%)	76,113,113	2.71	26 (34%)
37	CLA	14	302	-	65,73,73	2.01	18 (27%)	76,113,113	2.63	26 (34%)
48	A86	35	319	-	44,50,50	4.03	23 (52%)	51,76,76	7.39	21 (41%)
48	A86	32	217	-	44,50,50	4.01	23 (52%)	51,76,76	8.24	20 (39%)
48	A86	17	320	-	44,50,50	3.99	23 (52%)	51,76,76	7.83	20 (39%)
37	CLA	39	301	32	65,73,73	2.00	16 (24%)	76,113,113	2.72	29 (38%)
47	KC1	14	304	27	48,53,53	3.43	24 (50%)	55,89,89	3.91	26 (47%)
37	CLA	b	506	-	65,73,73	1.89	15 (23%)	76,113,113	2.87	27 (35%)
37	CLA	19	307	43	65,73,73	1.98	16 (24%)	76,113,113	2.67	27 (35%)
37	CLA	32	206	-	65,73,73	1.98	15 (23%)	76,113,113	2.80	31 (40%)
37	CLA	40	205	-	56,64,73	2.15	16 (28%)	65,102,113	3.12	34 (52%)
37	CLA	b	507	52	65,73,73	1.98	15 (23%)	76,113,113	2.68	28 (36%)
47	KC1	31	309	24	48,53,53	3.34	22 (45%)	55,89,89	3.69	32 (58%)
48	A86	34	316	-	44,50,50	3.99	24 (54%)	51,76,76	7.54	21 (41%)
37	CLA	19	303	52	65,73,73	2.00	18 (27%)	76,113,113	2.79	26 (34%)
48	A86	16	313	-	44,50,50	4.10	21 (47%)	51,76,76	8.50	22 (43%)
47	KC1	18	205	31	48,53,53	3.51	26 (54%)	55,89,89	3.74	29 (52%)
47	KC1	12	206	25	48,53,53	3.34	22 (45%)	55,89,89	3.63	26 (47%)
44	DGD	C	517	-	63,63,67	1.21	8 (12%)	77,77,81	1.50	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	A86	18	213	-	44,50,50	3.99	22 (50%)	51,76,76	8.18	20 (39%)
47	KC1	36	304	29	48,53,53	3.47	27 (56%)	55,89,89	3.84	29 (52%)
37	CLA	c	506	-	65,73,73	1.97	16 (24%)	76,113,113	2.72	28 (36%)
37	CLA	18	208	31	53,61,73	2.24	17 (32%)	61,98,113	2.87	25 (40%)
37	CLA	12	207	52	50,58,73	2.29	17 (34%)	58,95,113	3.16	30 (51%)
37	CLA	35	308	52	65,73,73	2.03	16 (24%)	76,113,113	2.72	27 (35%)
43	LHG	19	314	37	48,48,48	0.28	0	51,54,54	0.32	0
48	A86	12	216	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
48	A86	18	215	-	44,50,50	4.02	23 (52%)	51,76,76	7.92	18 (35%)
47	KC1	32	212	25	48,53,53	3.39	23 (47%)	55,89,89	3.69	33 (60%)
48	A86	40	211	-	44,50,50	4.14	23 (52%)	51,76,76	8.57	14 (27%)
37	CLA	39	309	32	45,53,73	2.41	16 (35%)	52,89,113	3.14	24 (46%)
47	KC1	12	211	25	48,53,53	3.38	23 (47%)	55,89,89	3.68	33 (60%)
37	CLA	34	302	-	65,73,73	2.01	17 (26%)	76,113,113	2.63	26 (34%)
37	CLA	34	307	27	52,60,73	2.23	15 (28%)	60,97,113	2.90	29 (48%)
47	KC1	35	302	-	48,53,53	3.47	26 (54%)	55,89,89	3.82	30 (54%)
40	SQD	L	101	-	53,54,54	0.93	5 (9%)	62,65,65	1.68	9 (14%)
37	CLA	40	203	33	56,64,73	2.19	17 (30%)	65,102,113	3.06	28 (43%)
37	CLA	13	303	-	57,65,73	2.17	16 (28%)	66,103,113	2.93	30 (45%)
37	CLA	34	303	-	57,65,73	2.17	16 (28%)	66,103,113	3.07	32 (48%)
41	LMG	16	316	-	36,36,55	0.96	1 (2%)	44,44,63	1.21	4 (9%)
48	A86	34	312	-	44,50,50	3.95	23 (52%)	51,76,76	7.92	21 (41%)
41	LMG	11	316	-	42,42,55	1.06	3 (7%)	50,50,63	1.22	3 (6%)
37	CLA	c	505	-	65,73,73	1.90	15 (23%)	76,113,113	2.74	29 (38%)
44	DGD	j	101	-	63,63,67	1.08	9 (14%)	77,77,81	1.50	12 (15%)
48	A86	16	310	-	44,50,50	3.88	22 (50%)	51,76,76	7.70	22 (43%)
48	A86	36	310	-	44,50,50	3.89	23 (52%)	51,76,76	7.71	22 (43%)
47	KC1	31	307	24	48,53,53	3.37	22 (45%)	55,89,89	3.72	27 (49%)
47	KC1	13	306	26	48,53,53	3.39	24 (50%)	55,89,89	3.74	30 (54%)
47	KC1	37	305	30	48,53,53	3.46	25 (52%)	55,89,89	3.71	31 (56%)
45	PL9	d	406	-	55,55,55	1.81	9 (16%)	68,69,69	1.44	12 (17%)
37	CLA	14	307	27	52,60,73	2.23	16 (30%)	60,97,113	2.90	29 (48%)
48	A86	37	310	-	44,50,50	4.01	23 (52%)	51,76,76	7.62	19 (37%)
43	LHG	21	217	-	44,44,48	0.64	1 (2%)	47,50,54	1.18	3 (6%)
39	BCR	A	406	-	41,41,41	1.23	2 (4%)	56,56,56	1.30	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	A86	14	314	-	44,50,50	4.14	23 (52%)	51,76,76	8.44	18 (35%)
37	CLA	18	206	-	45,53,73	2.50	17 (37%)	52,89,113	3.19	25 (48%)
37	CLA	b	516	-	65,73,73	1.91	15 (23%)	76,113,113	2.79	30 (39%)
48	A86	34	315	-	44,50,50	3.98	23 (52%)	51,76,76	8.03	18 (35%)
47	KC1	12	208	25	48,53,53	3.33	23 (47%)	55,89,89	3.69	32 (58%)
40	SQD	17	301	-	48,49,54	1.01	5 (10%)	57,60,65	1.56	10 (17%)
37	CLA	32	202	52	65,73,73	1.96	16 (24%)	76,113,113	2.65	28 (36%)
38	PHO	D	403	-	51,69,69	1.03	5 (9%)	47,99,99	1.29	7 (14%)
37	CLA	c	502	-	65,73,73	1.89	15 (23%)	76,113,113	2.66	26 (34%)
37	CLA	D	405	-	65,73,73	1.88	16 (24%)	76,113,113	2.92	29 (38%)
37	CLA	C	509	-	65,73,73	2.01	15 (23%)	76,113,113	2.78	28 (36%)
48	A86	35	314	-	44,50,50	4.17	23 (52%)	51,76,76	8.46	20 (39%)
37	CLA	11	307	24	52,60,73	2.21	17 (32%)	60,97,113	3.11	27 (45%)
48	A86	17	311	-	44,50,50	4.02	23 (52%)	51,76,76	7.61	20 (39%)
37	CLA	c	511	3	65,73,73	1.97	17 (26%)	76,113,113	2.67	29 (38%)
48	A86	33	315	-	44,50,50	4.06	23 (52%)	51,76,76	7.68	19 (37%)
43	LHG	a	412	-	45,45,48	0.85	2 (4%)	48,51,54	1.23	7 (14%)
37	CLA	11	303	-	65,73,73	1.98	16 (24%)	76,113,113	2.81	32 (42%)
48	A86	31	319	-	44,50,50	3.83	23 (52%)	51,76,76	7.59	18 (35%)
37	CLA	18	201	52	65,73,73	2.01	17 (26%)	76,113,113	2.70	27 (35%)
38	PHO	a	406	-	51,69,69	1.02	5 (9%)	47,99,99	1.27	6 (12%)
37	CLA	32	204	25	65,73,73	1.95	17 (26%)	76,113,113	2.64	27 (35%)
41	LMG	d	409	-	51,51,55	0.88	4 (7%)	59,59,63	1.41	7 (11%)
47	KC1	38	207	31	48,53,53	3.49	26 (54%)	55,89,89	3.82	34 (61%)
37	CLA	b	513	-	65,73,73	1.94	16 (24%)	76,113,113	2.75	27 (35%)
48	A86	36	313	-	44,50,50	3.78	23 (52%)	51,76,76	7.71	18 (35%)
37	CLA	Z	101	52	65,73,73	2.06	16 (24%)	76,113,113	2.73	26 (34%)
37	CLA	19	305	32	51,59,73	2.23	15 (29%)	59,96,113	3.11	26 (44%)
37	CLA	C	510	-	65,73,73	1.98	16 (24%)	76,113,113	2.75	26 (34%)
37	CLA	41	202	34	57,65,73	2.21	18 (31%)	66,103,113	2.89	26 (39%)
40	SQD	36	315	-	48,49,54	1.00	5 (10%)	57,60,65	1.56	10 (17%)
37	CLA	16	309	-	45,53,73	2.44	17 (37%)	52,89,113	3.34	25 (48%)
37	CLA	34	310	-	45,53,73	2.45	17 (37%)	52,89,113	3.18	23 (44%)
37	CLA	20	303	-	56,64,73	2.15	17 (30%)	65,102,113	3.12	34 (52%)
37	CLA	39	307	43	65,73,73	2.03	17 (26%)	76,113,113	2.68	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
37	CLA	31	302	24	65,73,73	1.93	15 (23%)	76,113,113	2.71	27 (35%)
37	CLA	33	310	-	45,53,73	2.53	16 (35%)	52,89,113	3.18	23 (44%)
41	LMG	l	101	-	40,40,55	0.96	3 (7%)	48,48,63	1.32	4 (8%)
37	CLA	17	302	30	65,73,73	2.04	17 (26%)	76,113,113	2.50	23 (30%)
37	CLA	18	204	-	56,64,73	2.21	16 (28%)	65,102,113	3.10	32 (49%)
37	CLA	38	203	-	65,73,73	2.06	17 (26%)	76,113,113	2.69	29 (38%)
48	A86	32	215	-	44,50,50	3.89	23 (52%)	51,76,76	7.84	17 (33%)
37	CLA	C	502	-	65,73,73	1.89	15 (23%)	76,113,113	2.65	26 (34%)
48	A86	13	313	-	44,50,50	4.18	24 (54%)	51,76,76	8.70	20 (39%)
39	BCR	D	407	-	41,41,41	1.13	3 (7%)	56,56,56	1.27	7 (12%)
37	CLA	11	305	52	45,53,73	2.38	17 (37%)	52,89,113	3.14	25 (48%)
37	CLA	B	511	-	65,73,73	1.96	15 (23%)	76,113,113	2.77	28 (36%)
37	CLA	16	306	29	65,73,73	2.02	15 (23%)	76,113,113	2.64	28 (36%)
37	CLA	c	510	-	65,73,73	1.98	16 (24%)	76,113,113	2.74	26 (34%)
37	CLA	B	509	-	65,73,73	1.90	14 (21%)	76,113,113	2.74	29 (38%)
37	CLA	13	308	52	65,73,73	2.05	17 (26%)	76,113,113	2.68	26 (34%)
47	KC1	15	309	28	48,53,53	3.47	24 (50%)	55,89,89	3.63	31 (56%)
37	CLA	B	507	52	65,73,73	1.98	15 (23%)	76,113,113	2.68	28 (36%)
48	A86	12	215	-	44,50,50	4.12	22 (50%)	51,76,76	8.17	14 (27%)
37	CLA	40	210	-	47,55,73	2.39	17 (36%)	54,91,113	3.08	26 (48%)
37	CLA	A	403	-	65,73,73	1.99	15 (23%)	76,113,113	2.73	29 (38%)
37	CLA	b	501	52	65,73,73	1.97	17 (26%)	76,113,113	2.66	26 (34%)
37	CLA	14	301	27	65,73,73	1.97	16 (24%)	76,113,113	2.70	27 (35%)
37	CLA	31	304	-	65,73,73	1.98	16 (24%)	76,113,113	2.80	32 (42%)
48	A86	11	315	-	44,50,50	3.87	23 (52%)	51,76,76	7.78	17 (33%)
39	BCR	b	524	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	7 (12%)
37	CLA	12	209	25	52,60,73	2.22	17 (32%)	60,97,113	3.03	31 (51%)
37	CLA	B	514	-	62,70,73	1.96	16 (25%)	72,109,113	2.83	29 (40%)
48	A86	15	315	-	44,50,50	4.05	24 (54%)	51,76,76	7.84	22 (43%)
48	A86	12	214	-	44,50,50	3.90	23 (52%)	51,76,76	7.84	17 (33%)
50	DD6	40	214	-	39,45,45	6.84	22 (56%)	52,67,67	6.90	31 (59%)
37	CLA	21	204	-	58,66,73	2.21	16 (27%)	67,104,113	3.01	31 (46%)
37	CLA	39	302	-	65,73,73	1.99	18 (27%)	76,113,113	2.82	27 (35%)
37	CLA	17	309	52	65,73,73	2.12	16 (24%)	76,113,113	2.86	31 (40%)
37	CLA	35	310	-	45,53,73	2.51	16 (35%)	52,89,113	3.22	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	CLA	31	310	52	51,59,73	2.22	17 (33%)	59,96,113	2.99	27 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	B	502	-	1/1/15/20	9/37/115/115	-
48	A86	31	315	-	-	6/34/90/90	0/3/3/3
46	HEM	F	101	6,5	-	8/12/54/54	-
43	LHG	37	321	-	-	28/49/49/53	-
50	DD6	36	312	-	-	12/26/80/80	0/3/3/3
48	A86	15	316	-	-	15/34/90/90	0/3/3/3
51	LMU	39	315	-	-	6/21/61/61	0/2/2/2
37	CLA	B	508	-	-	5/37/115/115	-
43	LHG	21	201	-	-	21/38/38/53	-
48	A86	39	311	-	-	7/34/90/90	0/3/3/3
37	CLA	41	206	34	1/1/15/20	15/37/115/115	-
39	BCR	5	101	-	-	8/29/63/63	0/2/2/2
48	A86	14	311	-	-	7/34/90/90	0/3/3/3
43	LHG	B	523	-	-	19/53/53/53	-
47	KC1	36	308	29	-	4/15/71/71	-
50	DD6	20	310	-	-	14/26/80/80	0/3/3/3
37	CLA	18	209	52	1/1/15/20	10/37/115/115	-
37	CLA	D	402	52	-	14/37/115/115	-
37	CLA	21	210	-	-	4/13/91/115	-
41	LMG	31	317	-	-	14/27/47/70	0/1/1/1
46	HEM	f	101	6,5	-	8/12/54/54	-
48	A86	21	214	-	-	6/34/90/90	0/3/3/3
46	HEM	v	201	16	-	4/12/54/54	-
48	A86	37	313	-	-	8/34/90/90	0/3/3/3
37	CLA	16	301	29	-	9/37/115/115	-
39	BCR	K	101	-	-	16/29/63/63	0/2/2/2
43	LHG	17	316	-	-	29/48/48/53	-
47	KC1	18	207	31	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	40	208	33	1/1/12/20	6/19/97/115	-
37	CLA	36	301	29	-	9/37/115/115	-
37	CLA	15	307	28	1/1/12/20	12/22/100/115	-
48	A86	17	312	-	-	8/34/90/90	0/3/3/3
47	KC1	17	306	30	-	9/15/71/71	-
37	CLA	33	301	26	-	12/37/115/115	-
48	A86	32	221	-	-	9/34/90/90	0/3/3/3
50	DD6	21	216	-	-	15/26/80/80	0/3/3/3
37	CLA	b	510	52	1/1/15/20	8/37/115/115	-
37	CLA	b	512	-	1/1/15/20	8/37/115/115	-
47	KC1	35	304	28	-	6/15/71/71	-
47	KC1	35	306	28	-	7/15/71/71	-
39	BCR	C	519	-	-	7/29/63/63	0/2/2/2
37	CLA	20	308	-	1/1/11/20	2/16/94/115	-
47	KC1	11	309	24	-	8/15/71/71	-
37	CLA	12	203	25	1/1/15/20	12/37/115/115	-
37	CLA	C	506	-	1/1/15/20	14/37/115/115	-
37	CLA	c	513	-	1/1/15/20	7/37/115/115	-
47	KC1	11	306	24	-	9/15/71/71	-
37	CLA	A	405	-	-	6/37/115/115	-
37	CLA	c	507	52	1/1/15/20	7/37/115/115	-
37	CLA	b	509	-	1/1/15/20	10/37/115/115	-
44	DGD	H	102	-	-	16/51/91/95	0/2/2/2
48	A86	33	312	-	-	8/34/90/90	0/3/3/3
37	CLA	d	404	-	1/1/15/20	17/37/115/115	-
48	A86	15	312	-	-	7/34/90/90	0/3/3/3
37	CLA	32	213	-	1/1/11/20	8/13/91/115	-
47	KC1	21	207	34	-	5/15/71/71	-
47	KC1	15	306	28	-	7/15/71/71	-
41	LMG	A	408	-	-	32/46/66/70	0/1/1/1
37	CLA	13	305	-	1/1/11/20	2/13/91/115	-
37	CLA	W	101	-	1/1/15/20	17/37/115/115	-
48	A86	15	311	-	-	6/34/90/90	0/3/3/3
50	DD6	41	212	-	-	13/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	41	208	-	1/1/15/20	13/37/115/115	-
37	CLA	18	211	-	-	3/13/91/115	-
37	CLA	39	305	32	1/1/12/20	5/21/99/115	-
48	A86	12	202	-	-	14/34/90/90	0/3/3/3
37	CLA	40	209	33	1/1/11/20	6/13/91/115	-
48	A86	33	313	-	-	17/34/90/90	0/3/3/3
39	BCR	a	413	-	-	8/29/63/63	0/2/2/2
37	CLA	14	305	-	1/1/11/20	3/13/91/115	-
44	DGD	C	516	-	-	17/51/91/95	0/2/2/2
48	A86	20	309	-	-	6/34/90/90	0/3/3/3
48	A86	35	313	-	-	9/34/90/90	0/3/3/3
48	A86	38	215	-	-	13/34/90/90	0/3/3/3
41	LMG	c	518	-	-	25/46/66/70	0/1/1/1
47	KC1	17	305	30	-	6/15/71/71	-
47	KC1	38	210	31	-	8/15/71/71	-
37	CLA	C	507	52	1/1/15/20	7/37/115/115	-
43	LHG	D	409	-	-	28/53/53/53	-
37	CLA	16	303	-	1/1/13/20	8/28/106/115	-
43	LHG	b	522	-	-	19/53/53/53	-
37	CLA	B	506	-	1/1/15/20	8/37/115/115	-
37	CLA	b	505	-	1/1/15/20	10/37/115/115	-
37	CLA	21	205	34	1/1/11/20	7/13/91/115	-
43	LHG	39	314	37	-	28/53/53/53	-
37	CLA	36	309	-	1/1/11/20	8/13/91/115	-
47	KC1	34	306	27	-	6/15/71/71	-
47	KC1	37	307	30	-	5/15/71/71	-
48	A86	37	312	-	-	7/34/90/90	0/3/3/3
37	CLA	a	403	-	1/1/15/20	4/37/115/115	-
47	KC1	20	305	33	-	11/15/71/71	-
37	CLA	35	303	-	-	7/28/106/115	-
48	A86	19	311	-	-	7/34/90/90	0/3/3/3
48	A86	11	319	-	-	7/34/90/90	0/3/3/3
37	CLA	36	307	52	1/1/14/20	11/33/111/115	-
48	A86	41	213	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	KC1	37	304	30	-	6/15/71/71	-
37	CLA	38	206	-	-	4/13/91/115	-
47	KC1	31	305	24	-	4/15/71/71	-
48	A86	15	319	-	-	8/34/90/90	0/3/3/3
37	CLA	21	209	34	1/1/11/20	6/13/91/115	-
48	A86	13	315	-	-	10/34/90/90	0/3/3/3
37	CLA	31	308	24	-	7/22/100/115	-
47	KC1	14	306	27	-	6/15/71/71	-
47	KC1	20	302	-	-	8/15/71/71	-
37	CLA	35	301	28	-	8/37/115/115	-
37	CLA	B	513	-	1/1/15/20	9/37/115/115	-
43	LHG	D	411	-	-	26/50/50/53	-
47	KC1	13	309	26	-	5/15/71/71	-
48	A86	21	213	-	-	8/34/90/90	0/3/3/3
41	LMG	36	314	-	-	14/31/51/70	0/1/1/1
50	DD6	19	312	-	-	12/26/80/80	0/3/3/3
48	A86	14	312	-	-	4/34/90/90	0/3/3/3
37	CLA	d	401	52	-	14/37/115/115	-
44	DGD	c	516	-	-	17/51/91/95	0/2/2/2
48	A86	31	314	-	-	10/34/90/90	0/3/3/3
37	CLA	32	210	25	1/1/12/20	13/22/100/115	-
37	CLA	19	302	-	1/1/15/20	13/37/115/115	-
48	A86	11	312	-	-	6/34/90/90	0/3/3/3
37	CLA	21	208	-	1/1/15/20	13/37/115/115	-
48	A86	41	214	-	-	6/34/90/90	0/3/3/3
37	CLA	W	102	-	1/1/15/20	19/37/115/115	-
47	KC1	16	304	29	-	6/15/71/71	-
39	BCR	b	517	-	-	6/29/63/63	0/2/2/2
37	CLA	b	503	-	1/1/15/20	10/37/115/115	-
37	CLA	15	301	28	-	8/37/115/115	-
48	A86	32	203	-	-	14/34/90/90	0/3/3/3
47	KC1	34	304	27	-	6/15/71/71	-
37	CLA	b	514	-	1/1/14/20	14/34/112/115	-
48	A86	32	216	-	-	13/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	40	201	-	-	14/34/90/90	0/3/3/3
37	CLA	B	515	-	1/1/15/20	3/37/115/115	-
37	CLA	15	308	52	1/1/15/20	10/37/115/115	-
39	BCR	b	518	-	-	6/29/63/63	0/2/2/2
47	KC1	41	203	-	-	4/15/71/71	-
37	CLA	41	210	-	-	4/13/91/115	-
48	A86	31	313	-	-	6/34/90/90	1/3/3/3
37	CLA	14	303	-	-	4/28/106/115	-
37	CLA	34	308	52	1/1/15/20	13/37/115/115	-
39	BCR	c	514	-	-	6/29/63/63	0/2/2/2
40	SQD	B	519	-	-	25/49/69/69	0/1/1/1
47	KC1	40	204	-	-	8/15/71/71	-
48	A86	11	314	-	-	10/34/90/90	0/3/3/3
47	KC1	39	308	-	-	3/15/71/71	-
37	CLA	37	308	52	1/1/15/20	11/37/115/115	-
47	KC1	38	205	31	-	7/15/71/71	-
47	KC1	17	303	-	-	6/15/71/71	-
37	CLA	41	209	34	1/1/11/20	6/13/91/115	-
39	BCR	c	519	-	-	7/29/63/63	0/2/2/2
37	CLA	c	509	-	1/1/15/20	8/37/115/115	-
37	CLA	21	206	34	1/1/15/20	15/37/115/115	-
48	A86	14	313	-	-	12/34/90/90	0/3/3/3
41	LMG	B	521	-	-	24/46/66/70	0/1/1/1
47	KC1	19	308	-	-	3/15/71/71	-
37	CLA	C	505	-	1/1/15/20	13/37/115/115	-
47	KC1	18	210	31	-	8/15/71/71	-
48	A86	16	311	-	-	9/34/90/90	0/3/3/3
48	A86	36	311	-	-	9/34/90/90	0/3/3/3
37	CLA	c	501	-	1/1/15/20	11/37/115/115	-
41	LMG	b	519	-	-	15/46/66/70	0/1/1/1
37	CLA	c	504	52	1/1/15/20	9/37/115/115	-
37	CLA	19	310	32	1/1/15/20	7/37/115/115	-
43	LHG	d	408	-	-	27/53/53/53	-
39	BCR	d	405	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	15	314	-	-	14/34/90/90	0/3/3/3
37	CLA	36	306	29	1/1/15/20	14/37/115/115	-
37	CLA	15	305	-	1/1/11/20	4/13/91/115	-
40	SQD	A	407	-	-	17/49/69/69	0/1/1/1
48	A86	38	213	-	-	9/34/90/90	0/3/3/3
47	KC1	14	309	27	-	8/15/71/71	-
37	CLA	B	524	-	1/1/15/20	12/37/115/115	-
48	A86	39	313	-	-	7/34/90/90	0/3/3/3
37	CLA	b	504	-	1/1/15/20	4/37/115/115	-
43	LHG	37	315	-	-	29/48/48/53	-
37	CLA	b	508	-	-	5/37/115/115	-
37	CLA	16	307	52	1/1/14/20	11/33/111/115	-
37	CLA	15	303	-	-	8/28/106/115	-
41	LMG	L	102	-	-	14/35/55/70	0/1/1/1
38	PHO	A	404	-	-	6/37/103/103	0/5/6/6
39	BCR	a	408	-	-	8/29/63/63	0/2/2/2
39	BCR	B	517	-	-	6/29/63/63	0/2/2/2
37	CLA	33	307	26	1/1/12/20	11/22/100/115	-
37	CLA	D	406	-	1/1/15/20	17/37/115/115	-
37	CLA	34	305	-	1/1/11/20	3/13/91/115	-
37	CLA	11	310	52	1/1/12/20	6/21/99/115	-
48	A86	18	214	-	-	13/34/90/90	0/3/3/3
37	CLA	21	202	34	1/1/13/20	7/28/106/115	-
39	BCR	A	410	-	-	8/29/63/63	0/2/2/2
37	CLA	C	501	-	1/1/15/20	11/37/115/115	-
40	SQD	B	522	-	-	12/32/52/69	0/1/1/1
37	CLA	17	304	-	1/1/13/20	9/27/105/115	-
47	KC1	17	308	30	-	5/15/71/71	-
37	CLA	37	301	30	-	10/37/115/115	-
45	PL9	d	402	-	-	17/53/73/73	0/1/1/1
37	CLA	39	306	32	-	6/37/115/115	-
39	BCR	0	101	-	-	8/29/63/63	0/2/2/2
37	CLA	14	308	52	1/1/15/20	13/37/115/115	-
48	A86	31	311	-	-	7/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	B	510	52	1/1/15/20	8/37/115/115	-
37	CLA	39	310	32	1/1/15/20	7/37/115/115	-
37	CLA	11	308	52	1/1/15/20	15/37/115/115	-
39	BCR	C	514	-	-	6/29/63/63	0/2/2/2
47	KC1	13	304	26	-	7/15/71/71	-
37	CLA	18	203	-	1/1/15/20	7/37/115/115	-
41	LMG	D	412	-	-	14/46/66/70	0/1/1/1
47	KC1	37	302	-	-	6/15/71/71	-
37	CLA	13	310	-	-	2/13/91/115	-
48	A86	17	310	-	-	12/34/90/90	0/3/3/3
48	A86	14	316	-	-	15/34/90/90	0/3/3/3
39	BCR	B	525	-	-	17/29/63/63	0/2/2/2
37	CLA	c	512	-	1/1/15/20	8/37/115/115	-
37	CLA	C	503	-	1/1/15/20	20/37/115/115	-
48	A86	13	314	-	-	9/34/90/90	0/3/3/3
47	KC1	40	206	33	-	7/15/71/71	-
48	A86	32	214	-	-	5/34/90/90	0/3/3/3
41	LMG	11	317	-	-	14/27/47/70	0/1/1/1
44	DGD	J	101	-	-	16/51/91/95	0/2/2/2
46	HEM	V	201	16	-	4/12/54/54	-
48	A86	21	211	-	-	9/34/90/90	0/3/3/3
37	CLA	a	404	52	1/1/15/20	8/37/115/115	-
41	LMG	C	518	-	-	25/46/66/70	0/1/1/1
37	CLA	B	516	-	1/1/15/20	13/37/115/115	-
37	CLA	35	307	28	1/1/12/20	12/22/100/115	-
48	A86	15	313	-	-	9/34/90/90	0/3/3/3
37	CLA	15	310	-	1/1/11/20	2/13/91/115	-
37	CLA	B	501	52	1/1/15/20	16/37/115/115	-
39	BCR	h	101	-	-	8/29/63/63	0/2/2/2
40	SQD	b	521	-	-	12/32/52/69	0/1/1/1
48	A86	37	311	-	-	8/34/90/90	0/3/3/3
37	CLA	38	204	-	1/1/13/20	10/27/105/115	-
37	CLA	B	504	-	1/1/15/20	4/37/115/115	-
37	CLA	39	304	32	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	13	312	-	-	8/34/90/90	0/3/3/3
45	PL9	D	408	-	-	10/53/73/73	0/1/1/1
39	BCR	y	101	-	-	16/29/63/63	0/2/2/2
44	DGD	h	102	-	-	16/51/91/95	0/2/2/2
37	CLA	w	101	-	1/1/15/20	17/37/115/115	-
41	LMG	b	520	-	-	24/46/66/70	0/1/1/1
48	A86	19	313	-	-	9/34/90/90	0/3/3/3
37	CLA	37	306	30	1/1/12/20	8/22/100/115	-
37	CLA	31	301	-	1/1/15/20	19/37/115/115	-
47	KC1	31	303	-	-	2/15/71/71	-
48	A86	16	314	-	-	8/34/90/90	0/3/3/3
37	CLA	B	512	-	1/1/15/20	8/37/115/115	-
37	CLA	19	301	32	1/1/15/20	10/37/115/115	-
48	A86	12	213	-	-	5/34/90/90	0/3/3/3
38	PHO	a	405	-	-	10/37/103/103	0/5/6/6
48	A86	34	314	-	-	14/34/90/90	0/3/3/3
47	KC1	40	207	33	-	11/15/71/71	-
37	CLA	12	205	-	1/1/15/20	11/37/115/115	-
37	CLA	13	307	26	1/1/12/20	11/22/100/115	-
37	CLA	33	305	-	1/1/11/20	2/13/91/115	-
48	A86	38	214	-	-	13/34/90/90	0/3/3/3
47	KC1	32	209	25	-	4/15/71/71	-
47	KC1	16	308	29	-	4/15/71/71	-
41	LMG	32	201	-	-	13/34/54/70	0/1/1/1
37	CLA	B	505	-	1/1/15/20	10/37/115/115	-
48	A86	17	315	-	-	13/34/90/90	0/3/3/3
37	CLA	20	306	33	1/1/12/20	6/19/97/115	-
37	CLA	33	303	-	1/1/13/20	13/28/106/115	-
37	CLA	d	403	-	1/1/15/20	7/37/115/115	-
40	SQD	40	202	-	-	25/49/69/69	0/1/1/1
47	KC1	11	304	24	-	4/15/71/71	-
40	SQD	16	315	-	-	25/49/69/69	0/1/1/1
41	LMG	12	201	-	-	13/34/54/70	0/1/1/1
47	KC1	33	304	26	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	c	503	-	1/1/15/20	20/37/115/115	-
47	KC1	33	306	26	-	6/15/71/71	-
41	LMG	17	317	-	-	15/32/52/70	0/1/1/1
37	CLA	C	511	3	1/1/15/20	6/37/115/115	-
37	CLA	C	504	52	1/1/15/20	9/37/115/115	-
48	A86	35	315	-	-	8/34/90/90	0/3/3/3
37	CLA	13	301	26	-	12/37/115/115	-
44	DGD	c	517	-	-	20/51/91/95	0/2/2/2
47	KC1	20	304	33	-	7/15/71/71	-
37	CLA	38	209	52	1/1/15/20	10/37/115/115	-
37	CLA	12	210	52	-	9/37/115/115	-
37	CLA	38	201	52	1/1/15/20	7/37/115/115	-
50	DD6	16	312	-	-	12/26/80/80	0/3/3/3
48	A86	12	220	-	-	9/34/90/90	0/3/3/3
48	A86	37	319	-	-	8/34/90/90	0/3/3/3
37	CLA	12	204	-	1/1/15/20	10/37/115/115	-
37	CLA	32	208	52	1/1/12/20	0/19/97/115	-
37	CLA	36	303	-	1/1/13/20	8/28/106/115	-
43	LHG	D	410	-	-	27/53/53/53	-
41	LMG	a	410	-	-	32/46/66/70	0/1/1/1
47	KC1	13	302	-	-	5/15/71/71	-
37	CLA	38	202	31	-	13/37/115/115	-
37	CLA	b	502	-	1/1/15/20	9/37/115/115	-
37	CLA	38	211	-	-	3/13/91/115	-
47	KC1	34	309	27	-	8/15/71/71	-
37	CLA	20	301	33	-	11/27/105/115	-
37	CLA	z	102	33	1/1/11/20	4/13/91/115	-
37	CLA	35	305	-	1/1/11/20	4/13/91/115	-
47	KC1	16	305	29	-	6/15/71/71	-
41	LMG	B	520	-	-	15/46/66/70	0/1/1/1
48	A86	11	313	-	-	7/34/90/90	1/3/3/3
43	LHG	41	201	-	-	20/38/38/53	-
41	LMG	37	316	-	-	15/32/52/70	0/1/1/1
48	A86	38	212	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	KC1	11	302	-	-	2/15/71/71	-
48	A86	33	311	-	-	6/34/90/90	0/3/3/3
48	A86	37	309	-	-	12/34/90/90	0/3/3/3
48	A86	34	313	-	-	12/34/90/90	0/3/3/3
47	KC1	15	302	-	-	6/15/71/71	-
37	CLA	19	309	32	1/1/11/20	3/13/91/115	-
47	KC1	15	304	28	-	6/15/71/71	-
39	BCR	C	515	-	-	7/29/63/63	0/2/2/2
50	DD6	39	312	-	-	12/26/80/80	0/3/3/3
48	A86	13	311	-	-	6/34/90/90	0/3/3/3
37	CLA	C	508	-	1/1/15/20	10/37/115/115	-
48	A86	34	311	-	-	7/34/90/90	0/3/3/3
37	CLA	39	303	52	1/1/15/20	15/37/115/115	-
37	CLA	41	204	-	-	13/29/107/115	-
37	CLA	b	515	-	1/1/15/20	3/37/115/115	-
48	A86	37	314	-	-	13/34/90/90	0/3/3/3
37	CLA	D	401	52	1/1/15/20	8/37/115/115	-
39	BCR	H	101	-	-	8/29/63/63	0/2/2/2
48	A86	17	313	-	-	8/34/90/90	0/3/3/3
37	CLA	Z	102	33	1/1/11/20	4/13/91/115	-
37	CLA	38	208	31	1/1/12/20	10/23/101/115	-
48	A86	35	311	-	-	6/34/90/90	0/3/3/3
37	CLA	B	503	-	1/1/15/20	10/37/115/115	-
47	KC1	32	207	25	-	6/15/71/71	-
47	KC1	33	309	26	-	5/15/71/71	-
39	BCR	B	518	-	-	6/29/63/63	0/2/2/2
37	CLA	20	307	33	1/1/11/20	6/13/91/115	-
51	LMU	19	315	-	-	6/21/61/61	0/2/2/2
47	KC1	35	309	28	-	6/15/71/71	-
48	A86	35	312	-	-	7/34/90/90	0/3/3/3
48	A86	14	315	-	-	6/34/90/90	0/3/3/3
48	A86	41	211	-	-	9/34/90/90	0/3/3/3
43	LHG	d	407	-	-	28/53/53/53	-
50	DD6	20	312	-	-	12/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	11	301	24	-	10/37/115/115	-
37	CLA	19	306	32	1/1/15/20	6/37/115/115	-
47	KC1	41	207	34	-	5/15/71/71	-
37	CLA	12	212	-	1/1/11/20	8/13/91/115	-
37	CLA	37	303	-	1/1/13/20	9/27/105/115	-
48	A86	41	215	-	-	6/34/90/90	0/3/3/3
37	CLA	32	211	52	-	9/37/115/115	-
48	A86	21	215	-	-	6/34/90/90	0/3/3/3
50	DD6	41	216	-	-	15/26/80/80	0/3/3/3
37	CLA	b	523	-	1/1/15/20	12/37/115/115	-
37	CLA	b	511	-	1/1/15/20	12/37/115/115	-
37	CLA	14	310	-	1/1/11/20	2/13/91/115	-
45	PL9	D	404	-	-	17/53/73/73	0/1/1/1
39	BCR	c	515	-	-	7/29/63/63	0/2/2/2
37	CLA	c	508	-	1/1/15/20	10/37/115/115	-
37	CLA	19	304	32	1/1/11/20	4/13/91/115	-
50	DD6	21	212	-	-	13/26/80/80	0/3/3/3
47	KC1	21	203	-	-	4/15/71/71	-
48	A86	40	213	-	-	16/34/90/90	0/3/3/3
37	CLA	z	101	52	1/1/15/20	18/37/115/115	-
37	CLA	17	307	30	1/1/12/20	8/22/100/115	-
48	A86	17	314	-	-	8/34/90/90	0/3/3/3
37	CLA	32	205	-	1/1/15/20	10/37/115/115	-
48	A86	31	312	-	-	6/34/90/90	0/3/3/3
37	CLA	18	202	31	-	13/37/115/115	-
47	KC1	36	305	29	-	6/15/71/71	-
48	A86	35	316	-	-	15/34/90/90	0/3/3/3
40	SQD	a	409	-	-	16/49/69/69	0/1/1/1
37	CLA	C	512	-	1/1/15/20	8/37/115/115	-
41	LMG	31	316	-	-	19/37/57/70	0/1/1/1
48	A86	18	212	-	-	8/34/90/90	0/3/3/3
48	A86	11	311	-	-	7/34/90/90	0/3/3/3
37	CLA	33	308	52	-	10/37/115/115	-
48	A86	20	311	-	-	16/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	12	217	-	-	15/34/90/90	0/3/3/3
37	CLA	C	513	-	1/1/15/20	7/37/115/115	-
47	KC1	16	302	-	-	2/15/71/71	-
47	KC1	36	302	-	-	2/15/71/71	-
37	CLA	41	205	34	1/1/11/20	7/13/91/115	-
37	CLA	a	407	-	-	6/37/115/115	-
47	KC1	33	302	-	-	5/15/71/71	-
37	CLA	31	306	52	1/1/11/20	2/13/91/115	-
48	A86	32	218	-	-	15/34/90/90	0/3/3/3
50	DD6	40	212	-	-	14/26/80/80	0/3/3/3
48	A86	33	314	-	-	9/34/90/90	0/3/3/3
37	CLA	34	301	27	-	13/37/115/115	-
37	CLA	14	302	-	1/1/15/20	17/37/115/115	-
48	A86	35	319	-	-	8/34/90/90	0/3/3/3
48	A86	32	217	-	-	10/34/90/90	0/3/3/3
48	A86	17	320	-	-	8/34/90/90	0/3/3/3
37	CLA	39	301	32	1/1/15/20	10/37/115/115	-
47	KC1	14	304	27	-	6/15/71/71	-
37	CLA	b	506	-	1/1/15/20	8/37/115/115	-
37	CLA	19	307	43	1/1/15/20	8/37/115/115	-
37	CLA	32	206	-	1/1/15/20	11/37/115/115	-
37	CLA	40	205	-	1/1/13/20	10/27/105/115	-
37	CLA	b	507	52	1/1/15/20	10/37/115/115	-
47	KC1	31	309	24	-	8/15/71/71	-
48	A86	34	316	-	-	15/34/90/90	0/3/3/3
37	CLA	19	303	52	1/1/15/20	15/37/115/115	-
48	A86	16	313	-	-	14/34/90/90	0/3/3/3
47	KC1	18	205	31	-	7/15/71/71	-
47	KC1	12	206	25	-	6/15/71/71	-
44	DGD	C	517	-	-	20/51/91/95	0/2/2/2
48	A86	18	213	-	-	9/34/90/90	0/3/3/3
47	KC1	36	304	29	-	6/15/71/71	-
37	CLA	c	506	-	1/1/15/20	14/37/115/115	-
37	CLA	18	208	31	1/1/12/20	11/23/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	12	207	52	1/1/12/20	0/19/97/115	-
37	CLA	35	308	52	-	10/37/115/115	-
43	LHG	19	314	37	-	28/53/53/53	-
48	A86	12	216	-	-	10/34/90/90	0/3/3/3
48	A86	18	215	-	-	13/34/90/90	0/3/3/3
47	KC1	32	212	25	-	5/15/71/71	-
48	A86	40	211	-	-	6/34/90/90	0/3/3/3
37	CLA	39	309	32	1/1/11/20	3/13/91/115	-
47	KC1	12	211	25	-	5/15/71/71	-
37	CLA	34	302	-	1/1/15/20	18/37/115/115	-
37	CLA	34	307	27	1/1/12/20	12/22/100/115	-
47	KC1	35	302	-	-	6/15/71/71	-
40	SQD	L	101	-	-	25/49/69/69	0/1/1/1
37	CLA	40	203	33	-	11/27/105/115	-
37	CLA	13	303	-	1/1/13/20	13/28/106/115	-
37	CLA	34	303	-	-	4/28/106/115	-
41	LMG	16	316	-	-	14/31/51/70	0/1/1/1
48	A86	34	312	-	-	4/34/90/90	0/3/3/3
41	LMG	11	316	-	-	19/37/57/70	0/1/1/1
37	CLA	c	505	-	1/1/15/20	13/37/115/115	-
44	DGD	j	101	-	-	16/51/91/95	0/2/2/2
48	A86	16	310	-	-	6/34/90/90	0/3/3/3
48	A86	36	310	-	-	6/34/90/90	0/3/3/3
47	KC1	31	307	24	-	9/15/71/71	-
47	KC1	13	306	26	-	6/15/71/71	-
47	KC1	37	305	30	-	9/15/71/71	-
45	PL9	d	406	-	-	10/53/73/73	0/1/1/1
37	CLA	14	307	27	1/1/12/20	11/22/100/115	-
48	A86	37	310	-	-	8/34/90/90	0/3/3/3
43	LHG	21	217	-	-	28/49/49/53	-
39	BCR	A	406	-	-	8/29/63/63	0/2/2/2
48	A86	14	314	-	-	14/34/90/90	0/3/3/3
37	CLA	18	206	-	1/1/11/20	4/13/91/115	-
37	CLA	b	516	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	34	315	-	-	6/34/90/90	0/3/3/3
47	KC1	12	208	25	-	4/15/71/71	-
40	SQD	17	301	-	-	25/44/64/69	0/1/1/1
37	CLA	32	202	52	1/1/15/20	15/37/115/115	-
38	PHO	D	403	-	-	10/37/103/103	0/5/6/6
37	CLA	c	502	-	1/1/15/20	8/37/115/115	-
37	CLA	D	405	-	1/1/15/20	7/37/115/115	-
37	CLA	C	509	-	1/1/15/20	8/37/115/115	-
48	A86	35	314	-	-	14/34/90/90	0/3/3/3
37	CLA	11	307	24	-	7/22/100/115	-
48	A86	17	311	-	-	8/34/90/90	0/3/3/3
37	CLA	c	511	3	1/1/15/20	6/37/115/115	-
48	A86	33	315	-	-	10/34/90/90	0/3/3/3
43	LHG	a	412	-	-	26/50/50/53	-
37	CLA	11	303	-	1/1/15/20	8/37/115/115	-
48	A86	31	319	-	-	7/34/90/90	0/3/3/3
37	CLA	18	201	52	1/1/15/20	8/37/115/115	-
38	PHO	a	406	-	-	6/37/103/103	0/5/6/6
37	CLA	32	204	25	1/1/15/20	12/37/115/115	-
41	LMG	d	409	-	-	14/46/66/70	0/1/1/1
47	KC1	38	207	31	-	5/15/71/71	-
37	CLA	b	513	-	1/1/15/20	9/37/115/115	-
48	A86	36	313	-	-	8/34/90/90	0/3/3/3
37	CLA	Z	101	52	1/1/15/20	18/37/115/115	-
37	CLA	19	305	32	1/1/12/20	5/21/99/115	-
37	CLA	C	510	-	1/1/15/20	15/37/115/115	-
37	CLA	41	202	34	1/1/13/20	7/28/106/115	-
40	SQD	36	315	-	-	25/44/64/69	0/1/1/1
37	CLA	16	309	-	1/1/11/20	7/13/91/115	-
37	CLA	34	310	-	1/1/11/20	2/13/91/115	-
37	CLA	20	303	-	1/1/13/20	10/27/105/115	-
37	CLA	39	307	43	1/1/15/20	8/37/115/115	-
37	CLA	31	302	24	-	10/37/115/115	-
37	CLA	33	310	-	-	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LMG	l	101	-	-	14/35/55/70	0/1/1/1
37	CLA	17	302	30	-	11/37/115/115	-
37	CLA	18	204	-	1/1/13/20	12/27/105/115	-
37	CLA	38	203	-	1/1/15/20	7/37/115/115	-
48	A86	32	215	-	-	3/34/90/90	0/3/3/3
37	CLA	C	502	-	1/1/15/20	8/37/115/115	-
48	A86	13	313	-	-	17/34/90/90	0/3/3/3
39	BCR	D	407	-	-	12/29/63/63	0/2/2/2
37	CLA	11	305	52	1/1/11/20	2/13/91/115	-
37	CLA	B	511	-	1/1/15/20	12/37/115/115	-
37	CLA	16	306	29	1/1/15/20	14/37/115/115	-
37	CLA	c	510	-	1/1/15/20	15/37/115/115	-
37	CLA	B	509	-	1/1/15/20	10/37/115/115	-
37	CLA	13	308	52	-	10/37/115/115	-
47	KC1	15	309	28	-	6/15/71/71	-
37	CLA	B	507	52	1/1/15/20	10/37/115/115	-
48	A86	12	215	-	-	13/34/90/90	0/3/3/3
37	CLA	40	210	-	1/1/11/20	2/16/94/115	-
37	CLA	A	403	-	1/1/15/20	4/37/115/115	-
37	CLA	b	501	52	1/1/15/20	16/37/115/115	-
37	CLA	31	304	-	1/1/15/20	8/37/115/115	-
37	CLA	14	301	27	-	13/37/115/115	-
48	A86	11	315	-	-	6/34/90/90	0/3/3/3
39	BCR	b	524	-	-	17/29/63/63	0/2/2/2
37	CLA	12	209	25	1/1/12/20	13/22/100/115	-
37	CLA	B	514	-	1/1/14/20	14/34/112/115	-
48	A86	15	315	-	-	8/34/90/90	0/3/3/3
48	A86	12	214	-	-	3/34/90/90	0/3/3/3
50	DD6	40	214	-	-	12/26/80/80	0/3/3/3
37	CLA	21	204	-	-	13/29/107/115	-
37	CLA	39	302	-	1/1/15/20	13/37/115/115	-
37	CLA	17	309	52	1/1/15/20	11/37/115/115	-
37	CLA	35	310	-	1/1/11/20	2/13/91/115	-
37	CLA	31	310	52	1/1/12/20	6/21/99/115	-

All (8303) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	20	312	DD6	C10-C11	25.78	1.70	1.35
50	40	214	DD6	C10-C11	25.69	1.69	1.35
50	41	212	DD6	C10-C11	25.53	1.69	1.35
50	39	312	DD6	C10-C11	25.49	1.69	1.35
50	41	216	DD6	C10-C11	25.49	1.69	1.35
50	19	312	DD6	C10-C11	25.47	1.69	1.35
50	21	212	DD6	C10-C11	25.46	1.69	1.35
50	21	216	DD6	C10-C11	25.42	1.69	1.35
50	20	310	DD6	C10-C11	25.38	1.69	1.35
50	40	212	DD6	C10-C11	25.34	1.69	1.35
50	16	312	DD6	C10-C11	25.04	1.69	1.35
50	36	312	DD6	C10-C11	24.99	1.68	1.35
50	40	214	DD6	C5-C6	17.65	1.59	1.35
50	20	312	DD6	C5-C6	17.62	1.59	1.35
50	41	216	DD6	C5-C6	17.50	1.59	1.35
50	21	216	DD6	C5-C6	17.49	1.59	1.35
50	20	310	DD6	C5-C6	17.47	1.58	1.35
50	40	212	DD6	C5-C6	17.40	1.58	1.35
50	16	312	DD6	C5-C6	17.28	1.58	1.35
50	36	312	DD6	C5-C6	17.24	1.58	1.35
50	21	212	DD6	C5-C6	17.22	1.58	1.35
50	41	212	DD6	C5-C6	17.20	1.58	1.35
50	19	312	DD6	C5-C6	17.06	1.58	1.35
50	39	312	DD6	C5-C6	17.03	1.58	1.35
48	40	213	A86	C14-C13	14.87	1.69	1.51
48	39	313	A86	C14-C13	14.87	1.69	1.51
48	20	311	A86	C14-C13	14.87	1.69	1.51
48	35	319	A86	C14-C13	14.72	1.69	1.51
48	15	319	A86	C14-C13	14.72	1.69	1.51
48	40	211	A86	C14-C13	14.61	1.68	1.51
48	20	309	A86	C14-C13	14.59	1.68	1.51
48	19	313	A86	C14-C13	14.58	1.68	1.51
48	41	214	A86	C14-C13	14.58	1.68	1.51
48	21	211	A86	C14-C13	14.57	1.68	1.51
48	41	211	A86	C14-C13	14.56	1.68	1.51
48	21	214	A86	C14-C13	14.56	1.68	1.51
48	37	312	A86	C14-C13	14.53	1.68	1.51
50	20	312	DD6	C36-C31	14.49	1.51	1.34
48	18	214	A86	C14-C13	14.48	1.68	1.51
48	38	214	A86	C14-C13	14.48	1.68	1.51
50	40	214	DD6	C36-C31	14.47	1.51	1.34
48	35	314	A86	C14-C13	14.46	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	15	314	A86	C14-C13	14.45	1.68	1.51
48	41	213	A86	C14-C13	14.44	1.68	1.51
48	17	313	A86	C14-C13	14.43	1.68	1.51
48	21	213	A86	C14-C13	14.42	1.68	1.51
48	14	314	A86	C14-C13	14.40	1.68	1.51
48	34	314	A86	C14-C13	14.40	1.68	1.51
48	32	221	A86	C14-C13	14.23	1.68	1.51
48	17	310	A86	C14-C13	14.22	1.68	1.51
48	13	314	A86	C14-C13	14.22	1.68	1.51
48	15	315	A86	C14-C13	14.21	1.68	1.51
48	37	309	A86	C14-C13	14.20	1.68	1.51
48	37	319	A86	C14-C13	14.20	1.68	1.51
48	34	312	A86	C14-C13	14.20	1.68	1.51
48	14	312	A86	C14-C13	14.18	1.68	1.51
48	12	220	A86	C14-C13	14.17	1.68	1.51
48	15	311	A86	C14-C13	14.16	1.68	1.51
48	35	311	A86	C14-C13	14.15	1.68	1.51
48	13	315	A86	C14-C13	14.14	1.68	1.51
48	33	315	A86	C14-C13	14.14	1.68	1.51
48	33	314	A86	C14-C13	14.13	1.68	1.51
48	17	320	A86	C14-C13	14.13	1.68	1.51
48	12	216	A86	C14-C13	14.11	1.68	1.51
48	35	315	A86	C14-C13	14.11	1.68	1.51
48	32	217	A86	C14-C13	14.10	1.68	1.51
48	36	311	A86	C14-C13	14.08	1.68	1.51
50	16	312	DD6	C36-C31	14.06	1.50	1.34
48	19	311	A86	C14-C13	14.05	1.68	1.51
48	39	311	A86	C14-C13	14.05	1.68	1.51
48	15	316	A86	C14-C13	14.05	1.68	1.51
48	16	311	A86	C14-C13	14.03	1.68	1.51
48	38	213	A86	C14-C13	14.00	1.68	1.51
50	36	312	DD6	C36-C31	13.99	1.50	1.34
48	14	315	A86	C14-C13	13.99	1.68	1.51
48	33	312	A86	C14-C13	13.99	1.68	1.51
48	34	315	A86	C14-C13	13.98	1.68	1.51
48	34	311	A86	C14-C13	13.97	1.68	1.51
48	37	310	A86	C14-C13	13.96	1.68	1.51
48	17	312	A86	C14-C13	13.95	1.68	1.51
48	14	311	A86	C14-C13	13.94	1.68	1.51
48	37	311	A86	C14-C13	13.94	1.68	1.51
48	13	313	A86	C14-C13	13.93	1.68	1.51
48	13	311	A86	C14-C13	13.90	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	35	316	A86	C14-C13	13.90	1.68	1.51
48	33	313	A86	C14-C13	13.90	1.68	1.51
48	13	312	A86	C14-C13	13.89	1.68	1.51
48	38	212	A86	C14-C13	13.86	1.68	1.51
48	32	218	A86	C14-C13	13.86	1.68	1.51
48	15	312	A86	C14-C13	13.86	1.68	1.51
48	32	214	A86	C14-C13	13.84	1.68	1.51
48	18	213	A86	C14-C13	13.84	1.68	1.51
48	33	311	A86	C14-C13	13.83	1.67	1.51
48	35	312	A86	C14-C13	13.83	1.67	1.51
48	31	314	A86	C14-C13	13.83	1.67	1.51
48	36	310	A86	C14-C13	13.83	1.67	1.51
48	12	217	A86	C14-C13	13.82	1.67	1.51
48	17	311	A86	C14-C13	13.80	1.67	1.51
48	37	313	A86	C14-C13	13.80	1.67	1.51
48	14	316	A86	C14-C13	13.79	1.67	1.51
48	34	313	A86	C14-C13	13.79	1.67	1.51
48	34	316	A86	C14-C13	13.79	1.67	1.51
48	11	314	A86	C14-C13	13.77	1.67	1.51
48	11	315	A86	C14-C13	13.77	1.67	1.51
48	32	203	A86	C14-C13	13.76	1.67	1.51
48	17	315	A86	C14-C13	13.76	1.67	1.51
48	16	310	A86	C14-C13	13.75	1.67	1.51
48	17	314	A86	C14-C13	13.75	1.67	1.51
50	21	212	DD6	C36-C31	13.75	1.50	1.34
48	14	313	A86	C14-C13	13.74	1.67	1.51
48	12	213	A86	C14-C13	13.73	1.67	1.51
48	18	212	A86	C14-C13	13.73	1.67	1.51
48	37	314	A86	C14-C13	13.72	1.67	1.51
50	41	212	DD6	C36-C31	13.72	1.50	1.34
48	31	315	A86	C14-C13	13.72	1.67	1.51
48	40	201	A86	C14-C13	13.70	1.67	1.51
48	12	215	A86	C14-C13	13.68	1.67	1.51
48	32	216	A86	C14-C13	13.68	1.67	1.51
48	12	202	A86	C14-C13	13.68	1.67	1.51
48	16	313	A86	C14-C13	13.67	1.67	1.51
50	20	310	DD6	C36-C31	13.66	1.50	1.34
48	38	215	A86	C14-C13	13.64	1.67	1.51
50	40	212	DD6	C36-C31	13.62	1.50	1.34
48	11	319	A86	C14-C13	13.61	1.67	1.51
48	31	319	A86	C14-C13	13.54	1.67	1.51
48	31	312	A86	C14-C13	13.54	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	18	215	A86	C14-C13	13.49	1.67	1.51
50	41	216	DD6	C36-C31	13.49	1.50	1.34
48	11	312	A86	C14-C13	13.49	1.67	1.51
50	21	216	DD6	C36-C31	13.46	1.49	1.34
48	11	311	A86	C14-C13	13.38	1.67	1.51
48	31	311	A86	C14-C13	13.33	1.67	1.51
48	35	313	A86	C14-C13	13.33	1.67	1.51
48	15	313	A86	C14-C13	13.29	1.67	1.51
48	32	215	A86	C14-C13	13.21	1.67	1.51
48	12	214	A86	C14-C13	13.21	1.67	1.51
48	36	313	A86	C14-C13	13.15	1.67	1.51
48	16	314	A86	C14-C13	13.15	1.67	1.51
48	31	313	A86	C14-C13	13.08	1.67	1.51
48	11	313	A86	C14-C13	13.04	1.67	1.51
50	39	312	DD6	C36-C31	12.74	1.49	1.34
50	19	312	DD6	C36-C31	12.73	1.49	1.34
48	41	215	A86	C14-C13	12.06	1.65	1.51
48	21	215	A86	C14-C13	12.05	1.65	1.51
47	18	205	KC1	C1D-ND	10.23	1.44	1.35
47	38	205	KC1	C1D-ND	10.23	1.44	1.35
47	20	304	KC1	C1D-ND	10.20	1.44	1.35
47	40	206	KC1	C1D-ND	10.18	1.44	1.35
47	16	302	KC1	C1D-ND	10.18	1.44	1.35
47	35	304	KC1	C1D-ND	10.16	1.44	1.35
47	36	302	KC1	C1D-ND	10.09	1.44	1.35
47	15	304	KC1	C1D-ND	10.09	1.44	1.35
47	16	304	KC1	C1D-ND	10.07	1.44	1.35
47	37	304	KC1	C1D-ND	10.00	1.44	1.35
47	18	210	KC1	C1D-ND	9.99	1.44	1.35
47	38	210	KC1	C1D-ND	9.99	1.44	1.35
47	37	307	KC1	C1D-ND	9.95	1.44	1.35
47	17	308	KC1	C1D-ND	9.95	1.44	1.35
47	36	304	KC1	C1D-ND	9.94	1.44	1.35
47	15	306	KC1	C1D-ND	9.92	1.44	1.35
47	40	204	KC1	C1D-ND	9.91	1.44	1.35
47	20	302	KC1	C1D-ND	9.90	1.44	1.35
47	38	207	KC1	C1D-ND	9.89	1.44	1.35
47	41	207	KC1	C1D-ND	9.88	1.44	1.35
47	35	302	KC1	C1D-ND	9.88	1.44	1.35
47	21	207	KC1	C1D-ND	9.84	1.44	1.35
47	35	306	KC1	C1D-ND	9.84	1.44	1.35
47	41	203	KC1	C1D-ND	9.82	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	21	203	KC1	C1D-ND	9.80	1.43	1.35
47	15	302	KC1	C1D-ND	9.78	1.43	1.35
47	36	305	KC1	C1D-ND	9.77	1.43	1.35
47	34	304	KC1	C1D-ND	9.76	1.43	1.35
47	16	308	KC1	C1D-ND	9.75	1.43	1.35
47	36	308	KC1	C1D-ND	9.75	1.43	1.35
47	37	305	KC1	C1D-ND	9.75	1.43	1.35
47	13	302	KC1	C1D-ND	9.73	1.43	1.35
47	33	302	KC1	C1D-ND	9.73	1.43	1.35
47	16	305	KC1	C1D-ND	9.72	1.43	1.35
47	35	309	KC1	C1D-ND	9.67	1.43	1.35
47	17	305	KC1	C1D-ND	9.66	1.43	1.35
47	37	302	KC1	C1D-ND	9.65	1.43	1.35
47	17	306	KC1	C1D-ND	9.64	1.43	1.35
47	18	207	KC1	C1D-ND	9.63	1.43	1.35
47	40	207	KC1	C1D-ND	9.62	1.43	1.35
47	17	303	KC1	C1D-ND	9.57	1.43	1.35
47	14	304	KC1	C1D-ND	9.57	1.43	1.35
47	15	309	KC1	C1D-ND	9.56	1.43	1.35
47	34	306	KC1	C1D-ND	9.55	1.43	1.35
47	33	304	KC1	C1D-ND	9.55	1.43	1.35
47	20	305	KC1	C1D-ND	9.53	1.43	1.35
47	14	306	KC1	C1D-ND	9.51	1.43	1.35
47	13	304	KC1	C1D-ND	9.49	1.43	1.35
47	11	304	KC1	C1D-ND	9.47	1.43	1.35
48	40	201	A86	C30-C29	9.45	1.47	1.32
48	16	313	A86	C30-C29	9.44	1.47	1.32
47	32	212	KC1	C1D-ND	9.41	1.43	1.35
47	14	309	KC1	C1D-ND	9.40	1.43	1.35
47	34	309	KC1	C1D-ND	9.40	1.43	1.35
48	21	213	A86	C30-C29	9.36	1.47	1.32
47	11	306	KC1	C1D-ND	9.35	1.43	1.35
47	33	306	KC1	C1D-ND	9.34	1.43	1.35
48	41	213	A86	C30-C29	9.33	1.47	1.32
47	31	305	KC1	C1D-ND	9.33	1.43	1.35
47	12	211	KC1	C1D-ND	9.33	1.43	1.35
47	11	309	KC1	C1D-ND	9.32	1.43	1.35
47	31	309	KC1	C1D-ND	9.30	1.43	1.35
47	31	307	KC1	C1D-ND	9.29	1.43	1.35
47	13	306	KC1	C1D-ND	9.28	1.43	1.35
48	35	313	A86	C30-C29	9.28	1.47	1.32
47	13	309	KC1	C1D-ND	9.27	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	33	309	KC1	C1D-ND	9.27	1.43	1.35
48	13	312	A86	C30-C29	9.26	1.47	1.32
48	35	314	A86	C30-C29	9.26	1.47	1.32
48	15	313	A86	C30-C29	9.25	1.47	1.32
48	13	313	A86	C30-C29	9.24	1.47	1.32
48	15	314	A86	C30-C29	9.23	1.47	1.32
48	33	312	A86	C30-C29	9.22	1.47	1.32
48	33	313	A86	C30-C29	9.22	1.47	1.32
48	32	216	A86	C30-C29	9.20	1.47	1.32
47	31	303	KC1	C1D-ND	9.19	1.43	1.35
47	19	308	KC1	C1D-ND	9.18	1.43	1.35
47	12	208	KC1	C1D-ND	9.18	1.43	1.35
47	39	308	KC1	C1D-ND	9.17	1.43	1.35
48	12	215	A86	C30-C29	9.16	1.47	1.32
47	11	302	KC1	C1D-ND	9.16	1.43	1.35
48	41	215	A86	C30-C29	9.06	1.47	1.32
48	34	313	A86	C30-C29	9.03	1.47	1.32
48	13	314	A86	C30-C29	9.03	1.47	1.32
48	21	215	A86	C30-C29	9.02	1.47	1.32
48	18	215	A86	C30-C29	9.01	1.47	1.32
47	32	209	KC1	C1D-ND	9.00	1.43	1.35
48	14	313	A86	C30-C29	9.00	1.46	1.32
48	33	314	A86	C30-C29	8.99	1.46	1.32
48	38	215	A86	C30-C29	8.96	1.46	1.32
50	21	216	DD6	C23-C16	8.95	1.71	1.53
48	21	214	A86	C30-C29	8.94	1.46	1.32
48	34	314	A86	C30-C29	8.93	1.46	1.32
48	41	214	A86	C30-C29	8.93	1.46	1.32
50	16	312	DD6	C13-C11	-8.93	1.26	1.45
50	41	216	DD6	C23-C16	8.91	1.71	1.53
50	36	312	DD6	C13-C11	-8.89	1.26	1.45
48	14	314	A86	C30-C29	8.88	1.46	1.32
48	37	311	A86	C30-C29	8.87	1.46	1.32
48	17	312	A86	C30-C29	8.87	1.46	1.32
48	18	212	A86	C30-C29	8.85	1.46	1.32
48	18	214	A86	C30-C29	8.83	1.46	1.32
48	38	214	A86	C30-C29	8.82	1.46	1.32
48	38	212	A86	C30-C29	8.82	1.46	1.32
48	15	316	A86	C30-C29	8.81	1.46	1.32
48	35	312	A86	C30-C29	8.77	1.46	1.32
48	41	211	A86	C30-C29	8.76	1.46	1.32
48	38	213	A86	C30-C29	8.76	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	18	213	A86	C30-C29	8.74	1.46	1.32
48	21	211	A86	C30-C29	8.74	1.46	1.32
48	34	316	A86	C30-C29	8.74	1.46	1.32
48	13	315	A86	C30-C29	8.72	1.46	1.32
48	14	316	A86	C30-C29	8.69	1.46	1.32
48	40	211	A86	C30-C29	8.68	1.46	1.32
48	35	316	A86	C30-C29	8.68	1.46	1.32
48	37	309	A86	C30-C29	8.68	1.46	1.32
48	15	312	A86	C30-C29	8.67	1.46	1.32
48	12	217	A86	C30-C29	8.67	1.46	1.32
48	20	309	A86	C30-C29	8.67	1.46	1.32
48	33	315	A86	C30-C29	8.66	1.46	1.32
47	12	206	KC1	C1D-ND	8.65	1.42	1.35
48	35	311	A86	C30-C29	8.65	1.46	1.32
48	32	218	A86	C30-C29	8.64	1.46	1.32
48	17	310	A86	C30-C29	8.64	1.46	1.32
48	35	315	A86	C30-C29	8.63	1.46	1.32
48	15	319	A86	C30-C29	8.62	1.46	1.32
48	39	313	A86	C30-C29	8.58	1.46	1.32
50	40	214	DD6	C2-C1	8.58	1.47	1.35
48	17	311	A86	C30-C29	8.57	1.46	1.32
48	35	319	A86	C30-C29	8.56	1.46	1.32
48	37	312	A86	C30-C29	8.56	1.46	1.32
47	32	207	KC1	C1D-ND	8.56	1.42	1.35
48	19	313	A86	C30-C29	8.55	1.46	1.32
48	17	313	A86	C30-C29	8.55	1.46	1.32
48	17	315	A86	C30-C29	8.55	1.46	1.32
48	14	312	A86	C30-C29	8.54	1.46	1.32
48	34	312	A86	C30-C29	8.54	1.46	1.32
48	15	311	A86	C30-C29	8.54	1.46	1.32
48	12	216	A86	C30-C29	8.54	1.46	1.32
50	20	312	DD6	C2-C1	8.54	1.47	1.35
48	37	310	A86	C30-C29	8.54	1.46	1.32
48	15	315	A86	C30-C29	8.53	1.46	1.32
48	14	311	A86	C30-C29	8.53	1.46	1.32
48	34	311	A86	C30-C29	8.53	1.46	1.32
50	21	212	DD6	C13-C11	-8.52	1.27	1.45
50	41	212	DD6	C13-C11	-8.52	1.27	1.45
48	31	314	A86	C30-C29	8.51	1.46	1.32
48	37	314	A86	C30-C29	8.51	1.46	1.32
48	32	217	A86	C30-C29	8.49	1.46	1.32
48	31	313	A86	C30-C29	8.47	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	17	320	A86	C30-C29	8.47	1.46	1.32
48	11	314	A86	C30-C29	8.46	1.46	1.32
48	32	214	A86	C30-C29	8.46	1.46	1.32
48	12	214	A86	C30-C29	8.44	1.46	1.32
48	12	213	A86	C30-C29	8.43	1.46	1.32
48	37	319	A86	C30-C29	8.42	1.46	1.32
50	20	312	DD6	C23-C16	8.42	1.70	1.53
50	40	212	DD6	C23-C16	8.41	1.70	1.53
50	40	214	DD6	C23-C16	8.40	1.70	1.53
48	20	311	A86	C30-C29	8.37	1.45	1.32
48	13	311	A86	C30-C29	8.37	1.45	1.32
50	20	310	DD6	C23-C16	8.37	1.70	1.53
48	40	213	A86	C30-C29	8.37	1.45	1.32
50	21	212	DD6	C2-C1	8.36	1.46	1.35
48	32	215	A86	C30-C29	8.36	1.45	1.32
50	21	216	DD6	C2-C1	8.35	1.46	1.35
48	11	312	A86	C30-C29	8.33	1.45	1.32
50	36	312	DD6	C23-C16	8.32	1.70	1.53
48	33	311	A86	C30-C29	8.31	1.45	1.32
50	16	312	DD6	C23-C16	8.31	1.70	1.53
50	41	216	DD6	C13-C11	-8.30	1.28	1.45
50	41	212	DD6	C2-C1	8.30	1.46	1.35
50	41	216	DD6	C2-C1	8.30	1.46	1.35
48	31	312	A86	C30-C29	8.29	1.45	1.32
50	21	216	DD6	C13-C11	-8.28	1.28	1.45
48	37	313	A86	C30-C29	8.26	1.45	1.32
48	36	313	A86	C30-C29	8.25	1.45	1.32
48	31	311	A86	C30-C29	8.24	1.45	1.32
48	31	315	A86	C30-C29	8.24	1.45	1.32
48	14	315	A86	C30-C29	8.21	1.45	1.32
48	16	314	A86	C30-C29	8.20	1.45	1.32
48	11	311	A86	C30-C29	8.20	1.45	1.32
50	20	312	DD6	C13-C11	-8.19	1.28	1.45
48	11	315	A86	C30-C29	8.19	1.45	1.32
50	40	214	DD6	C13-C11	-8.18	1.28	1.45
50	41	212	DD6	C23-C16	8.16	1.69	1.53
48	32	203	A86	C30-C29	8.15	1.45	1.32
48	12	202	A86	C30-C29	8.14	1.45	1.32
48	17	314	A86	C30-C29	8.14	1.45	1.32
50	21	212	DD6	C23-C16	8.13	1.69	1.53
48	16	311	A86	C30-C29	8.13	1.45	1.32
50	41	212	DD6	C19-C20	8.13	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	34	315	A86	C30-C29	8.13	1.45	1.32
50	19	312	DD6	C13-C11	-8.12	1.28	1.45
50	21	212	DD6	C19-C20	8.11	1.63	1.52
48	11	313	A86	C30-C29	8.11	1.45	1.32
48	36	311	A86	C30-C29	8.10	1.45	1.32
47	36	308	KC1	C2A-C3A	8.10	1.53	1.37
50	39	312	DD6	C13-C11	-8.08	1.28	1.45
50	41	216	DD6	C19-C20	8.08	1.63	1.52
47	16	308	KC1	C2A-C3A	8.06	1.53	1.37
50	40	212	DD6	C13-C11	-8.02	1.28	1.45
50	21	216	DD6	C19-C20	8.01	1.63	1.52
50	16	312	DD6	C2-C1	8.01	1.46	1.35
50	36	312	DD6	C2-C1	8.00	1.46	1.35
50	20	310	DD6	C13-C11	-8.00	1.28	1.45
48	39	311	A86	C30-C29	7.99	1.45	1.32
48	19	311	A86	C30-C29	7.98	1.45	1.32
47	17	308	KC1	C2A-C3A	7.95	1.53	1.37
47	37	307	KC1	C2A-C3A	7.95	1.53	1.37
47	32	209	KC1	C2A-C3A	7.94	1.53	1.37
48	38	213	A86	C19-C20	7.94	1.63	1.52
47	36	302	KC1	C2A-C3A	7.91	1.53	1.37
47	12	208	KC1	C2A-C3A	7.90	1.53	1.37
47	16	302	KC1	C2A-C3A	7.89	1.53	1.37
47	15	309	KC1	C2A-C3A	7.86	1.53	1.37
50	19	312	DD6	C19-C20	7.86	1.63	1.52
50	39	312	DD6	C19-C20	7.86	1.63	1.52
48	15	315	A86	C19-C20	7.85	1.63	1.52
50	16	312	DD6	C19-C20	7.84	1.63	1.52
50	40	212	DD6	C2-C1	7.84	1.46	1.35
47	17	306	KC1	C2A-C3A	7.84	1.53	1.37
48	36	310	A86	C30-C29	7.83	1.45	1.32
50	20	310	DD6	C2-C1	7.83	1.46	1.35
47	35	309	KC1	C2A-C3A	7.82	1.53	1.37
50	19	312	DD6	C23-C16	7.82	1.69	1.53
48	16	310	A86	C30-C29	7.81	1.45	1.32
48	12	220	A86	C30-C29	7.81	1.45	1.32
48	32	221	A86	C30-C29	7.81	1.45	1.32
47	17	303	KC1	C2A-C3A	7.81	1.53	1.37
47	37	302	KC1	C2A-C3A	7.81	1.53	1.37
50	39	312	DD6	C23-C16	7.81	1.69	1.53
48	35	315	A86	C19-C20	7.80	1.63	1.52
48	11	319	A86	C30-C29	7.79	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	37	305	KC1	C2A-C3A	7.79	1.53	1.37
50	36	312	DD6	C19-C20	7.79	1.63	1.52
48	31	319	A86	C30-C29	7.77	1.44	1.32
47	32	212	KC1	C2A-C3A	7.75	1.53	1.37
48	15	316	A86	C4-C5	7.75	1.67	1.43
47	38	210	KC1	C2A-C3A	7.74	1.53	1.37
48	18	213	A86	C19-C20	7.74	1.63	1.52
47	21	203	KC1	C2A-C3A	7.73	1.52	1.37
47	12	211	KC1	C2A-C3A	7.73	1.52	1.37
48	35	316	A86	C4-C5	7.72	1.67	1.43
47	14	306	KC1	C2A-C3A	7.71	1.52	1.37
47	34	306	KC1	C2A-C3A	7.71	1.52	1.37
47	41	203	KC1	C2A-C3A	7.71	1.52	1.37
47	18	210	KC1	C2A-C3A	7.70	1.52	1.37
50	39	312	DD6	C2-C1	7.70	1.46	1.35
48	13	313	A86	C4-C5	7.67	1.67	1.43
48	33	314	A86	C4-C5	7.66	1.67	1.43
50	19	312	DD6	C2-C1	7.66	1.45	1.35
48	33	313	A86	C4-C5	7.66	1.67	1.43
47	16	305	KC1	C2A-C3A	7.64	1.52	1.37
48	16	313	A86	C4-C5	7.64	1.67	1.43
47	11	302	KC1	C2A-C3A	7.63	1.52	1.37
47	31	303	KC1	C2A-C3A	7.63	1.52	1.37
48	13	314	A86	C4-C5	7.63	1.67	1.43
48	40	201	A86	C4-C5	7.63	1.67	1.43
47	37	304	KC1	C2A-C3A	7.62	1.52	1.37
47	33	309	KC1	C2A-C3A	7.62	1.52	1.37
47	18	207	KC1	C2A-C3A	7.62	1.52	1.37
47	38	207	KC1	C2A-C3A	7.62	1.52	1.37
48	34	314	A86	C19-C20	7.62	1.62	1.52
48	21	213	A86	C4-C5	7.62	1.67	1.43
47	11	309	KC1	C2A-C3A	7.62	1.52	1.37
47	20	305	KC1	C2A-C3A	7.61	1.52	1.37
48	21	211	A86	C4-C5	7.60	1.67	1.43
48	40	213	A86	C4-C5	7.59	1.67	1.43
48	41	211	A86	C4-C5	7.59	1.67	1.43
48	41	213	A86	C4-C5	7.59	1.67	1.43
47	13	309	KC1	C2A-C3A	7.59	1.52	1.37
48	15	313	A86	C4-C5	7.59	1.66	1.43
48	20	311	A86	C4-C5	7.58	1.66	1.43
47	13	306	KC1	C2A-C3A	7.58	1.52	1.37
47	33	306	KC1	C2A-C3A	7.58	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	35	313	A86	C4-C5	7.58	1.66	1.43
47	31	309	KC1	C2A-C3A	7.58	1.52	1.37
47	36	305	KC1	C2A-C3A	7.58	1.52	1.37
48	33	314	A86	C8-C6	7.58	1.62	1.45
48	38	215	A86	C4-C5	7.57	1.66	1.43
47	17	305	KC1	C2A-C3A	7.56	1.52	1.37
48	21	215	A86	C4-C5	7.56	1.66	1.43
48	39	313	A86	C19-C20	7.56	1.62	1.52
47	40	207	KC1	C2A-C3A	7.56	1.52	1.37
48	40	211	A86	C4-C5	7.55	1.66	1.43
48	33	313	A86	C8-C6	7.55	1.62	1.45
48	13	314	A86	C8-C6	7.55	1.62	1.45
47	11	306	KC1	C2A-C3A	7.55	1.52	1.37
50	40	214	DD6	C9-C10	7.55	1.66	1.43
48	14	313	A86	C4-C5	7.55	1.66	1.43
50	20	312	DD6	C9-C10	7.55	1.66	1.43
48	16	313	A86	C8-C6	7.55	1.62	1.45
48	40	213	A86	C19-C20	7.54	1.62	1.52
48	41	215	A86	C4-C5	7.54	1.66	1.43
48	20	309	A86	C4-C5	7.54	1.66	1.43
50	41	216	DD6	C9-C10	7.54	1.66	1.43
48	21	214	A86	C19-C20	7.53	1.62	1.52
50	21	216	DD6	C9-C10	7.53	1.66	1.43
48	34	313	A86	C4-C5	7.53	1.66	1.43
48	14	314	A86	C19-C20	7.53	1.62	1.52
48	13	313	A86	C8-C6	7.53	1.62	1.45
48	14	316	A86	C4-C5	7.52	1.66	1.43
48	34	316	A86	C4-C5	7.52	1.66	1.43
48	19	313	A86	C4-C5	7.52	1.66	1.43
48	12	217	A86	C4-C5	7.52	1.66	1.43
48	40	201	A86	C8-C6	7.51	1.62	1.45
48	40	213	A86	C8-C6	7.51	1.62	1.45
47	35	302	KC1	C2A-C3A	7.51	1.52	1.37
48	20	311	A86	C8-C6	7.51	1.62	1.45
48	18	215	A86	C4-C5	7.51	1.66	1.43
48	32	218	A86	C4-C5	7.51	1.66	1.43
50	20	310	DD6	C9-C10	7.50	1.66	1.43
48	18	212	A86	C8-C6	7.50	1.62	1.45
48	39	313	A86	C4-C5	7.50	1.66	1.43
48	38	212	A86	C8-C6	7.50	1.62	1.45
47	31	307	KC1	C2A-C3A	7.50	1.52	1.37
48	41	214	A86	C19-C20	7.50	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	35	306	KC1	C2A-C3A	7.49	1.52	1.37
47	11	304	KC1	C2A-C3A	7.49	1.52	1.37
50	20	312	DD6	C19-C20	7.49	1.62	1.52
48	21	213	A86	C8-C6	7.49	1.62	1.45
50	16	312	DD6	C9-C10	7.49	1.66	1.43
48	20	311	A86	C19-C20	7.49	1.62	1.52
48	33	312	A86	C4-C5	7.49	1.66	1.43
48	40	211	A86	C8-C6	7.49	1.62	1.45
50	40	212	DD6	C9-C10	7.48	1.66	1.43
50	41	212	DD6	C9-C10	7.48	1.66	1.43
48	32	216	A86	C4-C5	7.48	1.66	1.43
48	37	314	A86	C4-C5	7.48	1.66	1.43
48	15	314	A86	C19-C20	7.47	1.62	1.52
48	13	312	A86	C4-C5	7.47	1.66	1.43
50	40	212	DD6	C19-C20	7.47	1.62	1.52
50	40	214	DD6	C19-C20	7.47	1.62	1.52
48	35	314	A86	C4-C5	7.47	1.66	1.43
50	20	310	DD6	C19-C20	7.47	1.62	1.52
47	32	207	KC1	C2A-C3A	7.47	1.52	1.37
47	14	309	KC1	C2A-C3A	7.47	1.52	1.37
50	36	312	DD6	C9-C10	7.46	1.66	1.43
50	21	212	DD6	C9-C10	7.46	1.66	1.43
47	15	306	KC1	C2A-C3A	7.46	1.52	1.37
48	41	213	A86	C8-C6	7.46	1.62	1.45
48	38	214	A86	C19-C20	7.46	1.62	1.52
48	14	314	A86	C4-C5	7.46	1.66	1.43
48	17	315	A86	C4-C5	7.46	1.66	1.43
47	34	309	KC1	C2A-C3A	7.46	1.52	1.37
47	12	206	KC1	C2A-C3A	7.45	1.52	1.37
48	15	314	A86	C4-C5	7.45	1.66	1.43
48	15	316	A86	C8-C6	7.45	1.61	1.45
48	34	314	A86	C4-C5	7.45	1.66	1.43
48	12	215	A86	C4-C5	7.44	1.66	1.43
47	31	305	KC1	C2A-C3A	7.43	1.52	1.37
50	19	312	DD6	C9-C10	7.43	1.66	1.43
48	17	312	A86	C4-C5	7.43	1.66	1.43
48	35	312	A86	C4-C5	7.43	1.66	1.43
48	20	309	A86	C8-C6	7.43	1.61	1.45
47	40	206	KC1	C2A-C3A	7.43	1.52	1.37
47	15	302	KC1	C2A-C3A	7.43	1.52	1.37
48	37	311	A86	C4-C5	7.42	1.66	1.43
48	35	316	A86	C8-C6	7.42	1.61	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	38	214	A86	C4-C5	7.42	1.66	1.43
48	15	312	A86	C4-C5	7.42	1.66	1.43
50	39	312	DD6	C9-C10	7.41	1.66	1.43
48	18	214	A86	C4-C5	7.41	1.66	1.43
48	37	314	A86	C8-C6	7.41	1.61	1.45
48	41	214	A86	C4-C5	7.41	1.66	1.43
48	18	212	A86	C4-C5	7.41	1.66	1.43
48	15	311	A86	C4-C5	7.41	1.66	1.43
48	18	214	A86	C19-C20	7.39	1.62	1.52
48	38	215	A86	C8-C6	7.39	1.61	1.45
47	18	205	KC1	C2A-C3A	7.39	1.52	1.37
48	19	313	A86	C8-C6	7.39	1.61	1.45
48	38	212	A86	C4-C5	7.39	1.66	1.43
47	20	304	KC1	C2A-C3A	7.38	1.52	1.37
48	21	214	A86	C4-C5	7.38	1.66	1.43
48	17	315	A86	C8-C6	7.38	1.61	1.45
47	38	205	KC1	C2A-C3A	7.38	1.52	1.37
47	13	302	KC1	C2A-C3A	7.37	1.52	1.37
48	13	315	A86	C4-C5	7.37	1.66	1.43
48	33	315	A86	C4-C5	7.37	1.66	1.43
48	15	313	A86	C8-C6	7.37	1.61	1.45
48	35	311	A86	C4-C5	7.37	1.66	1.43
48	14	313	A86	C8-C6	7.36	1.61	1.45
47	20	302	KC1	C2A-C3A	7.36	1.52	1.37
48	12	215	A86	C8-C6	7.35	1.61	1.45
48	32	216	A86	C8-C6	7.35	1.61	1.45
48	37	312	A86	C4-C5	7.35	1.66	1.43
48	19	313	A86	C19-C20	7.35	1.62	1.52
48	17	313	A86	C4-C5	7.34	1.66	1.43
48	17	311	A86	C4-C5	7.34	1.66	1.43
48	34	313	A86	C8-C6	7.34	1.61	1.45
48	35	313	A86	C8-C6	7.34	1.61	1.45
48	17	310	A86	C19-C20	7.34	1.62	1.52
48	33	315	A86	C8-C6	7.34	1.61	1.45
47	33	302	KC1	C2A-C3A	7.34	1.52	1.37
47	40	204	KC1	C2A-C3A	7.34	1.52	1.37
48	37	309	A86	C19-C20	7.34	1.62	1.52
48	21	215	A86	C8-C6	7.33	1.61	1.45
48	18	215	A86	C8-C6	7.33	1.61	1.45
48	11	313	A86	C4-C5	7.33	1.66	1.43
48	32	217	A86	C4-C5	7.32	1.66	1.43
48	35	314	A86	C19-C20	7.32	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	14	315	A86	C4-C5	7.32	1.66	1.43
48	13	314	A86	C19-C20	7.31	1.62	1.52
48	39	313	A86	C8-C6	7.31	1.61	1.45
48	37	310	A86	C4-C5	7.31	1.66	1.43
48	33	314	A86	C19-C20	7.31	1.62	1.52
48	41	215	A86	C8-C6	7.31	1.61	1.45
48	34	315	A86	C4-C5	7.31	1.66	1.43
48	33	312	A86	C8-C6	7.30	1.61	1.45
48	14	316	A86	C8-C6	7.30	1.61	1.45
48	15	314	A86	C8-C6	7.30	1.61	1.45
48	31	313	A86	C4-C5	7.29	1.66	1.43
48	12	216	A86	C4-C5	7.29	1.66	1.43
48	17	310	A86	C4-C5	7.29	1.66	1.43
48	37	319	A86	C4-C5	7.29	1.66	1.43
48	35	314	A86	C8-C6	7.29	1.61	1.45
48	37	309	A86	C4-C5	7.29	1.66	1.43
48	13	312	A86	C8-C6	7.28	1.61	1.45
48	13	315	A86	C8-C6	7.28	1.61	1.45
48	34	316	A86	C8-C6	7.28	1.61	1.45
48	35	319	A86	C4-C5	7.27	1.66	1.43
48	17	320	A86	C4-C5	7.27	1.66	1.43
48	12	217	A86	C8-C6	7.27	1.61	1.45
48	13	311	A86	C4-C5	7.27	1.66	1.43
48	21	211	A86	C8-C6	7.27	1.61	1.45
48	15	315	A86	C4-C5	7.27	1.66	1.43
48	20	309	A86	C19-C20	7.27	1.62	1.52
48	41	211	A86	C8-C6	7.26	1.61	1.45
48	12	213	A86	C4-C5	7.26	1.65	1.43
48	18	214	A86	C8-C6	7.25	1.61	1.45
47	19	308	KC1	C2A-C3A	7.25	1.52	1.37
48	15	319	A86	C4-C5	7.25	1.65	1.43
48	40	211	A86	C19-C20	7.25	1.62	1.52
47	33	304	KC1	C2A-C3A	7.25	1.52	1.37
48	32	218	A86	C8-C6	7.24	1.61	1.45
48	34	314	A86	C8-C6	7.24	1.61	1.45
48	35	315	A86	C4-C5	7.24	1.65	1.43
48	16	310	A86	C4-C5	7.24	1.65	1.43
48	17	312	A86	C8-C6	7.24	1.61	1.45
48	15	312	A86	C8-C6	7.24	1.61	1.45
48	36	310	A86	C4-C5	7.24	1.65	1.43
48	35	312	A86	C8-C6	7.23	1.61	1.45
47	13	304	KC1	C2A-C3A	7.23	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	13	313	A86	C19-C20	7.22	1.62	1.52
48	21	211	A86	C19-C20	7.22	1.62	1.52
48	33	311	A86	C4-C5	7.22	1.65	1.43
48	14	314	A86	C8-C6	7.22	1.61	1.45
48	11	311	A86	C4-C5	7.22	1.65	1.43
47	39	308	KC1	C2A-C3A	7.22	1.51	1.37
48	38	214	A86	C8-C6	7.21	1.61	1.45
48	11	314	A86	C4-C5	7.21	1.65	1.43
48	37	313	A86	C4-C5	7.21	1.65	1.43
48	19	311	A86	C4-C5	7.20	1.65	1.43
47	15	304	KC1	C2A-C3A	7.20	1.51	1.37
48	32	203	A86	C4-C5	7.20	1.65	1.43
48	33	313	A86	C19-C20	7.20	1.62	1.52
48	31	311	A86	C4-C5	7.20	1.65	1.43
48	12	202	A86	C4-C5	7.19	1.65	1.43
47	35	304	KC1	C2A-C3A	7.19	1.51	1.37
48	32	214	A86	C4-C5	7.19	1.65	1.43
50	41	212	DD6	C24-C1	7.19	1.61	1.45
48	17	314	A86	C8-C6	7.19	1.61	1.45
48	31	314	A86	C4-C5	7.19	1.65	1.43
48	39	311	A86	C4-C5	7.19	1.65	1.43
48	38	213	A86	C4-C5	7.19	1.65	1.43
48	37	313	A86	C8-C6	7.19	1.61	1.45
48	16	314	A86	C4-C5	7.18	1.65	1.43
48	36	313	A86	C4-C5	7.18	1.65	1.43
48	41	211	A86	C19-C20	7.18	1.62	1.52
48	18	213	A86	C4-C5	7.18	1.65	1.43
48	31	314	A86	C19-C20	7.17	1.62	1.52
50	21	212	DD6	C24-C1	7.17	1.61	1.45
48	17	314	A86	C4-C5	7.17	1.65	1.43
48	21	215	A86	C19-C20	7.16	1.62	1.52
47	36	304	KC1	C2A-C3A	7.16	1.51	1.37
48	37	313	A86	C19-C20	7.16	1.62	1.52
48	37	311	A86	C8-C6	7.15	1.61	1.45
48	11	314	A86	C19-C20	7.15	1.62	1.52
47	16	304	KC1	C2A-C3A	7.15	1.51	1.37
48	41	214	A86	C8-C6	7.14	1.61	1.45
48	11	319	A86	C4-C5	7.14	1.65	1.43
48	41	215	A86	C19-C20	7.14	1.62	1.52
48	21	214	A86	C8-C6	7.14	1.61	1.45
48	37	312	A86	C19-C20	7.13	1.62	1.52
48	11	312	A86	C4-C5	7.13	1.65	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	18	212	A86	C19-C20	7.13	1.62	1.52
48	31	319	A86	C4-C5	7.13	1.65	1.43
48	17	314	A86	C19-C20	7.13	1.62	1.52
48	12	214	A86	C4-C5	7.13	1.65	1.43
48	32	215	A86	C4-C5	7.13	1.65	1.43
48	17	313	A86	C8-C6	7.12	1.61	1.45
48	31	312	A86	C4-C5	7.12	1.65	1.43
48	33	311	A86	C8-C6	7.11	1.61	1.45
48	35	311	A86	C8-C6	7.11	1.61	1.45
48	37	312	A86	C8-C6	7.11	1.61	1.45
47	21	207	KC1	C2A-C3A	7.11	1.51	1.37
47	41	207	KC1	C2A-C3A	7.10	1.51	1.37
48	17	313	A86	C19-C20	7.09	1.62	1.52
48	11	315	A86	C4-C5	7.09	1.65	1.43
50	40	214	DD6	C24-C1	7.08	1.61	1.45
48	14	312	A86	C4-C5	7.08	1.65	1.43
48	34	312	A86	C4-C5	7.08	1.65	1.43
48	13	311	A86	C8-C6	7.08	1.61	1.45
48	14	311	A86	C8-C6	7.08	1.61	1.45
48	31	315	A86	C4-C5	7.08	1.65	1.43
48	38	212	A86	C19-C20	7.07	1.62	1.52
48	15	311	A86	C8-C6	7.07	1.61	1.45
50	20	312	DD6	C24-C1	7.06	1.61	1.45
48	35	312	A86	C25-C26	7.06	1.65	1.43
50	40	212	DD6	C24-C1	7.05	1.61	1.45
48	38	213	A86	C8-C6	7.05	1.61	1.45
50	20	310	DD6	C24-C1	7.05	1.61	1.45
48	16	311	A86	C4-C5	7.05	1.65	1.43
48	35	319	A86	C8-C6	7.04	1.61	1.45
48	34	311	A86	C8-C6	7.04	1.61	1.45
48	36	311	A86	C4-C5	7.04	1.65	1.43
48	15	319	A86	C8-C6	7.04	1.61	1.45
48	11	313	A86	C8-C6	7.04	1.61	1.45
48	32	203	A86	C8-C6	7.04	1.61	1.45
48	12	215	A86	C19-C20	7.03	1.62	1.52
48	32	216	A86	C19-C20	7.03	1.62	1.52
48	15	312	A86	C25-C26	7.03	1.65	1.43
48	12	202	A86	C8-C6	7.03	1.61	1.45
47	14	304	KC1	C2A-C3A	7.02	1.51	1.37
47	34	304	KC1	C2A-C3A	7.02	1.51	1.37
48	31	313	A86	C8-C6	7.02	1.61	1.45
48	33	312	A86	C19-C20	7.02	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	12	214	A86	C25-C26	7.02	1.65	1.43
48	12	216	A86	C19-C20	7.02	1.62	1.52
48	37	319	A86	C19-C20	7.01	1.62	1.52
48	37	319	A86	C8-C6	7.01	1.61	1.45
48	17	320	A86	C8-C6	7.01	1.61	1.45
48	32	215	A86	C25-C26	7.01	1.65	1.43
48	14	315	A86	C8-C6	7.01	1.61	1.45
48	34	315	A86	C8-C6	7.01	1.61	1.45
48	40	201	A86	C19-C20	6.99	1.62	1.52
48	14	311	A86	C4-C5	6.99	1.65	1.43
48	34	311	A86	C4-C5	6.99	1.65	1.43
48	37	310	A86	C8-C6	6.99	1.61	1.45
48	19	311	A86	C8-C6	6.98	1.60	1.45
48	39	311	A86	C8-C6	6.98	1.60	1.45
48	13	312	A86	C19-C20	6.98	1.62	1.52
48	32	217	A86	C8-C6	6.98	1.60	1.45
48	12	216	A86	C8-C6	6.97	1.60	1.45
48	15	313	A86	C25-C26	6.97	1.65	1.43
48	16	313	A86	C19-C20	6.96	1.62	1.52
48	12	220	A86	C4-C5	6.96	1.65	1.43
48	35	313	A86	C25-C26	6.96	1.65	1.43
48	16	314	A86	C8-C6	6.96	1.60	1.45
48	35	312	A86	C19-C20	6.95	1.62	1.52
48	32	221	A86	C4-C5	6.95	1.65	1.43
48	37	309	A86	C8-C6	6.94	1.60	1.45
48	17	310	A86	C8-C6	6.94	1.60	1.45
48	15	312	A86	C19-C20	6.93	1.61	1.52
50	19	312	DD6	C24-C1	6.93	1.60	1.45
48	12	213	A86	C19-C20	6.93	1.61	1.52
48	14	312	A86	C8-C6	6.92	1.60	1.45
48	34	312	A86	C8-C6	6.92	1.60	1.45
48	36	313	A86	C8-C6	6.92	1.60	1.45
48	32	217	A86	C19-C20	6.92	1.61	1.52
48	17	311	A86	C8-C6	6.92	1.60	1.45
48	41	213	A86	C19-C20	6.92	1.61	1.52
48	13	312	A86	C25-C26	6.92	1.64	1.43
50	41	212	DD6	C30-C29	6.91	1.40	1.20
48	35	315	A86	C8-C6	6.91	1.60	1.45
48	33	312	A86	C25-C26	6.91	1.64	1.43
48	12	213	A86	C8-C6	6.91	1.60	1.45
48	14	313	A86	C25-C26	6.91	1.64	1.43
48	21	213	A86	C19-C20	6.91	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	32	214	A86	C19-C20	6.91	1.61	1.52
50	21	212	DD6	C30-C29	6.90	1.40	1.20
48	17	311	A86	C19-C20	6.90	1.61	1.52
48	35	311	A86	C19-C20	6.90	1.61	1.52
48	13	313	A86	C25-C26	6.90	1.64	1.43
48	33	313	A86	C25-C26	6.90	1.64	1.43
48	15	315	A86	C8-C6	6.90	1.60	1.45
50	41	216	DD6	C24-C1	6.89	1.60	1.45
48	16	311	A86	C8-C6	6.89	1.60	1.45
48	37	311	A86	C25-C26	6.89	1.64	1.43
48	15	311	A86	C19-C20	6.89	1.61	1.52
48	32	214	A86	C8-C6	6.89	1.60	1.45
50	39	312	DD6	C24-C1	6.88	1.60	1.45
48	34	313	A86	C25-C26	6.88	1.64	1.43
48	36	311	A86	C8-C6	6.88	1.60	1.45
48	12	215	A86	C25-C26	6.88	1.64	1.43
48	13	311	A86	C19-C20	6.87	1.61	1.52
48	17	312	A86	C25-C26	6.87	1.64	1.43
48	32	216	A86	C25-C26	6.87	1.64	1.43
50	21	216	DD6	C24-C1	6.87	1.60	1.45
50	41	216	DD6	C30-C29	6.87	1.40	1.20
48	17	311	A86	C25-C26	6.87	1.64	1.43
48	41	213	A86	C25-C26	6.86	1.64	1.43
48	33	311	A86	C19-C20	6.86	1.61	1.52
48	18	213	A86	C8-C6	6.86	1.60	1.45
50	21	216	DD6	C30-C29	6.86	1.40	1.20
48	21	213	A86	C25-C26	6.86	1.64	1.43
48	16	310	A86	C8-C6	6.85	1.60	1.45
48	34	315	A86	C19-C20	6.85	1.61	1.52
48	20	311	A86	C25-C26	6.84	1.64	1.43
48	15	316	A86	C19-C20	6.84	1.61	1.52
50	36	312	DD6	C30-C29	6.84	1.40	1.20
48	36	310	A86	C8-C6	6.84	1.60	1.45
50	16	312	DD6	C30-C29	6.83	1.40	1.20
48	37	310	A86	C19-C20	6.83	1.61	1.52
48	40	213	A86	C25-C26	6.83	1.64	1.43
48	31	314	A86	C8-C6	6.82	1.60	1.45
45	d	406	PL9	C7-C3	-6.82	1.44	1.51
48	12	214	A86	C19-C20	6.82	1.61	1.52
48	37	310	A86	C25-C26	6.80	1.64	1.43
48	41	215	A86	C25-C26	6.80	1.64	1.43
48	11	314	A86	C8-C6	6.80	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	21	215	A86	C25-C26	6.79	1.64	1.43
48	32	215	A86	C19-C20	6.78	1.61	1.52
48	15	311	A86	C25-C26	6.77	1.64	1.43
48	15	313	A86	C19-C20	6.77	1.61	1.52
50	16	312	DD6	C24-C1	6.77	1.60	1.45
48	35	313	A86	C19-C20	6.76	1.61	1.52
47	16	308	KC1	CBA-CAA	6.75	1.53	1.33
48	14	315	A86	C19-C20	6.75	1.61	1.52
47	36	308	KC1	CBA-CAA	6.75	1.53	1.33
48	13	314	A86	C25-C26	6.75	1.64	1.43
50	36	312	DD6	C24-C1	6.75	1.60	1.45
48	31	312	A86	C8-C6	6.75	1.60	1.45
48	11	312	A86	C8-C6	6.75	1.60	1.45
48	15	314	A86	C25-C26	6.75	1.64	1.43
48	18	212	A86	C25-C26	6.74	1.64	1.43
48	18	215	A86	C25-C26	6.74	1.64	1.43
48	33	314	A86	C25-C26	6.74	1.64	1.43
48	31	311	A86	C8-C6	6.73	1.60	1.45
48	21	211	A86	C25-C26	6.73	1.64	1.43
48	11	319	A86	C8-C6	6.73	1.60	1.45
48	31	319	A86	C8-C6	6.73	1.60	1.45
48	35	311	A86	C25-C26	6.72	1.64	1.43
48	41	211	A86	C25-C26	6.72	1.64	1.43
48	21	214	A86	C25-C26	6.72	1.64	1.43
48	38	215	A86	C25-C26	6.72	1.64	1.43
48	35	314	A86	C25-C26	6.72	1.64	1.43
48	14	311	A86	C19-C20	6.71	1.61	1.52
48	34	311	A86	C19-C20	6.71	1.61	1.52
48	35	316	A86	C19-C20	6.71	1.61	1.52
50	40	214	DD6	C30-C29	6.71	1.39	1.20
48	38	212	A86	C25-C26	6.71	1.64	1.43
50	20	312	DD6	C30-C29	6.71	1.39	1.20
45	D	408	PL9	C7-C3	-6.70	1.44	1.51
48	41	214	A86	C25-C26	6.70	1.64	1.43
48	18	214	A86	C25-C26	6.70	1.64	1.43
48	11	311	A86	C8-C6	6.70	1.60	1.45
48	15	316	A86	C25-C26	6.69	1.64	1.43
48	38	214	A86	C25-C26	6.69	1.64	1.43
48	14	314	A86	C25-C26	6.69	1.64	1.43
48	34	314	A86	C25-C26	6.69	1.64	1.43
47	13	304	KC1	CBA-CAA	6.68	1.53	1.33
47	20	305	KC1	CBA-CAA	6.67	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	32	215	A86	C8-C6	6.67	1.60	1.45
47	40	207	KC1	CBA-CAA	6.67	1.53	1.33
48	11	315	A86	C25-C26	6.66	1.64	1.43
48	31	315	A86	C25-C26	6.66	1.64	1.43
48	36	310	A86	C19-C20	6.66	1.61	1.52
47	33	304	KC1	CBA-CAA	6.66	1.53	1.33
48	35	316	A86	C25-C26	6.66	1.64	1.43
48	31	313	A86	C25-C26	6.66	1.64	1.43
47	18	207	KC1	CBA-CAA	6.65	1.53	1.33
47	38	207	KC1	CBA-CAA	6.65	1.53	1.33
48	14	312	A86	C19-C20	6.65	1.61	1.52
48	34	312	A86	C19-C20	6.65	1.61	1.52
48	11	312	A86	C25-C26	6.65	1.64	1.43
48	14	315	A86	C25-C26	6.65	1.64	1.43
48	12	214	A86	C8-C6	6.65	1.60	1.45
48	14	316	A86	C25-C26	6.65	1.64	1.43
48	16	313	A86	C25-C26	6.64	1.64	1.43
48	34	315	A86	C25-C26	6.64	1.64	1.43
47	37	307	KC1	CBA-CAA	6.64	1.53	1.33
48	31	312	A86	C25-C26	6.64	1.64	1.43
48	40	201	A86	C25-C26	6.64	1.64	1.43
48	12	217	A86	C25-C26	6.64	1.64	1.43
47	17	308	KC1	CBA-CAA	6.64	1.53	1.33
48	39	313	A86	C25-C26	6.64	1.64	1.43
50	20	310	DD6	C30-C29	6.63	1.39	1.20
48	19	313	A86	C25-C26	6.63	1.64	1.43
48	20	309	A86	C25-C26	6.63	1.64	1.43
48	32	218	A86	C25-C26	6.63	1.64	1.43
48	35	315	A86	C25-C26	6.63	1.64	1.43
47	37	304	KC1	CBA-CAA	6.62	1.53	1.33
48	19	311	A86	C19-C20	6.62	1.61	1.52
48	39	311	A86	C19-C20	6.62	1.61	1.52
48	33	315	A86	C25-C26	6.62	1.64	1.43
48	34	316	A86	C25-C26	6.62	1.64	1.43
48	17	313	A86	C25-C26	6.62	1.63	1.43
50	40	212	DD6	C30-C29	6.62	1.39	1.20
48	11	319	A86	C25-C26	6.61	1.63	1.43
48	15	315	A86	C25-C26	6.61	1.63	1.43
48	17	315	A86	C25-C26	6.61	1.63	1.43
48	40	211	A86	C25-C26	6.61	1.63	1.43
48	16	310	A86	C19-C20	6.61	1.61	1.52
47	17	305	KC1	CBA-CAA	6.61	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	37	305	KC1	CBA-CAA	6.60	1.53	1.33
47	19	308	KC1	CBA-CAA	6.60	1.53	1.33
48	37	314	A86	C19-C20	6.60	1.61	1.52
48	31	315	A86	C8-C6	6.60	1.60	1.45
47	35	309	KC1	CBA-CAA	6.60	1.53	1.33
48	13	315	A86	C25-C26	6.60	1.63	1.43
47	16	305	KC1	CBA-CAA	6.60	1.53	1.33
47	36	305	KC1	CBA-CAA	6.59	1.53	1.33
48	17	315	A86	C19-C20	6.59	1.61	1.52
48	37	314	A86	C25-C26	6.59	1.63	1.43
47	39	308	KC1	CBA-CAA	6.59	1.53	1.33
47	15	309	KC1	CBA-CAA	6.59	1.53	1.33
48	37	312	A86	C25-C26	6.59	1.63	1.43
47	20	302	KC1	CBA-CAA	6.59	1.53	1.33
48	11	315	A86	C8-C6	6.59	1.60	1.45
48	19	311	A86	C25-C26	6.59	1.63	1.43
48	31	319	A86	C25-C26	6.58	1.63	1.43
48	17	320	A86	C19-C20	6.58	1.61	1.52
48	15	319	A86	C25-C26	6.58	1.63	1.43
47	17	306	KC1	CBA-CAA	6.58	1.53	1.33
48	35	319	A86	C25-C26	6.58	1.63	1.43
47	21	207	KC1	CBA-CAA	6.58	1.52	1.33
47	40	204	KC1	CBA-CAA	6.57	1.52	1.33
48	37	309	A86	C25-C26	6.57	1.63	1.43
47	41	207	KC1	CBA-CAA	6.57	1.52	1.33
48	12	220	A86	C8-C6	6.57	1.60	1.45
47	16	302	KC1	CBA-CAA	6.57	1.52	1.33
47	36	302	KC1	CBA-CAA	6.57	1.52	1.33
47	18	210	KC1	CBA-CAA	6.56	1.52	1.33
48	14	313	A86	C19-C20	6.56	1.61	1.52
47	35	302	KC1	CBA-CAA	6.56	1.52	1.33
48	32	217	A86	C25-C26	6.56	1.63	1.43
48	32	221	A86	C8-C6	6.56	1.60	1.45
47	15	302	KC1	CBA-CAA	6.56	1.52	1.33
47	38	210	KC1	CBA-CAA	6.55	1.52	1.33
47	15	304	KC1	CBA-CAA	6.55	1.52	1.33
47	12	206	KC1	CBA-CAA	6.55	1.52	1.33
47	32	207	KC1	CBA-CAA	6.55	1.52	1.33
48	11	314	A86	C25-C26	6.55	1.63	1.43
47	13	306	KC1	CBA-CAA	6.55	1.52	1.33
48	39	311	A86	C25-C26	6.54	1.63	1.43
48	11	311	A86	C25-C26	6.54	1.63	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	17	320	A86	C25-C26	6.54	1.63	1.43
48	17	310	A86	C25-C26	6.54	1.63	1.43
48	34	313	A86	C19-C20	6.54	1.61	1.52
47	14	304	KC1	CBA-CAA	6.54	1.52	1.33
47	11	304	KC1	CBA-CAA	6.54	1.52	1.33
47	34	306	KC1	CBA-CAA	6.54	1.52	1.33
47	34	304	KC1	CBA-CAA	6.53	1.52	1.33
48	33	311	A86	C25-C26	6.53	1.63	1.43
48	12	216	A86	C25-C26	6.53	1.63	1.43
47	14	306	KC1	CBA-CAA	6.53	1.52	1.33
47	35	304	KC1	CBA-CAA	6.53	1.52	1.33
48	13	311	A86	C25-C26	6.53	1.63	1.43
48	37	319	A86	C25-C26	6.53	1.63	1.43
47	31	305	KC1	CBA-CAA	6.53	1.52	1.33
47	33	306	KC1	CBA-CAA	6.53	1.52	1.33
47	31	307	KC1	CBA-CAA	6.52	1.52	1.33
48	33	315	A86	C19-C20	6.52	1.61	1.52
48	31	311	A86	C25-C26	6.52	1.63	1.43
47	36	304	KC1	CBA-CAA	6.51	1.52	1.33
47	18	205	KC1	CBA-CAA	6.51	1.52	1.33
48	36	311	A86	C25-C26	6.51	1.63	1.43
48	16	311	A86	C25-C26	6.51	1.63	1.43
48	32	221	A86	C19-C20	6.51	1.61	1.52
47	11	306	KC1	CBA-CAA	6.51	1.52	1.33
50	19	312	DD6	C21-C20	-6.51	1.41	1.51
48	13	315	A86	C19-C20	6.50	1.61	1.52
47	16	304	KC1	CBA-CAA	6.50	1.52	1.33
48	11	313	A86	C25-C26	6.50	1.63	1.43
50	39	312	DD6	C21-C20	-6.50	1.41	1.51
47	33	309	KC1	CBA-CAA	6.50	1.52	1.33
47	38	205	KC1	CBA-CAA	6.50	1.52	1.33
48	14	312	A86	C25-C26	6.49	1.63	1.43
48	12	220	A86	C19-C20	6.49	1.61	1.52
47	37	302	KC1	CBA-CAA	6.49	1.52	1.33
47	17	303	KC1	CBA-CAA	6.49	1.52	1.33
48	31	314	A86	C25-C26	6.48	1.63	1.43
47	12	211	KC1	CBA-CAA	6.48	1.52	1.33
47	35	306	KC1	CBA-CAA	6.48	1.52	1.33
47	32	212	KC1	CBA-CAA	6.48	1.52	1.33
47	31	303	KC1	CBA-CAA	6.47	1.52	1.33
48	38	213	A86	C25-C26	6.47	1.63	1.43
48	34	312	A86	C25-C26	6.46	1.63	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	37	311	A86	C19-C20	6.46	1.61	1.52
47	15	306	KC1	CBA-CAA	6.46	1.52	1.33
47	11	302	KC1	CBA-CAA	6.45	1.52	1.33
47	13	309	KC1	CBA-CAA	6.45	1.52	1.33
50	20	312	DD6	C21-C20	-6.44	1.41	1.51
47	13	302	KC1	CBA-CAA	6.44	1.52	1.33
47	33	302	KC1	CBA-CAA	6.44	1.52	1.33
50	40	214	DD6	C21-C20	-6.43	1.41	1.51
48	18	213	A86	C25-C26	6.43	1.63	1.43
48	34	311	A86	C25-C26	6.43	1.63	1.43
47	20	304	KC1	CBA-CAA	6.43	1.52	1.33
50	21	212	DD6	C30-C31	6.42	1.55	1.42
48	32	214	A86	C25-C26	6.42	1.63	1.43
47	21	203	KC1	CBA-CAA	6.42	1.52	1.33
47	41	203	KC1	CBA-CAA	6.42	1.52	1.33
47	40	206	KC1	CBA-CAA	6.42	1.52	1.33
47	14	309	KC1	CBA-CAA	6.42	1.52	1.33
48	37	313	A86	C25-C26	6.41	1.63	1.43
48	36	311	A86	C19-C20	6.41	1.61	1.52
48	14	311	A86	C25-C26	6.40	1.63	1.43
50	36	312	DD6	C30-C31	6.40	1.55	1.42
50	41	212	DD6	C30-C31	6.40	1.55	1.42
48	17	312	A86	C19-C20	6.40	1.61	1.52
47	34	309	KC1	CBA-CAA	6.40	1.52	1.33
50	39	312	DD6	C30-C29	6.39	1.38	1.20
48	16	311	A86	C19-C20	6.37	1.61	1.52
50	16	312	DD6	C30-C31	6.37	1.55	1.42
50	19	312	DD6	C30-C29	6.36	1.38	1.20
48	35	319	A86	C19-C20	6.36	1.61	1.52
48	15	319	A86	C19-C20	6.36	1.61	1.52
48	12	220	A86	C25-C26	6.35	1.63	1.43
48	36	313	A86	C25-C26	6.35	1.63	1.43
48	32	221	A86	C25-C26	6.34	1.63	1.43
47	31	309	KC1	CBA-CAA	6.33	1.52	1.33
48	17	314	A86	C25-C26	6.33	1.63	1.43
47	11	309	KC1	CBA-CAA	6.33	1.52	1.33
48	12	202	A86	C25-C26	6.33	1.63	1.43
48	32	203	A86	C25-C26	6.33	1.63	1.43
48	12	202	A86	C19-C20	6.33	1.61	1.52
48	16	314	A86	C25-C26	6.33	1.63	1.43
48	12	213	A86	C25-C26	6.32	1.63	1.43
48	32	203	A86	C19-C20	6.32	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	41	216	DD6	C21-C20	-6.32	1.41	1.51
50	21	216	DD6	C21-C20	-6.29	1.42	1.51
48	16	310	A86	C25-C26	6.29	1.62	1.43
48	36	310	A86	C25-C26	6.28	1.62	1.43
50	20	312	DD6	C30-C31	6.28	1.55	1.42
50	40	214	DD6	C30-C31	6.27	1.55	1.42
48	14	316	A86	C19-C20	6.27	1.61	1.52
48	31	312	A86	C19-C20	6.25	1.61	1.52
50	36	312	DD6	C21-C20	-6.24	1.42	1.51
37	Z	101	CLA	C3B-C2B	6.23	1.49	1.40
50	16	312	DD6	C21-C20	-6.23	1.42	1.51
50	21	216	DD6	C30-C31	6.22	1.55	1.42
48	11	312	A86	C19-C20	6.21	1.60	1.52
37	z	101	CLA	C3B-C2B	6.20	1.49	1.40
48	34	316	A86	C19-C20	6.20	1.60	1.52
50	41	216	DD6	C30-C31	6.20	1.55	1.42
47	12	208	KC1	CBA-CAA	6.20	1.51	1.33
47	32	209	KC1	CBA-CAA	6.18	1.51	1.33
37	31	301	CLA	C3B-C2B	6.18	1.48	1.40
37	W	102	CLA	C3B-C2B	6.17	1.48	1.40
50	40	212	DD6	C21-C20	-6.16	1.42	1.51
48	38	215	A86	C19-C20	6.15	1.60	1.52
50	20	310	DD6	C21-C20	-6.11	1.42	1.51
48	12	217	A86	C19-C20	6.10	1.60	1.52
48	18	215	A86	C19-C20	6.08	1.60	1.52
37	13	310	CLA	C3B-C2B	6.06	1.48	1.40
48	32	218	A86	C19-C20	6.05	1.60	1.52
48	31	319	A86	C19-C20	6.04	1.60	1.52
48	11	319	A86	C19-C20	6.03	1.60	1.52
48	11	315	A86	C19-C20	6.03	1.60	1.52
48	31	315	A86	C19-C20	6.03	1.60	1.52
37	33	310	CLA	C3B-C2B	6.02	1.48	1.40
48	31	311	A86	C19-C20	6.02	1.60	1.52
37	b	513	CLA	C3B-C2B	6.00	1.48	1.40
37	38	211	CLA	C3B-C2B	6.00	1.48	1.40
50	41	216	DD6	C13-C14	6.00	1.45	1.32
48	11	311	A86	C19-C20	6.00	1.60	1.52
37	18	211	CLA	C3B-C2B	6.00	1.48	1.40
50	21	216	DD6	C13-C14	5.99	1.45	1.32
37	Z	102	CLA	C3B-C2B	5.99	1.48	1.40
37	B	512	CLA	C3B-C2B	5.98	1.48	1.40
37	z	102	CLA	C3B-C2B	5.98	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	38	206	CLA	C3B-C2B	5.98	1.48	1.40
37	18	208	CLA	C3B-C2B	5.97	1.48	1.40
37	b	512	CLA	C3B-C2B	5.97	1.48	1.40
50	21	212	DD6	C21-C20	-5.97	1.42	1.51
37	38	208	CLA	C3B-C2B	5.95	1.48	1.40
47	15	302	KC1	O2A-CGA	5.95	1.45	1.30
37	B	513	CLA	C3B-C2B	5.95	1.48	1.40
37	35	310	CLA	C3B-C2B	5.94	1.48	1.40
47	17	306	KC1	O2A-CGA	5.94	1.45	1.30
47	18	205	KC1	O2A-CGA	5.93	1.45	1.30
47	38	205	KC1	O2A-CGA	5.93	1.45	1.30
47	15	304	KC1	O2A-CGA	5.93	1.45	1.30
47	35	302	KC1	O2A-CGA	5.93	1.45	1.30
47	20	304	KC1	O2A-CGA	5.93	1.45	1.30
37	15	310	CLA	C3B-C2B	5.92	1.48	1.40
37	37	308	CLA	C3B-C2B	5.92	1.48	1.40
47	21	203	KC1	O2A-CGA	5.92	1.45	1.30
37	38	204	CLA	C3B-C2B	5.92	1.48	1.40
50	41	212	DD6	C21-C20	-5.92	1.42	1.51
47	40	206	KC1	O2A-CGA	5.91	1.45	1.30
37	40	210	CLA	C3B-C2B	5.91	1.48	1.40
47	15	306	KC1	O2A-CGA	5.91	1.45	1.30
47	35	306	KC1	O2A-CGA	5.91	1.45	1.30
37	21	205	CLA	C3B-C2B	5.90	1.48	1.40
47	35	309	KC1	O2A-CGA	5.90	1.45	1.30
47	41	203	KC1	O2A-CGA	5.90	1.45	1.30
47	13	306	KC1	O2A-CGA	5.90	1.45	1.30
37	20	308	CLA	C3B-C2B	5.90	1.48	1.40
37	18	204	CLA	C3B-C2B	5.90	1.48	1.40
50	40	212	DD6	C30-C31	5.90	1.54	1.42
37	41	208	CLA	C3B-C2B	5.89	1.48	1.40
47	41	203	KC1	C3B-C2B	5.89	1.49	1.37
47	20	305	KC1	O2A-CGA	5.89	1.45	1.30
48	11	313	A86	C19-C20	5.89	1.60	1.52
48	16	314	A86	C19-C20	5.89	1.60	1.52
37	14	308	CLA	C3B-C2B	5.89	1.48	1.40
47	37	305	KC1	O2A-CGA	5.89	1.45	1.30
47	35	304	KC1	O2A-CGA	5.89	1.45	1.30
37	41	209	CLA	C3B-C2B	5.88	1.48	1.40
47	40	204	KC1	O2A-CGA	5.88	1.45	1.30
47	36	302	KC1	O2A-CGA	5.88	1.45	1.30
50	20	310	DD6	C30-C31	5.88	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	21	207	KC1	O2A-CGA	5.88	1.45	1.30
47	40	207	KC1	O2A-CGA	5.88	1.45	1.30
47	36	304	KC1	O2A-CGA	5.88	1.45	1.30
37	34	308	CLA	C3B-C2B	5.88	1.48	1.40
47	33	302	KC1	O2A-CGA	5.88	1.45	1.30
47	21	203	KC1	C3B-C2B	5.88	1.49	1.37
37	20	307	CLA	C3B-C2B	5.88	1.48	1.40
37	40	209	CLA	C3B-C2B	5.88	1.48	1.40
47	16	304	KC1	O2A-CGA	5.87	1.45	1.30
47	16	308	KC1	O2A-CGA	5.87	1.45	1.30
37	41	205	CLA	C3B-C2B	5.87	1.48	1.40
37	17	307	CLA	C3B-C2B	5.87	1.48	1.40
47	15	309	KC1	O2A-CGA	5.87	1.45	1.30
47	19	308	KC1	O2A-CGA	5.87	1.45	1.30
37	37	306	CLA	C3B-C2B	5.87	1.48	1.40
47	36	308	KC1	O2A-CGA	5.87	1.45	1.30
47	38	207	KC1	O2A-CGA	5.87	1.45	1.30
47	34	306	KC1	O2A-CGA	5.86	1.45	1.30
48	31	313	A86	C19-C20	5.86	1.60	1.52
50	20	312	DD6	C13-C14	5.86	1.45	1.32
50	40	214	DD6	C13-C14	5.86	1.45	1.32
47	17	308	KC1	O2A-CGA	5.86	1.45	1.30
47	41	207	KC1	O2A-CGA	5.86	1.45	1.30
47	20	302	KC1	O2A-CGA	5.86	1.45	1.30
37	A	403	CLA	C3B-C2B	5.86	1.48	1.40
47	13	302	KC1	O2A-CGA	5.85	1.45	1.30
47	13	304	KC1	O2A-CGA	5.85	1.45	1.30
47	16	305	KC1	O2A-CGA	5.85	1.45	1.30
47	33	304	KC1	O2A-CGA	5.85	1.45	1.30
37	35	303	CLA	C3B-C2B	5.85	1.48	1.40
37	15	305	CLA	C3B-C2B	5.85	1.48	1.40
37	21	208	CLA	C3B-C2B	5.85	1.48	1.40
47	37	307	KC1	O2A-CGA	5.85	1.45	1.30
47	18	207	KC1	O2A-CGA	5.85	1.45	1.30
47	33	306	KC1	O2A-CGA	5.85	1.45	1.30
47	17	305	KC1	O2A-CGA	5.85	1.45	1.30
37	35	308	CLA	C3B-C2B	5.85	1.48	1.40
47	16	302	KC1	O2A-CGA	5.84	1.45	1.30
37	15	303	CLA	C3B-C2B	5.84	1.48	1.40
47	39	308	KC1	O2A-CGA	5.84	1.45	1.30
37	13	305	CLA	C3B-C2B	5.83	1.48	1.40
37	33	305	CLA	C3B-C2B	5.83	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	37	304	KC1	O2A-CGA	5.83	1.45	1.30
37	34	305	CLA	C3B-C2B	5.83	1.48	1.40
37	15	308	CLA	C3B-C2B	5.82	1.48	1.40
47	36	305	KC1	O2A-CGA	5.82	1.45	1.30
48	36	313	A86	C19-C20	5.82	1.60	1.52
37	21	209	CLA	C3B-C2B	5.82	1.48	1.40
37	a	403	CLA	C3B-C2B	5.81	1.48	1.40
37	B	511	CLA	C3B-C2B	5.81	1.48	1.40
37	b	511	CLA	C3B-C2B	5.81	1.48	1.40
47	14	306	KC1	O2A-CGA	5.81	1.45	1.30
37	17	309	CLA	C3B-C2B	5.81	1.48	1.40
47	38	210	KC1	O2A-CGA	5.81	1.45	1.30
47	11	304	KC1	O2A-CGA	5.80	1.45	1.30
47	18	210	KC1	O2A-CGA	5.80	1.45	1.30
37	37	303	CLA	C3B-C2B	5.80	1.48	1.40
47	31	305	KC1	O2A-CGA	5.79	1.45	1.30
47	17	303	KC1	O2A-CGA	5.79	1.45	1.30
47	37	302	KC1	O2A-CGA	5.79	1.45	1.30
37	c	510	CLA	C3B-C2B	5.79	1.48	1.40
47	13	309	KC1	O2A-CGA	5.78	1.45	1.30
37	17	304	CLA	C3B-C2B	5.78	1.48	1.40
47	14	304	KC1	O2A-CGA	5.77	1.45	1.30
37	C	510	CLA	C3B-C2B	5.77	1.48	1.40
37	21	204	CLA	C3B-C2B	5.77	1.48	1.40
37	c	507	CLA	C3B-C2B	5.77	1.48	1.40
37	14	305	CLA	C3B-C2B	5.77	1.48	1.40
37	35	307	CLA	C3B-C2B	5.77	1.48	1.40
37	38	202	CLA	C3B-C2B	5.76	1.48	1.40
37	33	308	CLA	C3B-C2B	5.75	1.48	1.40
37	41	204	CLA	C3B-C2B	5.75	1.48	1.40
47	33	309	KC1	O2A-CGA	5.75	1.45	1.30
37	C	507	CLA	C3B-C2B	5.75	1.48	1.40
47	31	307	KC1	O2A-CGA	5.74	1.45	1.30
37	15	307	CLA	C3B-C2B	5.74	1.48	1.40
37	16	307	CLA	C3B-C2B	5.74	1.48	1.40
47	11	306	KC1	O2A-CGA	5.74	1.45	1.30
47	34	304	KC1	O2A-CGA	5.74	1.45	1.30
37	36	307	CLA	C3B-C2B	5.73	1.48	1.40
37	40	205	CLA	C3B-C2B	5.73	1.48	1.40
37	38	203	CLA	C3B-C2B	5.72	1.48	1.40
37	19	302	CLA	C3B-C2B	5.72	1.48	1.40
37	31	310	CLA	C3B-C2B	5.72	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	39	302	CLA	C3B-C2B	5.72	1.48	1.40
37	C	509	CLA	C3B-C2B	5.71	1.48	1.40
37	11	310	CLA	C3B-C2B	5.71	1.48	1.40
47	34	309	KC1	O2A-CGA	5.70	1.45	1.30
37	13	308	CLA	C3B-C2B	5.70	1.48	1.40
37	16	309	CLA	C3B-C2B	5.70	1.48	1.40
37	19	304	CLA	C3B-C2B	5.70	1.48	1.40
37	17	309	CLA	C3C-C2C	5.70	1.48	1.36
37	35	305	CLA	C3B-C2B	5.69	1.48	1.40
47	14	309	KC1	O2A-CGA	5.69	1.45	1.30
47	11	302	KC1	C3B-C2B	5.69	1.48	1.37
47	31	303	KC1	C3B-C2B	5.69	1.48	1.37
37	13	307	CLA	C3B-C2B	5.69	1.48	1.40
47	12	206	KC1	O2A-CGA	5.68	1.45	1.30
47	32	207	KC1	O2A-CGA	5.68	1.45	1.30
47	31	303	KC1	O2A-CGA	5.68	1.45	1.30
47	32	212	KC1	O2A-CGA	5.68	1.45	1.30
37	36	309	CLA	C3B-C2B	5.68	1.48	1.40
47	11	302	KC1	O2A-CGA	5.67	1.45	1.30
37	18	202	CLA	C3B-C2B	5.67	1.48	1.40
37	20	303	CLA	C3B-C2B	5.67	1.48	1.40
37	35	301	CLA	C3B-C2B	5.67	1.48	1.40
37	21	206	CLA	C3B-C2B	5.67	1.48	1.40
37	19	303	CLA	C3B-C2B	5.67	1.48	1.40
47	12	206	KC1	C3C-C2C	5.67	1.48	1.36
37	18	206	CLA	C3B-C2B	5.66	1.48	1.40
47	12	211	KC1	O2A-CGA	5.65	1.45	1.30
37	c	511	CLA	C3B-C2B	5.65	1.48	1.40
37	c	509	CLA	C3B-C2B	5.64	1.48	1.40
48	35	312	A86	C26-C27	5.64	1.43	1.35
37	34	310	CLA	C3B-C2B	5.64	1.48	1.40
37	12	205	CLA	C3B-C2B	5.64	1.48	1.40
37	39	304	CLA	C3B-C2B	5.64	1.48	1.40
37	D	401	CLA	C3B-C2B	5.64	1.48	1.40
37	16	303	CLA	C3B-C2B	5.63	1.48	1.40
48	15	312	A86	C26-C27	5.63	1.43	1.35
37	32	206	CLA	C3B-C2B	5.63	1.48	1.40
37	20	301	CLA	C3B-C2B	5.63	1.48	1.40
37	36	303	CLA	C3B-C2B	5.63	1.48	1.40
47	32	207	KC1	C3C-C2C	5.63	1.48	1.36
47	41	203	KC1	C3D-C2D	5.62	1.49	1.39
37	17	302	CLA	C3B-C2B	5.62	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	39	303	CLA	C3B-C2B	5.62	1.48	1.40
47	35	304	KC1	C3D-C2D	5.61	1.49	1.39
37	15	301	CLA	C3B-C2B	5.61	1.48	1.40
47	16	304	KC1	C3B-C2B	5.61	1.48	1.37
47	20	305	KC1	C3B-C2B	5.60	1.48	1.37
37	41	210	CLA	C3B-C2B	5.60	1.48	1.40
37	33	307	CLA	C3B-C2B	5.60	1.48	1.40
37	14	310	CLA	C3B-C2B	5.60	1.48	1.40
47	31	309	KC1	O2A-CGA	5.60	1.44	1.30
47	36	304	KC1	C3B-C2B	5.60	1.48	1.37
47	40	207	KC1	C3B-C2B	5.60	1.48	1.37
47	11	309	KC1	O2A-CGA	5.59	1.44	1.30
37	37	301	CLA	C3B-C2B	5.59	1.48	1.40
47	13	309	KC1	C3D-C2D	5.59	1.49	1.39
47	21	203	KC1	C3D-C2D	5.59	1.49	1.39
37	18	203	CLA	C3B-C2B	5.59	1.48	1.40
37	37	308	CLA	C3C-C2C	5.58	1.48	1.36
37	41	206	CLA	C3B-C2B	5.58	1.48	1.40
37	a	404	CLA	C3B-C2B	5.58	1.48	1.40
37	19	309	CLA	C3B-C2B	5.58	1.48	1.40
37	39	309	CLA	C3B-C2B	5.58	1.48	1.40
37	38	211	CLA	C3C-C2C	5.58	1.48	1.36
37	C	511	CLA	C3B-C2B	5.57	1.48	1.40
47	33	309	KC1	C3D-C2D	5.57	1.49	1.39
37	12	212	CLA	C3B-C2B	5.57	1.48	1.40
37	37	301	CLA	C3C-C2C	5.57	1.48	1.36
50	19	312	DD6	C13-C14	5.57	1.44	1.32
37	33	303	CLA	C3B-C2B	5.56	1.48	1.40
37	40	203	CLA	C3B-C2B	5.56	1.48	1.40
47	18	205	KC1	C3B-C2B	5.56	1.48	1.37
37	34	303	CLA	C3B-C2B	5.56	1.48	1.40
50	39	312	DD6	C13-C14	5.55	1.44	1.32
47	35	304	KC1	C3B-C2B	5.55	1.48	1.37
37	12	210	CLA	C3B-C2B	5.55	1.48	1.40
37	31	308	CLA	C3C-C2C	5.54	1.48	1.36
37	21	210	CLA	C3B-C2B	5.54	1.48	1.40
47	15	304	KC1	C3B-C2B	5.54	1.48	1.37
37	11	303	CLA	C3B-C2B	5.53	1.48	1.40
37	31	304	CLA	C3B-C2B	5.53	1.48	1.40
37	11	307	CLA	C3C-C2C	5.53	1.48	1.36
47	38	205	KC1	C3B-C2B	5.53	1.48	1.37
47	36	305	KC1	C3D-C2D	5.53	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	16	302	KC1	C3D-C2D	5.53	1.49	1.39
37	38	209	CLA	C3B-C2B	5.53	1.48	1.40
47	15	304	KC1	C3D-C2D	5.53	1.49	1.39
37	32	213	CLA	C3B-C2B	5.53	1.48	1.40
47	16	305	KC1	C3D-C2D	5.53	1.49	1.39
37	18	209	CLA	C3B-C2B	5.52	1.48	1.40
47	36	302	KC1	C3D-C2D	5.52	1.49	1.39
37	c	508	CLA	C3B-C2B	5.52	1.48	1.40
46	v	201	HEM	C3C-C2C	-5.52	1.32	1.40
47	14	304	KC1	C3C-C2C	5.52	1.48	1.36
37	16	306	CLA	C3B-C2B	5.51	1.48	1.40
47	35	309	KC1	C3D-C2D	5.51	1.49	1.39
37	35	310	CLA	C3C-C2C	5.51	1.48	1.36
37	17	302	CLA	C3C-C2C	5.51	1.48	1.36
47	34	304	KC1	C3C-C2C	5.50	1.48	1.36
47	18	205	KC1	C3D-C2D	5.50	1.49	1.39
37	32	211	CLA	C3B-C2B	5.50	1.48	1.40
47	40	207	KC1	C3D-C2D	5.50	1.49	1.39
47	37	307	KC1	C3D-C2D	5.49	1.49	1.39
46	V	201	HEM	C3C-C2C	-5.49	1.32	1.40
37	14	303	CLA	C3B-C2B	5.49	1.48	1.40
47	15	309	KC1	C3D-C2D	5.48	1.49	1.39
37	15	310	CLA	C3C-C2C	5.48	1.48	1.36
37	41	202	CLA	C3C-C2C	5.48	1.48	1.36
37	33	307	CLA	O2D-CGD	5.48	1.46	1.33
37	21	202	CLA	C3C-C2C	5.47	1.48	1.36
47	17	308	KC1	C3D-C2D	5.47	1.49	1.39
47	15	306	KC1	C3D-C2D	5.47	1.49	1.39
47	15	306	KC1	C3B-C2B	5.47	1.48	1.37
37	36	306	CLA	C3B-C2B	5.47	1.48	1.40
47	38	205	KC1	C3D-C2D	5.47	1.49	1.39
47	14	304	KC1	C3D-C2D	5.47	1.49	1.39
47	15	302	KC1	C3D-C2D	5.46	1.49	1.39
37	13	307	CLA	O2D-CGD	5.46	1.46	1.33
47	20	305	KC1	C3D-C2D	5.46	1.49	1.39
37	33	310	CLA	C1D-ND	5.46	1.44	1.37
47	18	210	KC1	C3D-C2D	5.46	1.49	1.39
37	40	208	CLA	C3B-C2B	5.46	1.47	1.40
37	21	210	CLA	C3C-C2C	5.46	1.48	1.36
37	13	303	CLA	C3B-C2B	5.46	1.47	1.40
47	38	210	KC1	C3D-C2D	5.46	1.49	1.39
47	18	207	KC1	C3D-C2D	5.46	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	508	CLA	C3B-C2B	5.46	1.47	1.40
37	32	204	CLA	C3B-C2B	5.46	1.47	1.40
37	41	210	CLA	C3C-C2C	5.45	1.48	1.36
47	39	308	KC1	C3B-C2B	5.45	1.48	1.37
47	16	304	KC1	C3D-C2D	5.45	1.49	1.39
47	38	207	KC1	C3D-C2D	5.45	1.49	1.39
47	21	207	KC1	C3D-C2D	5.45	1.49	1.39
47	35	302	KC1	C3D-C2D	5.45	1.49	1.39
47	17	303	KC1	C3D-C2D	5.44	1.49	1.39
47	37	302	KC1	C3D-C2D	5.44	1.49	1.39
37	41	202	CLA	C3B-C2B	5.44	1.47	1.40
47	34	304	KC1	C3D-C2D	5.44	1.49	1.39
37	B	524	CLA	C3B-C2B	5.43	1.47	1.40
47	15	309	KC1	C3B-C2B	5.43	1.48	1.37
47	35	309	KC1	C3B-C2B	5.43	1.48	1.37
37	12	203	CLA	C3B-C2B	5.43	1.47	1.40
47	40	206	KC1	C3D-C2D	5.43	1.49	1.39
37	20	306	CLA	C3B-C2B	5.43	1.47	1.40
37	19	310	CLA	C3B-C2B	5.43	1.47	1.40
47	35	306	KC1	C3D-C2D	5.43	1.49	1.39
47	19	308	KC1	C3B-C2B	5.43	1.48	1.37
47	35	306	KC1	C3B-C2B	5.42	1.48	1.37
47	33	304	KC1	C3B-C2B	5.42	1.48	1.37
37	12	207	CLA	C3B-C2B	5.42	1.47	1.40
37	32	208	CLA	C3B-C2B	5.42	1.47	1.40
47	41	207	KC1	C3D-C2D	5.42	1.49	1.39
37	39	310	CLA	C3B-C2B	5.42	1.47	1.40
47	20	304	KC1	C3D-C2D	5.41	1.49	1.39
47	17	306	KC1	C3C-C2C	5.41	1.48	1.36
47	37	305	KC1	C3C-C2C	5.41	1.48	1.36
37	18	211	CLA	C1D-ND	5.41	1.44	1.37
47	18	210	KC1	C3B-C2B	5.41	1.48	1.37
37	21	202	CLA	C3B-C2B	5.41	1.47	1.40
47	17	303	KC1	C3B-C2B	5.40	1.48	1.37
47	13	304	KC1	C3B-C2B	5.40	1.48	1.37
47	11	302	KC1	C3D-C2D	5.40	1.49	1.39
47	31	303	KC1	C3D-C2D	5.40	1.49	1.39
47	38	207	KC1	C3B-C2B	5.40	1.48	1.37
45	D	404	PL9	C7-C3	-5.39	1.45	1.51
50	19	312	DD6	C30-C31	5.39	1.53	1.42
47	38	210	KC1	C3B-C2B	5.39	1.48	1.37
47	36	304	KC1	C3D-C2D	5.39	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	36	301	CLA	C3B-C2B	5.39	1.47	1.40
47	14	304	KC1	C3B-C2B	5.39	1.48	1.37
50	39	312	DD6	C30-C31	5.38	1.53	1.42
37	31	301	CLA	C3C-C2C	5.38	1.48	1.36
47	32	209	KC1	O2A-CGA	5.37	1.44	1.30
37	z	101	CLA	C3C-C2C	5.37	1.48	1.36
37	d	403	CLA	C3B-C2B	5.37	1.47	1.40
47	33	306	KC1	C3D-C2D	5.37	1.49	1.39
37	34	301	CLA	C3B-C2B	5.37	1.47	1.40
47	37	305	KC1	C3D-C2D	5.37	1.49	1.39
47	20	305	KC1	C3C-C2C	5.36	1.48	1.36
37	D	405	CLA	C3B-C2B	5.36	1.47	1.40
37	z	102	CLA	O2D-CGD	5.36	1.46	1.33
37	d	404	CLA	C3B-C2B	5.36	1.47	1.40
47	12	208	KC1	O2A-CGA	5.36	1.44	1.30
37	35	305	CLA	C3C-C2C	5.36	1.48	1.36
37	Z	102	CLA	O2D-CGD	5.36	1.46	1.33
45	d	402	PL9	C7-C3	-5.36	1.45	1.51
37	32	210	CLA	C3B-C2B	5.36	1.47	1.40
37	D	406	CLA	C3B-C2B	5.35	1.47	1.40
37	Z	102	CLA	C3C-C2C	5.35	1.48	1.36
37	D	401	CLA	C3C-C2C	5.35	1.48	1.36
37	b	523	CLA	C3B-C2B	5.35	1.47	1.40
47	17	306	KC1	C3D-C2D	5.35	1.49	1.39
37	35	301	CLA	C3C-C2C	5.35	1.48	1.36
45	D	408	PL9	C3-C4	-5.35	1.40	1.49
47	34	304	KC1	C3B-C2B	5.35	1.48	1.37
47	37	304	KC1	C3B-C2B	5.35	1.48	1.37
37	38	206	CLA	C3C-C2C	5.35	1.48	1.36
47	15	302	KC1	C3C-C2C	5.35	1.48	1.36
47	39	308	KC1	C3D-C2D	5.35	1.49	1.39
37	Z	101	CLA	C3C-C2C	5.35	1.48	1.36
47	13	306	KC1	C3D-C2D	5.34	1.49	1.39
37	B	502	CLA	C3B-C2B	5.34	1.47	1.40
37	B	506	CLA	C3B-C2B	5.34	1.47	1.40
37	a	404	CLA	C3C-C2C	5.34	1.48	1.36
45	d	406	PL9	C3-C4	-5.34	1.40	1.49
47	16	305	KC1	C3C-C2C	5.34	1.48	1.36
37	14	301	CLA	C3B-C2B	5.34	1.47	1.40
37	13	310	CLA	C1D-ND	5.34	1.44	1.37
37	18	206	CLA	C3C-C2C	5.34	1.48	1.36
50	20	312	DD6	C3-C2	5.34	1.60	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	102	CLA	C3C-C2C	5.34	1.48	1.36
47	41	207	KC1	C3B-C2B	5.33	1.48	1.37
37	z	102	CLA	C3C-C2C	5.33	1.48	1.36
47	37	305	KC1	C3B-C2B	5.33	1.48	1.37
37	15	305	CLA	C3C-C2C	5.33	1.48	1.36
47	11	304	KC1	C3B-C2B	5.33	1.48	1.37
47	31	305	KC1	C3B-C2B	5.33	1.48	1.37
37	b	506	CLA	C3B-C2B	5.33	1.47	1.40
37	21	209	CLA	C3C-C2C	5.33	1.48	1.36
37	41	209	CLA	C3C-C2C	5.32	1.48	1.36
47	19	308	KC1	C3D-C2D	5.32	1.49	1.39
37	21	209	CLA	C1D-ND	5.32	1.44	1.37
47	34	306	KC1	C3D-C2D	5.32	1.49	1.39
37	35	305	CLA	C1D-ND	5.32	1.44	1.37
37	39	304	CLA	C3C-C2C	5.32	1.48	1.36
47	13	306	KC1	C3B-C2B	5.32	1.48	1.37
37	38	201	CLA	C3C-C2C	5.32	1.48	1.36
47	35	304	KC1	CHD-C4C	5.32	1.48	1.35
47	11	304	KC1	C3D-C2D	5.32	1.49	1.39
37	b	502	CLA	C3B-C2B	5.32	1.47	1.40
37	16	301	CLA	C3B-C2B	5.32	1.47	1.40
37	34	310	CLA	C3C-C2C	5.32	1.48	1.36
37	41	210	CLA	C1D-ND	5.31	1.44	1.37
48	37	310	A86	C26-C27	5.31	1.42	1.35
37	12	209	CLA	C3B-C2B	5.31	1.47	1.40
47	37	302	KC1	C3B-C2B	5.31	1.48	1.37
47	21	207	KC1	C3B-C2B	5.31	1.48	1.37
37	41	209	CLA	C1D-ND	5.31	1.44	1.37
37	38	204	CLA	O2D-CGD	5.31	1.46	1.33
37	15	301	CLA	C3C-C2C	5.31	1.48	1.36
50	40	214	DD6	C3-C2	5.31	1.59	1.43
47	31	305	KC1	C3D-C2D	5.30	1.48	1.39
37	20	307	CLA	C3C-C2C	5.30	1.48	1.36
37	W	101	CLA	C3B-C2B	5.30	1.47	1.40
37	38	211	CLA	C1D-ND	5.30	1.44	1.37
37	19	304	CLA	C3C-C2C	5.30	1.48	1.36
47	37	304	KC1	CHD-C4C	5.30	1.48	1.35
47	40	207	KC1	C3C-C2C	5.30	1.48	1.36
47	15	304	KC1	CHD-C4C	5.30	1.48	1.35
37	16	309	CLA	C3C-C2C	5.30	1.48	1.36
47	17	308	KC1	C3B-C2B	5.30	1.48	1.37
37	13	310	CLA	C3C-C2C	5.29	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	14	306	KC1	C3D-C2D	5.29	1.48	1.39
37	b	510	CLA	C3B-C2B	5.29	1.47	1.40
47	33	306	KC1	C3B-C2B	5.29	1.48	1.37
37	15	305	CLA	C1D-ND	5.29	1.44	1.37
47	18	205	KC1	C3C-C2C	5.29	1.48	1.36
37	14	307	CLA	C3B-C2B	5.29	1.47	1.40
37	c	512	CLA	C3C-C2C	5.28	1.48	1.36
37	34	307	CLA	C3B-C2B	5.28	1.47	1.40
37	38	203	CLA	C1D-ND	5.28	1.44	1.37
37	14	310	CLA	C3C-C2C	5.28	1.48	1.36
47	36	305	KC1	C3C-C2C	5.28	1.48	1.36
37	21	202	CLA	C1D-ND	5.28	1.44	1.37
37	38	209	CLA	C3C-C2C	5.28	1.47	1.36
37	40	209	CLA	C3C-C2C	5.28	1.47	1.36
37	B	510	CLA	C3B-C2B	5.28	1.47	1.40
37	36	309	CLA	C3C-C2C	5.28	1.47	1.36
47	40	206	KC1	C3B-C2B	5.28	1.48	1.37
48	17	311	A86	C26-C27	5.28	1.42	1.35
37	18	204	CLA	O2D-CGD	5.28	1.46	1.33
37	w	101	CLA	C3B-C2B	5.27	1.47	1.40
47	35	302	KC1	C3C-C2C	5.27	1.47	1.36
47	11	306	KC1	C3D-C2D	5.27	1.48	1.39
37	12	212	CLA	C3C-C2C	5.27	1.47	1.36
37	21	204	CLA	C1D-ND	5.27	1.44	1.37
50	21	212	DD6	C13-C14	5.27	1.44	1.32
50	16	312	DD6	C13-C14	5.27	1.44	1.32
47	17	306	KC1	C3B-C2B	5.27	1.48	1.37
37	39	305	CLA	C3B-C2B	5.27	1.47	1.40
37	18	203	CLA	C1D-ND	5.26	1.44	1.37
37	35	303	CLA	C1D-ND	5.26	1.44	1.37
47	33	302	KC1	C3D-C2D	5.26	1.48	1.39
37	37	308	CLA	O2D-CGD	5.26	1.46	1.33
47	37	307	KC1	C3B-C2B	5.26	1.47	1.37
50	21	216	DD6	C3-C2	5.26	1.59	1.43
37	C	512	CLA	C3C-C2C	5.26	1.47	1.36
37	33	310	CLA	C3C-C2C	5.26	1.47	1.36
50	41	212	DD6	C13-C14	5.26	1.44	1.32
37	b	501	CLA	C3B-C2B	5.26	1.47	1.40
37	21	209	CLA	O2D-CGD	5.26	1.46	1.33
37	39	306	CLA	CHC-C1C	5.26	1.48	1.35
37	21	205	CLA	C3C-C2C	5.25	1.47	1.36
37	33	305	CLA	C3C-C2C	5.25	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	38	201	CLA	CHC-C1C	5.25	1.48	1.35
47	13	302	KC1	C3D-C2D	5.25	1.48	1.39
37	33	301	CLA	C3B-C2B	5.25	1.47	1.40
50	41	216	DD6	C3-C2	5.25	1.59	1.43
37	13	301	CLA	C3B-C2B	5.25	1.47	1.40
37	13	305	CLA	C1D-ND	5.25	1.44	1.37
37	41	208	CLA	C1D-ND	5.25	1.44	1.37
37	14	305	CLA	C3C-C2C	5.25	1.47	1.36
37	21	208	CLA	C3C-C2C	5.25	1.47	1.36
37	34	305	CLA	C3C-C2C	5.25	1.47	1.36
47	20	304	KC1	C3B-C2B	5.25	1.47	1.37
37	15	303	CLA	C3C-C2C	5.25	1.47	1.36
37	13	301	CLA	C1D-ND	5.25	1.44	1.37
37	33	301	CLA	C1D-ND	5.25	1.44	1.37
37	20	303	CLA	O2D-CGD	5.24	1.46	1.33
47	38	205	KC1	C3C-C2C	5.24	1.47	1.36
37	37	303	CLA	C3C-C2C	5.24	1.47	1.36
37	B	501	CLA	C3B-C2B	5.24	1.47	1.40
47	13	304	KC1	C3D-C2D	5.24	1.48	1.39
47	15	304	KC1	C3C-C2C	5.24	1.47	1.36
50	36	312	DD6	C13-C14	5.24	1.44	1.32
37	39	301	CLA	C3B-C2B	5.24	1.47	1.40
37	21	208	CLA	C1D-ND	5.24	1.44	1.37
47	31	307	KC1	C3D-C2D	5.24	1.48	1.39
47	21	203	KC1	C3C-C2C	5.24	1.47	1.36
37	41	205	CLA	C3C-C2C	5.24	1.47	1.36
37	33	305	CLA	C1D-ND	5.24	1.44	1.37
47	36	304	KC1	C3C-C2C	5.24	1.47	1.36
37	32	213	CLA	C3C-C2C	5.24	1.47	1.36
37	41	208	CLA	C3C-C2C	5.23	1.47	1.36
47	41	203	KC1	C3C-C2C	5.23	1.47	1.36
37	41	209	CLA	O2D-CGD	5.23	1.46	1.33
47	16	305	KC1	C3B-C2B	5.23	1.47	1.37
37	13	305	CLA	C3C-C2C	5.23	1.47	1.36
37	19	301	CLA	C3B-C2B	5.23	1.47	1.40
47	41	207	KC1	O2D-CGD	5.23	1.46	1.33
37	18	209	CLA	C3C-C2C	5.23	1.47	1.36
37	19	306	CLA	CHC-C1C	5.23	1.48	1.35
37	41	204	CLA	C1D-ND	5.23	1.44	1.37
37	38	209	CLA	O2D-CGD	5.23	1.46	1.33
37	35	303	CLA	C3C-C2C	5.22	1.47	1.36
37	D	402	CLA	C3C-C2C	5.22	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	18	209	CLA	O2D-CGD	5.22	1.45	1.33
37	36	307	CLA	C3C-C2C	5.22	1.47	1.36
47	16	304	KC1	C3C-C2C	5.22	1.47	1.36
47	33	304	KC1	C3D-C2D	5.22	1.48	1.39
37	40	205	CLA	O2D-CGD	5.22	1.45	1.33
37	d	401	CLA	C3C-C2C	5.22	1.47	1.36
50	20	310	DD6	C13-C14	5.22	1.44	1.32
37	17	304	CLA	C3C-C2C	5.22	1.47	1.36
37	16	307	CLA	C3C-C2C	5.21	1.47	1.36
47	15	306	KC1	C3C-C2C	5.21	1.47	1.36
47	35	304	KC1	C3C-C2C	5.21	1.47	1.36
47	32	212	KC1	C3B-C2B	5.21	1.47	1.37
47	21	207	KC1	O2D-CGD	5.21	1.45	1.33
37	18	211	CLA	C3C-C2C	5.21	1.47	1.36
37	14	303	CLA	C3C-C2C	5.21	1.47	1.36
37	41	202	CLA	C1D-ND	5.21	1.44	1.37
37	21	210	CLA	C1D-ND	5.21	1.44	1.37
37	38	202	CLA	O2D-CGD	5.21	1.45	1.33
47	20	302	KC1	C3D-C2D	5.21	1.48	1.39
47	20	304	KC1	CHD-C4C	5.21	1.48	1.35
47	36	305	KC1	C3B-C2B	5.20	1.47	1.37
37	B	515	CLA	C3B-C2B	5.20	1.47	1.40
37	20	307	CLA	C1D-ND	5.20	1.44	1.37
37	19	305	CLA	C3B-C2B	5.20	1.47	1.40
37	15	303	CLA	C1D-ND	5.20	1.44	1.37
47	17	305	KC1	C3B-C2B	5.20	1.47	1.37
37	33	308	CLA	C3C-C2C	5.20	1.47	1.36
37	17	309	CLA	O2D-CGD	5.20	1.45	1.33
37	z	102	CLA	C1D-ND	5.20	1.44	1.37
37	C	505	CLA	C3B-C2B	5.20	1.47	1.40
50	40	212	DD6	C13-C14	5.20	1.43	1.32
37	b	515	CLA	C3B-C2B	5.20	1.47	1.40
47	33	302	KC1	C3C-C2C	5.19	1.47	1.36
47	37	302	KC1	CHD-C4C	5.19	1.48	1.35
37	33	303	CLA	C3C-C2C	5.19	1.47	1.36
47	35	306	KC1	C3C-C2C	5.19	1.47	1.36
47	40	204	KC1	C3D-C2D	5.19	1.48	1.39
47	18	207	KC1	C3B-C2B	5.19	1.47	1.37
37	21	204	CLA	C3C-C2C	5.19	1.47	1.36
47	15	302	KC1	CHD-C4C	5.18	1.48	1.35
47	40	206	KC1	CHD-C4C	5.18	1.48	1.35
47	19	308	KC1	C3C-C2C	5.18	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	18	204	CLA	CHC-C1C	5.18	1.48	1.35
37	13	303	CLA	C3C-C2C	5.18	1.47	1.36
37	C	513	CLA	C3B-C2B	5.18	1.47	1.40
47	31	307	KC1	C3C-C2C	5.18	1.47	1.36
37	34	303	CLA	C3C-C2C	5.18	1.47	1.36
37	15	310	CLA	O2D-CGD	5.18	1.45	1.33
37	40	203	CLA	C1D-ND	5.18	1.44	1.37
47	36	302	KC1	C3C-C2C	5.18	1.47	1.36
47	16	308	KC1	C3C-C2C	5.18	1.47	1.36
37	32	208	CLA	C3C-C2C	5.18	1.47	1.36
37	20	308	CLA	C3C-C2C	5.18	1.47	1.36
37	20	301	CLA	C1D-ND	5.18	1.44	1.37
47	11	306	KC1	C3B-C2B	5.17	1.47	1.37
47	31	307	KC1	C3B-C2B	5.17	1.47	1.37
37	18	201	CLA	C3B-C2B	5.17	1.47	1.40
37	18	206	CLA	C1D-ND	5.17	1.44	1.37
47	14	309	KC1	C3B-C2B	5.17	1.47	1.37
37	15	301	CLA	O2D-CGD	5.17	1.45	1.33
37	15	308	CLA	O2D-CGD	5.17	1.45	1.33
37	41	204	CLA	C3C-C2C	5.17	1.47	1.36
37	11	305	CLA	C3B-C2B	5.17	1.47	1.40
37	35	301	CLA	O2D-CGD	5.16	1.45	1.33
37	13	308	CLA	C3C-C2C	5.16	1.47	1.36
47	11	309	KC1	C3D-C2D	5.16	1.48	1.39
37	38	206	CLA	C1D-ND	5.16	1.44	1.37
37	38	204	CLA	CHC-C1C	5.16	1.48	1.35
37	35	310	CLA	O2D-CGD	5.16	1.45	1.33
37	31	302	CLA	CHC-C1C	5.16	1.48	1.35
37	18	203	CLA	O2D-CGD	5.16	1.45	1.33
37	35	301	CLA	CHC-C1C	5.16	1.48	1.35
47	38	205	KC1	CHD-C4C	5.16	1.48	1.35
37	11	301	CLA	CHC-C1C	5.16	1.48	1.35
47	36	308	KC1	C3B-C2B	5.16	1.47	1.37
37	13	303	CLA	O2D-CGD	5.16	1.45	1.33
37	21	202	CLA	O2D-CGD	5.16	1.45	1.33
37	18	202	CLA	C3C-C2C	5.16	1.47	1.36
47	16	308	KC1	C3B-C2B	5.16	1.47	1.37
37	b	514	CLA	C3B-C2B	5.16	1.47	1.40
37	12	207	CLA	C3C-C2C	5.16	1.47	1.36
37	40	209	CLA	C1D-ND	5.16	1.44	1.37
37	38	203	CLA	O2D-CGD	5.16	1.45	1.33
47	13	302	KC1	C3C-C2C	5.16	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	34	309	KC1	C3B-C2B	5.16	1.47	1.37
37	34	301	CLA	CHC-C1C	5.16	1.48	1.35
47	18	205	KC1	CHD-C4C	5.15	1.48	1.35
47	17	303	KC1	CHD-C4C	5.15	1.48	1.35
37	15	301	CLA	CHC-C1C	5.15	1.48	1.35
37	18	202	CLA	O2D-CGD	5.15	1.45	1.33
47	17	305	KC1	CHD-C4C	5.15	1.48	1.35
37	38	204	CLA	C3C-C2C	5.15	1.47	1.36
47	35	302	KC1	CHD-C4C	5.15	1.48	1.35
37	31	310	CLA	C3C-C2C	5.15	1.47	1.36
37	40	210	CLA	C3C-C2C	5.15	1.47	1.36
37	C	501	CLA	C3B-C2B	5.15	1.47	1.40
37	20	301	CLA	CHC-C1C	5.15	1.48	1.35
37	40	203	CLA	CHC-C1C	5.15	1.48	1.35
47	38	205	KC1	O2D-CGD	5.15	1.45	1.33
47	11	306	KC1	C3C-C2C	5.15	1.47	1.36
47	34	309	KC1	C3D-C2D	5.15	1.48	1.39
47	21	207	KC1	CHD-C4C	5.15	1.48	1.35
37	13	305	CLA	O2D-CGD	5.14	1.45	1.33
47	32	212	KC1	C3D-C2D	5.14	1.48	1.39
37	21	205	CLA	O2D-CGD	5.14	1.45	1.33
37	17	309	CLA	C1D-ND	5.14	1.44	1.37
37	41	206	CLA	C1D-ND	5.14	1.44	1.37
47	39	308	KC1	C3C-C2C	5.14	1.47	1.36
37	19	302	CLA	C3C-C2C	5.14	1.47	1.36
37	z	101	CLA	O2D-CGD	5.14	1.45	1.33
37	18	206	CLA	O2D-CGD	5.14	1.45	1.33
47	36	302	KC1	CHD-C4C	5.14	1.48	1.35
47	13	309	KC1	C3B-C2B	5.14	1.47	1.37
47	33	309	KC1	C3B-C2B	5.14	1.47	1.37
37	B	514	CLA	C3B-C2B	5.14	1.47	1.40
37	39	302	CLA	C3C-C2C	5.14	1.47	1.36
37	33	305	CLA	O2D-CGD	5.14	1.45	1.33
37	11	301	CLA	C3B-C2B	5.14	1.47	1.40
37	Z	101	CLA	O2D-CGD	5.14	1.45	1.33
37	37	301	CLA	O2D-CGD	5.14	1.45	1.33
37	c	513	CLA	C3B-C2B	5.14	1.47	1.40
37	31	302	CLA	C3B-C2B	5.14	1.47	1.40
47	16	304	KC1	CHD-C4C	5.13	1.48	1.35
37	21	208	CLA	O2D-CGD	5.13	1.45	1.33
47	36	308	KC1	C3C-C2C	5.13	1.47	1.36
47	35	304	KC1	O2D-CGD	5.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	302	CLA	C3C-C2C	5.13	1.47	1.36
37	40	203	CLA	C3C-C2C	5.13	1.47	1.36
37	17	302	CLA	O2D-CGD	5.13	1.45	1.33
48	13	312	A86	C26-C27	5.13	1.42	1.35
47	36	304	KC1	CHD-C4C	5.13	1.48	1.35
48	35	313	A86	C26-C27	5.13	1.42	1.35
47	12	211	KC1	C3D-C2D	5.13	1.48	1.39
37	14	305	CLA	C1D-ND	5.13	1.44	1.37
37	34	305	CLA	C1D-ND	5.13	1.44	1.37
37	18	204	CLA	C3C-C2C	5.13	1.47	1.36
37	38	202	CLA	C1D-ND	5.13	1.44	1.37
47	12	211	KC1	C3B-C2B	5.13	1.47	1.37
37	41	205	CLA	O2D-CGD	5.13	1.45	1.33
37	20	301	CLA	C3C-C2C	5.13	1.47	1.36
47	21	203	KC1	CHD-C4C	5.12	1.48	1.35
37	41	206	CLA	C3C-C2C	5.12	1.47	1.36
37	18	203	CLA	C3C-C2C	5.12	1.47	1.36
37	c	501	CLA	C3B-C2B	5.12	1.47	1.40
47	20	302	KC1	CHD-C4C	5.12	1.48	1.35
47	14	304	KC1	CHD-C4C	5.12	1.48	1.35
47	34	304	KC1	CHD-C4C	5.12	1.48	1.35
37	19	306	CLA	C3B-C2B	5.12	1.47	1.40
48	15	313	A86	C26-C27	5.12	1.42	1.35
47	41	207	KC1	CHD-C4C	5.12	1.48	1.35
47	35	302	KC1	O2D-CGD	5.12	1.45	1.33
37	14	301	CLA	CHC-C1C	5.12	1.48	1.35
37	21	206	CLA	C1D-ND	5.12	1.44	1.37
47	16	302	KC1	CHD-C4C	5.12	1.48	1.35
37	11	310	CLA	C3C-C2C	5.12	1.47	1.36
47	41	203	KC1	CHD-C4C	5.12	1.48	1.35
37	35	308	CLA	C1D-ND	5.12	1.44	1.37
37	38	206	CLA	O2D-CGD	5.12	1.45	1.33
47	18	207	KC1	C3C-C2C	5.12	1.47	1.36
37	31	306	CLA	C3B-C2B	5.11	1.47	1.40
37	39	306	CLA	C3B-C2B	5.11	1.47	1.40
37	15	308	CLA	C1D-ND	5.11	1.44	1.37
37	c	505	CLA	C3B-C2B	5.11	1.47	1.40
47	31	309	KC1	C3D-C2D	5.11	1.48	1.39
47	18	205	KC1	O2D-CGD	5.11	1.45	1.33
47	38	210	KC1	C3C-C2C	5.11	1.47	1.36
37	38	203	CLA	C3C-C2C	5.11	1.47	1.36
37	Z	102	CLA	C1D-ND	5.11	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	32	213	CLA	C1D-ND	5.11	1.44	1.37
37	41	205	CLA	C1D-ND	5.11	1.44	1.37
37	38	211	CLA	O2D-CGD	5.11	1.45	1.33
37	B	508	CLA	C3C-C2C	5.11	1.47	1.36
47	12	206	KC1	C3B-C2B	5.11	1.47	1.37
47	32	207	KC1	C3B-C2B	5.11	1.47	1.37
37	34	302	CLA	C3C-C2C	5.11	1.47	1.36
37	38	201	CLA	C3B-C2B	5.11	1.47	1.40
37	41	202	CLA	O2D-CGD	5.11	1.45	1.33
37	31	301	CLA	O2D-CGD	5.10	1.45	1.33
37	38	202	CLA	C3C-C2C	5.10	1.47	1.36
37	37	306	CLA	O2D-CGD	5.10	1.45	1.33
37	35	310	CLA	C1D-ND	5.10	1.44	1.37
37	18	211	CLA	O2D-CGD	5.10	1.45	1.33
47	16	302	KC1	C3C-C2C	5.10	1.47	1.36
47	41	207	KC1	C4D-ND	5.10	1.39	1.35
37	35	305	CLA	O2D-CGD	5.10	1.45	1.33
37	39	301	CLA	C3C-C2C	5.10	1.47	1.36
37	11	307	CLA	C3B-C2B	5.10	1.47	1.40
47	38	207	KC1	C3C-C2C	5.10	1.47	1.36
37	17	307	CLA	O2D-CGD	5.10	1.45	1.33
37	16	301	CLA	O2D-CGD	5.09	1.45	1.33
37	16	306	CLA	O2D-CGD	5.09	1.45	1.33
37	38	202	CLA	CHC-C1C	5.09	1.48	1.35
47	15	306	KC1	CHD-C4C	5.09	1.48	1.35
47	14	304	KC1	O2D-CGD	5.09	1.45	1.33
37	17	304	CLA	O2D-CGD	5.09	1.45	1.33
37	b	508	CLA	C3C-C2C	5.09	1.47	1.36
37	W	102	CLA	O2D-CGD	5.09	1.45	1.33
37	C	513	CLA	CHC-C1C	5.09	1.48	1.35
48	32	216	A86	C26-C27	5.09	1.42	1.35
37	20	307	CLA	O2D-CGD	5.09	1.45	1.33
37	31	308	CLA	C3B-C2B	5.09	1.47	1.40
37	36	306	CLA	O2D-CGD	5.09	1.45	1.33
47	11	304	KC1	CHD-C4C	5.09	1.48	1.35
47	40	204	KC1	CHD-C4C	5.09	1.48	1.35
37	d	401	CLA	C3B-C2B	5.09	1.47	1.40
37	18	201	CLA	CHC-C1C	5.09	1.48	1.35
37	39	301	CLA	CHC-C1C	5.09	1.48	1.35
47	12	211	KC1	CHD-C4C	5.08	1.48	1.35
37	15	307	CLA	CHC-C1C	5.08	1.48	1.35
47	14	306	KC1	C3B-C2B	5.08	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	402	CLA	C3B-C2B	5.08	1.47	1.40
48	40	213	A86	C9-C8	5.08	1.47	1.34
37	34	302	CLA	C3B-C2B	5.08	1.47	1.40
47	40	206	KC1	O2D-CGD	5.08	1.45	1.33
37	19	301	CLA	C3C-C2C	5.08	1.47	1.36
37	19	303	CLA	C3C-C2C	5.08	1.47	1.36
37	39	303	CLA	C3C-C2C	5.08	1.47	1.36
47	35	306	KC1	O2D-CGD	5.08	1.45	1.33
47	16	305	KC1	CHD-C4C	5.08	1.48	1.35
47	34	304	KC1	O2D-CGD	5.08	1.45	1.33
37	19	310	CLA	C3C-C2C	5.08	1.47	1.36
47	14	309	KC1	C3D-C2D	5.08	1.48	1.39
37	a	407	CLA	C3B-C2B	5.08	1.47	1.40
37	16	307	CLA	O2D-CGD	5.08	1.45	1.33
37	41	208	CLA	O2D-CGD	5.08	1.45	1.33
37	35	307	CLA	CHC-C1C	5.08	1.48	1.35
47	18	210	KC1	C3C-C2C	5.08	1.47	1.36
37	20	308	CLA	C1D-ND	5.07	1.44	1.37
37	c	513	CLA	CHC-C1C	5.07	1.48	1.35
37	40	209	CLA	O2D-CGD	5.07	1.45	1.33
48	33	313	A86	C9-C8	5.07	1.47	1.34
47	15	306	KC1	O2D-CGD	5.07	1.45	1.33
47	20	302	KC1	C3B-C2B	5.07	1.47	1.37
37	33	310	CLA	O2D-CGD	5.07	1.45	1.33
47	12	208	KC1	C3D-C2D	5.07	1.48	1.39
47	32	209	KC1	C3D-C2D	5.07	1.48	1.39
48	21	213	A86	C26-C27	5.07	1.42	1.35
48	37	311	A86	C26-C27	5.07	1.42	1.35
48	13	313	A86	C9-C8	5.07	1.47	1.34
37	21	206	CLA	C3C-C2C	5.07	1.47	1.36
37	35	308	CLA	C3C-C2C	5.07	1.47	1.36
47	14	306	KC1	C3C-C2C	5.07	1.47	1.36
47	34	306	KC1	C3C-C2C	5.07	1.47	1.36
47	18	210	KC1	CHD-C4C	5.07	1.48	1.35
47	38	210	KC1	CHD-C4C	5.07	1.48	1.35
47	13	302	KC1	O2D-CGD	5.07	1.45	1.33
47	31	305	KC1	CHD-C4C	5.06	1.48	1.35
47	40	204	KC1	C3B-C2B	5.06	1.47	1.37
37	38	209	CLA	C1D-ND	5.06	1.44	1.37
47	20	304	KC1	O2D-CGD	5.06	1.45	1.33
47	35	306	KC1	CHD-C4C	5.06	1.47	1.35
37	21	206	CLA	O2D-CGD	5.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	41	210	CLA	O2D-CGD	5.06	1.45	1.33
48	20	311	A86	C9-C8	5.06	1.47	1.34
47	36	304	KC1	O2D-CGD	5.06	1.45	1.33
37	15	305	CLA	O2D-CGD	5.06	1.45	1.33
47	34	306	KC1	C3B-C2B	5.06	1.47	1.37
37	11	305	CLA	O2D-CGD	5.06	1.45	1.33
37	40	208	CLA	CHC-C1C	5.06	1.47	1.35
37	18	201	CLA	C1D-ND	5.06	1.44	1.37
37	19	303	CLA	CHC-C1C	5.06	1.47	1.35
37	39	303	CLA	CHC-C1C	5.06	1.47	1.35
37	18	201	CLA	O2D-CGD	5.06	1.45	1.33
47	35	302	KC1	C3B-C2B	5.06	1.47	1.37
37	14	305	CLA	O2D-CGD	5.06	1.45	1.33
37	13	310	CLA	O2D-CGD	5.06	1.45	1.33
37	33	308	CLA	O2D-CGD	5.06	1.45	1.33
37	b	507	CLA	C3B-C2B	5.06	1.47	1.40
37	15	307	CLA	O2D-CGD	5.06	1.45	1.33
48	39	313	A86	C9-C8	5.06	1.47	1.34
47	36	305	KC1	CHD-C4C	5.05	1.47	1.35
47	15	302	KC1	O2D-CGD	5.05	1.45	1.33
48	21	213	A86	C9-C8	5.05	1.47	1.34
37	37	303	CLA	O2D-CGD	5.05	1.45	1.33
37	37	308	CLA	C1D-ND	5.05	1.44	1.37
37	38	204	CLA	C1D-ND	5.05	1.44	1.37
50	20	310	DD6	C3-C2	5.05	1.59	1.43
37	21	210	CLA	CHC-C1C	5.05	1.47	1.35
37	21	205	CLA	C1D-ND	5.05	1.44	1.37
47	15	304	KC1	O2D-CGD	5.05	1.45	1.33
37	C	511	CLA	C3C-C2C	5.05	1.47	1.36
37	C	504	CLA	C3B-C2B	5.05	1.47	1.40
37	11	308	CLA	C3B-C2B	5.05	1.47	1.40
37	31	306	CLA	O2D-CGD	5.05	1.45	1.33
37	36	307	CLA	O2D-CGD	5.05	1.45	1.33
37	13	301	CLA	C3C-C2C	5.05	1.47	1.36
37	33	301	CLA	C3C-C2C	5.05	1.47	1.36
47	17	305	KC1	C3C-C2C	5.05	1.47	1.36
47	40	204	KC1	C3C-C2C	5.05	1.47	1.36
37	14	302	CLA	C3B-C2B	5.05	1.47	1.40
37	16	301	CLA	CHC-C1C	5.05	1.47	1.35
48	15	314	A86	C9-C8	5.05	1.47	1.34
37	11	305	CLA	C3C-C2C	5.05	1.47	1.36
37	31	306	CLA	C3C-C2C	5.05	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	39	310	CLA	C3C-C2C	5.05	1.47	1.36
37	40	210	CLA	C1D-ND	5.05	1.44	1.37
48	13	315	A86	C9-C8	5.05	1.47	1.34
37	13	308	CLA	O2D-CGD	5.05	1.45	1.33
37	21	210	CLA	O2D-CGD	5.05	1.45	1.33
47	17	305	KC1	O2D-CGD	5.05	1.45	1.33
48	41	213	A86	C9-C8	5.04	1.47	1.34
48	41	213	A86	C26-C27	5.04	1.42	1.35
37	18	209	CLA	C1D-ND	5.04	1.44	1.37
37	37	301	CLA	C1D-ND	5.04	1.44	1.37
37	41	210	CLA	CHC-C1C	5.04	1.47	1.35
50	16	312	DD6	C3-C2	5.04	1.59	1.43
37	34	302	CLA	O2D-CGD	5.04	1.45	1.33
37	19	304	CLA	CHC-C1C	5.04	1.47	1.35
37	39	304	CLA	CHC-C1C	5.04	1.47	1.35
37	19	301	CLA	CHC-C1C	5.04	1.47	1.35
37	36	301	CLA	O2D-CGD	5.04	1.45	1.33
47	13	304	KC1	C3C-C2C	5.04	1.47	1.36
37	20	306	CLA	CHC-C1C	5.04	1.47	1.35
37	39	309	CLA	C3C-C2C	5.04	1.47	1.36
47	37	302	KC1	C3C-C2C	5.04	1.47	1.36
48	35	314	A86	C9-C8	5.04	1.47	1.34
37	36	301	CLA	CHC-C1C	5.04	1.47	1.35
47	32	212	KC1	CHD-C4C	5.04	1.47	1.35
37	12	210	CLA	O2D-CGD	5.04	1.45	1.33
37	34	310	CLA	C1D-ND	5.04	1.44	1.37
37	19	305	CLA	C3C-C2C	5.04	1.47	1.36
37	39	305	CLA	C3C-C2C	5.04	1.47	1.36
47	16	302	KC1	C3B-C2B	5.04	1.47	1.37
37	41	206	CLA	O2D-CGD	5.04	1.45	1.33
50	40	212	DD6	C3-C2	5.03	1.59	1.43
37	18	202	CLA	CHC-C1C	5.03	1.47	1.35
47	17	308	KC1	C3C-C2C	5.03	1.47	1.36
37	35	307	CLA	O2D-CGD	5.03	1.45	1.33
37	19	307	CLA	C3C-C2C	5.03	1.47	1.36
37	39	307	CLA	C3C-C2C	5.03	1.47	1.36
48	17	312	A86	C26-C27	5.03	1.42	1.35
48	33	312	A86	C26-C27	5.03	1.42	1.35
48	18	212	A86	C9-C8	5.03	1.47	1.34
47	15	309	KC1	O2D-CGD	5.03	1.45	1.33
47	37	304	KC1	O2D-CGD	5.03	1.45	1.33
37	16	306	CLA	CHC-C1C	5.03	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c	511	CLA	C3C-C2C	5.03	1.47	1.36
37	34	305	CLA	O2D-CGD	5.03	1.45	1.33
47	40	204	KC1	O2D-CGD	5.03	1.45	1.33
47	17	308	KC1	CHD-C4C	5.03	1.47	1.35
47	37	307	KC1	CHD-C4C	5.03	1.47	1.35
37	B	507	CLA	C3C-C2C	5.03	1.47	1.36
37	16	303	CLA	C3C-C2C	5.03	1.47	1.36
47	33	304	KC1	C3C-C2C	5.03	1.47	1.36
37	38	201	CLA	C1D-ND	5.03	1.44	1.37
47	21	207	KC1	C4D-ND	5.03	1.39	1.35
37	c	504	CLA	C3B-C2B	5.03	1.47	1.40
47	16	304	KC1	O2D-CGD	5.03	1.45	1.33
47	20	302	KC1	O2D-CGD	5.03	1.45	1.33
37	W	102	CLA	C1D-ND	5.03	1.44	1.37
47	33	309	KC1	C3C-C2C	5.02	1.47	1.36
50	36	312	DD6	C3-C2	5.02	1.59	1.43
37	12	204	CLA	C3C-C2C	5.02	1.47	1.36
37	32	205	CLA	C3C-C2C	5.02	1.47	1.36
47	19	308	KC1	O2D-CGD	5.02	1.45	1.33
37	40	210	CLA	O2D-CGD	5.02	1.45	1.33
37	38	201	CLA	O2D-CGD	5.02	1.45	1.33
48	12	215	A86	C26-C27	5.02	1.42	1.35
37	19	309	CLA	C3C-C2C	5.02	1.47	1.36
47	13	309	KC1	CHD-C4C	5.02	1.47	1.35
47	33	309	KC1	CHD-C4C	5.02	1.47	1.35
37	34	308	CLA	O2D-CGD	5.02	1.45	1.33
47	11	309	KC1	C3B-C2B	5.02	1.47	1.37
37	40	203	CLA	O2D-CGD	5.02	1.45	1.33
47	20	302	KC1	C3C-C2C	5.02	1.47	1.36
47	13	309	KC1	C3C-C2C	5.02	1.47	1.36
37	14	302	CLA	O2D-CGD	5.02	1.45	1.33
37	15	301	CLA	C1D-ND	5.02	1.44	1.37
37	35	301	CLA	C1D-ND	5.02	1.44	1.37
48	33	314	A86	C9-C8	5.02	1.47	1.34
37	18	208	CLA	O2D-CGD	5.02	1.45	1.33
37	36	303	CLA	C3C-C2C	5.02	1.47	1.36
47	31	305	KC1	C3C-C2C	5.02	1.47	1.36
37	36	303	CLA	O2D-CGD	5.02	1.45	1.33
47	36	305	KC1	O2D-CGD	5.02	1.45	1.33
37	11	303	CLA	C3C-C2C	5.02	1.47	1.36
47	33	302	KC1	O2D-CGD	5.02	1.45	1.33
37	35	308	CLA	O2D-CGD	5.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	39	308	KC1	O2D-CGD	5.01	1.45	1.33
37	b	507	CLA	C3C-C2C	5.01	1.47	1.36
37	15	310	CLA	C1D-ND	5.01	1.43	1.37
47	38	207	KC1	CHD-C4C	5.01	1.47	1.35
48	34	313	A86	C9-C8	5.01	1.47	1.34
37	c	512	CLA	C3B-C2B	5.01	1.47	1.40
47	13	309	KC1	O2D-CGD	5.01	1.45	1.33
37	16	306	CLA	C3C-C2C	5.01	1.47	1.36
47	16	305	KC1	O2D-CGD	5.01	1.45	1.33
47	33	302	KC1	CHD-C4C	5.01	1.47	1.35
37	36	306	CLA	CHC-C1C	5.01	1.47	1.35
48	33	315	A86	C9-C8	5.01	1.47	1.34
37	21	206	CLA	CHC-C1C	5.01	1.47	1.35
37	41	204	CLA	O2D-CGD	5.01	1.45	1.33
37	C	512	CLA	C3B-C2B	5.01	1.47	1.40
47	16	308	KC1	C3D-C2D	5.01	1.48	1.39
48	38	212	A86	C9-C8	5.00	1.47	1.34
37	37	306	CLA	C3C-C2C	5.00	1.47	1.36
37	38	208	CLA	C3C-C2C	5.00	1.47	1.36
47	36	302	KC1	C3B-C2B	5.00	1.47	1.37
37	21	204	CLA	O2D-CGD	5.00	1.45	1.33
47	18	210	KC1	O2D-CGD	5.00	1.45	1.33
47	13	306	KC1	C3C-C2C	5.00	1.47	1.36
37	33	303	CLA	O2D-CGD	5.00	1.45	1.33
47	13	302	KC1	CHD-C4C	5.00	1.47	1.35
48	13	314	A86	C9-C8	5.00	1.47	1.34
47	36	308	KC1	CHD-C4C	5.00	1.47	1.35
47	17	306	KC1	CHD-C4C	5.00	1.47	1.35
37	32	211	CLA	O2D-CGD	5.00	1.45	1.33
37	B	507	CLA	C3B-C2B	5.00	1.47	1.40
37	32	202	CLA	C3B-C2B	5.00	1.47	1.40
37	41	204	CLA	CHC-C1C	5.00	1.47	1.35
37	20	303	CLA	C3C-C2C	5.00	1.47	1.36
48	38	214	A86	C9-C8	5.00	1.47	1.34
37	31	301	CLA	C1D-ND	5.00	1.43	1.37
37	14	301	CLA	O2D-CGD	5.00	1.45	1.33
37	13	305	CLA	CHC-C1C	5.00	1.47	1.35
47	16	308	KC1	CHD-C4C	5.00	1.47	1.35
47	37	307	KC1	O2D-CGD	5.00	1.45	1.33
47	15	309	KC1	C3C-C2C	5.00	1.47	1.36
47	16	302	KC1	O2D-CGD	5.00	1.45	1.33
47	41	207	KC1	C3C-C2C	5.00	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	w	101	CLA	C3C-C2C	5.00	1.47	1.36
47	41	203	KC1	O2D-CGD	5.00	1.45	1.33
37	20	307	CLA	CHC-C1C	4.99	1.47	1.35
47	18	207	KC1	CHD-C4C	4.99	1.47	1.35
37	14	308	CLA	O2D-CGD	4.99	1.45	1.33
37	40	209	CLA	CHC-C1C	4.99	1.47	1.35
47	33	306	KC1	C3C-C2C	4.99	1.47	1.36
37	35	307	CLA	C3C-C2C	4.99	1.47	1.36
47	31	309	KC1	C3B-C2B	4.99	1.47	1.37
37	20	308	CLA	O2D-CGD	4.99	1.45	1.33
47	35	309	KC1	CHD-C4C	4.99	1.47	1.35
47	35	309	KC1	C3C-C2C	4.99	1.47	1.36
37	39	309	CLA	O2D-CGD	4.99	1.45	1.33
47	11	304	KC1	O2D-CGD	4.99	1.45	1.33
47	37	307	KC1	C3C-C2C	4.99	1.47	1.36
37	12	204	CLA	C3B-C2B	4.99	1.47	1.40
37	c	507	CLA	C3C-C2C	4.99	1.47	1.36
47	17	308	KC1	O2D-CGD	4.99	1.45	1.33
37	16	303	CLA	O2D-CGD	4.99	1.45	1.33
47	11	304	KC1	C3C-C2C	4.99	1.47	1.36
47	38	207	KC1	O2D-CGD	4.99	1.45	1.33
47	37	304	KC1	C3C-C2C	4.99	1.47	1.36
37	33	305	CLA	CHC-C1C	4.99	1.47	1.35
47	32	212	KC1	C3C-C2C	4.99	1.47	1.36
37	35	303	CLA	O2D-CGD	4.99	1.45	1.33
37	19	310	CLA	O2D-CGD	4.98	1.45	1.33
47	17	303	KC1	O2D-CGD	4.98	1.45	1.33
47	21	207	KC1	C3C-C2C	4.98	1.47	1.36
37	b	503	CLA	C3C-C2C	4.98	1.47	1.36
37	36	306	CLA	C3C-C2C	4.98	1.47	1.36
37	c	508	CLA	C3C-C2C	4.98	1.47	1.36
37	31	304	CLA	C3C-C2C	4.98	1.47	1.36
47	31	305	KC1	O2D-CGD	4.98	1.45	1.33
37	17	307	CLA	C3C-C2C	4.98	1.47	1.36
37	18	202	CLA	C1D-ND	4.98	1.43	1.37
37	31	301	CLA	CHC-C1C	4.98	1.47	1.35
47	36	302	KC1	O2D-CGD	4.98	1.45	1.33
47	14	304	KC1	C1A-NA	-4.98	1.28	1.38
37	40	205	CLA	C3C-C2C	4.98	1.47	1.36
47	34	304	KC1	C1A-NA	-4.98	1.28	1.38
37	12	212	CLA	C1D-ND	4.98	1.43	1.37
37	40	205	CLA	C1D-ND	4.98	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	20	306	CLA	O2D-CGD	4.98	1.45	1.33
37	B	503	CLA	C3C-C2C	4.98	1.47	1.36
37	C	505	CLA	C3C-C2C	4.98	1.47	1.36
37	12	205	CLA	C3C-C2C	4.98	1.47	1.36
47	37	302	KC1	O2D-CGD	4.98	1.45	1.33
37	41	209	CLA	CHC-C1C	4.98	1.47	1.35
47	15	309	KC1	CHD-C4C	4.98	1.47	1.35
47	37	305	KC1	CHD-C4C	4.98	1.47	1.35
47	38	210	KC1	O2D-CGD	4.98	1.45	1.33
37	12	210	CLA	C3C-C2C	4.98	1.47	1.36
47	16	308	KC1	O2D-CGD	4.98	1.45	1.33
37	C	507	CLA	C3C-C2C	4.98	1.47	1.36
37	b	502	CLA	C3C-C2C	4.98	1.47	1.36
37	14	303	CLA	O2D-CGD	4.98	1.45	1.33
37	A	405	CLA	C3B-C2B	4.98	1.47	1.40
37	20	303	CLA	CHC-C1C	4.98	1.47	1.35
37	21	204	CLA	CHC-C1C	4.98	1.47	1.35
37	41	206	CLA	CHC-C1C	4.98	1.47	1.35
37	20	301	CLA	O2D-CGD	4.98	1.45	1.33
37	W	101	CLA	C3C-C2C	4.98	1.47	1.36
37	14	310	CLA	C1D-ND	4.97	1.43	1.37
37	38	206	CLA	CHC-C1C	4.97	1.47	1.35
48	14	313	A86	C9-C8	4.97	1.47	1.34
37	15	308	CLA	C3C-C2C	4.97	1.47	1.36
37	17	302	CLA	CHC-C1C	4.97	1.47	1.35
37	34	307	CLA	CHC-C1C	4.97	1.47	1.35
47	12	206	KC1	C3D-C2D	4.97	1.48	1.39
37	38	208	CLA	CHC-C1C	4.97	1.47	1.35
37	15	307	CLA	C3C-C2C	4.97	1.47	1.36
37	14	307	CLA	CHC-C1C	4.97	1.47	1.35
37	40	208	CLA	O2D-CGD	4.97	1.45	1.33
48	35	314	A86	C26-C27	4.97	1.42	1.35
47	36	308	KC1	C3D-C2D	4.97	1.48	1.39
37	19	309	CLA	O2D-CGD	4.97	1.45	1.33
48	35	313	A86	C9-C8	4.96	1.47	1.34
37	D	406	CLA	C3C-C2C	4.96	1.47	1.36
47	33	304	KC1	O2D-CGD	4.96	1.45	1.33
37	18	208	CLA	CHC-C1C	4.96	1.47	1.35
47	31	309	KC1	C3C-C2C	4.96	1.47	1.36
37	21	205	CLA	CHC-C1C	4.96	1.47	1.35
37	21	208	CLA	CHC-C1C	4.96	1.47	1.35
37	35	308	CLA	CHC-C1C	4.96	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	32	211	CLA	C3C-C2C	4.96	1.47	1.36
37	12	212	CLA	CHC-C1C	4.96	1.47	1.35
37	18	206	CLA	CHC-C1C	4.96	1.47	1.35
47	17	303	KC1	C3C-C2C	4.96	1.47	1.36
37	c	503	CLA	C3C-C2C	4.96	1.47	1.36
47	13	302	KC1	C1A-NA	-4.96	1.28	1.38
47	33	302	KC1	C1A-NA	-4.96	1.28	1.38
47	13	306	KC1	O2D-CGD	4.96	1.45	1.33
47	33	306	KC1	O2D-CGD	4.96	1.45	1.33
37	c	505	CLA	C3C-C2C	4.96	1.47	1.36
47	36	308	KC1	O2D-CGD	4.96	1.45	1.33
37	34	301	CLA	O2D-CGD	4.96	1.45	1.33
37	b	523	CLA	C3C-C2C	4.96	1.47	1.36
37	34	303	CLA	O2D-CGD	4.96	1.45	1.33
37	C	508	CLA	C3C-C2C	4.96	1.47	1.36
50	21	212	DD6	C3-C2	4.96	1.58	1.43
47	11	309	KC1	C3C-C2C	4.96	1.47	1.36
48	13	313	A86	C26-C27	4.96	1.42	1.35
37	20	303	CLA	C1D-ND	4.96	1.43	1.37
37	B	524	CLA	C3C-C2C	4.96	1.47	1.36
37	21	209	CLA	CHC-C1C	4.96	1.47	1.35
48	32	215	A86	C26-C27	4.95	1.42	1.35
48	18	214	A86	C9-C8	4.95	1.47	1.34
37	d	404	CLA	C3C-C2C	4.95	1.47	1.36
37	c	509	CLA	C3C-C2C	4.95	1.47	1.36
37	18	208	CLA	C3C-C2C	4.95	1.47	1.36
47	33	309	KC1	O2D-CGD	4.95	1.45	1.33
47	13	304	KC1	O2D-CGD	4.95	1.45	1.33
37	41	205	CLA	CHC-C1C	4.95	1.47	1.35
47	21	203	KC1	O2D-CGD	4.95	1.45	1.33
37	37	301	CLA	CHC-C1C	4.95	1.47	1.35
37	W	102	CLA	CHC-C1C	4.95	1.47	1.35
47	40	206	KC1	C3C-C2C	4.95	1.47	1.36
48	12	214	A86	C26-C27	4.95	1.42	1.35
37	19	302	CLA	C1D-ND	4.95	1.43	1.37
47	21	207	KC1	OBD-CAD	4.95	1.29	1.22
50	41	212	DD6	C3-C2	4.95	1.58	1.43
37	39	305	CLA	O2D-CGD	4.95	1.45	1.33
37	41	202	CLA	CHC-C1C	4.95	1.47	1.35
48	12	202	A86	C17-C18	-4.95	1.45	1.52
47	18	207	KC1	O2D-CGD	4.95	1.45	1.33
37	34	305	CLA	CHC-C1C	4.95	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	12	209	CLA	CHC-C1C	4.95	1.47	1.35
37	13	310	CLA	CHC-C1C	4.94	1.47	1.35
37	40	205	CLA	CHC-C1C	4.94	1.47	1.35
37	C	509	CLA	C3C-C2C	4.94	1.47	1.36
37	B	502	CLA	C3C-C2C	4.94	1.47	1.36
47	15	302	KC1	C3B-C2B	4.94	1.47	1.37
37	41	208	CLA	CHC-C1C	4.94	1.47	1.35
37	19	305	CLA	O2D-CGD	4.94	1.45	1.33
37	C	510	CLA	C3C-C2C	4.94	1.47	1.36
47	14	306	KC1	CHD-C4C	4.94	1.47	1.35
47	19	308	KC1	CHD-C4C	4.94	1.47	1.35
48	32	203	A86	C17-C18	-4.94	1.45	1.52
37	36	309	CLA	CHC-C1C	4.94	1.47	1.35
37	14	307	CLA	C3C-C2C	4.94	1.47	1.36
37	34	307	CLA	C3C-C2C	4.94	1.47	1.36
48	40	201	A86	C9-C8	4.94	1.47	1.34
37	38	208	CLA	O2D-CGD	4.94	1.45	1.33
37	39	310	CLA	O2D-CGD	4.94	1.45	1.33
48	19	313	A86	C9-C8	4.94	1.47	1.34
47	11	302	KC1	CHD-C4C	4.94	1.47	1.35
47	31	303	KC1	CHD-C4C	4.94	1.47	1.35
37	32	210	CLA	C3C-C2C	4.94	1.47	1.36
48	38	215	A86	C9-C8	4.94	1.47	1.34
47	12	211	KC1	C3C-C2C	4.94	1.47	1.36
48	33	313	A86	C26-C27	4.93	1.42	1.35
37	14	308	CLA	C3C-C2C	4.93	1.47	1.36
37	16	309	CLA	CHC-C1C	4.93	1.47	1.35
37	21	202	CLA	CHC-C1C	4.93	1.47	1.35
47	11	309	KC1	CHD-C4C	4.93	1.47	1.35
47	31	309	KC1	CHD-C4C	4.93	1.47	1.35
37	C	506	CLA	C3C-C2C	4.93	1.47	1.36
37	15	303	CLA	O2D-CGD	4.93	1.45	1.33
48	15	313	A86	C9-C8	4.93	1.47	1.34
37	13	301	CLA	CHC-C1C	4.93	1.47	1.35
37	32	213	CLA	CHC-C1C	4.93	1.47	1.35
37	33	301	CLA	CHC-C1C	4.93	1.47	1.35
47	39	308	KC1	CHD-C4C	4.93	1.47	1.35
48	34	313	A86	C26-C27	4.93	1.42	1.35
48	16	313	A86	C9-C8	4.93	1.47	1.34
47	14	309	KC1	CHD-C4C	4.93	1.47	1.35
37	13	308	CLA	C1D-ND	4.93	1.43	1.37
37	33	308	CLA	C1D-ND	4.93	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	11	304	KC1	C1A-NA	-4.93	1.28	1.38
47	19	308	KC1	C1A-NA	-4.93	1.28	1.38
47	39	308	KC1	C1A-NA	-4.93	1.28	1.38
37	C	503	CLA	C3C-C2C	4.93	1.47	1.36
47	31	305	KC1	C1A-NA	-4.93	1.28	1.38
37	35	305	CLA	CHC-C1C	4.92	1.47	1.35
47	32	207	KC1	C3D-C2D	4.92	1.48	1.39
37	16	307	CLA	C1D-ND	4.92	1.43	1.37
37	16	303	CLA	CHC-C1C	4.92	1.47	1.35
48	14	313	A86	C26-C27	4.92	1.42	1.35
37	12	209	CLA	C3C-C2C	4.92	1.47	1.36
37	A	405	CLA	C3C-C2C	4.92	1.47	1.36
37	a	407	CLA	C3C-C2C	4.92	1.47	1.36
37	32	210	CLA	CHC-C1C	4.92	1.47	1.35
47	41	207	KC1	OBD-CAD	4.92	1.29	1.22
47	20	304	KC1	C3C-C2C	4.92	1.47	1.36
37	39	302	CLA	C1D-ND	4.92	1.43	1.37
37	B	513	CLA	C3C-C2C	4.92	1.47	1.36
37	c	506	CLA	C3C-C2C	4.92	1.47	1.36
37	14	305	CLA	CHC-C1C	4.92	1.47	1.35
37	33	310	CLA	CHC-C1C	4.91	1.47	1.35
37	c	510	CLA	C3C-C2C	4.91	1.47	1.36
37	15	310	CLA	CHC-C1C	4.91	1.47	1.35
37	17	309	CLA	CHC-C1C	4.91	1.47	1.35
48	37	314	A86	C9-C8	4.91	1.47	1.34
47	34	309	KC1	CHD-C4C	4.91	1.47	1.35
37	A	403	CLA	C3C-C2C	4.91	1.47	1.36
37	34	308	CLA	C3C-C2C	4.91	1.47	1.36
37	18	201	CLA	C3C-C2C	4.91	1.47	1.36
37	15	305	CLA	CHC-C1C	4.91	1.47	1.35
37	b	513	CLA	C3C-C2C	4.91	1.47	1.36
37	36	303	CLA	CHC-C1C	4.91	1.47	1.35
47	35	309	KC1	O2D-CGD	4.91	1.45	1.33
48	11	319	A86	C17-C18	-4.91	1.45	1.52
48	31	319	A86	C17-C18	-4.91	1.45	1.52
37	39	306	CLA	C3C-C2C	4.91	1.47	1.36
37	34	310	CLA	O2D-CGD	4.91	1.45	1.33
37	14	310	CLA	O2D-CGD	4.90	1.45	1.33
37	D	402	CLA	CHC-C1C	4.90	1.47	1.35
37	C	513	CLA	C3C-C2C	4.90	1.47	1.36
37	32	202	CLA	C3C-C2C	4.90	1.47	1.36
48	15	314	A86	C26-C27	4.90	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Z	101	CLA	C1D-ND	4.90	1.43	1.37
37	39	307	CLA	O2D-CGD	4.90	1.45	1.33
37	37	308	CLA	CHC-C1C	4.90	1.47	1.35
37	C	503	CLA	C3B-C2B	4.90	1.47	1.40
37	36	303	CLA	C1D-ND	4.90	1.43	1.37
37	32	205	CLA	C3B-C2B	4.90	1.47	1.40
48	15	311	A86	C26-C27	4.90	1.42	1.35
37	18	203	CLA	CHC-C1C	4.90	1.47	1.35
47	34	306	KC1	CHD-C4C	4.89	1.47	1.35
37	14	302	CLA	CHC-C1C	4.89	1.47	1.35
37	18	209	CLA	CHC-C1C	4.89	1.47	1.35
37	35	310	CLA	CHC-C1C	4.89	1.47	1.35
37	38	209	CLA	CHC-C1C	4.89	1.47	1.35
37	32	206	CLA	C3C-C2C	4.89	1.47	1.36
37	c	503	CLA	C3B-C2B	4.89	1.47	1.40
47	31	303	KC1	C3C-C2C	4.89	1.47	1.36
37	38	203	CLA	CHC-C1C	4.89	1.47	1.35
37	36	307	CLA	C1D-ND	4.89	1.43	1.37
37	39	304	CLA	O2D-CGD	4.89	1.45	1.33
37	b	514	CLA	C3C-C2C	4.89	1.47	1.36
37	11	305	CLA	CHC-C1C	4.89	1.47	1.35
37	c	506	CLA	C3B-C2B	4.89	1.47	1.40
37	a	403	CLA	C3C-C2C	4.88	1.47	1.36
37	C	506	CLA	C3B-C2B	4.88	1.47	1.40
37	C	513	CLA	O2D-CGD	4.88	1.45	1.33
37	c	513	CLA	O2D-CGD	4.88	1.45	1.33
37	18	211	CLA	CHC-C1C	4.88	1.47	1.35
47	13	304	KC1	CHD-C4C	4.88	1.47	1.35
37	19	307	CLA	C3B-C2B	4.88	1.47	1.40
47	36	304	KC1	C1A-NA	-4.88	1.28	1.38
37	d	401	CLA	CHC-C1C	4.88	1.47	1.35
48	17	315	A86	C9-C8	4.88	1.47	1.34
47	33	304	KC1	CHD-C4C	4.88	1.47	1.35
37	19	307	CLA	O2D-CGD	4.87	1.45	1.33
48	18	215	A86	C9-C8	4.87	1.47	1.34
37	Z	102	CLA	CHC-C1C	4.87	1.47	1.35
47	14	309	KC1	C3C-C2C	4.87	1.47	1.36
37	37	303	CLA	CHC-C1C	4.87	1.47	1.35
47	17	305	KC1	C3D-C2D	4.87	1.48	1.39
47	14	309	KC1	O2D-CGD	4.87	1.45	1.33
47	34	309	KC1	O2D-CGD	4.87	1.45	1.33
47	31	307	KC1	CHD-C4C	4.87	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	505	CLA	CHC-C1C	4.87	1.47	1.35
37	12	203	CLA	O2D-CGD	4.87	1.45	1.33
37	b	523	CLA	CHC-C1C	4.87	1.47	1.35
47	37	304	KC1	C1A-NA	-4.87	1.28	1.38
37	32	204	CLA	O2D-CGD	4.87	1.45	1.33
37	12	203	CLA	CHC-C1C	4.87	1.47	1.35
37	b	515	CLA	C3C-C2C	4.87	1.47	1.36
47	16	304	KC1	C1A-NA	-4.87	1.28	1.38
37	19	310	CLA	CHC-C1C	4.87	1.47	1.35
37	14	307	CLA	O2D-CGD	4.87	1.45	1.33
37	34	307	CLA	O2D-CGD	4.87	1.45	1.33
37	20	306	CLA	C3C-C2C	4.87	1.47	1.36
37	11	308	CLA	C3C-C2C	4.87	1.47	1.36
37	13	301	CLA	O2D-CGD	4.87	1.45	1.33
37	33	301	CLA	O2D-CGD	4.87	1.45	1.33
37	34	302	CLA	CHC-C1C	4.86	1.47	1.35
37	B	515	CLA	C3C-C2C	4.86	1.47	1.36
37	14	302	CLA	C1D-ND	4.86	1.43	1.37
50	39	312	DD6	C3-C2	4.86	1.58	1.43
37	17	307	CLA	CHC-C1C	4.86	1.47	1.35
48	21	215	A86	C9-C8	4.86	1.47	1.34
48	41	215	A86	C9-C8	4.86	1.47	1.34
37	18	204	CLA	C1D-ND	4.86	1.43	1.37
37	12	205	CLA	O2D-CGD	4.86	1.45	1.33
37	34	301	CLA	C3C-C2C	4.86	1.47	1.36
37	12	207	CLA	CHC-C1C	4.86	1.47	1.35
37	32	204	CLA	CHC-C1C	4.86	1.47	1.35
37	B	524	CLA	CHC-C1C	4.86	1.47	1.35
50	19	312	DD6	C3-C2	4.86	1.58	1.43
37	19	306	CLA	O2D-CGD	4.86	1.45	1.33
37	b	508	CLA	C3B-C2B	4.86	1.47	1.40
37	31	306	CLA	CHC-C1C	4.86	1.47	1.35
48	18	212	A86	C17-C18	-4.86	1.45	1.52
37	39	310	CLA	CHC-C1C	4.86	1.47	1.35
37	36	307	CLA	CHC-C1C	4.86	1.47	1.35
48	13	314	A86	C26-C27	4.85	1.42	1.35
37	39	307	CLA	C3B-C2B	4.85	1.47	1.40
47	11	302	KC1	C3C-C2C	4.85	1.47	1.36
37	c	513	CLA	C3C-C2C	4.85	1.47	1.36
37	32	208	CLA	CHC-C1C	4.85	1.47	1.35
48	35	311	A86	C26-C27	4.85	1.42	1.35
47	12	208	KC1	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	32	209	KC1	C3C-C2C	4.85	1.47	1.36
37	32	202	CLA	O2D-CGD	4.85	1.45	1.33
48	34	314	A86	C26-C27	4.85	1.42	1.35
47	17	305	KC1	C1A-NA	-4.84	1.28	1.38
37	b	507	CLA	O2D-CGD	4.84	1.45	1.33
37	19	304	CLA	O2D-CGD	4.84	1.45	1.33
37	14	301	CLA	C1D-ND	4.84	1.43	1.37
37	34	301	CLA	C1D-ND	4.84	1.43	1.37
47	11	306	KC1	CHD-C4C	4.84	1.47	1.35
37	16	301	CLA	C1D-ND	4.84	1.43	1.37
37	b	505	CLA	CHC-C1C	4.84	1.47	1.35
37	37	306	CLA	CHC-C1C	4.84	1.47	1.35
37	c	509	CLA	O2D-CGD	4.84	1.45	1.33
37	19	305	CLA	C1D-ND	4.84	1.43	1.37
48	34	314	A86	C9-C8	4.84	1.47	1.34
37	17	304	CLA	CHC-C1C	4.84	1.47	1.35
37	12	212	CLA	O2D-CGD	4.84	1.45	1.33
37	B	505	CLA	C3C-C2C	4.84	1.47	1.36
37	33	303	CLA	C1D-ND	4.84	1.43	1.37
37	40	208	CLA	C3C-C2C	4.84	1.47	1.36
37	16	303	CLA	C1D-ND	4.84	1.43	1.37
37	z	102	CLA	CHC-C1C	4.84	1.47	1.35
47	32	209	KC1	C3B-C2B	4.84	1.47	1.37
47	20	302	KC1	C1A-NA	-4.84	1.28	1.38
37	32	206	CLA	O2D-CGD	4.84	1.45	1.33
37	15	303	CLA	CHC-C1C	4.84	1.47	1.35
37	11	308	CLA	O2D-CGD	4.84	1.45	1.33
47	34	309	KC1	C3C-C2C	4.84	1.47	1.36
37	C	504	CLA	CHC-C1C	4.84	1.47	1.35
37	12	205	CLA	CHC-C1C	4.84	1.47	1.35
37	B	514	CLA	C3C-C2C	4.84	1.47	1.36
37	b	501	CLA	C3C-C2C	4.84	1.47	1.36
47	40	207	KC1	CHD-C4C	4.84	1.47	1.35
37	16	307	CLA	CHC-C1C	4.83	1.47	1.35
37	B	509	CLA	O2D-CGD	4.83	1.45	1.33
37	b	515	CLA	O2D-CGD	4.83	1.45	1.33
37	34	302	CLA	C1D-ND	4.83	1.43	1.37
47	13	306	KC1	CHD-C4C	4.83	1.47	1.35
47	20	305	KC1	CHD-C4C	4.83	1.47	1.35
47	33	306	KC1	CHD-C4C	4.83	1.47	1.35
37	z	101	CLA	C1D-ND	4.83	1.43	1.37
37	b	509	CLA	O2D-CGD	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	17	304	CLA	C1D-ND	4.83	1.43	1.37
37	c	504	CLA	CHC-C1C	4.83	1.47	1.35
37	39	305	CLA	CHC-C1C	4.83	1.47	1.35
37	d	403	CLA	CHC-C1C	4.83	1.47	1.35
37	35	303	CLA	CHC-C1C	4.83	1.47	1.35
37	39	306	CLA	O2D-CGD	4.83	1.45	1.33
47	40	204	KC1	C1A-NA	-4.83	1.28	1.38
37	19	306	CLA	C3C-C2C	4.82	1.47	1.36
37	D	402	CLA	O2D-CGD	4.82	1.45	1.33
37	39	309	CLA	CHC-C1C	4.82	1.47	1.35
37	B	507	CLA	O2D-CGD	4.82	1.45	1.33
48	12	215	A86	C9-C8	4.82	1.47	1.34
48	32	216	A86	C9-C8	4.82	1.47	1.34
37	34	303	CLA	C1D-ND	4.82	1.43	1.37
47	37	305	KC1	O2D-CGD	4.82	1.45	1.33
37	c	503	CLA	CHC-C1C	4.82	1.47	1.35
37	B	510	CLA	C3C-C2C	4.82	1.47	1.36
47	12	206	KC1	C1A-NA	-4.82	1.28	1.38
47	32	207	KC1	C1A-NA	-4.82	1.28	1.38
37	12	207	CLA	O2D-CGD	4.82	1.45	1.33
37	32	206	CLA	CHC-C1C	4.82	1.47	1.35
37	b	510	CLA	C3C-C2C	4.82	1.47	1.36
37	14	301	CLA	C3C-C2C	4.82	1.47	1.36
48	17	312	A86	C9-C8	4.82	1.47	1.34
48	37	311	A86	C9-C8	4.82	1.47	1.34
37	19	309	CLA	CHC-C1C	4.82	1.47	1.35
37	B	508	CLA	C3B-C2B	4.81	1.47	1.40
47	12	208	KC1	C3B-C2B	4.81	1.47	1.37
37	D	405	CLA	CHC-C1C	4.81	1.47	1.35
48	14	314	A86	C9-C8	4.81	1.47	1.34
37	38	211	CLA	CHC-C1C	4.81	1.47	1.35
37	C	509	CLA	O2D-CGD	4.81	1.44	1.33
48	12	214	A86	C17-C18	-4.81	1.45	1.52
37	d	401	CLA	O2D-CGD	4.81	1.44	1.33
37	19	305	CLA	CHC-C1C	4.81	1.47	1.35
37	b	512	CLA	O2D-CGD	4.81	1.44	1.33
37	32	213	CLA	O2D-CGD	4.81	1.44	1.33
48	15	316	A86	C9-C8	4.81	1.47	1.34
47	15	304	KC1	C1A-NA	-4.81	1.28	1.38
48	18	214	A86	C26-C27	4.81	1.42	1.35
37	c	511	CLA	O2D-CGD	4.81	1.44	1.33
47	17	306	KC1	O2D-CGD	4.81	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	19	307	CLA	C1D-ND	4.80	1.43	1.37
37	11	303	CLA	O2D-CGD	4.80	1.44	1.33
47	34	306	KC1	O2D-CGD	4.80	1.44	1.33
37	b	514	CLA	CHC-C1C	4.80	1.47	1.35
47	14	306	KC1	O2D-CGD	4.80	1.44	1.33
37	b	509	CLA	C3C-C2C	4.80	1.46	1.36
37	c	502	CLA	C3C-C2C	4.80	1.46	1.36
37	B	501	CLA	C3C-C2C	4.80	1.46	1.36
37	b	505	CLA	C3C-C2C	4.80	1.46	1.36
37	32	208	CLA	O2D-CGD	4.80	1.44	1.33
47	32	209	KC1	O2D-CGD	4.80	1.44	1.33
37	B	512	CLA	O2D-CGD	4.80	1.44	1.33
47	12	211	KC1	O2D-CGD	4.79	1.44	1.33
37	C	511	CLA	O2D-CGD	4.79	1.44	1.33
48	14	314	A86	C26-C27	4.79	1.42	1.35
37	32	205	CLA	O2D-CGD	4.79	1.44	1.33
47	35	304	KC1	OBD-CAD	4.79	1.29	1.22
47	35	304	KC1	C1A-NA	-4.79	1.28	1.38
37	C	503	CLA	CHC-C1C	4.79	1.47	1.35
37	B	514	CLA	CHC-C1C	4.79	1.47	1.35
37	31	304	CLA	O2D-CGD	4.79	1.44	1.33
37	c	512	CLA	CHC-C1C	4.79	1.47	1.35
37	B	515	CLA	O2D-CGD	4.79	1.44	1.33
37	a	404	CLA	O2D-CGD	4.79	1.44	1.33
48	38	212	A86	C17-C18	-4.78	1.45	1.52
37	14	303	CLA	CHC-C1C	4.78	1.47	1.35
37	34	303	CLA	CHC-C1C	4.78	1.47	1.35
37	36	309	CLA	C1D-ND	4.78	1.43	1.37
37	C	502	CLA	C3C-C2C	4.78	1.46	1.36
47	13	304	KC1	C1A-NA	-4.78	1.28	1.38
48	31	315	A86	C17-C18	-4.78	1.45	1.52
37	16	309	CLA	C1D-ND	4.78	1.43	1.37
37	36	301	CLA	C1D-ND	4.78	1.43	1.37
48	33	312	A86	C9-C8	4.78	1.46	1.34
37	16	309	CLA	O2D-CGD	4.78	1.44	1.33
37	a	407	CLA	CHC-C1C	4.78	1.47	1.35
47	31	303	KC1	C1A-NA	-4.78	1.28	1.38
37	13	307	CLA	C3C-C2C	4.78	1.46	1.36
37	33	307	CLA	C3C-C2C	4.78	1.46	1.36
37	B	502	CLA	CHC-C1C	4.78	1.47	1.35
37	b	502	CLA	CHC-C1C	4.77	1.47	1.35
48	41	211	A86	C26-C27	4.77	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	32	212	KC1	O2D-CGD	4.77	1.44	1.33
37	C	512	CLA	CHC-C1C	4.77	1.47	1.35
37	39	307	CLA	C1D-ND	4.77	1.43	1.37
47	18	205	KC1	C1A-NA	-4.77	1.28	1.38
47	38	205	KC1	C1A-NA	-4.77	1.28	1.38
48	21	215	A86	C26-C27	4.77	1.42	1.35
37	14	310	CLA	CHC-C1C	4.77	1.47	1.35
37	37	303	CLA	C1D-ND	4.77	1.43	1.37
37	36	309	CLA	O2D-CGD	4.77	1.44	1.33
48	32	215	A86	C17-C18	-4.77	1.45	1.52
37	C	501	CLA	C3C-C2C	4.77	1.46	1.36
47	11	302	KC1	C1A-NA	-4.77	1.28	1.38
37	b	501	CLA	CHC-C1C	4.77	1.47	1.35
47	32	209	KC1	CHD-C4C	4.77	1.47	1.35
37	39	301	CLA	C1D-ND	4.77	1.43	1.37
37	14	303	CLA	C1D-ND	4.77	1.43	1.37
37	A	405	CLA	O2D-CGD	4.77	1.44	1.33
48	15	312	A86	C9-C8	4.77	1.46	1.34
37	11	307	CLA	O2D-CGD	4.77	1.44	1.33
37	31	308	CLA	O2D-CGD	4.77	1.44	1.33
37	d	403	CLA	C3C-C2C	4.77	1.46	1.36
37	14	308	CLA	C1D-ND	4.76	1.43	1.37
37	34	308	CLA	C1D-ND	4.76	1.43	1.37
37	D	401	CLA	O2D-CGD	4.76	1.44	1.33
37	z	101	CLA	CHC-C1C	4.76	1.47	1.35
37	12	204	CLA	CHC-C1C	4.76	1.47	1.35
37	32	205	CLA	CHC-C1C	4.76	1.47	1.35
47	12	208	KC1	O2D-CGD	4.76	1.44	1.33
48	21	211	A86	C9-C8	4.76	1.46	1.34
48	11	311	A86	C17-C18	-4.76	1.45	1.52
48	31	311	A86	C17-C18	-4.76	1.45	1.52
47	12	208	KC1	CHD-C4C	4.76	1.47	1.35
48	37	319	A86	C9-C8	4.76	1.46	1.34
48	37	312	A86	C9-C8	4.76	1.46	1.34
37	31	308	CLA	CHC-C1C	4.76	1.47	1.35
37	C	510	CLA	O2D-CGD	4.76	1.44	1.33
47	12	206	KC1	O2D-CGD	4.76	1.44	1.33
37	A	405	CLA	CHC-C1C	4.76	1.47	1.35
37	39	305	CLA	C1D-ND	4.76	1.43	1.37
37	12	204	CLA	O2D-CGD	4.76	1.44	1.33
47	32	207	KC1	O2D-CGD	4.76	1.44	1.33
37	B	501	CLA	CHC-C1C	4.76	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	14	315	A86	C9-C8	4.76	1.46	1.34
48	34	315	A86	C9-C8	4.76	1.46	1.34
37	Z	101	CLA	CHC-C1C	4.76	1.47	1.35
37	w	101	CLA	CHC-C1C	4.76	1.47	1.35
37	D	405	CLA	C3C-C2C	4.76	1.46	1.36
48	38	215	A86	C26-C27	4.76	1.42	1.35
37	B	509	CLA	C3C-C2C	4.76	1.46	1.36
37	B	506	CLA	C3C-C2C	4.76	1.46	1.36
48	20	309	A86	C9-C8	4.76	1.46	1.34
37	19	301	CLA	O2D-CGD	4.75	1.44	1.33
37	39	301	CLA	O2D-CGD	4.75	1.44	1.33
47	15	302	KC1	C1A-NA	-4.75	1.28	1.38
37	c	501	CLA	C3C-C2C	4.75	1.46	1.36
48	35	316	A86	C9-C8	4.75	1.46	1.34
37	b	515	CLA	CHC-C1C	4.75	1.47	1.35
48	33	314	A86	C26-C27	4.75	1.42	1.35
48	13	312	A86	C9-C8	4.75	1.46	1.34
48	17	310	A86	C9-C8	4.75	1.46	1.34
48	41	215	A86	C26-C27	4.74	1.42	1.35
48	18	215	A86	C26-C27	4.74	1.42	1.35
37	11	307	CLA	CHC-C1C	4.74	1.47	1.35
48	41	215	A86	C17-C18	-4.74	1.45	1.52
37	19	301	CLA	C1D-ND	4.74	1.43	1.37
37	39	302	CLA	CHC-C1C	4.74	1.47	1.35
37	b	506	CLA	C3C-C2C	4.74	1.46	1.36
47	32	212	KC1	C1A-NA	-4.74	1.28	1.38
47	33	304	KC1	C1A-NA	-4.74	1.28	1.38
37	20	308	CLA	CHC-C1C	4.74	1.47	1.35
47	11	309	KC1	O2D-CGD	4.74	1.44	1.33
47	31	309	KC1	O2D-CGD	4.74	1.44	1.33
48	35	312	A86	C9-C8	4.74	1.46	1.34
48	37	309	A86	C9-C8	4.74	1.46	1.34
37	32	204	CLA	C1D-ND	4.73	1.43	1.37
48	37	311	A86	C17-C18	-4.73	1.45	1.52
37	c	505	CLA	CHC-C1C	4.73	1.47	1.35
37	c	504	CLA	O2D-CGD	4.73	1.44	1.33
48	41	211	A86	C9-C8	4.73	1.46	1.34
37	W	101	CLA	CHC-C1C	4.73	1.47	1.35
47	21	207	KC1	CHC-C4B	4.73	1.47	1.38
47	41	207	KC1	CHC-C4B	4.73	1.47	1.38
37	D	406	CLA	CHC-C1C	4.73	1.47	1.35
48	40	211	A86	C9-C8	4.73	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	38	214	A86	C26-C27	4.73	1.42	1.35
37	c	504	CLA	C3C-C2C	4.73	1.46	1.36
48	21	214	A86	C9-C8	4.73	1.46	1.34
37	a	407	CLA	O2D-CGD	4.73	1.44	1.33
48	32	218	A86	C9-C8	4.73	1.46	1.34
48	15	311	A86	C9-C8	4.73	1.46	1.34
37	d	404	CLA	CHC-C1C	4.73	1.47	1.35
37	c	510	CLA	O2D-CGD	4.73	1.44	1.33
37	C	504	CLA	O2D-CGD	4.73	1.44	1.33
37	b	501	CLA	O2D-CGD	4.73	1.44	1.33
37	11	310	CLA	O2D-CGD	4.73	1.44	1.33
48	12	217	A86	C9-C8	4.73	1.46	1.34
48	41	214	A86	C9-C8	4.73	1.46	1.34
37	C	511	CLA	CHC-C1C	4.73	1.47	1.35
37	31	310	CLA	O2D-CGD	4.72	1.44	1.33
47	35	302	KC1	OBD-CAD	4.72	1.28	1.22
37	20	306	CLA	C1D-ND	4.72	1.43	1.37
48	11	315	A86	C17-C18	-4.72	1.45	1.52
37	34	310	CLA	CHC-C1C	4.72	1.47	1.35
37	B	515	CLA	CHC-C1C	4.72	1.47	1.35
37	B	505	CLA	O2D-CGD	4.72	1.44	1.33
37	B	516	CLA	O2D-CGD	4.72	1.44	1.33
48	21	215	A86	C17-C18	-4.72	1.45	1.52
48	17	313	A86	C9-C8	4.72	1.46	1.34
47	18	210	KC1	C4D-ND	4.72	1.39	1.35
37	B	501	CLA	O2D-CGD	4.72	1.44	1.33
48	35	315	A86	C9-C8	4.72	1.46	1.34
37	31	302	CLA	O2D-CGD	4.72	1.44	1.33
48	11	319	A86	C26-C27	4.71	1.42	1.35
48	31	319	A86	C26-C27	4.71	1.42	1.35
47	13	302	KC1	C3B-C2B	4.71	1.46	1.37
37	B	508	CLA	CHC-C1C	4.71	1.47	1.35
37	b	523	CLA	O2D-CGD	4.71	1.44	1.33
37	b	505	CLA	O2D-CGD	4.71	1.44	1.33
48	41	213	A86	O4-C38	4.71	1.45	1.35
48	38	213	A86	C9-C8	4.71	1.46	1.34
37	C	505	CLA	CHC-C1C	4.71	1.47	1.35
37	40	210	CLA	CHC-C1C	4.71	1.47	1.35
47	12	211	KC1	C1A-NA	-4.71	1.28	1.38
37	C	504	CLA	C3C-C2C	4.71	1.46	1.36
37	19	302	CLA	O2D-CGD	4.71	1.44	1.33
37	c	506	CLA	O2D-CGD	4.71	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c	511	CLA	CHC-C1C	4.71	1.47	1.35
48	31	313	A86	C17-C18	-4.70	1.45	1.52
37	39	302	CLA	O2D-CGD	4.70	1.44	1.33
47	38	207	KC1	OBD-CAD	4.70	1.28	1.22
48	34	315	A86	C26-C27	4.70	1.42	1.35
37	B	508	CLA	O2D-CGD	4.70	1.44	1.33
48	13	313	A86	O4-C38	4.70	1.45	1.35
47	33	302	KC1	C3B-C2B	4.70	1.46	1.37
37	b	508	CLA	CHC-C1C	4.70	1.47	1.35
37	19	302	CLA	CHC-C1C	4.70	1.47	1.35
48	13	315	A86	C17-C18	-4.70	1.45	1.52
48	19	311	A86	C9-C8	4.70	1.46	1.34
47	35	306	KC1	C1A-NA	-4.70	1.28	1.38
48	12	202	A86	C9-C8	4.70	1.46	1.34
48	32	203	A86	C9-C8	4.70	1.46	1.34
48	35	311	A86	C9-C8	4.70	1.46	1.34
37	34	308	CLA	CHC-C1C	4.70	1.47	1.35
37	B	524	CLA	O2D-CGD	4.70	1.44	1.33
37	12	203	CLA	C1D-ND	4.70	1.43	1.37
37	15	308	CLA	CHC-C1C	4.70	1.47	1.35
48	13	311	A86	C9-C8	4.69	1.46	1.34
48	33	311	A86	C9-C8	4.69	1.46	1.34
37	C	506	CLA	O2D-CGD	4.69	1.44	1.33
37	11	301	CLA	O2D-CGD	4.69	1.44	1.33
48	17	314	A86	C9-C8	4.69	1.46	1.34
48	16	313	A86	C26-C27	4.69	1.42	1.35
48	14	313	A86	O4-C38	4.69	1.45	1.35
47	14	304	KC1	OBD-CAD	4.69	1.28	1.22
47	34	304	KC1	OBD-CAD	4.69	1.28	1.22
48	15	315	A86	C9-C8	4.69	1.46	1.34
37	12	207	CLA	C1D-ND	4.69	1.43	1.37
37	18	208	CLA	C1D-ND	4.69	1.43	1.37
37	38	208	CLA	C1D-ND	4.69	1.43	1.37
48	33	315	A86	C17-C18	-4.68	1.45	1.52
37	b	516	CLA	O2D-CGD	4.68	1.44	1.33
37	d	403	CLA	O2D-CGD	4.68	1.44	1.33
37	D	405	CLA	O2D-CGD	4.68	1.44	1.33
37	12	210	CLA	C1D-ND	4.68	1.43	1.37
37	32	211	CLA	C1D-ND	4.68	1.43	1.37
37	c	505	CLA	O2D-CGD	4.68	1.44	1.33
37	15	307	CLA	C1D-ND	4.68	1.43	1.37
37	b	516	CLA	C3B-C2B	4.68	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	502	CLA	O2D-CGD	4.68	1.44	1.33
37	33	308	CLA	CHC-C1C	4.68	1.47	1.35
48	21	213	A86	O4-C38	4.68	1.45	1.35
48	37	310	A86	C9-C8	4.68	1.46	1.34
47	38	207	KC1	C4D-ND	4.67	1.39	1.35
37	19	310	CLA	C1D-ND	4.67	1.43	1.37
37	13	303	CLA	C1D-ND	4.67	1.43	1.37
37	11	308	CLA	CHC-C1C	4.67	1.46	1.35
37	b	511	CLA	C3C-C2C	4.67	1.46	1.36
48	34	313	A86	O4-C38	4.67	1.45	1.35
48	14	313	A86	C17-C18	-4.67	1.45	1.52
37	32	208	CLA	C1D-ND	4.67	1.43	1.37
47	14	309	KC1	C1A-NA	-4.67	1.28	1.38
47	34	309	KC1	C1A-NA	-4.67	1.28	1.38
48	14	315	A86	C26-C27	4.67	1.42	1.35
37	B	502	CLA	O2D-CGD	4.67	1.44	1.33
37	14	308	CLA	CHC-C1C	4.67	1.46	1.35
48	33	313	A86	O4-C38	4.67	1.45	1.35
37	B	511	CLA	C3C-C2C	4.67	1.46	1.36
48	34	316	A86	C9-C8	4.67	1.46	1.34
37	b	512	CLA	CHC-C1C	4.67	1.46	1.35
47	11	309	KC1	C1A-NA	-4.67	1.28	1.38
37	C	505	CLA	O2D-CGD	4.67	1.44	1.33
47	32	207	KC1	CHD-C4C	4.67	1.46	1.35
37	c	511	CLA	C1D-ND	4.67	1.43	1.37
48	38	212	A86	C26-C27	4.67	1.42	1.35
37	c	503	CLA	C1D-ND	4.66	1.43	1.37
37	b	508	CLA	O2D-CGD	4.66	1.44	1.33
47	15	306	KC1	C1A-NA	-4.66	1.28	1.38
37	13	308	CLA	CHC-C1C	4.66	1.46	1.35
37	C	503	CLA	C1D-ND	4.66	1.43	1.37
48	37	309	A86	O4-C38	4.66	1.45	1.35
48	39	311	A86	C9-C8	4.66	1.46	1.34
48	17	320	A86	C9-C8	4.66	1.46	1.34
37	B	506	CLA	O2D-CGD	4.66	1.44	1.33
48	40	201	A86	C26-C27	4.66	1.42	1.35
37	B	505	CLA	C3B-C2B	4.66	1.46	1.40
37	C	501	CLA	CHC-C1C	4.66	1.46	1.35
37	C	508	CLA	O2D-CGD	4.65	1.44	1.33
37	B	507	CLA	CHC-C1C	4.65	1.46	1.35
48	21	211	A86	C26-C27	4.65	1.42	1.35
47	31	309	KC1	C1A-NA	-4.65	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	31	302	CLA	C3C-C2C	4.65	1.46	1.36
37	B	516	CLA	C3B-C2B	4.65	1.46	1.40
37	b	503	CLA	C3B-C2B	4.65	1.46	1.40
37	33	303	CLA	CHC-C1C	4.65	1.46	1.35
37	B	512	CLA	CHC-C1C	4.65	1.46	1.35
37	c	501	CLA	CHC-C1C	4.65	1.46	1.35
47	35	302	KC1	C1A-NA	-4.65	1.28	1.38
47	40	207	KC1	O2D-CGD	4.65	1.44	1.33
37	b	505	CLA	C3B-C2B	4.65	1.46	1.40
37	40	208	CLA	C1D-ND	4.65	1.43	1.37
37	C	501	CLA	O2D-CGD	4.65	1.44	1.33
37	16	301	CLA	C3C-C2C	4.64	1.46	1.36
37	11	301	CLA	C3C-C2C	4.64	1.46	1.36
48	37	313	A86	C9-C8	4.64	1.46	1.34
47	12	206	KC1	CHD-C4C	4.64	1.46	1.35
48	35	313	A86	O4-C38	4.64	1.45	1.35
37	c	501	CLA	O2D-CGD	4.64	1.44	1.33
47	15	302	KC1	OBD-CAD	4.64	1.28	1.22
47	40	206	KC1	C1A-NA	-4.64	1.29	1.38
48	34	311	A86	C9-C8	4.64	1.46	1.34
47	33	302	KC1	CHC-C4B	4.64	1.47	1.38
47	13	302	KC1	CHC-C4B	4.64	1.47	1.38
47	18	207	KC1	OBD-CAD	4.64	1.28	1.22
48	14	316	A86	C9-C8	4.64	1.46	1.34
37	33	307	CLA	CHC-C1C	4.64	1.46	1.35
47	41	207	KC1	C1A-NA	-4.64	1.29	1.38
47	40	204	KC1	OBD-CAD	4.64	1.28	1.22
37	C	513	CLA	C1D-ND	4.64	1.43	1.37
37	11	308	CLA	C1D-ND	4.64	1.43	1.37
37	32	202	CLA	C1D-ND	4.64	1.43	1.37
47	12	208	KC1	C1A-NA	-4.64	1.29	1.38
47	32	209	KC1	C1A-NA	-4.64	1.29	1.38
37	19	307	CLA	CHC-C1C	4.63	1.46	1.35
48	15	313	A86	O4-C38	4.63	1.45	1.35
37	b	506	CLA	O2D-CGD	4.63	1.44	1.33
37	36	301	CLA	C3C-C2C	4.63	1.46	1.36
37	C	502	CLA	CHC-C1C	4.63	1.46	1.35
37	35	307	CLA	C1D-ND	4.63	1.43	1.37
37	39	310	CLA	C1D-ND	4.63	1.43	1.37
47	36	304	KC1	CHC-C4B	4.63	1.47	1.38
37	B	516	CLA	C1D-ND	4.63	1.43	1.37
37	39	303	CLA	C1D-ND	4.63	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	34	313	A86	C17-C18	-4.63	1.45	1.52
37	13	307	CLA	CHC-C1C	4.63	1.46	1.35
37	38	211	CLA	CHD-C1D	4.63	1.47	1.38
48	17	310	A86	O4-C38	4.63	1.45	1.35
48	17	315	A86	C17-C18	-4.63	1.45	1.52
37	c	502	CLA	O2D-CGD	4.63	1.44	1.33
37	11	303	CLA	CHC-C1C	4.62	1.46	1.35
37	c	508	CLA	O2D-CGD	4.62	1.44	1.33
37	32	210	CLA	O2D-CGD	4.62	1.44	1.33
47	13	306	KC1	C1A-NA	-4.62	1.29	1.38
47	20	304	KC1	C1A-NA	-4.62	1.29	1.38
37	32	211	CLA	CHC-C1C	4.62	1.46	1.35
48	12	215	A86	O4-C38	4.62	1.45	1.35
47	19	308	KC1	CHC-C4B	4.62	1.47	1.38
47	12	206	KC1	CHC-C4B	4.62	1.47	1.38
47	32	207	KC1	CHC-C4B	4.62	1.47	1.38
48	17	312	A86	C17-C18	-4.62	1.45	1.52
37	32	202	CLA	CHC-C1C	4.62	1.46	1.35
47	21	207	KC1	C1A-NA	-4.62	1.29	1.38
47	35	306	KC1	CHC-C4B	4.62	1.47	1.38
47	18	207	KC1	CHB-C1B	4.62	1.47	1.38
48	14	311	A86	C9-C8	4.62	1.46	1.34
48	12	217	A86	C17-C18	-4.62	1.45	1.52
37	12	209	CLA	O2D-CGD	4.62	1.44	1.33
48	32	218	A86	C17-C18	-4.62	1.45	1.52
47	18	205	KC1	CHC-C4B	4.62	1.47	1.38
47	38	205	KC1	CHC-C4B	4.62	1.47	1.38
47	11	306	KC1	O2D-CGD	4.62	1.44	1.33
37	b	507	CLA	CHC-C1C	4.62	1.46	1.35
48	32	216	A86	O4-C38	4.62	1.45	1.35
37	11	301	CLA	C1D-ND	4.62	1.43	1.37
37	31	302	CLA	C1D-ND	4.62	1.43	1.37
37	12	210	CLA	CHC-C1C	4.61	1.46	1.35
37	11	310	CLA	CHC-C1C	4.61	1.46	1.35
37	31	310	CLA	CHC-C1C	4.61	1.46	1.35
37	b	514	CLA	O2D-CGD	4.61	1.44	1.33
47	16	304	KC1	OBD-CAD	4.61	1.28	1.22
47	11	302	KC1	O2D-CGD	4.61	1.44	1.33
47	21	203	KC1	C1A-NA	-4.61	1.29	1.38
47	31	303	KC1	O2D-CGD	4.61	1.44	1.33
37	19	303	CLA	C1D-ND	4.61	1.43	1.37
48	41	214	A86	C26-C27	4.61	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	11	313	A86	C17-C18	-4.61	1.45	1.52
47	37	302	KC1	OBD-CAD	4.61	1.28	1.22
47	41	203	KC1	C1A-NA	-4.61	1.29	1.38
48	32	217	A86	C9-C8	4.61	1.46	1.34
48	13	312	A86	C2-C1	4.61	1.41	1.35
37	B	501	CLA	C1D-ND	4.61	1.43	1.37
47	20	305	KC1	O2D-CGD	4.60	1.44	1.33
37	c	513	CLA	C1D-ND	4.60	1.43	1.37
37	B	503	CLA	CHC-C1C	4.60	1.46	1.35
37	b	503	CLA	CHC-C1C	4.60	1.46	1.35
37	a	404	CLA	C1D-ND	4.60	1.43	1.37
47	11	309	KC1	C1B-NB	-4.60	1.32	1.37
47	31	303	KC1	C1B-NB	-4.60	1.32	1.37
47	34	309	KC1	C1B-NB	-4.60	1.32	1.37
47	20	302	KC1	OBD-CAD	4.60	1.28	1.22
37	C	508	CLA	CHC-C1C	4.60	1.46	1.35
47	31	307	KC1	O2D-CGD	4.60	1.44	1.33
47	39	308	KC1	CHC-C4B	4.60	1.47	1.38
37	b	501	CLA	C1D-ND	4.60	1.43	1.37
48	15	319	A86	C9-C8	4.60	1.46	1.34
47	33	306	KC1	C1A-NA	-4.60	1.29	1.38
48	15	312	A86	C2-C1	4.60	1.41	1.35
37	32	204	CLA	C3C-C2C	4.60	1.46	1.36
48	12	216	A86	C9-C8	4.60	1.46	1.34
48	36	310	A86	C9-C8	4.60	1.46	1.34
47	16	304	KC1	CHC-C4B	4.59	1.47	1.38
47	15	304	KC1	OBD-CAD	4.59	1.28	1.22
47	36	304	KC1	OBD-CAD	4.59	1.28	1.22
48	18	212	A86	C26-C27	4.59	1.41	1.35
37	B	514	CLA	O2D-CGD	4.59	1.44	1.33
37	13	310	CLA	CHD-C1D	4.59	1.47	1.38
47	15	306	KC1	CHC-C4B	4.59	1.47	1.38
37	C	502	CLA	O2D-CGD	4.59	1.44	1.33
47	18	207	KC1	C4D-ND	4.59	1.39	1.35
47	38	210	KC1	C4D-ND	4.59	1.39	1.35
37	C	511	CLA	C1D-ND	4.59	1.43	1.37
47	31	307	KC1	CHC-C4B	4.59	1.47	1.38
48	38	213	A86	C17-C18	-4.59	1.45	1.52
47	13	309	KC1	C1A-NA	-4.59	1.29	1.38
37	B	503	CLA	C3B-C2B	4.59	1.46	1.40
37	c	502	CLA	CHC-C1C	4.59	1.46	1.35
48	33	312	A86	C17-C18	-4.58	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	13	303	CLA	CHC-C1C	4.58	1.46	1.35
48	33	312	A86	C2-C1	4.58	1.41	1.35
47	11	306	KC1	CHC-C4B	4.58	1.47	1.38
47	18	205	KC1	OBD-CAD	4.58	1.28	1.22
37	39	307	CLA	CHC-C1C	4.58	1.46	1.35
37	a	404	CLA	CHC-C1C	4.58	1.46	1.35
48	11	311	A86	C26-C27	4.58	1.41	1.35
48	17	314	A86	C17-C18	-4.58	1.45	1.52
37	b	516	CLA	C1D-ND	4.58	1.43	1.37
48	35	319	A86	C9-C8	4.58	1.46	1.34
47	33	304	KC1	CHC-C4B	4.58	1.47	1.38
48	16	310	A86	C9-C8	4.58	1.46	1.34
37	31	304	CLA	CHC-C1C	4.58	1.46	1.35
47	40	206	KC1	OBD-CAD	4.58	1.28	1.22
37	c	508	CLA	CHC-C1C	4.58	1.46	1.35
37	C	510	CLA	CHC-C1C	4.58	1.46	1.35
48	37	314	A86	C17-C18	-4.57	1.45	1.52
37	c	502	CLA	C1D-ND	4.57	1.43	1.37
45	d	406	PL9	C6-C1	-4.57	1.40	1.48
37	33	310	CLA	CHD-C1D	4.57	1.47	1.38
48	15	313	A86	C2-C1	4.57	1.41	1.35
48	35	312	A86	C2-C1	4.57	1.41	1.35
37	a	403	CLA	CHC-C1C	4.57	1.46	1.35
47	36	305	KC1	OBD-CAD	4.57	1.28	1.22
37	D	401	CLA	CHC-C1C	4.57	1.46	1.35
47	33	309	KC1	C1A-NA	-4.57	1.29	1.38
48	11	315	A86	C26-C27	4.57	1.41	1.35
37	b	516	CLA	C3C-C2C	4.57	1.46	1.36
47	12	211	KC1	C1B-NB	-4.57	1.32	1.37
37	39	304	CLA	O2A-CGA	4.57	1.46	1.30
47	14	309	KC1	C1B-NB	-4.57	1.32	1.37
37	c	509	CLA	CHC-C1C	4.56	1.46	1.35
47	11	302	KC1	C1B-NB	-4.56	1.32	1.37
47	31	309	KC1	C1B-NB	-4.56	1.32	1.37
47	38	205	KC1	OBD-CAD	4.56	1.28	1.22
48	21	213	A86	C2-C1	4.56	1.41	1.35
37	C	509	CLA	CHC-C1C	4.56	1.46	1.35
37	c	507	CLA	CHC-C1C	4.56	1.46	1.35
47	16	305	KC1	OBD-CAD	4.56	1.28	1.22
48	21	214	A86	C26-C27	4.56	1.41	1.35
48	36	313	A86	C9-C8	4.56	1.46	1.34
37	c	510	CLA	CHC-C1C	4.56	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	11	306	KC1	C1A-NA	-4.56	1.29	1.38
37	B	513	CLA	CHC-C1C	4.56	1.46	1.35
37	B	516	CLA	C3C-C2C	4.56	1.46	1.36
37	37	306	CLA	C1D-ND	4.56	1.43	1.37
37	C	507	CLA	CHC-C1C	4.56	1.46	1.35
47	13	304	KC1	CHC-C4B	4.56	1.47	1.38
48	15	311	A86	O4-C38	4.56	1.45	1.35
37	19	304	CLA	O2A-CGA	4.56	1.46	1.30
48	39	311	A86	C26-C27	4.56	1.41	1.35
47	32	212	KC1	C1B-NB	-4.56	1.32	1.37
48	13	313	A86	C2-C1	4.56	1.41	1.35
45	D	408	PL9	C6-C1	-4.55	1.40	1.48
37	12	203	CLA	C3C-C2C	4.55	1.46	1.36
47	37	304	KC1	C3D-C2D	4.55	1.47	1.39
37	A	403	CLA	CHC-C1C	4.55	1.46	1.35
37	39	309	CLA	C1D-ND	4.55	1.43	1.37
48	17	311	A86	C9-C8	4.55	1.46	1.34
47	36	302	KC1	OBD-CAD	4.55	1.28	1.22
37	D	401	CLA	C1D-ND	4.55	1.43	1.37
37	33	308	CLA	O2A-CGA	4.55	1.46	1.33
47	38	210	KC1	CHC-C4B	4.55	1.47	1.38
48	14	312	A86	C9-C8	4.55	1.46	1.34
37	C	507	CLA	O2D-CGD	4.54	1.44	1.33
37	b	513	CLA	CHC-C1C	4.54	1.46	1.35
37	B	502	CLA	C1D-ND	4.54	1.43	1.37
48	13	314	A86	C2-C1	4.54	1.41	1.35
48	33	314	A86	C2-C1	4.54	1.41	1.35
47	12	206	KC1	C1B-NB	-4.54	1.32	1.37
37	19	309	CLA	O2A-CGA	4.54	1.46	1.30
48	39	313	A86	C19-C18	4.54	1.58	1.52
48	37	311	A86	O4-C38	4.54	1.45	1.35
37	C	512	CLA	O2D-CGD	4.54	1.44	1.33
37	13	308	CLA	O2A-CGA	4.54	1.46	1.33
47	35	309	KC1	OBD-CAD	4.54	1.28	1.22
37	C	502	CLA	C1D-ND	4.54	1.43	1.37
48	16	314	A86	C9-C8	4.54	1.46	1.34
37	c	512	CLA	O2D-CGD	4.54	1.44	1.33
48	37	313	A86	C17-C18	-4.54	1.45	1.52
48	17	313	A86	C26-C27	4.53	1.41	1.35
47	15	309	KC1	CHC-C4B	4.53	1.47	1.38
47	38	207	KC1	CHC-C4B	4.53	1.47	1.38
48	18	213	A86	C9-C8	4.53	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	32	207	KC1	C1B-NB	-4.53	1.32	1.37
37	13	307	CLA	C1D-ND	4.53	1.43	1.37
37	33	307	CLA	C1D-ND	4.53	1.43	1.37
48	31	313	A86	C9-C8	4.53	1.46	1.34
48	15	316	A86	C26-C27	4.53	1.41	1.35
37	14	310	CLA	O2A-CGA	4.53	1.46	1.30
37	34	310	CLA	O2A-CGA	4.53	1.46	1.30
37	b	506	CLA	CHC-C1C	4.53	1.46	1.35
48	11	313	A86	C9-C8	4.53	1.46	1.34
47	16	302	KC1	OBD-CAD	4.53	1.28	1.22
37	c	507	CLA	O2D-CGD	4.53	1.44	1.33
48	13	312	A86	C17-C18	-4.53	1.45	1.52
37	17	307	CLA	C1D-ND	4.53	1.43	1.37
37	b	507	CLA	C1D-ND	4.52	1.43	1.37
48	41	213	A86	C2-C1	4.52	1.41	1.35
48	17	312	A86	O4-C38	4.52	1.45	1.35
48	31	311	A86	C26-C27	4.52	1.41	1.35
37	B	507	CLA	C1D-ND	4.52	1.43	1.37
37	38	211	CLA	O2A-CGA	4.52	1.45	1.30
37	39	309	CLA	O2A-CGA	4.52	1.45	1.30
48	34	312	A86	C9-C8	4.52	1.46	1.34
47	17	303	KC1	OBD-CAD	4.52	1.28	1.22
47	15	302	KC1	CHC-C4B	4.52	1.47	1.38
37	C	501	CLA	C1D-ND	4.52	1.43	1.37
37	32	213	CLA	O2A-CGA	4.52	1.45	1.30
37	b	509	CLA	C3B-C2B	4.52	1.46	1.40
37	b	504	CLA	O2D-CGD	4.52	1.44	1.33
37	19	309	CLA	C1D-ND	4.52	1.43	1.37
37	b	516	CLA	CHC-C1C	4.52	1.46	1.35
47	14	304	KC1	CHC-C4B	4.52	1.47	1.38
37	b	511	CLA	CHC-C1C	4.52	1.46	1.35
47	35	309	KC1	CHC-C4B	4.52	1.47	1.38
48	12	213	A86	C9-C8	4.52	1.46	1.34
37	d	404	CLA	O2D-CGD	4.52	1.44	1.33
37	B	513	CLA	O2D-CGD	4.52	1.44	1.33
48	15	316	A86	C21-C20	4.52	1.58	1.51
37	19	304	CLA	C1D-ND	4.52	1.43	1.37
37	39	304	CLA	C1D-ND	4.52	1.43	1.37
47	31	307	KC1	C1A-NA	-4.52	1.29	1.38
48	12	216	A86	C26-C27	4.51	1.41	1.35
37	B	506	CLA	CHC-C1C	4.51	1.46	1.35
37	B	516	CLA	CHC-C1C	4.51	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	34	306	KC1	C1A-NA	-4.51	1.29	1.38
37	21	209	CLA	O2A-CGA	4.51	1.45	1.30
48	32	214	A86	C9-C8	4.51	1.46	1.34
47	20	304	KC1	OBD-CAD	4.51	1.28	1.22
47	12	208	KC1	C1B-NB	-4.51	1.32	1.37
47	32	209	KC1	C1B-NB	-4.51	1.32	1.37
37	b	502	CLA	C1D-ND	4.51	1.43	1.37
37	41	204	CLA	CHD-C1D	4.51	1.47	1.38
48	19	313	A86	O4-C38	4.51	1.45	1.35
48	31	313	A86	C26-C27	4.51	1.41	1.35
37	41	210	CLA	O2A-CGA	4.50	1.45	1.30
47	18	210	KC1	OBD-CAD	4.50	1.28	1.22
48	31	315	A86	C26-C27	4.50	1.41	1.35
47	40	207	KC1	C1A-NA	-4.50	1.29	1.38
48	12	220	A86	C9-C8	4.50	1.46	1.34
48	35	313	A86	C2-C1	4.50	1.41	1.35
37	18	211	CLA	O2A-CGA	4.50	1.45	1.30
48	17	311	A86	C2-C1	4.50	1.41	1.35
48	37	314	A86	C26-C27	4.50	1.41	1.35
48	37	312	A86	C26-C27	4.50	1.41	1.35
47	17	303	KC1	C1A-NA	-4.50	1.29	1.38
48	33	313	A86	C2-C1	4.50	1.41	1.35
37	35	310	CLA	O2A-CGA	4.50	1.45	1.30
37	40	209	CLA	O2A-CGA	4.50	1.45	1.30
37	32	206	CLA	C1D-ND	4.50	1.43	1.37
37	15	310	CLA	O2A-CGA	4.50	1.45	1.30
47	15	309	KC1	OBD-CAD	4.49	1.28	1.22
37	12	212	CLA	O2A-CGA	4.49	1.45	1.30
37	Z	101	CLA	O2A-CGA	4.49	1.46	1.33
47	17	308	KC1	C1A-NA	-4.49	1.29	1.38
37	B	512	CLA	C3C-C2C	4.49	1.46	1.36
37	B	504	CLA	O2D-CGD	4.49	1.44	1.33
47	14	306	KC1	C1A-NA	-4.49	1.29	1.38
37	15	305	CLA	O2A-CGA	4.49	1.45	1.30
48	36	311	A86	C9-C8	4.49	1.46	1.34
37	38	206	CLA	O2A-CGA	4.49	1.45	1.30
47	15	304	KC1	CHC-C4B	4.49	1.47	1.38
47	16	305	KC1	CHC-C4B	4.49	1.47	1.38
37	B	511	CLA	CHC-C1C	4.49	1.46	1.35
37	35	305	CLA	O2A-CGA	4.49	1.45	1.30
37	20	307	CLA	O2A-CGA	4.49	1.45	1.30
47	38	210	KC1	OBD-CAD	4.49	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	39	313	A86	O4-C38	4.49	1.45	1.35
47	20	305	KC1	C1A-NA	-4.48	1.29	1.38
47	37	304	KC1	CHC-C4B	4.48	1.47	1.38
37	34	305	CLA	O2A-CGA	4.48	1.45	1.30
48	19	311	A86	C26-C27	4.48	1.41	1.35
37	D	406	CLA	C1D-ND	4.48	1.43	1.37
47	35	306	KC1	OBD-CAD	4.48	1.28	1.22
47	38	207	KC1	CHB-C1B	4.48	1.47	1.38
37	21	204	CLA	CHD-C1D	4.48	1.47	1.38
48	14	313	A86	C2-C1	4.48	1.41	1.35
37	33	310	CLA	O2A-CGA	4.48	1.45	1.30
47	34	304	KC1	CHC-C4B	4.48	1.47	1.38
47	11	306	KC1	CHB-C1B	4.48	1.47	1.38
37	b	503	CLA	O2D-CGD	4.48	1.44	1.33
37	21	210	CLA	O2A-CGA	4.48	1.45	1.30
37	11	305	CLA	C1D-ND	4.48	1.43	1.37
37	14	305	CLA	O2A-CGA	4.48	1.45	1.30
47	35	302	KC1	CHC-C4B	4.48	1.47	1.38
37	D	406	CLA	O2D-CGD	4.47	1.44	1.33
37	b	513	CLA	O2D-CGD	4.47	1.44	1.33
37	13	310	CLA	O2A-CGA	4.47	1.45	1.30
37	18	204	CLA	O2A-CGA	4.47	1.46	1.33
47	35	304	KC1	CHC-C4B	4.47	1.47	1.38
37	41	209	CLA	O2A-CGA	4.47	1.45	1.30
37	21	205	CLA	O2A-CGA	4.47	1.45	1.30
47	40	204	KC1	CHC-C4B	4.47	1.47	1.38
37	c	509	CLA	O2A-CGA	4.47	1.46	1.33
37	z	101	CLA	O2A-CGA	4.47	1.46	1.33
37	B	510	CLA	O2D-CGD	4.47	1.44	1.33
37	b	510	CLA	O2D-CGD	4.47	1.44	1.33
47	15	306	KC1	OBD-CAD	4.47	1.28	1.22
48	16	311	A86	C9-C8	4.47	1.46	1.34
37	C	509	CLA	O2A-CGA	4.47	1.46	1.33
47	20	302	KC1	CHC-C4B	4.46	1.47	1.38
47	34	306	KC1	OBD-CAD	4.46	1.28	1.22
37	c	501	CLA	C1D-ND	4.46	1.43	1.37
37	31	306	CLA	C1D-ND	4.46	1.43	1.37
48	17	315	A86	C26-C27	4.46	1.41	1.35
48	32	221	A86	C9-C8	4.46	1.46	1.34
37	c	504	CLA	C1D-ND	4.46	1.43	1.37
48	35	316	A86	C26-C27	4.46	1.41	1.35
37	36	309	CLA	O2A-CGA	4.46	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	41	205	CLA	O2A-CGA	4.46	1.45	1.30
48	40	213	A86	C7-C6	4.46	1.60	1.50
47	31	307	KC1	CHB-C1B	4.46	1.47	1.38
37	b	512	CLA	C3C-C2C	4.46	1.46	1.36
37	13	305	CLA	O2A-CGA	4.46	1.45	1.30
48	20	311	A86	C7-C6	4.46	1.60	1.50
47	18	210	KC1	CHC-C4B	4.46	1.47	1.38
37	15	310	CLA	CHD-C1D	4.45	1.47	1.38
48	32	217	A86	C26-C27	4.45	1.41	1.35
37	17	302	CLA	C1D-ND	4.45	1.43	1.37
47	14	309	KC1	CHC-C4B	4.45	1.47	1.38
37	B	510	CLA	CHC-C1C	4.45	1.46	1.35
47	37	302	KC1	C1A-NA	-4.45	1.29	1.38
47	18	207	KC1	CHC-C4B	4.45	1.47	1.38
37	18	211	CLA	CHD-C1D	4.45	1.47	1.38
37	b	510	CLA	CHC-C1C	4.45	1.46	1.35
37	41	204	CLA	O2A-CGA	4.45	1.46	1.33
47	37	307	KC1	C1A-NA	-4.45	1.29	1.38
37	35	305	CLA	CHD-C1D	4.45	1.47	1.38
47	36	305	KC1	CHC-C4B	4.45	1.47	1.38
48	15	316	A86	O4-C38	4.45	1.45	1.35
47	16	305	KC1	C1A-NA	-4.45	1.29	1.38
48	13	315	A86	C26-C27	4.44	1.41	1.35
37	31	306	CLA	O2A-CGA	4.44	1.45	1.30
37	21	204	CLA	O2A-CGA	4.44	1.46	1.33
37	d	401	CLA	C1D-ND	4.44	1.43	1.37
37	B	509	CLA	C3B-C2B	4.44	1.46	1.40
47	20	304	KC1	CHB-C1B	4.44	1.47	1.38
37	38	204	CLA	O2A-CGA	4.44	1.46	1.33
37	34	307	CLA	C1D-ND	4.44	1.43	1.37
37	16	309	CLA	O2A-CGA	4.44	1.45	1.30
48	34	313	A86	C2-C1	4.44	1.41	1.35
37	12	205	CLA	C1D-ND	4.44	1.43	1.37
47	14	306	KC1	OBD-CAD	4.44	1.28	1.22
37	C	512	CLA	O2A-CGA	4.44	1.46	1.33
37	37	306	CLA	O2A-CGA	4.44	1.46	1.33
47	17	305	KC1	CHC-C4B	4.44	1.47	1.38
37	40	205	CLA	O2A-CGA	4.43	1.46	1.33
47	18	205	KC1	C4D-ND	4.43	1.39	1.35
37	18	206	CLA	O2A-CGA	4.43	1.45	1.30
47	14	306	KC1	CHC-C4B	4.43	1.47	1.38
37	d	404	CLA	C1D-ND	4.43	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	11	314	A86	C9-C8	4.43	1.46	1.34
48	37	310	A86	C2-C1	4.43	1.41	1.35
48	40	213	A86	C2-C1	4.43	1.41	1.35
47	20	305	KC1	OBD-CAD	4.43	1.28	1.22
37	B	503	CLA	O2D-CGD	4.43	1.44	1.33
48	35	316	A86	C21-C20	4.43	1.58	1.51
37	c	512	CLA	O2A-CGA	4.43	1.46	1.33
37	17	309	CLA	CHD-C1D	4.43	1.47	1.38
48	21	215	A86	O4-C38	4.43	1.45	1.35
48	35	316	A86	O4-C38	4.43	1.45	1.35
37	33	305	CLA	O2A-CGA	4.42	1.45	1.30
37	19	303	CLA	O2D-CGD	4.42	1.44	1.33
47	40	206	KC1	CHB-C1B	4.42	1.47	1.38
37	C	502	CLA	C3B-C2B	4.42	1.46	1.40
37	C	504	CLA	C1D-ND	4.42	1.43	1.37
37	b	505	CLA	C1D-ND	4.42	1.43	1.37
48	32	216	A86	C2-C1	4.42	1.41	1.35
37	11	305	CLA	O2A-CGA	4.42	1.45	1.30
48	35	315	A86	C7-C6	4.42	1.60	1.50
37	B	515	CLA	C1D-ND	4.42	1.43	1.37
48	12	202	A86	O4-C38	4.42	1.45	1.35
48	32	203	A86	O4-C38	4.42	1.45	1.35
48	12	215	A86	C2-C1	4.42	1.41	1.35
48	16	310	A86	C17-C18	-4.42	1.46	1.52
37	B	505	CLA	C1D-ND	4.42	1.43	1.37
37	19	306	CLA	C1D-ND	4.42	1.43	1.37
37	39	306	CLA	C1D-ND	4.42	1.43	1.37
37	37	301	CLA	CHD-C1D	4.42	1.47	1.38
37	20	303	CLA	O2A-CGA	4.42	1.46	1.33
48	38	212	A86	C2-C1	4.42	1.41	1.35
37	B	511	CLA	O2D-CGD	4.42	1.44	1.33
47	15	309	KC1	C4D-ND	4.42	1.39	1.35
48	35	313	A86	C17-C18	-4.41	1.46	1.52
48	33	315	A86	C26-C27	4.41	1.41	1.35
37	15	303	CLA	CHD-C1D	4.41	1.47	1.38
37	c	509	CLA	C1D-ND	4.41	1.43	1.37
48	21	215	A86	C7-C6	4.41	1.60	1.50
37	W	101	CLA	C1D-ND	4.41	1.43	1.37
37	C	503	CLA	O2D-CGD	4.41	1.44	1.33
37	15	305	CLA	CHD-C1D	4.41	1.47	1.38
37	35	310	CLA	CHD-C1D	4.41	1.47	1.38
48	31	314	A86	C9-C8	4.41	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	20	311	A86	C2-C1	4.41	1.41	1.35
37	13	303	CLA	O2A-CGA	4.41	1.46	1.33
37	B	509	CLA	CHC-C1C	4.41	1.46	1.35
37	b	511	CLA	O2D-CGD	4.41	1.43	1.33
37	21	202	CLA	CHD-C1D	4.40	1.46	1.38
47	34	309	KC1	CHC-C4B	4.40	1.46	1.38
47	13	306	KC1	CHC-C4B	4.40	1.46	1.38
47	33	306	KC1	CHC-C4B	4.40	1.46	1.38
47	36	308	KC1	CHC-C4B	4.40	1.46	1.38
48	15	313	A86	C17-C18	-4.40	1.46	1.52
37	c	503	CLA	O2D-CGD	4.40	1.43	1.33
47	35	304	KC1	CHB-C1B	4.40	1.46	1.38
47	17	308	KC1	CHC-C4B	4.40	1.46	1.38
47	21	203	KC1	CHC-C4B	4.40	1.46	1.38
48	40	213	A86	C26-C27	4.40	1.41	1.35
47	13	302	KC1	OBD-CAD	4.40	1.28	1.22
37	14	307	CLA	C1D-ND	4.40	1.43	1.37
37	b	504	CLA	C3C-C2C	4.40	1.46	1.36
48	36	310	A86	C17-C18	-4.40	1.46	1.52
37	w	101	CLA	C1D-ND	4.40	1.43	1.37
37	11	303	CLA	C1D-ND	4.40	1.43	1.37
47	34	306	KC1	CHC-C4B	4.40	1.46	1.38
37	38	208	CLA	O2A-CGA	4.40	1.46	1.33
48	41	215	A86	O4-C38	4.39	1.45	1.35
37	33	308	CLA	CHD-C1D	4.39	1.46	1.38
47	40	207	KC1	OBD-CAD	4.39	1.28	1.22
48	12	215	A86	C17-C18	-4.39	1.46	1.52
48	32	216	A86	C17-C18	-4.39	1.46	1.52
47	37	304	KC1	OBD-CAD	4.39	1.28	1.22
37	39	303	CLA	O2D-CGD	4.39	1.43	1.33
47	36	305	KC1	C1A-NA	-4.39	1.29	1.38
48	31	319	A86	C9-C8	4.39	1.45	1.34
48	19	311	A86	O4-C38	4.39	1.45	1.35
47	15	304	KC1	CHB-C1B	4.39	1.46	1.38
47	16	308	KC1	CHC-C4B	4.39	1.46	1.38
37	b	509	CLA	CHC-C1C	4.39	1.46	1.35
37	37	308	CLA	CHD-C1D	4.39	1.46	1.38
48	18	212	A86	C2-C1	4.39	1.41	1.35
48	13	311	A86	C17-C18	-4.39	1.46	1.52
48	34	316	A86	C26-C27	4.39	1.41	1.35
48	16	313	A86	O4-C38	4.39	1.45	1.35
48	11	319	A86	C9-C8	4.39	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	33	303	CLA	O2A-CGA	4.39	1.46	1.33
47	36	308	KC1	OBD-CAD	4.39	1.28	1.22
48	11	314	A86	O4-C38	4.39	1.45	1.35
47	13	309	KC1	CHC-C4B	4.39	1.46	1.38
47	37	307	KC1	CHC-C4B	4.39	1.46	1.38
37	B	504	CLA	C3C-C2C	4.38	1.46	1.36
48	11	315	A86	C9-C8	4.38	1.45	1.34
37	18	208	CLA	O2A-CGA	4.38	1.46	1.33
37	37	303	CLA	O2A-CGA	4.38	1.46	1.33
37	17	307	CLA	O2A-CGA	4.38	1.46	1.33
37	d	404	CLA	O2A-CGA	4.38	1.46	1.33
48	41	215	A86	C7-C6	4.38	1.59	1.50
37	38	203	CLA	CHD-C1D	4.38	1.46	1.38
48	39	311	A86	O4-C38	4.38	1.45	1.35
48	41	211	A86	C2-C1	4.38	1.41	1.35
47	40	207	KC1	CHC-C4B	4.38	1.46	1.38
47	20	305	KC1	CHC-C4B	4.38	1.46	1.38
37	b	515	CLA	C1D-ND	4.38	1.43	1.37
48	31	315	A86	C9-C8	4.38	1.45	1.34
47	41	203	KC1	CHC-C4B	4.38	1.46	1.38
48	14	316	A86	O4-C38	4.38	1.45	1.35
48	34	316	A86	O4-C38	4.38	1.45	1.35
48	35	311	A86	O4-C38	4.38	1.45	1.35
37	D	402	CLA	C1D-ND	4.37	1.43	1.37
48	32	218	A86	O4-C38	4.37	1.45	1.35
48	15	315	A86	C7-C6	4.37	1.59	1.50
47	35	304	KC1	C4D-ND	4.37	1.39	1.35
37	13	303	CLA	CHD-C1D	4.37	1.46	1.38
37	C	509	CLA	C1D-ND	4.37	1.43	1.37
37	c	502	CLA	C3B-C2B	4.37	1.46	1.40
37	b	509	CLA	C1D-ND	4.37	1.43	1.37
48	40	201	A86	O4-C38	4.37	1.45	1.35
48	35	315	A86	O4-C38	4.37	1.45	1.35
48	35	314	A86	C2-C1	4.37	1.41	1.35
48	31	311	A86	O4-C38	4.37	1.45	1.35
47	33	304	KC1	CHB-C1B	4.37	1.46	1.38
48	41	214	A86	C2-C1	4.36	1.41	1.35
48	21	214	A86	C2-C1	4.36	1.41	1.35
48	41	214	A86	O4-C38	4.36	1.45	1.35
37	41	202	CLA	CHD-C1D	4.36	1.46	1.38
37	16	303	CLA	CHD-C1D	4.36	1.46	1.38
37	21	210	CLA	CHD-C1D	4.36	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	35	315	A86	C26-C27	4.36	1.41	1.35
37	w	101	CLA	O2D-CGD	4.36	1.43	1.33
48	11	311	A86	O4-C38	4.36	1.45	1.35
37	B	511	CLA	C1D-ND	4.36	1.43	1.37
37	W	101	CLA	O2D-CGD	4.36	1.43	1.33
48	18	213	A86	O4-C38	4.36	1.45	1.35
37	a	403	CLA	O2D-CGD	4.36	1.43	1.33
47	35	306	KC1	CHB-C1B	4.36	1.46	1.38
47	12	211	KC1	CHC-C4B	4.36	1.46	1.38
47	32	212	KC1	CHC-C4B	4.36	1.46	1.38
37	13	308	CLA	CHD-C1D	4.35	1.46	1.38
48	13	315	A86	C7-C6	4.35	1.59	1.50
37	35	303	CLA	CHD-C1D	4.35	1.46	1.38
37	A	403	CLA	O2D-CGD	4.35	1.43	1.33
37	41	209	CLA	CHD-C1D	4.35	1.46	1.38
37	17	304	CLA	O2A-CGA	4.35	1.46	1.33
47	16	308	KC1	OBD-CAD	4.35	1.28	1.22
48	16	314	A86	O4-C38	4.35	1.45	1.35
37	12	209	CLA	C1D-ND	4.35	1.43	1.37
37	D	402	CLA	O2A-CGA	4.35	1.46	1.33
48	14	316	A86	C26-C27	4.35	1.41	1.35
48	20	311	A86	C26-C27	4.35	1.41	1.35
37	b	511	CLA	C1D-ND	4.35	1.43	1.37
37	19	307	CLA	O2A-CGA	4.35	1.46	1.33
48	13	315	A86	O4-C38	4.35	1.45	1.35
48	21	214	A86	O4-C38	4.35	1.45	1.35
48	20	309	A86	O4-C38	4.35	1.45	1.35
47	17	306	KC1	CHB-C1B	4.34	1.46	1.38
48	32	218	A86	C26-C27	4.34	1.41	1.35
37	11	307	CLA	C1D-ND	4.34	1.43	1.37
37	b	514	CLA	O2A-CGA	4.34	1.46	1.33
47	35	309	KC1	C4D-ND	4.34	1.39	1.35
47	40	207	KC1	C4D-ND	4.34	1.39	1.35
48	12	217	A86	C26-C27	4.34	1.41	1.35
48	17	310	A86	C26-C27	4.34	1.41	1.35
48	37	309	A86	C26-C27	4.34	1.41	1.35
37	38	206	CLA	CHD-C1D	4.34	1.46	1.38
47	11	304	KC1	OBD-CAD	4.34	1.28	1.22
37	d	401	CLA	O2A-CGA	4.34	1.46	1.33
37	31	308	CLA	C1D-ND	4.34	1.43	1.37
48	17	312	A86	C2-C1	4.34	1.41	1.35
37	A	405	CLA	O2A-CGA	4.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	31	311	A86	C9-C8	4.34	1.45	1.34
48	11	311	A86	C9-C8	4.34	1.45	1.34
37	Z	102	CLA	CHD-C1D	4.34	1.46	1.38
47	33	309	KC1	CHC-C4B	4.34	1.46	1.38
48	14	315	A86	C2-C1	4.34	1.41	1.35
48	37	314	A86	C7-C6	4.34	1.59	1.50
37	B	509	CLA	C1D-ND	4.34	1.43	1.37
48	12	217	A86	O4-C38	4.34	1.45	1.35
48	15	315	A86	O4-C38	4.34	1.45	1.35
37	c	510	CLA	C1D-ND	4.34	1.43	1.37
48	12	213	A86	C17-C18	-4.34	1.46	1.52
48	35	316	A86	C17-C18	-4.34	1.46	1.52
37	18	203	CLA	CHD-C1D	4.34	1.46	1.38
37	31	304	CLA	C1D-ND	4.34	1.43	1.37
48	18	215	A86	C2-C1	4.33	1.41	1.35
48	17	313	A86	C7-C6	4.33	1.59	1.50
47	40	206	KC1	C4D-ND	4.33	1.39	1.35
47	16	308	KC1	C1A-NA	-4.33	1.29	1.38
48	38	215	A86	C2-C1	4.33	1.41	1.35
47	33	309	KC1	C1B-NB	-4.33	1.32	1.37
48	21	211	A86	C2-C1	4.33	1.41	1.35
48	16	311	A86	C17-C18	-4.33	1.46	1.52
37	18	206	CLA	CHD-C1D	4.33	1.46	1.38
37	a	407	CLA	O2A-CGA	4.33	1.46	1.33
37	16	306	CLA	C1D-ND	4.33	1.43	1.37
48	12	214	A86	C9-C8	4.33	1.45	1.34
37	z	102	CLA	CHD-C1D	4.33	1.46	1.38
37	36	306	CLA	C1D-ND	4.33	1.43	1.37
37	36	303	CLA	CHD-C1D	4.33	1.46	1.38
48	37	319	A86	C17-C18	-4.33	1.46	1.52
48	15	314	A86	C2-C1	4.33	1.41	1.35
48	41	215	A86	C2-C1	4.33	1.41	1.35
37	D	406	CLA	O2A-CGA	4.33	1.46	1.33
37	33	303	CLA	CHD-C1D	4.33	1.46	1.38
37	C	510	CLA	C1D-ND	4.32	1.43	1.37
48	36	313	A86	O4-C38	4.32	1.45	1.35
37	21	209	CLA	CHD-C1D	4.32	1.46	1.38
47	31	305	KC1	OBD-CAD	4.32	1.28	1.22
48	32	214	A86	C17-C18	-4.32	1.46	1.52
37	39	307	CLA	O2A-CGA	4.32	1.46	1.33
47	33	304	KC1	OBD-CAD	4.32	1.28	1.22
47	37	305	KC1	CHB-C1B	4.32	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	19	308	KC1	OBD-CAD	4.32	1.28	1.22
37	40	210	CLA	O2A-CGA	4.32	1.46	1.33
37	34	305	CLA	CHD-C1D	4.32	1.46	1.38
48	17	315	A86	C7-C6	4.32	1.59	1.50
48	33	315	A86	O4-C38	4.32	1.45	1.35
47	37	305	KC1	OBD-CAD	4.32	1.28	1.22
37	B	514	CLA	O2A-CGA	4.32	1.46	1.33
47	13	304	KC1	CHB-C1B	4.32	1.46	1.38
37	41	208	CLA	CHD-C1D	4.32	1.46	1.38
47	16	302	KC1	CHC-C4B	4.32	1.46	1.38
47	37	305	KC1	C1A-NA	-4.32	1.29	1.38
48	38	213	A86	C7-C6	4.32	1.59	1.50
37	21	208	CLA	O2A-CGA	4.32	1.46	1.33
48	40	211	A86	C26-C27	4.31	1.41	1.35
48	37	310	A86	C17-C18	-4.31	1.46	1.52
48	21	211	A86	O4-C38	4.31	1.44	1.35
48	37	314	A86	O4-C38	4.31	1.44	1.35
48	40	211	A86	O4-C38	4.31	1.44	1.35
48	12	220	A86	C17-C18	-4.31	1.46	1.52
48	11	312	A86	C9-C8	4.31	1.45	1.34
47	36	302	KC1	CHC-C4B	4.31	1.46	1.38
47	37	302	KC1	C4D-ND	4.31	1.39	1.35
48	17	315	A86	O4-C38	4.31	1.44	1.35
48	17	311	A86	C17-C18	-4.31	1.46	1.52
37	41	210	CLA	CHD-C1D	4.31	1.46	1.38
48	14	314	A86	C7-C6	4.31	1.59	1.50
48	34	314	A86	C7-C6	4.31	1.59	1.50
47	33	302	KC1	OBD-CAD	4.31	1.28	1.22
47	36	308	KC1	C1A-NA	-4.31	1.29	1.38
47	17	303	KC1	C1B-NB	-4.31	1.32	1.37
47	38	205	KC1	C4D-ND	4.31	1.39	1.35
37	21	208	CLA	CHD-C1D	4.31	1.46	1.38
47	39	308	KC1	CHB-C1B	4.31	1.46	1.38
37	18	203	CLA	O2A-CGA	4.31	1.45	1.33
48	35	311	A86	C17-C18	-4.31	1.46	1.52
48	31	319	A86	O4-C38	4.30	1.44	1.35
48	38	213	A86	O4-C38	4.30	1.44	1.35
48	41	211	A86	O4-C38	4.30	1.44	1.35
47	40	207	KC1	CHB-C1B	4.30	1.46	1.38
48	15	311	A86	C2-C1	4.30	1.41	1.35
48	35	316	A86	C2-C1	4.30	1.41	1.35
48	35	319	A86	C7-C6	4.30	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	13	306	KC1	OBD-CAD	4.30	1.28	1.22
47	17	306	KC1	OBD-CAD	4.30	1.28	1.22
47	33	306	KC1	OBD-CAD	4.30	1.28	1.22
48	14	314	A86	O4-C38	4.30	1.44	1.35
48	34	314	A86	O4-C38	4.30	1.44	1.35
37	D	401	CLA	O2A-CGA	4.30	1.45	1.33
48	15	311	A86	C17-C18	-4.30	1.46	1.52
47	13	304	KC1	OBD-CAD	4.30	1.28	1.22
47	15	306	KC1	CHB-C1B	4.30	1.46	1.38
37	14	302	CLA	O2A-CGA	4.30	1.45	1.33
37	41	208	CLA	O2A-CGA	4.30	1.45	1.33
48	37	311	A86	C2-C1	4.30	1.41	1.35
48	15	315	A86	C26-C27	4.30	1.41	1.35
37	15	301	CLA	O2A-CGA	4.30	1.45	1.33
47	17	306	KC1	C4D-ND	4.30	1.39	1.35
37	32	205	CLA	O2A-CGA	4.30	1.45	1.33
37	38	209	CLA	O2A-CGA	4.30	1.45	1.33
48	32	215	A86	C9-C8	4.30	1.45	1.34
47	18	210	KC1	C1A-NA	-4.30	1.29	1.38
37	17	302	CLA	CHD-C1D	4.30	1.46	1.38
47	11	304	KC1	C1B-NB	-4.30	1.32	1.37
48	15	314	A86	C7-C6	4.30	1.59	1.50
47	33	306	KC1	CHB-C1B	4.30	1.46	1.38
48	31	312	A86	C9-C8	4.30	1.45	1.34
48	32	221	A86	O4-C38	4.30	1.44	1.35
47	36	305	KC1	CHB-C1B	4.29	1.46	1.38
48	18	214	A86	C7-C6	4.29	1.59	1.50
37	W	101	CLA	O2A-CGA	4.29	1.45	1.33
48	11	319	A86	O4-C38	4.29	1.44	1.35
37	15	303	CLA	O2A-CGA	4.29	1.45	1.33
47	33	309	KC1	OBD-CAD	4.29	1.28	1.22
37	20	308	CLA	O2A-CGA	4.29	1.45	1.33
47	11	304	KC1	CHC-C4B	4.29	1.46	1.38
48	13	314	A86	O4-C38	4.29	1.44	1.35
47	38	210	KC1	C1A-NA	-4.29	1.29	1.38
48	15	316	A86	C17-C18	-4.29	1.46	1.52
47	17	306	KC1	C1A-NA	-4.29	1.29	1.38
48	15	316	A86	C2-C1	4.29	1.41	1.35
48	35	311	A86	C2-C1	4.29	1.41	1.35
48	38	214	A86	C2-C1	4.29	1.41	1.35
48	33	314	A86	C7-C6	4.29	1.59	1.50
48	35	312	A86	C17-C18	-4.29	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	13	305	CLA	CHD-C1D	4.29	1.46	1.38
47	19	308	KC1	CHB-C1B	4.29	1.46	1.38
48	12	216	A86	O4-C38	4.29	1.44	1.35
48	32	221	A86	C17-C18	-4.29	1.46	1.52
37	a	404	CLA	O2A-CGA	4.29	1.45	1.33
48	37	312	A86	O4-C38	4.29	1.44	1.35
48	40	213	A86	O4-C38	4.29	1.44	1.35
47	20	305	KC1	CHB-C1B	4.29	1.46	1.38
37	11	310	CLA	C1D-ND	4.28	1.43	1.37
37	39	302	CLA	O2A-CGA	4.28	1.45	1.33
37	14	305	CLA	CHD-C1D	4.28	1.46	1.38
37	34	310	CLA	CHD-C1D	4.28	1.46	1.38
47	20	305	KC1	C4D-ND	4.28	1.39	1.35
48	37	313	A86	O4-C38	4.28	1.44	1.35
37	B	504	CLA	CHC-C1C	4.28	1.45	1.35
48	35	312	A86	C7-C6	4.28	1.59	1.50
37	33	305	CLA	CHD-C1D	4.28	1.46	1.38
37	34	302	CLA	O2A-CGA	4.28	1.45	1.33
48	33	315	A86	C7-C6	4.28	1.59	1.50
47	39	308	KC1	OBD-CAD	4.28	1.28	1.22
37	32	210	CLA	C1D-ND	4.28	1.43	1.37
47	18	207	KC1	C1A-NA	-4.28	1.29	1.38
48	13	314	A86	C7-C6	4.28	1.59	1.50
48	14	314	A86	C2-C1	4.28	1.41	1.35
48	31	314	A86	C26-C27	4.28	1.41	1.35
48	33	311	A86	C17-C18	-4.28	1.46	1.52
48	36	311	A86	C17-C18	-4.28	1.46	1.52
48	40	201	A86	C7-C6	4.28	1.59	1.50
37	w	101	CLA	O2A-CGA	4.28	1.45	1.33
47	16	305	KC1	CHB-C1B	4.28	1.46	1.38
48	21	215	A86	C2-C1	4.28	1.41	1.35
48	38	213	A86	C26-C27	4.28	1.41	1.35
37	31	310	CLA	C1D-ND	4.28	1.43	1.37
48	19	313	A86	C2-C1	4.28	1.41	1.35
37	12	212	CLA	CHD-C1D	4.27	1.46	1.38
47	37	302	KC1	C1B-NB	-4.27	1.32	1.37
37	12	204	CLA	O2A-CGA	4.27	1.45	1.33
47	17	305	KC1	OBD-CAD	4.27	1.28	1.22
48	33	314	A86	O4-C38	4.27	1.44	1.35
48	17	320	A86	C21-C20	4.27	1.58	1.51
37	c	506	CLA	O2A-CGA	4.27	1.45	1.33
47	31	305	KC1	CHC-C4B	4.27	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	40	203	CLA	CHD-C1D	4.27	1.46	1.38
48	16	313	A86	C7-C6	4.27	1.59	1.50
48	34	313	A86	C7-C6	4.27	1.59	1.50
37	20	306	CLA	O2A-CGA	4.27	1.45	1.33
48	17	320	A86	C17-C18	-4.27	1.46	1.52
48	12	220	A86	O4-C38	4.27	1.44	1.35
37	40	208	CLA	O2A-CGA	4.27	1.45	1.33
48	15	319	A86	C26-C27	4.27	1.41	1.35
48	38	214	A86	O4-C38	4.27	1.44	1.35
37	15	308	CLA	O2A-CGA	4.27	1.45	1.33
48	36	313	A86	C7-C6	4.27	1.59	1.50
48	20	309	A86	C7-C6	4.27	1.59	1.50
37	31	301	CLA	CHD-C1D	4.27	1.46	1.38
48	20	309	A86	C26-C27	4.27	1.41	1.35
37	C	506	CLA	C1B-NB	-4.27	1.31	1.35
48	38	215	A86	O4-C38	4.27	1.44	1.35
37	20	301	CLA	CHD-C1D	4.26	1.46	1.38
48	34	315	A86	C2-C1	4.26	1.41	1.35
47	38	207	KC1	C1A-NA	-4.26	1.29	1.38
37	36	303	CLA	O2A-CGA	4.26	1.45	1.33
48	11	314	A86	C26-C27	4.26	1.41	1.35
47	14	306	KC1	CHB-C1B	4.26	1.46	1.38
48	15	319	A86	C7-C6	4.26	1.59	1.50
48	14	313	A86	C7-C6	4.26	1.59	1.50
48	21	214	A86	C7-C6	4.26	1.59	1.50
47	13	309	KC1	C1B-NB	-4.26	1.32	1.37
37	b	504	CLA	CHC-C1C	4.26	1.45	1.35
48	20	311	A86	O4-C38	4.26	1.44	1.35
37	35	303	CLA	O2A-CGA	4.26	1.45	1.33
47	15	309	KC1	C1A-NA	-4.26	1.29	1.38
37	14	303	CLA	CHD-C1D	4.26	1.46	1.38
37	35	301	CLA	O2A-CGA	4.26	1.45	1.33
48	15	312	A86	C17-C18	-4.26	1.46	1.52
48	13	313	A86	C7-C6	4.26	1.59	1.50
48	18	214	A86	C2-C1	4.26	1.41	1.35
48	17	320	A86	O4-C38	4.25	1.44	1.35
37	A	403	CLA	C1D-ND	4.25	1.43	1.37
48	17	313	A86	O4-C38	4.25	1.44	1.35
37	20	307	CLA	CHD-C1D	4.25	1.46	1.38
47	17	303	KC1	CHB-C1B	4.25	1.46	1.38
37	39	303	CLA	O2A-CGA	4.25	1.45	1.33
47	12	206	KC1	OBD-CAD	4.25	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	34	303	CLA	CHD-C1D	4.25	1.46	1.38
37	18	202	CLA	O2A-CGA	4.25	1.45	1.33
48	19	311	A86	C17-C18	-4.25	1.46	1.52
48	39	311	A86	C17-C18	-4.25	1.46	1.52
48	17	314	A86	C7-C6	4.25	1.59	1.50
48	41	214	A86	C7-C6	4.25	1.59	1.50
37	a	403	CLA	C1D-ND	4.25	1.43	1.37
48	13	312	A86	O4-C38	4.25	1.44	1.35
47	20	304	KC1	C4D-ND	4.25	1.39	1.35
48	16	314	A86	C7-C6	4.25	1.59	1.50
48	35	313	A86	C7-C6	4.25	1.59	1.50
48	38	212	A86	C7-C6	4.25	1.59	1.50
48	40	213	A86	C5-C6	4.25	1.41	1.35
48	17	312	A86	C7-C6	4.25	1.59	1.50
37	20	301	CLA	O2A-CGA	4.25	1.45	1.33
48	13	311	A86	O4-C38	4.25	1.44	1.35
48	20	311	A86	C5-C6	4.25	1.41	1.35
48	39	313	A86	C9-C10	4.25	1.56	1.43
47	13	306	KC1	CHB-C1B	4.25	1.46	1.38
48	18	213	A86	C26-C27	4.25	1.41	1.35
48	35	314	A86	C7-C6	4.25	1.59	1.50
37	40	203	CLA	O2A-CGA	4.25	1.45	1.33
48	12	213	A86	O4-C38	4.25	1.44	1.35
48	32	214	A86	O4-C38	4.25	1.44	1.35
48	14	315	A86	C17-C18	-4.25	1.46	1.52
37	18	209	CLA	O2A-CGA	4.25	1.45	1.33
48	37	319	A86	O4-C38	4.25	1.44	1.35
47	16	302	KC1	C4D-ND	4.24	1.39	1.35
47	35	309	KC1	C1A-NA	-4.24	1.29	1.38
37	16	303	CLA	O2A-CGA	4.24	1.45	1.33
37	33	307	CLA	O2A-CGA	4.24	1.45	1.33
37	14	310	CLA	CHD-C1D	4.24	1.46	1.38
48	15	314	A86	O4-C38	4.24	1.44	1.35
48	32	217	A86	O4-C38	4.24	1.44	1.35
37	Z	102	CLA	O2A-CGA	4.24	1.45	1.30
37	38	201	CLA	CHD-C1D	4.24	1.46	1.38
47	21	203	KC1	OBD-CAD	4.24	1.28	1.22
37	C	506	CLA	O2A-CGA	4.24	1.45	1.33
37	34	302	CLA	CHD-C1D	4.24	1.46	1.38
37	38	204	CLA	CHD-C1D	4.24	1.46	1.38
37	40	209	CLA	CHD-C1D	4.24	1.46	1.38
47	32	207	KC1	OBD-CAD	4.24	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	37	303	CLA	CHD-C1D	4.24	1.46	1.38
37	34	303	CLA	O2A-CGA	4.24	1.45	1.33
48	34	315	A86	C17-C18	-4.24	1.46	1.52
48	18	214	A86	O4-C38	4.24	1.44	1.35
48	37	311	A86	C7-C6	4.24	1.59	1.50
47	41	203	KC1	OBD-CAD	4.23	1.28	1.22
48	15	312	A86	C7-C6	4.23	1.59	1.50
47	36	304	KC1	CHB-C1B	4.23	1.46	1.38
48	17	311	A86	C7-C6	4.23	1.59	1.50
37	13	301	CLA	O2A-CGA	4.23	1.45	1.33
47	34	306	KC1	CHB-C1B	4.23	1.46	1.38
47	17	303	KC1	C4D-ND	4.23	1.39	1.35
37	14	303	CLA	O2A-CGA	4.23	1.45	1.33
37	16	307	CLA	O2A-CGA	4.23	1.45	1.33
47	35	302	KC1	CHB-C1B	4.23	1.46	1.38
47	40	206	KC1	CHC-C4B	4.23	1.46	1.38
48	34	316	A86	C17-C18	-4.23	1.46	1.52
37	12	210	CLA	CHD-C1D	4.23	1.46	1.38
48	37	319	A86	C21-C20	4.23	1.58	1.51
48	21	213	A86	C17-C18	-4.23	1.46	1.52
47	15	306	KC1	C4D-ND	4.23	1.39	1.35
47	35	306	KC1	C4D-ND	4.23	1.39	1.35
37	35	308	CLA	O2A-CGA	4.23	1.45	1.33
48	18	212	A86	C21-C20	4.23	1.58	1.51
48	40	211	A86	C7-C6	4.23	1.59	1.50
37	33	301	CLA	O2A-CGA	4.23	1.45	1.33
47	18	205	KC1	CHB-C1B	4.23	1.46	1.38
47	38	205	KC1	CHB-C1B	4.23	1.46	1.38
37	W	102	CLA	CHD-C1D	4.23	1.46	1.38
37	36	307	CLA	O2A-CGA	4.23	1.45	1.33
48	17	314	A86	O4-C38	4.23	1.44	1.35
48	18	215	A86	O4-C38	4.23	1.44	1.35
48	14	316	A86	C17-C18	-4.22	1.46	1.52
37	32	206	CLA	O2A-CGA	4.22	1.45	1.33
47	16	305	KC1	C4D-ND	4.22	1.39	1.35
47	31	309	KC1	CHC-C4B	4.22	1.46	1.38
37	12	205	CLA	O2A-CGA	4.22	1.45	1.33
37	19	303	CLA	O2A-CGA	4.22	1.45	1.33
37	B	513	CLA	C1D-ND	4.22	1.43	1.37
48	37	313	A86	C7-C6	4.22	1.59	1.50
48	37	310	A86	C7-C6	4.22	1.59	1.50
37	13	307	CLA	O2A-CGA	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	11	303	CLA	O2A-CGA	4.22	1.45	1.33
37	31	304	CLA	O2A-CGA	4.22	1.45	1.33
48	35	319	A86	C26-C27	4.22	1.41	1.35
47	11	302	KC1	OBD-CAD	4.22	1.28	1.22
48	36	310	A86	C7-C6	4.22	1.59	1.50
37	14	302	CLA	CHD-C1D	4.22	1.46	1.38
47	37	307	KC1	OBD-CAD	4.22	1.28	1.22
37	c	506	CLA	C1B-NB	-4.22	1.31	1.35
37	38	201	CLA	O2A-CGA	4.22	1.45	1.33
48	38	214	A86	C7-C6	4.22	1.59	1.50
48	34	314	A86	C2-C1	4.22	1.41	1.35
48	33	311	A86	O4-C38	4.22	1.44	1.35
48	14	312	A86	O4-C38	4.22	1.44	1.35
37	C	507	CLA	O2A-CGA	4.21	1.45	1.33
48	35	319	A86	O4-C38	4.21	1.44	1.35
48	31	314	A86	O4-C38	4.21	1.44	1.35
47	16	304	KC1	CHB-C1B	4.21	1.46	1.38
47	16	302	KC1	CHB-C1B	4.21	1.46	1.38
48	33	313	A86	C7-C6	4.21	1.59	1.50
48	15	313	A86	C7-C6	4.21	1.59	1.50
37	B	501	CLA	O2A-CGA	4.21	1.45	1.33
37	z	102	CLA	O2A-CGA	4.21	1.44	1.30
37	C	506	CLA	CHC-C1C	4.21	1.45	1.35
37	18	204	CLA	CHD-C1D	4.21	1.46	1.38
37	b	501	CLA	O2A-CGA	4.21	1.45	1.33
48	39	313	A86	C2-C1	4.21	1.41	1.35
47	17	306	KC1	C1A-CHA	4.21	1.51	1.40
47	37	305	KC1	C1A-CHA	4.21	1.51	1.40
48	19	313	A86	C7-C6	4.21	1.59	1.50
37	36	301	CLA	O2A-CGA	4.21	1.45	1.33
37	c	506	CLA	CHC-C1C	4.21	1.45	1.35
37	17	304	CLA	CHD-C1D	4.21	1.46	1.38
37	32	213	CLA	CHD-C1D	4.20	1.46	1.38
37	39	301	CLA	O2A-CGA	4.20	1.45	1.33
48	12	214	A86	O4-C38	4.20	1.44	1.35
48	32	215	A86	O4-C38	4.20	1.44	1.35
47	36	308	KC1	C1B-NB	-4.20	1.32	1.37
47	37	302	KC1	CHB-C1B	4.20	1.46	1.38
37	32	211	CLA	CHD-C1D	4.20	1.46	1.38
37	c	507	CLA	O2A-CGA	4.20	1.45	1.33
37	15	307	CLA	O2A-CGA	4.20	1.45	1.33
47	18	207	KC1	C1A-CHA	4.20	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	35	302	KC1	C4D-ND	4.20	1.39	1.35
48	16	310	A86	C7-C6	4.20	1.59	1.50
47	38	210	KC1	C1A-CHA	4.20	1.51	1.40
48	35	314	A86	O4-C38	4.20	1.44	1.35
48	11	313	A86	C7-C6	4.20	1.59	1.50
47	17	305	KC1	CHB-C1B	4.20	1.46	1.38
47	37	305	KC1	C4D-ND	4.19	1.39	1.35
47	12	208	KC1	CHC-C4B	4.19	1.46	1.38
47	17	308	KC1	OBD-CAD	4.19	1.28	1.22
47	18	210	KC1	C1A-CHA	4.19	1.51	1.40
37	35	307	CLA	O2A-CGA	4.19	1.45	1.33
48	18	212	A86	C7-C6	4.19	1.59	1.50
48	33	312	A86	C7-C6	4.19	1.59	1.50
37	c	513	CLA	O2A-CGA	4.19	1.45	1.33
37	37	301	CLA	O2A-CGA	4.19	1.45	1.33
47	20	304	KC1	CHC-C4B	4.19	1.46	1.38
48	39	311	A86	C7-C6	4.19	1.59	1.50
48	36	311	A86	C21-C20	4.19	1.58	1.51
37	13	301	CLA	CHD-C1D	4.19	1.46	1.38
37	14	307	CLA	O2A-CGA	4.19	1.45	1.33
37	19	301	CLA	O2A-CGA	4.19	1.45	1.33
37	17	309	CLA	O2A-CGA	4.19	1.45	1.33
37	18	201	CLA	O2A-CGA	4.19	1.45	1.33
48	33	312	A86	O4-C38	4.19	1.44	1.35
37	19	302	CLA	O2A-CGA	4.19	1.45	1.33
37	34	307	CLA	O2A-CGA	4.19	1.45	1.33
37	39	302	CLA	CHD-C1D	4.19	1.46	1.38
48	31	314	A86	C17-C18	-4.19	1.46	1.52
37	21	206	CLA	O2A-CGA	4.19	1.45	1.33
37	33	301	CLA	CHD-C1D	4.19	1.46	1.38
47	36	302	KC1	CHB-C1B	4.19	1.46	1.38
47	36	305	KC1	C4D-ND	4.19	1.38	1.35
37	32	208	CLA	CHD-C1D	4.19	1.46	1.38
47	13	309	KC1	OBD-CAD	4.19	1.28	1.22
37	38	203	CLA	O2A-CGA	4.19	1.45	1.33
37	41	206	CLA	O2A-CGA	4.18	1.45	1.33
48	19	313	A86	C10-C11	4.18	1.46	1.34
47	31	303	KC1	OBD-CAD	4.18	1.28	1.22
47	36	302	KC1	C1A-NA	-4.18	1.29	1.38
37	C	513	CLA	O2A-CGA	4.18	1.45	1.33
47	36	302	KC1	C1A-CHA	4.18	1.51	1.40
37	31	301	CLA	O2A-CGA	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	17	310	A86	C7-C6	4.18	1.59	1.50
48	39	313	A86	C7-C6	4.18	1.59	1.50
48	41	213	A86	C17-C18	-4.18	1.46	1.52
47	41	203	KC1	CHB-C1B	4.18	1.46	1.38
48	16	311	A86	C21-C20	4.18	1.58	1.51
47	38	207	KC1	C1A-CHA	4.18	1.51	1.40
37	17	302	CLA	O2A-CGA	4.18	1.45	1.33
48	41	211	A86	C10-C11	4.18	1.46	1.34
48	13	312	A86	C7-C6	4.18	1.59	1.50
37	W	102	CLA	O2A-CGA	4.18	1.45	1.33
47	16	302	KC1	C1A-NA	-4.18	1.29	1.38
48	41	211	A86	C5-C6	4.18	1.41	1.35
48	40	201	A86	C10-C11	4.18	1.46	1.34
37	12	207	CLA	O2A-CGA	4.18	1.45	1.33
37	16	301	CLA	O2A-CGA	4.17	1.45	1.33
37	c	506	CLA	C1D-ND	4.17	1.42	1.37
48	16	313	A86	C9-C10	4.17	1.56	1.43
47	34	304	KC1	CHB-C1B	4.17	1.46	1.38
48	41	211	A86	C7-C6	4.17	1.59	1.50
47	35	309	KC1	C1A-CHA	4.17	1.51	1.40
37	39	305	CLA	O2A-CGA	4.17	1.45	1.33
47	17	308	KC1	C1B-NB	-4.17	1.32	1.37
47	16	308	KC1	C1B-NB	-4.17	1.32	1.37
47	15	302	KC1	C4D-ND	4.17	1.38	1.35
47	37	304	KC1	CHB-C1B	4.17	1.46	1.38
37	14	308	CLA	O2A-CGA	4.17	1.45	1.33
37	34	308	CLA	O2A-CGA	4.17	1.45	1.33
37	38	202	CLA	O2A-CGA	4.17	1.45	1.33
47	16	305	KC1	C1A-CHA	4.17	1.51	1.40
47	36	305	KC1	C1A-CHA	4.17	1.51	1.40
47	36	302	KC1	C4D-ND	4.17	1.38	1.35
37	d	401	CLA	CHD-C1D	4.17	1.46	1.38
37	17	307	CLA	CHD-C1D	4.17	1.46	1.38
37	37	306	CLA	CHD-C1D	4.17	1.46	1.38
48	40	201	A86	C2-C1	4.17	1.41	1.35
48	21	211	A86	C7-C6	4.17	1.59	1.50
37	11	303	CLA	CHD-C1D	4.17	1.46	1.38
48	12	216	A86	C7-C6	4.17	1.59	1.50
37	36	306	CLA	O2A-CGA	4.17	1.45	1.33
47	32	209	KC1	CHC-C4B	4.17	1.46	1.38
48	33	311	A86	C7-C6	4.17	1.59	1.50
47	11	304	KC1	CHB-C1B	4.17	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	11	309	KC1	CHC-C4B	4.17	1.46	1.38
48	16	313	A86	C2-C1	4.17	1.41	1.35
48	19	313	A86	C9-C10	4.17	1.56	1.43
47	32	209	KC1	C1A-CHA	4.16	1.51	1.40
48	11	314	A86	C7-C6	4.16	1.59	1.50
37	19	305	CLA	O2A-CGA	4.16	1.45	1.33
48	39	313	A86	C10-C11	4.16	1.46	1.34
48	15	319	A86	O4-C38	4.16	1.44	1.35
47	17	306	KC1	C1B-NB	-4.16	1.32	1.37
37	18	201	CLA	CHD-C1D	4.16	1.46	1.38
37	19	302	CLA	CHD-C1D	4.16	1.46	1.38
37	19	303	CLA	CHD-C1D	4.16	1.46	1.38
37	39	303	CLA	CHD-C1D	4.16	1.46	1.38
47	31	305	KC1	CHB-C1B	4.16	1.46	1.38
48	11	314	A86	C17-C18	-4.16	1.46	1.52
48	13	314	A86	C5-C6	4.16	1.41	1.35
48	17	315	A86	C21-C20	4.16	1.58	1.51
48	40	213	A86	C21-C20	4.16	1.58	1.51
48	35	311	A86	C7-C6	4.16	1.59	1.50
48	20	311	A86	C21-C20	4.16	1.58	1.51
48	12	220	A86	C7-C6	4.16	1.59	1.50
48	34	312	A86	O4-C38	4.16	1.44	1.35
47	16	302	KC1	C1A-CHA	4.16	1.51	1.40
48	33	311	A86	C26-C27	4.16	1.41	1.35
48	37	313	A86	C21-C20	4.16	1.58	1.51
47	37	302	KC1	CHC-C4B	4.16	1.46	1.38
37	21	202	CLA	O2A-CGA	4.16	1.45	1.33
47	31	305	KC1	C1B-NB	-4.16	1.32	1.37
48	11	315	A86	C7-C6	4.16	1.59	1.50
47	32	207	KC1	CHB-C1B	4.16	1.46	1.38
37	21	204	CLA	CHD-C4C	4.15	1.48	1.39
37	b	513	CLA	C1D-ND	4.15	1.42	1.37
48	16	313	A86	C10-C11	4.15	1.46	1.34
48	17	313	A86	C2-C1	4.15	1.41	1.35
48	40	211	A86	C21-C20	4.15	1.58	1.51
48	31	313	A86	C7-C6	4.15	1.59	1.50
37	32	208	CLA	O2A-CGA	4.15	1.45	1.33
48	34	315	A86	C7-C6	4.15	1.59	1.50
37	37	308	CLA	O2A-CGA	4.15	1.45	1.33
47	35	306	KC1	C1A-CHA	4.15	1.51	1.40
37	b	501	CLA	CHD-C1D	4.15	1.46	1.38
47	16	304	KC1	C4D-ND	4.15	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	17	308	KC1	C4D-ND	4.15	1.38	1.35
37	16	306	CLA	O2A-CGA	4.15	1.45	1.33
48	37	309	A86	C7-C6	4.15	1.59	1.50
47	37	307	KC1	C1B-NB	-4.15	1.32	1.37
37	39	307	CLA	CHD-C1D	4.15	1.46	1.38
48	32	221	A86	C7-C6	4.15	1.59	1.50
48	21	211	A86	C10-C11	4.15	1.46	1.34
37	41	202	CLA	O2A-CGA	4.15	1.45	1.33
48	17	314	A86	C21-C20	4.15	1.58	1.51
37	Z	101	CLA	CHD-C1D	4.15	1.46	1.38
48	20	309	A86	C21-C20	4.15	1.58	1.51
47	41	203	KC1	C4D-ND	4.15	1.38	1.35
48	13	311	A86	C7-C6	4.15	1.59	1.50
48	19	311	A86	C7-C6	4.15	1.59	1.50
37	D	402	CLA	CHD-C1D	4.15	1.46	1.38
47	15	304	KC1	C4D-ND	4.14	1.38	1.35
47	15	309	KC1	C1A-CHA	4.14	1.51	1.40
37	31	308	CLA	O2A-CGA	4.14	1.45	1.33
37	35	308	CLA	CHD-C1D	4.14	1.46	1.38
37	12	207	CLA	CHD-C1D	4.14	1.46	1.38
47	17	303	KC1	CHC-C4B	4.14	1.46	1.38
47	21	203	KC1	CHB-C1B	4.14	1.46	1.38
48	14	311	A86	C17-C18	-4.14	1.46	1.52
47	14	304	KC1	CHB-C1B	4.14	1.46	1.38
37	19	306	CLA	O2A-CGA	4.14	1.45	1.33
37	C	506	CLA	C1D-ND	4.14	1.42	1.37
48	40	201	A86	C9-C10	4.14	1.56	1.43
37	z	101	CLA	CHD-C1D	4.14	1.46	1.38
48	14	315	A86	C7-C6	4.14	1.59	1.50
37	19	307	CLA	CHD-C1D	4.14	1.46	1.38
48	33	315	A86	C2-C1	4.14	1.41	1.35
48	37	314	A86	C21-C20	4.14	1.58	1.51
37	36	306	CLA	CHD-C1D	4.14	1.46	1.38
48	20	309	A86	C2-C1	4.13	1.41	1.35
37	B	501	CLA	CHD-C1D	4.13	1.46	1.38
48	41	215	A86	C21-C20	4.13	1.58	1.51
37	b	507	CLA	O2A-CGA	4.13	1.45	1.33
37	31	304	CLA	CHD-C1D	4.13	1.46	1.38
47	12	206	KC1	CHB-C1B	4.13	1.46	1.38
47	31	307	KC1	OBD-CAD	4.13	1.28	1.22
37	B	524	CLA	O2A-CGA	4.13	1.45	1.33
47	17	303	KC1	C1A-CHA	4.13	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	37	302	KC1	C1A-CHA	4.13	1.51	1.40
48	36	310	A86	C26-C27	4.13	1.41	1.35
48	37	309	A86	C2-C1	4.13	1.41	1.35
37	41	204	CLA	CHD-C4C	4.13	1.48	1.39
48	17	310	A86	C2-C1	4.13	1.41	1.35
48	17	320	A86	C7-C6	4.13	1.59	1.50
47	12	208	KC1	C1A-CHA	4.13	1.51	1.40
37	20	308	CLA	CHD-C1D	4.13	1.46	1.38
48	13	315	A86	C2-C1	4.13	1.41	1.35
48	21	211	A86	C5-C6	4.13	1.41	1.35
48	31	314	A86	C7-C6	4.13	1.59	1.50
48	37	312	A86	C2-C1	4.13	1.41	1.35
37	39	306	CLA	O2A-CGA	4.12	1.45	1.33
48	16	310	A86	O4-C38	4.12	1.44	1.35
37	16	309	CLA	CHD-C1D	4.12	1.46	1.38
48	13	311	A86	C26-C27	4.12	1.41	1.35
48	33	314	A86	C5-C6	4.12	1.41	1.35
37	a	407	CLA	C1D-ND	4.12	1.42	1.37
48	18	215	A86	C7-C6	4.12	1.59	1.50
37	B	502	CLA	CHD-C1D	4.12	1.46	1.38
37	A	405	CLA	C1D-ND	4.12	1.42	1.37
48	32	217	A86	C7-C6	4.12	1.59	1.50
37	39	310	CLA	CHD-C1D	4.12	1.46	1.38
37	b	504	CLA	C1D-ND	4.12	1.42	1.37
48	12	214	A86	C7-C6	4.12	1.59	1.50
48	14	312	A86	C7-C6	4.12	1.59	1.50
37	B	507	CLA	O2A-CGA	4.12	1.45	1.33
47	15	302	KC1	CHB-C1B	4.12	1.46	1.38
47	15	306	KC1	C1A-CHA	4.11	1.51	1.40
37	11	307	CLA	O2A-CGA	4.11	1.45	1.33
37	b	523	CLA	O2A-CGA	4.11	1.45	1.33
47	34	306	KC1	C1A-CHA	4.11	1.51	1.40
48	36	310	A86	O4-C38	4.11	1.44	1.35
37	34	308	CLA	CHD-C1D	4.11	1.46	1.38
48	14	312	A86	C19-C18	4.11	1.58	1.52
37	39	310	CLA	O2A-CGA	4.11	1.45	1.33
48	21	211	A86	C21-C20	4.11	1.58	1.51
48	37	319	A86	C7-C6	4.11	1.59	1.50
47	14	306	KC1	C1A-CHA	4.11	1.51	1.40
37	b	508	CLA	C1D-ND	4.11	1.42	1.37
37	c	512	CLA	C1D-ND	4.11	1.42	1.37
47	37	305	KC1	C1B-NB	-4.11	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	308	CLA	CHD-C1D	4.11	1.46	1.38
48	15	312	A86	O4-C38	4.11	1.44	1.35
48	40	211	A86	C2-C1	4.11	1.41	1.35
48	12	202	A86	C7-C6	4.11	1.59	1.50
48	32	203	A86	C7-C6	4.11	1.59	1.50
48	32	216	A86	C7-C6	4.11	1.59	1.50
37	B	504	CLA	C1D-ND	4.11	1.42	1.37
48	21	215	A86	C21-C20	4.11	1.58	1.51
48	38	212	A86	C21-C20	4.11	1.58	1.51
48	35	313	A86	C21-C20	4.10	1.58	1.51
47	12	208	KC1	OBD-CAD	4.10	1.28	1.22
48	34	311	A86	C17-C18	-4.10	1.46	1.52
48	12	215	A86	C7-C6	4.10	1.59	1.50
48	21	213	A86	C7-C6	4.10	1.59	1.50
37	38	211	CLA	CHD-C4C	4.10	1.48	1.39
47	17	305	KC1	C1B-NB	-4.10	1.32	1.37
48	17	315	A86	C2-C1	4.10	1.41	1.35
37	34	301	CLA	O2A-CGA	4.10	1.45	1.33
37	33	307	CLA	CHD-C1D	4.10	1.46	1.38
37	33	310	CLA	CHD-C4C	4.10	1.48	1.39
48	15	313	A86	C21-C20	4.10	1.58	1.51
48	38	214	A86	C17-C18	-4.10	1.46	1.52
48	38	215	A86	C7-C6	4.10	1.59	1.50
48	35	311	A86	C21-C20	4.10	1.58	1.51
37	b	509	CLA	O2A-CGA	4.10	1.45	1.33
48	32	215	A86	C7-C6	4.10	1.59	1.50
37	15	303	CLA	CHD-C4C	4.10	1.48	1.39
48	39	313	A86	C26-C27	4.10	1.41	1.35
37	32	210	CLA	O2A-CGA	4.10	1.45	1.33
48	16	311	A86	C7-C6	4.10	1.59	1.50
37	14	307	CLA	CHD-C1D	4.10	1.46	1.38
37	40	210	CLA	CHD-C1D	4.10	1.46	1.38
48	15	311	A86	C7-C6	4.10	1.59	1.50
48	18	213	A86	C21-C20	4.10	1.58	1.51
48	34	312	A86	C7-C6	4.10	1.59	1.50
47	36	304	KC1	C4D-ND	4.10	1.38	1.35
37	36	309	CLA	CHD-C1D	4.10	1.46	1.38
48	15	316	A86	C7-C6	4.10	1.59	1.50
48	18	214	A86	C21-C20	4.10	1.58	1.51
37	19	310	CLA	O2A-CGA	4.10	1.45	1.33
37	C	504	CLA	O2A-CGA	4.09	1.45	1.33
48	11	312	A86	C7-C6	4.09	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	512	CLA	C1D-ND	4.09	1.42	1.37
37	40	208	CLA	CHD-C1D	4.09	1.46	1.38
37	c	504	CLA	O2A-CGA	4.09	1.45	1.33
48	13	314	A86	C17-C18	-4.09	1.46	1.52
37	19	310	CLA	CHD-C1D	4.09	1.46	1.38
48	35	314	A86	C17-C18	-4.09	1.46	1.52
37	12	209	CLA	O2A-CGA	4.09	1.45	1.33
47	21	203	KC1	C4D-ND	4.09	1.38	1.35
48	31	315	A86	O4-C38	4.09	1.44	1.35
48	19	313	A86	C19-C18	4.09	1.58	1.52
48	11	315	A86	O4-C38	4.09	1.44	1.35
37	12	210	CLA	O2A-CGA	4.09	1.45	1.33
48	31	315	A86	C7-C6	4.09	1.59	1.50
48	16	310	A86	C26-C27	4.09	1.41	1.35
48	41	213	A86	C5-C6	4.09	1.41	1.35
37	15	301	CLA	CHD-C1D	4.09	1.46	1.38
37	16	306	CLA	CHD-C1D	4.09	1.46	1.38
37	35	301	CLA	CHD-C1D	4.09	1.46	1.38
48	18	215	A86	C21-C20	4.09	1.58	1.51
48	37	314	A86	C2-C1	4.09	1.41	1.35
48	18	214	A86	C17-C18	-4.09	1.46	1.52
37	B	516	CLA	O2A-CGA	4.08	1.45	1.33
37	B	508	CLA	O2A-CGA	4.08	1.45	1.33
48	41	215	A86	C5-C6	4.08	1.41	1.35
37	14	301	CLA	O2A-CGA	4.08	1.45	1.33
48	35	316	A86	C7-C6	4.08	1.59	1.50
37	35	303	CLA	CHD-C4C	4.08	1.48	1.39
48	32	214	A86	C7-C6	4.08	1.59	1.50
37	b	515	CLA	O2A-CGA	4.08	1.45	1.33
48	35	312	A86	O4-C38	4.08	1.44	1.35
48	12	213	A86	C7-C6	4.08	1.59	1.50
37	20	306	CLA	CHD-C1D	4.08	1.46	1.38
47	17	308	KC1	C1A-CHA	4.08	1.51	1.40
37	15	308	CLA	CHD-C1D	4.08	1.46	1.38
37	b	508	CLA	O2A-CGA	4.08	1.45	1.33
37	B	502	CLA	O2A-CGA	4.08	1.45	1.33
37	38	208	CLA	CHD-C1D	4.08	1.46	1.38
48	40	213	A86	C10-C11	4.08	1.46	1.34
48	11	313	A86	C26-C27	4.08	1.41	1.35
37	18	209	CLA	CHD-C1D	4.08	1.46	1.38
37	38	209	CLA	CHD-C1D	4.08	1.46	1.38
48	34	311	A86	C7-C6	4.08	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	20	311	A86	C10-C11	4.08	1.46	1.34
48	41	213	A86	C7-C6	4.08	1.59	1.50
37	38	204	CLA	CHD-C4C	4.08	1.48	1.39
37	B	515	CLA	O2A-CGA	4.08	1.45	1.33
37	18	204	CLA	CHD-C4C	4.08	1.48	1.39
48	31	312	A86	C7-C6	4.08	1.59	1.50
48	41	211	A86	C21-C20	4.08	1.58	1.51
48	36	311	A86	C7-C6	4.08	1.59	1.50
37	b	502	CLA	CHD-C1D	4.08	1.46	1.38
37	b	516	CLA	O2A-CGA	4.07	1.45	1.33
48	38	214	A86	C21-C20	4.07	1.58	1.51
48	37	319	A86	C26-C27	4.07	1.41	1.35
37	B	503	CLA	O2A-CGA	4.07	1.45	1.33
37	21	209	CLA	CHD-C4C	4.07	1.48	1.39
37	13	307	CLA	CHD-C1D	4.07	1.46	1.38
37	B	508	CLA	C1D-ND	4.07	1.42	1.37
48	40	213	A86	C17-C18	-4.07	1.46	1.52
37	B	509	CLA	O2A-CGA	4.07	1.45	1.33
48	21	214	A86	C17-C18	-4.07	1.46	1.52
48	21	211	A86	C9-C10	4.07	1.56	1.43
37	19	305	CLA	CHD-C1D	4.07	1.46	1.38
48	39	311	A86	C21-C20	4.07	1.58	1.51
37	31	306	CLA	CHD-C1D	4.07	1.46	1.38
37	39	309	CLA	CHD-C1D	4.07	1.46	1.38
37	A	403	CLA	CHD-C1D	4.07	1.46	1.38
37	c	508	CLA	C1D-ND	4.07	1.42	1.37
48	34	312	A86	C19-C18	4.07	1.58	1.52
48	37	312	A86	C7-C6	4.07	1.59	1.50
48	35	315	A86	C2-C1	4.07	1.41	1.35
47	37	307	KC1	C1A-CHA	4.07	1.51	1.40
48	12	213	A86	C21-C20	4.07	1.58	1.51
48	32	214	A86	C21-C20	4.07	1.58	1.51
48	15	319	A86	C2-C1	4.06	1.41	1.35
48	19	313	A86	C26-C27	4.06	1.41	1.35
48	34	311	A86	O4-C38	4.06	1.44	1.35
47	13	306	KC1	C1B-NB	-4.06	1.32	1.37
47	33	306	KC1	C1B-NB	-4.06	1.32	1.37
47	37	307	KC1	C4D-ND	4.06	1.38	1.35
48	12	216	A86	C17-C18	-4.06	1.46	1.52
47	32	209	KC1	OBD-CAD	4.06	1.28	1.22
48	16	310	A86	C21-C20	4.06	1.58	1.51
37	41	209	CLA	CHD-C4C	4.06	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	41	203	KC1	C1B-NB	-4.06	1.32	1.37
37	b	502	CLA	O2A-CGA	4.06	1.45	1.33
37	17	309	CLA	CHD-C4C	4.06	1.48	1.39
37	b	503	CLA	C1D-ND	4.06	1.42	1.37
37	12	205	CLA	CHD-C1D	4.06	1.46	1.38
37	32	211	CLA	O2A-CGA	4.06	1.45	1.33
47	20	305	KC1	C1B-NB	-4.06	1.32	1.37
48	38	215	A86	C21-C20	4.06	1.58	1.51
47	20	302	KC1	C1B-NB	-4.06	1.32	1.37
47	11	306	KC1	OBD-CAD	4.06	1.28	1.22
47	40	207	KC1	C1B-NB	-4.05	1.32	1.37
47	31	303	KC1	CHC-C4B	4.05	1.46	1.38
37	C	508	CLA	O2A-CGA	4.05	1.45	1.33
37	11	305	CLA	CHD-C1D	4.05	1.46	1.38
47	20	304	KC1	C1A-CHA	4.05	1.51	1.40
37	21	210	CLA	CHD-C4C	4.05	1.48	1.39
37	34	307	CLA	CHD-C1D	4.05	1.46	1.38
37	C	505	CLA	C1D-ND	4.05	1.42	1.37
37	21	205	CLA	CHD-C1D	4.05	1.46	1.38
47	40	204	KC1	C1B-NB	-4.05	1.32	1.37
37	41	205	CLA	CHD-C1D	4.05	1.46	1.38
48	36	310	A86	C21-C20	4.05	1.58	1.51
37	39	305	CLA	CHD-C1D	4.05	1.46	1.38
47	40	206	KC1	C1A-CHA	4.05	1.51	1.40
47	34	306	KC1	C4D-ND	4.05	1.38	1.35
48	14	311	A86	O4-C38	4.05	1.44	1.35
37	C	508	CLA	C1D-ND	4.05	1.42	1.37
37	c	508	CLA	O2A-CGA	4.05	1.45	1.33
48	41	211	A86	C9-C10	4.05	1.56	1.43
48	32	217	A86	C21-C20	4.05	1.58	1.51
37	b	503	CLA	O2A-CGA	4.05	1.45	1.33
48	32	217	A86	C2-C1	4.04	1.41	1.35
37	11	308	CLA	CHD-C1D	4.04	1.46	1.38
37	32	202	CLA	CHD-C1D	4.04	1.46	1.38
37	b	510	CLA	C1D-ND	4.04	1.42	1.37
48	13	315	A86	C21-C20	4.04	1.58	1.51
47	13	309	KC1	C4D-ND	4.04	1.38	1.35
47	33	309	KC1	C4D-ND	4.04	1.38	1.35
48	37	312	A86	C17-C18	-4.04	1.46	1.52
48	17	320	A86	C26-C27	4.04	1.41	1.35
37	a	403	CLA	CHD-C1D	4.04	1.46	1.38
48	33	315	A86	C9-C10	4.04	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	18	213	A86	C17-C18	-4.04	1.46	1.52
37	B	513	CLA	O2A-CGA	4.04	1.45	1.33
47	16	302	KC1	C1B-NB	-4.04	1.32	1.37
47	21	203	KC1	C1B-NB	-4.04	1.32	1.37
37	41	208	CLA	CHD-C4C	4.04	1.48	1.39
37	c	501	CLA	CHD-C1D	4.04	1.46	1.38
37	35	310	CLA	CHD-C4C	4.04	1.48	1.39
37	18	208	CLA	CHD-C1D	4.04	1.46	1.38
48	19	311	A86	C21-C20	4.03	1.58	1.51
48	34	316	A86	C2-C1	4.03	1.41	1.35
48	15	315	A86	C2-C1	4.03	1.41	1.35
37	19	309	CLA	CHD-C1D	4.03	1.46	1.38
48	38	212	A86	C10-C11	4.03	1.46	1.34
37	b	513	CLA	O2A-CGA	4.03	1.45	1.33
37	B	507	CLA	CHD-C1D	4.03	1.46	1.38
37	c	503	CLA	O2A-CGA	4.03	1.45	1.33
47	16	308	KC1	CHB-C1B	4.03	1.46	1.38
48	41	214	A86	C17-C18	-4.03	1.46	1.52
47	35	309	KC1	CHB-C1B	4.03	1.46	1.38
47	31	307	KC1	C1A-CHA	4.03	1.51	1.40
48	12	217	A86	C7-C6	4.03	1.59	1.50
47	35	309	KC1	C1B-NB	-4.03	1.32	1.37
47	37	304	KC1	C4D-ND	4.03	1.38	1.35
37	C	511	CLA	O2A-CGA	4.03	1.45	1.33
37	41	202	CLA	CHD-C4C	4.03	1.48	1.39
37	21	208	CLA	CHD-C4C	4.03	1.48	1.39
48	32	217	A86	C17-C18	-4.03	1.46	1.52
48	12	216	A86	C2-C1	4.03	1.41	1.35
47	18	210	KC1	CHB-C1B	4.03	1.46	1.38
48	13	312	A86	C21-C20	4.03	1.58	1.51
48	33	312	A86	C21-C20	4.03	1.58	1.51
37	13	310	CLA	CHD-C4C	4.03	1.48	1.39
47	38	210	KC1	CHB-C1B	4.03	1.46	1.38
48	11	312	A86	O4-C38	4.03	1.44	1.35
37	C	501	CLA	CHD-C1D	4.03	1.46	1.38
47	11	302	KC1	CHB-C1B	4.03	1.46	1.38
48	35	319	A86	C2-C1	4.03	1.41	1.35
47	14	306	KC1	C1B-NB	-4.02	1.32	1.37
47	34	306	KC1	C1B-NB	-4.02	1.32	1.37
48	15	314	A86	C21-C20	4.02	1.58	1.51
48	15	313	A86	C5-C6	4.02	1.41	1.35
48	35	313	A86	C5-C6	4.02	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	38	213	A86	C21-C20	4.02	1.58	1.51
37	41	210	CLA	CHD-C4C	4.02	1.48	1.39
48	21	214	A86	C21-C20	4.02	1.58	1.51
48	13	315	A86	C9-C10	4.02	1.55	1.43
37	38	201	CLA	CHD-C4C	4.02	1.48	1.39
47	11	302	KC1	CHC-C4B	4.02	1.46	1.38
37	b	507	CLA	CHD-C1D	4.02	1.46	1.38
37	21	206	CLA	CHD-C1D	4.02	1.46	1.38
47	31	303	KC1	CHB-C1B	4.02	1.46	1.38
47	11	302	KC1	C4B-NB	-4.02	1.32	1.37
47	31	303	KC1	C4B-NB	-4.02	1.32	1.37
37	36	307	CLA	CHD-C1D	4.02	1.46	1.38
37	19	304	CLA	CHD-C4C	4.02	1.48	1.39
48	39	311	A86	C2-C1	4.02	1.41	1.35
48	15	311	A86	C21-C20	4.02	1.58	1.51
37	B	503	CLA	C1D-ND	4.01	1.42	1.37
37	38	206	CLA	CHD-C4C	4.01	1.48	1.39
48	14	311	A86	C7-C6	4.01	1.59	1.50
47	12	208	KC1	CHB-C1B	4.01	1.46	1.38
47	32	209	KC1	CHB-C1B	4.01	1.46	1.38
48	21	215	A86	C5-C6	4.01	1.41	1.35
37	C	503	CLA	O2A-CGA	4.01	1.45	1.33
37	35	305	CLA	CHD-C4C	4.01	1.48	1.39
37	38	202	CLA	CHD-C1D	4.01	1.46	1.38
48	15	314	A86	C17-C18	-4.01	1.46	1.52
48	16	313	A86	C19-C18	4.01	1.58	1.52
47	15	309	KC1	C1B-NB	-4.01	1.32	1.37
37	13	303	CLA	CHD-C4C	4.01	1.48	1.39
37	37	301	CLA	CHD-C4C	4.01	1.48	1.39
48	17	311	A86	O4-C38	4.01	1.44	1.35
47	16	308	KC1	C1A-CHA	4.01	1.51	1.40
37	37	308	CLA	CHD-C4C	4.01	1.48	1.39
48	14	315	A86	C21-C20	4.01	1.58	1.51
37	B	510	CLA	C1D-ND	4.01	1.42	1.37
48	14	316	A86	C7-C6	4.01	1.59	1.50
48	12	220	A86	C21-C20	4.01	1.58	1.51
48	32	221	A86	C21-C20	4.01	1.58	1.51
47	11	302	KC1	C1A-CHA	4.01	1.51	1.40
47	12	206	KC1	C1A-CHA	4.01	1.51	1.40
37	B	504	CLA	C3B-C2B	4.01	1.45	1.40
48	41	214	A86	C21-C20	4.01	1.58	1.51
48	36	313	A86	C21-C20	4.00	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	31	303	KC1	C1A-CHA	4.00	1.51	1.40
37	18	203	CLA	CHD-C4C	4.00	1.48	1.39
47	36	308	KC1	C1A-CHA	4.00	1.51	1.40
37	c	511	CLA	O2A-CGA	4.00	1.45	1.33
48	34	316	A86	C7-C6	4.00	1.59	1.50
47	13	306	KC1	C1A-CHA	4.00	1.51	1.40
37	15	307	CLA	CHD-C1D	4.00	1.46	1.38
37	15	305	CLA	CHD-C4C	4.00	1.48	1.39
48	14	312	A86	C21-C20	4.00	1.58	1.51
48	34	312	A86	C21-C20	4.00	1.58	1.51
47	11	306	KC1	C1A-CHA	4.00	1.51	1.40
37	21	202	CLA	CHD-C4C	4.00	1.48	1.39
37	c	510	CLA	CHD-C1D	4.00	1.46	1.38
48	14	316	A86	C2-C1	4.00	1.41	1.35
48	15	314	A86	C9-C10	4.00	1.55	1.43
48	34	313	A86	C10-C11	4.00	1.46	1.34
37	32	206	CLA	CHD-C1D	3.99	1.46	1.38
48	12	216	A86	C21-C20	3.99	1.58	1.51
48	13	313	A86	C5-C6	3.99	1.41	1.35
48	33	313	A86	C5-C6	3.99	1.41	1.35
48	13	313	A86	C9-C10	3.99	1.55	1.43
48	33	313	A86	C9-C10	3.99	1.55	1.43
47	17	305	KC1	C4D-ND	3.99	1.38	1.35
37	C	510	CLA	O2A-CGA	3.99	1.45	1.33
48	32	218	A86	C7-C6	3.99	1.59	1.50
48	11	319	A86	C7-C6	3.99	1.59	1.50
37	b	504	CLA	CHD-C1D	3.99	1.46	1.38
48	35	312	A86	C21-C20	3.99	1.58	1.51
47	36	308	KC1	CHB-C1B	3.99	1.46	1.38
48	33	315	A86	C21-C20	3.99	1.58	1.51
37	35	307	CLA	CHD-C1D	3.99	1.46	1.38
37	33	305	CLA	CHD-C4C	3.99	1.48	1.39
48	31	312	A86	O4-C38	3.99	1.44	1.35
37	11	310	CLA	O2A-CGA	3.99	1.45	1.33
37	34	310	CLA	CHD-C4C	3.99	1.48	1.39
37	39	304	CLA	CHD-C4C	3.99	1.48	1.39
48	21	213	A86	C21-C20	3.99	1.58	1.51
48	35	313	A86	C10-C11	3.99	1.46	1.34
48	40	211	A86	C9-C10	3.99	1.55	1.43
48	40	213	A86	C9-C10	3.99	1.55	1.43
37	15	310	CLA	CHD-C4C	3.99	1.48	1.39
37	B	511	CLA	O2A-CGA	3.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	504	CLA	CHD-C1D	3.98	1.46	1.38
37	16	307	CLA	CHD-C1D	3.98	1.46	1.38
48	14	315	A86	O4-C38	3.98	1.44	1.35
48	34	315	A86	O4-C38	3.98	1.44	1.35
37	c	505	CLA	C1D-ND	3.98	1.42	1.37
37	16	303	CLA	CHD-C4C	3.98	1.48	1.39
48	20	311	A86	C17-C18	-3.98	1.46	1.52
48	33	314	A86	C17-C18	-3.98	1.46	1.52
37	14	310	CLA	CHD-C4C	3.98	1.48	1.39
47	33	306	KC1	C1A-CHA	3.98	1.51	1.40
48	16	314	A86	C21-C20	3.98	1.58	1.51
47	11	306	KC1	C4D-ND	3.98	1.38	1.35
47	31	307	KC1	C4D-ND	3.98	1.38	1.35
48	34	312	A86	C26-C27	3.98	1.41	1.35
48	12	217	A86	C2-C1	3.98	1.41	1.35
37	18	206	CLA	CHD-C4C	3.98	1.48	1.39
37	14	305	CLA	CHD-C4C	3.98	1.48	1.39
47	36	302	KC1	C1B-NB	-3.98	1.32	1.37
48	14	313	A86	C10-C11	3.98	1.46	1.34
47	38	205	KC1	C1A-CHA	3.98	1.51	1.40
37	C	510	CLA	CHD-C1D	3.98	1.46	1.38
48	20	311	A86	C9-C10	3.98	1.55	1.43
48	18	212	A86	C10-C11	3.98	1.46	1.34
37	c	510	CLA	O2A-CGA	3.98	1.45	1.33
37	41	206	CLA	CHD-C1D	3.97	1.46	1.38
47	18	205	KC1	C1A-CHA	3.97	1.51	1.40
47	20	305	KC1	C1A-CHA	3.97	1.51	1.40
37	33	303	CLA	CHD-C4C	3.97	1.48	1.39
47	32	207	KC1	C1A-CHA	3.97	1.51	1.40
37	12	203	CLA	O2A-CGA	3.97	1.45	1.33
37	31	310	CLA	O2A-CGA	3.97	1.45	1.33
48	20	309	A86	C9-C10	3.97	1.55	1.43
37	b	504	CLA	C3B-C2B	3.97	1.45	1.40
37	12	209	CLA	CHD-C1D	3.97	1.46	1.38
37	32	210	CLA	CHD-C1D	3.97	1.46	1.38
48	13	315	A86	C10-C11	3.97	1.46	1.34
48	15	313	A86	C10-C11	3.97	1.46	1.34
48	17	315	A86	C10-C11	3.97	1.46	1.34
48	37	314	A86	C10-C11	3.97	1.46	1.34
37	c	506	CLA	CHD-C1D	3.97	1.46	1.38
47	15	309	KC1	CHB-C1B	3.97	1.46	1.38
48	17	310	A86	C21-C20	3.97	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	17	313	A86	C17-C18	-3.97	1.46	1.52
37	b	511	CLA	O2A-CGA	3.97	1.44	1.33
48	14	311	A86	C21-C20	3.97	1.58	1.51
48	34	311	A86	C21-C20	3.97	1.58	1.51
47	21	207	KC1	C1A-CHA	3.97	1.51	1.40
47	40	207	KC1	C1A-CHA	3.97	1.51	1.40
48	31	319	A86	C7-C6	3.97	1.59	1.50
48	17	310	A86	C10-C11	3.97	1.46	1.34
48	33	315	A86	C10-C11	3.97	1.46	1.34
48	41	211	A86	C17-C18	-3.97	1.46	1.52
48	35	314	A86	C9-C10	3.97	1.55	1.43
48	34	315	A86	C21-C20	3.97	1.58	1.51
48	38	214	A86	C9-C10	3.97	1.55	1.43
37	36	303	CLA	CHD-C4C	3.96	1.48	1.39
48	12	202	A86	C26-C27	3.96	1.41	1.35
48	21	213	A86	C5-C6	3.96	1.41	1.35
48	40	201	A86	C19-C18	3.96	1.58	1.52
47	41	207	KC1	CHC-C1C	3.96	1.48	1.39
48	32	218	A86	C2-C1	3.96	1.41	1.35
47	17	306	KC1	CHC-C4B	3.96	1.46	1.38
47	37	305	KC1	CHC-C4B	3.96	1.46	1.38
37	13	305	CLA	CHD-C4C	3.96	1.48	1.39
48	37	309	A86	C21-C20	3.96	1.58	1.51
48	34	313	A86	C5-C6	3.96	1.41	1.35
48	21	211	A86	C17-C18	-3.96	1.46	1.52
47	15	302	KC1	C1A-CHA	3.96	1.51	1.40
48	15	312	A86	C21-C20	3.96	1.58	1.51
48	38	215	A86	C9-C10	3.96	1.55	1.43
47	35	302	KC1	C1A-CHA	3.96	1.51	1.40
48	38	215	A86	C5-C6	3.95	1.41	1.35
48	35	314	A86	C10-C11	3.95	1.46	1.34
48	21	213	A86	C9-C10	3.95	1.55	1.43
37	34	305	CLA	CHD-C4C	3.95	1.48	1.39
37	C	503	CLA	CHD-C1D	3.95	1.46	1.38
37	c	503	CLA	CHD-C1D	3.95	1.46	1.38
47	14	306	KC1	C4D-ND	3.95	1.38	1.35
48	11	313	A86	C2-C1	3.95	1.41	1.35
47	21	207	KC1	CHC-C1C	3.95	1.48	1.39
37	32	204	CLA	CHD-C1D	3.95	1.46	1.38
37	37	303	CLA	CHD-C4C	3.95	1.48	1.39
48	37	311	A86	C10-C11	3.95	1.46	1.34
37	D	401	CLA	CHD-C1D	3.95	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	17	304	CLA	CHD-C4C	3.95	1.48	1.39
37	a	404	CLA	CHD-C1D	3.95	1.46	1.38
48	35	319	A86	C21-C20	3.94	1.58	1.51
37	c	507	CLA	C1D-ND	3.94	1.42	1.37
37	12	203	CLA	CHD-C1D	3.94	1.46	1.38
47	41	207	KC1	C1A-CHA	3.94	1.51	1.40
48	20	309	A86	C5-C6	3.94	1.41	1.35
47	16	308	KC1	C4D-ND	3.94	1.38	1.35
48	31	312	A86	C26-C27	3.94	1.41	1.35
48	37	309	A86	C10-C11	3.94	1.46	1.34
47	13	304	KC1	C1B-NB	-3.94	1.32	1.37
37	C	506	CLA	CHD-C1D	3.94	1.46	1.38
37	40	209	CLA	CHD-C4C	3.94	1.48	1.39
47	33	302	KC1	C4B-NB	-3.94	1.32	1.37
48	31	313	A86	O4-C38	3.94	1.44	1.35
48	15	319	A86	C21-C20	3.94	1.58	1.51
48	40	211	A86	C5-C6	3.94	1.41	1.35
37	38	203	CLA	CHD-C4C	3.94	1.48	1.39
48	33	314	A86	C10-C11	3.94	1.46	1.34
37	D	406	CLA	CHD-C1D	3.94	1.46	1.38
37	19	301	CLA	CHD-C1D	3.94	1.46	1.38
37	39	301	CLA	CHD-C1D	3.94	1.46	1.38
48	19	311	A86	C2-C1	3.94	1.41	1.35
48	11	311	A86	C7-C6	3.94	1.59	1.50
48	31	311	A86	C7-C6	3.94	1.59	1.50
48	35	315	A86	C21-C20	3.94	1.58	1.51
37	C	507	CLA	C1D-ND	3.94	1.42	1.37
48	14	313	A86	C5-C6	3.94	1.41	1.35
37	32	204	CLA	O2A-CGA	3.94	1.44	1.33
47	19	308	KC1	C1B-NB	-3.93	1.32	1.37
37	16	309	CLA	CHD-C4C	3.93	1.48	1.39
48	15	314	A86	C10-C11	3.93	1.46	1.34
47	20	304	KC1	C1B-NB	-3.93	1.32	1.37
47	33	304	KC1	C1B-NB	-3.93	1.32	1.37
48	37	310	A86	O4-C38	3.93	1.44	1.35
37	18	211	CLA	CHD-C4C	3.93	1.48	1.39
48	33	314	A86	C9-C10	3.93	1.55	1.43
47	33	304	KC1	C1A-CHA	3.93	1.51	1.40
47	13	304	KC1	C1A-CHA	3.93	1.51	1.40
37	36	309	CLA	CHD-C4C	3.93	1.48	1.39
37	a	407	CLA	CHD-C1D	3.93	1.46	1.38
47	32	212	KC1	OBD-CAD	3.93	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	36	311	A86	C2-C1	3.93	1.41	1.35
48	41	213	A86	C21-C20	3.93	1.58	1.51
37	A	405	CLA	CHD-C1D	3.93	1.46	1.38
37	C	501	CLA	O2A-CGA	3.93	1.44	1.33
48	17	315	A86	C9-C10	3.93	1.55	1.43
48	33	311	A86	C21-C20	3.93	1.58	1.51
37	14	303	CLA	CHD-C4C	3.92	1.48	1.39
37	B	515	CLA	CHD-C1D	3.92	1.46	1.38
48	20	309	A86	C17-C18	-3.92	1.46	1.52
48	41	213	A86	C9-C10	3.92	1.55	1.43
47	17	308	KC1	CHB-C1B	3.92	1.46	1.38
48	37	314	A86	C9-C10	3.92	1.55	1.43
48	14	312	A86	C26-C27	3.92	1.41	1.35
48	31	312	A86	C17-C18	-3.92	1.46	1.52
37	20	307	CLA	CHD-C4C	3.92	1.48	1.39
37	11	308	CLA	O2A-CGA	3.92	1.44	1.33
48	13	314	A86	C10-C11	3.92	1.45	1.34
47	14	304	KC1	C4D-ND	3.92	1.38	1.35
47	34	304	KC1	C4D-ND	3.92	1.38	1.35
47	34	304	KC1	C1B-NB	-3.92	1.33	1.37
48	33	314	A86	C21-C20	3.92	1.58	1.51
48	11	312	A86	C17-C18	-3.92	1.46	1.52
37	13	308	CLA	CHD-C4C	3.92	1.48	1.39
47	14	309	KC1	OBD-CAD	3.92	1.27	1.22
47	11	304	KC1	C1A-CHA	3.92	1.51	1.40
47	31	309	KC1	C1A-CHA	3.91	1.51	1.40
48	17	311	A86	C21-C20	3.91	1.58	1.51
48	11	314	A86	C2-C1	3.91	1.41	1.35
47	13	302	KC1	C1B-NB	-3.91	1.33	1.37
47	33	302	KC1	C1B-NB	-3.91	1.33	1.37
37	41	205	CLA	CHD-C4C	3.91	1.48	1.39
48	18	214	A86	C9-C10	3.91	1.55	1.43
48	13	314	A86	C9-C10	3.91	1.55	1.43
48	21	213	A86	C10-C11	3.91	1.45	1.34
48	38	213	A86	C10-C11	3.91	1.45	1.34
48	18	215	A86	C9-C10	3.91	1.55	1.43
48	37	313	A86	C2-C1	3.91	1.41	1.35
47	34	309	KC1	OBD-CAD	3.91	1.27	1.22
47	11	309	KC1	C1A-CHA	3.91	1.51	1.40
48	35	319	A86	C17-C18	-3.91	1.46	1.52
37	35	308	CLA	CHD-C4C	3.91	1.48	1.39
47	16	304	KC1	C1A-CHA	3.91	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	36	304	KC1	C1A-CHA	3.91	1.51	1.40
37	34	301	CLA	CHD-C1D	3.91	1.46	1.38
48	20	309	A86	C10-C11	3.91	1.45	1.34
37	B	514	CLA	C1D-ND	3.91	1.42	1.37
47	39	308	KC1	C4D-ND	3.91	1.38	1.35
48	41	213	A86	C10-C11	3.91	1.45	1.34
47	33	309	KC1	CHB-C1B	3.91	1.46	1.38
37	d	404	CLA	CHD-C1D	3.91	1.46	1.38
48	12	217	A86	C9-C10	3.91	1.55	1.43
47	41	203	KC1	C1A-CHA	3.90	1.51	1.40
47	36	308	KC1	C4D-ND	3.90	1.38	1.35
48	17	312	A86	C10-C11	3.90	1.45	1.34
37	32	202	CLA	O2A-CGA	3.90	1.44	1.33
37	d	403	CLA	O2A-CGA	3.90	1.44	1.33
48	34	314	A86	C19-C18	3.90	1.57	1.52
47	41	207	KC1	C1B-NB	-3.90	1.33	1.37
48	34	316	A86	C21-C20	3.90	1.57	1.51
48	40	213	A86	C19-C18	3.90	1.57	1.52
37	C	513	CLA	CHD-C1D	3.90	1.46	1.38
48	33	311	A86	C2-C1	3.90	1.41	1.35
48	17	313	A86	C21-C20	3.90	1.57	1.51
37	c	501	CLA	O2A-CGA	3.90	1.44	1.33
48	12	202	A86	C21-C20	3.90	1.57	1.51
48	31	319	A86	C21-C20	3.90	1.57	1.51
48	32	203	A86	C26-C27	3.90	1.40	1.35
48	14	314	A86	C19-C18	3.90	1.57	1.52
37	19	302	CLA	CHD-C4C	3.90	1.48	1.39
48	31	314	A86	C2-C1	3.90	1.40	1.35
48	16	311	A86	C2-C1	3.89	1.40	1.35
48	38	214	A86	C10-C11	3.89	1.45	1.34
48	40	211	A86	C17-C18	-3.89	1.46	1.52
48	40	201	A86	C21-C20	3.89	1.57	1.51
37	W	101	CLA	CHD-C1D	3.89	1.45	1.38
47	39	308	KC1	C1B-NB	-3.89	1.33	1.37
47	21	203	KC1	C1A-CHA	3.89	1.51	1.40
48	14	313	A86	C9-C10	3.89	1.55	1.43
37	B	510	CLA	O2A-CGA	3.89	1.44	1.33
37	33	308	CLA	CHD-C4C	3.89	1.48	1.39
37	D	405	CLA	O2A-CGA	3.89	1.44	1.33
37	b	514	CLA	C1D-ND	3.88	1.42	1.37
37	39	302	CLA	CHD-C4C	3.88	1.48	1.39
47	40	206	KC1	C1B-NB	-3.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	11	312	A86	C26-C27	3.88	1.40	1.35
37	b	510	CLA	O2A-CGA	3.88	1.44	1.33
48	13	313	A86	C10-C11	3.88	1.45	1.34
48	33	313	A86	C10-C11	3.88	1.45	1.34
48	13	311	A86	C2-C1	3.88	1.40	1.35
48	40	211	A86	C10-C11	3.88	1.45	1.34
37	b	515	CLA	CHD-C1D	3.88	1.45	1.38
47	34	309	KC1	C1A-CHA	3.88	1.51	1.40
47	13	302	KC1	C4B-NB	-3.88	1.33	1.37
48	38	212	A86	O4-C38	3.88	1.44	1.35
37	b	512	CLA	O2A-CGA	3.88	1.44	1.33
47	32	212	KC1	C1A-CHA	3.88	1.51	1.40
37	16	301	CLA	CHD-C1D	3.88	1.45	1.38
48	13	311	A86	C21-C20	3.88	1.57	1.51
48	32	218	A86	C9-C10	3.88	1.55	1.43
48	11	312	A86	C2-C1	3.88	1.40	1.35
48	14	316	A86	C9-C10	3.88	1.55	1.43
48	34	316	A86	C9-C10	3.88	1.55	1.43
47	41	207	KC1	CHB-C1B	3.88	1.45	1.38
47	20	302	KC1	C1A-CHA	3.88	1.51	1.40
50	40	212	DD6	C35-C34	3.88	1.58	1.52
47	36	305	KC1	C1B-NB	-3.88	1.33	1.37
46	f	101	HEM	C3C-C2C	-3.88	1.35	1.40
47	37	307	KC1	CHB-C1B	3.88	1.45	1.38
37	21	205	CLA	CHD-C4C	3.87	1.48	1.39
47	31	309	KC1	C4B-NB	-3.87	1.33	1.37
37	33	310	CLA	C3D-C2D	3.87	1.49	1.39
37	12	207	CLA	CHD-C4C	3.87	1.48	1.39
37	B	512	CLA	O2A-CGA	3.87	1.44	1.33
48	34	313	A86	C9-C10	3.87	1.55	1.43
47	13	309	KC1	CHB-C1B	3.87	1.45	1.38
47	14	304	KC1	C1B-NB	-3.87	1.33	1.37
37	w	101	CLA	CHD-C1D	3.87	1.45	1.38
37	C	509	CLA	CHD-C1D	3.87	1.45	1.38
37	31	310	CLA	CHD-C1D	3.87	1.45	1.38
47	37	304	KC1	C1B-NB	-3.87	1.33	1.37
48	37	312	A86	C21-C20	3.87	1.57	1.51
48	11	313	A86	O4-C38	3.87	1.43	1.35
48	38	212	A86	C9-C10	3.87	1.55	1.43
47	19	308	KC1	C4D-ND	3.87	1.38	1.35
47	13	309	KC1	C1A-CHA	3.87	1.51	1.40
47	33	309	KC1	C1A-CHA	3.87	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	508	CLA	CHD-C1D	3.87	1.45	1.38
37	36	301	CLA	CHD-C1D	3.87	1.45	1.38
47	31	305	KC1	C1A-CHA	3.87	1.51	1.40
48	32	216	A86	C9-C10	3.86	1.55	1.43
47	21	207	KC1	C1B-NB	-3.86	1.33	1.37
48	14	316	A86	C21-C20	3.86	1.57	1.51
50	20	310	DD6	C35-C34	3.86	1.58	1.52
37	c	509	CLA	CHD-C1D	3.86	1.45	1.38
37	37	306	CLA	CHD-C4C	3.86	1.48	1.39
47	40	204	KC1	C1A-CHA	3.86	1.51	1.40
37	34	303	CLA	CHD-C4C	3.86	1.48	1.39
37	c	513	CLA	CHD-C1D	3.86	1.45	1.38
47	14	309	KC1	C1A-CHA	3.86	1.50	1.40
48	17	310	A86	C17-C18	-3.86	1.46	1.52
48	12	215	A86	C9-C10	3.86	1.55	1.43
37	39	310	CLA	CHD-C4C	3.86	1.48	1.39
48	14	315	A86	C9-C10	3.86	1.55	1.43
48	34	315	A86	C9-C10	3.86	1.55	1.43
37	c	504	CLA	CHD-C4C	3.86	1.48	1.39
47	40	204	KC1	C4D-ND	3.86	1.38	1.35
37	15	308	CLA	CHD-C4C	3.86	1.48	1.39
46	f	101	HEM	C3C-CAC	3.86	1.55	1.47
37	19	303	CLA	CHD-C4C	3.85	1.48	1.39
48	16	310	A86	C2-C1	3.85	1.40	1.35
48	37	309	A86	C9-C10	3.85	1.55	1.43
37	14	301	CLA	CHD-C1D	3.85	1.45	1.38
48	11	319	A86	C21-C20	3.85	1.57	1.51
37	17	307	CLA	CHD-C4C	3.85	1.48	1.39
48	15	319	A86	C17-C18	-3.85	1.46	1.52
37	19	310	CLA	CHD-C4C	3.85	1.48	1.39
48	15	311	A86	C10-C11	3.85	1.45	1.34
37	15	301	CLA	CHD-C4C	3.85	1.48	1.39
48	16	311	A86	O4-C38	3.85	1.43	1.35
37	39	303	CLA	CHD-C4C	3.85	1.48	1.39
37	b	506	CLA	C1D-ND	3.85	1.42	1.37
37	c	505	CLA	O2A-CGA	3.85	1.44	1.33
48	35	311	A86	C10-C11	3.85	1.45	1.34
48	37	309	A86	C17-C18	-3.85	1.46	1.52
48	14	314	A86	C17-C18	-3.85	1.46	1.52
48	34	314	A86	C17-C18	-3.85	1.46	1.52
48	12	217	A86	C21-C20	3.85	1.57	1.51
48	37	309	A86	C19-C18	3.84	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	13	301	CLA	CHD-C4C	3.84	1.48	1.39
47	18	210	KC1	C1B-NB	-3.84	1.33	1.37
48	16	314	A86	C26-C27	3.84	1.40	1.35
48	18	212	A86	O4-C38	3.84	1.43	1.35
48	36	311	A86	O4-C38	3.84	1.43	1.35
37	C	504	CLA	CHD-C4C	3.84	1.48	1.39
48	18	212	A86	C9-C10	3.84	1.55	1.43
37	z	102	CLA	CHD-C4C	3.84	1.48	1.39
48	20	311	A86	C19-C18	3.84	1.57	1.52
48	32	203	A86	C21-C20	3.84	1.57	1.51
37	35	301	CLA	CHD-C4C	3.84	1.48	1.39
47	12	211	KC1	C4D-ND	3.84	1.38	1.35
37	a	404	CLA	CHD-C4C	3.84	1.48	1.39
47	12	211	KC1	C1A-CHA	3.84	1.50	1.40
48	17	310	A86	C9-C10	3.84	1.55	1.43
37	D	402	CLA	CHD-C4C	3.84	1.48	1.39
47	20	302	KC1	C4D-ND	3.84	1.38	1.35
37	Z	102	CLA	CHD-C4C	3.83	1.48	1.39
48	36	310	A86	C2-C1	3.83	1.40	1.35
48	15	313	A86	C9-C10	3.83	1.55	1.43
37	C	505	CLA	O2A-CGA	3.83	1.44	1.33
48	15	315	A86	C21-C20	3.83	1.57	1.51
37	32	208	CLA	CHD-C4C	3.83	1.48	1.39
47	13	302	KC1	C1A-CHA	3.83	1.50	1.40
47	33	302	KC1	C1A-CHA	3.83	1.50	1.40
37	17	302	CLA	CHD-C4C	3.83	1.48	1.39
46	F	101	HEM	C3C-CAC	3.83	1.55	1.47
47	16	305	KC1	C1B-NB	-3.83	1.33	1.37
47	12	211	KC1	OBD-CAD	3.83	1.27	1.22
37	B	506	CLA	C1D-ND	3.83	1.42	1.37
48	16	313	A86	C21-C20	3.83	1.57	1.51
47	20	302	KC1	CHB-C1B	3.83	1.45	1.38
37	C	502	CLA	O2A-CGA	3.83	1.44	1.33
47	15	304	KC1	C1A-CHA	3.82	1.50	1.40
37	11	310	CLA	CHD-C1D	3.82	1.45	1.38
37	21	206	CLA	CHD-C4C	3.82	1.48	1.39
48	31	319	A86	C2-C1	3.82	1.40	1.35
47	14	309	KC1	C4D-ND	3.82	1.38	1.35
46	F	101	HEM	C3C-C2C	-3.82	1.35	1.40
48	11	312	A86	C21-C20	3.82	1.57	1.51
37	b	505	CLA	CHD-C1D	3.82	1.45	1.38
47	21	207	KC1	CHB-C1B	3.82	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	21	214	A86	C19-C18	3.82	1.57	1.52
37	z	102	CLA	OBD-CAD	3.82	1.29	1.22
37	41	210	CLA	C3D-C2D	3.82	1.49	1.39
37	B	514	CLA	CHD-C1D	3.82	1.45	1.38
48	17	320	A86	C2-C1	3.82	1.40	1.35
37	B	508	CLA	CHD-C1D	3.82	1.45	1.38
37	34	302	CLA	CHD-C4C	3.82	1.47	1.39
48	32	216	A86	C21-C20	3.81	1.57	1.51
37	C	502	CLA	CHD-C1D	3.81	1.45	1.38
37	33	301	CLA	CHD-C4C	3.81	1.47	1.39
48	11	314	A86	C21-C20	3.81	1.57	1.51
47	40	204	KC1	CHB-C1B	3.81	1.45	1.38
37	38	209	CLA	C3D-C2D	3.81	1.49	1.39
47	16	304	KC1	C1B-NB	-3.81	1.33	1.37
37	B	505	CLA	CHD-C1D	3.81	1.45	1.38
37	14	308	CLA	CHD-C4C	3.81	1.47	1.39
37	18	201	CLA	CHD-C4C	3.81	1.47	1.39
37	c	502	CLA	O2A-CGA	3.81	1.44	1.33
47	31	303	KC1	C4D-ND	3.81	1.38	1.35
37	40	203	CLA	CHD-C4C	3.81	1.47	1.39
47	35	304	KC1	C1A-CHA	3.81	1.50	1.40
37	32	210	CLA	C1B-NB	-3.81	1.31	1.35
37	39	309	CLA	CHD-C4C	3.81	1.47	1.39
48	14	314	A86	C21-C20	3.81	1.57	1.51
48	31	314	A86	C21-C20	3.81	1.57	1.51
37	C	504	CLA	CHD-C1D	3.81	1.45	1.38
37	c	504	CLA	CHD-C1D	3.81	1.45	1.38
48	17	314	A86	C9-C10	3.81	1.55	1.43
48	37	313	A86	C9-C10	3.81	1.55	1.43
48	11	319	A86	C2-C1	3.81	1.40	1.35
48	36	311	A86	C26-C27	3.81	1.40	1.35
48	14	314	A86	C9-C10	3.81	1.55	1.43
48	35	313	A86	C9-C10	3.81	1.55	1.43
48	12	202	A86	C10-C11	3.81	1.45	1.34
48	37	311	A86	C21-C20	3.81	1.57	1.51
37	11	301	CLA	O2A-CGA	3.81	1.44	1.33
48	35	316	A86	C5-C6	3.80	1.40	1.35
48	11	311	A86	C2-C1	3.80	1.40	1.35
48	37	319	A86	C2-C1	3.80	1.40	1.35
37	40	210	CLA	CHD-C4C	3.80	1.47	1.39
48	32	203	A86	C10-C11	3.80	1.45	1.34
48	17	314	A86	C10-C11	3.80	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	18	202	CLA	CHD-C4C	3.80	1.47	1.39
37	b	504	CLA	O2A-CGA	3.80	1.44	1.33
48	12	215	A86	C10-C11	3.80	1.45	1.34
37	B	504	CLA	O2A-CGA	3.80	1.44	1.33
37	41	206	CLA	CHD-C4C	3.80	1.47	1.39
37	C	511	CLA	CHD-C1D	3.80	1.45	1.38
37	B	511	CLA	CHD-C1D	3.80	1.45	1.38
47	12	211	KC1	CHB-C1B	3.80	1.45	1.38
47	32	212	KC1	CHB-C1B	3.80	1.45	1.38
37	D	401	CLA	CHD-C4C	3.80	1.47	1.39
48	33	314	A86	C19-C18	3.80	1.57	1.52
48	13	314	A86	C21-C20	3.79	1.57	1.51
48	37	313	A86	C10-C11	3.79	1.45	1.34
47	18	207	KC1	C1B-NB	-3.79	1.33	1.37
37	12	210	CLA	CHD-C4C	3.79	1.47	1.39
37	c	502	CLA	CHD-C1D	3.79	1.45	1.38
48	12	215	A86	C21-C20	3.79	1.57	1.51
37	21	210	CLA	C3D-C2D	3.79	1.49	1.39
48	18	213	A86	C19-C18	3.79	1.57	1.52
37	18	209	CLA	C3D-C2D	3.79	1.49	1.39
37	14	302	CLA	CHD-C4C	3.79	1.47	1.39
37	c	511	CLA	CHD-C1D	3.79	1.45	1.38
37	31	302	CLA	O2A-CGA	3.79	1.44	1.33
37	z	101	CLA	CHD-C4C	3.79	1.47	1.39
47	14	304	KC1	C1A-CHA	3.79	1.50	1.40
47	34	304	KC1	C1A-CHA	3.79	1.50	1.40
37	32	213	CLA	CHD-C4C	3.79	1.47	1.39
37	40	208	CLA	CHD-C4C	3.79	1.47	1.39
48	17	314	A86	C2-C1	3.79	1.40	1.35
48	38	214	A86	C19-C18	3.79	1.57	1.52
37	16	306	CLA	CHD-C4C	3.79	1.47	1.39
37	W	102	CLA	CHD-C4C	3.79	1.47	1.39
37	31	304	CLA	CHD-C4C	3.79	1.47	1.39
48	17	310	A86	C19-C18	3.79	1.57	1.52
48	34	314	A86	C9-C10	3.78	1.55	1.43
48	15	312	A86	C9-C10	3.78	1.55	1.43
48	36	313	A86	C26-C27	3.78	1.40	1.35
48	13	312	A86	C9-C10	3.78	1.55	1.43
48	15	314	A86	C19-C18	3.78	1.57	1.52
37	b	502	CLA	CHD-C4C	3.78	1.47	1.39
48	31	312	A86	C21-C20	3.78	1.57	1.51
37	d	401	CLA	CHD-C4C	3.78	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	37	313	A86	C26-C27	3.78	1.40	1.35
48	35	312	A86	C10-C11	3.78	1.45	1.34
37	37	308	CLA	OBD-CAD	3.78	1.29	1.22
37	Z	102	CLA	OBD-CAD	3.78	1.29	1.22
37	15	303	CLA	C3D-C2D	3.78	1.49	1.39
37	15	307	CLA	C3D-C2D	3.78	1.49	1.39
48	34	311	A86	C26-C27	3.78	1.40	1.35
37	12	212	CLA	CHD-C4C	3.78	1.47	1.39
37	20	308	CLA	CHD-C4C	3.78	1.47	1.39
37	38	202	CLA	CHD-C4C	3.77	1.47	1.39
37	b	514	CLA	CHD-C1D	3.77	1.45	1.38
37	12	209	CLA	C1B-NB	-3.77	1.31	1.35
37	15	307	CLA	CHD-C4C	3.77	1.47	1.39
37	19	309	CLA	CHD-C4C	3.77	1.47	1.39
37	b	503	CLA	CHD-C1D	3.77	1.45	1.38
37	b	511	CLA	CHD-C1D	3.77	1.45	1.38
37	20	301	CLA	CHD-C4C	3.77	1.47	1.39
37	36	306	CLA	CHD-C4C	3.77	1.47	1.39
37	B	503	CLA	CHD-C1D	3.77	1.45	1.38
37	15	308	CLA	C3D-C2D	3.77	1.49	1.39
48	14	312	A86	C2-C1	3.77	1.40	1.35
48	31	312	A86	C2-C1	3.77	1.40	1.35
48	15	312	A86	C10-C11	3.77	1.45	1.34
48	17	312	A86	C9-C10	3.77	1.55	1.43
48	13	314	A86	C19-C18	3.77	1.57	1.52
37	B	501	CLA	CHD-C4C	3.77	1.47	1.39
48	12	202	A86	C9-C10	3.77	1.55	1.43
37	15	305	CLA	C3D-C2D	3.77	1.49	1.39
48	32	216	A86	C10-C11	3.77	1.45	1.34
37	20	307	CLA	OBD-CAD	3.77	1.29	1.22
48	17	312	A86	C21-C20	3.77	1.57	1.51
47	11	309	KC1	C4B-NB	-3.77	1.33	1.37
47	15	302	KC1	C1B-NB	-3.77	1.33	1.37
37	38	211	CLA	C3D-C2D	3.77	1.49	1.39
50	21	216	DD6	C35-C34	3.77	1.58	1.52
48	37	311	A86	C9-C10	3.76	1.55	1.43
37	35	305	CLA	C3D-C2D	3.76	1.49	1.39
37	b	501	CLA	CHD-C4C	3.76	1.47	1.39
48	16	311	A86	C26-C27	3.76	1.40	1.35
37	17	309	CLA	OBD-CAD	3.76	1.29	1.22
37	38	203	CLA	OBD-CAD	3.76	1.29	1.22
37	39	301	CLA	CHD-C4C	3.76	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	13	303	CLA	C3D-C2D	3.76	1.49	1.39
37	32	211	CLA	CHD-C4C	3.76	1.47	1.39
50	41	212	DD6	C35-C34	3.76	1.58	1.52
48	41	214	A86	C19-C18	3.76	1.57	1.52
37	B	502	CLA	CHD-C4C	3.76	1.47	1.39
37	20	306	CLA	CHD-C4C	3.76	1.47	1.39
37	35	307	CLA	C3D-C2D	3.76	1.49	1.39
47	18	205	KC1	C1B-NB	-3.76	1.33	1.37
48	33	312	A86	C9-C10	3.76	1.55	1.43
37	A	403	CLA	O2A-CGA	3.76	1.44	1.33
37	11	303	CLA	CHD-C4C	3.76	1.47	1.39
47	36	304	KC1	C1B-NB	-3.76	1.33	1.37
47	35	302	KC1	C1B-NB	-3.76	1.33	1.37
48	32	218	A86	C21-C20	3.76	1.57	1.51
48	18	213	A86	C10-C11	3.76	1.45	1.34
48	33	311	A86	C10-C11	3.76	1.45	1.34
48	32	203	A86	C9-C10	3.76	1.55	1.43
48	18	214	A86	C10-C11	3.76	1.45	1.34
48	38	215	A86	C10-C11	3.76	1.45	1.34
37	41	204	CLA	C3D-C2D	3.76	1.49	1.39
48	21	211	A86	C19-C18	3.76	1.57	1.52
37	20	303	CLA	CHD-C1D	3.75	1.45	1.38
37	40	209	CLA	OBD-CAD	3.75	1.28	1.22
37	a	403	CLA	O2A-CGA	3.75	1.44	1.33
48	18	215	A86	C17-C18	-3.75	1.46	1.52
37	Z	101	CLA	CHD-C4C	3.75	1.47	1.39
48	34	314	A86	C21-C20	3.75	1.57	1.51
48	14	314	A86	C5-C6	3.75	1.40	1.35
48	34	314	A86	C5-C6	3.75	1.40	1.35
37	b	516	CLA	CHD-C1D	3.75	1.45	1.38
37	40	209	CLA	C3D-C2D	3.75	1.49	1.39
37	34	308	CLA	CHD-C4C	3.75	1.47	1.39
48	37	310	A86	C21-C20	3.75	1.57	1.51
47	32	212	KC1	C4D-ND	3.75	1.38	1.35
37	20	307	CLA	C3D-C2D	3.75	1.49	1.39
37	33	303	CLA	C3D-C2D	3.75	1.49	1.39
48	35	312	A86	C9-C10	3.75	1.55	1.43
37	C	503	CLA	CHD-C4C	3.75	1.47	1.39
48	13	311	A86	C9-C10	3.75	1.55	1.43
48	33	311	A86	C9-C10	3.75	1.55	1.43
37	B	516	CLA	CHD-C1D	3.75	1.45	1.38
48	40	211	A86	C19-C18	3.75	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	13	313	A86	C21-C20	3.75	1.57	1.51
47	38	210	KC1	C1B-NB	-3.75	1.33	1.37
47	13	302	KC1	CHB-C1B	3.75	1.45	1.38
50	41	216	DD6	C35-C34	3.75	1.58	1.52
48	13	312	A86	C10-C11	3.74	1.45	1.34
48	33	312	A86	C10-C11	3.74	1.45	1.34
37	c	503	CLA	CHD-C4C	3.74	1.47	1.39
48	35	316	A86	C9-C10	3.74	1.55	1.43
48	13	311	A86	C10-C11	3.74	1.45	1.34
48	39	311	A86	C9-C10	3.74	1.55	1.43
37	31	301	CLA	CHD-C4C	3.74	1.47	1.39
48	35	311	A86	C9-C10	3.74	1.55	1.43
48	37	319	A86	C10-C11	3.74	1.45	1.34
37	b	507	CLA	CHD-C4C	3.74	1.47	1.39
37	17	309	CLA	C3D-C2D	3.74	1.49	1.39
37	21	204	CLA	C3D-C2D	3.74	1.49	1.39
48	31	311	A86	C2-C1	3.74	1.40	1.35
37	15	310	CLA	OBD-CAD	3.74	1.28	1.22
37	35	307	CLA	CHD-C4C	3.74	1.47	1.39
48	35	315	A86	C9-C10	3.74	1.55	1.43
48	18	215	A86	C5-C6	3.74	1.40	1.35
37	c	508	CLA	C3D-C2D	3.74	1.49	1.39
37	C	508	CLA	C3D-C2D	3.74	1.49	1.39
37	31	308	CLA	CHD-C1D	3.74	1.45	1.38
37	19	301	CLA	CHD-C4C	3.73	1.47	1.39
37	19	307	CLA	CHD-C4C	3.73	1.47	1.39
37	20	306	CLA	C3D-C2D	3.73	1.49	1.39
48	11	315	A86	C21-C20	3.73	1.57	1.51
48	31	315	A86	C21-C20	3.73	1.57	1.51
37	35	303	CLA	C3D-C2D	3.73	1.49	1.39
37	11	307	CLA	CHD-C1D	3.73	1.45	1.38
48	15	316	A86	C5-C6	3.73	1.40	1.35
37	c	508	CLA	CHD-C1D	3.73	1.45	1.38
37	18	208	CLA	CHD-C4C	3.73	1.47	1.39
37	35	303	CLA	OBD-CAD	3.73	1.28	1.22
37	18	211	CLA	C3D-C2D	3.73	1.49	1.39
48	41	214	A86	C9-C10	3.73	1.55	1.43
37	40	205	CLA	CHD-C1D	3.73	1.45	1.38
48	17	313	A86	C9-C10	3.73	1.55	1.43
48	41	211	A86	C19-C18	3.73	1.57	1.52
37	39	307	CLA	CHD-C4C	3.73	1.47	1.39
37	B	507	CLA	CHD-C4C	3.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	15	303	CLA	OBD-CAD	3.73	1.28	1.22
37	21	208	CLA	OBD-CAD	3.73	1.28	1.22
37	21	209	CLA	C3D-C2D	3.73	1.49	1.39
37	11	301	CLA	CHD-C1D	3.73	1.45	1.38
37	31	302	CLA	CHD-C1D	3.73	1.45	1.38
37	39	302	CLA	C3D-C2D	3.73	1.49	1.39
47	17	305	KC1	C1A-CHA	3.73	1.50	1.40
37	41	208	CLA	OBD-CAD	3.73	1.28	1.22
47	11	306	KC1	C1B-NB	-3.73	1.33	1.37
48	19	311	A86	C9-C10	3.72	1.55	1.43
37	35	301	CLA	OBD-CAD	3.72	1.28	1.22
48	34	312	A86	C2-C1	3.72	1.40	1.35
37	35	308	CLA	C3D-C2D	3.72	1.49	1.39
37	B	509	CLA	CHD-C1D	3.72	1.45	1.38
37	19	305	CLA	CHD-C4C	3.72	1.47	1.39
37	b	510	CLA	CHD-C1D	3.72	1.45	1.38
37	11	305	CLA	CHD-C4C	3.72	1.47	1.39
37	14	310	CLA	OBD-CAD	3.72	1.28	1.22
37	21	209	CLA	OBD-CAD	3.72	1.28	1.22
37	34	310	CLA	OBD-CAD	3.72	1.28	1.22
37	35	310	CLA	OBD-CAD	3.72	1.28	1.22
37	16	307	CLA	CHD-C4C	3.72	1.47	1.39
37	18	203	CLA	OBD-CAD	3.72	1.28	1.22
48	16	313	A86	C5-C6	3.72	1.40	1.35
37	B	510	CLA	CHD-C1D	3.72	1.45	1.38
37	36	307	CLA	CHD-C4C	3.72	1.47	1.39
37	37	308	CLA	C3D-C2D	3.72	1.49	1.39
37	40	208	CLA	C3D-C2D	3.72	1.49	1.39
37	41	209	CLA	C3D-C2D	3.72	1.49	1.39
37	B	505	CLA	O2A-CGA	3.71	1.44	1.33
48	15	319	A86	C9-C10	3.71	1.55	1.43
37	38	203	CLA	C3D-C2D	3.71	1.49	1.39
48	14	314	A86	C10-C11	3.71	1.45	1.34
48	37	312	A86	C9-C10	3.71	1.54	1.43
47	11	302	KC1	C4D-ND	3.71	1.38	1.35
47	13	302	KC1	C4D-ND	3.71	1.38	1.35
47	33	302	KC1	C4D-ND	3.71	1.38	1.35
48	20	309	A86	C19-C18	3.71	1.57	1.52
37	17	304	CLA	C3D-C2D	3.71	1.49	1.39
37	B	503	CLA	C1B-NB	-3.71	1.31	1.35
37	39	305	CLA	CHD-C4C	3.71	1.47	1.39
47	37	304	KC1	C1A-CHA	3.71	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	40	201	A86	C5-C6	3.71	1.40	1.35
47	38	205	KC1	C1B-NB	-3.71	1.33	1.37
37	18	211	CLA	OBD-CAD	3.71	1.28	1.22
37	31	306	CLA	CHD-C4C	3.71	1.47	1.39
37	B	506	CLA	O2A-CGA	3.71	1.44	1.33
37	C	512	CLA	CHD-C1D	3.71	1.45	1.38
37	12	204	CLA	CHD-C1D	3.71	1.45	1.38
48	18	215	A86	C10-C11	3.71	1.45	1.34
37	c	512	CLA	CHD-C1D	3.70	1.45	1.38
37	34	307	CLA	C1B-NB	-3.70	1.31	1.35
48	12	214	A86	C2-C1	3.70	1.40	1.35
50	21	212	DD6	C35-C34	3.70	1.58	1.52
37	d	404	CLA	CHD-C4C	3.70	1.47	1.39
37	41	202	CLA	C3D-C2D	3.70	1.49	1.39
37	21	202	CLA	C3D-C2D	3.70	1.49	1.39
48	15	315	A86	C9-C10	3.70	1.54	1.43
37	c	501	CLA	CHD-C4C	3.70	1.47	1.39
48	38	213	A86	C9-C10	3.70	1.54	1.43
37	C	508	CLA	CHD-C1D	3.70	1.45	1.38
48	38	213	A86	C19-C18	3.70	1.57	1.52
37	b	505	CLA	O2A-CGA	3.70	1.44	1.33
47	33	302	KC1	CHB-C1B	3.70	1.45	1.38
37	b	509	CLA	CHD-C1D	3.70	1.45	1.38
48	38	213	A86	C2-C1	3.70	1.40	1.35
48	41	214	A86	C10-C11	3.70	1.45	1.34
37	13	310	CLA	C3D-C2D	3.70	1.49	1.39
37	D	406	CLA	CHD-C4C	3.70	1.47	1.39
37	b	515	CLA	CHD-C4C	3.70	1.47	1.39
48	11	311	A86	C21-C20	3.70	1.57	1.51
37	41	209	CLA	OBD-CAD	3.69	1.28	1.22
37	18	206	CLA	C3D-C2D	3.69	1.49	1.39
48	15	311	A86	C9-C10	3.69	1.54	1.43
48	15	314	A86	C5-C6	3.69	1.40	1.35
37	37	303	CLA	C3D-C2D	3.69	1.49	1.39
37	Z	101	CLA	OBD-CAD	3.69	1.28	1.22
37	18	206	CLA	OBD-CAD	3.69	1.28	1.22
48	21	215	A86	C10-C11	3.69	1.45	1.34
48	34	314	A86	C10-C11	3.69	1.45	1.34
37	14	303	CLA	C3D-C2D	3.69	1.49	1.39
37	34	303	CLA	C3D-C2D	3.69	1.49	1.39
37	C	501	CLA	CHD-C4C	3.69	1.47	1.39
48	33	313	A86	C21-C20	3.69	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	19	302	CLA	C3D-C2D	3.69	1.49	1.39
47	35	304	KC1	C1B-NB	-3.69	1.33	1.37
37	c	510	CLA	CHD-C4C	3.69	1.47	1.39
37	15	301	CLA	OBD-CAD	3.69	1.28	1.22
47	36	305	KC1	CHC-C1C	3.69	1.47	1.39
37	a	403	CLA	CHD-C4C	3.69	1.47	1.39
37	b	506	CLA	O2A-CGA	3.69	1.44	1.33
48	11	312	A86	C19-C18	3.69	1.57	1.52
37	41	210	CLA	OBD-CAD	3.69	1.28	1.22
47	16	305	KC1	CHC-C1C	3.69	1.47	1.39
37	36	303	CLA	C3D-C2D	3.69	1.49	1.39
48	14	311	A86	C26-C27	3.69	1.40	1.35
37	B	505	CLA	CHD-C4C	3.69	1.47	1.39
37	38	208	CLA	CHD-C4C	3.69	1.47	1.39
37	19	304	CLA	CHD-C1D	3.69	1.45	1.38
47	31	307	KC1	C1B-NB	-3.69	1.33	1.37
48	33	313	A86	C19-C18	3.69	1.57	1.52
37	13	305	CLA	OBD-CAD	3.69	1.28	1.22
37	33	305	CLA	OBD-CAD	3.69	1.28	1.22
37	16	303	CLA	C3D-C2D	3.69	1.49	1.39
48	39	311	A86	C10-C11	3.69	1.45	1.34
37	39	304	CLA	CHD-C1D	3.69	1.45	1.38
48	12	216	A86	C9-C10	3.69	1.54	1.43
48	32	217	A86	C9-C10	3.69	1.54	1.43
48	35	319	A86	C9-C10	3.68	1.54	1.43
48	12	213	A86	C26-C27	3.68	1.40	1.35
37	38	211	CLA	OBD-CAD	3.68	1.28	1.22
48	31	311	A86	C21-C20	3.68	1.57	1.51
48	21	214	A86	C10-C11	3.68	1.45	1.34
47	31	309	KC1	OBD-CAD	3.68	1.27	1.22
47	39	308	KC1	C1A-CHA	3.68	1.50	1.40
37	b	505	CLA	CHD-C4C	3.68	1.47	1.39
37	34	307	CLA	CHD-C4C	3.68	1.47	1.39
48	15	316	A86	C9-C10	3.68	1.54	1.43
48	32	214	A86	C9-C10	3.68	1.54	1.43
48	11	315	A86	C2-C1	3.68	1.40	1.35
37	14	302	CLA	C3D-C2D	3.68	1.49	1.39
37	34	302	CLA	C3D-C2D	3.68	1.49	1.39
47	18	210	KC1	CHC-C1C	3.68	1.47	1.39
48	21	214	A86	C9-C10	3.68	1.54	1.43
37	b	511	CLA	C1B-NB	-3.68	1.31	1.35
37	16	301	CLA	C3D-C2D	3.68	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	11	308	CLA	CHD-C4C	3.68	1.47	1.39
37	32	202	CLA	CHD-C4C	3.68	1.47	1.39
37	39	301	CLA	C3D-C2D	3.68	1.49	1.39
37	c	508	CLA	C1B-NB	-3.68	1.31	1.35
37	z	101	CLA	OBD-CAD	3.68	1.28	1.22
48	19	311	A86	C10-C11	3.68	1.45	1.34
48	38	215	A86	C17-C18	-3.68	1.47	1.52
37	39	310	CLA	C3D-C2D	3.68	1.49	1.39
37	15	301	CLA	C3D-C2D	3.68	1.49	1.39
37	35	301	CLA	C3D-C2D	3.68	1.49	1.39
48	35	314	A86	C19-C18	3.68	1.57	1.52
37	C	512	CLA	CHD-C4C	3.68	1.47	1.39
37	12	205	CLA	CHD-C4C	3.68	1.47	1.39
37	41	208	CLA	C3D-C2D	3.68	1.49	1.39
37	12	203	CLA	CHD-C4C	3.67	1.47	1.39
48	18	214	A86	C19-C18	3.67	1.57	1.52
37	18	203	CLA	C3D-C2D	3.67	1.49	1.39
37	15	310	CLA	C3D-C2D	3.67	1.49	1.39
37	C	510	CLA	CHD-C4C	3.67	1.47	1.39
48	17	314	A86	C26-C27	3.67	1.40	1.35
37	18	209	CLA	CHD-C4C	3.67	1.47	1.39
37	38	206	CLA	C3D-C2D	3.67	1.49	1.39
37	32	213	CLA	OBD-CAD	3.67	1.28	1.22
48	13	313	A86	C19-C18	3.67	1.57	1.52
37	18	208	CLA	OBD-CAD	3.67	1.28	1.22
47	15	306	KC1	CHC-C1C	3.67	1.47	1.39
37	14	307	CLA	C1B-NB	-3.67	1.31	1.35
48	21	215	A86	C9-C10	3.67	1.54	1.43
37	33	301	CLA	C3D-C2D	3.67	1.49	1.39
37	14	307	CLA	CHD-C4C	3.67	1.47	1.39
47	19	308	KC1	C1A-CHA	3.66	1.50	1.40
37	33	310	CLA	OBD-CAD	3.66	1.28	1.22
48	12	214	A86	C21-C20	3.66	1.57	1.51
48	32	215	A86	C21-C20	3.66	1.57	1.51
47	31	309	KC1	CHB-C1B	3.66	1.45	1.38
48	41	215	A86	C10-C11	3.66	1.45	1.34
47	14	304	KC1	CHC-C1C	3.66	1.47	1.39
37	36	301	CLA	C3D-C2D	3.66	1.49	1.39
47	11	309	KC1	CHB-C1B	3.66	1.45	1.38
37	B	515	CLA	CHD-C4C	3.66	1.47	1.39
37	12	209	CLA	CHD-C4C	3.66	1.47	1.39
37	A	403	CLA	CHD-C4C	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	z	102	CLA	C3D-C2D	3.66	1.49	1.39
48	12	213	A86	C9-C10	3.66	1.54	1.43
37	11	305	CLA	C3D-C2D	3.66	1.49	1.39
37	15	305	CLA	OBD-CAD	3.66	1.28	1.22
37	20	306	CLA	OBD-CAD	3.65	1.28	1.22
48	41	215	A86	C9-C10	3.65	1.54	1.43
37	13	301	CLA	C3D-C2D	3.65	1.49	1.39
37	35	305	CLA	OBD-CAD	3.65	1.28	1.22
37	37	306	CLA	C3D-C2D	3.65	1.49	1.39
37	14	305	CLA	OBD-CAD	3.65	1.28	1.22
37	34	305	CLA	OBD-CAD	3.65	1.28	1.22
48	34	311	A86	C9-C10	3.65	1.54	1.43
37	12	212	CLA	OBD-CAD	3.65	1.28	1.22
48	35	316	A86	C10-C11	3.65	1.45	1.34
37	32	204	CLA	CHD-C4C	3.65	1.47	1.39
37	b	512	CLA	C1B-NB	-3.65	1.32	1.35
37	40	210	CLA	C3D-C2D	3.65	1.49	1.39
47	14	309	KC1	CHB-C1B	3.65	1.45	1.38
48	15	316	A86	C10-C11	3.65	1.45	1.34
37	36	306	CLA	C3D-C2D	3.65	1.49	1.39
48	14	311	A86	C9-C10	3.65	1.54	1.43
48	14	313	A86	C21-C20	3.65	1.57	1.51
48	35	314	A86	C5-C6	3.65	1.40	1.35
37	19	310	CLA	C3D-C2D	3.65	1.49	1.39
37	38	209	CLA	OBD-CAD	3.65	1.28	1.22
47	34	309	KC1	C4D-ND	3.64	1.38	1.35
50	36	312	DD6	C35-C34	3.64	1.58	1.52
37	38	208	CLA	OBD-CAD	3.64	1.28	1.22
48	12	217	A86	C10-C11	3.64	1.45	1.34
37	b	503	CLA	C1B-NB	-3.64	1.32	1.35
48	31	312	A86	C19-C18	3.64	1.57	1.52
47	38	210	KC1	CHC-C1C	3.64	1.47	1.39
37	c	507	CLA	CHD-C1D	3.64	1.45	1.38
37	32	205	CLA	CHD-C1D	3.64	1.45	1.38
37	38	209	CLA	CHD-C4C	3.64	1.47	1.39
48	37	319	A86	C9-C10	3.64	1.54	1.43
48	37	312	A86	C10-C11	3.64	1.45	1.34
37	20	301	CLA	C3D-C2D	3.64	1.49	1.39
48	17	320	A86	C10-C11	3.64	1.45	1.34
37	c	505	CLA	CHD-C1D	3.64	1.45	1.38
37	A	405	CLA	CHD-C4C	3.64	1.47	1.39
37	32	210	CLA	CHD-C4C	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	16	311	A86	C10-C11	3.64	1.45	1.34
37	21	210	CLA	OBD-CAD	3.64	1.28	1.22
47	34	304	KC1	CHC-C1C	3.64	1.47	1.39
47	15	306	KC1	C1B-NB	-3.64	1.33	1.37
37	c	509	CLA	CHD-C4C	3.64	1.47	1.39
37	40	208	CLA	OBD-CAD	3.64	1.28	1.22
48	17	312	A86	C5-C6	3.64	1.40	1.35
37	Z	102	CLA	C3D-C2D	3.63	1.49	1.39
37	32	206	CLA	CHD-C4C	3.63	1.47	1.39
37	31	306	CLA	C3D-C2D	3.63	1.49	1.39
37	B	513	CLA	CHD-C1D	3.63	1.45	1.38
37	38	201	CLA	C3D-C2D	3.63	1.49	1.39
37	c	513	CLA	CHD-C4C	3.63	1.47	1.39
47	36	304	KC1	CHC-C1C	3.63	1.47	1.39
48	14	316	A86	C10-C11	3.63	1.45	1.34
47	16	304	KC1	CHC-C1C	3.63	1.47	1.39
37	14	305	CLA	C3D-C2D	3.63	1.49	1.39
37	34	305	CLA	C3D-C2D	3.63	1.49	1.39
48	18	213	A86	C9-C10	3.63	1.54	1.43
37	c	512	CLA	CHD-C4C	3.63	1.47	1.39
37	18	209	CLA	OBD-CAD	3.63	1.28	1.22
37	40	203	CLA	C3D-C2D	3.63	1.49	1.39
48	35	315	A86	C19-C18	3.63	1.57	1.52
48	37	311	A86	C5-C6	3.63	1.40	1.35
37	C	506	CLA	CHD-C4C	3.63	1.47	1.39
37	a	407	CLA	CHD-C4C	3.63	1.47	1.39
37	b	507	CLA	C1B-NB	-3.63	1.32	1.35
37	36	309	CLA	C3D-C2D	3.63	1.49	1.39
48	14	311	A86	C10-C11	3.63	1.45	1.34
48	34	311	A86	C10-C11	3.63	1.45	1.34
37	19	301	CLA	OBD-CAD	3.63	1.28	1.22
37	21	208	CLA	C3D-C2D	3.63	1.49	1.39
37	b	506	CLA	CHD-C1D	3.62	1.45	1.38
37	17	307	CLA	C3D-C2D	3.62	1.49	1.39
48	31	313	A86	C10-C11	3.62	1.45	1.34
48	34	316	A86	C10-C11	3.62	1.45	1.34
37	16	306	CLA	C3D-C2D	3.62	1.49	1.39
37	C	505	CLA	CHD-C1D	3.62	1.45	1.38
48	17	313	A86	C10-C11	3.62	1.45	1.34
37	20	308	CLA	C3D-C2D	3.62	1.49	1.39
47	13	306	KC1	C4D-ND	3.62	1.38	1.35
47	33	306	KC1	C4D-ND	3.62	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	11	309	KC1	OBD-CAD	3.62	1.27	1.22
47	41	203	KC1	CHC-C1C	3.62	1.47	1.39
48	32	214	A86	C26-C27	3.62	1.40	1.35
37	B	506	CLA	CHD-C1D	3.62	1.45	1.38
47	15	304	KC1	C1B-NB	-3.62	1.33	1.37
37	16	309	CLA	C3D-C2D	3.62	1.49	1.39
37	40	205	CLA	CHD-C4C	3.62	1.47	1.39
48	36	311	A86	C9-C10	3.62	1.54	1.43
37	Z	101	CLA	C3D-C2D	3.62	1.49	1.39
48	12	213	A86	C2-C1	3.62	1.40	1.35
37	18	201	CLA	C3D-C2D	3.62	1.49	1.39
37	32	213	CLA	C3D-C2D	3.62	1.49	1.39
37	C	508	CLA	C1B-NB	-3.62	1.32	1.35
37	13	310	CLA	OBD-CAD	3.62	1.28	1.22
37	19	301	CLA	C3D-C2D	3.62	1.49	1.39
37	19	305	CLA	C3D-C2D	3.62	1.49	1.39
48	32	218	A86	C10-C11	3.62	1.45	1.34
48	31	315	A86	C2-C1	3.62	1.40	1.35
37	13	307	CLA	CHD-C4C	3.61	1.47	1.39
37	33	307	CLA	CHD-C4C	3.61	1.47	1.39
37	c	506	CLA	CHD-C4C	3.61	1.47	1.39
37	21	205	CLA	C3D-C2D	3.61	1.49	1.39
48	15	312	A86	C5-C6	3.61	1.40	1.35
48	31	313	A86	C2-C1	3.61	1.40	1.35
37	19	306	CLA	C3D-C2D	3.61	1.49	1.39
37	35	310	CLA	C3D-C2D	3.61	1.49	1.39
48	36	311	A86	C10-C11	3.61	1.45	1.34
50	16	312	DD6	C35-C34	3.61	1.58	1.52
48	32	214	A86	C2-C1	3.61	1.40	1.35
48	12	213	A86	C10-C11	3.61	1.45	1.34
47	34	309	KC1	CHB-C1B	3.61	1.45	1.38
37	z	101	CLA	C3D-C2D	3.61	1.49	1.39
47	37	304	KC1	CHC-C1C	3.61	1.47	1.39
48	12	216	A86	C19-C18	3.61	1.57	1.52
48	14	312	A86	C9-C10	3.61	1.54	1.43
37	41	205	CLA	C3D-C2D	3.61	1.49	1.39
37	39	301	CLA	OBD-CAD	3.61	1.28	1.22
37	19	306	CLA	CHD-C1D	3.60	1.45	1.38
37	39	306	CLA	C3D-C2D	3.60	1.49	1.39
37	B	512	CLA	C1B-NB	-3.60	1.32	1.35
47	14	309	KC1	CHC-C1C	3.60	1.47	1.39
48	32	215	A86	C2-C1	3.60	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	513	CLA	CHD-C4C	3.60	1.47	1.39
37	39	307	CLA	MG-ND	-3.60	1.98	2.05
37	39	307	CLA	C3D-C2D	3.60	1.49	1.39
37	C	507	CLA	CHD-C1D	3.60	1.45	1.38
47	34	309	KC1	CHC-C1C	3.60	1.47	1.39
48	16	314	A86	C2-C1	3.60	1.40	1.35
37	12	212	CLA	C3D-C2D	3.60	1.49	1.39
47	18	205	KC1	CHC-C1C	3.60	1.47	1.39
47	37	307	KC1	CHC-C1C	3.60	1.47	1.39
37	C	509	CLA	CHD-C4C	3.60	1.47	1.39
37	13	305	CLA	C3D-C2D	3.60	1.48	1.39
37	33	305	CLA	C3D-C2D	3.60	1.48	1.39
48	36	310	A86	C10-C11	3.60	1.45	1.34
48	32	214	A86	C10-C11	3.60	1.45	1.34
47	35	306	KC1	C1B-NB	-3.60	1.33	1.37
37	36	307	CLA	C3D-C2D	3.60	1.48	1.39
37	b	513	CLA	CHD-C1D	3.60	1.45	1.38
48	11	311	A86	C10-C11	3.60	1.45	1.34
48	16	311	A86	C9-C10	3.60	1.54	1.43
37	38	202	CLA	OBD-CAD	3.60	1.28	1.22
48	34	313	A86	C21-C20	3.60	1.57	1.51
48	11	313	A86	C10-C11	3.60	1.45	1.34
48	32	203	A86	C2-C1	3.59	1.40	1.35
37	19	307	CLA	C3D-C2D	3.59	1.48	1.39
47	35	306	KC1	CHC-C1C	3.59	1.47	1.39
48	36	313	A86	C2-C1	3.59	1.40	1.35
37	35	307	CLA	OBD-CAD	3.59	1.28	1.22
37	12	209	CLA	C3D-C2D	3.59	1.48	1.39
48	17	311	A86	C10-C11	3.59	1.45	1.34
48	17	311	A86	C9-C10	3.59	1.54	1.43
48	32	217	A86	C19-C18	3.59	1.57	1.52
48	34	312	A86	C9-C10	3.59	1.54	1.43
37	39	305	CLA	C3D-C2D	3.59	1.48	1.39
37	14	301	CLA	CHD-C4C	3.59	1.47	1.39
48	35	319	A86	C10-C11	3.59	1.45	1.34
47	11	304	KC1	C4D-ND	3.59	1.38	1.35
47	31	305	KC1	C4D-ND	3.59	1.38	1.35
48	21	214	A86	C5-C6	3.59	1.40	1.35
48	32	216	A86	C5-C6	3.59	1.40	1.35
37	34	301	CLA	OBD-CAD	3.59	1.28	1.22
48	15	315	A86	C19-C18	3.59	1.57	1.52
48	15	311	A86	C5-C6	3.58	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	v	201	HEM	C3C-CAC	3.58	1.55	1.47
37	34	301	CLA	CHD-C4C	3.58	1.47	1.39
37	39	306	CLA	CHD-C1D	3.58	1.45	1.38
48	12	215	A86	C5-C6	3.58	1.40	1.35
37	19	306	CLA	OBD-CAD	3.58	1.28	1.22
48	36	310	A86	C9-C10	3.58	1.54	1.43
37	20	303	CLA	CHD-C4C	3.58	1.47	1.39
47	35	309	KC1	CHC-C1C	3.58	1.47	1.39
37	14	303	CLA	OBD-CAD	3.58	1.28	1.22
37	C	512	CLA	C3D-C2D	3.58	1.48	1.39
48	31	311	A86	C10-C11	3.58	1.45	1.34
37	W	102	CLA	C3D-C2D	3.58	1.48	1.39
47	35	304	KC1	CHC-C1C	3.58	1.47	1.39
47	17	305	KC1	CHC-C1C	3.58	1.47	1.39
37	18	201	CLA	OBD-CAD	3.57	1.28	1.22
37	38	206	CLA	OBD-CAD	3.57	1.28	1.22
47	12	211	KC1	CHC-C1C	3.57	1.47	1.39
48	34	316	A86	C5-C6	3.57	1.40	1.35
37	34	302	CLA	OBD-CAD	3.57	1.28	1.22
47	21	203	KC1	CHC-C1C	3.57	1.47	1.39
47	38	207	KC1	C1B-NB	-3.57	1.33	1.37
37	B	508	CLA	CHD-C4C	3.57	1.47	1.39
48	13	313	A86	C17-C18	-3.57	1.47	1.52
37	17	302	CLA	C3D-C2D	3.57	1.48	1.39
37	31	304	CLA	C3D-C2D	3.57	1.48	1.39
47	17	308	KC1	CHC-C1C	3.57	1.47	1.39
47	31	307	KC1	CHC-C1C	3.57	1.47	1.39
48	31	313	A86	C9-C10	3.57	1.54	1.43
48	15	319	A86	C10-C11	3.57	1.44	1.34
37	12	205	CLA	C3D-C2D	3.57	1.48	1.39
37	12	210	CLA	C3D-C2D	3.57	1.48	1.39
37	B	507	CLA	C1B-NB	-3.57	1.32	1.35
37	33	301	CLA	OBD-CAD	3.57	1.28	1.22
37	41	205	CLA	OBD-CAD	3.57	1.28	1.22
48	35	311	A86	C5-C6	3.57	1.40	1.35
37	B	511	CLA	C1B-NB	-3.57	1.32	1.35
48	18	212	A86	C5-C6	3.57	1.40	1.35
37	13	301	CLA	OBD-CAD	3.57	1.28	1.22
48	14	315	A86	C10-C11	3.57	1.44	1.34
37	31	301	CLA	C3D-C2D	3.57	1.48	1.39
37	32	206	CLA	C3D-C2D	3.57	1.48	1.39
48	35	315	A86	C10-C11	3.57	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	13	304	KC1	CHC-C1C	3.57	1.47	1.39
37	21	205	CLA	OBD-CAD	3.57	1.28	1.22
37	36	309	CLA	OBD-CAD	3.57	1.28	1.22
47	15	302	KC1	CHC-C1C	3.57	1.47	1.39
37	C	502	CLA	C3D-C2D	3.57	1.48	1.39
37	b	508	CLA	CHD-C4C	3.57	1.47	1.39
37	38	202	CLA	C3D-C2D	3.56	1.48	1.39
46	V	201	HEM	C3C-CAC	3.56	1.55	1.47
48	21	213	A86	C19-C18	3.56	1.57	1.52
48	41	214	A86	C5-C6	3.56	1.40	1.35
48	18	213	A86	C2-C1	3.56	1.40	1.35
37	36	301	CLA	CHD-C4C	3.56	1.47	1.39
37	41	206	CLA	C3D-C2D	3.56	1.48	1.39
48	11	314	A86	C19-C18	3.56	1.57	1.52
48	31	314	A86	C19-C18	3.56	1.57	1.52
37	19	303	CLA	C3D-C2D	3.56	1.48	1.39
37	39	303	CLA	C3D-C2D	3.56	1.48	1.39
48	16	310	A86	C10-C11	3.56	1.44	1.34
48	34	315	A86	C10-C11	3.56	1.44	1.34
47	38	205	KC1	CHC-C1C	3.56	1.47	1.39
37	21	204	CLA	OBD-CAD	3.56	1.28	1.22
48	35	312	A86	C5-C6	3.56	1.40	1.35
37	31	302	CLA	CHD-C4C	3.56	1.47	1.39
37	32	210	CLA	C3D-C2D	3.56	1.48	1.39
37	14	307	CLA	C3D-C2D	3.56	1.48	1.39
37	14	301	CLA	OBD-CAD	3.56	1.28	1.22
48	33	313	A86	C17-C18	-3.55	1.47	1.52
37	17	302	CLA	OBD-CAD	3.55	1.28	1.22
48	19	313	A86	C5-C6	3.55	1.40	1.35
37	34	303	CLA	OBD-CAD	3.55	1.28	1.22
48	12	216	A86	C10-C11	3.55	1.44	1.34
47	15	304	KC1	CHC-C1C	3.55	1.47	1.39
37	31	308	CLA	C3D-C2D	3.55	1.48	1.39
47	15	309	KC1	CHC-C1C	3.55	1.47	1.39
48	38	212	A86	C5-C6	3.55	1.40	1.35
37	c	502	CLA	C3D-C2D	3.55	1.48	1.39
48	16	310	A86	C9-C10	3.55	1.54	1.43
37	14	301	CLA	C3D-C2D	3.55	1.48	1.39
37	34	301	CLA	C3D-C2D	3.55	1.48	1.39
37	11	301	CLA	CHD-C4C	3.55	1.47	1.39
48	18	212	A86	C19-C18	3.55	1.57	1.52
48	38	214	A86	C5-C6	3.55	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	32	211	CLA	C3D-C2D	3.55	1.48	1.39
37	c	512	CLA	C3D-C2D	3.55	1.48	1.39
47	33	304	KC1	CHC-C1C	3.55	1.47	1.39
48	37	310	A86	C10-C11	3.55	1.44	1.34
37	38	201	CLA	OBD-CAD	3.55	1.28	1.22
48	11	314	A86	C9-C10	3.55	1.54	1.43
48	31	314	A86	C9-C10	3.55	1.54	1.43
37	D	405	CLA	CHD-C4C	3.55	1.47	1.39
37	b	501	CLA	C3D-C2D	3.55	1.48	1.39
48	11	313	A86	C9-C10	3.55	1.54	1.43
48	17	320	A86	C9-C10	3.55	1.54	1.43
37	34	307	CLA	C3D-C2D	3.55	1.48	1.39
48	18	213	A86	C7-C6	3.55	1.58	1.50
37	11	303	CLA	C3D-C2D	3.55	1.48	1.39
37	37	301	CLA	C3D-C2D	3.55	1.48	1.39
37	11	307	CLA	C3D-C2D	3.54	1.48	1.39
37	16	307	CLA	C3D-C2D	3.54	1.48	1.39
47	33	309	KC1	CHC-C1C	3.54	1.47	1.39
37	b	508	CLA	C1B-NB	-3.54	1.32	1.35
37	21	206	CLA	C3D-C2D	3.54	1.48	1.39
47	12	206	KC1	CHC-C1C	3.54	1.47	1.39
37	C	509	CLA	C1B-NB	-3.54	1.32	1.35
48	12	220	A86	C26-C27	3.54	1.40	1.35
48	32	221	A86	C26-C27	3.54	1.40	1.35
50	20	312	DD6	C-C1	3.54	1.58	1.50
47	20	302	KC1	CHC-C1C	3.54	1.47	1.39
37	12	204	CLA	OBD-CAD	3.54	1.28	1.22
37	32	205	CLA	OBD-CAD	3.54	1.28	1.22
37	b	511	CLA	CHD-C4C	3.54	1.47	1.39
48	39	313	A86	C21-C20	3.54	1.57	1.51
37	B	501	CLA	C3D-C2D	3.54	1.48	1.39
48	34	311	A86	C2-C1	3.54	1.40	1.35
47	39	308	KC1	CHC-C1C	3.54	1.47	1.39
37	32	208	CLA	C3D-C2D	3.54	1.48	1.39
37	16	309	CLA	OBD-CAD	3.54	1.28	1.22
37	15	307	CLA	OBD-CAD	3.54	1.28	1.22
47	13	304	KC1	C4D-ND	3.54	1.38	1.35
37	41	204	CLA	OBD-CAD	3.54	1.28	1.22
48	18	214	A86	C5-C6	3.54	1.40	1.35
48	37	310	A86	C9-C10	3.53	1.54	1.43
37	32	205	CLA	C3D-C2D	3.53	1.48	1.39
37	B	503	CLA	CHD-C4C	3.53	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	14	302	CLA	OBD-CAD	3.53	1.28	1.22
47	40	204	KC1	CHC-C1C	3.53	1.47	1.39
37	c	509	CLA	C1B-NB	-3.53	1.32	1.35
37	d	403	CLA	CHD-C4C	3.53	1.47	1.39
37	12	207	CLA	C3D-C2D	3.53	1.48	1.39
48	15	315	A86	C10-C11	3.53	1.44	1.34
37	b	509	CLA	C3D-C2D	3.53	1.48	1.39
37	36	307	CLA	OBD-CAD	3.53	1.28	1.22
48	16	314	A86	C9-C10	3.53	1.54	1.43
37	14	308	CLA	OBD-CAD	3.53	1.28	1.22
37	34	308	CLA	OBD-CAD	3.53	1.28	1.22
37	32	204	CLA	C3D-C2D	3.52	1.48	1.39
48	32	217	A86	C10-C11	3.52	1.44	1.34
37	31	308	CLA	CHD-C4C	3.52	1.47	1.39
37	b	503	CLA	CHD-C4C	3.52	1.47	1.39
37	11	305	CLA	OBD-CAD	3.52	1.28	1.22
48	17	313	A86	C19-C18	3.52	1.57	1.52
48	37	312	A86	C19-C18	3.52	1.57	1.52
37	12	204	CLA	C3D-C2D	3.52	1.48	1.39
37	B	509	CLA	C3D-C2D	3.52	1.48	1.39
37	12	210	CLA	OBD-CAD	3.52	1.28	1.22
37	31	306	CLA	OBD-CAD	3.52	1.28	1.22
37	c	511	CLA	CHD-C4C	3.52	1.47	1.39
37	B	506	CLA	C1B-NB	-3.52	1.32	1.35
37	16	301	CLA	CHD-C4C	3.51	1.47	1.39
47	11	306	KC1	CHC-C1C	3.51	1.47	1.39
50	40	214	DD6	C-C1	3.51	1.58	1.50
37	32	205	CLA	C1B-NB	-3.51	1.32	1.35
37	32	211	CLA	OBD-CAD	3.51	1.28	1.22
37	B	511	CLA	CHD-C4C	3.51	1.47	1.39
37	b	508	CLA	C3D-C2D	3.51	1.48	1.39
37	B	508	CLA	C3D-C2D	3.51	1.48	1.39
37	W	101	CLA	CHD-C4C	3.51	1.47	1.39
37	C	511	CLA	CHD-C4C	3.51	1.47	1.39
37	19	304	CLA	C3D-C2D	3.51	1.48	1.39
37	39	304	CLA	C3D-C2D	3.51	1.48	1.39
48	14	312	A86	C10-C11	3.51	1.44	1.34
37	19	309	CLA	C3D-C2D	3.51	1.48	1.39
37	11	307	CLA	CHD-C4C	3.51	1.47	1.39
37	39	306	CLA	CHD-C4C	3.51	1.47	1.39
48	14	316	A86	C5-C6	3.50	1.40	1.35
37	b	506	CLA	C1B-NB	-3.50	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	16	308	KC1	CHC-C1C	3.50	1.47	1.39
37	39	306	CLA	OBD-CAD	3.50	1.28	1.22
47	32	207	KC1	CHC-C1C	3.50	1.47	1.39
48	41	213	A86	C19-C18	3.50	1.57	1.52
50	41	216	DD6	O2-C18	3.50	1.53	1.43
48	34	312	A86	C10-C11	3.50	1.44	1.34
48	36	313	A86	C17-C18	-3.50	1.47	1.52
47	19	308	KC1	CHC-C1C	3.50	1.47	1.39
37	B	513	CLA	CHD-C4C	3.50	1.47	1.39
48	12	202	A86	C2-C1	3.50	1.40	1.35
37	20	308	CLA	OBD-CAD	3.50	1.28	1.22
37	37	301	CLA	OBD-CAD	3.50	1.28	1.22
37	16	307	CLA	OBD-CAD	3.50	1.28	1.22
48	17	320	A86	C5-C6	3.50	1.40	1.35
37	18	202	CLA	CHD-C1D	3.50	1.45	1.38
37	40	210	CLA	OBD-CAD	3.50	1.28	1.22
48	32	218	A86	C5-C6	3.50	1.40	1.35
37	b	513	CLA	CHD-C4C	3.50	1.47	1.39
37	w	101	CLA	CHD-C4C	3.50	1.47	1.39
47	13	309	KC1	CHC-C1C	3.50	1.47	1.39
48	17	314	A86	C19-C18	3.49	1.57	1.52
47	36	308	KC1	CHC-C1C	3.49	1.47	1.39
48	15	315	A86	C5-C6	3.49	1.40	1.35
48	35	315	A86	C5-C6	3.49	1.40	1.35
47	14	309	KC1	C4B-NB	-3.49	1.33	1.37
37	19	306	CLA	CHD-C4C	3.49	1.47	1.39
48	14	311	A86	C2-C1	3.49	1.40	1.35
48	38	212	A86	C19-C18	3.49	1.57	1.52
48	11	319	A86	C9-C10	3.49	1.54	1.43
48	31	319	A86	C9-C10	3.49	1.54	1.43
37	c	505	CLA	C1B-NB	-3.49	1.32	1.35
48	31	315	A86	C10-C11	3.49	1.44	1.34
37	12	203	CLA	C3D-C2D	3.49	1.48	1.39
48	19	313	A86	C21-C20	3.49	1.57	1.51
48	37	314	A86	C5-C6	3.49	1.40	1.35
47	17	305	KC1	C4B-NB	-3.49	1.33	1.37
37	18	202	CLA	OBD-CAD	3.49	1.28	1.22
37	c	506	CLA	C3D-C2D	3.49	1.48	1.39
47	31	305	KC1	C4B-NB	-3.49	1.33	1.37
37	37	306	CLA	OBD-CAD	3.48	1.28	1.22
37	C	506	CLA	C3D-C2D	3.48	1.48	1.39
47	11	309	KC1	C4D-ND	3.48	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	39	313	A86	C14-C15	3.48	1.59	1.52
48	11	315	A86	C10-C11	3.48	1.44	1.34
50	21	216	DD6	O2-C18	3.48	1.53	1.43
47	11	304	KC1	C4B-NB	-3.48	1.33	1.37
39	y	101	BCR	C1-C6	-3.48	1.49	1.53
37	B	524	CLA	CHD-C1D	3.48	1.45	1.38
48	36	313	A86	C9-C10	3.48	1.54	1.43
37	13	308	CLA	C3D-C2D	3.47	1.48	1.39
37	31	310	CLA	C3D-C2D	3.47	1.48	1.39
48	11	315	A86	C9-C10	3.47	1.54	1.43
47	33	304	KC1	C4D-ND	3.47	1.38	1.35
48	16	313	A86	C17-C18	-3.47	1.47	1.52
48	12	217	A86	C5-C6	3.47	1.40	1.35
47	35	302	KC1	CHC-C1C	3.47	1.47	1.39
47	18	207	KC1	CHC-C1C	3.47	1.47	1.39
48	31	315	A86	C9-C10	3.47	1.54	1.43
37	39	309	CLA	OBD-CAD	3.47	1.28	1.22
48	17	315	A86	C5-C6	3.47	1.40	1.35
48	36	313	A86	C10-C11	3.47	1.44	1.34
48	16	314	A86	C17-C18	-3.47	1.47	1.52
37	11	310	CLA	CHD-C4C	3.47	1.47	1.39
37	B	504	CLA	CHD-C4C	3.47	1.47	1.39
37	18	202	CLA	C3D-C2D	3.47	1.48	1.39
48	19	311	A86	C5-C6	3.46	1.40	1.35
47	32	209	KC1	C4D-ND	3.46	1.38	1.35
37	D	406	CLA	C3D-C2D	3.46	1.48	1.39
37	17	307	CLA	OBD-CAD	3.46	1.28	1.22
37	39	309	CLA	C3D-C2D	3.46	1.48	1.39
39	K	101	BCR	C1-C6	-3.46	1.49	1.53
37	18	208	CLA	C3D-C2D	3.46	1.48	1.39
37	32	202	CLA	C3D-C2D	3.46	1.48	1.39
48	40	201	A86	C17-C18	-3.46	1.47	1.52
37	b	523	CLA	CHD-C1D	3.46	1.45	1.38
47	38	207	KC1	CHC-C1C	3.46	1.47	1.39
37	11	308	CLA	C3D-C2D	3.46	1.48	1.39
48	39	311	A86	C5-C6	3.45	1.40	1.35
48	15	319	A86	C5-C6	3.45	1.40	1.35
37	38	208	CLA	C3D-C2D	3.45	1.48	1.39
37	11	310	CLA	C3D-C2D	3.45	1.48	1.39
37	14	310	CLA	C3D-C2D	3.45	1.48	1.39
37	34	310	CLA	C3D-C2D	3.45	1.48	1.39
37	b	514	CLA	CHD-C4C	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	515	CLA	C3D-C2D	3.45	1.48	1.39
47	36	302	KC1	CHC-C1C	3.45	1.47	1.39
37	b	507	CLA	C3D-C2D	3.45	1.48	1.39
47	34	309	KC1	C4B-NB	-3.45	1.33	1.37
48	17	314	A86	C5-C6	3.45	1.40	1.35
48	35	314	A86	C21-C20	3.45	1.57	1.51
48	37	313	A86	C19-C18	3.45	1.57	1.52
47	32	212	KC1	CHC-C1C	3.44	1.47	1.39
48	16	314	A86	C10-C11	3.44	1.44	1.34
47	12	208	KC1	C4D-ND	3.44	1.38	1.35
48	11	311	A86	C9-C10	3.44	1.54	1.43
48	31	311	A86	C9-C10	3.44	1.54	1.43
48	34	315	A86	C5-C6	3.44	1.40	1.35
37	a	407	CLA	C3D-C2D	3.44	1.48	1.39
37	14	308	CLA	C3D-C2D	3.44	1.48	1.39
37	B	508	CLA	C1B-NB	-3.44	1.32	1.35
37	b	510	CLA	CHD-C4C	3.44	1.47	1.39
37	b	504	CLA	CHD-C4C	3.44	1.47	1.39
47	14	306	KC1	CHC-C1C	3.44	1.47	1.39
48	13	312	A86	C5-C6	3.44	1.40	1.35
48	12	214	A86	C9-C10	3.44	1.54	1.43
48	32	215	A86	C9-C10	3.44	1.54	1.43
48	12	220	A86	C9-C10	3.44	1.54	1.43
48	32	221	A86	C9-C10	3.44	1.54	1.43
37	b	516	CLA	C3D-C2D	3.44	1.48	1.39
37	39	303	CLA	OBD-CAD	3.44	1.28	1.22
37	B	507	CLA	C3D-C2D	3.44	1.48	1.39
37	31	310	CLA	CHD-C4C	3.44	1.47	1.39
37	C	503	CLA	C3D-C2D	3.43	1.48	1.39
48	11	319	A86	C10-C11	3.43	1.44	1.34
48	17	313	A86	C5-C6	3.43	1.40	1.35
37	12	204	CLA	C1B-NB	-3.43	1.32	1.35
47	13	302	KC1	CHC-C1C	3.43	1.47	1.39
47	16	302	KC1	CHC-C1C	3.43	1.47	1.39
37	36	306	CLA	OBD-CAD	3.43	1.28	1.22
37	D	401	CLA	C3D-C2D	3.43	1.48	1.39
37	19	305	CLA	OBD-CAD	3.43	1.28	1.22
37	A	405	CLA	C3D-C2D	3.43	1.48	1.39
37	b	516	CLA	CHD-C4C	3.43	1.47	1.39
47	33	302	KC1	CHC-C1C	3.43	1.47	1.39
37	d	404	CLA	C3D-C2D	3.43	1.48	1.39
37	W	102	CLA	OBD-CAD	3.43	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	20	301	CLA	OBD-CAD	3.43	1.28	1.22
48	33	312	A86	C5-C6	3.43	1.40	1.35
48	15	315	A86	C17-C18	-3.43	1.47	1.52
47	32	209	KC1	CHC-C1C	3.43	1.47	1.39
37	39	310	CLA	OBD-CAD	3.43	1.28	1.22
37	B	510	CLA	CHD-C4C	3.43	1.47	1.39
37	19	310	CLA	OBD-CAD	3.43	1.28	1.22
37	33	308	CLA	C3D-C2D	3.43	1.48	1.39
48	37	313	A86	C5-C6	3.43	1.40	1.35
37	c	503	CLA	C3D-C2D	3.43	1.48	1.39
37	b	509	CLA	C1B-NB	-3.42	1.32	1.35
37	C	502	CLA	CHD-C4C	3.42	1.47	1.39
37	a	404	CLA	C3D-C2D	3.42	1.48	1.39
37	B	514	CLA	CHD-C4C	3.42	1.47	1.39
37	19	309	CLA	OBD-CAD	3.42	1.28	1.22
37	39	305	CLA	OBD-CAD	3.42	1.28	1.22
37	B	515	CLA	C3D-C2D	3.42	1.48	1.39
48	32	217	A86	C5-C6	3.42	1.40	1.35
48	37	310	A86	C5-C6	3.42	1.40	1.35
37	B	516	CLA	C3D-C2D	3.42	1.48	1.39
37	C	513	CLA	C3D-C2D	3.42	1.48	1.39
48	11	313	A86	C5-C6	3.42	1.40	1.35
37	41	202	CLA	OBD-CAD	3.42	1.28	1.22
37	16	306	CLA	OBD-CAD	3.42	1.28	1.22
37	40	203	CLA	OBD-CAD	3.42	1.28	1.22
48	13	312	A86	C19-C18	3.42	1.57	1.52
37	C	505	CLA	C1B-NB	-3.42	1.32	1.35
48	31	312	A86	C9-C10	3.42	1.54	1.43
48	33	312	A86	C19-C18	3.42	1.57	1.52
47	31	305	KC1	CHC-C1C	3.42	1.47	1.39
37	B	516	CLA	C1B-NB	-3.42	1.32	1.35
37	21	202	CLA	OBD-CAD	3.41	1.28	1.22
48	12	213	A86	C5-C6	3.41	1.40	1.35
37	c	508	CLA	CHD-C4C	3.41	1.47	1.39
37	11	301	CLA	C3D-C2D	3.41	1.48	1.39
37	c	502	CLA	CHD-C4C	3.41	1.47	1.39
37	31	302	CLA	C3D-C2D	3.41	1.48	1.39
48	33	315	A86	C5-C6	3.41	1.40	1.35
37	32	205	CLA	C1D-ND	3.41	1.42	1.37
37	14	307	CLA	OBD-CAD	3.41	1.28	1.22
37	34	307	CLA	OBD-CAD	3.41	1.28	1.22
48	39	313	A86	C5-C6	3.41	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	14	311	A86	C19-C18	3.41	1.57	1.52
48	37	319	A86	C19-C18	3.41	1.57	1.52
47	40	207	KC1	CHC-C1C	3.41	1.47	1.39
37	b	510	CLA	C3D-C2D	3.40	1.48	1.39
48	31	319	A86	C10-C11	3.40	1.44	1.34
50	16	312	DD6	C-C1	3.40	1.57	1.50
37	c	513	CLA	C3D-C2D	3.40	1.48	1.39
39	B	517	BCR	C1-C6	-3.40	1.49	1.53
39	b	517	BCR	C1-C6	-3.40	1.49	1.53
37	C	504	CLA	C3D-C2D	3.40	1.48	1.39
37	31	301	CLA	OBD-CAD	3.40	1.28	1.22
37	b	514	CLA	C3D-C2D	3.40	1.48	1.39
37	13	308	CLA	OBD-CAD	3.40	1.28	1.22
48	32	221	A86	C10-C11	3.40	1.44	1.34
48	12	216	A86	C5-C6	3.40	1.40	1.35
47	34	306	KC1	CHC-C1C	3.40	1.47	1.39
47	31	309	KC1	C4D-ND	3.40	1.38	1.35
37	C	512	CLA	OBD-CAD	3.40	1.28	1.22
50	36	312	DD6	C-C1	3.40	1.57	1.50
47	15	302	KC1	C4B-NB	-3.39	1.33	1.37
37	B	516	CLA	CHD-C4C	3.39	1.47	1.39
37	C	508	CLA	CHD-C4C	3.39	1.47	1.39
48	11	312	A86	C9-C10	3.39	1.54	1.43
48	12	213	A86	C19-C18	3.39	1.57	1.52
48	32	214	A86	C19-C18	3.39	1.57	1.52
50	20	312	DD6	C35-C34	3.39	1.58	1.52
37	34	308	CLA	C3D-C2D	3.39	1.48	1.39
37	B	514	CLA	C3D-C2D	3.39	1.48	1.39
48	31	313	A86	C5-C6	3.39	1.40	1.35
37	c	505	CLA	CHD-C4C	3.39	1.47	1.39
37	33	307	CLA	C1B-NB	-3.39	1.32	1.35
48	12	220	A86	C10-C11	3.39	1.44	1.34
48	11	314	A86	C10-C11	3.39	1.44	1.34
37	c	507	CLA	CHD-C4C	3.39	1.47	1.39
37	b	502	CLA	C3D-C2D	3.39	1.48	1.39
47	37	304	KC1	C4B-NB	-3.39	1.33	1.37
48	12	215	A86	C19-C18	3.39	1.57	1.52
37	B	502	CLA	C3D-C2D	3.38	1.48	1.39
48	32	216	A86	C19-C18	3.38	1.57	1.52
48	31	314	A86	C10-C11	3.38	1.44	1.34
47	20	305	KC1	CHC-C1C	3.38	1.47	1.39
37	D	405	CLA	C1D-ND	3.38	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	38	204	CLA	OBD-CAD	3.38	1.28	1.22
37	36	301	CLA	OBD-CAD	3.38	1.28	1.22
37	C	507	CLA	CHD-C4C	3.38	1.46	1.39
48	13	315	A86	C5-C6	3.38	1.40	1.35
50	40	214	DD6	C35-C34	3.38	1.58	1.52
37	C	513	CLA	OBD-CAD	3.38	1.28	1.22
37	19	307	CLA	OBD-CAD	3.38	1.28	1.22
37	39	307	CLA	OBD-CAD	3.38	1.28	1.22
37	B	510	CLA	C3D-C2D	3.38	1.48	1.39
50	41	212	DD6	O2-C18	3.38	1.53	1.43
37	12	204	CLA	C1D-ND	3.37	1.41	1.37
37	d	403	CLA	C1D-ND	3.37	1.41	1.37
37	c	512	CLA	OBD-CAD	3.37	1.28	1.22
48	12	214	A86	C10-C11	3.37	1.44	1.34
37	13	307	CLA	C3D-C2D	3.37	1.48	1.39
37	33	307	CLA	C3D-C2D	3.37	1.48	1.39
48	35	319	A86	C5-C6	3.37	1.40	1.35
37	B	509	CLA	C1B-NB	-3.37	1.32	1.35
50	20	310	DD6	O2-C18	3.37	1.53	1.43
37	33	308	CLA	OBD-CAD	3.37	1.28	1.22
47	32	209	KC1	C4B-NB	-3.37	1.33	1.37
48	32	214	A86	C5-C6	3.37	1.40	1.35
50	21	212	DD6	O2-C18	3.37	1.53	1.43
48	31	312	A86	C10-C11	3.37	1.44	1.34
51	39	315	LMU	O5B-C1B	3.37	1.50	1.41
47	12	208	KC1	CHC-C1C	3.37	1.46	1.39
37	c	513	CLA	OBD-CAD	3.37	1.28	1.22
37	c	507	CLA	C3D-C2D	3.37	1.48	1.39
37	A	403	CLA	C1B-NB	-3.37	1.32	1.35
37	13	307	CLA	C1B-NB	-3.37	1.32	1.35
51	19	315	LMU	O5B-C1B	3.36	1.50	1.41
48	11	312	A86	C10-C11	3.36	1.44	1.34
48	14	315	A86	C5-C6	3.36	1.40	1.35
37	19	303	CLA	OBD-CAD	3.36	1.28	1.22
37	B	511	CLA	C3D-C2D	3.36	1.48	1.39
37	18	204	CLA	OBD-CAD	3.36	1.28	1.22
37	C	505	CLA	CHD-C4C	3.36	1.46	1.39
37	B	501	CLA	OBD-CAD	3.36	1.28	1.22
37	b	501	CLA	OBD-CAD	3.36	1.28	1.22
37	c	504	CLA	C3D-C2D	3.36	1.48	1.39
47	13	306	KC1	CHC-C1C	3.36	1.46	1.39
48	17	320	A86	C19-C18	3.36	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	507	CLA	C3D-C2D	3.36	1.48	1.39
47	11	304	KC1	CHC-C1C	3.36	1.46	1.39
37	12	207	CLA	OBD-CAD	3.36	1.28	1.22
47	16	308	KC1	C4B-NB	-3.35	1.33	1.37
47	36	308	KC1	C4B-NB	-3.35	1.33	1.37
48	19	311	A86	C19-C18	3.35	1.57	1.52
48	39	311	A86	C19-C18	3.35	1.57	1.52
50	40	212	DD6	O2-C18	3.35	1.53	1.43
37	32	210	CLA	OBD-CAD	3.35	1.28	1.22
47	32	212	KC1	C4B-NB	-3.35	1.33	1.37
37	16	301	CLA	OBD-CAD	3.35	1.28	1.22
37	C	503	CLA	OBD-CAD	3.34	1.28	1.22
47	31	303	KC1	CHC-C1C	3.34	1.46	1.39
37	b	516	CLA	C1B-NB	-3.34	1.32	1.35
37	w	101	CLA	C3D-C2D	3.34	1.48	1.39
48	37	309	A86	C5-C6	3.34	1.40	1.35
37	B	524	CLA	C1B-NB	-3.34	1.32	1.35
48	32	215	A86	C10-C11	3.34	1.44	1.34
37	32	208	CLA	OBD-CAD	3.34	1.28	1.22
37	39	304	CLA	OBD-CAD	3.34	1.28	1.22
47	31	309	KC1	CHC-C1C	3.34	1.46	1.39
48	17	310	A86	C5-C6	3.33	1.40	1.35
48	35	311	A86	C19-C18	3.33	1.57	1.52
47	20	304	KC1	CHC-C1C	3.33	1.46	1.39
37	b	511	CLA	C3D-C2D	3.33	1.48	1.39
37	C	501	CLA	C3D-C2D	3.33	1.48	1.39
37	W	101	CLA	C3D-C2D	3.33	1.48	1.39
37	12	209	CLA	OBD-CAD	3.33	1.28	1.22
37	31	308	CLA	OBD-CAD	3.33	1.28	1.22
48	34	311	A86	C19-C18	3.33	1.57	1.52
50	20	312	DD6	O2-C18	3.33	1.53	1.43
50	40	214	DD6	O2-C18	3.33	1.53	1.43
48	37	319	A86	C5-C6	3.33	1.40	1.35
47	12	211	KC1	C4B-NB	-3.32	1.33	1.37
48	14	313	A86	C25-C24	3.32	1.43	1.34
37	11	301	CLA	OBD-CAD	3.32	1.28	1.22
37	31	302	CLA	OBD-CAD	3.32	1.28	1.22
37	32	204	CLA	OBD-CAD	3.32	1.28	1.22
37	12	203	CLA	OBD-CAD	3.32	1.28	1.22
37	b	509	CLA	CHD-C4C	3.32	1.46	1.39
48	18	215	A86	C19-C18	3.32	1.57	1.52
37	36	303	CLA	OBD-CAD	3.32	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	37	302	KC1	C4B-NB	-3.32	1.33	1.37
37	d	401	CLA	C3D-C2D	3.32	1.48	1.39
48	33	311	A86	C19-C18	3.32	1.57	1.52
48	35	313	A86	C19-C18	3.32	1.57	1.52
47	33	306	KC1	CHC-C1C	3.32	1.46	1.39
37	31	308	CLA	C1B-NB	-3.31	1.32	1.35
37	c	503	CLA	OBD-CAD	3.31	1.28	1.22
48	37	310	A86	C19-C18	3.31	1.57	1.52
37	b	513	CLA	C3D-C2D	3.31	1.48	1.39
47	40	206	KC1	CHC-C1C	3.31	1.46	1.39
47	11	302	KC1	CHC-C1C	3.31	1.46	1.39
37	16	306	CLA	C1B-NB	-3.31	1.32	1.35
47	11	309	KC1	CHC-C1C	3.31	1.46	1.39
37	B	515	CLA	OBD-CAD	3.31	1.28	1.22
48	17	311	A86	C19-C18	3.31	1.57	1.52
48	34	313	A86	C25-C24	3.31	1.43	1.34
37	33	303	CLA	OBD-CAD	3.31	1.28	1.22
50	36	312	DD6	O2-C18	3.31	1.53	1.43
37	C	509	CLA	C3D-C2D	3.31	1.48	1.39
37	11	307	CLA	OBD-CAD	3.31	1.28	1.22
37	B	509	CLA	CHD-C4C	3.31	1.46	1.39
47	17	308	KC1	C4B-NB	-3.30	1.33	1.37
47	37	302	KC1	CHC-C1C	3.30	1.46	1.39
37	19	304	CLA	OBD-CAD	3.30	1.28	1.22
47	14	304	KC1	C4B-NB	-3.30	1.33	1.37
37	a	403	CLA	C1B-NB	-3.30	1.32	1.35
48	37	312	A86	C5-C6	3.30	1.40	1.35
37	c	501	CLA	C3D-C2D	3.29	1.48	1.39
37	D	402	CLA	C3D-C2D	3.29	1.48	1.39
50	16	312	DD6	O2-C18	3.29	1.53	1.43
48	11	313	A86	C21-C20	3.29	1.57	1.51
37	B	506	CLA	C3D-C2D	3.29	1.48	1.39
37	c	510	CLA	OBD-CAD	3.29	1.28	1.22
48	15	311	A86	C19-C18	3.29	1.57	1.52
48	35	319	A86	C19-C18	3.29	1.57	1.52
48	33	311	A86	C5-C6	3.28	1.40	1.35
48	13	311	A86	C19-C18	3.28	1.57	1.52
39	H	101	BCR	C1-C6	-3.28	1.49	1.53
37	c	509	CLA	C3D-C2D	3.28	1.48	1.39
47	20	305	KC1	C4B-NB	-3.28	1.33	1.37
48	31	313	A86	C21-C20	3.28	1.57	1.51
37	11	307	CLA	C1B-NB	-3.28	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	11	310	CLA	OBD-CAD	3.28	1.28	1.22
37	D	401	CLA	OBD-CAD	3.28	1.28	1.22
37	a	404	CLA	OBD-CAD	3.28	1.28	1.22
37	b	506	CLA	C3D-C2D	3.28	1.48	1.39
47	12	208	KC1	C4B-NB	-3.28	1.33	1.37
37	b	523	CLA	C1B-NB	-3.28	1.32	1.35
37	B	513	CLA	C3D-C2D	3.28	1.48	1.39
45	D	408	PL9	C52-C5	-3.28	1.43	1.50
37	D	402	CLA	OBD-CAD	3.28	1.28	1.22
47	17	306	KC1	C4B-NB	-3.28	1.33	1.37
47	37	305	KC1	C4B-NB	-3.28	1.33	1.37
48	38	215	A86	C19-C18	3.28	1.57	1.52
37	B	524	CLA	C1D-ND	3.27	1.41	1.37
37	11	310	CLA	C1B-NB	-3.27	1.32	1.35
37	31	310	CLA	C1B-NB	-3.27	1.32	1.35
48	18	213	A86	O-C13	-3.27	1.16	1.23
47	40	206	KC1	C4B-NB	-3.27	1.33	1.37
37	b	505	CLA	C3D-C2D	3.27	1.48	1.39
37	32	202	CLA	OBD-CAD	3.27	1.28	1.22
37	11	308	CLA	C1B-NB	-3.27	1.32	1.35
37	C	511	CLA	C3D-C2D	3.27	1.48	1.39
48	13	311	A86	C5-C6	3.26	1.40	1.35
48	40	213	A86	C25-C24	3.26	1.43	1.34
47	41	203	KC1	C4B-NB	-3.26	1.33	1.37
48	35	313	A86	C25-C24	3.26	1.43	1.34
48	15	319	A86	C19-C18	3.26	1.57	1.52
48	20	311	A86	C25-C24	3.26	1.43	1.34
48	13	313	A86	C25-C24	3.26	1.43	1.34
48	33	313	A86	C25-C24	3.26	1.43	1.34
37	12	204	CLA	CHD-C4C	3.26	1.46	1.39
37	32	205	CLA	CHD-C4C	3.26	1.46	1.39
37	b	503	CLA	C3D-C2D	3.26	1.48	1.39
48	15	313	A86	C25-C24	3.26	1.43	1.34
47	36	304	KC1	C4B-NB	-3.26	1.33	1.37
37	B	516	CLA	C1C-NC	-3.26	1.32	1.37
47	17	303	KC1	CHC-C1C	3.25	1.46	1.39
37	c	511	CLA	C3D-C2D	3.25	1.48	1.39
48	38	213	A86	O-C13	-3.25	1.16	1.23
37	16	303	CLA	OBD-CAD	3.25	1.28	1.22
48	14	312	A86	C17-C18	-3.25	1.47	1.52
37	B	503	CLA	C3D-C2D	3.25	1.48	1.39
37	20	303	CLA	C3D-C2D	3.25	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	40	205	CLA	C3D-C2D	3.25	1.48	1.39
37	D	406	CLA	OBD-CAD	3.25	1.28	1.22
47	17	303	KC1	C4B-NB	-3.25	1.33	1.37
48	31	315	A86	C5-C6	3.25	1.40	1.35
37	B	502	CLA	OBD-CAD	3.25	1.28	1.22
47	14	306	KC1	C4B-NB	-3.25	1.33	1.37
37	B	505	CLA	C3D-C2D	3.25	1.48	1.39
37	b	515	CLA	OBD-CAD	3.25	1.28	1.22
48	15	313	A86	C19-C18	3.24	1.57	1.52
37	d	404	CLA	OBD-CAD	3.24	1.28	1.22
47	35	302	KC1	C4B-NB	-3.24	1.33	1.37
37	31	310	CLA	OBD-CAD	3.24	1.28	1.22
45	d	406	PL9	C52-C5	-3.24	1.43	1.50
47	20	304	KC1	C4B-NB	-3.24	1.33	1.37
37	b	502	CLA	OBD-CAD	3.24	1.28	1.22
37	B	524	CLA	OBD-CAD	3.24	1.28	1.22
37	C	510	CLA	OBD-CAD	3.24	1.28	1.22
37	d	401	CLA	OBD-CAD	3.24	1.28	1.22
47	37	307	KC1	C4B-NB	-3.23	1.33	1.37
48	34	312	A86	C17-C18	-3.23	1.47	1.52
37	d	403	CLA	C3D-C2D	3.23	1.47	1.39
37	A	405	CLA	OBD-CAD	3.23	1.28	1.22
37	b	523	CLA	OBD-CAD	3.23	1.28	1.22
37	C	504	CLA	OBD-CAD	3.23	1.28	1.22
37	a	407	CLA	OBD-CAD	3.23	1.28	1.22
48	21	213	A86	C25-C24	3.23	1.42	1.34
39	c	514	BCR	C30-C25	-3.23	1.49	1.53
37	B	512	CLA	CHD-C1D	3.23	1.44	1.38
47	21	203	KC1	C4B-NB	-3.23	1.33	1.37
48	15	316	A86	C19-C18	3.22	1.57	1.52
37	B	507	CLA	OBD-CAD	3.22	1.28	1.22
37	b	507	CLA	OBD-CAD	3.22	1.28	1.22
37	W	101	CLA	OBD-CAD	3.22	1.28	1.22
37	c	504	CLA	OBD-CAD	3.22	1.28	1.22
47	16	304	KC1	C4B-NB	-3.22	1.33	1.37
47	40	207	KC1	C4B-NB	-3.22	1.33	1.37
37	C	510	CLA	C1B-NB	-3.22	1.32	1.35
37	b	516	CLA	C1C-NC	-3.22	1.33	1.37
48	16	311	A86	C19-C18	3.22	1.57	1.52
48	15	312	A86	C25-C24	3.22	1.42	1.34
47	35	309	KC1	C4B-NB	-3.22	1.33	1.37
37	36	306	CLA	C1B-NB	-3.22	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	w	101	CLA	OBD-CAD	3.21	1.28	1.22
47	34	304	KC1	C4B-NB	-3.21	1.33	1.37
37	b	523	CLA	C1D-ND	3.21	1.41	1.37
50	41	216	DD6	C-C1	3.21	1.57	1.50
50	20	310	DD6	C-C1	3.21	1.57	1.50
37	D	405	CLA	C3D-C2D	3.21	1.47	1.39
48	12	214	A86	C25-C24	3.21	1.42	1.34
37	11	308	CLA	OBD-CAD	3.21	1.28	1.22
48	11	311	A86	C5-C6	3.21	1.40	1.35
48	31	311	A86	C5-C6	3.21	1.40	1.35
47	15	309	KC1	C4B-NB	-3.21	1.33	1.37
37	32	202	CLA	C1B-NB	-3.21	1.32	1.35
50	19	312	DD6	C-C1	3.20	1.57	1.50
39	C	514	BCR	C30-C25	-3.20	1.49	1.53
47	16	302	KC1	C2A-C1A	3.20	1.54	1.44
39	b	517	BCR	C30-C25	-3.20	1.49	1.53
48	41	213	A86	C25-C24	3.20	1.42	1.34
48	35	314	A86	C25-C24	3.20	1.42	1.34
48	34	315	A86	C19-C18	3.20	1.56	1.52
37	13	303	CLA	OBD-CAD	3.20	1.28	1.22
48	31	314	A86	C5-C6	3.20	1.40	1.35
37	c	510	CLA	C1B-NB	-3.19	1.32	1.35
51	19	315	LMU	O5'-C1'	3.19	1.50	1.41
48	35	312	A86	C25-C24	3.19	1.42	1.34
37	b	506	CLA	OBD-CAD	3.19	1.28	1.22
47	38	205	KC1	C4B-NB	-3.19	1.33	1.37
39	h	101	BCR	C1-C6	-3.19	1.49	1.53
40	40	202	SQD	O48-C23	3.19	1.42	1.33
48	36	311	A86	C19-C18	3.19	1.56	1.52
48	32	215	A86	C25-C24	3.19	1.42	1.34
48	14	315	A86	C19-C18	3.19	1.56	1.52
47	33	306	KC1	C4B-NB	-3.19	1.33	1.37
37	41	206	CLA	OBD-CAD	3.19	1.28	1.22
47	15	306	KC1	C4B-NB	-3.19	1.33	1.37
47	39	308	KC1	C4B-NB	-3.19	1.33	1.37
44	c	517	DGD	O1G-C1G	-3.19	1.37	1.45
47	12	206	KC1	C4B-NB	-3.19	1.33	1.37
47	32	207	KC1	C4B-NB	-3.19	1.33	1.37
37	B	506	CLA	OBD-CAD	3.19	1.28	1.22
37	c	512	CLA	C1B-NB	-3.19	1.32	1.35
37	B	509	CLA	OBD-CAD	3.19	1.28	1.22
48	13	314	A86	C25-C24	3.18	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	39	312	DD6	C-C1	3.18	1.57	1.50
44	C	517	DGD	O1G-C1G	-3.18	1.37	1.45
37	B	510	CLA	OBD-CAD	3.18	1.28	1.22
37	b	512	CLA	CHD-C1D	3.18	1.44	1.38
48	12	214	A86	C19-C18	3.18	1.56	1.52
37	b	510	CLA	C1B-NB	-3.18	1.32	1.35
48	11	315	A86	C5-C6	3.18	1.40	1.35
37	21	206	CLA	OBD-CAD	3.18	1.28	1.22
40	16	315	SQD	O48-C23	3.18	1.42	1.33
48	16	310	A86	C5-C6	3.18	1.40	1.35
47	34	306	KC1	C4B-NB	-3.18	1.33	1.37
48	15	314	A86	C25-C24	3.17	1.42	1.34
37	b	523	CLA	CHD-C4C	3.17	1.46	1.39
37	c	507	CLA	OBD-CAD	3.17	1.27	1.22
48	17	311	A86	C5-C6	3.17	1.40	1.35
37	a	404	CLA	C1B-NB	-3.17	1.32	1.35
47	36	302	KC1	C2A-C1A	3.17	1.54	1.44
37	b	505	CLA	OBD-CAD	3.17	1.27	1.22
50	21	216	DD6	C-C1	3.17	1.57	1.50
47	13	306	KC1	C4B-NB	-3.17	1.33	1.37
39	B	517	BCR	C30-C25	-3.17	1.49	1.53
37	C	507	CLA	C4B-NB	-3.16	1.32	1.35
47	18	205	KC1	C4B-NB	-3.16	1.33	1.37
37	B	510	CLA	C1B-NB	-3.16	1.32	1.35
37	A	403	CLA	OBD-CAD	3.16	1.27	1.22
48	36	310	A86	C19-C18	3.16	1.56	1.52
37	B	524	CLA	CHD-C4C	3.16	1.46	1.39
48	11	314	A86	C5-C6	3.16	1.40	1.35
48	35	316	A86	C19-C18	3.15	1.56	1.52
50	40	212	DD6	C-C1	3.15	1.57	1.50
37	b	510	CLA	OBD-CAD	3.15	1.27	1.22
37	c	506	CLA	OBD-CAD	3.15	1.27	1.22
47	17	306	KC1	CHC-C1C	3.15	1.46	1.39
47	37	305	KC1	CHC-C1C	3.15	1.46	1.39
48	33	314	A86	C25-C24	3.15	1.42	1.34
48	36	310	A86	C5-C6	3.15	1.40	1.35
37	B	513	CLA	C1B-NB	-3.15	1.32	1.35
37	C	512	CLA	C1B-NB	-3.15	1.32	1.35
37	C	507	CLA	OBD-CAD	3.15	1.27	1.22
48	21	215	A86	C19-C18	3.15	1.56	1.52
48	18	215	A86	C25-C24	3.15	1.42	1.34
40	17	301	SQD	O48-C23	3.15	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	D	407	BCR	C1-C6	-3.15	1.49	1.53
37	b	504	CLA	C3D-C2D	3.15	1.47	1.39
37	a	403	CLA	OBD-CAD	3.15	1.27	1.22
37	15	307	CLA	C1B-NB	-3.15	1.32	1.35
37	B	508	CLA	OBD-CAD	3.14	1.27	1.22
48	12	215	A86	C25-C24	3.14	1.42	1.34
44	c	517	DGD	O6D-C5D	-3.14	1.36	1.44
37	d	403	CLA	CHD-C1D	3.14	1.44	1.38
39	C	519	BCR	C30-C25	-3.14	1.49	1.53
40	36	315	SQD	O48-C23	3.14	1.42	1.33
44	C	517	DGD	O6D-C5D	-3.14	1.36	1.44
37	D	405	CLA	CHD-C1D	3.14	1.44	1.38
47	35	306	KC1	C4B-NB	-3.14	1.33	1.37
37	b	509	CLA	OBD-CAD	3.14	1.27	1.22
48	35	312	A86	C19-C18	3.14	1.56	1.52
37	B	524	CLA	C3D-C2D	3.14	1.47	1.39
48	21	214	A86	C25-C24	3.13	1.42	1.34
48	15	312	A86	C19-C18	3.13	1.56	1.52
37	B	505	CLA	OBD-CAD	3.13	1.27	1.22
37	17	304	CLA	OBD-CAD	3.13	1.27	1.22
37	b	504	CLA	C1B-NB	-3.13	1.32	1.35
37	b	512	CLA	C4B-NB	-3.13	1.32	1.35
37	B	511	CLA	OBD-CAD	3.13	1.27	1.22
37	b	508	CLA	OBD-CAD	3.13	1.27	1.22
48	37	311	A86	C25-C24	3.13	1.42	1.34
48	41	214	A86	C25-C24	3.13	1.42	1.34
37	b	523	CLA	C3D-C2D	3.13	1.47	1.39
37	D	401	CLA	C1B-NB	-3.13	1.32	1.35
51	39	315	LMU	O5'-C1'	3.13	1.49	1.41
37	B	504	CLA	C3D-C2D	3.13	1.47	1.39
39	B	525	BCR	C1-C6	-3.13	1.49	1.53
37	C	506	CLA	OBD-CAD	3.12	1.27	1.22
39	c	519	BCR	C30-C25	-3.12	1.49	1.53
47	20	302	KC1	C4B-NB	-3.12	1.33	1.37
37	B	504	CLA	OBD-CAD	3.12	1.27	1.22
37	C	501	CLA	OBD-CAD	3.12	1.27	1.22
37	c	507	CLA	C1B-NB	-3.12	1.32	1.35
37	b	511	CLA	OBD-CAD	3.12	1.27	1.22
48	32	221	A86	C2-C1	3.12	1.39	1.35
39	c	515	BCR	C1-C6	-3.12	1.49	1.53
37	B	504	CLA	C1B-NB	-3.12	1.32	1.35
37	37	303	CLA	OBD-CAD	3.11	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	31	307	KC1	C4B-NB	-3.11	1.34	1.37
37	15	308	CLA	OBD-CAD	3.11	1.27	1.22
48	41	215	A86	C25-C24	3.11	1.42	1.34
37	b	504	CLA	OBD-CAD	3.11	1.27	1.22
48	32	215	A86	C19-C18	3.11	1.56	1.52
37	c	501	CLA	OBD-CAD	3.11	1.27	1.22
48	32	216	A86	C25-C24	3.11	1.42	1.34
48	38	215	A86	C25-C24	3.11	1.42	1.34
47	19	308	KC1	C4B-NB	-3.10	1.34	1.37
48	12	220	A86	C2-C1	3.10	1.39	1.35
48	18	214	A86	C25-C24	3.10	1.42	1.34
37	C	509	CLA	OBD-CAD	3.10	1.27	1.22
37	17	307	CLA	C1B-NB	-3.10	1.32	1.35
39	b	524	BCR	C1-C6	-3.10	1.49	1.53
37	35	308	CLA	OBD-CAD	3.10	1.27	1.22
37	c	507	CLA	C4B-NB	-3.10	1.32	1.35
47	13	304	KC1	C4B-NB	-3.10	1.34	1.37
48	41	215	A86	C19-C18	3.10	1.56	1.52
37	B	514	CLA	C1B-NB	-3.10	1.32	1.35
48	14	314	A86	C25-C24	3.09	1.42	1.34
48	38	214	A86	C25-C24	3.09	1.42	1.34
48	21	215	A86	C25-C24	3.09	1.42	1.34
37	38	204	CLA	C3D-C2D	3.09	1.47	1.39
37	32	206	CLA	OBD-CAD	3.09	1.27	1.22
48	17	312	A86	C25-C24	3.09	1.42	1.34
48	34	314	A86	C25-C24	3.09	1.42	1.34
48	35	315	A86	C17-C18	-3.09	1.47	1.52
37	12	205	CLA	C1B-NB	-3.09	1.32	1.35
37	C	510	CLA	C3D-C4D	-3.09	1.37	1.44
39	d	405	BCR	C1-C6	-3.09	1.49	1.53
37	12	205	CLA	OBD-CAD	3.08	1.27	1.22
37	b	513	CLA	C1B-NB	-3.08	1.32	1.35
37	c	505	CLA	OBD-CAD	3.08	1.27	1.22
37	18	204	CLA	C3D-C2D	3.08	1.47	1.39
47	11	306	KC1	C4B-NB	-3.08	1.34	1.37
37	32	206	CLA	C1B-NB	-3.08	1.32	1.35
48	34	312	A86	C5-C6	3.08	1.39	1.35
37	c	510	CLA	C3D-C4D	-3.08	1.37	1.44
48	33	312	A86	C25-C24	3.08	1.42	1.34
39	a	408	BCR	C30-C25	-3.08	1.49	1.53
48	16	310	A86	C19-C18	3.08	1.56	1.52
47	35	304	KC1	C4B-NB	-3.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	37	306	CLA	C1B-NB	-3.07	1.32	1.35
37	c	509	CLA	OBD-CAD	3.07	1.27	1.22
37	35	307	CLA	C1B-NB	-3.07	1.32	1.35
48	19	313	A86	C14-C15	3.07	1.58	1.52
39	A	406	BCR	C30-C25	-3.07	1.49	1.53
37	B	512	CLA	C4B-NB	-3.07	1.32	1.35
37	b	512	CLA	OBD-CAD	3.07	1.27	1.22
48	31	319	A86	C5-C6	3.07	1.39	1.35
48	17	312	A86	C19-C18	3.06	1.56	1.52
48	36	313	A86	C19-C18	3.06	1.56	1.52
47	33	304	KC1	C4B-NB	-3.06	1.34	1.37
37	11	303	CLA	OBD-CAD	3.06	1.27	1.22
47	13	309	KC1	C4B-NB	-3.06	1.34	1.37
47	16	305	KC1	C4B-NB	-3.06	1.34	1.37
37	B	512	CLA	OBD-CAD	3.06	1.27	1.22
47	40	204	KC1	C4B-NB	-3.06	1.34	1.37
37	a	403	CLA	C3D-C2D	3.06	1.47	1.39
37	A	403	CLA	C3D-C2D	3.05	1.47	1.39
37	C	505	CLA	OBD-CAD	3.05	1.27	1.22
37	31	304	CLA	OBD-CAD	3.05	1.27	1.22
48	37	311	A86	C19-C18	3.05	1.56	1.52
39	C	515	BCR	C1-C6	-3.05	1.49	1.53
48	31	312	A86	O-C13	-3.05	1.16	1.23
47	36	305	KC1	C4B-NB	-3.05	1.34	1.37
48	11	311	A86	O-C13	-3.05	1.16	1.23
48	31	311	A86	O-C13	-3.05	1.16	1.23
48	13	312	A86	C25-C24	3.05	1.42	1.34
48	16	314	A86	C19-C18	3.04	1.56	1.52
48	13	315	A86	C19-C18	3.04	1.56	1.52
47	31	309	KC1	CHB-C4A	-3.03	1.32	1.39
37	c	508	CLA	OBD-CAD	3.03	1.27	1.22
48	34	316	A86	C19-C18	3.03	1.56	1.52
48	32	221	A86	C19-C18	3.03	1.56	1.52
48	41	213	A86	C14-C15	3.03	1.58	1.52
47	13	302	KC1	CHB-C4A	-3.02	1.32	1.39
37	C	508	CLA	OBD-CAD	3.02	1.27	1.22
37	b	514	CLA	C1B-NB	-3.02	1.32	1.35
48	14	312	A86	C5-C6	3.02	1.39	1.35
48	11	319	A86	C5-C6	3.02	1.39	1.35
47	15	304	KC1	C4B-NB	-3.01	1.34	1.37
50	21	216	DD6	C9-C8	3.01	1.42	1.34
47	16	302	KC1	C4B-NB	-3.01	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	14	316	A86	C19-C18	3.01	1.56	1.52
48	38	213	A86	C5-C6	3.01	1.39	1.35
48	21	213	A86	C14-C15	3.01	1.58	1.52
48	40	201	A86	C25-C24	3.01	1.42	1.34
48	17	320	A86	O-C13	-3.01	1.17	1.23
48	15	319	A86	C14-C15	3.01	1.58	1.52
48	18	212	A86	C25-C24	3.01	1.42	1.34
48	16	313	A86	C25-C24	3.01	1.42	1.34
48	35	316	A86	C25-C24	3.01	1.42	1.34
50	41	216	DD6	C9-C8	3.00	1.42	1.34
37	B	512	CLA	C1D-ND	3.00	1.41	1.37
37	B	512	CLA	C3D-C2D	3.00	1.47	1.39
37	13	307	CLA	OBD-CAD	3.00	1.27	1.22
48	35	319	A86	C14-C15	3.00	1.58	1.52
47	11	309	KC1	CHB-C4A	-3.00	1.32	1.39
47	14	309	KC1	CHB-C4A	-3.00	1.32	1.39
47	33	309	KC1	C4B-NB	-3.00	1.34	1.37
37	C	507	CLA	C1B-NB	-3.00	1.32	1.35
47	33	302	KC1	CHB-C4A	-2.99	1.32	1.39
37	33	307	CLA	OBD-CAD	2.99	1.27	1.22
37	c	511	CLA	OBD-CAD	2.99	1.27	1.22
48	38	212	A86	C25-C24	2.99	1.42	1.34
47	12	206	KC1	C4D-ND	2.99	1.37	1.35
37	b	503	CLA	OBD-CAD	2.99	1.27	1.22
37	b	512	CLA	C1D-ND	2.99	1.41	1.37
48	37	314	A86	C19-C18	2.99	1.56	1.52
44	c	516	DGD	O1G-C1G	-2.98	1.38	1.45
44	C	516	DGD	O1G-C1G	-2.98	1.38	1.45
50	40	214	DD6	C9-C8	2.98	1.42	1.34
47	34	309	KC1	CHB-C4A	-2.98	1.32	1.39
48	17	310	A86	C25-C24	2.98	1.42	1.34
48	33	315	A86	C19-C18	2.98	1.56	1.52
47	41	207	KC1	C4B-NB	-2.98	1.34	1.37
48	11	312	A86	C5-C6	2.98	1.39	1.35
48	35	312	A86	O-C13	-2.98	1.17	1.23
46	f	101	HEM	CAB-C3B	2.98	1.55	1.47
48	31	313	A86	C25-C24	2.98	1.42	1.34
48	34	313	A86	C19-C18	2.98	1.56	1.52
40	L	101	SQD	O48-C23	2.97	1.42	1.33
50	21	212	DD6	C9-C8	2.97	1.42	1.34
48	11	312	A86	O-C13	-2.97	1.17	1.23
37	C	505	CLA	C3D-C2D	2.97	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	15	316	A86	C14-C15	2.97	1.58	1.52
48	40	211	A86	C25-C24	2.97	1.42	1.34
47	36	302	KC1	C4B-NB	-2.97	1.34	1.37
48	16	314	A86	C5-C6	2.97	1.39	1.35
48	13	315	A86	C25-C24	2.97	1.42	1.34
50	19	312	DD6	O2-C18	2.97	1.52	1.43
50	39	312	DD6	O2-C18	2.97	1.52	1.43
48	37	309	A86	C25-C24	2.97	1.42	1.34
37	a	407	CLA	C1B-NB	-2.97	1.32	1.35
43	d	408	LHG	O7-C5	-2.97	1.39	1.46
48	31	312	A86	C5-C6	2.97	1.39	1.35
47	38	207	KC1	C4B-NB	-2.97	1.34	1.37
48	36	313	A86	C5-C6	2.97	1.39	1.35
48	12	217	A86	C25-C24	2.97	1.42	1.34
48	32	218	A86	C25-C24	2.97	1.42	1.34
37	B	512	CLA	CHD-C4C	2.97	1.46	1.39
50	20	312	DD6	C9-C8	2.96	1.42	1.34
40	B	519	SQD	O48-C23	2.96	1.42	1.33
37	B	506	CLA	CHD-C4C	2.96	1.46	1.39
48	17	313	A86	C25-C24	2.96	1.42	1.34
50	21	212	DD6	C-C1	2.96	1.57	1.50
48	37	312	A86	C25-C24	2.96	1.42	1.34
48	15	316	A86	C25-C24	2.96	1.42	1.34
37	c	502	CLA	C1B-NB	-2.96	1.32	1.35
48	17	315	A86	C19-C18	2.96	1.56	1.52
46	F	101	HEM	CAB-C3B	2.96	1.55	1.47
48	37	314	A86	C25-C24	2.96	1.42	1.34
50	41	212	DD6	C9-C8	2.96	1.42	1.34
37	b	512	CLA	C3D-C2D	2.95	1.47	1.39
37	C	511	CLA	C1B-NB	-2.95	1.32	1.35
37	b	512	CLA	C3D-C4D	-2.95	1.37	1.44
50	41	212	DD6	C-C1	2.95	1.57	1.50
37	c	509	CLA	C4B-NB	-2.95	1.32	1.35
48	17	314	A86	O-C13	-2.95	1.17	1.23
48	18	214	A86	C14-C15	2.95	1.58	1.52
37	b	512	CLA	CHD-C4C	2.95	1.46	1.39
39	A	406	BCR	C1-C6	-2.95	1.49	1.53
43	D	410	LHG	O7-C5	-2.95	1.39	1.46
48	12	214	A86	C5-C6	2.95	1.39	1.35
48	11	314	A86	C25-C24	2.95	1.42	1.34
47	41	207	KC1	CHB-C4A	-2.95	1.32	1.39
48	14	313	A86	C19-C18	2.95	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	506	CLA	CHD-C4C	2.95	1.46	1.39
48	12	215	A86	O-C13	-2.95	1.17	1.23
37	c	505	CLA	C3D-C2D	2.94	1.47	1.39
47	32	207	KC1	C4D-ND	2.94	1.37	1.35
48	33	315	A86	C25-C24	2.94	1.42	1.34
48	32	215	A86	O-C13	-2.94	1.17	1.23
48	40	213	A86	C14-C15	2.94	1.58	1.52
37	B	503	CLA	OBD-CAD	2.94	1.27	1.22
37	B	512	CLA	C3D-C4D	-2.94	1.37	1.44
37	a	407	CLA	C3D-C4D	-2.94	1.37	1.44
37	d	403	CLA	OBD-CAD	2.94	1.27	1.22
48	16	311	A86	C25-C24	2.94	1.42	1.34
48	32	215	A86	C5-C6	2.94	1.39	1.35
37	D	405	CLA	OBD-CAD	2.94	1.27	1.22
37	C	511	CLA	OBD-CAD	2.94	1.27	1.22
37	B	502	CLA	C1B-NB	-2.93	1.32	1.35
37	D	405	CLA	C1B-NB	-2.93	1.32	1.35
47	18	207	KC1	C4B-NB	-2.93	1.34	1.37
48	20	309	A86	C25-C24	2.93	1.42	1.34
48	12	220	A86	C19-C18	2.93	1.56	1.52
37	D	402	CLA	C1B-NB	-2.93	1.32	1.35
37	D	406	CLA	C1B-NB	-2.93	1.32	1.35
48	17	315	A86	C25-C24	2.93	1.42	1.34
48	35	315	A86	C25-C24	2.93	1.42	1.34
48	35	319	A86	C25-C24	2.93	1.42	1.34
48	15	312	A86	O-C13	-2.93	1.17	1.23
48	37	311	A86	C14-C15	2.93	1.58	1.52
48	35	313	A86	C24-C1	2.93	1.52	1.45
48	12	214	A86	O-C13	-2.93	1.17	1.23
37	d	401	CLA	C1B-NB	-2.93	1.32	1.35
48	20	311	A86	C14-C15	2.93	1.58	1.52
48	31	314	A86	C25-C24	2.92	1.42	1.34
37	A	403	CLA	C3D-C4D	-2.92	1.37	1.44
48	15	315	A86	C25-C24	2.92	1.42	1.34
46	V	201	HEM	CAB-C3B	2.92	1.55	1.47
46	v	201	HEM	CAB-C3B	2.92	1.55	1.47
48	15	319	A86	C25-C24	2.92	1.42	1.34
47	21	207	KC1	CHB-C4A	-2.92	1.32	1.39
48	37	313	A86	O-C13	-2.92	1.17	1.23
37	a	403	CLA	C3D-C4D	-2.92	1.37	1.44
48	35	314	A86	C14-C15	2.92	1.58	1.52
37	a	403	CLA	C4B-NB	-2.92	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	15	313	A86	C24-C1	2.92	1.52	1.45
40	B	522	SQD	O48-C23	2.92	1.41	1.33
39	C	519	BCR	C1-C6	-2.91	1.49	1.53
48	12	216	A86	C25-C24	2.91	1.42	1.34
37	A	405	CLA	C1B-NB	-2.91	1.32	1.35
47	17	303	KC1	C2A-C1A	2.91	1.53	1.44
48	36	311	A86	C5-C6	2.91	1.39	1.35
37	B	513	CLA	OBD-CAD	2.91	1.27	1.22
48	31	313	A86	C19-C18	2.90	1.56	1.52
37	C	502	CLA	C1C-NC	-2.90	1.33	1.37
48	41	211	A86	C14-C15	2.90	1.58	1.52
48	36	311	A86	C25-C24	2.90	1.42	1.34
48	32	217	A86	C25-C24	2.90	1.42	1.34
37	C	502	CLA	C1B-NB	-2.90	1.32	1.35
48	33	313	A86	C24-C1	2.90	1.52	1.45
48	17	311	A86	C25-C24	2.90	1.42	1.34
48	38	214	A86	C14-C15	2.90	1.58	1.52
39	a	413	BCR	C1-C6	-2.90	1.49	1.53
37	38	211	CLA	C4C-C3C	2.90	1.50	1.45
37	C	509	CLA	C4B-NB	-2.90	1.32	1.35
40	b	521	SQD	O48-C23	2.89	1.41	1.33
48	17	312	A86	C14-C15	2.89	1.58	1.52
50	39	312	DD6	C26-C27	-2.89	1.30	1.37
45	d	406	PL9	C7-C8	-2.89	1.46	1.50
48	21	213	A86	C24-C1	2.89	1.52	1.45
37	d	404	CLA	C1B-NB	-2.89	1.32	1.35
48	41	213	A86	C24-C1	2.89	1.52	1.45
37	d	403	CLA	C1B-NB	-2.89	1.32	1.35
39	A	410	BCR	C1-C6	-2.89	1.49	1.53
48	14	313	A86	C14-C15	2.89	1.58	1.52
48	34	313	A86	C14-C15	2.89	1.58	1.52
47	12	206	KC1	CHB-C4A	-2.89	1.32	1.39
47	32	207	KC1	CHB-C4A	-2.89	1.32	1.39
47	37	302	KC1	C2A-C1A	2.89	1.53	1.44
50	19	312	DD6	C26-C27	-2.89	1.30	1.37
48	13	313	A86	C24-C1	2.88	1.52	1.45
37	18	206	CLA	C1B-NB	-2.88	1.32	1.35
39	C	514	BCR	C1-C6	-2.88	1.49	1.53
48	41	211	A86	C25-C24	2.88	1.42	1.34
48	32	216	A86	O-C13	-2.88	1.17	1.23
48	11	313	A86	C19-C18	2.88	1.56	1.52
47	21	207	KC1	C4B-NB	-2.88	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	518	BCR	C1-C6	-2.88	1.49	1.53
48	14	313	A86	C24-C1	2.88	1.52	1.45
37	b	501	CLA	C1B-NB	-2.88	1.32	1.35
37	c	511	CLA	C1B-NB	-2.88	1.32	1.35
37	A	405	CLA	C3D-C4D	-2.87	1.37	1.44
37	b	502	CLA	C1B-NB	-2.87	1.32	1.35
37	C	510	CLA	C3D-C2D	2.87	1.47	1.39
37	c	509	CLA	C3D-C4D	-2.87	1.37	1.44
40	a	409	SQD	O48-C23	2.87	1.41	1.33
48	21	211	A86	C14-C15	2.87	1.58	1.52
47	16	308	KC1	C4A-C3A	2.87	1.50	1.44
39	b	518	BCR	C1-C6	-2.87	1.49	1.53
48	14	314	A86	C14-C15	2.87	1.58	1.52
48	34	314	A86	C14-C15	2.87	1.58	1.52
37	b	513	CLA	OBD-CAD	2.87	1.27	1.22
48	11	312	A86	C25-C24	2.87	1.42	1.34
40	A	407	SQD	O48-C23	2.86	1.41	1.33
48	16	311	A86	C5-C6	2.86	1.39	1.35
37	W	101	CLA	C1B-NB	-2.86	1.32	1.35
37	A	403	CLA	C4B-NB	-2.86	1.32	1.35
37	b	504	CLA	C3D-C4D	-2.86	1.37	1.44
47	36	308	KC1	C4A-C3A	2.86	1.50	1.44
37	B	504	CLA	C3D-C4D	-2.86	1.37	1.44
48	35	316	A86	C14-C15	2.85	1.58	1.52
37	c	510	CLA	C3D-C2D	2.85	1.46	1.39
39	a	408	BCR	C1-C6	-2.85	1.49	1.53
37	b	511	CLA	C4B-NB	-2.85	1.32	1.35
47	32	212	KC1	CHB-C4A	-2.85	1.32	1.39
47	40	206	KC1	C4A-C3A	2.85	1.50	1.44
48	15	312	A86	C24-C1	2.85	1.52	1.45
37	17	304	CLA	C1B-NB	-2.85	1.32	1.35
47	12	211	KC1	CHB-C4A	-2.85	1.32	1.39
37	c	503	CLA	C1B-NB	-2.85	1.32	1.35
37	B	502	CLA	C3D-C4D	-2.85	1.37	1.44
48	15	314	A86	C14-C15	2.85	1.58	1.52
37	B	515	CLA	C1B-NB	-2.85	1.32	1.35
37	C	501	CLA	C1B-NB	-2.85	1.32	1.35
48	19	313	A86	C17-C18	-2.84	1.48	1.52
48	31	319	A86	C19-C18	2.84	1.56	1.52
37	C	509	CLA	C3D-C4D	-2.84	1.37	1.44
44	J	101	DGD	O2G-C2G	-2.84	1.39	1.46
40	L	101	SQD	O47-C7	2.84	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	525	BCR	C30-C25	-2.84	1.49	1.53
48	15	315	A86	C14-C15	2.84	1.58	1.52
47	16	302	KC1	C4A-C3A	2.84	1.50	1.44
48	11	319	A86	C19-C18	2.84	1.56	1.52
37	c	511	CLA	C3D-C4D	-2.84	1.37	1.44
48	37	310	A86	O-C13	-2.84	1.17	1.23
48	33	314	A86	C-C1	2.84	1.56	1.50
48	34	313	A86	C24-C1	2.84	1.52	1.45
47	20	304	KC1	C4A-C3A	2.84	1.50	1.44
37	C	503	CLA	C1B-NB	-2.84	1.32	1.35
37	c	502	CLA	C1C-NC	-2.83	1.33	1.37
44	j	101	DGD	O2G-C2G	-2.83	1.39	1.46
45	D	408	PL9	C7-C8	-2.83	1.46	1.50
50	21	216	DD6	C35-C36	2.83	1.55	1.51
39	b	524	BCR	C30-C25	-2.83	1.49	1.53
37	B	501	CLA	C1B-NB	-2.83	1.32	1.35
37	37	303	CLA	C1B-NB	-2.83	1.32	1.35
40	B	519	SQD	O47-C7	2.83	1.42	1.34
47	18	210	KC1	C4B-NB	-2.83	1.34	1.37
47	16	308	KC1	C2A-C1A	2.83	1.53	1.44
48	21	211	A86	C25-C24	2.83	1.41	1.34
48	31	312	A86	C25-C24	2.83	1.41	1.34
39	c	514	BCR	C1-C6	-2.83	1.49	1.53
48	11	319	A86	O-C13	-2.83	1.17	1.23
50	41	216	DD6	C35-C36	2.83	1.55	1.51
47	38	210	KC1	C4B-NB	-2.83	1.34	1.37
38	a	405	PHO	CAC-C3C	-2.83	1.47	1.52
47	36	302	KC1	C4A-C3A	2.83	1.50	1.44
37	B	510	CLA	C1C-NC	-2.82	1.33	1.37
37	11	303	CLA	C4B-NB	-2.82	1.32	1.35
37	31	304	CLA	C4B-NB	-2.82	1.32	1.35
47	15	309	KC1	C2A-C1A	2.82	1.53	1.44
48	17	311	A86	O-C13	-2.82	1.17	1.23
48	15	311	A86	C25-C24	2.82	1.41	1.34
48	35	315	A86	O-C13	-2.82	1.17	1.23
37	b	502	CLA	C3D-C4D	-2.82	1.37	1.44
37	C	511	CLA	C3D-C4D	-2.82	1.37	1.44
37	D	402	CLA	C3D-C4D	-2.82	1.37	1.44
48	21	214	A86	C14-C15	2.82	1.58	1.52
39	c	519	BCR	C1-C6	-2.82	1.49	1.53
47	17	306	KC1	C2A-C1A	2.82	1.53	1.44
47	37	305	KC1	C2A-C1A	2.82	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	39	313	A86	C25-C24	2.82	1.41	1.34
38	D	403	PHO	CAC-C3C	-2.82	1.47	1.52
48	31	313	A86	O-C13	-2.82	1.17	1.23
48	13	311	A86	C25-C24	2.81	1.41	1.34
48	31	314	A86	O-C13	-2.81	1.17	1.23
41	c	518	LMG	O1-C7	-2.81	1.38	1.43
37	b	510	CLA	C1C-NC	-2.81	1.33	1.37
48	35	312	A86	C24-C1	2.81	1.52	1.45
48	19	313	A86	C25-C24	2.81	1.41	1.34
47	12	208	KC1	C2A-C1A	2.81	1.53	1.44
48	31	319	A86	O-C13	-2.81	1.17	1.23
48	33	314	A86	C24-C1	2.81	1.52	1.45
47	36	308	KC1	C2A-C1A	2.81	1.53	1.44
48	18	213	A86	C25-C24	2.80	1.41	1.34
48	13	314	A86	C-C1	2.80	1.56	1.50
37	31	304	CLA	C1B-NB	-2.80	1.32	1.35
47	35	309	KC1	C2A-C1A	2.80	1.53	1.44
48	41	214	A86	C14-C15	2.80	1.58	1.52
37	B	503	CLA	C3D-C4D	-2.80	1.37	1.44
48	11	314	A86	O-C13	-2.80	1.17	1.23
48	15	315	A86	O-C13	-2.80	1.17	1.23
48	38	213	A86	C25-C24	2.80	1.41	1.34
48	37	319	A86	C25-C24	2.80	1.41	1.34
37	w	101	CLA	C1B-NB	-2.80	1.32	1.35
48	14	316	A86	C25-C24	2.80	1.41	1.34
48	34	316	A86	C25-C24	2.80	1.41	1.34
47	41	203	KC1	C2A-C1A	2.80	1.53	1.44
48	40	213	A86	C24-C1	2.80	1.51	1.45
48	21	215	A86	C24-C1	2.79	1.51	1.45
37	19	309	CLA	C1B-NB	-2.79	1.32	1.35
37	b	510	CLA	C3D-C4D	-2.79	1.37	1.44
48	17	320	A86	C25-C24	2.79	1.41	1.34
48	13	314	A86	C24-C1	2.79	1.51	1.45
37	C	507	CLA	C3D-C4D	-2.79	1.37	1.44
43	a	412	LHG	O8-C6	-2.79	1.38	1.45
48	33	311	A86	C25-C24	2.79	1.41	1.34
47	40	204	KC1	CHB-C4A	-2.79	1.32	1.39
37	d	401	CLA	C3D-C4D	-2.79	1.37	1.44
48	14	312	A86	C14-C15	2.79	1.58	1.52
43	D	411	LHG	O8-C6	-2.78	1.38	1.45
48	14	312	A86	O-C13	-2.78	1.17	1.23
48	34	312	A86	O-C13	-2.78	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	11	315	A86	O-C13	-2.78	1.17	1.23
47	21	203	KC1	C2A-C1A	2.78	1.53	1.44
48	34	312	A86	C14-C15	2.78	1.58	1.52
48	37	313	A86	C25-C24	2.78	1.41	1.34
37	b	515	CLA	C1B-NB	-2.78	1.32	1.35
48	11	313	A86	O-C13	-2.78	1.17	1.23
48	14	311	A86	C5-C6	2.78	1.39	1.35
37	c	507	CLA	C3D-C4D	-2.78	1.37	1.44
50	36	312	DD6	C35-C36	2.78	1.55	1.51
37	b	515	CLA	C3D-C4D	-2.78	1.37	1.44
50	41	216	DD6	C26-C27	-2.78	1.31	1.37
48	35	315	A86	C14-C15	2.78	1.58	1.52
37	B	514	CLA	C3D-C4D	-2.78	1.37	1.44
47	41	203	KC1	C4A-C3A	2.78	1.49	1.44
48	33	312	A86	C24-C1	2.78	1.51	1.45
50	21	216	DD6	C26-C27	-2.78	1.31	1.37
48	11	315	A86	C25-C24	2.78	1.41	1.34
37	B	510	CLA	C3D-C4D	-2.77	1.37	1.44
48	34	313	A86	C-C1	2.77	1.56	1.50
41	C	518	LMG	O1-C7	-2.77	1.38	1.43
47	32	209	KC1	C2A-C1A	2.77	1.53	1.44
41	a	410	LMG	O7-C8	-2.77	1.39	1.46
48	16	311	A86	C14-C15	2.77	1.58	1.52
48	35	312	A86	C-C1	2.77	1.56	1.50
47	35	309	KC1	C4A-C3A	2.77	1.49	1.44
48	36	310	A86	O-C13	-2.77	1.17	1.23
37	38	203	CLA	C4D-CHA	2.77	1.48	1.38
47	38	210	KC1	C4A-C3A	2.77	1.49	1.44
41	A	408	LMG	O7-C8	-2.77	1.39	1.46
40	17	301	SQD	O47-C7	2.77	1.42	1.34
47	21	203	KC1	C4A-C3A	2.77	1.49	1.44
48	13	312	A86	C24-C1	2.77	1.51	1.45
37	c	501	CLA	C1B-NB	-2.77	1.32	1.35
48	37	312	A86	C14-C15	2.77	1.58	1.52
50	19	312	DD6	C35-C34	2.77	1.57	1.52
48	34	311	A86	C5-C6	2.77	1.39	1.35
48	33	313	A86	C-C1	2.77	1.56	1.50
50	19	312	DD6	C9-C8	2.77	1.41	1.34
37	B	511	CLA	C4B-NB	-2.77	1.32	1.35
37	39	309	CLA	C1B-NB	-2.77	1.32	1.35
48	16	310	A86	O-C13	-2.77	1.17	1.23
47	20	302	KC1	CHB-C4A	-2.77	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	32	216	A86	C14-C15	2.77	1.58	1.52
47	15	309	KC1	C4A-C3A	2.77	1.49	1.44
37	18	203	CLA	C4D-CHA	2.77	1.48	1.38
37	b	508	CLA	C3D-C4D	-2.76	1.37	1.44
48	35	311	A86	C25-C24	2.76	1.41	1.34
50	20	310	DD6	C9-C8	2.76	1.41	1.34
47	36	302	KC1	C4D-CHA	2.76	1.48	1.45
48	15	314	A86	C-C1	2.76	1.56	1.50
47	34	304	KC1	CHB-C4A	-2.76	1.32	1.39
37	b	505	CLA	C1B-NB	-2.76	1.32	1.35
37	B	507	CLA	C1C-NC	-2.76	1.33	1.37
47	16	305	KC1	C4A-C3A	2.76	1.49	1.44
48	37	310	A86	C25-C24	2.76	1.41	1.34
48	37	312	A86	C-C1	2.76	1.56	1.50
50	39	312	DD6	C9-C8	2.76	1.41	1.34
47	37	307	KC1	C2A-C1A	2.75	1.53	1.44
37	B	508	CLA	C3D-C4D	-2.75	1.38	1.44
50	39	312	DD6	C35-C34	2.75	1.57	1.52
37	b	516	CLA	C3D-C4D	-2.75	1.38	1.44
48	15	319	A86	C-C1	2.75	1.56	1.50
48	20	311	A86	C24-C1	2.75	1.51	1.45
37	31	306	CLA	C1B-NB	-2.75	1.32	1.35
37	D	405	CLA	C3D-C4D	-2.75	1.38	1.44
48	17	313	A86	C-C1	2.75	1.56	1.50
37	b	503	CLA	C3D-C4D	-2.75	1.38	1.44
50	36	312	DD6	C9-C8	2.75	1.41	1.34
48	38	214	A86	C-C1	2.75	1.56	1.50
37	c	506	CLA	C3D-C4D	-2.75	1.38	1.44
48	31	315	A86	O-C13	-2.75	1.17	1.23
48	17	312	A86	C-C1	2.75	1.56	1.50
47	17	308	KC1	C2A-C1A	2.74	1.53	1.44
50	16	312	DD6	C9-C8	2.74	1.41	1.34
37	b	505	CLA	C3D-C4D	-2.74	1.38	1.44
37	B	515	CLA	C3D-C4D	-2.74	1.38	1.44
48	11	313	A86	C25-C24	2.74	1.41	1.34
48	35	314	A86	C-C1	2.74	1.56	1.50
48	32	203	A86	C19-C18	2.74	1.56	1.52
47	18	210	KC1	C2A-C1A	2.74	1.53	1.44
47	16	302	KC1	C4D-CHA	2.74	1.48	1.45
37	33	307	CLA	C3D-C4D	-2.74	1.38	1.44
48	12	217	A86	C19-C18	2.74	1.56	1.52
48	17	313	A86	C14-C15	2.74	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	15	312	A86	C-C1	2.74	1.56	1.50
47	18	210	KC1	C4A-C3A	2.74	1.49	1.44
37	B	516	CLA	C3D-C4D	-2.74	1.38	1.44
47	11	304	KC1	CHB-C4A	-2.74	1.33	1.39
47	17	308	KC1	CHB-C4A	-2.74	1.33	1.39
47	31	305	KC1	CHB-C4A	-2.74	1.33	1.39
47	37	307	KC1	CHB-C4A	-2.74	1.33	1.39
50	40	212	DD6	C9-C8	2.74	1.41	1.34
48	14	314	A86	C-C1	2.73	1.56	1.50
48	34	314	A86	C-C1	2.73	1.56	1.50
47	36	305	KC1	C4A-C3A	2.73	1.49	1.44
48	17	314	A86	C25-C24	2.73	1.41	1.34
48	17	313	A86	O-C13	-2.73	1.17	1.23
37	d	403	CLA	C3D-C4D	-2.73	1.38	1.44
37	12	210	CLA	C1B-NB	-2.73	1.32	1.35
48	31	315	A86	C25-C24	2.73	1.41	1.34
37	C	506	CLA	C3D-C4D	-2.73	1.38	1.44
37	d	404	CLA	C3D-C4D	-2.73	1.38	1.44
48	12	216	A86	O-C13	-2.73	1.17	1.23
37	b	514	CLA	C3D-C4D	-2.73	1.38	1.44
48	12	215	A86	C14-C15	2.73	1.58	1.52
47	38	207	KC1	C2A-C1A	2.73	1.53	1.44
48	18	214	A86	C-C1	2.73	1.56	1.50
47	12	208	KC1	CHB-C4A	-2.73	1.33	1.39
45	d	402	PL9	C3-C4	-2.73	1.45	1.49
50	16	312	DD6	C35-C36	2.73	1.55	1.51
37	B	507	CLA	C3D-C4D	-2.73	1.38	1.44
37	C	501	CLA	C3D-C4D	-2.73	1.38	1.44
37	13	307	CLA	C3D-C4D	-2.73	1.38	1.44
37	B	505	CLA	C3D-C4D	-2.73	1.38	1.44
39	5	101	BCR	C30-C25	-2.73	1.50	1.53
48	41	215	A86	C24-C1	2.72	1.51	1.45
48	12	215	A86	C-C1	2.72	1.56	1.50
37	c	505	CLA	C3D-C4D	-2.72	1.38	1.44
47	32	209	KC1	CHB-C4A	-2.72	1.33	1.39
47	33	304	KC1	CHB-C4A	-2.72	1.33	1.39
48	37	311	A86	C-C1	2.72	1.56	1.50
48	33	312	A86	O-C13	-2.72	1.17	1.23
48	32	216	A86	C24-C1	2.72	1.51	1.45
47	38	210	KC1	C2A-C1A	2.72	1.53	1.44
48	35	319	A86	C-C1	2.72	1.56	1.50
37	B	511	CLA	C3D-C4D	-2.72	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	19	304	CLA	C4C-C3C	2.72	1.49	1.45
40	36	315	SQD	O47-C7	2.72	1.42	1.34
44	c	517	DGD	O5D-C6D	-2.72	1.38	1.43
37	D	406	CLA	C3D-C4D	-2.72	1.38	1.44
37	C	510	CLA	C4B-NB	-2.72	1.32	1.35
37	B	505	CLA	C1B-NB	-2.72	1.32	1.35
47	14	304	KC1	CHB-C4A	-2.71	1.33	1.39
48	35	313	A86	O-C13	-2.71	1.17	1.23
39	0	101	BCR	C1-C6	-2.71	1.50	1.53
37	c	501	CLA	C3D-C4D	-2.71	1.38	1.44
48	14	315	A86	O-C13	-2.71	1.17	1.23
47	17	306	KC1	C4A-C3A	2.71	1.49	1.44
47	11	302	KC1	C2A-C1A	2.71	1.53	1.44
37	11	303	CLA	C1B-NB	-2.71	1.32	1.35
48	16	310	A86	C14-C15	2.71	1.58	1.52
47	37	305	KC1	C4A-C3A	2.71	1.49	1.44
48	12	202	A86	C19-C18	2.71	1.56	1.52
48	37	314	A86	O-C13	-2.71	1.17	1.23
37	39	304	CLA	C4C-C3C	2.71	1.49	1.45
48	14	313	A86	C-C1	2.71	1.56	1.50
37	B	516	CLA	OBD-CAD	2.71	1.27	1.22
48	41	215	A86	C-C1	2.71	1.56	1.50
45	D	404	PL9	C3-C4	-2.71	1.45	1.49
37	13	308	CLA	C1B-NB	-2.71	1.32	1.35
41	c	518	LMG	O8-C9	-2.70	1.39	1.45
48	13	313	A86	C-C1	2.70	1.56	1.50
44	C	517	DGD	O5D-C6D	-2.70	1.38	1.43
48	19	311	A86	C14-C15	2.70	1.58	1.52
48	36	310	A86	C14-C15	2.70	1.58	1.52
48	37	309	A86	C14-C15	2.70	1.58	1.52
48	39	311	A86	C14-C15	2.70	1.58	1.52
48	18	213	A86	C-C1	2.70	1.56	1.50
47	16	304	KC1	CHB-C4A	-2.70	1.33	1.39
44	j	101	DGD	O3D-C3D	-2.70	1.36	1.43
48	32	203	A86	O-C13	-2.70	1.17	1.23
47	36	304	KC1	CHB-C4A	-2.70	1.33	1.39
48	17	310	A86	C14-C15	2.70	1.58	1.52
48	15	313	A86	C-C1	2.70	1.56	1.50
48	35	313	A86	C-C1	2.70	1.56	1.50
48	40	211	A86	C14-C15	2.70	1.58	1.52
48	36	311	A86	C14-C15	2.70	1.58	1.52
48	37	314	A86	C-C1	2.70	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	20	303	CLA	C1B-NB	-2.70	1.32	1.35
47	31	303	KC1	C2A-C1A	2.70	1.52	1.44
37	D	401	CLA	C3D-C4D	-2.70	1.38	1.44
48	21	214	A86	C-C1	2.70	1.56	1.50
47	37	302	KC1	C4A-C3A	2.69	1.49	1.44
37	38	204	CLA	C3D-C4D	-2.69	1.38	1.44
37	12	212	CLA	C4D-CHA	2.69	1.48	1.38
37	18	209	CLA	C4D-CHA	2.69	1.48	1.38
41	D	412	LMG	O7-C8	-2.69	1.39	1.46
37	40	205	CLA	C3D-C4D	-2.69	1.38	1.44
37	32	213	CLA	C4D-CHA	2.69	1.48	1.38
48	21	215	A86	C-C1	2.69	1.56	1.50
37	b	516	CLA	OBD-CAD	2.69	1.27	1.22
48	20	309	A86	C14-C15	2.69	1.58	1.52
37	B	524	CLA	C3D-C4D	-2.69	1.38	1.44
48	19	311	A86	O-C13	-2.69	1.17	1.23
37	18	204	CLA	C3D-C4D	-2.69	1.38	1.44
39	0	101	BCR	C30-C25	-2.69	1.50	1.53
37	15	305	CLA	C4D-CHA	2.69	1.47	1.38
47	33	306	KC1	CHB-C4A	-2.69	1.33	1.39
47	40	207	KC1	C4C-C3C	2.69	1.49	1.45
47	13	304	KC1	CHB-C4A	-2.69	1.33	1.39
48	15	313	A86	O-C13	-2.69	1.17	1.23
48	32	221	A86	C5-C6	2.69	1.39	1.35
48	32	214	A86	O-C13	-2.69	1.17	1.23
37	D	401	CLA	C4B-NB	-2.68	1.32	1.35
37	C	505	CLA	C3D-C4D	-2.68	1.38	1.44
37	b	513	CLA	C3D-C4D	-2.68	1.38	1.44
48	18	215	A86	C-C1	2.68	1.56	1.50
37	17	309	CLA	C4C-C3C	2.68	1.49	1.45
48	32	217	A86	O-C13	-2.68	1.17	1.23
47	13	304	KC1	C2A-C1A	2.68	1.52	1.44
48	39	313	A86	O-C13	-2.68	1.17	1.23
48	35	316	A86	C-C1	2.68	1.56	1.50
47	16	305	KC1	C2A-C1A	2.68	1.52	1.44
37	35	305	CLA	C4D-CHA	2.68	1.47	1.38
37	C	504	CLA	C1B-NB	-2.68	1.32	1.35
37	c	504	CLA	C1B-NB	-2.68	1.32	1.35
37	20	303	CLA	C3D-C4D	-2.68	1.38	1.44
44	C	517	DGD	O2G-C2G	-2.68	1.39	1.46
44	c	517	DGD	O2G-C2G	-2.68	1.39	1.46
48	32	216	A86	C-C1	2.68	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	12	206	KC1	C2A-C1A	2.68	1.52	1.44
47	32	207	KC1	C2A-C1A	2.68	1.52	1.44
37	41	208	CLA	C4D-CHA	2.68	1.47	1.38
37	38	209	CLA	C4D-CHA	2.68	1.47	1.38
39	5	101	BCR	C1-C6	-2.68	1.50	1.53
48	36	311	A86	O-C13	-2.68	1.17	1.23
47	18	207	KC1	C2A-C1A	2.68	1.52	1.44
48	34	315	A86	C25-C24	2.68	1.41	1.34
48	35	316	A86	C24-C1	2.68	1.51	1.45
37	14	302	CLA	C4D-CHA	2.68	1.47	1.38
37	b	511	CLA	C3D-C4D	-2.68	1.38	1.44
37	c	510	CLA	C4B-NB	-2.68	1.32	1.35
41	d	409	LMG	O7-C8	-2.68	1.39	1.46
47	33	304	KC1	C2A-C1A	2.68	1.52	1.44
48	32	218	A86	O-C13	-2.68	1.17	1.23
41	C	518	LMG	O8-C9	-2.68	1.39	1.45
48	34	315	A86	O-C13	-2.68	1.17	1.23
48	34	313	A86	O-C13	-2.67	1.17	1.23
37	19	306	CLA	C1B-NB	-2.67	1.32	1.35
48	18	215	A86	C24-C1	2.67	1.51	1.45
48	41	214	A86	C24-C1	2.67	1.51	1.45
47	37	304	KC1	C4A-C3A	2.67	1.49	1.44
44	J	101	DGD	O3D-C3D	-2.67	1.36	1.43
47	35	302	KC1	C2A-C1A	2.67	1.52	1.44
48	38	215	A86	C-C1	2.67	1.56	1.50
48	15	316	A86	C-C1	2.67	1.56	1.50
37	b	523	CLA	C3D-C4D	-2.67	1.38	1.44
48	37	319	A86	C14-C15	2.67	1.57	1.52
48	32	218	A86	C19-C18	2.67	1.56	1.52
37	18	211	CLA	C4D-CHA	2.67	1.47	1.38
37	36	307	CLA	C1B-NB	-2.67	1.32	1.35
47	20	305	KC1	C4C-C3C	2.67	1.49	1.45
37	38	211	CLA	C4D-CHA	2.67	1.47	1.38
47	36	305	KC1	C2A-C1A	2.67	1.52	1.44
44	J	101	DGD	O1G-C1G	-2.67	1.39	1.45
48	15	312	A86	C14-C15	2.67	1.57	1.52
37	b	506	CLA	C3D-C4D	-2.67	1.38	1.44
48	41	214	A86	C-C1	2.67	1.56	1.50
37	B	513	CLA	C4B-NB	-2.67	1.32	1.35
48	32	217	A86	C-C1	2.67	1.56	1.50
48	13	315	A86	C-C1	2.67	1.56	1.50
48	36	313	A86	C-C1	2.67	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	15	306	KC1	C4A-C3A	2.66	1.49	1.44
37	B	506	CLA	C3D-C4D	-2.66	1.38	1.44
47	15	302	KC1	CHB-C4A	-2.66	1.33	1.39
37	b	507	CLA	C1C-NC	-2.66	1.33	1.37
48	35	313	A86	C14-C15	2.66	1.57	1.52
48	35	312	A86	C14-C15	2.66	1.57	1.52
37	a	404	CLA	C4B-NB	-2.66	1.32	1.35
48	17	311	A86	C14-C15	2.66	1.57	1.52
37	C	508	CLA	C1C-NC	-2.66	1.33	1.37
48	12	202	A86	C5-C6	2.66	1.39	1.35
48	21	214	A86	C24-C1	2.66	1.51	1.45
37	C	506	CLA	C1C-NC	-2.66	1.33	1.37
48	41	213	A86	C-C1	2.66	1.56	1.50
47	17	303	KC1	C4A-C3A	2.66	1.49	1.44
48	12	215	A86	C24-C1	2.66	1.51	1.45
37	b	507	CLA	C3D-C4D	-2.66	1.38	1.44
47	21	203	KC1	CHB-C4A	-2.66	1.33	1.39
48	21	213	A86	C-C1	2.66	1.56	1.50
37	13	307	CLA	C4D-CHA	2.66	1.47	1.38
47	35	306	KC1	C4A-C3A	2.66	1.49	1.44
48	35	314	A86	C24-C1	2.66	1.51	1.45
48	37	310	A86	C14-C15	2.66	1.57	1.52
41	11	316	LMG	C3-C2	2.66	1.59	1.52
47	41	203	KC1	CHB-C4A	-2.66	1.33	1.39
47	11	309	KC1	C2A-C1A	2.66	1.52	1.44
47	31	309	KC1	C2A-C1A	2.66	1.52	1.44
48	12	213	A86	O-C13	-2.66	1.17	1.23
37	11	305	CLA	C1B-NB	-2.66	1.32	1.35
48	38	213	A86	C-C1	2.66	1.56	1.50
48	17	315	A86	O-C13	-2.66	1.17	1.23
37	34	302	CLA	C4D-CHA	2.66	1.47	1.38
47	33	306	KC1	C4A-C3A	2.66	1.49	1.44
48	12	202	A86	O-C13	-2.66	1.17	1.23
47	18	207	KC1	C4A-C3A	2.66	1.49	1.44
37	B	513	CLA	C3D-C4D	-2.66	1.38	1.44
37	c	508	CLA	C1C-NC	-2.66	1.33	1.37
48	14	315	A86	C25-C24	2.66	1.41	1.34
47	14	309	KC1	C2A-C1A	2.66	1.52	1.44
47	34	309	KC1	C2A-C1A	2.66	1.52	1.44
48	38	215	A86	C24-C1	2.65	1.51	1.45
37	a	404	CLA	C3D-C4D	-2.65	1.38	1.44
47	13	309	KC1	CHB-C4A	-2.65	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	33	309	KC1	CHB-C4A	-2.65	1.33	1.39
37	40	208	CLA	C1B-NB	-2.65	1.32	1.35
37	33	307	CLA	C4D-CHA	2.65	1.47	1.38
43	D	411	LHG	O7-C5	-2.65	1.40	1.46
44	j	101	DGD	O1G-C1G	-2.65	1.39	1.45
37	21	208	CLA	C4D-CHA	2.65	1.47	1.38
47	40	207	KC1	C2A-C1A	2.65	1.52	1.44
48	18	215	A86	O-C13	-2.65	1.17	1.23
37	38	202	CLA	C4D-CHA	2.65	1.47	1.38
47	37	305	KC1	C4D-CHA	2.65	1.48	1.45
47	20	304	KC1	C2A-C1A	2.65	1.52	1.44
47	20	305	KC1	C2A-C1A	2.65	1.52	1.44
48	20	311	A86	C-C1	2.65	1.56	1.50
48	37	312	A86	O-C13	-2.65	1.17	1.23
47	15	302	KC1	C2A-C1A	2.65	1.52	1.44
48	17	320	A86	C14-C15	2.65	1.57	1.52
48	31	315	A86	C19-C18	2.65	1.56	1.52
47	17	303	KC1	CHB-C4A	-2.65	1.33	1.39
48	33	311	A86	C14-C15	2.65	1.57	1.52
37	13	303	CLA	C1B-NB	-2.65	1.32	1.35
43	a	412	LHG	O7-C5	-2.65	1.40	1.46
48	12	220	A86	C5-C6	2.65	1.39	1.35
48	12	216	A86	C-C1	2.65	1.56	1.50
47	12	211	KC1	C2A-C1A	2.65	1.52	1.44
48	13	311	A86	C14-C15	2.65	1.57	1.52
37	b	512	CLA	C1C-NC	-2.65	1.33	1.37
37	39	306	CLA	C1B-NB	-2.64	1.32	1.35
48	12	217	A86	O-C13	-2.64	1.17	1.23
48	39	313	A86	C-C1	2.64	1.56	1.50
37	20	306	CLA	C1B-NB	-2.64	1.32	1.35
48	15	314	A86	C24-C1	2.64	1.51	1.45
48	13	312	A86	O-C13	-2.64	1.17	1.23
48	40	213	A86	C-C1	2.64	1.56	1.50
47	15	304	KC1	C4A-C3A	2.64	1.49	1.44
48	39	311	A86	O-C13	-2.64	1.17	1.23
37	20	307	CLA	C4D-CHA	2.64	1.47	1.38
48	17	315	A86	C-C1	2.64	1.56	1.50
48	14	312	A86	C25-C24	2.64	1.41	1.34
37	32	211	CLA	C1B-NB	-2.64	1.32	1.35
41	11	316	LMG	C4-C5	2.64	1.58	1.53
37	31	304	CLA	C3D-C4D	-2.64	1.38	1.44
47	35	309	KC1	CHB-C4A	-2.64	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	40	205	CLA	C4D-CHA	2.64	1.47	1.38
41	31	316	LMG	C3-C2	2.64	1.59	1.52
48	19	313	A86	O-C13	-2.64	1.17	1.23
37	b	513	CLA	C4B-NB	-2.64	1.32	1.35
48	31	314	A86	C14-C15	2.64	1.57	1.52
37	41	205	CLA	C4D-CHA	2.64	1.47	1.38
37	15	301	CLA	C1C-C2C	2.64	1.49	1.44
47	32	212	KC1	C2A-C1A	2.64	1.52	1.44
47	13	306	KC1	CHB-C4A	-2.64	1.33	1.39
47	19	308	KC1	CHB-C4A	-2.64	1.33	1.39
48	34	314	A86	O-C13	-2.64	1.17	1.23
37	c	508	CLA	C3D-C4D	-2.63	1.38	1.44
37	12	204	CLA	C3D-C4D	-2.63	1.38	1.44
37	32	205	CLA	C3D-C4D	-2.63	1.38	1.44
47	38	205	KC1	CHB-C4A	-2.63	1.33	1.39
48	14	314	A86	O-C13	-2.63	1.17	1.23
48	32	218	A86	C-C1	2.63	1.56	1.50
37	C	502	CLA	C3D-C4D	-2.63	1.38	1.44
37	20	303	CLA	C4D-CHA	2.63	1.47	1.38
50	20	310	DD6	C35-C36	2.63	1.55	1.51
47	17	306	KC1	C4C-C3C	2.63	1.49	1.45
47	40	206	KC1	C2A-C1A	2.63	1.52	1.44
48	11	314	A86	C14-C15	2.63	1.57	1.52
47	37	305	KC1	C4C-C3C	2.63	1.49	1.45
37	12	203	CLA	C1B-NB	-2.63	1.32	1.35
48	15	316	A86	C24-C1	2.63	1.51	1.45
48	16	314	A86	C-C1	2.63	1.56	1.50
47	14	306	KC1	C2A-C1A	2.63	1.52	1.44
37	21	205	CLA	C4D-CHA	2.63	1.47	1.38
47	39	308	KC1	CHB-C4A	-2.63	1.33	1.39
48	12	217	A86	C-C1	2.63	1.56	1.50
48	17	312	A86	O-C13	-2.63	1.17	1.23
37	33	310	CLA	C4D-CHA	2.63	1.47	1.38
37	11	307	CLA	C4B-NB	-2.63	1.32	1.35
47	37	302	KC1	CHB-C4A	-2.63	1.33	1.39
48	19	313	A86	C-C1	2.63	1.56	1.50
48	34	311	A86	C25-C24	2.62	1.41	1.34
48	34	312	A86	C25-C24	2.62	1.41	1.34
37	20	308	CLA	C4D-CHA	2.62	1.47	1.38
47	13	309	KC1	C2A-C1A	2.62	1.52	1.44
47	33	309	KC1	C2A-C1A	2.62	1.52	1.44
47	15	309	KC1	CHB-C4A	-2.62	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	508	CLA	C3D-C4D	-2.62	1.38	1.44
48	36	313	A86	C25-C24	2.62	1.41	1.34
48	14	316	A86	C-C1	2.62	1.56	1.50
48	34	316	A86	C-C1	2.62	1.56	1.50
48	12	220	A86	C25-C24	2.62	1.41	1.34
39	C	515	BCR	C30-C25	-2.62	1.50	1.53
37	33	305	CLA	C4D-CHA	2.62	1.47	1.38
37	33	308	CLA	C1B-NB	-2.62	1.32	1.35
47	37	307	KC1	C4A-C3A	2.62	1.49	1.44
48	38	212	A86	C14-C15	2.62	1.57	1.52
48	16	311	A86	O-C13	-2.62	1.17	1.23
47	13	306	KC1	C4A-C3A	2.62	1.49	1.44
48	37	311	A86	O-C13	-2.62	1.17	1.23
37	15	307	CLA	C4D-CHA	2.62	1.47	1.38
37	35	307	CLA	C4D-CHA	2.62	1.47	1.38
47	35	304	KC1	C4A-C3A	2.62	1.49	1.44
48	12	202	A86	C25-C24	2.62	1.41	1.34
48	32	221	A86	C25-C24	2.62	1.41	1.34
37	39	307	CLA	C4D-CHA	2.62	1.47	1.38
48	13	312	A86	C14-C15	2.62	1.57	1.52
47	16	308	KC1	CHB-C4A	-2.62	1.33	1.39
47	33	302	KC1	C2A-C1A	2.62	1.52	1.44
47	31	307	KC1	CHB-C4A	-2.61	1.33	1.39
48	11	315	A86	C14-C15	2.61	1.57	1.52
48	33	315	A86	C-C1	2.61	1.56	1.50
37	13	301	CLA	C4D-CHA	2.61	1.47	1.38
37	33	301	CLA	C4D-CHA	2.61	1.47	1.38
43	B	523	LHG	O7-C5	-2.61	1.40	1.46
48	12	216	A86	C14-C15	2.61	1.57	1.52
48	35	315	A86	C-C1	2.61	1.56	1.50
48	15	313	A86	C14-C15	2.61	1.57	1.52
37	c	502	CLA	C3D-C4D	-2.61	1.38	1.44
47	20	304	KC1	CHB-C4A	-2.61	1.33	1.39
40	a	409	SQD	O47-C7	2.61	1.41	1.34
47	17	305	KC1	C4A-C3A	2.61	1.49	1.44
39	c	515	BCR	C30-C25	-2.61	1.50	1.53
47	13	302	KC1	C2A-C1A	2.61	1.52	1.44
43	b	522	LHG	O7-C5	-2.61	1.40	1.46
48	31	315	A86	C14-C15	2.61	1.57	1.52
48	14	313	A86	O-C13	-2.61	1.17	1.23
37	18	206	CLA	C4D-CHA	2.61	1.47	1.38
37	40	205	CLA	C1B-NB	-2.61	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	37	319	A86	O-C13	-2.61	1.17	1.23
50	40	212	DD6	C35-C36	2.61	1.55	1.51
37	15	308	CLA	C4D-CHA	2.61	1.47	1.38
37	c	506	CLA	C1C-NC	-2.61	1.33	1.37
48	17	320	A86	C-C1	2.61	1.56	1.50
48	16	314	A86	C25-C24	2.61	1.41	1.34
37	37	306	CLA	C4D-CHA	2.61	1.47	1.38
48	32	203	A86	C25-C24	2.60	1.41	1.34
47	18	205	KC1	CHB-C4A	-2.60	1.33	1.39
37	40	210	CLA	C4D-CHA	2.60	1.47	1.38
48	37	319	A86	C-C1	2.60	1.56	1.50
37	13	305	CLA	C4D-CHA	2.60	1.47	1.38
48	14	311	A86	C25-C24	2.60	1.41	1.34
40	A	407	SQD	O47-C7	2.60	1.41	1.34
47	40	207	KC1	C4A-C3A	2.60	1.49	1.44
48	11	314	A86	C-C1	2.60	1.56	1.50
37	32	206	CLA	C3D-C4D	-2.60	1.38	1.44
37	C	502	CLA	OBD-CAD	2.60	1.27	1.22
37	31	301	CLA	C4D-CHA	2.60	1.47	1.38
47	34	306	KC1	C2A-C1A	2.60	1.52	1.44
37	40	209	CLA	C4D-CHA	2.60	1.47	1.38
48	11	315	A86	C19-C18	2.60	1.56	1.52
48	38	213	A86	C14-C15	2.60	1.57	1.52
47	18	207	KC1	C4D-CHA	2.60	1.48	1.45
41	C	518	LMG	O7-C8	-2.60	1.40	1.46
47	14	306	KC1	C4A-C3A	2.60	1.49	1.44
48	18	214	A86	C24-C1	2.60	1.51	1.45
47	13	304	KC1	C4A-C3A	2.60	1.49	1.44
47	17	308	KC1	C4A-C3A	2.60	1.49	1.44
47	33	304	KC1	C4A-C3A	2.60	1.49	1.44
37	35	310	CLA	C4D-CHA	2.60	1.47	1.38
37	37	308	CLA	C4C-C3C	2.60	1.49	1.45
41	d	409	LMG	O1-C7	-2.60	1.39	1.43
37	16	307	CLA	C4D-CHA	2.60	1.47	1.38
47	17	305	KC1	CHB-C4A	-2.60	1.33	1.39
48	32	203	A86	C5-C6	2.60	1.39	1.35
37	B	501	CLA	C4D-CHA	2.60	1.47	1.38
37	19	310	CLA	C4D-CHA	2.60	1.47	1.38
37	39	310	CLA	C4D-CHA	2.60	1.47	1.38
37	11	303	CLA	C3D-C4D	-2.60	1.38	1.44
37	33	308	CLA	C4C-C3C	2.60	1.49	1.45
41	31	316	LMG	C4-C5	2.60	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	33	311	A86	O-C13	-2.60	1.17	1.23
47	40	206	KC1	CHB-C4A	-2.60	1.33	1.39
37	18	211	CLA	C4C-C3C	2.59	1.49	1.45
37	C	509	CLA	C1C-NC	-2.59	1.33	1.37
37	19	307	CLA	C4D-CHA	2.59	1.47	1.38
47	38	207	KC1	C4A-C3A	2.59	1.49	1.44
37	15	310	CLA	C4D-CHA	2.59	1.47	1.38
37	c	502	CLA	OBD-CAD	2.59	1.26	1.22
37	35	301	CLA	C1C-C2C	2.59	1.49	1.44
48	18	212	A86	O-C13	-2.59	1.17	1.23
47	38	205	KC1	C4A-C3A	2.59	1.49	1.44
37	b	501	CLA	C4D-CHA	2.59	1.47	1.38
37	16	307	CLA	C1B-NB	-2.59	1.32	1.35
48	31	313	A86	C-C1	2.59	1.56	1.50
47	14	306	KC1	CHB-C4A	-2.59	1.33	1.39
47	18	210	KC1	C4D-CHA	2.59	1.48	1.45
48	37	311	A86	C24-C1	2.59	1.51	1.45
37	33	303	CLA	C1B-NB	-2.59	1.32	1.35
48	32	217	A86	C14-C15	2.59	1.57	1.52
47	20	305	KC1	C4A-C3A	2.59	1.49	1.44
47	38	207	KC1	C4D-CHA	2.58	1.48	1.45
37	B	509	CLA	C3D-C4D	-2.58	1.38	1.44
37	z	102	CLA	C4D-CHA	2.58	1.47	1.38
48	13	312	A86	C-C1	2.58	1.56	1.50
37	38	206	CLA	C4D-CHA	2.58	1.47	1.38
37	19	307	CLA	C1B-NB	-2.58	1.32	1.35
37	41	209	CLA	C4D-CHA	2.58	1.47	1.38
48	17	310	A86	C-C1	2.58	1.56	1.50
37	B	506	CLA	C1C-NC	-2.58	1.34	1.37
37	W	102	CLA	C4D-CHA	2.58	1.47	1.38
37	36	307	CLA	C4D-CHA	2.58	1.47	1.38
47	18	205	KC1	C4A-C3A	2.58	1.49	1.44
37	31	308	CLA	C4B-NB	-2.58	1.32	1.35
37	15	303	CLA	C4D-CHA	2.58	1.47	1.38
37	B	514	CLA	OBD-CAD	2.58	1.26	1.22
47	35	304	KC1	CHB-C4A	-2.58	1.33	1.39
48	38	212	A86	C-C1	2.58	1.56	1.50
48	41	214	A86	O-C13	-2.58	1.17	1.23
37	37	308	CLA	C4D-CHA	2.58	1.47	1.38
37	13	303	CLA	C4B-NB	-2.58	1.32	1.35
48	13	311	A86	O-C13	-2.58	1.17	1.23
48	31	314	A86	C-C1	2.58	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	c	518	LMG	O7-C8	-2.58	1.40	1.46
37	13	310	CLA	C4D-CHA	2.58	1.47	1.38
37	12	212	CLA	C1B-NB	-2.58	1.32	1.35
37	32	213	CLA	C1B-NB	-2.58	1.32	1.35
37	a	404	CLA	C1C-NC	-2.58	1.34	1.37
48	15	315	A86	C-C1	2.58	1.56	1.50
37	b	514	CLA	OBD-CAD	2.58	1.26	1.22
37	35	308	CLA	C4C-C3C	2.58	1.49	1.45
48	37	309	A86	C-C1	2.58	1.56	1.50
47	36	308	KC1	CHB-C4A	-2.58	1.33	1.39
48	33	312	A86	C-C1	2.57	1.56	1.50
47	17	306	KC1	C4D-CHA	2.57	1.48	1.45
37	Z	102	CLA	C4D-CHA	2.57	1.47	1.38
37	18	202	CLA	C4D-CHA	2.57	1.47	1.38
37	w	101	CLA	C1C-NC	-2.57	1.34	1.37
48	17	315	A86	C24-C1	2.57	1.51	1.45
37	17	307	CLA	C4D-CHA	2.57	1.47	1.38
37	21	202	CLA	C4D-CHA	2.57	1.47	1.38
37	b	506	CLA	C1C-NC	-2.57	1.34	1.37
47	20	302	KC1	C2A-C1A	2.57	1.52	1.44
47	11	302	KC1	CHB-C4A	-2.57	1.33	1.39
47	31	303	KC1	CHB-C4A	-2.57	1.33	1.39
41	D	412	LMG	O1-C7	-2.57	1.39	1.43
37	b	507	CLA	C4D-CHA	2.57	1.47	1.38
37	21	209	CLA	C4D-CHA	2.57	1.47	1.38
37	B	512	CLA	C1C-NC	-2.57	1.34	1.37
37	32	208	CLA	C3D-C4D	-2.57	1.38	1.44
48	18	214	A86	O-C13	-2.57	1.17	1.23
48	21	213	A86	O-C13	-2.57	1.17	1.23
37	12	203	CLA	C4D-CHA	2.57	1.47	1.38
37	32	204	CLA	C4D-CHA	2.57	1.47	1.38
47	11	306	KC1	CHB-C4A	-2.57	1.33	1.39
37	35	308	CLA	C4D-CHA	2.57	1.47	1.38
37	14	307	CLA	C4D-CHA	2.57	1.47	1.38
48	17	312	A86	C24-C1	2.57	1.51	1.45
48	38	214	A86	C24-C1	2.57	1.51	1.45
37	14	305	CLA	C4D-CHA	2.57	1.47	1.38
37	17	309	CLA	C4D-CHA	2.57	1.47	1.38
37	34	305	CLA	C4D-CHA	2.57	1.47	1.38
37	15	308	CLA	C4C-C3C	2.57	1.49	1.45
47	37	304	KC1	CHB-C4A	-2.57	1.33	1.39
48	17	310	A86	O-C13	-2.57	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	37	309	A86	O-C13	-2.57	1.17	1.23
48	14	315	A86	C14-C15	2.57	1.57	1.52
48	34	315	A86	C14-C15	2.57	1.57	1.52
37	16	306	CLA	C4D-CHA	2.56	1.47	1.38
37	C	504	CLA	C3D-C4D	-2.56	1.38	1.44
47	15	304	KC1	CHB-C4A	-2.56	1.33	1.39
48	33	312	A86	C14-C15	2.56	1.57	1.52
48	33	315	A86	C24-C1	2.56	1.51	1.45
47	34	306	KC1	C4A-C3A	2.56	1.49	1.44
48	11	312	A86	C14-C15	2.56	1.57	1.52
50	40	212	DD6	C26-C27	-2.56	1.31	1.37
37	31	306	CLA	C4D-CHA	2.56	1.47	1.38
47	38	210	KC1	C4D-CHA	2.56	1.48	1.45
37	41	204	CLA	C4D-CHA	2.56	1.47	1.38
40	B	522	SQD	O47-C7	2.56	1.41	1.34
37	B	515	CLA	C4B-NB	-2.56	1.32	1.35
37	38	204	CLA	C1B-NB	-2.56	1.32	1.35
37	34	307	CLA	C4D-CHA	2.56	1.47	1.38
37	b	509	CLA	C3D-C4D	-2.56	1.38	1.44
37	12	205	CLA	C3D-C4D	-2.56	1.38	1.44
37	33	303	CLA	C4B-NB	-2.56	1.32	1.35
47	11	304	KC1	C4A-C3A	2.56	1.49	1.44
48	39	313	A86	C17-C18	-2.56	1.48	1.52
37	c	502	CLA	C4B-NB	-2.56	1.32	1.35
37	39	302	CLA	C3D-C4D	-2.56	1.38	1.44
37	38	201	CLA	C4D-CHA	2.56	1.47	1.38
48	41	215	A86	O-C13	-2.56	1.17	1.23
37	B	507	CLA	C4D-CHA	2.56	1.47	1.38
37	C	503	CLA	C3D-C4D	-2.56	1.38	1.44
48	14	316	A86	O-C13	-2.56	1.17	1.23
47	15	306	KC1	CHB-C4A	-2.56	1.33	1.39
37	21	204	CLA	C4D-CHA	2.56	1.47	1.38
37	32	211	CLA	C4D-CHA	2.56	1.47	1.38
48	34	316	A86	O-C13	-2.56	1.17	1.23
37	c	504	CLA	C3D-C4D	-2.56	1.38	1.44
48	13	315	A86	C24-C1	2.56	1.51	1.45
47	35	302	KC1	CHB-C4A	-2.56	1.33	1.39
37	39	302	CLA	C4D-CHA	2.56	1.47	1.38
50	40	214	DD6	C35-C36	2.56	1.55	1.51
37	W	101	CLA	C4B-NB	-2.55	1.32	1.35
47	31	305	KC1	C2A-C1A	2.55	1.52	1.44
37	18	201	CLA	C4D-CHA	2.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	13	308	CLA	C4C-C3C	2.55	1.49	1.45
47	40	204	KC1	C2A-C1A	2.55	1.52	1.44
37	36	306	CLA	C4D-CHA	2.55	1.47	1.38
38	a	406	PHO	CAC-C3C	-2.55	1.47	1.52
48	39	311	A86	C25-C24	2.55	1.41	1.34
48	41	213	A86	O-C13	-2.55	1.17	1.23
37	D	401	CLA	C1C-NC	-2.55	1.34	1.37
44	C	517	DGD	O4E-C4E	-2.55	1.37	1.43
48	32	214	A86	C25-C24	2.55	1.41	1.34
37	13	303	CLA	C3D-C4D	-2.55	1.38	1.44
37	c	509	CLA	C1C-NC	-2.55	1.34	1.37
37	40	208	CLA	C4D-CHA	2.55	1.47	1.38
37	c	508	CLA	C4B-NB	-2.55	1.32	1.35
37	39	303	CLA	C3D-C4D	-2.55	1.38	1.44
48	21	214	A86	O-C13	-2.55	1.17	1.23
48	13	313	A86	O-C13	-2.55	1.17	1.23
37	c	503	CLA	C3D-C4D	-2.55	1.38	1.44
37	b	515	CLA	C4B-NB	-2.55	1.32	1.35
47	11	306	KC1	C2A-C1A	2.55	1.52	1.44
37	14	308	CLA	C4D-CHA	2.55	1.47	1.38
37	11	310	CLA	C3D-C4D	-2.55	1.38	1.44
44	c	517	DGD	O4E-C4E	-2.55	1.37	1.43
37	W	101	CLA	C1C-NC	-2.55	1.34	1.37
48	14	311	A86	O-C13	-2.55	1.17	1.23
48	34	311	A86	O-C13	-2.55	1.17	1.23
47	38	210	KC1	CHB-C4A	-2.55	1.33	1.39
48	33	313	A86	O-C13	-2.55	1.17	1.23
37	21	206	CLA	C4D-CHA	2.55	1.47	1.38
47	11	304	KC1	C2A-C1A	2.55	1.52	1.44
37	11	301	CLA	C4D-CHA	2.54	1.47	1.38
37	12	207	CLA	C3D-C4D	-2.54	1.38	1.44
37	41	206	CLA	C4D-CHA	2.54	1.47	1.38
37	12	207	CLA	C1B-NB	-2.54	1.32	1.35
37	32	208	CLA	C1B-NB	-2.54	1.32	1.35
48	11	313	A86	C-C1	2.54	1.56	1.50
37	32	210	CLA	C4D-CHA	2.54	1.47	1.38
37	35	303	CLA	C4D-CHA	2.54	1.47	1.38
47	15	306	KC1	C4D-CHA	2.54	1.48	1.45
37	31	302	CLA	C4D-CHA	2.54	1.47	1.38
40	b	521	SQD	O47-C7	2.54	1.41	1.34
50	20	310	DD6	O1-C20	2.54	1.49	1.46
48	32	203	A86	C-C1	2.54	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	31	305	KC1	C4A-C3A	2.54	1.49	1.44
37	31	304	CLA	C4D-CHA	2.54	1.47	1.38
40	16	315	SQD	O47-C7	2.54	1.41	1.34
37	11	305	CLA	C4D-CHA	2.54	1.47	1.38
37	34	308	CLA	C4D-CHA	2.54	1.47	1.38
37	z	101	CLA	C3D-C4D	-2.54	1.38	1.44
37	19	302	CLA	C4D-CHA	2.54	1.47	1.38
37	17	304	CLA	C4D-CHA	2.54	1.47	1.38
37	37	303	CLA	C4D-CHA	2.54	1.47	1.38
40	40	202	SQD	O47-C7	2.54	1.41	1.34
37	12	210	CLA	C4D-CHA	2.54	1.47	1.38
37	34	301	CLA	C4D-CHA	2.54	1.47	1.38
47	34	306	KC1	CHB-C4A	-2.54	1.33	1.39
37	34	310	CLA	C4D-CHA	2.54	1.47	1.38
37	12	209	CLA	C4D-CHA	2.53	1.47	1.38
37	41	202	CLA	C4D-CHA	2.53	1.47	1.38
37	C	502	CLA	C4B-NB	-2.53	1.32	1.35
48	37	314	A86	C24-C1	2.53	1.51	1.45
48	21	215	A86	O-C13	-2.53	1.18	1.23
38	A	404	PHO	CAC-C3C	-2.53	1.47	1.52
37	11	307	CLA	C4D-CHA	2.53	1.47	1.38
50	20	310	DD6	C26-C27	-2.53	1.31	1.37
50	40	212	DD6	O1-C20	2.53	1.49	1.46
37	18	208	CLA	C4D-CHA	2.53	1.47	1.38
37	38	208	CLA	C4D-CHA	2.53	1.47	1.38
50	20	312	DD6	C35-C36	2.53	1.55	1.51
47	40	207	KC1	CHB-C4A	-2.53	1.33	1.39
48	14	312	A86	C-C1	2.53	1.56	1.50
37	37	301	CLA	C4D-CHA	2.53	1.47	1.38
48	12	202	A86	C-C1	2.53	1.56	1.50
37	c	502	CLA	C4D-CHA	2.53	1.47	1.38
37	w	101	CLA	C4D-CHA	2.53	1.47	1.38
48	17	311	A86	C-C1	2.53	1.56	1.50
37	39	302	CLA	OBD-CAD	2.53	1.26	1.22
50	21	216	DD6	C4-C5	2.53	1.51	1.43
37	c	507	CLA	C1C-NC	-2.53	1.34	1.37
48	31	311	A86	C25-C24	2.53	1.41	1.34
37	32	204	CLA	C1B-NB	-2.53	1.33	1.35
37	41	205	CLA	C4C-C3C	2.53	1.49	1.45
37	41	210	CLA	C4D-CHA	2.53	1.47	1.38
47	12	211	KC1	C4A-C3A	2.53	1.49	1.44
47	32	212	KC1	C4A-C3A	2.53	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	21	208	CLA	C4C-C3C	2.53	1.49	1.45
37	b	511	CLA	C1C-NC	-2.53	1.34	1.37
47	31	307	KC1	C4A-C3A	2.53	1.49	1.44
48	19	311	A86	C25-C24	2.53	1.41	1.34
44	j	101	DGD	O5D-C6D	-2.53	1.39	1.43
37	14	303	CLA	C4D-CHA	2.53	1.47	1.38
37	34	303	CLA	C4D-CHA	2.53	1.47	1.38
37	19	302	CLA	OBD-CAD	2.53	1.26	1.22
37	B	515	CLA	C4D-CHA	2.53	1.47	1.38
47	18	205	KC1	C2A-C1A	2.53	1.52	1.44
37	38	202	CLA	C4B-CHC	2.53	1.48	1.41
37	32	202	CLA	C3D-C4D	-2.53	1.38	1.44
37	b	515	CLA	C4D-CHA	2.53	1.47	1.38
37	19	303	CLA	C3D-C4D	-2.53	1.38	1.44
37	20	306	CLA	C4D-CHA	2.53	1.47	1.38
37	B	507	CLA	C4B-NB	-2.52	1.33	1.35
37	35	301	CLA	C4D-CHA	2.52	1.47	1.38
37	a	403	CLA	C1C-NC	-2.52	1.34	1.37
37	b	504	CLA	C4D-CHA	2.52	1.47	1.38
37	C	508	CLA	C4B-NB	-2.52	1.33	1.35
48	32	221	A86	O-C13	-2.52	1.18	1.23
47	31	307	KC1	C2A-C1A	2.52	1.52	1.44
48	34	312	A86	C-C1	2.52	1.56	1.50
37	14	310	CLA	C4D-CHA	2.52	1.47	1.38
48	18	212	A86	C14-C15	2.52	1.57	1.52
37	B	509	CLA	C4D-CHA	2.52	1.47	1.38
37	39	307	CLA	C1B-NB	-2.52	1.33	1.35
37	11	303	CLA	C4D-CHA	2.52	1.47	1.38
37	14	301	CLA	C4D-CHA	2.52	1.47	1.38
37	b	509	CLA	C4D-CHA	2.52	1.47	1.38
48	31	313	A86	C24-C1	2.52	1.51	1.45
47	18	210	KC1	CHB-C4A	-2.52	1.33	1.39
37	21	210	CLA	C4D-CHA	2.52	1.47	1.38
37	19	309	CLA	C4D-CHA	2.52	1.47	1.38
37	c	511	CLA	C4D-CHA	2.52	1.47	1.38
50	41	216	DD6	C4-C5	2.52	1.51	1.43
37	19	302	CLA	C3D-C4D	-2.52	1.38	1.44
48	38	212	A86	O-C13	-2.52	1.18	1.23
37	31	308	CLA	C4D-CHA	2.52	1.47	1.38
37	C	502	CLA	C4D-CHA	2.51	1.47	1.38
37	39	309	CLA	C4D-CHA	2.51	1.47	1.38
37	Z	101	CLA	C3D-C4D	-2.51	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	A	403	CLA	C1C-NC	-2.51	1.34	1.37
47	16	302	KC1	CHB-C4A	-2.51	1.33	1.39
39	D	407	BCR	C30-C25	-2.51	1.50	1.53
39	K	101	BCR	C30-C25	-2.51	1.50	1.53
37	W	101	CLA	C4D-CHA	2.51	1.47	1.38
48	12	220	A86	O-C13	-2.51	1.18	1.23
39	y	101	BCR	C30-C25	-2.51	1.50	1.53
37	12	204	CLA	C4D-CHA	2.51	1.47	1.38
37	32	205	CLA	C4D-CHA	2.51	1.47	1.38
48	40	211	A86	C-C1	2.51	1.56	1.50
47	16	305	KC1	CHB-C4A	-2.51	1.33	1.39
47	12	206	KC1	C4A-C3A	2.51	1.49	1.44
47	32	207	KC1	C4A-C3A	2.51	1.49	1.44
37	C	511	CLA	C4D-CHA	2.51	1.47	1.38
47	36	302	KC1	CHB-C4A	-2.51	1.33	1.39
37	21	202	CLA	C4C-C3C	2.51	1.49	1.45
37	13	308	CLA	C4D-CHA	2.51	1.47	1.38
37	19	309	CLA	C3D-C4D	-2.51	1.38	1.44
50	19	312	DD6	C29-C27	-2.51	1.37	1.42
47	38	205	KC1	C2A-C1A	2.51	1.52	1.44
37	15	310	CLA	C4C-C3C	2.51	1.49	1.45
37	19	301	CLA	C1B-NB	-2.51	1.33	1.35
37	C	507	CLA	C1C-NC	-2.50	1.34	1.37
47	35	306	KC1	C4D-CHA	2.50	1.48	1.45
37	15	303	CLA	C4C-C3C	2.50	1.49	1.45
37	33	308	CLA	C4D-CHA	2.50	1.47	1.38
37	39	301	CLA	C1B-NB	-2.50	1.33	1.35
37	21	205	CLA	C4C-C3C	2.50	1.49	1.45
37	c	505	CLA	C1C-NC	-2.50	1.34	1.37
47	35	306	KC1	CHB-C4A	-2.50	1.33	1.39
37	w	101	CLA	C4B-NB	-2.50	1.33	1.35
37	11	301	CLA	C1B-NB	-2.50	1.33	1.35
37	31	302	CLA	C1B-NB	-2.50	1.33	1.35
47	15	306	KC1	C2A-C1A	2.50	1.52	1.44
48	18	212	A86	C24-C1	2.50	1.51	1.45
37	14	310	CLA	C3D-C4D	-2.50	1.38	1.44
48	38	212	A86	C24-C1	2.50	1.51	1.45
48	18	213	A86	C5-C6	2.50	1.39	1.35
37	16	306	CLA	C3D-C4D	-2.50	1.38	1.44
37	36	306	CLA	C3D-C4D	-2.50	1.38	1.44
48	32	214	A86	C-C1	2.50	1.56	1.50
48	36	313	A86	O-C13	-2.50	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	31	312	A86	C14-C15	2.50	1.57	1.52
47	35	304	KC1	C4C-C3C	2.50	1.49	1.45
48	11	311	A86	C25-C24	2.50	1.41	1.34
37	15	301	CLA	C4D-CHA	2.50	1.47	1.38
47	15	304	KC1	C4C-C3C	2.50	1.49	1.45
37	c	512	CLA	C3D-C4D	-2.50	1.38	1.44
37	C	512	CLA	C3D-C4D	-2.50	1.38	1.44
37	36	303	CLA	C1B-NB	-2.50	1.33	1.35
37	B	504	CLA	C4D-CHA	2.50	1.47	1.38
37	31	310	CLA	C3D-C4D	-2.50	1.38	1.44
48	16	313	A86	C24-C1	2.50	1.51	1.45
39	h	101	BCR	C30-C25	-2.49	1.50	1.53
37	13	310	CLA	C4C-C3C	2.49	1.49	1.45
48	13	314	A86	C14-C15	2.49	1.57	1.52
37	b	502	CLA	C1C-NC	-2.49	1.34	1.37
37	38	208	CLA	C1B-NB	-2.49	1.33	1.35
37	16	303	CLA	C4D-CHA	2.49	1.47	1.38
37	40	203	CLA	C3D-C4D	-2.49	1.38	1.44
47	16	304	KC1	C4A-C3A	2.49	1.49	1.44
47	35	306	KC1	C2A-C1A	2.49	1.52	1.44
37	11	308	CLA	C4D-CHA	2.49	1.47	1.38
48	34	315	A86	C-C1	2.49	1.56	1.50
48	37	313	A86	C-C1	2.49	1.56	1.50
37	B	508	CLA	C1C-NC	-2.49	1.34	1.37
37	B	511	CLA	C1C-NC	-2.49	1.34	1.37
37	b	508	CLA	C1C-NC	-2.49	1.34	1.37
37	20	301	CLA	C3D-C4D	-2.49	1.38	1.44
48	16	311	A86	O4-C34	-2.49	1.40	1.46
47	21	207	KC1	C1C-C2C	2.49	1.49	1.44
48	16	314	A86	O-C13	-2.49	1.18	1.23
47	33	306	KC1	C2A-C1A	2.49	1.52	1.44
37	39	309	CLA	C3D-C4D	-2.49	1.38	1.44
50	20	312	DD6	C4-C5	2.49	1.51	1.43
37	13	303	CLA	C4C-C3C	2.49	1.49	1.45
50	40	214	DD6	C4-C5	2.49	1.51	1.43
37	14	301	CLA	C4B-CHC	2.49	1.47	1.41
47	41	207	KC1	C1C-C2C	2.49	1.49	1.44
37	19	305	CLA	C4D-CHA	2.49	1.47	1.38
46	F	101	HEM	CAA-C2A	2.49	1.55	1.52
37	16	309	CLA	C4D-CHA	2.49	1.47	1.38
41	l	101	LMG	O8-C9	-2.49	1.39	1.45
47	35	302	KC1	C4A-C3A	2.48	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	33	314	A86	C14-C15	2.48	1.57	1.52
47	15	304	KC1	C2A-C1A	2.48	1.52	1.44
47	13	309	KC1	C4A-C3A	2.48	1.49	1.44
39	d	405	BCR	C30-C25	-2.48	1.50	1.53
37	32	206	CLA	C4D-CHA	2.48	1.47	1.38
48	15	311	A86	C-C1	2.48	1.56	1.50
37	C	507	CLA	C4D-CHA	2.48	1.47	1.38
37	c	507	CLA	C4D-CHA	2.48	1.47	1.38
48	20	309	A86	C-C1	2.48	1.56	1.50
48	12	213	A86	C25-C24	2.48	1.41	1.34
37	36	303	CLA	C4D-CHA	2.48	1.47	1.38
48	40	201	A86	C24-C1	2.48	1.51	1.45
48	13	315	A86	O-C13	-2.48	1.18	1.23
37	39	305	CLA	C4D-CHA	2.48	1.47	1.38
47	36	305	KC1	CHB-C4A	-2.48	1.33	1.39
37	13	307	CLA	C4B-NB	-2.48	1.33	1.35
37	18	208	CLA	C1B-NB	-2.48	1.33	1.35
48	20	309	A86	C24-C1	2.48	1.51	1.45
37	13	303	CLA	C4D-CHA	2.48	1.47	1.38
37	35	301	CLA	C4B-CHC	2.48	1.47	1.41
37	34	310	CLA	C3D-C4D	-2.48	1.38	1.44
48	12	213	A86	C14-C15	2.48	1.57	1.52
48	21	211	A86	C24-C1	2.48	1.51	1.45
37	C	505	CLA	C1C-NC	-2.48	1.34	1.37
47	13	306	KC1	C2A-C1A	2.48	1.52	1.44
40	A	407	SQD	O2-C2	-2.48	1.37	1.43
50	39	312	DD6	C29-C27	-2.48	1.37	1.42
37	B	501	CLA	C3D-C4D	-2.48	1.38	1.44
37	B	514	CLA	C4D-CHA	2.48	1.47	1.38
48	40	211	A86	C24-C1	2.48	1.51	1.45
47	35	302	KC1	C4C-C3C	2.48	1.49	1.45
48	17	314	A86	C14-C15	2.48	1.57	1.52
44	H	102	DGD	O2G-C2G	-2.48	1.40	1.46
37	18	204	CLA	C1B-NB	-2.48	1.33	1.35
37	34	302	CLA	C1B-NB	-2.48	1.33	1.35
37	34	308	CLA	C1B-NB	-2.48	1.33	1.35
37	32	202	CLA	C4D-CHA	2.48	1.47	1.38
37	11	305	CLA	C3D-C4D	-2.47	1.38	1.44
37	33	303	CLA	C4D-CHA	2.47	1.47	1.38
48	17	314	A86	C-C1	2.47	1.56	1.50
47	17	305	KC1	C2A-C1A	2.47	1.52	1.44
47	37	304	KC1	C2A-C1A	2.47	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	17	309	CLA	C3D-C4D	-2.47	1.38	1.44
37	37	308	CLA	C3D-C4D	-2.47	1.38	1.44
44	C	516	DGD	O5D-C6D	-2.47	1.39	1.43
48	38	214	A86	O-C13	-2.47	1.18	1.23
37	C	503	CLA	C4D-CHA	2.47	1.47	1.38
37	11	308	CLA	C3D-C4D	-2.47	1.38	1.44
37	12	209	CLA	C3D-C4D	-2.47	1.38	1.44
37	32	210	CLA	C3D-C4D	-2.47	1.38	1.44
44	J	101	DGD	O5D-C6D	-2.47	1.39	1.43
47	36	304	KC1	C4A-C3A	2.47	1.49	1.44
47	15	302	KC1	C4C-C3C	2.47	1.49	1.45
48	34	314	A86	C24-C1	2.47	1.51	1.45
37	16	301	CLA	C4D-CHA	2.47	1.47	1.38
37	41	202	CLA	C4C-C3C	2.47	1.49	1.45
37	36	309	CLA	C4D-CHA	2.47	1.47	1.38
47	39	308	KC1	C4A-C3A	2.47	1.49	1.44
37	32	206	CLA	C4B-NB	-2.47	1.33	1.35
37	b	513	CLA	C4D-CHA	2.47	1.47	1.38
47	40	207	KC1	C4D-CHA	2.47	1.48	1.45
47	11	306	KC1	C4A-C3A	2.47	1.49	1.44
37	35	303	CLA	C4C-C3C	2.47	1.49	1.45
37	12	205	CLA	C4D-CHA	2.47	1.47	1.38
37	16	303	CLA	C1B-NB	-2.47	1.33	1.35
47	32	209	KC1	C4A-C3A	2.47	1.49	1.44
48	37	313	A86	C14-C15	2.47	1.57	1.52
47	35	309	KC1	C4D-CHA	2.47	1.48	1.45
37	c	503	CLA	C4D-CHA	2.47	1.47	1.38
48	33	315	A86	O-C13	-2.46	1.18	1.23
37	11	307	CLA	C3D-C4D	-2.46	1.38	1.44
37	31	308	CLA	C3D-C4D	-2.46	1.38	1.44
44	h	102	DGD	O2G-C2G	-2.46	1.40	1.46
37	34	301	CLA	C4B-CHC	2.46	1.47	1.41
37	12	210	CLA	C4C-C3C	2.46	1.49	1.45
37	36	303	CLA	C3D-C4D	-2.46	1.38	1.44
47	11	309	KC1	C4A-C3A	2.46	1.49	1.44
37	20	301	CLA	C4D-CHA	2.46	1.47	1.38
48	14	315	A86	C-C1	2.46	1.56	1.50
37	31	306	CLA	C3D-C4D	-2.46	1.38	1.44
40	a	409	SQD	O2-C2	-2.46	1.37	1.43
37	b	501	CLA	C3D-C4D	-2.46	1.38	1.44
47	20	304	KC1	C4C-C3C	2.46	1.49	1.45
37	B	510	CLA	C4D-CHA	2.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	504	CLA	C4D-CHA	2.46	1.47	1.38
37	32	211	CLA	C4C-C3C	2.46	1.49	1.45
37	41	208	CLA	C4C-C3C	2.46	1.49	1.45
48	36	311	A86	O4-C34	-2.46	1.40	1.46
37	13	301	CLA	C1B-NB	-2.46	1.33	1.35
37	14	303	CLA	C1B-NB	-2.46	1.33	1.35
37	33	301	CLA	C1B-NB	-2.46	1.33	1.35
37	34	303	CLA	C1B-NB	-2.46	1.33	1.35
37	c	506	CLA	C4D-CHA	2.46	1.47	1.38
37	c	513	CLA	C4D-CHA	2.45	1.47	1.38
37	17	302	CLA	C3D-C4D	-2.45	1.38	1.44
46	f	101	HEM	CAA-C2A	2.45	1.55	1.52
41	L	102	LMG	O8-C9	-2.45	1.39	1.45
37	39	306	CLA	C4B-CHC	2.45	1.47	1.41
37	b	514	CLA	C4D-CHA	2.45	1.47	1.38
48	15	319	A86	O-C13	-2.45	1.18	1.23
47	20	305	KC1	CHB-C4A	-2.45	1.33	1.39
47	33	309	KC1	C4A-C3A	2.45	1.49	1.44
47	31	309	KC1	C4A-C3A	2.45	1.49	1.44
37	33	307	CLA	O1D-CGD	2.45	1.27	1.21
37	b	510	CLA	C4D-CHA	2.45	1.47	1.38
48	32	214	A86	C14-C15	2.45	1.57	1.52
47	40	206	KC1	C4C-C3C	2.45	1.49	1.45
48	16	311	A86	C-C1	2.45	1.55	1.50
37	17	302	CLA	C4D-CHA	2.45	1.47	1.38
37	20	308	CLA	C4C-C3C	2.45	1.49	1.45
48	13	311	A86	C-C1	2.45	1.55	1.50
37	B	502	CLA	C1C-NC	-2.45	1.34	1.37
37	c	504	CLA	C4D-CHA	2.45	1.47	1.38
37	40	203	CLA	C4D-CHA	2.45	1.47	1.38
37	c	513	CLA	C3D-C4D	-2.45	1.38	1.44
48	33	311	A86	C-C1	2.45	1.55	1.50
37	11	308	CLA	C1C-NC	-2.45	1.34	1.37
37	20	307	CLA	C4C-C3C	2.45	1.49	1.45
47	36	305	KC1	C4C-C3C	2.45	1.49	1.45
47	38	207	KC1	CHB-C4A	-2.45	1.33	1.39
47	35	304	KC1	C2A-C1A	2.45	1.52	1.44
37	35	310	CLA	C4C-C3C	2.45	1.49	1.45
50	16	312	DD6	C26-C27	-2.45	1.31	1.37
48	15	311	A86	O-C13	-2.44	1.18	1.23
37	39	301	CLA	C4D-CHA	2.44	1.47	1.38
48	35	311	A86	C-C1	2.44	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	33	303	CLA	C3D-C4D	-2.44	1.38	1.44
50	36	312	DD6	C26-C27	-2.44	1.31	1.37
37	B	513	CLA	C4D-CHA	2.44	1.47	1.38
39	H	101	BCR	C30-C25	-2.44	1.50	1.53
37	36	301	CLA	C4D-CHA	2.44	1.47	1.38
37	33	307	CLA	C4B-NB	-2.44	1.33	1.35
47	36	302	KC1	CAA-C2A	2.44	1.54	1.46
48	13	315	A86	C14-C15	2.44	1.57	1.52
48	20	309	A86	O-C13	-2.44	1.18	1.23
47	15	309	KC1	C4D-CHA	2.44	1.48	1.45
37	39	307	CLA	C3D-C4D	-2.44	1.38	1.44
37	B	514	CLA	C4B-NB	-2.44	1.33	1.35
37	b	507	CLA	C4B-NB	-2.44	1.33	1.35
47	17	303	KC1	C4D-CHA	2.44	1.48	1.45
47	15	302	KC1	C4A-C3A	2.44	1.49	1.44
47	16	302	KC1	CAA-C2A	2.44	1.54	1.46
37	40	209	CLA	C4C-C3C	2.44	1.49	1.45
37	41	204	CLA	C1B-NB	-2.44	1.33	1.35
47	14	309	KC1	C4A-C3A	2.44	1.49	1.44
37	19	301	CLA	C4D-CHA	2.44	1.47	1.38
48	35	311	A86	O-C13	-2.44	1.18	1.23
37	b	516	CLA	C4D-CHA	2.44	1.47	1.38
37	C	513	CLA	C4D-CHA	2.44	1.47	1.38
48	18	212	A86	C-C1	2.44	1.55	1.50
47	19	308	KC1	C4A-C3A	2.44	1.49	1.44
48	32	218	A86	C24-C1	2.44	1.51	1.45
41	16	316	LMG	C4-C5	2.44	1.58	1.53
37	33	310	CLA	C4C-C3C	2.43	1.49	1.45
37	C	506	CLA	C4D-CHA	2.43	1.47	1.38
48	33	315	A86	C14-C15	2.43	1.57	1.52
37	C	513	CLA	C3D-C4D	-2.43	1.38	1.44
43	D	409	LHG	O7-C5	-2.43	1.40	1.46
37	15	301	CLA	C4B-CHC	2.43	1.47	1.41
37	31	302	CLA	C3D-C4D	-2.43	1.38	1.44
37	39	304	CLA	C4D-CHA	2.43	1.47	1.38
48	37	309	A86	C24-C1	2.43	1.51	1.45
37	b	503	CLA	C1C-NC	-2.43	1.34	1.37
48	14	314	A86	C24-C1	2.43	1.51	1.45
47	41	203	KC1	C4D-CHA	2.43	1.48	1.45
45	d	402	PL9	C53-C6	-2.43	1.45	1.50
37	35	307	CLA	C4B-CHC	2.43	1.47	1.41
47	13	302	KC1	C4A-C3A	2.43	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	12	220	A86	C14-C15	2.43	1.57	1.52
37	40	203	CLA	C4B-CHC	2.43	1.47	1.41
48	40	211	A86	O-C13	-2.43	1.18	1.23
37	16	309	CLA	C3D-C4D	-2.43	1.38	1.44
48	12	217	A86	C24-C1	2.43	1.51	1.45
37	d	404	CLA	C4D-CHA	2.43	1.47	1.38
37	38	201	CLA	C1B-NB	-2.43	1.33	1.35
47	17	305	KC1	C4C-C3C	2.43	1.49	1.45
47	11	302	KC1	C4A-C3A	2.42	1.49	1.44
37	40	205	CLA	OBD-CAD	2.42	1.26	1.22
37	19	306	CLA	C4B-CHC	2.42	1.47	1.41
37	14	307	CLA	C3D-C4D	-2.42	1.38	1.44
37	16	303	CLA	C3D-C4D	-2.42	1.38	1.44
37	34	307	CLA	C3D-C4D	-2.42	1.38	1.44
48	32	221	A86	C14-C15	2.42	1.57	1.52
37	b	504	CLA	C1C-NC	-2.42	1.34	1.37
37	B	502	CLA	C4B-NB	-2.42	1.33	1.35
48	17	310	A86	C24-C1	2.42	1.51	1.45
37	c	512	CLA	C4D-CHA	2.42	1.47	1.38
48	11	319	A86	C14-C15	2.42	1.57	1.52
48	18	213	A86	C14-C15	2.42	1.57	1.52
48	31	319	A86	C14-C15	2.42	1.57	1.52
48	12	214	A86	C-C1	2.42	1.55	1.50
37	20	303	CLA	OBD-CAD	2.42	1.26	1.22
37	11	310	CLA	C4D-CHA	2.42	1.47	1.38
37	20	301	CLA	C4B-CHC	2.42	1.47	1.41
48	14	315	A86	O4-C34	-2.42	1.40	1.46
48	34	315	A86	O4-C34	-2.42	1.40	1.46
37	D	406	CLA	C4D-CHA	2.42	1.47	1.38
37	17	302	CLA	C1B-NB	-2.42	1.33	1.35
47	17	308	KC1	C4D-CHA	2.42	1.48	1.45
43	d	407	LHG	O7-C5	-2.42	1.40	1.46
37	14	302	CLA	C1B-NB	-2.42	1.33	1.35
37	15	307	CLA	C4B-CHC	2.42	1.47	1.41
47	20	305	KC1	C4D-CHA	2.42	1.48	1.45
37	33	308	CLA	C3D-C4D	-2.42	1.38	1.44
37	C	512	CLA	C4D-CHA	2.42	1.47	1.38
47	37	304	KC1	C4C-C3C	2.42	1.49	1.45
47	12	208	KC1	C4A-C3A	2.42	1.49	1.44
37	18	202	CLA	C4B-CHC	2.42	1.47	1.41
48	36	311	A86	C-C1	2.42	1.55	1.50
37	19	307	CLA	C3D-C4D	-2.42	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	516	CLA	C4D-CHA	2.42	1.47	1.38
37	B	505	CLA	C1C-NC	-2.42	1.34	1.37
48	32	215	A86	C-C1	2.42	1.55	1.50
37	36	309	CLA	C4C-C3C	2.42	1.49	1.45
48	37	312	A86	C24-C1	2.41	1.51	1.45
37	19	304	CLA	C4D-CHA	2.41	1.47	1.38
37	32	211	CLA	C3D-C4D	-2.41	1.38	1.44
48	41	211	A86	C24-C1	2.41	1.51	1.45
37	39	303	CLA	C4D-CHA	2.41	1.47	1.38
47	14	306	KC1	C4D-CHA	2.41	1.48	1.45
48	35	319	A86	O-C13	-2.41	1.18	1.23
37	19	306	CLA	C4D-CHA	2.41	1.47	1.38
37	B	503	CLA	C1C-NC	-2.41	1.34	1.37
37	B	511	CLA	C4D-CHA	2.41	1.47	1.38
37	12	210	CLA	C3D-C4D	-2.41	1.38	1.44
44	c	516	DGD	O5D-C6D	-2.41	1.39	1.43
45	D	404	PL9	C53-C6	-2.41	1.45	1.50
37	B	504	CLA	C1C-NC	-2.41	1.34	1.37
37	19	310	CLA	C1B-NB	-2.41	1.33	1.35
41	36	314	LMG	C4-C5	2.41	1.58	1.53
37	14	303	CLA	C4B-NB	-2.41	1.33	1.35
37	34	303	CLA	C4B-NB	-2.41	1.33	1.35
37	19	310	CLA	C3D-C4D	-2.41	1.38	1.44
39	a	413	BCR	C30-C25	-2.41	1.50	1.53
37	37	301	CLA	C3D-C4D	-2.41	1.38	1.44
37	13	307	CLA	O1D-CGD	2.41	1.27	1.21
37	z	102	CLA	C3D-C4D	-2.41	1.38	1.44
37	14	303	CLA	C3D-C4D	-2.41	1.38	1.44
50	21	212	DD6	C35-C36	2.40	1.54	1.51
37	32	202	CLA	C1C-NC	-2.40	1.34	1.37
40	16	315	SQD	O2-C2	-2.40	1.37	1.43
37	a	404	CLA	C4D-CHA	2.40	1.46	1.38
37	b	506	CLA	C4D-CHA	2.40	1.46	1.38
37	39	310	CLA	C3D-C4D	-2.40	1.38	1.44
37	41	209	CLA	C4C-C3C	2.40	1.49	1.45
48	35	315	A86	C24-C1	2.40	1.51	1.45
37	19	303	CLA	C4D-CHA	2.40	1.46	1.38
37	39	306	CLA	C4D-CHA	2.40	1.46	1.38
50	40	212	DD6	C4-C5	2.40	1.50	1.43
47	21	203	KC1	C4D-CHA	2.40	1.48	1.45
37	41	210	CLA	C1C-C2C	2.40	1.49	1.44
37	19	307	CLA	C4B-CHC	2.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	35	319	A86	C24-C1	2.40	1.51	1.45
37	31	310	CLA	C4D-CHA	2.40	1.46	1.38
37	z	101	CLA	C1B-NB	-2.40	1.33	1.35
37	15	305	CLA	C4C-C3C	2.40	1.49	1.45
37	40	210	CLA	C4C-C3C	2.40	1.49	1.45
47	16	305	KC1	C4C-C3C	2.40	1.49	1.45
37	33	303	CLA	C4C-C3C	2.40	1.49	1.45
37	b	505	CLA	C1C-NC	-2.40	1.34	1.37
37	21	204	CLA	C4C-C3C	2.40	1.49	1.45
48	38	215	A86	C14-C15	2.40	1.57	1.52
47	34	309	KC1	C4A-C3A	2.40	1.49	1.44
37	Z	102	CLA	C3D-C4D	-2.40	1.38	1.44
47	40	204	KC1	C4A-C3A	2.40	1.49	1.44
40	40	202	SQD	O2-C2	-2.40	1.37	1.43
37	B	513	CLA	C1C-NC	-2.40	1.34	1.37
37	16	309	CLA	C1B-NB	-2.40	1.33	1.35
47	11	306	KC1	C4D-CHA	2.40	1.48	1.45
47	31	307	KC1	C4D-CHA	2.40	1.48	1.45
37	D	401	CLA	C4D-CHA	2.40	1.46	1.38
47	31	303	KC1	C4A-C3A	2.39	1.49	1.44
37	36	309	CLA	C3D-C4D	-2.39	1.38	1.44
48	17	313	A86	C24-C1	2.39	1.51	1.45
47	37	307	KC1	C4D-CHA	2.39	1.48	1.45
37	B	524	CLA	C1C-C2C	2.39	1.49	1.44
37	b	511	CLA	C4D-CHA	2.39	1.46	1.38
48	12	216	A86	C24-C1	2.39	1.51	1.45
48	32	217	A86	C24-C1	2.39	1.51	1.45
37	19	306	CLA	C3D-C4D	-2.39	1.38	1.44
37	B	506	CLA	C4D-CHA	2.39	1.46	1.38
39	A	410	BCR	C30-C25	-2.39	1.50	1.53
50	21	212	DD6	C4-C5	2.39	1.50	1.43
50	41	212	DD6	C4-C5	2.39	1.50	1.43
39	B	518	BCR	C30-C25	-2.39	1.50	1.53
37	41	204	CLA	C4C-C3C	2.39	1.49	1.45
39	b	518	BCR	C30-C25	-2.39	1.50	1.53
39	y	101	BCR	C33-C5	-2.39	1.47	1.50
48	15	315	A86	C24-C1	2.39	1.51	1.45
37	b	502	CLA	C4D-CHA	2.39	1.46	1.38
37	34	303	CLA	C3D-C4D	-2.39	1.38	1.44
37	20	307	CLA	C4B-CHC	2.39	1.47	1.41
37	33	305	CLA	C4B-CHC	2.39	1.47	1.41
48	12	220	A86	C-C1	2.39	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	39	312	DD6	C22-C16	-2.39	1.49	1.53
37	14	308	CLA	C1B-NB	-2.39	1.33	1.35
37	38	204	CLA	C4D-CHA	2.39	1.46	1.38
48	39	313	A86	C24-C1	2.39	1.51	1.45
37	19	301	CLA	C4B-CHC	2.39	1.47	1.41
37	14	310	CLA	C1B-NB	-2.39	1.33	1.35
37	B	510	CLA	C4B-NB	-2.38	1.33	1.35
37	36	306	CLA	C1C-C2C	2.38	1.49	1.44
50	19	312	DD6	C22-C16	-2.38	1.49	1.53
48	17	311	A86	C24-C1	2.38	1.51	1.45
37	B	505	CLA	C4D-CHA	2.38	1.46	1.38
48	15	319	A86	C24-C1	2.38	1.51	1.45
37	36	301	CLA	C4B-CHC	2.38	1.47	1.41
37	41	204	CLA	C3D-C4D	-2.38	1.38	1.44
37	36	309	CLA	C1B-NB	-2.38	1.33	1.35
37	16	309	CLA	C4C-C3C	2.38	1.49	1.45
45	d	406	PL9	C53-C6	-2.38	1.45	1.50
47	33	302	KC1	C4A-C3A	2.38	1.49	1.44
47	38	205	KC1	C4C-C3C	2.38	1.49	1.45
37	11	301	CLA	C3D-C4D	-2.38	1.38	1.44
47	37	302	KC1	C4D-CHA	2.38	1.48	1.45
37	B	502	CLA	C4D-CHA	2.38	1.46	1.38
37	13	305	CLA	C4B-CHC	2.38	1.47	1.41
37	A	405	CLA	C4D-CHA	2.38	1.46	1.38
37	31	301	CLA	C3D-C4D	-2.38	1.38	1.44
48	31	311	A86	C14-C15	2.38	1.57	1.52
37	32	208	CLA	C4D-CHA	2.38	1.46	1.38
45	D	408	PL9	C53-C6	-2.38	1.45	1.50
37	21	209	CLA	C4B-CHC	2.38	1.47	1.41
47	21	207	KC1	C2A-C1A	2.37	1.51	1.44
47	37	305	KC1	CHB-C4A	-2.37	1.33	1.39
50	20	310	DD6	C4-C5	2.37	1.50	1.43
37	11	301	CLA	C4B-CHC	2.37	1.47	1.41
37	31	302	CLA	C4B-CHC	2.37	1.47	1.41
37	36	309	CLA	C4B-CHC	2.37	1.47	1.41
37	38	201	CLA	C1C-C2C	2.37	1.49	1.44
41	A	408	LMG	O8-C9	-2.37	1.39	1.45
37	38	203	CLA	C4C-C3C	2.37	1.49	1.45
47	18	207	KC1	CHB-C4A	-2.37	1.33	1.39
37	19	304	CLA	C3D-C4D	-2.37	1.38	1.44
48	11	312	A86	O4-C34	-2.37	1.40	1.46
41	32	201	LMG	O4-C4	-2.37	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	21	209	CLA	C4C-C3C	2.37	1.49	1.45
37	39	304	CLA	C1B-NB	-2.37	1.33	1.35
48	11	319	A86	C-C1	2.37	1.55	1.50
37	16	306	CLA	C1C-C2C	2.37	1.49	1.44
37	21	210	CLA	C1C-C2C	2.37	1.49	1.44
48	32	221	A86	C-C1	2.37	1.55	1.50
47	36	304	KC1	C2A-C1A	2.37	1.51	1.44
47	41	207	KC1	C2A-C1A	2.37	1.51	1.44
37	Z	101	CLA	C1B-NB	-2.37	1.33	1.35
37	b	505	CLA	C4D-CHA	2.37	1.46	1.38
37	b	502	CLA	C4B-NB	-2.37	1.33	1.35
37	a	407	CLA	C4D-CHA	2.37	1.46	1.38
37	39	306	CLA	C3D-C4D	-2.37	1.38	1.44
37	17	304	CLA	C3D-C4D	-2.37	1.38	1.44
37	37	303	CLA	C3D-C4D	-2.37	1.38	1.44
37	34	310	CLA	C4C-C3C	2.37	1.49	1.45
37	d	401	CLA	C4D-CHA	2.37	1.46	1.38
37	40	209	CLA	C4B-CHC	2.37	1.47	1.41
39	K	101	BCR	C33-C5	-2.36	1.47	1.50
37	16	303	CLA	C4C-C3C	2.36	1.49	1.45
47	16	304	KC1	C2A-C1A	2.36	1.51	1.44
44	H	102	DGD	O1G-C1G	-2.36	1.39	1.45
37	12	205	CLA	C4B-NB	-2.36	1.33	1.35
37	b	508	CLA	C4D-CHA	2.36	1.46	1.38
44	h	102	DGD	O1G-C1G	-2.36	1.39	1.45
47	16	302	KC1	C4C-C3C	2.36	1.49	1.45
37	W	102	CLA	C3D-C4D	-2.36	1.38	1.44
37	d	404	CLA	C1C-NC	-2.36	1.34	1.37
41	17	317	LMG	O8-C9	-2.36	1.39	1.45
47	35	302	KC1	C4D-CHA	2.36	1.48	1.45
37	13	308	CLA	C3D-C4D	-2.36	1.38	1.44
48	34	316	A86	C14-C15	2.36	1.57	1.52
48	15	314	A86	O-C13	-2.36	1.18	1.23
50	41	212	DD6	C35-C36	2.36	1.54	1.51
37	12	207	CLA	C4D-CHA	2.36	1.46	1.38
48	14	316	A86	C14-C15	2.36	1.57	1.52
37	a	403	CLA	C4D-CHA	2.36	1.46	1.38
37	34	302	CLA	C3D-C4D	-2.36	1.38	1.44
37	C	508	CLA	C4D-CHA	2.36	1.46	1.38
37	21	204	CLA	C3D-C4D	-2.36	1.38	1.44
37	39	301	CLA	C4B-CHC	2.36	1.47	1.41
48	21	211	A86	C-C1	2.36	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	a	410	LMG	O8-C9	-2.36	1.39	1.45
37	16	309	CLA	C4B-CHC	2.36	1.47	1.41
37	39	307	CLA	C4B-CHC	2.36	1.47	1.41
37	12	209	CLA	C4B-NB	-2.36	1.33	1.35
47	18	207	KC1	C4C-C3C	2.36	1.49	1.45
37	c	508	CLA	C4D-CHA	2.36	1.46	1.38
48	11	313	A86	O4-C34	-2.36	1.40	1.46
48	37	310	A86	O4-C34	-2.36	1.40	1.46
37	39	304	CLA	C4B-CHC	2.36	1.47	1.41
48	11	313	A86	C24-C1	2.36	1.51	1.45
37	38	208	CLA	C3D-C4D	-2.36	1.38	1.44
48	16	310	A86	C25-C24	2.36	1.40	1.34
48	21	215	A86	O1-C20	2.36	1.49	1.46
48	14	311	A86	C-C1	2.35	1.55	1.50
48	34	311	A86	C-C1	2.35	1.55	1.50
37	39	307	CLA	C1C-NC	-2.35	1.34	1.37
37	41	210	CLA	C4C-C3C	2.35	1.49	1.45
37	38	209	CLA	C4B-CHC	2.35	1.47	1.41
37	18	204	CLA	C4D-CHA	2.35	1.46	1.38
47	36	302	KC1	C4C-C3C	2.35	1.49	1.45
44	j	101	DGD	O3G-C3G	-2.35	1.39	1.43
37	41	209	CLA	C4B-CHC	2.35	1.47	1.41
37	16	301	CLA	C4B-CHC	2.35	1.47	1.41
37	41	206	CLA	C4B-CHC	2.35	1.47	1.41
37	B	508	CLA	C4D-CHA	2.35	1.46	1.38
37	13	310	CLA	C1B-NB	-2.35	1.33	1.35
37	39	310	CLA	C1B-NB	-2.35	1.33	1.35
37	21	206	CLA	C4B-CHC	2.35	1.47	1.41
37	A	403	CLA	C4D-CHA	2.35	1.46	1.38
37	14	308	CLA	C3D-C4D	-2.35	1.38	1.44
37	39	304	CLA	C3D-C4D	-2.35	1.38	1.44
37	b	523	CLA	C1C-C2C	2.35	1.49	1.44
37	38	206	CLA	C1B-NB	-2.35	1.33	1.35
37	18	204	CLA	C4B-CHC	2.35	1.47	1.41
48	41	211	A86	C-C1	2.35	1.55	1.50
37	31	301	CLA	C4B-CHC	2.35	1.47	1.41
37	14	302	CLA	C3D-C4D	-2.35	1.38	1.44
48	41	215	A86	O1-C20	2.35	1.49	1.46
37	D	402	CLA	C4D-CHA	2.35	1.46	1.38
41	12	201	LMG	O4-C4	-2.35	1.37	1.43
47	17	306	KC1	CHB-C4A	-2.35	1.33	1.39
48	31	312	A86	O4-C34	-2.35	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	38	201	CLA	C4B-CHC	2.35	1.47	1.41
37	35	301	CLA	C3D-C4D	-2.35	1.38	1.44
48	36	310	A86	C25-C24	2.35	1.40	1.34
37	38	206	CLA	C4B-CHC	2.35	1.47	1.41
37	z	101	CLA	C4D-CHA	2.35	1.46	1.38
47	34	306	KC1	C4D-CHA	2.35	1.48	1.45
37	38	202	CLA	C1C-C2C	2.34	1.49	1.44
47	20	302	KC1	C4A-C3A	2.34	1.49	1.44
37	35	305	CLA	C4C-C3C	2.34	1.49	1.45
41	37	316	LMG	O8-C9	-2.34	1.39	1.45
37	36	303	CLA	C4C-C3C	2.34	1.49	1.45
37	C	509	CLA	C4D-CHA	2.34	1.46	1.38
37	21	204	CLA	C1B-NB	-2.34	1.33	1.35
48	19	313	A86	C24-C1	2.34	1.51	1.45
37	D	402	CLA	C1C-NC	-2.34	1.34	1.37
37	32	204	CLA	C3D-C4D	-2.34	1.38	1.44
48	31	319	A86	C25-C24	2.34	1.40	1.34
37	12	203	CLA	C3D-C4D	-2.34	1.38	1.44
37	41	208	CLA	C4B-CHC	2.34	1.47	1.41
37	18	208	CLA	C3D-C4D	-2.34	1.38	1.44
48	40	201	A86	C14-C15	2.34	1.57	1.52
37	W	102	CLA	C4B-CHC	2.34	1.47	1.41
37	C	501	CLA	C1C-NC	-2.34	1.34	1.37
48	40	201	A86	O-C13	-2.34	1.18	1.23
37	19	307	CLA	C1C-NC	-2.34	1.34	1.37
48	17	311	A86	O4-C34	-2.34	1.40	1.46
37	Z	101	CLA	C4D-CHA	2.33	1.46	1.38
37	12	212	CLA	C4B-CHC	2.33	1.47	1.41
37	32	213	CLA	C4B-CHC	2.33	1.47	1.41
37	40	208	CLA	C3D-C4D	-2.33	1.38	1.44
48	31	319	A86	C-C1	2.33	1.55	1.50
37	d	401	CLA	C1C-NC	-2.33	1.34	1.37
37	19	304	CLA	C4B-CHC	2.33	1.47	1.41
37	11	307	CLA	C1C-NC	-2.33	1.34	1.37
48	19	313	A86	C22-C16	2.33	1.58	1.53
48	38	215	A86	O-C13	-2.33	1.18	1.23
48	11	311	A86	C14-C15	2.33	1.57	1.52
37	34	308	CLA	C3D-C4D	-2.33	1.38	1.44
37	20	306	CLA	C3D-C4D	-2.33	1.38	1.44
37	D	406	CLA	C1C-NC	-2.33	1.34	1.37
37	B	503	CLA	C4D-CHA	2.33	1.46	1.38
48	15	311	A86	C24-C1	2.33	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	18	209	CLA	C4B-CHC	2.33	1.47	1.41
37	C	506	CLA	C4B-NB	-2.33	1.33	1.35
37	B	509	CLA	C1C-NC	-2.33	1.34	1.37
48	39	313	A86	C22-C16	2.33	1.58	1.53
37	b	501	CLA	C1C-NC	-2.33	1.34	1.37
48	11	319	A86	C25-C24	2.33	1.40	1.34
48	31	315	A86	O4-C34	-2.33	1.40	1.46
37	b	513	CLA	C1C-NC	-2.33	1.34	1.37
37	b	523	CLA	C4D-CHA	2.33	1.46	1.38
37	20	301	CLA	C1C-C2C	2.32	1.49	1.44
37	17	309	CLA	C4B-CHC	2.32	1.47	1.41
37	14	305	CLA	C4B-CHC	2.32	1.47	1.41
37	37	308	CLA	C4B-CHC	2.32	1.47	1.41
38	A	404	PHO	CMC-C2C	-2.32	1.46	1.51
41	11	316	LMG	O7-C8	-2.32	1.40	1.46
41	31	316	LMG	O7-C8	-2.32	1.40	1.46
37	b	509	CLA	C1C-NC	-2.32	1.34	1.37
37	34	305	CLA	C4B-CHC	2.32	1.47	1.41
37	40	203	CLA	C1C-C2C	2.32	1.49	1.44
37	21	210	CLA	C4C-C3C	2.32	1.49	1.45
47	18	205	KC1	C4C-C3C	2.32	1.49	1.45
37	c	509	CLA	C4D-CHA	2.32	1.46	1.38
37	17	309	CLA	C1C-NC	-2.32	1.34	1.37
37	17	307	CLA	C3D-C4D	-2.32	1.38	1.44
37	37	306	CLA	C3D-C4D	-2.32	1.38	1.44
37	38	209	CLA	C1C-C2C	2.32	1.49	1.44
48	31	319	A86	O4-C34	-2.32	1.40	1.46
48	20	311	A86	O-C13	-2.32	1.18	1.23
37	b	523	CLA	C4B-CHC	2.32	1.47	1.41
37	b	510	CLA	C4B-NB	-2.32	1.33	1.35
37	b	514	CLA	C4B-NB	-2.32	1.33	1.35
43	41	201	LHG	O7-C5	-2.32	1.40	1.46
37	15	301	CLA	C3D-C4D	-2.32	1.38	1.44
47	19	308	KC1	C2A-C1A	2.32	1.51	1.44
47	39	308	KC1	C2A-C1A	2.32	1.51	1.44
48	12	213	A86	C-C1	2.32	1.55	1.50
37	18	206	CLA	C4C-C3C	2.32	1.49	1.45
37	14	301	CLA	C1C-C2C	2.32	1.49	1.44
47	14	304	KC1	C4A-C3A	2.32	1.49	1.44
37	c	501	CLA	C4D-CHA	2.31	1.46	1.38
37	15	307	CLA	C1C-C2C	2.31	1.49	1.44
37	18	209	CLA	C1C-C2C	2.31	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	35	307	CLA	C1C-C2C	2.31	1.49	1.44
37	18	201	CLA	C4B-CHC	2.31	1.47	1.41
37	19	304	CLA	C1B-NB	-2.31	1.33	1.35
37	B	524	CLA	C4B-CHC	2.31	1.47	1.41
48	37	319	A86	C24-C1	2.31	1.50	1.45
47	14	304	KC1	C2A-C1A	2.31	1.51	1.44
47	34	304	KC1	C2A-C1A	2.31	1.51	1.44
38	a	406	PHO	CMC-C2C	-2.31	1.46	1.51
37	c	510	CLA	C4D-CHA	2.31	1.46	1.38
37	18	209	CLA	C1B-CHB	2.31	1.47	1.41
37	C	505	CLA	C4D-CHA	2.31	1.46	1.38
44	J	101	DGD	O3G-C3G	-2.31	1.39	1.43
37	33	305	CLA	C1C-C2C	2.31	1.49	1.44
37	32	210	CLA	C4B-NB	-2.31	1.33	1.35
48	35	314	A86	O-C13	-2.31	1.18	1.23
37	c	501	CLA	C1C-NC	-2.31	1.34	1.37
37	18	204	CLA	C1C-C2C	2.31	1.49	1.44
48	11	315	A86	O4-C34	-2.31	1.40	1.46
37	38	204	CLA	C4B-CHC	2.31	1.47	1.41
37	b	503	CLA	C4D-CHA	2.31	1.46	1.38
48	13	312	A86	O4-C34	-2.31	1.40	1.46
37	c	513	CLA	C1B-NB	-2.31	1.33	1.35
37	17	302	CLA	C4B-NB	-2.31	1.33	1.35
37	B	524	CLA	C4D-CHA	2.31	1.46	1.38
37	20	306	CLA	C4B-CHC	2.31	1.47	1.41
48	33	313	A86	C14-C15	2.30	1.57	1.52
37	C	510	CLA	C4D-CHA	2.30	1.46	1.38
37	19	302	CLA	C1B-NB	-2.30	1.33	1.35
37	39	302	CLA	C1B-NB	-2.30	1.33	1.35
48	16	313	A86	O-C13	-2.30	1.18	1.23
37	21	208	CLA	C4B-CHC	2.30	1.47	1.41
48	31	311	A86	C19-C18	2.30	1.55	1.52
37	c	511	CLA	C1C-NC	-2.30	1.34	1.37
37	18	202	CLA	C1B-NB	-2.30	1.33	1.35
48	40	213	A86	O-C13	-2.30	1.18	1.23
37	14	305	CLA	C3D-C4D	-2.30	1.39	1.44
37	34	305	CLA	C3D-C4D	-2.30	1.39	1.44
37	11	303	CLA	C1C-NC	-2.30	1.34	1.37
47	15	302	KC1	C4D-CHA	2.30	1.47	1.45
44	H	102	DGD	O5D-C6D	-2.30	1.39	1.43
37	14	310	CLA	C4C-C3C	2.30	1.49	1.45
41	l	101	LMG	O2-C2	-2.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	36	312	DD6	C4-C5	2.30	1.50	1.43
37	W	101	CLA	C4B-CHC	2.30	1.47	1.41
37	40	208	CLA	C4B-CHC	2.30	1.47	1.41
48	12	217	A86	C14-C15	2.30	1.57	1.52
37	13	305	CLA	C3D-C4D	-2.30	1.39	1.44
37	33	305	CLA	C3D-C4D	-2.30	1.39	1.44
37	34	301	CLA	C3D-C4D	-2.30	1.39	1.44
38	D	403	PHO	CMC-C2C	-2.30	1.46	1.51
50	21	212	DD6	O1-C20	2.30	1.49	1.46
37	b	503	CLA	C4B-NB	-2.30	1.33	1.35
37	33	310	CLA	C1B-NB	-2.30	1.33	1.35
48	31	315	A86	C-C1	2.30	1.55	1.50
41	L	102	LMG	O2-C2	-2.30	1.37	1.43
37	C	511	CLA	C1C-NC	-2.30	1.34	1.37
37	c	503	CLA	C4B-NB	-2.29	1.33	1.35
37	12	207	CLA	C1C-NC	-2.29	1.34	1.37
37	32	208	CLA	C1C-NC	-2.29	1.34	1.37
48	16	313	A86	C14-C15	2.29	1.57	1.52
37	11	310	CLA	C1C-NC	-2.29	1.34	1.37
37	31	310	CLA	C1C-NC	-2.29	1.34	1.37
48	34	316	A86	C24-C1	2.29	1.50	1.45
37	18	203	CLA	C4C-C3C	2.29	1.49	1.45
48	12	213	A86	O4-C34	-2.29	1.40	1.46
47	21	207	KC1	C4A-C3A	2.29	1.49	1.44
37	34	310	CLA	C1B-NB	-2.29	1.33	1.35
37	34	308	CLA	C1B-CHB	2.29	1.47	1.41
37	38	206	CLA	C3D-C4D	-2.29	1.39	1.44
48	41	211	A86	O-C13	-2.29	1.18	1.23
48	35	311	A86	C14-C15	2.29	1.57	1.52
50	40	214	DD6	C22-C16	-2.29	1.49	1.53
37	13	310	CLA	C3D-C4D	-2.29	1.39	1.44
47	41	203	KC1	C1C-C2C	2.29	1.49	1.44
37	c	506	CLA	C4B-NB	-2.29	1.33	1.35
50	20	312	DD6	C22-C16	-2.29	1.49	1.53
48	11	319	A86	O4-C34	-2.29	1.40	1.46
48	11	311	A86	C19-C18	2.28	1.55	1.52
37	31	308	CLA	C1C-NC	-2.28	1.34	1.37
48	18	215	A86	C14-C15	2.28	1.57	1.52
37	36	306	CLA	C4B-CHC	2.28	1.47	1.41
37	Z	102	CLA	C4B-CHC	2.28	1.47	1.41
37	w	101	CLA	C4B-CHC	2.28	1.47	1.41
37	c	505	CLA	C4D-CHA	2.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	13	305	CLA	C1C-C2C	2.28	1.49	1.44
37	C	501	CLA	C4D-CHA	2.28	1.46	1.38
50	41	212	DD6	O1-C20	2.28	1.49	1.46
38	a	405	PHO	CMC-C2C	-2.28	1.46	1.51
44	J	101	DGD	O2E-C2E	-2.28	1.37	1.43
37	Z	102	CLA	CAA-C2A	-2.28	1.49	1.54
37	16	306	CLA	C4B-CHC	2.28	1.47	1.41
37	31	301	CLA	C1B-CHB	2.28	1.47	1.41
50	16	312	DD6	C4-C5	2.28	1.50	1.43
37	C	513	CLA	C1B-NB	-2.28	1.33	1.35
48	33	312	A86	O4-C34	-2.28	1.40	1.46
48	14	316	A86	C24-C1	2.28	1.50	1.45
37	z	102	CLA	C4B-CHC	2.28	1.47	1.41
37	35	305	CLA	C1C-C2C	2.28	1.49	1.44
37	17	304	CLA	C4B-NB	-2.28	1.33	1.35
47	41	207	KC1	C4A-C3A	2.27	1.49	1.44
48	37	314	A86	C35-C34	2.27	1.55	1.51
47	37	304	KC1	C3D-C4D	-2.27	1.38	1.40
48	32	214	A86	O4-C34	-2.27	1.40	1.46
37	18	201	CLA	C1C-C2C	2.27	1.49	1.44
37	19	305	CLA	C3D-C4D	-2.27	1.39	1.44
44	H	102	DGD	O2D-C2D	-2.27	1.37	1.43
37	15	303	CLA	C3D-C4D	-2.27	1.39	1.44
44	h	102	DGD	O5D-C6D	-2.27	1.39	1.43
44	h	102	DGD	O2D-C2D	-2.27	1.37	1.43
48	17	320	A86	C24-C1	2.27	1.50	1.45
44	j	101	DGD	O2E-C2E	-2.27	1.37	1.43
37	34	303	CLA	C4C-C3C	2.27	1.48	1.45
47	34	304	KC1	C4A-C3A	2.27	1.49	1.44
48	15	312	A86	O4-C34	-2.27	1.40	1.46
47	35	306	KC1	C1C-C2C	2.27	1.49	1.44
48	11	315	A86	C-C1	2.27	1.55	1.50
37	32	206	CLA	C1C-NC	-2.27	1.34	1.37
37	38	202	CLA	C1B-NB	-2.27	1.33	1.35
37	21	205	CLA	C4B-CHC	2.27	1.47	1.41
47	21	203	KC1	C1C-C2C	2.27	1.49	1.44
50	39	312	DD6	C4-C5	2.27	1.50	1.43
37	39	302	CLA	C4C-C3C	2.27	1.48	1.45
37	40	210	CLA	C4B-CHC	2.27	1.47	1.41
48	16	314	A86	C14-C15	2.27	1.57	1.52
37	37	308	CLA	C1C-NC	-2.27	1.34	1.37
37	a	407	CLA	C1C-NC	-2.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	31	313	A86	O4-C34	-2.26	1.40	1.46
48	11	311	A86	O4-C34	-2.26	1.40	1.46
37	c	506	CLA	C4C-C3C	2.26	1.48	1.45
37	20	308	CLA	C4B-CHC	2.26	1.47	1.41
37	31	301	CLA	C1C-C2C	2.26	1.48	1.44
37	21	210	CLA	C4B-CHC	2.26	1.47	1.41
37	B	501	CLA	C1C-NC	-2.26	1.34	1.37
37	15	305	CLA	C1C-C2C	2.26	1.48	1.44
37	21	206	CLA	C1C-C2C	2.26	1.48	1.44
43	21	201	LHG	O7-C5	-2.26	1.40	1.46
37	41	210	CLA	C4B-CHC	2.26	1.47	1.41
37	w	101	CLA	C3D-C4D	-2.26	1.39	1.44
48	35	311	A86	C24-C1	2.26	1.50	1.45
45	D	408	PL9	C46-C44	-2.26	1.46	1.51
37	35	303	CLA	C4B-CHC	2.26	1.47	1.41
47	41	207	KC1	C4D-CHA	2.26	1.47	1.45
38	D	403	PHO	CMD-C2D	-2.26	1.46	1.51
37	c	511	CLA	C4B-NB	-2.26	1.33	1.35
37	18	203	CLA	C1B-NB	-2.26	1.33	1.35
48	31	311	A86	O4-C34	-2.26	1.40	1.46
40	B	522	SQD	O2-C2	-2.26	1.37	1.43
50	21	212	DD6	C26-C27	-2.26	1.32	1.37
50	41	212	DD6	C26-C27	-2.26	1.32	1.37
37	W	102	CLA	C1B-CHB	2.26	1.47	1.41
37	18	201	CLA	C1B-NB	-2.26	1.33	1.35
37	20	307	CLA	C1C-C2C	2.26	1.48	1.44
38	a	405	PHO	CMD-C2D	-2.26	1.46	1.51
37	12	212	CLA	C3D-C4D	-2.26	1.39	1.44
37	32	213	CLA	C3D-C4D	-2.26	1.39	1.44
37	35	303	CLA	C3D-C4D	-2.26	1.39	1.44
37	35	310	CLA	C3D-C4D	-2.26	1.39	1.44
37	40	205	CLA	C1C-C2C	2.26	1.48	1.44
37	13	310	CLA	C4B-CHC	2.26	1.47	1.41
48	21	211	A86	O-C13	-2.26	1.18	1.23
47	41	207	KC1	C3B-C4B	2.26	1.50	1.46
40	b	521	SQD	O2-C2	-2.26	1.37	1.43
37	38	203	CLA	C1B-NB	-2.26	1.33	1.35
37	35	307	CLA	C3D-C4D	-2.26	1.39	1.44
37	40	210	CLA	C1C-C2C	2.26	1.48	1.44
48	32	218	A86	C14-C15	2.26	1.57	1.52
37	14	301	CLA	C3D-C4D	-2.25	1.39	1.44
47	11	309	KC1	C4D-CHA	2.25	1.47	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	31	309	KC1	C4D-CHA	2.25	1.47	1.45
37	34	302	CLA	C4B-CHC	2.25	1.47	1.41
37	39	303	CLA	C4B-CHC	2.25	1.47	1.41
37	35	310	CLA	C4B-CHC	2.25	1.47	1.41
48	11	319	A86	C39-C38	2.25	1.57	1.49
37	38	206	CLA	C4C-C3C	2.25	1.48	1.45
37	41	202	CLA	C3D-C4D	-2.25	1.39	1.44
47	38	207	KC1	C4C-C3C	2.25	1.48	1.45
41	32	201	LMG	O8-C9	-2.25	1.40	1.45
37	38	209	CLA	C1B-CHB	2.25	1.47	1.41
37	41	206	CLA	C3D-C4D	-2.25	1.39	1.44
37	11	310	CLA	C4B-CHC	2.25	1.47	1.41
37	20	308	CLA	C3D-C4D	-2.25	1.39	1.44
37	15	305	CLA	C4B-CHC	2.25	1.47	1.41
48	37	313	A86	C24-C1	2.25	1.50	1.45
37	C	503	CLA	C4B-NB	-2.25	1.33	1.35
48	31	319	A86	C39-C38	2.25	1.57	1.49
47	15	304	KC1	CAA-C2A	2.25	1.53	1.46
37	W	102	CLA	C1C-C2C	2.25	1.48	1.44
37	35	305	CLA	C4B-CHC	2.25	1.47	1.41
37	38	203	CLA	C4B-CHC	2.25	1.47	1.41
37	C	510	CLA	C1C-NC	-2.25	1.34	1.37
37	17	304	CLA	C4C-C3C	2.25	1.48	1.45
37	37	303	CLA	C4C-C3C	2.25	1.48	1.45
40	a	409	SQD	O4-C4	-2.25	1.37	1.43
47	13	302	KC1	C4C-C3C	2.25	1.48	1.45
47	33	302	KC1	C4C-C3C	2.25	1.48	1.45
37	34	301	CLA	C1C-C2C	2.25	1.48	1.44
37	W	101	CLA	C3D-C4D	-2.25	1.39	1.44
37	41	205	CLA	C4B-CHC	2.25	1.47	1.41
37	19	302	CLA	C4C-C3C	2.25	1.48	1.45
48	15	311	A86	C14-C15	2.24	1.57	1.52
50	19	312	DD6	C4-C5	2.24	1.50	1.43
37	13	307	CLA	C1C-NC	-2.24	1.34	1.37
37	33	307	CLA	C1C-NC	-2.24	1.34	1.37
37	36	307	CLA	C4B-CHC	2.24	1.47	1.41
40	B	519	SQD	O2-C2	-2.24	1.37	1.43
37	21	206	CLA	C3D-C4D	-2.24	1.39	1.44
37	14	308	CLA	C1B-CHB	2.24	1.47	1.41
37	21	202	CLA	C1C-NC	-2.24	1.34	1.37
37	19	303	CLA	C4B-CHC	2.24	1.47	1.41
37	14	302	CLA	C4B-CHC	2.24	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	11	307	CLA	C1C-C2C	2.24	1.48	1.44
37	18	206	CLA	C1C-C2C	2.24	1.48	1.44
48	13	313	A86	C14-C15	2.24	1.57	1.52
47	39	308	KC1	CAA-C2A	2.24	1.53	1.46
37	16	301	CLA	C3D-C4D	-2.24	1.39	1.44
48	16	310	A86	O4-C34	-2.24	1.41	1.46
37	16	307	CLA	C4B-CHC	2.24	1.47	1.41
37	41	209	CLA	C3D-C4D	-2.24	1.39	1.44
37	A	405	CLA	C1C-NC	-2.24	1.34	1.37
47	21	203	KC1	C4C-C3C	2.24	1.48	1.45
37	C	511	CLA	C4B-NB	-2.24	1.33	1.35
37	40	210	CLA	C3D-C4D	-2.24	1.39	1.44
37	39	306	CLA	C1C-C2C	2.24	1.48	1.44
37	38	203	CLA	C3D-C4D	-2.24	1.39	1.44
37	21	209	CLA	C3D-C4D	-2.24	1.39	1.44
37	20	308	CLA	C1B-CHB	2.23	1.47	1.41
44	c	516	DGD	O3G-C3G	-2.23	1.39	1.43
37	34	305	CLA	C4C-C3C	2.23	1.48	1.45
37	18	203	CLA	C4B-CHC	2.23	1.47	1.41
48	11	314	A86	C24-C1	2.23	1.50	1.45
45	d	406	PL9	C46-C44	-2.23	1.46	1.51
37	20	303	CLA	C1C-C2C	2.23	1.48	1.44
47	13	309	KC1	C4D-CHA	2.23	1.47	1.45
47	33	309	KC1	C4D-CHA	2.23	1.47	1.45
38	a	406	PHO	CMD-C2D	-2.23	1.46	1.51
37	15	303	CLA	C4B-CHC	2.23	1.47	1.41
37	31	310	CLA	C4B-CHC	2.23	1.47	1.41
37	39	310	CLA	C4B-CHC	2.23	1.47	1.41
44	C	516	DGD	O3G-C3G	-2.23	1.39	1.43
37	15	307	CLA	C3D-C4D	-2.23	1.39	1.44
40	A	407	SQD	O4-C4	-2.23	1.37	1.43
47	16	308	KC1	C4D-CHA	2.23	1.47	1.45
37	c	512	CLA	C1C-NC	-2.23	1.34	1.37
48	35	312	A86	O4-C34	-2.23	1.41	1.46
37	C	504	CLA	C4B-NB	-2.23	1.33	1.35
37	36	301	CLA	C1C-C2C	2.23	1.48	1.44
37	41	206	CLA	C1C-C2C	2.23	1.48	1.44
47	18	207	KC1	CAA-C2A	2.23	1.53	1.46
37	15	310	CLA	C4B-CHC	2.23	1.47	1.41
37	34	302	CLA	C1C-C2C	2.23	1.48	1.44
44	c	516	DGD	O2G-C2G	-2.23	1.41	1.46
37	B	514	CLA	C1C-NC	-2.23	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	33	310	CLA	C4B-CHC	2.23	1.47	1.41
47	36	305	KC1	C4D-CHA	2.23	1.47	1.45
37	15	308	CLA	C3D-C4D	-2.23	1.39	1.44
47	21	207	KC1	C3B-C4B	2.23	1.50	1.46
37	20	307	CLA	C3D-C4D	-2.23	1.39	1.44
37	14	302	CLA	C1C-C2C	2.23	1.48	1.44
47	41	203	KC1	C4C-C3C	2.23	1.48	1.45
37	A	405	CLA	C4B-NB	-2.23	1.33	1.35
37	d	401	CLA	C4B-NB	-2.23	1.33	1.35
48	32	215	A86	C24-C1	2.23	1.50	1.45
37	C	512	CLA	C1C-NC	-2.22	1.34	1.37
40	B	522	SQD	O4-C4	-2.22	1.37	1.43
37	39	305	CLA	C3D-C4D	-2.22	1.39	1.44
47	18	210	KC1	C4C-C3C	2.22	1.48	1.45
37	15	310	CLA	C3D-C4D	-2.22	1.39	1.44
48	38	213	A86	C24-C1	2.22	1.50	1.45
37	36	307	CLA	C3D-C4D	-2.22	1.39	1.44
37	19	306	CLA	C1C-C2C	2.22	1.48	1.44
37	C	504	CLA	C1C-NC	-2.22	1.34	1.37
37	b	514	CLA	C1C-NC	-2.22	1.34	1.37
37	19	310	CLA	C4B-CHC	2.22	1.47	1.41
47	16	305	KC1	C1C-C2C	2.22	1.48	1.44
37	14	305	CLA	C4C-C3C	2.22	1.48	1.45
48	36	313	A86	C14-C15	2.22	1.57	1.52
37	14	303	CLA	C4C-C3C	2.22	1.48	1.45
48	31	314	A86	C24-C1	2.22	1.50	1.45
40	b	521	SQD	O3-C3	-2.22	1.37	1.43
48	36	310	A86	O4-C34	-2.22	1.41	1.46
37	18	206	CLA	C4B-CHC	2.22	1.47	1.41
37	21	205	CLA	C3D-C4D	-2.22	1.39	1.44
37	41	205	CLA	C3D-C4D	-2.22	1.39	1.44
47	21	207	KC1	C4D-CHA	2.22	1.47	1.45
37	40	209	CLA	C3D-C4D	-2.22	1.39	1.44
47	33	302	KC1	C4D-CHA	2.22	1.47	1.45
37	18	203	CLA	C3D-C4D	-2.22	1.39	1.44
37	17	302	CLA	C1C-NC	-2.22	1.34	1.37
38	A	404	PHO	CMD-C2D	-2.22	1.46	1.51
37	32	213	CLA	C1C-C2C	2.22	1.48	1.44
37	18	211	CLA	C3D-C4D	-2.22	1.39	1.44
37	21	202	CLA	C3D-C4D	-2.22	1.39	1.44
48	34	311	A86	O4-C34	-2.22	1.41	1.46
37	40	209	CLA	C1B-CHB	2.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	z	102	CLA	CAA-C2A	-2.22	1.50	1.54
37	19	301	CLA	C3D-C4D	-2.22	1.39	1.44
37	13	301	CLA	C3D-C4D	-2.22	1.39	1.44
37	38	206	CLA	C1C-C2C	2.21	1.48	1.44
47	40	206	KC1	C4D-CHA	2.21	1.47	1.45
48	37	313	A86	O4-C34	-2.21	1.41	1.46
47	36	305	KC1	C1C-C2C	2.21	1.48	1.44
37	33	301	CLA	C3D-C4D	-2.21	1.39	1.44
47	32	212	KC1	C4D-CHA	2.21	1.47	1.45
37	41	202	CLA	C1C-NC	-2.21	1.34	1.37
37	15	305	CLA	C3D-C4D	-2.21	1.39	1.44
37	C	506	CLA	C4C-C3C	2.21	1.48	1.45
37	37	301	CLA	C1B-NB	-2.21	1.33	1.35
37	c	504	CLA	C1C-NC	-2.21	1.34	1.37
37	d	403	CLA	C1C-NC	-2.21	1.34	1.37
48	14	312	A86	O4-C34	-2.21	1.41	1.46
37	40	210	CLA	C1B-CHB	2.21	1.47	1.41
40	A	407	SQD	O3-C3	-2.21	1.37	1.43
47	16	305	KC1	CAA-C2A	2.21	1.53	1.46
40	L	101	SQD	O2-C2	-2.21	1.37	1.43
37	c	510	CLA	C1B-CHB	2.21	1.47	1.41
37	18	206	CLA	C3D-C4D	-2.21	1.39	1.44
47	19	308	KC1	CAA-C2A	2.21	1.53	1.46
37	16	307	CLA	C3D-C4D	-2.21	1.39	1.44
40	B	522	SQD	O3-C3	-2.21	1.37	1.43
37	38	208	CLA	C4B-CHC	2.21	1.47	1.41
37	37	301	CLA	C4B-CHC	2.21	1.47	1.41
48	34	312	A86	O4-C34	-2.21	1.41	1.46
37	13	305	CLA	C4C-C3C	2.21	1.48	1.45
37	33	305	CLA	C4C-C3C	2.21	1.48	1.45
47	16	305	KC1	C4D-CHA	2.21	1.47	1.45
44	C	516	DGD	O2G-C2G	-2.21	1.41	1.46
40	b	521	SQD	O4-C4	-2.21	1.37	1.43
47	38	210	KC1	C4C-C3C	2.21	1.48	1.45
48	12	214	A86	C24-C1	2.21	1.50	1.45
37	35	308	CLA	C4B-CHC	2.21	1.47	1.41
37	38	211	CLA	C4B-CHC	2.21	1.47	1.41
47	35	304	KC1	C1D-CHD	2.21	1.47	1.41
37	B	504	CLA	C1B-CHB	2.21	1.47	1.41
48	34	315	A86	C24-C1	2.21	1.50	1.45
37	D	405	CLA	C4D-CHA	2.21	1.46	1.38
40	17	301	SQD	O2-C2	-2.20	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	12	212	CLA	C1C-C2C	2.20	1.48	1.44
37	18	211	CLA	C4B-CHC	2.20	1.47	1.41
37	20	307	CLA	C1B-CHB	2.20	1.47	1.41
47	36	308	KC1	C4D-CHA	2.20	1.47	1.45
37	31	304	CLA	C1C-NC	-2.20	1.34	1.37
37	31	306	CLA	C1C-NC	-2.20	1.34	1.37
37	D	405	CLA	C1C-NC	-2.20	1.34	1.37
37	36	301	CLA	C3D-C4D	-2.20	1.39	1.44
37	B	508	CLA	C4B-CHC	2.20	1.47	1.41
37	18	209	CLA	C4C-C3C	2.20	1.48	1.45
37	b	504	CLA	C1B-CHB	2.20	1.47	1.41
47	37	304	KC1	CAA-C2A	2.20	1.53	1.46
37	11	305	CLA	C1C-NC	-2.20	1.34	1.37
47	35	304	KC1	CAA-C2A	2.20	1.53	1.46
37	c	511	CLA	C1B-CHB	2.20	1.47	1.41
47	13	302	KC1	C4D-CHA	2.20	1.47	1.45
47	36	305	KC1	CAA-C2A	2.20	1.53	1.46
37	C	513	CLA	C4B-CHC	2.20	1.47	1.41
37	39	301	CLA	C3D-C4D	-2.20	1.39	1.44
37	16	301	CLA	C1C-C2C	2.20	1.48	1.44
47	15	304	KC1	C1D-CHD	2.20	1.47	1.41
37	B	503	CLA	C4B-NB	-2.20	1.33	1.35
44	h	102	DGD	O3G-C3G	-2.20	1.39	1.43
37	19	309	CLA	C1C-NC	-2.20	1.34	1.37
37	12	207	CLA	C4B-CHC	2.20	1.47	1.41
37	D	402	CLA	C4B-NB	-2.20	1.33	1.35
48	14	311	A86	O4-C34	-2.20	1.41	1.46
48	17	315	A86	C35-C34	2.20	1.55	1.51
37	37	306	CLA	C4B-CHC	2.20	1.47	1.41
37	33	310	CLA	C3D-C4D	-2.19	1.39	1.44
37	38	211	CLA	C3D-C4D	-2.19	1.39	1.44
37	40	209	CLA	C1C-C2C	2.19	1.48	1.44
37	20	303	CLA	C4B-CHC	2.19	1.47	1.41
37	12	210	CLA	C1C-NC	-2.19	1.34	1.37
47	17	303	KC1	CAA-C2A	2.19	1.53	1.46
37	C	510	CLA	C1B-CHB	2.19	1.47	1.41
37	21	210	CLA	C3D-C4D	-2.19	1.39	1.44
37	12	204	CLA	C4B-CHC	2.19	1.47	1.41
37	32	205	CLA	C4B-CHC	2.19	1.47	1.41
47	20	304	KC1	C4D-CHA	2.19	1.47	1.45
41	12	201	LMG	O8-C9	-2.19	1.40	1.45
47	41	207	KC1	CAA-C2A	2.19	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	41	210	CLA	C3D-C4D	-2.19	1.39	1.44
50	20	312	DD6	C26-C27	-2.19	1.32	1.37
37	c	513	CLA	C4B-CHC	2.19	1.47	1.41
37	13	308	CLA	C1B-CHB	2.19	1.47	1.41
48	13	314	A86	O4-C34	-2.19	1.41	1.46
48	33	314	A86	O4-C34	-2.19	1.41	1.46
47	35	304	KC1	C4D-CHA	2.19	1.47	1.45
37	35	305	CLA	C3D-C4D	-2.19	1.39	1.44
37	20	308	CLA	C1C-C2C	2.19	1.48	1.44
37	B	501	CLA	C4B-NB	-2.19	1.33	1.35
37	34	302	CLA	C4B-NB	-2.19	1.33	1.35
37	b	508	CLA	C4B-CHC	2.19	1.47	1.41
47	35	309	KC1	C4C-C3C	2.19	1.48	1.45
37	c	505	CLA	C4B-CHC	2.19	1.47	1.41
37	19	303	CLA	C1B-CHB	2.19	1.47	1.41
37	c	510	CLA	C1C-NC	-2.19	1.34	1.37
37	31	308	CLA	C1C-C2C	2.19	1.48	1.44
37	21	208	CLA	C1B-CHB	2.19	1.47	1.41
37	15	308	CLA	C4B-CHC	2.19	1.47	1.41
37	37	308	CLA	C1B-NB	-2.19	1.33	1.35
47	37	307	KC1	C4C-C3C	2.18	1.48	1.45
47	21	207	KC1	CAA-C2A	2.18	1.53	1.46
40	36	315	SQD	O2-C2	-2.18	1.37	1.43
44	H	102	DGD	O3G-C3G	-2.18	1.39	1.43
47	15	302	KC1	C1C-C2C	2.18	1.48	1.44
37	19	305	CLA	C4B-CHC	2.18	1.47	1.41
37	39	305	CLA	C4B-CHC	2.18	1.47	1.41
40	a	409	SQD	O3-C3	-2.18	1.37	1.43
37	B	510	CLA	C4B-CHC	2.18	1.47	1.41
37	15	308	CLA	C1B-CHB	2.18	1.47	1.41
37	b	510	CLA	C4B-CHC	2.18	1.47	1.41
37	17	307	CLA	C4B-CHC	2.18	1.47	1.41
37	37	303	CLA	C4B-NB	-2.18	1.33	1.35
37	41	202	CLA	C1B-NB	-2.18	1.33	1.35
37	18	208	CLA	C4B-CHC	2.18	1.47	1.41
48	11	312	A86	C-C1	2.18	1.55	1.50
48	32	215	A86	O4-C34	-2.18	1.41	1.46
37	19	309	CLA	C4B-CHC	2.18	1.47	1.41
37	39	309	CLA	C4B-CHC	2.18	1.47	1.41
37	41	202	CLA	C1C-C2C	2.18	1.48	1.44
47	15	306	KC1	C1C-C2C	2.18	1.48	1.44
39	d	405	BCR	C33-C5	-2.18	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	13	308	CLA	C4B-CHC	2.18	1.47	1.41
37	33	308	CLA	C4B-CHC	2.18	1.47	1.41
37	41	206	CLA	C1B-NB	-2.18	1.33	1.35
48	17	314	A86	O4-C34	-2.18	1.41	1.46
37	39	307	CLA	C4C-C3C	2.18	1.48	1.45
47	37	302	KC1	C4C-C3C	2.18	1.48	1.45
37	35	310	CLA	C1C-C2C	2.18	1.48	1.44
37	32	208	CLA	C4B-CHC	2.18	1.47	1.41
48	13	311	A86	O4-C34	-2.18	1.41	1.46
47	20	302	KC1	C4D-CHA	2.18	1.47	1.45
37	d	403	CLA	C4D-CHA	2.18	1.46	1.38
47	36	304	KC1	C4C-C3C	2.18	1.48	1.45
37	17	302	CLA	C4B-CHC	2.18	1.47	1.41
40	40	202	SQD	O4-C4	-2.18	1.37	1.43
37	21	205	CLA	C1B-CHB	2.17	1.47	1.41
37	32	210	CLA	C4B-CHC	2.17	1.47	1.41
37	39	309	CLA	C1C-NC	-2.17	1.34	1.37
48	32	215	A86	C14-C15	2.17	1.57	1.52
41	l	101	LMG	O4-C4	-2.17	1.37	1.43
37	39	303	CLA	C1B-CHB	2.17	1.47	1.41
47	13	309	KC1	C4C-C3C	2.17	1.48	1.45
50	40	214	DD6	C26-C27	-2.17	1.32	1.37
37	33	308	CLA	C1B-CHB	2.17	1.47	1.41
37	B	512	CLA	C4D-CHA	2.17	1.46	1.38
47	15	309	KC1	C4C-C3C	2.17	1.48	1.45
47	16	304	KC1	C4C-C3C	2.17	1.48	1.45
47	38	207	KC1	C3B-C4B	2.17	1.50	1.46
48	35	316	A86	O-C13	-2.17	1.18	1.23
47	37	302	KC1	CAA-C2A	2.17	1.53	1.46
48	14	315	A86	C24-C1	2.17	1.50	1.45
37	c	504	CLA	C4B-NB	-2.17	1.33	1.35
48	14	314	A86	O4-C34	-2.17	1.41	1.46
37	11	307	CLA	C4B-CHC	2.17	1.47	1.41
37	11	301	CLA	C1C-C2C	2.17	1.48	1.44
37	19	307	CLA	C4C-C3C	2.17	1.48	1.45
41	L	102	LMG	O4-C4	-2.17	1.37	1.43
37	38	204	CLA	C1C-C2C	2.17	1.48	1.44
37	17	309	CLA	C1B-NB	-2.17	1.33	1.35
48	32	221	A86	O4-C34	-2.17	1.41	1.46
47	40	204	KC1	C4D-CHA	2.17	1.47	1.45
40	16	315	SQD	O4-C4	-2.17	1.37	1.43
37	12	209	CLA	C4B-CHC	2.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	40	205	CLA	C4B-CHC	2.17	1.47	1.41
37	38	211	CLA	C1B-CHB	2.17	1.47	1.41
37	38	201	CLA	C4C-C3C	2.17	1.48	1.45
47	34	309	KC1	C4D-CHA	2.17	1.47	1.45
41	D	412	LMG	O4-C4	-2.17	1.37	1.43
48	33	311	A86	O4-C34	-2.17	1.41	1.46
37	35	308	CLA	C3D-C4D	-2.16	1.39	1.44
41	37	316	LMG	C4-C5	2.16	1.57	1.53
37	C	511	CLA	C1B-CHB	2.16	1.47	1.41
37	14	308	CLA	C4B-CHC	2.16	1.47	1.41
37	41	204	CLA	C4B-CHC	2.16	1.47	1.41
37	38	209	CLA	C4C-C3C	2.16	1.48	1.45
47	18	205	KC1	C1C-C2C	2.16	1.48	1.44
47	31	305	KC1	C4D-CHA	2.16	1.47	1.45
37	21	204	CLA	C4B-CHC	2.16	1.47	1.41
48	18	212	A86	O4-C34	-2.16	1.41	1.46
37	20	303	CLA	C1B-CHB	2.16	1.47	1.41
37	21	202	CLA	C1C-C2C	2.16	1.48	1.44
47	34	304	KC1	CAA-C2A	2.16	1.53	1.46
47	37	304	KC1	C1D-CHD	2.16	1.47	1.41
41	b	520	LMG	O4-C4	-2.16	1.37	1.43
37	11	310	CLA	C4B-NB	-2.16	1.33	1.35
37	18	211	CLA	C1C-NC	-2.16	1.34	1.37
48	12	214	A86	O4-C34	-2.16	1.41	1.46
37	35	308	CLA	C1B-CHB	2.16	1.47	1.41
41	b	519	LMG	O7-C8	-2.16	1.41	1.46
48	37	314	A86	C14-C15	2.16	1.57	1.52
37	32	204	CLA	C4B-CHC	2.16	1.47	1.41
37	b	512	CLA	C4D-CHA	2.16	1.46	1.38
41	d	409	LMG	O4-C4	-2.16	1.37	1.43
48	12	220	A86	O4-C34	-2.16	1.41	1.46
44	C	517	DGD	O3D-C3D	-2.16	1.37	1.43
37	C	505	CLA	C4B-CHC	2.16	1.47	1.41
37	12	203	CLA	C4B-CHC	2.16	1.47	1.41
37	33	301	CLA	C4B-CHC	2.16	1.47	1.41
37	C	501	CLA	C1B-CHB	2.16	1.47	1.41
40	40	202	SQD	O47-C45	-2.16	1.41	1.46
47	15	306	KC1	C4C-C3C	2.16	1.48	1.45
37	14	307	CLA	C4B-CHC	2.16	1.47	1.41
37	z	101	CLA	C1C-NC	-2.16	1.34	1.37
37	21	202	CLA	C4B-NB	-2.16	1.33	1.35
37	31	308	CLA	C4B-CHC	2.16	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	31	302	CLA	C1C-C2C	2.15	1.48	1.44
47	38	207	KC1	CAA-C2A	2.15	1.53	1.46
37	21	202	CLA	C1B-NB	-2.15	1.33	1.35
40	16	315	SQD	O47-C45	-2.15	1.41	1.46
48	15	314	A86	O4-C34	-2.15	1.41	1.46
48	40	213	A86	O4-C34	-2.15	1.41	1.46
47	38	210	KC1	C3B-C4B	2.15	1.50	1.46
48	17	314	A86	C24-C1	2.15	1.50	1.45
50	36	312	DD6	O1-C20	2.15	1.49	1.46
48	32	214	A86	C24-C1	2.15	1.50	1.45
48	31	312	A86	C-C1	2.15	1.55	1.50
37	14	302	CLA	C4B-NB	-2.15	1.33	1.35
37	15	303	CLA	C1B-CHB	2.15	1.47	1.41
37	35	303	CLA	C1B-CHB	2.15	1.47	1.41
37	38	206	CLA	C1B-CHB	2.15	1.47	1.41
38	a	406	PHO	C1C-NC	-2.15	1.31	1.38
37	33	308	CLA	C1C-NC	-2.15	1.34	1.37
37	38	204	CLA	C4C-C3C	2.15	1.48	1.45
37	34	310	CLA	C4B-CHC	2.15	1.47	1.41
47	35	306	KC1	CAA-C2A	2.15	1.53	1.46
37	C	503	CLA	C4C-C3C	2.15	1.48	1.45
47	16	308	KC1	C4C-C3C	2.15	1.48	1.45
37	B	506	CLA	C4B-CHC	2.15	1.47	1.41
37	34	308	CLA	C4B-CHC	2.15	1.47	1.41
47	12	208	KC1	C4D-CHA	2.15	1.47	1.45
47	13	304	KC1	CAA-C2A	2.15	1.53	1.46
47	33	304	KC1	CAA-C2A	2.15	1.53	1.46
47	38	207	KC1	C1C-C2C	2.15	1.48	1.44
37	41	205	CLA	C1B-CHB	2.15	1.47	1.41
37	33	303	CLA	C1C-NC	-2.15	1.34	1.37
37	18	204	CLA	C4C-C3C	2.15	1.48	1.45
37	34	307	CLA	C4B-CHC	2.15	1.47	1.41
37	21	208	CLA	C3D-C4D	-2.15	1.39	1.44
39	D	407	BCR	C33-C5	-2.15	1.47	1.50
37	d	401	CLA	C4B-CHC	2.15	1.47	1.41
37	41	208	CLA	C1B-CHB	2.15	1.47	1.41
47	17	305	KC1	CAA-C2A	2.15	1.53	1.46
37	b	506	CLA	C4B-CHC	2.15	1.47	1.41
37	39	301	CLA	C1C-NC	-2.15	1.34	1.37
48	35	314	A86	O4-C34	-2.15	1.41	1.46
47	36	302	KC1	C1D-CHD	2.15	1.47	1.41
37	c	513	CLA	C1C-C2C	2.15	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	36	308	KC1	C4C-C3C	2.14	1.48	1.45
37	21	209	CLA	C1B-CHB	2.14	1.47	1.41
48	38	212	A86	O4-C34	-2.14	1.41	1.46
37	19	309	CLA	C4C-C3C	2.14	1.48	1.45
37	b	523	CLA	C1C-NC	-2.14	1.34	1.37
37	15	303	CLA	C1C-C2C	2.14	1.48	1.44
37	38	211	CLA	C1C-C2C	2.14	1.48	1.44
37	32	211	CLA	C1C-NC	-2.14	1.34	1.37
37	15	310	CLA	C1C-C2C	2.14	1.48	1.44
38	A	404	PHO	C1C-NC	-2.14	1.31	1.38
37	35	303	CLA	C1B-NB	-2.14	1.33	1.35
47	14	309	KC1	C4D-CHA	2.14	1.47	1.45
47	12	211	KC1	C4D-CHA	2.14	1.47	1.45
47	17	303	KC1	C4C-C3C	2.14	1.48	1.45
37	W	102	CLA	C4C-C3C	2.14	1.48	1.45
47	18	210	KC1	C3B-C4B	2.14	1.49	1.46
47	40	206	KC1	C1D-CHD	2.14	1.46	1.41
47	15	306	KC1	CAA-C2A	2.14	1.53	1.46
37	36	301	CLA	C1C-NC	-2.14	1.34	1.37
37	41	208	CLA	C1C-C2C	2.14	1.48	1.44
37	c	512	CLA	C4B-CHC	2.14	1.46	1.41
48	14	311	A86	C14-C15	2.14	1.56	1.52
37	C	513	CLA	C1C-C2C	2.14	1.48	1.44
41	17	317	LMG	C4-C5	2.14	1.57	1.53
37	18	211	CLA	C1B-CHB	2.14	1.46	1.41
48	31	311	A86	C-C1	2.14	1.55	1.50
37	b	501	CLA	C4B-NB	-2.14	1.33	1.35
37	35	301	CLA	C1B-CHB	2.14	1.46	1.41
48	35	315	A86	O4-C34	-2.14	1.41	1.46
47	16	302	KC1	C1D-CHD	2.14	1.46	1.41
37	39	305	CLA	C1C-NC	-2.14	1.34	1.37
47	14	304	KC1	CAA-C2A	2.14	1.53	1.46
37	C	512	CLA	C4B-CHC	2.14	1.46	1.41
37	15	308	CLA	C1B-NB	-2.14	1.33	1.35
50	40	212	DD6	C29-C27	-2.14	1.38	1.42
37	15	301	CLA	C1B-CHB	2.14	1.46	1.41
37	B	524	CLA	C1C-NC	-2.13	1.34	1.37
48	34	314	A86	O4-C34	-2.13	1.41	1.46
37	14	310	CLA	C4B-CHC	2.13	1.46	1.41
37	13	301	CLA	C4B-CHC	2.13	1.46	1.41
37	40	205	CLA	C1B-CHB	2.13	1.46	1.41
37	Z	101	CLA	C1C-NC	-2.13	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	13	311	A86	C24-C1	2.13	1.50	1.45
45	D	408	PL9	C26-C24	-2.13	1.46	1.51
37	41	210	CLA	C1B-CHB	2.13	1.46	1.41
47	33	309	KC1	C4C-C3C	2.13	1.48	1.45
47	37	305	KC1	CAA-C2A	2.13	1.53	1.46
47	15	309	KC1	C1C-C2C	2.13	1.48	1.44
47	20	304	KC1	C1D-CHD	2.13	1.46	1.41
47	20	302	KC1	C3B-C4B	2.13	1.49	1.46
37	41	208	CLA	C3D-C4D	-2.13	1.39	1.44
37	15	308	CLA	C1C-NC	-2.13	1.34	1.37
48	20	311	A86	O4-C34	-2.13	1.41	1.46
37	32	205	CLA	C1C-NC	-2.13	1.34	1.37
37	18	201	CLA	C1B-CHB	2.13	1.46	1.41
41	B	521	LMG	O4-C4	-2.13	1.38	1.43
47	38	210	KC1	CAA-C2A	2.13	1.53	1.46
37	19	301	CLA	C1C-C2C	2.13	1.48	1.44
37	D	402	CLA	C4B-CHC	2.13	1.46	1.41
37	35	310	CLA	C1B-CHB	2.13	1.46	1.41
47	15	302	KC1	CAA-C2A	2.13	1.53	1.46
37	32	208	CLA	C1C-C2C	2.13	1.48	1.44
37	D	405	CLA	C4B-CHC	2.13	1.46	1.41
48	15	316	A86	C35-C34	2.13	1.55	1.51
47	17	308	KC1	C4C-C3C	2.13	1.48	1.45
37	13	303	CLA	C1C-NC	-2.13	1.34	1.37
47	17	306	KC1	CAA-C2A	2.13	1.53	1.46
47	38	205	KC1	C1D-CHD	2.13	1.46	1.41
38	a	405	PHO	C1C-NC	-2.13	1.32	1.38
37	14	310	CLA	C1B-CHB	2.13	1.46	1.41
48	11	311	A86	C-C1	2.13	1.55	1.50
50	20	310	DD6	C29-C27	-2.13	1.38	1.42
40	17	301	SQD	O4-C4	-2.13	1.38	1.43
37	Z	101	CLA	C4B-CHC	2.13	1.46	1.41
45	d	406	PL9	C26-C24	-2.12	1.46	1.51
48	20	309	A86	C35-C34	2.12	1.55	1.51
48	37	310	A86	C-C1	2.12	1.55	1.50
47	35	302	KC1	CAA-C2A	2.12	1.53	1.46
37	34	305	CLA	C1B-NB	-2.12	1.33	1.35
47	35	309	KC1	C1C-C2C	2.12	1.48	1.44
37	z	101	CLA	C4B-CHC	2.12	1.46	1.41
47	18	205	KC1	C4D-CHA	2.12	1.47	1.45
41	B	520	LMG	O7-C8	-2.12	1.41	1.46
47	11	304	KC1	CAA-C2A	2.12	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	31	301	CLA	C4C-C3C	2.12	1.48	1.45
37	41	202	CLA	C4B-NB	-2.12	1.33	1.35
48	35	319	A86	O4-C34	-2.12	1.41	1.46
47	15	304	KC1	C4D-CHA	2.12	1.47	1.45
47	31	305	KC1	CAA-C2A	2.12	1.53	1.46
48	12	214	A86	C14-C15	2.12	1.56	1.52
37	19	302	CLA	C4B-CHC	2.12	1.46	1.41
48	15	315	A86	O4-C34	-2.12	1.41	1.46
37	20	306	CLA	C4C-C3C	2.12	1.48	1.45
37	32	202	CLA	C4B-CHC	2.12	1.46	1.41
37	z	102	CLA	C1B-NB	-2.12	1.33	1.35
48	16	314	A86	O4-C34	-2.12	1.41	1.46
48	37	312	A86	O4-C34	-2.12	1.41	1.46
37	12	204	CLA	C1C-NC	-2.12	1.34	1.37
41	B	521	LMG	C7-C8	2.12	1.57	1.50
40	B	519	SQD	O3-C3	-2.12	1.38	1.43
44	c	517	DGD	O3D-C3D	-2.12	1.38	1.43
37	14	302	CLA	C4C-C3C	2.12	1.48	1.45
48	13	313	A86	C33-C34	2.12	1.55	1.51
37	B	505	CLA	C4B-CHC	2.12	1.46	1.41
37	b	505	CLA	C4B-CHC	2.12	1.46	1.41
48	12	216	A86	O4-C34	-2.12	1.41	1.46
47	13	302	KC1	C1C-C2C	2.12	1.48	1.44
37	41	209	CLA	C1B-CHB	2.12	1.46	1.41
41	B	521	LMG	C4-C5	2.12	1.57	1.53
47	38	205	KC1	C4D-CHA	2.12	1.47	1.45
41	b	520	LMG	C7-C8	2.12	1.57	1.50
47	38	205	KC1	C1C-C2C	2.12	1.48	1.44
48	17	315	A86	C14-C15	2.12	1.56	1.52
37	b	516	CLA	C4B-NB	-2.11	1.33	1.35
37	32	205	CLA	MG-ND	-2.11	2.01	2.05
37	c	501	CLA	C1B-CHB	2.11	1.46	1.41
44	J	101	DGD	O2D-C2D	-2.11	1.38	1.43
37	21	210	CLA	C1B-CHB	2.11	1.46	1.41
37	12	209	CLA	C1C-NC	-2.11	1.34	1.37
37	d	403	CLA	C4B-CHC	2.11	1.46	1.41
37	15	310	CLA	C1B-CHB	2.11	1.46	1.41
37	16	301	CLA	C1C-NC	-2.11	1.34	1.37
38	D	403	PHO	C1C-NC	-2.11	1.32	1.38
47	20	305	KC1	CAA-C2A	2.11	1.53	1.46
37	20	301	CLA	C1B-CHB	2.11	1.46	1.41
37	34	310	CLA	C1B-CHB	2.11	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	31	310	CLA	C1C-C2C	2.11	1.48	1.44
47	18	205	KC1	C1D-CHD	2.11	1.46	1.41
41	C	518	LMG	O4-C4	-2.11	1.38	1.43
44	J	101	DGD	O4D-C4D	-2.11	1.38	1.43
37	19	302	CLA	C1B-CHB	2.11	1.46	1.41
37	35	303	CLA	C1C-C2C	2.11	1.48	1.44
48	11	315	A86	C24-C1	2.11	1.50	1.45
48	31	315	A86	C24-C1	2.11	1.50	1.45
37	15	305	CLA	C1B-CHB	2.11	1.46	1.41
50	16	312	DD6	O1-C20	2.11	1.49	1.46
37	18	202	CLA	C1B-CHB	2.11	1.46	1.41
37	34	305	CLA	C1B-CHB	2.11	1.46	1.41
37	13	301	CLA	C1C-C2C	2.11	1.48	1.44
47	33	302	KC1	C1C-C2C	2.11	1.48	1.44
48	17	313	A86	O4-C34	-2.11	1.41	1.46
37	39	309	CLA	C4C-C3C	2.11	1.48	1.45
37	b	515	CLA	C1C-NC	-2.11	1.34	1.37
37	21	209	CLA	C1C-C2C	2.11	1.48	1.44
37	41	209	CLA	C1C-C2C	2.11	1.48	1.44
47	18	207	KC1	C1C-C2C	2.11	1.48	1.44
40	36	315	SQD	O4-C4	-2.11	1.38	1.43
47	11	302	KC1	C4D-CHA	2.11	1.47	1.45
47	16	304	KC1	C4D-CHA	2.11	1.47	1.45
47	31	303	KC1	C4D-CHA	2.11	1.47	1.45
37	b	501	CLA	C4B-CHC	2.10	1.46	1.41
37	11	308	CLA	C4B-CHC	2.10	1.46	1.41
37	B	515	CLA	C1C-NC	-2.10	1.34	1.37
37	40	203	CLA	C1B-CHB	2.10	1.46	1.41
37	39	301	CLA	C1C-C2C	2.10	1.48	1.44
37	12	207	CLA	C4B-NB	-2.10	1.33	1.35
37	32	208	CLA	C4B-NB	-2.10	1.33	1.35
48	36	310	A86	C-C1	2.10	1.55	1.50
48	36	313	A86	O4-C34	-2.10	1.41	1.46
48	40	211	A86	C35-C34	2.10	1.55	1.51
44	c	516	DGD	O4E-C4E	-2.10	1.38	1.43
48	34	311	A86	C14-C15	2.10	1.56	1.52
37	14	305	CLA	C1C-C2C	2.10	1.48	1.44
37	12	210	CLA	C4B-CHC	2.10	1.46	1.41
37	38	201	CLA	C3D-C4D	-2.10	1.39	1.44
48	34	312	A86	C24-C1	2.10	1.50	1.45
44	C	516	DGD	O4E-C4E	-2.10	1.38	1.43
37	13	301	CLA	C4B-NB	-2.10	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	z	102	CLA	C1C-C2C	2.10	1.48	1.44
41	b	520	LMG	C4-C5	2.10	1.57	1.53
48	41	213	A86	C35-C34	2.10	1.55	1.51
41	b	520	LMG	O2-C2	-2.10	1.38	1.43
37	b	515	CLA	C4C-C3C	2.10	1.48	1.45
37	39	302	CLA	C4B-CHC	2.10	1.46	1.41
40	40	202	SQD	O3-C3	-2.10	1.38	1.43
48	14	316	A86	O4-C34	-2.10	1.41	1.46
48	34	316	A86	O4-C34	-2.10	1.41	1.46
40	L	101	SQD	O4-C4	-2.10	1.38	1.43
48	16	310	A86	C-C1	2.10	1.55	1.50
37	A	405	CLA	C4B-CHC	2.10	1.46	1.41
41	B	521	LMG	O2-C2	-2.10	1.38	1.43
37	33	305	CLA	C1B-NB	-2.10	1.33	1.35
44	j	101	DGD	O4E-C4E	-2.10	1.38	1.43
47	40	207	KC1	CAA-C2A	2.10	1.53	1.46
48	38	214	A86	O4-C34	-2.10	1.41	1.46
48	35	316	A86	C35-C34	2.10	1.55	1.51
37	B	501	CLA	C4B-CHC	2.10	1.46	1.41
40	16	315	SQD	O3-C3	-2.10	1.38	1.43
44	J	101	DGD	O4E-C4E	-2.10	1.38	1.43
38	a	405	PHO	CMB-C2B	-2.10	1.46	1.51
37	11	310	CLA	C1C-C2C	2.09	1.48	1.44
37	21	204	CLA	C1C-C2C	2.09	1.48	1.44
37	Z	102	CLA	C1B-NB	-2.09	1.33	1.35
37	34	305	CLA	C1C-C2C	2.09	1.48	1.44
48	32	218	A86	O4-C34	-2.09	1.41	1.46
47	35	306	KC1	C4C-C3C	2.09	1.48	1.45
37	21	208	CLA	C1C-C2C	2.09	1.48	1.44
47	40	204	KC1	C3B-C4B	2.09	1.49	1.46
48	17	320	A86	O4-C34	-2.09	1.41	1.46
48	37	319	A86	O4-C34	-2.09	1.41	1.46
38	D	403	PHO	CMB-C2B	-2.09	1.46	1.51
40	L	101	SQD	O3-C3	-2.09	1.38	1.43
47	17	308	KC1	CAA-C2A	2.09	1.53	1.46
47	18	210	KC1	CAA-C2A	2.09	1.53	1.46
37	18	202	CLA	C3D-C4D	-2.09	1.39	1.44
37	c	503	CLA	C4C-C3C	2.09	1.48	1.45
48	32	218	A86	C35-C34	2.09	1.55	1.51
37	14	301	CLA	C1B-NB	-2.09	1.33	1.35
37	34	301	CLA	C1B-NB	-2.09	1.33	1.35
47	21	203	KC1	CAA-C2A	2.09	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	18	205	KC1	CAA-C2A	2.09	1.53	1.46
37	33	310	CLA	C1B-CHB	2.09	1.46	1.41
37	12	207	CLA	C1C-C2C	2.09	1.48	1.44
37	41	202	CLA	C1B-CHB	2.09	1.46	1.41
47	32	207	KC1	C1C-C2C	2.09	1.48	1.44
37	18	201	CLA	C4C-C3C	2.09	1.48	1.45
37	19	305	CLA	C1C-NC	-2.09	1.34	1.37
37	12	204	CLA	MG-ND	-2.09	2.01	2.05
37	19	301	CLA	C1C-NC	-2.09	1.34	1.37
40	B	522	SQD	O47-C45	-2.09	1.41	1.46
48	32	217	A86	O4-C34	-2.09	1.41	1.46
48	33	313	A86	C33-C34	2.09	1.55	1.51
44	j	101	DGD	O2D-C2D	-2.09	1.38	1.43
37	B	515	CLA	C4C-C3C	2.08	1.48	1.45
48	14	312	A86	C24-C1	2.08	1.50	1.45
44	c	516	DGD	O2E-C2E	-2.08	1.38	1.43
37	14	305	CLA	C1B-CHB	2.08	1.46	1.41
37	19	303	CLA	C1C-C2C	2.08	1.48	1.44
37	35	308	CLA	C1C-C2C	2.08	1.48	1.44
37	39	303	CLA	C1C-C2C	2.08	1.48	1.44
48	18	213	A86	C24-C1	2.08	1.50	1.45
47	39	308	KC1	C3B-C4B	2.08	1.49	1.46
37	31	306	CLA	C4B-CHC	2.08	1.46	1.41
37	12	205	CLA	C1C-NC	-2.08	1.34	1.37
37	13	308	CLA	C1C-NC	-2.08	1.34	1.37
37	B	524	CLA	MG-ND	-2.08	2.01	2.05
40	B	519	SQD	O4-C4	-2.08	1.38	1.43
48	21	215	A86	O4-C34	-2.08	1.41	1.46
47	16	308	KC1	C1C-C2C	2.08	1.48	1.44
48	33	315	A86	O4-C34	-2.08	1.41	1.46
37	a	407	CLA	C4B-NB	-2.08	1.33	1.35
39	H	101	BCR	C33-C5	-2.08	1.47	1.50
37	B	513	CLA	C1B-CHB	2.08	1.46	1.41
37	16	307	CLA	C1C-C2C	2.08	1.48	1.44
40	17	301	SQD	O3-C3	-2.08	1.38	1.43
47	41	203	KC1	CAA-C2A	2.08	1.53	1.46
37	37	301	CLA	C4B-NB	-2.08	1.33	1.35
47	20	305	KC1	C1D-CHD	2.08	1.46	1.41
37	33	301	CLA	C1C-C2C	2.08	1.48	1.44
37	34	303	CLA	C1C-NC	-2.08	1.34	1.37
40	b	521	SQD	O47-C45	-2.08	1.41	1.46
50	36	312	DD6	C22-C16	-2.08	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	39	313	A86	O1-C20	2.08	1.49	1.46
37	39	302	CLA	C1B-CHB	2.08	1.46	1.41
47	15	302	KC1	C1D-CHD	2.08	1.46	1.41
37	16	303	CLA	C4B-CHC	2.08	1.46	1.41
37	18	201	CLA	C3D-C4D	-2.08	1.39	1.44
37	32	205	CLA	C4C-C3C	2.08	1.48	1.45
37	19	305	CLA	C1B-CHB	2.08	1.46	1.41
48	18	214	A86	O4-C34	-2.08	1.41	1.46
37	35	305	CLA	C1B-CHB	2.08	1.46	1.41
47	35	302	KC1	C1D-CHD	2.08	1.46	1.41
37	36	309	CLA	C1C-C2C	2.08	1.48	1.44
47	31	305	KC1	C4C-C3C	2.08	1.48	1.45
47	36	304	KC1	C4D-CHA	2.08	1.47	1.45
48	21	213	A86	C35-C34	2.08	1.55	1.51
48	15	319	A86	O4-C34	-2.08	1.41	1.46
37	37	301	CLA	C1C-NC	-2.08	1.34	1.37
37	b	512	CLA	C4B-CHC	2.07	1.46	1.41
41	D	412	LMG	O2-C2	-2.07	1.38	1.43
37	12	203	CLA	C4B-NB	-2.07	1.33	1.35
47	11	304	KC1	C4D-CHA	2.07	1.47	1.45
37	11	305	CLA	C4B-CHC	2.07	1.46	1.41
37	32	210	CLA	C1C-NC	-2.07	1.34	1.37
47	36	304	KC1	CAA-C2A	2.07	1.52	1.46
37	39	304	CLA	C1B-CHB	2.07	1.46	1.41
37	33	301	CLA	C4B-NB	-2.07	1.33	1.35
37	16	309	CLA	C1C-C2C	2.07	1.48	1.44
37	41	204	CLA	C1C-C2C	2.07	1.48	1.44
37	b	513	CLA	C1B-CHB	2.07	1.46	1.41
47	36	302	KC1	C3B-C4B	2.07	1.49	1.46
37	a	407	CLA	C4B-CHC	2.07	1.46	1.41
48	33	314	A86	O-C13	-2.07	1.18	1.23
38	a	406	PHO	CMB-C2B	-2.07	1.46	1.51
48	12	217	A86	C35-C34	2.07	1.55	1.51
48	33	311	A86	C24-C1	2.07	1.50	1.45
37	13	310	CLA	C1B-CHB	2.07	1.46	1.41
37	b	512	CLA	MG-ND	-2.07	2.01	2.05
37	16	303	CLA	C1C-C2C	2.07	1.48	1.44
48	12	217	A86	O4-C34	-2.07	1.41	1.46
48	16	314	A86	C24-C1	2.07	1.50	1.45
37	B	524	CLA	C1B-CHB	2.07	1.46	1.41
37	36	307	CLA	C1C-C2C	2.07	1.48	1.44
37	38	208	CLA	C1C-C2C	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	12	206	KC1	C1C-C2C	2.07	1.48	1.44
47	35	302	KC1	C1C-C2C	2.07	1.48	1.44
37	21	206	CLA	C1B-NB	-2.07	1.33	1.35
37	19	304	CLA	C1B-CHB	2.07	1.46	1.41
44	j	101	DGD	O4D-C4D	-2.07	1.38	1.43
37	d	403	CLA	C1B-CHB	2.07	1.46	1.41
37	12	210	CLA	C1B-CHB	2.07	1.46	1.41
48	17	315	A86	O4-C34	-2.07	1.41	1.46
48	37	314	A86	O4-C34	-2.07	1.41	1.46
37	36	301	CLA	C1B-CHB	2.07	1.46	1.41
37	C	513	CLA	C1C-NC	-2.07	1.34	1.37
37	39	302	CLA	C1C-NC	-2.07	1.34	1.37
37	31	306	CLA	C4C-C3C	2.07	1.48	1.45
47	16	302	KC1	C3B-C4B	2.07	1.49	1.46
37	36	309	CLA	C1C-NC	-2.07	1.34	1.37
37	12	203	CLA	C1C-NC	-2.07	1.34	1.37
37	B	512	CLA	C4B-CHC	2.07	1.46	1.41
37	21	202	CLA	C1B-CHB	2.07	1.46	1.41
40	36	315	SQD	O3-C3	-2.07	1.38	1.43
47	17	305	KC1	C1C-C2C	2.06	1.48	1.44
37	15	303	CLA	C1B-NB	-2.06	1.33	1.35
48	38	215	A86	O4-C34	-2.06	1.41	1.46
37	D	405	CLA	C1B-CHB	2.06	1.46	1.41
47	17	306	KC1	C1D-CHD	2.06	1.46	1.41
47	38	205	KC1	CAA-C2A	2.06	1.52	1.46
48	21	211	A86	C35-C34	2.06	1.55	1.51
37	18	209	CLA	C1A-CHA	2.06	1.51	1.43
47	36	308	KC1	C1C-C2C	2.06	1.48	1.44
47	21	207	KC1	C4C-C3C	2.06	1.48	1.45
41	c	518	LMG	O4-C4	-2.06	1.38	1.43
44	C	516	DGD	O2E-C2E	-2.06	1.38	1.43
37	41	205	CLA	C1C-C2C	2.06	1.48	1.44
47	33	304	KC1	C1C-C2C	2.06	1.48	1.44
37	41	208	CLA	C1A-CHA	2.06	1.51	1.43
48	37	310	A86	C24-C1	2.06	1.50	1.45
47	37	307	KC1	CAA-C2A	2.06	1.52	1.46
48	13	313	A86	C35-C34	2.06	1.55	1.51
47	37	305	KC1	C1D-CHD	2.06	1.46	1.41
37	18	203	CLA	C1A-CHA	2.06	1.51	1.43
37	32	211	CLA	C4B-CHC	2.06	1.46	1.41
37	39	305	CLA	C1B-CHB	2.06	1.46	1.41
37	38	202	CLA	C3D-C4D	-2.06	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	40	208	CLA	C4C-C3C	2.06	1.48	1.45
41	12	201	LMG	C7-C8	2.06	1.57	1.50
37	Z	102	CLA	C1C-C2C	2.06	1.48	1.44
37	40	208	CLA	C1C-C2C	2.06	1.48	1.44
37	18	208	CLA	C1B-CHB	2.06	1.46	1.41
37	18	208	CLA	C1C-C2C	2.06	1.48	1.44
47	35	304	KC1	C1C-C2C	2.06	1.48	1.44
37	c	513	CLA	C1C-NC	-2.06	1.34	1.37
37	12	204	CLA	C4C-C3C	2.06	1.48	1.45
37	38	209	CLA	C1A-CHA	2.06	1.51	1.43
37	32	211	CLA	C1B-CHB	2.06	1.46	1.41
48	41	211	A86	C35-C34	2.06	1.55	1.51
38	A	404	PHO	CBD-CGD	-2.06	1.49	1.52
37	21	205	CLA	C1C-C2C	2.06	1.48	1.44
37	33	305	CLA	C1B-CHB	2.05	1.46	1.41
37	36	303	CLA	C4B-CHC	2.05	1.46	1.41
47	13	302	KC1	C1D-CHD	2.05	1.46	1.41
47	19	308	KC1	C3B-C4B	2.05	1.49	1.46
37	B	516	CLA	C4B-NB	-2.05	1.33	1.35
37	31	310	CLA	C4B-NB	-2.05	1.33	1.35
47	11	304	KC1	C4C-C3C	2.05	1.48	1.45
47	41	207	KC1	C1D-CHD	2.05	1.46	1.41
37	B	504	CLA	C4B-NB	-2.05	1.33	1.35
37	39	303	CLA	C1B-NB	-2.05	1.33	1.35
37	B	501	CLA	C4C-C3C	2.05	1.48	1.45
37	11	303	CLA	C4C-C3C	2.05	1.48	1.45
37	31	304	CLA	C4C-C3C	2.05	1.48	1.45
37	16	309	CLA	C1C-NC	-2.05	1.34	1.37
37	14	301	CLA	C1B-CHB	2.05	1.46	1.41
37	34	301	CLA	C1B-CHB	2.05	1.46	1.41
37	20	301	CLA	C1D-C2D	2.05	1.49	1.45
48	19	311	A86	O4-C34	-2.05	1.41	1.46
37	11	305	CLA	C4C-C3C	2.05	1.48	1.45
41	11	317	LMG	O7-C8	-2.05	1.41	1.46
37	14	303	CLA	C1C-NC	-2.05	1.34	1.37
48	31	314	A86	O4-C34	-2.05	1.41	1.46
37	19	302	CLA	C1C-C2C	2.05	1.48	1.44
37	38	208	CLA	C1B-CHB	2.05	1.46	1.41
37	19	303	CLA	C1C-NC	-2.05	1.34	1.37
47	16	304	KC1	CAA-C2A	2.05	1.52	1.46
37	16	301	CLA	C1B-CHB	2.05	1.46	1.41
37	b	523	CLA	MG-ND	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	12	208	KC1	CAA-C2A	2.05	1.52	1.46
48	41	215	A86	O4-C34	-2.05	1.41	1.46
47	19	308	KC1	C1C-C2C	2.05	1.48	1.44
37	b	501	CLA	C4C-C3C	2.05	1.48	1.45
47	33	306	KC1	C4C-C3C	2.05	1.48	1.45
37	z	101	CLA	C1B-CHB	2.05	1.46	1.41
50	16	312	DD6	C22-C16	-2.05	1.49	1.53
41	A	408	LMG	O4-C4	-2.05	1.38	1.43
37	b	523	CLA	C1B-CHB	2.05	1.46	1.41
37	21	206	CLA	C1B-CHB	2.05	1.46	1.41
47	12	211	KC1	C3B-C4B	2.05	1.49	1.46
37	39	302	CLA	C1C-C2C	2.05	1.48	1.44
37	20	306	CLA	C1C-C2C	2.05	1.48	1.44
37	19	303	CLA	C4C-C3C	2.05	1.48	1.45
37	39	303	CLA	C4C-C3C	2.05	1.48	1.45
37	12	210	CLA	C4B-NB	-2.05	1.33	1.35
41	d	409	LMG	O2-C2	-2.05	1.38	1.43
37	B	512	CLA	MG-ND	-2.05	2.01	2.05
48	14	313	A86	C35-C34	2.04	1.55	1.51
48	34	313	A86	C35-C34	2.04	1.55	1.51
37	38	203	CLA	C1A-CHA	2.04	1.51	1.43
37	19	304	CLA	C1C-C2C	2.04	1.48	1.44
47	14	304	KC1	C1C-C2C	2.04	1.48	1.44
47	13	306	KC1	CAA-C2A	2.04	1.52	1.46
37	32	204	CLA	C4B-NB	-2.04	1.33	1.35
37	21	208	CLA	C1A-CHA	2.04	1.51	1.43
37	12	203	CLA	C1C-C2C	2.04	1.48	1.44
45	d	402	PL9	C36-C34	-2.04	1.47	1.51
37	34	308	CLA	C4C-C3C	2.04	1.48	1.45
47	34	306	KC1	C4C-C3C	2.04	1.48	1.45
37	18	206	CLA	C1B-CHB	2.04	1.46	1.41
47	18	210	KC1	C1D-CHD	2.04	1.46	1.41
47	21	207	KC1	C1D-CHD	2.04	1.46	1.41
40	a	409	SQD	O47-C45	-2.04	1.41	1.46
37	18	209	CLA	C1B-NB	-2.04	1.33	1.35
37	C	511	CLA	C4B-CHC	2.04	1.46	1.41
48	14	316	A86	C35-C34	2.04	1.55	1.51
48	34	316	A86	C35-C34	2.04	1.55	1.51
37	14	308	CLA	C1C-NC	-2.04	1.34	1.37
37	34	308	CLA	C1C-NC	-2.04	1.34	1.37
48	36	313	A86	C24-C1	2.04	1.50	1.45
37	38	208	CLA	C4C-C3C	2.04	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	32	209	KC1	C4D-CHA	2.04	1.47	1.45
37	36	303	CLA	C1C-C2C	2.04	1.48	1.44
37	40	203	CLA	C4C-C3C	2.04	1.48	1.45
37	36	306	CLA	C4C-C3C	2.04	1.48	1.45
47	13	306	KC1	C4D-CHA	2.04	1.47	1.45
37	Z	101	CLA	C1B-CHB	2.04	1.46	1.41
47	32	209	KC1	CAA-C2A	2.04	1.52	1.46
37	39	304	CLA	C1C-C2C	2.04	1.48	1.44
37	C	501	CLA	C4B-CHC	2.04	1.46	1.41
47	40	207	KC1	C1D-CHD	2.04	1.46	1.41
44	C	517	DGD	O4D-C4D	-2.04	1.38	1.43
38	A	404	PHO	CMB-C2B	-2.04	1.46	1.51
47	40	204	KC1	CAA-C2A	2.04	1.52	1.46
47	36	308	KC1	CAA-C2A	2.04	1.52	1.46
47	17	305	KC1	C1D-CHD	2.04	1.46	1.41
37	14	307	CLA	C4B-NB	-2.04	1.33	1.35
37	34	302	CLA	C4C-C3C	2.04	1.48	1.45
37	c	503	CLA	C1C-NC	-2.04	1.34	1.37
37	36	307	CLA	C1C-NC	-2.04	1.34	1.37
47	33	306	KC1	CAA-C2A	2.03	1.52	1.46
37	18	202	CLA	C1C-NC	-2.03	1.34	1.37
48	21	214	A86	O4-C34	-2.03	1.41	1.46
48	39	311	A86	C39-C38	2.03	1.56	1.49
37	17	304	CLA	C1C-C2C	2.03	1.48	1.44
37	c	501	CLA	C4B-CHC	2.03	1.46	1.41
37	d	404	CLA	C4B-CHC	2.03	1.46	1.41
47	33	306	KC1	C4D-CHA	2.03	1.47	1.45
48	13	314	A86	O-C13	-2.03	1.19	1.23
47	18	207	KC1	C1B-C2B	2.03	1.49	1.45
47	13	304	KC1	C1C-C2C	2.03	1.48	1.44
47	16	304	KC1	C1C-C2C	2.03	1.48	1.44
37	d	404	CLA	C4B-NB	-2.03	1.33	1.35
37	c	511	CLA	C4B-CHC	2.03	1.46	1.41
37	20	301	CLA	C4C-C3C	2.03	1.48	1.45
37	13	305	CLA	C1B-CHB	2.03	1.46	1.41
47	13	306	KC1	C4C-C3C	2.03	1.48	1.45
47	39	308	KC1	C1C-C2C	2.03	1.48	1.44
41	32	201	LMG	C7-C8	2.03	1.56	1.50
47	15	304	KC1	C1C-C2C	2.03	1.48	1.44
47	41	203	KC1	C1D-CHD	2.03	1.46	1.41
47	15	306	KC1	C1D-CHD	2.03	1.46	1.41
37	17	307	CLA	C1C-C2C	2.03	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	37	306	CLA	C1C-C2C	2.03	1.48	1.44
37	D	406	CLA	C4B-CHC	2.03	1.46	1.41
37	40	208	CLA	C1C-NC	-2.03	1.34	1.37
37	17	307	CLA	C4C-C3C	2.03	1.48	1.45
37	37	306	CLA	C4C-C3C	2.03	1.48	1.45
47	41	207	KC1	C4C-C3C	2.03	1.48	1.45
47	32	212	KC1	C3B-C4B	2.03	1.49	1.46
47	36	304	KC1	C1C-C2C	2.03	1.48	1.44
37	37	301	CLA	C4C-C3C	2.03	1.48	1.45
48	13	315	A86	O4-C34	-2.03	1.41	1.46
47	33	309	KC1	C1D-CHD	2.03	1.46	1.41
43	37	321	LHG	O7-C5	-2.03	1.41	1.46
48	41	214	A86	O4-C34	-2.03	1.41	1.46
37	41	206	CLA	C1B-CHB	2.03	1.46	1.41
37	20	308	CLA	C1A-CHA	2.03	1.51	1.43
37	40	210	CLA	C1A-CHA	2.03	1.51	1.43
39	h	101	BCR	C33-C5	-2.03	1.47	1.50
37	41	205	CLA	C1C-NC	-2.03	1.34	1.37
37	41	204	CLA	C1D-C2D	2.03	1.49	1.45
44	c	517	DGD	O4D-C4D	-2.03	1.38	1.43
37	Z	102	CLA	C1C-NC	-2.02	1.34	1.37
37	a	407	CLA	C1C-C2C	2.02	1.48	1.44
37	B	514	CLA	C1B-CHB	2.02	1.46	1.41
48	18	215	A86	O4-C34	-2.02	1.41	1.46
44	C	517	DGD	O2E-C2E	-2.02	1.38	1.43
48	12	202	A86	C24-C1	2.02	1.50	1.45
48	38	213	A86	O4-C34	-2.02	1.41	1.46
37	16	301	CLA	C1B-NB	-2.02	1.33	1.35
47	36	304	KC1	C1D-CHD	2.02	1.46	1.41
37	36	303	CLA	C1B-CHB	2.02	1.46	1.41
37	39	310	CLA	C4C-C3C	2.02	1.48	1.45
47	33	302	KC1	C1D-CHD	2.02	1.46	1.41
37	20	303	CLA	C1C-NC	-2.02	1.34	1.37
47	13	302	KC1	CAA-C2A	2.02	1.52	1.46
47	33	302	KC1	CAA-C2A	2.02	1.52	1.46
37	34	310	CLA	C1C-NC	-2.02	1.34	1.37
37	17	304	CLA	C4B-CHC	2.02	1.46	1.41
37	34	307	CLA	C1C-C2C	2.02	1.48	1.44
47	13	302	KC1	C3B-C4B	2.02	1.49	1.46
37	19	303	CLA	C1B-NB	-2.02	1.33	1.35
48	39	311	A86	O4-C34	-2.02	1.41	1.46
48	14	313	A86	C33-C34	2.02	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	512	CLA	C1B-CHB	2.02	1.46	1.41
37	b	504	CLA	C4B-NB	-2.02	1.33	1.35
37	36	307	CLA	C1B-CHB	2.02	1.46	1.41
37	37	308	CLA	C1C-C2C	2.02	1.48	1.44
37	c	504	CLA	C4B-CHC	2.02	1.46	1.41
47	21	203	KC1	C1D-CHD	2.02	1.46	1.41
48	19	311	A86	C24-C1	2.02	1.50	1.45
37	16	307	CLA	C1C-NC	-2.02	1.34	1.37
37	18	208	CLA	C4C-C3C	2.02	1.48	1.45
41	a	410	LMG	O4-C4	-2.02	1.38	1.43
44	C	516	DGD	O3G-C1D	-2.02	1.36	1.40
44	c	516	DGD	O3G-C1D	-2.02	1.36	1.40
47	11	306	KC1	CAA-C2A	2.01	1.52	1.46
48	19	311	A86	C-C1	2.01	1.55	1.50
45	d	406	PL9	C31-C29	-2.01	1.47	1.51
48	36	310	A86	C24-C1	2.01	1.50	1.45
37	17	302	CLA	C4C-C3C	2.01	1.48	1.45
47	14	304	KC1	C4C-C3C	2.01	1.48	1.45
47	34	304	KC1	C4C-C3C	2.01	1.48	1.45
37	40	203	CLA	C1D-C2D	2.01	1.49	1.45
47	16	304	KC1	C3B-C4B	2.01	1.49	1.46
48	14	313	A86	C39-C38	2.01	1.56	1.49
48	12	213	A86	C24-C1	2.01	1.50	1.45
48	15	315	A86	C39-C38	2.01	1.56	1.49
47	17	305	KC1	C4D-CHA	2.01	1.47	1.45
37	16	307	CLA	C1B-CHB	2.01	1.46	1.41
37	C	504	CLA	C4B-CHC	2.01	1.46	1.41
48	39	313	A86	O4-C34	-2.01	1.41	1.46
47	33	302	KC1	C3B-C4B	2.01	1.49	1.46
37	19	302	CLA	C1C-NC	-2.01	1.34	1.37
48	33	313	A86	C35-C34	2.01	1.55	1.51
41	31	317	LMG	O7-C8	-2.01	1.41	1.46
37	38	203	CLA	C1B-CHB	2.01	1.46	1.41
47	37	304	KC1	C1C-C2C	2.01	1.48	1.44
37	32	204	CLA	C1C-NC	-2.01	1.34	1.37
47	20	302	KC1	CAA-C2A	2.01	1.52	1.46
37	14	307	CLA	C1C-C2C	2.01	1.48	1.44
37	21	205	CLA	C1C-NC	-2.01	1.34	1.37
47	17	303	KC1	C1D-CHD	2.01	1.46	1.41
37	12	209	CLA	C1C-C2C	2.01	1.48	1.44
47	36	304	KC1	C3B-C4B	2.01	1.49	1.46
44	c	517	DGD	O2E-C2E	-2.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	13	309	KC1	C3B-C4B	2.01	1.49	1.46
37	11	308	CLA	C4C-C3C	2.01	1.48	1.45
37	11	305	CLA	C4B-NB	-2.01	1.33	1.35
37	13	305	CLA	C1B-NB	-2.01	1.33	1.35
37	31	306	CLA	C4B-NB	-2.01	1.33	1.35
37	19	310	CLA	C4C-C3C	2.01	1.48	1.45
37	14	302	CLA	C1C-NC	-2.01	1.34	1.37
37	b	523	CLA	C4B-NB	-2.01	1.33	1.35
37	15	310	CLA	C1B-NB	-2.01	1.33	1.35
48	19	311	A86	C39-C38	2.01	1.56	1.49
48	35	315	A86	C39-C38	2.01	1.56	1.49
37	19	310	CLA	C1B-CHB	2.01	1.46	1.41
43	21	217	LHG	O7-C5	-2.00	1.41	1.46
37	32	202	CLA	C4C-C3C	2.00	1.48	1.45
48	39	311	A86	C-C1	2.00	1.55	1.50
46	F	101	HEM	CMB-C2B	2.00	1.55	1.50
47	35	306	KC1	C1D-CHD	2.00	1.46	1.41
45	D	404	PL9	C10-C9	-2.00	1.45	1.50
47	16	308	KC1	CAA-C2A	2.00	1.52	1.46
47	34	304	KC1	C1C-C2C	2.00	1.48	1.44
40	A	407	SQD	O47-C45	-2.00	1.41	1.46
48	19	313	A86	O4-C34	-2.00	1.41	1.46
47	40	204	KC1	C4C-C3C	2.00	1.48	1.45
47	11	309	KC1	C3D-C4D	-2.00	1.38	1.40
47	13	309	KC1	C1D-CHD	2.00	1.46	1.41
47	14	306	KC1	CAA-C2A	2.00	1.52	1.46
37	A	405	CLA	C1C-C2C	2.00	1.48	1.44
37	32	204	CLA	C1C-C2C	2.00	1.48	1.44
37	14	310	CLA	C1C-NC	-2.00	1.34	1.37

All (11167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	17	314	A86	O1-C20-C19	57.83	156.82	113.38
48	37	313	A86	O1-C20-C19	57.77	156.78	113.38
48	39	313	A86	O1-C20-C19	57.61	156.66	113.38
48	40	213	A86	O1-C20-C19	57.29	156.42	113.38
48	20	311	A86	O1-C20-C19	57.26	156.40	113.38
48	19	313	A86	O1-C20-C19	57.25	156.39	113.38
48	13	313	A86	O1-C20-C19	56.80	156.05	113.38
48	33	313	A86	O1-C20-C19	56.77	156.03	113.38
48	40	211	A86	O1-C20-C19	56.74	156.00	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	20	309	A86	O1-C20-C19	56.70	155.98	113.38
48	33	314	A86	O1-C20-C19	56.37	155.73	113.38
48	13	314	A86	O1-C20-C19	56.33	155.69	113.38
48	35	314	A86	O1-C20-C19	55.77	155.28	113.38
48	14	314	A86	O1-C20-C19	55.72	155.24	113.38
48	34	314	A86	O1-C20-C19	55.64	155.18	113.38
48	17	310	A86	O1-C20-C19	55.48	155.06	113.38
48	37	309	A86	O1-C20-C19	55.38	154.98	113.38
48	21	214	A86	O1-C20-C19	55.31	154.93	113.38
48	41	214	A86	O1-C20-C19	55.27	154.90	113.38
48	15	314	A86	O1-C20-C19	55.17	154.83	113.38
48	37	312	A86	O1-C20-C19	55.14	154.80	113.38
48	34	311	A86	O1-C20-C19	55.02	154.71	113.38
48	17	313	A86	O1-C20-C19	55.00	154.70	113.38
48	14	311	A86	O1-C20-C19	54.99	154.69	113.38
48	41	215	A86	O1-C20-C19	54.92	154.64	113.38
48	21	215	A86	O1-C20-C19	54.83	154.57	113.38
48	40	201	A86	O1-C20-C19	54.42	154.26	113.38
48	16	313	A86	O1-C20-C19	54.37	154.22	113.38
48	31	314	A86	O1-C20-C19	54.36	154.22	113.38
48	11	314	A86	O1-C20-C19	54.33	154.19	113.38
48	41	211	A86	O1-C20-C19	54.25	154.13	113.38
48	21	211	A86	O1-C20-C19	54.25	154.13	113.38
48	12	215	A86	O1-C20-C19	54.15	154.06	113.38
48	32	216	A86	O1-C20-C19	54.08	154.01	113.38
48	38	214	A86	O1-C20-C19	53.98	153.93	113.38
48	21	213	A86	O1-C20-C19	53.97	153.92	113.38
48	18	212	A86	O1-C20-C19	53.94	153.90	113.38
48	38	212	A86	O1-C20-C19	53.92	153.89	113.38
48	41	213	A86	O1-C20-C19	53.91	153.88	113.38
48	32	217	A86	O1-C20-C19	53.79	153.79	113.38
48	12	216	A86	O1-C20-C19	53.76	153.77	113.38
48	18	214	A86	O1-C20-C19	53.55	153.61	113.38
48	14	315	A86	O1-C20-C19	53.40	153.50	113.38
48	34	315	A86	O1-C20-C19	53.36	153.47	113.38
48	32	214	A86	O1-C20-C19	53.24	153.38	113.38
48	12	213	A86	O1-C20-C19	53.18	153.33	113.38
48	18	213	A86	O1-C20-C19	52.54	152.85	113.38
48	33	311	A86	O1-C20-C19	52.44	152.78	113.38
48	13	311	A86	O1-C20-C19	52.42	152.76	113.38
48	13	312	A86	O1-C20-C19	52.32	152.68	113.38
48	33	312	A86	O1-C20-C19	52.26	152.64	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	32	221	A86	O1-C20-C19	52.16	152.57	113.38
48	38	213	A86	O1-C20-C19	52.13	152.54	113.38
48	12	220	A86	O1-C20-C19	52.11	152.53	113.38
48	15	311	A86	O1-C20-C19	52.05	152.48	113.38
48	35	311	A86	O1-C20-C19	52.01	152.46	113.38
48	34	312	A86	O1-C20-C19	51.74	152.25	113.38
48	14	312	A86	O1-C20-C19	51.71	152.23	113.38
48	15	312	A86	O1-C20-C19	51.41	152.00	113.38
48	35	312	A86	O1-C20-C19	51.40	151.99	113.38
48	32	215	A86	O1-C20-C19	51.37	151.97	113.38
48	12	214	A86	O1-C20-C19	51.35	151.96	113.38
48	39	311	A86	O1-C20-C19	51.29	151.91	113.38
48	19	311	A86	O1-C20-C19	51.27	151.89	113.38
48	15	315	A86	O1-C20-C19	51.26	151.89	113.38
48	18	215	A86	O1-C20-C19	51.10	151.77	113.38
48	35	315	A86	O1-C20-C19	51.06	151.74	113.38
48	17	320	A86	O1-C20-C19	51.04	151.72	113.38
48	38	215	A86	O1-C20-C19	50.90	151.62	113.38
48	17	315	A86	O1-C20-C19	50.90	151.62	113.38
48	37	314	A86	O1-C20-C19	50.86	151.59	113.38
48	37	319	A86	O1-C20-C19	50.84	151.57	113.38
48	11	312	A86	O1-C20-C19	50.74	151.50	113.38
48	11	315	A86	O1-C20-C19	50.74	151.50	113.38
48	31	315	A86	O1-C20-C19	50.73	151.49	113.38
48	31	312	A86	O1-C20-C19	50.71	151.48	113.38
48	35	316	A86	O1-C20-C19	50.26	151.14	113.38
48	15	316	A86	O1-C20-C19	50.17	151.07	113.38
48	12	202	A86	O1-C20-C19	50.03	150.96	113.38
48	32	203	A86	O1-C20-C19	49.98	150.93	113.38
48	37	310	A86	O1-C20-C19	49.65	150.68	113.38
48	13	315	A86	O1-C20-C19	49.58	150.62	113.38
48	36	313	A86	O1-C20-C19	49.52	150.58	113.38
48	36	310	A86	O1-C20-C19	49.52	150.58	113.38
48	33	315	A86	O1-C20-C19	49.49	150.56	113.38
48	16	310	A86	O1-C20-C19	49.47	150.54	113.38
48	16	314	A86	O1-C20-C19	49.46	150.53	113.38
48	17	311	A86	O1-C20-C19	49.45	150.53	113.38
48	15	313	A86	O1-C20-C19	49.19	150.33	113.38
48	35	313	A86	O1-C20-C19	49.18	150.33	113.38
48	31	319	A86	O1-C20-C19	49.15	150.31	113.38
48	14	313	A86	O1-C20-C19	49.11	150.27	113.38
48	11	319	A86	O1-C20-C19	49.08	150.25	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	34	313	A86	O1-C20-C19	49.05	150.23	113.38
48	36	311	A86	O1-C20-C19	49.03	150.22	113.38
48	16	311	A86	O1-C20-C19	48.99	150.18	113.38
48	11	311	A86	O1-C20-C19	48.68	149.95	113.38
48	31	311	A86	O1-C20-C19	48.65	149.93	113.38
48	32	218	A86	O1-C20-C19	48.30	149.67	113.38
48	12	217	A86	O1-C20-C19	48.25	149.63	113.38
48	17	312	A86	O1-C20-C19	48.24	149.62	113.38
48	37	311	A86	O1-C20-C19	48.14	149.54	113.38
48	34	316	A86	O1-C20-C19	47.84	149.32	113.38
48	14	316	A86	O1-C20-C19	47.81	149.29	113.38
48	15	319	A86	O1-C20-C19	47.62	149.15	113.38
48	35	319	A86	O1-C20-C19	47.60	149.14	113.38
48	31	313	A86	O1-C20-C19	45.49	147.55	113.38
48	11	313	A86	O1-C20-C19	45.41	147.50	113.38
50	20	310	DD6	O1-C20-C19	31.61	137.13	113.38
50	40	212	DD6	O1-C20-C19	31.51	137.05	113.38
50	41	212	DD6	O1-C20-C19	31.41	136.97	113.38
50	21	212	DD6	O1-C20-C19	31.34	136.93	113.38
50	21	216	DD6	O1-C20-C19	31.03	136.69	113.38
50	41	216	DD6	O1-C20-C19	30.99	136.66	113.38
50	40	214	DD6	O1-C20-C19	30.10	135.99	113.38
50	20	312	DD6	O1-C20-C19	30.07	135.97	113.38
50	16	312	DD6	O1-C20-C19	27.09	133.74	113.38
50	36	312	DD6	O1-C20-C19	26.98	133.65	113.38
50	19	312	DD6	O1-C20-C19	24.38	131.69	113.38
50	39	312	DD6	O1-C20-C19	24.35	131.67	113.38
50	41	216	DD6	C28-C27-C29	18.61	153.70	116.84
50	21	216	DD6	C28-C27-C29	18.59	153.66	116.84
50	19	312	DD6	C28-C27-C29	17.07	150.66	116.84
50	39	312	DD6	C28-C27-C29	17.07	150.65	116.84
50	16	312	DD6	C28-C27-C29	16.37	149.26	116.84
50	36	312	DD6	C28-C27-C29	16.36	149.24	116.84
50	40	212	DD6	C28-C27-C29	16.33	149.19	116.84
50	20	310	DD6	C28-C27-C29	16.33	149.17	116.84
50	20	310	DD6	C29-C30-C31	-16.31	134.13	175.43
50	40	212	DD6	C29-C30-C31	-16.29	134.17	175.43
50	40	214	DD6	C28-C27-C29	15.68	147.89	116.84
50	20	312	DD6	C28-C27-C29	15.67	147.86	116.84
50	41	212	DD6	C28-C27-C29	15.15	146.84	116.84
50	21	212	DD6	C28-C27-C29	15.11	146.76	116.84
50	39	312	DD6	C29-C30-C31	-14.93	137.63	175.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	19	312	DD6	C29-C30-C31	-14.90	137.69	175.43
50	21	212	DD6	C29-C30-C31	-14.86	137.80	175.43
50	41	212	DD6	C29-C30-C31	-14.86	137.80	175.43
50	40	214	DD6	C29-C30-C31	-14.70	138.20	175.43
50	20	312	DD6	C29-C30-C31	-14.69	138.23	175.43
50	36	312	DD6	C29-C30-C31	-13.79	140.51	175.43
50	16	312	DD6	C29-C30-C31	-13.79	140.52	175.43
48	20	311	A86	O1-C20-C21	-13.42	98.97	115.06
48	40	213	A86	O1-C20-C21	-13.39	99.02	115.06
50	21	216	DD6	C29-C30-C31	-12.47	143.85	175.43
50	41	216	DD6	C29-C30-C31	-12.46	143.89	175.43
48	19	313	A86	O1-C20-C21	-12.39	100.21	115.06
50	41	216	DD6	C37-C36-C31	-12.36	107.55	124.35
50	21	216	DD6	C37-C36-C31	-12.35	107.57	124.35
48	13	313	A86	C21-C20-C19	-12.34	100.40	114.28
48	33	313	A86	C21-C20-C19	-12.31	100.43	114.28
50	20	310	DD6	C3-C2-C1	-12.26	109.81	127.31
50	40	212	DD6	C3-C2-C1	-12.25	109.82	127.31
50	40	214	DD6	C37-C36-C31	-12.25	107.70	124.35
48	17	314	A86	C21-C20-C19	-12.25	100.50	114.28
50	20	312	DD6	C37-C36-C31	-12.24	107.72	124.35
50	39	312	DD6	C37-C36-C31	-12.11	107.89	124.35
48	37	313	A86	C21-C20-C19	-12.08	100.69	114.28
48	40	211	A86	O1-C20-C21	-12.08	100.58	115.06
50	19	312	DD6	C37-C36-C31	-12.07	107.94	124.35
48	20	309	A86	O1-C20-C21	-12.07	100.59	115.06
50	16	312	DD6	C37-C36-C31	-12.03	108.00	124.35
47	40	204	KC1	CMA-C3A-C4A	-12.02	106.73	125.04
48	34	316	A86	C17-C16-C15	12.02	121.43	109.16
50	36	312	DD6	C37-C36-C31	-11.99	108.06	124.35
47	20	302	KC1	CMA-C3A-C4A	-11.98	106.80	125.04
48	14	316	A86	C17-C16-C15	11.94	121.34	109.16
48	14	314	A86	O1-C20-C21	-11.94	100.75	115.06
48	34	314	A86	O1-C20-C21	-11.87	100.83	115.06
47	14	309	KC1	C2A-C3A-C4A	-11.85	97.70	106.49
48	33	314	A86	C21-C20-C19	-11.83	100.97	114.28
47	34	309	KC1	C2A-C3A-C4A	-11.79	97.74	106.49
48	13	314	A86	C21-C20-C19	-11.76	101.05	114.28
48	41	215	A86	O1-C20-C21	-11.72	101.01	115.06
48	21	215	A86	O1-C20-C21	-11.67	101.08	115.06
47	14	304	KC1	CMA-C3A-C4A	-11.65	107.30	125.04
47	34	304	KC1	CMA-C3A-C4A	-11.61	107.36	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	41	207	KC1	CMA-C3A-C4A	-11.58	107.40	125.04
47	21	207	KC1	CMA-C3A-C4A	-11.58	107.41	125.04
48	31	314	A86	O1-C20-C21	-11.57	101.19	115.06
48	11	314	A86	O1-C20-C21	-11.55	101.22	115.06
48	39	313	A86	O1-C20-C21	-11.54	101.23	115.06
48	11	311	A86	C21-C20-C19	-11.52	101.32	114.28
48	31	311	A86	C21-C20-C19	-11.50	101.34	114.28
48	32	218	A86	C17-C16-C15	11.49	120.88	109.16
48	41	214	A86	O1-C20-C21	-11.48	101.30	115.06
48	21	214	A86	O1-C20-C21	-11.47	101.31	115.06
48	12	217	A86	C17-C16-C15	11.46	120.85	109.16
50	20	310	DD6	C12-C11-C10	-11.41	106.94	122.92
48	18	214	A86	O1-C20-C21	-11.40	101.39	115.06
50	40	212	DD6	C12-C11-C10	-11.40	106.96	122.92
48	38	214	A86	O1-C20-C21	-11.40	101.40	115.06
48	35	314	A86	C21-C20-C19	-11.39	101.46	114.28
48	38	215	A86	C17-C16-C15	11.34	120.73	109.16
50	20	310	DD6	C37-C36-C31	-11.22	109.11	124.35
50	20	312	DD6	C3-C2-C1	-11.21	111.31	127.31
50	40	214	DD6	C3-C2-C1	-11.21	111.32	127.31
50	40	212	DD6	C37-C36-C31	-11.20	109.14	124.35
47	15	309	KC1	C2A-C3A-C4A	-11.19	98.18	106.49
47	38	210	KC1	C2A-C3A-C4A	-11.19	98.19	106.49
47	18	210	KC1	C2A-C3A-C4A	-11.18	98.19	106.49
48	41	211	A86	O1-C20-C21	-11.16	101.69	115.06
47	11	309	KC1	C2A-C3A-C4A	-11.15	98.22	106.49
48	17	310	A86	O1-C20-C21	-11.14	101.71	115.06
50	20	310	DD6	C9-C10-C11	-11.14	111.41	127.31
48	21	211	A86	O1-C20-C21	-11.14	101.71	115.06
47	35	309	KC1	C2A-C3A-C4A	-11.13	98.23	106.49
47	17	308	KC1	C2A-C3A-C4A	-11.13	98.23	106.49
48	39	313	A86	C21-C20-C19	-11.12	101.77	114.28
47	15	304	KC1	CMA-C3A-C4A	-11.12	108.10	125.04
48	40	201	A86	C33-C32-C31	11.12	120.02	109.21
47	37	307	KC1	C2A-C3A-C4A	-11.11	98.24	106.49
50	40	212	DD6	C9-C10-C11	-11.11	111.45	127.31
48	16	313	A86	C33-C32-C31	11.09	119.99	109.21
48	15	314	A86	O1-C20-C21	-11.09	101.77	115.06
47	31	309	KC1	C2A-C3A-C4A	-11.08	98.26	106.49
48	18	215	A86	C17-C16-C15	11.08	120.46	109.16
48	37	309	A86	O1-C20-C21	-11.05	101.82	115.06
47	39	308	KC1	CMA-C3A-C4A	-11.03	108.23	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	41	216	DD6	C12-C11-C10	-11.03	107.47	122.92
47	19	308	KC1	CMA-C3A-C4A	-11.03	108.24	125.04
48	37	312	A86	O1-C20-C21	-11.02	101.86	115.06
50	21	216	DD6	C12-C11-C10	-11.01	107.50	122.92
47	35	304	KC1	CMA-C3A-C4A	-10.97	108.33	125.04
48	37	313	A86	O1-C20-C21	-10.97	101.91	115.06
48	32	203	A86	C21-C20-C19	-10.97	101.94	114.28
48	12	202	A86	C21-C20-C19	-10.96	101.95	114.28
48	17	313	A86	O1-C20-C21	-10.95	101.93	115.06
48	15	319	A86	C17-C16-C15	10.95	120.33	109.16
50	20	310	DD6	C4-C5-C6	-10.91	111.74	127.31
48	32	216	A86	O1-C20-C21	-10.90	101.99	115.06
48	35	319	A86	C17-C16-C15	10.90	120.28	109.16
50	40	212	DD6	C4-C5-C6	-10.89	111.77	127.31
48	14	311	A86	C21-C20-C19	-10.89	102.03	114.28
48	34	311	A86	C21-C20-C19	-10.89	102.03	114.28
48	12	215	A86	O1-C20-C21	-10.85	102.06	115.06
48	17	314	A86	O1-C20-C21	-10.85	102.06	115.06
48	17	315	A86	C21-C20-C19	-10.84	102.08	114.28
50	21	216	DD6	C9-C10-C11	-10.83	111.85	127.31
50	41	216	DD6	C9-C10-C11	-10.83	111.85	127.31
37	18	202	CLA	C1D-ND-C4D	-10.82	98.65	106.33
47	16	304	KC1	CMA-C3A-C4A	-10.82	108.57	125.04
50	41	212	DD6	C12-C11-C10	-10.81	107.78	122.92
48	37	309	A86	C21-C20-C19	-10.81	102.12	114.28
48	37	314	A86	C21-C20-C19	-10.81	102.12	114.28
50	21	212	DD6	C12-C11-C10	-10.80	107.79	122.92
50	41	212	DD6	C37-C36-C31	-10.80	109.67	124.35
47	36	304	KC1	CMA-C3A-C4A	-10.80	108.59	125.04
50	21	212	DD6	C37-C36-C31	-10.79	109.69	124.35
48	17	310	A86	C21-C20-C19	-10.78	102.15	114.28
48	13	315	A86	C21-C20-C19	-10.78	102.16	114.28
48	35	314	A86	O1-C20-C21	-10.77	102.15	115.06
48	33	315	A86	C21-C20-C19	-10.75	102.19	114.28
47	15	302	KC1	CMA-C3A-C4A	-10.73	108.69	125.04
48	13	314	A86	O1-C20-C21	-10.73	102.20	115.06
48	33	314	A86	O1-C20-C21	-10.72	102.21	115.06
48	16	313	A86	C21-C20-C19	-10.71	102.23	114.28
48	12	216	A86	O1-C20-C21	-10.71	102.22	115.06
48	40	201	A86	C21-C20-C19	-10.71	102.23	114.28
48	32	217	A86	O1-C20-C21	-10.71	102.23	115.06
48	17	313	A86	C21-C20-C19	-10.69	102.26	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	37	312	A86	C21-C20-C19	-10.69	102.26	114.28
48	32	214	A86	O1-C20-C21	-10.68	102.26	115.06
48	12	213	A86	O1-C20-C21	-10.67	102.27	115.06
48	15	314	A86	C21-C20-C19	-10.67	102.28	114.28
47	35	302	KC1	CMA-C3A-C4A	-10.67	108.80	125.04
48	18	212	A86	O1-C20-C21	-10.65	102.29	115.06
48	16	311	A86	C17-C16-C15	10.65	120.03	109.16
48	36	311	A86	C17-C16-C15	10.65	120.03	109.16
48	34	311	A86	O1-C20-C21	-10.62	102.34	115.06
48	38	212	A86	O1-C20-C21	-10.60	102.36	115.06
48	15	315	A86	O1-C20-C21	-10.60	102.36	115.06
48	19	313	A86	C21-C20-C19	-10.60	102.36	114.28
48	14	311	A86	O1-C20-C21	-10.58	102.37	115.06
48	16	314	A86	C17-C16-C15	10.55	119.92	109.16
47	40	204	KC1	C2A-C3A-C4A	-10.54	98.67	106.49
47	20	302	KC1	C2A-C3A-C4A	-10.52	98.68	106.49
48	21	213	A86	C21-C20-C19	-10.50	102.47	114.28
48	36	313	A86	C17-C16-C15	10.49	119.86	109.16
48	38	215	A86	C21-C20-C19	-10.49	102.48	114.28
48	21	213	A86	O1-C20-C21	-10.48	102.50	115.06
48	41	213	A86	O1-C20-C21	-10.47	102.51	115.06
48	34	315	A86	C21-C20-C19	-10.46	102.51	114.28
48	32	215	A86	O1-C20-C21	-10.46	102.52	115.06
48	41	213	A86	C21-C20-C19	-10.46	102.52	114.28
37	D	405	CLA	C1D-ND-C4D	-10.45	98.91	106.33
48	12	214	A86	O1-C20-C21	-10.44	102.55	115.06
48	14	315	A86	C21-C20-C19	-10.44	102.54	114.28
48	35	315	A86	O1-C20-C21	-10.41	102.58	115.06
48	17	313	A86	C33-C32-C31	10.38	119.30	109.21
48	13	313	A86	O1-C20-C21	-10.36	102.64	115.06
37	d	403	CLA	C1D-ND-C4D	-10.36	98.98	106.33
48	33	313	A86	O1-C20-C21	-10.35	102.65	115.06
48	37	312	A86	C33-C32-C31	10.33	119.25	109.21
47	33	302	KC1	C2A-C3A-C4A	-10.32	98.83	106.49
48	38	212	A86	C21-C20-C19	-10.31	102.68	114.28
47	13	302	KC1	C2A-C3A-C4A	-10.31	98.84	106.49
48	12	215	A86	C21-C20-C19	-10.30	102.69	114.28
48	40	201	A86	O1-C20-C21	-10.29	102.73	115.06
48	32	221	A86	C21-C20-C19	-10.29	102.71	114.28
48	18	213	A86	O1-C20-C21	-10.27	102.76	115.06
48	12	220	A86	C21-C20-C19	-10.26	102.74	114.28
48	16	313	A86	O1-C20-C21	-10.25	102.77	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	40	214	DD6	C12-C11-C10	-10.25	108.56	122.92
48	21	214	A86	C21-C20-C19	-10.25	102.75	114.28
48	40	211	A86	C21-C20-C19	-10.24	102.76	114.28
50	20	312	DD6	C12-C11-C10	-10.24	108.58	122.92
48	14	315	A86	O1-C20-C21	-10.24	102.79	115.06
48	20	309	A86	C21-C20-C19	-10.24	102.76	114.28
47	36	304	KC1	C2A-C3A-C4A	-10.23	98.89	106.49
48	15	312	A86	C21-C20-C19	-10.23	102.77	114.28
48	35	312	A86	C21-C20-C19	-10.22	102.78	114.28
48	41	214	A86	C21-C20-C19	-10.22	102.78	114.28
48	18	213	A86	C21-C20-C19	-10.22	102.78	114.28
47	16	304	KC1	C2A-C3A-C4A	-10.22	98.91	106.49
47	33	309	KC1	C2A-C3A-C4A	-10.22	98.91	106.49
48	32	216	A86	C21-C20-C19	-10.21	102.79	114.28
47	13	309	KC1	C2A-C3A-C4A	-10.21	98.91	106.49
48	15	316	A86	C21-C20-C19	-10.21	102.80	114.28
48	35	316	A86	C21-C20-C19	-10.21	102.80	114.28
48	34	312	A86	O1-C20-C21	-10.20	102.83	115.06
48	14	312	A86	O1-C20-C21	-10.20	102.83	115.06
47	13	304	KC1	C2A-C3A-C4A	-10.19	98.92	106.49
48	38	213	A86	O1-C20-C21	-10.19	102.84	115.06
47	31	305	KC1	C2A-C3A-C4A	-10.19	98.93	106.49
48	34	315	A86	O1-C20-C21	-10.18	102.86	115.06
47	11	304	KC1	C2A-C3A-C4A	-10.17	98.94	106.49
47	18	205	KC1	C2A-C3A-C4A	-10.17	98.94	106.49
48	18	212	A86	C21-C20-C19	-10.16	102.85	114.28
48	34	314	A86	C21-C20-C19	-10.16	102.85	114.28
47	38	205	KC1	C2A-C3A-C4A	-10.16	98.95	106.49
48	32	217	A86	C21-C20-C19	-10.15	102.86	114.28
47	33	304	KC1	C2A-C3A-C4A	-10.15	98.96	106.49
48	14	314	A86	C21-C20-C19	-10.15	102.87	114.28
48	39	311	A86	C21-C20-C19	-10.14	102.87	114.28
48	12	216	A86	C21-C20-C19	-10.14	102.88	114.28
48	33	311	A86	C21-C20-C19	-10.12	102.90	114.28
48	19	311	A86	C21-C20-C19	-10.12	102.90	114.28
47	21	203	KC1	C2A-C3A-C4A	-10.12	98.98	106.49
50	19	312	DD6	C9-C10-C11	-10.11	112.88	127.31
48	13	312	A86	O1-C20-C21	-10.11	102.95	115.06
47	12	211	KC1	C2A-C3A-C4A	-10.11	98.99	106.49
47	34	304	KC1	C2A-C3A-C4A	-10.10	98.99	106.49
50	16	312	DD6	C12-C11-C10	-10.10	108.78	122.92
50	21	212	DD6	C7-C6-C5	-10.10	108.78	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	41	212	DD6	C7-C6-C5	-10.10	108.78	122.92
50	20	312	DD6	C9-C10-C11	-10.10	112.90	127.31
48	13	311	A86	C21-C20-C19	-10.10	102.92	114.28
50	36	312	DD6	C12-C11-C10	-10.09	108.78	122.92
47	14	304	KC1	C2A-C3A-C4A	-10.09	99.00	106.49
50	40	214	DD6	C9-C10-C11	-10.09	112.92	127.31
47	32	209	KC1	C2A-C3A-C4A	-10.08	99.00	106.49
48	37	314	A86	C17-C16-C15	10.08	119.45	109.16
47	32	212	KC1	C2A-C3A-C4A	-10.08	99.01	106.49
48	35	311	A86	O1-C20-C21	-10.07	102.99	115.06
47	40	206	KC1	C2A-C3A-C4A	-10.07	99.01	106.49
47	12	208	KC1	C2A-C3A-C4A	-10.07	99.01	106.49
47	41	203	KC1	C2A-C3A-C4A	-10.07	99.02	106.49
50	39	312	DD6	C9-C10-C11	-10.07	112.94	127.31
48	15	311	A86	O1-C20-C21	-10.07	103.00	115.06
48	18	215	A86	C21-C20-C19	-10.06	102.96	114.28
48	38	213	A86	C21-C20-C19	-10.06	102.97	114.28
50	36	312	DD6	C3-C2-C1	-10.06	112.96	127.31
48	33	312	A86	O1-C20-C21	-10.05	103.02	115.06
37	18	202	CLA	C2D-C1D-ND	10.05	117.51	110.10
47	36	308	KC1	C2A-C3A-C4A	-10.04	99.04	106.49
50	16	312	DD6	C3-C2-C1	-10.04	112.99	127.31
37	16	301	CLA	C1D-ND-C4D	-10.04	99.21	106.33
47	15	306	KC1	C2A-C3A-C4A	-10.03	99.04	106.49
48	17	315	A86	C17-C16-C15	10.03	119.39	109.16
48	13	311	A86	O1-C20-C21	-10.02	103.05	115.06
48	33	311	A86	O1-C20-C21	-10.02	103.05	115.06
48	33	312	A86	C21-C20-C19	-10.01	103.02	114.28
48	13	312	A86	C21-C20-C19	-9.99	103.05	114.28
48	12	217	A86	C21-C20-C19	-9.99	103.05	114.28
50	41	216	DD6	C7-C6-C5	-9.98	108.95	122.92
48	21	215	A86	C21-C20-C19	-9.97	103.06	114.28
48	41	215	A86	C21-C20-C19	-9.97	103.06	114.28
50	21	216	DD6	C7-C6-C5	-9.97	108.96	122.92
47	16	308	KC1	C2A-C3A-C4A	-9.97	99.09	106.49
37	15	301	CLA	C1D-ND-C4D	-9.96	99.26	106.33
37	35	301	CLA	C1D-ND-C4D	-9.96	99.26	106.33
37	36	301	CLA	C1D-ND-C4D	-9.95	99.26	106.33
47	32	207	KC1	C2A-C3A-C4A	-9.95	99.10	106.49
48	11	312	A86	C21-C20-C19	-9.94	103.09	114.28
47	31	307	KC1	CMA-C3A-C4A	-9.94	109.89	125.04
48	14	313	A86	C21-C20-C19	-9.94	103.10	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	32	218	A86	C21-C20-C19	-9.94	103.10	114.28
48	31	312	A86	C21-C20-C19	-9.94	103.10	114.28
47	20	304	KC1	C2A-C3A-C4A	-9.94	99.11	106.49
47	12	206	KC1	C2A-C3A-C4A	-9.93	99.12	106.49
47	11	306	KC1	CMA-C3A-C4A	-9.92	109.92	125.04
47	13	302	KC1	CMA-C3A-C4A	-9.92	109.92	125.04
48	34	313	A86	C21-C20-C19	-9.92	103.12	114.28
47	33	302	KC1	CMA-C3A-C4A	-9.91	109.94	125.04
47	35	306	KC1	C2A-C3A-C4A	-9.91	99.14	106.49
48	15	311	A86	C21-C20-C19	-9.90	103.15	114.28
37	38	202	CLA	C1D-ND-C4D	-9.88	99.31	106.33
48	32	214	A86	C21-C20-C19	-9.86	103.18	114.28
48	21	211	A86	C21-C20-C19	-9.86	103.19	114.28
50	36	312	DD6	C13-C11-C10	-9.86	103.82	118.94
48	12	213	A86	C21-C20-C19	-9.85	103.19	114.28
50	40	212	DD6	C-C1-C2	-9.85	109.12	122.92
48	41	211	A86	C21-C20-C19	-9.85	103.20	114.28
50	20	310	DD6	C-C1-C2	-9.85	109.13	122.92
50	16	312	DD6	C13-C11-C10	-9.84	103.83	118.94
48	34	316	A86	C21-C20-C19	-9.83	103.22	114.28
47	15	302	KC1	C2A-C3A-C4A	-9.83	99.19	106.49
48	33	315	A86	C17-C16-C15	9.83	119.19	109.16
48	35	311	A86	C21-C20-C19	-9.83	103.22	114.28
37	19	304	CLA	C1D-ND-C4D	-9.82	99.36	106.33
47	31	303	KC1	C2A-C3A-C4A	-9.82	99.20	106.49
37	39	304	CLA	C1D-ND-C4D	-9.81	99.36	106.33
48	13	315	A86	C17-C16-C15	9.81	119.17	109.16
48	35	315	A86	C21-C20-C19	-9.81	103.24	114.28
48	14	316	A86	C21-C20-C19	-9.80	103.25	114.28
48	16	314	A86	C21-C20-C19	-9.79	103.27	114.28
48	17	311	A86	O1-C20-C21	-9.78	103.33	115.06
48	17	320	A86	O1-C20-C21	-9.78	103.33	115.06
47	11	302	KC1	C2A-C3A-C4A	-9.78	99.23	106.49
37	40	203	CLA	C1D-ND-C4D	-9.78	99.39	106.33
47	16	302	KC1	C2A-C3A-C4A	-9.77	99.24	106.49
47	37	304	KC1	C2A-C3A-C4A	-9.77	99.24	106.49
47	18	207	KC1	CMA-C3A-C4A	-9.76	110.17	125.04
48	36	313	A86	C21-C20-C19	-9.75	103.31	114.28
48	15	315	A86	C21-C20-C19	-9.74	103.32	114.28
47	36	302	KC1	C2A-C3A-C4A	-9.74	99.26	106.49
47	34	306	KC1	CMA-C3A-C4A	-9.74	110.21	125.04
47	14	306	KC1	CMA-C3A-C4A	-9.73	110.21	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	19	305	CLA	C1D-ND-C4D	-9.73	99.42	106.33
47	38	207	KC1	CMA-C3A-C4A	-9.72	110.24	125.04
48	36	310	A86	C21-C20-C19	-9.71	103.36	114.28
37	41	210	CLA	C1D-ND-C4D	-9.71	99.44	106.33
37	20	301	CLA	C1D-ND-C4D	-9.70	99.45	106.33
48	38	214	A86	C21-C20-C19	-9.69	103.38	114.28
50	41	212	DD6	C13-C11-C10	-9.69	104.08	118.94
47	20	305	KC1	C2A-C3A-C4A	-9.68	99.31	106.49
37	D	405	CLA	C2D-C1D-ND	9.67	117.23	110.10
50	21	212	DD6	C13-C11-C10	-9.66	104.11	118.94
37	21	210	CLA	C1D-ND-C4D	-9.66	99.47	106.33
37	39	305	CLA	C1D-ND-C4D	-9.66	99.47	106.33
37	d	403	CLA	C2D-C1D-ND	9.65	117.22	110.10
48	32	221	A86	O1-C20-C21	-9.65	103.49	115.06
48	16	310	A86	C21-C20-C19	-9.65	103.42	114.28
48	11	314	A86	C21-C20-C19	-9.65	103.42	114.28
47	17	305	KC1	C2A-C3A-C4A	-9.65	99.33	106.49
48	31	314	A86	C33-C32-C31	9.65	118.59	109.21
48	31	314	A86	C21-C20-C19	-9.64	103.44	114.28
48	37	319	A86	O1-C20-C21	-9.64	103.51	115.06
48	17	312	A86	C21-C20-C19	-9.63	103.44	114.28
47	35	304	KC1	C2A-C3A-C4A	-9.63	99.34	106.49
48	12	220	A86	O1-C20-C21	-9.63	103.51	115.06
48	19	311	A86	O1-C20-C21	-9.63	103.52	115.06
47	15	304	KC1	C2A-C3A-C4A	-9.63	99.34	106.49
37	34	301	CLA	C1D-ND-C4D	-9.63	99.50	106.33
50	39	312	DD6	C12-C11-C10	-9.62	109.44	122.92
37	C	513	CLA	C1D-ND-C4D	-9.62	99.50	106.33
48	35	313	A86	C21-C20-C19	-9.62	103.46	114.28
47	40	207	KC1	C2A-C3A-C4A	-9.62	99.35	106.49
50	21	216	DD6	C4-C5-C6	-9.61	113.59	127.31
50	19	312	DD6	C12-C11-C10	-9.61	109.46	122.92
47	36	305	KC1	CMA-C3A-C4A	-9.61	110.40	125.04
48	11	315	A86	O1-C20-C21	-9.61	103.54	115.06
50	20	312	DD6	C4-C5-C6	-9.61	113.60	127.31
48	31	315	A86	O1-C20-C21	-9.60	103.55	115.06
48	39	311	A86	O1-C20-C21	-9.60	103.55	115.06
47	16	305	KC1	CMA-C3A-C4A	-9.60	110.42	125.04
37	c	513	CLA	C1D-ND-C4D	-9.60	99.52	106.33
37	18	201	CLA	C1D-ND-C4D	-9.59	99.52	106.33
50	41	216	DD6	C4-C5-C6	-9.59	113.62	127.31
50	41	212	DD6	C9-C10-C11	-9.59	113.63	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	35	302	KC1	C2A-C3A-C4A	-9.59	99.37	106.49
50	40	214	DD6	C4-C5-C6	-9.58	113.63	127.31
48	15	313	A86	C21-C20-C19	-9.58	103.50	114.28
47	11	306	KC1	C2A-C3A-C4A	-9.58	99.38	106.49
37	19	306	CLA	C1D-ND-C4D	-9.58	99.53	106.33
50	21	212	DD6	C32-C31-C36	-9.58	109.11	122.63
47	38	205	KC1	CMA-C3A-C4A	-9.58	110.45	125.04
37	39	306	CLA	C1D-ND-C4D	-9.58	99.53	106.33
50	21	212	DD6	C9-C10-C11	-9.57	113.64	127.31
47	31	307	KC1	C2A-C3A-C4A	-9.57	99.38	106.49
50	41	212	DD6	C32-C31-C36	-9.57	109.12	122.63
48	37	319	A86	C21-C20-C19	-9.57	103.51	114.28
47	18	205	KC1	CMA-C3A-C4A	-9.56	110.47	125.04
47	40	207	KC1	CMA-C3A-C4A	-9.56	110.48	125.04
48	17	320	A86	C21-C20-C19	-9.56	103.53	114.28
37	16	309	CLA	C1D-ND-C4D	-9.55	99.55	106.33
47	20	305	KC1	CMA-C3A-C4A	-9.55	110.49	125.04
37	14	301	CLA	C1D-ND-C4D	-9.55	99.55	106.33
47	21	207	KC1	C2A-C3A-C4A	-9.55	99.40	106.49
48	18	214	A86	C21-C20-C19	-9.54	103.55	114.28
48	15	316	A86	C17-C16-C15	9.53	118.88	109.16
37	39	301	CLA	C1D-ND-C4D	-9.52	99.57	106.33
47	38	207	KC1	C2A-C3A-C4A	-9.52	99.42	106.49
37	36	309	CLA	C1D-ND-C4D	-9.52	99.57	106.33
47	41	207	KC1	C2A-C3A-C4A	-9.51	99.43	106.49
37	a	404	CLA	C1D-ND-C4D	-9.51	99.58	106.33
48	37	310	A86	O1-C20-C21	-9.51	103.66	115.06
48	37	311	A86	C21-C20-C19	-9.51	103.59	114.28
37	D	401	CLA	C1D-ND-C4D	-9.50	99.58	106.33
48	31	319	A86	C21-C20-C19	-9.50	103.59	114.28
37	b	506	CLA	C1D-ND-C4D	-9.50	99.59	106.33
48	35	316	A86	C17-C16-C15	9.49	118.85	109.16
48	11	319	A86	C21-C20-C19	-9.49	103.60	114.28
37	19	301	CLA	C1D-ND-C4D	-9.49	99.60	106.33
37	D	406	CLA	C1D-ND-C4D	-9.48	99.60	106.33
47	18	207	KC1	C2A-C3A-C4A	-9.47	99.46	106.49
47	13	306	KC1	CMA-C3A-C4A	-9.47	110.62	125.04
47	34	306	KC1	C2A-C3A-C4A	-9.47	99.46	106.49
47	33	306	KC1	CMA-C3A-C4A	-9.47	110.62	125.04
47	11	304	KC1	CMA-C3A-C4A	-9.46	110.62	125.04
37	B	506	CLA	C1D-ND-C4D	-9.46	99.61	106.33
50	21	216	DD6	C3-C2-C1	-9.46	113.81	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	36	305	KC1	C2A-C3A-C4A	-9.46	99.47	106.49
47	31	305	KC1	CMA-C3A-C4A	-9.46	110.63	125.04
47	16	305	KC1	C2A-C3A-C4A	-9.46	99.47	106.49
37	A	405	CLA	C1D-ND-C4D	-9.46	99.62	106.33
47	41	203	KC1	CMA-C3A-C4A	-9.45	110.64	125.04
37	c	504	CLA	C1D-ND-C4D	-9.45	99.62	106.33
48	11	315	A86	C17-C16-C15	9.45	118.80	109.16
48	31	315	A86	C17-C16-C15	9.45	118.80	109.16
37	a	407	CLA	C1D-ND-C4D	-9.45	99.62	106.33
50	41	216	DD6	C3-C2-C1	-9.44	113.84	127.31
47	32	209	KC1	CMA-C3A-C4A	-9.44	110.67	125.04
47	13	306	KC1	C2A-C3A-C4A	-9.43	99.49	106.49
48	37	311	A86	C17-C16-C15	9.42	118.78	109.16
47	14	306	KC1	C2A-C3A-C4A	-9.42	99.50	106.49
47	21	203	KC1	CMA-C3A-C4A	-9.42	110.70	125.04
47	17	306	KC1	C2A-C3A-C4A	-9.41	99.51	106.49
47	12	208	KC1	CMA-C3A-C4A	-9.41	110.72	125.04
37	d	404	CLA	C1D-ND-C4D	-9.40	99.65	106.33
37	D	402	CLA	C1D-ND-C4D	-9.40	99.66	106.33
48	12	216	A86	C33-C32-C31	9.40	118.34	109.21
48	32	217	A86	C33-C32-C31	9.40	118.34	109.21
37	d	401	CLA	C1D-ND-C4D	-9.39	99.66	106.33
37	C	504	CLA	C1D-ND-C4D	-9.39	99.66	106.33
50	20	310	DD6	C7-C6-C5	-9.39	109.77	122.92
37	b	505	CLA	C1D-ND-C4D	-9.39	99.67	106.33
37	B	505	CLA	C1D-ND-C4D	-9.38	99.67	106.33
47	33	306	KC1	C2A-C3A-C4A	-9.38	99.53	106.49
48	15	312	A86	O1-C20-C21	-9.38	103.81	115.06
47	17	303	KC1	C2A-C3A-C4A	-9.38	99.53	106.49
47	37	305	KC1	CMA-C3A-C4A	-9.38	110.76	125.04
48	11	314	A86	C33-C32-C31	9.38	118.32	109.21
47	11	302	KC1	CMA-C3A-C4A	-9.38	110.76	125.04
37	21	206	CLA	C1D-ND-C4D	-9.37	99.68	106.33
47	17	306	KC1	CMA-C3A-C4A	-9.37	110.77	125.04
48	14	312	A86	C21-C20-C19	-9.37	103.74	114.28
48	34	312	A86	C21-C20-C19	-9.37	103.74	114.28
50	40	212	DD6	C7-C6-C5	-9.37	109.80	122.92
48	35	312	A86	O1-C20-C21	-9.36	103.84	115.06
37	41	206	CLA	C1D-ND-C4D	-9.36	99.69	106.33
37	b	508	CLA	C1D-ND-C4D	-9.35	99.69	106.33
37	32	208	CLA	C1D-ND-C4D	-9.35	99.69	106.33
37	12	207	CLA	C1D-ND-C4D	-9.35	99.69	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	31	303	KC1	CMA-C3A-C4A	-9.34	110.81	125.04
37	38	201	CLA	C1D-ND-C4D	-9.34	99.70	106.33
47	37	305	KC1	C2A-C3A-C4A	-9.34	99.56	106.49
37	c	501	CLA	C1D-ND-C4D	-9.33	99.71	106.33
37	C	501	CLA	C1D-ND-C4D	-9.32	99.71	106.33
47	37	302	KC1	C2A-C3A-C4A	-9.31	99.58	106.49
37	39	303	CLA	C1D-ND-C4D	-9.30	99.73	106.33
37	B	508	CLA	C1D-ND-C4D	-9.30	99.73	106.33
48	17	312	A86	C17-C16-C15	9.30	118.65	109.16
48	37	310	A86	C21-C20-C19	-9.30	103.82	114.28
37	37	301	CLA	C1D-ND-C4D	-9.30	99.73	106.33
37	18	204	CLA	C1D-ND-C4D	-9.30	99.73	106.33
37	W	101	CLA	C1D-ND-C4D	-9.27	99.75	106.33
37	38	204	CLA	C1D-ND-C4D	-9.27	99.75	106.33
37	19	303	CLA	C1D-ND-C4D	-9.27	99.75	106.33
37	41	208	CLA	C1D-ND-C4D	-9.26	99.76	106.33
48	12	214	A86	C21-C20-C19	-9.25	103.87	114.28
37	31	302	CLA	C1D-ND-C4D	-9.25	99.76	106.33
50	16	312	DD6	C9-C10-C11	-9.25	114.11	127.31
50	36	312	DD6	C9-C10-C11	-9.25	114.11	127.31
50	20	312	DD6	C7-C6-C5	-9.24	109.98	122.92
37	C	512	CLA	C1D-ND-C4D	-9.23	99.78	106.33
37	38	206	CLA	C1D-ND-C4D	-9.23	99.78	106.33
37	36	307	CLA	C1D-ND-C4D	-9.23	99.78	106.33
48	32	215	A86	C21-C20-C19	-9.23	103.90	114.28
37	11	310	CLA	C1D-ND-C4D	-9.22	99.78	106.33
50	40	214	DD6	C7-C6-C5	-9.22	110.01	122.92
37	16	307	CLA	C1D-ND-C4D	-9.21	99.79	106.33
47	19	308	KC1	C2A-C3A-C4A	-9.21	99.65	106.49
47	39	308	KC1	C2A-C3A-C4A	-9.21	99.66	106.49
37	11	301	CLA	C1D-ND-C4D	-9.20	99.80	106.33
37	31	310	CLA	C1D-ND-C4D	-9.19	99.80	106.33
48	11	312	A86	O1-C20-C21	-9.19	104.04	115.06
47	13	304	KC1	CMA-C3A-C4A	-9.19	111.05	125.04
48	12	217	A86	C4-C5-C6	-9.19	114.20	127.31
48	31	312	A86	O1-C20-C21	-9.18	104.05	115.06
48	11	313	A86	C17-C16-C15	9.18	118.53	109.16
48	12	202	A86	C17-C16-C15	9.18	118.53	109.16
37	B	513	CLA	C1D-ND-C4D	-9.17	99.82	106.33
48	32	218	A86	C4-C5-C6	-9.17	114.23	127.31
47	33	304	KC1	CMA-C3A-C4A	-9.16	111.08	125.04
48	16	311	A86	O1-C20-C21	-9.16	104.08	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	33	305	CLA	C1D-ND-C4D	-9.16	99.83	106.33
50	39	312	DD6	C3-C2-C1	-9.16	114.24	127.31
37	21	208	CLA	C1D-ND-C4D	-9.16	99.83	106.33
37	C	505	CLA	C1D-ND-C4D	-9.15	99.83	106.33
37	18	211	CLA	C1D-ND-C4D	-9.15	99.84	106.33
48	36	311	A86	O1-C20-C21	-9.15	104.10	115.06
50	41	216	DD6	C32-C31-C36	-9.14	109.73	122.63
37	41	205	CLA	C1D-ND-C4D	-9.14	99.84	106.33
50	16	312	DD6	C7-C6-C5	-9.14	110.12	122.92
37	c	512	CLA	C1D-ND-C4D	-9.13	99.85	106.33
37	w	101	CLA	C1D-ND-C4D	-9.13	99.85	106.33
50	19	312	DD6	C3-C2-C1	-9.13	114.28	127.31
50	21	216	DD6	C32-C31-C36	-9.13	109.75	122.63
50	36	312	DD6	C7-C6-C5	-9.13	110.14	122.92
48	11	319	A86	C17-C16-C15	9.13	118.47	109.16
48	11	315	A86	C21-C20-C19	-9.11	104.03	114.28
48	31	315	A86	C21-C20-C19	-9.11	104.03	114.28
37	C	503	CLA	C1D-ND-C4D	-9.11	99.86	106.33
48	32	203	A86	C17-C16-C15	9.11	118.46	109.16
37	21	205	CLA	C1D-ND-C4D	-9.11	99.86	106.33
37	33	308	CLA	C1D-ND-C4D	-9.11	99.86	106.33
37	c	503	CLA	C1D-ND-C4D	-9.10	99.87	106.33
37	c	505	CLA	C1D-ND-C4D	-9.10	99.87	106.33
48	31	319	A86	C17-C16-C15	9.09	118.44	109.16
37	B	515	CLA	C1D-ND-C4D	-9.09	99.88	106.33
47	35	306	KC1	CMA-C3A-C4A	-9.09	111.20	125.04
37	b	513	CLA	C1D-ND-C4D	-9.09	99.88	106.33
48	18	213	A86	C33-C32-C31	9.09	118.04	109.21
48	17	311	A86	C21-C20-C19	-9.09	104.06	114.28
50	19	312	DD6	C7-C6-C5	-9.08	110.20	122.92
37	34	310	CLA	C1D-ND-C4D	-9.08	99.89	106.33
37	B	502	CLA	C1D-ND-C4D	-9.08	99.89	106.33
37	13	305	CLA	C1D-ND-C4D	-9.07	99.89	106.33
37	35	303	CLA	C1D-ND-C4D	-9.07	99.89	106.33
50	21	212	DD6	C-C1-C2	-9.07	110.22	122.92
37	b	515	CLA	C1D-ND-C4D	-9.07	99.89	106.33
50	39	312	DD6	C7-C6-C5	-9.06	110.22	122.92
37	35	310	CLA	C1D-ND-C4D	-9.06	99.90	106.33
48	40	213	A86	C21-C20-C19	-9.06	104.08	114.28
37	14	310	CLA	C1D-ND-C4D	-9.06	99.90	106.33
48	38	213	A86	C33-C32-C31	9.06	118.02	109.21
47	13	309	KC1	CMA-C3A-C4A	-9.06	111.25	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	41	212	DD6	C-C1-C2	-9.05	110.25	122.92
37	21	204	CLA	C1D-ND-C4D	-9.04	99.91	106.33
37	15	308	CLA	C1D-ND-C4D	-9.04	99.91	106.33
37	41	204	CLA	C1D-ND-C4D	-9.04	99.92	106.33
47	33	309	KC1	CMA-C3A-C4A	-9.04	111.28	125.04
47	17	305	KC1	CMA-C3A-C4A	-9.03	111.28	125.04
37	35	308	CLA	C1D-ND-C4D	-9.03	99.92	106.33
37	16	301	CLA	C2D-C1D-ND	9.03	116.76	110.10
47	15	306	KC1	CMA-C3A-C4A	-9.03	111.29	125.04
37	36	301	CLA	C2D-C1D-ND	9.03	116.76	110.10
37	13	308	CLA	C1D-ND-C4D	-9.03	99.92	106.33
48	31	313	A86	C17-C16-C15	9.02	118.36	109.16
37	b	502	CLA	C1D-ND-C4D	-9.02	99.93	106.33
37	15	310	CLA	C1D-ND-C4D	-9.02	99.93	106.33
48	20	311	A86	C21-C20-C19	-9.02	104.13	114.28
37	41	209	CLA	C1D-ND-C4D	-9.02	99.93	106.33
37	B	511	CLA	C1D-ND-C4D	-9.02	99.93	106.33
37	15	303	CLA	C1D-ND-C4D	-9.01	99.93	106.33
37	18	209	CLA	C1D-ND-C4D	-9.01	99.94	106.33
47	37	304	KC1	CMA-C3A-C4A	-9.00	111.33	125.04
50	41	212	DD6	C4-C5-C6	-9.00	114.47	127.31
50	21	212	DD6	C4-C5-C6	-9.00	114.47	127.31
37	21	209	CLA	C1D-ND-C4D	-8.99	99.95	106.33
48	19	313	A86	C33-C32-C31	8.99	117.95	109.21
48	39	313	A86	C33-C32-C31	8.99	117.95	109.21
50	39	312	DD6	C4-C5-C6	-8.99	114.48	127.31
37	33	310	CLA	C1D-ND-C4D	-8.98	99.96	106.33
37	b	511	CLA	C1D-ND-C4D	-8.97	99.97	106.33
50	19	312	DD6	C4-C5-C6	-8.96	114.52	127.31
37	15	305	CLA	C1D-ND-C4D	-8.95	99.97	106.33
37	14	305	CLA	C1D-ND-C4D	-8.95	99.98	106.33
37	34	305	CLA	C1D-ND-C4D	-8.95	99.98	106.33
48	34	313	A86	C17-C16-C15	8.94	118.28	109.16
37	14	308	CLA	C1D-ND-C4D	-8.94	99.99	106.33
37	21	202	CLA	C1D-ND-C4D	-8.94	99.99	106.33
37	38	209	CLA	C1D-ND-C4D	-8.94	99.99	106.33
37	32	202	CLA	C1D-ND-C4D	-8.93	99.99	106.33
37	13	310	CLA	C1D-ND-C4D	-8.93	99.99	106.33
37	11	308	CLA	C1D-ND-C4D	-8.93	99.99	106.33
48	15	319	A86	O1-C20-C21	-8.93	104.36	115.06
48	35	319	A86	O1-C20-C21	-8.93	104.36	115.06
48	14	313	A86	C17-C16-C15	8.93	118.27	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	38	202	CLA	C2D-C1D-ND	8.93	116.68	110.10
37	11	307	CLA	C1D-ND-C4D	-8.92	100.00	106.33
37	18	206	CLA	C1D-ND-C4D	-8.91	100.00	106.33
37	16	303	CLA	C1D-ND-C4D	-8.91	100.00	106.33
37	17	302	CLA	C1D-ND-C4D	-8.91	100.00	106.33
48	36	311	A86	C21-C20-C19	-8.91	104.26	114.28
37	34	308	CLA	C1D-ND-C4D	-8.90	100.02	106.33
48	34	316	A86	C4-C5-C6	-8.89	114.62	127.31
37	36	303	CLA	C1D-ND-C4D	-8.89	100.02	106.33
37	B	516	CLA	C1D-ND-C4D	-8.89	100.02	106.33
37	b	516	CLA	C1D-ND-C4D	-8.88	100.02	106.33
37	12	210	CLA	C1D-ND-C4D	-8.88	100.03	106.33
37	32	211	CLA	C1D-ND-C4D	-8.88	100.03	106.33
37	13	301	CLA	C1D-ND-C4D	-8.88	100.03	106.33
37	31	308	CLA	C1D-ND-C4D	-8.88	100.03	106.33
37	33	301	CLA	C1D-ND-C4D	-8.87	100.03	106.33
48	18	215	A86	O1-C20-C21	-8.87	104.42	115.06
48	13	314	A86	C17-C16-C15	8.87	118.21	109.16
48	14	316	A86	C4-C5-C6	-8.86	114.66	127.31
37	20	307	CLA	C1D-ND-C4D	-8.84	100.05	106.33
37	41	202	CLA	C1D-ND-C4D	-8.84	100.05	106.33
48	16	311	A86	C21-C20-C19	-8.84	104.34	114.28
37	19	304	CLA	C2D-C1D-ND	8.82	116.61	110.10
48	36	310	A86	C17-C16-C15	8.82	118.16	109.16
48	16	310	A86	O1-C20-C21	-8.82	104.49	115.06
48	31	319	A86	O1-C20-C21	-8.81	104.49	115.06
48	16	310	A86	C17-C16-C15	8.81	118.15	109.16
37	b	510	CLA	C1D-ND-C4D	-8.81	100.08	106.33
37	40	209	CLA	C1D-ND-C4D	-8.81	100.08	106.33
48	36	310	A86	O1-C20-C21	-8.80	104.51	115.06
48	17	320	A86	C17-C16-C15	8.80	118.14	109.16
37	39	304	CLA	C2D-C1D-ND	8.79	116.58	110.10
37	B	513	CLA	C2D-C1D-ND	8.79	116.58	110.10
48	16	311	A86	C33-C32-C31	8.79	117.75	109.21
48	11	319	A86	O1-C20-C21	-8.78	104.53	115.06
37	14	303	CLA	C1D-ND-C4D	-8.78	100.10	106.33
37	b	512	CLA	C1D-ND-C4D	-8.77	100.11	106.33
37	38	211	CLA	C1D-ND-C4D	-8.76	100.11	106.33
37	39	302	CLA	C1D-ND-C4D	-8.76	100.11	106.33
48	36	311	A86	C33-C32-C31	8.76	117.72	109.21
37	B	510	CLA	C1D-ND-C4D	-8.76	100.11	106.33
37	B	512	CLA	C1D-ND-C4D	-8.76	100.11	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	37	303	CLA	C1D-ND-C4D	-8.75	100.12	106.33
48	33	314	A86	C33-C32-C31	8.75	117.72	109.21
37	39	301	CLA	C2D-C1D-ND	8.75	116.55	110.10
50	36	312	DD6	C4-C5-C6	-8.75	114.82	127.31
50	16	312	DD6	C4-C5-C6	-8.74	114.84	127.31
37	38	204	CLA	CMD-C2D-C1D	8.74	140.11	124.71
48	20	311	A86	C33-C32-C31	8.73	117.70	109.21
48	40	213	A86	C33-C32-C31	8.73	117.70	109.21
37	b	513	CLA	C2D-C1D-ND	8.73	116.54	110.10
48	13	314	A86	C33-C32-C31	8.73	117.70	109.21
37	19	302	CLA	C1D-ND-C4D	-8.73	100.13	106.33
37	35	305	CLA	C1D-ND-C4D	-8.73	100.14	106.33
48	15	313	A86	O1-C20-C21	-8.72	104.61	115.06
37	18	204	CLA	CMD-C2D-C1D	8.72	140.08	124.71
37	17	304	CLA	C1D-ND-C4D	-8.71	100.15	106.33
37	20	306	CLA	C1D-ND-C4D	-8.71	100.15	106.33
37	40	208	CLA	C1D-ND-C4D	-8.71	100.15	106.33
37	34	303	CLA	C1D-ND-C4D	-8.70	100.15	106.33
37	39	307	CLA	C1D-ND-C4D	-8.70	100.15	106.33
50	40	212	DD6	C32-C31-C36	-8.70	110.35	122.63
48	15	316	A86	C4-C5-C6	-8.70	114.90	127.31
48	35	311	A86	C33-C32-C31	8.69	117.66	109.21
37	37	308	CLA	C1D-ND-C4D	-8.69	100.16	106.33
50	20	310	DD6	C32-C31-C36	-8.69	110.36	122.63
37	17	307	CLA	C1D-ND-C4D	-8.69	100.16	106.33
37	c	508	CLA	C1D-ND-C4D	-8.69	100.17	106.33
48	35	313	A86	O1-C20-C21	-8.68	104.66	115.06
37	32	213	CLA	C1D-ND-C4D	-8.66	100.18	106.33
37	17	309	CLA	C1D-ND-C4D	-8.66	100.18	106.33
50	21	216	DD6	C-C1-C2	-8.65	110.80	122.92
50	41	216	DD6	C-C1-C2	-8.65	110.81	122.92
37	19	301	CLA	C2D-C1D-ND	8.64	116.47	110.10
37	19	309	CLA	C1D-ND-C4D	-8.63	100.20	106.33
37	34	301	CLA	C2D-C1D-ND	8.63	116.46	110.10
37	C	508	CLA	C1D-ND-C4D	-8.62	100.21	106.33
37	19	307	CLA	C1D-ND-C4D	-8.62	100.21	106.33
48	33	313	A86	C33-C32-C31	8.62	117.58	109.21
37	31	306	CLA	C1D-ND-C4D	-8.61	100.22	106.33
37	39	309	CLA	C1D-ND-C4D	-8.61	100.22	106.33
37	12	212	CLA	C1D-ND-C4D	-8.61	100.22	106.33
48	35	316	A86	C4-C5-C6	-8.61	115.02	127.31
37	39	306	CLA	C2D-C1D-ND	8.61	116.45	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	37	306	CLA	C1D-ND-C4D	-8.60	100.22	106.33
37	B	514	CLA	C1D-ND-C4D	-8.60	100.22	106.33
37	20	308	CLA	C1D-ND-C4D	-8.60	100.22	106.33
50	20	310	DD6	C13-C11-C10	-8.60	105.75	118.94
47	37	302	KC1	CMA-C3A-C4A	-8.60	111.95	125.04
37	18	209	CLA	C2D-C1D-ND	8.60	116.44	110.10
37	14	301	CLA	C2D-C1D-ND	8.58	116.43	110.10
37	19	306	CLA	C2D-C1D-ND	8.58	116.43	110.10
37	38	208	CLA	C1D-ND-C4D	-8.57	100.24	106.33
50	40	212	DD6	C13-C11-C10	-8.57	105.79	118.94
37	32	204	CLA	C1D-ND-C4D	-8.57	100.25	106.33
37	12	203	CLA	C1D-ND-C4D	-8.57	100.25	106.33
37	15	307	CLA	C1D-ND-C4D	-8.57	100.25	106.33
48	13	313	A86	C33-C32-C31	8.56	117.53	109.21
48	14	313	A86	O1-C20-C21	-8.56	104.80	115.06
37	40	210	CLA	C1D-ND-C4D	-8.56	100.26	106.33
37	38	209	CLA	C2D-C1D-ND	8.56	116.41	110.10
47	17	303	KC1	CMA-C3A-C4A	-8.56	112.01	125.04
47	34	309	KC1	C2B-C1B-NB	8.55	116.41	110.10
37	11	305	CLA	C1D-ND-C4D	-8.55	100.26	106.33
37	39	305	CLA	C2D-C1D-ND	8.55	116.40	110.10
37	b	514	CLA	C1D-ND-C4D	-8.55	100.26	106.33
37	c	511	CLA	C1D-ND-C4D	-8.55	100.26	106.33
37	15	301	CLA	C2D-C1D-ND	8.54	116.40	110.10
37	a	403	CLA	C1D-ND-C4D	-8.54	100.27	106.33
37	18	208	CLA	C1D-ND-C4D	-8.54	100.27	106.33
48	35	312	A86	C17-C16-C15	8.54	117.87	109.16
37	Z	101	CLA	C1D-ND-C4D	-8.53	100.27	106.33
47	14	309	KC1	C2B-C1B-NB	8.53	116.39	110.10
37	C	511	CLA	C1D-ND-C4D	-8.53	100.28	106.33
48	34	313	A86	O1-C20-C21	-8.53	104.84	115.06
37	c	502	CLA	C1D-ND-C4D	-8.53	100.28	106.33
48	15	312	A86	C17-C16-C15	8.52	117.86	109.16
37	19	305	CLA	C2D-C1D-ND	8.52	116.38	110.10
48	12	213	A86	C33-C32-C31	8.52	117.49	109.21
37	32	206	CLA	C1D-ND-C4D	-8.52	100.28	106.33
37	b	509	CLA	C1D-ND-C4D	-8.52	100.29	106.33
48	35	316	A86	O1-C20-C21	-8.51	104.86	115.06
37	35	301	CLA	C2D-C1D-ND	8.51	116.38	110.10
48	37	310	A86	C17-C16-C15	8.51	117.85	109.16
37	C	513	CLA	C2D-C1D-ND	8.51	116.38	110.10
47	41	203	KC1	C2B-C1B-NB	8.51	116.38	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	A	403	CLA	C1D-ND-C4D	-8.51	100.29	106.33
37	B	509	CLA	C1D-ND-C4D	-8.51	100.29	106.33
37	35	307	CLA	C1D-ND-C4D	-8.50	100.30	106.33
48	16	314	A86	C4-C5-C6	-8.49	115.19	127.31
37	31	302	CLA	C2D-C1D-ND	8.49	116.36	110.10
37	20	303	CLA	C1D-ND-C4D	-8.49	100.31	106.33
37	c	509	CLA	C1D-ND-C4D	-8.48	100.31	106.33
37	c	513	CLA	C2D-C1D-ND	8.48	116.35	110.10
47	21	203	KC1	C2B-C1B-NB	8.48	116.35	110.10
37	z	101	CLA	C1D-ND-C4D	-8.48	100.31	106.33
48	36	313	A86	C4-C5-C6	-8.48	115.21	127.31
37	C	502	CLA	C1D-ND-C4D	-8.48	100.31	106.33
37	40	205	CLA	C1D-ND-C4D	-8.48	100.31	106.33
48	15	316	A86	O1-C20-C21	-8.47	104.91	115.06
37	b	506	CLA	C2D-C1D-ND	8.47	116.34	110.10
48	32	214	A86	C33-C32-C31	8.47	117.44	109.21
37	B	506	CLA	C2D-C1D-ND	8.46	116.34	110.10
47	20	302	KC1	C2B-C1B-NB	8.46	116.34	110.10
37	B	501	CLA	C1D-ND-C4D	-8.46	100.32	106.33
37	C	509	CLA	C1D-ND-C4D	-8.46	100.32	106.33
37	C	512	CLA	C2D-C1D-ND	8.46	116.34	110.10
47	11	309	KC1	C2B-C1B-NB	8.46	116.34	110.10
37	11	301	CLA	C2D-C1D-ND	8.45	116.33	110.10
47	40	204	KC1	C2B-C1B-NB	8.44	116.33	110.10
37	b	501	CLA	C1D-ND-C4D	-8.44	100.34	106.33
37	12	205	CLA	C1D-ND-C4D	-8.44	100.34	106.33
47	33	302	KC1	C2B-C1B-NB	8.42	116.31	110.10
48	17	310	A86	C33-C32-C31	8.42	117.39	109.21
47	31	309	KC1	C2B-C1B-NB	8.42	116.31	110.10
37	11	307	CLA	C2D-C1D-ND	8.40	116.29	110.10
47	13	302	KC1	C2B-C1B-NB	8.40	116.29	110.10
37	z	102	CLA	C1D-ND-C4D	-8.39	100.37	106.33
48	37	314	A86	O1-C20-C21	-8.39	105.00	115.06
48	38	215	A86	O1-C20-C21	-8.39	105.00	115.06
37	B	507	CLA	C1D-ND-C4D	-8.39	100.37	106.33
37	18	201	CLA	C2D-C1D-ND	8.39	116.29	110.10
48	37	309	A86	C33-C32-C31	8.39	117.36	109.21
48	17	315	A86	O1-C20-C21	-8.39	105.01	115.06
37	33	303	CLA	C1D-ND-C4D	-8.39	100.38	106.33
37	B	503	CLA	C1D-ND-C4D	-8.38	100.38	106.33
37	c	508	CLA	C2D-C1D-ND	8.38	116.28	110.10
37	38	203	CLA	C1D-ND-C4D	-8.38	100.38	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	16	312	DD6	C-C1-C2	-8.37	111.19	122.92
48	33	314	A86	C17-C16-C15	8.37	117.70	109.16
37	39	310	CLA	C1D-ND-C4D	-8.37	100.39	106.33
47	12	211	KC1	C2B-C1B-NB	8.37	116.27	110.10
37	34	302	CLA	C1D-ND-C4D	-8.36	100.39	106.33
37	c	512	CLA	C2D-C1D-ND	8.36	116.27	110.10
37	19	310	CLA	C1D-ND-C4D	-8.35	100.40	106.33
48	34	311	A86	C33-C32-C31	8.35	117.33	109.21
37	W	101	CLA	C2D-C1D-ND	8.35	116.26	110.10
37	C	508	CLA	C2D-C1D-ND	8.35	116.26	110.10
37	C	510	CLA	C1D-ND-C4D	-8.35	100.40	106.33
50	36	312	DD6	C-C1-C2	-8.35	111.23	122.92
48	18	215	A86	C4-C5-C6	-8.35	115.40	127.31
37	31	308	CLA	C2D-C1D-ND	8.34	116.25	110.10
47	32	212	KC1	C2B-C1B-NB	8.34	116.25	110.10
37	b	507	CLA	C1D-ND-C4D	-8.33	100.42	106.33
47	21	207	KC1	C2B-C1B-NB	8.33	116.24	110.10
37	Z	102	CLA	C1D-ND-C4D	-8.33	100.42	106.33
47	17	308	KC1	C2B-C1B-NB	8.33	116.24	110.10
48	14	311	A86	C33-C32-C31	8.33	117.31	109.21
37	14	302	CLA	C1D-ND-C4D	-8.33	100.42	106.33
37	36	306	CLA	C1D-ND-C4D	-8.33	100.42	106.33
37	b	503	CLA	C1D-ND-C4D	-8.32	100.42	106.33
50	40	214	DD6	C-C1-C2	-8.32	111.27	122.92
47	41	207	KC1	C2B-C1B-NB	8.32	116.24	110.10
37	11	303	CLA	C1D-ND-C4D	-8.31	100.43	106.33
50	20	312	DD6	C-C1-C2	-8.31	111.28	122.92
37	c	510	CLA	C1D-ND-C4D	-8.31	100.43	106.33
47	18	210	KC1	CMA-C3A-C4A	-8.30	112.40	125.04
48	16	313	A86	C4-C5-C6	-8.30	115.47	127.31
48	15	319	A86	C21-C20-C19	-8.30	104.95	114.28
48	11	313	A86	C21-C20-C19	-8.29	104.95	114.28
37	16	306	CLA	C1D-ND-C4D	-8.29	100.45	106.33
48	35	319	A86	C21-C20-C19	-8.29	104.95	114.28
37	c	510	CLA	CMD-C2D-C1D	8.28	139.31	124.71
37	C	510	CLA	CMD-C2D-C1D	8.28	139.31	124.71
48	38	215	A86	C4-C5-C6	-8.28	115.49	127.31
48	31	313	A86	C21-C20-C19	-8.28	104.97	114.28
37	18	203	CLA	C1D-ND-C4D	-8.28	100.45	106.33
47	37	307	KC1	C2B-C1B-NB	8.28	116.20	110.10
50	16	312	DD6	C8-C6-C5	-8.27	106.25	118.94
50	21	212	DD6	C3-C2-C1	-8.26	115.52	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	36	312	DD6	C8-C6-C5	-8.26	106.27	118.94
48	40	201	A86	C4-C5-C6	-8.25	115.53	127.31
37	13	303	CLA	C1D-ND-C4D	-8.25	100.47	106.33
37	36	309	CLA	C2D-C1D-ND	8.25	116.19	110.10
37	31	310	CLA	C2D-C1D-ND	8.25	116.19	110.10
47	38	210	KC1	CMA-C3A-C4A	-8.25	112.48	125.04
37	16	309	CLA	C2D-C1D-ND	8.25	116.18	110.10
37	c	506	CLA	C1D-ND-C4D	-8.24	100.48	106.33
37	31	304	CLA	C1D-ND-C4D	-8.24	100.48	106.33
37	w	101	CLA	C2D-C1D-ND	8.24	116.18	110.10
48	18	213	A86	C4-C5-C6	-8.23	115.56	127.31
37	c	504	CLA	C2D-C1D-ND	8.23	116.17	110.10
37	B	524	CLA	C1D-ND-C4D	-8.23	100.49	106.33
48	17	311	A86	C17-C16-C15	8.23	117.56	109.16
47	11	302	KC1	C2B-C1B-NB	8.23	116.17	110.10
50	41	212	DD6	C3-C2-C1	-8.23	115.57	127.31
37	21	206	CLA	C2D-C1D-ND	8.23	116.17	110.10
48	36	313	A86	O1-C20-C21	-8.22	105.20	115.06
48	37	311	A86	O1-C20-C21	-8.22	105.21	115.06
37	C	504	CLA	C2D-C1D-ND	8.22	116.16	110.10
37	11	310	CLA	C2D-C1D-ND	8.22	116.16	110.10
47	31	303	KC1	C2B-C1B-NB	8.22	116.16	110.10
37	36	307	CLA	C2D-C1D-ND	8.21	116.15	110.10
37	32	210	CLA	C1D-ND-C4D	-8.21	100.51	106.33
48	12	214	A86	C17-C16-C15	8.20	117.53	109.16
37	21	210	CLA	C2D-C1D-ND	8.20	116.15	110.10
37	41	210	CLA	C2D-C1D-ND	8.20	116.15	110.10
37	41	206	CLA	C2D-C1D-ND	8.19	116.14	110.10
37	b	523	CLA	C1D-ND-C4D	-8.19	100.52	106.33
48	32	215	A86	C17-C16-C15	8.19	117.52	109.16
48	17	312	A86	O1-C20-C21	-8.18	105.25	115.06
37	C	506	CLA	C1D-ND-C4D	-8.18	100.53	106.33
37	12	209	CLA	C1D-ND-C4D	-8.17	100.53	106.33
37	21	205	CLA	C2D-C1D-ND	8.17	116.12	110.10
37	D	406	CLA	C2D-C1D-ND	8.16	116.12	110.10
37	a	404	CLA	C2D-C1D-ND	8.16	116.11	110.10
37	b	505	CLA	C2D-C1D-ND	8.15	116.11	110.10
48	16	314	A86	O1-C20-C21	-8.15	105.29	115.06
37	D	401	CLA	C2D-C1D-ND	8.15	116.11	110.10
37	41	205	CLA	C2D-C1D-ND	8.15	116.11	110.10
50	19	312	DD6	C8-C6-C5	-8.14	106.45	118.94
50	39	312	DD6	C8-C6-C5	-8.14	106.45	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	A	405	CLA	C2D-C1D-ND	8.13	116.10	110.10
37	16	307	CLA	C2D-C1D-ND	8.13	116.10	110.10
37	d	404	CLA	C2D-C1D-ND	8.12	116.09	110.10
48	35	313	A86	C17-C16-C15	8.12	117.44	109.16
37	20	303	CLA	C2D-C1D-ND	8.11	116.08	110.10
37	31	301	CLA	C1D-ND-C4D	-8.10	100.58	106.33
48	16	310	A86	C33-C32-C31	8.09	117.08	109.21
37	a	407	CLA	C2D-C1D-ND	8.09	116.07	110.10
37	B	516	CLA	C2D-C1D-ND	8.08	116.06	110.10
48	15	313	A86	C17-C16-C15	8.08	117.41	109.16
37	B	505	CLA	C2D-C1D-ND	8.08	116.06	110.10
37	B	509	CLA	C2D-C1D-ND	8.07	116.05	110.10
37	40	205	CLA	C2D-C1D-ND	8.07	116.05	110.10
37	b	516	CLA	C2D-C1D-ND	8.07	116.05	110.10
37	b	509	CLA	C2D-C1D-ND	8.06	116.04	110.10
48	36	310	A86	C33-C32-C31	8.06	117.04	109.21
48	31	312	A86	C3-C2-C1	-8.05	115.82	127.31
50	16	312	DD6	C32-C31-C36	-8.05	111.27	122.63
48	31	311	A86	C17-C16-C15	8.05	117.37	109.16
37	W	102	CLA	C1D-ND-C4D	-8.04	100.62	106.33
48	11	312	A86	C3-C2-C1	-8.04	115.83	127.31
48	39	313	A86	C4-C5-C6	-8.04	115.83	127.31
37	c	502	CLA	C2D-C1D-ND	8.04	116.03	110.10
50	36	312	DD6	C32-C31-C36	-8.03	111.29	122.63
37	c	507	CLA	C1D-ND-C4D	-8.03	100.63	106.33
37	C	502	CLA	C2D-C1D-ND	8.03	116.02	110.10
37	B	515	CLA	C2D-C1D-ND	8.03	116.02	110.10
48	11	311	A86	C17-C16-C15	8.03	117.35	109.16
48	14	312	A86	C33-C32-C31	8.01	117.00	109.21
37	b	515	CLA	C2D-C1D-ND	8.01	116.00	110.10
50	41	216	DD6	C-C1-C24	-7.99	105.49	118.08
37	C	503	CLA	C2D-C1D-ND	7.98	115.99	110.10
37	33	301	CLA	C2D-C1D-ND	7.98	115.99	110.10
37	c	503	CLA	C2D-C1D-ND	7.98	115.98	110.10
47	38	210	KC1	C2B-C1B-NB	7.98	115.98	110.10
37	13	301	CLA	C2D-C1D-ND	7.97	115.98	110.10
48	34	312	A86	C33-C32-C31	7.97	116.96	109.21
37	B	511	CLA	C2D-C1D-ND	7.97	115.98	110.10
37	40	203	CLA	C2D-C1D-ND	7.97	115.98	110.10
50	39	312	DD6	C-C1-C2	-7.96	111.77	122.92
37	b	511	CLA	C2D-C1D-ND	7.96	115.97	110.10
37	38	201	CLA	C2D-C1D-ND	7.96	115.97	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	19	312	DD6	C-C1-C2	-7.96	111.77	122.92
37	39	307	CLA	C2D-C1D-ND	7.96	115.97	110.10
50	21	216	DD6	C-C1-C24	-7.96	105.54	118.08
37	C	507	CLA	C1D-ND-C4D	-7.96	100.68	106.33
47	34	304	KC1	CMA-C3A-C2A	-7.93	108.89	128.30
47	18	210	KC1	C2B-C1B-NB	7.92	115.94	110.10
37	14	307	CLA	C1D-ND-C4D	-7.92	100.71	106.33
47	14	304	KC1	CMA-C3A-C2A	-7.92	108.90	128.30
37	15	308	CLA	C2D-C1D-ND	7.92	115.94	110.10
37	B	514	CLA	C2D-C1D-ND	7.91	115.93	110.10
37	20	301	CLA	C2D-C1D-ND	7.91	115.93	110.10
37	34	307	CLA	C1D-ND-C4D	-7.91	100.72	106.33
48	15	311	A86	C33-C32-C31	7.90	116.89	109.21
37	b	514	CLA	C2D-C1D-ND	7.90	115.93	110.10
48	41	215	A86	C17-C16-C15	7.90	117.22	109.16
47	35	309	KC1	C2B-C1B-NB	7.89	115.92	110.10
48	12	202	A86	O1-C20-C21	-7.89	105.60	115.06
37	B	508	CLA	C2D-C1D-ND	7.88	115.91	110.10
48	21	215	A86	C17-C16-C15	7.88	117.20	109.16
37	19	307	CLA	C2D-C1D-ND	7.88	115.91	110.10
37	b	510	CLA	C2D-C1D-ND	7.87	115.90	110.10
37	b	508	CLA	C2D-C1D-ND	7.87	115.90	110.10
37	41	208	CLA	C2D-C1D-ND	7.86	115.90	110.10
48	13	315	A86	O1-C20-C21	-7.86	105.63	115.06
47	15	309	KC1	C2B-C1B-NB	7.86	115.90	110.10
48	32	203	A86	O1-C20-C21	-7.86	105.64	115.06
48	32	218	A86	O1-C20-C21	-7.85	105.65	115.06
37	12	212	CLA	C2D-C1D-ND	7.84	115.88	110.10
48	33	315	A86	O1-C20-C21	-7.84	105.66	115.06
37	B	510	CLA	C2D-C1D-ND	7.84	115.88	110.10
37	33	305	CLA	C2D-C1D-ND	7.83	115.88	110.10
48	19	313	A86	C4-C5-C6	-7.83	116.14	127.31
37	32	208	CLA	C2D-C1D-ND	7.82	115.87	110.10
47	37	304	KC1	CMD-C2D-C1D	7.82	140.48	128.46
48	18	212	A86	C33-C32-C31	7.81	116.81	109.21
37	12	203	CLA	C2D-C1D-ND	7.81	115.86	110.10
37	14	303	CLA	CAA-C2A-C3A	-7.81	91.40	112.78
37	34	303	CLA	CAA-C2A-C3A	-7.81	91.40	112.78
37	12	207	CLA	C2D-C1D-ND	7.80	115.86	110.10
48	18	214	A86	C33-C32-C31	7.80	116.79	109.21
48	12	217	A86	O1-C20-C21	-7.80	105.71	115.06
37	32	213	CLA	C2D-C1D-ND	7.80	115.85	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	38	212	A86	C33-C32-C31	7.79	116.78	109.21
47	34	304	KC1	C2B-C1B-NB	7.79	115.84	110.10
47	33	309	KC1	C2B-C1B-NB	7.79	115.84	110.10
37	32	204	CLA	C2D-C1D-ND	7.79	115.84	110.10
48	38	214	A86	C33-C32-C31	7.78	116.78	109.21
37	35	308	CLA	C2D-C1D-ND	7.76	115.82	110.10
48	11	319	A86	C3-C2-C1	-7.76	116.23	127.31
37	34	302	CLA	C2D-C1D-ND	7.76	115.82	110.10
48	12	202	A86	C4-C5-C6	-7.75	116.25	127.31
37	21	208	CLA	C2D-C1D-ND	7.75	115.81	110.10
48	32	203	A86	C4-C5-C6	-7.75	116.25	127.31
37	13	305	CLA	C2D-C1D-ND	7.74	115.81	110.10
37	15	307	CLA	C2D-C1D-ND	7.74	115.81	110.10
37	11	308	CLA	C2D-C1D-ND	7.74	115.81	110.10
37	32	202	CLA	C2D-C1D-ND	7.74	115.81	110.10
47	13	309	KC1	C2B-C1B-NB	7.73	115.80	110.10
47	14	304	KC1	C2B-C1B-NB	7.73	115.80	110.10
48	31	319	A86	C3-C2-C1	-7.73	116.28	127.31
37	12	209	CLA	C2D-C1D-ND	7.73	115.80	110.10
47	16	308	KC1	C2B-C1B-NB	7.73	115.80	110.10
37	37	301	CLA	C2D-C1D-ND	7.72	115.80	110.10
37	35	307	CLA	C2D-C1D-ND	7.72	115.79	110.10
37	17	307	CLA	C2D-C1D-ND	7.71	115.78	110.10
37	32	210	CLA	C2D-C1D-ND	7.71	115.78	110.10
37	39	303	CLA	C2D-C1D-ND	7.70	115.78	110.10
47	36	308	KC1	C2B-C1B-NB	7.70	115.78	110.10
37	c	507	CLA	C2D-C1D-ND	7.70	115.78	110.10
37	40	210	CLA	C2D-C1D-ND	7.69	115.77	110.10
37	37	303	CLA	C2D-C1D-ND	7.68	115.77	110.10
37	C	511	CLA	C2D-C1D-ND	7.67	115.76	110.10
37	20	308	CLA	C2D-C1D-ND	7.67	115.76	110.10
37	15	305	CLA	C2D-C1D-ND	7.67	115.76	110.10
37	19	303	CLA	C2D-C1D-ND	7.67	115.76	110.10
37	14	302	CLA	C2D-C1D-ND	7.67	115.76	110.10
48	31	313	A86	C36-C31-C32	-7.67	112.09	119.70
37	31	306	CLA	C2D-C1D-ND	7.66	115.75	110.10
37	12	210	CLA	C2D-C1D-ND	7.65	115.74	110.10
37	39	302	CLA	C2D-C1D-ND	7.65	115.74	110.10
37	40	208	CLA	C2D-C1D-ND	7.65	115.74	110.10
37	38	206	CLA	C2D-C1D-ND	7.64	115.74	110.10
37	D	402	CLA	C2D-C1D-ND	7.64	115.73	110.10
37	20	306	CLA	C2D-C1D-ND	7.64	115.73	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	32	211	CLA	C2D-C1D-ND	7.63	115.73	110.10
47	20	305	KC1	C2B-C1B-NB	7.63	115.73	110.10
37	13	307	CLA	C1D-ND-C4D	-7.63	100.91	106.33
37	33	307	CLA	C1D-ND-C4D	-7.63	100.91	106.33
37	37	306	CLA	C2D-C1D-ND	7.63	115.73	110.10
47	15	306	KC1	C2B-C1B-NB	7.63	115.73	110.10
48	13	315	A86	C4-C5-C6	-7.61	116.44	127.31
37	12	204	CLA	C1D-ND-C4D	-7.61	100.93	106.33
37	14	308	CLA	C2D-C1D-ND	7.61	115.71	110.10
37	B	502	CLA	C2D-C1D-ND	7.61	115.71	110.10
48	33	315	A86	C4-C5-C6	-7.61	116.45	127.31
37	d	401	CLA	C2D-C1D-ND	7.61	115.71	110.10
47	36	304	KC1	C2B-C1B-NB	7.61	115.71	110.10
37	32	205	CLA	C1D-ND-C4D	-7.61	100.93	106.33
47	15	302	KC1	C2B-C1B-NB	7.60	115.71	110.10
37	17	304	CLA	C2D-C1D-ND	7.60	115.71	110.10
47	40	207	KC1	C2B-C1B-NB	7.60	115.71	110.10
37	C	507	CLA	C2D-C1D-ND	7.60	115.70	110.10
37	c	511	CLA	C2D-C1D-ND	7.59	115.70	110.10
37	33	310	CLA	C2D-C1D-ND	7.59	115.70	110.10
37	b	502	CLA	C2D-C1D-ND	7.59	115.70	110.10
37	C	501	CLA	C2D-C1D-ND	7.59	115.70	110.10
37	19	302	CLA	C2D-C1D-ND	7.59	115.70	110.10
37	14	303	CLA	C2D-C1D-ND	7.59	115.69	110.10
37	35	303	CLA	C2D-C1D-ND	7.59	115.69	110.10
37	c	501	CLA	C2D-C1D-ND	7.58	115.69	110.10
37	21	209	CLA	C2D-C1D-ND	7.58	115.69	110.10
37	18	211	CLA	C2D-C1D-ND	7.58	115.69	110.10
48	13	313	A86	C17-C16-C15	7.58	116.90	109.16
37	a	403	CLA	CMD-C2D-C1D	7.58	138.07	124.71
37	11	305	CLA	C2D-C1D-ND	7.57	115.68	110.10
37	A	403	CLA	CMD-C2D-C1D	7.56	138.04	124.71
37	40	209	CLA	C2D-C1D-ND	7.56	115.68	110.10
37	41	209	CLA	C2D-C1D-ND	7.56	115.68	110.10
48	33	313	A86	C17-C16-C15	7.56	116.88	109.16
37	20	307	CLA	C2D-C1D-ND	7.56	115.67	110.10
37	W	101	CLA	O2D-CGD-CBD	7.55	124.69	111.27
37	13	308	CLA	C2D-C1D-ND	7.55	115.67	110.10
37	33	308	CLA	C2D-C1D-ND	7.55	115.67	110.10
37	14	305	CLA	C2D-C1D-ND	7.55	115.67	110.10
37	34	305	CLA	C2D-C1D-ND	7.55	115.67	110.10
48	37	314	A86	C4-C5-C6	-7.55	116.54	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	15	303	CLA	C2D-C1D-ND	7.54	115.66	110.10
37	34	308	CLA	C2D-C1D-ND	7.54	115.66	110.10
47	16	304	KC1	C2B-C1B-NB	7.54	115.66	110.10
47	14	309	KC1	CHB-C4A-C3A	-7.54	113.20	124.98
37	c	506	CLA	C2D-C1D-ND	7.54	115.66	110.10
47	37	304	KC1	C2B-C1B-NB	7.54	115.66	110.10
48	34	313	A86	C33-C32-C31	7.53	116.53	109.21
48	17	311	A86	C33-C32-C31	7.53	116.53	109.21
48	17	315	A86	C4-C5-C6	-7.53	116.57	127.31
37	w	101	CLA	O2D-CGD-CBD	7.52	124.64	111.27
37	34	303	CLA	C2D-C1D-ND	7.52	115.65	110.10
37	35	305	CLA	C2D-C1D-ND	7.52	115.65	110.10
47	35	302	KC1	C2B-C1B-NB	7.52	115.65	110.10
47	17	308	KC1	CMA-C3A-C4A	-7.52	113.59	125.04
47	34	309	KC1	CHB-C4A-C3A	-7.51	113.25	124.98
47	37	307	KC1	CMA-C3A-C4A	-7.51	113.60	125.04
47	15	304	KC1	CMA-C3A-C2A	-7.51	109.92	128.30
48	14	313	A86	C33-C32-C31	7.51	116.51	109.21
48	37	310	A86	C33-C32-C31	7.51	116.51	109.21
37	B	501	CLA	C2D-C1D-ND	7.50	115.63	110.10
48	14	314	A86	C33-C32-C31	7.49	116.49	109.21
37	C	506	CLA	C2D-C1D-ND	7.49	115.62	110.10
37	B	512	CLA	C2D-C1D-ND	7.48	115.62	110.10
37	b	501	CLA	C2D-C1D-ND	7.47	115.61	110.10
37	B	507	CLA	C2D-C1D-ND	7.47	115.61	110.10
48	14	316	A86	O1-C20-C21	-7.47	106.11	115.06
48	34	314	A86	C33-C32-C31	7.46	116.47	109.21
47	15	304	KC1	C2B-C1B-NB	7.46	115.60	110.10
37	b	504	CLA	C1D-ND-C4D	-7.46	101.04	106.33
37	32	206	CLA	C2D-C1D-ND	7.45	115.60	110.10
37	40	205	CLA	CMD-C2D-C1D	7.45	137.84	124.71
37	b	507	CLA	C2D-C1D-ND	7.45	115.59	110.10
37	21	202	CLA	C2D-C1D-ND	7.45	115.59	110.10
37	20	303	CLA	CMD-C2D-C1D	7.44	137.82	124.71
48	34	316	A86	O1-C20-C21	-7.44	106.15	115.06
50	39	312	DD6	C13-C11-C10	-7.43	107.53	118.94
37	B	504	CLA	C1D-ND-C4D	-7.43	101.06	106.33
47	35	306	KC1	C2B-C1B-NB	7.43	115.58	110.10
48	11	312	A86	C33-C32-C31	7.43	116.43	109.21
37	12	205	CLA	C2D-C1D-ND	7.43	115.58	110.10
47	13	302	KC1	CHB-C4A-C3A	-7.42	113.39	124.98
50	19	312	DD6	C13-C11-C10	-7.42	107.56	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	35	304	KC1	CMA-C3A-C2A	-7.42	110.14	128.30
37	38	203	CLA	C2D-C1D-ND	7.41	115.57	110.10
37	b	512	CLA	C2D-C1D-ND	7.41	115.56	110.10
47	14	306	KC1	C2B-C1B-NB	7.41	115.56	110.10
48	16	313	A86	C17-C16-C15	7.41	116.72	109.16
47	33	302	KC1	CHB-C4A-C3A	-7.41	113.41	124.98
37	16	303	CLA	C2D-C1D-ND	7.40	115.56	110.10
47	34	306	KC1	C2B-C1B-NB	7.40	115.56	110.10
48	33	311	A86	C33-C32-C31	7.40	116.40	109.21
37	39	310	CLA	C2D-C1D-ND	7.40	115.56	110.10
48	21	213	A86	C33-C32-C31	7.39	116.40	109.21
48	31	312	A86	C33-C32-C31	7.39	116.39	109.21
48	41	213	A86	C33-C32-C31	7.39	116.39	109.21
37	15	310	CLA	C2D-C1D-ND	7.39	115.55	110.10
47	18	210	KC1	CHB-C4A-C3A	-7.38	113.45	124.98
48	40	201	A86	C17-C16-C15	7.38	116.69	109.16
37	35	310	CLA	C2D-C1D-ND	7.37	115.54	110.10
37	41	202	CLA	C2D-C1D-ND	7.36	115.53	110.10
48	13	311	A86	C33-C32-C31	7.35	116.36	109.21
47	16	308	KC1	CMA-C3A-C4A	-7.35	113.84	125.04
47	38	210	KC1	CHB-C4A-C3A	-7.35	113.50	124.98
47	20	302	KC1	C3A-C4A-NA	7.34	118.59	110.57
37	19	309	CLA	C2D-C1D-ND	7.34	115.51	110.10
37	b	505	CLA	CMD-C2D-C1D	7.34	137.65	124.71
37	11	303	CLA	C2D-C1D-ND	7.34	115.51	110.10
47	11	309	KC1	CHB-C4A-C3A	-7.34	113.52	124.98
47	33	302	KC1	C3A-C4A-NA	7.34	118.58	110.57
37	18	206	CLA	C2D-C1D-ND	7.33	115.50	110.10
47	36	308	KC1	CMA-C3A-C4A	-7.33	113.88	125.04
37	B	505	CLA	CMD-C2D-C1D	7.32	137.62	124.71
37	19	310	CLA	C2D-C1D-ND	7.32	115.50	110.10
47	18	205	KC1	C2B-C1B-NB	7.32	115.50	110.10
37	36	303	CLA	C2D-C1D-ND	7.32	115.50	110.10
47	15	309	KC1	CHB-C4A-C3A	-7.32	113.55	124.98
37	39	309	CLA	C2D-C1D-ND	7.31	115.49	110.10
37	41	204	CLA	C2D-C1D-ND	7.31	115.49	110.10
37	31	304	CLA	C2D-C1D-ND	7.31	115.49	110.10
47	35	309	KC1	CHB-C4A-C3A	-7.31	113.57	124.98
47	40	204	KC1	C3A-C4A-NA	7.30	118.55	110.57
47	31	309	KC1	CHB-C4A-C3A	-7.30	113.58	124.98
47	17	308	KC1	CHB-C4A-C3A	-7.29	113.58	124.98
47	32	212	KC1	CMA-C3A-C4A	-7.29	113.93	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	35	314	A86	C33-C32-C31	7.29	116.30	109.21
47	13	302	KC1	C3A-C4A-NA	7.29	118.53	110.57
37	21	204	CLA	C2D-C1D-ND	7.29	115.48	110.10
37	C	503	CLA	CMD-C2D-C1D	7.29	137.56	124.71
37	c	503	CLA	CMD-C2D-C1D	7.29	137.56	124.71
47	12	211	KC1	CMA-C3A-C4A	-7.29	113.94	125.04
47	35	304	KC1	C2B-C1B-NB	7.29	115.47	110.10
47	37	307	KC1	CHB-C4A-C3A	-7.29	113.60	124.98
48	31	313	A86	O1-C20-C21	-7.28	106.33	115.06
48	35	311	A86	C17-C16-C15	7.28	116.59	109.16
37	14	310	CLA	C2D-C1D-ND	7.27	115.46	110.10
48	36	311	A86	C3-C2-C1	-7.27	116.93	127.31
48	15	314	A86	C33-C32-C31	7.27	116.28	109.21
37	36	306	CLA	C2D-C1D-ND	7.27	115.46	110.10
48	15	311	A86	C17-C16-C15	7.26	116.57	109.16
37	D	402	CLA	CMD-C2D-C1D	7.26	137.50	124.71
37	34	310	CLA	C2D-C1D-ND	7.26	115.45	110.10
47	38	205	KC1	C2B-C1B-NB	7.26	115.45	110.10
47	36	302	KC1	C2B-C1B-NB	7.26	115.45	110.10
47	17	303	KC1	C2B-C1B-NB	7.25	115.45	110.10
37	37	308	CLA	C2D-C1D-ND	7.25	115.44	110.10
48	11	313	A86	O1-C20-C21	-7.25	106.37	115.06
37	13	310	CLA	C2D-C1D-ND	7.24	115.44	110.10
47	16	302	KC1	C2B-C1B-NB	7.24	115.44	110.10
48	40	211	A86	C33-C32-C31	7.24	116.25	109.21
48	16	311	A86	C3-C2-C1	-7.24	116.97	127.31
37	18	203	CLA	C2D-C1D-ND	7.24	115.44	110.10
37	d	401	CLA	CMD-C2D-C1D	7.24	137.47	124.71
37	C	505	CLA	C2D-C1D-ND	7.24	115.44	110.10
37	C	509	CLA	C2D-C1D-ND	7.23	115.44	110.10
47	37	302	KC1	C2B-C1B-NB	7.23	115.43	110.10
47	11	306	KC1	C2B-C1B-NB	7.23	115.43	110.10
37	c	509	CLA	C2D-C1D-ND	7.22	115.42	110.10
48	21	211	A86	C33-C32-C31	7.22	116.22	109.21
48	20	309	A86	C33-C32-C31	7.21	116.22	109.21
37	c	505	CLA	C2D-C1D-ND	7.20	115.41	110.10
47	20	302	KC1	CHB-C4A-C3A	-7.20	113.73	124.98
47	16	305	KC1	C2B-C1B-NB	7.20	115.41	110.10
47	36	305	KC1	C2B-C1B-NB	7.20	115.41	110.10
47	14	309	KC1	C3A-C4A-NA	7.19	118.42	110.57
37	Z	101	CLA	C2D-C1D-ND	7.19	115.40	110.10
47	40	204	KC1	CHB-C4A-C3A	-7.18	113.76	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	40	203	CLA	CMD-C2D-C1D	7.18	137.37	124.71
37	16	306	CLA	C2D-C1D-ND	7.18	115.40	110.10
47	34	309	KC1	C3A-C4A-NA	7.18	118.41	110.57
48	31	311	A86	C33-C32-C31	7.18	116.19	109.21
48	11	311	A86	C33-C32-C31	7.17	116.18	109.21
47	19	308	KC1	C1A-C2A-C3A	-7.17	101.42	107.11
37	20	301	CLA	CMD-C2D-C1D	7.17	137.34	124.71
47	19	308	KC1	CMA-C3A-C2A	-7.17	110.76	128.30
48	41	211	A86	C33-C32-C31	7.16	116.17	109.21
37	z	101	CLA	C2D-C1D-ND	7.16	115.38	110.10
37	17	309	CLA	C2D-C1D-ND	7.16	115.38	110.10
47	39	308	KC1	CMA-C3A-C2A	-7.16	110.77	128.30
47	15	302	KC1	CHB-C4A-C3A	-7.15	113.81	124.98
37	38	211	CLA	C2D-C1D-ND	7.14	115.37	110.10
47	33	306	KC1	C2B-C1B-NB	7.14	115.37	110.10
47	39	308	KC1	C1A-C2A-C3A	-7.14	101.44	107.11
37	C	511	CLA	CMD-C2D-C1D	7.14	137.30	124.71
37	B	503	CLA	C2D-C1D-ND	7.14	115.36	110.10
47	13	306	KC1	C2B-C1B-NB	7.14	115.36	110.10
37	c	511	CLA	CMD-C2D-C1D	7.12	137.26	124.71
47	21	203	KC1	C3A-C4A-NA	7.12	118.34	110.57
37	b	503	CLA	C2D-C1D-ND	7.12	115.35	110.10
48	35	312	A86	C3-C2-C1	-7.11	117.16	127.31
50	20	310	DD6	C8-C6-C5	-7.11	108.02	118.94
47	41	203	KC1	C3A-C4A-NA	7.11	118.34	110.57
47	19	308	KC1	C2B-C1B-NB	7.11	115.34	110.10
47	31	307	KC1	C2B-C1B-NB	7.11	115.34	110.10
50	40	212	DD6	C8-C6-C5	-7.11	108.03	118.94
47	16	304	KC1	CMA-C3A-C2A	-7.11	110.90	128.30
37	38	208	CLA	C2D-C1D-ND	7.11	115.34	110.10
47	37	302	KC1	C1A-C2A-C3A	-7.10	101.48	107.11
47	36	304	KC1	CMA-C3A-C2A	-7.09	110.94	128.30
37	b	506	CLA	CMD-C2D-C1D	7.09	137.21	124.71
37	C	501	CLA	CMD-C2D-C1D	7.09	137.21	124.71
37	b	502	CLA	CMD-C2D-C1D	7.09	137.21	124.71
50	21	216	DD6	C13-C11-C10	-7.09	108.06	118.94
47	39	308	KC1	C2B-C1B-NB	7.08	115.32	110.10
50	36	312	DD6	C-C1-C24	-7.08	106.92	118.08
37	B	502	CLA	CMD-C2D-C1D	7.08	137.19	124.71
47	38	207	KC1	O2D-CGD-CBD	7.08	123.84	111.27
48	13	313	A86	C4-C5-C6	-7.08	117.21	127.31
50	41	216	DD6	C13-C11-C10	-7.07	108.09	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	506	CLA	CMD-C2D-C1D	7.07	137.17	124.71
37	c	501	CLA	CMD-C2D-C1D	7.07	137.17	124.71
47	38	207	KC1	C2B-C1B-NB	7.07	115.31	110.10
48	37	319	A86	C17-C16-C15	7.07	116.37	109.16
50	16	312	DD6	C-C1-C24	-7.07	106.94	118.08
47	17	303	KC1	C1A-C2A-C3A	-7.06	101.51	107.11
47	33	309	KC1	CHB-C4A-C3A	-7.06	113.94	124.98
47	33	304	KC1	CMA-C3A-C2A	-7.06	111.01	128.30
37	33	303	CLA	C2D-C1D-ND	7.06	115.31	110.10
47	12	211	KC1	CHB-C4A-C3A	-7.06	113.95	124.98
47	13	304	KC1	CMA-C3A-C2A	-7.06	111.02	128.30
48	33	313	A86	C4-C5-C6	-7.06	117.24	127.31
37	19	302	CLA	O2D-CGD-CBD	7.05	123.80	111.27
47	13	309	KC1	CHB-C4A-C3A	-7.05	113.97	124.98
47	16	302	KC1	CHB-C4A-C3A	-7.05	113.97	124.98
47	12	208	KC1	C3A-C4A-NA	7.05	118.26	110.57
37	14	307	CLA	C2D-C1D-ND	7.04	115.30	110.10
37	Z	101	CLA	CMD-C2D-C1D	7.04	137.12	124.71
37	C	505	CLA	O2D-CGD-CBD	7.04	123.77	111.27
47	20	302	KC1	CMA-C3A-C2A	-7.04	111.08	128.30
47	40	204	KC1	CMA-C3A-C2A	-7.03	111.08	128.30
47	32	212	KC1	CHB-C4A-C3A	-7.03	113.99	124.98
37	14	310	CLA	CMD-C2D-C1D	7.03	137.10	124.71
48	33	311	A86	C17-C16-C15	7.03	116.33	109.16
37	c	505	CLA	O2D-CGD-CBD	7.03	123.76	111.27
47	40	207	KC1	O2D-CGD-CBD	7.03	123.76	111.27
37	z	101	CLA	CMD-C2D-C1D	7.03	137.10	124.71
37	34	310	CLA	CMD-C2D-C1D	7.03	137.10	124.71
37	18	208	CLA	C2D-C1D-ND	7.02	115.28	110.10
47	20	305	KC1	O2D-CGD-CBD	7.02	123.75	111.27
47	36	302	KC1	CHB-C4A-C3A	-7.02	114.01	124.98
47	21	207	KC1	CHB-C4A-C3A	-7.02	114.02	124.98
47	32	209	KC1	C3A-C4A-NA	7.02	118.23	110.57
37	39	302	CLA	O2D-CGD-CBD	7.01	123.73	111.27
50	20	312	DD6	C13-C11-C10	-7.00	108.20	118.94
48	19	313	A86	C17-C16-C15	7.00	116.31	109.16
47	32	209	KC1	C2B-C1B-NB	7.00	115.26	110.10
47	41	207	KC1	CHB-C4A-C3A	-7.00	114.05	124.98
37	b	507	CLA	CMD-C2D-C1D	7.00	137.04	124.71
37	17	302	CLA	C2D-C1D-ND	7.00	115.26	110.10
47	18	207	KC1	O2D-CGD-CBD	7.00	123.70	111.27
37	33	301	CLA	CMD-C2D-C1D	6.99	137.04	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	13	301	CLA	CMD-C2D-C1D	6.99	137.04	124.71
48	13	311	A86	C17-C16-C15	6.99	116.30	109.16
37	z	102	CLA	C2D-C1D-ND	6.99	115.25	110.10
37	34	307	CLA	C2D-C1D-ND	6.99	115.25	110.10
47	12	208	KC1	C2B-C1B-NB	6.99	115.25	110.10
37	Z	102	CLA	C2D-C1D-ND	6.98	115.25	110.10
50	40	214	DD6	C13-C11-C10	-6.98	108.22	118.94
48	15	312	A86	C3-C2-C1	-6.98	117.35	127.31
47	32	207	KC1	C3C-C4C-NC	6.97	116.44	109.88
37	B	507	CLA	CMD-C2D-C1D	6.97	137.00	124.71
48	11	311	A86	O1-C20-C21	-6.97	106.70	115.06
47	18	210	KC1	C3A-C4A-NA	6.97	118.18	110.57
47	15	302	KC1	C3A-C4A-NA	6.97	118.18	110.57
47	32	209	KC1	CHB-C4A-C3A	-6.97	114.10	124.98
47	35	302	KC1	CHB-C4A-C3A	-6.96	114.10	124.98
47	11	304	KC1	C2B-C1B-NB	6.96	115.23	110.10
47	20	304	KC1	CMA-C3A-C4A	-6.96	114.44	125.04
37	b	503	CLA	O2D-CGD-CBD	6.96	123.63	111.27
48	11	313	A86	C36-C31-C32	-6.96	112.79	119.70
47	12	206	KC1	C3C-C4C-NC	6.96	116.43	109.88
37	C	504	CLA	CMD-C2D-C1D	6.95	136.97	124.71
37	37	301	CLA	CMD-C2D-C1D	6.95	136.97	124.71
47	12	208	KC1	CHB-C4A-C3A	-6.95	114.12	124.98
37	39	304	CLA	CMD-C2D-C1D	6.95	136.96	124.71
37	B	503	CLA	O2D-CGD-CBD	6.95	123.61	111.27
37	33	305	CLA	CMD-C2D-C1D	6.94	136.95	124.71
48	11	314	A86	C40-C32-C31	-6.94	104.26	110.47
48	31	311	A86	O1-C20-C21	-6.94	106.74	115.06
37	B	511	CLA	CMD-C2D-C1D	6.94	136.94	124.71
47	31	305	KC1	C3A-C4A-NA	6.94	118.14	110.57
37	41	208	CLA	CMD-C2D-C1D	6.93	136.94	124.71
47	21	207	KC1	CMA-C3A-C2A	-6.93	111.33	128.30
47	33	302	KC1	C3B-C2B-C1B	-6.93	100.46	107.08
47	41	207	KC1	CMA-C3A-C2A	-6.93	111.33	128.30
47	16	302	KC1	CMA-C3A-C4A	-6.93	114.48	125.04
37	13	305	CLA	CMD-C2D-C1D	6.93	136.93	124.71
37	c	504	CLA	CMD-C2D-C1D	6.93	136.92	124.71
47	40	206	KC1	CMA-C3A-C4A	-6.93	114.49	125.04
37	41	206	CLA	CMD-C2D-C1D	6.93	136.92	124.71
37	21	206	CLA	CMD-C2D-C1D	6.93	136.92	124.71
47	31	305	KC1	C2B-C1B-NB	6.92	115.21	110.10
37	18	201	CLA	CMD-C2D-C1D	6.92	136.91	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	308	CLA	CMD-C2D-C1D	6.92	136.91	124.71
37	19	304	CLA	CMD-C2D-C1D	6.92	136.91	124.71
47	36	302	KC1	CMA-C3A-C4A	-6.92	114.50	125.04
48	35	314	A86	C25-C26-C27	-6.92	117.44	127.31
47	11	304	KC1	C3A-C4A-NA	6.91	118.12	110.57
37	31	301	CLA	C2D-C1D-ND	6.91	115.20	110.10
47	38	210	KC1	C3A-C4A-NA	6.91	118.12	110.57
47	13	304	KC1	CHB-C4A-C3A	-6.91	114.18	124.98
37	C	509	CLA	CMD-C2D-C1D	6.91	136.89	124.71
37	21	209	CLA	CMD-C2D-C1D	6.91	136.89	124.71
37	W	101	CLA	CMD-C2D-C1D	6.91	136.88	124.71
47	33	306	KC1	C1A-C2A-C3A	-6.90	101.63	107.11
47	15	309	KC1	C3A-C4A-NA	6.90	118.11	110.57
47	33	304	KC1	CHB-C4A-C3A	-6.90	114.20	124.98
50	20	312	DD6	C-C1-C24	-6.90	107.20	118.08
37	21	208	CLA	CMD-C2D-C1D	6.90	136.88	124.71
37	b	511	CLA	CMD-C2D-C1D	6.90	136.88	124.71
47	31	303	KC1	CHB-C4A-C3A	-6.90	114.20	124.98
47	17	305	KC1	C2B-C1B-NB	6.90	115.19	110.10
47	13	304	KC1	C3A-C4A-NA	6.90	118.10	110.57
37	12	204	CLA	C2D-C1D-ND	6.90	115.19	110.10
47	20	305	KC1	CHB-C4A-C3A	-6.90	114.20	124.98
37	w	101	CLA	CMD-C2D-C1D	6.89	136.86	124.71
37	C	506	CLA	C2C-C1C-NC	6.89	116.43	109.97
37	34	308	CLA	CMD-C2D-C1D	6.89	136.86	124.71
37	c	509	CLA	CMD-C2D-C1D	6.89	136.85	124.71
37	41	209	CLA	CMD-C2D-C1D	6.89	136.85	124.71
48	15	314	A86	C25-C26-C27	-6.89	117.48	127.31
47	12	206	KC1	CMA-C3A-C4A	-6.89	114.55	125.04
50	40	214	DD6	C-C1-C24	-6.89	107.23	118.08
47	35	309	KC1	C3A-C4A-NA	6.88	118.09	110.57
47	32	207	KC1	CMA-C3A-C4A	-6.88	114.56	125.04
47	37	307	KC1	C3A-C4A-NA	6.88	118.09	110.57
47	33	304	KC1	C3A-C4A-NA	6.88	118.08	110.57
37	38	201	CLA	CMD-C2D-C1D	6.88	136.84	124.71
47	11	302	KC1	CHB-C4A-C3A	-6.88	114.23	124.98
47	38	207	KC1	CHB-C4A-C3A	-6.88	114.23	124.98
47	37	304	KC1	C1A-C2A-C3A	-6.88	101.66	107.11
47	13	306	KC1	C1A-C2A-C3A	-6.87	101.66	107.11
37	c	506	CLA	C2C-C1C-NC	6.87	116.41	109.97
37	W	102	CLA	C2D-C1D-ND	6.87	115.16	110.10
47	33	309	KC1	C3A-C4A-NA	6.86	118.06	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	17	308	KC1	C3A-C4A-NA	6.86	118.06	110.57
37	13	303	CLA	C2D-C1D-ND	6.86	115.16	110.10
47	40	207	KC1	CHB-C4A-C3A	-6.85	114.27	124.98
47	14	304	KC1	CHB-C4A-C3A	-6.85	114.27	124.98
47	34	304	KC1	C3A-C4A-NA	6.85	118.05	110.57
37	B	506	CLA	CHD-C1D-ND	-6.85	118.16	124.45
37	32	205	CLA	C2D-C1D-ND	6.85	115.15	110.10
37	b	506	CLA	CHD-C1D-ND	-6.85	118.16	124.45
48	31	314	A86	C40-C32-C31	-6.85	104.34	110.47
37	18	202	CLA	CMD-C2D-C1D	6.85	136.78	124.71
47	36	308	KC1	CHB-C4A-C3A	-6.84	114.29	124.98
47	38	205	KC1	CHB-C4A-C3A	-6.84	114.29	124.98
50	40	214	DD6	C8-C6-C5	-6.84	108.44	118.94
47	16	304	KC1	CHB-C4A-C3A	-6.84	114.29	124.98
48	41	214	A86	C33-C32-C31	6.84	115.86	109.21
47	36	304	KC1	CHB-C4A-C3A	-6.84	114.30	124.98
50	20	312	DD6	C8-C6-C5	-6.84	108.45	118.94
48	21	214	A86	C33-C32-C31	6.84	115.86	109.21
47	16	308	KC1	CHB-C4A-C3A	-6.83	114.30	124.98
37	21	202	CLA	CMD-C2D-C1D	6.83	136.75	124.71
47	34	304	KC1	CHB-C4A-C3A	-6.83	114.31	124.98
47	17	303	KC1	CHB-C4A-C3A	-6.83	114.31	124.98
47	13	309	KC1	C3A-C4A-NA	6.83	118.03	110.57
47	15	306	KC1	CHB-C4A-C3A	-6.83	114.31	124.98
47	18	205	KC1	CHB-C4A-C3A	-6.83	114.31	124.98
37	b	523	CLA	C2D-C1D-ND	6.83	115.14	110.10
37	b	513	CLA	CMD-C2D-C1D	6.83	136.74	124.71
37	40	203	CLA	CHD-C1D-ND	-6.83	118.18	124.45
37	B	524	CLA	C2D-C1D-ND	6.83	115.13	110.10
47	37	304	KC1	CHB-C4A-C3A	-6.82	114.32	124.98
47	17	305	KC1	CHB-C4A-C3A	-6.82	114.32	124.98
47	14	309	KC1	CMA-C3A-C4A	-6.82	114.65	125.04
47	34	309	KC1	CMA-C3A-C4A	-6.82	114.65	125.04
37	38	203	CLA	CMD-C2D-C1D	6.82	136.73	124.71
47	13	302	KC1	C3B-C2B-C1B	-6.82	100.57	107.08
37	z	102	CLA	CMD-C2D-C1D	6.82	136.72	124.71
37	41	202	CLA	CMD-C2D-C1D	6.82	136.72	124.71
37	20	301	CLA	CHD-C1D-ND	-6.81	118.20	124.45
37	B	513	CLA	CMD-C2D-C1D	6.81	136.71	124.71
47	14	304	KC1	C3A-C4A-NA	6.81	118.00	110.57
37	Z	102	CLA	CMD-C2D-C1D	6.80	136.70	124.71
47	17	306	KC1	CHB-C4A-C3A	-6.80	114.35	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	11	309	KC1	C3A-C4A-NA	6.79	117.99	110.57
48	13	312	A86	C17-C16-C15	6.79	116.09	109.16
47	35	302	KC1	C3A-C4A-NA	6.78	117.98	110.57
48	13	312	A86	C3-C2-C1	-6.78	117.64	127.31
47	37	302	KC1	CHB-C4A-C3A	-6.78	114.39	124.98
47	37	305	KC1	CHB-C4A-C3A	-6.77	114.40	124.98
37	16	303	CLA	CMD-C2D-C1D	6.77	136.64	124.71
48	38	215	A86	C33-C32-C31	6.76	115.78	109.21
37	18	203	CLA	CMD-C2D-C1D	6.76	136.63	124.71
37	37	308	CLA	CMD-C2D-C1D	6.76	136.62	124.71
47	17	305	KC1	C1A-C2A-C3A	-6.76	101.75	107.11
47	31	309	KC1	C3A-C4A-NA	6.75	117.94	110.57
47	11	304	KC1	CHB-C4A-C3A	-6.75	114.43	124.98
50	21	216	DD6	C8-C6-C5	-6.75	108.58	118.94
47	33	304	KC1	C2B-C1B-NB	6.75	115.08	110.10
37	40	209	CLA	CMD-C2D-C1D	6.75	136.61	124.71
47	18	205	KC1	C3A-C4A-NA	6.75	117.94	110.57
37	41	204	CLA	CMD-C2D-C1D	6.75	136.60	124.71
37	38	202	CLA	CMD-C2D-C1D	6.75	136.60	124.71
48	18	215	A86	C33-C32-C31	6.75	115.77	109.21
47	38	205	KC1	C3A-C4A-NA	6.74	117.93	110.57
47	34	306	KC1	CHB-C4A-C3A	-6.74	114.44	124.98
47	31	305	KC1	CHB-C4A-C3A	-6.74	114.45	124.98
50	41	216	DD6	C8-C6-C5	-6.74	108.60	118.94
37	36	303	CLA	CMD-C2D-C1D	6.74	136.59	124.71
37	38	206	CLA	CMD-C2D-C1D	6.74	136.59	124.71
48	37	313	A86	C4-C5-C6	-6.74	117.69	127.31
37	21	204	CLA	CMD-C2D-C1D	6.74	136.59	124.71
47	32	207	KC1	C3A-C4A-NA	6.74	117.93	110.57
37	37	308	CLA	O2D-CGD-CBD	6.73	123.23	111.27
37	13	308	CLA	CMD-C2D-C1D	6.73	136.58	124.71
37	33	308	CLA	CMD-C2D-C1D	6.73	136.58	124.71
47	12	206	KC1	C3A-C4A-NA	6.73	117.92	110.57
37	39	309	CLA	CMD-C2D-C1D	6.73	136.57	124.71
37	c	513	CLA	CMD-C2D-C1D	6.73	136.57	124.71
37	20	307	CLA	CMD-C2D-C1D	6.73	136.57	124.71
47	14	306	KC1	CHB-C4A-C3A	-6.72	114.47	124.98
37	14	305	CLA	CMD-C2D-C1D	6.72	136.56	124.71
37	34	305	CLA	CMD-C2D-C1D	6.72	136.56	124.71
37	32	204	CLA	CMD-C2D-C1D	6.72	136.56	124.71
37	35	310	CLA	CMD-C2D-C1D	6.72	136.56	124.71
47	35	306	KC1	CHB-C4A-C3A	-6.72	114.48	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	513	CLA	CMD-C2D-C1D	6.72	136.56	124.71
48	33	312	A86	C17-C16-C15	6.72	116.02	109.16
47	21	207	KC1	C3A-C4A-NA	6.72	117.91	110.57
47	31	303	KC1	C3B-C2B-C1B	-6.72	100.66	107.08
37	18	206	CLA	CMD-C2D-C1D	6.72	136.55	124.71
37	35	303	CLA	CMD-C2D-C1D	6.72	136.55	124.71
47	12	211	KC1	C3A-C4A-NA	6.71	117.90	110.57
37	12	203	CLA	CMD-C2D-C1D	6.71	136.54	124.71
37	21	205	CLA	CMD-C2D-C1D	6.71	136.54	124.71
47	11	302	KC1	C3B-C2B-C1B	-6.71	100.67	107.08
48	13	312	A86	C33-C32-C31	6.71	115.73	109.21
47	20	305	KC1	C3A-C4A-NA	6.71	117.89	110.57
37	12	207	CLA	CMD-C2D-C1D	6.70	136.53	124.71
37	18	211	CLA	CMD-C2D-C1D	6.70	136.53	124.71
37	17	309	CLA	O2D-CGD-CBD	6.70	123.17	111.27
37	37	303	CLA	CMD-C2D-C1D	6.70	136.52	124.71
47	35	309	KC1	CMA-C3A-C4A	-6.70	114.84	125.04
47	12	206	KC1	CHB-C4A-C3A	-6.69	114.52	124.98
47	32	207	KC1	CHB-C4A-C3A	-6.69	114.52	124.98
37	41	205	CLA	CMD-C2D-C1D	6.69	136.51	124.71
37	32	208	CLA	CMD-C2D-C1D	6.69	136.51	124.71
37	18	204	CLA	C2D-C1D-ND	6.69	115.03	110.10
47	31	307	KC1	CHB-C4A-C3A	-6.69	114.53	124.98
37	17	309	CLA	CMD-C2D-C1D	6.69	136.50	124.71
47	41	207	KC1	C3A-C4A-NA	6.68	117.87	110.57
47	11	306	KC1	CHB-C4A-C3A	-6.68	114.54	124.98
47	32	212	KC1	C3A-C4A-NA	6.68	117.86	110.57
37	15	303	CLA	CMD-C2D-C1D	6.68	136.49	124.71
47	32	212	KC1	C1A-C2A-C3A	-6.68	101.81	107.11
48	33	312	A86	C3-C2-C1	-6.67	117.78	127.31
47	15	309	KC1	CMA-C3A-C4A	-6.67	114.88	125.04
37	17	304	CLA	CMD-C2D-C1D	6.67	136.47	124.71
47	37	304	KC1	C3A-C4A-NA	6.67	117.85	110.57
37	31	302	CLA	CMD-C2D-C1D	6.67	136.47	124.71
50	21	212	DD6	C8-C6-C5	-6.67	108.71	118.94
47	15	304	KC1	CHB-C4A-C3A	-6.66	114.57	124.98
50	41	212	DD6	C8-C6-C5	-6.66	108.72	118.94
37	a	404	CLA	CMD-C2D-C1D	6.66	136.46	124.71
47	16	305	KC1	CHB-C4A-C3A	-6.66	114.58	124.98
47	17	306	KC1	C2B-C1B-NB	6.66	115.01	110.10
47	15	306	KC1	C3A-C4A-NA	6.66	117.84	110.57
37	D	401	CLA	CMD-C2D-C1D	6.65	136.44	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	33	307	CLA	C2D-C1D-ND	6.65	115.00	110.10
47	35	302	KC1	C1A-C2A-C3A	-6.65	101.84	107.11
47	37	305	KC1	C2B-C1B-NB	6.65	115.00	110.10
47	17	303	KC1	C3A-C4A-NA	6.65	117.83	110.57
47	35	304	KC1	CHB-C4A-C3A	-6.65	114.60	124.98
47	38	207	KC1	C3A-C4A-NA	6.64	117.83	110.57
47	36	305	KC1	CHB-C4A-C3A	-6.64	114.60	124.98
37	13	307	CLA	C2D-C1D-ND	6.64	115.00	110.10
47	35	304	KC1	C3A-C4A-NA	6.64	117.82	110.57
37	11	301	CLA	CMD-C2D-C1D	6.63	136.40	124.71
47	36	304	KC1	C3A-C4A-NA	6.63	117.81	110.57
47	40	207	KC1	C3A-C4A-NA	6.63	117.81	110.57
37	38	211	CLA	CMD-C2D-C1D	6.63	136.40	124.71
37	D	406	CLA	CMD-C2D-C1D	6.63	136.39	124.71
48	31	313	A86	C4-C5-C6	-6.62	117.86	127.31
50	16	312	DD6	C12-C11-C13	-6.62	107.64	118.08
37	a	404	CLA	CHD-C1D-ND	-6.62	118.37	124.45
47	16	304	KC1	C3A-C4A-NA	6.62	117.80	110.57
48	33	312	A86	C33-C32-C31	6.62	115.64	109.21
47	20	305	KC1	C3C-C4C-NC	6.62	116.11	109.88
37	d	404	CLA	CMD-C2D-C1D	6.61	136.37	124.71
47	12	211	KC1	C1A-C2A-C3A	-6.61	101.86	107.11
47	17	306	KC1	O2D-CGD-CBD	6.61	123.02	111.27
47	11	306	KC1	C3A-C4A-NA	6.61	117.79	110.57
50	36	312	DD6	C12-C11-C13	-6.61	107.66	118.08
47	13	304	KC1	C2B-C1B-NB	6.61	114.97	110.10
47	18	207	KC1	CHB-C4A-C3A	-6.61	114.66	124.98
47	13	306	KC1	CHB-C4A-C3A	-6.61	114.66	124.98
47	40	206	KC1	CHB-C4A-C3A	-6.61	114.66	124.98
47	32	209	KC1	C1A-C2A-C3A	-6.60	101.87	107.11
47	41	203	KC1	C1A-C2A-C3A	-6.60	101.87	107.11
37	19	305	CLA	CHD-C1D-ND	-6.60	118.39	124.45
37	39	305	CLA	CMD-C2D-C1D	6.60	136.34	124.71
37	38	204	CLA	C2D-C1D-ND	6.60	114.97	110.10
37	B	512	CLA	CHD-C4C-C3C	-6.59	115.15	124.84
47	37	302	KC1	C3A-C4A-NA	6.59	117.77	110.57
47	21	203	KC1	CHB-C4A-C3A	-6.59	114.68	124.98
47	33	306	KC1	CHB-C4A-C3A	-6.59	114.68	124.98
47	40	207	KC1	C3C-C4C-NC	6.59	116.08	109.88
47	31	307	KC1	C3A-C4A-NA	6.59	117.77	110.57
47	41	203	KC1	CHB-C4A-C3A	-6.59	114.69	124.98
37	12	205	CLA	CMD-C2D-C1D	6.59	136.32	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	15	301	CLA	CMD-C2D-C1D	6.59	136.32	124.71
47	36	308	KC1	C3A-C4A-NA	6.59	117.76	110.57
37	D	401	CLA	CHD-C1D-ND	-6.58	118.41	124.45
47	36	302	KC1	C1A-C2A-C3A	-6.58	101.89	107.11
37	32	202	CLA	CMD-C2D-C1D	6.58	136.31	124.71
37	32	206	CLA	CMD-C2D-C1D	6.58	136.31	124.71
37	35	301	CLA	CMD-C2D-C1D	6.58	136.31	124.71
47	31	303	KC1	C3A-C4A-NA	6.58	117.75	110.57
37	11	308	CLA	CMD-C2D-C1D	6.58	136.30	124.71
37	15	305	CLA	CMD-C2D-C1D	6.58	136.30	124.71
47	20	304	KC1	CHB-C4A-C3A	-6.57	114.71	124.98
47	16	302	KC1	C3A-C4A-NA	6.57	117.74	110.57
37	a	403	CLA	C2D-C1D-ND	6.57	114.94	110.10
47	16	302	KC1	C1A-C2A-C3A	-6.56	101.90	107.11
47	37	305	KC1	O2D-CGD-CBD	6.56	122.93	111.27
37	19	304	CLA	CHD-C1D-ND	-6.56	118.42	124.45
47	36	305	KC1	C3A-C4A-NA	6.56	117.73	110.57
37	39	305	CLA	CHD-C1D-ND	-6.56	118.42	124.45
47	11	302	KC1	C3A-C4A-NA	6.56	117.73	110.57
37	b	512	CLA	CHD-C4C-C3C	-6.56	115.20	124.84
47	37	305	KC1	C1A-C2A-C3A	-6.56	101.91	107.11
47	32	207	KC1	C2B-C1B-NB	6.56	114.94	110.10
37	39	304	CLA	CHD-C1D-ND	-6.56	118.43	124.45
37	15	308	CLA	CMD-C2D-C1D	6.55	136.26	124.71
37	18	202	CLA	CHD-C1D-ND	-6.55	118.43	124.45
47	17	306	KC1	C1A-C2A-C3A	-6.55	101.91	107.11
37	33	303	CLA	CMD-C2D-C1D	6.55	136.26	124.71
47	12	208	KC1	C1A-C2A-C3A	-6.55	101.91	107.11
47	21	203	KC1	C1A-C2A-C3A	-6.55	101.91	107.11
50	39	312	DD6	C24-C1-C2	-6.55	108.89	118.94
47	35	306	KC1	C3A-C4A-NA	6.54	117.72	110.57
47	16	308	KC1	C1A-C2A-C3A	-6.54	101.92	107.11
37	37	303	CLA	CHD-C1D-ND	-6.54	118.44	124.45
37	32	213	CLA	O2D-CGD-CBD	6.54	122.89	111.27
47	36	308	KC1	C1A-C2A-C3A	-6.54	101.92	107.11
47	18	207	KC1	C3A-C4A-NA	6.53	117.71	110.57
47	17	305	KC1	CMD-C2D-C1D	6.53	138.50	128.46
37	35	305	CLA	CMD-C2D-C1D	6.53	136.22	124.71
47	15	304	KC1	C3A-C4A-NA	6.53	117.70	110.57
37	40	210	CLA	CMD-C2D-C1D	6.53	136.22	124.71
47	13	306	KC1	C3A-C4A-NA	6.53	117.70	110.57
47	15	302	KC1	C1A-C2A-C3A	-6.53	101.93	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	16	305	KC1	C1A-C2A-C3A	-6.53	101.93	107.11
47	35	304	KC1	C1A-C2A-C3A	-6.53	101.93	107.11
50	19	312	DD6	C24-C1-C2	-6.53	108.93	118.94
37	31	308	CLA	CHD-C4C-C3C	-6.52	115.25	124.84
47	16	308	KC1	C3A-C4A-NA	6.52	117.69	110.57
47	17	305	KC1	C3A-C4A-NA	6.52	117.69	110.57
37	13	310	CLA	CMD-C2D-C1D	6.52	136.21	124.71
47	36	302	KC1	C3A-C4A-NA	6.52	117.69	110.57
47	40	206	KC1	C3A-C4A-NA	6.52	117.69	110.57
37	B	501	CLA	CMD-C2D-C1D	6.51	136.19	124.71
47	20	304	KC1	C2B-C1B-NB	6.51	114.90	110.10
37	17	304	CLA	CHD-C1D-ND	-6.51	118.47	124.45
47	16	305	KC1	C3A-C4A-NA	6.51	117.68	110.57
37	C	505	CLA	CMD-C2D-C1D	6.51	136.19	124.71
37	11	307	CLA	CHD-C4C-C3C	-6.51	115.27	124.84
37	36	309	CLA	CMD-C2D-C1D	6.51	136.18	124.71
37	37	301	CLA	CHD-C1D-ND	-6.51	118.47	124.45
37	20	308	CLA	CMD-C2D-C1D	6.51	136.18	124.71
47	39	308	KC1	CHB-C4A-C3A	-6.50	114.82	124.98
37	b	501	CLA	CMD-C2D-C1D	6.50	136.18	124.71
37	31	302	CLA	CHD-C4C-C3C	-6.50	115.28	124.84
37	16	309	CLA	CMD-C2D-C1D	6.50	136.17	124.71
37	12	212	CLA	CMD-C2D-C1D	6.50	136.17	124.71
47	33	306	KC1	C3A-C4A-NA	6.49	117.66	110.57
37	A	403	CLA	C2D-C1D-ND	6.49	114.89	110.10
48	33	315	A86	C33-C32-C31	6.49	115.52	109.21
37	12	212	CLA	O2D-CGD-CBD	6.49	122.81	111.27
37	32	213	CLA	CMD-C2D-C1D	6.49	136.15	124.71
48	13	315	A86	C33-C32-C31	6.49	115.52	109.21
47	17	306	KC1	C3A-C4A-NA	6.49	117.66	110.57
37	19	305	CLA	CMD-C2D-C1D	6.49	136.15	124.71
37	c	505	CLA	CMD-C2D-C1D	6.49	136.15	124.71
47	19	308	KC1	CHB-C4A-C3A	-6.48	114.85	124.98
37	14	303	CLA	CMD-C2D-C1D	6.48	136.14	124.71
37	34	303	CLA	CMD-C2D-C1D	6.48	136.14	124.71
37	D	402	CLA	CHD-C1D-ND	-6.48	118.50	124.45
37	d	401	CLA	CHD-C1D-ND	-6.48	118.50	124.45
37	12	209	CLA	O2D-CGD-CBD	6.48	122.78	111.27
47	36	305	KC1	C1A-C2A-C3A	-6.48	101.97	107.11
37	34	301	CLA	CMD-C2D-C1D	6.47	136.12	124.71
47	12	206	KC1	C1A-C2A-C3A	-6.47	101.98	107.11
37	c	503	CLA	CHD-C1D-ND	-6.47	118.51	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	16	308	KC1	O2D-CGD-CBD	6.47	122.77	111.27
37	39	302	CLA	CMD-C2D-C1D	6.47	136.12	124.71
37	11	301	CLA	CHD-C4C-C3C	-6.47	115.33	124.84
47	12	206	KC1	C2B-C1B-NB	6.47	114.87	110.10
47	18	210	KC1	O2D-CGD-CBD	6.47	122.76	111.27
47	11	302	KC1	C1A-C2A-C3A	-6.46	101.98	107.11
37	C	503	CLA	CHD-C1D-ND	-6.46	118.52	124.45
48	12	220	A86	C17-C16-C15	6.46	115.75	109.16
47	40	206	KC1	C2B-C1B-NB	6.46	114.86	110.10
48	32	221	A86	C17-C16-C15	6.46	115.75	109.16
48	11	312	A86	C17-C16-C15	6.46	115.75	109.16
47	14	306	KC1	C1A-C2A-C3A	-6.46	101.99	107.11
47	36	308	KC1	O2D-CGD-CBD	6.45	122.74	111.27
47	19	308	KC1	C3A-C4A-NA	6.45	117.62	110.57
37	15	301	CLA	CHD-C1D-ND	-6.45	118.52	124.45
37	35	301	CLA	CHD-C1D-ND	-6.45	118.52	124.45
48	17	314	A86	C4-C5-C6	-6.45	118.10	127.31
47	32	207	KC1	C1A-C2A-C3A	-6.45	101.99	107.11
37	b	504	CLA	CMD-C2D-C1D	6.45	136.08	124.71
47	20	304	KC1	C3A-C4A-NA	6.45	117.61	110.57
47	11	306	KC1	C1A-C2A-C3A	-6.44	102.00	107.11
48	16	310	A86	C3-C2-C1	-6.44	118.12	127.31
48	15	314	A86	C3-C2-C1	-6.44	118.12	127.31
48	31	312	A86	C17-C16-C15	6.44	115.73	109.16
37	b	523	CLA	CHD-C4C-C3C	-6.44	115.38	124.84
37	c	506	CLA	CMD-C2D-C1D	6.43	136.05	124.71
37	14	301	CLA	CMD-C2D-C1D	6.43	136.05	124.71
48	15	313	A86	C33-C32-C31	6.43	115.47	109.21
47	34	306	KC1	C1A-C2A-C3A	-6.43	102.01	107.11
47	39	308	KC1	C3A-C4A-NA	6.43	117.59	110.57
37	C	506	CLA	CMD-C2D-C1D	6.43	136.04	124.71
47	37	305	KC1	C3A-C4A-NA	6.43	117.59	110.57
37	19	302	CLA	CMD-C2D-C1D	6.43	136.04	124.71
48	34	315	A86	C17-C16-C15	6.42	115.72	109.16
37	31	306	CLA	CMD-C2D-C1D	6.42	136.03	124.71
37	B	524	CLA	CHD-C4C-C3C	-6.42	115.40	124.84
48	36	310	A86	C3-C2-C1	-6.42	118.15	127.31
37	31	304	CLA	CMD-C2D-C1D	6.42	136.02	124.71
37	15	310	CLA	CMD-C2D-C1D	6.42	136.02	124.71
47	11	309	KC1	C3B-C2B-C1B	-6.41	100.95	107.08
37	B	504	CLA	CMD-C2D-C1D	6.41	136.01	124.71
37	36	307	CLA	CMD-C2D-C1D	6.41	136.01	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	38	201	CLA	CHD-C1D-ND	-6.41	118.56	124.45
47	18	207	KC1	C2B-C1B-NB	6.41	114.83	110.10
37	11	303	CLA	CMD-C2D-C1D	6.40	136.00	124.71
47	31	303	KC1	C1A-C2A-C3A	-6.40	102.03	107.11
48	17	312	A86	C33-C32-C31	6.40	115.43	109.21
37	11	305	CLA	CMD-C2D-C1D	6.40	136.00	124.71
47	13	302	KC1	C1A-C2A-C3A	-6.40	102.03	107.11
47	31	307	KC1	C1A-C2A-C3A	-6.40	102.03	107.11
37	21	210	CLA	CMD-C2D-C1D	6.40	135.99	124.71
48	14	315	A86	C17-C16-C15	6.39	115.68	109.16
37	16	307	CLA	CMD-C2D-C1D	6.39	135.97	124.71
37	41	210	CLA	CMD-C2D-C1D	6.39	135.97	124.71
47	15	304	KC1	C1A-C2A-C3A	-6.39	102.04	107.11
37	19	307	CLA	CMD-C2D-C1D	6.39	135.97	124.71
37	39	307	CLA	CMD-C2D-C1D	6.39	135.97	124.71
47	20	305	KC1	C1A-C2A-C3A	-6.38	102.05	107.11
37	B	503	CLA	CMD-C2D-C1D	6.38	135.96	124.71
37	19	303	CLA	CMD-C2D-C1D	6.38	135.96	124.71
37	39	303	CLA	CMD-C2D-C1D	6.38	135.96	124.71
48	13	314	A86	C3-C2-C1	-6.38	118.21	127.31
37	21	206	CLA	CHD-C4C-C3C	-6.38	115.47	124.84
37	41	206	CLA	CHD-C4C-C3C	-6.38	115.47	124.84
37	14	308	CLA	C2C-C1C-NC	6.37	115.94	109.97
37	34	308	CLA	C2C-C1C-NC	6.37	115.94	109.97
37	32	210	CLA	O2D-CGD-CBD	6.37	122.59	111.27
47	38	205	KC1	CMA-C3A-C2A	-6.37	112.71	128.30
37	34	302	CLA	CMD-C2D-C1D	6.37	135.94	124.71
47	33	302	KC1	C1A-C2A-C3A	-6.37	102.06	107.11
37	13	303	CLA	CMD-C2D-C1D	6.37	135.94	124.71
47	41	207	KC1	C1A-C2A-C3A	-6.37	102.06	107.11
37	19	306	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
37	b	503	CLA	CMD-C2D-C1D	6.37	135.93	124.71
47	34	306	KC1	O2D-CGD-CBD	6.36	122.58	111.27
37	b	515	CLA	CMD-C2D-C1D	6.36	135.93	124.71
47	18	205	KC1	CMA-C3A-C2A	-6.36	112.72	128.30
47	40	207	KC1	C1A-C2A-C3A	-6.36	102.07	107.11
37	14	302	CLA	CMD-C2D-C1D	6.36	135.92	124.71
47	38	210	KC1	O2D-CGD-CBD	6.36	122.56	111.27
48	33	314	A86	C3-C2-C1	-6.36	118.24	127.31
37	B	509	CLA	C2C-C1C-NC	6.36	115.93	109.97
37	c	507	CLA	O2D-CGD-CBD	6.36	122.56	111.27
37	c	504	CLA	CHD-C1D-ND	-6.36	118.61	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	18	202	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
47	21	207	KC1	C1A-C2A-C3A	-6.35	102.07	107.11
37	B	515	CLA	CMD-C2D-C1D	6.35	135.90	124.71
37	B	502	CLA	CHD-C1D-ND	-6.35	118.62	124.45
37	b	509	CLA	C2C-C1C-NC	6.35	115.92	109.97
37	b	516	CLA	O2D-CGD-CBD	6.35	122.55	111.27
37	39	306	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
47	34	306	KC1	C3A-C4A-NA	6.34	117.50	110.57
47	14	306	KC1	O2D-CGD-CBD	6.34	122.54	111.27
48	35	315	A86	C33-C32-C31	6.34	115.37	109.21
37	16	301	CLA	CMD-C2D-C1D	6.34	135.88	124.71
37	b	512	CLA	O2D-CGD-CBD	6.34	122.53	111.27
37	C	507	CLA	O2D-CGD-CBD	6.34	122.53	111.27
48	37	319	A86	C4-C5-C6	-6.33	118.27	127.31
47	31	309	KC1	C3B-C2B-C1B	-6.33	101.03	107.08
37	38	202	CLA	CHD-C4C-C3C	-6.33	115.53	124.84
37	D	405	CLA	CHD-C1D-ND	-6.33	118.64	124.45
48	35	313	A86	C33-C32-C31	6.33	115.36	109.21
37	40	205	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
48	35	314	A86	C3-C2-C1	-6.33	118.28	127.31
37	19	309	CLA	CMD-C2D-C1D	6.33	135.86	124.71
37	35	308	CLA	CHD-C1D-ND	-6.32	118.64	124.45
47	34	309	KC1	C3B-C2B-C1B	-6.32	101.04	107.08
47	11	304	KC1	C1A-C2A-C3A	-6.32	102.09	107.11
37	21	202	CLA	CHD-C1D-ND	-6.32	118.64	124.45
37	34	301	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
37	36	301	CLA	CMD-C2D-C1D	6.32	135.85	124.71
37	B	516	CLA	O2D-CGD-CBD	6.32	122.50	111.27
37	14	301	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
48	17	320	A86	C33-C32-C31	6.32	115.35	109.21
37	d	403	CLA	CHD-C1D-ND	-6.32	118.65	124.45
37	C	504	CLA	CHD-C1D-ND	-6.31	118.66	124.45
47	14	306	KC1	C3A-C4A-NA	6.31	117.46	110.57
37	B	512	CLA	O2D-CGD-CBD	6.31	122.48	111.27
47	38	210	KC1	CBA-CAA-C2A	-6.31	101.22	125.27
48	17	311	A86	C3-C2-C1	-6.31	118.31	127.31
47	18	210	KC1	CBA-CAA-C2A	-6.30	101.24	125.27
47	18	207	KC1	C1A-C2A-C3A	-6.30	102.11	107.11
37	39	310	CLA	CMD-C2D-C1D	6.30	135.81	124.71
37	39	301	CLA	CMD-C2D-C1D	6.29	135.80	124.71
48	37	319	A86	C33-C32-C31	6.29	115.33	109.21
48	15	312	A86	C33-C32-C31	6.29	115.33	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	20	303	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
48	35	312	A86	C33-C32-C31	6.29	115.32	109.21
37	36	309	CLA	CHD-C1D-ND	-6.29	118.68	124.45
37	16	309	CLA	CHD-C1D-ND	-6.28	118.68	124.45
37	32	208	CLA	CHD-C1D-ND	-6.28	118.68	124.45
47	14	309	KC1	C3B-C2B-C1B	-6.28	101.08	107.08
37	31	304	CLA	O2D-CGD-CBD	6.28	122.42	111.27
47	34	304	KC1	C3B-C2B-C1B	-6.27	101.08	107.08
48	15	315	A86	C33-C32-C31	6.27	115.31	109.21
47	35	309	KC1	C3B-C2B-C1B	-6.27	101.09	107.08
47	38	207	KC1	C1A-C2A-C3A	-6.27	102.14	107.11
48	39	313	A86	O4-C38-C39	6.27	122.62	111.09
37	C	507	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
37	11	303	CLA	O2D-CGD-CBD	6.27	122.41	111.27
37	A	405	CLA	CMD-C2D-C1D	6.26	135.75	124.71
37	b	502	CLA	CHD-C1D-ND	-6.26	118.70	124.45
47	15	309	KC1	C3B-C2B-C1B	-6.26	101.10	107.08
37	c	507	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
48	40	213	A86	C4-C5-C6	-6.26	118.38	127.31
37	21	204	CLA	CHD-C1D-ND	-6.25	118.71	124.45
37	19	301	CLA	CMD-C2D-C1D	6.25	135.72	124.71
48	34	312	A86	C17-C16-C15	6.25	115.54	109.16
37	b	505	CLA	CHD-C1D-ND	-6.25	118.71	124.45
47	31	305	KC1	C1A-C2A-C3A	-6.25	102.16	107.11
37	19	310	CLA	CMD-C2D-C1D	6.24	135.72	124.71
37	33	310	CLA	CMD-C2D-C1D	6.24	135.72	124.71
47	41	207	KC1	C3B-C2B-C1B	-6.24	101.12	107.08
47	15	306	KC1	C3B-C2B-C1B	-6.24	101.12	107.08
48	20	311	A86	C4-C5-C6	-6.24	118.41	127.31
47	21	207	KC1	C3B-C2B-C1B	-6.24	101.12	107.08
48	32	221	A86	C4-C5-C6	-6.24	118.41	127.31
48	11	319	A86	O4-C38-C39	6.24	122.57	111.09
37	41	202	CLA	CHD-C1D-ND	-6.24	118.72	124.45
37	a	407	CLA	CMD-C2D-C1D	6.24	135.70	124.71
37	12	207	CLA	CHD-C1D-ND	-6.24	118.72	124.45
37	41	204	CLA	CHD-C1D-ND	-6.23	118.73	124.45
37	31	301	CLA	CMD-C2D-C1D	6.23	135.70	124.71
37	W	101	CLA	CHD-C1D-ND	-6.23	118.73	124.45
48	12	220	A86	C4-C5-C6	-6.23	118.42	127.31
48	31	315	A86	C3-C2-C1	-6.23	118.42	127.31
37	d	403	CLA	CMD-C2D-C1D	6.23	135.69	124.71
48	11	315	A86	C3-C2-C1	-6.23	118.42	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	507	CLA	CMD-C2D-C1D	6.23	135.69	124.71
48	19	313	A86	O4-C38-C39	6.23	122.55	111.09
47	17	308	KC1	C3B-C2B-C1B	-6.23	101.13	107.08
47	35	302	KC1	CMA-C3A-C2A	-6.22	113.06	128.30
37	35	308	CLA	CMD-C2D-C1D	6.22	135.67	124.71
37	D	405	CLA	CMD-C2D-C1D	6.22	135.67	124.71
47	14	304	KC1	C3B-C2B-C1B	-6.22	101.14	107.08
37	c	505	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
48	31	319	A86	O4-C38-C39	6.21	122.52	111.09
37	21	206	CLA	CHD-C1D-ND	-6.21	118.75	124.45
48	40	211	A86	C4-C5-C6	-6.21	118.45	127.31
37	16	303	CLA	CHD-C1D-ND	-6.21	118.75	124.45
48	35	313	A86	C4-C5-C6	-6.21	118.45	127.31
37	W	102	CLA	CMD-C2D-C1D	6.21	135.65	124.71
48	15	313	A86	C4-C5-C6	-6.21	118.45	127.31
37	C	507	CLA	CMD-C2D-C1D	6.20	135.65	124.71
48	37	311	A86	C33-C32-C31	6.20	115.24	109.21
47	15	302	KC1	C3B-C2B-C1B	-6.20	101.15	107.08
37	C	505	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
37	c	513	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
37	41	210	CLA	CHD-C1D-ND	-6.20	118.76	124.45
37	B	505	CLA	CHD-C1D-ND	-6.19	118.77	124.45
37	C	513	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
37	36	301	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
37	16	301	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
37	36	303	CLA	CHD-C1D-ND	-6.18	118.77	124.45
37	B	513	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
37	b	509	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
47	34	309	KC1	CBA-CAA-C2A	-6.18	101.72	125.27
37	b	516	CLA	CMD-C2D-C1D	6.18	135.60	124.71
37	40	203	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
37	b	511	CLA	CHD-C1D-ND	-6.17	118.78	124.45
37	18	201	CLA	CHD-C1D-ND	-6.17	118.78	124.45
47	14	309	KC1	CBA-CAA-C2A	-6.17	101.75	125.27
37	21	210	CLA	CHD-C1D-ND	-6.17	118.78	124.45
37	41	206	CLA	CHD-C1D-ND	-6.16	118.79	124.45
37	B	509	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
48	14	312	A86	C17-C16-C15	6.16	115.45	109.16
37	B	511	CLA	CHD-C1D-ND	-6.16	118.79	124.45
37	38	204	CLA	CHD-C1D-ND	-6.16	118.79	124.45
47	15	302	KC1	CMA-C3A-C2A	-6.16	113.22	128.30
37	20	301	CLA	CHD-C4C-C3C	-6.16	115.79	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	513	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
37	B	516	CLA	CMD-C2D-C1D	6.15	135.56	124.71
37	12	210	CLA	C2C-C1C-NC	6.15	115.74	109.97
37	B	504	CLA	O2D-CGD-CBD	6.15	122.20	111.27
37	b	510	CLA	CMD-C2D-C1D	6.15	135.56	124.71
48	20	309	A86	C4-C5-C6	-6.15	118.53	127.31
47	37	307	KC1	C3B-C2B-C1B	-6.15	101.20	107.08
48	18	213	A86	C3-C2-C1	-6.15	118.54	127.31
47	35	306	KC1	C3B-C2B-C1B	-6.15	101.21	107.08
37	32	211	CLA	C2C-C1C-NC	6.14	115.72	109.97
37	21	209	CLA	CHD-C1D-ND	-6.14	118.81	124.45
37	41	208	CLA	CHD-C1D-ND	-6.14	118.81	124.45
48	12	214	A86	C33-C32-C31	6.13	115.17	109.21
37	w	101	CLA	CHD-C1D-ND	-6.13	118.82	124.45
37	B	510	CLA	CMD-C2D-C1D	6.13	135.52	124.71
37	41	209	CLA	CHD-C1D-ND	-6.13	118.82	124.45
37	b	504	CLA	O2D-CGD-CBD	6.13	122.16	111.27
37	C	501	CLA	CHD-C1D-ND	-6.13	118.82	124.45
37	18	204	CLA	CHD-C1D-ND	-6.13	118.82	124.45
37	C	510	CLA	C2D-C1D-ND	6.13	114.62	110.10
48	13	314	A86	C25-C26-C27	-6.13	118.56	127.31
37	38	208	CLA	CMD-C2D-C1D	6.13	135.51	124.71
37	b	504	CLA	C2D-C1D-ND	6.13	114.62	110.10
37	39	301	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
50	20	310	DD6	C7-C6-C8	-6.12	108.43	118.08
37	19	301	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
37	c	501	CLA	CHD-C1D-ND	-6.12	118.83	124.45
47	13	302	KC1	CMA-C3A-C2A	-6.12	113.32	128.30
48	12	202	A86	C3-C2-C1	-6.12	118.58	127.31
37	B	516	CLA	C4A-NA-C1A	-6.12	103.95	106.71
47	11	306	KC1	C3B-C2B-C1B	-6.12	101.23	107.08
37	15	308	CLA	CHD-C1D-ND	-6.12	118.83	124.45
50	40	212	DD6	C7-C6-C8	-6.12	108.44	118.08
37	c	512	CLA	O2D-CGD-CBD	6.11	122.12	111.27
48	32	215	A86	C33-C32-C31	6.11	115.15	109.21
37	c	510	CLA	C2D-C1D-ND	6.11	114.60	110.10
48	32	203	A86	C3-C2-C1	-6.11	118.60	127.31
37	C	513	CLA	CHD-C1D-ND	-6.10	118.84	124.45
37	11	307	CLA	O2D-CGD-CBD	6.10	122.11	111.27
37	33	303	CLA	CHD-C1D-ND	-6.10	118.85	124.45
47	11	309	KC1	O2D-CGD-CBD	6.10	122.11	111.27
48	33	314	A86	C25-C26-C27	-6.10	118.60	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	33	302	KC1	CMA-C3A-C2A	-6.10	113.37	128.30
47	20	302	KC1	C3B-C2B-C1B	-6.09	101.26	107.08
37	C	512	CLA	O2D-CGD-CBD	6.09	122.10	111.27
37	B	504	CLA	C2D-C1D-ND	6.09	114.59	110.10
37	20	308	CLA	C2C-C1C-NC	6.09	115.68	109.97
47	35	302	KC1	C3B-C2B-C1B	-6.09	101.26	107.08
37	31	308	CLA	O2D-CGD-CBD	6.09	122.09	111.27
48	39	311	A86	C3-C2-C1	-6.09	118.62	127.31
47	35	306	KC1	C1A-C2A-C3A	-6.09	102.28	107.11
37	35	307	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
37	32	211	CLA	CMD-C2D-C1D	6.08	135.44	124.71
47	37	304	KC1	C3B-C2B-C1B	-6.08	101.27	107.08
47	16	305	KC1	C3C-C4C-NC	6.08	115.61	109.88
37	b	508	CLA	CMD-C2D-C1D	6.08	135.44	124.71
37	c	513	CLA	CHD-C1D-ND	-6.08	118.86	124.45
37	12	210	CLA	CMD-C2D-C1D	6.08	135.43	124.71
37	B	508	CLA	CMD-C2D-C1D	6.08	135.43	124.71
47	31	307	KC1	C3B-C2B-C1B	-6.08	101.27	107.08
50	41	216	DD6	C12-C11-C13	-6.08	108.50	118.08
37	38	211	CLA	C2C-C1C-NC	6.08	115.66	109.97
37	39	307	CLA	C2C-C1C-NC	6.07	115.66	109.97
47	40	204	KC1	C3B-C2B-C1B	-6.07	101.28	107.08
48	15	315	A86	C17-C16-C15	6.07	115.36	109.16
37	21	208	CLA	CHD-C1D-ND	-6.07	118.88	124.45
47	33	309	KC1	C1A-C2A-C3A	-6.07	102.30	107.11
47	36	305	KC1	C3C-C4C-NC	6.07	115.59	109.88
37	b	504	CLA	C2C-C1C-NC	6.06	115.65	109.97
37	b	514	CLA	O2D-CGD-CBD	6.06	122.04	111.27
37	31	310	CLA	CMD-C2D-C1D	6.06	135.39	124.71
50	21	216	DD6	C12-C11-C13	-6.06	108.53	118.08
37	11	310	CLA	CMD-C2D-C1D	6.06	135.39	124.71
47	31	309	KC1	O2D-CGD-CBD	6.06	122.03	111.27
48	19	311	A86	C3-C2-C1	-6.06	118.67	127.31
37	15	307	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
37	B	514	CLA	O2D-CGD-CBD	6.05	122.02	111.27
37	B	504	CLA	C2C-C1C-NC	6.05	115.64	109.97
48	17	320	A86	C4-C5-C6	-6.05	118.68	127.31
37	16	301	CLA	CHD-C1D-ND	-6.05	118.90	124.45
47	13	309	KC1	C1A-C2A-C3A	-6.05	102.31	107.11
37	D	406	CLA	CHD-C1D-ND	-6.04	118.90	124.45
37	36	301	CLA	CHD-C1D-ND	-6.04	118.90	124.45
50	41	212	DD6	C7-C6-C8	-6.04	108.56	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	21	203	KC1	C3B-C2B-C1B	-6.04	101.31	107.08
47	12	211	KC1	C3B-C2B-C1B	-6.04	101.31	107.08
37	c	508	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
37	15	308	CLA	C2C-C1C-NC	6.04	115.63	109.97
50	21	212	DD6	C7-C6-C8	-6.04	108.56	118.08
37	35	301	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
37	35	303	CLA	CHD-C1D-ND	-6.03	118.91	124.45
37	40	210	CLA	C2C-C1C-NC	6.03	115.62	109.97
48	12	215	A86	C33-C32-C31	6.03	115.07	109.21
37	d	404	CLA	CHD-C1D-ND	-6.03	118.91	124.45
37	19	303	CLA	CHD-C1D-ND	-6.03	118.91	124.45
37	38	202	CLA	CHD-C1D-ND	-6.03	118.92	124.45
47	32	212	KC1	C3B-C2B-C1B	-6.03	101.32	107.08
48	12	216	A86	C3-C2-C1	-6.02	118.72	127.31
37	19	307	CLA	C2C-C1C-NC	6.02	115.61	109.97
37	18	208	CLA	CMD-C2D-C1D	6.02	135.32	124.71
37	B	506	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
37	13	303	CLA	C2C-C1C-NC	6.02	115.61	109.97
48	31	311	A86	O4-C38-C39	6.02	122.16	111.09
48	34	314	A86	C3-C2-C1	-6.02	118.72	127.31
37	39	303	CLA	CHD-C1D-ND	-6.02	118.93	124.45
47	41	203	KC1	C3B-C2B-C1B	-6.01	101.34	107.08
48	14	314	A86	C3-C2-C1	-6.01	118.73	127.31
37	35	303	CLA	O2D-CGD-CBD	6.01	121.95	111.27
37	15	301	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
37	C	510	CLA	C2C-C1C-NC	6.01	115.60	109.97
47	14	304	KC1	C1A-C2A-C3A	-6.01	102.35	107.11
47	34	304	KC1	C1A-C2A-C3A	-6.01	102.35	107.11
37	c	511	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
48	32	216	A86	C33-C32-C31	6.00	115.05	109.21
37	19	310	CLA	C2C-C1C-NC	6.00	115.60	109.97
37	b	506	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
48	11	311	A86	O4-C38-C39	6.00	122.12	111.09
37	14	310	CLA	C2C-C1C-NC	6.00	115.59	109.97
37	C	508	CLA	CHD-C4C-C3C	-6.00	116.03	124.84
37	31	310	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
37	a	403	CLA	CHD-C1D-ND	-5.99	118.95	124.45
37	12	205	CLA	CHD-C1D-ND	-5.99	118.95	124.45
37	C	511	CLA	CHD-C4C-C3C	-5.98	116.04	124.84
37	34	310	CLA	C2C-C1C-NC	5.98	115.58	109.97
37	12	212	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
48	37	309	A86	O4-C38-C39	5.98	122.09	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	13	308	CLA	C2C-C1C-NC	5.98	115.57	109.97
47	15	306	KC1	C1A-C2A-C3A	-5.98	102.37	107.11
37	11	310	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
48	38	214	A86	C3-C2-C1	-5.97	118.79	127.31
47	35	306	KC1	CMA-C3A-C2A	-5.97	113.68	128.30
48	31	313	A86	C25-C26-C27	-5.97	118.79	127.31
37	36	306	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
37	15	303	CLA	CHD-C1D-ND	-5.97	118.97	124.45
48	34	316	A86	O4-C38-C39	5.97	122.07	111.09
48	14	316	A86	O4-C38-C39	5.97	122.07	111.09
47	20	302	KC1	C1A-C2A-C3A	-5.97	102.38	107.11
37	c	510	CLA	C2C-C1C-NC	5.97	115.56	109.97
37	Z	101	CLA	CHD-C1D-ND	-5.97	118.97	124.45
37	39	310	CLA	C2C-C1C-NC	5.96	115.56	109.97
37	b	510	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
48	32	217	A86	C3-C2-C1	-5.96	118.80	127.31
48	12	214	A86	C3-C2-C1	-5.96	118.80	127.31
48	38	212	A86	C17-C16-C15	5.96	115.24	109.16
37	32	204	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
37	B	513	CLA	CHD-C1D-ND	-5.96	118.98	124.45
37	33	308	CLA	C2C-C1C-NC	5.96	115.55	109.97
37	B	510	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
37	32	205	CLA	C2C-C1C-NC	5.95	115.55	109.97
37	16	306	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
37	w	101	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
47	31	309	KC1	CMA-C3A-C4A	-5.95	115.98	125.04
48	17	310	A86	O4-C38-C39	5.95	122.03	111.09
37	b	516	CLA	C4A-NA-C1A	-5.95	104.03	106.71
47	11	309	KC1	CMA-C3A-C4A	-5.94	115.99	125.04
37	C	502	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
37	32	205	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
37	19	303	CLA	CAA-C2A-C3A	-5.94	96.51	112.78
37	40	208	CLA	CMD-C2D-C1D	5.94	135.18	124.71
37	d	403	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
37	33	305	CLA	CHD-C1D-ND	-5.94	119.00	124.45
37	12	203	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
37	39	301	CLA	CHD-C1D-ND	-5.93	119.00	124.45
37	c	509	CLA	O2D-CGD-CBD	5.93	121.81	111.27
37	32	213	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
37	20	306	CLA	CMD-C2D-C1D	5.93	135.17	124.71
37	A	403	CLA	CHD-C1D-ND	-5.93	119.00	124.45
37	z	102	CLA	CHD-C4C-C3C	-5.93	116.12	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	13	305	CLA	CHD-C1D-ND	-5.93	119.00	124.45
37	W	101	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
48	32	215	A86	C3-C2-C1	-5.93	118.85	127.31
37	z	101	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
37	38	208	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
37	C	509	CLA	O2D-CGD-CBD	5.92	121.80	111.27
37	c	502	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
37	12	204	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
37	Z	102	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
37	D	405	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
37	C	507	CLA	C2C-C1C-NC	5.92	115.52	109.97
37	39	303	CLA	CAA-C2A-C3A	-5.92	96.57	112.78
37	39	302	CLA	CHD-C1D-ND	-5.92	119.02	124.45
37	39	303	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
37	12	204	CLA	C2C-C1C-NC	5.92	115.52	109.97
37	21	204	CLA	O2D-CGD-CBD	5.92	121.78	111.27
47	12	206	KC1	CHD-C4C-C3C	-5.91	114.23	125.33
37	13	307	CLA	CMD-C2D-C1D	5.91	135.13	124.71
47	40	204	KC1	C1A-C2A-C3A	-5.91	102.42	107.11
37	19	303	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
48	19	311	A86	C33-C32-C31	5.91	114.96	109.21
47	32	207	KC1	CHD-C4C-C3C	-5.91	114.23	125.33
47	41	207	KC1	O2D-CGD-CBD	5.91	121.77	111.27
48	16	314	A86	C3-C2-C1	-5.91	118.88	127.31
37	14	302	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
37	18	201	CLA	CHD-C4C-C3C	-5.90	116.16	124.84
37	B	507	CLA	CHD-C1D-ND	-5.90	119.03	124.45
37	33	303	CLA	C2C-C1C-NC	5.90	115.50	109.97
37	12	209	CLA	CMD-C2D-C1D	5.90	135.12	124.71
37	18	208	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
37	38	211	CLA	CHD-C1D-ND	-5.90	119.03	124.45
48	39	311	A86	C33-C32-C31	5.90	114.94	109.21
47	13	306	KC1	CMA-C3A-C2A	-5.90	113.87	128.30
47	33	306	KC1	CMA-C3A-C2A	-5.90	113.87	128.30
37	13	303	CLA	CHD-C1D-ND	-5.90	119.04	124.45
37	z	101	CLA	CHD-C1D-ND	-5.89	119.04	124.45
37	33	301	CLA	CHD-C1D-ND	-5.89	119.04	124.45
37	16	309	CLA	CAA-C2A-C3A	-5.89	96.64	112.78
37	19	301	CLA	CHD-C1D-ND	-5.89	119.04	124.45
37	c	507	CLA	C2C-C1C-NC	5.89	115.49	109.97
37	37	306	CLA	CMD-C2D-C1D	5.89	135.10	124.71
37	34	302	CLA	CHD-C4C-C3C	-5.89	116.18	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	32	206	CLA	CHD-C1D-ND	-5.89	119.04	124.45
37	41	204	CLA	O2D-CGD-CBD	5.89	121.73	111.27
37	14	307	CLA	CMD-C2D-C1D	5.89	135.09	124.71
47	21	207	KC1	O2D-CGD-CBD	5.89	121.73	111.27
37	33	307	CLA	CMD-C2D-C1D	5.89	135.09	124.71
37	B	501	CLA	O2D-CGD-CBD	5.89	121.73	111.27
37	B	510	CLA	O2D-CGD-CBD	5.88	121.72	111.27
47	18	207	KC1	CMA-C3A-C2A	-5.88	113.89	128.30
37	18	209	CLA	CMD-C2D-C1D	5.88	135.08	124.71
37	b	513	CLA	CHD-C1D-ND	-5.88	119.05	124.45
37	36	307	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
47	20	304	KC1	C1A-C2A-C3A	-5.88	102.45	107.11
37	Z	101	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
37	36	309	CLA	CAA-C2A-C3A	-5.88	96.68	112.78
48	35	319	A86	C20-C19-C18	-5.88	101.12	112.75
47	17	303	KC1	C3B-C2B-C1B	-5.88	101.46	107.08
37	17	307	CLA	CMD-C2D-C1D	5.88	135.07	124.71
48	36	313	A86	C3-C2-C1	-5.88	118.92	127.31
48	15	319	A86	C20-C19-C18	-5.88	101.12	112.75
48	12	217	A86	O4-C38-C39	5.87	121.90	111.09
37	b	510	CLA	O2D-CGD-CBD	5.87	121.70	111.27
37	34	307	CLA	CMD-C2D-C1D	5.87	135.06	124.71
37	b	501	CLA	O2D-CGD-CBD	5.87	121.70	111.27
37	A	405	CLA	CHD-C1D-ND	-5.87	119.06	124.45
37	19	305	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
37	39	305	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
48	32	218	A86	O4-C38-C39	5.87	121.89	111.09
37	11	303	CLA	C2C-C1C-NC	5.87	115.47	109.97
37	38	209	CLA	CMD-C2D-C1D	5.87	135.05	124.71
37	a	404	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
48	34	312	A86	C25-C26-C27	-5.86	118.94	127.31
37	18	204	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
48	18	212	A86	C17-C16-C15	5.86	115.14	109.16
47	38	205	KC1	C1A-C2A-C3A	-5.86	102.46	107.11
37	11	307	CLA	CMD-C2D-C1D	5.85	135.03	124.71
37	b	507	CLA	CHD-C1D-ND	-5.85	119.07	124.45
37	13	301	CLA	CHD-C1D-ND	-5.85	119.07	124.45
37	14	303	CLA	CHD-C1D-ND	-5.85	119.07	124.45
37	34	308	CLA	CHD-C1D-ND	-5.85	119.07	124.45
47	37	302	KC1	C3B-C2B-C1B	-5.85	101.49	107.08
37	B	503	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
37	a	407	CLA	CHD-C1D-ND	-5.85	119.08	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	20	311	A86	C17-C16-C15	5.85	115.13	109.16
37	13	308	CLA	CHD-C1D-ND	-5.85	119.08	124.45
48	15	311	A86	O4-C38-C39	5.85	121.85	111.09
37	16	307	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
48	14	312	A86	C25-C26-C27	-5.85	118.96	127.31
47	15	306	KC1	CMA-C3A-C2A	-5.85	113.98	128.30
37	D	401	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
37	b	516	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
47	18	205	KC1	C3B-C2B-C1B	-5.84	101.50	107.08
37	B	505	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
37	b	503	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
37	19	302	CLA	CHD-C1D-ND	-5.84	119.09	124.45
50	16	312	DD6	C24-C1-C2	-5.84	109.98	118.94
47	36	304	KC1	C3B-C2B-C1B	-5.84	101.50	107.08
37	38	206	CLA	CHD-C1D-ND	-5.84	119.09	124.45
47	40	206	KC1	C1A-C2A-C3A	-5.84	102.48	107.11
48	38	213	A86	C4-C5-C6	-5.84	118.98	127.31
37	33	310	CLA	CHD-C1D-ND	-5.84	119.09	124.45
37	A	405	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
37	34	303	CLA	CHD-C1D-ND	-5.83	119.09	124.45
37	B	514	CLA	CMD-C2D-C1D	5.83	135.00	124.71
48	39	311	A86	O4-C38-C39	5.83	121.82	111.09
48	40	213	A86	C17-C16-C15	5.83	115.11	109.16
37	32	206	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
37	31	308	CLA	CMD-C2D-C1D	5.83	134.99	124.71
37	32	210	CLA	CMD-C2D-C1D	5.83	134.99	124.71
37	33	308	CLA	CHD-C1D-ND	-5.83	119.09	124.45
47	18	205	KC1	C1A-C2A-C3A	-5.83	102.49	107.11
37	b	505	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
48	18	214	A86	C3-C2-C1	-5.83	118.99	127.31
37	35	310	CLA	CHD-C1D-ND	-5.83	119.10	124.45
47	32	212	KC1	O2D-CGD-CBD	5.83	121.62	111.27
47	33	304	KC1	C1A-C2A-C3A	-5.83	102.49	107.11
37	15	310	CLA	C2C-C1C-NC	5.83	115.43	109.97
37	a	407	CLA	CHD-C4C-C3C	-5.83	116.28	124.84
37	b	514	CLA	CMD-C2D-C1D	5.83	134.98	124.71
48	19	311	A86	O4-C38-C39	5.83	121.81	111.09
37	32	210	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
37	34	310	CLA	CHD-C1D-ND	-5.82	119.10	124.45
47	38	207	KC1	C3C-C4C-NC	5.82	115.36	109.88
37	14	308	CLA	CHD-C1D-ND	-5.82	119.10	124.45
37	38	209	CLA	CHD-C4C-C3C	-5.82	116.28	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	310	CLA	CHD-C1D-ND	-5.82	119.11	124.45
47	13	304	KC1	C1A-C2A-C3A	-5.82	102.50	107.11
47	12	211	KC1	O2D-CGD-CBD	5.82	121.60	111.27
37	12	209	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
37	31	304	CLA	C2C-C1C-NC	5.81	115.42	109.97
37	20	307	CLA	CHD-C1D-ND	-5.81	119.11	124.45
37	B	516	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
47	20	305	KC1	CMA-C3A-C2A	-5.81	114.07	128.30
47	11	306	KC1	O2D-CGD-CBD	5.81	121.59	111.27
48	35	311	A86	C41-C32-C31	-5.81	105.27	110.47
50	36	312	DD6	C24-C1-C2	-5.81	110.03	118.94
47	20	305	KC1	C3B-C2B-C1B	-5.81	101.53	107.08
47	38	205	KC1	C3B-C2B-C1B	-5.80	101.54	107.08
37	18	209	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
47	16	308	KC1	C3B-C2B-C1B	-5.80	101.54	107.08
37	38	203	CLA	C2C-C1C-NC	5.80	115.40	109.97
47	16	304	KC1	C3B-C2B-C1B	-5.79	101.55	107.08
47	31	307	KC1	O2D-CGD-CBD	5.79	121.56	111.27
37	40	209	CLA	CHD-C1D-ND	-5.79	119.13	124.45
47	38	210	KC1	C3B-C2B-C1B	-5.79	101.55	107.08
47	40	207	KC1	CMA-C3A-C2A	-5.78	114.14	128.30
37	14	305	CLA	CHD-C1D-ND	-5.78	119.14	124.45
37	11	307	CLA	C2C-C1C-NC	5.78	115.39	109.97
50	20	310	DD6	C-C1-C24	-5.78	108.97	118.08
37	40	205	CLA	CAA-C2A-C3A	-5.78	96.95	112.78
37	38	211	CLA	O2D-CGD-CBD	5.78	121.54	111.27
37	36	306	CLA	C4A-NA-C1A	-5.78	104.11	106.71
37	31	308	CLA	C2C-C1C-NC	5.78	115.38	109.97
37	38	204	CLA	O2D-CGD-CBD	5.77	121.53	111.27
47	15	304	KC1	C3B-C2B-C1B	-5.77	101.56	107.08
47	40	207	KC1	C3B-C2B-C1B	-5.77	101.56	107.08
37	37	308	CLA	CHD-C1D-ND	-5.77	119.15	124.45
37	18	211	CLA	CHD-C1D-ND	-5.77	119.15	124.45
37	18	203	CLA	C2C-C1C-NC	5.77	115.38	109.97
37	35	310	CLA	C2C-C1C-NC	5.77	115.38	109.97
37	11	303	CLA	CHD-C1D-ND	-5.77	119.15	124.45
37	20	303	CLA	CAA-C2A-C3A	-5.77	96.99	112.78
37	34	305	CLA	CHD-C1D-ND	-5.77	119.16	124.45
37	c	502	CLA	CMD-C2D-C1D	5.76	134.87	124.71
37	36	306	CLA	CMD-C2D-C1D	5.76	134.87	124.71
47	17	308	KC1	CBA-CAA-C2A	-5.76	103.30	125.27
50	40	212	DD6	C-C1-C24	-5.76	109.00	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	37	307	KC1	CBA-CAA-C2A	-5.76	103.30	125.27
37	33	305	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
37	17	309	CLA	CHD-C1D-ND	-5.76	119.16	124.45
37	C	502	CLA	CMD-C2D-C1D	5.76	134.87	124.71
47	36	308	KC1	C3B-C2B-C1B	-5.76	101.58	107.08
48	36	310	A86	C41-C32-C31	-5.76	105.32	110.47
37	13	305	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
47	33	304	KC1	C3C-C4C-NC	5.76	115.30	109.88
48	16	310	A86	C41-C32-C31	-5.76	105.32	110.47
37	38	203	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
37	14	307	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
37	16	306	CLA	C4A-NA-C1A	-5.75	104.12	106.71
37	39	307	CLA	CHD-C1D-ND	-5.75	119.17	124.45
47	18	207	KC1	C3C-C4C-NC	5.75	115.29	109.88
47	13	304	KC1	C3C-C4C-NC	5.75	115.29	109.88
48	13	315	A86	O4-C38-C39	5.75	121.67	111.09
50	39	312	DD6	C32-C31-C36	-5.75	114.52	122.63
48	12	220	A86	C3-C2-C1	-5.75	119.11	127.31
37	13	310	CLA	CHD-C1D-ND	-5.75	119.17	124.45
37	36	307	CLA	CHD-C1D-ND	-5.75	119.17	124.45
47	38	207	KC1	CMA-C3A-C2A	-5.74	114.24	128.30
37	18	203	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
37	20	306	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
47	40	206	KC1	CMA-C3A-C2A	-5.74	114.24	128.30
37	19	307	CLA	CHD-C1D-ND	-5.74	119.18	124.45
47	18	210	KC1	C3B-C2B-C1B	-5.74	101.59	107.08
37	19	310	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
47	34	306	KC1	C3B-C2B-C1B	-5.74	101.59	107.08
47	20	304	KC1	CMA-C3A-C2A	-5.74	114.25	128.30
37	16	306	CLA	CMD-C2D-C1D	5.74	134.83	124.71
37	11	308	CLA	CHD-C1D-ND	-5.74	119.18	124.45
37	32	202	CLA	CHD-C1D-ND	-5.74	119.18	124.45
47	17	306	KC1	CHC-C1C-C2C	-5.74	116.02	124.98
47	37	305	KC1	CHC-C1C-C2C	-5.74	116.02	124.98
37	39	310	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
37	15	305	CLA	CHD-C1D-ND	-5.73	119.18	124.45
37	32	208	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
37	35	310	CLA	O2D-CGD-CBD	5.73	121.45	111.27
48	33	315	A86	O4-C38-C39	5.73	121.63	111.09
48	37	310	A86	C3-C2-C1	-5.73	119.13	127.31
48	35	316	A86	O4-C38-C39	5.73	121.63	111.09
37	B	514	CLA	CHD-C4C-C3C	-5.73	116.42	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	34	307	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
48	32	221	A86	C3-C2-C1	-5.72	119.14	127.31
47	32	209	KC1	C3C-C4C-NC	5.72	115.27	109.88
37	13	301	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
37	B	511	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
37	16	307	CLA	CHD-C1D-ND	-5.72	119.20	124.45
37	C	509	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
37	b	511	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
37	15	303	CLA	C2C-C1C-NC	5.72	115.33	109.97
37	38	204	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
50	40	214	DD6	C12-C11-C13	-5.71	109.07	118.08
37	18	209	CLA	C2C-C1C-NC	5.71	115.32	109.97
47	35	306	KC1	O2D-CGD-CBD	5.71	121.42	111.27
37	18	204	CLA	O2D-CGD-CBD	5.71	121.42	111.27
37	B	509	CLA	CMD-C2D-C1D	5.71	134.78	124.71
37	c	509	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
50	19	312	DD6	C32-C31-C36	-5.71	114.57	122.63
37	d	404	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
37	b	514	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
37	12	205	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
37	40	208	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
47	12	208	KC1	C3C-C4C-NC	5.71	115.25	109.88
50	20	312	DD6	C12-C11-C13	-5.71	109.08	118.08
37	B	508	CLA	CHD-C1D-ND	-5.71	119.21	124.45
37	c	506	CLA	CHD-C1D-ND	-5.71	119.21	124.45
37	W	102	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
37	31	306	CLA	CHD-C1D-ND	-5.70	119.21	124.45
37	14	301	CLA	CHD-C1D-ND	-5.70	119.21	124.45
37	35	308	CLA	CED-O2D-CGD	5.70	128.83	115.94
37	12	203	CLA	CHD-C1D-ND	-5.70	119.22	124.45
37	15	303	CLA	O2D-CGD-CBD	5.70	121.40	111.27
37	12	207	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
37	15	310	CLA	O2D-CGD-CBD	5.70	121.39	111.27
47	14	306	KC1	C3B-C2B-C1B	-5.70	101.64	107.08
37	C	512	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
47	33	309	KC1	C3B-C2B-C1B	-5.69	101.64	107.08
37	17	309	CLA	C2C-C1C-NC	5.69	115.31	109.97
37	14	308	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
48	14	313	A86	C4-C5-C6	-5.69	119.19	127.31
37	20	308	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
37	D	406	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
37	32	206	CLA	O2D-CGD-CBD	5.69	121.37	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	34	313	A86	C4-C5-C6	-5.68	119.20	127.31
47	35	304	KC1	C3B-C2B-C1B	-5.68	101.65	107.08
47	15	306	KC1	O2D-CGD-CBD	5.68	121.36	111.27
37	33	301	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
37	c	509	CLA	C2C-C1C-NC	5.68	115.30	109.97
37	31	301	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
37	C	501	CLA	C2C-C1C-NC	5.68	115.29	109.97
37	b	509	CLA	CMD-C2D-C1D	5.68	134.72	124.71
37	34	308	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
37	b	508	CLA	CHD-C1D-ND	-5.68	119.24	124.45
37	z	102	CLA	CHD-C1D-ND	-5.68	119.24	124.45
37	39	302	CLA	C2C-C1C-NC	5.68	115.29	109.97
48	15	316	A86	O4-C38-C39	5.68	121.53	111.09
48	35	315	A86	C17-C16-C15	5.67	114.95	109.16
37	a	404	CLA	C2C-C1C-NC	5.67	115.29	109.97
37	c	501	CLA	C2C-C1C-NC	5.67	115.28	109.97
37	13	307	CLA	C2C-C1C-NC	5.67	115.28	109.97
37	33	307	CLA	C2C-C1C-NC	5.67	115.28	109.97
47	16	308	KC1	CMD-C2D-C1D	5.67	137.18	128.46
37	39	310	CLA	CHD-C1D-ND	-5.67	119.24	124.45
37	35	305	CLA	CHD-C1D-ND	-5.67	119.24	124.45
37	C	506	CLA	CHD-C1D-ND	-5.67	119.25	124.45
37	c	512	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
47	11	304	KC1	C3B-C2B-C1B	-5.67	101.66	107.08
37	34	301	CLA	CHD-C1D-ND	-5.67	119.25	124.45
37	12	205	CLA	O2D-CGD-CBD	5.67	121.34	111.27
37	40	210	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
37	31	304	CLA	CHD-C1D-ND	-5.67	119.25	124.45
37	18	206	CLA	CHD-C1D-ND	-5.66	119.25	124.45
37	35	303	CLA	C2C-C1C-NC	5.66	115.28	109.97
37	11	301	CLA	CHD-C1D-ND	-5.66	119.25	124.45
37	31	302	CLA	CHD-C1D-ND	-5.66	119.25	124.45
37	C	509	CLA	C2C-C1C-NC	5.66	115.27	109.97
47	13	309	KC1	C3B-C2B-C1B	-5.66	101.67	107.08
37	19	302	CLA	C2C-C1C-NC	5.66	115.27	109.97
37	38	209	CLA	C2C-C1C-NC	5.66	115.27	109.97
37	B	515	CLA	CHD-C1D-ND	-5.66	119.26	124.45
37	13	307	CLA	CHD-C4C-C3C	-5.66	116.53	124.84
37	Z	102	CLA	CHD-C1D-ND	-5.65	119.26	124.45
37	C	504	CLA	O2D-CGD-CBD	5.65	121.31	111.27
37	19	310	CLA	CHD-C1D-ND	-5.65	119.26	124.45
37	33	307	CLA	CHD-C4C-C3C	-5.65	116.54	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	502	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
47	16	305	KC1	CMA-C3A-C2A	-5.65	114.48	128.30
47	31	305	KC1	C3B-C2B-C1B	-5.64	101.69	107.08
47	31	305	KC1	CMA-C3A-C2A	-5.64	114.50	128.30
47	36	308	KC1	CMD-C2D-C1D	5.64	137.13	128.46
48	35	315	A86	C4-C5-C6	-5.64	119.27	127.31
37	c	504	CLA	O2D-CGD-CBD	5.63	121.28	111.27
47	16	305	KC1	C3B-C2B-C1B	-5.63	101.70	107.08
37	b	502	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
37	38	206	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
37	b	515	CLA	CHD-C1D-ND	-5.63	119.28	124.45
37	b	508	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
48	41	213	A86	C25-C26-C27	-5.63	119.27	127.31
37	B	513	CLA	C2C-C1C-NC	5.63	115.25	109.97
47	36	305	KC1	C3B-C2B-C1B	-5.63	101.70	107.08
37	b	506	CLA	C2C-C1C-NC	5.63	115.25	109.97
50	21	216	DD6	C7-C6-C8	-5.63	109.21	118.08
37	B	508	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
37	11	305	CLA	CHD-C1D-ND	-5.62	119.28	124.45
37	21	205	CLA	CHD-C1D-ND	-5.62	119.28	124.45
47	36	305	KC1	CMA-C3A-C2A	-5.62	114.53	128.30
37	31	310	CLA	CHD-C1D-ND	-5.62	119.29	124.45
37	15	310	CLA	CHD-C1D-ND	-5.62	119.29	124.45
37	14	305	CLA	O2D-CGD-CBD	5.62	121.26	111.27
47	21	203	KC1	O2D-CGD-CBD	5.62	121.26	111.27
37	b	515	CLA	C2C-C1C-NC	5.62	115.24	109.97
37	D	401	CLA	C2C-C1C-NC	5.62	115.24	109.97
50	41	216	DD6	C7-C6-C8	-5.62	109.22	118.08
37	39	309	CLA	CHD-C1D-ND	-5.62	119.29	124.45
37	32	204	CLA	CHD-C1D-ND	-5.62	119.29	124.45
48	21	213	A86	C25-C26-C27	-5.62	119.30	127.31
37	c	510	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
37	18	206	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
47	11	304	KC1	CMA-C3A-C2A	-5.61	114.57	128.30
37	34	305	CLA	O2D-CGD-CBD	5.61	121.23	111.27
47	41	203	KC1	C3C-C4C-NC	5.61	115.16	109.88
37	41	205	CLA	CHD-C1D-ND	-5.61	119.30	124.45
37	15	305	CLA	C2C-C1C-NC	5.61	115.22	109.97
47	11	309	KC1	CBA-CAA-C2A	-5.60	103.90	125.27
37	14	302	CLA	C2C-C1C-NC	5.60	115.22	109.97
37	b	513	CLA	C2C-C1C-NC	5.60	115.22	109.97
37	39	305	CLA	C2C-C1C-NC	5.60	115.22	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	19	307	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
37	37	308	CLA	C2C-C1C-NC	5.60	115.22	109.97
37	18	203	CLA	CHD-C1D-ND	-5.59	119.31	124.45
37	38	203	CLA	CHD-C1D-ND	-5.59	119.31	124.45
47	31	309	KC1	CBA-CAA-C2A	-5.59	103.94	125.27
37	18	211	CLA	O2D-CGD-CBD	5.59	121.21	111.27
47	41	203	KC1	O2D-CGD-CBD	5.59	121.21	111.27
48	15	315	A86	C4-C5-C6	-5.59	119.33	127.31
37	z	101	CLA	C4A-NA-C1A	-5.59	104.19	106.71
37	D	406	CLA	O2D-CGD-CBD	5.59	121.20	111.27
37	41	202	CLA	C2C-C1C-NC	5.59	115.21	109.97
37	b	501	CLA	CHD-C1D-ND	-5.59	119.32	124.45
37	c	508	CLA	O2D-CGD-CBD	5.59	121.20	111.27
37	21	202	CLA	C2C-C1C-NC	5.59	115.21	109.97
37	39	309	CLA	C2C-C1C-NC	5.58	115.20	109.97
48	17	315	A86	C3-C2-C1	-5.58	119.34	127.31
37	b	507	CLA	O2D-CGD-CBD	5.58	121.19	111.27
37	Z	101	CLA	C4A-NA-C1A	-5.58	104.20	106.71
37	C	510	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
37	B	507	CLA	O2D-CGD-CBD	5.58	121.19	111.27
37	40	209	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
37	b	503	CLA	C2C-C1C-NC	5.57	115.19	109.97
47	21	203	KC1	C3C-C4C-NC	5.57	115.12	109.88
37	d	404	CLA	O2D-CGD-CBD	5.57	121.17	111.27
48	31	314	A86	C3-C2-C1	-5.57	119.36	127.31
47	35	309	KC1	CBA-CAA-C2A	-5.57	104.02	125.27
37	14	305	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
37	C	508	CLA	O2D-CGD-CBD	5.57	121.17	111.27
37	11	310	CLA	CHD-C1D-ND	-5.57	119.34	124.45
47	17	305	KC1	C3B-C2B-C1B	-5.57	101.76	107.08
37	B	506	CLA	C2C-C1C-NC	5.57	115.19	109.97
37	B	515	CLA	C2C-C1C-NC	5.57	115.19	109.97
37	B	501	CLA	CHD-C1D-ND	-5.57	119.34	124.45
37	34	305	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
37	B	524	CLA	O2D-CGD-CBD	5.56	121.15	111.27
37	A	403	CLA	C2C-C1C-NC	5.56	115.18	109.97
37	37	303	CLA	C2C-C1C-NC	5.56	115.18	109.97
47	17	306	KC1	C3C-C4C-NC	5.56	115.11	109.88
47	15	309	KC1	CBA-CAA-C2A	-5.56	104.08	125.27
48	11	314	A86	C3-C2-C1	-5.56	119.38	127.31
37	a	403	CLA	C2C-C1C-NC	5.56	115.18	109.97
37	c	509	CLA	CHD-C1D-ND	-5.55	119.35	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	20	307	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
47	15	309	KC1	C3C-C4C-NC	5.55	115.11	109.88
37	C	509	CLA	CHD-C1D-ND	-5.55	119.35	124.45
37	z	102	CLA	C4A-NA-C1A	-5.55	104.21	106.71
37	B	510	CLA	C2C-C1C-NC	5.55	115.17	109.97
37	19	309	CLA	C2C-C1C-NC	5.55	115.17	109.97
47	16	304	KC1	C1A-C2A-C3A	-5.55	102.71	107.11
37	z	101	CLA	C2C-C1C-NC	5.55	115.17	109.97
47	36	304	KC1	C1A-C2A-C3A	-5.55	102.71	107.11
37	11	305	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
47	13	309	KC1	O2D-CGD-CBD	5.55	121.12	111.27
37	39	307	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
37	33	310	CLA	O2D-CGD-CBD	5.55	121.12	111.27
47	38	205	KC1	CMD-C2D-C1D	5.55	136.99	128.46
37	b	502	CLA	O2D-CGD-CBD	5.54	121.12	111.27
47	33	309	KC1	O2D-CGD-CBD	5.54	121.12	111.27
37	21	210	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
48	12	216	A86	C17-C16-C15	5.54	114.82	109.16
37	B	503	CLA	C2C-C1C-NC	5.54	115.16	109.97
48	37	314	A86	C3-C2-C1	-5.54	119.41	127.31
47	37	305	KC1	C3C-C4C-NC	5.54	115.09	109.88
47	14	306	KC1	C3C-C4C-NC	5.53	115.09	109.88
47	14	306	KC1	CMA-C3A-C2A	-5.53	114.76	128.30
47	34	306	KC1	CMA-C3A-C2A	-5.53	114.76	128.30
47	13	306	KC1	C3C-C4C-NC	5.53	115.08	109.88
40	a	409	SQD	O6-C1-C2	5.53	116.93	108.30
47	19	308	KC1	C3B-C2B-C1B	-5.53	101.80	107.08
37	c	503	CLA	C2C-C1C-NC	5.53	115.15	109.97
37	b	523	CLA	O2D-CGD-CBD	5.52	121.08	111.27
48	32	217	A86	C17-C16-C15	5.52	114.80	109.16
47	16	308	KC1	C3C-C4C-NC	5.52	115.07	109.88
37	17	304	CLA	C2C-C1C-NC	5.52	115.14	109.97
47	19	308	KC1	C3C-C4C-NC	5.52	115.07	109.88
37	34	303	CLA	C2C-C1C-NC	5.52	115.14	109.97
37	41	210	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
37	35	305	CLA	C2C-C1C-NC	5.52	115.14	109.97
37	21	210	CLA	O2D-CGD-CBD	5.52	121.07	111.27
37	14	303	CLA	C2C-C1C-NC	5.52	115.14	109.97
47	13	306	KC1	C3B-C2B-C1B	-5.51	101.81	107.08
40	A	407	SQD	O6-C1-C2	5.51	116.91	108.30
37	14	303	CLA	C4A-NA-C1A	-5.51	104.23	106.71
47	34	306	KC1	C3C-C4C-NC	5.51	115.06	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Z	101	CLA	C2C-C1C-NC	5.51	115.13	109.97
37	41	210	CLA	O2D-CGD-CBD	5.51	121.06	111.27
37	b	511	CLA	C2C-C1C-NC	5.51	115.13	109.97
48	40	211	A86	C25-C26-C27	-5.51	119.45	127.31
37	B	502	CLA	O2D-CGD-CBD	5.50	121.05	111.27
37	31	306	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
47	36	308	KC1	C3C-C4C-NC	5.50	115.06	109.88
47	35	309	KC1	C3C-C4C-NC	5.50	115.06	109.88
37	C	503	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
37	34	302	CLA	C2C-C1C-NC	5.50	115.12	109.97
47	39	308	KC1	C3B-C2B-C1B	-5.50	101.83	107.08
48	38	213	A86	C3-C2-C1	-5.50	119.47	127.31
48	20	309	A86	C25-C26-C27	-5.49	119.47	127.31
48	11	314	A86	O4-C38-C39	5.49	121.19	111.09
37	37	306	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
47	33	306	KC1	C3B-C2B-C1B	-5.49	101.83	107.08
37	c	508	CLA	CHD-C1D-ND	-5.49	119.41	124.45
48	21	215	A86	O4-C38-C39	5.49	121.19	111.09
37	c	503	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
37	B	511	CLA	C2C-C1C-NC	5.48	115.11	109.97
37	C	508	CLA	CHD-C1D-ND	-5.48	119.42	124.45
37	19	305	CLA	C2C-C1C-NC	5.48	115.10	109.97
48	17	310	A86	C4-C5-C6	-5.48	119.49	127.31
48	41	215	A86	O4-C38-C39	5.48	121.17	111.09
37	38	201	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
37	37	308	CLA	CAA-C2A-C3A	-5.47	97.79	112.78
37	w	101	CLA	C2C-C1C-NC	5.47	115.10	109.97
47	15	309	KC1	O2D-CGD-CBD	5.47	120.99	111.27
47	21	207	KC1	C3C-C4C-NC	5.47	115.03	109.88
47	37	307	KC1	O2D-CGD-CBD	5.47	120.99	111.27
37	19	309	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
47	33	306	KC1	C3C-C4C-NC	5.47	115.03	109.88
48	37	309	A86	C4-C5-C6	-5.47	119.50	127.31
37	A	403	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
47	17	308	KC1	O2D-CGD-CBD	5.47	120.98	111.27
37	b	510	CLA	C2C-C1C-NC	5.47	115.09	109.97
37	c	510	CLA	CHD-C1D-ND	-5.47	119.43	124.45
37	b	515	CLA	CHD-C4C-C3C	-5.47	116.81	124.84
37	16	309	CLA	C4A-NA-C1A	-5.47	104.25	106.71
37	12	204	CLA	O2D-CGD-CBD	5.46	120.98	111.27
37	17	307	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
48	41	213	A86	C17-C16-C15	5.46	114.74	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	41	207	KC1	C3C-C4C-NC	5.46	115.02	109.88
37	15	305	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
48	34	313	A86	O4-C38-C39	5.46	121.13	111.09
37	a	403	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
37	17	307	CLA	CHD-C1D-ND	-5.46	119.44	124.45
48	15	311	A86	C41-C32-C31	-5.46	105.59	110.47
37	C	510	CLA	CHD-C1D-ND	-5.46	119.44	124.45
48	11	311	A86	C3-C4-C5	-5.46	112.30	123.47
47	40	206	KC1	CMD-C2D-C1D	5.45	136.85	128.46
37	33	310	CLA	C4A-NA-C1A	-5.45	104.25	106.71
37	35	305	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
37	31	310	CLA	C2C-C1C-NC	5.45	115.08	109.97
37	34	305	CLA	C2C-C1C-NC	5.45	115.08	109.97
37	11	308	CLA	C2C-C1C-NC	5.45	115.08	109.97
37	21	205	CLA	C2C-C1C-NC	5.45	115.08	109.97
48	21	213	A86	C17-C16-C15	5.44	114.72	109.16
47	39	308	KC1	C3C-C4C-NC	5.44	115.00	109.88
47	36	304	KC1	O2D-CGD-CBD	5.44	120.94	111.27
37	B	515	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
37	32	205	CLA	O2D-CGD-CBD	5.44	120.94	111.27
37	34	303	CLA	C4A-NA-C1A	-5.44	104.26	106.71
47	35	306	KC1	C3C-C4C-NC	5.44	115.00	109.88
37	B	507	CLA	C2C-C1C-NC	5.44	115.07	109.97
47	31	309	KC1	C1A-C2A-C3A	-5.44	102.80	107.11
47	14	309	KC1	O2D-CGD-CBD	5.44	120.93	111.27
47	16	304	KC1	O2D-CGD-CBD	5.44	120.93	111.27
48	39	313	A86	C17-C16-C15	5.44	114.71	109.16
37	18	206	CLA	C2C-C1C-NC	5.44	115.06	109.97
37	31	301	CLA	C2C-C1C-NC	5.44	115.06	109.97
37	34	302	CLA	CHD-C1D-ND	-5.44	119.46	124.45
47	11	306	KC1	C3C-C4C-NC	5.43	114.99	109.88
37	13	310	CLA	O2D-CGD-CBD	5.43	120.92	111.27
37	11	310	CLA	C2C-C1C-NC	5.43	115.06	109.97
37	41	205	CLA	C2C-C1C-NC	5.43	115.06	109.97
47	11	309	KC1	C1A-C2A-C3A	-5.43	102.80	107.11
48	14	313	A86	O4-C38-C39	5.43	121.08	111.09
37	Z	102	CLA	C4A-NA-C1A	-5.43	104.27	106.71
50	21	212	DD6	C12-C11-C13	-5.43	109.52	118.08
47	20	304	KC1	CMD-C2D-C1D	5.43	136.81	128.46
37	C	512	CLA	CMD-C2D-C1D	5.43	134.28	124.71
47	18	205	KC1	CMD-C2D-C1D	5.43	136.81	128.46
37	B	516	CLA	CHD-C1D-ND	-5.43	119.47	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	13	310	CLA	C4A-NA-C1A	-5.43	104.27	106.71
37	C	503	CLA	C2C-C1C-NC	5.42	115.05	109.97
37	c	512	CLA	CMD-C2D-C1D	5.42	134.27	124.71
47	31	307	KC1	C3C-C4C-NC	5.42	114.98	109.88
47	33	304	KC1	C3B-C2B-C1B	-5.42	101.90	107.08
37	17	304	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
37	39	309	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
37	b	507	CLA	C2C-C1C-NC	5.42	115.05	109.97
50	41	212	DD6	C12-C11-C13	-5.42	109.54	118.08
48	31	311	A86	C3-C4-C5	-5.42	112.38	123.47
37	32	202	CLA	C2C-C1C-NC	5.42	115.05	109.97
37	C	501	CLA	O2D-CGD-CBD	5.42	120.89	111.27
47	15	304	KC1	CMD-C2D-C1D	5.42	136.79	128.46
37	18	211	CLA	CHD-C4C-C3C	-5.41	116.88	124.84
37	16	303	CLA	C2C-C1C-NC	5.41	115.04	109.97
37	W	102	CLA	C2C-C1C-NC	5.41	115.04	109.97
37	36	309	CLA	C4A-NA-C1A	-5.41	104.27	106.71
47	34	309	KC1	O2D-CGD-CBD	5.41	120.88	111.27
37	18	202	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
48	35	315	A86	O4-C38-C39	5.41	121.04	111.09
37	W	101	CLA	C2C-C1C-NC	5.41	115.04	109.97
37	34	303	CLA	O2D-CGD-CBD	5.41	120.88	111.27
47	11	302	KC1	O2D-CGD-CBD	5.41	120.88	111.27
48	15	315	A86	O4-C38-C39	5.41	121.04	111.09
37	18	206	CLA	O2D-CGD-CBD	5.41	120.87	111.27
37	D	402	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
37	17	309	CLA	CAA-C2A-C3A	-5.40	97.98	112.78
37	19	306	CLA	CMD-C2D-C1D	5.40	134.24	124.71
47	35	309	KC1	O2D-CGD-CBD	5.40	120.87	111.27
48	32	216	A86	C3-C2-C1	-5.40	119.60	127.31
47	32	209	KC1	O2D-CGD-CBD	5.40	120.87	111.27
37	41	209	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
37	C	512	CLA	CHD-C1D-ND	-5.40	119.49	124.45
37	38	206	CLA	O2D-CGD-CBD	5.40	120.86	111.27
48	31	315	A86	O4-C38-C39	5.40	121.02	111.09
48	33	313	A86	O4-C38-C39	5.40	121.02	111.09
37	37	306	CLA	CHD-C1D-ND	-5.40	119.49	124.45
37	37	303	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
37	19	309	CLA	CHD-C1D-ND	-5.39	119.50	124.45
47	15	306	KC1	C3C-C4C-NC	5.39	114.95	109.88
37	21	209	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
37	14	302	CLA	CHD-C1D-ND	-5.39	119.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	Z	102	CLA	C2C-C1C-NC	5.39	115.02	109.97
48	12	215	A86	C3-C2-C1	-5.39	119.61	127.31
47	12	208	KC1	O2D-CGD-CBD	5.39	120.85	111.27
37	39	302	CLA	C4A-NA-C1A	-5.39	104.28	106.71
37	20	303	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
37	40	205	CLA	CHD-C1D-ND	-5.39	119.50	124.45
37	14	305	CLA	C2C-C1C-NC	5.39	115.02	109.97
47	41	203	KC1	CMA-C3A-C2A	-5.39	115.11	128.30
37	20	303	CLA	CHD-C1D-ND	-5.39	119.50	124.45
37	36	303	CLA	C2C-C1C-NC	5.39	115.02	109.97
37	39	306	CLA	CMD-C2D-C1D	5.38	134.20	124.71
37	d	401	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
47	11	306	KC1	CMA-C3A-C2A	-5.38	115.12	128.30
37	14	303	CLA	O2D-CGD-CBD	5.38	120.83	111.27
47	16	304	KC1	CMD-C2D-C1D	5.38	136.74	128.46
37	c	512	CLA	C4A-NA-C1A	-5.38	104.29	106.71
37	b	516	CLA	CHD-C1D-ND	-5.38	119.51	124.45
37	b	523	CLA	CAA-C2A-C3A	-5.38	98.05	112.78
37	z	102	CLA	C2C-C1C-NC	5.37	115.01	109.97
47	31	303	KC1	O2D-CGD-CBD	5.37	120.82	111.27
37	c	501	CLA	O2D-CGD-CBD	5.37	120.82	111.27
37	21	208	CLA	C2C-C1C-NC	5.37	115.01	109.97
48	11	315	A86	O4-C38-C39	5.37	120.97	111.09
37	C	512	CLA	C4A-NA-C1A	-5.37	104.29	106.71
37	13	310	CLA	C2C-C1C-NC	5.37	115.00	109.97
47	31	307	KC1	CMA-C3A-C2A	-5.37	115.16	128.30
48	36	313	A86	O4-C38-C39	5.37	120.97	111.09
47	21	203	KC1	CMA-C3A-C2A	-5.36	115.17	128.30
48	13	313	A86	O4-C38-C39	5.36	120.96	111.09
37	34	310	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
47	17	306	KC1	C2C-C1C-NC	5.36	116.42	110.57
47	37	305	KC1	C2C-C1C-NC	5.36	116.42	110.57
47	36	304	KC1	CMD-C2D-C1D	5.36	136.70	128.46
37	B	505	CLA	O2D-CGD-CBD	5.35	120.78	111.27
37	c	508	CLA	CMD-C2D-C1D	5.35	134.15	124.71
47	34	309	KC1	CMD-C2D-C1D	5.35	136.69	128.46
37	12	212	CLA	CHD-C1D-ND	-5.35	119.54	124.45
37	40	205	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
37	b	501	CLA	C2C-C1C-NC	5.35	114.98	109.97
37	38	206	CLA	C2C-C1C-NC	5.35	114.98	109.97
37	C	508	CLA	CMD-C2D-C1D	5.35	134.14	124.71
37	17	309	CLA	C4A-NA-C1A	-5.35	104.30	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	32	213	CLA	CHD-C1D-ND	-5.35	119.54	124.45
37	21	210	CLA	C2C-C1C-NC	5.34	114.98	109.97
37	41	210	CLA	C2C-C1C-NC	5.34	114.98	109.97
37	39	302	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
37	33	310	CLA	C2C-C1C-NC	5.34	114.97	109.97
48	16	314	A86	O4-C38-C39	5.34	120.91	111.09
47	12	206	KC1	O2D-CGD-CBD	5.34	120.75	111.27
50	39	312	DD6	C12-C11-C13	-5.34	109.67	118.08
48	32	216	A86	C17-C16-C15	5.34	114.61	109.16
37	b	514	CLA	C2C-C1C-NC	5.34	114.97	109.97
37	41	208	CLA	C2C-C1C-NC	5.34	114.97	109.97
48	12	215	A86	C17-C16-C15	5.33	114.60	109.16
48	41	211	A86	C17-C16-C15	5.33	114.60	109.16
37	B	514	CLA	C2C-C1C-NC	5.33	114.97	109.97
37	19	302	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
47	13	302	KC1	C3C-C4C-NC	5.33	114.89	109.88
47	33	302	KC1	C3C-C4C-NC	5.33	114.89	109.88
37	C	511	CLA	C2C-C1C-NC	5.33	114.96	109.97
48	21	211	A86	C17-C16-C15	5.33	114.60	109.16
50	41	212	DD6	C21-C20-C19	-5.33	108.29	114.28
37	11	307	CLA	CHD-C1D-ND	-5.33	119.56	124.45
47	13	304	KC1	C3B-C2B-C1B	-5.33	101.99	107.08
37	C	501	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
48	21	213	A86	C3-C2-C1	-5.32	119.71	127.31
37	b	523	CLA	C2C-C1C-NC	5.32	114.96	109.97
37	32	211	CLA	CHD-C1D-ND	-5.32	119.56	124.45
37	b	505	CLA	O2D-CGD-CBD	5.32	120.73	111.27
37	31	304	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
42	A	409	BCT	O2-C-O1	5.32	133.35	119.55
37	B	501	CLA	C2C-C1C-NC	5.32	114.95	109.97
37	11	305	CLA	C2C-C1C-NC	5.32	114.95	109.97
37	35	308	CLA	C2C-C1C-NC	5.32	114.95	109.97
37	20	306	CLA	CHD-C1D-ND	-5.32	119.57	124.45
50	21	212	DD6	C21-C20-C19	-5.32	108.30	114.28
37	c	505	CLA	C2C-C1C-NC	5.32	114.95	109.97
42	a	411	BCT	O2-C-O1	5.32	133.34	119.55
37	c	512	CLA	CHD-C1D-ND	-5.32	119.57	124.45
48	41	213	A86	C3-C2-C1	-5.31	119.73	127.31
37	c	501	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
37	11	303	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
37	31	306	CLA	C2C-C1C-NC	5.31	114.94	109.97
37	B	507	CLA	CHD-C4C-C3C	-5.31	117.04	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	524	CLA	C2C-C1C-NC	5.31	114.94	109.97
37	17	302	CLA	C2C-C1C-NC	5.31	114.94	109.97
37	35	310	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
50	19	312	DD6	C12-C11-C13	-5.30	109.72	118.08
37	18	209	CLA	CHD-C1D-ND	-5.30	119.58	124.45
47	14	309	KC1	CMD-C2D-C1D	5.30	136.61	128.46
47	12	208	KC1	C3B-C2B-C1B	-5.30	102.02	107.08
37	15	310	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
37	21	202	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
37	41	205	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
37	20	307	CLA	C2C-C1C-NC	5.29	114.93	109.97
37	b	507	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
37	41	202	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
37	33	303	CLA	O2D-CGD-CBD	5.29	120.67	111.27
37	B	508	CLA	C2C-C1C-NC	5.29	114.93	109.97
37	c	511	CLA	C2C-C1C-NC	5.29	114.92	109.97
47	39	308	KC1	O2D-CGD-CBD	5.29	120.66	111.27
37	14	303	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
37	19	302	CLA	C4A-NA-C1A	-5.28	104.33	106.71
37	40	209	CLA	C2C-C1C-NC	5.28	114.92	109.97
37	C	512	CLA	C2C-C1C-NC	5.28	114.92	109.97
37	c	512	CLA	C2C-C1C-NC	5.28	114.92	109.97
48	41	211	A86	O4-C38-C39	5.28	120.80	111.09
37	21	205	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
47	37	305	KC1	C3B-C2B-C1B	-5.28	102.03	107.08
37	35	307	CLA	O2D-CGD-CBD	5.28	120.65	111.27
37	21	204	CLA	C2C-C1C-NC	5.28	114.92	109.97
48	21	211	A86	O4-C38-C39	5.28	120.80	111.09
37	13	303	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
47	19	308	KC1	O2D-CGD-CBD	5.28	120.64	111.27
37	34	303	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
37	c	511	CLA	CHD-C1D-ND	-5.27	119.61	124.45
37	a	407	CLA	C2C-C1C-NC	5.27	114.91	109.97
37	C	511	CLA	CHD-C1D-ND	-5.27	119.61	124.45
37	14	310	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
47	32	207	KC1	O2D-CGD-CBD	5.27	120.63	111.27
37	37	301	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
37	D	406	CLA	C2C-C1C-NC	5.27	114.91	109.97
37	31	308	CLA	CHD-C1D-ND	-5.27	119.61	124.45
37	12	210	CLA	CHD-C1D-ND	-5.27	119.61	124.45
47	33	302	KC1	C1A-NA-C4A	-5.27	104.34	106.71
37	41	204	CLA	C2C-C1C-NC	5.27	114.91	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	40	208	CLA	CHD-C1D-ND	-5.27	119.61	124.45
48	11	313	A86	C3-C2-C1	-5.27	119.79	127.31
47	35	304	KC1	CMD-C2D-C1D	5.27	136.56	128.46
47	37	302	KC1	CHC-C1C-C2C	-5.26	116.75	124.98
47	32	209	KC1	C3B-C2B-C1B	-5.26	102.05	107.08
37	c	508	CLA	C2C-C1C-NC	5.26	114.90	109.97
47	14	309	KC1	C3C-C4C-NC	5.26	114.83	109.88
47	31	307	KC1	CHD-C4C-C3C	-5.26	115.45	125.33
37	C	508	CLA	C2C-C1C-NC	5.26	114.90	109.97
47	38	207	KC1	C3B-C2B-C1B	-5.26	102.06	107.08
37	38	201	CLA	C4A-NA-C1A	-5.26	104.34	106.71
37	A	405	CLA	C2C-C1C-NC	5.26	114.89	109.97
37	C	505	CLA	C2C-C1C-NC	5.25	114.89	109.97
47	31	305	KC1	CMD-C2D-C1D	5.25	136.54	128.46
48	35	311	A86	O4-C38-C39	5.25	120.75	111.09
37	41	209	CLA	C2C-C1C-NC	5.25	114.89	109.97
47	20	302	KC1	CMD-C2D-C1D	5.25	136.53	128.46
37	B	513	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
37	B	524	CLA	CAA-C2A-C3A	-5.25	98.41	112.78
37	21	209	CLA	C2C-C1C-NC	5.25	114.89	109.97
48	31	313	A86	C3-C2-C1	-5.25	119.82	127.31
37	38	209	CLA	CHD-C1D-ND	-5.25	119.63	124.45
37	17	302	CLA	CHD-C4C-C3C	-5.25	117.13	124.84
37	d	404	CLA	C2C-C1C-NC	5.24	114.89	109.97
37	37	301	CLA	C2C-C1C-NC	5.24	114.88	109.97
48	32	217	A86	C25-C26-C27	-5.24	119.83	127.31
37	16	303	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
37	b	513	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
47	11	306	KC1	CHD-C4C-C3C	-5.24	115.49	125.33
47	17	306	KC1	C3B-C2B-C1B	-5.24	102.07	107.08
47	11	304	KC1	CMD-C2D-C1D	5.24	136.51	128.46
48	12	216	A86	C25-C26-C27	-5.24	119.83	127.31
37	B	504	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
37	19	304	CLA	C2C-C1C-NC	5.24	114.88	109.97
47	40	204	KC1	CMD-C2D-C1D	5.24	136.51	128.46
37	39	304	CLA	C2C-C1C-NC	5.23	114.87	109.97
47	38	210	KC1	C3C-C4C-NC	5.23	114.80	109.88
37	12	209	CLA	CHD-C1D-ND	-5.23	119.65	124.45
37	15	303	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
37	c	510	CLA	O2D-CGD-CBD	5.23	120.56	111.27
37	21	208	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
48	31	313	A86	C20-C19-C18	-5.22	102.42	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	18	210	KC1	C3C-C4C-NC	5.22	114.79	109.88
37	16	307	CLA	C2C-C1C-NC	5.22	114.86	109.97
37	37	308	CLA	C4A-NA-C1A	-5.22	104.36	106.71
37	37	303	CLA	O2D-CGD-CBD	5.22	120.54	111.27
37	36	303	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
48	32	221	A86	O4-C38-C39	5.22	120.69	111.09
48	32	215	A86	C4-C5-C6	-5.22	119.87	127.31
37	36	307	CLA	C2C-C1C-NC	5.22	114.86	109.97
37	b	504	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
37	15	307	CLA	O2D-CGD-CBD	5.22	120.53	111.27
37	b	508	CLA	C2C-C1C-NC	5.21	114.86	109.97
37	35	303	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
37	32	210	CLA	CHD-C1D-ND	-5.21	119.66	124.45
47	37	307	KC1	C1A-C2A-C3A	-5.21	102.98	107.11
48	34	311	A86	C41-C32-C31	-5.21	105.81	110.47
37	11	305	CLA	O2D-CGD-CBD	5.20	120.51	111.27
48	14	311	A86	C41-C32-C31	-5.20	105.82	110.47
47	34	309	KC1	C3C-C4C-NC	5.20	114.78	109.88
48	12	213	A86	C17-C16-C15	5.20	114.47	109.16
37	20	303	CLA	C2C-C1C-NC	5.20	114.84	109.97
37	b	502	CLA	C2C-C1C-NC	5.20	114.84	109.97
37	33	303	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
48	11	313	A86	C20-C19-C18	-5.20	102.47	112.75
37	B	503	CLA	CHD-C1D-ND	-5.20	119.68	124.45
47	17	303	KC1	CHC-C1C-C2C	-5.20	116.86	124.98
48	16	313	A86	C28-C27-C26	-5.20	115.64	122.92
37	b	503	CLA	CHD-C1D-ND	-5.19	119.68	124.45
37	17	304	CLA	O2D-CGD-CBD	5.19	120.50	111.27
37	41	208	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
48	32	214	A86	C17-C16-C15	5.19	114.46	109.16
37	13	310	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
37	15	308	CLA	CED-O2D-CGD	5.19	127.68	115.94
37	b	501	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
37	C	510	CLA	O2D-CGD-CBD	5.19	120.49	111.27
48	36	313	A86	C33-C32-C31	5.19	114.25	109.21
48	12	214	A86	C4-C5-C6	-5.19	119.91	127.31
47	17	308	KC1	C1A-C2A-C3A	-5.19	103.00	107.11
47	41	203	KC1	C1A-NA-C4A	-5.18	104.38	106.71
37	31	306	CLA	O2D-CGD-CBD	5.18	120.48	111.27
37	15	305	CLA	O2D-CGD-CBD	5.18	120.48	111.27
47	13	302	KC1	C1A-NA-C4A	-5.18	104.38	106.71
37	16	309	CLA	CHD-C4C-C3C	-5.18	117.23	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	17	302	CLA	CMD-C2D-C1D	5.18	133.84	124.71
48	37	313	A86	C25-C26-C27	-5.18	119.92	127.31
37	13	308	CLA	C4A-NA-C1A	-5.18	104.38	106.71
37	35	305	CLA	O2D-CGD-CBD	5.18	120.46	111.27
47	37	305	KC1	CMA-C3A-C2A	-5.17	115.63	128.30
48	15	314	A86	C17-C16-C15	5.17	114.44	109.16
48	32	203	A86	C33-C32-C31	5.17	114.24	109.21
37	40	205	CLA	O2D-CGD-CBD	5.17	120.46	111.27
37	C	502	CLA	C2C-C1C-NC	5.17	114.82	109.97
37	16	309	CLA	C2C-C1C-NC	5.17	114.82	109.97
47	17	306	KC1	CMA-C3A-C2A	-5.17	115.65	128.30
40	L	101	SQD	O7-S-C6	5.17	113.08	106.94
37	B	502	CLA	C2C-C1C-NC	5.17	114.81	109.97
37	18	208	CLA	C2C-C1C-NC	5.16	114.81	109.97
47	13	304	KC1	O2D-CGD-CBD	5.16	120.44	111.27
48	16	314	A86	C33-C32-C31	5.16	114.23	109.21
37	13	303	CLA	O2D-CGD-CBD	5.16	120.44	111.27
47	40	206	KC1	C3B-C2B-C1B	-5.16	102.15	107.08
37	B	506	CLA	C3C-C4C-NC	5.16	116.36	110.57
47	33	302	KC1	CMD-C2D-C1D	5.16	136.40	128.46
37	c	502	CLA	C2C-C1C-NC	5.16	114.81	109.97
40	B	519	SQD	O7-S-C6	5.16	113.07	106.94
37	A	405	CLA	O2D-CGD-CBD	5.16	120.43	111.27
37	36	309	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
37	33	305	CLA	C2C-C1C-NC	5.15	114.80	109.97
37	B	514	CLA	CHD-C1D-ND	-5.15	119.72	124.45
37	B	501	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
47	33	304	KC1	O2D-CGD-CBD	5.15	120.42	111.27
47	38	210	KC1	CMA-C3A-C2A	-5.15	115.69	128.30
48	33	312	A86	O4-C38-C39	5.15	120.56	111.09
47	18	210	KC1	CMA-C3A-C2A	-5.15	115.70	128.30
37	41	204	CLA	CHD-C4C-C3C	-5.15	117.28	124.84
37	a	407	CLA	O2D-CGD-CBD	5.15	120.41	111.27
37	21	204	CLA	CHD-C4C-C3C	-5.15	117.28	124.84
37	d	403	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
48	13	312	A86	O4-C38-C39	5.14	120.56	111.09
40	B	519	SQD	O9-S-C6	5.14	113.05	106.94
37	c	502	CLA	O2D-CGD-CBD	5.14	120.41	111.27
47	31	309	KC1	C3C-C4C-NC	5.14	114.72	109.88
47	36	302	KC1	C3C-C4C-NC	5.14	114.72	109.88
37	36	309	CLA	C2C-C1C-NC	5.14	114.79	109.97
47	20	304	KC1	C3B-C2B-C1B	-5.14	102.17	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	33	310	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
48	12	220	A86	O4-C38-C39	5.14	120.55	111.09
37	20	303	CLA	O2D-CGD-CBD	5.14	120.40	111.27
47	13	302	KC1	CMD-C2D-C1D	5.14	136.36	128.46
48	40	201	A86	C28-C27-C26	-5.14	115.73	122.92
47	21	203	KC1	C1A-NA-C4A	-5.14	104.40	106.71
48	12	202	A86	C33-C32-C31	5.14	114.20	109.21
37	C	502	CLA	O2D-CGD-CBD	5.14	120.39	111.27
37	D	405	CLA	C3D-C2D-C1D	-5.13	98.82	105.83
37	40	205	CLA	C2C-C1C-NC	5.13	114.78	109.97
47	13	304	KC1	CHD-C4C-C3C	-5.13	115.69	125.33
48	31	314	A86	O4-C38-C39	5.13	120.53	111.09
50	41	212	DD6	C26-C25-C24	5.13	139.23	123.22
48	38	213	A86	C17-C16-C15	5.13	114.40	109.16
47	12	211	KC1	CMD-C2D-C1D	5.13	136.35	128.46
50	21	212	DD6	C26-C25-C24	5.13	139.22	123.22
47	11	304	KC1	C3C-C4C-NC	5.13	114.70	109.88
37	13	305	CLA	C2C-C1C-NC	5.12	114.77	109.97
48	35	314	A86	C17-C16-C15	5.12	114.39	109.16
48	14	313	A86	C41-C32-C31	-5.12	105.89	110.47
37	c	504	CLA	C2C-C1C-NC	5.12	114.77	109.97
47	40	206	KC1	CHC-C1C-C2C	-5.12	116.98	124.98
40	L	101	SQD	O9-S-C6	5.12	113.02	106.94
47	33	304	KC1	CHD-C4C-C3C	-5.12	115.72	125.33
47	31	305	KC1	C3C-C4C-NC	5.12	114.70	109.88
37	11	308	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
37	33	303	CLA	C4A-NA-C1A	-5.11	104.41	106.71
47	36	302	KC1	C3B-C2B-C1B	-5.11	102.19	107.08
37	c	506	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
37	32	202	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
47	35	304	KC1	O2D-CGD-CBD	5.11	120.35	111.27
37	c	502	CLA	CHD-C1D-ND	-5.11	119.76	124.45
47	36	302	KC1	CHC-C1C-C2C	-5.11	117.00	124.98
37	b	509	CLA	C4A-NA-C1A	-5.11	104.41	106.71
50	20	312	DD6	C7-C6-C8	-5.11	110.03	118.08
37	35	308	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
37	C	504	CLA	C2C-C1C-NC	5.11	114.76	109.97
47	40	207	KC1	CHC-C1C-C2C	-5.11	117.00	124.98
47	16	302	KC1	C3B-C2B-C1B	-5.11	102.20	107.08
47	16	305	KC1	O2D-CGD-CBD	5.11	120.34	111.27
37	c	503	CLA	C4A-NA-C1A	-5.10	104.41	106.71
48	15	319	A86	O4-C38-C39	5.10	120.48	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	37	306	CLA	O2D-CGD-CBD	5.10	120.34	111.27
37	37	308	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
37	b	514	CLA	CHD-C1D-ND	-5.10	119.77	124.45
37	C	506	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
48	37	311	A86	C4-C5-C6	-5.10	120.04	127.31
37	b	506	CLA	C3C-C4C-NC	5.10	116.29	110.57
47	20	305	KC1	CHC-C1C-C2C	-5.10	117.02	124.98
47	32	212	KC1	CMD-C2D-C1D	5.09	136.29	128.46
48	20	311	A86	C25-C26-C27	-5.09	120.04	127.31
48	34	313	A86	C41-C32-C31	-5.09	105.91	110.47
47	20	304	KC1	CHC-C1C-C2C	-5.09	117.02	124.98
37	C	502	CLA	CHD-C1D-ND	-5.09	119.77	124.45
37	31	301	CLA	O2D-CGD-CBD	5.09	120.32	111.27
48	12	220	A86	C12-C11-C13	5.09	124.57	116.02
47	16	302	KC1	C3C-C4C-NC	5.09	114.67	109.88
48	35	319	A86	O4-C38-C39	5.09	120.45	111.09
47	18	205	KC1	C3C-C4C-NC	5.09	114.67	109.88
37	33	308	CLA	C4A-NA-C1A	-5.09	104.42	106.71
37	34	307	CLA	C2C-C1C-NC	5.09	114.74	109.97
37	12	205	CLA	C4A-NA-C1A	-5.08	104.42	106.71
48	33	315	A86	C3-C2-C1	-5.08	120.05	127.31
37	17	307	CLA	C2C-C1C-NC	5.08	114.73	109.97
47	11	309	KC1	C3C-C4C-NC	5.08	114.66	109.88
50	40	214	DD6	C7-C6-C8	-5.08	110.07	118.08
37	W	102	CLA	O2D-CGD-CBD	5.08	120.29	111.27
37	37	303	CLA	C4A-NA-C1A	-5.08	104.42	106.71
40	40	202	SQD	O7-S-C6	5.08	112.97	106.94
48	11	314	A86	C17-C16-C15	5.08	114.34	109.16
48	40	213	A86	C25-C26-C27	-5.07	120.07	127.31
47	38	205	KC1	O2D-CGD-CBD	5.07	120.28	111.27
48	41	211	A86	C41-C32-C31	-5.07	105.93	110.47
47	18	205	KC1	O2D-CGD-CBD	5.07	120.28	111.27
37	15	308	CLA	CHD-C4C-C3C	-5.07	117.38	124.84
47	31	309	KC1	CMD-C2D-C1D	5.07	136.26	128.46
37	17	309	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
47	36	305	KC1	O2D-CGD-CBD	5.07	120.28	111.27
48	21	211	A86	C41-C32-C31	-5.07	105.94	110.47
48	39	311	A86	C17-C16-C15	5.07	114.33	109.16
48	14	315	A86	C3-C2-C1	-5.07	120.08	127.31
47	17	308	KC1	C3C-C4C-NC	5.07	114.65	109.88
47	21	207	KC1	CHD-C4C-C3C	-5.07	115.82	125.33
37	36	306	CLA	CHD-C1D-ND	-5.07	119.80	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	32	221	A86	C12-C11-C13	5.07	124.53	116.02
37	17	307	CLA	O2D-CGD-CBD	5.07	120.27	111.27
37	18	211	CLA	C2C-C1C-NC	5.07	114.72	109.97
48	40	201	A86	C3-C2-C1	-5.06	120.08	127.31
47	37	307	KC1	C3C-C4C-NC	5.06	114.64	109.88
40	16	315	SQD	O7-S-C6	5.06	112.96	106.94
48	31	314	A86	C17-C16-C15	5.06	114.33	109.16
37	37	306	CLA	C2C-C1C-NC	5.06	114.71	109.97
47	41	207	KC1	CHD-C4C-C3C	-5.06	115.83	125.33
47	11	309	KC1	CMD-C2D-C1D	5.06	136.24	128.46
48	19	311	A86	C17-C16-C15	5.06	114.32	109.16
47	16	302	KC1	CHC-C1C-C2C	-5.06	117.08	124.98
48	34	315	A86	C3-C2-C1	-5.05	120.10	127.31
47	32	209	KC1	CHD-C4C-C3C	-5.05	115.85	125.33
47	35	309	KC1	C1A-C2A-C3A	-5.05	103.11	107.11
48	16	313	A86	C3-C2-C1	-5.05	120.11	127.31
37	B	506	CLA	O2D-CGD-CBD	5.05	120.24	111.27
37	b	506	CLA	O2D-CGD-CBD	5.05	120.24	111.27
37	Z	101	CLA	O2D-CGD-CBD	5.05	120.23	111.27
37	16	306	CLA	CHD-C1D-ND	-5.05	119.82	124.45
48	13	315	A86	C3-C2-C1	-5.04	120.11	127.31
37	20	306	CLA	C4A-NA-C1A	-5.04	104.44	106.71
37	33	308	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
37	40	208	CLA	O2D-CGD-CBD	5.04	120.22	111.27
48	34	314	A86	C25-C26-C27	-5.04	120.12	127.31
37	c	504	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
47	35	302	KC1	CMD-C2D-C1D	5.04	136.21	128.46
37	D	405	CLA	CAA-C2A-C3A	-5.04	98.98	112.78
37	d	401	CLA	C2C-C1C-NC	5.04	114.69	109.97
37	C	504	CLA	CHD-C4C-C3C	-5.04	117.44	124.84
37	d	403	CLA	CAA-C2A-C3A	-5.04	98.99	112.78
37	20	306	CLA	O2D-CGD-CBD	5.04	120.22	111.27
47	12	208	KC1	CHD-C4C-C3C	-5.04	115.88	125.33
37	z	102	CLA	CAA-C2A-C3A	-5.03	98.99	112.78
48	13	311	A86	O4-C38-C39	5.03	120.35	111.09
37	z	101	CLA	O2D-CGD-CBD	5.03	120.21	111.27
47	15	302	KC1	C3C-C4C-NC	5.03	114.61	109.88
48	12	216	A86	O4-C38-C39	5.03	120.34	111.09
48	14	314	A86	C25-C26-C27	-5.03	120.13	127.31
37	32	213	CLA	C2C-C1C-NC	5.03	114.68	109.97
37	31	304	CLA	C4A-NA-C1A	-5.03	104.45	106.71
37	38	206	CLA	C4A-NA-C1A	-5.03	104.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	12	210	CLA	CHD-C4C-C3C	-5.03	117.45	124.84
37	12	212	CLA	C2C-C1C-NC	5.03	114.68	109.97
47	11	302	KC1	C3C-C4C-NC	5.03	114.61	109.88
37	33	301	CLA	C2C-C1C-NC	5.02	114.68	109.97
37	b	523	CLA	C4A-NA-C1A	-5.02	104.45	106.71
37	16	301	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
48	18	213	A86	C23-C16-C22	-5.02	99.96	107.37
37	35	308	CLA	C4A-NA-C1A	-5.02	104.45	106.71
37	13	308	CLA	CHD-C4C-C3C	-5.02	117.47	124.84
47	32	212	KC1	C3C-C4C-NC	5.02	114.60	109.88
37	Z	102	CLA	CAA-C2A-C3A	-5.02	99.04	112.78
37	41	208	CLA	O2D-CGD-CBD	5.02	120.18	111.27
45	D	404	PL9	C7-C3-C4	5.02	120.95	116.88
47	39	308	KC1	CHD-C4C-C3C	-5.01	115.92	125.33
37	C	503	CLA	C4A-NA-C1A	-5.01	104.45	106.71
47	15	309	KC1	C1A-C2A-C3A	-5.01	103.14	107.11
37	38	202	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
48	17	314	A86	C25-C26-C27	-5.01	120.16	127.31
47	17	305	KC1	CMA-C3A-C2A	-5.01	116.03	128.30
47	19	308	KC1	CHD-C4C-C3C	-5.01	115.93	125.33
50	16	312	DD6	C21-C20-C15	-5.01	113.87	122.26
37	14	307	CLA	C2C-C1C-NC	5.01	114.66	109.97
37	B	524	CLA	C4A-NA-C1A	-5.01	104.45	106.71
48	33	311	A86	O4-C38-C39	5.01	120.30	111.09
37	14	307	CLA	CHD-C1D-ND	-5.01	119.85	124.45
37	D	402	CLA	C2C-C1C-NC	5.00	114.66	109.97
47	20	304	KC1	O2D-CGD-CBD	5.00	120.16	111.27
47	40	206	KC1	O2D-CGD-CBD	5.00	120.16	111.27
50	36	312	DD6	C21-C20-C15	-5.00	113.88	122.26
48	32	217	A86	O4-C38-C39	5.00	120.29	111.09
37	20	301	CLA	O2D-CGD-CBD	5.00	120.16	111.27
37	38	208	CLA	C2C-C1C-NC	5.00	114.66	109.97
50	36	312	DD6	C7-C6-C8	-5.00	110.20	118.08
37	17	304	CLA	C4A-NA-C1A	-5.00	104.46	106.71
37	36	301	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
37	32	211	CLA	CHD-C4C-C3C	-5.00	117.50	124.84
37	c	507	CLA	CHD-C1D-ND	-5.00	119.86	124.45
37	34	307	CLA	CHD-C1D-ND	-5.00	119.86	124.45
37	12	207	CLA	C2C-C1C-NC	5.00	114.65	109.97
47	31	305	KC1	O2D-CGD-CBD	5.00	120.15	111.27
37	b	503	CLA	C4A-NA-C1A	-5.00	104.46	106.71
37	32	208	CLA	C2C-C1C-NC	5.00	114.65	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	36	304	KC1	C3C-C4C-NC	5.00	114.58	109.88
37	B	512	CLA	C3C-C4C-NC	5.00	116.17	110.57
37	B	503	CLA	C4A-NA-C1A	-4.99	104.46	106.71
37	11	303	CLA	C4A-NA-C1A	-4.99	104.46	106.71
37	21	208	CLA	O2D-CGD-CBD	4.99	120.14	111.27
37	41	202	CLA	O2D-CGD-CBD	4.99	120.14	111.27
47	20	304	KC1	CBA-CAA-C2A	-4.99	106.26	125.27
47	33	309	KC1	CHC-C1C-C2C	-4.99	117.19	124.98
37	41	209	CLA	O2D-CGD-CBD	4.99	120.13	111.27
47	37	302	KC1	CMD-C2D-C1D	4.98	136.12	128.46
48	41	211	A86	C25-C26-C27	-4.98	120.20	127.31
48	12	216	A86	C40-C32-C31	-4.98	106.01	110.47
48	32	217	A86	C40-C32-C31	-4.98	106.01	110.47
45	d	402	PL9	C7-C3-C4	4.98	120.93	116.88
47	16	304	KC1	C3C-C4C-NC	4.98	114.57	109.88
47	31	303	KC1	C3C-C4C-NC	4.98	114.57	109.88
37	18	206	CLA	C4A-NA-C1A	-4.98	104.47	106.71
50	21	216	DD6	C24-C1-C2	-4.98	111.30	118.94
47	13	309	KC1	CHC-C1C-C2C	-4.98	117.20	124.98
47	40	206	KC1	CBA-CAA-C2A	-4.98	106.29	125.27
37	b	523	CLA	C3C-C4C-NC	4.98	116.15	110.57
50	41	216	DD6	C24-C1-C2	-4.98	111.31	118.94
37	b	510	CLA	CHD-C1D-ND	-4.98	119.88	124.45
37	c	508	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
37	32	206	CLA	C4A-NA-C1A	-4.98	104.47	106.71
37	c	503	CLA	O2D-CGD-CBD	4.98	120.11	111.27
47	32	207	KC1	CAC-C3C-C2C	4.97	136.04	127.53
47	15	302	KC1	CMD-C2D-C1D	4.97	136.11	128.46
48	40	211	A86	O4-C38-C39	4.97	120.24	111.09
37	B	510	CLA	CHD-C1D-ND	-4.97	119.88	124.45
48	38	214	A86	C17-C16-C15	4.97	114.24	109.16
48	34	312	A86	O4-C38-C39	4.97	120.24	111.09
47	37	304	KC1	CMA-C3A-C2A	-4.97	116.13	128.30
37	19	304	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
47	35	302	KC1	C3C-C4C-NC	4.97	114.56	109.88
47	11	304	KC1	O2D-CGD-CBD	4.97	120.10	111.27
47	35	306	KC1	CMD-C2D-C1D	4.97	136.10	128.46
48	17	312	A86	C4-C5-C6	-4.97	120.22	127.31
47	12	206	KC1	CAC-C3C-C2C	4.97	136.03	127.53
50	16	312	DD6	C7-C6-C8	-4.97	110.25	118.08
37	b	506	CLA	C4A-NA-C1A	-4.97	104.47	106.71
47	35	304	KC1	C1A-NA-C4A	-4.97	104.47	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	502	CLA	CAA-C2A-C3A	-4.97	99.18	112.78
47	34	304	KC1	O2D-CGD-CBD	4.97	120.09	111.27
37	B	524	CLA	C3C-C4C-NC	4.97	116.14	110.57
37	b	502	CLA	CAA-C2A-C3A	-4.97	99.18	112.78
37	21	202	CLA	O2D-CGD-CBD	4.97	120.09	111.27
50	19	312	DD6	C-C1-C24	-4.97	110.25	118.08
48	40	211	A86	C3-C2-C1	-4.97	120.22	127.31
37	B	506	CLA	C4A-NA-C1A	-4.96	104.47	106.71
37	35	307	CLA	CMD-C2D-C1D	4.96	133.46	124.71
48	20	309	A86	C3-C2-C1	-4.96	120.23	127.31
48	20	309	A86	O4-C38-C39	4.96	120.22	111.09
47	37	302	KC1	C2C-C1C-NC	4.96	115.99	110.57
47	17	303	KC1	CMD-C2D-C1D	4.96	136.09	128.46
37	12	205	CLA	C2C-C1C-NC	4.96	114.62	109.97
48	21	211	A86	C25-C26-C27	-4.96	120.23	127.31
47	20	302	KC1	C1A-NA-C4A	-4.96	104.48	106.71
37	b	512	CLA	C2C-C1C-NC	4.96	114.62	109.97
37	36	303	CLA	O2D-CGD-CBD	4.96	120.08	111.27
37	13	301	CLA	C2C-C1C-NC	4.96	114.61	109.97
37	40	203	CLA	O2D-CGD-CBD	4.96	120.07	111.27
37	C	503	CLA	O2D-CGD-CBD	4.95	120.07	111.27
37	C	508	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
47	15	306	KC1	CMD-C2D-C1D	4.95	136.08	128.46
37	B	512	CLA	C2C-C1C-NC	4.95	114.61	109.97
37	39	309	CLA	C4A-NA-C1A	-4.95	104.48	106.71
47	41	203	KC1	C4B-C3B-C2B	-4.95	102.69	106.75
37	39	304	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
47	18	207	KC1	C3B-C2B-C1B	-4.95	102.35	107.08
37	B	516	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
37	C	502	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
37	19	303	CLA	C2C-C1C-NC	4.95	114.61	109.97
48	14	312	A86	O4-C38-C39	4.94	120.19	111.09
37	13	305	CLA	O2D-CGD-CBD	4.94	120.05	111.27
48	40	211	A86	C17-C16-C15	4.94	114.20	109.16
37	16	303	CLA	O2D-CGD-CBD	4.94	120.05	111.27
48	35	311	A86	C3-C4-C5	-4.94	113.36	123.47
47	13	309	KC1	C3C-C4C-NC	4.94	114.53	109.88
37	B	509	CLA	C4A-NA-C1A	-4.94	104.49	106.71
37	40	208	CLA	C4A-NA-C1A	-4.94	104.49	106.71
37	39	301	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
47	35	306	KC1	CHD-C4C-C3C	-4.94	116.06	125.33
47	33	309	KC1	C3C-C4C-NC	4.94	114.53	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	512	CLA	C3C-C4C-NC	4.94	116.11	110.57
37	D	401	CLA	O2D-CGD-CBD	4.94	120.04	111.27
37	A	403	CLA	C4A-NA-C1A	-4.94	104.49	106.71
37	21	209	CLA	O2D-CGD-CBD	4.93	120.04	111.27
47	14	304	KC1	O2D-CGD-CBD	4.93	120.04	111.27
37	37	303	CLA	CAA-C2A-C3A	-4.93	99.27	112.78
44	c	516	DGD	O3G-C3G-C2G	-4.93	98.99	110.90
48	15	311	A86	C3-C4-C5	-4.93	113.37	123.47
37	a	404	CLA	O2D-CGD-CBD	4.93	120.03	111.27
47	37	304	KC1	O2D-CGD-CBD	4.93	120.03	111.27
48	20	309	A86	C17-C16-C15	4.93	114.19	109.16
37	C	507	CLA	CHD-C1D-ND	-4.93	119.93	124.45
47	15	304	KC1	O2D-CGD-CBD	4.93	120.02	111.27
47	18	210	KC1	CMD-C2D-C1D	4.93	136.04	128.46
47	12	211	KC1	C3C-C4C-NC	4.93	114.52	109.88
37	33	305	CLA	O2D-CGD-CBD	4.93	120.02	111.27
47	40	207	KC1	C2C-C1C-NC	4.92	115.95	110.57
44	C	516	DGD	O3G-C3G-C2G	-4.92	99.02	110.90
47	18	207	KC1	C2C-C1C-NC	4.92	115.95	110.57
37	19	303	CLA	C4A-NA-C1A	-4.92	104.49	106.71
37	39	303	CLA	C4A-NA-C1A	-4.92	104.49	106.71
37	36	306	CLA	O2D-CGD-CBD	4.92	120.01	111.27
48	17	312	A86	O4-C38-C39	4.92	120.14	111.09
47	20	305	KC1	C2C-C1C-NC	4.92	115.94	110.57
37	36	309	CLA	O2D-CGD-CBD	4.92	120.01	111.27
37	b	516	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
50	39	312	DD6	C-C1-C24	-4.92	110.33	118.08
37	D	405	CLA	C2C-C1C-NC	4.92	114.58	109.97
48	14	311	A86	O4-C38-C39	4.92	120.14	111.09
48	11	313	A86	C4-C5-C6	-4.92	120.29	127.31
37	32	210	CLA	C2C-C1C-NC	4.92	114.58	109.97
47	38	205	KC1	C3C-C4C-NC	4.91	114.50	109.88
47	34	309	KC1	CHD-C4C-C3C	-4.91	116.11	125.33
47	17	303	KC1	C2C-C1C-NC	4.91	115.94	110.57
47	14	309	KC1	CHD-C4C-C3C	-4.91	116.11	125.33
37	b	505	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
37	15	307	CLA	CMD-C2D-C1D	4.91	133.37	124.71
37	39	303	CLA	C2C-C1C-NC	4.91	114.57	109.97
37	35	303	CLA	C4A-NA-C1A	-4.91	104.50	106.71
47	17	303	KC1	O2D-CGD-CBD	4.91	119.99	111.27
47	41	207	KC1	CMD-C2D-C1D	4.91	136.01	128.46
37	c	502	CLA	C3D-C2D-C1D	-4.91	99.13	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	16	309	CLA	O2D-CGD-CBD	4.91	119.99	111.27
48	17	313	A86	O4-C38-C39	4.91	120.11	111.09
47	40	206	KC1	C2C-C1C-NC	4.90	115.93	110.57
37	16	306	CLA	O2D-CGD-CBD	4.90	119.98	111.27
47	37	302	KC1	O2D-CGD-CBD	4.90	119.98	111.27
48	34	311	A86	O4-C38-C39	4.90	120.11	111.09
47	21	207	KC1	CMD-C2D-C1D	4.90	136.00	128.46
48	41	211	A86	C3-C2-C1	-4.90	120.32	127.31
48	37	311	A86	O4-C38-C39	4.90	120.10	111.09
48	37	312	A86	O4-C38-C39	4.90	120.10	111.09
48	13	314	A86	O4-C38-C39	4.90	120.10	111.09
47	20	304	KC1	C2C-C1C-NC	4.90	115.92	110.57
37	d	403	CLA	C2C-C1C-NC	4.90	114.56	109.97
47	37	307	KC1	CMD-C2D-C1D	4.90	135.99	128.46
47	14	304	KC1	C3C-C4C-NC	4.90	114.49	109.88
47	34	304	KC1	C3C-C4C-NC	4.90	114.49	109.88
48	33	314	A86	O4-C38-C39	4.89	120.09	111.09
37	41	204	CLA	CAA-C2A-C3A	-4.89	99.38	112.78
37	19	301	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
47	32	207	KC1	C3B-C2B-C1B	-4.89	102.41	107.08
37	39	304	CLA	C4A-NA-C1A	-4.89	104.51	106.71
47	12	206	KC1	C3B-C2B-C1B	-4.89	102.41	107.08
48	21	211	A86	C3-C2-C1	-4.89	120.33	127.31
47	38	207	KC1	CHD-C4C-C3C	-4.89	116.15	125.33
48	13	312	A86	C36-C31-C32	-4.89	114.85	119.70
47	35	302	KC1	O2D-CGD-CBD	4.89	119.95	111.27
37	17	304	CLA	CAA-C2A-C3A	-4.89	99.40	112.78
37	38	211	CLA	CHD-C4C-C3C	-4.88	117.66	124.84
48	33	312	A86	C36-C31-C32	-4.88	114.85	119.70
47	31	305	KC1	CHC-C1C-C2C	-4.88	117.35	124.98
47	21	203	KC1	C4B-C3B-C2B	-4.88	102.74	106.75
37	19	309	CLA	C4A-NA-C1A	-4.88	104.51	106.71
47	15	306	KC1	CHD-C4C-C3C	-4.88	116.17	125.33
37	19	307	CLA	C4A-NA-C1A	-4.88	104.51	106.71
47	17	305	KC1	O2D-CGD-CBD	4.88	119.94	111.27
48	12	213	A86	C25-C26-C27	-4.88	120.35	127.31
37	31	302	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
37	C	503	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
50	41	216	DD6	C21-C20-C19	-4.87	108.80	114.28
37	21	209	CLA	C4A-NA-C1A	-4.87	104.52	106.71
48	38	214	A86	O4-C38-C39	4.87	120.06	111.09
37	34	307	CLA	O2D-CGD-CBD	4.87	119.93	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	40	210	CLA	CHD-C1D-ND	-4.87	119.98	124.45
48	18	215	A86	O4-C38-C39	4.87	120.05	111.09
37	21	204	CLA	CAA-C2A-C3A	-4.87	99.44	112.78
37	17	302	CLA	CHD-C1D-ND	-4.87	119.98	124.45
37	B	505	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
47	11	304	KC1	CHC-C1C-C2C	-4.87	117.37	124.98
48	37	319	A86	O4-C38-C39	4.87	120.05	111.09
37	12	209	CLA	C2C-C1C-NC	4.87	114.53	109.97
48	17	320	A86	O4-C38-C39	4.87	120.04	111.09
37	D	401	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
47	12	206	KC1	CMD-C2D-C1D	4.87	135.94	128.46
47	41	203	KC1	CHD-C4C-C3C	-4.87	116.20	125.33
47	38	207	KC1	C2C-C1C-NC	4.86	115.88	110.57
37	B	509	CLA	O2D-CGD-CBD	4.86	119.91	111.27
48	38	215	A86	O4-C38-C39	4.86	120.03	111.09
47	21	203	KC1	CHD-C4C-C3C	-4.86	116.20	125.33
47	35	304	KC1	CHC-C1C-C2C	-4.86	117.38	124.98
47	40	204	KC1	C1A-NA-C4A	-4.86	104.52	106.71
48	18	214	A86	C17-C16-C15	4.86	114.12	109.16
50	21	216	DD6	C21-C20-C19	-4.86	108.81	114.28
37	11	301	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
37	13	301	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
47	13	304	KC1	CMD-C2D-C1D	4.86	135.93	128.46
47	14	304	KC1	CMD-C2D-C1D	4.86	135.93	128.46
37	20	308	CLA	CHD-C1D-ND	-4.86	119.99	124.45
37	32	205	CLA	C3C-C4C-NC	4.86	116.02	110.57
37	14	307	CLA	O2D-CGD-CBD	4.85	119.89	111.27
48	14	314	A86	O4-C38-C39	4.85	120.02	111.09
48	16	313	A86	C26-C25-C24	-4.85	108.07	123.22
48	34	314	A86	O4-C38-C39	4.85	120.02	111.09
47	15	302	KC1	O2D-CGD-CBD	4.85	119.89	111.27
47	15	304	KC1	CHC-C1C-C2C	-4.85	117.40	124.98
48	18	214	A86	O4-C38-C39	4.85	120.02	111.09
37	34	301	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
37	c	503	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
37	21	206	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
47	17	308	KC1	CMD-C2D-C1D	4.85	135.91	128.46
37	41	206	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
47	32	207	KC1	CMD-C2D-C1D	4.85	135.91	128.46
37	b	509	CLA	O2D-CGD-CBD	4.85	119.88	111.27
47	36	302	KC1	C2C-C1C-NC	4.84	115.86	110.57
48	40	201	A86	C26-C25-C24	-4.84	108.10	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	15	301	CLA	C2C-C1C-NC	4.84	114.51	109.97
48	32	216	A86	O4-C38-C39	4.84	120.00	111.09
37	21	206	CLA	C2C-C1C-NC	4.84	114.51	109.97
47	13	309	KC1	CMA-C3A-C2A	-4.84	116.45	128.30
37	B	509	CLA	CHD-C1D-ND	-4.84	120.00	124.45
37	b	509	CLA	CHD-C1D-ND	-4.84	120.00	124.45
37	39	307	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
47	33	309	KC1	CMA-C3A-C2A	-4.84	116.45	128.30
37	41	206	CLA	C2C-C1C-NC	4.84	114.50	109.97
47	33	304	KC1	CMD-C2D-C1D	4.84	135.90	128.46
37	C	511	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
37	15	303	CLA	C4A-NA-C1A	-4.84	104.53	106.71
48	31	313	A86	O4-C38-C39	4.84	119.99	111.09
37	a	404	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
37	12	204	CLA	C3C-C4C-NC	4.83	115.99	110.57
47	16	305	KC1	CHD-C4C-C3C	-4.83	116.26	125.33
47	17	305	KC1	C3C-C4C-NC	4.83	114.42	109.88
37	b	511	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
37	B	511	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
37	39	306	CLA	CHD-C1D-ND	-4.83	120.02	124.45
37	14	301	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
48	12	215	A86	O4-C38-C39	4.83	119.97	111.09
37	33	301	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
37	15	307	CLA	C4A-NA-C1A	-4.82	104.54	106.71
48	17	315	A86	C25-C26-C27	-4.82	120.43	127.31
48	15	312	A86	O4-C38-C39	4.82	119.96	111.09
37	32	208	CLA	O2D-CGD-CBD	4.82	119.84	111.27
47	36	305	KC1	CHD-C4C-C3C	-4.82	116.28	125.33
37	C	513	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
37	c	513	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
47	31	303	KC1	CHC-C1C-C2C	-4.82	117.45	124.98
37	35	301	CLA	C2C-C1C-NC	4.82	114.48	109.97
37	12	207	CLA	O2D-CGD-CBD	4.82	119.83	111.27
37	38	209	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
37	11	307	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
47	38	210	KC1	CMD-C2D-C1D	4.81	135.86	128.46
37	19	306	CLA	CHD-C1D-ND	-4.81	120.03	124.45
48	18	214	A86	C25-C26-C27	-4.81	120.44	127.31
47	31	303	KC1	CMA-C3A-C2A	-4.81	116.53	128.30
47	11	302	KC1	CMA-C3A-C2A	-4.81	116.53	128.30
47	34	304	KC1	CMD-C2D-C1D	4.81	135.85	128.46
37	19	307	CLA	C3D-C2D-C1D	-4.81	99.27	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	35	312	A86	O4-C38-C39	4.81	119.93	111.09
48	37	314	A86	C25-C26-C27	-4.80	120.46	127.31
47	31	309	KC1	CHC-C1C-C2C	-4.80	117.48	124.98
48	35	314	A86	O4-C38-C39	4.80	119.92	111.09
47	17	306	KC1	C4B-C3B-C2B	-4.80	102.81	106.75
37	a	403	CLA	C4A-NA-C1A	-4.80	104.55	106.71
37	19	304	CLA	C4A-NA-C1A	-4.80	104.55	106.71
37	18	209	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
47	14	306	KC1	CHD-C4C-C3C	-4.80	116.32	125.33
37	19	309	CLA	O2D-CGD-CBD	4.80	119.79	111.27
37	c	511	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
37	39	305	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
37	39	309	CLA	O2D-CGD-CBD	4.79	119.79	111.27
37	14	307	CLA	C4A-NA-C1A	-4.79	104.55	106.71
48	17	314	A86	C17-C16-C15	4.79	114.05	109.16
37	B	509	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
37	15	301	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
50	16	312	DD6	C15-C14-C13	-4.79	115.87	125.99
48	15	314	A86	O4-C38-C39	4.79	119.90	111.09
48	31	319	A86	C20-C19-C18	-4.79	103.28	112.75
47	37	302	KC1	C3C-C4C-NC	4.79	114.39	109.88
47	34	306	KC1	CHD-C4C-C3C	-4.79	116.34	125.33
47	16	308	KC1	CHD-C4C-C3C	-4.79	116.34	125.33
48	37	314	A86	O4-C38-C39	4.79	119.90	111.09
37	B	506	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
37	c	506	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
37	31	308	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
48	16	313	A86	O4-C38-C39	4.79	119.89	111.09
37	B	516	CLA	C2C-C1C-NC	4.78	114.45	109.97
37	16	306	CLA	C2C-C1C-NC	4.78	114.45	109.97
48	21	214	A86	O4-C38-C39	4.78	119.89	111.09
37	20	301	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
50	36	312	DD6	C15-C14-C13	-4.78	115.89	125.99
48	40	201	A86	O4-C38-C39	4.78	119.88	111.09
37	13	307	CLA	CED-O2D-CGD	4.78	126.74	115.94
37	21	205	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
37	b	506	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
47	11	302	KC1	CHC-C1C-C2C	-4.78	117.52	124.98
37	35	301	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
37	d	403	CLA	C4A-NA-C1A	-4.78	104.56	106.71
37	b	509	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
48	17	315	A86	O4-C38-C39	4.78	119.88	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	d	404	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
37	19	305	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
47	17	303	KC1	C3C-C4C-NC	4.77	114.37	109.88
37	39	307	CLA	C4A-NA-C1A	-4.77	104.56	106.71
37	d	401	CLA	O2D-CGD-CBD	4.77	119.75	111.27
47	37	305	KC1	CMD-C2D-C1D	4.77	135.80	128.46
37	w	101	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
48	11	315	A86	C33-C32-C31	4.77	113.85	109.21
48	17	314	A86	O4-C38-C39	4.77	119.86	111.09
48	32	214	A86	O4-C38-C39	4.77	119.86	111.09
47	15	309	KC1	CHD-C4C-C3C	-4.77	116.38	125.33
47	17	306	KC1	CMD-C2D-C1D	4.77	135.79	128.46
47	37	307	KC1	CHD-C4C-C3C	-4.77	116.38	125.33
48	21	213	A86	O4-C38-C39	4.76	119.86	111.09
47	13	306	KC1	CHD-C4C-C3C	-4.76	116.39	125.33
48	41	214	A86	O4-C38-C39	4.76	119.85	111.09
47	36	308	KC1	CHD-C4C-C3C	-4.76	116.39	125.33
48	38	214	A86	C25-C26-C27	-4.76	120.51	127.31
37	34	302	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
37	B	510	CLA	C4A-NA-C1A	-4.76	104.56	106.71
47	11	309	KC1	CHC-C1C-C2C	-4.76	117.54	124.98
37	40	203	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
37	C	506	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
37	33	307	CLA	CED-O2D-CGD	4.76	126.70	115.94
37	41	209	CLA	C4A-NA-C1A	-4.76	104.57	106.71
37	32	206	CLA	C2C-C1C-NC	4.76	114.43	109.97
48	11	319	A86	C20-C19-C18	-4.76	103.33	112.75
47	35	309	KC1	CHD-C4C-C3C	-4.76	116.40	125.33
37	W	101	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
37	b	508	CLA	O2D-CGD-CBD	4.76	119.72	111.27
37	B	514	CLA	C4A-NA-C1A	-4.76	104.57	106.71
37	34	307	CLA	C4A-NA-C1A	-4.76	104.57	106.71
47	16	302	KC1	C2C-C1C-NC	4.75	115.76	110.57
37	36	306	CLA	C2C-C1C-NC	4.75	114.43	109.97
47	33	306	KC1	CHD-C4C-C3C	-4.75	116.41	125.33
47	17	308	KC1	CHD-C4C-C3C	-4.75	116.41	125.33
48	41	213	A86	O4-C38-C39	4.75	119.83	111.09
37	D	406	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
37	41	205	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
37	18	204	CLA	C4A-NA-C1A	-4.75	104.57	106.71
37	B	507	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
37	C	513	CLA	O2D-CGD-CBD	4.75	119.71	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	35	307	CLA	C2C-C1C-NC	4.75	114.42	109.97
48	38	213	A86	O4-C38-C39	4.75	119.83	111.09
37	34	310	CLA	O2D-CGD-CBD	4.75	119.70	111.27
37	b	516	CLA	C2C-C1C-NC	4.75	114.42	109.97
47	11	302	KC1	CHD-C4C-C3C	-4.75	116.42	125.33
47	37	305	KC1	C4B-C3B-C2B	-4.74	102.86	106.75
47	14	304	KC1	CHD-C4C-C3C	-4.74	116.42	125.33
47	34	304	KC1	CHD-C4C-C3C	-4.74	116.42	125.33
37	B	508	CLA	O2D-CGD-CBD	4.74	119.70	111.27
37	c	507	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
48	12	213	A86	O4-C38-C39	4.74	119.81	111.09
37	19	304	CLA	O2D-CGD-CBD	4.74	119.69	111.27
37	14	302	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
47	18	207	KC1	CHD-C4C-C3C	-4.74	116.43	125.33
37	16	303	CLA	CAA-C2A-C3A	-4.74	99.80	112.78
37	36	303	CLA	CAA-C2A-C3A	-4.74	99.80	112.78
37	B	515	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
37	c	513	CLA	O2D-CGD-CBD	4.74	119.69	111.27
37	12	212	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
47	11	306	KC1	CMD-C2D-C1D	4.74	135.75	128.46
37	18	201	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
37	38	208	CLA	C4A-NA-C1A	-4.74	104.58	106.71
37	40	203	CLA	C2C-C1C-NC	4.74	114.41	109.97
37	20	301	CLA	C2C-C1C-NC	4.74	114.41	109.97
47	20	305	KC1	CMD-C2D-C1D	4.74	135.74	128.46
37	C	504	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
37	18	208	CLA	C4A-NA-C1A	-4.74	104.58	106.71
47	13	306	KC1	C2C-C1C-NC	4.74	115.74	110.57
47	31	303	KC1	CHD-C4C-C3C	-4.73	116.44	125.33
47	40	207	KC1	CMD-C2D-C1D	4.73	135.74	128.46
37	c	504	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
37	38	204	CLA	C4A-NA-C1A	-4.73	104.58	106.71
37	C	513	CLA	C2C-C1C-NC	4.73	114.40	109.97
37	b	515	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
37	D	402	CLA	O2D-CGD-CBD	4.72	119.66	111.27
37	36	309	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
47	34	304	KC1	C1A-NA-C4A	-4.72	104.58	106.71
47	16	302	KC1	C4B-C3B-C2B	-4.72	102.87	106.75
37	16	309	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
48	37	313	A86	C17-C16-C15	4.72	113.98	109.16
47	31	307	KC1	CMD-C2D-C1D	4.72	135.72	128.46
37	C	511	CLA	O2D-CGD-CBD	4.72	119.66	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	31	301	CLA	CHD-C1D-ND	-4.72	120.12	124.45
37	14	310	CLA	O2D-CGD-CBD	4.72	119.65	111.27
47	15	304	KC1	C3C-C4C-NC	4.72	114.32	109.88
48	31	312	A86	O4-C38-C39	4.72	119.77	111.09
37	b	512	CLA	C1D-CHD-C4C	-4.72	115.88	126.06
48	16	310	A86	O4-C38-C39	4.72	119.77	111.09
37	b	507	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
47	18	210	KC1	CHC-C1C-C2C	-4.72	117.61	124.98
37	b	514	CLA	C4A-NA-C1A	-4.72	104.59	106.71
37	c	505	CLA	C4A-NA-C1A	-4.72	104.59	106.71
37	B	505	CLA	C2C-C1C-NC	4.71	114.39	109.97
47	38	210	KC1	CHC-C1C-C2C	-4.71	117.61	124.98
37	B	512	CLA	C1D-CHD-C4C	-4.71	115.89	126.06
37	C	507	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
48	12	215	A86	C25-C26-C27	-4.71	120.59	127.31
37	39	302	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
37	c	511	CLA	O2D-CGD-CBD	4.71	119.64	111.27
47	35	302	KC1	CHC-C1C-C2C	-4.71	117.62	124.98
48	12	214	A86	O4-C38-C39	4.71	119.75	111.09
48	32	215	A86	O4-C38-C39	4.71	119.75	111.09
37	W	102	CLA	CHD-C1D-ND	-4.71	120.13	124.45
47	19	308	KC1	C1A-NA-C4A	-4.71	104.59	106.71
47	39	308	KC1	C1A-NA-C4A	-4.71	104.59	106.71
48	31	315	A86	C33-C32-C31	4.71	113.78	109.21
48	40	213	A86	O4-C38-C39	4.71	119.75	111.09
37	21	210	CLA	C4A-NA-C1A	-4.70	104.59	106.71
48	18	213	A86	O4-C38-C39	4.70	119.74	111.09
37	32	204	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
48	32	216	A86	C25-C26-C27	-4.70	120.60	127.31
37	12	203	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
37	37	303	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
47	33	306	KC1	O2D-CGD-CBD	4.70	119.62	111.27
48	40	201	A86	C24-C1-C2	4.70	126.15	118.94
47	14	304	KC1	CHC-C1C-C2C	-4.70	117.64	124.98
48	20	311	A86	O4-C38-C39	4.70	119.73	111.09
37	20	308	CLA	O2D-CGD-CBD	4.70	119.61	111.27
48	11	312	A86	O4-C38-C39	4.70	119.73	111.09
47	13	306	KC1	O2D-CGD-CBD	4.70	119.61	111.27
48	13	313	A86	C25-C26-C27	-4.69	120.61	127.31
37	40	210	CLA	O2D-CGD-CBD	4.69	119.61	111.27
50	19	312	DD6	C21-C20-C19	-4.69	109.00	114.28
37	32	213	CLA	C3D-C2D-C1D	-4.69	99.43	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	18	213	A86	C40-C32-C31	-4.69	106.27	110.47
48	32	216	A86	C4-C5-C6	-4.69	120.62	127.31
47	20	302	KC1	C3C-C4C-NC	4.69	114.29	109.88
48	33	313	A86	C25-C26-C27	-4.69	120.62	127.31
48	36	310	A86	O4-C38-C39	4.69	119.71	111.09
37	39	304	CLA	O2D-CGD-CBD	4.69	119.60	111.27
47	18	207	KC1	CHC-C1C-C2C	-4.69	117.66	124.98
47	33	306	KC1	C2C-C1C-NC	4.69	115.69	110.57
48	37	309	A86	C25-C26-C27	-4.68	120.62	127.31
48	16	313	A86	C24-C1-C2	4.68	126.13	118.94
47	40	204	KC1	C3C-C4C-NC	4.68	114.29	109.88
47	38	210	KC1	CHD-C4C-C3C	-4.68	116.54	125.33
48	14	313	A86	C3-C2-C1	-4.68	120.63	127.31
47	12	211	KC1	CHD-C4C-C3C	-4.68	116.54	125.33
48	37	312	A86	C3-C2-C1	-4.68	120.63	127.31
37	19	302	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
48	38	213	A86	C40-C32-C31	-4.68	106.28	110.47
48	33	311	A86	C25-C26-C27	-4.68	120.63	127.31
37	17	304	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
37	b	505	CLA	C2C-C1C-NC	4.68	114.35	109.97
37	b	502	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
37	15	307	CLA	C2C-C1C-NC	4.67	114.35	109.97
37	15	310	CLA	C4A-NA-C1A	-4.67	104.61	106.71
47	34	304	KC1	CHC-C1C-C2C	-4.67	117.68	124.98
37	a	407	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
47	41	203	KC1	CMD-C2D-C1D	4.67	135.64	128.46
47	17	308	KC1	CHC-C1C-C2C	-4.67	117.68	124.98
37	35	307	CLA	C4A-NA-C1A	-4.67	104.61	106.71
50	39	312	DD6	C21-C20-C15	-4.67	114.44	122.26
37	41	204	CLA	C4A-NA-C1A	-4.66	104.61	106.71
47	21	203	KC1	CMD-C2D-C1D	4.66	135.63	128.46
47	35	304	KC1	C3C-C4C-NC	4.66	114.27	109.88
48	17	310	A86	C25-C26-C27	-4.66	120.65	127.31
37	12	209	CLA	C4A-NA-C1A	-4.66	104.61	106.71
47	20	304	KC1	C3C-C4C-NC	4.66	114.27	109.88
48	15	319	A86	C4-C5-C6	-4.66	120.66	127.31
48	12	215	A86	C4-C5-C6	-4.66	120.66	127.31
48	37	312	A86	C17-C16-C15	4.66	113.92	109.16
37	C	505	CLA	C4A-NA-C1A	-4.66	104.61	106.71
37	D	405	CLA	C4A-NA-C1A	-4.66	104.61	106.71
37	b	510	CLA	C4A-NA-C1A	-4.66	104.61	106.71
37	41	210	CLA	C4A-NA-C1A	-4.66	104.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	39	312	DD6	C21-C20-C19	-4.66	109.04	114.28
37	33	305	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
37	A	405	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
37	a	404	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
47	18	210	KC1	CHD-C4C-C3C	-4.66	116.59	125.33
50	41	212	DD6	C24-C1-C2	-4.66	111.80	118.94
47	14	306	KC1	CHC-C1C-C2C	-4.65	117.71	124.98
37	40	208	CLA	C2C-C1C-NC	4.65	114.33	109.97
47	32	212	KC1	CHD-C4C-C3C	-4.65	116.60	125.33
50	19	312	DD6	C21-C20-C15	-4.65	114.47	122.26
48	41	215	A86	C4-C5-C6	-4.65	120.67	127.31
37	19	310	CLA	O2D-CGD-CBD	4.65	119.53	111.27
37	b	508	CLA	C4A-NA-C1A	-4.65	104.61	106.71
48	36	313	A86	C12-C11-C13	4.65	123.83	116.02
48	35	319	A86	C4-C5-C6	-4.65	120.67	127.31
37	36	307	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
37	15	308	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
47	36	302	KC1	CMD-C2D-C1D	4.65	135.61	128.46
48	34	313	A86	C3-C2-C1	-4.65	120.68	127.31
50	21	212	DD6	C24-C1-C2	-4.65	111.81	118.94
47	18	210	KC1	C1A-C2A-C3A	-4.64	103.43	107.11
37	39	310	CLA	O2D-CGD-CBD	4.64	119.52	111.27
37	20	306	CLA	C2C-C1C-NC	4.64	114.32	109.97
37	38	208	CLA	O2D-CGD-CBD	4.64	119.52	111.27
47	15	302	KC1	C1A-NA-C4A	-4.64	104.62	106.71
47	40	206	KC1	C3C-C4C-NC	4.64	114.25	109.88
37	41	210	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
37	c	513	CLA	C2C-C1C-NC	4.64	114.32	109.97
48	39	313	A86	C36-C31-C32	-4.64	115.09	119.70
37	12	209	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
37	21	210	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
48	21	215	A86	C36-C31-C32	-4.64	115.09	119.70
47	34	306	KC1	CHC-C1C-C2C	-4.64	117.74	124.98
37	13	305	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
47	36	302	KC1	C4B-C3B-C2B	-4.64	102.94	106.75
37	B	502	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
47	18	207	KC1	C4B-C3B-C2B	-4.63	102.95	106.75
47	16	302	KC1	CMD-C2D-C1D	4.63	135.58	128.46
37	32	208	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
37	16	307	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
37	18	204	CLA	C2C-C1C-NC	4.63	114.31	109.97
48	41	215	A86	C36-C31-C32	-4.63	115.10	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	21	204	CLA	C4A-NA-C1A	-4.63	104.62	106.71
47	31	305	KC1	C2C-C1C-NC	4.63	115.62	110.57
37	38	204	CLA	C2C-C1C-NC	4.63	114.31	109.97
37	D	401	CLA	C1C-C2C-C3C	-4.63	102.09	106.96
37	b	514	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
47	40	204	KC1	CHC-C1C-C2C	-4.62	117.75	124.98
48	14	316	A86	C20-C19-C18	-4.62	103.60	112.75
47	16	305	KC1	CHC-C1C-C2C	-4.62	117.76	124.98
47	37	302	KC1	C1C-C2C-C3C	-4.62	102.10	106.96
37	z	101	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
48	21	214	A86	C3-C2-C1	-4.62	120.71	127.31
37	B	514	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
47	38	210	KC1	C1A-C2A-C3A	-4.62	103.45	107.11
47	20	302	KC1	CHC-C1C-C2C	-4.62	117.76	124.98
48	16	314	A86	C12-C11-C13	4.62	123.78	116.02
37	12	205	CLA	CAA-C2A-C3A	-4.62	100.13	112.78
37	b	510	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
48	17	313	A86	C17-C16-C15	4.62	113.87	109.16
37	33	303	CLA	CAA-C2A-C3A	-4.62	100.14	112.78
37	11	310	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
47	37	307	KC1	CHC-C1C-C2C	-4.62	117.77	124.98
37	18	208	CLA	CHD-C1D-ND	-4.61	120.21	124.45
48	34	316	A86	C20-C19-C18	-4.61	103.62	112.75
48	35	315	A86	C25-C26-C27	-4.61	120.73	127.31
48	21	215	A86	C4-C5-C6	-4.61	120.73	127.31
37	40	209	CLA	C4A-NA-C1A	-4.61	104.63	106.71
37	B	515	CLA	O2D-CGD-CBD	4.61	119.46	111.27
47	16	305	KC1	C2C-C1C-NC	4.61	115.60	110.57
37	32	206	CLA	CAA-C2A-C3A	-4.61	100.16	112.78
37	C	510	CLA	C4A-NA-C1A	-4.61	104.64	106.71
47	36	304	KC1	CHD-C4C-C3C	-4.61	116.68	125.33
37	B	510	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
47	20	304	KC1	C4B-C3B-C2B	-4.60	102.97	106.75
37	b	515	CLA	O2D-CGD-CBD	4.60	119.45	111.27
48	19	313	A86	C36-C31-C32	-4.60	115.13	119.70
37	12	207	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
48	21	213	A86	C41-C32-C31	-4.60	106.36	110.47
37	32	204	CLA	C2C-C1C-NC	4.60	114.28	109.97
37	12	203	CLA	C2C-C1C-NC	4.60	114.28	109.97
47	31	305	KC1	CHD-C4C-C3C	-4.60	116.70	125.33
37	38	203	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
47	16	304	KC1	CHD-C4C-C3C	-4.60	116.70	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	19	301	CLA	C2C-C1C-NC	4.60	114.28	109.97
48	41	214	A86	C3-C2-C1	-4.60	120.75	127.31
48	34	311	A86	C17-C16-C15	4.59	113.85	109.16
37	B	524	CLA	C1D-CHD-C4C	-4.59	116.15	126.06
37	b	523	CLA	C1D-CHD-C4C	-4.59	116.15	126.06
37	32	210	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
37	41	208	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
47	17	303	KC1	C1C-C2C-C3C	-4.59	102.13	106.96
37	Z	101	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
37	39	301	CLA	C2C-C1C-NC	4.59	114.27	109.97
37	31	310	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
48	15	313	A86	O4-C38-C39	4.59	119.53	111.09
37	20	301	CLA	C3D-C4D-ND	4.59	117.66	110.24
37	40	203	CLA	C3D-C4D-ND	4.59	117.66	110.24
47	38	207	KC1	CHC-C1C-C2C	-4.59	117.81	124.98
37	37	301	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
47	40	206	KC1	C4B-C3B-C2B	-4.59	102.98	106.75
47	38	205	KC1	CHC-C1C-C2C	-4.59	117.81	124.98
48	11	313	A86	C25-C24-C1	-4.59	113.53	126.42
48	35	313	A86	O4-C38-C39	4.58	119.52	111.09
47	11	304	KC1	CHD-C4C-C3C	-4.58	116.73	125.33
37	13	303	CLA	CAA-C2A-C3A	-4.58	100.23	112.78
37	20	308	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
47	11	304	KC1	C2C-C1C-NC	4.58	115.57	110.57
47	14	306	KC1	C2C-C1C-NC	4.58	115.57	110.57
37	32	206	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
37	c	512	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
37	38	208	CLA	CHD-C1D-ND	-4.58	120.25	124.45
37	d	401	CLA	C4A-NA-C1A	-4.58	104.65	106.71
37	C	512	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
37	39	306	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
37	32	210	CLA	C4A-NA-C1A	-4.58	104.65	106.71
47	21	207	KC1	C1A-NA-C4A	-4.58	104.65	106.71
37	40	210	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
48	13	311	A86	C41-C32-C31	-4.58	106.38	110.47
37	B	508	CLA	C4A-NA-C1A	-4.58	104.65	106.71
37	20	307	CLA	C4A-NA-C1A	-4.58	104.65	106.71
37	31	304	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
47	36	304	KC1	CHC-C1C-C2C	-4.57	117.83	124.98
48	16	314	A86	C25-C26-C27	-4.57	120.78	127.31
48	34	311	A86	C25-C26-C27	-4.57	120.78	127.31
48	36	313	A86	C25-C26-C27	-4.57	120.78	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	16	308	KC1	CHC-C1C-C2C	-4.57	117.84	124.98
47	11	309	KC1	CHD-C4C-C3C	-4.57	116.75	125.33
47	13	302	KC1	CHD-C4C-C3C	-4.57	116.75	125.33
47	31	309	KC1	CHD-C4C-C3C	-4.57	116.75	125.33
48	13	311	A86	C25-C26-C27	-4.57	120.79	127.31
48	21	214	A86	C17-C16-C15	4.57	113.83	109.16
37	32	211	CLA	C4A-NA-C1A	-4.57	104.65	106.71
47	14	304	KC1	C1A-NA-C4A	-4.57	104.65	106.71
37	38	202	CLA	C2C-C1C-NC	4.57	114.25	109.97
47	36	305	KC1	CHC-C1C-C2C	-4.57	117.84	124.98
37	21	208	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
48	17	313	A86	C3-C2-C1	-4.57	120.79	127.31
37	12	205	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
48	41	214	A86	C17-C16-C15	4.57	113.82	109.16
37	38	203	CLA	O2D-CGD-CBD	4.57	119.38	111.27
37	20	307	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
37	D	402	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
47	33	302	KC1	O2D-CGD-CBD	4.56	119.38	111.27
48	37	313	A86	O4-C38-C39	4.56	119.49	111.09
47	36	305	KC1	C2C-C1C-NC	4.56	115.55	110.57
37	21	209	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
37	16	303	CLA	C4A-NA-C1A	-4.56	104.66	106.71
47	34	309	KC1	C1A-C2A-C3A	-4.56	103.49	107.11
37	D	402	CLA	C4A-NA-C1A	-4.56	104.66	106.71
37	12	212	CLA	C4A-NA-C1A	-4.56	104.66	106.71
37	32	213	CLA	C4A-NA-C1A	-4.56	104.66	106.71
48	36	311	A86	C20-C19-C18	-4.56	103.73	112.75
47	32	212	KC1	CHC-C1C-C2C	-4.56	117.86	124.98
48	15	315	A86	C25-C26-C27	-4.56	120.80	127.31
37	19	306	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
47	16	304	KC1	CHC-C1C-C2C	-4.56	117.86	124.98
37	36	303	CLA	C4A-NA-C1A	-4.56	104.66	106.71
37	38	201	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
37	B	524	CLA	CBA-CAA-C2A	4.56	127.31	113.86
37	32	202	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
37	B	502	CLA	C4A-NA-C1A	-4.56	104.66	106.71
37	35	303	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
47	19	308	KC1	C2A-C1A-NA	4.55	116.71	109.40
47	39	308	KC1	C2A-C1A-NA	4.55	116.71	109.40
37	11	303	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
48	20	311	A86	C40-C32-C31	-4.55	106.40	110.47
37	B	501	CLA	C3D-C2D-C1D	-4.55	99.62	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	14	311	A86	C25-C26-C27	-4.55	120.81	127.31
48	35	316	A86	C41-C32-C31	-4.55	106.40	110.47
37	31	306	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
37	18	203	CLA	O2D-CGD-CBD	4.55	119.36	111.27
37	40	209	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
37	d	401	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
48	13	313	A86	C3-C2-C1	-4.55	120.82	127.31
37	19	304	CLA	CHD-C4C-C3C	-4.55	118.16	124.84
50	40	212	DD6	C25-C24-C1	-4.55	113.65	126.42
48	33	313	A86	C3-C2-C1	-4.54	120.82	127.31
50	20	310	DD6	C25-C24-C1	-4.54	113.65	126.42
37	b	502	CLA	C4A-NA-C1A	-4.54	104.66	106.71
47	33	302	KC1	CHD-C4C-C3C	-4.54	116.80	125.33
47	17	303	KC1	CBC-CAC-C3C	-4.54	99.91	112.43
47	36	308	KC1	CHC-C1C-C2C	-4.54	117.88	124.98
48	41	213	A86	C41-C32-C31	-4.54	106.41	110.47
47	32	209	KC1	CMD-C2D-C1D	4.54	135.44	128.46
48	37	312	A86	C40-C32-C31	-4.54	106.41	110.47
48	16	311	A86	C20-C19-C18	-4.54	103.77	112.75
47	12	211	KC1	CHC-C1C-C2C	-4.54	117.89	124.98
37	14	303	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
37	34	303	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
47	34	306	KC1	CMD-C2D-C1D	4.54	135.44	128.46
47	20	302	KC1	CHD-C4C-C3C	-4.54	116.81	125.33
47	37	302	KC1	CBC-CAC-C3C	-4.53	99.93	112.43
37	c	509	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
37	35	307	CLA	CHD-C1D-ND	-4.53	120.29	124.45
50	40	214	DD6	C15-C14-C13	4.53	135.58	125.99
47	40	204	KC1	CHD-C4C-C3C	-4.53	116.82	125.33
48	35	319	A86	C3-C2-C1	-4.53	120.84	127.31
37	11	308	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
37	35	310	CLA	C4A-NA-C1A	-4.53	104.67	106.71
47	15	304	KC1	C1A-NA-C4A	-4.53	104.67	106.71
47	15	302	KC1	CHC-C1C-C2C	-4.53	117.90	124.98
37	W	102	CLA	C1D-CHD-C4C	-4.53	116.29	126.06
48	33	311	A86	C41-C32-C31	-4.53	106.42	110.47
47	35	304	KC1	C2C-C1C-NC	4.53	115.51	110.57
37	18	201	CLA	C4A-NA-C1A	-4.52	104.67	106.71
37	15	303	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
48	15	319	A86	C3-C2-C1	-4.52	120.86	127.31
48	18	213	A86	C36-C31-C32	-4.52	115.21	119.70
37	b	501	CLA	C3D-C2D-C1D	-4.52	99.66	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	35	302	KC1	C2C-C1C-NC	4.52	115.51	110.57
37	C	505	CLA	CHD-C1D-ND	-4.52	120.30	124.45
48	17	313	A86	C40-C32-C31	-4.52	106.43	110.47
37	C	509	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
37	11	307	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
37	41	209	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
50	20	312	DD6	C15-C14-C13	4.52	135.55	125.99
47	14	309	KC1	C1A-C2A-C3A	-4.52	103.53	107.11
47	13	302	KC1	O2D-CGD-CBD	4.52	119.30	111.27
47	35	302	KC1	CHD-C4C-C3C	-4.52	116.85	125.33
37	c	510	CLA	C4A-NA-C1A	-4.52	104.67	106.71
37	12	207	CLA	C4A-NA-C1A	-4.52	104.67	106.71
47	37	302	KC1	CMA-C3A-C2A	-4.52	117.24	128.30
47	14	306	KC1	CMD-C2D-C1D	4.52	135.41	128.46
47	34	306	KC1	C2C-C1C-NC	4.52	115.50	110.57
37	15	307	CLA	CHD-C1D-ND	-4.52	120.30	124.45
47	12	208	KC1	CMD-C2D-C1D	4.52	135.40	128.46
47	18	205	KC1	CHC-C1C-C2C	-4.51	117.93	124.98
50	39	312	DD6	C7-C6-C8	-4.51	110.97	118.08
47	18	205	KC1	CHD-C4C-C3C	-4.51	116.86	125.33
37	14	302	CLA	O2D-CGD-CBD	4.51	119.29	111.27
47	33	306	KC1	CHC-C1C-C2C	-4.51	117.93	124.98
47	33	306	KC1	CMD-C2D-C1D	4.51	135.40	128.46
37	35	305	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
47	12	208	KC1	CHC-C1C-C2C	-4.51	117.93	124.98
37	15	305	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
37	11	305	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
37	32	208	CLA	C4A-NA-C1A	-4.51	104.68	106.71
37	31	301	CLA	C1D-CHD-C4C	-4.51	116.33	126.06
48	38	213	A86	C36-C31-C32	-4.51	115.22	119.70
48	41	214	A86	C4-C5-C6	-4.51	120.88	127.31
48	40	213	A86	C40-C32-C31	-4.51	106.44	110.47
47	38	207	KC1	C4B-C3B-C2B	-4.51	103.05	106.75
37	b	523	CLA	CBA-CAA-C2A	4.51	127.16	113.86
37	18	208	CLA	O2D-CGD-CBD	4.50	119.27	111.27
37	41	210	CLA	C3D-C4D-ND	4.50	117.52	110.24
48	17	310	A86	C41-C32-C31	-4.50	106.44	110.47
50	19	312	DD6	C7-C6-C8	-4.50	110.98	118.08
37	19	306	CLA	C4A-NA-C1A	-4.50	104.68	106.71
37	34	302	CLA	O2D-CGD-CBD	4.50	119.27	111.27
47	32	209	KC1	CHC-C1C-C2C	-4.50	117.95	124.98
37	39	304	CLA	CHD-C4C-C3C	-4.50	118.22	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	18	211	CLA	C4A-NA-C1A	-4.50	104.68	106.71
47	41	207	KC1	C1A-NA-C4A	-4.50	104.68	106.71
47	13	306	KC1	CMD-C2D-C1D	4.50	135.38	128.46
47	20	302	KC1	O2D-CGD-CBD	4.50	119.26	111.27
47	33	302	KC1	C2C-C1C-NC	4.50	115.48	110.57
47	17	303	KC1	CMA-C3A-C2A	-4.50	117.29	128.30
37	14	305	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
37	34	305	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
47	15	302	KC1	CHD-C4C-C3C	-4.50	116.88	125.33
47	15	304	KC1	C2C-C1C-NC	4.50	115.48	110.57
47	13	309	KC1	CBA-CAA-C2A	-4.50	108.13	125.27
47	33	309	KC1	CBA-CAA-C2A	-4.50	108.13	125.27
37	C	501	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
37	35	301	CLA	C3D-C4D-ND	4.49	117.51	110.24
47	37	304	KC1	C1A-NA-C4A	-4.49	104.69	106.71
37	c	501	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
37	38	211	CLA	C4A-NA-C1A	-4.49	104.69	106.71
48	21	214	A86	C4-C5-C6	-4.49	120.90	127.31
37	18	203	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
37	D	405	CLA	C3D-C4D-ND	4.49	117.50	110.24
48	11	313	A86	O4-C38-C39	4.49	119.35	111.09
37	19	302	CLA	O2D-CGD-O1D	-4.49	115.06	123.84
37	15	301	CLA	C3D-C4D-ND	4.49	117.50	110.24
37	21	210	CLA	C3D-C4D-ND	4.48	117.49	110.24
37	d	404	CLA	C4A-NA-C1A	-4.48	104.69	106.71
37	c	513	CLA	C4A-NA-C1A	-4.48	104.69	106.71
37	13	303	CLA	C4A-NA-C1A	-4.48	104.69	106.71
48	14	311	A86	C17-C16-C15	4.48	113.73	109.16
47	40	204	KC1	O2D-CGD-CBD	4.48	119.23	111.27
47	13	306	KC1	CHC-C1C-C2C	-4.48	117.98	124.98
37	33	310	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
37	38	204	CLA	C3D-C4D-ND	4.48	117.48	110.24
37	12	204	CLA	C1D-CHD-C4C	-4.48	116.40	126.06
37	c	505	CLA	CHD-C1D-ND	-4.48	120.34	124.45
48	34	314	A86	C17-C16-C15	4.47	113.73	109.16
37	18	204	CLA	C3D-C4D-ND	4.47	117.48	110.24
37	39	306	CLA	C4A-NA-C1A	-4.47	104.70	106.71
37	39	303	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
37	31	308	CLA	C3C-C4C-NC	4.47	115.58	110.57
47	38	205	KC1	CHD-C4C-C3C	-4.47	116.94	125.33
47	36	305	KC1	CMD-C2D-C1D	4.47	135.33	128.46
37	32	205	CLA	C1D-CHD-C4C	-4.47	116.42	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	41	204	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
47	36	302	KC1	CHD-C4C-C3C	-4.46	116.95	125.33
37	19	303	CLA	C3D-C4D-ND	4.46	117.46	110.24
37	33	308	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
37	31	308	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
47	37	304	KC1	CHC-C1C-C2C	-4.46	118.01	124.98
47	40	204	KC1	C2C-C1C-NC	4.46	115.44	110.57
48	32	214	A86	C25-C26-C27	-4.46	120.94	127.31
37	38	206	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
37	18	201	CLA	C2C-C1C-NC	4.46	114.15	109.97
47	39	308	KC1	CMD-C2D-C1D	4.46	135.32	128.46
47	37	302	KC1	CHD-C4C-C3C	-4.46	116.96	125.33
48	12	217	A86	C20-C19-C18	-4.46	103.93	112.75
37	40	203	CLA	C4A-NA-C1A	-4.46	104.70	106.71
47	19	308	KC1	CMD-C2D-C1D	4.46	135.31	128.46
47	15	302	KC1	C2C-C1C-NC	4.46	115.44	110.57
37	14	308	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
37	C	506	CLA	C4A-NA-C1A	-4.46	104.70	106.71
37	40	205	CLA	C4A-NA-C1A	-4.46	104.70	106.71
37	c	506	CLA	C4A-NA-C1A	-4.45	104.70	106.71
37	39	303	CLA	C3D-C4D-ND	4.45	117.44	110.24
37	13	308	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
37	21	202	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
48	32	218	A86	C20-C19-C18	-4.45	103.95	112.75
47	16	305	KC1	CMD-C2D-C1D	4.45	135.30	128.46
37	d	401	CLA	C3D-C4D-ND	4.45	117.43	110.24
37	d	403	CLA	C3D-C4D-ND	4.45	117.43	110.24
37	36	303	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
37	19	303	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
47	20	305	KC1	CHD-C4C-C3C	-4.45	116.98	125.33
47	20	302	KC1	C2C-C1C-NC	4.45	115.42	110.57
48	15	313	A86	C3-C2-C1	-4.44	120.97	127.31
48	35	311	A86	C3-C2-C1	-4.44	120.97	127.31
37	11	307	CLA	C3C-C4C-NC	4.44	115.55	110.57
37	37	308	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
47	17	303	KC1	CHD-C4C-C3C	-4.44	116.99	125.33
47	33	309	KC1	C2C-C1C-NC	4.44	115.42	110.57
48	37	309	A86	C41-C32-C31	-4.44	106.50	110.47
48	14	314	A86	C17-C16-C15	4.44	113.69	109.16
37	16	301	CLA	C3D-C4D-ND	4.44	117.42	110.24
37	b	508	CLA	C3D-C4D-ND	4.44	117.42	110.24
47	37	304	KC1	C2A-C1A-NA	4.44	116.52	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	514	CLA	C1-O2A-CGA	4.44	128.09	116.44
48	31	315	A86	C4-C5-C6	-4.44	120.98	127.31
40	b	521	SQD	O8-S-C6	4.43	112.81	105.74
37	21	204	CLA	C3D-C4D-ND	4.43	117.41	110.24
37	41	204	CLA	C3D-C4D-ND	4.43	117.41	110.24
37	34	308	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
47	15	306	KC1	C2C-C1C-NC	4.43	115.41	110.57
37	16	303	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
37	35	308	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
47	13	309	KC1	C2C-C1C-NC	4.43	115.41	110.57
37	18	211	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
48	37	319	A86	C3-C2-C1	-4.43	120.99	127.31
37	21	204	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
48	17	311	A86	O4-C38-C39	4.43	119.23	111.09
37	B	514	CLA	C1-O2A-CGA	4.43	128.06	116.44
48	21	215	A86	O1-C15-C14	-4.42	104.33	113.21
37	c	501	CLA	C3D-C4D-ND	4.42	117.39	110.24
37	35	305	CLA	C4A-NA-C1A	-4.42	104.72	106.71
50	20	310	DD6	C21-C20-C19	-4.42	109.30	114.28
37	39	302	CLA	O2D-CGD-O1D	-4.42	115.19	123.84
37	41	202	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
40	B	522	SQD	O8-S-C6	4.42	112.79	105.74
47	35	309	KC1	CHC-C1C-C2C	-4.42	118.07	124.98
37	33	303	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
37	C	513	CLA	C4A-NA-C1A	-4.42	104.72	106.71
47	16	302	KC1	CHD-C4C-C3C	-4.42	117.04	125.33
40	B	522	SQD	O7-S-C6	4.41	112.19	106.94
37	12	207	CLA	C3D-C4D-ND	4.41	117.38	110.24
37	C	509	CLA	C4A-NA-C1A	-4.41	104.72	106.71
47	40	207	KC1	CHD-C4C-C3C	-4.41	117.05	125.33
37	c	507	CLA	C3C-C4C-NC	4.41	115.52	110.57
47	14	309	KC1	CHC-C1C-C2C	-4.41	118.09	124.98
37	Z	102	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
37	D	402	CLA	C3D-C4D-ND	4.41	117.37	110.24
40	b	521	SQD	O7-S-C6	4.41	112.18	106.94
48	37	311	A86	C20-C19-C18	-4.41	104.03	112.75
37	20	303	CLA	C4A-NA-C1A	-4.41	104.72	106.71
37	C	507	CLA	C3C-C4C-NC	4.41	115.52	110.57
37	32	208	CLA	C3D-C4D-ND	4.41	117.37	110.24
37	z	102	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
37	C	501	CLA	C3D-C4D-ND	4.41	117.37	110.24
37	12	210	CLA	C4A-NA-C1A	-4.41	104.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	31	309	KC1	C2C-C1C-NC	4.40	115.38	110.57
47	33	304	KC1	CBA-CAA-C2A	-4.40	108.48	125.27
48	35	313	A86	C3-C2-C1	-4.40	121.03	127.31
48	11	315	A86	C4-C5-C6	-4.40	121.03	127.31
37	20	301	CLA	C4A-NA-C1A	-4.40	104.73	106.71
37	11	301	CLA	O2D-CGD-CBD	4.40	119.09	111.27
37	17	307	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
37	B	508	CLA	C3D-C4D-ND	4.40	117.36	110.24
37	17	302	CLA	C3D-C4D-ND	4.40	117.36	110.24
48	41	215	A86	O1-C15-C14	-4.40	104.38	113.21
47	32	209	KC1	CMA-C3A-C2A	-4.40	117.53	128.30
47	13	304	KC1	CBA-CAA-C2A	-4.40	108.51	125.27
37	17	309	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
37	12	203	CLA	O2D-CGD-CBD	4.39	119.08	111.27
47	12	208	KC1	CMA-C3A-C2A	-4.39	117.55	128.30
47	32	209	KC1	C2C-C1C-NC	4.39	115.37	110.57
47	33	304	KC1	CHC-C1C-C2C	-4.39	118.12	124.98
37	37	306	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
37	38	204	CLA	CBA-CAA-C2A	4.39	126.81	113.86
37	39	310	CLA	C3D-C2D-C1D	-4.39	99.85	105.83
47	13	302	KC1	C2C-C1C-NC	4.39	115.36	110.57
37	14	310	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
47	35	306	KC1	C2C-C1C-NC	4.38	115.36	110.57
37	A	405	CLA	C3D-C4D-ND	4.38	117.33	110.24
37	C	510	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
37	32	211	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
37	34	301	CLA	C2C-C1C-NC	4.38	114.08	109.97
37	a	407	CLA	C3D-C4D-ND	4.38	117.32	110.24
47	13	309	KC1	CHD-C4C-C3C	-4.38	117.11	125.33
48	17	312	A86	C20-C19-C18	-4.38	104.09	112.75
48	31	319	A86	C28-C27-C26	4.38	129.06	122.92
37	14	301	CLA	C2C-C1C-NC	4.38	114.07	109.97
37	c	508	CLA	C3C-C4C-NC	4.38	115.48	110.57
37	B	508	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
48	34	316	A86	C35-C34-C33	4.38	117.51	109.88
48	15	311	A86	C3-C2-C1	-4.38	121.07	127.31
37	36	301	CLA	C3D-C4D-ND	4.37	117.31	110.24
48	18	213	A86	C17-C16-C15	4.37	113.63	109.16
37	12	210	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
37	38	201	CLA	C2C-C1C-NC	4.37	114.07	109.97
37	39	304	CLA	CAC-C3C-C4C	4.37	130.48	124.81
47	15	309	KC1	CHC-C1C-C2C	-4.37	118.15	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	40	212	DD6	C21-C20-C19	-4.37	109.36	114.28
37	19	310	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
37	34	310	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
47	13	304	KC1	C2C-C1C-NC	4.37	115.34	110.57
47	33	309	KC1	CHD-C4C-C3C	-4.37	117.13	125.33
47	35	304	KC1	C2A-C1A-NA	4.37	116.41	109.40
37	19	304	CLA	CAC-C3C-C4C	4.37	130.48	124.81
48	18	213	A86	C25-C26-C27	-4.36	121.08	127.31
37	W	101	CLA	C3C-C4C-NC	4.36	115.46	110.57
48	20	311	A86	C3-C2-C1	-4.36	121.08	127.31
47	13	304	KC1	CHC-C1C-C2C	-4.36	118.17	124.98
37	40	208	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
47	33	304	KC1	C2C-C1C-NC	4.36	115.33	110.57
37	20	306	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
48	40	213	A86	C3-C2-C1	-4.36	121.09	127.31
37	b	508	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
37	31	302	CLA	O2D-CGD-CBD	4.36	119.01	111.27
47	31	303	KC1	C2C-C1C-NC	4.36	115.33	110.57
37	B	512	CLA	CMB-C2B-C3B	4.36	132.83	124.68
37	b	512	CLA	CMB-C2B-C3B	4.36	132.83	124.68
37	32	204	CLA	O2D-CGD-CBD	4.36	119.01	111.27
48	11	311	A86	C41-C32-C31	-4.36	106.57	110.47
47	34	309	KC1	CHC-C1C-C2C	-4.36	118.17	124.98
37	14	310	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
37	34	310	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
48	14	316	A86	C35-C34-C33	4.35	117.47	109.88
47	16	308	KC1	C2C-C1C-NC	4.35	115.32	110.57
37	D	401	CLA	C3D-C4D-ND	4.35	117.28	110.24
37	16	309	CLA	C3D-C4D-ND	4.35	117.27	110.24
37	20	307	CLA	O2D-CGD-CBD	4.35	118.99	111.27
48	31	311	A86	C41-C32-C31	-4.35	106.58	110.47
37	39	309	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
37	18	202	CLA	C3D-C4D-ND	4.35	117.27	110.24
37	19	305	CLA	C3D-C4D-ND	4.35	117.27	110.24
37	a	404	CLA	C3D-C4D-ND	4.34	117.27	110.24
37	40	209	CLA	O2D-CGD-CBD	4.34	118.99	111.27
37	c	510	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
37	w	101	CLA	C3C-C4C-NC	4.34	115.44	110.57
48	11	319	A86	C28-C27-C26	4.34	129.01	122.92
47	41	203	KC1	C2C-C1C-NC	4.34	115.31	110.57
37	11	310	CLA	C3C-C4C-NC	4.34	115.44	110.57
47	11	309	KC1	C2C-C1C-NC	4.34	115.31	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	509	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
47	31	303	KC1	CMD-C2D-C1D	4.33	135.13	128.46
37	a	403	CLA	CAA-C2A-C3A	-4.33	100.91	112.78
37	38	206	CLA	C3D-C4D-ND	4.33	117.25	110.24
47	37	304	KC1	C3C-C4C-NC	4.33	113.96	109.88
47	12	208	KC1	C2C-C1C-NC	4.33	115.30	110.57
37	35	307	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
47	36	308	KC1	C2C-C1C-NC	4.33	115.30	110.57
37	36	303	CLA	C3D-C4D-ND	4.33	117.24	110.24
37	36	309	CLA	C3D-C4D-ND	4.33	117.24	110.24
37	15	310	CLA	C3D-C4D-ND	4.33	117.24	110.24
37	D	406	CLA	C4A-NA-C1A	-4.33	104.76	106.71
37	41	202	CLA	C3B-C4B-NB	4.33	114.80	109.21
37	16	303	CLA	C3D-C4D-ND	4.33	117.24	110.24
47	20	302	KC1	C1C-C2C-C3C	-4.33	102.41	106.96
37	b	516	CLA	C1D-CHD-C4C	-4.33	116.73	126.06
37	16	301	CLA	C2C-C1C-NC	4.32	114.02	109.97
37	c	501	CLA	C4A-NA-C1A	-4.32	104.76	106.71
37	c	505	CLA	C1D-CHD-C4C	-4.32	116.73	126.06
38	a	406	PHO	CMB-C2B-C3B	4.32	132.77	124.68
37	36	301	CLA	C2C-C1C-NC	4.32	114.02	109.97
37	C	507	CLA	C1D-CHD-C4C	-4.32	116.74	126.06
37	A	403	CLA	CAA-C2A-C3A	-4.32	100.95	112.78
47	16	302	KC1	O2D-CGD-CBD	4.32	118.94	111.27
37	15	308	CLA	C4A-NA-C1A	-4.32	104.77	106.71
37	D	406	CLA	C3D-C4D-ND	4.32	117.22	110.24
48	11	315	A86	C20-C19-C18	-4.32	104.21	112.75
37	35	301	CLA	O2D-CGD-CBD	4.32	118.94	111.27
37	B	509	CLA	C3C-C4C-NC	4.32	115.41	110.57
37	b	509	CLA	C3C-C4C-NC	4.32	115.41	110.57
37	15	301	CLA	O2D-CGD-CBD	4.31	118.94	111.27
37	21	202	CLA	C3B-C4B-NB	4.31	114.79	109.21
37	39	304	CLA	C3D-C4D-ND	4.31	117.22	110.24
37	B	509	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
37	40	205	CLA	C1D-CHD-C4C	-4.31	116.75	126.06
37	31	310	CLA	C3C-C4C-NC	4.31	115.41	110.57
37	B	505	CLA	C4A-NA-C1A	-4.31	104.77	106.71
47	31	305	KC1	C1A-NA-C4A	-4.31	104.77	106.71
48	31	315	A86	C20-C19-C18	-4.31	104.22	112.75
37	20	303	CLA	C1D-CHD-C4C	-4.31	116.76	126.06
47	36	302	KC1	O2D-CGD-CBD	4.31	118.93	111.27
37	19	306	CLA	C3D-C4D-ND	4.31	117.21	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	511	CLA	C3C-C4C-NC	4.31	115.40	110.57
37	19	306	CLA	C1D-CHD-C4C	-4.31	116.77	126.06
37	40	205	CLA	C3C-C4C-NC	4.31	115.40	110.57
37	13	310	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
37	39	305	CLA	C3D-C4D-ND	4.30	117.20	110.24
37	16	306	CLA	C3C-C4C-NC	4.30	115.40	110.57
47	11	302	KC1	CMD-C2D-C1D	4.30	135.08	128.46
37	c	511	CLA	C3C-C4C-NC	4.30	115.40	110.57
47	14	304	KC1	C2C-C1C-NC	4.30	115.27	110.57
37	39	306	CLA	C3D-C4D-ND	4.30	117.20	110.24
48	14	312	A86	C3-C2-C1	-4.30	121.17	127.31
47	33	302	KC1	CHC-C1C-C2C	-4.30	118.26	124.98
37	C	505	CLA	C3C-C4C-NC	4.30	115.40	110.57
47	21	203	KC1	C2C-C1C-NC	4.30	115.27	110.57
37	18	204	CLA	CBA-CAA-C2A	4.30	126.56	113.86
47	13	306	KC1	C4B-C3B-C2B	-4.30	103.22	106.75
37	c	507	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
37	C	505	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
47	40	207	KC1	C4B-C3B-C2B	-4.30	103.22	106.75
37	11	308	CLA	C4A-NA-C1A	-4.30	104.77	106.71
37	15	303	CLA	C3D-C4D-ND	4.30	117.19	110.24
38	A	404	PHO	CMB-C2B-C3B	4.30	132.72	124.68
37	35	310	CLA	C3D-C4D-ND	4.30	117.19	110.24
47	38	205	KC1	C2C-C1C-NC	4.30	115.27	110.57
37	B	516	CLA	C1D-CHD-C4C	-4.30	116.79	126.06
47	40	204	KC1	C1C-C2C-C3C	-4.30	102.44	106.96
47	37	305	KC1	CHD-C4C-C3C	-4.30	117.26	125.33
37	c	505	CLA	C3C-C4C-NC	4.30	115.39	110.57
47	20	305	KC1	C4B-C3B-C2B	-4.30	103.22	106.75
47	33	306	KC1	C2A-C1A-NA	4.30	116.29	109.40
50	41	212	DD6	C-C1-C24	-4.30	111.31	118.08
47	40	206	KC1	C1C-C2C-C3C	-4.30	102.44	106.96
48	34	312	A86	C3-C2-C1	-4.30	121.18	127.31
37	11	303	CLA	CAA-C2A-C3A	-4.29	101.02	112.78
37	31	304	CLA	CAA-C2A-C3A	-4.29	101.02	112.78
43	d	408	LHG	O4-P-O5	4.29	133.47	112.24
47	15	304	KC1	CHD-C4C-C3C	-4.29	117.27	125.33
37	19	304	CLA	C3D-C4D-ND	4.29	117.18	110.24
47	32	209	KC1	C4B-C3B-C2B	-4.29	103.23	106.75
37	b	515	CLA	C4A-NA-C1A	-4.29	104.78	106.71
37	w	101	CLA	C4A-NA-C1A	-4.29	104.78	106.71
37	18	206	CLA	C3D-C2D-C1D	-4.29	99.98	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	508	CLA	C3C-C4C-NC	4.29	115.38	110.57
47	17	306	KC1	CHD-C4C-C3C	-4.29	117.28	125.33
48	13	313	A86	C41-C32-C31	-4.29	106.63	110.47
37	19	309	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
48	33	313	A86	C41-C32-C31	-4.29	106.63	110.47
50	21	216	DD6	C15-C14-C13	4.29	135.06	125.99
47	13	306	KC1	C2A-C1A-NA	4.29	116.28	109.40
47	34	304	KC1	C2C-C1C-NC	4.29	115.25	110.57
37	35	310	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
43	D	410	LHG	O4-P-O5	4.29	133.43	112.24
43	d	407	LHG	O4-P-O5	4.28	133.42	112.24
37	39	306	CLA	C1D-CHD-C4C	-4.28	116.81	126.06
37	35	303	CLA	C3D-C4D-ND	4.28	117.17	110.24
48	16	311	A86	O4-C38-C39	4.28	118.97	111.09
37	38	201	CLA	C3D-C4D-ND	4.28	117.17	110.24
37	35	308	CLA	CAC-C3C-C4C	4.28	130.37	124.81
37	B	511	CLA	C4A-NA-C1A	-4.28	104.78	106.71
47	11	304	KC1	C1A-NA-C4A	-4.28	104.78	106.71
50	41	216	DD6	C15-C14-C13	4.28	135.04	125.99
37	C	506	CLA	C3B-C4B-NB	4.28	114.74	109.21
43	b	522	LHG	O4-P-O5	4.28	133.40	112.24
47	33	306	KC1	C4B-C3B-C2B	-4.28	103.24	106.75
47	18	205	KC1	C2C-C1C-NC	4.28	115.24	110.57
47	31	307	KC1	CHC-C1C-C2C	-4.28	118.30	124.98
43	D	409	LHG	O4-P-O5	4.28	133.38	112.24
47	15	306	KC1	CHC-C1C-C2C	-4.27	118.30	124.98
37	B	504	CLA	CAC-C3C-C4C	4.27	130.35	124.81
43	B	523	LHG	O4-P-O5	4.27	133.37	112.24
37	13	303	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
37	34	310	CLA	C3D-C4D-ND	4.27	117.15	110.24
47	17	305	KC1	C2A-C1A-NA	4.27	116.25	109.40
37	34	301	CLA	O2D-CGD-CBD	4.27	118.86	111.27
37	18	211	CLA	C3D-C4D-ND	4.27	117.14	110.24
37	37	301	CLA	C3D-C4D-ND	4.27	117.14	110.24
47	17	305	KC1	CHC-C1C-C2C	-4.27	118.31	124.98
48	14	316	A86	C25-C26-C27	-4.27	121.22	127.31
50	21	212	DD6	C-C1-C24	-4.27	111.35	118.08
37	15	307	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
37	36	306	CLA	C3C-C4C-NC	4.27	115.36	110.57
37	W	101	CLA	C4A-NA-C1A	-4.27	104.79	106.71
37	b	511	CLA	C4A-NA-C1A	-4.27	104.79	106.71
47	13	302	KC1	CHC-C1C-C2C	-4.27	118.31	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	35	306	KC1	CHC-C1C-C2C	-4.27	118.31	124.98
37	d	404	CLA	C3D-C4D-ND	4.26	117.14	110.24
47	12	206	KC1	C2C-C1C-NC	4.26	115.23	110.57
47	41	203	KC1	C2A-C1A-NA	4.26	116.24	109.40
48	36	311	A86	O4-C38-C39	4.26	118.93	111.09
48	17	311	A86	C3-C4-C5	-4.26	114.75	123.47
37	18	201	CLA	C3D-C4D-ND	4.26	117.13	110.24
37	32	202	CLA	C4A-NA-C1A	-4.26	104.79	106.71
47	14	304	KC1	C1C-C2C-C3C	-4.26	102.48	106.96
37	18	206	CLA	C3D-C4D-ND	4.26	117.12	110.24
47	11	302	KC1	C2C-C1C-NC	4.25	115.22	110.57
37	b	504	CLA	CAC-C3C-C4C	4.25	130.33	124.81
47	32	207	KC1	C4B-C3B-C2B	-4.25	103.26	106.75
47	32	212	KC1	C2C-C1C-NC	4.25	115.22	110.57
37	13	310	CLA	C3D-C4D-ND	4.25	117.12	110.24
37	c	509	CLA	C4A-NA-C1A	-4.25	104.79	106.71
47	15	304	KC1	C2A-C1A-NA	4.25	116.22	109.40
37	14	301	CLA	O2D-CGD-CBD	4.25	118.82	111.27
47	18	210	KC1	C4B-C3B-C2B	-4.25	103.26	106.75
47	21	203	KC1	C2A-C1A-NA	4.25	116.22	109.40
37	38	204	CLA	CAA-C2A-C3A	-4.25	101.15	112.78
37	39	303	CLA	CBA-CAA-C2A	4.25	126.40	113.86
48	31	311	A86	C20-C19-C18	-4.24	104.35	112.75
37	B	515	CLA	C4A-NA-C1A	-4.24	104.80	106.71
37	13	303	CLA	C3D-C4D-ND	4.24	117.10	110.24
37	31	308	CLA	C4A-NA-C1A	-4.24	104.80	106.71
47	33	306	KC1	C1C-C2C-C3C	-4.24	102.50	106.96
37	14	310	CLA	C3D-C4D-ND	4.24	117.10	110.24
37	11	307	CLA	C4A-NA-C1A	-4.24	104.80	106.71
47	11	306	KC1	CHC-C1C-C2C	-4.24	118.36	124.98
37	c	506	CLA	C3B-C4B-NB	4.24	114.69	109.21
37	15	307	CLA	C1D-CHD-C4C	-4.24	116.92	126.06
48	36	310	A86	C12-C11-C13	4.24	123.14	116.02
37	16	301	CLA	O2D-CGD-CBD	4.24	118.80	111.27
37	41	208	CLA	C3D-C4D-ND	4.24	117.09	110.24
37	35	307	CLA	C1D-CHD-C4C	-4.24	116.92	126.06
37	19	303	CLA	CBA-CAA-C2A	4.23	126.36	113.86
37	31	302	CLA	C3C-C4C-NC	4.23	115.32	110.57
37	b	514	CLA	C3C-C4C-NC	4.23	115.32	110.57
47	40	204	KC1	CBC-CAC-C3C	-4.23	100.76	112.43
47	13	302	KC1	C2A-C1A-NA	4.23	116.19	109.40
48	11	311	A86	C20-C19-C18	-4.23	104.38	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	38	211	CLA	C3D-C4D-ND	4.23	117.08	110.24
37	38	211	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
48	11	315	A86	C12-C11-C13	4.23	123.13	116.02
37	38	208	CLA	C1D-CHD-C4C	-4.23	116.93	126.06
37	36	301	CLA	O2D-CGD-CBD	4.23	118.78	111.27
50	39	312	DD6	C23-C16-C22	-4.23	101.13	107.37
47	35	304	KC1	CHD-C4C-C3C	-4.23	117.39	125.33
47	32	207	KC1	CMA-C3A-C2A	-4.23	117.95	128.30
48	31	315	A86	C12-C11-C13	4.23	123.12	116.02
47	12	206	KC1	C4B-C3B-C2B	-4.22	103.28	106.75
50	19	312	DD6	C23-C16-C22	-4.22	101.14	107.37
48	14	316	A86	C4-C3-C2	-4.22	114.82	123.47
47	17	306	KC1	C1C-C2C-C3C	-4.22	102.52	106.96
47	37	305	KC1	C1C-C2C-C3C	-4.22	102.52	106.96
47	35	309	KC1	C2C-C1C-NC	4.22	115.18	110.57
47	35	302	KC1	C1A-NA-C4A	-4.22	104.81	106.71
37	b	504	CLA	CHD-C1D-ND	-4.22	120.58	124.45
47	18	205	KC1	CBA-CAA-C2A	-4.22	109.18	125.27
48	34	316	A86	C25-C26-C27	-4.22	121.29	127.31
48	34	316	A86	C4-C3-C2	-4.22	114.83	123.47
37	b	503	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
37	A	405	CLA	C4A-NA-C1A	-4.22	104.81	106.71
37	C	501	CLA	C4A-NA-C1A	-4.22	104.81	106.71
47	38	205	KC1	CBA-CAA-C2A	-4.22	109.19	125.27
37	B	505	CLA	C3D-C4D-ND	4.22	117.06	110.24
43	37	315	LHG	O4-P-O5	4.22	133.10	112.24
37	B	504	CLA	CHD-C1D-ND	-4.22	120.58	124.45
37	c	506	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
47	20	304	KC1	C1C-C2C-C3C	-4.22	102.52	106.96
37	20	303	CLA	C3C-C4C-NC	4.22	115.30	110.57
37	B	503	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
37	18	208	CLA	C1D-CHD-C4C	-4.22	116.96	126.06
47	33	302	KC1	C2A-C1A-NA	4.22	116.16	109.40
47	13	306	KC1	C1C-C2C-C3C	-4.22	102.53	106.96
47	12	206	KC1	CMA-C3A-C2A	-4.21	117.98	128.30
48	41	214	A86	C36-C31-C32	-4.21	115.51	119.70
37	21	202	CLA	C3D-C4D-ND	4.21	117.06	110.24
37	B	514	CLA	C3C-C4C-NC	4.21	115.30	110.57
37	41	209	CLA	C3D-C4D-ND	4.21	117.05	110.24
37	b	513	CLA	C3B-C4B-NB	4.21	114.66	109.21
48	33	314	A86	C41-C32-C31	-4.21	106.70	110.47
37	C	502	CLA	C3C-C4C-NC	4.21	115.29	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	21	214	A86	C36-C31-C32	-4.21	115.52	119.70
37	C	513	CLA	C3D-C4D-ND	4.21	117.05	110.24
37	31	301	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
48	16	310	A86	C12-C11-C13	4.21	123.09	116.02
37	33	310	CLA	C3D-C4D-ND	4.21	117.05	110.24
47	34	304	KC1	C1C-C2C-C3C	-4.21	102.53	106.96
47	35	309	KC1	CMD-C2D-C1D	4.21	134.93	128.46
47	32	207	KC1	C2C-C1C-NC	4.21	115.17	110.57
48	17	320	A86	C25-C26-C27	-4.21	121.31	127.31
37	b	502	CLA	C3D-C4D-ND	4.21	117.04	110.24
47	15	309	KC1	C2C-C1C-NC	4.21	115.16	110.57
37	C	504	CLA	C3D-C4D-ND	4.20	117.04	110.24
47	38	207	KC1	CMD-C2D-C1D	4.20	134.92	128.46
47	20	302	KC1	CBC-CAC-C3C	-4.20	100.85	112.43
37	B	502	CLA	C3D-C4D-ND	4.20	117.03	110.24
47	12	208	KC1	C4B-C3B-C2B	-4.20	103.30	106.75
37	15	305	CLA	C4A-NA-C1A	-4.20	104.82	106.71
43	37	321	LHG	O4-P-O5	4.20	133.00	112.24
37	33	303	CLA	C3D-C4D-ND	4.20	117.03	110.24
43	17	316	LHG	O4-P-O5	4.20	133.00	112.24
37	17	304	CLA	C3D-C4D-ND	4.20	117.03	110.24
37	C	506	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
37	c	513	CLA	C3D-C4D-ND	4.20	117.03	110.24
37	19	305	CLA	C3C-C4C-NC	4.20	115.28	110.57
37	14	303	CLA	C3D-C4D-ND	4.19	117.02	110.24
37	35	308	CLA	C3D-C4D-ND	4.19	117.02	110.24
37	41	202	CLA	C3D-C4D-ND	4.19	117.02	110.24
47	18	207	KC1	CMD-C2D-C1D	4.19	134.91	128.46
37	C	505	CLA	C3D-C4D-ND	4.19	117.02	110.24
37	15	310	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
37	11	301	CLA	C3C-C4C-NC	4.19	115.27	110.57
48	35	316	A86	C4-C3-C2	-4.19	114.89	123.47
37	21	209	CLA	C3D-C4D-ND	4.19	117.02	110.24
43	21	217	LHG	O4-P-O5	4.19	132.96	112.24
37	34	301	CLA	C3D-C4D-ND	4.19	117.02	110.24
37	38	202	CLA	C3D-C4D-ND	4.19	117.02	110.24
40	A	407	SQD	O9-S-C6	4.19	111.92	106.94
37	36	306	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
37	38	202	CLA	C3C-C4C-NC	4.19	115.27	110.57
37	B	506	CLA	C3D-C4D-ND	4.19	117.01	110.24
37	c	504	CLA	C3D-C4D-ND	4.19	117.01	110.24
37	b	506	CLA	C3D-C4D-ND	4.19	117.01	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	41	201	LHG	O4-P-O5	4.19	132.94	112.24
37	17	307	CLA	CMB-C2B-C3B	4.19	132.51	124.68
47	38	210	KC1	C4B-C3B-C2B	-4.19	103.31	106.75
43	a	412	LHG	O4-P-O5	4.19	132.93	112.24
37	B	513	CLA	C3B-C4B-NB	4.18	114.62	109.21
43	D	411	LHG	O4-P-O5	4.18	132.93	112.24
37	15	308	CLA	C3D-C4D-ND	4.18	117.00	110.24
37	b	515	CLA	C3C-C4C-NC	4.18	115.26	110.57
37	b	505	CLA	C3D-C4D-ND	4.18	117.00	110.24
37	b	510	CLA	CAA-C2A-C3A	-4.18	101.33	112.78
37	21	208	CLA	C3D-C4D-ND	4.18	117.00	110.24
37	37	303	CLA	C3D-C4D-ND	4.18	117.00	110.24
37	b	505	CLA	C4A-NA-C1A	-4.18	104.83	106.71
37	14	308	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
47	19	308	KC1	CHC-C1C-C2C	-4.18	118.45	124.98
37	20	307	CLA	C3D-C4D-ND	4.18	117.00	110.24
37	B	510	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
37	38	202	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
47	35	304	KC1	C4B-C3B-C2B	-4.18	103.32	106.75
37	d	403	CLA	O2D-CGD-CBD	4.18	118.69	111.27
48	15	316	A86	C4-C3-C2	-4.18	114.92	123.47
37	34	303	CLA	C3D-C4D-ND	4.18	116.99	110.24
47	39	308	KC1	CHC-C1C-C2C	-4.17	118.46	124.98
37	d	403	CLA	C3C-C4C-NC	4.17	115.25	110.57
48	31	312	A86	C3-C4-C5	-4.17	114.93	123.47
37	W	102	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
47	13	309	KC1	C4B-C3B-C2B	-4.17	103.33	106.75
48	13	311	A86	C4-C5-C6	-4.17	121.36	127.31
37	C	502	CLA	C1D-CHD-C4C	-4.17	117.06	126.06
37	c	502	CLA	C3C-C4C-NC	4.17	115.25	110.57
37	c	502	CLA	C1D-CHD-C4C	-4.17	117.06	126.06
37	39	301	CLA	C3D-C4D-ND	4.17	116.98	110.24
37	18	209	CLA	C3C-C4C-NC	4.17	115.25	110.57
37	39	305	CLA	C3C-C4C-NC	4.17	115.25	110.57
37	41	206	CLA	C3D-C4D-ND	4.17	116.98	110.24
47	36	304	KC1	C2C-C1C-NC	4.17	115.12	110.57
47	16	304	KC1	C2C-C1C-NC	4.17	115.12	110.57
37	16	306	CLA	C3D-C2D-C1D	-4.17	100.15	105.83
48	14	315	A86	O4-C38-C39	4.16	118.75	111.09
48	34	315	A86	O4-C38-C39	4.16	118.75	111.09
48	37	310	A86	O4-C38-C39	4.16	118.75	111.09
37	37	306	CLA	CMB-C2B-C3B	4.16	132.47	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	21	201	LHG	O4-P-O5	4.16	132.82	112.24
47	36	308	KC1	C4B-C3B-C2B	-4.16	103.33	106.75
48	33	311	A86	C4-C5-C6	-4.16	121.37	127.31
37	c	505	CLA	C3D-C4D-ND	4.16	116.97	110.24
48	11	312	A86	C3-C4-C5	-4.16	114.95	123.47
37	Z	102	CLA	C1D-CHD-C4C	-4.16	117.09	126.06
37	D	405	CLA	O2D-CGD-CBD	4.16	118.66	111.27
37	34	308	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
37	33	308	CLA	C3D-C4D-ND	4.16	116.96	110.24
37	38	209	CLA	C3C-C4C-NC	4.15	115.23	110.57
47	20	304	KC1	CHD-C4C-C3C	-4.15	117.53	125.33
37	14	305	CLA	C3D-C4D-ND	4.15	116.96	110.24
37	34	305	CLA	C3D-C4D-ND	4.15	116.96	110.24
37	14	301	CLA	C3D-C4D-ND	4.15	116.95	110.24
47	40	206	KC1	CHD-C4C-C3C	-4.15	117.53	125.33
37	b	523	CLA	CMD-C2D-C1D	4.15	132.03	124.71
37	19	301	CLA	C3D-C4D-ND	4.15	116.95	110.24
37	D	405	CLA	C3C-C4C-NC	4.15	115.22	110.57
37	z	102	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
37	39	306	CLA	C2C-C1C-NC	4.15	113.86	109.97
37	A	403	CLA	C3D-C4D-ND	4.15	116.95	110.24
37	40	203	CLA	C3C-C4C-NC	4.15	115.22	110.57
37	c	508	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
37	z	101	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
37	b	509	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
48	13	314	A86	C41-C32-C31	-4.15	106.76	110.47
37	39	306	CLA	C3C-C4C-NC	4.15	115.22	110.57
37	C	508	CLA	C3B-C4B-NB	4.14	114.57	109.21
47	11	304	KC1	C2A-C1A-NA	4.14	116.05	109.40
48	18	213	A86	C7-C6-C8	4.14	124.61	118.08
37	19	306	CLA	C3C-C4C-NC	4.14	115.22	110.57
48	38	213	A86	C25-C26-C27	-4.14	121.40	127.31
37	21	206	CLA	C3D-C4D-ND	4.14	116.94	110.24
37	B	524	CLA	CMD-C2D-C1D	4.14	132.01	124.71
37	a	407	CLA	C4A-NA-C1A	-4.14	104.84	106.71
37	C	508	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
37	Z	101	CLA	C3D-C4D-ND	4.14	116.94	110.24
37	32	204	CLA	C1D-CHD-C4C	-4.14	117.13	126.06
37	c	508	CLA	C3B-C4B-NB	4.14	114.56	109.21
37	C	507	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
48	37	319	A86	C25-C26-C27	-4.14	121.40	127.31
37	40	209	CLA	C3D-C4D-ND	4.14	116.93	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	13	308	CLA	C3D-C4D-ND	4.14	116.93	110.24
37	B	509	CLA	C1D-CHD-C4C	-4.14	117.13	126.06
47	15	309	KC1	CMD-C2D-C1D	4.14	134.82	128.46
47	33	309	KC1	C4B-C3B-C2B	-4.13	103.36	106.75
37	18	211	CLA	C3C-C4C-NC	4.13	115.21	110.57
37	40	210	CLA	C3C-C4C-NC	4.13	115.21	110.57
48	18	212	A86	C41-C32-C31	-4.13	106.77	110.47
40	a	409	SQD	O9-S-C6	4.13	111.85	106.94
37	35	307	CLA	CMB-C2B-C3B	4.13	132.41	124.68
47	16	308	KC1	C4B-C3B-C2B	-4.13	103.36	106.75
47	15	302	KC1	C2A-C1A-NA	4.13	116.03	109.40
47	32	207	KC1	CBA-CAA-C2A	-4.13	109.52	125.27
37	b	511	CLA	C3B-C4B-NB	4.13	114.55	109.21
37	37	308	CLA	C3D-C4D-ND	4.13	116.92	110.24
48	15	315	A86	C3-C2-C1	-4.13	121.41	127.31
47	12	206	KC1	CBA-CAA-C2A	-4.13	109.52	125.27
37	a	403	CLA	C3D-C4D-ND	4.13	116.92	110.24
37	C	512	CLA	C3D-C4D-ND	4.13	116.92	110.24
37	17	309	CLA	C3D-C4D-ND	4.13	116.92	110.24
37	20	301	CLA	C3C-C4C-NC	4.13	115.20	110.57
37	B	515	CLA	C3C-C4C-NC	4.13	115.20	110.57
37	b	503	CLA	C3C-C4C-NC	4.13	115.20	110.57
37	20	306	CLA	C3D-C4D-ND	4.13	116.91	110.24
48	17	313	A86	C41-C32-C31	-4.13	106.78	110.47
37	z	101	CLA	C3D-C4D-ND	4.13	116.91	110.24
37	B	511	CLA	C3B-C4B-NB	4.13	114.54	109.21
37	b	513	CLA	C3C-C4C-NC	4.12	115.20	110.57
47	32	212	KC1	C4B-C3B-C2B	-4.12	103.36	106.75
47	35	304	KC1	C1C-C2C-C3C	-4.12	102.62	106.96
37	40	208	CLA	C3D-C4D-ND	4.12	116.91	110.24
47	13	304	KC1	C4B-C3B-C2B	-4.12	103.37	106.75
37	B	504	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
37	14	307	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
37	39	306	CLA	O2D-CGD-CBD	4.12	118.59	111.27
37	B	503	CLA	C3C-C4C-NC	4.12	115.19	110.57
47	13	306	KC1	C1A-NA-C4A	-4.12	104.85	106.71
37	11	310	CLA	C3D-C4D-ND	4.12	116.90	110.24
37	c	510	CLA	C3B-C4B-NB	4.12	114.53	109.21
37	16	306	CLA	CMB-C2B-C3B	4.12	132.38	124.68
48	31	314	A86	C3-C4-C5	-4.12	115.04	123.47
37	Z	101	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
37	12	210	CLA	C3D-C4D-ND	4.12	116.90	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	14	306	KC1	CBA-CAA-C2A	-4.12	109.57	125.27
47	34	306	KC1	CBA-CAA-C2A	-4.12	109.57	125.27
48	37	312	A86	C41-C32-C31	-4.12	106.79	110.47
48	35	315	A86	C3-C2-C1	-4.11	121.44	127.31
37	b	510	CLA	C3C-C4C-NC	4.11	115.19	110.57
37	20	308	CLA	C3C-C4C-NC	4.11	115.19	110.57
37	C	503	CLA	C3D-C4D-ND	4.11	116.89	110.24
37	32	211	CLA	C3D-C4D-ND	4.11	116.89	110.24
37	15	307	CLA	CMB-C2B-C3B	4.11	132.38	124.68
37	36	307	CLA	C3D-C4D-ND	4.11	116.89	110.24
50	39	312	DD6	C15-C14-C13	4.11	134.69	125.99
37	14	308	CLA	C3C-C4C-NC	4.11	115.18	110.57
37	b	511	CLA	CMB-C2B-C3B	4.11	132.37	124.68
37	B	512	CLA	C4A-NA-C1A	-4.11	104.86	106.71
37	B	510	CLA	C3C-C4C-NC	4.11	115.18	110.57
47	39	308	KC1	C2C-C1C-NC	4.11	115.06	110.57
37	40	205	CLA	CBA-CAA-C2A	4.11	126.00	113.86
37	b	504	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
37	31	301	CLA	C4A-NA-C1A	-4.11	104.86	106.71
37	c	507	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
37	20	303	CLA	CBA-CAA-C2A	4.11	126.00	113.86
37	41	206	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
48	21	215	A86	C3-C2-C1	-4.11	121.44	127.31
37	34	307	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
48	15	319	A86	C33-C32-C31	4.11	113.20	109.21
47	31	305	KC1	C2A-C1A-NA	4.11	115.99	109.40
37	33	305	CLA	C3D-C4D-ND	4.11	116.88	110.24
37	31	310	CLA	C4A-NA-C1A	-4.11	104.86	106.71
37	B	513	CLA	C3C-C4C-NC	4.11	115.18	110.57
37	B	511	CLA	CMB-C2B-C3B	4.11	132.36	124.68
37	C	506	CLA	CAA-C2A-C3A	-4.11	101.53	112.78
37	12	203	CLA	C1D-CHD-C4C	-4.11	117.20	126.06
37	15	305	CLA	C3D-C4D-ND	4.11	116.88	110.24
37	b	510	CLA	C1D-CHD-C4C	-4.11	117.20	126.06
47	34	304	KC1	C2A-C1A-NA	4.11	115.99	109.40
37	C	510	CLA	C3B-C4B-NB	4.10	114.52	109.21
37	19	306	CLA	O2D-CGD-CBD	4.10	118.56	111.27
48	41	215	A86	C3-C2-C1	-4.10	121.45	127.31
47	16	304	KC1	C4B-C3B-C2B	-4.10	103.38	106.75
48	19	311	A86	C3-C4-C5	-4.10	115.07	123.47
37	B	511	CLA	C3D-C4D-ND	4.10	116.88	110.24
47	31	303	KC1	C1C-C2C-C3C	-4.10	102.64	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	21	206	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
37	33	307	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
37	31	308	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
37	31	310	CLA	C3D-C4D-ND	4.10	116.87	110.24
37	B	510	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
37	16	307	CLA	C3D-C4D-ND	4.10	116.87	110.24
48	15	316	A86	C41-C32-C31	-4.10	106.80	110.47
37	b	511	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
37	b	512	CLA	C4A-NA-C1A	-4.10	104.86	106.71
47	33	306	KC1	C1A-NA-C4A	-4.10	104.86	106.71
48	35	319	A86	C33-C32-C31	4.10	113.19	109.21
37	c	512	CLA	C3D-C4D-ND	4.10	116.87	110.24
37	B	511	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
37	34	302	CLA	C3C-C4C-NC	4.10	115.17	110.57
37	14	308	CLA	C3D-C4D-ND	4.10	116.87	110.24
47	12	206	KC1	CHC-C1C-C2C	-4.10	118.58	124.98
37	c	513	CLA	C3C-C4C-NC	4.10	115.17	110.57
37	34	301	CLA	C3C-C4C-NC	4.10	115.17	110.57
50	19	312	DD6	C15-C14-C13	4.10	134.66	125.99
48	11	314	A86	C3-C4-C5	-4.10	115.08	123.47
37	13	307	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
37	19	302	CLA	C3D-C4D-ND	4.10	116.86	110.24
37	14	301	CLA	C3C-C4C-NC	4.10	115.16	110.57
48	37	309	A86	C17-C16-C15	4.10	113.34	109.16
37	W	102	CLA	C4A-NA-C1A	-4.09	104.86	106.71
37	39	302	CLA	C3D-C4D-ND	4.09	116.86	110.24
37	20	308	CLA	C1D-CHD-C4C	-4.09	117.22	126.06
48	38	215	A86	C3-C2-C1	-4.09	121.47	127.31
48	41	215	A86	C25-C26-C27	-4.09	121.47	127.31
37	40	203	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
37	c	506	CLA	CAA-C2A-C3A	-4.09	101.57	112.78
47	21	207	KC1	C2A-C1A-NA	4.09	115.96	109.40
37	13	305	CLA	C3D-C4D-ND	4.09	116.86	110.24
37	13	307	CLA	C3C-C4C-NC	4.09	115.16	110.57
47	31	305	KC1	C1C-C2C-C3C	-4.09	102.66	106.96
48	16	313	A86	C10-C9-C8	-4.09	110.46	123.22
47	14	304	KC1	C2A-C1A-NA	4.09	115.96	109.40
47	35	302	KC1	C2A-C1A-NA	4.09	115.96	109.40
37	17	302	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
37	a	403	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
48	21	215	A86	C25-C26-C27	-4.09	121.48	127.31
37	11	307	CLA	C1D-CHD-C4C	-4.09	117.24	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	41	207	KC1	C2A-C1A-NA	4.08	115.95	109.40
37	36	306	CLA	CMB-C2B-C3B	4.08	132.32	124.68
47	18	210	KC1	C2C-C1C-NC	4.08	115.03	110.57
37	C	513	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
37	c	513	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
47	15	304	KC1	C4B-C3B-C2B	-4.08	103.40	106.75
47	33	304	KC1	C4B-C3B-C2B	-4.08	103.40	106.75
37	A	403	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
37	c	503	CLA	C3D-C4D-ND	4.08	116.84	110.24
37	B	503	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
47	15	306	KC1	C1C-C2C-C3C	-4.08	102.67	106.96
37	13	301	CLA	O2D-CGD-CBD	4.08	118.52	111.27
37	33	301	CLA	O2D-CGD-CBD	4.08	118.52	111.27
37	35	303	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
37	20	301	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
47	35	306	KC1	C1C-C2C-C3C	-4.08	102.67	106.96
37	35	301	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
48	40	201	A86	C10-C9-C8	-4.08	110.49	123.22
47	39	308	KC1	C4B-C3B-C2B	-4.08	103.40	106.75
47	13	309	KC1	CMD-C2D-C1D	4.08	134.73	128.46
37	b	515	CLA	C1D-CHD-C4C	-4.08	117.27	126.06
47	32	207	KC1	CHC-C1C-C2C	-4.07	118.61	124.98
37	B	515	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
37	19	307	CLA	C3C-C4C-NC	4.07	115.14	110.57
47	17	303	KC1	C4B-C3B-C2B	-4.07	103.41	106.75
37	19	309	CLA	C3D-C4D-ND	4.07	116.83	110.24
47	16	305	KC1	C2A-C1A-NA	4.07	115.93	109.40
48	39	311	A86	C3-C4-C5	-4.07	115.13	123.47
37	12	210	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
50	16	312	DD6	C21-C20-C19	-4.07	109.70	114.28
37	40	210	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
37	W	101	CLA	C3D-C4D-ND	4.07	116.82	110.24
37	14	308	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
47	38	210	KC1	C2C-C1C-NC	4.07	115.01	110.57
47	14	306	KC1	C1C-C2C-C3C	-4.07	102.68	106.96
47	17	305	KC1	CAC-C3C-C4C	4.07	130.09	124.81
37	b	503	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
48	11	319	A86	C12-C11-C13	4.07	122.85	116.02
48	15	316	A86	C35-C34-C33	4.07	116.97	109.88
37	b	510	CLA	C3D-C4D-ND	4.07	116.82	110.24
37	33	307	CLA	C3C-C4C-NC	4.07	115.13	110.57
37	18	202	CLA	C1D-CHD-C4C	-4.07	117.28	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	17	305	KC1	CHD-C4C-C3C	-4.07	117.69	125.33
48	38	212	A86	C41-C32-C31	-4.07	106.83	110.47
37	c	509	CLA	C3C-C4C-NC	4.07	115.13	110.57
47	12	211	KC1	C2C-C1C-NC	4.06	115.01	110.57
37	34	308	CLA	C3D-C4D-ND	4.06	116.81	110.24
47	15	302	KC1	C1C-C2C-C3C	-4.06	102.68	106.96
47	36	304	KC1	C4B-C3B-C2B	-4.06	103.42	106.75
37	11	308	CLA	C3D-C4D-ND	4.06	116.81	110.24
37	18	209	CLA	C1D-CHD-C4C	-4.06	117.29	126.06
47	36	305	KC1	C2A-C1A-NA	4.06	115.92	109.40
48	16	314	A86	C20-C19-C18	-4.06	104.71	112.75
37	19	306	CLA	C2C-C1C-NC	4.06	113.78	109.97
48	36	313	A86	C20-C19-C18	-4.06	104.71	112.75
47	15	304	KC1	C1C-C2C-C3C	-4.06	102.69	106.96
37	39	307	CLA	C3C-C4C-NC	4.06	115.12	110.57
37	34	308	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
47	33	309	KC1	CMD-C2D-C1D	4.06	134.70	128.46
48	37	310	A86	C3-C4-C5	-4.06	115.16	123.47
47	18	207	KC1	C1C-C2C-C3C	-4.06	102.69	106.96
48	32	203	A86	O4-C38-C39	4.06	118.56	111.09
47	33	309	KC1	C1C-C2C-C3C	-4.06	102.69	106.96
47	36	302	KC1	C1C-C2C-C3C	-4.06	102.69	106.96
37	15	301	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
37	38	209	CLA	C1D-CHD-C4C	-4.06	117.31	126.06
37	B	513	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
37	c	501	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
37	34	308	CLA	C3C-C4C-NC	4.06	115.12	110.57
37	19	307	CLA	C1D-CHD-C4C	-4.06	117.31	126.06
48	15	315	A86	C12-C11-C13	4.06	122.84	116.02
37	b	511	CLA	C3D-C4D-ND	4.06	116.80	110.24
37	C	509	CLA	C3C-C4C-NC	4.06	115.12	110.57
48	17	310	A86	C17-C16-C15	4.06	113.30	109.16
37	38	202	CLA	C4A-NA-C1A	-4.05	104.88	106.71
37	39	307	CLA	C1D-CHD-C4C	-4.05	117.31	126.06
37	18	202	CLA	C2C-C1C-NC	4.05	113.77	109.97
44	c	517	DGD	O3G-C3G-C2G	-4.05	101.12	110.90
48	33	314	A86	C36-C31-C32	-4.05	115.67	119.70
37	35	308	CLA	C3B-C4B-NB	4.05	114.45	109.21
37	33	308	CLA	O2D-CGD-CBD	4.05	118.47	111.27
37	12	210	CLA	CAC-C3C-C4C	4.05	130.07	124.81
44	C	517	DGD	O3G-C3G-C2G	-4.05	101.13	110.90
37	13	308	CLA	C3C-C4C-NC	4.05	115.11	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	16	302	KC1	CBA-CAA-C2A	-4.05	109.83	125.27
37	31	302	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
37	C	513	CLA	C3C-C4C-NC	4.05	115.11	110.57
47	36	302	KC1	CBA-CAA-C2A	-4.05	109.83	125.27
37	32	206	CLA	C3D-C4D-ND	4.05	116.79	110.24
37	13	308	CLA	O2D-CGD-CBD	4.05	118.46	111.27
47	11	304	KC1	C1C-C2C-C3C	-4.05	102.70	106.96
48	31	319	A86	C12-C11-C13	4.05	122.82	116.02
47	19	308	KC1	C2C-C1C-NC	4.05	114.99	110.57
37	b	515	CLA	C3D-C4D-ND	4.05	116.78	110.24
48	12	202	A86	O4-C38-C39	4.05	118.53	111.09
37	11	301	CLA	C1D-CHD-C4C	-4.05	117.33	126.06
47	11	302	KC1	C1C-C2C-C3C	-4.05	102.70	106.96
47	35	302	KC1	C1C-C2C-C3C	-4.04	102.70	106.96
37	32	202	CLA	C3D-C4D-ND	4.04	116.78	110.24
37	C	501	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
37	b	513	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
47	11	304	KC1	C4B-C3B-C2B	-4.04	103.43	106.75
37	z	102	CLA	C3D-C4D-ND	4.04	116.78	110.24
37	32	211	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
37	A	403	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
37	34	301	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
37	39	309	CLA	C3D-C4D-ND	4.04	116.78	110.24
37	C	503	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
37	C	512	CLA	C3C-C4C-NC	4.04	115.10	110.57
37	14	302	CLA	C3C-C4C-NC	4.04	115.10	110.57
37	w	101	CLA	C3D-C4D-ND	4.04	116.77	110.24
37	39	302	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
37	c	503	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
37	15	301	CLA	C3C-C4C-NC	4.04	115.10	110.57
37	b	512	CLA	C3D-C4D-ND	4.04	116.77	110.24
37	17	309	CLA	O2D-CGD-O1D	-4.04	115.95	123.84
47	34	306	KC1	C1C-C2C-C3C	-4.04	102.71	106.96
37	c	508	CLA	C4A-NA-C1A	-4.03	104.89	106.71
37	36	301	CLA	C3C-C4C-NC	4.03	115.10	110.57
37	B	512	CLA	C3D-C4D-ND	4.03	116.76	110.24
37	13	301	CLA	C4A-NA-C1A	-4.03	104.89	106.71
37	33	301	CLA	C4A-NA-C1A	-4.03	104.89	106.71
47	12	211	KC1	C4B-C3B-C2B	-4.03	103.44	106.75
47	38	207	KC1	C1C-C2C-C3C	-4.03	102.72	106.96
37	B	510	CLA	C3D-C4D-ND	4.03	116.76	110.24
37	14	301	CLA	C1D-CHD-C4C	-4.03	117.36	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	524	CLA	CAA-C2A-C1A	4.03	125.19	111.97
47	37	302	KC1	C4B-C3B-C2B	-4.03	103.44	106.75
37	19	310	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
37	38	204	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
47	31	305	KC1	C4B-C3B-C2B	-4.03	103.44	106.75
37	38	209	CLA	C4A-NA-C1A	-4.03	104.89	106.71
37	a	403	CLA	C1D-CHD-C4C	-4.03	117.37	126.06
37	16	301	CLA	C3C-C4C-NC	4.03	115.09	110.57
37	11	305	CLA	C3D-C4D-ND	4.03	116.75	110.24
37	39	310	CLA	C3C-C4C-NC	4.03	115.09	110.57
37	C	508	CLA	CMB-C2B-C3B	4.03	132.21	124.68
37	11	310	CLA	C4A-NA-C1A	-4.03	104.90	106.71
37	B	515	CLA	C3D-C4D-ND	4.02	116.75	110.24
37	c	508	CLA	C3D-C4D-ND	4.02	116.75	110.24
37	16	306	CLA	C3D-C4D-ND	4.02	116.75	110.24
37	35	305	CLA	C3D-C4D-ND	4.02	116.75	110.24
37	19	310	CLA	C3C-C4C-NC	4.02	115.08	110.57
37	33	308	CLA	C3C-C4C-NC	4.02	115.08	110.57
37	35	310	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
47	13	309	KC1	C1C-C2C-C3C	-4.02	102.73	106.96
48	17	311	A86	C36-C31-C32	-4.02	115.71	119.70
37	c	512	CLA	C3C-C4C-NC	4.02	115.08	110.57
40	36	315	SQD	O9-S-C6	4.02	111.72	106.94
37	C	510	CLA	C3D-C4D-ND	4.02	116.74	110.24
37	18	208	CLA	C3D-C4D-ND	4.02	116.74	110.24
40	a	409	SQD	O7-S-C6	4.02	111.72	106.94
37	34	310	CLA	C4A-NA-C1A	-4.02	104.90	106.71
37	37	308	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
37	39	301	CLA	C3C-C4C-NC	4.02	115.08	110.57
37	12	205	CLA	C3D-C4D-ND	4.02	116.73	110.24
37	c	508	CLA	CMB-C2B-C3B	4.02	132.19	124.68
47	36	305	KC1	C1A-NA-C4A	-4.01	104.90	106.71
47	37	304	KC1	CHD-C4C-C3C	-4.01	117.79	125.33
37	11	303	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
37	38	202	CLA	O2D-CGD-CBD	4.01	118.40	111.27
37	31	306	CLA	C3D-C4D-ND	4.01	116.73	110.24
50	36	312	DD6	C21-C20-C19	-4.01	109.77	114.28
48	36	310	A86	C4-C5-C6	-4.01	121.59	127.31
37	39	301	CLA	C4A-NA-C1A	-4.01	104.90	106.71
37	36	306	CLA	C3D-C4D-ND	4.01	116.72	110.24
37	40	209	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
37	19	302	CLA	C1C-C2C-C3C	-4.01	102.74	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	14	306	KC1	C4B-C3B-C2B	-4.01	103.46	106.75
40	17	301	SQD	O9-S-C6	4.01	111.70	106.94
48	16	310	A86	C4-C5-C6	-4.01	121.59	127.31
48	37	313	A86	C9-C10-C11	-4.01	114.83	126.61
37	18	204	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
37	17	307	CLA	C3D-C4D-ND	4.01	116.72	110.24
47	13	302	KC1	CBA-CAA-C2A	-4.01	109.99	125.27
47	33	302	KC1	CBA-CAA-C2A	-4.01	109.99	125.27
37	37	306	CLA	C3D-C4D-ND	4.01	116.72	110.24
37	41	205	CLA	C3D-C4D-ND	4.01	116.72	110.24
37	b	516	CLA	C3C-C4C-NC	4.01	115.06	110.57
40	A	407	SQD	O7-S-C6	4.01	111.70	106.94
48	16	311	A86	C12-C11-C13	4.01	122.75	116.02
47	37	302	KC1	C2A-C1A-NA	4.00	115.83	109.40
37	38	208	CLA	C3D-C2D-C1D	-4.00	100.37	105.83
47	31	307	KC1	C2A-C1A-NA	4.00	115.82	109.40
37	39	310	CLA	C1D-CHD-C4C	-4.00	117.42	126.06
37	15	308	CLA	CAC-C3C-C4C	4.00	130.00	124.81
37	38	208	CLA	C3D-C4D-ND	4.00	116.71	110.24
37	C	509	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
47	38	205	KC1	C1A-NA-C4A	-4.00	104.91	106.71
37	32	211	CLA	CAC-C3C-C4C	4.00	130.00	124.81
48	19	313	A86	C40-C32-C31	-4.00	106.89	110.47
47	20	302	KC1	C2A-C1A-NA	4.00	115.81	109.40
37	c	509	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
37	C	508	CLA	C3D-C4D-ND	4.00	116.71	110.24
37	33	307	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
37	19	307	CLA	O2D-CGD-CBD	4.00	118.37	111.27
37	41	209	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
37	35	301	CLA	C3C-C4C-NC	4.00	115.05	110.57
37	19	310	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
37	38	208	CLA	C3C-C4C-NC	4.00	115.05	110.57
37	39	310	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
37	Z	102	CLA	C3D-C4D-ND	4.00	116.70	110.24
37	14	310	CLA	C4A-NA-C1A	-3.99	104.91	106.71
37	b	523	CLA	CAA-C2A-C1A	3.99	125.07	111.97
47	11	302	KC1	C4B-C3B-C2B	-3.99	103.47	106.75
47	31	303	KC1	C4B-C3B-C2B	-3.99	103.47	106.75
48	13	314	A86	C36-C31-C32	-3.99	115.73	119.70
37	19	301	CLA	C3C-C4C-NC	3.99	115.05	110.57
37	13	307	CLA	C3D-C2D-C1D	-3.99	100.38	105.83
37	c	510	CLA	C3D-C4D-ND	3.99	116.70	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	16	310	A86	C34-O4-C38	-3.99	110.46	117.90
47	35	306	KC1	CBA-CAA-C2A	-3.99	110.06	125.27
47	35	306	KC1	C2A-C1A-NA	3.99	115.80	109.40
47	16	302	KC1	C1C-C2C-C3C	-3.99	102.76	106.96
37	41	205	CLA	O2D-CGD-CBD	3.99	118.36	111.27
37	17	302	CLA	C4A-NA-C1A	-3.99	104.91	106.71
37	34	302	CLA	C4A-NA-C1A	-3.99	104.91	106.71
47	18	205	KC1	C1A-NA-C4A	-3.99	104.91	106.71
48	36	310	A86	C34-O4-C38	-3.99	110.46	117.90
37	15	307	CLA	C3D-C4D-ND	3.99	116.69	110.24
37	21	205	CLA	C3D-C4D-ND	3.99	116.69	110.24
37	B	513	CLA	C4A-NA-C1A	-3.99	104.91	106.71
48	18	215	A86	C3-C2-C1	-3.99	121.62	127.31
40	40	202	SQD	O6-C1-C2	3.99	114.53	108.30
37	11	301	CLA	C2C-C1C-NC	3.98	113.70	109.97
37	21	205	CLA	O2D-CGD-CBD	3.98	118.35	111.27
47	19	308	KC1	C4B-C3B-C2B	-3.98	103.48	106.75
37	14	302	CLA	C1D-CHD-C4C	-3.98	117.46	126.06
47	11	306	KC1	C2A-C1A-NA	3.98	115.79	109.40
37	a	403	CLA	C3B-C4B-NB	3.98	114.36	109.21
37	18	208	CLA	C3C-C4C-NC	3.98	115.04	110.57
48	41	213	A86	C4-C5-C6	-3.98	121.63	127.31
50	21	216	DD6	O1-C20-C21	-3.98	110.29	115.06
37	20	307	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
37	11	303	CLA	C3D-C4D-ND	3.98	116.68	110.24
37	21	209	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
47	15	306	KC1	CBA-CAA-C2A	-3.98	110.10	125.27
47	41	203	KC1	CHC-C1C-C2C	-3.98	118.76	124.98
47	17	303	KC1	C2A-C1A-NA	3.98	115.78	109.40
47	40	204	KC1	C2A-C1A-NA	3.98	115.78	109.40
37	31	304	CLA	C3D-C4D-ND	3.98	116.67	110.24
37	37	301	CLA	C4A-NA-C1A	-3.98	104.92	106.71
47	20	305	KC1	C2A-C1A-NA	3.98	115.78	109.40
37	b	513	CLA	C4A-NA-C1A	-3.97	104.92	106.71
47	31	307	KC1	CBA-CAA-C2A	-3.97	110.12	125.27
37	35	305	CLA	C1D-CHD-C4C	-3.97	117.48	126.06
37	31	304	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
47	21	203	KC1	CHC-C1C-C2C	-3.97	118.77	124.98
37	17	304	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
48	12	217	A86	C3-C2-C1	-3.97	121.64	127.31
37	31	301	CLA	C3C-C4C-NC	3.97	115.02	110.57
47	17	305	KC1	C1A-NA-C4A	-3.97	104.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	36	306	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
37	34	302	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
50	40	212	DD6	C24-C1-C2	-3.97	112.85	118.94
37	B	516	CLA	C3C-C4C-NC	3.97	115.02	110.57
37	40	208	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
37	39	301	CLA	C1-C2-C3	-3.97	119.18	126.04
37	39	307	CLA	O2D-CGD-CBD	3.97	118.31	111.27
37	32	210	CLA	C3C-C4C-NC	3.97	115.02	110.57
47	40	207	KC1	C2A-C1A-NA	3.96	115.76	109.40
48	12	217	A86	C35-C34-C33	3.96	116.79	109.88
37	W	102	CLA	C3C-C4C-NC	3.96	115.02	110.57
50	20	310	DD6	C24-C1-C2	-3.96	112.86	118.94
48	21	213	A86	C4-C5-C6	-3.96	121.66	127.31
37	20	306	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
37	C	501	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
48	36	310	A86	C20-C19-C18	-3.96	104.92	112.75
37	13	305	CLA	C4A-NA-C1A	-3.96	104.93	106.71
37	c	501	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
37	31	302	CLA	C2C-C1C-NC	3.96	113.68	109.97
37	A	403	CLA	C3B-C4B-NB	3.96	114.33	109.21
48	32	218	A86	C3-C2-C1	-3.96	121.66	127.31
50	20	310	DD6	O1-C20-C21	-3.96	110.31	115.06
37	32	213	CLA	C3C-C4C-NC	3.96	115.01	110.57
47	15	306	KC1	C2A-C1A-NA	3.96	115.75	109.40
48	14	312	A86	C4-C5-C6	-3.96	121.67	127.31
48	34	312	A86	C4-C5-C6	-3.95	121.67	127.31
37	18	203	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
37	B	524	CLA	C3D-C4D-ND	3.95	116.63	110.24
48	31	319	A86	C25-C26-C27	3.95	132.95	127.31
37	19	301	CLA	C1-C2-C3	-3.95	119.21	126.04
37	b	516	CLA	C3D-C4D-ND	3.95	116.63	110.24
37	16	306	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
50	40	212	DD6	O1-C20-C21	-3.95	110.32	115.06
48	35	315	A86	C12-C11-C13	3.95	122.66	116.02
48	37	311	A86	C3-C2-C1	-3.95	121.67	127.31
37	B	511	CLA	C3C-C4C-NC	3.95	115.00	110.57
37	38	203	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
37	12	212	CLA	C3C-C4C-NC	3.95	115.00	110.57
47	38	205	KC1	C2A-C1A-NA	3.95	115.74	109.40
37	13	301	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
37	15	310	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
47	17	305	KC1	C2C-C1C-NC	3.95	114.88	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	17	308	KC1	C2C-C1C-NC	3.95	114.88	110.57
47	16	305	KC1	C4B-C3B-C2B	-3.95	103.51	106.75
47	11	306	KC1	CBA-CAA-C2A	-3.95	110.22	125.27
37	33	303	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
48	18	215	A86	C41-C32-C31	-3.95	106.94	110.47
47	14	304	KC1	CBA-CAA-C2A	-3.95	110.22	125.27
37	39	303	CLA	C3C-C4C-NC	3.95	115.00	110.57
37	38	209	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
48	31	313	A86	O1-C15-C14	-3.95	105.29	113.21
37	12	209	CLA	C3C-C4C-NC	3.95	115.00	110.57
40	16	315	SQD	O6-C1-C2	3.95	114.46	108.30
48	16	310	A86	C20-C19-C18	-3.95	104.94	112.75
37	18	209	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
47	33	302	KC1	C1C-C2C-C3C	-3.94	102.81	106.96
37	18	201	CLA	C3C-C4C-NC	3.94	115.00	110.57
37	19	310	CLA	C3D-C4D-ND	3.94	116.62	110.24
37	39	310	CLA	C3D-C4D-ND	3.94	116.62	110.24
48	11	319	A86	C25-C26-C27	3.94	132.94	127.31
47	34	304	KC1	CBA-CAA-C2A	-3.94	110.23	125.27
47	37	304	KC1	C2C-C1C-NC	3.94	114.88	110.57
37	37	303	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
48	34	315	A86	C3-C4-C5	-3.94	115.40	123.47
50	41	216	DD6	O1-C20-C21	-3.94	110.33	115.06
37	35	307	CLA	C3D-C4D-ND	3.94	116.61	110.24
48	36	311	A86	C12-C11-C13	3.94	122.64	116.02
48	32	218	A86	C35-C34-C33	3.94	116.75	109.88
37	18	209	CLA	C4A-NA-C1A	-3.94	104.93	106.71
37	19	301	CLA	C4A-NA-C1A	-3.94	104.93	106.71
37	33	305	CLA	C4A-NA-C1A	-3.94	104.93	106.71
47	32	212	KC1	CBA-CAA-C2A	-3.94	110.25	125.27
48	38	215	A86	C41-C32-C31	-3.94	106.95	110.47
37	b	523	CLA	C3D-C4D-ND	3.94	116.61	110.24
37	b	511	CLA	C3C-C4C-NC	3.94	114.99	110.57
37	15	305	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
47	36	305	KC1	C4B-C3B-C2B	-3.94	103.52	106.75
48	34	315	A86	C41-C32-C31	-3.94	106.95	110.47
37	31	302	CLA	C3D-C4D-ND	3.94	116.61	110.24
48	17	320	A86	C12-C11-C13	3.94	122.64	116.02
37	37	301	CLA	O2D-CGD-CBD	3.94	118.27	111.27
37	11	301	CLA	C3D-C4D-ND	3.94	116.61	110.24
50	20	312	DD6	C23-C16-C15	3.94	120.67	110.05
47	12	211	KC1	CBA-CAA-C2A	-3.94	110.26	125.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	18	207	KC1	CBA-CAA-C2A	-3.94	110.27	125.27
37	c	510	CLA	C3D-C2D-C1D	-3.93	100.46	105.83
47	33	304	KC1	C1A-NA-C4A	-3.93	104.94	106.71
48	17	314	A86	C9-C10-C11	-3.93	115.05	126.61
47	18	205	KC1	C2A-C1A-NA	3.93	115.71	109.40
37	15	303	CLA	CAA-C2A-C3A	-3.93	102.01	112.78
48	16	314	A86	C9-C8-C6	-3.93	115.37	126.42
37	11	307	CLA	C3D-C4D-ND	3.93	116.60	110.24
50	40	214	DD6	C23-C16-C15	3.93	120.66	110.05
37	C	508	CLA	C4A-NA-C1A	-3.93	104.94	106.71
37	13	301	CLA	C3D-C4D-ND	3.93	116.59	110.24
48	14	315	A86	C41-C32-C31	-3.93	106.95	110.47
37	33	301	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
37	15	303	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
37	33	301	CLA	C3D-C4D-ND	3.93	116.59	110.24
47	38	207	KC1	CBA-CAA-C2A	-3.93	110.30	125.27
47	31	307	KC1	C1C-C2C-C3C	-3.93	102.83	106.96
47	32	212	KC1	C1C-C2C-C3C	-3.93	102.83	106.96
47	37	307	KC1	C4B-C3B-C2B	-3.93	103.53	106.75
48	14	315	A86	C3-C4-C5	-3.92	115.43	123.47
37	C	509	CLA	C3D-C4D-ND	3.92	116.58	110.24
37	B	516	CLA	C3D-C4D-ND	3.92	116.58	110.24
37	31	308	CLA	C3D-C4D-ND	3.92	116.58	110.24
37	12	212	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
47	35	304	KC1	CBA-CAA-C2A	-3.92	110.33	125.27
37	16	307	CLA	C4A-NA-C1A	-3.92	104.94	106.71
48	18	213	A86	C7-C6-C5	-3.92	117.43	122.92
37	32	210	CLA	CMB-C2B-C3B	3.92	132.01	124.68
37	35	305	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
37	31	302	CLA	CAA-CBA-CGA	-3.92	101.80	113.25
48	40	211	A86	C41-C32-C31	-3.92	106.97	110.47
48	36	313	A86	C9-C8-C6	-3.92	115.42	126.42
47	38	205	KC1	C1C-C2C-C3C	-3.92	102.84	106.96
37	b	504	CLA	C4A-NA-C1A	-3.91	104.95	106.71
37	36	307	CLA	C4A-NA-C1A	-3.91	104.95	106.71
47	31	303	KC1	CBC-CAC-C3C	-3.91	101.64	112.43
37	c	509	CLA	C3D-C4D-ND	3.91	116.57	110.24
37	18	208	CLA	C3D-C2D-C1D	-3.91	100.49	105.83
37	36	301	CLA	C1D-CHD-C4C	-3.91	117.61	126.06
37	c	503	CLA	C3C-C4C-NC	3.91	114.96	110.57
37	19	303	CLA	C3C-C4C-NC	3.91	114.96	110.57
48	17	315	A86	C35-C34-C33	3.91	116.70	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	36	307	CLA	O2D-CGD-CBD	3.91	118.22	111.27
47	17	308	KC1	C4B-C3B-C2B	-3.91	103.54	106.75
37	40	210	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
47	11	302	KC1	CBC-CAC-C3C	-3.91	101.65	112.43
37	C	510	CLA	C3D-C2D-C1D	-3.91	100.50	105.83
47	15	304	KC1	CBA-CAA-C2A	-3.91	110.37	125.27
37	B	514	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
37	33	308	CLA	CAC-C3C-C4C	3.91	129.88	124.81
37	13	303	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
48	37	314	A86	C35-C34-C33	3.91	116.69	109.88
37	35	303	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
37	11	301	CLA	CAA-CBA-CGA	-3.90	101.84	113.25
37	b	514	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
37	16	301	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
37	34	310	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
48	35	319	A86	C12-C11-C13	3.90	122.58	116.02
37	21	210	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
37	38	211	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
47	41	203	KC1	CBA-CAA-C2A	-3.90	110.40	125.27
37	C	504	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
40	A	407	SQD	O9-S-O7	-3.90	100.45	113.95
40	a	409	SQD	O9-S-O7	-3.90	100.45	113.95
47	21	203	KC1	CBA-CAA-C2A	-3.90	110.41	125.27
37	16	307	CLA	O2D-CGD-CBD	3.90	118.20	111.27
47	31	309	KC1	C4B-C3B-C2B	-3.90	103.55	106.75
48	36	311	A86	C40-C32-C31	-3.90	106.98	110.47
47	34	306	KC1	C4B-C3B-C2B	-3.90	103.55	106.75
48	35	313	A86	C41-C32-C31	-3.90	106.99	110.47
37	20	308	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
37	18	203	CLA	C3C-C4C-NC	3.89	114.94	110.57
48	20	309	A86	C41-C32-C31	-3.89	106.99	110.47
48	39	313	A86	C40-C32-C31	-3.89	106.99	110.47
37	12	210	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
47	20	305	KC1	C1A-NA-C4A	-3.89	104.96	106.71
48	15	319	A86	C12-C11-C13	3.89	122.56	116.02
50	21	212	DD6	C37-C36-C35	-3.89	107.14	114.36
37	13	308	CLA	CAC-C3C-C4C	3.89	129.86	124.81
37	17	307	CLA	C4A-NA-C1A	-3.89	104.96	106.71
37	c	510	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
37	32	213	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
37	b	501	CLA	C3D-C4D-ND	3.89	116.53	110.24
37	15	305	CLA	C1C-C2C-C3C	-3.89	102.87	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	18	205	KC1	C1C-C2C-C3C	-3.89	102.87	106.96
37	12	209	CLA	CMB-C2B-C3B	3.89	131.95	124.68
37	15	307	CLA	C3C-C4C-NC	3.89	114.93	110.57
37	c	506	CLA	CHC-C1C-C2C	-3.89	115.97	126.72
37	c	504	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
37	38	203	CLA	C3C-C4C-NC	3.89	114.93	110.57
37	19	305	CLA	O2D-CGD-CBD	3.89	118.17	111.27
37	14	307	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
37	35	307	CLA	C3C-C4C-NC	3.89	114.93	110.57
37	31	306	CLA	C4A-NA-C1A	-3.89	104.96	106.71
50	21	212	DD6	O1-C20-C21	-3.88	110.40	115.06
37	B	501	CLA	C3D-C4D-ND	3.88	116.52	110.24
50	41	212	DD6	O1-C20-C21	-3.88	110.40	115.06
37	39	307	CLA	C3D-C4D-ND	3.88	116.52	110.24
37	C	510	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
37	B	503	CLA	C3D-C4D-ND	3.88	116.52	110.24
47	36	304	KC1	CBA-CAA-C2A	-3.88	110.47	125.27
48	11	313	A86	O1-C15-C14	-3.88	105.42	113.21
37	13	310	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
37	14	310	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
37	C	506	CLA	CHC-C1C-C2C	-3.88	115.99	126.72
47	16	304	KC1	CBA-CAA-C2A	-3.88	110.48	125.27
37	34	307	CLA	C3C-C4C-NC	3.88	114.92	110.57
37	c	504	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
44	j	101	DGD	O3G-C3G-C2G	-3.88	101.54	110.90
47	32	212	KC1	C2A-C1A-NA	3.88	115.62	109.40
37	C	503	CLA	C3C-C4C-NC	3.88	114.92	110.57
47	17	305	KC1	C4B-C3B-C2B	-3.88	103.57	106.75
48	16	311	A86	C40-C32-C31	-3.88	107.00	110.47
37	36	307	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
37	12	207	CLA	CAA-C2A-C3A	-3.88	102.16	112.78
37	21	210	CLA	C3C-C4C-NC	3.88	114.92	110.57
47	12	206	KC1	C2A-C1A-NA	3.88	115.62	109.40
47	32	207	KC1	C2A-C1A-NA	3.88	115.62	109.40
50	41	212	DD6	C37-C36-C35	-3.87	107.18	114.36
37	41	210	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
37	31	310	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
37	14	302	CLA	C4A-NA-C1A	-3.87	104.97	106.71
47	20	305	KC1	C4C-C3C-C2C	-3.87	101.25	106.90
47	32	209	KC1	C1C-C2C-C3C	-3.87	102.89	106.96
37	33	310	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
37	34	307	CLA	C1D-CHD-C4C	-3.87	117.71	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	13	304	KC1	C1A-NA-C4A	-3.87	104.97	106.71
37	15	310	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
47	31	307	KC1	C2C-C1C-NC	3.87	114.80	110.57
47	33	306	KC1	CBA-CAA-C2A	-3.87	110.52	125.27
37	39	303	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
37	14	307	CLA	C3C-C4C-NC	3.87	114.91	110.57
37	41	210	CLA	C3C-C4C-NC	3.87	114.91	110.57
37	39	309	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
47	13	304	KC1	C1C-C2C-C3C	-3.87	102.89	106.96
47	12	206	KC1	C1C-C2C-C3C	-3.87	102.89	106.96
37	39	305	CLA	O2D-CGD-CBD	3.87	118.14	111.27
47	37	307	KC1	C2C-C1C-NC	3.87	114.79	110.57
37	36	307	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
37	18	206	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
37	18	202	CLA	C3C-C4C-NC	3.87	114.91	110.57
37	11	310	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
47	38	205	KC1	C4B-C3B-C2B	-3.87	103.58	106.75
47	16	304	KC1	C2A-C1A-NA	3.87	115.60	109.40
37	z	102	CLA	O2D-CGD-CBD	3.86	118.13	111.27
47	12	208	KC1	C1C-C2C-C3C	-3.86	102.89	106.96
37	B	507	CLA	C3B-C4B-NB	3.86	114.20	109.21
44	J	101	DGD	O3G-C3G-C2G	-3.86	101.58	110.90
37	C	504	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
37	17	309	CLA	C3C-C4C-NC	3.86	114.90	110.57
37	19	303	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
37	12	204	CLA	C4A-NA-C1A	-3.86	104.97	106.71
37	41	208	CLA	C4A-NA-C1A	-3.86	104.97	106.71
37	c	511	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
37	c	506	CLA	C3D-C4D-ND	3.86	116.48	110.24
37	16	307	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
37	Z	102	CLA	O2D-CGD-CBD	3.86	118.12	111.27
37	Z	102	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
47	13	302	KC1	C1C-C2C-C3C	-3.86	102.90	106.96
37	A	405	CLA	C3C-C4C-NC	3.86	114.90	110.57
37	b	503	CLA	C3D-C4D-ND	3.86	116.48	110.24
47	13	306	KC1	CBA-CAA-C2A	-3.86	110.56	125.27
48	18	212	A86	C4-C5-C6	-3.86	121.81	127.31
37	16	307	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
37	18	211	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
48	37	319	A86	C12-C11-C13	3.86	122.50	116.02
37	32	208	CLA	CAA-C2A-C3A	-3.85	102.22	112.78
37	32	206	CLA	C3C-C4C-NC	3.85	114.89	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	36	311	A86	C35-C34-C33	3.85	116.60	109.88
47	40	207	KC1	C4C-C3C-C2C	-3.85	101.28	106.90
37	33	307	CLA	C4A-NA-C1A	-3.85	104.97	106.71
37	20	308	CLA	C3D-C4D-ND	3.85	116.47	110.24
37	b	504	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
48	17	312	A86	C3-C2-C1	-3.85	121.81	127.31
37	19	307	CLA	C3D-C4D-ND	3.85	116.47	110.24
48	16	311	A86	C35-C34-C33	3.85	116.59	109.88
37	C	511	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
37	16	303	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
37	21	204	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
48	35	312	A86	C3-C4-C5	-3.85	115.59	123.47
47	37	305	KC1	C2A-C1A-NA	3.85	115.58	109.40
37	34	305	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
47	16	305	KC1	C1A-NA-C4A	-3.85	104.98	106.71
50	39	312	DD6	C19-C18-C17	3.85	118.20	110.77
37	z	102	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
48	14	315	A86	C4-C5-C6	-3.85	121.82	127.31
47	18	207	KC1	C2A-C1A-NA	3.85	115.57	109.40
47	16	304	KC1	C1A-NA-C4A	-3.85	104.98	106.71
37	12	210	CLA	C3C-C4C-NC	3.85	114.88	110.57
48	33	313	A86	C36-C31-C32	-3.85	115.88	119.70
47	18	205	KC1	C4B-C3B-C2B	-3.85	103.59	106.75
48	17	314	A86	C4-C3-C2	-3.84	115.60	123.47
47	36	304	KC1	C2A-C1A-NA	3.84	115.57	109.40
48	34	315	A86	C4-C5-C6	-3.84	121.82	127.31
48	15	312	A86	C3-C4-C5	-3.84	115.60	123.47
47	32	207	KC1	C1C-C2C-C3C	-3.84	102.92	106.96
37	C	506	CLA	O2D-CGD-CBD	3.84	118.09	111.27
37	a	407	CLA	C3C-C4C-NC	3.84	114.88	110.57
37	32	211	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
39	0	101	BCR	C2-C1-C6	3.84	116.39	110.48
47	17	306	KC1	C2A-C1A-NA	3.84	115.56	109.40
37	B	514	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
48	37	310	A86	C36-C31-C32	-3.84	115.89	119.70
47	39	308	KC1	C1C-C2C-C3C	-3.84	102.92	106.96
48	34	314	A86	C41-C32-C31	-3.84	107.04	110.47
37	37	306	CLA	C4A-NA-C1A	-3.84	104.98	106.71
50	19	312	DD6	C19-C18-C17	3.84	118.19	110.77
37	d	404	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
48	18	213	A86	C3-C4-C5	-3.84	115.61	123.47
37	33	305	CLA	C1D-CHD-C4C	-3.84	117.78	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	38	206	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
37	17	302	CLA	O2D-CGD-CBD	3.84	118.09	111.27
47	12	211	KC1	C2A-C1A-NA	3.84	115.56	109.40
47	11	306	KC1	C1C-C2C-C3C	-3.84	102.92	106.96
37	D	406	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
37	32	206	CLA	CBA-CAA-C2A	3.84	125.19	113.86
37	b	507	CLA	C3B-C4B-NB	3.83	114.17	109.21
37	11	303	CLA	CBA-CAA-C2A	3.83	125.18	113.86
37	17	302	CLA	C3C-C4C-NC	3.83	114.87	110.57
37	b	516	CLA	C4C-C3C-C2C	-3.83	101.31	106.90
47	31	309	KC1	C1C-C2C-C3C	-3.83	102.93	106.96
40	40	202	SQD	O9-S-O7	-3.83	100.68	113.95
37	b	514	CLA	O2D-CGD-O1D	-3.83	116.34	123.84
37	32	204	CLA	C3D-C4D-ND	3.83	116.44	110.24
47	12	211	KC1	C1C-C2C-C3C	-3.83	102.93	106.96
37	C	506	CLA	C3D-C4D-ND	3.83	116.44	110.24
37	41	205	CLA	C4A-NA-C1A	-3.83	104.98	106.71
37	14	305	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
47	33	304	KC1	C1C-C2C-C3C	-3.83	102.93	106.96
37	40	210	CLA	C3D-C4D-ND	3.83	116.43	110.24
37	12	209	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
40	16	315	SQD	O9-S-O7	-3.83	100.70	113.95
37	32	211	CLA	C3C-C4C-NC	3.83	114.86	110.57
37	B	504	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
37	15	308	CLA	C1C-C2C-C3C	-3.83	102.94	106.96
47	36	304	KC1	C1C-C2C-C3C	-3.83	102.94	106.96
47	40	206	KC1	C2A-C1A-NA	3.82	115.54	109.40
37	21	205	CLA	C3C-C4C-NC	3.82	114.86	110.57
37	41	205	CLA	C3C-C4C-NC	3.82	114.86	110.57
37	18	206	CLA	C3B-C4B-NB	3.82	114.15	109.21
37	B	514	CLA	C3D-C4D-ND	3.82	116.42	110.24
37	12	205	CLA	CBA-CAA-C2A	3.82	125.15	113.86
37	41	204	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
48	17	312	A86	C12-C11-C13	3.82	122.44	116.02
37	B	516	CLA	C4C-C3C-C2C	-3.82	101.33	106.90
37	13	305	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
37	11	301	CLA	C4A-NA-C1A	-3.82	104.99	106.71
47	31	307	KC1	C1A-NA-C4A	-3.82	104.99	106.71
47	16	304	KC1	C1C-C2C-C3C	-3.82	102.94	106.96
39	5	101	BCR	C2-C1-C6	3.82	116.36	110.48
47	11	306	KC1	C2C-C1C-NC	3.82	114.74	110.57
37	b	507	CLA	C1D-CHD-C4C	-3.82	117.82	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	17	301	SQD	O7-S-C6	3.82	111.48	106.94
40	36	315	SQD	O7-S-C6	3.82	111.48	106.94
48	19	311	A86	C25-C24-C1	-3.82	115.69	126.42
37	19	305	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
37	31	304	CLA	CBA-CAA-C2A	3.82	125.13	113.86
48	13	315	A86	C25-C26-C27	-3.82	121.86	127.31
48	32	221	A86	C10-C9-C8	-3.82	111.31	123.22
37	35	310	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
37	19	309	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
37	C	506	CLA	C3C-C4C-NC	3.82	114.85	110.57
37	14	303	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
37	32	210	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
47	20	304	KC1	C2A-C1A-NA	3.81	115.52	109.40
37	15	310	CLA	CAA-C2A-C3A	-3.81	102.33	112.78
48	14	314	A86	C41-C32-C31	-3.81	107.06	110.47
37	31	301	CLA	C3D-C4D-ND	3.81	116.41	110.24
47	32	209	KC1	C2A-C1A-NA	3.81	115.52	109.40
37	35	310	CLA	CAA-C2A-C3A	-3.81	102.34	112.78
37	11	305	CLA	C4A-NA-C1A	-3.81	104.99	106.71
48	17	320	A86	C3-C2-C1	-3.81	121.87	127.31
37	19	309	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
48	34	315	A86	C25-C24-C1	-3.81	115.71	126.42
37	b	514	CLA	C3D-C4D-ND	3.81	116.40	110.24
37	B	502	CLA	C3B-C4B-NB	3.81	114.14	109.21
37	B	507	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
37	c	506	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
37	18	204	CLA	CAA-C2A-C3A	-3.81	102.35	112.78
37	18	209	CLA	C3D-C4D-ND	3.81	116.40	110.24
37	38	209	CLA	C3D-C4D-ND	3.81	116.40	110.24
37	14	302	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
50	20	312	DD6	C21-C20-C19	-3.81	110.00	114.28
47	15	306	KC1	C1A-NA-C4A	-3.81	104.99	106.71
37	36	303	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
48	11	312	A86	C26-C25-C24	-3.81	111.33	123.22
47	33	304	KC1	C2A-C1A-NA	3.81	115.51	109.40
37	c	506	CLA	O2D-CGD-CBD	3.81	118.03	111.27
37	39	305	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
48	14	315	A86	C25-C24-C1	-3.81	115.72	126.42
47	38	207	KC1	C2A-C1A-NA	3.81	115.50	109.40
37	12	203	CLA	C3D-C4D-ND	3.80	116.39	110.24
48	31	312	A86	C26-C25-C24	-3.80	111.34	123.22
37	34	305	CLA	C1C-C2C-C3C	-3.80	102.96	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	19	308	KC1	C1C-C2C-C3C	-3.80	102.96	106.96
47	41	203	KC1	C1C-C2C-C3C	-3.80	102.96	106.96
37	D	401	CLA	C3B-C4B-NB	3.80	114.13	109.21
47	14	309	KC1	C2C-C1C-NC	3.80	114.72	110.57
37	14	302	CLA	C3D-C4D-ND	3.80	116.39	110.24
37	38	209	CLA	O2D-CGD-CBD	3.80	118.03	111.27
47	20	304	KC1	CAC-C3C-C4C	3.80	129.74	124.81
37	38	201	CLA	O2D-CGD-CBD	3.80	118.02	111.27
37	B	504	CLA	C4A-NA-C1A	-3.80	105.00	106.71
37	c	506	CLA	C3C-C4C-NC	3.80	114.83	110.57
48	39	311	A86	C25-C24-C1	-3.80	115.74	126.42
37	34	303	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
47	40	207	KC1	C1A-NA-C4A	-3.80	105.00	106.71
37	C	506	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
37	21	208	CLA	C4A-NA-C1A	-3.80	105.00	106.71
37	31	302	CLA	C4A-NA-C1A	-3.80	105.00	106.71
37	20	306	CLA	C3C-C4C-NC	3.80	114.83	110.57
37	18	206	CLA	C3C-C4C-NC	3.80	114.83	110.57
47	11	309	KC1	C4B-C3B-C2B	-3.79	103.64	106.75
47	40	206	KC1	CAC-C3C-C4C	3.79	129.73	124.81
37	41	202	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
37	18	201	CLA	O2D-CGD-CBD	3.79	118.01	111.27
37	W	102	CLA	C3D-C4D-ND	3.79	116.37	110.24
37	32	213	CLA	C3D-C4D-ND	3.79	116.37	110.24
48	33	315	A86	C25-C26-C27	-3.79	121.90	127.31
47	13	304	KC1	C2A-C1A-NA	3.79	115.48	109.40
37	18	203	CLA	C3D-C4D-ND	3.79	116.37	110.24
48	39	313	A86	C19-C18-C17	3.79	118.09	110.77
37	38	203	CLA	C3D-C4D-ND	3.79	116.37	110.24
48	12	220	A86	C10-C9-C8	-3.79	111.39	123.22
37	z	101	CLA	C3C-C4C-NC	3.79	114.82	110.57
47	41	207	KC1	CHC-C1C-C2C	-3.79	119.06	124.98
50	40	214	DD6	C21-C20-C19	-3.79	110.02	114.28
37	c	505	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
46	f	101	HEM	CMC-C2C-C3C	3.79	131.76	124.68
37	38	204	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
37	41	204	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
48	40	201	A86	C8-C6-C5	3.79	124.75	118.94
47	34	306	KC1	C2A-C1A-NA	3.79	115.47	109.40
37	B	512	CLA	CMD-C2D-C1D	3.79	131.39	124.71
37	33	308	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
48	13	313	A86	C36-C31-C32	-3.78	115.94	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	12	217	A86	C25-C26-C27	-3.78	121.91	127.31
47	21	203	KC1	C1C-C2C-C3C	-3.78	102.98	106.96
48	12	217	A86	C12-C11-C13	3.78	122.38	116.02
37	b	507	CLA	C3D-C4D-ND	3.78	116.36	110.24
48	31	311	A86	C35-C34-C33	3.78	116.48	109.88
47	16	308	KC1	C1C-C2C-C3C	-3.78	102.98	106.96
50	21	212	DD6	C35-C36-C31	-3.78	111.99	120.57
37	C	505	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
48	15	314	A86	C36-C31-C32	-3.78	115.94	119.70
37	B	507	CLA	C3D-C4D-ND	3.78	116.35	110.24
47	12	208	KC1	C2A-C1A-NA	3.78	115.46	109.40
37	b	504	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
48	11	311	A86	C35-C34-C33	3.78	116.47	109.88
37	32	202	CLA	O2D-CGD-CBD	3.78	117.98	111.27
48	32	218	A86	C25-C26-C27	-3.78	121.92	127.31
37	14	308	CLA	O2D-CGD-CBD	3.78	117.98	111.27
37	B	508	CLA	C1C-C2C-C3C	-3.78	102.99	106.96
47	11	309	KC1	C1C-C2C-C3C	-3.78	102.99	106.96
47	14	306	KC1	C2A-C1A-NA	3.78	115.46	109.40
37	34	302	CLA	C3D-C4D-ND	3.77	116.34	110.24
37	a	404	CLA	C3B-C4B-NB	3.77	114.09	109.21
37	21	202	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
37	21	204	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
47	36	304	KC1	C1A-NA-C4A	-3.77	105.01	106.71
48	15	313	A86	C41-C32-C31	-3.77	107.09	110.47
37	A	405	CLA	CAA-C2A-C3A	-3.77	102.44	112.78
37	34	308	CLA	O2D-CGD-CBD	3.77	117.97	111.27
47	18	207	KC1	O2D-CGD-O1D	-3.77	116.47	123.84
37	11	308	CLA	O2D-CGD-CBD	3.77	117.97	111.27
37	B	504	CLA	C3D-C2D-C1D	-3.77	100.69	105.83
37	14	305	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
37	11	305	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
48	18	212	A86	O4-C38-C39	3.77	118.02	111.09
37	13	308	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
37	b	502	CLA	C3B-C4B-NB	3.77	114.08	109.21
37	37	308	CLA	C3C-C4C-NC	3.77	114.80	110.57
48	38	212	A86	O4-C38-C39	3.77	118.02	111.09
37	b	505	CLA	C4-C3-C5	3.77	121.61	115.27
37	B	508	CLA	C3C-C4C-NC	3.77	114.80	110.57
37	a	407	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
47	21	207	KC1	CHC-C1C-C2C	-3.77	119.09	124.98
37	B	513	CLA	C1D-CHD-C4C	-3.77	117.93	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	41	212	DD6	C35-C36-C31	-3.77	112.02	120.57
37	34	302	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
37	34	305	CLA	C4A-NA-C1A	-3.77	105.01	106.71
37	b	513	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
37	b	512	CLA	CMD-C2D-C1D	3.76	131.35	124.71
37	32	205	CLA	C4A-NA-C1A	-3.76	105.01	106.71
37	A	405	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
37	b	515	CLA	CAC-C3C-C4C	3.76	129.69	124.81
50	40	214	DD6	O1-C20-C21	-3.76	110.55	115.06
37	D	401	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
47	37	304	KC1	CAC-C3C-C4C	3.76	129.69	124.81
37	32	206	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
37	c	502	CLA	C3D-C4D-ND	3.76	116.32	110.24
37	b	508	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
48	21	214	A86	C25-C26-C27	-3.76	121.94	127.31
37	18	204	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
37	39	309	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
46	F	101	HEM	CMC-C2C-C3C	3.76	131.71	124.68
48	37	313	A86	C4-C3-C2	-3.76	115.77	123.47
48	11	314	A86	C10-C9-C8	-3.76	111.49	123.22
37	B	505	CLA	C4-C3-C5	3.76	121.59	115.27
37	C	509	CLA	C3B-C4B-NB	3.76	114.07	109.21
37	39	307	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
37	11	305	CLA	C3C-C4C-NC	3.76	114.78	110.57
37	c	509	CLA	C3B-C4B-NB	3.76	114.07	109.21
37	12	212	CLA	C3D-C4D-ND	3.76	116.31	110.24
37	37	301	CLA	C3C-C4C-NC	3.76	114.78	110.57
37	a	407	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
48	31	314	A86	C10-C9-C8	-3.76	111.49	123.22
37	a	407	CLA	CAA-C2A-C3A	-3.76	102.49	112.78
37	40	208	CLA	C3C-C4C-NC	3.75	114.78	110.57
37	17	304	CLA	CBA-CAA-C2A	3.75	124.95	113.86
48	11	314	A86	C25-C26-C27	-3.75	121.95	127.31
37	a	404	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
48	35	314	A86	C36-C31-C32	-3.75	115.97	119.70
47	34	309	KC1	C2C-C1C-NC	3.75	114.67	110.57
50	40	212	DD6	C33-C34-C35	3.75	115.44	110.30
48	35	316	A86	C35-C34-C33	3.75	116.42	109.88
37	b	513	CLA	C3D-C4D-ND	3.75	116.31	110.24
47	37	304	KC1	C1C-C2C-C3C	-3.75	103.01	106.96
37	32	210	CLA	C3D-C4D-ND	3.75	116.30	110.24
37	21	206	CLA	C3C-C4C-NC	3.75	114.78	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	20	306	CLA	CAC-C3C-C4C	3.75	129.67	124.81
37	32	202	CLA	CAC-C3C-C4C	3.75	129.67	124.81
48	32	218	A86	C12-C11-C13	3.75	122.32	116.02
40	L	101	SQD	C1-O5-C5	3.75	121.04	113.69
48	37	311	A86	C12-C11-C13	3.75	122.31	116.02
47	36	308	KC1	C1C-C2C-C3C	-3.75	103.02	106.96
37	13	307	CLA	C4A-NA-C1A	-3.75	105.02	106.71
37	15	310	CLA	C3C-C4C-NC	3.75	114.77	110.57
37	14	307	CLA	C3D-C4D-ND	3.75	116.30	110.24
37	34	307	CLA	C3D-C4D-ND	3.75	116.30	110.24
37	C	502	CLA	C3D-C4D-ND	3.74	116.29	110.24
37	C	509	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
37	41	204	CLA	CBA-CAA-C2A	3.74	124.91	113.86
37	c	509	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
37	41	202	CLA	C3C-C4C-NC	3.74	114.77	110.57
37	12	203	CLA	C4A-NA-C1A	-3.74	105.02	106.71
37	21	204	CLA	CBA-CAA-C2A	3.74	124.91	113.86
48	16	313	A86	C8-C6-C5	3.74	124.68	118.94
37	31	306	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
37	37	303	CLA	CBA-CAA-C2A	3.74	124.90	113.86
37	B	515	CLA	CAC-C3C-C4C	3.74	129.66	124.81
37	B	513	CLA	C3D-C4D-ND	3.74	116.28	110.24
48	31	314	A86	C25-C26-C27	-3.74	121.97	127.31
47	14	309	KC1	C4B-C3B-C2B	-3.74	103.68	106.75
50	20	312	DD6	O1-C20-C21	-3.74	110.58	115.06
37	40	208	CLA	CAC-C3C-C4C	3.74	129.66	124.81
37	12	207	CLA	C3C-C4C-NC	3.74	114.76	110.57
37	19	310	CLA	C4A-NA-C1A	-3.74	105.03	106.71
48	38	215	A86	C25-C26-C27	-3.74	121.98	127.31
37	18	209	CLA	O2D-CGD-CBD	3.74	117.91	111.27
37	14	303	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
37	11	308	CLA	CAC-C3C-C4C	3.74	129.66	124.81
37	b	508	CLA	C3C-C4C-NC	3.74	114.76	110.57
37	13	307	CLA	CHD-C1D-ND	-3.74	121.02	124.45
37	20	307	CLA	C3C-C4C-NC	3.74	114.76	110.57
47	21	207	KC1	CAA-CBA-CGA	-3.73	108.07	127.26
37	38	206	CLA	C3C-C4C-NC	3.73	114.76	110.57
37	19	301	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
50	41	216	DD6	C33-C34-C35	3.73	115.41	110.30
47	41	207	KC1	CAA-CBA-CGA	-3.73	108.08	127.26
37	15	301	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
37	35	301	CLA	C1C-C2C-C3C	-3.73	103.03	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	16	307	CLA	C3C-C4C-NC	3.73	114.75	110.57
37	31	304	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
50	21	216	DD6	C33-C34-C35	3.73	115.41	110.30
40	a	409	SQD	O47-C7-C8	3.73	119.54	111.50
37	13	307	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
37	33	307	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
37	37	301	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
37	34	301	CLA	C4A-NA-C1A	-3.73	105.03	106.71
48	11	311	A86	C3-C2-C1	-3.73	121.99	127.31
40	17	301	SQD	O9-S-O7	-3.73	101.05	113.95
50	40	214	DD6	C33-C32-C31	3.73	117.17	109.62
37	b	501	CLA	CAC-C3C-C4C	3.73	129.65	124.81
37	Z	101	CLA	C3C-C4C-NC	3.73	114.75	110.57
37	31	306	CLA	C3C-C4C-NC	3.73	114.75	110.57
37	12	209	CLA	C3D-C4D-ND	3.73	116.27	110.24
48	14	314	A86	C3-C4-C5	-3.72	115.84	123.47
37	38	206	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
48	41	214	A86	C25-C26-C27	-3.72	122.00	127.31
40	36	315	SQD	O9-S-O7	-3.72	101.06	113.95
37	18	211	CLA	CAC-C3C-C4C	3.72	129.64	124.81
37	19	302	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
37	A	405	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
37	11	308	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
37	39	305	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
47	36	308	KC1	C2A-C1A-NA	3.72	115.37	109.40
37	21	204	CLA	CAC-C3C-C4C	3.72	129.64	124.81
37	32	202	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
37	21	202	CLA	C3C-C4C-NC	3.72	114.75	110.57
37	33	307	CLA	CHD-C1D-ND	-3.72	121.03	124.45
37	41	202	CLA	C4A-NA-C1A	-3.72	105.03	106.71
40	B	519	SQD	C1-O5-C5	3.72	120.99	113.69
37	32	208	CLA	C3C-C4C-NC	3.72	114.74	110.57
37	39	301	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
47	16	308	KC1	C2A-C1A-NA	3.72	115.37	109.40
48	11	312	A86	C25-C26-C27	-3.72	122.00	127.31
37	C	512	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
48	34	314	A86	C3-C4-C5	-3.72	115.86	123.47
37	13	303	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
37	b	503	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
37	41	206	CLA	C3C-C4C-NC	3.72	114.74	110.57
40	A	407	SQD	O47-C7-C8	3.72	119.51	111.50
37	c	512	CLA	C1D-CHD-C4C	-3.72	118.04	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	516	CLA	CAC-C3C-C4C	3.72	129.63	124.81
50	19	312	DD6	C35-C36-C31	-3.72	112.14	120.57
48	37	312	A86	C3-C4-C5	-3.71	115.86	123.47
37	B	501	CLA	C1D-CHD-C4C	-3.71	118.04	126.06
37	B	502	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
37	13	301	CLA	C3C-C4C-NC	3.71	114.74	110.57
37	B	502	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
37	b	501	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
37	41	204	CLA	CAC-C3C-C4C	3.71	129.63	124.81
37	39	302	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
37	b	502	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
37	11	308	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
37	32	202	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
48	18	214	A86	C41-C32-C31	-3.71	107.15	110.47
37	38	203	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
47	35	309	KC1	C1C-C2C-C3C	-3.71	103.05	106.96
48	18	215	A86	C25-C26-C27	-3.71	122.01	127.31
37	B	504	CLA	C3C-C4C-NC	3.71	114.73	110.57
37	14	305	CLA	C4A-NA-C1A	-3.71	105.04	106.71
37	21	205	CLA	C4A-NA-C1A	-3.71	105.04	106.71
48	18	214	A86	C3-C4-C5	-3.71	115.87	123.47
47	38	207	KC1	O2D-CGD-O1D	-3.71	116.59	123.84
37	41	208	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
47	11	306	KC1	C1A-NA-C4A	-3.71	105.04	106.71
50	39	312	DD6	C35-C36-C31	-3.71	112.15	120.57
37	b	502	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
48	12	214	A86	C12-C11-C13	3.71	122.25	116.02
37	z	101	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
37	B	503	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
37	b	501	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
37	21	210	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
47	17	303	KC1	CBA-CAA-C2A	-3.70	111.15	125.27
50	20	310	DD6	C33-C34-C35	3.70	115.37	110.30
48	32	215	A86	C12-C11-C13	3.70	122.24	116.02
47	37	302	KC1	CBA-CAA-C2A	-3.70	111.16	125.27
47	20	302	KC1	C4B-C3B-C2B	-3.70	103.71	106.75
37	15	303	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
37	41	205	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
37	17	302	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
37	11	303	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
47	40	204	KC1	C4B-C3B-C2B	-3.70	103.71	106.75
37	B	501	CLA	C1C-C2C-C3C	-3.70	103.07	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	38	214	A86	C41-C32-C31	-3.70	107.16	110.47
37	b	508	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
37	19	309	CLA	C3C-C4C-NC	3.70	114.72	110.57
37	38	201	CLA	C3C-C4C-NC	3.70	114.72	110.57
50	20	312	DD6	C33-C32-C31	3.70	117.11	109.62
37	41	210	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
37	18	203	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
37	33	305	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
37	b	504	CLA	C3C-C4C-NC	3.70	114.72	110.57
37	A	403	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
48	15	316	A86	C25-C26-C27	-3.70	122.04	127.31
37	19	307	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
37	21	208	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
37	16	303	CLA	C3B-C4B-NB	3.69	113.98	109.21
37	36	303	CLA	C3B-C4B-NB	3.69	113.98	109.21
47	16	305	KC1	C1C-C2C-C3C	-3.69	103.08	106.96
40	B	519	SQD	O47-C7-C8	3.69	119.46	111.50
37	18	206	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
37	37	306	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
37	32	204	CLA	C4A-NA-C1A	-3.69	105.05	106.71
48	31	311	A86	C3-C2-C1	-3.69	122.04	127.31
37	15	308	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
37	B	516	CLA	CAC-C3C-C4C	3.69	129.60	124.81
37	18	201	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
48	35	313	A86	C25-C26-C27	-3.69	122.05	127.31
37	41	205	CLA	CAC-C3C-C4C	3.69	129.60	124.81
37	12	205	CLA	C3C-C4C-NC	3.69	114.70	110.57
37	40	209	CLA	C3C-C4C-NC	3.69	114.70	110.57
37	35	303	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
37	w	101	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
47	11	304	KC1	CBA-CAA-C2A	-3.68	111.22	125.27
37	36	307	CLA	C3C-C4C-NC	3.68	114.70	110.57
37	Z	101	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
48	14	313	A86	C20-C19-C18	-3.68	105.46	112.75
37	21	205	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
37	34	303	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
37	32	204	CLA	CMC-C2C-C1C	3.68	130.65	125.04
39	C	519	BCR	C24-C23-C22	-3.68	120.67	126.23
37	35	310	CLA	C3C-C4C-NC	3.68	114.70	110.57
48	12	213	A86	C4-C5-C6	-3.68	122.06	127.31
37	15	301	CLA	C4A-NA-C1A	-3.68	105.05	106.71
39	c	519	BCR	C24-C23-C22	-3.68	120.67	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	32	214	A86	C4-C5-C6	-3.68	122.06	127.31
37	B	508	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
37	21	205	CLA	CAC-C3C-C4C	3.68	129.59	124.81
37	a	403	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
50	41	212	DD6	C25-C26-C27	3.68	137.27	126.58
37	38	204	CLA	CMB-C2B-C3B	3.68	131.56	124.68
37	36	301	CLA	CAC-C3C-C4C	3.68	129.58	124.81
47	34	309	KC1	C4B-C3B-C2B	-3.68	103.73	106.75
37	b	505	CLA	C3C-C4C-NC	3.68	114.70	110.57
48	34	314	A86	C36-C31-C32	-3.68	116.05	119.70
47	13	309	KC1	C2A-C1A-NA	3.68	115.30	109.40
37	d	401	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
37	21	202	CLA	C4A-NA-C1A	-3.67	105.05	106.71
48	31	312	A86	C25-C26-C27	-3.67	122.07	127.31
47	31	305	KC1	CBA-CAA-C2A	-3.67	111.26	125.27
37	B	505	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
37	B	509	CLA	C3D-C4D-ND	3.67	116.18	110.24
37	12	203	CLA	CMC-C2C-C1C	3.67	130.63	125.04
37	33	301	CLA	C3C-C4C-NC	3.67	114.69	110.57
37	17	307	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
37	37	308	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
37	B	501	CLA	CAC-C3C-C4C	3.67	129.57	124.81
48	35	316	A86	C33-C32-C31	3.67	112.78	109.21
37	d	404	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
37	b	509	CLA	C3D-C4D-ND	3.67	116.17	110.24
37	z	102	CLA	C3C-C4C-NC	3.67	114.68	110.57
37	c	511	CLA	C3B-C4B-NB	3.67	113.95	109.21
37	16	301	CLA	CAC-C3C-C4C	3.67	129.57	124.81
47	18	207	KC1	CMB-C2B-C1B	3.67	131.17	124.71
37	B	505	CLA	C3C-C4C-NC	3.67	114.68	110.57
47	35	306	KC1	C1A-NA-C4A	-3.67	105.06	106.71
47	35	309	KC1	C4B-C3B-C2B	-3.66	103.74	106.75
47	31	303	KC1	CBA-CAA-C2A	-3.66	111.30	125.27
47	11	302	KC1	CBA-CAA-C2A	-3.66	111.30	125.27
37	C	502	CLA	C4C-C3C-C2C	-3.66	101.56	106.90
37	c	502	CLA	C4C-C3C-C2C	-3.66	101.56	106.90
37	37	301	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
47	15	309	KC1	C1C-C2C-C3C	-3.66	103.11	106.96
48	38	212	A86	C4-C5-C6	-3.66	122.08	127.31
48	11	314	A86	C12-C11-C13	3.66	122.17	116.02
37	36	301	CLA	CMC-C2C-C1C	3.66	130.62	125.04
37	13	305	CLA	C3C-C4C-NC	3.66	114.68	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	33	305	CLA	C3C-C4C-NC	3.66	114.68	110.57
37	18	211	CLA	C4C-C3C-C2C	-3.66	101.56	106.90
48	38	215	A86	C20-C19-C18	-3.66	105.51	112.75
47	33	309	KC1	C2A-C1A-NA	3.66	115.27	109.40
37	34	307	CLA	CMB-C2B-C3B	3.66	131.53	124.68
37	D	402	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
48	15	316	A86	C20-C19-C18	-3.66	105.51	112.75
48	15	313	A86	C25-C26-C27	-3.66	122.09	127.31
37	D	406	CLA	C3C-C4C-NC	3.66	114.67	110.57
37	17	304	CLA	C3B-C4B-NB	3.66	113.94	109.21
37	W	101	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
37	b	505	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
37	31	301	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
37	32	208	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
37	32	205	CLA	C3D-C4D-ND	3.66	116.15	110.24
48	14	314	A86	C36-C31-C32	-3.66	116.07	119.70
50	20	310	DD6	C35-C36-C31	-3.66	112.27	120.57
37	a	403	CLA	CMB-C2B-C3B	3.66	131.52	124.68
37	15	305	CLA	C3C-C4C-NC	3.65	114.67	110.57
50	21	212	DD6	C25-C26-C27	3.65	137.19	126.58
37	16	309	CLA	C3C-C4C-NC	3.65	114.67	110.57
37	19	305	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
48	35	315	A86	O2-C18-C17	3.65	117.06	109.80
48	32	218	A86	C41-C32-C31	-3.65	107.20	110.47
37	39	309	CLA	C3C-C4C-NC	3.65	114.67	110.57
47	11	302	KC1	C2A-C1A-NA	3.65	115.26	109.40
48	34	313	A86	C20-C19-C18	-3.65	105.52	112.75
37	D	406	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
37	15	308	CLA	C3C-C4C-NC	3.65	114.67	110.57
48	11	311	A86	C36-C31-C32	-3.65	116.07	119.70
48	31	311	A86	C36-C31-C32	-3.65	116.07	119.70
37	31	306	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
47	20	302	KC1	CBA-CAA-C2A	-3.65	111.35	125.27
47	40	204	KC1	CBA-CAA-C2A	-3.65	111.36	125.27
37	c	512	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
40	L	101	SQD	O47-C7-C8	3.65	119.36	111.50
37	13	305	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
37	35	308	CLA	C3C-C4C-NC	3.65	114.66	110.57
37	c	509	CLA	CAA-C2A-C3A	-3.65	102.79	112.78
48	37	310	A86	C28-C27-C26	3.65	128.03	122.92
37	C	512	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
37	14	301	CLA	C4A-NA-C1A	-3.65	105.07	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	511	CLA	C3B-C4B-NB	3.65	113.92	109.21
37	12	205	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
47	37	304	KC1	CBA-CAA-C2A	-3.64	111.38	125.27
37	D	402	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
47	31	303	KC1	C2A-C1A-NA	3.64	115.24	109.40
37	14	308	CLA	C4A-NA-C1A	-3.64	105.07	106.71
37	16	301	CLA	CMC-C2C-C1C	3.64	130.58	125.04
37	b	511	CLA	O2D-CGD-CBD	3.64	117.74	111.27
37	12	207	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
37	w	101	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
37	12	204	CLA	C3D-C4D-ND	3.64	116.12	110.24
37	d	401	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
46	F	101	HEM	CBA-CAA-C2A	3.64	118.83	112.62
47	13	309	KC1	C1A-NA-C4A	-3.64	105.07	106.71
48	31	314	A86	C12-C11-C13	3.64	122.13	116.02
37	Z	102	CLA	C3C-C4C-NC	3.64	114.65	110.57
37	13	303	CLA	C3B-C4B-NB	3.64	113.91	109.21
46	f	101	HEM	CBA-CAA-C2A	3.64	118.83	112.62
37	14	307	CLA	CMB-C2B-C3B	3.64	131.48	124.68
47	15	309	KC1	C4B-C3B-C2B	-3.64	103.77	106.75
47	38	207	KC1	C1A-NA-C4A	-3.64	105.07	106.71
37	38	211	CLA	C1D-CHD-C4C	-3.64	118.22	126.06
37	17	302	CLA	C3D-C2D-C1D	-3.63	100.87	105.83
37	B	501	CLA	C4A-NA-C1A	-3.63	105.07	106.71
50	40	212	DD6	C35-C36-C31	-3.63	112.32	120.57
37	37	306	CLA	C3C-C4C-NC	3.63	114.65	110.57
37	38	211	CLA	C3C-C4C-NC	3.63	114.65	110.57
37	c	511	CLA	C3D-C4D-ND	3.63	116.12	110.24
37	b	504	CLA	O2A-CGA-CBA	3.63	123.31	111.91
37	21	206	CLA	C4A-NA-C1A	-3.63	105.07	106.71
37	39	306	CLA	C1-C2-C3	-3.63	119.76	126.04
37	17	309	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
37	C	509	CLA	CAA-C2A-C3A	-3.63	102.83	112.78
37	d	404	CLA	C3C-C4C-NC	3.63	114.64	110.57
48	12	220	A86	C25-C26-C27	-3.63	122.13	127.31
47	17	305	KC1	CBA-CAA-C2A	-3.63	111.44	125.27
37	11	305	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
37	41	202	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
48	38	213	A86	C23-C16-C22	-3.63	102.02	107.37
37	A	403	CLA	CMB-C2B-C3B	3.63	131.46	124.68
37	32	208	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
37	18	204	CLA	C3C-C4C-NC	3.62	114.64	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	34	303	CLA	C3B-C4B-NB	3.62	113.90	109.21
37	36	309	CLA	C3C-C4C-NC	3.62	114.63	110.57
37	B	504	CLA	O2A-CGA-CBA	3.62	123.27	111.91
37	14	303	CLA	C3B-C4B-NB	3.62	113.89	109.21
37	21	208	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
37	12	203	CLA	C3C-C4C-NC	3.62	114.63	110.57
37	14	305	CLA	C3C-C4C-NC	3.62	114.63	110.57
37	19	306	CLA	C1-C2-C3	-3.62	119.78	126.04
48	33	311	A86	C12-C11-C13	3.62	122.10	116.02
37	18	211	CLA	C3B-C4B-NB	3.62	113.89	109.21
37	37	303	CLA	C3B-C4B-NB	3.62	113.89	109.21
37	33	308	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
37	35	308	CLA	C1-C2-C3	-3.62	119.79	126.04
48	32	221	A86	C4-C3-C2	-3.62	116.07	123.47
37	B	513	CLA	O2D-CGD-CBD	3.62	117.69	111.27
37	33	303	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
37	35	308	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
48	13	311	A86	C3-C2-C1	-3.61	122.15	127.31
50	36	312	DD6	C37-C36-C35	-3.61	107.66	114.36
37	17	307	CLA	C3C-C4C-NC	3.61	114.62	110.57
37	B	514	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
37	W	102	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
50	41	212	DD6	C21-C20-C15	-3.61	116.21	122.26
37	C	511	CLA	C3D-C4D-ND	3.61	116.08	110.24
48	12	220	A86	C4-C3-C2	-3.61	116.08	123.47
37	B	511	CLA	O2D-CGD-CBD	3.61	117.68	111.27
37	16	301	CLA	C4A-NA-C1A	-3.61	105.08	106.71
37	41	206	CLA	C4A-NA-C1A	-3.61	105.08	106.71
37	B	515	CLA	C3B-C4B-NB	3.61	113.88	109.21
37	21	209	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
37	32	204	CLA	C3C-C4C-NC	3.61	114.62	110.57
37	b	513	CLA	O2D-CGD-CBD	3.61	117.68	111.27
37	B	524	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
37	21	202	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
37	18	202	CLA	O2D-CGD-CBD	3.61	117.67	111.27
37	D	405	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
37	C	502	CLA	C3B-C4B-NB	3.61	113.87	109.21
37	W	101	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
37	b	515	CLA	C3B-C4B-NB	3.60	113.87	109.21
47	36	305	KC1	C1C-C2C-C3C	-3.60	103.17	106.96
47	13	302	KC1	CAA-CBA-CGA	-3.60	108.75	127.26
48	35	316	A86	C25-C26-C27	-3.60	122.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	12	213	A86	C25-C24-C1	-3.60	116.30	126.42
37	41	208	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
37	A	403	CLA	C3C-C4C-NC	3.60	114.61	110.57
44	H	102	DGD	O3G-C3G-C2G	-3.60	102.21	110.90
47	33	309	KC1	C1A-NA-C4A	-3.60	105.09	106.71
37	18	204	CLA	CMB-C2B-C3B	3.60	131.41	124.68
37	12	207	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
37	13	308	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
37	a	403	CLA	C3C-C4C-NC	3.60	114.61	110.57
48	12	217	A86	C41-C32-C31	-3.60	107.25	110.47
37	c	503	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
47	33	302	KC1	CAA-CBA-CGA	-3.60	108.78	127.26
48	12	217	A86	C4-C3-C2	-3.60	116.11	123.47
37	17	304	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
37	31	310	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
37	c	502	CLA	C3B-C4B-NB	3.59	113.86	109.21
47	12	206	KC1	C4C-C3C-C2C	-3.59	101.66	106.90
37	37	303	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
37	11	310	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
48	32	221	A86	C25-C26-C27	-3.59	122.19	127.31
47	32	207	KC1	C4C-C3C-C2C	-3.59	101.67	106.90
37	c	510	CLA	C3C-C4C-NC	3.59	114.59	110.57
37	31	304	CLA	C3C-C4C-NC	3.59	114.59	110.57
37	38	211	CLA	C3B-C4B-NB	3.59	113.85	109.21
37	35	301	CLA	C4A-NA-C1A	-3.59	105.09	106.71
37	b	514	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
37	16	309	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
37	21	206	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
48	13	311	A86	C12-C11-C13	3.58	122.04	116.02
50	16	312	DD6	C37-C36-C35	-3.58	107.72	114.36
37	B	510	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
37	b	502	CLA	C3C-C4C-NC	3.58	114.59	110.57
48	32	221	A86	C7-C6-C8	3.58	123.71	118.08
37	B	511	CLA	CAC-C3C-C4C	3.58	129.45	124.81
47	32	212	KC1	C1A-NA-C4A	-3.58	105.10	106.71
37	41	209	CLA	C1C-C2C-C3C	-3.58	103.20	106.96
44	h	102	DGD	O3G-C3G-C2G	-3.57	102.27	110.90
48	12	220	A86	C7-C6-C8	3.57	123.71	118.08
37	34	305	CLA	C3C-C4C-NC	3.57	114.58	110.57
37	35	305	CLA	C3C-C4C-NC	3.57	114.58	110.57
48	17	311	A86	C20-C19-C18	-3.57	105.68	112.75
37	11	301	CLA	CMC-C2C-C1C	3.57	130.48	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	511	CLA	CAC-C3C-C4C	3.57	129.44	124.81
37	39	310	CLA	C4A-NA-C1A	-3.57	105.10	106.71
37	36	309	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
37	b	504	CLA	C3D-C4D-ND	3.57	116.02	110.24
37	C	503	CLA	C3B-C4B-NB	3.57	113.83	109.21
50	21	212	DD6	C21-C20-C15	-3.57	116.28	122.26
37	31	302	CLA	CMC-C2C-C1C	3.57	130.47	125.04
37	11	303	CLA	C3C-C4C-NC	3.57	114.57	110.57
47	12	211	KC1	C1A-NA-C4A	-3.57	105.10	106.71
37	35	303	CLA	CBA-CAA-C2A	3.57	124.39	113.86
37	c	507	CLA	C3D-C4D-ND	3.57	116.01	110.24
37	32	213	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
37	b	510	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
48	18	215	A86	C20-C19-C18	-3.57	105.69	112.75
47	34	309	KC1	CMA-C3A-C2A	-3.57	119.57	128.30
37	b	523	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
44	C	517	DGD	O6D-C1D-O3G	-3.57	101.53	109.97
37	33	303	CLA	C3B-C4B-NB	3.56	113.81	109.21
47	14	309	KC1	CMA-C3A-C2A	-3.56	119.58	128.30
37	d	403	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
37	C	503	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
37	41	204	CLA	C3B-C4B-NB	3.56	113.81	109.21
48	19	313	A86	C19-C18-C17	3.56	117.64	110.77
48	36	310	A86	C26-C25-C24	-3.56	112.12	123.22
47	37	302	KC1	C1A-NA-C4A	-3.56	105.11	106.71
37	B	504	CLA	C3D-C4D-ND	3.56	115.99	110.24
37	B	506	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
37	16	303	CLA	CBA-CAA-C2A	3.56	124.36	113.86
37	B	502	CLA	C3C-C4C-NC	3.55	114.56	110.57
37	37	308	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
37	b	506	CLA	C4C-C3C-C2C	-3.55	101.72	106.90
37	c	503	CLA	C3B-C4B-NB	3.55	113.80	109.21
37	B	503	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
37	C	507	CLA	C3D-C4D-ND	3.55	115.98	110.24
48	12	202	A86	C25-C26-C27	-3.55	122.24	127.31
48	16	310	A86	C26-C25-C24	-3.55	112.14	123.22
37	33	301	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
37	15	303	CLA	CBA-CAA-C2A	3.55	124.34	113.86
37	18	203	CLA	C4A-NA-C1A	-3.55	105.11	106.71
37	36	303	CLA	CBA-CAA-C2A	3.55	124.33	113.86
44	c	517	DGD	O6D-C1D-O3G	-3.55	101.57	109.97
37	21	204	CLA	C3B-C4B-NB	3.55	113.80	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	41	206	CLA	CHD-C4C-NC	3.55	129.79	124.20
48	21	211	A86	C4-C5-C6	-3.55	122.25	127.31
37	b	503	CLA	O2D-CGD-O1D	-3.55	116.91	123.84
37	B	512	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
37	B	506	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
37	12	212	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
37	b	509	CLA	C3B-C4B-NB	3.54	113.79	109.21
37	41	206	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
37	B	504	CLA	C3B-C4B-NB	3.54	113.79	109.21
37	39	309	CLA	CAA-C2A-C3A	-3.54	103.08	112.78
37	14	310	CLA	CAA-C2A-C3A	-3.54	103.09	112.78
48	17	320	A86	C10-C9-C8	-3.54	112.17	123.22
37	B	509	CLA	C3B-C4B-NB	3.54	113.78	109.21
37	21	208	CLA	CAC-C3C-C4C	3.54	129.40	124.81
48	32	218	A86	C4-C3-C2	-3.54	116.23	123.47
48	32	203	A86	C25-C26-C27	-3.54	122.26	127.31
37	36	301	CLA	C4A-NA-C1A	-3.54	105.12	106.71
47	17	303	KC1	C1A-NA-C4A	-3.54	105.12	106.71
48	32	214	A86	C3-C2-C1	-3.54	122.26	127.31
37	12	212	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
40	16	315	SQD	O47-C7-C8	3.54	119.12	111.50
37	41	206	CLA	O2D-CGD-CBD	3.54	117.55	111.27
48	17	310	A86	C3-C2-C1	-3.53	122.27	127.31
37	11	308	CLA	C3C-C4C-NC	3.53	114.53	110.57
37	38	204	CLA	C3C-C4C-NC	3.53	114.53	110.57
47	20	304	KC1	CAA-CBA-CGA	-3.53	109.10	127.26
47	31	307	KC1	CHD-C4C-NC	3.53	129.56	124.20
37	17	307	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
37	a	404	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
37	13	310	CLA	C3C-C4C-NC	3.53	114.53	110.57
48	41	211	A86	C4-C5-C6	-3.53	122.27	127.31
37	C	510	CLA	C3C-C4C-NC	3.53	114.53	110.57
37	20	307	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
37	34	310	CLA	CAA-C2A-C3A	-3.53	103.12	112.78
37	21	206	CLA	O2D-CGD-CBD	3.53	117.54	111.27
37	38	203	CLA	C4A-NA-C1A	-3.53	105.12	106.71
37	32	202	CLA	C3C-C4C-NC	3.53	114.53	110.57
47	18	207	KC1	CHB-C1B-NB	-3.53	121.21	124.45
47	40	206	KC1	CAA-CBA-CGA	-3.53	109.14	127.26
48	14	316	A86	C33-C32-C31	3.53	112.64	109.21
40	40	202	SQD	O47-C7-C8	3.53	119.10	111.50
50	40	214	DD6	C21-C20-C15	-3.53	116.35	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	303	CLA	C3C-C4C-NC	3.52	114.52	110.57
37	b	503	CLA	C4-C3-C5	3.52	121.20	115.27
37	41	208	CLA	CAC-C3C-C4C	3.52	129.38	124.81
37	21	206	CLA	CHD-C4C-NC	3.52	129.76	124.20
37	D	402	CLA	C3C-C4C-NC	3.52	114.52	110.57
37	c	508	CLA	C4C-C3C-C2C	-3.52	101.76	106.90
48	14	311	A86	C12-C11-C13	3.52	121.94	116.02
48	32	216	A86	C41-C32-C31	-3.52	107.32	110.47
37	16	303	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
37	13	301	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
37	17	309	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
37	19	304	CLA	C3C-C4C-NC	3.52	114.52	110.57
47	32	207	KC1	C1A-NA-C4A	-3.52	105.12	106.71
37	b	504	CLA	C3B-C4B-NB	3.52	113.76	109.21
37	D	401	CLA	CAA-C2A-C3A	-3.52	103.14	112.78
41	d	409	LMG	C1-C2-C3	-3.52	102.67	110.00
37	19	302	CLA	CAA-C2A-C3A	-3.52	103.15	112.78
50	21	216	DD6	C35-C36-C31	-3.52	112.59	120.57
47	37	304	KC1	C4B-C3B-C2B	-3.52	103.86	106.75
37	15	308	CLA	C3B-C4B-NB	3.51	113.75	109.21
48	33	311	A86	C3-C2-C1	-3.51	122.29	127.31
48	12	215	A86	C41-C32-C31	-3.51	107.33	110.47
37	37	306	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
37	40	209	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
47	14	309	KC1	C1C-C2C-C3C	-3.51	103.26	106.96
48	34	316	A86	C33-C32-C31	3.51	112.63	109.21
37	12	205	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
37	31	302	CLA	CAC-C3C-C4C	3.51	129.37	124.81
37	b	506	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
37	38	204	CLA	CMD-C2D-C3D	-3.51	119.54	127.61
37	B	503	CLA	C4-C3-C5	3.51	121.18	115.27
37	32	213	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
37	C	508	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
37	36	303	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
37	18	204	CLA	CMD-C2D-C3D	-3.51	119.54	127.61
47	41	207	KC1	CMC-C2C-C1C	3.51	130.38	125.04
47	18	207	KC1	C1A-NA-C4A	-3.51	105.13	106.71
37	20	303	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
48	17	312	A86	C40-C32-C31	-3.51	107.33	110.47
45	D	404	PL9	C7-C3-C2	-3.50	118.69	123.30
48	34	311	A86	C12-C11-C13	3.50	121.91	116.02
41	D	412	LMG	C1-C2-C3	-3.50	102.70	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	d	402	PL9	C7-C3-C2	-3.50	118.69	123.30
50	20	312	DD6	C21-C20-C15	-3.50	116.39	122.26
48	37	319	A86	C10-C9-C8	-3.50	112.28	123.22
47	12	206	KC1	C1A-NA-C4A	-3.50	105.13	106.71
50	41	216	DD6	C35-C36-C31	-3.50	112.62	120.57
44	J	101	DGD	O6D-C1D-O3G	-3.50	101.68	109.97
37	b	501	CLA	C4A-NA-C1A	-3.50	105.13	106.71
37	B	512	CLA	C3B-C4B-NB	3.50	113.74	109.21
37	19	309	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
47	11	306	KC1	CHD-C4C-NC	3.50	129.51	124.20
48	14	312	A86	C36-C31-C32	-3.50	116.22	119.70
44	j	101	DGD	O6D-C1D-O3G	-3.50	101.69	109.97
45	d	406	PL9	C7-C3-C4	3.50	119.72	116.88
48	15	315	A86	O2-C18-C17	3.50	116.75	109.80
37	b	523	CLA	O2A-CGA-CBA	3.50	122.88	111.91
48	12	216	A86	C12-C11-C13	3.50	121.89	116.02
48	34	315	A86	C12-C11-C13	3.50	121.89	116.02
48	13	315	A86	C35-C34-C33	3.50	115.97	109.88
37	39	304	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
37	b	512	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
37	b	512	CLA	C3B-C4B-NB	3.49	113.72	109.21
47	15	302	KC1	CBA-CAA-C2A	-3.49	111.96	125.27
47	38	210	KC1	C1C-C2C-C3C	-3.49	103.29	106.96
48	14	316	A86	C41-C32-C31	-3.49	107.35	110.47
37	34	307	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
37	15	303	CLA	C3C-C4C-NC	3.49	114.48	110.57
47	37	307	KC1	CAC-C3C-C4C	3.49	129.34	124.81
37	32	205	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
37	33	310	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
47	41	207	KC1	C2C-C1C-NC	3.49	114.38	110.57
37	41	209	CLA	C3C-C4C-NC	3.49	114.48	110.57
47	17	305	KC1	C1C-C2C-C3C	-3.48	103.29	106.96
48	32	215	A86	C41-C32-C31	-3.48	107.35	110.47
47	35	306	KC1	C4B-C3B-C2B	-3.48	103.89	106.75
37	39	302	CLA	CAA-C2A-C3A	-3.48	103.24	112.78
37	b	507	CLA	C3C-C4C-NC	3.48	114.48	110.57
37	b	503	CLA	CAA-C2A-C3A	-3.48	103.24	112.78
47	17	308	KC1	C1C-C2C-C3C	-3.48	103.30	106.96
37	16	309	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
37	35	303	CLA	C3C-C4C-NC	3.48	114.47	110.57
37	13	303	CLA	C3C-C4C-NC	3.48	114.47	110.57
37	33	303	CLA	C3C-C4C-NC	3.48	114.47	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	37	309	A86	C3-C2-C1	-3.48	122.34	127.31
47	35	302	KC1	CBA-CAA-C2A	-3.48	112.01	125.27
48	34	315	A86	C33-C32-C31	3.48	112.59	109.21
48	33	315	A86	C35-C34-C33	3.48	115.94	109.88
37	38	201	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
37	11	301	CLA	CAC-C3C-C4C	3.48	129.32	124.81
47	14	306	KC1	CHB-C1B-NB	-3.48	121.26	124.45
37	B	512	CLA	C3D-C2D-C1D	-3.48	101.09	105.83
37	b	514	CLA	CAC-C3C-C4C	3.48	129.32	124.81
37	14	307	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
37	B	507	CLA	C3C-C4C-NC	3.47	114.47	110.57
37	12	203	CLA	CAC-C3C-C4C	3.47	129.32	124.81
37	32	204	CLA	CAC-C3C-C4C	3.47	129.32	124.81
48	32	217	A86	C12-C11-C13	3.47	121.86	116.02
47	40	206	KC1	C1A-NA-C4A	-3.47	105.14	106.71
37	d	401	CLA	C3C-C4C-NC	3.47	114.46	110.57
40	16	315	SQD	O5-C5-C4	3.47	116.00	109.69
37	12	204	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
37	B	514	CLA	CAC-C3C-C4C	3.47	129.31	124.81
37	34	303	CLA	C3C-C4C-NC	3.47	114.46	110.57
38	D	403	PHO	CMB-C2B-C3B	3.47	131.16	124.68
47	21	207	KC1	CMC-C2C-C1C	3.47	130.32	125.04
48	31	312	A86	C4-C5-C6	-3.47	122.36	127.31
48	15	316	A86	C33-C32-C31	3.47	112.58	109.21
37	21	209	CLA	C3C-C4C-NC	3.47	114.46	110.57
37	c	501	CLA	C3B-C4B-NB	3.46	113.69	109.21
47	15	306	KC1	C4B-C3B-C2B	-3.46	103.91	106.75
48	14	315	A86	C12-C11-C13	3.46	121.84	116.02
37	19	304	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
37	B	503	CLA	CAA-C2A-C3A	-3.46	103.29	112.78
40	40	202	SQD	O5-C5-C4	3.46	115.98	109.69
37	36	309	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
47	34	309	KC1	C1C-C2C-C3C	-3.46	103.32	106.96
37	19	302	CLA	C3C-C4C-NC	3.46	114.45	110.57
48	34	312	A86	C36-C31-C32	-3.46	116.26	119.70
40	B	519	SQD	O9-S-O7	-3.46	101.97	113.95
37	C	504	CLA	C3B-C4B-NB	3.46	113.68	109.21
40	L	101	SQD	O9-S-O7	-3.46	101.97	113.95
48	37	312	A86	C25-C26-C27	-3.46	122.37	127.31
37	12	209	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
37	34	308	CLA	C4A-NA-C1A	-3.46	105.15	106.71
48	34	312	A86	C3-C4-C5	-3.46	116.39	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	33	303	CLA	CBA-CAA-C2A	3.46	124.07	113.86
37	c	503	CLA	CAC-C3C-C4C	3.46	129.29	124.81
48	14	312	A86	C3-C4-C5	-3.46	116.39	123.47
37	39	302	CLA	C3C-C4C-NC	3.46	114.45	110.57
48	17	313	A86	C3-C4-C5	-3.46	116.39	123.47
37	32	210	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
37	c	504	CLA	C3B-C4B-NB	3.45	113.68	109.21
37	38	208	CLA	CAC-C3C-C4C	3.45	129.29	124.81
47	15	304	KC1	CAA-CBA-CGA	-3.45	109.52	127.26
37	C	509	CLA	CMB-C2B-C3B	3.45	131.14	124.68
37	37	303	CLA	C3C-C4C-NC	3.45	114.44	110.57
37	B	504	CLA	CHC-C1C-C2C	-3.45	117.17	126.72
37	40	205	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
37	17	304	CLA	CMB-C2B-C3B	3.45	131.13	124.68
47	21	207	KC1	C2C-C1C-NC	3.45	114.34	110.57
37	b	504	CLA	CHC-C1C-C2C	-3.45	117.18	126.72
37	31	306	CLA	CAA-C2A-C3A	-3.45	103.33	112.78
48	38	214	A86	C3-C4-C5	-3.45	116.41	123.47
37	11	305	CLA	CAA-C2A-C3A	-3.45	103.33	112.78
37	b	513	CLA	CMB-C2B-C3B	3.45	131.13	124.68
38	a	405	PHO	CMB-C2B-C3B	3.45	131.13	124.68
48	17	320	A86	C20-C19-C18	-3.45	105.92	112.75
37	B	524	CLA	O2A-CGA-CBA	3.45	122.73	111.91
47	34	306	KC1	CHB-C1B-NB	-3.45	121.28	124.45
48	16	311	A86	C34-O4-C38	-3.45	111.47	117.90
37	b	512	CLA	C3D-C2D-C1D	-3.45	101.13	105.83
37	15	305	CLA	C3B-C4B-NB	3.45	113.67	109.21
48	36	311	A86	C34-O4-C38	-3.45	111.47	117.90
37	b	511	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
37	C	502	CLA	CHC-C1C-C2C	-3.45	117.19	126.72
48	14	315	A86	C33-C32-C31	3.45	112.56	109.21
48	12	213	A86	C12-C11-C13	3.44	121.81	116.02
48	17	313	A86	C25-C26-C27	-3.44	122.39	127.31
47	35	309	KC1	CMA-C3A-C2A	-3.44	119.87	128.30
37	12	204	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
37	32	205	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
48	11	312	A86	C36-C31-C32	-3.44	116.28	119.70
37	17	304	CLA	C3C-C4C-NC	3.44	114.43	110.57
37	b	507	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
37	B	511	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
48	12	213	A86	C41-C32-C31	-3.44	107.39	110.47
48	21	213	A86	C35-C34-C33	3.44	115.88	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	12	210	CLA	C3B-C4B-NB	3.44	113.66	109.21
37	35	310	CLA	C3B-C4B-NB	3.44	113.66	109.21
37	C	503	CLA	CAC-C3C-C4C	3.44	129.27	124.81
47	35	304	KC1	CAA-CBA-CGA	-3.44	109.59	127.26
37	c	502	CLA	CHC-C1C-C2C	-3.44	117.21	126.72
37	W	101	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
37	15	307	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
48	32	221	A86	C33-C32-C31	3.44	112.55	109.21
37	39	304	CLA	C3C-C4C-NC	3.44	114.42	110.57
37	B	506	CLA	CAC-C3C-C4C	3.44	129.27	124.81
37	C	501	CLA	C3B-C4B-NB	3.44	113.65	109.21
37	37	303	CLA	CMB-C2B-C3B	3.44	131.10	124.68
48	12	214	A86	C41-C32-C31	-3.43	107.40	110.47
48	32	214	A86	C41-C32-C31	-3.43	107.40	110.47
48	36	311	A86	C4-C3-C2	-3.43	116.44	123.47
48	41	213	A86	C35-C34-C33	3.43	115.87	109.88
37	18	203	CLA	CHC-C1C-C2C	-3.43	117.22	126.72
37	B	507	CLA	CHC-C1C-C2C	-3.43	117.22	126.72
37	B	513	CLA	CMB-C2B-C3B	3.43	131.10	124.68
37	B	507	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
37	c	504	CLA	CAC-C3C-C4C	3.43	129.26	124.81
37	c	505	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
47	16	304	KC1	CAA-CBA-CGA	-3.43	109.62	127.26
48	35	315	A86	C41-C32-C31	-3.43	107.40	110.47
47	36	304	KC1	CAA-CBA-CGA	-3.43	109.63	127.26
48	34	311	A86	C3-C4-C5	-3.43	116.45	123.47
37	41	210	CLA	C3B-C4B-NB	3.43	113.64	109.21
37	35	307	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
47	15	309	KC1	CMA-C3A-C2A	-3.43	119.91	128.30
37	C	505	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
47	18	210	KC1	C1C-C2C-C3C	-3.43	103.35	106.96
47	20	304	KC1	C1A-NA-C4A	-3.43	105.17	106.71
37	15	310	CLA	C3B-C4B-NB	3.42	113.64	109.21
48	16	310	A86	C3-C4-C5	-3.42	116.46	123.47
47	17	308	KC1	CAC-C3C-C4C	3.42	129.25	124.81
48	34	316	A86	C41-C32-C31	-3.42	107.41	110.47
37	13	310	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
37	13	303	CLA	CBA-CAA-C2A	3.42	123.96	113.86
45	D	408	PL9	C7-C3-C4	3.42	119.66	116.88
48	11	312	A86	C4-C5-C6	-3.42	122.43	127.31
37	18	201	CLA	CAC-C3C-C4C	3.42	129.25	124.81
37	32	206	CLA	C3B-C4B-NB	3.42	113.63	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	38	204	CLA	C3B-C4B-NB	3.42	113.63	109.21
37	15	308	CLA	CHC-C1C-C2C	-3.42	117.27	126.72
48	32	214	A86	C12-C11-C13	3.42	121.76	116.02
50	16	312	DD6	C19-C18-C17	3.42	117.37	110.77
48	41	215	A86	C34-O4-C38	-3.42	111.53	117.90
37	B	505	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
37	b	515	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
37	32	211	CLA	C3B-C4B-NB	3.41	113.62	109.21
37	21	205	CLA	C3B-C4B-NB	3.41	113.62	109.21
48	31	312	A86	C36-C31-C32	-3.41	116.31	119.70
48	18	214	A86	C4-C5-C6	-3.41	122.44	127.31
37	33	310	CLA	C3C-C4C-NC	3.41	114.40	110.57
48	14	311	A86	C3-C4-C5	-3.41	116.48	123.47
37	D	401	CLA	CHD-C4C-NC	3.41	129.58	124.20
37	18	202	CLA	CHD-C4C-NC	3.41	129.58	124.20
48	11	313	A86	C34-O4-C38	-3.41	111.54	117.90
37	a	407	CLA	C3B-C4B-NB	3.41	113.62	109.21
37	c	509	CLA	CMB-C2B-C3B	3.41	131.06	124.68
37	A	405	CLA	C3B-C4B-NB	3.41	113.62	109.21
37	16	303	CLA	CAC-C3C-C4C	3.41	129.24	124.81
37	11	308	CLA	C3B-C4B-NB	3.41	113.62	109.21
50	36	312	DD6	C19-C18-C17	3.41	117.36	110.77
37	w	101	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
37	19	303	CLA	O2D-CGD-CBD	3.41	117.32	111.27
48	16	311	A86	C4-C5-C6	-3.41	122.45	127.31
37	b	507	CLA	CHC-C1C-C2C	-3.41	117.30	126.72
37	33	310	CLA	C3B-C4B-NB	3.41	113.61	109.21
47	40	207	KC1	O2D-CGD-O1D	-3.41	117.18	123.84
37	c	510	CLA	CAA-C2A-C3A	-3.41	103.45	112.78
48	11	315	A86	C10-C9-C8	-3.40	112.59	123.22
37	13	310	CLA	C3B-C4B-NB	3.40	113.61	109.21
37	32	211	CLA	O2D-CGD-CBD	3.40	117.31	111.27
48	31	315	A86	C10-C9-C8	-3.40	112.60	123.22
37	21	205	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
48	18	215	A86	C4-C3-C2	-3.40	116.51	123.47
37	16	303	CLA	C3C-C4C-NC	3.40	114.39	110.57
47	37	307	KC1	C1C-C2C-C3C	-3.40	103.38	106.96
48	36	311	A86	C4-C5-C6	-3.40	122.46	127.31
37	C	510	CLA	CAA-C2A-C3A	-3.40	103.47	112.78
48	32	203	A86	C35-C34-C33	3.40	115.81	109.88
37	36	303	CLA	C3C-C4C-NC	3.40	114.38	110.57
37	21	206	CLA	CAA-C2A-C3A	-3.40	103.47	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	16	311	A86	C4-C3-C2	-3.40	116.51	123.47
37	D	405	CLA	C3B-C4B-NB	3.40	113.60	109.21
48	37	310	A86	C20-C19-C18	-3.40	106.03	112.75
37	36	303	CLA	CAC-C3C-C4C	3.40	129.22	124.81
48	35	312	A86	C36-C31-C32	-3.40	116.33	119.70
48	21	215	A86	C34-O4-C38	-3.40	111.57	117.90
47	31	303	KC1	CAA-CBA-CGA	-3.39	109.82	127.26
37	a	404	CLA	CHD-C4C-NC	3.39	129.55	124.20
37	41	206	CLA	CAA-C2A-C3A	-3.39	103.49	112.78
37	C	511	CLA	C4A-NA-C1A	-3.39	105.18	106.71
37	32	202	CLA	C3B-C4B-NB	3.39	113.59	109.21
37	41	209	CLA	C3B-C4B-NB	3.39	113.59	109.21
47	11	302	KC1	CAA-CBA-CGA	-3.39	109.83	127.26
37	12	204	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
37	20	303	CLA	C3B-C4B-NB	3.39	113.59	109.21
37	33	308	CLA	C3B-C4B-NB	3.39	113.59	109.21
48	38	214	A86	C4-C5-C6	-3.39	122.47	127.31
37	c	505	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
37	41	205	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
37	B	516	CLA	C3B-C4B-NB	3.39	113.59	109.21
37	C	504	CLA	CAC-C3C-C4C	3.39	129.21	124.81
37	c	509	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
37	C	513	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
37	41	208	CLA	C3C-C4C-NC	3.39	114.37	110.57
48	38	215	A86	C4-C3-C2	-3.39	116.53	123.47
47	12	206	KC1	CHD-C4C-NC	3.39	129.34	124.20
48	36	310	A86	C3-C4-C5	-3.39	116.53	123.47
37	32	206	CLA	CMB-C2B-C3B	3.39	131.02	124.68
37	d	403	CLA	C3B-C4B-NB	3.39	113.59	109.21
37	11	303	CLA	C3B-C4B-NB	3.39	113.59	109.21
37	21	210	CLA	C3B-C4B-NB	3.39	113.59	109.21
37	31	304	CLA	C3B-C4B-NB	3.39	113.59	109.21
37	b	516	CLA	C3B-C4B-NB	3.38	113.58	109.21
47	40	204	KC1	CAA-CBA-CGA	-3.38	109.87	127.26
37	B	515	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
37	32	205	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
37	C	507	CLA	CMB-C2B-C3B	3.38	131.01	124.68
48	18	214	A86	C36-C31-C32	-3.38	116.34	119.70
48	37	312	A86	C12-C11-C13	3.38	121.70	116.02
47	36	302	KC1	C2A-C1A-NA	3.38	114.83	109.40
48	12	202	A86	C35-C34-C33	3.38	115.78	109.88
48	38	214	A86	C36-C31-C32	-3.38	116.34	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	38	203	CLA	CHC-C1C-C2C	-3.38	117.37	126.72
47	20	302	KC1	CAA-CBA-CGA	-3.38	109.89	127.26
48	17	311	A86	C28-C27-C26	3.38	127.65	122.92
37	16	306	CLA	CAC-C3C-C4C	3.38	129.19	124.81
37	12	205	CLA	C3B-C4B-NB	3.37	113.57	109.21
47	32	207	KC1	CHD-C4C-NC	3.37	129.32	124.20
37	a	403	CLA	O2D-CGD-CBD	3.37	117.26	111.27
37	36	306	CLA	CAC-C3C-C4C	3.37	129.19	124.81
37	A	403	CLA	O2D-CGD-CBD	3.37	117.26	111.27
37	C	509	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
47	35	304	KC1	CAC-C3C-C4C	3.37	129.19	124.81
37	b	506	CLA	CAC-C3C-C4C	3.37	129.19	124.81
37	17	309	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
37	38	209	CLA	C3B-C4B-NB	3.37	113.56	109.21
48	32	214	A86	C25-C24-C1	-3.37	116.95	126.42
37	13	308	CLA	C3B-C4B-NB	3.37	113.56	109.21
37	21	208	CLA	C3C-C4C-NC	3.37	114.35	110.57
37	a	404	CLA	CMB-C2B-C3B	3.37	130.97	124.68
37	38	206	CLA	C3B-C4B-NB	3.36	113.56	109.21
37	13	307	CLA	C3D-C4D-ND	3.36	115.68	110.24
48	17	315	A86	C33-C32-C31	3.36	112.48	109.21
48	31	315	A86	C25-C24-C1	-3.36	116.97	126.42
47	20	305	KC1	O2D-CGD-O1D	-3.36	117.26	123.84
48	13	315	A86	C41-C32-C31	-3.36	107.46	110.47
48	11	315	A86	C25-C24-C1	-3.36	116.97	126.42
37	20	308	CLA	C4A-NA-C1A	-3.36	105.19	106.71
48	12	220	A86	C33-C32-C31	3.36	112.48	109.21
37	40	205	CLA	C3B-C4B-NB	3.36	113.55	109.21
37	b	505	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
37	32	213	CLA	CAA-C2A-C3A	-3.36	103.58	112.78
48	37	314	A86	C9-C8-C6	-3.36	116.98	126.42
37	C	501	CLA	C1-C2-C3	-3.36	120.23	126.04
47	16	302	KC1	C2A-C1A-NA	3.36	114.79	109.40
37	C	505	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
37	11	310	CLA	O2D-CGD-CBD	3.36	117.23	111.27
48	37	311	A86	C4-C3-C2	-3.36	116.60	123.47
48	16	313	A86	C36-C31-C32	-3.36	116.37	119.70
47	14	304	KC1	C4B-C3B-C2B	-3.36	104.00	106.75
48	37	314	A86	C33-C32-C31	3.36	112.47	109.21
37	c	507	CLA	CMB-C2B-C3B	3.35	130.95	124.68
37	33	307	CLA	C3D-C4D-ND	3.35	115.66	110.24
37	34	308	CLA	CHC-C1C-C2C	-3.35	117.44	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	501	CLA	C3C-C4C-NC	3.35	114.33	110.57
37	13	308	CLA	O2A-CGA-CBA	3.35	122.43	111.91
37	41	205	CLA	C3B-C4B-NB	3.35	113.54	109.21
41	16	316	LMG	O6-C1-O1	-3.35	102.04	109.97
37	B	506	CLA	O2A-CGA-CBA	3.35	122.42	111.91
37	b	506	CLA	O2A-CGA-CBA	3.35	122.42	111.91
37	12	205	CLA	CMB-C2B-C3B	3.35	130.95	124.68
47	36	308	KC1	CBA-CAA-C2A	-3.35	112.50	125.27
37	14	308	CLA	CHC-C1C-C2C	-3.35	117.45	126.72
37	15	303	CLA	C3B-C4B-NB	3.35	113.54	109.21
37	21	209	CLA	C3B-C4B-NB	3.35	113.54	109.21
37	41	208	CLA	C3B-C4B-NB	3.35	113.54	109.21
37	18	209	CLA	C3B-C4B-NB	3.35	113.54	109.21
37	12	203	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
37	34	310	CLA	CHC-C1C-C2C	-3.35	117.46	126.72
48	35	316	A86	C40-C32-C31	3.35	113.47	110.47
37	12	212	CLA	CAA-C2A-C3A	-3.35	103.61	112.78
37	21	204	CLA	C4-C3-C5	3.35	120.90	115.27
37	B	514	CLA	C3B-C4B-NB	3.35	113.54	109.21
48	18	212	A86	C34-O4-C38	-3.35	111.66	117.90
37	33	308	CLA	O2A-CGA-CBA	3.34	122.40	111.91
37	14	310	CLA	C3B-C4B-NB	3.34	113.53	109.21
37	14	310	CLA	CHC-C1C-C2C	-3.34	117.47	126.72
47	13	306	KC1	CBC-CAC-C3C	-3.34	103.22	112.43
41	36	314	LMG	O6-C1-O1	-3.34	102.06	109.97
37	13	310	CLA	CAC-C3C-C4C	3.34	129.15	124.81
47	16	308	KC1	CBA-CAA-C2A	-3.34	112.53	125.27
37	40	210	CLA	C4A-NA-C1A	-3.34	105.20	106.71
37	c	513	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
37	35	308	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
48	40	201	A86	C36-C31-C32	-3.34	116.38	119.70
37	D	401	CLA	CMB-C2B-C3B	3.34	130.93	124.68
48	17	315	A86	C9-C8-C6	-3.34	117.04	126.42
37	35	303	CLA	C3B-C4B-NB	3.34	113.53	109.21
37	19	302	CLA	C3B-C4B-NB	3.34	113.53	109.21
40	40	202	SQD	O9-S-C6	3.34	110.91	106.94
37	40	210	CLA	C3B-C4B-NB	3.34	113.52	109.21
37	C	511	CLA	C4C-C3C-C2C	-3.34	102.04	106.90
48	36	311	A86	C36-C31-C32	-3.33	116.39	119.70
47	35	302	KC1	CAA-CBA-CGA	-3.33	110.13	127.26
48	12	216	A86	C3-C4-C5	-3.33	116.65	123.47
37	32	205	CLA	CAA-C2A-C1A	3.33	122.90	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	15	302	KC1	CAA-CBA-CGA	-3.33	110.14	127.26
37	c	501	CLA	C1-C2-C3	-3.33	120.28	126.04
37	b	514	CLA	C3B-C4B-NB	3.33	113.52	109.21
47	41	207	KC1	C1C-C2C-C3C	-3.33	103.45	106.96
37	33	310	CLA	CAC-C3C-C4C	3.33	129.13	124.81
37	31	310	CLA	O2D-CGD-CBD	3.33	117.19	111.27
48	33	315	A86	C41-C32-C31	-3.33	107.49	110.47
47	33	306	KC1	CBC-CAC-C3C	-3.33	103.25	112.43
37	34	301	CLA	CMC-C2C-C1C	3.33	130.11	125.04
37	C	503	CLA	O2A-CGA-CBA	3.33	122.36	111.91
48	38	214	A86	C9-C8-C6	-3.33	117.07	126.42
37	38	203	CLA	C3B-C4B-NB	3.33	113.51	109.21
48	16	311	A86	C36-C31-C32	-3.33	116.39	119.70
37	19	303	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
37	39	303	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
48	34	312	A86	C41-C32-C31	-3.33	107.50	110.47
47	37	302	KC1	CAA-CBA-CGA	-3.33	110.17	127.26
37	18	204	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
37	12	204	CLA	C3D-C2D-C1D	-3.32	101.30	105.83
37	12	204	CLA	CAA-C2A-C1A	3.32	122.87	111.97
37	34	310	CLA	C3B-C4B-NB	3.32	113.51	109.21
37	c	511	CLA	C4C-C3C-C2C	-3.32	102.05	106.90
37	20	308	CLA	C3B-C4B-NB	3.32	113.50	109.21
37	c	503	CLA	O2A-CGA-CBA	3.32	122.33	111.91
37	C	507	CLA	C3B-C4B-NB	3.32	113.50	109.21
37	18	201	CLA	CMC-C2C-C1C	3.32	130.09	125.04
37	c	502	CLA	C4A-NA-C1A	-3.32	105.21	106.71
37	21	208	CLA	C3B-C4B-NB	3.32	113.50	109.21
48	14	312	A86	C41-C32-C31	-3.32	107.50	110.47
48	19	313	A86	C26-C25-C24	-3.32	112.87	123.22
37	34	301	CLA	CAC-C3C-C4C	3.32	129.11	124.81
47	36	305	KC1	CBA-CAA-C2A	-3.32	112.63	125.27
47	16	305	KC1	CBA-CAA-C2A	-3.32	112.63	125.27
37	B	501	CLA	C3C-C4C-NC	3.32	114.29	110.57
37	32	204	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
37	40	210	CLA	CAC-C3C-C4C	3.31	129.11	124.81
37	41	204	CLA	C4-C3-C5	3.31	120.85	115.27
48	35	316	A86	C20-C19-C18	-3.31	106.19	112.75
37	14	301	CLA	CAC-C3C-C4C	3.31	129.11	124.81
37	b	523	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
37	18	208	CLA	CAC-C3C-C4C	3.31	129.11	124.81
37	20	308	CLA	CAC-C3C-C4C	3.31	129.11	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	21	203	KC1	CAA-CBA-CGA	-3.31	110.24	127.26
48	32	217	A86	C3-C4-C5	-3.31	116.69	123.47
47	12	208	KC1	C1A-NA-C4A	-3.31	105.22	106.71
48	17	313	A86	C12-C11-C13	3.31	121.58	116.02
37	c	501	CLA	C3C-C4C-NC	3.31	114.28	110.57
47	41	203	KC1	CAA-CBA-CGA	-3.31	110.25	127.26
37	18	208	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
48	37	319	A86	C20-C19-C18	-3.31	106.20	112.75
47	17	303	KC1	CAA-CBA-CGA	-3.31	110.26	127.26
47	12	208	KC1	CBA-CAA-C2A	-3.31	112.66	125.27
37	35	305	CLA	C3B-C4B-NB	3.31	113.49	109.21
48	11	313	A86	C12-C11-C13	3.31	121.58	116.02
48	15	312	A86	C36-C31-C32	-3.31	116.41	119.70
37	39	302	CLA	C3B-C4B-NB	3.31	113.48	109.21
37	C	501	CLA	C3C-C4C-NC	3.31	114.28	110.57
37	c	511	CLA	C4A-NA-C1A	-3.31	105.22	106.71
37	c	507	CLA	C3B-C4B-NB	3.31	113.48	109.21
48	38	212	A86	C34-O4-C38	-3.30	111.74	117.90
37	a	404	CLA	CHC-C1C-C2C	-3.30	117.58	126.72
37	C	502	CLA	CAC-C3C-C4C	3.30	129.09	124.81
37	b	503	CLA	O2A-CGA-CBA	3.30	122.27	111.91
37	14	301	CLA	CMC-C2C-C1C	3.30	130.07	125.04
37	34	310	CLA	C3C-C4C-NC	3.30	114.27	110.57
37	32	205	CLA	C3D-C2D-C1D	-3.30	101.33	105.83
47	32	209	KC1	CBA-CAA-C2A	-3.30	112.70	125.27
37	b	503	CLA	C3B-C4B-NB	3.30	113.47	109.21
37	20	303	CLA	C3D-C4D-ND	3.30	115.57	110.24
37	33	303	CLA	CAC-C3C-C4C	3.30	129.09	124.81
37	11	301	CLA	CHD-C4C-NC	3.29	129.39	124.20
37	31	302	CLA	CHD-C4C-NC	3.29	129.39	124.20
37	19	305	CLA	CAA-C2A-C3A	-3.29	103.76	112.78
37	34	308	CLA	C3B-C4B-NB	3.29	113.47	109.21
37	B	503	CLA	O2A-CGA-CBA	3.29	122.24	111.91
37	19	310	CLA	CHC-C1C-C2C	-3.29	117.61	126.72
47	41	207	KC1	C4B-C3B-C2B	-3.29	104.05	106.75
37	z	101	CLA	CHC-C1C-C2C	-3.29	117.62	126.72
37	C	505	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
37	40	205	CLA	C3D-C4D-ND	3.29	115.56	110.24
48	36	311	A86	C26-C25-C24	-3.29	112.95	123.22
48	35	319	A86	C25-C24-C1	-3.29	117.18	126.42
37	b	509	CLA	CHC-C1C-C2C	-3.29	117.63	126.72
48	32	203	A86	C12-C11-C13	3.29	121.54	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	308	CLA	C3B-C4B-NB	3.29	113.46	109.21
37	D	405	CLA	CMC-C2C-C1C	3.29	130.04	125.04
48	16	311	A86	C26-C25-C24	-3.29	112.96	123.22
37	D	401	CLA	CHC-C1C-C2C	-3.29	117.63	126.72
37	12	210	CLA	CHC-C1C-C2C	-3.29	117.63	126.72
48	15	319	A86	C36-C31-C32	-3.28	116.44	119.70
37	d	403	CLA	CMC-C2C-C1C	3.28	130.04	125.04
40	16	315	SQD	O9-S-C6	3.28	110.84	106.94
47	15	304	KC1	CAC-C3C-C4C	3.28	129.07	124.81
37	b	516	CLA	CHC-C1C-C2C	-3.28	117.64	126.72
48	15	313	A86	C12-C11-C13	3.28	121.53	116.02
47	36	302	KC1	CAC-C3C-C4C	3.28	129.07	124.81
48	15	319	A86	C10-C9-C8	-3.28	112.98	123.22
37	c	505	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
37	B	516	CLA	CHC-C1C-C2C	-3.28	117.65	126.72
37	37	308	CLA	CED-O2D-CGD	3.28	123.36	115.94
48	15	319	A86	C25-C24-C1	-3.28	117.20	126.42
37	B	509	CLA	CHC-C1C-C2C	-3.28	117.65	126.72
37	39	310	CLA	CHC-C1C-C2C	-3.28	117.65	126.72
47	21	207	KC1	CAC-C3C-C4C	3.28	129.06	124.81
48	37	319	A86	C4-C3-C2	-3.28	116.76	123.47
48	39	313	A86	C26-C25-C24	-3.28	112.99	123.22
37	B	524	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
47	33	302	KC1	CAC-C3C-C4C	3.28	129.06	124.81
37	11	307	CLA	CAC-C3C-C2C	3.28	133.13	127.53
37	Z	101	CLA	CHC-C1C-C2C	-3.28	117.66	126.72
48	13	314	A86	C4-C5-C6	-3.27	122.64	127.31
37	B	503	CLA	C3B-C4B-NB	3.27	113.44	109.21
47	20	305	KC1	C1C-C2C-C3C	-3.27	103.52	106.96
48	11	313	A86	C25-C26-C27	-3.27	122.64	127.31
47	19	308	KC1	CBA-CAA-C2A	-3.27	112.80	125.27
48	13	314	A86	C12-C11-C13	3.27	121.52	116.02
47	21	207	KC1	C1C-C2C-C3C	-3.27	103.52	106.96
48	35	314	A86	C41-C32-C31	-3.27	107.55	110.47
37	b	501	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
37	21	206	CLA	C3B-C4B-NB	3.27	113.44	109.21
48	35	319	A86	C10-C9-C8	-3.27	113.02	123.22
37	B	501	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
47	40	207	KC1	C1C-C2C-C3C	-3.27	103.52	106.96
37	a	403	CLA	CAC-C3C-C4C	3.27	129.05	124.81
37	c	502	CLA	CAC-C3C-C4C	3.27	129.05	124.81
47	13	309	KC1	CAC-C3C-C4C	3.27	129.05	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	a	404	CLA	C3C-C4C-NC	3.26	114.23	110.57
48	14	311	A86	C4-C3-C2	-3.26	116.79	123.47
47	21	207	KC1	CHD-C4C-NC	3.26	129.16	124.20
47	36	302	KC1	CMA-C3A-C2A	-3.26	120.31	128.30
48	34	311	A86	C4-C3-C2	-3.26	116.79	123.47
37	18	204	CLA	C3B-C4B-NB	3.26	113.43	109.21
48	15	314	A86	C41-C32-C31	-3.26	107.55	110.47
37	c	511	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
47	39	308	KC1	CBA-CAA-C2A	-3.26	112.83	125.27
37	14	310	CLA	C3C-C4C-NC	3.26	114.23	110.57
37	39	303	CLA	O2D-CGD-CBD	3.26	117.06	111.27
37	C	506	CLA	CAC-C3C-C4C	3.26	129.04	124.81
48	12	202	A86	C12-C11-C13	3.26	121.50	116.02
47	13	302	KC1	CAC-C3C-C4C	3.26	129.04	124.81
37	32	211	CLA	CHC-C1C-C2C	-3.26	117.71	126.72
47	41	207	KC1	CHD-C4C-NC	3.26	129.15	124.20
37	31	308	CLA	CAC-C3C-C2C	3.26	133.10	127.53
37	C	501	CLA	CHC-C1C-C2C	-3.26	117.71	126.72
37	12	210	CLA	O2D-CGD-CBD	3.26	117.05	111.27
37	c	501	CLA	CHC-C1C-C2C	-3.26	117.72	126.72
37	13	307	CLA	C3B-C4B-NB	3.25	113.42	109.21
37	A	403	CLA	CAC-C3C-C4C	3.25	129.03	124.81
47	41	207	KC1	CAC-C3C-C4C	3.25	129.03	124.81
37	C	511	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
48	35	319	A86	C36-C31-C32	-3.25	116.47	119.70
47	18	210	KC1	CAC-C3C-C4C	3.25	129.03	124.81
48	37	313	A86	C25-C24-C1	-3.25	117.28	126.42
47	36	305	KC1	C4C-C3C-C2C	-3.25	102.16	106.90
37	39	305	CLA	CAA-C2A-C3A	-3.25	103.88	112.78
37	c	510	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
37	37	306	CLA	C3B-C4B-NB	3.25	113.41	109.21
47	32	209	KC1	C1A-NA-C4A	-3.25	105.25	106.71
37	b	501	CLA	C3B-C4B-NB	3.25	113.41	109.21
37	D	406	CLA	C3B-C4B-NB	3.25	113.41	109.21
37	C	510	CLA	CHC-C1C-C2C	-3.25	117.74	126.72
37	Z	101	CLA	C3B-C4B-NB	3.24	113.41	109.21
47	33	309	KC1	CBC-CAC-C3C	-3.24	103.49	112.43
47	16	302	KC1	CMA-C3A-C2A	-3.24	120.36	128.30
37	w	101	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
37	31	302	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
37	11	307	CLA	C4-C3-C5	3.24	120.73	115.27
48	39	313	A86	C9-C8-C6	-3.24	117.31	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	37	308	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
37	W	101	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
47	34	304	KC1	C4B-C3B-C2B	-3.24	104.09	106.75
48	31	313	A86	C12-C11-C13	3.24	121.47	116.02
48	33	314	A86	C4-C5-C6	-3.24	122.69	127.31
37	33	307	CLA	C3B-C4B-NB	3.24	113.40	109.21
47	33	309	KC1	CAC-C3C-C4C	3.24	129.01	124.81
47	15	306	KC1	CAA-CBA-CGA	-3.24	110.61	127.26
37	c	506	CLA	CAC-C3C-C4C	3.24	129.01	124.81
37	13	303	CLA	CAC-C3C-C4C	3.24	129.01	124.81
37	32	206	CLA	CAC-C3C-C4C	3.24	129.01	124.81
37	A	403	CLA	CHC-C1C-C2C	-3.24	117.76	126.72
37	33	308	CLA	CHC-C1C-C2C	-3.24	117.76	126.72
44	C	516	DGD	O6D-C1D-O3G	-3.24	102.31	109.97
47	16	305	KC1	C4C-C3C-C2C	-3.24	102.18	106.90
47	33	302	KC1	CMB-C2B-C1B	3.24	130.42	124.71
48	32	215	A86	C3-C4-C5	-3.24	116.85	123.47
37	b	512	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
37	19	309	CLA	C3B-C4B-NB	3.23	113.39	109.21
37	38	202	CLA	CAC-C3C-C4C	3.23	129.01	124.81
37	19	306	CLA	CHD-C4C-NC	3.23	129.30	124.20
47	21	207	KC1	C4B-C3B-C2B	-3.23	104.10	106.75
47	13	309	KC1	CBC-CAC-C3C	-3.23	103.52	112.43
37	d	404	CLA	C3B-C4B-NB	3.23	113.39	109.21
37	32	204	CLA	CHD-C4C-NC	3.23	129.30	124.20
48	12	214	A86	C3-C4-C5	-3.23	116.85	123.47
37	14	308	CLA	CAC-C3C-C4C	3.23	129.00	124.81
37	W	101	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
48	31	314	A86	C8-C6-C5	-3.23	113.98	118.94
37	38	208	CLA	CMB-C2B-C3B	3.23	130.72	124.68
48	21	213	A86	C36-C31-C32	-3.23	116.49	119.70
47	17	306	KC1	C1A-NA-C4A	-3.23	105.25	106.71
37	z	101	CLA	C3B-C4B-NB	3.23	113.39	109.21
48	14	311	A86	C7-C6-C8	3.23	123.17	118.08
37	38	204	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
37	37	308	CLA	C3B-C4B-NB	3.23	113.38	109.21
37	C	501	CLA	CAC-C3C-C4C	3.23	129.00	124.81
47	35	306	KC1	CAA-CBA-CGA	-3.23	110.67	127.26
47	34	309	KC1	CHD-C4C-NC	3.23	129.10	124.20
37	C	510	CLA	CMD-C2D-C3D	-3.23	120.19	127.61
37	w	101	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
37	16	309	CLA	CAC-C3C-C4C	3.23	129.00	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	18	208	CLA	CMB-C2B-C3B	3.23	130.71	124.68
37	41	202	CLA	CAC-C3C-C4C	3.22	128.99	124.81
48	17	312	A86	C4-C3-C2	-3.22	116.87	123.47
37	16	306	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
47	35	302	KC1	C4B-C3B-C2B	-3.22	104.10	106.75
37	34	301	CLA	CHD-C4C-NC	3.22	129.28	124.20
48	33	311	A86	C34-O4-C38	-3.22	111.89	117.90
37	13	308	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
37	14	301	CLA	CHD-C4C-NC	3.22	129.28	124.20
37	a	403	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
48	31	319	A86	C3-C4-C5	-3.22	116.88	123.47
48	14	312	A86	C40-C32-C31	-3.22	107.59	110.47
44	c	516	DGD	O6D-C1D-O3G	-3.22	102.35	109.97
37	d	403	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
47	14	304	KC1	CHD-C4C-NC	3.22	129.09	124.20
47	34	304	KC1	CHD-C4C-NC	3.22	129.09	124.20
37	39	309	CLA	C3B-C4B-NB	3.22	113.37	109.21
48	34	311	A86	C7-C6-C8	3.22	123.15	118.08
37	36	306	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
48	34	312	A86	C40-C32-C31	-3.22	107.59	110.47
37	D	405	CLA	C1D-CHD-C4C	-3.22	119.12	126.06
47	18	207	KC1	CAC-C3C-C4C	3.22	128.99	124.81
37	31	301	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
37	c	503	CLA	O2A-C1-C2	3.22	117.09	108.64
47	39	308	KC1	CHD-C4C-NC	3.22	129.08	124.20
37	B	506	CLA	C3B-C4B-NB	3.21	113.37	109.21
37	C	502	CLA	C4A-NA-C1A	-3.21	105.26	106.71
47	37	305	KC1	C1A-NA-C4A	-3.21	105.26	106.71
37	41	206	CLA	C3B-C4B-NB	3.21	113.36	109.21
37	39	306	CLA	CHD-C4C-NC	3.21	129.27	124.20
48	12	220	A86	C26-C25-C24	-3.21	113.19	123.22
37	17	309	CLA	CHC-C1C-C2C	-3.21	117.83	126.72
37	34	305	CLA	CHC-C1C-C2C	-3.21	117.83	126.72
37	11	301	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
37	13	303	CLA	CHC-C1C-C2C	-3.21	117.83	126.72
37	15	308	CLA	C1-C2-C3	-3.21	120.49	126.04
37	b	504	CLA	C1-C2-C3	-3.21	120.49	126.04
37	D	401	CLA	C3C-C4C-NC	3.21	114.17	110.57
47	32	212	KC1	CMA-C3A-C2A	-3.21	120.44	128.30
37	c	510	CLA	CMD-C2D-C3D	-3.21	120.23	127.61
37	32	205	CLA	CAC-C3C-C4C	3.21	128.98	124.81
37	36	309	CLA	CAC-C3C-C4C	3.21	128.98	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	14	306	KC1	CMB-C2B-C1B	3.21	130.37	124.71
37	C	503	CLA	O2A-C1-C2	3.21	117.07	108.64
48	31	312	A86	C41-C32-C31	-3.21	107.60	110.47
48	31	315	A86	C3-C4-C5	-3.21	116.90	123.47
37	14	305	CLA	C3B-C4B-NB	3.21	113.36	109.21
37	12	204	CLA	CHC-C1C-C2C	-3.21	117.84	126.72
37	32	205	CLA	CHC-C1C-C2C	-3.21	117.84	126.72
47	16	302	KC1	CAC-C3C-C4C	3.21	128.97	124.81
37	b	510	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
48	11	315	A86	C3-C4-C5	-3.21	116.90	123.47
37	21	209	CLA	CAC-C3C-C4C	3.21	128.97	124.81
37	17	309	CLA	C3B-C4B-NB	3.21	113.36	109.21
48	35	313	A86	C12-C11-C13	3.21	121.41	116.02
48	14	316	A86	C7-C6-C5	-3.21	118.43	122.92
47	36	308	KC1	C1A-NA-C4A	-3.21	105.27	106.71
37	34	305	CLA	C3B-C4B-NB	3.20	113.35	109.21
48	14	312	A86	C12-C11-C13	3.20	121.41	116.02
48	37	310	A86	C12-C11-C13	3.20	121.41	116.02
37	33	303	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
37	12	203	CLA	CHD-C4C-NC	3.20	129.25	124.20
37	W	102	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
37	33	308	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
37	21	202	CLA	CAC-C3C-C4C	3.20	128.97	124.81
37	12	209	CLA	C4-C3-C5	3.20	120.66	115.27
37	18	203	CLA	C3B-C4B-NB	3.20	113.35	109.21
37	19	305	CLA	C4-C3-C5	3.20	119.64	115.98
37	39	306	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
37	c	501	CLA	CAC-C3C-C4C	3.20	128.96	124.81
37	b	523	CLA	C3D-C2D-C1D	-3.20	101.46	105.83
48	37	313	A86	C33-C32-C31	3.20	112.32	109.21
37	B	510	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
48	39	311	A86	C12-C11-C13	3.20	121.40	116.02
37	38	211	CLA	CHC-C1C-C2C	-3.20	117.87	126.72
37	32	210	CLA	C4-C3-C5	3.20	120.65	115.27
47	38	210	KC1	CAC-C3C-C4C	3.20	128.96	124.81
37	14	305	CLA	CHC-C1C-C2C	-3.20	117.87	126.72
37	20	306	CLA	CAA-C2A-C3A	-3.20	104.02	112.78
48	19	311	A86	C12-C11-C13	3.20	121.39	116.02
37	B	507	CLA	CMB-C2B-C3B	3.20	130.66	124.68
48	38	213	A86	C3-C4-C5	-3.20	116.92	123.47
47	36	305	KC1	CAA-CBA-CGA	-3.20	110.83	127.26
37	B	512	CLA	O2D-CGD-O1D	-3.20	117.59	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	19	306	CLA	C4C-C3C-C2C	-3.20	102.24	106.90
47	16	305	KC1	CAA-CBA-CGA	-3.20	110.83	127.26
48	32	203	A86	C41-C32-C31	-3.20	107.61	110.47
47	31	309	KC1	CAC-C3C-C4C	3.20	128.96	124.81
37	17	307	CLA	C3B-C4B-NB	3.20	113.34	109.21
37	38	201	CLA	C1C-C2C-C3C	-3.20	103.60	106.96
37	B	501	CLA	C3B-C4B-NB	3.19	113.34	109.21
48	32	221	A86	C26-C25-C24	-3.19	113.25	123.22
48	37	312	A86	C4-C5-C6	-3.19	122.75	127.31
37	40	208	CLA	CAA-C2A-C3A	-3.19	104.03	112.78
37	B	511	CLA	CHC-C1C-C2C	-3.19	117.89	126.72
37	b	511	CLA	CHC-C1C-C2C	-3.19	117.89	126.72
37	31	304	CLA	CMB-C2B-C3B	3.19	130.65	124.68
47	14	309	KC1	CAC-C3C-C4C	3.19	128.95	124.81
37	11	303	CLA	CHC-C1C-C2C	-3.19	117.89	126.72
37	13	305	CLA	C3B-C4B-NB	3.19	113.34	109.21
48	19	311	A86	C4-C5-C6	-3.19	122.75	127.31
37	B	524	CLA	C3D-C2D-C1D	-3.19	101.48	105.83
37	b	506	CLA	C3B-C4B-NB	3.19	113.33	109.21
37	40	203	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
48	13	311	A86	C34-O4-C38	-3.19	111.95	117.90
37	Z	102	CLA	CHC-C1C-C2C	-3.19	117.90	126.72
48	11	312	A86	C41-C32-C31	-3.19	107.62	110.47
48	34	316	A86	C7-C6-C5	-3.19	118.45	122.92
47	14	309	KC1	CHD-C4C-NC	3.19	129.04	124.20
37	15	310	CLA	CHC-C1C-C2C	-3.19	117.90	126.72
48	11	314	A86	C8-C6-C5	-3.19	114.05	118.94
37	41	208	CLA	CHC-C1C-C2C	-3.19	117.90	126.72
37	13	308	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
37	39	307	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
47	17	308	KC1	CBC-CAC-C3C	-3.19	103.64	112.43
48	11	319	A86	C3-C4-C5	-3.19	116.94	123.47
37	18	202	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
48	13	311	A86	C10-C9-C8	-3.19	113.27	123.22
48	33	311	A86	C10-C9-C8	-3.19	113.27	123.22
47	11	309	KC1	CAC-C3C-C4C	3.19	128.95	124.81
37	38	208	CLA	C1C-C2C-C3C	-3.19	103.61	106.96
48	33	314	A86	C12-C11-C13	3.19	121.38	116.02
37	B	516	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
37	34	308	CLA	CAC-C3C-C4C	3.19	128.94	124.81
37	11	303	CLA	CMB-C2B-C3B	3.18	130.64	124.68
37	21	208	CLA	CHC-C1C-C2C	-3.18	117.91	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	19	307	CLA	CAA-C2A-C3A	-3.18	104.06	112.78
47	34	306	KC1	CMB-C2B-C1B	3.18	130.32	124.71
48	14	315	A86	C10-C9-C8	-3.18	113.28	123.22
48	34	315	A86	C10-C9-C8	-3.18	113.28	123.22
47	17	306	KC1	O2D-CGD-O1D	-3.18	117.61	123.84
48	16	314	A86	C4-C3-C2	-3.18	116.95	123.47
37	18	202	CLA	C4A-NA-C1A	-3.18	105.28	106.71
37	14	305	CLA	CAA-C2A-C3A	-3.18	104.06	112.78
37	34	305	CLA	CAA-C2A-C3A	-3.18	104.06	112.78
37	19	301	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
47	34	309	KC1	CAC-C3C-C4C	3.18	128.94	124.81
48	19	313	A86	C9-C8-C6	-3.18	117.48	126.42
48	31	319	A86	C25-C24-C1	-3.18	117.48	126.42
37	w	101	CLA	O2A-CGA-CBA	3.18	121.89	111.91
47	15	309	KC1	CAC-C3C-C4C	3.18	128.94	124.81
37	37	308	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
37	Z	102	CLA	CHD-C4C-NC	3.18	129.22	124.20
48	41	213	A86	C36-C31-C32	-3.18	116.54	119.70
48	16	311	A86	C41-C32-C31	-3.18	107.63	110.47
37	z	102	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
37	b	512	CLA	CMC-C2C-C1C	3.18	129.88	125.04
37	20	307	CLA	CAC-C3C-C4C	3.18	128.94	124.81
37	c	507	CLA	C4-C3-C5	3.18	120.62	115.27
37	39	301	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
48	13	312	A86	C12-C11-C13	3.18	121.36	116.02
37	C	508	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
37	D	402	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
47	12	211	KC1	CMA-C3A-C2A	-3.18	120.52	128.30
48	17	320	A86	C4-C3-C2	-3.18	116.96	123.47
37	b	515	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
37	39	305	CLA	C4-C3-C5	3.18	119.62	115.98
37	38	202	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
37	d	401	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
37	W	101	CLA	O2A-CGA-CBA	3.18	121.87	111.91
47	16	302	KC1	CBC-CAC-C3C	-3.18	103.68	112.43
37	32	206	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
37	14	303	CLA	CBA-CAA-C2A	3.17	123.23	113.86
37	34	303	CLA	CBA-CAA-C2A	3.17	123.23	113.86
37	41	209	CLA	CAC-C3C-C4C	3.17	128.93	124.81
50	40	214	DD6	C14-C13-C11	-3.17	120.61	125.53
37	12	204	CLA	CAC-C3C-C4C	3.17	128.93	124.81
37	39	306	CLA	CMC-C2C-C1C	3.17	129.87	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	33	305	CLA	C3B-C4B-NB	3.17	113.31	109.21
48	17	314	A86	C25-C24-C1	-3.17	117.50	126.42
37	40	209	CLA	CAC-C3C-C4C	3.17	128.93	124.81
37	39	302	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
48	34	312	A86	C12-C11-C13	3.17	121.35	116.02
48	32	218	A86	C7-C6-C5	-3.17	118.48	122.92
48	11	319	A86	C25-C24-C1	-3.17	117.51	126.42
48	36	311	A86	C41-C32-C31	-3.17	107.63	110.47
47	13	304	KC1	CHD-C4C-NC	3.17	129.01	124.20
48	37	312	A86	C10-C9-C8	-3.17	113.32	123.22
37	b	516	CLA	CAA-C2A-C3A	-3.17	104.10	112.78
37	B	504	CLA	C1-C2-C3	-3.17	120.56	126.04
37	17	304	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
37	35	310	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
37	B	512	CLA	CMC-C2C-C1C	3.17	129.86	125.04
39	A	406	BCR	C24-C23-C22	-3.17	121.45	126.23
37	z	102	CLA	CHD-C4C-NC	3.17	129.19	124.20
37	31	308	CLA	CMB-C2B-C3B	3.17	130.60	124.68
50	20	312	DD6	C14-C13-C11	-3.17	120.62	125.53
37	b	507	CLA	CMB-C2B-C3B	3.17	130.60	124.68
47	13	302	KC1	CMB-C2B-C1B	3.17	130.29	124.71
37	21	205	CLA	CHC-C1C-C2C	-3.17	117.96	126.72
37	38	202	CLA	CHD-C4C-NC	3.17	129.19	124.20
37	41	205	CLA	CHC-C1C-C2C	-3.17	117.97	126.72
47	36	302	KC1	CBC-CAC-C3C	-3.17	103.70	112.43
37	31	301	CLA	C3B-C4B-NB	3.17	113.30	109.21
37	c	508	CLA	CAA-C2A-C3A	-3.16	104.11	112.78
37	B	512	CLA	CAC-C3C-C4C	3.16	128.92	124.81
37	21	204	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
37	15	307	CLA	CMC-C2C-C1C	3.16	129.86	125.04
37	c	508	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
37	31	304	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
48	33	312	A86	C12-C11-C13	3.16	121.33	116.02
47	20	305	KC1	CBA-CAA-C2A	-3.16	113.22	125.27
47	19	308	KC1	CHD-C4C-NC	3.16	129.00	124.20
37	37	303	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
37	39	301	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
37	20	301	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
48	12	217	A86	C7-C6-C5	-3.16	118.50	122.92
48	36	313	A86	C4-C3-C2	-3.16	117.00	123.47
40	b	521	SQD	O47-C7-C8	3.16	118.31	111.50
37	C	508	CLA	CHC-C1C-C2C	-3.16	117.98	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	503	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
37	40	203	CLA	C4-C3-C5	3.16	120.58	115.27
47	16	302	KC1	CMB-C2B-C1B	3.16	130.28	124.71
37	B	515	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
37	35	307	CLA	CHD-C4C-NC	3.16	129.18	124.20
39	a	408	BCR	C24-C23-C22	-3.16	121.47	126.23
37	31	310	CLA	C3B-C4B-NB	3.16	113.29	109.21
37	11	310	CLA	CMB-C2B-C3B	3.15	130.58	124.68
37	11	307	CLA	CHD-C4C-NC	3.15	129.17	124.20
47	31	303	KC1	CHD-C4C-NC	3.15	128.99	124.20
37	38	203	CLA	CAA-C2A-C1A	3.15	122.31	111.97
37	11	310	CLA	C3B-C4B-NB	3.15	113.29	109.21
37	b	502	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
37	19	309	CLA	CAC-C3C-C4C	3.15	128.90	124.81
48	12	202	A86	C41-C32-C31	-3.15	107.65	110.47
37	b	501	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
47	33	304	KC1	CHD-C4C-NC	3.15	128.98	124.20
37	31	308	CLA	CHD-C4C-NC	3.15	129.17	124.20
47	36	302	KC1	CMB-C2B-C1B	3.15	130.26	124.71
37	C	507	CLA	C4-C3-C5	3.15	120.57	115.27
37	20	301	CLA	C4-C3-C5	3.15	120.57	115.27
47	11	302	KC1	O2D-CGD-O1D	-3.15	117.68	123.84
37	35	307	CLA	CMC-C2C-C1C	3.15	129.83	125.04
37	32	205	CLA	O2A-CGA-CBA	3.15	121.79	111.91
48	11	319	A86	C10-C9-C8	-3.15	113.39	123.22
37	41	205	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
37	16	307	CLA	C3B-C4B-NB	3.15	113.28	109.21
47	40	207	KC1	CBA-CAA-C2A	-3.15	113.27	125.27
37	39	309	CLA	CHC-C1C-C2C	-3.15	118.02	126.72
37	11	310	CLA	C4-C3-C5	3.15	119.58	115.98
47	37	305	KC1	O2D-CGD-O1D	-3.15	117.69	123.84
48	31	319	A86	C10-C9-C8	-3.15	113.40	123.22
48	39	311	A86	C4-C5-C6	-3.14	122.82	127.31
48	19	311	A86	C28-C27-C26	3.14	127.33	122.92
37	20	307	CLA	C3B-C4B-NB	3.14	113.28	109.21
37	19	309	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
47	35	309	KC1	CAC-C3C-C4C	3.14	128.89	124.81
37	C	512	CLA	C3B-C4B-NB	3.14	113.27	109.21
37	41	204	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
37	15	303	CLA	CAC-C3C-C4C	3.14	128.89	124.81
37	31	310	CLA	CMB-C2B-C3B	3.14	130.56	124.68
37	19	302	CLA	CHC-C1C-C2C	-3.14	118.03	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	12	217	A86	C33-C32-C31	3.14	112.27	109.21
37	39	306	CLA	CAC-C3C-C4C	3.14	128.89	124.81
47	11	306	KC1	O2D-CGD-O1D	-3.14	117.70	123.84
47	11	302	KC1	CHD-C4C-NC	3.14	128.97	124.20
37	35	308	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
37	c	508	CLA	C1C-C2C-C3C	-3.14	103.65	106.96
37	16	301	CLA	CHD-C4C-NC	3.14	129.15	124.20
40	B	522	SQD	O47-C7-C8	3.14	118.27	111.50
47	38	207	KC1	CAC-C3C-C4C	3.14	128.88	124.81
37	12	204	CLA	O2A-CGA-CBA	3.14	121.76	111.91
37	11	305	CLA	C3B-C4B-NB	3.14	113.27	109.21
47	37	307	KC1	CHD-C4C-NC	3.14	128.97	124.20
37	36	301	CLA	CHD-C4C-NC	3.14	129.15	124.20
37	11	307	CLA	CMB-C2B-C3B	3.14	130.55	124.68
37	31	306	CLA	CHC-C1C-C2C	-3.14	118.05	126.72
37	18	208	CLA	C3B-C4B-NB	3.14	113.27	109.21
37	B	507	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
37	21	205	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
48	12	213	A86	C10-C9-C8	-3.14	113.43	123.22
48	17	311	A86	C34-O4-C38	-3.14	112.05	117.90
37	B	510	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
37	B	501	CLA	CHC-C1C-C2C	-3.14	118.05	126.72
37	C	503	CLA	CHC-C1C-C2C	-3.14	118.05	126.72
37	40	209	CLA	C3B-C4B-NB	3.13	113.26	109.21
37	C	513	CLA	CHD-C4C-NC	3.13	129.14	124.20
37	31	306	CLA	C3B-C4B-NB	3.13	113.26	109.21
37	W	101	CLA	O1D-CGD-CBD	-3.13	118.08	124.48
37	w	101	CLA	O1D-CGD-CBD	-3.13	118.08	124.48
37	38	208	CLA	C3B-C4B-NB	3.13	113.26	109.21
37	B	507	CLA	C4A-NA-C1A	-3.13	105.30	106.71
37	b	510	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
37	19	303	CLA	C1-C2-C3	-3.13	120.63	126.04
37	W	101	CLA	C3B-C4B-NB	3.13	113.26	109.21
37	36	307	CLA	C3B-C4B-NB	3.13	113.26	109.21
37	18	204	CLA	CHD-C4C-NC	3.13	129.14	124.20
37	19	301	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
37	11	305	CLA	CHC-C1C-C2C	-3.13	118.06	126.72
37	16	307	CLA	C1-C2-C3	-3.13	120.63	126.04
37	c	512	CLA	C3B-C4B-NB	3.13	113.26	109.21
37	19	306	CLA	CMC-C2C-C1C	3.13	129.81	125.04
41	c	518	LMG	O1-C7-C8	-3.13	103.35	110.90
48	39	311	A86	C28-C27-C26	3.13	127.31	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	39	309	CLA	CAC-C3C-C4C	3.13	128.87	124.81
37	20	301	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
37	16	306	CLA	CMC-C2C-C1C	3.13	129.80	125.04
47	16	308	KC1	C1A-NA-C4A	-3.13	105.30	106.71
37	C	504	CLA	CHC-C1C-C2C	-3.13	118.07	126.72
48	37	319	A86	C36-C31-C32	-3.13	116.59	119.70
37	33	310	CLA	CHC-C1C-C2C	-3.13	118.07	126.72
37	39	307	CLA	CHC-C1C-C2C	-3.13	118.07	126.72
50	21	216	DD6	C23-C16-C15	3.13	118.49	110.05
37	W	102	CLA	C3B-C4B-NB	3.13	113.25	109.21
37	36	307	CLA	C1-C2-C3	-3.13	120.64	126.04
48	32	218	A86	C33-C32-C31	3.13	112.25	109.21
37	40	203	CLA	C1C-C2C-C3C	-3.12	103.67	106.96
37	12	207	CLA	C3B-C4B-NB	3.12	113.25	109.21
37	32	208	CLA	C3B-C4B-NB	3.12	113.25	109.21
48	32	217	A86	C4-C5-C6	-3.12	122.85	127.31
47	12	211	KC1	CHD-C4C-NC	3.12	128.94	124.20
37	17	309	CLA	CED-O2D-CGD	3.12	123.00	115.94
37	40	210	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
37	b	503	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
37	15	307	CLA	CHD-C4C-NC	3.12	129.12	124.20
37	B	502	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
41	C	518	LMG	O1-C7-C8	-3.12	103.37	110.90
37	39	303	CLA	C1-C2-C3	-3.12	120.64	126.04
48	40	201	A86	C7-C6-C5	-3.12	118.55	122.92
47	17	308	KC1	CHD-C4C-NC	3.12	128.94	124.20
47	35	306	KC1	CHD-C4C-NC	3.12	128.94	124.20
48	31	314	A86	C34-O4-C38	-3.12	112.08	117.90
50	41	216	DD6	C23-C16-C15	3.12	118.47	110.05
37	19	303	CLA	CAC-C3C-C4C	3.12	128.86	124.81
47	31	303	KC1	O2D-CGD-O1D	-3.12	117.74	123.84
37	b	502	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
37	c	504	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
48	37	311	A86	C36-C31-C32	-3.12	116.60	119.70
37	B	502	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
37	B	503	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
48	17	313	A86	C10-C9-C8	-3.12	113.48	123.22
50	41	212	DD6	C23-C16-C17	-3.12	103.56	108.98
37	19	306	CLA	CAC-C3C-C4C	3.12	128.86	124.81
37	39	307	CLA	CAC-C3C-C4C	3.12	128.86	124.81
37	31	310	CLA	C4-C3-C5	3.12	119.55	115.98
37	19	307	CLA	CAC-C3C-C4C	3.12	128.85	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	504	CLA	C3C-C4C-NC	3.12	114.07	110.57
47	15	302	KC1	CMB-C2B-C1B	3.11	130.20	124.71
37	19	307	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
37	19	303	CLA	C3B-C4B-NB	3.11	113.24	109.21
37	19	301	CLA	CHD-C4C-NC	3.11	129.11	124.20
47	31	307	KC1	O2D-CGD-O1D	-3.11	117.75	123.84
37	20	308	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
37	c	513	CLA	CHD-C4C-NC	3.11	129.11	124.20
37	c	507	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
37	17	302	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
37	20	303	CLA	CHD-C4C-NC	3.11	129.10	124.20
37	13	310	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
37	14	303	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
47	16	302	KC1	CAA-CBA-CGA	-3.11	111.28	127.26
37	18	201	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
48	32	214	A86	C10-C9-C8	-3.11	113.52	123.22
37	36	307	CLA	CHD-C4C-NC	3.11	129.10	124.20
37	36	306	CLA	CMC-C2C-C1C	3.11	129.77	125.04
37	17	309	CLA	C1-C2-C3	-3.11	120.67	126.04
48	15	316	A86	C9-C10-C11	-3.11	117.47	126.61
37	b	510	CLA	O2A-CGA-CBA	3.11	121.66	111.91
37	20	306	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
37	40	205	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
37	b	512	CLA	CAC-C3C-C4C	3.11	128.84	124.81
37	32	210	CLA	CAC-C3C-C4C	3.11	128.84	124.81
50	21	212	DD6	C23-C16-C17	-3.10	103.59	108.98
37	21	202	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
37	32	204	CLA	C3B-C4B-NB	3.10	113.22	109.21
37	39	303	CLA	C3B-C4B-NB	3.10	113.22	109.21
37	20	306	CLA	C1-C2-C3	-3.10	121.73	126.75
48	33	312	A86	C3-C4-C5	-3.10	117.11	123.47
37	16	301	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
37	38	208	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
37	33	301	CLA	C3B-C4B-NB	3.10	113.22	109.21
48	38	213	A86	C7-C6-C8	3.10	122.97	118.08
37	B	510	CLA	O2A-CGA-CBA	3.10	121.65	111.91
48	12	213	A86	C3-C2-C1	-3.10	122.88	127.31
47	32	212	KC1	CAC-C3C-C4C	3.10	128.84	124.81
47	36	302	KC1	CAA-CBA-CGA	-3.10	111.31	127.26
37	c	512	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
48	12	216	A86	C4-C5-C6	-3.10	122.88	127.31
37	C	508	CLA	C1C-C2C-C3C	-3.10	103.69	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	16	313	A86	C40-C32-C31	-3.10	107.70	110.47
48	19	313	A86	C25-C26-C27	-3.10	122.88	127.31
47	34	306	KC1	O2D-CGD-O1D	-3.10	117.78	123.84
50	39	312	DD6	C37-C36-C35	-3.10	108.61	114.36
48	17	320	A86	C36-C31-C32	-3.10	116.62	119.70
37	C	512	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
48	32	221	A86	C-C1-C24	3.10	122.96	118.08
37	34	303	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
37	37	301	CLA	C3B-C4B-NB	3.10	113.22	109.21
37	19	307	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
37	w	101	CLA	C3B-C4B-NB	3.10	113.22	109.21
37	39	301	CLA	CHD-C4C-NC	3.10	129.08	124.20
48	11	311	A86	C12-C11-C13	3.10	121.22	116.02
37	39	307	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
37	21	209	CLA	CHC-C1C-C2C	-3.10	118.16	126.72
37	40	208	CLA	C1-C2-C3	-3.10	121.74	126.75
45	D	408	PL9	C7-C8-C9	-3.10	121.64	126.79
37	17	307	CLA	CAA-C2A-C1A	3.09	122.12	111.97
48	19	313	A86	C7-C6-C5	-3.09	118.59	122.92
37	35	303	CLA	CAC-C3C-C4C	3.09	128.82	124.81
47	35	302	KC1	CAC-C3C-C4C	3.09	128.82	124.81
37	b	515	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
48	32	203	A86	C3-C4-C5	-3.09	117.14	123.47
37	20	301	CLA	C1-C2-C3	-3.09	120.69	126.04
37	39	303	CLA	CAC-C3C-C4C	3.09	128.82	124.81
37	B	503	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
37	40	203	CLA	C1-C2-C3	-3.09	120.70	126.04
37	d	404	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
50	19	312	DD6	C37-C36-C35	-3.09	108.63	114.36
48	16	313	A86	C7-C6-C5	-3.09	118.59	122.92
37	b	507	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
37	b	511	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
37	C	512	CLA	CMA-C3A-C4A	-3.09	103.47	111.77
37	41	209	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
37	B	513	CLA	CHD-C4C-NC	3.09	129.07	124.20
47	32	209	KC1	CHD-C4C-NC	3.09	128.89	124.20
37	B	515	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
37	D	406	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
47	20	302	KC1	CHD-C4C-NC	3.09	128.88	124.20
47	40	204	KC1	CHD-C4C-NC	3.09	128.88	124.20
37	41	202	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
37	B	505	CLA	CHD-C4C-NC	3.09	129.06	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	c	514	BCR	C15-C16-C17	-3.09	117.15	123.47
48	12	202	A86	C3-C4-C5	-3.09	117.15	123.47
37	14	307	CLA	CAC-C3C-C4C	3.09	128.81	124.81
37	39	305	CLA	C3B-C4B-NB	3.08	113.20	109.21
39	B	525	BCR	C24-C23-C22	-3.08	121.57	126.23
37	b	514	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
48	13	312	A86	C3-C4-C5	-3.08	117.16	123.47
37	C	509	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
37	c	512	CLA	CMA-C3A-C4A	-3.08	103.48	111.77
37	21	202	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
37	b	514	CLA	CAA-C2A-C3A	-3.08	104.33	112.78
41	c	518	LMG	O6-C1-O1	-3.08	102.67	109.97
37	b	507	CLA	C4A-NA-C1A	-3.08	105.32	106.71
37	C	505	CLA	C3B-C4B-NB	3.08	113.19	109.21
48	37	310	A86	C34-O4-C38	-3.08	112.15	117.90
37	B	511	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
37	36	301	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
37	32	208	CLA	O2A-CGA-CBA	3.08	121.58	111.91
37	41	202	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
47	14	306	KC1	O2D-CGD-O1D	-3.08	117.81	123.84
37	40	205	CLA	CHD-C4C-NC	3.08	129.06	124.20
37	b	503	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
48	31	311	A86	C12-C11-C13	3.08	121.20	116.02
37	C	507	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
37	z	101	CLA	CMB-C2B-C3B	3.08	130.44	124.68
37	13	307	CLA	CAC-C3C-C4C	3.08	128.81	124.81
48	17	312	A86	C36-C31-C32	-3.08	116.64	119.70
37	18	203	CLA	C1-C2-C3	-3.08	120.72	126.04
47	15	306	KC1	CHD-C4C-NC	3.08	128.88	124.20
37	36	307	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
37	C	504	CLA	C3C-C4C-NC	3.08	114.02	110.57
37	Z	102	CLA	C3B-C4B-NB	3.08	113.19	109.21
47	11	309	KC1	C2A-C1A-NA	3.08	114.34	109.40
47	12	208	KC1	CHD-C4C-NC	3.08	128.87	124.20
37	19	303	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
37	39	303	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
37	c	505	CLA	C3B-C4B-NB	3.08	113.19	109.21
37	34	301	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
37	Z	101	CLA	CHD-C4C-NC	3.08	129.05	124.20
37	c	509	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
37	17	302	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
37	31	310	CLA	C4C-C3C-C2C	-3.08	102.41	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	z	101	CLA	CHD-C4C-NC	3.08	129.05	124.20
37	b	512	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
48	32	218	A86	C8-C6-C5	3.08	123.66	118.94
48	13	315	A86	C20-C19-C18	-3.08	106.67	112.75
48	18	213	A86	C35-C34-C33	3.08	115.24	109.88
48	12	220	A86	C-C1-C24	3.08	122.92	118.08
37	40	203	CLA	CAC-C3C-C4C	3.07	128.80	124.81
37	16	303	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
39	b	524	BCR	C24-C23-C22	-3.07	121.59	126.23
37	C	509	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
48	36	310	A86	C35-C34-C33	3.07	115.24	109.88
47	39	308	KC1	CAA-CBA-CGA	-3.07	111.46	127.26
48	16	310	A86	C35-C34-C33	3.07	115.24	109.88
37	12	209	CLA	CAC-C3C-C4C	3.07	128.80	124.81
37	16	307	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
47	37	307	KC1	C2A-C1A-NA	3.07	114.33	109.40
37	33	307	CLA	CAC-C3C-C4C	3.07	128.80	124.81
39	C	514	BCR	C15-C16-C17	-3.07	117.18	123.47
47	19	308	KC1	CAA-CBA-CGA	-3.07	111.48	127.26
37	c	509	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
37	12	207	CLA	O2A-CGA-CBA	3.07	121.54	111.91
37	34	307	CLA	CAC-C3C-C4C	3.07	128.79	124.81
37	37	301	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
37	37	306	CLA	CAA-C2A-C1A	3.07	122.03	111.97
37	19	304	CLA	C1D-CHD-C4C	-3.07	119.44	126.06
37	12	203	CLA	C3B-C4B-NB	3.07	113.18	109.21
37	Z	101	CLA	CMB-C2B-C3B	3.07	130.42	124.68
48	37	309	A86	C23-C16-C22	-3.07	102.84	107.37
37	14	302	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
37	B	514	CLA	CAA-C2A-C3A	-3.07	104.38	112.78
37	40	208	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
48	14	311	A86	C3-C2-C1	-3.07	122.93	127.31
37	14	307	CLA	C4-C3-C5	3.07	120.43	115.27
48	38	213	A86	C35-C34-C33	3.07	115.23	109.88
37	11	310	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
48	34	311	A86	C3-C2-C1	-3.06	122.94	127.31
37	38	202	CLA	C1C-C2C-C3C	-3.06	103.73	106.96
47	17	308	KC1	C2A-C1A-NA	3.06	114.32	109.40
48	37	319	A86	C41-C32-C31	-3.06	107.73	110.47
37	B	507	CLA	CAC-C3C-C4C	3.06	128.78	124.81
47	31	309	KC1	C2A-C1A-NA	3.06	114.31	109.40
37	14	301	CLA	C4C-C3C-C2C	-3.06	102.43	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	12	211	KC1	CAC-C3C-C4C	3.06	128.78	124.81
39	a	413	BCR	C11-C10-C9	-3.06	122.94	127.31
37	37	308	CLA	C1-C2-C3	-3.06	120.75	126.04
37	33	307	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
37	b	505	CLA	CHD-C4C-NC	3.06	129.03	124.20
37	D	406	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
37	B	506	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
37	18	204	CLA	CAC-C3C-C4C	3.06	128.78	124.81
37	39	304	CLA	C1D-CHD-C4C	-3.06	119.46	126.06
37	38	204	CLA	CHD-C4C-NC	3.06	129.02	124.20
37	36	303	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
37	13	307	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
37	39	305	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
37	b	507	CLA	CAC-C3C-C4C	3.06	128.78	124.81
37	d	403	CLA	CBC-CAC-C3C	-3.06	104.01	112.43
48	35	316	A86	C9-C10-C11	-3.06	117.63	126.61
37	20	301	CLA	CAC-C3C-C4C	3.06	128.77	124.81
47	15	302	KC1	C4B-C3B-C2B	-3.05	104.24	106.75
37	20	303	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
37	34	303	CLA	O2A-CGA-CBA	3.05	121.49	111.91
37	19	305	CLA	C3B-C4B-NB	3.05	113.16	109.21
37	c	502	CLA	C1-C2-C3	-3.05	120.77	126.04
37	D	405	CLA	CBC-CAC-C3C	-3.05	104.02	112.43
37	14	303	CLA	O2A-CGA-CBA	3.05	121.48	111.91
48	12	202	A86	C20-C19-C18	-3.05	106.71	112.75
37	b	506	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
37	15	303	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
37	b	513	CLA	CHD-C4C-NC	3.05	129.01	124.20
48	18	213	A86	C26-C25-C24	-3.05	113.70	123.22
48	39	313	A86	C25-C26-C27	-3.05	122.96	127.31
47	31	307	KC1	C4B-C3B-C2B	-3.05	104.25	106.75
37	b	502	CLA	C1-C2-C3	-3.05	120.77	126.04
37	14	307	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
48	18	214	A86	C12-C11-C13	3.05	121.14	116.02
48	13	311	A86	C7-C6-C8	3.05	122.88	118.08
37	34	302	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
37	20	301	CLA	CHD-C4C-NC	3.05	129.01	124.20
37	40	203	CLA	CHD-C4C-NC	3.05	129.01	124.20
37	31	304	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
41	C	518	LMG	O6-C1-O1	-3.05	102.75	109.97
37	20	307	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
48	12	217	A86	C8-C6-C5	3.05	123.62	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	19	305	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
37	16	307	CLA	CHD-C4C-NC	3.05	129.00	124.20
37	11	303	CLA	CAC-C3C-C4C	3.05	128.76	124.81
37	B	514	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
37	11	303	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
37	18	206	CLA	CMA-C3A-C2A	-3.05	101.54	113.83
37	34	307	CLA	C4-C3-C5	3.05	120.39	115.27
37	12	209	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
37	19	304	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
37	19	305	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
37	16	306	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
37	32	206	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
37	c	508	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
37	18	206	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
37	21	204	CLA	CMB-C2B-C3B	3.04	130.37	124.68
47	18	205	KC1	CAA-CBA-CGA	-3.04	111.62	127.26
37	21	204	CLA	C3C-C4C-NC	3.04	113.98	110.57
48	39	313	A86	C4-C3-C2	-3.04	117.24	123.47
37	B	502	CLA	C1-C2-C3	-3.04	120.78	126.04
40	36	315	SQD	O47-C7-C8	3.04	118.06	111.50
47	35	302	KC1	CMB-C2B-C1B	3.04	130.08	124.71
47	36	308	KC1	CMA-C3A-C2A	-3.04	120.85	128.30
37	32	210	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
37	38	203	CLA	C1-C2-C3	-3.04	120.78	126.04
48	33	315	A86	C20-C19-C18	-3.04	106.73	112.75
37	B	513	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
37	c	513	CLA	C3B-C4B-NB	3.04	113.14	109.21
37	A	405	CLA	CAC-C3C-C4C	3.04	128.76	124.81
37	34	307	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
37	41	204	CLA	C3C-C4C-NC	3.04	113.98	110.57
37	C	513	CLA	C3B-C4B-NB	3.04	113.14	109.21
37	z	102	CLA	C3B-C4B-NB	3.04	113.14	109.21
37	d	401	CLA	C3B-C4B-NB	3.04	113.14	109.21
37	17	302	CLA	C3B-C4B-NB	3.04	113.14	109.21
37	18	208	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
37	d	404	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
48	18	214	A86	C9-C8-C6	-3.04	117.88	126.42
37	13	301	CLA	C3B-C4B-NB	3.04	113.14	109.21
37	12	205	CLA	CAC-C3C-C4C	3.04	128.75	124.81
48	32	203	A86	C20-C19-C18	-3.04	106.74	112.75
37	33	307	CLA	C4-C3-C5	3.04	120.38	115.27
37	41	204	CLA	CMB-C2B-C3B	3.04	130.36	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	38	204	CLA	CAC-C3C-C4C	3.04	128.75	124.81
47	11	306	KC1	C4B-C3B-C2B	-3.04	104.26	106.75
37	b	506	CLA	C1D-CHD-C4C	-3.04	119.51	126.06
37	40	209	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
47	38	205	KC1	CAA-CBA-CGA	-3.04	111.66	127.26
37	31	304	CLA	CAC-C3C-C4C	3.04	128.75	124.81
37	36	309	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
37	14	303	CLA	CAC-C3C-C4C	3.04	128.75	124.81
47	38	205	KC1	CAC-C3C-C4C	3.04	128.75	124.81
37	16	309	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
47	37	307	KC1	CBC-CAC-C3C	-3.03	104.06	112.43
39	b	517	BCR	C11-C10-C9	-3.03	122.98	127.31
37	19	304	CLA	C3B-C4B-NB	3.03	113.13	109.21
37	39	304	CLA	C3B-C4B-NB	3.03	113.13	109.21
37	a	407	CLA	CAC-C3C-C4C	3.03	128.75	124.81
47	17	306	KC1	C4C-C3C-C2C	-3.03	102.48	106.90
37	14	301	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
37	36	306	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
37	35	303	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
37	B	506	CLA	C1D-CHD-C4C	-3.03	119.52	126.06
40	17	301	SQD	O47-C7-C8	3.03	118.03	111.50
37	35	308	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
39	A	410	BCR	C11-C10-C9	-3.03	122.98	127.31
45	d	406	PL9	C7-C8-C9	-3.03	121.75	126.79
48	17	311	A86	C12-C11-C13	3.03	121.11	116.02
47	32	212	KC1	CHD-C4C-NC	3.03	128.80	124.20
37	18	203	CLA	CAA-C2A-C1A	3.03	121.90	111.97
48	33	311	A86	C7-C6-C8	3.03	122.85	118.08
37	C	502	CLA	C1-C2-C3	-3.03	120.81	126.04
37	38	203	CLA	C4-C3-C5	3.03	120.36	115.27
48	40	201	A86	C40-C32-C31	-3.03	107.76	110.47
39	B	517	BCR	C11-C10-C9	-3.03	122.99	127.31
48	34	315	A86	C36-C31-C32	-3.03	116.69	119.70
37	18	211	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
37	A	405	CLA	C4-C3-C5	3.03	120.36	115.27
48	34	311	A86	C25-C24-C1	-3.03	117.92	126.42
39	c	514	BCR	C11-C10-C9	-3.02	122.99	127.31
37	a	407	CLA	C4-C3-C5	3.02	120.36	115.27
37	37	308	CLA	CAA-C2A-C1A	-3.02	102.06	111.97
37	D	402	CLA	C3B-C4B-NB	3.02	113.12	109.21
47	33	304	KC1	CAA-CBA-CGA	-3.02	111.72	127.26
37	B	505	CLA	CAC-C3C-C4C	3.02	128.73	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	13	304	KC1	CAA-CBA-CGA	-3.02	111.72	127.26
47	37	305	KC1	C4C-C3C-C2C	-3.02	102.49	106.90
37	b	513	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
39	C	514	BCR	C11-C10-C9	-3.02	123.00	127.31
37	40	205	CLA	CAC-C3C-C4C	3.02	128.73	124.81
37	B	505	CLA	CMC-C2C-C1C	3.02	129.64	125.04
38	A	404	PHO	O1D-CGD-CBD	3.02	129.77	124.74
37	19	310	CLA	C3B-C4B-NB	3.02	113.12	109.21
37	c	511	CLA	CAC-C3C-C4C	3.02	128.73	124.81
37	35	301	CLA	CHD-C4C-NC	3.02	128.97	124.20
47	18	210	KC1	C4C-C3C-C2C	-3.02	102.49	106.90
47	16	308	KC1	CMA-C3A-C2A	-3.02	120.90	128.30
48	32	217	A86	C41-C32-C31	-3.02	107.77	110.47
37	34	301	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
47	37	305	KC1	CBA-CAA-C2A	-3.02	113.75	125.27
50	36	312	DD6	C3-C4-C5	-3.02	117.29	123.47
37	39	310	CLA	C3B-C4B-NB	3.02	113.11	109.21
37	39	305	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
47	32	212	KC1	CAA-CBA-CGA	-3.02	111.75	127.26
37	C	511	CLA	CAC-C3C-C4C	3.02	128.73	124.81
37	19	304	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
37	11	307	CLA	O2A-CGA-CBA	3.02	121.38	111.91
50	16	312	DD6	C3-C4-C5	-3.02	117.29	123.47
37	C	508	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
37	34	303	CLA	CAC-C3C-C4C	3.02	128.72	124.81
48	15	316	A86	C3-C2-C1	-3.02	123.00	127.31
37	39	304	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
37	31	308	CLA	C4-C3-C5	3.02	120.34	115.27
37	37	301	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
48	17	320	A86	C41-C32-C31	-3.01	107.77	110.47
37	12	212	CLA	CHD-C4C-NC	3.01	128.95	124.20
37	c	512	CLA	CHC-C1C-C2C	-3.01	118.38	126.72
48	32	217	A86	C10-C9-C8	-3.01	113.81	123.22
40	B	519	SQD	O5-C5-C4	3.01	115.17	109.69
37	33	305	CLA	CHD-C4C-NC	3.01	128.95	124.20
47	12	211	KC1	CAA-CBA-CGA	-3.01	111.78	127.26
37	C	503	CLA	CAA-C2A-C3A	-3.01	104.53	112.78
37	13	310	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
47	18	205	KC1	CAC-C3C-C4C	3.01	128.72	124.81
48	12	216	A86	C10-C9-C8	-3.01	113.82	123.22
47	17	306	KC1	CBA-CAA-C2A	-3.01	113.80	125.27
37	b	506	CLA	C1-C2-C3	-3.01	120.84	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	35	305	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
48	11	315	A86	C36-C31-C32	-3.01	116.71	119.70
37	13	305	CLA	CHD-C4C-NC	3.01	128.94	124.20
37	B	512	CLA	C1C-C2C-C3C	-3.01	103.80	106.96
37	15	305	CLA	CHC-C1C-C2C	-3.01	118.41	126.72
37	B	506	CLA	C1-C2-C3	-3.01	120.84	126.04
47	16	308	KC1	CAC-C3C-C4C	3.01	128.71	124.81
37	C	507	CLA	CHC-C1C-C2C	-3.01	118.41	126.72
47	11	306	KC1	CMB-C2B-C1B	3.01	130.01	124.71
38	a	405	PHO	O2D-CGD-O1D	-3.01	117.96	123.84
47	32	209	KC1	CMB-C2B-C1B	3.00	130.01	124.71
47	16	308	KC1	O2D-CGD-O1D	-3.00	117.96	123.84
37	31	308	CLA	O2A-CGA-CBA	3.00	121.34	111.91
40	A	407	SQD	O5-C5-C4	3.00	115.15	109.69
40	b	521	SQD	O9-S-O7	-3.00	103.55	113.95
48	37	314	A86	C22-C16-C17	-3.00	103.76	108.98
48	17	315	A86	C41-C32-C31	-3.00	107.78	110.47
48	14	311	A86	C25-C24-C1	-3.00	117.98	126.42
48	34	312	A86	C4-C3-C2	-3.00	117.32	123.47
37	b	505	CLA	CAC-C3C-C4C	3.00	128.71	124.81
44	h	102	DGD	C1D-C2D-C3D	-3.00	103.74	110.00
38	D	403	PHO	O2D-CGD-O1D	-3.00	117.97	123.84
37	b	505	CLA	CMC-C2C-C1C	3.00	129.61	125.04
40	B	522	SQD	O9-S-O7	-3.00	103.56	113.95
43	21	201	LHG	O8-C23-C24	3.00	121.33	111.91
37	C	512	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
48	14	312	A86	C4-C3-C2	-3.00	117.33	123.47
40	17	301	SQD	C4-C3-C2	3.00	116.06	110.82
37	B	504	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
37	B	524	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
47	12	208	KC1	CMB-C2B-C1B	3.00	130.00	124.71
37	c	507	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
37	c	511	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
37	20	303	CLA	CAC-C3C-C4C	3.00	128.70	124.81
37	18	203	CLA	CBA-CAA-C2A	-3.00	105.02	113.86
47	35	309	KC1	C2A-C1A-NA	3.00	114.21	109.40
37	39	304	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
37	C	511	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
48	33	312	A86	C4-C5-C6	-3.00	123.03	127.31
48	31	315	A86	C36-C31-C32	-3.00	116.72	119.70
37	W	102	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
47	38	210	KC1	C4C-C3C-C2C	-3.00	102.53	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	507	CLA	CHC-C1C-C2C	-3.00	118.44	126.72
44	c	516	DGD	C3G-C2G-C1G	-3.00	104.70	111.79
48	12	214	A86	C36-C31-C32	-2.99	116.72	119.70
37	b	504	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
37	c	503	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
48	19	313	A86	C4-C3-C2	-2.99	117.34	123.47
37	32	202	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
47	18	210	KC1	O2D-CGD-O1D	-2.99	117.98	123.84
37	39	305	CLA	CHB-C4A-NA	2.99	128.65	124.51
37	c	513	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
37	20	308	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
37	40	208	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
48	41	214	A86	C4-C3-C2	-2.99	117.34	123.47
37	31	301	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
41	17	317	LMG	C1-C2-C3	-2.99	103.76	110.00
44	H	102	DGD	C1D-C2D-C3D	-2.99	103.76	110.00
48	38	214	A86	C7-C6-C8	2.99	122.79	118.08
44	C	516	DGD	C3G-C2G-C1G	-2.99	104.71	111.79
37	c	505	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
47	18	210	KC1	C2A-C1A-NA	2.99	114.20	109.40
37	36	301	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
37	13	307	CLA	C4-C3-C5	2.99	120.30	115.27
48	18	214	A86	C7-C6-C8	2.99	122.79	118.08
37	B	508	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
48	36	311	A86	C10-C9-C8	-2.99	113.89	123.22
37	12	212	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
37	c	504	CLA	C4A-NA-C1A	-2.99	105.36	106.71
37	C	506	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
47	36	304	KC1	CHD-C4C-NC	2.99	128.74	124.20
48	40	201	A86	C12-C11-C10	-2.99	116.19	123.42
48	35	315	A86	C36-C31-C32	-2.99	116.73	119.70
48	12	216	A86	C41-C32-C31	-2.99	107.80	110.47
37	11	308	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
37	C	507	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
48	15	316	A86	C40-C32-C31	2.99	113.14	110.47
40	36	315	SQD	C4-C3-C2	2.99	116.04	110.82
37	b	523	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
45	D	404	PL9	C40-C39-C41	2.99	120.29	115.27
47	16	304	KC1	CHD-C4C-NC	2.99	128.73	124.20
37	C	509	CLA	C1-O2A-CGA	2.99	124.28	116.44
37	d	404	CLA	CHD-C4C-NC	2.99	128.91	124.20
48	17	315	A86	C20-C19-C18	-2.98	106.84	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	21	214	A86	C4-C3-C2	-2.98	117.36	123.47
47	38	210	KC1	C2A-C1A-NA	2.98	114.19	109.40
50	21	216	DD6	C21-C20-C15	-2.98	117.26	122.26
37	21	202	CLA	C1-C2-C3	-2.98	120.88	126.04
37	32	206	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
48	37	314	A86	C20-C19-C18	-2.98	106.85	112.75
47	12	208	KC1	CAA-CBA-CGA	-2.98	111.93	127.26
38	a	406	PHO	O1D-CGD-CBD	2.98	129.71	124.74
47	32	209	KC1	CAA-CBA-CGA	-2.98	111.94	127.26
37	B	502	CLA	CHD-C4C-NC	2.98	128.90	124.20
40	a	409	SQD	O5-C5-C4	2.98	115.11	109.69
37	38	206	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
37	31	308	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
37	18	203	CLA	C4-C3-C5	2.98	120.29	115.27
37	z	101	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
37	b	508	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
48	16	313	A86	C12-C11-C10	-2.98	116.22	123.42
48	17	315	A86	C36-C31-C32	-2.98	116.74	119.70
37	19	305	CLA	CHB-C4A-NA	2.98	128.63	124.51
37	15	301	CLA	CMC-C2C-C1C	2.98	129.57	125.04
37	38	208	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
37	20	303	CLA	C1-O2A-CGA	2.98	124.26	116.44
40	L	101	SQD	O5-C5-C4	2.98	115.10	109.69
37	38	202	CLA	CMC-C2C-C1C	2.98	129.57	125.04
47	31	307	KC1	CMB-C2B-C1B	2.98	129.96	124.71
37	c	501	CLA	CAA-C2A-C3A	-2.98	104.63	112.78
48	35	313	A86	C36-C31-C32	-2.98	116.74	119.70
47	14	304	KC1	CAA-CBA-CGA	-2.98	111.96	127.26
37	C	513	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
37	B	505	CLA	C3B-C4B-NB	2.97	113.06	109.21
48	37	314	A86	C36-C31-C32	-2.97	116.74	119.70
37	c	505	CLA	CHD-C4C-NC	2.97	128.89	124.20
47	34	304	KC1	CAA-CBA-CGA	-2.97	111.98	127.26
48	35	316	A86	C3-C2-C1	-2.97	123.07	127.31
37	19	303	CLA	CHD-C4C-NC	2.97	128.89	124.20
37	41	202	CLA	C1-C2-C3	-2.97	120.90	126.04
50	39	312	DD6	C14-C13-C11	-2.97	120.92	125.53
37	40	205	CLA	C1-O2A-CGA	2.97	124.24	116.44
37	32	213	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
47	38	207	KC1	C4C-C3C-C2C	-2.97	102.56	106.90
48	37	314	A86	C41-C32-C31	-2.97	107.81	110.47
48	34	313	A86	C35-C34-C33	2.97	115.06	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	36	309	CLA	C3B-C4B-NB	2.97	113.05	109.21
39	0	101	BCR	C11-C10-C9	-2.97	123.07	127.31
37	c	510	CLA	C1-C2-C3	-2.97	120.90	126.04
37	40	210	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
47	16	308	KC1	C4C-C3C-C2C	-2.97	102.57	106.90
37	C	505	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
37	b	505	CLA	C3B-C4B-NB	2.97	113.05	109.21
48	18	212	A86	C25-C26-C27	-2.97	123.07	127.31
37	39	301	CLA	O2D-CGD-CBD	2.97	116.55	111.27
48	14	312	A86	C26-C25-C24	-2.97	113.95	123.22
37	C	501	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
37	15	301	CLA	CHD-C4C-NC	2.97	128.88	124.20
37	38	211	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
48	16	311	A86	C10-C9-C8	-2.97	113.95	123.22
37	D	402	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
37	11	307	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
37	20	303	CLA	C4-C3-C5	2.97	120.26	115.27
37	18	201	CLA	C1C-C2C-C3C	-2.97	103.84	106.96
37	c	503	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
37	d	403	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
41	37	316	LMG	C1-C2-C3	-2.97	103.82	110.00
37	b	504	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
48	14	316	A86	C3-C2-C1	-2.97	123.08	127.31
37	12	212	CLA	C3B-C4B-NB	2.97	113.05	109.21
48	32	215	A86	C36-C31-C32	-2.97	116.75	119.70
48	17	315	A86	C22-C16-C17	-2.97	103.83	108.98
48	34	312	A86	C26-C25-C24	-2.96	113.97	123.22
37	11	303	CLA	C4-C3-C5	2.96	120.26	115.27
45	d	402	PL9	C40-C39-C41	2.96	120.26	115.27
47	36	308	KC1	O2D-CGD-O1D	-2.96	118.04	123.84
48	39	311	A86	C41-C32-C31	-2.96	107.82	110.47
47	35	306	KC1	CMB-C2B-C1B	2.96	129.94	124.71
48	14	315	A86	C36-C31-C32	-2.96	116.75	119.70
47	31	305	KC1	CAC-C3C-C4C	2.96	128.66	124.81
37	39	301	CLA	C3B-C4B-NB	2.96	113.04	109.21
37	c	506	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
37	31	306	CLA	CHB-C4A-NA	2.96	128.61	124.51
37	32	213	CLA	CHD-C4C-NC	2.96	128.87	124.20
37	C	503	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
37	11	305	CLA	CAC-C3C-C4C	2.96	128.65	124.81
47	36	308	KC1	CAC-C3C-C4C	2.96	128.65	124.81
47	15	309	KC1	C2A-C1A-NA	2.96	114.15	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	505	CLA	CHD-C4C-NC	2.96	128.87	124.20
37	C	501	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
37	c	501	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
37	12	212	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
37	18	208	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
48	14	313	A86	C35-C34-C33	2.96	115.04	109.88
50	20	310	DD6	C21-C20-C15	-2.96	117.30	122.26
48	31	314	A86	C7-C6-C8	2.96	122.74	118.08
37	32	210	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
37	c	509	CLA	C1-O2A-CGA	2.96	124.21	116.44
37	20	306	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
37	40	205	CLA	C4-C3-C5	2.96	120.25	115.27
48	36	313	A86	C26-C25-C24	-2.96	113.98	123.22
37	19	301	CLA	C3B-C4B-NB	2.96	113.03	109.21
37	B	504	CLA	CAA-C2A-C3A	-2.96	104.68	112.78
37	17	309	CLA	CAA-C2A-C1A	-2.96	102.28	111.97
47	21	203	KC1	O2D-CGD-O1D	-2.96	118.06	123.84
37	19	301	CLA	O2D-CGD-CBD	2.96	116.52	111.27
48	38	213	A86	C26-C25-C24	-2.96	113.99	123.22
37	38	201	CLA	CAC-C3C-C4C	2.96	128.65	124.81
37	31	304	CLA	C4-C3-C5	2.96	120.25	115.27
37	21	210	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
37	d	401	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
44	C	517	DGD	CDB-CCB-CBB	-2.96	99.42	114.42
37	31	301	CLA	CMB-C2B-C3B	2.96	130.21	124.68
48	39	311	A86	C35-C34-C33	2.96	115.03	109.88
47	15	302	KC1	CAC-C3C-C4C	2.96	128.65	124.81
37	13	303	CLA	C4-C3-C5	2.96	120.24	115.27
44	c	517	DGD	CDB-CCB-CBB	-2.96	99.42	114.42
37	13	307	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
37	20	307	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
37	39	303	CLA	CHD-C4C-NC	2.96	128.86	124.20
37	38	206	CLA	CMA-C3A-C2A	-2.96	101.91	113.83
37	40	208	CLA	C3B-C4B-NB	2.95	113.03	109.21
48	19	311	A86	C35-C34-C33	2.95	115.03	109.88
37	20	303	CLA	CAA-C2A-C1A	2.95	121.65	111.97
37	19	302	CLA	CAC-C3C-C4C	2.95	128.64	124.81
48	15	315	A86	C41-C32-C31	-2.95	107.83	110.47
47	18	207	KC1	C4C-C3C-C2C	-2.95	102.59	106.90
37	11	305	CLA	CHB-C4A-NA	2.95	128.59	124.51
37	31	306	CLA	CAC-C3C-C4C	2.95	128.64	124.81
48	15	314	A86	C3-C4-C5	-2.95	117.43	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	17	313	A86	C4-C5-C6	-2.95	123.10	127.31
37	11	305	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
37	12	207	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
47	13	306	KC1	CAA-CBA-CGA	-2.95	112.09	127.26
37	B	508	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
37	41	210	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
47	36	308	KC1	C4C-C3C-C2C	-2.95	102.60	106.90
50	40	212	DD6	C21-C20-C15	-2.95	117.31	122.26
37	b	502	CLA	CHD-C4C-NC	2.95	128.85	124.20
37	40	209	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
37	C	507	CLA	CHD-C4C-NC	2.95	128.85	124.20
37	16	309	CLA	C3B-C4B-NB	2.95	113.02	109.21
48	11	314	A86	C7-C6-C8	2.95	122.72	118.08
37	38	201	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
37	d	404	CLA	C4-C3-C5	2.95	120.23	115.27
37	C	502	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
37	33	307	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
37	32	213	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
48	12	220	A86	C8-C6-C5	-2.95	114.42	118.94
47	11	304	KC1	CAC-C3C-C4C	2.95	128.63	124.81
37	C	510	CLA	C1-C2-C3	-2.95	120.94	126.04
48	15	319	A86	C7-C6-C8	2.95	122.72	118.08
37	B	504	CLA	CMB-C2B-C1B	2.95	132.99	128.46
48	14	314	A86	C10-C9-C8	-2.95	114.02	123.22
37	Z	101	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
47	33	302	KC1	C4C-C3C-C2C	-2.95	102.60	106.90
47	33	304	KC1	C4C-C3C-C2C	-2.95	102.60	106.90
37	16	301	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
37	40	205	CLA	CAA-C2A-C1A	2.95	121.63	111.97
48	16	314	A86	C26-C25-C24	-2.95	114.02	123.22
37	a	407	CLA	CHD-C4C-NC	2.95	128.84	124.20
47	21	203	KC1	CHD-C4C-NC	2.94	128.67	124.20
47	13	302	KC1	C4C-C3C-C2C	-2.94	102.61	106.90
37	D	406	CLA	C4-C3-C5	2.94	120.22	115.27
37	32	208	CLA	CHD-C4C-NC	2.94	128.84	124.20
48	34	316	A86	C3-C2-C1	-2.94	123.11	127.31
37	12	205	CLA	CHD-C4C-NC	2.94	128.84	124.20
47	19	308	KC1	C4C-C3C-C2C	-2.94	102.61	106.90
37	18	209	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
37	18	203	CLA	CAC-C3C-C4C	2.94	128.63	124.81
37	D	406	CLA	CHD-C4C-NC	2.94	128.84	124.20
37	18	201	CLA	CHD-C4C-NC	2.94	128.84	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	a	404	CLA	C1-C2-C3	-2.94	120.95	126.04
37	12	207	CLA	CAA-C2A-C1A	-2.94	102.33	111.97
37	37	301	CLA	C4-C3-C5	2.94	120.22	115.27
37	A	405	CLA	CHD-C4C-NC	2.94	128.84	124.20
37	C	504	CLA	CHB-C4A-NA	2.94	128.58	124.51
37	36	309	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
37	35	301	CLA	CMC-C2C-C1C	2.94	129.52	125.04
47	33	306	KC1	CAA-CBA-CGA	-2.94	112.14	127.26
37	13	305	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
48	35	319	A86	C4-C3-C2	-2.94	117.45	123.47
37	12	209	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
39	5	101	BCR	C11-C10-C9	-2.94	123.11	127.31
47	38	210	KC1	O2D-CGD-O1D	-2.94	118.09	123.84
50	41	216	DD6	C21-C20-C15	-2.94	117.33	122.26
40	17	301	SQD	C44-O6-C1	2.94	119.48	113.74
37	38	204	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
37	C	510	CLA	CHD-C4C-NC	2.94	128.84	124.20
37	c	507	CLA	CHD-C4C-NC	2.94	128.84	124.20
37	33	305	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
37	D	401	CLA	C1-C2-C3	-2.94	120.96	126.04
48	12	215	A86	C36-C31-C32	-2.94	116.78	119.70
37	12	210	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
37	13	301	CLA	CHD-C4C-NC	2.94	128.83	124.20
48	13	312	A86	C4-C5-C6	-2.94	123.12	127.31
47	41	203	KC1	CAC-C3C-C4C	2.94	128.62	124.81
48	13	314	A86	C25-C24-C1	-2.94	118.17	126.42
37	38	209	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
37	18	201	CLA	C3B-C4B-NB	2.94	113.01	109.21
50	19	312	DD6	C14-C13-C11	-2.94	120.97	125.53
37	32	206	CLA	CHD-C4C-NC	2.94	128.83	124.20
47	15	309	KC1	C4C-C3C-C2C	-2.94	102.62	106.90
37	18	204	CLA	CMC-C2C-C1C	2.94	129.51	125.04
48	32	216	A86	C36-C31-C32	-2.94	116.78	119.70
37	39	302	CLA	CAC-C3C-C4C	2.94	128.62	124.81
37	32	211	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
48	34	314	A86	C10-C9-C8	-2.94	114.06	123.22
47	38	210	KC1	CHD-C4C-NC	2.94	128.66	124.20
48	15	319	A86	C4-C3-C2	-2.93	117.46	123.47
48	36	311	A86	C7-C6-C8	2.93	122.70	118.08
37	c	502	CLA	CAA-C2A-C3A	-2.93	104.74	112.78
37	37	306	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
37	D	405	CLA	C4C-C3C-C2C	-2.93	102.62	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	508	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
37	16	309	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
37	18	203	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
37	14	303	CLA	CMB-C2B-C3B	2.93	130.17	124.68
47	41	203	KC1	O2D-CGD-O1D	-2.93	118.10	123.84
47	37	302	KC1	CHD-C4C-NC	2.93	128.65	124.20
37	b	509	CLA	CHD-C4C-NC	2.93	128.82	124.20
37	32	213	CLA	C3B-C4B-NB	2.93	113.00	109.21
37	32	208	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
37	d	404	CLA	CAC-C3C-C4C	2.93	128.61	124.81
37	32	208	CLA	CAA-C2A-C1A	-2.93	102.37	111.97
37	33	301	CLA	CHD-C4C-NC	2.93	128.82	124.20
37	13	303	CLA	CMB-C2B-C3B	2.93	130.16	124.68
48	35	319	A86	C7-C6-C8	2.93	122.69	118.08
47	38	207	KC1	CMB-C2B-C1B	2.93	129.88	124.71
37	W	102	CLA	CMB-C2B-C3B	2.93	130.16	124.68
37	32	210	CLA	C3B-C4B-NB	2.93	113.00	109.21
40	36	315	SQD	C44-O6-C1	2.93	119.46	113.74
48	18	212	A86	C25-C24-C1	-2.93	118.19	126.42
37	B	510	CLA	C3B-C4B-NB	2.93	113.00	109.21
37	c	510	CLA	CHD-C4C-NC	2.93	128.82	124.20
47	21	207	KC1	C4C-C3C-C2C	-2.93	102.63	106.90
37	31	306	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
37	31	301	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
47	41	203	KC1	CHD-C4C-NC	2.93	128.65	124.20
48	33	314	A86	C25-C24-C1	-2.93	118.19	126.42
37	20	306	CLA	C3B-C4B-NB	2.93	112.99	109.21
48	35	312	A86	C20-C19-C18	-2.93	106.96	112.75
37	21	202	CLA	CHB-C4A-NA	2.93	128.56	124.51
37	38	209	CLA	C1-C2-C3	-2.93	120.98	126.04
47	13	304	KC1	C4C-C3C-C2C	-2.93	102.63	106.90
37	38	204	CLA	C4-C3-C5	2.92	120.19	115.27
37	11	307	CLA	C3B-C4B-NB	2.92	112.99	109.21
47	36	304	KC1	CAC-C3C-C4C	2.92	128.60	124.81
37	38	208	CLA	CHD-C4C-NC	2.92	128.81	124.20
47	37	307	KC1	C4C-C3C-C2C	-2.92	102.64	106.90
37	17	304	CLA	CAC-C3C-C4C	2.92	128.60	124.81
37	37	303	CLA	CAC-C3C-C4C	2.92	128.60	124.81
37	b	509	CLA	CBC-CAC-C3C	-2.92	104.37	112.43
40	B	519	SQD	O6-C1-C2	2.92	112.86	108.30
47	17	303	KC1	CHD-C4C-NC	2.92	128.64	124.20
37	D	406	CLA	CAC-C3C-C4C	2.92	128.60	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	L	101	SQD	O6-C1-C2	2.92	112.86	108.30
37	15	310	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
37	31	308	CLA	C3B-C4B-NB	2.92	112.99	109.21
37	18	202	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
37	a	403	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
37	B	509	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
37	14	302	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
37	b	501	CLA	O2A-CGA-CBA	2.92	121.07	111.91
47	31	309	KC1	CBC-CAC-C3C	-2.92	104.38	112.43
37	12	209	CLA	C3B-C4B-NB	2.92	112.98	109.21
48	32	217	A86	C36-C31-C32	-2.92	116.80	119.70
37	D	406	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
37	d	404	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
47	21	203	KC1	CAC-C3C-C4C	2.92	128.60	124.81
48	15	319	A86	C41-C32-C31	-2.92	107.86	110.47
48	19	311	A86	C41-C32-C31	-2.92	107.86	110.47
37	41	202	CLA	CHB-C4A-NA	2.92	128.55	124.51
37	38	203	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
37	38	209	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
37	17	307	CLA	CHC-C1C-C2C	-2.92	118.66	126.72
37	D	401	CLA	C4A-NA-C1A	-2.92	105.39	106.71
37	B	509	CLA	CHD-C4C-NC	2.92	128.80	124.20
48	18	212	A86	C7-C6-C8	2.92	122.67	118.08
37	35	301	CLA	C3B-C4B-NB	2.92	112.98	109.21
47	11	309	KC1	CBC-CAC-C3C	-2.91	104.39	112.43
37	c	501	CLA	O2A-CGA-CBA	2.91	121.06	111.91
47	39	308	KC1	C4C-C3C-C2C	-2.91	102.65	106.90
37	A	403	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
37	B	508	CLA	C3B-C4B-NB	2.91	112.98	109.21
37	17	302	CLA	C4-C3-C5	2.91	120.17	115.27
37	34	302	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
47	12	208	KC1	C4C-C3C-C2C	-2.91	102.65	106.90
47	32	209	KC1	C4C-C3C-C2C	-2.91	102.65	106.90
37	b	505	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
37	C	501	CLA	O2A-CGA-CBA	2.91	121.05	111.91
37	31	308	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
37	14	307	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
37	c	508	CLA	CAC-C3C-C4C	2.91	128.59	124.81
37	W	102	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
37	b	510	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
37	C	509	CLA	CAC-C3C-C4C	2.91	128.59	124.81
37	18	204	CLA	C4-C3-C5	2.91	120.17	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	510	CLA	C3B-C4B-NB	2.91	112.97	109.21
37	18	208	CLA	CHD-C4C-NC	2.91	128.79	124.20
37	34	303	CLA	CMB-C2B-C3B	2.91	130.12	124.68
37	36	301	CLA	C1-C2-C3	-2.91	121.01	126.04
48	15	315	A86	C4-C3-C2	-2.91	117.52	123.47
48	37	312	A86	C7-C6-C8	2.91	122.66	118.08
47	18	210	KC1	CHD-C4C-NC	2.91	128.61	124.20
37	d	403	CLA	CAC-C3C-C4C	2.91	128.58	124.81
37	33	301	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
48	14	316	A86	C12-C11-C13	2.91	120.90	116.02
47	35	309	KC1	C4C-C3C-C2C	-2.91	102.66	106.90
48	35	314	A86	C3-C4-C5	-2.91	117.52	123.47
37	c	504	CLA	CHB-C4A-NA	2.90	128.53	124.51
37	33	307	CLA	CMB-C2B-C3B	2.90	130.11	124.68
47	37	302	KC1	CAC-C3C-C4C	2.90	128.58	124.81
48	41	214	A86	C41-C32-C31	-2.90	107.87	110.47
37	34	307	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
37	12	207	CLA	CHD-C4C-NC	2.90	128.78	124.20
48	16	311	A86	C7-C6-C8	2.90	122.65	118.08
37	b	514	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
47	31	305	KC1	CHD-C4C-NC	2.90	128.61	124.20
37	12	205	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
37	c	512	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
37	18	209	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
48	32	221	A86	C8-C6-C5	-2.90	114.49	118.94
37	c	507	CLA	C4A-NA-C1A	-2.90	105.40	106.71
48	41	215	A86	C20-C19-C18	-2.90	107.01	112.75
48	12	216	A86	C36-C31-C32	-2.90	116.82	119.70
37	C	510	CLA	CMB-C2B-C3B	2.90	130.10	124.68
47	41	203	KC1	C4C-C3C-C2C	-2.90	102.67	106.90
37	20	306	CLA	CHD-C4C-NC	2.90	128.77	124.20
48	12	202	A86	C26-C25-C24	-2.90	114.17	123.22
47	36	308	KC1	CAA-CBA-CGA	-2.90	112.36	127.26
48	17	320	A86	C7-C6-C8	2.90	122.64	118.08
37	B	514	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
39	C	514	BCR	C2-C1-C6	2.90	114.94	110.48
37	13	310	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
37	40	208	CLA	CHD-C4C-NC	2.90	128.77	124.20
37	B	510	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
37	18	204	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
47	35	302	KC1	CHD-C4C-NC	2.90	128.60	124.20
37	34	310	CLA	CHD-C4C-NC	2.90	128.77	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	501	CLA	O2A-CGA-CBA	2.90	120.99	111.91
48	34	314	A86	C12-C11-C13	2.89	120.89	116.02
37	33	310	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
47	41	207	KC1	C4C-C3C-C2C	-2.89	102.68	106.90
37	13	301	CLA	CHC-C1C-C2C	-2.89	118.71	126.72
40	B	519	SQD	C44-O6-C1	2.89	119.39	113.74
47	34	306	KC1	CHD-C4C-NC	2.89	128.59	124.20
37	D	402	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
47	16	304	KC1	CAC-C3C-C4C	2.89	128.56	124.81
48	32	221	A86	C3-C4-C5	-2.89	117.55	123.47
37	C	504	CLA	C4A-NA-C1A	-2.89	105.41	106.71
37	B	505	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
37	32	206	CLA	CAA-C2A-C1A	2.89	121.45	111.97
48	34	316	A86	C12-C11-C13	2.89	120.88	116.02
47	21	203	KC1	C4C-C3C-C2C	-2.89	102.68	106.90
37	34	305	CLA	CHD-C4C-NC	2.89	128.76	124.20
48	35	314	A86	C7-C6-C8	2.89	122.63	118.08
47	14	306	KC1	CHD-C4C-NC	2.89	128.59	124.20
37	37	306	CLA	CAC-C3C-C4C	2.89	128.56	124.81
47	14	309	KC1	C4C-C3C-C2C	-2.89	102.69	106.90
48	35	315	A86	C4-C3-C2	-2.89	117.55	123.47
37	13	307	CLA	CMB-C2B-C3B	2.89	130.09	124.68
47	16	308	KC1	CAA-CBA-CGA	-2.89	112.41	127.26
47	33	306	KC1	CHB-C1B-NB	-2.89	121.80	124.45
37	36	307	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
39	A	406	BCR	C15-C16-C17	-2.89	117.56	123.47
37	c	510	CLA	CMB-C2B-C3B	2.89	130.08	124.68
48	15	312	A86	C20-C19-C18	-2.89	107.04	112.75
47	34	309	KC1	C4C-C3C-C2C	-2.89	102.69	106.90
48	32	203	A86	C26-C25-C24	-2.89	114.21	123.22
37	38	203	CLA	CBA-CAA-C2A	-2.89	105.34	113.86
37	33	303	CLA	C4-C3-C5	2.89	120.13	115.27
37	b	504	CLA	CMB-C2B-C1B	2.89	132.90	128.46
39	c	514	BCR	C2-C1-C6	2.89	114.92	110.48
48	14	314	A86	C12-C11-C13	2.89	120.87	116.02
37	b	508	CLA	C3B-C4B-NB	2.88	112.94	109.21
39	a	408	BCR	C15-C16-C17	-2.88	117.57	123.47
48	17	310	A86	C23-C16-C22	-2.88	103.12	107.37
47	11	309	KC1	CHD-C4C-NC	2.88	128.58	124.20
47	11	306	KC1	CAA-CBA-CGA	-2.88	112.44	127.26
37	A	405	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
37	17	307	CLA	CAC-C3C-C4C	2.88	128.55	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	523	CLA	C1-C2-C3	-2.88	121.06	126.04
48	38	212	A86	C25-C26-C27	-2.88	123.20	127.31
37	18	206	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
37	c	509	CLA	CAC-C3C-C4C	2.88	128.55	124.81
37	16	307	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
37	B	501	CLA	C4-C3-C5	2.88	120.12	115.27
37	D	406	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
47	17	308	KC1	C4C-C3C-C2C	-2.88	102.70	106.90
48	33	311	A86	C25-C24-C1	-2.88	118.32	126.42
47	38	207	KC1	CHB-C1B-NB	-2.88	121.81	124.45
37	41	204	CLA	CHD-C4C-NC	2.88	128.74	124.20
37	41	206	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
37	12	205	CLA	CAA-C2A-C1A	2.88	121.41	111.97
37	14	307	CLA	CAA-C2A-C1A	2.88	121.41	111.97
37	15	308	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
47	16	308	KC1	CHD-C4C-NC	2.88	128.57	124.20
37	14	307	CLA	C3B-C4B-NB	2.88	112.93	109.21
37	21	204	CLA	CHD-C4C-NC	2.88	128.74	124.20
37	34	307	CLA	C3B-C4B-NB	2.88	112.93	109.21
37	14	302	CLA	CHD-C4C-NC	2.88	128.74	124.20
47	33	306	KC1	CHD-C4C-NC	2.88	128.57	124.20
37	B	524	CLA	C1-C2-C3	-2.88	121.07	126.04
48	21	215	A86	C20-C19-C18	-2.88	107.06	112.75
50	40	212	DD6	C37-C36-C35	-2.88	109.02	114.36
37	a	407	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
37	21	206	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
47	11	304	KC1	CHD-C4C-NC	2.88	128.57	124.20
37	A	405	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
37	b	510	CLA	CHD-C4C-NC	2.88	128.74	124.20
37	B	524	CLA	CMC-C2C-C1C	2.88	129.42	125.04
37	40	205	CLA	CHC-C1C-C2C	-2.88	118.77	126.72
37	20	303	CLA	CHC-C1C-C2C	-2.87	118.77	126.72
40	L	101	SQD	C44-O6-C1	2.87	119.36	113.74
37	21	205	CLA	CAA-C2A-C3A	-2.87	104.91	112.78
37	19	302	CLA	CGD-CBD-CAD	-2.87	101.43	110.73
37	33	310	CLA	CAA-C2A-C3A	-2.87	104.91	112.78
37	D	405	CLA	CAC-C3C-C4C	2.87	128.54	124.81
48	17	313	A86	C25-C24-C1	-2.87	118.35	126.42
47	11	309	KC1	C4C-C3C-C2C	-2.87	102.71	106.90
37	34	307	CLA	CAA-C2A-C1A	2.87	121.38	111.97
37	C	508	CLA	CAC-C3C-C4C	2.87	128.53	124.81
37	C	512	CLA	O2D-CGD-O1D	-2.87	118.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	d	404	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
37	11	307	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
37	B	510	CLA	CHD-C4C-NC	2.87	128.73	124.20
37	33	303	CLA	CMB-C2B-C3B	2.87	130.05	124.68
50	20	310	DD6	C37-C36-C35	-2.87	109.04	114.36
48	12	214	A86	C20-C19-C18	-2.87	107.07	112.75
48	35	319	A86	C41-C32-C31	-2.87	107.91	110.47
47	38	205	KC1	CHD-C4C-NC	2.87	128.55	124.20
37	16	301	CLA	C1-C2-C3	-2.87	121.08	126.04
47	13	306	KC1	CAC-C3C-C4C	2.87	128.53	124.81
47	17	305	KC1	CAA-CBA-CGA	-2.87	112.53	127.26
47	37	304	KC1	CAA-CBA-CGA	-2.87	112.53	127.26
37	14	305	CLA	CHD-C4C-NC	2.87	128.72	124.20
37	b	510	CLA	CAC-C3C-C4C	2.87	128.53	124.81
47	14	306	KC1	C4C-C3C-C2C	-2.87	102.72	106.90
47	34	306	KC1	C4C-C3C-C2C	-2.87	102.72	106.90
48	21	214	A86	C41-C32-C31	-2.86	107.91	110.47
48	34	312	A86	C10-C9-C8	-2.86	114.28	123.22
47	17	303	KC1	CAC-C3C-C4C	2.86	128.53	124.81
47	17	308	KC1	CMA-C3A-C2A	-2.86	121.29	128.30
47	37	307	KC1	CMA-C3A-C2A	-2.86	121.29	128.30
48	13	311	A86	C25-C24-C1	-2.86	118.38	126.42
48	14	315	A86	C7-C6-C8	2.86	122.59	118.08
37	B	510	CLA	CAC-C3C-C4C	2.86	128.52	124.81
37	b	523	CLA	CMC-C2C-C1C	2.86	129.40	125.04
37	12	204	CLA	CMD-C2D-C1D	2.86	129.76	124.71
37	32	205	CLA	CMD-C2D-C1D	2.86	129.76	124.71
47	12	208	KC1	CAC-C3C-C4C	2.86	128.52	124.81
47	32	209	KC1	CAC-C3C-C4C	2.86	128.52	124.81
47	31	307	KC1	CAA-CBA-CGA	-2.86	112.56	127.26
48	37	312	A86	C25-C24-C1	-2.86	118.38	126.42
37	C	501	CLA	CHD-C4C-NC	2.86	128.71	124.20
37	12	209	CLA	CHD-C4C-NC	2.86	128.71	124.20
48	14	312	A86	C10-C9-C8	-2.86	114.29	123.22
37	12	207	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
47	33	306	KC1	CAC-C3C-C4C	2.86	128.52	124.81
48	17	314	A86	C3-C2-C1	-2.86	123.23	127.31
47	36	308	KC1	CHD-C4C-NC	2.86	128.54	124.20
37	12	205	CLA	C1-O2A-CGA	2.86	123.94	116.44
48	41	214	A86	C12-C11-C13	2.86	120.82	116.02
37	35	310	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
37	20	306	CLA	CHC-C1C-C2C	-2.86	118.82	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	40	208	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
37	B	524	CLA	CHD-C1D-ND	-2.86	121.83	124.45
50	40	212	DD6	C12-C11-C13	-2.86	113.58	118.08
37	41	205	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
48	12	202	A86	C7-C6-C5	-2.86	118.92	122.92
48	38	212	A86	C7-C6-C8	2.86	122.58	118.08
37	40	205	CLA	CMC-C2C-C1C	2.86	129.39	125.04
37	14	307	CLA	CHD-C4C-NC	2.86	128.70	124.20
37	C	510	CLA	CBC-CAC-C3C	-2.86	104.56	112.43
37	13	301	CLA	CHB-C4A-NA	2.86	128.46	124.51
48	36	310	A86	C10-C9-C8	-2.85	114.31	123.22
47	13	306	KC1	CHD-C4C-NC	2.85	128.53	124.20
37	14	305	CLA	CAC-C3C-C4C	2.85	128.51	124.81
37	32	210	CLA	CHD-C4C-NC	2.85	128.70	124.20
48	34	315	A86	C7-C6-C8	2.85	122.57	118.08
50	20	310	DD6	C12-C11-C13	-2.85	113.58	118.08
37	b	501	CLA	C4-C3-C5	2.85	120.07	115.27
37	35	307	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
37	17	304	CLA	CHD-C4C-NC	2.85	128.70	124.20
48	13	313	A86	C7-C6-C5	-2.85	118.93	122.92
48	32	215	A86	C20-C19-C18	-2.85	107.11	112.75
37	b	507	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
37	15	301	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
47	31	309	KC1	C4C-C3C-C2C	-2.85	102.74	106.90
44	H	102	DGD	O6D-C1D-O3G	-2.85	103.22	109.97
47	35	309	KC1	CHD-C4C-NC	2.85	128.53	124.20
37	18	202	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
37	B	513	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
44	h	102	DGD	O6D-C1D-O3G	-2.85	103.22	109.97
37	20	303	CLA	CMC-C2C-C1C	2.85	129.38	125.04
50	20	312	DD6	C19-C18-C17	2.85	116.28	110.77
47	13	306	KC1	CHB-C1B-NB	-2.85	121.84	124.45
37	34	305	CLA	CAC-C3C-C4C	2.85	128.51	124.81
37	b	512	CLA	CHD-C4C-NC	2.85	128.69	124.20
50	40	214	DD6	C19-C18-C17	2.85	116.27	110.77
37	12	205	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
37	C	513	CLA	CMC-C2C-C1C	2.85	129.38	125.04
37	b	523	CLA	CHD-C1D-ND	-2.85	121.84	124.45
37	b	502	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
37	b	516	CLA	CHD-C4C-NC	2.85	128.69	124.20
47	31	309	KC1	CHD-C4C-NC	2.85	128.52	124.20
37	32	208	CLA	CHC-C1C-C2C	-2.85	118.85	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	38	203	CLA	CHD-C4C-NC	2.85	128.69	124.20
48	34	311	A86	C10-C9-C8	-2.85	114.33	123.22
37	32	206	CLA	C1-O2A-CGA	2.85	123.91	116.44
37	38	203	CLA	CAC-C3C-C4C	2.85	128.50	124.81
37	d	401	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
37	34	303	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
37	41	209	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
37	19	303	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
37	39	303	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
48	40	201	A86	O4-C34-C35	2.85	114.68	107.59
48	40	201	A86	C25-C26-C27	2.85	131.37	127.31
37	C	512	CLA	O2A-CGA-CBA	2.85	120.84	111.91
37	w	101	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
37	a	407	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
37	38	206	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
37	38	209	CLA	CAC-C3C-C4C	2.84	128.50	124.81
37	18	203	CLA	CMB-C2B-C3B	2.84	130.00	124.68
48	16	310	A86	C10-C9-C8	-2.84	114.34	123.22
37	B	516	CLA	CHD-C4C-NC	2.84	128.68	124.20
37	37	303	CLA	C4-C3-C5	2.84	120.05	115.27
39	A	406	BCR	C11-C10-C9	-2.84	123.25	127.31
44	j	101	DGD	C3G-C2G-C1G	-2.84	105.06	111.79
37	13	301	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
37	38	206	CLA	CHD-C4C-NC	2.84	128.68	124.20
37	39	306	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
39	a	408	BCR	C11-C10-C9	-2.84	123.25	127.31
48	12	220	A86	C3-C4-C5	-2.84	117.65	123.47
37	B	512	CLA	CHD-C4C-NC	2.84	128.68	124.20
37	c	501	CLA	CHD-C4C-NC	2.84	128.68	124.20
37	11	301	CLA	C1-C2-C3	-2.84	121.13	126.04
37	c	510	CLA	CBC-CAC-C3C	-2.84	104.60	112.43
37	14	302	CLA	C3B-C4B-NB	2.84	112.88	109.21
37	35	307	CLA	CAC-C3C-C4C	2.84	128.49	124.81
37	14	303	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
37	19	309	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
48	32	203	A86	C7-C6-C5	-2.84	118.95	122.92
37	b	508	CLA	CHD-C4C-NC	2.84	128.68	124.20
37	12	209	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
37	39	302	CLA	CGD-CBD-CAD	-2.84	101.54	110.73
48	15	313	A86	C36-C31-C32	-2.84	116.88	119.70
37	B	515	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
37	14	310	CLA	CHD-C4C-NC	2.84	128.67	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	31	314	A86	C35-C34-C33	2.84	114.83	109.88
37	21	209	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
48	14	316	A86	C36-C31-C32	-2.84	116.88	119.70
37	20	306	CLA	CMB-C2B-C3B	2.83	129.98	124.68
37	18	202	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
37	b	509	CLA	CMC-C2C-C1C	2.83	129.36	125.04
48	21	214	A86	C12-C11-C13	2.83	120.78	116.02
37	41	210	CLA	CAA-C2A-C3A	-2.83	105.02	112.78
37	b	513	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
47	15	309	KC1	CHD-C4C-NC	2.83	128.50	124.20
48	14	311	A86	C10-C9-C8	-2.83	114.38	123.22
47	15	302	KC1	CHD-C4C-NC	2.83	128.50	124.20
47	16	305	KC1	CMB-C2B-C1B	2.83	129.71	124.71
37	35	301	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
37	A	405	CLA	CMC-C2C-C1C	2.83	129.35	125.04
37	18	203	CLA	CHD-C4C-NC	2.83	128.67	124.20
37	16	309	CLA	CMB-C2B-C3B	2.83	129.98	124.68
37	C	507	CLA	C4A-NA-C1A	-2.83	105.43	106.71
37	33	301	CLA	CHB-C4A-NA	2.83	128.43	124.51
37	Z	102	CLA	CED-O2D-CGD	2.83	122.34	115.94
48	38	212	A86	C25-C24-C1	-2.83	118.47	126.42
37	B	508	CLA	CMB-C2B-C3B	2.83	129.97	124.68
37	15	307	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
37	12	207	CLA	C1-C2-C3	-2.83	122.18	126.75
37	W	101	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
37	15	301	CLA	C3B-C4B-NB	2.83	112.87	109.21
48	33	313	A86	C7-C6-C5	-2.83	118.96	122.92
47	17	305	KC1	C4C-C3C-C2C	-2.83	102.78	106.90
37	z	102	CLA	CED-O2D-CGD	2.83	122.33	115.94
37	11	303	CLA	C1-O2A-CGA	2.83	123.86	116.44
37	31	304	CLA	C1-O2A-CGA	2.83	123.86	116.44
37	13	303	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
48	32	221	A86	C20-C19-C18	-2.83	107.16	112.75
37	b	515	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
37	36	301	CLA	C3B-C4B-NB	2.83	112.86	109.21
47	11	309	KC1	CMB-C2B-C1B	2.83	129.69	124.71
48	16	313	A86	O4-C34-C35	2.83	114.63	107.59
37	c	512	CLA	O2A-CGA-CBA	2.83	120.78	111.91
37	32	210	CLA	CHC-C1C-C2C	-2.83	118.91	126.72
37	B	507	CLA	CAA-C2A-C3A	-2.82	105.04	112.78
37	Z	101	CLA	O2A-CGA-CBA	2.82	120.77	111.91
37	41	208	CLA	CAA-C2A-C3A	-2.82	105.05	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	34	302	CLA	CHD-C4C-NC	2.82	128.65	124.20
37	32	208	CLA	C1-C2-C3	-2.82	122.18	126.75
37	21	210	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
47	38	207	KC1	CHD-C4C-NC	2.82	128.49	124.20
47	31	309	KC1	CMB-C2B-C1B	2.82	129.69	124.71
44	J	101	DGD	C3G-C2G-C1G	-2.82	105.11	111.79
37	34	302	CLA	C3B-C4B-NB	2.82	112.86	109.21
37	31	310	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
37	34	307	CLA	CHD-C4C-NC	2.82	128.65	124.20
37	37	303	CLA	CHD-C4C-NC	2.82	128.65	124.20
37	B	509	CLA	O2A-CGA-CBA	2.82	120.76	111.91
37	33	307	CLA	CHB-C4A-NA	2.82	128.41	124.51
37	b	514	CLA	CMC-C2C-C1C	2.82	129.34	125.04
43	41	201	LHG	O8-C23-C24	2.82	120.76	111.91
47	16	302	KC1	C1A-NA-C4A	-2.82	105.44	106.71
37	b	504	CLA	CMC-C2C-C1C	2.82	129.33	125.04
37	B	502	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
37	11	308	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
47	14	309	KC1	CBC-CAC-C3C	-2.82	104.66	112.43
37	B	509	CLA	CMC-C2C-C1C	2.82	129.33	125.04
37	40	208	CLA	CMC-C2C-C1C	2.82	129.33	125.04
39	c	515	BCR	C15-C16-C17	-2.82	117.70	123.47
37	38	211	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
37	a	404	CLA	C4A-NA-C1A	-2.82	105.44	106.71
37	40	209	CLA	CHD-C4C-NC	2.82	128.64	124.20
37	B	511	CLA	O2A-CGA-CBA	2.82	120.75	111.91
37	21	208	CLA	CAA-C2A-C3A	-2.82	105.06	112.78
47	11	306	KC1	C4C-C3C-C2C	-2.82	102.79	106.90
37	32	204	CLA	C4-C3-C5	2.82	120.01	115.27
37	15	305	CLA	CAC-C3C-C4C	2.82	128.47	124.81
48	39	313	A86	C7-C6-C5	-2.82	118.98	122.92
47	17	306	KC1	CAC-C3C-C4C	2.82	128.46	124.81
37	33	301	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
39	K	101	BCR	C24-C23-C22	-2.82	121.98	126.23
37	36	309	CLA	CMB-C2B-C3B	2.82	129.95	124.68
37	11	310	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
47	18	205	KC1	CHD-C4C-NC	2.82	128.47	124.20
37	D	405	CLA	CHD-C4C-NC	2.81	128.64	124.20
37	18	202	CLA	C3B-C4B-NB	2.81	112.85	109.21
48	16	313	A86	C25-C26-C27	2.81	131.33	127.31
50	20	312	DD6	C24-C1-C2	-2.81	114.62	118.94
47	11	302	KC1	CHB-C1B-NB	-2.81	121.87	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	32	202	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
37	d	403	CLA	CHD-C4C-NC	2.81	128.64	124.20
37	37	308	CLA	O2A-CGA-CBA	2.81	120.74	111.91
37	b	507	CLA	CHB-C4A-NA	2.81	128.40	124.51
37	b	508	CLA	CMB-C2B-C3B	2.81	129.94	124.68
37	20	306	CLA	CMC-C2C-C1C	2.81	129.32	125.04
37	32	202	CLA	CMC-C2C-C1C	2.81	129.32	125.04
48	17	310	A86	C4-C3-C2	-2.81	117.71	123.47
37	B	507	CLA	CHB-C4A-NA	2.81	128.40	124.51
48	15	314	A86	C4-C5-C6	-2.81	123.30	127.31
37	B	509	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
37	B	504	CLA	CMC-C2C-C1C	2.81	129.32	125.04
37	13	307	CLA	CHB-C4A-NA	2.81	128.40	124.51
37	38	211	CLA	CAC-C3C-C4C	2.81	128.46	124.81
37	B	508	CLA	CHD-C4C-NC	2.81	128.63	124.20
39	b	524	BCR	C15-C14-C13	-2.81	123.30	127.31
39	B	518	BCR	C15-C16-C17	-2.81	117.72	123.47
37	13	305	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
37	19	310	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
48	38	213	A86	C41-C32-C31	-2.81	107.96	110.47
48	12	220	A86	C20-C19-C18	-2.81	107.19	112.75
37	z	101	CLA	O2A-CGA-CBA	2.81	120.72	111.91
37	16	301	CLA	C3B-C4B-NB	2.81	112.84	109.21
37	16	306	CLA	C3B-C4B-NB	2.81	112.84	109.21
37	40	208	CLA	CMB-C2B-C3B	2.81	129.93	124.68
47	34	309	KC1	CBC-CAC-C3C	-2.81	104.69	112.43
37	B	512	CLA	CHD-C1D-ND	-2.81	121.87	124.45
48	15	314	A86	C7-C6-C8	2.81	122.50	118.08
45	D	404	PL9	C7-C8-C9	-2.81	122.12	126.79
37	C	511	CLA	C1-C2-C3	-2.81	121.19	126.04
50	40	214	DD6	C24-C1-C2	-2.81	114.64	118.94
37	31	302	CLA	C1-C2-C3	-2.81	121.19	126.04
47	37	305	KC1	CAC-C3C-C4C	2.81	128.45	124.81
37	21	209	CLA	CHD-C4C-NC	2.81	128.62	124.20
47	36	305	KC1	CMB-C2B-C1B	2.81	129.66	124.71
37	a	407	CLA	CMC-C2C-C1C	2.81	129.31	125.04
48	12	202	A86	C9-C8-C6	-2.81	118.54	126.42
37	b	509	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
37	32	204	CLA	CMB-C2B-C3B	2.80	129.93	124.68
37	b	511	CLA	O2A-CGA-CBA	2.80	120.71	111.91
47	36	302	KC1	C1A-NA-C4A	-2.80	105.44	106.71
48	37	313	A86	C41-C32-C31	-2.80	107.96	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	513	CLA	CMC-C2C-C1C	2.80	129.31	125.04
37	36	306	CLA	C3B-C4B-NB	2.80	112.83	109.21
48	37	309	A86	C4-C3-C2	-2.80	117.73	123.47
48	15	312	A86	C34-O4-C38	-2.80	112.67	117.90
39	C	515	BCR	C15-C16-C17	-2.80	117.73	123.47
37	39	310	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
37	21	210	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
37	c	502	CLA	CHD-C4C-NC	2.80	128.62	124.20
37	33	305	CLA	CAC-C3C-C4C	2.80	128.44	124.81
37	41	209	CLA	CHD-C4C-NC	2.80	128.62	124.20
39	b	518	BCR	C15-C16-C17	-2.80	117.74	123.47
47	31	307	KC1	C4C-C3C-C2C	-2.80	102.82	106.90
48	32	218	A86	C40-C32-C31	2.80	112.98	110.47
48	11	314	A86	C34-O4-C38	-2.80	112.68	117.90
47	15	306	KC1	CMB-C2B-C1B	2.80	129.65	124.71
48	18	215	A86	C12-C11-C13	2.80	120.72	116.02
37	b	514	CLA	O2A-C1-C2	-2.80	101.28	108.64
37	b	509	CLA	O2A-CGA-CBA	2.80	120.69	111.91
41	b	519	LMG	C1-C2-C3	-2.80	104.17	110.00
37	15	307	CLA	CAC-C3C-C4C	2.80	128.44	124.81
37	11	308	CLA	CMC-C2C-C1C	2.80	129.30	125.04
37	C	506	CLA	O2A-CGA-CBA	2.80	120.68	111.91
37	d	401	CLA	CHD-C4C-NC	2.80	128.61	124.20
37	41	210	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
47	13	306	KC1	C4C-C3C-C2C	-2.79	102.82	106.90
37	35	307	CLA	C3B-C4B-NB	2.79	112.82	109.21
48	32	217	A86	C25-C24-C1	-2.79	118.57	126.42
37	33	303	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
37	35	303	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
48	32	203	A86	C9-C8-C6	-2.79	118.57	126.42
37	36	307	CLA	CMB-C2B-C3B	2.79	129.90	124.68
48	33	311	A86	C3-C4-C5	-2.79	117.75	123.47
37	37	301	CLA	CHB-C4A-NA	2.79	128.37	124.51
48	37	319	A86	C7-C6-C8	2.79	122.47	118.08
37	B	514	CLA	O2A-C1-C2	-2.79	101.30	108.64
37	37	306	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
37	C	502	CLA	CHD-C4C-NC	2.79	128.60	124.20
47	32	212	KC1	O2D-CGD-O1D	-2.79	118.38	123.84
37	33	305	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
37	15	307	CLA	C3B-C4B-NB	2.79	112.82	109.21
37	39	301	CLA	CAC-C3C-C4C	2.79	128.43	124.81
40	a	409	SQD	O8-S-C6	2.79	110.19	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	35	309	KC1	C1A-NA-C4A	-2.79	105.45	106.71
37	14	305	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
37	20	303	CLA	OBD-CAD-C3D	-2.79	121.81	128.52
39	A	410	BCR	C15-C16-C17	-2.79	117.77	123.47
47	36	302	KC1	C4C-C3C-C2C	-2.79	102.84	106.90
48	13	311	A86	C3-C4-C5	-2.79	117.77	123.47
37	b	509	CLA	CAC-C3C-C4C	2.79	128.42	124.81
47	14	306	KC1	CAC-C3C-C4C	2.79	128.42	124.81
37	B	509	CLA	CAC-C3C-C4C	2.78	128.42	124.81
37	35	305	CLA	CHD-C4C-NC	2.78	128.59	124.20
37	B	514	CLA	CMC-C2C-C1C	2.78	129.28	125.04
37	c	511	CLA	CHD-C4C-NC	2.78	128.59	124.20
37	39	309	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
37	41	206	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
37	B	502	CLA	CMB-C2B-C3B	2.78	129.89	124.68
47	41	207	KC1	O2D-CGD-O1D	-2.78	118.40	123.84
37	A	403	CLA	CHD-C4C-NC	2.78	128.59	124.20
40	A	407	SQD	O8-S-C6	2.78	110.17	105.74
37	41	206	CLA	CMC-C2C-C1C	2.78	129.28	125.04
37	21	202	CLA	O2A-CGA-CBA	2.78	120.64	111.91
37	17	309	CLA	O2A-CGA-CBA	2.78	120.64	111.91
37	15	305	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
48	12	216	A86	C25-C24-C1	-2.78	118.60	126.42
41	B	520	LMG	C1-C2-C3	-2.78	104.20	110.00
37	12	203	CLA	C4-C3-C5	2.78	119.95	115.27
48	35	316	A86	C12-C11-C13	2.78	120.69	116.02
48	31	313	A86	C4-C3-C2	-2.78	117.78	123.47
47	18	205	KC1	C4C-C3C-C2C	-2.78	102.85	106.90
37	40	205	CLA	OBD-CAD-C3D	-2.78	121.83	128.52
37	C	508	CLA	CHD-C4C-NC	2.78	128.58	124.20
37	37	306	CLA	CHD-C4C-NC	2.78	128.58	124.20
37	13	305	CLA	CAC-C3C-C4C	2.78	128.42	124.81
37	41	202	CLA	O2A-CGA-CBA	2.78	120.63	111.91
37	16	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
37	17	307	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
37	12	203	CLA	CMB-C2B-C3B	2.78	129.88	124.68
37	19	301	CLA	CAC-C3C-C4C	2.78	128.41	124.81
39	B	525	BCR	C15-C14-C13	-2.78	123.35	127.31
48	32	214	A86	C34-O4-C38	-2.78	112.72	117.90
37	D	402	CLA	CHD-C4C-NC	2.78	128.58	124.20
37	B	510	CLA	CMB-C2B-C3B	2.78	129.87	124.68
41	a	410	LMG	C1-C2-C3	-2.78	104.21	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	18	206	CLA	CHD-C4C-NC	2.78	128.58	124.20
37	b	503	CLA	CAC-C3C-C4C	2.78	128.41	124.81
37	W	101	CLA	CAC-C3C-C4C	2.78	128.41	124.81
37	a	403	CLA	CHD-C4C-NC	2.77	128.58	124.20
48	12	213	A86	C34-O4-C38	-2.77	112.72	117.90
37	B	503	CLA	CAC-C3C-C4C	2.77	128.41	124.81
37	b	502	CLA	CMB-C2B-C3B	2.77	129.87	124.68
47	21	207	KC1	O2D-CGD-O1D	-2.77	118.41	123.84
37	14	308	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
37	w	101	CLA	CAC-C3C-C4C	2.77	128.41	124.81
37	13	301	CLA	CAC-C3C-C4C	2.77	128.41	124.81
37	36	306	CLA	CHD-C4C-NC	2.77	128.57	124.20
47	15	304	KC1	CHD-C4C-NC	2.77	128.41	124.20
37	19	301	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
48	36	313	A86	C41-C32-C31	-2.77	107.99	110.47
48	34	316	A86	C36-C31-C32	-2.77	116.94	119.70
37	c	506	CLA	O2A-CGA-CBA	2.77	120.61	111.91
47	11	304	KC1	CAA-CBA-CGA	-2.77	113.01	127.26
37	c	513	CLA	CAC-C3C-C4C	2.77	128.41	124.81
37	b	511	CLA	CHD-C4C-NC	2.77	128.57	124.20
48	35	311	A86	C12-C11-C13	2.77	120.68	116.02
37	18	211	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
47	11	309	KC1	CAA-CBA-CGA	-2.77	113.02	127.26
37	b	507	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
37	B	503	CLA	CHD-C4C-NC	2.77	128.57	124.20
45	d	402	PL9	C7-C8-C9	-2.77	122.18	126.79
37	17	307	CLA	CHD-C4C-NC	2.77	128.57	124.20
39	y	101	BCR	C24-C23-C22	-2.77	122.05	126.23
37	34	308	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
47	31	309	KC1	CAA-CBA-CGA	-2.77	113.03	127.26
47	36	304	KC1	C4C-C3C-C2C	-2.77	102.86	106.90
47	12	211	KC1	O2D-CGD-O1D	-2.77	118.43	123.84
37	Z	102	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
47	33	306	KC1	C4C-C3C-C2C	-2.77	102.86	106.90
48	15	315	A86	C20-C19-C18	-2.77	107.28	112.75
37	B	511	CLA	CHD-C4C-NC	2.77	128.56	124.20
37	39	302	CLA	CHD-C4C-NC	2.77	128.56	124.20
47	31	303	KC1	CHB-C1B-NB	-2.77	121.91	124.45
37	31	310	CLA	CHD-C4C-NC	2.77	128.56	124.20
48	15	312	A86	C7-C6-C8	2.77	122.44	118.08
37	34	305	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
48	15	316	A86	C12-C11-C13	2.77	120.67	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	302	CLA	CHB-C4A-NA	2.77	128.34	124.51
37	b	506	CLA	CMC-C2C-C1C	2.77	129.25	125.04
37	C	513	CLA	CHB-C4A-NA	2.76	128.34	124.51
47	40	204	KC1	CAC-C3C-C4C	2.76	128.40	124.81
37	z	102	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
48	31	311	A86	C10-C9-C8	-2.76	114.59	123.22
48	37	314	A86	C7-C6-C5	-2.76	119.05	122.92
48	35	315	A86	C20-C19-C18	-2.76	107.28	112.75
48	11	319	A86	C8-C6-C5	-2.76	114.70	118.94
47	14	309	KC1	C2A-C1A-NA	2.76	113.83	109.40
47	34	309	KC1	C2A-C1A-NA	2.76	113.83	109.40
37	20	307	CLA	CHD-C4C-NC	2.76	128.56	124.20
47	11	309	KC1	O2D-CGD-O1D	-2.76	118.44	123.84
48	17	315	A86	C7-C6-C5	-2.76	119.05	122.92
44	J	101	DGD	CDB-CCB-CBB	-2.76	100.40	114.42
37	40	203	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
47	16	304	KC1	C4C-C3C-C2C	-2.76	102.87	106.90
37	C	505	CLA	CAC-C3C-C4C	2.76	128.39	124.81
37	17	304	CLA	O1D-CGD-CBD	-2.76	118.83	124.48
44	j	101	DGD	CDB-CCB-CBB	-2.76	100.41	114.42
48	15	315	A86	C36-C31-C32	-2.76	116.96	119.70
39	a	413	BCR	C15-C16-C17	-2.76	117.82	123.47
48	34	314	A86	C40-C32-C31	-2.76	108.00	110.47
37	C	511	CLA	CHD-C4C-NC	2.76	128.55	124.20
48	14	316	A86	C8-C6-C5	2.76	123.18	118.94
47	16	302	KC1	C4C-C3C-C2C	-2.76	102.87	106.90
37	b	510	CLA	CMB-C2B-C3B	2.76	129.84	124.68
37	20	301	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
37	20	306	CLA	O2A-CGA-CBA	2.76	120.57	111.91
37	b	505	CLA	CHB-C4A-NA	2.76	128.33	124.51
47	32	207	KC1	CAA-CBA-CGA	-2.76	113.08	127.26
37	B	505	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
37	39	301	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
47	34	306	KC1	CAC-C3C-C4C	2.76	128.39	124.81
37	18	202	CLA	C1-C2-C3	-2.76	121.27	126.04
37	11	307	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
37	c	508	CLA	CHD-C4C-NC	2.76	128.55	124.20
47	31	305	KC1	CAA-CBA-CGA	-2.76	113.09	127.26
39	D	407	BCR	C24-C23-C22	-2.76	122.07	126.23
47	20	305	KC1	CAC-C3C-C4C	2.76	128.39	124.81
47	36	308	KC1	CMB-C2B-C1B	2.76	129.57	124.71
37	14	301	CLA	C3B-C4B-NB	2.76	112.78	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	17	301	SQD	O8-S-C6	2.76	110.13	105.74
47	14	309	KC1	C1A-NA-C4A	-2.76	105.47	106.71
47	34	309	KC1	C1A-NA-C4A	-2.76	105.47	106.71
47	20	302	KC1	CMB-C2B-C1B	2.76	129.57	124.71
37	b	503	CLA	CHD-C4C-NC	2.76	128.55	124.20
37	18	209	CLA	CAC-C3C-C4C	2.76	128.38	124.81
37	33	301	CLA	C4-C3-C5	2.76	119.91	115.27
37	35	303	CLA	C1-C2-C3	-2.76	121.28	126.04
37	b	512	CLA	CHD-C1D-ND	-2.75	121.92	124.45
41	A	408	LMG	C1-C2-C3	-2.75	104.26	110.00
37	38	202	CLA	CMB-C2B-C3B	2.75	129.83	124.68
47	19	308	KC1	CAA-C2A-C1A	-2.75	112.09	124.75
37	11	303	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
37	21	206	CLA	CMC-C2C-C1C	2.75	129.23	125.04
37	B	516	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
37	35	305	CLA	CAC-C3C-C4C	2.75	128.38	124.81
37	19	306	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
47	39	308	KC1	CAA-C2A-C1A	-2.75	112.09	124.75
37	16	307	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
37	21	208	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
37	B	506	CLA	CMC-C2C-C1C	2.75	129.23	125.04
48	34	312	A86	C7-C6-C8	2.75	122.41	118.08
47	12	206	KC1	CAA-CBA-CGA	-2.75	113.11	127.26
48	11	311	A86	C10-C9-C8	-2.75	114.63	123.22
37	37	306	CLA	CHB-C4A-NA	2.75	128.32	124.51
48	33	314	A86	C40-C32-C31	-2.75	108.01	110.47
37	19	302	CLA	CHD-C4C-NC	2.75	128.54	124.20
47	16	308	KC1	CMB-C2B-C1B	2.75	129.56	124.71
37	b	516	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
37	b	505	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
37	C	504	CLA	CHD-C4C-NC	2.75	128.54	124.20
37	39	305	CLA	CHD-C4C-NC	2.75	128.54	124.20
48	11	314	A86	C36-C31-C32	-2.75	116.97	119.70
37	21	206	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
47	15	306	KC1	CAC-C3C-C4C	2.75	128.38	124.81
37	36	307	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
37	40	208	CLA	O2A-CGA-CBA	2.75	120.53	111.91
39	d	405	BCR	C24-C23-C22	-2.75	122.08	126.23
50	40	214	DD6	C32-C31-C36	-2.75	118.75	122.63
48	20	311	A86	C41-C32-C31	-2.75	108.01	110.47
37	13	301	CLA	C4-C3-C5	2.75	119.89	115.27
37	c	513	CLA	CHB-C4A-NA	2.75	128.31	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	14	313	A86	C25-C24-C1	-2.75	118.70	126.42
37	37	303	CLA	O1D-CGD-CBD	-2.75	118.86	124.48
37	b	504	CLA	C4-C3-C5	2.75	119.89	115.27
37	17	307	CLA	C4-C3-C5	2.75	119.89	115.27
48	12	217	A86	C40-C32-C31	2.75	112.93	110.47
37	C	513	CLA	CAC-C3C-C4C	2.75	128.37	124.81
37	W	102	CLA	CHD-C4C-NC	2.75	128.53	124.20
40	A	407	SQD	C1-C2-C3	-2.75	104.28	110.00
48	31	319	A86	C8-C6-C5	-2.74	114.73	118.94
37	31	304	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
37	33	301	CLA	CAC-C3C-C4C	2.74	128.37	124.81
37	11	305	CLA	CHD-C4C-NC	2.74	128.53	124.20
41	D	412	LMG	C6-C5-C4	-2.74	106.58	113.00
48	13	314	A86	C40-C32-C31	-2.74	108.02	110.47
37	38	201	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
37	b	515	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
37	31	301	CLA	CAC-C3C-C4C	2.74	128.37	124.81
47	20	302	KC1	CAC-C3C-C4C	2.74	128.37	124.81
41	d	409	LMG	O6-C1-O1	-2.74	103.48	109.97
37	c	511	CLA	C1-C2-C3	-2.74	121.31	126.04
47	13	302	KC1	CHD-C4C-NC	2.74	128.36	124.20
40	36	315	SQD	O8-S-C6	2.74	110.11	105.74
48	17	311	A86	C25-C24-C1	-2.74	118.72	126.42
47	13	309	KC1	CHD-C4C-NC	2.74	128.36	124.20
48	14	314	A86	C40-C32-C31	-2.74	108.02	110.47
37	W	102	CLA	CAC-C3C-C4C	2.74	128.36	124.81
37	c	505	CLA	CAC-C3C-C4C	2.74	128.36	124.81
37	31	308	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
37	39	301	CLA	CHB-C4A-NA	2.74	128.30	124.51
48	18	212	A86	C10-C9-C8	-2.74	114.67	123.22
37	Z	102	CLA	CMB-C2B-C3B	2.74	129.80	124.68
37	15	303	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
37	B	504	CLA	C4-C3-C5	2.74	119.88	115.27
37	A	405	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
41	31	316	LMG	C1-O6-C5	-2.74	108.32	113.69
37	19	305	CLA	CAC-C3C-C4C	2.74	128.36	124.81
48	35	312	A86	C7-C6-C8	2.74	122.39	118.08
37	B	507	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
37	19	310	CLA	CHD-C4C-NC	2.74	128.51	124.20
48	14	312	A86	C7-C6-C8	2.74	122.39	118.08
48	13	314	A86	C22-C16-C17	-2.74	104.23	108.98
37	B	506	CLA	O2A-CGA-O1A	-2.74	116.69	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	515	CLA	O2A-CGA-O1A	-2.74	116.69	123.59
48	16	314	A86	C41-C32-C31	-2.74	108.02	110.47
41	11	317	LMG	O6-C1-O1	-2.73	103.50	109.97
48	32	218	A86	C36-C31-C32	-2.73	116.98	119.70
37	34	302	CLA	CAC-C3C-C4C	2.73	128.36	124.81
37	15	305	CLA	CHD-C4C-NC	2.73	128.51	124.20
37	33	301	CLA	CMC-C2C-C1C	2.73	129.20	125.04
37	38	202	CLA	C3B-C4B-NB	2.73	112.74	109.21
48	40	213	A86	C41-C32-C31	-2.73	108.03	110.47
37	B	504	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
37	13	310	CLA	CMB-C2B-C3B	2.73	129.79	124.68
37	D	405	CLA	C4-C3-C5	2.73	119.87	115.27
48	12	213	A86	C23-C16-C22	-2.73	103.34	107.37
40	a	409	SQD	C1-C2-C3	-2.73	104.31	110.00
37	19	305	CLA	CHD-C4C-NC	2.73	128.51	124.20
37	16	306	CLA	CHD-C4C-NC	2.73	128.51	124.20
37	34	301	CLA	C3B-C4B-NB	2.73	112.74	109.21
37	40	203	CLA	CMC-C2C-C1C	2.73	129.20	125.04
47	37	304	KC1	CMD-C2D-C3D	-2.73	119.57	124.68
48	11	312	A86	C12-C11-C13	2.73	120.61	116.02
37	B	506	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
50	16	312	DD6	C33-C34-C35	2.73	114.04	110.30
48	35	313	A86	C20-C19-C18	-2.73	107.35	112.75
47	32	212	KC1	CBC-CAC-C3C	-2.73	104.91	112.43
37	39	310	CLA	CHD-C4C-NC	2.73	128.50	124.20
47	35	302	KC1	CBC-CAC-C3C	-2.73	104.91	112.43
47	35	304	KC1	CHD-C4C-NC	2.73	128.34	124.20
47	21	207	KC1	CBA-CAA-C2A	-2.73	114.87	125.27
37	39	305	CLA	CAC-C3C-C4C	2.73	128.35	124.81
37	b	501	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
37	17	304	CLA	CBC-CAC-C3C	-2.73	104.91	112.43
37	12	204	CLA	C3B-C4B-NB	2.73	112.73	109.21
48	15	311	A86	C12-C11-C13	2.73	120.60	116.02
37	z	102	CLA	CMB-C2B-C3B	2.73	129.78	124.68
47	33	309	KC1	CHD-C4C-NC	2.73	128.34	124.20
37	c	504	CLA	CHD-C4C-NC	2.73	128.50	124.20
37	11	310	CLA	CHD-C4C-NC	2.73	128.50	124.20
37	31	306	CLA	CHD-C4C-NC	2.73	128.50	124.20
37	w	101	CLA	CGD-CBD-CAD	2.73	119.56	110.73
37	15	303	CLA	C1-C2-C3	-2.73	121.33	126.04
37	19	301	CLA	CHB-C4A-NA	2.72	128.28	124.51
37	37	303	CLA	CBC-CAC-C3C	-2.72	104.92	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	12	217	A86	C36-C31-C32	-2.72	116.99	119.70
50	20	312	DD6	C32-C31-C36	-2.72	118.79	122.63
48	32	214	A86	C3-C4-C5	-2.72	117.89	123.47
47	12	211	KC1	CBC-CAC-C3C	-2.72	104.92	112.43
37	B	524	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
37	B	501	CLA	CHB-C4A-NA	2.72	128.28	124.51
37	37	308	CLA	CMB-C2B-C3B	2.72	129.77	124.68
41	d	409	LMG	C6-C5-C4	-2.72	106.63	113.00
47	18	210	KC1	C1A-NA-C4A	-2.72	105.48	106.71
37	B	507	CLA	CHD-C4C-NC	2.72	128.49	124.20
37	21	208	CLA	CHD-C4C-NC	2.72	128.49	124.20
37	19	310	CLA	C1-C2-C3	-2.72	121.34	126.04
37	38	201	CLA	CHD-C4C-NC	2.72	128.49	124.20
37	b	523	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
37	W	101	CLA	CGD-CBD-CAD	2.72	119.55	110.73
48	18	213	A86	C41-C32-C31	-2.72	108.04	110.47
47	31	309	KC1	O2D-CGD-O1D	-2.72	118.52	123.84
47	36	302	KC1	CHD-C4C-NC	2.72	128.33	124.20
47	38	205	KC1	C4C-C3C-C2C	-2.72	102.93	106.90
37	39	302	CLA	C4-C3-C5	2.72	119.85	115.27
48	37	309	A86	C25-C24-C1	-2.72	118.78	126.42
41	11	316	LMG	C1-O6-C5	-2.72	108.35	113.69
41	D	412	LMG	O6-C1-O1	-2.72	103.53	109.97
37	12	209	CLA	CMC-C2C-C1C	2.72	129.18	125.04
48	17	313	A86	C7-C6-C8	2.72	122.36	118.08
48	12	214	A86	C10-C9-C8	-2.72	114.73	123.22
37	b	506	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
48	15	313	A86	C20-C19-C18	-2.72	107.37	112.75
48	32	215	A86	C10-C9-C8	-2.72	114.73	123.22
48	35	312	A86	C34-O4-C38	-2.72	112.83	117.90
47	14	309	KC1	CMC-C2C-C1C	2.72	129.18	125.04
37	C	509	CLA	C4-C3-C5	2.72	119.84	115.27
47	41	207	KC1	CBA-CAA-C2A	-2.72	114.91	125.27
37	32	204	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
48	34	316	A86	C8-C6-C5	2.72	123.11	118.94
37	13	307	CLA	CGD-CBD-CAD	-2.72	101.93	110.73
48	15	314	A86	C34-O4-C38	-2.72	112.83	117.90
47	40	204	KC1	CMB-C2B-C1B	2.72	129.50	124.71
48	34	313	A86	C25-C24-C1	-2.72	118.78	126.42
37	37	306	CLA	C1-C2-C3	-2.72	121.34	126.04
37	a	404	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
37	31	301	CLA	CHD-C4C-NC	2.72	128.48	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	31	312	A86	C12-C11-C13	2.72	120.58	116.02
37	17	309	CLA	CMB-C2B-C3B	2.72	129.76	124.68
37	13	301	CLA	CMC-C2C-C1C	2.72	129.18	125.04
47	34	309	KC1	CMC-C2C-C1C	2.72	129.17	125.04
37	41	208	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
37	19	309	CLA	CHD-C4C-NC	2.71	128.48	124.20
37	38	209	CLA	CHD-C4C-NC	2.71	128.48	124.20
37	19	310	CLA	CAC-C3C-C4C	2.71	128.33	124.81
37	35	305	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
48	11	319	A86	O4-C38-O5	-2.71	117.57	122.96
37	b	506	CLA	CHC-C1C-C2C	-2.71	119.21	126.72
37	16	303	CLA	CHD-C4C-NC	2.71	128.48	124.20
47	31	303	KC1	CAC-C3C-C4C	2.71	128.33	124.81
37	20	301	CLA	CMC-C2C-C1C	2.71	129.17	125.04
37	b	504	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
37	c	510	CLA	O2A-CGA-CBA	2.71	120.42	111.91
37	11	310	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
37	31	310	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
48	15	312	A86	C12-C11-C13	2.71	120.58	116.02
37	C	513	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
37	17	304	CLA	C4-C3-C5	2.71	119.83	115.27
37	35	303	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
47	37	307	KC1	O2D-CGD-O1D	-2.71	118.54	123.84
48	37	309	A86	C9-C10-C11	-2.71	118.64	126.61
48	18	213	A86	C12-C11-C13	2.71	120.57	116.02
47	11	302	KC1	CAC-C3C-C4C	2.71	128.32	124.81
37	C	503	CLA	CHB-C4A-NA	2.71	128.26	124.51
37	12	203	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
37	20	301	CLA	C3B-C4B-NB	2.71	112.71	109.21
47	12	208	KC1	CHB-C1B-NB	-2.71	121.97	124.45
47	32	209	KC1	CHB-C1B-NB	-2.71	121.97	124.45
37	37	308	CLA	CAA-CBA-CGA	-2.71	105.34	113.25
37	B	505	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
37	B	506	CLA	CMB-C2B-C3B	2.71	129.74	124.68
47	15	302	KC1	CBC-CAC-C3C	-2.71	104.97	112.43
37	21	208	CLA	C4-C3-C5	2.71	119.82	115.27
37	32	210	CLA	CHB-C4A-NA	2.71	128.25	124.51
37	b	523	CLA	CHD-C4C-NC	2.71	128.47	124.20
37	11	308	CLA	CBC-CAC-C3C	-2.71	104.97	112.43
48	21	215	A86	C12-C11-C13	2.71	120.57	116.02
37	d	403	CLA	C4-C3-C5	2.71	119.82	115.27
37	17	307	CLA	CHB-C4A-NA	2.71	128.25	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	35	306	KC1	CAC-C3C-C4C	2.71	128.32	124.81
47	33	302	KC1	CHD-C4C-NC	2.71	128.31	124.20
47	33	309	KC1	CMB-C2B-C1B	2.70	129.48	124.71
37	33	307	CLA	CGD-CBD-CAD	-2.70	101.97	110.73
37	b	501	CLA	CHB-C4A-NA	2.70	128.25	124.51
37	w	101	CLA	CHD-C4C-NC	2.70	128.47	124.20
47	40	207	KC1	CAC-C3C-C4C	2.70	128.32	124.81
37	c	509	CLA	C4-C3-C5	2.70	119.82	115.27
37	14	302	CLA	CAC-C3C-C4C	2.70	128.32	124.81
37	C	510	CLA	O2A-CGA-CBA	2.70	120.39	111.91
37	a	407	CLA	CHB-C4A-NA	2.70	128.25	124.51
37	C	502	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
37	b	507	CLA	CHD-C4C-NC	2.70	128.46	124.20
37	b	506	CLA	CMB-C2B-C3B	2.70	129.73	124.68
37	39	310	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
50	36	312	DD6	C33-C34-C35	2.70	114.00	110.30
37	39	309	CLA	CHD-C4C-NC	2.70	128.46	124.20
50	21	216	DD6	C37-C36-C35	-2.70	109.35	114.36
47	11	309	KC1	CHB-C4A-NA	2.70	128.46	124.20
47	17	308	KC1	O2D-CGD-O1D	-2.70	118.56	123.84
37	16	306	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
37	B	524	CLA	CHD-C4C-NC	2.70	128.46	124.20
37	39	305	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
37	38	209	CLA	C4-C3-C5	2.70	119.81	115.27
37	32	205	CLA	C3B-C4B-NB	2.70	112.70	109.21
39	B	517	BCR	C15-C16-C17	-2.70	117.95	123.47
37	b	501	CLA	CHD-C4C-NC	2.70	128.46	124.20
37	C	503	CLA	C4-C3-C5	2.70	119.81	115.27
37	41	208	CLA	C4-C3-C5	2.70	119.81	115.27
48	31	319	A86	O4-C38-O5	-2.70	117.60	122.96
37	34	303	CLA	CHD-C4C-NC	2.70	128.45	124.20
37	21	208	CLA	O2A-CGA-CBA	2.70	120.37	111.91
39	b	524	BCR	C15-C16-C17	-2.70	117.95	123.47
37	C	502	CLA	CHB-C4A-NA	2.70	128.24	124.51
37	19	310	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
50	41	216	DD6	C37-C36-C35	-2.70	109.36	114.36
39	b	517	BCR	C15-C16-C17	-2.70	117.95	123.47
47	15	302	KC1	C4C-C3C-C2C	-2.70	102.97	106.90
47	15	306	KC1	C4C-C3C-C2C	-2.69	102.97	106.90
47	35	302	KC1	C4C-C3C-C2C	-2.69	102.97	106.90
39	B	525	BCR	C15-C16-C17	-2.69	117.96	123.47
37	B	524	CLA	CAC-C3C-C4C	2.69	128.31	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	15	309	KC1	C1A-NA-C4A	-2.69	105.50	106.71
37	b	516	CLA	O1D-CGD-CBD	-2.69	118.97	124.48
48	34	314	A86	C25-C24-C1	-2.69	118.85	126.42
37	C	509	CLA	CHD-C4C-NC	2.69	128.45	124.20
47	16	302	KC1	CHD-C4C-NC	2.69	128.29	124.20
37	36	303	CLA	CHD-C4C-NC	2.69	128.45	124.20
41	31	317	LMG	O6-C1-O1	-2.69	103.60	109.97
47	37	305	KC1	CHB-C1B-NB	-2.69	121.98	124.45
37	18	208	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
37	B	505	CLA	CHB-C4A-NA	2.69	128.23	124.51
37	39	306	CLA	O2A-CGA-CBA	2.69	120.35	111.91
47	20	305	KC1	O1D-CGD-CBD	-2.69	118.98	124.48
37	c	511	CLA	O2A-CGA-CBA	2.69	120.35	111.91
37	36	306	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
48	39	311	A86	C7-C6-C8	2.69	122.31	118.08
37	B	501	CLA	CHD-C4C-NC	2.69	128.44	124.20
37	13	303	CLA	CHD-C4C-NC	2.69	128.44	124.20
37	36	303	CLA	C1-C2-C3	-2.69	121.39	126.04
48	35	314	A86	C34-O4-C38	-2.69	112.89	117.90
37	b	512	CLA	C4-C3-C5	2.69	119.79	115.27
48	37	310	A86	C25-C24-C1	-2.69	118.86	126.42
48	35	319	A86	C-C1-C24	2.69	122.31	118.08
37	a	407	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
47	13	309	KC1	CMB-C2B-C1B	2.69	129.45	124.71
47	14	309	KC1	CAA-CBA-CGA	-2.69	113.45	127.26
37	B	501	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
48	15	319	A86	C-C1-C24	2.69	122.31	118.08
37	c	505	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
47	18	207	KC1	CHD-C4C-NC	2.69	128.28	124.20
48	35	312	A86	C12-C11-C13	2.69	120.53	116.02
37	c	513	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
37	b	513	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
37	b	501	CLA	CMC-C2C-C1C	2.69	129.13	125.04
37	17	302	CLA	CMB-C2B-C3B	2.69	129.70	124.68
37	c	503	CLA	CHB-C4A-NA	2.69	128.22	124.51
37	12	212	CLA	CHB-C4A-NA	2.69	128.22	124.51
37	32	210	CLA	CMC-C2C-C1C	2.68	129.13	125.04
47	31	309	KC1	CHB-C4A-NA	2.68	128.43	124.20
39	B	517	BCR	C7-C8-C9	-2.68	122.18	126.23
37	17	302	CLA	CHB-C4A-NA	2.68	128.22	124.51
47	17	306	KC1	CHC-C4B-C3B	-2.68	120.67	125.26
47	31	305	KC1	C4C-C3C-C2C	-2.68	102.99	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	11	309	KC1	C1A-NA-C4A	-2.68	105.50	106.71
37	32	202	CLA	CBC-CAC-C3C	-2.68	105.04	112.43
50	41	212	DD6	C19-C18-C17	2.68	115.95	110.77
37	18	209	CLA	CHD-C4C-NC	2.68	128.43	124.20
37	35	308	CLA	CBC-CAC-C3C	-2.68	105.04	112.43
47	11	304	KC1	C4C-C3C-C2C	-2.68	102.99	106.90
47	35	306	KC1	C4C-C3C-C2C	-2.68	102.99	106.90
37	C	512	CLA	CHD-C4C-NC	2.68	128.43	124.20
48	14	311	A86	C34-O4-C38	-2.68	112.90	117.90
37	B	513	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
37	34	302	CLA	CHB-C4A-NA	2.68	128.22	124.51
37	11	301	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
47	13	309	KC1	O2D-CGD-O1D	-2.68	118.60	123.84
37	b	523	CLA	CAC-C3C-C4C	2.68	128.29	124.81
37	C	511	CLA	O2A-CGA-CBA	2.68	120.32	111.91
48	19	311	A86	C7-C6-C8	2.68	122.30	118.08
40	40	202	SQD	O48-C23-C24	2.68	120.32	111.91
40	a	409	SQD	O48-C23-C24	2.68	120.32	111.91
47	34	309	KC1	CAA-CBA-CGA	-2.68	113.49	127.26
40	16	315	SQD	O8-S-C6	2.68	110.01	105.74
37	D	401	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
37	12	209	CLA	CHB-C4A-NA	2.68	128.22	124.51
37	c	509	CLA	CHD-C4C-NC	2.68	128.42	124.20
37	b	505	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
37	37	303	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
48	34	311	A86	C34-O4-C38	-2.68	112.91	117.90
39	b	517	BCR	C7-C8-C9	-2.68	122.19	126.23
37	12	203	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
37	B	512	CLA	C4-C3-C5	2.68	119.77	115.27
48	14	314	A86	C25-C24-C1	-2.68	118.90	126.42
37	41	208	CLA	CHD-C4C-NC	2.68	128.42	124.20
37	41	208	CLA	O2A-CGA-CBA	2.68	120.31	111.91
37	38	209	CLA	O2A-CGA-CBA	2.68	120.31	111.91
37	39	310	CLA	CAC-C3C-C4C	2.68	128.28	124.81
37	19	306	CLA	O2A-CGA-CBA	2.68	120.31	111.91
48	41	215	A86	C12-C11-C13	2.68	120.52	116.02
37	c	502	CLA	CHB-C4A-NA	2.68	128.21	124.51
37	38	201	CLA	C3B-C4B-NB	2.68	112.67	109.21
47	38	210	KC1	CAA-CBA-CGA	-2.68	113.51	127.26
37	33	310	CLA	CMB-C2B-C3B	2.67	129.68	124.68
47	18	210	KC1	CAA-CBA-CGA	-2.67	113.52	127.26
46	V	201	HEM	CMB-C2B-C1B	-2.67	120.97	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	40	203	CLA	C3B-C4B-NB	2.67	112.67	109.21
48	32	214	A86	C23-C16-C22	-2.67	103.43	107.37
43	D	409	LHG	C11-C10-C9	-2.67	100.86	114.42
37	16	303	CLA	C1-C2-C3	-2.67	121.42	126.04
37	C	504	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
48	17	310	A86	C9-C10-C11	-2.67	118.75	126.61
37	38	203	CLA	CMB-C2B-C3B	2.67	129.68	124.68
46	v	201	HEM	CMB-C2B-C1B	-2.67	120.97	125.04
37	35	307	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
40	40	202	SQD	O8-S-C6	2.67	110.00	105.74
37	36	306	CLA	C2A-C3A-C4A	-2.67	97.55	101.87
39	a	408	BCR	C15-C14-C13	-2.67	123.50	127.31
37	c	502	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
37	21	210	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
47	14	306	KC1	CAA-CBA-CGA	-2.67	113.54	127.26
47	13	309	KC1	CAA-CBA-CGA	-2.67	113.54	127.26
47	34	306	KC1	CAA-CBA-CGA	-2.67	113.54	127.26
37	38	203	CLA	CHB-C4A-NA	2.67	128.20	124.51
37	c	503	CLA	C4-C3-C5	2.67	119.76	115.27
37	W	101	CLA	CHD-C4C-NC	2.67	128.41	124.20
37	16	306	CLA	C2A-C3A-C4A	-2.67	97.56	101.87
48	17	310	A86	C25-C24-C1	-2.67	118.92	126.42
37	c	512	CLA	CHD-C4C-NC	2.67	128.41	124.20
37	D	406	CLA	O2A-CGA-CBA	2.67	120.28	111.91
47	37	304	KC1	CHD-C4C-NC	2.67	128.25	124.20
47	14	309	KC1	O2D-CGD-O1D	-2.67	118.62	123.84
37	B	516	CLA	O1D-CGD-CBD	-2.67	119.03	124.48
37	33	307	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
37	14	303	CLA	CHD-C4C-NC	2.67	128.41	124.20
37	12	203	CLA	CHB-C4A-NA	2.67	128.20	124.51
43	d	407	LHG	C11-C10-C9	-2.67	100.89	114.42
37	c	504	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
37	c	502	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
47	37	305	KC1	CHC-C4B-C3B	-2.67	120.70	125.26
47	15	309	KC1	CAA-CBA-CGA	-2.67	113.56	127.26
47	38	210	KC1	CBC-CAC-C3C	-2.66	105.08	112.43
37	38	204	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
40	A	407	SQD	O48-C23-C24	2.66	120.27	111.91
47	33	309	KC1	CAA-CBA-CGA	-2.66	113.57	127.26
37	C	505	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
47	32	212	KC1	C4C-C3C-C2C	-2.66	103.02	106.90
37	C	501	CLA	CBC-CAC-C3C	-2.66	105.09	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	13	307	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
37	41	210	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
37	32	213	CLA	CHB-C4A-NA	2.66	128.19	124.51
48	34	311	A86	C23-C16-C22	-2.66	103.44	107.37
37	15	303	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
37	19	305	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
37	35	301	CLA	C1-C2-C3	-2.66	121.44	126.04
37	c	501	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
37	d	404	CLA	O2A-CGA-CBA	2.66	120.26	111.91
40	16	315	SQD	O48-C23-C24	2.66	120.26	111.91
37	C	502	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
47	18	210	KC1	CBC-CAC-C3C	-2.66	105.10	112.43
47	37	304	KC1	CMB-C2B-C1B	2.66	129.40	124.71
47	12	206	KC1	O2D-CGD-O1D	-2.66	118.64	123.84
37	b	523	CLA	C3B-C4B-NB	2.66	112.65	109.21
48	38	215	A86	C35-C34-C33	2.66	114.52	109.88
37	15	307	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
47	35	309	KC1	CAA-CBA-CGA	-2.66	113.60	127.26
50	21	212	DD6	C19-C18-C17	2.66	115.91	110.77
47	34	309	KC1	O2D-CGD-O1D	-2.66	118.64	123.84
37	11	303	CLA	CHD-C4C-NC	2.66	128.39	124.20
37	17	304	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
48	19	313	A86	C22-C16-C17	-2.66	104.37	108.98
37	37	301	CLA	CMB-C2B-C3B	2.66	129.65	124.68
44	H	102	DGD	CDB-CCB-CBB	-2.66	100.94	114.42
44	h	102	DGD	CDB-CCB-CBB	-2.66	100.94	114.42
37	c	504	CLA	C4-C3-C5	2.66	119.74	115.27
37	31	304	CLA	CHD-C4C-NC	2.66	128.39	124.20
37	15	301	CLA	C1-C2-C3	-2.66	121.45	126.04
37	21	210	CLA	CHD-C4C-NC	2.65	128.39	124.20
37	34	308	CLA	CHD-C4C-NC	2.65	128.39	124.20
37	18	203	CLA	CHB-C4A-NA	2.65	128.18	124.51
37	41	208	CLA	CHB-C4A-NA	2.65	128.18	124.51
47	12	211	KC1	C4C-C3C-C2C	-2.65	103.03	106.90
37	32	204	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
48	38	215	A86	C7-C6-C5	-2.65	119.20	122.92
37	A	405	CLA	CHB-C4A-NA	2.65	128.18	124.51
37	21	208	CLA	CHB-C4A-NA	2.65	128.18	124.51
37	C	504	CLA	C4-C3-C5	2.65	119.73	115.27
37	18	201	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
47	40	207	KC1	O1D-CGD-CBD	-2.65	119.06	124.48
37	12	210	CLA	CED-O2D-CGD	2.65	121.94	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	18	215	A86	C35-C34-C33	2.65	114.50	109.88
47	38	210	KC1	CHB-C4A-NA	2.65	128.38	124.20
50	41	216	DD6	C34-C35-C36	2.65	117.14	111.85
37	b	508	CLA	C1-C2-C3	-2.65	121.46	126.04
37	b	523	CLA	CHA-C1A-NA	-2.65	120.33	126.40
47	20	304	KC1	CMB-C2B-C1B	2.65	129.38	124.71
37	C	501	CLA	C4-C3-C5	2.65	119.73	115.27
48	15	314	A86	C25-C24-C1	-2.65	118.97	126.42
48	32	214	A86	C4-C3-C2	-2.65	118.05	123.47
37	32	202	CLA	C1-C2-C3	-2.65	121.46	126.04
37	38	202	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
39	b	518	BCR	C15-C14-C13	-2.65	123.53	127.31
37	11	303	CLA	CAA-C2A-C1A	2.65	120.65	111.97
37	31	304	CLA	CAA-C2A-C1A	2.65	120.65	111.97
48	38	212	A86	C10-C9-C8	-2.65	114.95	123.22
37	39	306	CLA	C4-C3-C5	2.65	119.72	115.27
47	17	306	KC1	CHB-C1B-NB	-2.65	122.02	124.45
39	A	406	BCR	C15-C14-C13	-2.65	123.53	127.31
47	31	309	KC1	C1A-NA-C4A	-2.65	105.52	106.71
37	15	305	CLA	CHB-C4A-NA	2.65	128.17	124.51
50	21	216	DD6	C34-C35-C36	2.65	117.12	111.85
37	B	524	CLA	C3B-C4B-NB	2.65	112.63	109.21
47	40	206	KC1	CHD-C4C-NC	2.65	128.22	124.20
47	40	206	KC1	CMB-C2B-C1B	2.64	129.37	124.71
37	18	202	CLA	CMB-C2B-C3B	2.64	129.63	124.68
37	b	512	CLA	CHB-C4A-NA	2.64	128.17	124.51
37	B	524	CLA	CHA-C1A-NA	-2.64	120.34	126.40
47	33	306	KC1	CMB-C2B-C1B	2.64	129.37	124.71
37	39	302	CLA	C4C-C3C-C2C	-2.64	103.04	106.90
37	d	403	CLA	CHC-C1C-C2C	-2.64	119.41	126.72
44	c	516	DGD	O5D-C6D-C5D	-2.64	104.16	109.05
37	B	501	CLA	CMC-C2C-C1C	2.64	129.06	125.04
37	19	306	CLA	C4-C3-C5	2.64	119.72	115.27
37	17	309	CLA	CAA-CBA-CGA	-2.64	105.53	113.25
37	b	506	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
37	B	512	CLA	CHB-C4A-NA	2.64	128.17	124.51
48	34	313	A86	C9-C8-C6	-2.64	118.99	126.42
48	16	310	A86	C36-C31-C32	-2.64	117.07	119.70
37	C	505	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
37	17	304	CLA	CHB-C4A-NA	2.64	128.16	124.51
37	21	205	CLA	CHB-C4A-NA	2.64	128.16	124.51
37	32	204	CLA	CHB-C4A-NA	2.64	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	506	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
37	35	305	CLA	CHB-C4A-NA	2.64	128.16	124.51
37	15	308	CLA	CBC-CAC-C3C	-2.64	105.16	112.43
47	18	210	KC1	CHB-C4A-NA	2.64	128.36	124.20
47	34	306	KC1	C1A-NA-C4A	-2.64	105.52	106.71
37	13	307	CLA	CMC-C2C-C1C	2.64	129.06	125.04
37	21	208	CLA	CMB-C2B-C3B	2.64	129.61	124.68
44	C	516	DGD	O5D-C6D-C5D	-2.64	104.17	109.05
37	41	210	CLA	CHD-C4C-NC	2.64	128.36	124.20
48	13	311	A86	C4-C3-C2	-2.64	118.07	123.47
37	11	308	CLA	C1-C2-C3	-2.64	121.48	126.04
37	14	308	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
37	34	308	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
37	11	303	CLA	CBC-CAC-C3C	-2.64	105.16	112.43
37	19	302	CLA	CBC-CAC-C3C	-2.64	105.16	112.43
47	20	304	KC1	CHD-C4C-NC	2.64	128.20	124.20
47	16	305	KC1	CAC-C3C-C4C	2.64	128.23	124.81
37	19	302	CLA	C4C-C3C-C2C	-2.64	103.06	106.90
47	16	302	KC1	CAB-C3B-C4B	2.64	131.26	124.90
37	15	303	CLA	CHD-C4C-NC	2.64	128.36	124.20
37	31	302	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
47	33	309	KC1	O2D-CGD-O1D	-2.63	118.69	123.84
37	38	206	CLA	CMB-C2B-C3B	2.63	129.61	124.68
47	14	309	KC1	CHB-C4A-NA	2.63	128.35	124.20
48	14	313	A86	C9-C8-C6	-2.63	119.02	126.42
39	b	518	BCR	C27-C26-C25	2.63	126.55	122.73
48	35	314	A86	C25-C24-C1	-2.63	119.02	126.42
48	13	312	A86	C25-C24-C1	-2.63	119.02	126.42
39	0	101	BCR	C3-C4-C5	-2.63	109.38	114.08
37	c	505	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
47	35	309	KC1	CMC-C2C-C1C	2.63	129.04	125.04
47	32	207	KC1	O2D-CGD-O1D	-2.63	118.69	123.84
37	D	405	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
47	17	308	KC1	CMB-C2B-C1B	2.63	129.35	124.71
37	21	204	CLA	CHB-C4A-NA	2.63	128.15	124.51
37	19	307	CLA	CHB-C4A-NA	2.63	128.15	124.51
37	39	304	CLA	CHB-C4A-NA	2.63	128.15	124.51
37	31	304	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
37	39	302	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
37	35	303	CLA	CHD-C4C-NC	2.63	128.34	124.20
37	B	524	CLA	C4-C3-C5	2.63	119.69	115.27
37	14	308	CLA	CHD-C4C-NC	2.63	128.34	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	308	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
43	D	409	LHG	O8-C23-C24	2.63	120.15	111.91
37	33	307	CLA	CMC-C2C-C1C	2.63	129.04	125.04
37	D	406	CLA	CMB-C2B-C3B	2.63	129.59	124.68
48	33	311	A86	C4-C3-C2	-2.63	118.09	123.47
37	b	505	CLA	CAA-C2A-C3A	-2.63	105.59	112.78
37	34	305	CLA	CMB-C2B-C3B	2.63	129.59	124.68
37	41	208	CLA	CMB-C2B-C3B	2.63	129.59	124.68
37	b	512	CLA	CHC-C1C-C2C	-2.63	119.46	126.72
47	13	309	KC1	C4C-C3C-C2C	-2.63	103.07	106.90
37	b	513	CLA	C1-C2-C3	-2.63	121.50	126.04
47	18	207	KC1	CAA-CBA-CGA	-2.62	113.77	127.26
37	19	302	CLA	C4-C3-C5	2.62	119.69	115.27
43	d	407	LHG	O8-C23-C24	2.62	120.14	111.91
37	d	404	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
37	20	308	CLA	CHD-C4C-NC	2.62	128.34	124.20
47	13	306	KC1	CMB-C2B-C1B	2.62	129.34	124.71
37	d	404	CLA	CHB-C4A-NA	2.62	128.14	124.51
37	B	508	CLA	C1-C2-C3	-2.62	121.51	126.04
47	17	308	KC1	CHB-C4A-NA	2.62	128.34	124.20
48	19	313	A86	C-C1-C24	2.62	122.21	118.08
44	h	102	DGD	CBB-CAB-C9B	-2.62	101.11	114.42
37	18	211	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
48	11	311	A86	O1-C15-C14	-2.62	107.95	113.21
48	40	211	A86	C4-C3-C2	-2.62	118.10	123.47
37	39	307	CLA	CHB-C4A-NA	2.62	128.14	124.51
44	H	102	DGD	CBB-CAB-C9B	-2.62	101.12	114.42
48	38	214	A86	C12-C11-C13	2.62	120.42	116.02
50	16	312	DD6	C25-C24-C1	-2.62	119.06	126.42
47	31	303	KC1	C1A-NA-C4A	-2.62	105.53	106.71
37	D	406	CLA	CHB-C4A-NA	2.62	128.13	124.51
37	c	501	CLA	C4-C3-C5	2.62	119.68	115.27
37	40	203	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
37	D	406	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
48	36	310	A86	C36-C31-C32	-2.62	117.10	119.70
37	17	307	CLA	O2A-CGA-CBA	2.62	120.12	111.91
50	39	312	DD6	C4-C3-C2	-2.62	118.11	123.47
37	33	307	CLA	CHD-C4C-NC	2.62	128.33	124.20
37	39	303	CLA	CMC-C2C-C1C	2.62	129.03	125.04
48	13	315	A86	C7-C6-C5	-2.62	119.26	122.92
37	41	206	CLA	O2A-CGA-CBA	2.62	120.12	111.91
37	38	206	CLA	CAC-C3C-C4C	2.62	128.21	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	33	303	CLA	CHD-C4C-NC	2.62	128.33	124.20
47	34	309	KC1	CHB-C4A-NA	2.62	128.33	124.20
37	39	301	CLA	CMC-C2C-C1C	2.62	129.02	125.04
39	C	514	BCR	C15-C14-C13	-2.62	123.58	127.31
37	B	505	CLA	CAA-C2A-C3A	-2.62	105.62	112.78
37	21	206	CLA	O2A-CGA-CBA	2.61	120.11	111.91
37	38	208	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
48	32	217	A86	C34-O4-C38	-2.61	113.03	117.90
47	35	309	KC1	CHB-C4A-NA	2.61	128.32	124.20
48	38	215	A86	C36-C31-C32	-2.61	117.10	119.70
37	39	309	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
37	C	503	CLA	CHD-C4C-NC	2.61	128.32	124.20
47	34	304	KC1	C4C-C3C-C2C	-2.61	103.09	106.90
37	34	307	CLA	CHB-C4A-NA	2.61	128.12	124.51
37	14	301	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
37	33	310	CLA	CHD-C4C-NC	2.61	128.32	124.20
37	B	513	CLA	C1-C2-C3	-2.61	121.53	126.04
37	B	507	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
48	13	315	A86	C12-C11-C13	2.61	120.41	116.02
47	38	210	KC1	C1A-NA-C4A	-2.61	105.53	106.71
37	37	303	CLA	CHB-C4A-NA	2.61	128.12	124.51
47	15	309	KC1	CHB-C4A-NA	2.61	128.32	124.20
37	34	301	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
37	d	404	CLA	CMB-C2B-C3B	2.61	129.56	124.68
37	33	305	CLA	CHB-C4A-NA	2.61	128.12	124.51
48	12	216	A86	C34-O4-C38	-2.61	113.03	117.90
47	36	305	KC1	CAC-C3C-C4C	2.61	128.20	124.81
48	33	315	A86	C12-C11-C13	2.61	120.41	116.02
47	35	309	KC1	CMB-C2B-C1B	2.61	129.31	124.71
39	c	514	BCR	C15-C14-C13	-2.61	123.58	127.31
37	16	306	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
37	31	310	CLA	O2A-CGA-CBA	2.61	120.10	111.91
37	40	210	CLA	CMB-C2B-C3B	2.61	129.56	124.68
48	33	313	A86	C35-C34-C33	2.61	114.43	109.88
37	b	507	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
39	B	518	BCR	C15-C14-C13	-2.61	123.59	127.31
37	34	305	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
47	21	207	KC1	CBC-CAC-C3C	-2.61	105.24	112.43
47	38	210	KC1	CMB-C2B-C1B	2.61	129.31	124.71
48	33	312	A86	C-C1-C2	-2.61	119.27	122.92
37	34	308	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
37	b	515	CLA	C4-C3-C5	2.61	119.66	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	20	309	A86	C4-C3-C2	-2.61	118.13	123.47
47	15	306	KC1	O2D-CGD-O1D	-2.61	118.74	123.84
37	19	304	CLA	CHB-C4A-NA	2.61	128.12	124.51
37	B	515	CLA	C4-C3-C5	2.61	119.66	115.27
37	13	307	CLA	CHD-C4C-NC	2.61	128.31	124.20
37	36	303	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
37	39	310	CLA	C1-C2-C3	-2.61	121.54	126.04
50	19	312	DD6	C4-C3-C2	-2.60	118.14	123.47
48	17	320	A86	C26-C25-C24	-2.60	115.09	123.22
37	C	512	CLA	CMB-C2B-C3B	2.60	129.55	124.68
47	39	308	KC1	O2D-CGD-O1D	-2.60	118.75	123.84
37	B	512	CLA	CHC-C1C-C2C	-2.60	119.52	126.72
37	39	310	CLA	CHB-C4A-NA	2.60	128.11	124.51
37	11	308	CLA	O2A-CGA-CBA	2.60	120.08	111.91
37	20	308	CLA	CMB-C2B-C3B	2.60	129.55	124.68
50	36	312	DD6	C25-C24-C1	-2.60	119.11	126.42
37	33	305	CLA	CMC-C2C-C1C	2.60	129.00	125.04
48	33	312	A86	C25-C24-C1	-2.60	119.11	126.42
37	41	205	CLA	CHB-C4A-NA	2.60	128.11	124.51
48	18	213	A86	C9-C8-C6	-2.60	119.11	126.42
37	16	303	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
47	36	302	KC1	CAB-C3B-C4B	2.60	131.18	124.90
37	32	202	CLA	O2A-CGA-CBA	2.60	120.06	111.91
47	37	307	KC1	CHB-C4A-NA	2.60	128.30	124.20
47	35	306	KC1	O2D-CGD-O1D	-2.60	118.76	123.84
48	35	315	A86	C10-C9-C8	-2.60	115.11	123.22
39	B	518	BCR	C27-C26-C25	2.60	126.50	122.73
48	12	215	A86	C12-C11-C13	2.60	120.39	116.02
37	13	305	CLA	CHB-C4A-NA	2.60	128.10	124.51
48	35	314	A86	C4-C5-C6	-2.60	123.60	127.31
37	36	306	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
48	17	313	A86	C34-O4-C38	-2.60	113.06	117.90
37	14	305	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
37	38	204	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
39	5	101	BCR	C3-C4-C5	-2.60	109.44	114.08
39	C	519	BCR	C27-C26-C25	2.60	126.50	122.73
37	17	307	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
48	18	215	A86	C36-C31-C32	-2.59	117.12	119.70
37	12	209	CLA	CAA-C2A-C1A	2.59	120.48	111.97
47	15	309	KC1	O2D-CGD-O1D	-2.59	118.77	123.84
37	14	310	CLA	CHB-C4A-NA	2.59	128.10	124.51
37	c	512	CLA	CMB-C2B-C3B	2.59	129.53	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	12	207	CLA	CHB-C4A-NA	2.59	128.10	124.51
48	13	312	A86	C7-C6-C8	2.59	122.16	118.08
47	41	207	KC1	CBC-CAC-C3C	-2.59	105.28	112.43
37	20	301	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
48	39	313	A86	C-C1-C24	2.59	122.16	118.08
37	21	206	CLA	CHB-C4A-NA	2.59	128.10	124.51
37	15	308	CLA	CMC-C2C-C1C	2.59	128.99	125.04
37	21	210	CLA	CAC-C3C-C4C	2.59	128.17	124.81
47	37	307	KC1	CMB-C2B-C1B	2.59	129.28	124.71
37	D	402	CLA	C4-C3-C5	2.59	119.63	115.27
47	35	306	KC1	CMC-C2C-C1C	2.59	128.99	125.04
47	33	309	KC1	C4C-C3C-C2C	-2.59	103.12	106.90
37	16	303	CLA	CBC-CAC-C3C	-2.59	105.29	112.43
37	13	305	CLA	CMC-C2C-C1C	2.59	128.99	125.04
37	32	210	CLA	CAA-C2A-C1A	2.59	120.47	111.97
47	36	305	KC1	CHD-C4C-NC	2.59	128.13	124.20
37	14	305	CLA	CMB-C2B-C3B	2.59	129.53	124.68
47	16	305	KC1	CHD-C4C-NC	2.59	128.13	124.20
37	z	102	CLA	O1D-CGD-CBD	-2.59	119.18	124.48
37	B	514	CLA	CHD-C4C-NC	2.59	128.28	124.20
48	31	311	A86	O1-C15-C14	-2.59	108.01	113.21
48	31	314	A86	C41-C32-C31	-2.59	108.15	110.47
37	19	303	CLA	CMC-C2C-C1C	2.59	128.98	125.04
47	21	207	KC1	CAA-C2A-C1A	-2.59	112.84	124.75
37	40	203	CLA	CMB-C2B-C3B	2.59	129.52	124.68
47	41	207	KC1	CAA-C2A-C1A	-2.59	112.85	124.75
37	14	303	CLA	C1-O2A-CGA	2.59	123.23	116.44
41	c	518	LMG	O1-C1-C2	-2.59	104.26	108.30
37	40	210	CLA	CHD-C4C-NC	2.59	128.28	124.20
48	18	212	A86	C12-C11-C13	2.59	120.37	116.02
37	19	310	CLA	CHB-C4A-NA	2.59	128.09	124.51
37	32	208	CLA	CHB-C4A-NA	2.59	128.09	124.51
47	14	304	KC1	C4C-C3C-C2C	-2.59	103.12	106.90
47	35	309	KC1	O2D-CGD-O1D	-2.59	118.78	123.84
37	14	307	CLA	C1-C2-C3	-2.59	121.57	126.04
37	32	208	CLA	CMB-C2B-C3B	2.59	129.52	124.68
47	36	304	KC1	O2D-CGD-O1D	-2.59	118.78	123.84
37	11	310	CLA	O2A-CGA-CBA	2.59	120.03	111.91
37	38	208	CLA	O2A-CGA-CBA	2.59	120.03	111.91
37	19	309	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
37	36	303	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
47	11	302	KC1	C1A-NA-C4A	-2.58	105.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	18	209	CLA	O2A-CGA-CBA	2.58	120.02	111.91
37	a	403	CLA	CMD-C2D-C3D	-2.58	121.67	127.61
39	c	514	BCR	C7-C8-C9	-2.58	122.33	126.23
48	35	312	A86	C25-C24-C1	-2.58	119.16	126.42
37	41	204	CLA	CHB-C4A-NA	2.58	128.08	124.51
48	11	312	A86	C23-C16-C22	-2.58	103.56	107.37
48	15	315	A86	C10-C9-C8	-2.58	115.16	123.22
47	36	302	KC1	CHB-C4A-NA	2.58	128.27	124.20
37	15	310	CLA	CAC-C3C-C4C	2.58	128.16	124.81
37	41	206	CLA	CHB-C4A-NA	2.58	128.08	124.51
37	37	306	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
37	41	210	CLA	CAC-C3C-C4C	2.58	128.16	124.81
37	32	211	CLA	C1-C2-C3	-2.58	121.58	126.04
37	b	506	CLA	C4-C3-C5	2.58	119.61	115.27
37	12	210	CLA	C1-C2-C3	-2.58	121.58	126.04
37	18	206	CLA	CBC-CAC-C3C	-2.58	105.32	112.43
48	32	216	A86	C12-C11-C13	2.58	120.36	116.02
48	31	314	A86	C25-C24-C1	-2.58	119.17	126.42
37	d	401	CLA	O2A-CGA-CBA	2.58	120.00	111.91
47	38	207	KC1	CAA-CBA-CGA	-2.58	114.00	127.26
48	11	314	A86	C25-C24-C1	-2.58	119.17	126.42
47	15	309	KC1	CMB-C2B-C1B	2.58	129.26	124.71
47	19	308	KC1	O2D-CGD-O1D	-2.58	118.80	123.84
48	34	315	A86	C35-C34-C33	2.58	114.38	109.88
37	14	303	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
47	36	308	KC1	O1D-CGD-CBD	-2.58	119.21	124.48
48	31	313	A86	C34-O4-C38	-2.58	113.09	117.90
47	21	203	KC1	CHB-C1B-C2B	-2.58	120.08	125.48
37	14	307	CLA	CHB-C4A-NA	2.58	128.07	124.51
37	33	303	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
46	V	201	HEM	C4D-ND-C1D	2.58	107.73	105.07
48	33	312	A86	C34-O4-C38	-2.58	113.09	117.90
48	14	311	A86	C23-C16-C22	-2.58	103.57	107.37
37	c	503	CLA	CHD-C4C-NC	2.58	128.26	124.20
37	B	506	CLA	C4-C3-C5	2.58	119.60	115.27
37	12	205	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
37	18	211	CLA	CMB-C2B-C3B	2.58	129.50	124.68
48	34	314	A86	C7-C6-C8	2.58	122.14	118.08
40	B	522	SQD	C1-O5-C5	2.58	118.74	113.69
37	31	302	CLA	CHB-C4A-NA	2.58	128.07	124.51
37	14	308	CLA	O2A-CGA-CBA	2.57	119.99	111.91
41	C	518	LMG	O1-C1-C2	-2.57	104.28	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	c	519	BCR	C27-C26-C25	2.57	126.47	122.73
37	13	310	CLA	CHD-C4C-NC	2.57	128.26	124.20
47	16	302	KC1	CHB-C4A-NA	2.57	128.26	124.20
37	B	505	CLA	C1-C2-C3	-2.57	121.59	126.04
37	39	302	CLA	CMB-C2B-C3B	2.57	129.49	124.68
37	34	303	CLA	C1-O2A-CGA	2.57	123.20	116.44
37	19	301	CLA	CMC-C2C-C1C	2.57	128.96	125.04
37	A	403	CLA	CMD-C2D-C3D	-2.57	121.69	127.61
47	15	304	KC1	C4C-C3C-C2C	-2.57	103.15	106.90
37	15	307	CLA	CHB-C4A-NA	2.57	128.07	124.51
39	c	515	BCR	C11-C10-C9	-2.57	123.64	127.31
47	32	212	KC1	CMC-C2C-C1C	2.57	128.96	125.04
37	34	302	CLA	CAA-C2A-C1A	2.57	120.41	111.97
37	B	502	CLA	CHB-C4A-NA	2.57	128.07	124.51
48	31	319	A86	C4-C5-C6	-2.57	123.64	127.31
47	15	306	KC1	CMC-C2C-C1C	2.57	128.96	125.04
37	D	402	CLA	O2A-CGA-CBA	2.57	119.98	111.91
37	34	310	CLA	CHB-C4A-NA	2.57	128.07	124.51
37	12	209	CLA	O1D-CGD-CBD	-2.57	119.22	124.48
48	11	319	A86	C4-C5-C6	-2.57	123.64	127.31
37	35	310	CLA	CHD-C4C-NC	2.57	128.25	124.20
37	34	305	CLA	CHB-C4A-NA	2.57	128.07	124.51
37	C	513	CLA	C1-C2-C3	-2.57	121.60	126.04
37	39	305	CLA	C1-O2A-CGA	2.57	123.19	116.44
37	32	206	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
37	34	303	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
37	B	510	CLA	C1-C2-C3	-2.57	121.60	126.04
37	b	510	CLA	C1-C2-C3	-2.57	121.60	126.04
50	36	312	DD6	C35-C36-C31	-2.57	114.74	120.57
47	16	304	KC1	O2D-CGD-O1D	-2.57	118.82	123.84
47	41	203	KC1	CHB-C1B-C2B	-2.57	120.09	125.48
37	Z	102	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
47	17	305	KC1	CMB-C2B-C1B	2.57	129.24	124.71
47	11	302	KC1	C4C-C3C-C2C	-2.57	103.16	106.90
50	19	312	DD6	C25-C24-C1	-2.57	119.20	126.42
37	c	504	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
40	36	315	SQD	C1-O5-C5	2.57	118.72	113.69
37	19	307	CLA	CHD-C4C-NC	2.57	128.25	124.20
37	32	213	CLA	CMB-C2B-C3B	2.57	129.48	124.68
40	b	521	SQD	C1-O5-C5	2.57	118.72	113.69
48	13	312	A86	C34-O4-C38	-2.56	113.12	117.90
37	19	302	CLA	CMB-C2B-C3B	2.56	129.48	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	a	404	CLA	CHB-C4A-NA	2.56	128.06	124.51
37	b	515	CLA	CHB-C4A-NA	2.56	128.06	124.51
37	14	302	CLA	CAA-C2A-C1A	2.56	120.38	111.97
37	36	307	CLA	CAC-C3C-C4C	2.56	128.14	124.81
37	34	307	CLA	CMC-C2C-C1C	2.56	128.94	125.04
48	33	315	A86	C7-C6-C5	-2.56	119.33	122.92
37	11	301	CLA	CHB-C4A-NA	2.56	128.06	124.51
37	18	209	CLA	C4-C3-C5	2.56	119.58	115.27
43	21	201	LHG	C11-C10-C9	-2.56	101.42	114.42
37	d	401	CLA	C4-C3-C5	2.56	119.58	115.27
37	38	211	CLA	CMB-C2B-C3B	2.56	129.47	124.68
37	14	305	CLA	CHB-C4A-NA	2.56	128.05	124.51
37	34	307	CLA	CHA-C1A-NA	-2.56	120.53	126.40
50	16	312	DD6	C35-C36-C31	-2.56	114.76	120.57
37	14	307	CLA	CHA-C1A-NA	-2.56	120.53	126.40
50	39	312	DD6	C25-C24-C1	-2.56	119.22	126.42
37	C	504	CLA	CBC-CAC-C3C	-2.56	105.37	112.43
37	20	301	CLA	CMB-C2B-C3B	2.56	129.47	124.68
48	31	312	A86	C10-C9-C8	-2.56	115.23	123.22
48	13	313	A86	C35-C34-C33	2.56	114.34	109.88
37	c	512	CLA	CHB-C4A-NA	2.56	128.05	124.51
37	12	205	CLA	C4-C3-C5	2.56	119.58	115.27
37	C	504	CLA	CMC-C2C-C1C	2.56	128.94	125.04
37	16	303	CLA	CMC-C2C-C1C	2.56	128.94	125.04
37	34	307	CLA	C1-C2-C3	-2.56	121.62	126.04
48	19	313	A86	C24-C1-C2	-2.56	115.02	118.94
37	21	209	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
39	C	519	BCR	C15-C16-C17	-2.56	118.23	123.47
37	34	308	CLA	O2A-CGA-CBA	2.56	119.94	111.91
47	14	306	KC1	C1A-NA-C4A	-2.56	105.56	106.71
37	b	514	CLA	CHD-C4C-NC	2.56	128.23	124.20
48	14	314	A86	C7-C6-C8	2.56	122.11	118.08
47	15	309	KC1	CMC-C2C-C1C	2.56	128.93	125.04
37	b	523	CLA	C4-C3-C5	2.56	119.57	115.27
37	12	207	CLA	CMB-C2B-C3B	2.56	129.46	124.68
37	13	310	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
38	A	404	PHO	O2D-CGD-O1D	-2.56	118.84	123.84
47	18	210	KC1	O1D-CGD-CBD	-2.56	119.25	124.48
38	a	405	PHO	O1D-CGD-CBD	2.56	129.00	124.74
39	C	515	BCR	C7-C8-C9	-2.56	122.37	126.23
37	b	505	CLA	C1-C2-C3	-2.56	121.62	126.04
37	c	513	CLA	C1-C2-C3	-2.56	121.62	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	35	306	KC1	CHB-C1B-NB	-2.55	122.11	124.45
37	C	512	CLA	CHB-C4A-NA	2.55	128.04	124.51
47	16	308	KC1	O1D-CGD-CBD	-2.55	119.26	124.48
40	17	301	SQD	C1-O5-C5	2.55	118.70	113.69
48	18	215	A86	C7-C6-C5	-2.55	119.34	122.92
37	41	209	CLA	CAA-C2A-C3A	-2.55	105.78	112.78
43	b	522	LHG	C11-C10-C9	-2.55	101.46	114.42
48	11	313	A86	C3-C4-C5	-2.55	118.24	123.47
37	19	305	CLA	C1-O2A-CGA	2.55	123.14	116.44
48	37	311	A86	C41-C32-C31	-2.55	108.19	110.47
48	31	312	A86	C23-C16-C22	-2.55	103.60	107.37
47	12	211	KC1	CMC-C2C-C1C	2.55	128.93	125.04
37	D	401	CLA	O2A-CGA-CBA	2.55	119.92	111.91
43	41	201	LHG	C11-C10-C9	-2.55	101.47	114.42
39	c	515	BCR	C7-C8-C9	-2.55	122.38	126.23
37	36	301	CLA	CHC-C1C-C2C	-2.55	119.66	126.72
47	31	303	KC1	C4C-C3C-C2C	-2.55	103.18	106.90
48	15	312	A86	C25-C24-C1	-2.55	119.25	126.42
37	B	515	CLA	CHB-C4A-NA	2.55	128.04	124.51
39	c	515	BCR	C15-C14-C13	-2.55	123.67	127.31
37	21	204	CLA	CMC-C2C-C1C	2.55	128.92	125.04
48	40	213	A86	C9-C8-C6	-2.55	119.25	126.42
48	11	312	A86	C10-C9-C8	-2.55	115.26	123.22
37	18	204	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
37	b	502	CLA	CHB-C4A-NA	2.55	128.04	124.51
37	b	507	CLA	C1-C2-C3	-2.55	121.63	126.04
37	c	504	CLA	CMC-C2C-C1C	2.55	128.92	125.04
48	17	311	A86	C10-C9-C8	-2.55	115.26	123.22
37	11	305	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
43	B	523	LHG	C11-C10-C9	-2.55	101.48	114.42
37	36	309	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
37	a	404	CLA	O2A-CGA-CBA	2.55	119.90	111.91
48	33	312	A86	C7-C6-C8	2.55	122.09	118.08
46	v	201	HEM	C4D-ND-C1D	2.55	107.70	105.07
37	16	309	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
48	13	312	A86	C-C1-C2	-2.54	119.36	122.92
37	12	212	CLA	CMB-C2B-C3B	2.54	129.44	124.68
37	14	307	CLA	CMC-C2C-C1C	2.54	128.91	125.04
37	36	303	CLA	CMC-C2C-C1C	2.54	128.91	125.04
48	17	313	A86	C36-C31-C32	-2.54	117.17	119.70
47	17	308	KC1	CAA-CBA-CGA	-2.54	114.19	127.26
37	b	502	CLA	C4-C3-C5	2.54	119.55	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	C	515	BCR	C15-C14-C13	-2.54	123.68	127.31
48	33	312	A86	C20-C19-C18	-2.54	107.72	112.75
50	41	212	DD6	C33-C34-C35	2.54	113.78	110.30
44	J	101	DGD	C1D-C2D-C3D	-2.54	104.70	110.00
48	21	215	A86	C19-C18-C17	-2.54	105.86	110.77
44	j	101	DGD	C1D-C2D-C3D	-2.54	104.70	110.00
48	11	315	A86	C41-C32-C31	-2.54	108.20	110.47
39	c	519	BCR	C15-C16-C17	-2.54	118.27	123.47
48	12	202	A86	C34-O4-C38	-2.54	113.16	117.90
48	32	203	A86	C34-O4-C38	-2.54	113.16	117.90
40	a	409	SQD	O48-C23-O10	-2.54	117.18	123.59
37	21	204	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
37	a	404	CLA	CBC-CAC-C3C	-2.54	105.43	112.43
37	16	307	CLA	CAC-C3C-C4C	2.54	128.10	124.81
37	32	206	CLA	C4-C3-C5	2.54	119.54	115.27
37	C	501	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
38	D	403	PHO	O1D-CGD-CBD	2.54	128.97	124.74
37	18	204	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
48	34	316	A86	C40-C32-C31	2.54	112.74	110.47
47	20	304	KC1	CHB-C1B-NB	-2.54	122.12	124.45
48	37	319	A86	C26-C25-C24	-2.54	115.30	123.22
37	B	507	CLA	C1-C2-C3	-2.54	121.65	126.04
48	12	213	A86	C3-C4-C5	-2.54	118.28	123.47
39	C	514	BCR	C7-C8-C9	-2.54	122.40	126.23
48	14	316	A86	C40-C32-C31	2.54	112.74	110.47
37	13	303	CLA	CHB-C4A-NA	2.54	128.02	124.51
47	35	309	KC1	CBC-CAC-C3C	-2.54	105.44	112.43
50	39	312	DD6	C23-C16-C15	2.54	116.89	110.05
37	39	304	CLA	CMB-C2B-C3B	2.54	129.42	124.68
47	40	206	KC1	CHB-C1B-NB	-2.54	122.12	124.45
48	33	315	A86	C36-C31-C32	-2.54	117.18	119.70
48	20	311	A86	C9-C8-C6	-2.54	119.29	126.42
48	14	315	A86	C35-C34-C33	2.54	114.30	109.88
37	18	201	CLA	C1-O2A-CGA	2.54	123.10	116.44
37	18	208	CLA	O2A-CGA-CBA	2.54	119.86	111.91
37	21	202	CLA	CHD-C4C-NC	2.54	128.20	124.20
37	16	301	CLA	CHC-C1C-C2C	-2.54	119.71	126.72
37	13	303	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
37	Z	101	CLA	C1-C2-C3	-2.53	121.66	126.04
37	B	502	CLA	C4-C3-C5	2.53	119.53	115.27
37	17	307	CLA	CMC-C2C-C1C	2.53	128.90	125.04
37	37	306	CLA	CMC-C2C-C1C	2.53	128.90	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	40	204	KC1	CHC-C4B-NB	-2.53	122.12	124.45
37	41	204	CLA	CMC-C2C-C1C	2.53	128.90	125.04
37	19	309	CLA	CMB-C2B-C3B	2.53	129.42	124.68
37	39	309	CLA	CMB-C2B-C3B	2.53	129.42	124.68
37	C	509	CLA	O2A-CGA-CBA	2.53	119.86	111.91
37	c	513	CLA	CBC-CAC-C3C	-2.53	105.45	112.43
37	z	101	CLA	C1-C2-C3	-2.53	121.66	126.04
48	15	311	A86	C20-C19-C18	-2.53	107.74	112.75
37	20	303	CLA	CHB-C4A-NA	2.53	128.01	124.51
47	18	210	KC1	CMB-C2B-C1B	2.53	129.18	124.71
47	32	209	KC1	O2D-CGD-O1D	-2.53	118.89	123.84
37	35	307	CLA	CHB-C4A-NA	2.53	128.01	124.51
48	34	314	A86	C8-C6-C5	-2.53	115.06	118.94
47	37	307	KC1	CAA-CBA-CGA	-2.53	114.26	127.26
37	41	204	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
37	36	309	CLA	CAA-CBA-CGA	-2.53	105.79	112.51
37	c	503	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
37	20	306	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
37	32	210	CLA	C1-C2-C3	-2.53	121.67	126.04
37	38	206	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
37	16	309	CLA	CAA-CBA-CGA	-2.53	105.80	112.51
48	13	314	A86	C34-O4-C38	-2.53	113.19	117.90
47	12	208	KC1	O2D-CGD-O1D	-2.53	118.90	123.84
50	21	212	DD6	C33-C34-C35	2.53	113.76	110.30
48	33	314	A86	C34-O4-C38	-2.53	113.19	117.90
37	39	307	CLA	CHD-C4C-NC	2.53	128.19	124.20
37	C	513	CLA	CBC-CAC-C3C	-2.53	105.47	112.43
48	15	311	A86	C10-C9-C8	-2.53	115.33	123.22
37	c	511	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
47	35	304	KC1	C4C-C3C-C2C	-2.53	103.22	106.90
50	19	312	DD6	C23-C16-C15	2.52	116.86	110.05
48	17	313	A86	C8-C6-C5	-2.52	115.07	118.94
39	C	515	BCR	C11-C10-C9	-2.52	123.71	127.31
48	17	315	A86	C12-C11-C13	2.52	120.26	116.02
37	12	209	CLA	CHA-C1A-NA	-2.52	120.62	126.40
48	35	311	A86	C10-C9-C8	-2.52	115.34	123.22
37	D	401	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
40	A	407	SQD	O48-C23-O10	-2.52	117.23	123.59
37	C	511	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
37	18	208	CLA	CMC-C2C-C1C	2.52	128.88	125.04
48	12	213	A86	C4-C3-C2	-2.52	118.31	123.47
37	15	310	CLA	CHD-C4C-NC	2.52	128.18	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	32	211	CLA	CED-O2D-CGD	2.52	121.64	115.94
41	L	102	LMG	O2-C2-C1	-2.52	103.92	110.05
37	31	308	CLA	CHA-C1A-NA	-2.52	120.63	126.40
37	18	204	CLA	C1-O2A-CGA	2.52	123.06	116.44
48	37	314	A86	C12-C11-C13	2.52	120.25	116.02
48	11	314	A86	C41-C32-C31	-2.52	108.22	110.47
37	32	211	CLA	O2A-CGA-CBA	2.52	119.81	111.91
41	b	519	LMG	C38-C37-C36	-2.52	101.64	114.42
37	31	308	CLA	CHB-C4A-NA	2.52	127.99	124.51
41	l	101	LMG	O2-C2-C1	-2.52	103.93	110.05
48	37	312	A86	C36-C31-C32	-2.52	117.20	119.70
37	c	510	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
37	41	202	CLA	CHD-C4C-NC	2.52	128.17	124.20
37	12	207	CLA	C5-C3-C4	2.52	120.16	114.60
41	B	520	LMG	C38-C37-C36	-2.52	101.65	114.42
37	34	310	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
37	40	203	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
43	d	407	LHG	C20-C19-C18	-2.51	101.66	114.42
43	D	409	LHG	C20-C19-C18	-2.51	101.66	114.42
37	41	204	CLA	O2A-CGA-CBA	2.51	119.80	111.91
37	d	403	CLA	O2A-CGA-CBA	2.51	119.80	111.91
37	D	405	CLA	O2A-CGA-CBA	2.51	119.80	111.91
37	c	509	CLA	O2A-CGA-CBA	2.51	119.79	111.91
48	37	312	A86	C34-O4-C38	-2.51	113.21	117.90
37	21	204	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
37	32	208	CLA	C5-C3-C4	2.51	120.15	114.60
47	20	302	KC1	CHC-C4B-NB	-2.51	122.14	124.45
37	11	307	CLA	CHA-C1A-NA	-2.51	120.64	126.40
37	20	307	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
37	Z	101	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
37	20	301	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
47	33	304	KC1	CMB-C2B-C1B	2.51	129.14	124.71
47	37	304	KC1	CMC-C2C-C1C	2.51	128.86	125.04
37	18	204	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
37	19	304	CLA	CMB-C2B-C3B	2.51	129.38	124.68
48	17	311	A86	C7-C6-C8	2.51	122.03	118.08
48	14	313	A86	C12-C11-C13	2.51	120.24	116.02
37	38	202	CLA	C1-C2-C3	-2.51	121.70	126.04
48	14	314	A86	C8-C6-C5	-2.51	115.09	118.94
48	21	215	A86	C40-C32-C31	2.51	112.72	110.47
37	35	303	CLA	CMB-C2B-C3B	2.51	129.38	124.68
37	38	206	CLA	CBC-CAC-C3C	-2.51	105.51	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	38	210	KC1	O1D-CGD-CBD	-2.51	119.35	124.48
37	19	301	CLA	CMA-C3A-C2A	-2.51	103.70	113.83
37	c	501	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
37	18	208	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
37	13	303	CLA	CAA-C2A-C1A	2.51	120.20	111.97
37	d	401	CLA	CMB-C2B-C3B	2.51	129.37	124.68
38	a	406	PHO	O2D-CGD-O1D	-2.51	118.93	123.84
37	38	204	CLA	C1-O2A-CGA	2.51	123.03	116.44
37	40	208	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
37	12	210	CLA	O2A-CGA-CBA	2.51	119.78	111.91
37	39	306	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
48	13	315	A86	C36-C31-C32	-2.51	117.21	119.70
47	15	309	KC1	CBC-CAC-C3C	-2.51	105.52	112.43
37	40	205	CLA	CHB-C4A-NA	2.51	127.98	124.51
37	32	210	CLA	CHA-C1A-NA	-2.51	120.66	126.40
48	35	312	A86	C10-C9-C8	-2.51	115.39	123.22
48	41	215	A86	C19-C18-C17	-2.51	105.93	110.77
47	17	306	KC1	O1D-CGD-CBD	-2.51	119.36	124.48
37	C	503	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
47	34	304	KC1	CMB-C2B-C1B	2.51	129.13	124.71
37	C	506	CLA	CMB-C2B-C3B	2.51	129.37	124.68
37	39	301	CLA	CMA-C3A-C4A	-2.50	105.04	111.77
37	15	303	CLA	CMB-C2B-C3B	2.50	129.36	124.68
48	13	312	A86	C20-C19-C18	-2.50	107.79	112.75
37	21	204	CLA	O2A-CGA-CBA	2.50	119.77	111.91
37	39	307	CLA	O2A-CGA-CBA	2.50	119.77	111.91
37	B	504	CLA	CAA-CBA-CGA	-2.50	105.94	113.25
37	11	308	CLA	CHD-C4C-NC	2.50	128.15	124.20
37	32	202	CLA	CHD-C4C-NC	2.50	128.15	124.20
47	17	303	KC1	CHB-C1B-NB	-2.50	122.15	124.45
44	c	516	DGD	CDB-CCB-CBB	-2.50	101.72	114.42
37	31	306	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
43	b	522	LHG	C20-C19-C18	-2.50	101.72	114.42
48	35	312	A86	C-C1-C2	-2.50	119.42	122.92
37	b	509	CLA	CHA-C1A-NA	-2.50	120.67	126.40
48	11	315	A86	C19-C18-C17	-2.50	105.94	110.77
43	B	523	LHG	C20-C19-C18	-2.50	101.73	114.42
47	20	304	KC1	C4C-C3C-C2C	-2.50	103.25	106.90
37	18	206	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
37	32	202	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
48	34	313	A86	C12-C11-C13	2.50	120.22	116.02
48	39	313	A86	C24-C1-C2	-2.50	115.10	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	41	204	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
37	C	502	CLA	CHC-C1C-NC	2.50	128.00	124.20
47	37	305	KC1	O1D-CGD-CBD	-2.50	119.37	124.48
47	14	304	KC1	CMB-C2B-C1B	2.50	129.12	124.71
47	34	309	KC1	CHB-C1B-C2B	-2.50	120.24	125.48
37	D	401	CLA	CHB-C4A-NA	2.50	127.97	124.51
48	37	310	A86	C8-C6-C5	-2.50	115.11	118.94
37	B	511	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
37	b	502	CLA	CAA-CBA-CGA	-2.50	105.95	113.25
48	35	311	A86	C20-C19-C18	-2.50	107.81	112.75
37	b	504	CLA	CAA-CBA-CGA	-2.50	105.95	113.25
47	14	309	KC1	CHB-C1B-C2B	-2.50	120.24	125.48
44	c	517	DGD	O5D-C6D-C5D	-2.50	104.43	109.05
37	11	307	CLA	CHB-C4A-NA	2.50	127.97	124.51
47	21	203	KC1	CBC-CAC-C3C	-2.50	105.55	112.43
47	37	304	KC1	C4C-C3C-C2C	-2.50	103.26	106.90
37	B	509	CLA	CHA-C1A-NA	-2.50	120.68	126.40
44	C	516	DGD	CDB-CCB-CBB	-2.50	101.75	114.42
37	11	308	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
48	31	315	A86	C41-C32-C31	-2.50	108.24	110.47
45	D	404	PL9	C41-C39-C38	-2.50	116.07	121.12
37	z	101	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
48	40	201	A86	C-C1-C2	-2.50	119.43	122.92
37	35	301	CLA	CHC-C1C-C2C	-2.50	119.82	126.72
37	b	508	CLA	O2A-CGA-CBA	2.50	119.74	111.91
47	16	302	KC1	CHC-C4B-NB	-2.50	122.16	124.45
48	41	215	A86	C40-C32-C31	2.50	112.70	110.47
37	B	502	CLA	CAA-CBA-CGA	-2.50	105.96	113.25
37	33	310	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
48	32	218	A86	C22-C16-C17	-2.49	104.65	108.98
37	35	308	CLA	CHB-C4A-NA	2.49	127.96	124.51
47	41	203	KC1	CBC-CAC-C3C	-2.49	105.56	112.43
37	W	102	CLA	C4-C3-C5	2.49	119.47	115.27
48	38	212	A86	C12-C11-C13	2.49	120.21	116.02
37	W	101	CLA	CMB-C2B-C3B	2.49	129.34	124.68
37	37	306	CLA	C4-C3-C5	2.49	119.47	115.27
39	0	101	BCR	C29-C30-C25	2.49	114.32	110.48
48	19	311	A86	C8-C6-C5	-2.49	115.12	118.94
37	34	302	CLA	O2A-CGA-CBA	2.49	119.73	111.91
45	d	402	PL9	C41-C39-C38	-2.49	116.07	121.12
37	40	209	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
47	17	306	KC1	CAA-CBA-CGA	-2.49	114.45	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	37	305	KC1	CAA-CBA-CGA	-2.49	114.46	127.26
37	19	305	CLA	C4A-NA-C1A	-2.49	105.59	106.71
37	c	502	CLA	CHC-C1C-NC	2.49	127.98	124.20
37	37	308	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
37	c	506	CLA	CMB-C2B-C3B	2.49	129.34	124.68
47	12	211	KC1	CHB-C4A-NA	2.49	128.13	124.20
37	B	508	CLA	O2A-CGA-CBA	2.49	119.72	111.91
37	15	301	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
48	31	315	A86	C19-C18-C17	-2.49	105.96	110.77
37	B	504	CLA	CHD-C4C-NC	2.49	128.13	124.20
47	36	302	KC1	CHC-C4B-NB	-2.49	122.17	124.45
48	37	319	A86	C40-C32-C31	-2.49	108.24	110.47
47	32	212	KC1	CHB-C4A-NA	2.49	128.13	124.20
48	11	314	A86	C35-C34-C33	2.49	114.22	109.88
37	19	307	CLA	O2A-CGA-CBA	2.49	119.72	111.91
44	C	517	DGD	O5D-C6D-C5D	-2.49	104.44	109.05
37	12	209	CLA	C1-C2-C3	-2.49	121.74	126.04
37	w	101	CLA	CMB-C2B-C3B	2.49	129.33	124.68
37	C	510	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
43	37	315	LHG	O8-C23-C24	2.49	119.71	111.91
37	39	305	CLA	C4A-NA-C1A	-2.49	105.59	106.71
37	31	301	CLA	C4-C3-C5	2.49	119.45	115.27
47	19	308	KC1	CMB-C2B-C1B	2.49	129.09	124.71
47	39	308	KC1	CMB-C2B-C1B	2.49	129.09	124.71
48	34	313	A86	C36-C31-C32	-2.49	117.23	119.70
37	19	301	CLA	CMA-C3A-C4A	-2.49	105.09	111.77
37	b	511	CLA	CAA-C2A-C3A	-2.49	105.97	112.78
37	c	510	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
37	D	402	CLA	CMB-C2B-C3B	2.48	129.33	124.68
37	34	307	CLA	CBC-CAC-C3C	-2.48	105.58	112.43
48	21	215	A86	C25-C24-C1	-2.48	119.44	126.42
48	15	312	A86	C-C1-C2	-2.48	119.44	122.92
37	A	403	CLA	C6-C7-C8	-2.48	107.89	115.92
39	D	407	BCR	C28-C27-C26	-2.48	109.64	114.08
37	40	210	CLA	O2A-CGA-CBA	2.48	119.69	111.91
37	14	302	CLA	O2A-CGA-CBA	2.48	119.69	111.91
37	18	206	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
37	11	305	CLA	CMB-C2B-C3B	2.48	129.32	124.68
37	21	204	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
37	41	204	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
39	5	101	BCR	C29-C30-C25	2.48	114.30	110.48
37	a	403	CLA	C6-C7-C8	-2.48	107.90	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	13	304	KC1	CMB-C2B-C1B	2.48	129.08	124.71
37	b	504	CLA	CHD-C4C-NC	2.48	128.11	124.20
37	b	511	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
37	37	301	CLA	CHD-C4C-NC	2.48	128.11	124.20
37	14	307	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
37	11	301	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
43	B	523	LHG	O8-C23-C24	2.48	119.68	111.91
37	16	307	CLA	O2A-CGA-CBA	2.48	119.68	111.91
37	39	301	CLA	CMA-C3A-C2A	-2.48	103.83	113.83
37	15	305	CLA	CMB-C2B-C3B	2.48	129.31	124.68
37	39	306	CLA	C3B-C4B-NB	2.48	112.41	109.21
48	12	213	A86	C7-C6-C8	2.48	121.98	118.08
37	13	305	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
37	A	403	CLA	C1-C2-C3	-2.48	121.76	126.04
37	20	308	CLA	O2A-CGA-CBA	2.48	119.68	111.91
43	b	522	LHG	O8-C23-C24	2.48	119.68	111.91
47	31	309	KC1	O1D-CGD-CBD	-2.48	119.42	124.48
37	36	307	CLA	O2A-CGA-CBA	2.47	119.67	111.91
37	16	309	CLA	CHD-C4C-NC	2.47	128.10	124.20
48	16	313	A86	C-C1-C2	-2.47	119.46	122.92
37	36	309	CLA	CHD-C4C-NC	2.47	128.10	124.20
37	38	206	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
48	12	217	A86	C22-C16-C17	-2.47	104.69	108.98
37	B	511	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
44	j	101	DGD	O5D-C6D-C5D	-2.47	104.47	109.05
37	b	502	CLA	CAC-C3C-C4C	2.47	128.02	124.81
37	41	206	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
37	32	210	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
47	11	309	KC1	O1D-CGD-CBD	-2.47	119.42	124.48
37	13	303	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
37	C	508	CLA	CHB-C4A-NA	2.47	127.93	124.51
43	17	316	LHG	O8-C23-C24	2.47	119.66	111.91
37	38	201	CLA	C1-O2A-CGA	2.47	122.93	116.44
37	b	503	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
37	12	205	CLA	CMC-C2C-C1C	2.47	128.80	125.04
48	14	313	A86	C36-C31-C32	-2.47	117.24	119.70
37	31	308	CLA	C1-C2-C3	-2.47	121.77	126.04
37	b	523	CLA	CMB-C2B-C3B	2.47	129.30	124.68
37	14	303	CLA	CHB-C4A-NA	2.47	127.93	124.51
44	J	101	DGD	O5D-C6D-C5D	-2.47	104.48	109.05
46	f	101	HEM	C4A-C3A-C2A	2.47	108.71	107.00
37	31	306	CLA	CBC-CAC-C3C	-2.47	105.62	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	15	311	A86	C8-C6-C5	-2.47	115.15	118.94
39	b	524	BCR	C11-C10-C9	-2.47	123.79	127.31
37	C	510	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
37	11	301	CLA	C3B-C4B-NB	2.47	112.40	109.21
37	31	302	CLA	C3B-C4B-NB	2.47	112.40	109.21
48	41	215	A86	C25-C24-C1	-2.47	119.48	126.42
37	39	302	CLA	O2A-CGA-CBA	2.47	119.65	111.91
39	d	405	BCR	C28-C27-C26	-2.47	109.67	114.08
37	13	307	CLA	C4D-CHA-C1A	-2.47	118.25	121.25
37	39	307	CLA	C3B-C4B-NB	2.47	112.40	109.21
48	39	311	A86	C8-C6-C5	-2.47	115.16	118.94
37	a	403	CLA	C1-C2-C3	-2.47	121.78	126.04
37	B	507	CLA	O2A-CGA-CBA	2.47	119.65	111.91
37	b	507	CLA	O2A-CGA-CBA	2.47	119.65	111.91
45	D	408	PL9	C22-C23-C24	-2.47	121.72	127.66
37	33	305	CLA	CAA-C2A-C3A	-2.47	106.03	112.78
37	19	306	CLA	C3B-C4B-NB	2.47	112.40	109.21
37	41	205	CLA	CHD-C4C-NC	2.47	128.09	124.20
37	a	403	CLA	CHB-C4A-NA	2.46	127.92	124.51
37	C	503	CLA	CMB-C2B-C3B	2.46	129.29	124.68
37	38	208	CLA	CMC-C2C-C1C	2.46	128.79	125.04
48	18	212	A86	C4-C3-C2	-2.46	118.43	123.47
37	B	508	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
37	16	303	CLA	CMB-C2B-C3B	2.46	129.29	124.68
50	41	216	DD6	C19-C18-C17	2.46	115.53	110.77
37	b	516	CLA	CHC-C1C-NC	2.46	127.94	124.20
48	33	311	A86	C20-C19-C18	-2.46	107.88	112.75
37	40	210	CLA	CMC-C2C-C1C	2.46	128.79	125.04
48	34	315	A86	C20-C19-C18	-2.46	107.88	112.75
37	14	310	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
37	11	308	CLA	C4-C3-C5	2.46	119.41	115.27
48	17	311	A86	C8-C6-C5	-2.46	115.16	118.94
37	15	308	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
37	36	301	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
47	13	302	KC1	CHB-C4A-NA	2.46	128.08	124.20
47	41	207	KC1	CHB-C4A-NA	2.46	128.08	124.20
37	31	306	CLA	CMB-C2B-C3B	2.46	129.28	124.68
48	21	211	A86	C9-C8-C6	-2.46	119.50	126.42
48	13	311	A86	C20-C19-C18	-2.46	107.88	112.75
50	21	216	DD6	C19-C18-C17	2.46	115.53	110.77
48	31	319	A86	C7-C6-C8	2.46	121.95	118.08
37	20	308	CLA	CMC-C2C-C1C	2.46	128.79	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	21	203	KC1	CMC-C2C-C1C	2.46	128.79	125.04
37	36	303	CLA	CHB-C4A-NA	2.46	127.91	124.51
48	32	214	A86	C7-C6-C8	2.46	121.95	118.08
37	19	310	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
37	19	310	CLA	CMB-C2B-C3B	2.46	129.28	124.68
37	11	305	CLA	CMA-C3A-C4A	-2.46	105.16	111.77
37	18	209	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
37	B	513	CLA	CMC-C2C-C1C	2.46	128.78	125.04
37	39	304	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
37	21	206	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
37	A	403	CLA	CHB-C4A-NA	2.46	127.91	124.51
41	A	408	LMG	C6-C5-C4	-2.46	107.25	113.00
50	41	212	DD6	C33-C32-C31	2.46	114.60	109.62
39	B	517	BCR	C27-C26-C25	2.46	126.30	122.73
37	19	306	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
39	D	407	BCR	C15-C16-C17	-2.46	118.44	123.47
45	d	406	PL9	C22-C23-C24	-2.46	121.74	127.66
47	33	304	KC1	CAC-C3C-C4C	2.46	128.00	124.81
37	B	508	CLA	C4-C3-C5	2.46	119.40	115.27
48	15	312	A86	C10-C9-C8	-2.46	115.55	123.22
37	35	310	CLA	CAC-C3C-C4C	2.46	128.00	124.81
39	d	405	BCR	C15-C16-C17	-2.46	118.44	123.47
37	B	503	CLA	O1D-CGD-CBD	-2.46	119.46	124.48
37	38	204	CLA	CMC-C2C-C1C	2.46	128.78	125.04
41	12	201	LMG	O3-C3-C2	-2.46	104.67	110.35
48	14	315	A86	C20-C19-C18	-2.46	107.89	112.75
48	17	320	A86	C40-C32-C31	-2.45	108.28	110.47
47	11	309	KC1	CMA-C3A-C2A	-2.45	122.29	128.30
37	35	310	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
48	11	319	A86	C7-C6-C8	2.45	121.94	118.08
48	37	310	A86	C10-C9-C8	-2.45	115.56	123.22
37	35	310	CLA	CMB-C2B-C3B	2.45	129.27	124.68
47	21	207	KC1	CHB-C4A-NA	2.45	128.07	124.20
37	c	507	CLA	CHB-C4A-NA	2.45	127.91	124.51
37	39	306	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
48	15	312	A86	C8-C6-C5	-2.45	115.18	118.94
45	d	406	PL9	C7-C3-C2	-2.45	120.07	123.30
37	D	402	CLA	CAC-C3C-C4C	2.45	127.99	124.81
37	b	508	CLA	C4-C3-C5	2.45	119.40	115.27
37	38	202	CLA	CBC-CAC-C3C	-2.45	105.67	112.43
37	c	511	CLA	CAA-CBA-CGA	-2.45	106.09	113.25
41	B	521	LMG	O6-C1-O1	-2.45	104.17	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	D	408	PL9	C7-C3-C2	-2.45	120.08	123.30
37	35	301	CLA	O2A-CGA-CBA	2.45	119.60	111.91
37	B	502	CLA	CAC-C3C-C4C	2.45	127.99	124.81
48	41	211	A86	C9-C8-C6	-2.45	119.53	126.42
47	40	206	KC1	C4C-C3C-C2C	-2.45	103.33	106.90
37	39	310	CLA	CMB-C2B-C3B	2.45	129.26	124.68
37	15	310	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
48	16	310	A86	C25-C26-C27	-2.45	123.81	127.31
48	17	314	A86	O-C13-C14	-2.45	116.68	121.66
47	14	306	KC1	CHB-C4A-NA	2.45	128.06	124.20
37	32	211	CLA	C4-C3-C5	2.45	119.39	115.27
37	B	506	CLA	CHB-C4A-NA	2.45	127.90	124.51
41	32	201	LMG	O3-C3-C2	-2.45	104.69	110.35
37	34	303	CLA	CHB-C4A-NA	2.45	127.90	124.51
41	b	520	LMG	O6-C1-O1	-2.45	104.18	109.97
37	21	205	CLA	CHD-C4C-NC	2.45	128.06	124.20
47	37	302	KC1	CHB-C1B-NB	-2.45	122.20	124.45
37	33	303	CLA	CHB-C4A-NA	2.45	127.90	124.51
37	31	302	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
37	38	208	CLA	CBC-CAC-C3C	-2.45	105.69	112.43
37	c	513	CLA	O2A-CGA-CBA	2.45	119.58	111.91
37	12	203	CLA	O2A-CGA-CBA	2.45	119.58	111.91
46	F	101	HEM	C4A-C3A-C2A	2.45	108.70	107.00
37	31	306	CLA	CMA-C3A-C4A	-2.45	105.20	111.77
37	32	204	CLA	O2A-CGA-CBA	2.45	119.58	111.91
37	33	307	CLA	C4D-CHA-C1A	-2.45	118.27	121.25
47	41	203	KC1	CMC-C2C-C1C	2.45	128.76	125.04
48	13	313	A86	C9-C10-C11	-2.44	119.42	126.61
48	33	313	A86	C9-C10-C11	-2.44	119.42	126.61
37	36	303	CLA	CMB-C2B-C3B	2.44	129.25	124.68
37	18	206	CLA	CAC-C3C-C4C	2.44	127.98	124.81
37	C	513	CLA	O2A-CGA-CBA	2.44	119.58	111.91
37	18	202	CLA	O2A-CGA-CBA	2.44	119.58	111.91
47	34	306	KC1	CHB-C4A-NA	2.44	128.05	124.20
37	C	504	CLA	C4C-C3C-C2C	-2.44	103.34	106.90
37	c	504	CLA	C4C-C3C-C2C	-2.44	103.34	106.90
37	19	304	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
39	b	518	BCR	C30-C25-C26	-2.44	119.17	122.61
41	a	410	LMG	C6-C5-C4	-2.44	107.28	113.00
37	C	505	CLA	O2A-CGA-CBA	2.44	119.57	111.91
37	c	505	CLA	O2A-CGA-CBA	2.44	119.57	111.91
37	38	209	CLA	C1-O2A-CGA	2.44	122.85	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	36	310	A86	C7-C6-C8	2.44	121.92	118.08
37	B	524	CLA	CMB-C2B-C3B	2.44	129.25	124.68
37	B	508	CLA	CAC-C3C-C4C	2.44	127.98	124.81
37	C	505	CLA	C1-C2-C3	-2.44	121.82	126.04
39	b	517	BCR	C27-C26-C25	2.44	126.27	122.73
38	a	405	PHO	C1B-NB-C4B	2.44	112.10	107.09
37	b	508	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
37	14	302	CLA	C4-C3-C5	2.44	119.38	115.27
48	36	310	A86	C25-C26-C27	-2.44	123.83	127.31
47	31	303	KC1	CHB-C4A-NA	2.44	128.05	124.20
50	21	212	DD6	C20-C19-C18	2.44	117.57	112.75
39	B	525	BCR	C11-C10-C9	-2.44	123.83	127.31
39	B	525	BCR	C27-C26-C25	2.44	126.27	122.73
37	11	305	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
37	15	301	CLA	O2A-CGA-CBA	2.44	119.56	111.91
37	C	511	CLA	CAA-CBA-CGA	-2.44	106.13	113.25
37	34	310	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
48	34	314	A86	C34-O4-C38	-2.44	113.36	117.90
47	37	305	KC1	CMB-C2B-C1B	2.44	129.01	124.71
43	d	408	LHG	O8-C23-C24	2.44	119.55	111.91
47	37	307	KC1	C1A-NA-C4A	-2.44	105.61	106.71
37	b	513	CLA	CMC-C2C-C1C	2.44	128.75	125.04
37	B	516	CLA	CHC-C1C-NC	2.44	127.90	124.20
47	40	207	KC1	CHB-C1B-NB	-2.44	122.22	124.45
37	13	307	CLA	O2A-CGA-CBA	2.43	119.55	111.91
37	33	301	CLA	CMB-C2B-C3B	2.43	129.23	124.68
47	20	305	KC1	CHB-C1B-NB	-2.43	122.22	124.45
47	31	309	KC1	CMA-C3A-C2A	-2.43	122.34	128.30
38	D	403	PHO	C1B-NB-C4B	2.43	112.09	107.09
37	C	507	CLA	CHB-C4A-NA	2.43	127.88	124.51
37	35	310	CLA	O1D-CGD-CBD	-2.43	119.50	124.48
37	37	301	CLA	C1-O2A-CGA	2.43	122.83	116.44
48	35	312	A86	C8-C6-C5	-2.43	115.21	118.94
48	15	316	A86	C36-C31-C32	-2.43	117.28	119.70
50	21	212	DD6	C33-C32-C31	2.43	114.55	109.62
37	39	310	CLA	CBC-CAC-C3C	-2.43	105.72	112.43
37	b	508	CLA	CAC-C3C-C4C	2.43	127.97	124.81
37	19	306	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
48	34	313	A86	C19-C18-C17	-2.43	106.08	110.77
48	17	312	A86	C41-C32-C31	-2.43	108.30	110.47
47	15	304	KC1	CMB-C2B-C1B	2.43	129.00	124.71
37	b	501	CLA	CBC-CAC-C3C	-2.43	105.73	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	12	205	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
37	c	503	CLA	CMB-C2B-C3B	2.43	129.22	124.68
37	33	303	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
47	11	302	KC1	CHB-C4A-NA	2.43	128.03	124.20
48	14	314	A86	C34-O4-C38	-2.43	113.37	117.90
37	16	303	CLA	CHB-C4A-NA	2.43	127.87	124.51
37	d	403	CLA	C1-C2-C3	-2.43	121.84	126.04
37	41	206	CLA	CMB-C2B-C3B	2.43	129.22	124.68
37	16	301	CLA	CBC-CAC-C3C	-2.43	105.74	112.43
37	12	210	CLA	C4-C3-C5	2.43	119.36	115.27
48	14	311	A86	C8-C6-C5	-2.43	115.22	118.94
45	D	404	PL9	C22-C23-C24	-2.43	121.81	127.66
37	39	310	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
47	33	304	KC1	O2D-CGD-O1D	-2.43	119.09	123.84
48	16	310	A86	C7-C6-C8	2.43	121.90	118.08
37	c	508	CLA	CHB-C4A-NA	2.43	127.87	124.51
47	14	309	KC1	CMB-C2B-C1B	2.43	128.99	124.71
48	38	215	A86	C8-C6-C5	2.43	122.66	118.94
37	11	307	CLA	C1-C2-C3	-2.43	121.85	126.04
37	32	202	CLA	C4-C3-C5	2.43	119.35	115.27
37	A	405	CLA	O2A-CGA-CBA	2.43	119.52	111.91
39	a	413	BCR	C15-C14-C13	-2.43	123.85	127.31
37	38	209	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
37	a	407	CLA	O2A-CGA-CBA	2.42	119.52	111.91
47	17	305	KC1	CHD-C4C-NC	2.42	127.88	124.20
37	c	505	CLA	C1-C2-C3	-2.42	121.85	126.04
37	D	405	CLA	C1-C2-C3	-2.42	121.85	126.04
48	35	311	A86	C8-C6-C5	-2.42	115.22	118.94
43	D	411	LHG	C20-C19-C18	-2.42	102.12	114.42
43	D	410	LHG	O8-C23-C24	2.42	119.51	111.91
43	a	412	LHG	C20-C19-C18	-2.42	102.13	114.42
37	C	501	CLA	CMC-C2C-C1C	2.42	128.73	125.04
39	b	524	BCR	C27-C26-C25	2.42	126.25	122.73
37	21	206	CLA	CMB-C2B-C3B	2.42	129.21	124.68
37	14	308	CLA	CED-O2D-CGD	2.42	121.41	115.94
37	20	301	CLA	CHB-C4A-NA	2.42	127.86	124.51
37	B	501	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
47	17	306	KC1	CMB-C2B-C1B	2.42	128.98	124.71
37	d	401	CLA	CAC-C3C-C4C	2.42	127.95	124.81
47	13	304	KC1	CAC-C3C-C4C	2.42	127.95	124.81
37	C	512	CLA	C4-C3-C5	2.42	119.34	115.27
37	33	305	CLA	CMB-C2B-C3B	2.42	129.20	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	12	212	CLA	CAC-C3C-C4C	2.42	127.95	124.81
37	B	509	CLA	CHB-C4A-NA	2.42	127.86	124.51
37	33	307	CLA	O2A-CGA-CBA	2.42	119.49	111.91
37	14	310	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
47	33	302	KC1	CHB-C4A-NA	2.42	128.01	124.20
39	B	517	BCR	C15-C14-C13	-2.42	123.86	127.31
37	34	302	CLA	C4-C3-C5	2.42	119.33	115.27
47	13	302	KC1	CBC-CAC-C3C	-2.42	105.77	112.43
37	11	303	CLA	C7-C6-C5	-2.42	106.80	113.36
37	13	301	CLA	CMB-C2B-C3B	2.42	129.20	124.68
37	21	208	CLA	CMC-C2C-C1C	2.42	128.72	125.04
37	W	101	CLA	CHB-C4A-NA	2.41	127.85	124.51
41	L	102	LMG	C1-C2-C3	-2.41	104.97	110.00
37	18	208	CLA	CHB-C4A-NA	2.41	127.85	124.51
47	15	302	KC1	CHB-C4A-NA	2.41	128.01	124.20
37	35	308	CLA	CHD-C4C-NC	2.41	128.01	124.20
37	35	310	CLA	CHB-C4A-NA	2.41	127.85	124.51
47	37	305	KC1	CHB-C4A-NA	2.41	128.00	124.20
48	14	313	A86	C19-C18-C17	-2.41	106.11	110.77
37	B	511	CLA	C7-C6-C5	-2.41	106.81	113.36
47	17	308	KC1	CMC-C2C-C1C	2.41	128.71	125.04
37	c	511	CLA	CMB-C2B-C3B	2.41	129.19	124.68
45	d	402	PL9	C22-C23-C24	-2.41	121.86	127.66
48	14	312	A86	C34-O4-C38	-2.41	113.41	117.90
47	13	309	KC1	CHB-C4A-NA	2.41	128.00	124.20
37	35	308	CLA	CMC-C2C-C1C	2.41	128.71	125.04
37	19	310	CLA	CBC-CAC-C3C	-2.41	105.79	112.43
37	b	511	CLA	C7-C6-C5	-2.41	106.82	113.36
48	15	311	A86	C7-C6-C8	2.41	121.87	118.08
37	15	310	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
50	41	212	DD6	C20-C19-C18	2.41	117.51	112.75
50	41	212	DD6	C22-C16-C17	2.41	113.17	108.98
47	32	209	KC1	CMC-C2C-C1C	2.41	128.71	125.04
48	32	216	A86	C3-C4-C5	-2.41	118.54	123.47
47	35	304	KC1	CAA-C2A-C1A	-2.41	113.68	124.75
37	b	506	CLA	CHB-C4A-NA	2.41	127.84	124.51
37	32	202	CLA	CAA-CBA-CGA	-2.41	106.22	113.25
37	c	511	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
48	35	312	A86	C41-C32-C31	-2.41	108.32	110.47
48	20	311	A86	C34-O4-C38	-2.41	113.41	117.90
47	33	302	KC1	CBC-CAC-C3C	-2.41	105.80	112.43
50	21	212	DD6	C4-C3-C2	-2.40	118.55	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B	518	BCR	C30-C25-C26	-2.40	119.23	122.61
47	33	309	KC1	CHB-C4A-NA	2.40	127.99	124.20
41	l	101	LMG	C1-C2-C3	-2.40	104.99	110.00
37	31	304	CLA	C7-C6-C5	-2.40	106.83	113.36
37	B	508	CLA	CHB-C4A-NA	2.40	127.84	124.51
37	C	511	CLA	CMB-C2B-C3B	2.40	129.18	124.68
47	34	309	KC1	CMB-C2B-C1B	2.40	128.95	124.71
48	32	217	A86	C7-C6-C8	2.40	121.86	118.08
37	w	101	CLA	CHB-C4A-NA	2.40	127.83	124.51
47	21	207	KC1	CMB-C2B-C1B	2.40	128.95	124.71
37	38	201	CLA	CMC-C2C-C1C	2.40	128.70	125.04
37	38	209	CLA	CMC-C2C-C1C	2.40	128.70	125.04
37	c	512	CLA	C4-C3-C5	2.40	119.31	115.27
47	12	208	KC1	CMC-C2C-C1C	2.40	128.70	125.04
37	17	302	CLA	CHD-C4C-NC	2.40	127.99	124.20
47	38	207	KC1	O1D-CGD-CBD	-2.40	119.57	124.48
47	17	306	KC1	CHB-C4A-NA	2.40	127.99	124.20
37	20	307	CLA	CMB-C2B-C3B	2.40	129.17	124.68
47	13	304	KC1	O2D-CGD-O1D	-2.40	119.14	123.84
37	11	310	CLA	CMC-C2C-C1C	2.40	128.69	125.04
41	L	102	LMG	O6-C1-O1	-2.40	104.29	109.97
47	17	305	KC1	CHB-C4A-NA	2.40	127.99	124.20
37	19	307	CLA	CMB-C2B-C3B	2.40	129.17	124.68
37	b	508	CLA	CHB-C4A-NA	2.40	127.83	124.51
47	37	307	KC1	CMC-C2C-C1C	2.40	128.69	125.04
37	15	310	CLA	CMB-C2B-C3B	2.40	129.17	124.68
47	16	308	KC1	CHB-C4A-NA	2.40	127.98	124.20
37	B	508	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
48	31	313	A86	C9-C8-C6	-2.40	119.68	126.42
39	b	517	BCR	C15-C14-C13	-2.40	123.89	127.31
47	17	305	KC1	O2D-CGD-O1D	-2.40	119.15	123.84
47	41	207	KC1	CMB-C2B-C1B	2.40	128.94	124.71
37	13	301	CLA	CBC-CAC-C3C	-2.40	105.83	112.43
43	21	217	LHG	C11-C10-C9	-2.40	102.26	114.42
48	40	213	A86	C34-O4-C38	-2.40	113.43	117.90
50	21	212	DD6	C22-C16-C17	2.40	113.15	108.98
43	37	321	LHG	C11-C10-C9	-2.40	102.26	114.42
37	16	307	CLA	CBC-CAC-C3C	-2.40	105.83	112.43
48	21	213	A86	C28-C27-C26	-2.40	119.57	122.92
37	19	307	CLA	C3B-C4B-NB	2.40	112.31	109.21
44	c	517	DGD	CBB-CAB-C9B	-2.40	102.27	114.42
37	C	511	CLA	O2D-CGD-O1D	-2.40	119.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	39	306	CLA	CBC-CAC-C3C	-2.39	105.83	112.43
37	W	102	CLA	CGD-CBD-CAD	-2.39	102.98	110.73
37	A	403	CLA	O2A-CGA-CBA	2.39	119.42	111.91
37	19	302	CLA	O2A-CGA-CBA	2.39	119.42	111.91
37	31	301	CLA	CGD-CBD-CAD	-2.39	102.98	110.73
37	39	302	CLA	CMC-C2C-C1C	2.39	128.68	125.04
37	11	308	CLA	CAA-CBA-CGA	-2.39	106.26	113.25
37	31	310	CLA	CMC-C2C-C1C	2.39	128.68	125.04
48	12	215	A86	C3-C4-C5	-2.39	118.57	123.47
37	b	511	CLA	C1-C2-C3	-2.39	121.91	126.04
37	40	209	CLA	CMB-C2B-C3B	2.39	129.15	124.68
47	35	304	KC1	CHB-C1B-NB	-2.39	122.26	124.45
44	C	517	DGD	CBB-CAB-C9B	-2.39	102.28	114.42
37	36	301	CLA	CHB-C4A-NA	2.39	127.82	124.51
37	39	307	CLA	C1-C2-C3	-2.39	121.91	126.04
37	13	305	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
41	L	102	LMG	O3-C3-C2	-2.39	104.82	110.35
47	32	209	KC1	CAB-C3B-C4B	2.39	130.67	124.90
39	A	410	BCR	C15-C14-C13	-2.39	123.90	127.31
47	16	304	KC1	O2A-CGA-O1A	-2.39	117.70	122.67
41	l	101	LMG	O6-C1-O1	-2.39	104.31	109.97
48	34	311	A86	C8-C6-C5	-2.39	115.27	118.94
37	34	308	CLA	CED-O2D-CGD	2.39	121.34	115.94
37	33	301	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
48	32	203	A86	C22-C16-C17	-2.39	104.83	108.98
37	15	303	CLA	CMC-C2C-C1C	2.39	128.68	125.04
37	b	508	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
41	l	101	LMG	O3-C3-C2	-2.39	104.83	110.35
37	c	506	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
37	14	308	CLA	CMC-C2C-C1C	2.39	128.68	125.04
37	B	510	CLA	CAA-CBA-CGA	-2.39	106.28	113.25
37	32	208	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
37	38	211	CLA	CHB-C4A-NA	2.39	127.81	124.51
37	a	403	CLA	O2A-CGA-CBA	2.39	119.40	111.91
43	41	201	LHG	O3-C3-C2	-2.39	99.48	109.69
50	41	212	DD6	C4-C3-C2	-2.39	118.58	123.47
37	12	204	CLA	CHA-C1A-NA	-2.39	120.93	126.40
37	19	306	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
37	21	209	CLA	CMB-C2B-C3B	2.39	129.14	124.68
47	14	306	KC1	O1D-CGD-CBD	-2.39	119.60	124.48
47	34	306	KC1	O1D-CGD-CBD	-2.39	119.60	124.48
37	20	301	CLA	O2A-CGA-CBA	2.39	119.40	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	32	212	KC1	CMB-C2B-C1B	2.39	128.92	124.71
48	37	313	A86	O-C13-C14	-2.39	116.81	121.66
47	36	304	KC1	O2A-CGA-O1A	-2.39	117.71	122.67
37	14	302	CLA	CMC-C2C-C1C	2.39	128.67	125.04
37	36	307	CLA	CBC-CAC-C3C	-2.39	105.86	112.43
48	35	314	A86	C28-C27-C26	-2.39	119.58	122.92
37	D	402	CLA	CHB-C4A-NA	2.38	127.81	124.51
48	32	216	A86	C23-C16-C22	-2.38	103.85	107.37
47	17	305	KC1	CMC-C2C-C1C	2.38	128.67	125.04
37	b	509	CLA	CHB-C4A-NA	2.38	127.81	124.51
37	40	203	CLA	CHB-C4A-NA	2.38	127.81	124.51
47	14	306	KC1	CBD-CHA-C1A	2.38	133.33	128.88
37	40	205	CLA	C1-C2-C3	-2.38	121.92	126.04
37	38	208	CLA	CHB-C4A-NA	2.38	127.81	124.51
48	37	311	A86	C40-C32-C31	-2.38	108.34	110.47
37	b	501	CLA	CMB-C2B-C3B	2.38	129.14	124.68
48	12	215	A86	C23-C16-C22	-2.38	103.86	107.37
43	D	410	LHG	C20-C19-C18	-2.38	102.33	114.42
44	J	101	DGD	O6E-C1E-O5D	-2.38	104.33	109.97
48	38	212	A86	C4-C3-C2	-2.38	118.59	123.47
37	B	515	CLA	CHD-C4C-NC	2.38	127.96	124.20
37	34	301	CLA	CHB-C4A-NA	2.38	127.81	124.51
37	12	207	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
37	38	208	CLA	C4-C3-C5	2.38	119.28	115.27
48	12	202	A86	C22-C16-C17	-2.38	104.85	108.98
37	33	303	CLA	CAA-C2A-C1A	2.38	119.78	111.97
37	41	202	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
47	33	304	KC1	CMC-C2C-C1C	2.38	128.66	125.04
37	b	510	CLA	CAA-CBA-CGA	-2.38	106.30	113.25
37	d	401	CLA	CHB-C4A-NA	2.38	127.80	124.51
37	36	307	CLA	CHB-C4A-NA	2.38	127.80	124.51
37	16	301	CLA	CBA-CAA-C2A	2.38	120.89	113.86
47	38	207	KC1	CMC-C2C-C1C	2.38	128.66	125.04
41	C	518	LMG	C40-C39-C38	-2.38	102.35	114.42
43	d	408	LHG	C20-C19-C18	-2.38	102.35	114.42
48	37	311	A86	O4-C34-C33	2.38	113.52	107.59
41	c	518	LMG	C40-C39-C38	-2.38	102.35	114.42
48	38	212	A86	C3-C4-C5	-2.38	118.60	123.47
48	15	314	A86	C8-C6-C5	-2.38	115.29	118.94
37	11	303	CLA	CHB-C4A-NA	2.38	127.80	124.51
46	F	101	HEM	CMB-C2B-C1B	-2.38	121.42	125.04
47	15	306	KC1	CHB-C1B-NB	-2.38	122.27	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	20	303	CLA	C1-C2-C3	-2.38	121.93	126.04
39	b	518	BCR	C40-C30-C25	2.38	114.16	110.30
37	c	501	CLA	CMC-C2C-C1C	2.38	128.66	125.04
48	17	312	A86	O4-C34-C33	2.38	113.51	107.59
47	12	211	KC1	CMB-C2B-C1B	2.38	128.90	124.71
37	15	308	CLA	CHD-C4C-NC	2.38	127.95	124.20
37	a	404	CLA	C4C-C3C-C2C	-2.38	103.43	106.90
48	35	314	A86	C8-C6-C5	-2.38	115.29	118.94
48	12	216	A86	C7-C6-C8	2.38	121.82	118.08
48	35	311	A86	C7-C6-C8	2.38	121.82	118.08
37	32	213	CLA	CAC-C3C-C4C	2.38	127.89	124.81
37	40	203	CLA	O2A-CGA-CBA	2.38	119.36	111.91
37	C	506	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
37	18	209	CLA	CMC-C2C-C1C	2.37	128.65	125.04
37	41	208	CLA	CMC-C2C-C1C	2.37	128.65	125.04
37	33	305	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
47	38	207	KC1	CHB-C4A-NA	2.37	127.94	124.20
37	17	302	CLA	C1-O2A-CGA	2.37	122.67	116.44
37	12	207	CLA	CAC-C3C-C4C	2.37	127.89	124.81
48	11	312	A86	C7-C6-C8	2.37	121.81	118.08
37	16	307	CLA	CMC-C2C-C1C	2.37	128.65	125.04
50	19	312	DD6	C10-C9-C8	-2.37	115.82	123.22
48	17	314	A86	C23-C16-C17	-2.37	104.86	108.98
37	12	210	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
37	32	205	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
37	c	503	CLA	CMC-C2C-C1C	2.37	128.65	125.04
37	19	302	CLA	CMC-C2C-C1C	2.37	128.65	125.04
48	34	312	A86	C34-O4-C38	-2.37	113.48	117.90
47	12	208	KC1	CAB-C3B-C4B	2.37	130.62	124.90
37	11	301	CLA	C4-C3-C5	2.37	119.26	115.27
48	37	313	A86	C23-C16-C17	-2.37	104.87	108.98
37	17	307	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
37	35	303	CLA	CMC-C2C-C1C	2.37	128.65	125.04
47	40	204	KC1	C4C-C3C-C2C	-2.37	103.44	106.90
37	34	302	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
37	14	303	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
50	39	312	DD6	C10-C9-C8	-2.37	115.83	123.22
37	36	301	CLA	CBA-CAA-C2A	2.37	120.85	113.86
37	32	205	CLA	CHA-C1A-NA	-2.37	120.98	126.40
37	Z	102	CLA	CAC-C3C-C4C	2.37	127.88	124.81
47	34	306	KC1	CBD-CHA-C1A	2.37	133.29	128.88
48	31	312	A86	C7-C6-C8	2.37	121.81	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	504	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
37	34	308	CLA	CMC-C2C-C1C	2.37	128.64	125.04
39	B	518	BCR	C40-C30-C25	2.37	114.14	110.30
37	16	307	CLA	CHB-C4A-NA	2.37	127.78	124.51
37	31	304	CLA	CHB-C4A-NA	2.37	127.78	124.51
37	41	210	CLA	CMB-C2B-C3B	2.37	129.10	124.68
47	36	308	KC1	CHB-C4A-NA	2.37	127.93	124.20
37	38	201	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
47	20	302	KC1	O2D-CGD-O1D	-2.37	119.21	123.84
37	15	310	CLA	CHB-C4A-NA	2.37	127.78	124.51
37	36	307	CLA	CMC-C2C-C1C	2.37	128.64	125.04
37	21	202	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
44	j	101	DGD	O6E-C1E-O5D	-2.37	104.37	109.97
37	B	511	CLA	C1-C2-C3	-2.36	121.95	126.04
37	19	307	CLA	C1-C2-C3	-2.36	121.95	126.04
37	b	515	CLA	CHD-C4C-NC	2.36	127.93	124.20
39	5	101	BCR	C24-C23-C22	-2.36	122.66	126.23
37	13	305	CLA	CMB-C2B-C3B	2.36	129.10	124.68
37	C	512	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
39	y	101	BCR	C37-C22-C21	-2.36	119.61	122.92
37	17	307	CLA	C1-C2-C3	-2.36	121.96	126.04
37	14	310	CLA	CMB-C2B-C3B	2.36	129.10	124.68
37	14	301	CLA	CHB-C4A-NA	2.36	127.78	124.51
37	20	308	CLA	CHB-C4A-NA	2.36	127.78	124.51
37	21	202	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
48	31	313	A86	C9-C10-C11	-2.36	119.66	126.61
50	41	216	DD6	C14-C13-C11	-2.36	121.86	125.53
37	D	401	CLA	C4C-C3C-C2C	-2.36	103.45	106.90
37	41	202	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
44	c	517	DGD	C3D-C4D-C5D	-2.36	106.03	110.24
37	35	307	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
37	b	509	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
37	41	209	CLA	CMB-C2B-C3B	2.36	129.09	124.68
48	31	314	A86	C36-C31-C32	-2.36	117.35	119.70
48	37	313	A86	C36-C31-C32	-2.36	117.35	119.70
48	15	315	A86	C40-C32-C31	-2.36	108.36	110.47
47	35	304	KC1	CMB-C2B-C1B	2.36	128.87	124.71
37	d	401	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
37	z	101	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
47	35	302	KC1	CHB-C4A-NA	2.36	127.92	124.20
37	C	507	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
37	16	301	CLA	CHB-C4A-NA	2.36	127.77	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C	517	DGD	O3E-C3E-C2E	-2.36	104.90	110.35
37	12	210	CLA	CMC-C2C-C1C	2.36	128.63	125.04
37	19	303	CLA	O2A-CGA-CBA	2.36	119.31	111.91
47	15	304	KC1	CAA-C2A-C1A	-2.36	113.91	124.75
37	21	209	CLA	CHB-C4A-NA	2.36	127.77	124.51
37	32	211	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
37	14	302	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
50	21	216	DD6	C14-C13-C11	-2.36	121.87	125.53
47	40	207	KC1	CHB-C4A-NA	2.36	127.92	124.20
48	39	313	A86	C41-C32-C31	-2.36	108.36	110.47
41	B	520	LMG	C40-C39-C38	-2.36	102.46	114.42
37	c	508	CLA	C1-C2-C3	-2.36	121.97	126.04
47	40	204	KC1	O2D-CGD-O1D	-2.36	119.23	123.84
41	17	317	LMG	O6-C1-O1	-2.36	104.39	109.97
48	41	213	A86	C28-C27-C26	-2.36	119.62	122.92
37	w	101	CLA	C4-C3-C5	2.35	119.23	115.27
37	32	208	CLA	CAC-C3C-C4C	2.35	127.86	124.81
37	b	515	CLA	CMC-C2C-C1C	2.35	128.62	125.04
48	35	311	A86	C23-C16-C22	-2.35	103.90	107.37
37	34	302	CLA	CMB-C2B-C3B	2.35	129.08	124.68
37	34	303	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
44	h	102	DGD	C3G-C2G-C1G	-2.35	106.22	111.79
37	37	306	CLA	CHA-C1A-NA	-2.35	121.01	126.40
47	17	308	KC1	C1A-NA-C4A	-2.35	105.65	106.71
37	18	201	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
47	20	302	KC1	C4C-C3C-C2C	-2.35	103.47	106.90
41	b	519	LMG	C40-C39-C38	-2.35	102.48	114.42
39	0	101	BCR	C24-C23-C22	-2.35	122.68	126.23
37	B	512	CLA	O2A-CGA-CBA	2.35	119.29	111.91
37	d	403	CLA	CMB-C2B-C3B	2.35	129.08	124.68
41	c	518	LMG	O3-C3-C2	-2.35	104.91	110.35
41	C	518	LMG	O3-C3-C2	-2.35	104.91	110.35
37	35	303	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
37	z	102	CLA	CAC-C3C-C4C	2.35	127.86	124.81
37	32	210	CLA	O2A-CGA-CBA	2.35	119.28	111.91
41	C	518	LMG	O2-C2-C1	-2.35	104.34	110.05
39	K	101	BCR	C37-C22-C21	-2.35	119.63	122.92
44	c	517	DGD	O3E-C3E-C2E	-2.35	104.92	110.35
37	31	302	CLA	C4-C3-C5	2.35	119.22	115.27
45	d	402	PL9	C20-C19-C21	2.35	119.22	115.27
37	18	211	CLA	CHD-C4C-NC	2.35	127.91	124.20
47	16	304	KC1	CHB-C4A-NA	2.35	127.91	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	501	CLA	CMB-C2B-C3B	2.35	129.07	124.68
37	32	206	CLA	CHB-C4A-NA	2.35	127.76	124.51
37	b	513	CLA	O2A-CGA-CBA	2.35	119.28	111.91
37	d	403	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
37	21	210	CLA	CMB-C2B-C3B	2.35	129.07	124.68
37	38	202	CLA	O2A-CGA-CBA	2.35	119.28	111.91
37	c	512	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
37	B	514	CLA	CMA-C3A-C2A	-2.35	104.36	113.83
37	37	308	CLA	CHB-C4A-NA	2.35	127.76	124.51
37	b	512	CLA	O2A-CGA-CBA	2.35	119.28	111.91
47	20	305	KC1	CHB-C4A-NA	2.35	127.90	124.20
48	33	315	A86	C4-C3-C2	-2.35	118.67	123.47
37	35	303	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
37	17	309	CLA	CHB-C4A-NA	2.35	127.76	124.51
37	38	209	CLA	CED-O2D-CGD	2.35	121.24	115.94
46	f	101	HEM	CMB-C2B-C1B	-2.35	121.47	125.04
48	17	312	A86	C25-C24-C1	-2.35	119.83	126.42
47	32	212	KC1	CGD-CBD-CAD	-2.35	103.14	110.73
37	c	507	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
37	38	204	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
37	12	209	CLA	O2A-CGA-CBA	2.35	119.27	111.91
44	H	102	DGD	C3G-C2G-C1G	-2.35	106.24	111.79
48	35	315	A86	C7-C6-C8	2.35	121.77	118.08
41	c	518	LMG	O2-C2-C1	-2.34	104.35	110.05
37	39	303	CLA	O2A-CGA-CBA	2.34	119.27	111.91
37	14	301	CLA	C1-C2-C3	-2.34	121.99	126.04
47	11	304	KC1	O2D-CGD-O1D	-2.34	119.25	123.84
37	20	306	CLA	CHB-C4A-NA	2.34	127.75	124.51
37	17	307	CLA	CHA-C1A-NA	-2.34	121.03	126.40
37	15	303	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
48	32	221	A86	C41-C32-C31	-2.34	108.37	110.47
47	31	303	KC1	CMC-C2C-C1C	2.34	128.61	125.04
37	D	402	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
37	31	304	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
47	15	304	KC1	CHB-C1B-NB	-2.34	122.30	124.45
37	32	211	CLA	CMC-C2C-C1C	2.34	128.61	125.04
37	Z	101	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
44	j	101	DGD	CAB-C9B-C8B	-2.34	102.53	114.42
47	15	306	KC1	CBC-CAC-C3C	-2.34	105.97	112.43
47	14	304	KC1	CAA-C2A-C1A	-2.34	113.98	124.75
37	C	513	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
37	b	511	CLA	CMC-C2C-C1C	2.34	128.61	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	514	CLA	CMA-C3A-C2A	-2.34	104.38	113.83
44	J	101	DGD	CAB-C9B-C8B	-2.34	102.53	114.42
37	B	504	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
37	37	306	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
37	12	204	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
47	36	304	KC1	CHB-C4A-NA	2.34	127.89	124.20
37	C	508	CLA	C1-C2-C3	-2.34	122.00	126.04
44	C	517	DGD	C3D-C4D-C5D	-2.34	106.06	110.24
37	11	303	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
47	12	211	KC1	CGD-CBD-CAD	-2.34	103.16	110.73
37	B	513	CLA	C4-C3-C5	2.34	119.21	115.27
37	C	506	CLA	CHA-C1A-NA	-2.34	121.04	126.40
37	B	509	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
37	21	208	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
47	31	305	KC1	O2D-CGD-O1D	-2.34	119.26	123.84
37	34	310	CLA	CMB-C2B-C3B	2.34	129.05	124.68
47	34	304	KC1	CAA-C2A-C1A	-2.34	114.00	124.75
41	a	410	LMG	C38-C37-C36	-2.34	102.56	114.42
43	B	523	LHG	C18-C17-C16	-2.34	102.56	114.42
37	14	308	CLA	C1-O2A-CGA	2.34	122.58	116.44
37	b	510	CLA	C4-C3-C5	2.34	119.20	115.27
37	19	310	CLA	C4-C3-C5	2.34	119.20	115.27
37	12	205	CLA	CHB-C4A-NA	2.34	127.74	124.51
37	40	210	CLA	CHB-C4A-NA	2.34	127.74	124.51
45	d	406	PL9	O1-C4-C3	-2.34	118.15	120.72
37	B	511	CLA	CMC-C2C-C1C	2.34	128.60	125.04
45	D	404	PL9	C20-C19-C21	2.34	119.20	115.27
37	D	405	CLA	CMB-C2B-C3B	2.34	129.05	124.68
37	w	101	CLA	CMC-C2C-C1C	2.34	128.60	125.04
37	18	204	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
37	38	204	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
48	17	312	A86	C19-C18-C17	-2.34	106.26	110.77
39	K	101	BCR	C35-C13-C14	-2.34	119.65	122.92
41	37	316	LMG	O6-C1-O1	-2.34	104.44	109.97
37	40	208	CLA	CHB-C4A-NA	2.34	127.74	124.51
48	41	214	A86	C10-C9-C8	-2.34	115.93	123.22
41	A	408	LMG	C38-C37-C36	-2.33	102.57	114.42
48	16	313	A86	C-C1-C24	-2.33	114.40	118.08
37	c	507	CLA	CBC-CAC-C3C	-2.33	105.99	112.43
37	B	510	CLA	C4-C3-C5	2.33	119.20	115.27
38	D	403	PHO	CMC-C2C-C3C	2.33	129.34	124.94
48	17	311	A86	C41-C32-C31	-2.33	108.38	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	35	306	KC1	CBC-CAC-C3C	-2.33	106.00	112.43
47	38	207	KC1	CHC-C4B-NB	-2.33	122.31	124.45
37	41	205	CLA	CMB-C2B-C3B	2.33	129.04	124.68
38	a	405	PHO	CMC-C2C-C3C	2.33	129.34	124.94
37	15	305	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
37	35	305	CLA	CMC-C2C-C1C	2.33	128.59	125.04
37	35	305	CLA	CMB-C2B-C3B	2.33	129.04	124.68
37	16	306	CLA	C1-C2-C3	-2.33	122.01	126.04
37	15	305	CLA	CMC-C2C-C1C	2.33	128.59	125.04
48	12	220	A86	C41-C32-C31	-2.33	108.39	110.47
37	c	513	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
37	20	301	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
37	D	401	CLA	CAC-C3C-C2C	2.33	131.52	127.53
37	39	310	CLA	C4-C3-C5	2.33	119.19	115.27
37	C	507	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
37	34	301	CLA	C1-C2-C3	-2.33	122.01	126.04
37	12	204	CLA	CHD-C4C-NC	2.33	127.88	124.20
37	32	205	CLA	CHD-C4C-NC	2.33	127.88	124.20
43	21	217	LHG	C27-C26-C25	-2.33	102.59	114.42
39	B	525	BCR	C7-C8-C9	-2.33	122.71	126.23
48	31	314	A86	C23-C16-C22	-2.33	103.93	107.37
47	34	304	KC1	O2D-CGD-O1D	-2.33	119.28	123.84
37	34	308	CLA	C1-O2A-CGA	2.33	122.56	116.44
50	20	310	DD6	C34-C35-C36	2.33	116.49	111.85
37	14	308	CLA	CMB-C2B-C3B	2.33	129.04	124.68
45	d	406	PL9	C46-C47-C48	-2.33	104.23	111.88
44	c	516	DGD	C1D-C2D-C3D	-2.33	105.15	110.00
48	40	201	A86	C-C1-C24	-2.33	114.41	118.08
43	37	321	LHG	C27-C26-C25	-2.33	102.60	114.42
37	16	306	CLA	C4-C3-C5	2.33	119.19	115.27
37	36	306	CLA	C4-C3-C5	2.33	119.19	115.27
48	31	312	A86	C40-C32-C31	-2.33	108.39	110.47
37	D	405	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
37	c	506	CLA	CHA-C1A-NA	-2.33	121.07	126.40
43	b	522	LHG	C18-C17-C16	-2.33	102.61	114.42
37	31	302	CLA	CMB-C2B-C3B	2.33	129.03	124.68
37	11	301	CLA	CMB-C2B-C3B	2.33	129.03	124.68
39	d	405	BCR	C33-C5-C6	-2.33	121.92	124.53
37	C	502	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
37	B	515	CLA	CMC-C2C-C1C	2.33	128.58	125.04
37	40	210	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
47	31	309	KC1	CHB-C1B-NB	-2.33	122.32	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	513	CLA	O2A-CGA-CBA	2.33	119.20	111.91
48	35	316	A86	C8-C6-C5	2.33	122.51	118.94
48	13	315	A86	C4-C3-C2	-2.33	118.71	123.47
37	41	209	CLA	CHB-C4A-NA	2.32	127.73	124.51
48	11	314	A86	C23-C16-C22	-2.32	103.94	107.37
48	15	316	A86	C22-C16-C17	-2.32	104.94	108.98
45	d	402	PL9	C36-C34-C33	-2.32	116.41	121.12
37	34	302	CLA	CMC-C2C-C1C	2.32	128.58	125.04
37	20	308	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
44	c	517	DGD	O6E-C1E-O5D	-2.32	104.47	109.97
39	y	101	BCR	C35-C13-C14	-2.32	119.67	122.92
37	18	209	CLA	CED-O2D-CGD	2.32	121.19	115.94
37	14	302	CLA	CMB-C2B-C3B	2.32	129.02	124.68
37	15	308	CLA	O2A-CGA-CBA	2.32	119.19	111.91
39	h	101	BCR	C15-C14-C13	-2.32	124.00	127.31
37	40	209	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
37	B	509	CLA	C1-C2-C3	-2.32	122.03	126.04
37	35	305	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
37	a	404	CLA	CAC-C3C-C2C	2.32	131.50	127.53
47	17	303	KC1	O2D-CGD-O1D	-2.32	119.30	123.84
47	11	309	KC1	CHB-C1B-NB	-2.32	122.32	124.45
37	C	506	CLA	CGD-CBD-CAD	-2.32	103.22	110.73
41	C	518	LMG	C38-C37-C36	-2.32	102.64	114.42
37	31	308	CLA	CAA-C2A-C1A	2.32	119.58	111.97
37	37	308	CLA	CHD-C4C-NC	2.32	127.86	124.20
48	31	319	A86	C19-C18-C17	-2.32	106.29	110.77
37	b	509	CLA	C1-C2-C3	-2.32	122.03	126.04
41	B	521	LMG	C1-C2-C3	-2.32	105.17	110.00
37	D	406	CLA	CMC-C2C-C1C	2.32	128.57	125.04
37	17	309	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
41	c	518	LMG	C38-C37-C36	-2.32	102.65	114.42
47	20	302	KC1	CMC-C2C-C1C	2.32	128.57	125.04
47	14	304	KC1	O2D-CGD-O1D	-2.32	119.31	123.84
37	b	513	CLA	C4-C3-C5	2.32	119.17	115.27
39	b	517	BCR	C33-C5-C6	-2.32	121.92	124.53
47	37	304	KC1	O2D-CGD-O1D	-2.32	119.31	123.84
47	39	308	KC1	CMC-C2C-C1C	2.32	128.57	125.04
47	40	206	KC1	CMC-C2C-C1C	2.32	128.57	125.04
50	20	312	DD6	C33-C34-C35	2.32	113.48	110.30
47	19	308	KC1	CBC-CAC-C3C	-2.32	106.04	112.43
47	17	303	KC1	CHB-C4A-NA	2.32	127.86	124.20
39	D	407	BCR	C11-C10-C9	-2.32	124.00	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	c	514	BCR	C27-C26-C25	2.32	126.09	122.73
37	36	309	CLA	CHB-C4A-NA	2.32	127.72	124.51
37	20	307	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
50	40	214	DD6	C33-C34-C35	2.32	113.47	110.30
37	b	511	CLA	CHB-C4A-NA	2.32	127.72	124.51
39	B	517	BCR	C33-C5-C6	-2.32	121.93	124.53
37	c	502	CLA	CBC-CAC-C3C	-2.32	106.05	112.43
37	36	306	CLA	C1-C2-C3	-2.32	122.04	126.04
47	39	308	KC1	CBC-CAC-C3C	-2.32	106.05	112.43
37	39	301	CLA	O2A-C1-C2	2.31	114.72	108.64
44	C	516	DGD	C1D-C2D-C3D	-2.31	105.17	110.00
48	13	315	A86	C23-C16-C17	-2.31	104.96	108.98
48	13	311	A86	C8-C6-C5	-2.31	115.39	118.94
47	37	302	KC1	CMC-C2C-C1C	2.31	128.56	125.04
37	35	307	CLA	CAA-C2A-C1A	2.31	119.56	111.97
37	37	303	CLA	C1-O2A-CGA	2.31	122.52	116.44
37	34	308	CLA	CMB-C2B-C3B	2.31	129.01	124.68
47	19	308	KC1	CHB-C1B-NB	-2.31	122.33	124.45
37	41	208	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
47	37	302	KC1	O2D-CGD-O1D	-2.31	119.31	123.84
48	21	215	A86	C10-C9-C8	-2.31	116.00	123.22
48	11	319	A86	C19-C18-C17	-2.31	106.31	110.77
37	20	303	CLA	CHA-C1A-NA	-2.31	121.10	126.40
37	19	307	CLA	C4-C3-C5	2.31	119.16	115.27
37	C	504	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
47	15	306	KC1	CHB-C4A-NA	2.31	127.85	124.20
37	W	101	CLA	CMC-C2C-C1C	2.31	128.56	125.04
37	11	307	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
48	14	311	A86	C4-C5-C6	-2.31	124.01	127.31
37	c	506	CLA	CGD-CBD-CAD	-2.31	103.25	110.73
37	C	507	CLA	O2A-CGA-CBA	2.31	119.16	111.91
47	18	207	KC1	O2A-CGA-O1A	-2.31	117.87	122.67
48	35	316	A86	C7-C6-C5	-2.31	119.69	122.92
47	13	304	KC1	CMC-C2C-C1C	2.31	128.56	125.04
47	40	204	KC1	CMC-C2C-C1C	2.31	128.56	125.04
37	19	301	CLA	O2A-C1-C2	2.31	114.71	108.64
37	40	205	CLA	CHA-C1A-NA	-2.31	121.11	126.40
37	c	507	CLA	O2A-CGA-CBA	2.31	119.16	111.91
37	B	507	CLA	CHC-C1C-NC	2.31	127.71	124.20
41	b	520	LMG	C1-C2-C3	-2.31	105.19	110.00
37	19	301	CLA	CMB-C2B-C3B	2.31	129.00	124.68
37	W	101	CLA	C4-C3-C5	2.31	119.16	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	16	303	CLA	C4-C3-C5	2.31	119.16	115.27
37	C	507	CLA	CMC-C2C-C1C	2.31	128.56	125.04
37	18	211	CLA	CHB-C4A-NA	2.31	127.70	124.51
37	18	209	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
48	15	312	A86	C41-C32-C31	-2.31	108.41	110.47
48	19	313	A86	C41-C32-C31	-2.31	108.41	110.47
48	21	214	A86	C10-C9-C8	-2.31	116.01	123.22
37	c	506	CLA	CHD-C4C-NC	2.31	127.84	124.20
39	C	514	BCR	C27-C26-C25	2.31	126.08	122.73
37	D	405	CLA	CMA-C3A-C2A	-2.31	104.52	113.83
37	C	512	CLA	CAA-C2A-C3A	-2.31	106.46	112.78
37	40	203	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
45	D	404	PL9	C36-C34-C33	-2.31	116.45	121.12
41	B	521	LMG	O3-C3-C2	-2.31	105.01	110.35
37	12	203	CLA	C1-C2-C3	-2.31	122.05	126.04
37	d	404	CLA	CMC-C2C-C1C	2.31	128.55	125.04
45	D	408	PL9	C46-C47-C48	-2.31	104.30	111.88
39	D	407	BCR	C29-C30-C25	2.31	114.03	110.48
48	35	316	A86	C36-C31-C32	-2.31	117.41	119.70
37	c	503	CLA	CAA-CBA-CGA	-2.31	106.51	113.25
37	C	503	CLA	CMC-C2C-C1C	2.31	128.55	125.04
47	15	306	KC1	CAA-C2A-C1A	-2.31	114.14	124.75
37	32	204	CLA	C1-C2-C3	-2.31	122.06	126.04
47	37	302	KC1	CHB-C4A-NA	2.31	127.84	124.20
40	b	521	SQD	O48-C23-O10	-2.31	117.77	123.59
37	11	310	CLA	CHB-C4A-NA	2.31	127.70	124.51
37	39	310	CLA	O2A-CGA-CBA	2.31	119.14	111.91
37	c	512	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
37	40	210	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
50	40	214	DD6	C37-C36-C35	-2.30	110.08	114.36
37	39	305	CLA	CMC-C2C-C1C	2.30	128.55	125.04
48	13	311	A86	C35-C34-C33	2.30	113.90	109.88
47	11	302	KC1	CMC-C2C-C1C	2.30	128.55	125.04
37	39	306	CLA	CHB-C4A-NA	2.30	127.70	124.51
48	11	312	A86	C40-C32-C31	-2.30	108.41	110.47
48	33	315	A86	C23-C16-C17	-2.30	104.98	108.98
37	B	502	CLA	O2A-CGA-CBA	2.30	119.13	111.91
37	39	307	CLA	C4-C3-C5	2.30	119.14	115.27
48	38	212	A86	C23-C16-C17	-2.30	104.98	108.98
39	D	407	BCR	C33-C5-C6	-2.30	121.94	124.53
41	d	409	LMG	C40-C39-C38	-2.30	102.74	114.42
50	40	212	DD6	C34-C35-C36	2.30	116.44	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	18	202	CLA	CED-O2D-CGD	2.30	121.14	115.94
37	18	209	CLA	C1-C2-C3	-2.30	122.06	126.04
37	33	307	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
39	H	101	BCR	C15-C14-C13	-2.30	124.03	127.31
37	c	511	CLA	CHB-C4A-NA	2.30	127.69	124.51
47	37	304	KC1	CHB-C4A-NA	2.30	127.83	124.20
47	13	302	KC1	C4B-C3B-C2B	-2.30	104.86	106.75
37	36	303	CLA	C4-C3-C5	2.30	119.14	115.27
48	15	314	A86	C28-C27-C26	-2.30	119.70	122.92
44	C	517	DGD	O6E-C1E-O5D	-2.30	104.53	109.97
47	35	306	KC1	CAA-C2A-C1A	-2.30	114.18	124.75
48	34	311	A86	C4-C5-C6	-2.30	124.03	127.31
37	13	307	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
41	D	412	LMG	C40-C39-C38	-2.30	102.76	114.42
37	21	205	CLA	CMB-C2B-C3B	2.30	128.98	124.68
37	31	301	CLA	O2A-CGA-CBA	2.30	119.12	111.91
37	d	403	CLA	CMA-C3A-C2A	-2.30	104.56	113.83
37	13	305	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
37	c	507	CLA	CMC-C2C-C1C	2.30	128.54	125.04
39	d	405	BCR	C29-C30-C25	2.30	114.02	110.48
37	15	307	CLA	CAA-C2A-C1A	2.30	119.50	111.97
47	20	304	KC1	CMC-C2C-C1C	2.30	128.54	125.04
47	33	302	KC1	CHB-C1B-C2B	-2.30	120.66	125.48
48	40	213	A86	C9-C10-C11	-2.30	119.86	126.61
48	33	311	A86	C35-C34-C33	2.30	113.88	109.88
39	b	524	BCR	C7-C8-C9	-2.30	122.77	126.23
37	B	504	CLA	O1D-CGD-CBD	-2.30	119.79	124.48
48	38	213	A86	C19-C18-C17	-2.29	106.34	110.77
37	W	102	CLA	O2A-CGA-CBA	2.29	119.11	111.91
37	11	307	CLA	CAA-C2A-C1A	2.29	119.50	111.97
37	C	512	CLA	CAC-C3C-C4C	2.29	127.79	124.81
37	34	302	CLA	CHA-C1A-NA	-2.29	121.14	126.40
50	20	312	DD6	C37-C36-C35	-2.29	110.11	114.36
47	19	308	KC1	CMC-C2C-C1C	2.29	128.53	125.04
45	D	404	PL9	C37-C38-C39	-2.29	122.14	127.66
40	B	522	SQD	O48-C23-O10	-2.29	117.81	123.59
50	41	212	DD6	C23-C16-C22	-2.29	103.99	107.37
48	15	319	A86	C8-C6-C5	-2.29	115.42	118.94
48	37	310	A86	C7-C6-C8	2.29	121.69	118.08
37	38	201	CLA	C4-C3-C5	2.29	119.13	115.27
47	35	306	KC1	O1D-CGD-CBD	-2.29	119.80	124.48
37	c	504	CLA	CAA-C2A-C3A	-2.29	106.50	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	509	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
37	b	502	CLA	O2A-CGA-CBA	2.29	119.10	111.91
37	c	505	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
37	31	308	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
37	c	509	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
48	18	212	A86	C3-C4-C5	-2.29	118.78	123.47
37	C	505	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
37	B	511	CLA	CHB-C4A-NA	2.29	127.68	124.51
45	D	408	PL9	C20-C19-C21	2.29	119.12	115.27
47	16	308	KC1	CMC-C2C-C1C	2.29	128.52	125.04
47	37	302	KC1	C4C-C3C-C2C	-2.29	103.56	106.90
37	b	509	CLA	C4-C3-C5	2.29	119.12	115.27
37	b	503	CLA	CMC-C2C-C1C	2.29	128.52	125.04
37	15	303	CLA	C4-C3-C5	2.29	119.12	115.27
45	D	408	PL9	O1-C4-C3	-2.29	118.20	120.72
48	20	311	A86	C9-C10-C11	-2.29	119.88	126.61
37	32	206	CLA	O1D-CGD-CBD	-2.29	119.81	124.48
37	37	308	CLA	CAC-C3C-C4C	2.29	127.78	124.81
37	C	503	CLA	CAA-CBA-CGA	-2.29	106.57	113.25
47	13	302	KC1	CHB-C1B-C2B	-2.29	120.68	125.48
37	32	211	CLA	CMB-C2B-C3B	2.29	128.96	124.68
37	15	307	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
41	31	316	LMG	O1-C7-C8	-2.29	105.38	110.90
37	35	303	CLA	C4-C3-C5	2.29	119.11	115.27
37	17	302	CLA	CAA-CBA-CGA	-2.28	106.58	113.25
37	37	308	CLA	C2A-C3A-C4A	-2.28	98.18	101.87
47	13	306	KC1	CMC-C2C-C1C	2.28	128.52	125.04
48	31	311	A86	C8-C6-C5	-2.28	115.44	118.94
37	b	503	CLA	CMB-C2B-C3B	2.28	128.95	124.68
48	14	313	A86	C4-C3-C2	-2.28	118.80	123.47
48	34	313	A86	C4-C3-C2	-2.28	118.80	123.47
37	C	506	CLA	CHD-C4C-NC	2.28	127.80	124.20
37	20	308	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
37	19	306	CLA	CHB-C4A-NA	2.28	127.67	124.51
47	35	306	KC1	CHB-C4A-NA	2.28	127.80	124.20
48	17	314	A86	C36-C31-C32	-2.28	117.43	119.70
37	16	309	CLA	CHB-C4A-NA	2.28	127.67	124.51
42	a	411	BCT	O3-C-O1	-2.28	113.63	119.55
37	35	308	CLA	O2A-CGA-CBA	2.28	119.07	111.91
41	b	520	LMG	O3-C3-C2	-2.28	105.07	110.35
48	35	315	A86	C40-C32-C31	-2.28	108.43	110.47
37	B	515	CLA	C1-C2-C3	-2.28	122.10	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	308	CLA	C1-C2-C3	-2.28	122.10	126.04
37	b	516	CLA	C4-C3-C5	2.28	119.11	115.27
48	16	311	A86	C8-C6-C5	-2.28	115.44	118.94
48	33	311	A86	C8-C6-C5	-2.28	115.44	118.94
37	41	206	CLA	CAC-C3C-C4C	2.28	127.77	124.81
37	38	206	CLA	CMC-C2C-C1C	2.28	128.51	125.04
37	21	208	CLA	C1-C2-C3	-2.28	122.10	126.04
37	31	310	CLA	CHB-C4A-NA	2.28	127.67	124.51
37	14	302	CLA	CHA-C1A-NA	-2.28	121.17	126.40
37	33	305	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
37	21	206	CLA	CAC-C3C-C4C	2.28	127.77	124.81
37	35	301	CLA	CHB-C4A-NA	2.28	127.67	124.51
37	b	504	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
47	18	207	KC1	CMC-C2C-C1C	2.28	128.51	125.04
48	37	311	A86	C19-C18-C17	-2.28	106.37	110.77
37	12	210	CLA	CHB-C4A-NA	2.28	127.66	124.51
39	a	413	BCR	C7-C8-C9	-2.28	122.79	126.23
37	B	503	CLA	CMC-C2C-C1C	2.28	128.51	125.04
47	16	308	KC1	CBC-CAC-C3C	-2.28	106.15	112.43
48	36	311	A86	C8-C6-C5	-2.28	115.44	118.94
39	d	405	BCR	C11-C10-C9	-2.28	124.06	127.31
47	33	306	KC1	CMC-C2C-C1C	2.28	128.51	125.04
48	13	315	A86	C22-C16-C17	-2.28	105.02	108.98
47	41	207	KC1	O1D-CGD-CBD	-2.28	119.82	124.48
48	11	312	A86	C19-C18-C17	2.28	115.17	110.77
37	b	511	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
37	B	503	CLA	CMB-C2B-C3B	2.28	128.94	124.68
37	c	509	CLA	CHB-C4A-NA	2.28	127.66	124.51
48	41	215	A86	C10-C9-C8	-2.28	116.11	123.22
48	35	319	A86	C8-C6-C5	-2.28	115.45	118.94
48	38	213	A86	C23-C16-C17	-2.28	105.03	108.98
48	37	312	A86	C-C1-C24	2.28	121.67	118.08
47	38	207	KC1	O2A-CGA-O1A	-2.28	117.94	122.67
37	41	208	CLA	C1-C2-C3	-2.28	122.11	126.04
48	17	311	A86	C4-C5-C6	-2.28	124.06	127.31
37	39	301	CLA	CMB-C2B-C3B	2.28	128.94	124.68
46	V	201	HEM	C4C-CHD-C1D	2.28	125.56	122.56
37	C	504	CLA	C1-C2-C3	-2.28	122.11	126.04
37	C	503	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
37	19	309	CLA	CBC-CAC-C3C	-2.28	106.16	112.43
37	B	514	CLA	CHB-C4A-NA	2.28	127.66	124.51
42	A	409	BCT	O3-C-O1	-2.27	113.64	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	b	515	CLA	C1-C2-C3	-2.27	122.11	126.04
47	38	205	KC1	O2D-CGD-O1D	-2.27	119.39	123.84
48	18	215	A86	C8-C6-C5	2.27	122.43	118.94
47	35	302	KC1	CHB-C1B-NB	-2.27	122.36	124.45
37	b	507	CLA	CHC-C1C-NC	2.27	127.65	124.20
37	B	509	CLA	C4-C3-C5	2.27	119.10	115.27
47	18	207	KC1	O1D-CGD-CBD	-2.27	119.83	124.48
37	c	504	CLA	C1-C2-C3	-2.27	122.11	126.04
41	11	316	LMG	O1-C7-C8	-2.27	105.42	110.90
48	11	311	A86	C8-C6-C5	-2.27	115.45	118.94
37	A	403	CLA	C11-C10-C8	-2.27	108.58	115.92
37	32	205	CLA	C4-C3-C5	2.27	119.09	115.27
50	39	312	DD6	C33-C32-C31	2.27	114.22	109.62
37	b	515	CLA	CMB-C2B-C3B	2.27	128.93	124.68
37	B	514	CLA	C4-C3-C5	2.27	119.09	115.27
43	D	410	LHG	C5-O7-C7	-2.27	112.20	117.79
50	21	212	DD6	C23-C16-C22	-2.27	104.02	107.37
45	d	402	PL9	O2-C1-C6	2.27	124.52	120.59
37	c	503	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
37	39	309	CLA	CMC-C2C-C1C	2.27	128.50	125.04
37	40	205	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
37	39	309	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
47	13	304	KC1	CBC-CAC-C3C	-2.27	106.17	112.43
47	36	308	KC1	CBC-CAC-C3C	-2.27	106.17	112.43
41	a	410	LMG	O2-C2-C1	-2.27	104.53	110.05
47	37	305	KC1	CHD-C4C-NC	2.27	127.65	124.20
50	19	312	DD6	C33-C32-C31	2.27	114.22	109.62
47	21	207	KC1	O1D-CGD-CBD	-2.27	119.84	124.48
45	d	406	PL9	C20-C19-C21	2.27	119.09	115.27
37	12	210	CLA	CMB-C2B-C3B	2.27	128.92	124.68
48	35	316	A86	C22-C16-C17	-2.27	105.04	108.98
48	31	314	A86	C4-C5-C6	-2.27	124.07	127.31
45	d	402	PL9	C37-C38-C39	-2.27	122.20	127.66
47	15	304	KC1	CBC-CAC-C3C	-2.27	106.18	112.43
37	15	308	CLA	CMB-C2B-C3B	2.27	128.92	124.68
37	18	201	CLA	C4-C3-C5	2.27	119.08	115.27
48	36	310	A86	C23-C16-C22	-2.27	104.03	107.37
48	39	313	A86	C3-C2-C1	-2.27	124.08	127.31
47	38	205	KC1	CHB-C4A-NA	2.27	127.78	124.20
37	15	308	CLA	C4-C3-C5	2.27	119.08	115.27
37	21	209	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
48	15	315	A86	C19-C18-C17	-2.27	106.40	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	33	315	A86	C22-C16-C17	-2.27	105.05	108.98
41	A	408	LMG	C40-C39-C38	-2.27	102.92	114.42
50	40	212	DD6	C3-C4-C5	-2.27	118.83	123.47
48	37	313	A86	C34-O4-C38	-2.27	113.67	117.90
43	37	315	LHG	C20-C19-C18	-2.27	102.92	114.42
37	a	403	CLA	C11-C10-C8	-2.27	108.60	115.92
37	z	102	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
37	15	307	CLA	CHA-C1A-NA	-2.26	121.21	126.40
37	34	310	CLA	CAC-C3C-C4C	2.26	127.75	124.81
37	12	205	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
37	B	515	CLA	CMB-C2B-C3B	2.26	128.91	124.68
50	20	310	DD6	C3-C4-C5	-2.26	118.84	123.47
48	19	311	A86	C10-C9-C8	-2.26	116.15	123.22
37	19	309	CLA	CHB-C4A-NA	2.26	127.64	124.51
37	41	206	CLA	C1-C2-C3	-2.26	122.13	126.04
37	34	308	CLA	C1-C2-C3	-2.26	122.13	126.04
37	19	309	CLA	CMC-C2C-C1C	2.26	128.48	125.04
47	36	308	KC1	CMC-C2C-C1C	2.26	128.48	125.04
48	39	311	A86	C10-C9-C8	-2.26	116.16	123.22
39	B	525	BCR	C33-C5-C6	-2.26	121.99	124.53
43	d	408	LHG	C5-O7-C7	-2.26	112.22	117.79
37	41	210	CLA	CHB-C4A-NA	2.26	127.64	124.51
37	37	301	CLA	CAA-CBA-CGA	-2.26	106.64	113.25
37	41	209	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
48	16	310	A86	C23-C16-C22	-2.26	104.03	107.37
37	B	516	CLA	C4-C3-C5	2.26	119.07	115.27
37	19	305	CLA	CMC-C2C-C1C	2.26	128.48	125.04
48	37	311	A86	C-C1-C24	2.26	121.64	118.08
47	18	205	KC1	CMB-C2B-C1B	2.26	128.69	124.71
37	c	512	CLA	CAC-C3C-C4C	2.26	127.74	124.81
41	a	410	LMG	C40-C39-C38	-2.26	102.96	114.42
48	20	309	A86	C25-C24-C1	-2.26	120.07	126.42
37	35	305	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
47	16	308	KC1	CBD-CHA-C1A	2.26	133.09	128.88
48	40	211	A86	C25-C24-C1	-2.26	120.08	126.42
41	A	408	LMG	O2-C2-C1	-2.26	104.56	110.05
37	35	307	CLA	CHA-C1A-NA	-2.26	121.23	126.40
47	17	303	KC1	C4C-C3C-C2C	-2.26	103.61	106.90
39	b	524	BCR	C33-C5-C6	-2.26	121.99	124.53
37	B	514	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
37	15	303	CLA	CAA-C2A-C1A	2.26	119.37	111.97
37	b	514	CLA	CBC-CAC-C3C	-2.26	106.21	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	31	312	A86	C19-C18-C17	2.26	115.13	110.77
47	15	306	KC1	O1D-CGD-CBD	-2.26	119.87	124.48
47	35	304	KC1	CED-O2D-CGD	2.26	121.04	115.94
37	34	307	CLA	O2A-CGA-CBA	2.26	118.98	111.91
37	41	209	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
43	17	316	LHG	C20-C19-C18	-2.25	102.98	114.42
37	C	509	CLA	CHB-C4A-NA	2.25	127.63	124.51
47	39	308	KC1	CHB-C1B-NB	-2.25	122.38	124.45
37	38	209	CLA	CAA-C2A-C3A	-2.25	106.60	112.78
37	Z	102	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
47	15	302	KC1	CGD-CBD-CAD	-2.25	103.43	110.73
46	v	201	HEM	C4C-CHD-C1D	2.25	125.53	122.56
37	39	309	CLA	CHB-C4A-NA	2.25	127.63	124.51
37	B	511	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
47	35	302	KC1	CGD-CBD-CAD	-2.25	103.43	110.73
37	18	206	CLA	CMC-C2C-C1C	2.25	128.47	125.04
37	c	506	CLA	CHC-C1C-NC	2.25	127.62	124.20
43	B	523	LHG	C27-C26-C25	-2.25	102.98	114.42
37	14	307	CLA	O2A-CGA-CBA	2.25	118.98	111.91
37	b	514	CLA	CHB-C4A-NA	2.25	127.63	124.51
37	C	510	CLA	CMC-C2C-C1C	2.25	128.47	125.04
37	41	208	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
37	19	307	CLA	CHA-C1A-NA	-2.25	121.24	126.40
37	b	514	CLA	C4-C3-C5	2.25	119.06	115.27
37	Z	102	CLA	CGD-CBD-CAD	-2.25	103.44	110.73
51	39	315	LMU	C1B-O1B-C4'	-2.25	112.39	117.96
47	38	205	KC1	CMC-C2C-C1C	2.25	128.47	125.04
37	33	308	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
37	35	303	CLA	CAA-C2A-C1A	2.25	119.35	111.97
48	33	314	A86	C-C1-C2	-2.25	119.77	122.92
37	17	304	CLA	C1-O2A-CGA	2.25	122.35	116.44
47	18	205	KC1	CHB-C4A-NA	2.25	127.75	124.20
51	19	315	LMU	C1B-O1B-C4'	-2.25	112.40	117.96
37	Z	101	CLA	C1-O2A-CGA	2.25	122.35	116.44
48	31	312	A86	C9-C10-C11	-2.25	119.99	126.61
37	C	511	CLA	CHB-C4A-NA	2.25	127.62	124.51
48	18	214	A86	C8-C6-C5	-2.25	115.49	118.94
37	12	205	CLA	O2A-CGA-CBA	2.25	118.96	111.91
48	31	314	A86	C-C1-C24	2.25	121.62	118.08
37	38	201	CLA	O2A-CGA-CBA	2.25	118.96	111.91
47	18	205	KC1	O2D-CGD-O1D	-2.25	119.44	123.84
37	13	308	CLA	CAA-C2A-C3A	-2.25	106.62	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	509	CLA	C7-C6-C5	-2.25	107.26	113.36
48	19	313	A86	C3-C2-C1	-2.25	124.10	127.31
37	12	204	CLA	C4-C3-C5	2.25	119.05	115.27
37	21	210	CLA	CMC-C2C-C1C	2.25	128.46	125.04
37	21	208	CLA	CBC-CAC-C3C	-2.25	106.24	112.43
47	17	306	KC1	CHD-C4C-NC	2.25	127.61	124.20
47	35	304	KC1	O2D-CGD-O1D	-2.25	119.45	123.84
48	38	212	A86	C3-C2-C1	-2.25	124.11	127.31
37	b	509	CLA	C7-C6-C5	-2.25	107.26	113.36
37	18	208	CLA	C4-C3-C5	2.25	119.05	115.27
37	34	310	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
47	36	308	KC1	CBD-CHA-C1A	2.24	133.07	128.88
37	35	307	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
37	c	506	CLA	C4-C3-C5	2.24	119.05	115.27
37	b	508	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
37	12	204	CLA	CHB-C4A-NA	2.24	127.61	124.51
37	38	209	CLA	CHB-C4A-NA	2.24	127.61	124.51
37	18	203	CLA	O2A-CGA-CBA	2.24	118.95	111.91
37	19	310	CLA	O2A-CGA-CBA	2.24	118.95	111.91
48	15	311	A86	C23-C16-C22	-2.24	104.06	107.37
37	11	308	CLA	CHB-C4A-NA	2.24	127.61	124.51
43	b	522	LHG	C27-C26-C25	-2.24	103.04	114.42
47	38	207	KC1	CAB-C3B-C4B	2.24	130.31	124.90
48	41	211	A86	C25-C24-C1	-2.24	120.12	126.42
37	32	206	CLA	O2A-CGA-CBA	2.24	118.94	111.91
43	d	407	LHG	C18-C17-C16	-2.24	103.04	114.42
47	33	304	KC1	CBC-CAC-C3C	-2.24	106.25	112.43
47	31	309	KC1	CGD-CBD-CAD	-2.24	103.47	110.73
47	16	305	KC1	CHB-C4A-NA	2.24	127.74	124.20
48	35	319	A86	C34-O4-C38	-2.24	113.72	117.90
37	B	508	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
37	39	307	CLA	CMB-C2B-C3B	2.24	128.87	124.68
37	32	210	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
48	20	309	A86	C7-C6-C5	-2.24	119.78	122.92
48	35	313	A86	C9-C8-C6	-2.24	120.12	126.42
37	32	211	CLA	CHB-C4A-NA	2.24	127.61	124.51
37	17	309	CLA	C2A-C3A-C4A	-2.24	98.25	101.87
43	D	409	LHG	C18-C17-C16	-2.24	103.06	114.42
43	17	316	LHG	C27-C26-C25	-2.24	103.06	114.42
43	21	201	LHG	O3-C3-C2	-2.24	100.12	109.69
37	12	203	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
48	17	313	A86	C-C1-C24	2.24	121.61	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	A	410	BCR	C7-C8-C9	-2.24	122.85	126.23
37	A	403	CLA	CMC-C2C-C1C	2.24	128.45	125.04
37	B	516	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
50	16	312	DD6	C34-C35-C36	2.24	116.31	111.85
37	38	202	CLA	CHA-C1A-NA	-2.24	121.27	126.40
37	38	202	CLA	CHB-C4A-NA	2.24	127.61	124.51
39	B	518	BCR	C11-C10-C9	-2.24	124.12	127.31
37	C	504	CLA	CMB-C2B-C3B	2.24	128.87	124.68
43	37	315	LHG	C27-C26-C25	-2.24	103.06	114.42
37	18	202	CLA	CAA-CBA-CGA	-2.24	106.72	113.25
37	d	401	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
47	37	302	KC1	CMB-C2B-C1B	2.24	128.66	124.71
47	15	304	KC1	CHB-C4A-NA	2.24	127.73	124.20
37	z	102	CLA	CGD-CBD-CAD	-2.24	103.49	110.73
37	D	402	CLA	CBC-CAC-C3C	-2.24	106.27	112.43
37	36	306	CLA	C1-O2A-CGA	2.24	122.31	116.44
37	39	307	CLA	CHA-C1A-NA	-2.24	121.28	126.40
48	11	314	A86	C-C1-C24	2.24	121.60	118.08
37	z	101	CLA	C1-O2A-CGA	2.24	122.31	116.44
37	31	310	CLA	CAC-C3C-C4C	2.24	127.71	124.81
47	32	212	KC1	CHC-C4B-NB	-2.24	122.40	124.45
37	21	206	CLA	C4-C3-C5	2.23	119.03	115.27
48	13	314	A86	C-C1-C2	-2.23	119.79	122.92
48	21	211	A86	C25-C24-C1	-2.23	120.14	126.42
37	15	305	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
37	12	204	CLA	CHD-C1D-ND	-2.23	122.40	124.45
47	19	308	KC1	CAC-C3C-C4C	2.23	127.71	124.81
48	32	217	A86	C8-C6-C5	-2.23	115.51	118.94
37	18	202	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
37	15	301	CLA	CHB-C4A-NA	2.23	127.60	124.51
37	33	310	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
37	C	506	CLA	C4-C3-C5	2.23	119.03	115.27
37	B	516	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
37	32	204	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
37	c	510	CLA	CMC-C2C-C1C	2.23	128.44	125.04
39	y	101	BCR	C34-C9-C10	-2.23	119.80	122.92
37	12	203	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
47	17	303	KC1	CMC-C2C-C1C	2.23	128.44	125.04
45	D	404	PL9	O2-C1-C6	2.23	124.45	120.59
47	33	304	KC1	CHB-C4A-NA	2.23	127.72	124.20
48	37	311	A86	C25-C24-C1	-2.23	120.15	126.42
37	18	206	CLA	CMB-C2B-C3B	2.23	128.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	15	307	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
39	a	408	BCR	C16-C15-C14	-2.23	118.91	123.47
48	19	311	A86	O4-C38-O5	-2.23	118.53	122.96
37	B	512	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
47	13	304	KC1	CHB-C4A-NA	2.23	127.72	124.20
37	18	202	CLA	CHB-C4A-NA	2.23	127.59	124.51
37	38	204	CLA	CHB-C4A-NA	2.23	127.59	124.51
39	K	101	BCR	C34-C9-C10	-2.23	119.80	122.92
37	b	516	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
47	38	210	KC1	CHB-C1B-NB	-2.23	122.41	124.45
47	16	305	KC1	O2D-CGD-O1D	-2.23	119.48	123.84
37	C	506	CLA	CHC-C1C-NC	2.23	127.58	124.20
47	14	304	KC1	CHB-C4A-NA	2.23	127.71	124.20
37	41	210	CLA	CMC-C2C-C1C	2.23	128.43	125.04
37	14	310	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
37	C	508	CLA	O2A-CGA-CBA	2.23	118.89	111.91
48	31	311	A86	C23-C16-C22	-2.23	104.09	107.37
37	B	512	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
37	32	202	CLA	CHB-C4A-NA	2.23	127.59	124.51
37	17	309	CLA	CHD-C4C-NC	2.23	127.71	124.20
37	14	310	CLA	CAC-C3C-C4C	2.23	127.70	124.81
47	38	205	KC1	CMB-C2B-C1B	2.22	128.63	124.71
37	41	209	CLA	CMC-C2C-C1C	2.22	128.43	125.04
41	16	316	LMG	O3-C3-C2	-2.22	105.21	110.35
47	11	309	KC1	CGD-CBD-CAD	-2.22	103.53	110.73
48	15	313	A86	C9-C8-C6	-2.22	120.17	126.42
37	17	307	CLA	CBA-CAA-C2A	-2.22	107.30	113.86
37	b	516	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
37	32	204	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
37	37	306	CLA	O2A-CGA-CBA	2.22	118.88	111.91
37	20	303	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
37	38	201	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
48	38	215	A86	C12-C11-C13	2.22	119.75	116.02
41	36	314	LMG	O3-C3-C2	-2.22	105.21	110.35
37	B	516	CLA	O2A-CGA-CBA	2.22	118.88	111.91
39	b	518	BCR	C11-C10-C9	-2.22	124.14	127.31
47	40	204	KC1	CAB-C3B-C4B	2.22	130.26	124.90
37	35	301	CLA	CMB-C2B-C3B	2.22	128.83	124.68
48	11	312	A86	C9-C10-C11	-2.22	120.08	126.61
47	16	304	KC1	CAA-C2A-C1A	-2.22	114.54	124.75
48	21	213	A86	C25-C24-C1	-2.22	120.18	126.42
41	b	519	LMG	O6-C1-O1	-2.22	104.72	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	D	410	LHG	C18-C17-C16	-2.22	103.16	114.42
47	31	307	KC1	CHB-C4A-NA	2.22	127.70	124.20
37	b	507	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
37	38	203	CLA	CHA-C1A-NA	-2.22	121.32	126.40
37	21	209	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
37	32	205	CLA	CHD-C1D-ND	-2.22	122.42	124.45
39	A	406	BCR	C16-C15-C14	-2.22	118.93	123.47
37	c	504	CLA	CMB-C2B-C3B	2.22	128.83	124.68
37	c	508	CLA	O2A-CGA-CBA	2.22	118.87	111.91
48	35	315	A86	C26-C25-C24	-2.22	116.29	123.22
47	33	309	KC1	CMC-C2C-C1C	2.22	128.42	125.04
37	11	310	CLA	CAC-C3C-C4C	2.22	127.69	124.81
48	38	214	A86	C40-C32-C31	-2.22	108.49	110.47
47	21	207	KC1	CHB-C1B-C2B	-2.22	120.83	125.48
37	35	308	CLA	C4-C3-C5	2.22	119.00	115.27
39	B	518	BCR	C38-C26-C27	-2.22	109.36	113.62
37	21	206	CLA	C1-C2-C3	-2.22	122.21	126.04
37	12	209	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
37	21	209	CLA	CMC-C2C-C1C	2.22	128.41	125.04
50	36	312	DD6	C34-C35-C36	2.22	116.27	111.85
48	11	314	A86	C4-C5-C6	-2.22	124.15	127.31
37	b	512	CLA	C1-C2-C3	-2.22	122.21	126.04
37	18	202	CLA	C4-C3-C5	2.22	119.00	115.27
37	32	206	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
40	17	301	SQD	O6-C1-C2	2.22	111.76	108.30
37	B	507	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
37	18	211	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
37	41	206	CLA	C4-C3-C5	2.21	119.00	115.27
37	C	513	CLA	CMB-C2B-C3B	2.21	128.82	124.68
47	31	305	KC1	CMC-C2C-C1C	2.21	128.41	125.04
37	b	512	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
47	17	303	KC1	CHC-C4B-C3B	-2.21	121.47	125.26
37	13	307	CLA	C1-C2-C3	-2.21	122.21	126.04
44	C	516	DGD	CBB-CAB-C9B	-2.21	103.18	114.42
47	12	211	KC1	O1D-CGD-CBD	-2.21	119.95	124.48
37	b	506	CLA	CHD-C4C-NC	2.21	127.69	124.20
41	B	520	LMG	O6-C1-O1	-2.21	104.73	109.97
37	32	205	CLA	CHB-C4A-NA	2.21	127.57	124.51
37	11	301	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
47	41	207	KC1	CHB-C1B-C2B	-2.21	120.84	125.48
48	15	319	A86	C34-O4-C38	-2.21	113.77	117.90
48	32	221	A86	C34-O4-C38	-2.21	113.77	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	18	204	CLA	CHB-C4A-NA	2.21	127.57	124.51
47	15	302	KC1	CMC-C2C-C1C	2.21	128.41	125.04
48	12	220	A86	C34-O4-C38	-2.21	113.77	117.90
37	38	211	CLA	CHD-C4C-NC	2.21	127.69	124.20
37	38	202	CLA	CAA-CBA-CGA	-2.21	106.79	113.25
47	20	302	KC1	CAB-C3B-C4B	2.21	130.24	124.90
48	16	314	A86	C3-C4-C5	-2.21	118.94	123.47
37	b	512	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
48	13	312	A86	C41-C32-C31	-2.21	108.49	110.47
39	d	405	BCR	C7-C8-C9	-2.21	122.89	126.23
37	18	203	CLA	CHA-C1A-NA	-2.21	121.33	126.40
37	20	303	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
44	c	516	DGD	CBB-CAB-C9B	-2.21	103.20	114.42
37	a	403	CLA	CMC-C2C-C1C	2.21	128.41	125.04
47	38	210	KC1	CBD-CHA-C1A	2.21	133.00	128.88
47	36	304	KC1	CAA-C2A-C1A	-2.21	114.59	124.75
37	11	308	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
47	18	210	KC1	CBD-CHA-C1A	2.21	133.00	128.88
37	39	303	CLA	CMB-C2B-C3B	2.21	128.81	124.68
37	19	307	CLA	CMC-C2C-C1C	2.21	128.40	125.04
37	C	513	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
48	21	214	A86	C25-C24-C1	-2.21	120.21	126.42
37	16	306	CLA	C1-O2A-CGA	2.21	122.24	116.44
47	40	204	KC1	CHB-C4A-NA	2.21	127.68	124.20
48	38	213	A86	C4-C3-C2	-2.21	118.95	123.47
37	17	309	CLA	OBD-CAD-C3D	-2.21	123.21	128.52
43	d	408	LHG	C18-C17-C16	-2.21	103.22	114.42
37	B	512	CLA	C1-C2-C3	-2.21	122.22	126.04
39	h	101	BCR	C7-C8-C9	-2.21	122.90	126.23
47	15	302	KC1	O1D-CGD-CBD	-2.21	119.97	124.48
37	19	303	CLA	CMB-C2B-C3B	2.21	128.81	124.68
48	11	311	A86	C23-C16-C22	-2.21	104.11	107.37
37	15	303	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
37	34	305	CLA	CBC-CAC-C3C	-2.21	106.35	112.43
37	13	303	CLA	C1-O2A-CGA	2.21	122.23	116.44
41	31	317	LMG	O1-C7-C8	-2.21	105.58	110.90
47	11	304	KC1	CMC-C2C-C1C	2.21	128.40	125.04
37	32	202	CLA	O2D-CGD-O1D	-2.21	119.53	123.84
39	b	518	BCR	C38-C26-C27	-2.21	109.38	113.62
37	14	305	CLA	CBC-CAC-C3C	-2.21	106.35	112.43
47	38	207	KC1	CBD-CHA-C1A	2.20	132.99	128.88
48	37	313	A86	C3-C2-C1	-2.20	124.16	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	13	309	KC1	CMC-C2C-C1C	2.20	128.40	125.04
37	13	308	CLA	CMB-C2B-C3B	2.20	128.80	124.68
37	40	205	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
37	11	310	CLA	C1-C2-C3	-2.20	122.23	126.04
37	b	516	CLA	O2A-CGA-CBA	2.20	118.82	111.91
47	32	212	KC1	O1D-CGD-CBD	-2.20	119.98	124.48
37	37	308	CLA	OBD-CAD-C3D	-2.20	123.22	128.52
47	17	306	KC1	CBD-CHA-C1A	2.20	132.99	128.88
47	37	305	KC1	CBD-CHA-C1A	2.20	132.99	128.88
47	12	208	KC1	CBC-CAC-C3C	-2.20	106.36	112.43
37	14	305	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
40	36	315	SQD	O48-C23-C24	2.20	118.82	111.91
47	13	309	KC1	CAB-C3B-C4B	2.20	130.21	124.90
47	15	304	KC1	O2D-CGD-O1D	-2.20	119.53	123.84
48	41	214	A86	C25-C24-C1	-2.20	120.23	126.42
37	21	205	CLA	CED-O2D-CGD	2.20	120.92	115.94
48	12	213	A86	C8-C6-C5	-2.20	115.56	118.94
48	37	310	A86	C41-C32-C31	-2.20	108.50	110.47
37	33	307	CLA	C1-C2-C3	-2.20	122.24	126.04
37	34	301	CLA	C4-C3-C5	2.20	118.97	115.27
48	15	315	A86	C26-C25-C24	-2.20	116.35	123.22
48	39	311	A86	O4-C38-O5	-2.20	118.59	122.96
48	18	214	A86	C40-C32-C31	-2.20	108.50	110.47
48	15	316	A86	C10-C9-C8	-2.20	116.36	123.22
48	31	315	A86	C8-C6-C5	-2.20	115.57	118.94
37	B	512	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
47	20	302	KC1	CHB-C4A-NA	2.20	127.67	124.20
37	20	303	CLA	CMB-C2B-C3B	2.20	128.79	124.68
37	14	303	CLA	C4-C3-C5	2.20	118.97	115.27
37	b	510	CLA	CHB-C4A-NA	2.20	127.55	124.51
37	31	302	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
47	11	306	KC1	CHB-C4A-NA	2.20	127.67	124.20
47	32	209	KC1	CHB-C4A-NA	2.20	127.67	124.20
37	a	407	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
41	b	520	LMG	C38-C37-C36	-2.20	103.27	114.42
41	17	317	LMG	O3-C3-C2	-2.20	105.27	110.35
47	17	303	KC1	CMB-C2B-C1B	2.20	128.58	124.71
48	41	213	A86	C25-C24-C1	-2.20	120.25	126.42
43	17	316	LHG	C18-C17-C16	-2.20	103.28	114.42
40	17	301	SQD	O48-C23-C24	2.20	118.80	111.91
41	D	412	LMG	C38-C37-C36	-2.20	103.28	114.42
37	41	204	CLA	C1-C2-C3	-2.20	122.25	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	14	301	CLA	C4-C3-C5	2.20	118.97	115.27
39	H	101	BCR	C7-C8-C9	-2.20	122.92	126.23
39	C	515	BCR	C27-C26-C25	2.20	125.92	122.73
48	11	315	A86	C8-C6-C5	-2.19	115.57	118.94
47	37	304	KC1	CHB-C1B-NB	-2.19	122.44	124.45
37	41	205	CLA	CED-O2D-CGD	2.19	120.90	115.94
37	12	210	CLA	CHD-C4C-NC	2.19	127.66	124.20
37	31	310	CLA	C1-C2-C3	-2.19	122.25	126.04
47	11	304	KC1	CMB-C2B-C1B	2.19	128.58	124.71
37	31	301	CLA	CMC-C2C-C1C	2.19	128.38	125.04
37	c	513	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
43	37	315	LHG	C18-C17-C16	-2.19	103.29	114.42
37	21	204	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
41	11	317	LMG	O1-C7-C8	-2.19	105.61	110.90
37	12	207	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
37	15	303	CLA	CHB-C4A-NA	2.19	127.54	124.51
37	21	210	CLA	CHB-C4A-NA	2.19	127.54	124.51
37	21	204	CLA	C1-C2-C3	-2.19	122.25	126.04
37	W	102	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
37	41	204	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
47	36	305	KC1	CHB-C4A-NA	2.19	127.66	124.20
48	15	316	A86	C8-C6-C5	2.19	122.30	118.94
37	c	513	CLA	CMB-C2B-C3B	2.19	128.78	124.68
37	40	205	CLA	CMB-C2B-C3B	2.19	128.78	124.68
48	32	214	A86	C8-C6-C5	-2.19	115.58	118.94
47	32	209	KC1	CBC-CAC-C3C	-2.19	106.39	112.43
40	36	315	SQD	O6-C1-C2	2.19	111.72	108.30
47	33	306	KC1	CHB-C4A-NA	2.19	127.65	124.20
48	37	314	A86	C25-C24-C1	-2.19	120.27	126.42
37	C	511	CLA	OBD-CAD-C3D	-2.19	123.25	128.52
37	32	208	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
37	c	510	CLA	CAC-C3C-C4C	2.19	127.65	124.81
37	19	310	CLA	CMC-C2C-C1C	2.19	128.37	125.04
39	C	514	BCR	C24-C23-C22	-2.19	122.93	126.23
39	c	514	BCR	C24-C23-C22	-2.19	122.93	126.23
47	20	304	KC1	CHB-C4A-NA	2.19	127.65	124.20
47	18	207	KC1	CBD-CHA-C1A	2.19	132.96	128.88
37	34	307	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
37	15	301	CLA	CMB-C2B-C3B	2.19	128.77	124.68
37	14	307	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
47	36	305	KC1	O2D-CGD-O1D	-2.19	119.56	123.84
39	c	515	BCR	C27-C26-C25	2.19	125.91	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	16	303	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
39	C	514	BCR	C31-C1-C6	2.19	113.84	110.30
37	33	308	CLA	CMB-C2B-C3B	2.19	128.77	124.68
37	15	308	CLA	CHB-C4A-NA	2.19	127.53	124.51
37	B	510	CLA	CMC-C2C-C1C	2.19	128.37	125.04
37	12	207	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
50	41	216	DD6	C9-C8-C6	-2.18	120.28	126.42
48	17	315	A86	C25-C24-C1	-2.18	120.28	126.42
48	36	313	A86	C3-C4-C5	-2.18	119.00	123.47
47	35	302	KC1	O1D-CGD-CBD	-2.18	120.02	124.48
41	d	409	LMG	C38-C37-C36	-2.18	103.34	114.42
48	11	313	A86	C-C1-C24	2.18	121.52	118.08
37	B	514	CLA	O2A-CGA-CBA	2.18	118.76	111.91
37	39	310	CLA	CMC-C2C-C1C	2.18	128.36	125.04
37	B	506	CLA	CHD-C4C-NC	2.18	127.64	124.20
37	19	305	CLA	O2A-CGA-CBA	2.18	118.76	111.91
37	b	512	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
37	34	303	CLA	C4-C3-C5	2.18	118.94	115.27
47	13	306	KC1	CHB-C4A-NA	2.18	127.64	124.20
47	33	309	KC1	CAB-C3B-C4B	2.18	130.17	124.90
47	13	302	KC1	CHC-C4B-NB	-2.18	122.45	124.45
48	15	319	A86	C3-C4-C5	-2.18	119.00	123.47
37	B	515	CLA	O2A-CGA-CBA	2.18	118.75	111.91
37	b	514	CLA	O2A-CGA-CBA	2.18	118.75	111.91
37	20	303	CLA	O2A-CGA-CBA	2.18	118.75	111.91
47	18	207	KC1	CBC-CAC-C3C	-2.18	106.42	112.43
37	35	307	CLA	C4-C3-C5	2.18	118.94	115.27
37	Z	102	CLA	CHB-C4A-NA	2.18	127.53	124.51
48	12	213	A86	C36-C31-C32	-2.18	117.53	119.70
41	B	521	LMG	C38-C37-C36	-2.18	103.36	114.42
47	20	302	KC1	CHB-C1B-C2B	-2.18	120.91	125.48
37	32	211	CLA	CHD-C4C-NC	2.18	127.64	124.20
37	38	211	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
37	A	405	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
37	B	510	CLA	CHB-C4A-NA	2.18	127.53	124.51
37	18	201	CLA	CHB-C4A-NA	2.18	127.53	124.51
47	31	305	KC1	CMB-C2B-C1B	2.18	128.55	124.71
37	34	305	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
47	18	207	KC1	CHB-C4A-NA	2.18	127.64	124.20
48	40	211	A86	C7-C6-C5	-2.18	119.87	122.92
48	12	216	A86	C8-C6-C5	-2.18	115.60	118.94
48	14	316	A86	C23-C16-C17	-2.18	105.20	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	20	307	CLA	CHB-C4A-NA	2.18	127.52	124.51
48	21	213	A86	C10-C9-C8	-2.18	116.42	123.22
37	18	209	CLA	CHB-C4A-NA	2.18	127.52	124.51
37	c	511	CLA	OBD-CAD-C3D	-2.18	123.28	128.52
37	31	301	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
41	37	316	LMG	O3-C3-C2	-2.18	105.32	110.35
48	11	311	A86	C9-C10-C11	-2.18	120.21	126.61
37	12	207	CLA	CMC-C2C-C1C	2.18	128.35	125.04
50	21	216	DD6	C9-C8-C6	-2.18	120.30	126.42
47	33	309	KC1	CHB-C1B-C2B	-2.18	120.92	125.48
44	j	101	DGD	CBB-CAB-C9B	-2.18	103.38	114.42
37	z	101	CLA	CAC-C3C-C4C	2.18	127.63	124.81
47	39	308	KC1	CAC-C3C-C4C	2.18	127.63	124.81
37	11	301	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
37	12	212	CLA	CMC-C2C-C1C	2.18	128.35	125.04
44	J	101	DGD	CBB-CAB-C9B	-2.18	103.38	114.42
45	d	402	PL9	O2-C1-C2	-2.18	116.80	121.78
37	35	303	CLA	CHB-C4A-NA	2.18	127.52	124.51
47	34	304	KC1	CHB-C4A-NA	2.17	127.63	124.20
47	40	206	KC1	CHB-C4A-NA	2.17	127.63	124.20
37	38	204	CLA	O2A-CGA-CBA	2.17	118.73	111.91
37	21	205	CLA	CHA-C1A-NA	-2.17	121.42	126.40
37	15	307	CLA	O1D-CGD-CBD	-2.17	120.03	124.48
47	18	205	KC1	CMC-C2C-C1C	2.17	128.35	125.04
37	40	205	CLA	O2A-CGA-CBA	2.17	118.73	111.91
37	39	307	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
47	35	304	KC1	CBC-CAC-C3C	-2.17	106.44	112.43
48	35	319	A86	C3-C4-C5	-2.17	119.02	123.47
37	31	302	CLA	CHA-C1A-NA	-2.17	121.42	126.40
37	b	515	CLA	O2A-CGA-CBA	2.17	118.73	111.91
37	41	204	CLA	CGD-CBD-CAD	-2.17	103.69	110.73
48	41	213	A86	C10-C9-C8	-2.17	116.43	123.22
37	35	308	CLA	CMB-C2B-C3B	2.17	128.74	124.68
37	32	208	CLA	CMC-C2C-C1C	2.17	128.35	125.04
37	36	303	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
40	16	315	SQD	C1-O5-C5	2.17	117.95	113.69
47	40	206	KC1	O2D-CGD-O1D	-2.17	119.59	123.84
47	40	207	KC1	CAA-CBA-CGA	-2.17	116.10	127.26
47	20	305	KC1	CAA-CBA-CGA	-2.17	116.10	127.26
37	34	301	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
37	B	516	CLA	C4-C3-C2	-2.17	118.11	123.68
39	c	514	BCR	C31-C1-C6	2.17	113.82	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	39	305	CLA	O2A-CGA-CBA	2.17	118.72	111.91
50	20	312	DD6	C3-C4-C5	-2.17	119.03	123.47
48	11	313	A86	C9-C10-C11	-2.17	120.23	126.61
48	17	320	A86	C22-C16-C17	-2.17	105.21	108.98
48	14	315	A86	C8-C6-C5	-2.17	115.61	118.94
37	41	202	CLA	C4-C3-C5	2.17	118.92	115.27
47	39	308	KC1	CAB-C3B-C4B	2.17	130.13	124.90
48	11	311	A86	C28-C27-C26	2.17	125.96	122.92
37	15	305	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
48	36	311	A86	C3-C4-C5	-2.17	119.03	123.47
37	31	302	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
48	32	214	A86	C36-C31-C32	-2.17	117.55	119.70
37	38	201	CLA	CMB-C2B-C3B	2.17	128.73	124.68
37	41	205	CLA	CHA-C1A-NA	-2.17	121.44	126.40
45	D	408	PL9	C50-C49-C48	-2.17	116.38	122.65
37	11	301	CLA	CHA-C1A-NA	-2.17	121.44	126.40
37	14	301	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
40	40	202	SQD	C1-O5-C5	2.17	117.94	113.69
37	b	513	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
37	20	303	CLA	CED-O2D-CGD	2.17	120.84	115.94
37	C	510	CLA	CAC-C3C-C4C	2.17	127.62	124.81
37	11	303	CLA	O2A-CGA-CBA	2.17	118.70	111.91
37	31	304	CLA	O2A-CGA-CBA	2.17	118.70	111.91
39	D	407	BCR	C7-C8-C9	-2.17	122.96	126.23
50	40	214	DD6	C3-C4-C5	-2.16	119.04	123.47
37	B	513	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
37	b	510	CLA	CMC-C2C-C1C	2.16	128.34	125.04
46	V	201	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
37	37	308	CLA	C4-C3-C5	2.16	118.91	115.27
37	19	307	CLA	CBC-CAC-C3C	-2.16	106.47	112.43
37	17	304	CLA	CMC-C2C-C1C	2.16	128.33	125.04
48	12	220	A86	C40-C32-C31	-2.16	108.54	110.47
43	D	411	LHG	C27-C26-C25	-2.16	103.44	114.42
47	36	305	KC1	CAA-C2A-C1A	-2.16	114.80	124.75
48	34	316	A86	C9-C10-C11	-2.16	120.25	126.61
37	37	303	CLA	CMC-C2C-C1C	2.16	128.33	125.04
37	32	206	CLA	CHA-C1A-NA	-2.16	121.44	126.40
48	17	314	A86	C23-C16-C22	-2.16	104.18	107.37
48	31	311	A86	C9-C10-C11	-2.16	120.25	126.61
47	12	208	KC1	CHB-C4A-NA	2.16	127.61	124.20
47	40	204	KC1	CHB-C1B-C2B	-2.16	120.94	125.48
48	32	221	A86	C40-C32-C31	-2.16	108.54	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	512	CLA	CMA-C3A-C2A	-2.16	105.11	113.83
38	A	404	PHO	CMC-C2C-C3C	2.16	129.02	124.94
48	17	310	A86	C3-C4-C5	-2.16	119.05	123.47
47	40	207	KC1	CBD-CHA-C1A	2.16	132.91	128.88
39	K	101	BCR	C1-C6-C5	-2.16	119.57	122.61
47	13	302	KC1	CAB-C3B-C4B	2.16	130.12	124.90
40	B	519	SQD	O48-C23-C24	2.16	118.69	111.91
37	W	101	CLA	C1-C2-C3	-2.16	122.31	126.04
48	34	316	A86	C23-C16-C17	-2.16	105.23	108.98
48	15	315	A86	C7-C6-C8	2.16	121.48	118.08
37	12	210	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
45	d	406	PL9	C50-C49-C48	-2.16	116.41	122.65
47	11	306	KC1	O2A-CGA-O1A	-2.16	118.18	122.67
47	16	305	KC1	CAA-C2A-C1A	-2.16	114.82	124.75
47	31	307	KC1	O2A-CGA-O1A	-2.16	118.19	122.67
48	17	312	A86	O1-C15-C14	-2.16	108.88	113.21
37	13	303	CLA	O2A-CGA-CBA	2.16	118.68	111.91
37	40	210	CLA	CHA-C1A-NA	-2.16	121.46	126.40
48	17	315	A86	C4-C3-C2	-2.16	119.05	123.47
43	a	412	LHG	C27-C26-C25	-2.16	103.47	114.42
37	32	208	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
37	35	307	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
37	z	102	CLA	CHB-C4A-NA	2.16	127.50	124.51
37	13	310	CLA	CHB-C4A-NA	2.16	127.50	124.51
37	39	302	CLA	CHB-C4A-NA	2.16	127.50	124.51
37	40	205	CLA	CED-O2D-CGD	2.16	120.82	115.94
37	32	213	CLA	CMC-C2C-C1C	2.16	128.32	125.04
37	C	504	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
37	b	512	CLA	CMA-C3A-C2A	-2.16	105.13	113.83
37	19	302	CLA	CHB-C4A-NA	2.16	127.49	124.51
47	20	304	KC1	O2D-CGD-O1D	-2.16	119.62	123.84
48	37	309	A86	C3-C4-C5	-2.16	119.06	123.47
47	38	207	KC1	CBC-CAC-C3C	-2.15	106.49	112.43
47	13	309	KC1	CHB-C1B-C2B	-2.15	120.96	125.48
37	21	204	CLA	CGD-CBD-CAD	-2.15	103.76	110.73
48	14	316	A86	C9-C10-C11	-2.15	120.27	126.61
37	12	205	CLA	CHA-C1A-NA	-2.15	121.47	126.40
39	y	101	BCR	C1-C6-C5	-2.15	119.58	122.61
48	33	315	A86	C26-C25-C24	-2.15	116.50	123.22
48	38	214	A86	C25-C24-C1	-2.15	120.37	126.42
37	B	504	CLA	CHB-C4A-NA	2.15	127.49	124.51
37	36	301	CLA	CMB-C2B-C3B	2.15	128.71	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B	517	BCR	C16-C15-C14	-2.15	119.06	123.47
43	D	411	LHG	C11-C10-C9	-2.15	103.49	114.42
47	33	302	KC1	CMC-C2C-C1C	2.15	128.32	125.04
37	13	307	CLA	OBD-CAD-C3D	-2.15	123.34	128.52
45	d	402	PL9	C50-C49-C48	-2.15	116.42	122.65
37	16	301	CLA	CMB-C2B-C3B	2.15	128.71	124.68
48	31	311	A86	C28-C27-C26	2.15	125.94	122.92
45	D	404	PL9	O2-C1-C2	-2.15	116.85	121.78
37	36	309	CLA	CAA-C2A-C1A	-2.15	104.92	111.97
37	35	308	CLA	C1-O2A-CGA	2.15	122.09	116.44
38	a	406	PHO	CMC-C2C-C3C	2.15	129.00	124.94
37	19	301	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
37	32	211	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
40	L	101	SQD	O48-C23-C24	2.15	118.66	111.91
46	f	101	HEM	C4D-ND-C1D	2.15	107.30	105.07
43	a	412	LHG	C11-C10-C9	-2.15	103.50	114.42
44	C	517	DGD	CAB-C9B-C8B	-2.15	103.50	114.42
37	C	511	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
48	36	313	A86	C7-C6-C5	-2.15	119.91	122.92
37	33	308	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
37	b	516	CLA	C4-C3-C2	-2.15	118.16	123.68
37	18	201	CLA	O2A-CGA-CBA	2.15	118.66	111.91
48	32	218	A86	C9-C8-C6	-2.15	120.38	126.42
48	11	312	A86	C34-O4-C38	-2.15	113.89	117.90
47	19	308	KC1	CAB-C3B-C4B	2.15	130.09	124.90
37	14	308	CLA	C4-C3-C5	2.15	118.89	115.27
47	39	308	KC1	CHB-C4A-NA	2.15	127.59	124.20
39	b	517	BCR	C16-C15-C14	-2.15	119.07	123.47
41	32	201	LMG	O2-C2-C1	-2.15	104.83	110.05
37	c	504	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
48	34	315	A86	C8-C6-C5	-2.15	115.65	118.94
37	20	308	CLA	CHA-C1A-NA	-2.15	121.48	126.40
47	38	210	KC1	CHC-C4B-NB	-2.15	122.48	124.45
37	Z	102	CLA	C2A-C3A-C4A	-2.15	98.40	101.87
41	31	316	LMG	O2-C2-C1	-2.15	104.83	110.05
48	13	315	A86	C26-C25-C24	-2.15	116.52	123.22
51	39	315	LMU	C2'-C3'-C4'	2.15	114.58	109.68
37	39	307	CLA	CMC-C2C-C1C	2.15	128.31	125.04
37	b	505	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
37	B	505	CLA	CBC-CAC-C3C	-2.15	106.52	112.43
47	32	207	KC1	CAB-C3B-C4B	2.15	130.08	124.90
47	33	306	KC1	CBD-CHA-C1A	2.15	132.88	128.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	512	CLA	CHA-C1A-NA	-2.15	121.48	126.40
44	c	517	DGD	CAB-C9B-C8B	-2.14	103.54	114.42
37	40	209	CLA	CMC-C2C-C1C	2.14	128.30	125.04
37	c	512	CLA	CHA-C1A-NA	-2.14	121.49	126.40
37	33	301	CLA	CHA-C1A-NA	-2.14	121.49	126.40
37	w	101	CLA	C1-C2-C3	-2.14	122.33	126.04
48	40	201	A86	C4-C3-C2	2.14	127.86	123.47
37	Z	102	CLA	CMC-C2C-C1C	2.14	128.30	125.04
47	20	305	KC1	CBD-CHA-C1A	2.14	132.88	128.88
48	16	311	A86	C3-C4-C5	-2.14	119.08	123.47
47	18	205	KC1	CHB-C1B-NB	-2.14	122.48	124.45
37	40	209	CLA	CHB-C4A-NA	2.14	127.47	124.51
47	35	302	KC1	CMC-C2C-C1C	2.14	128.30	125.04
47	35	304	KC1	CHB-C4A-NA	2.14	127.58	124.20
41	d	409	LMG	O3-C3-C2	-2.14	105.40	110.35
37	16	309	CLA	CAA-C2A-C1A	-2.14	104.96	111.97
47	18	210	KC1	CHB-C1B-NB	-2.14	122.49	124.45
37	33	307	CLA	OBD-CAD-C3D	-2.14	123.37	128.52
37	b	511	CLA	CHA-C1A-NA	-2.14	121.50	126.40
48	37	310	A86	C40-C32-C31	-2.14	108.56	110.47
37	12	207	CLA	CMA-C3A-C4A	-2.14	106.02	111.77
37	33	308	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
48	12	217	A86	C9-C8-C6	-2.14	120.40	126.42
37	38	201	CLA	CHB-C4A-NA	2.14	127.47	124.51
37	13	308	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
37	39	301	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
37	38	202	CLA	C4-C3-C5	2.14	118.87	115.27
39	H	101	BCR	C27-C26-C25	2.14	125.84	122.73
37	c	511	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
37	21	202	CLA	C4-C3-C5	2.14	118.87	115.27
47	13	306	KC1	CBD-CHA-C1A	2.14	132.87	128.88
37	b	523	CLA	CHB-C4A-NA	2.14	127.47	124.51
37	z	102	CLA	C2A-C3A-C4A	-2.14	98.41	101.87
45	D	408	PL9	C40-C39-C41	2.14	118.87	115.27
37	35	305	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
37	D	406	CLA	C1-C2-C3	-2.14	122.34	126.04
40	B	522	SQD	C44-O6-C1	2.14	117.92	113.74
37	W	102	CLA	CMC-C2C-C1C	2.14	128.29	125.04
43	37	315	LHG	C11-C10-C9	-2.14	103.57	114.42
48	13	314	A86	C3-C4-C5	-2.14	119.09	123.47
37	d	404	CLA	C1-C2-C3	-2.14	122.35	126.04
37	16	306	CLA	CMB-C2B-C1B	-2.14	125.18	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	41	201	LHG	C27-C26-C25	-2.14	103.58	114.42
37	20	303	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
47	37	302	KC1	CHC-C4B-C3B	-2.14	121.60	125.26
37	14	303	CLA	C1-C2-C3	-2.14	122.35	126.04
43	21	201	LHG	C27-C26-C25	-2.14	103.58	114.42
46	V	201	HEM	CAD-CBD-CGD	-2.14	109.01	113.60
37	D	405	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
48	16	314	A86	C7-C6-C5	-2.14	119.93	122.92
37	36	301	CLA	CED-O2D-CGD	2.14	120.77	115.94
41	17	317	LMG	O7-C10-O9	-2.14	118.54	123.70
47	33	302	KC1	CHC-C4B-NB	-2.13	122.49	124.45
37	20	307	CLA	CMC-C2C-C1C	2.13	128.29	125.04
48	37	309	A86	C12-C11-C13	2.13	119.61	116.02
41	11	316	LMG	O2-C2-C1	-2.13	104.86	110.05
37	39	303	CLA	C4-C3-C5	2.13	118.86	115.27
48	38	214	A86	C8-C6-C5	-2.13	115.67	118.94
37	b	504	CLA	CHB-C4A-NA	2.13	127.46	124.51
37	34	308	CLA	C4-C3-C5	2.13	118.86	115.27
48	36	310	A86	C8-C6-C5	-2.13	115.67	118.94
37	33	303	CLA	O2A-CGA-CBA	2.13	118.60	111.91
48	33	313	A86	C25-C24-C1	-2.13	120.43	126.42
37	b	501	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
48	37	319	A86	C19-C18-C17	-2.13	106.66	110.77
37	17	304	CLA	CHA-C1A-NA	-2.13	121.52	126.40
43	D	411	LHG	C18-C17-C16	-2.13	103.61	114.42
44	c	516	DGD	C1E-O6E-C5E	2.13	117.87	113.69
46	v	201	HEM	CAD-CBD-CGD	-2.13	109.02	113.60
39	h	101	BCR	C27-C26-C25	2.13	125.83	122.73
37	16	301	CLA	CED-O2D-CGD	2.13	120.76	115.94
43	a	412	LHG	C18-C17-C16	-2.13	103.61	114.42
48	40	213	A86	C3-C4-C5	-2.13	119.11	123.47
37	c	502	CLA	CHA-C1A-NA	-2.13	121.52	126.40
37	38	203	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
41	B	521	LMG	C40-C39-C38	-2.13	103.61	114.42
41	b	520	LMG	C40-C39-C38	-2.13	103.61	114.42
48	33	314	A86	C3-C4-C5	-2.13	119.11	123.47
37	36	301	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
48	32	215	A86	C34-O4-C38	-2.13	113.93	117.90
37	C	501	CLA	CHB-C4A-NA	2.13	127.46	124.51
45	D	404	PL9	C50-C49-C48	-2.13	116.49	122.65
37	c	509	CLA	CMC-C2C-C1C	2.13	128.28	125.04
48	21	213	A86	C-C1-C2	-2.13	119.94	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	12	203	CLA	CHA-C1A-NA	-2.13	121.52	126.40
47	17	306	KC1	CHC-C1C-NC	2.13	127.56	124.20
47	37	305	KC1	CHC-C1C-NC	2.13	127.56	124.20
37	b	504	CLA	C6-C7-C8	-2.13	109.04	115.92
48	21	213	A86	C12-C11-C13	2.13	119.60	116.02
37	13	301	CLA	CHA-C1A-NA	-2.13	121.53	126.40
46	v	201	HEM	CMA-C3A-C4A	-2.13	125.19	128.46
47	12	211	KC1	CHB-C1B-C2B	-2.13	121.02	125.48
47	35	309	KC1	CHB-C1B-C2B	-2.13	121.02	125.48
48	41	213	A86	C-C1-C2	-2.13	119.94	122.92
47	40	207	KC1	O2A-CGA-O1A	-2.13	118.25	122.67
48	40	211	A86	C9-C8-C6	-2.13	120.44	126.42
48	16	313	A86	C4-C3-C2	2.13	127.83	123.47
47	12	211	KC1	CHC-C4B-NB	-2.13	122.50	124.45
41	12	201	LMG	O2-C2-C1	-2.13	104.88	110.05
48	13	313	A86	C25-C24-C1	-2.13	120.44	126.42
47	12	206	KC1	CAB-C3B-C4B	2.13	130.03	124.90
37	37	303	CLA	CAA-C2A-C1A	2.13	118.94	111.97
50	21	212	DD6	C34-C35-C36	2.13	116.09	111.85
48	31	312	A86	C34-O4-C38	-2.13	113.94	117.90
37	38	211	CLA	O1D-CGD-CBD	-2.13	120.14	124.48
43	17	316	LHG	C11-C10-C9	-2.13	103.64	114.42
48	14	313	A86	O1-C15-C14	-2.13	108.94	113.21
48	34	313	A86	O1-C15-C14	-2.13	108.94	113.21
37	18	206	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
48	17	310	A86	C7-C6-C8	2.12	121.42	118.08
37	B	503	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
37	38	206	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
50	41	212	DD6	C34-C35-C36	2.12	116.09	111.85
44	C	516	DGD	C1E-O6E-C5E	2.12	117.86	113.69
37	36	306	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
47	33	302	KC1	CAB-C3B-C4B	2.12	130.03	124.90
48	12	214	A86	C34-O4-C38	-2.12	113.94	117.90
37	32	208	CLA	CMA-C3A-C4A	-2.12	106.06	111.77
37	B	504	CLA	C6-C7-C8	-2.12	109.06	115.92
37	13	307	CLA	CMA-C3A-C4A	-2.12	106.07	111.77
37	33	307	CLA	CMA-C3A-C4A	-2.12	106.07	111.77
47	32	212	KC1	CHB-C1B-NB	-2.12	122.50	124.45
37	16	303	CLA	O2A-CGA-CBA	2.12	118.57	111.91
48	13	314	A86	C28-C27-C26	-2.12	119.95	122.92
37	40	210	CLA	CAA-C2A-C1A	2.12	118.93	111.97
47	15	302	KC1	CHB-C1B-NB	-2.12	122.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	20	308	CLA	CAA-C2A-C1A	2.12	118.93	111.97
37	19	303	CLA	C4-C3-C5	2.12	118.84	115.27
48	20	311	A86	C3-C4-C5	-2.12	119.13	123.47
37	32	210	CLA	C6-C5-C3	-2.12	111.15	114.62
48	33	314	A86	C22-C16-C17	-2.12	105.30	108.98
48	37	311	A86	O1-C15-C14	-2.12	108.95	113.21
41	D	412	LMG	O3-C3-C2	-2.12	105.44	110.35
37	13	308	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
37	c	501	CLA	O2A-C1-C2	2.12	114.21	108.64
48	20	309	A86	C9-C8-C6	-2.12	120.46	126.42
47	38	205	KC1	CHB-C1B-NB	-2.12	122.50	124.45
43	D	410	LHG	O8-C6-C5	-2.12	102.26	108.43
47	14	309	KC1	CGD-CBD-CAD	-2.12	103.87	110.73
47	33	302	KC1	C4B-C3B-C2B	-2.12	105.01	106.75
41	37	316	LMG	O7-C10-O9	-2.12	118.58	123.70
37	38	204	CLA	C1-C2-C3	-2.12	122.38	126.04
37	c	505	CLA	C4-C3-C5	2.12	118.83	115.27
37	b	503	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
37	B	511	CLA	CHA-C1A-NA	-2.12	121.55	126.40
37	34	303	CLA	C1-C2-C3	-2.12	122.38	126.04
37	A	403	CLA	C11-C12-C13	-2.12	109.07	115.92
37	14	303	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
37	40	205	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
48	36	311	A86	C23-C16-C22	-2.12	104.25	107.37
37	Z	101	CLA	CAC-C3C-C4C	2.12	127.56	124.81
37	17	304	CLA	O2A-CGA-CBA	2.12	118.55	111.91
37	19	304	CLA	CMC-C2C-C1C	2.12	128.26	125.04
37	c	508	CLA	C4-C3-C5	2.12	118.83	115.27
37	C	501	CLA	O2A-C1-C2	2.12	114.20	108.64
48	17	314	A86	C34-O4-C38	-2.12	113.95	117.90
37	B	524	CLA	CHB-C4A-NA	2.12	127.44	124.51
48	15	316	A86	C7-C6-C5	-2.12	119.96	122.92
48	37	313	A86	C23-C16-C22	-2.12	104.25	107.37
37	d	403	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
37	20	307	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
41	37	316	LMG	C6-C5-C4	-2.12	108.05	113.00
48	39	311	A86	C23-C16-C22	-2.12	104.25	107.37
37	39	304	CLA	CMC-C2C-C1C	2.12	128.26	125.04
47	34	309	KC1	CGD-CBD-CAD	-2.11	103.88	110.73
48	35	314	A86	C12-C11-C13	2.11	119.58	116.02
37	36	303	CLA	O2A-CGA-CBA	2.11	118.54	111.91
37	18	204	CLA	CAA-C2A-C1A	2.11	118.90	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	41	213	A86	C12-C11-C13	2.11	119.57	116.02
47	19	308	KC1	CHB-C4A-NA	2.11	127.53	124.20
47	36	305	KC1	O1D-CGD-CBD	-2.11	120.16	124.48
47	12	206	KC1	CHB-C4A-NA	2.11	127.53	124.20
43	D	410	LHG	C27-C26-C25	-2.11	103.70	114.42
51	19	315	LMU	C2'-C3'-C4'	2.11	114.51	109.68
37	z	102	CLA	CMC-C2C-C1C	2.11	128.26	125.04
48	13	313	A86	O4-C34-C33	2.11	112.85	107.59
39	C	514	BCR	C16-C15-C14	-2.11	119.15	123.47
37	C	509	CLA	C12-C11-C10	-2.11	103.53	113.24
37	C	508	CLA	C4-C3-C5	2.11	118.83	115.27
50	39	312	DD6	C41-C32-C31	-2.11	107.11	110.47
37	C	502	CLA	CHA-C1A-NA	-2.11	121.56	126.40
37	a	407	CLA	CMB-C2B-C3B	2.11	128.63	124.68
48	37	309	A86	C7-C6-C8	2.11	121.41	118.08
40	b	521	SQD	C44-O6-C1	2.11	117.86	113.74
37	34	303	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
39	C	519	BCR	C15-C14-C13	-2.11	124.30	127.31
37	16	301	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
47	20	305	KC1	O2A-CGA-O1A	-2.11	118.28	122.67
37	B	501	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
37	38	208	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
47	14	306	KC1	CMC-C2C-C1C	2.11	128.25	125.04
48	37	314	A86	C4-C3-C2	-2.11	119.15	123.47
37	16	306	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
41	A	408	LMG	O3-C3-C2	-2.11	105.47	110.35
48	14	312	A86	C8-C6-C5	-2.11	115.70	118.94
48	35	312	A86	C4-C5-C6	-2.11	124.30	127.31
47	32	207	KC1	CHB-C4A-NA	2.11	127.53	124.20
48	34	312	A86	C8-C6-C5	-2.11	115.70	118.94
37	B	503	CLA	CHB-C4A-NA	2.11	127.43	124.51
37	A	405	CLA	CMB-C2B-C3B	2.11	128.62	124.68
50	16	312	DD6	C10-C9-C8	-2.11	116.64	123.22
43	d	408	LHG	C27-C26-C25	-2.11	103.72	114.42
37	37	306	CLA	CBA-CAA-C2A	-2.11	107.64	113.86
37	c	509	CLA	C12-C11-C10	-2.11	103.55	113.24
48	35	315	A86	C19-C18-C17	-2.11	106.70	110.77
48	14	316	A86	C26-C25-C24	-2.11	116.64	123.22
41	11	317	LMG	O3-C3-C2	-2.11	105.48	110.35
48	18	214	A86	C34-O4-C38	-2.11	113.97	117.90
47	16	305	KC1	O1D-CGD-CBD	-2.11	120.17	124.48
37	12	209	CLA	C6-C5-C3	-2.11	111.17	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	20	306	CLA	CHA-C1A-NA	-2.11	121.57	126.40
45	d	406	PL9	C40-C39-C41	2.11	118.81	115.27
37	18	203	CLA	CHC-C1C-NC	2.11	127.40	124.20
37	14	303	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
37	C	509	CLA	CMC-C2C-C1C	2.11	128.25	125.04
48	20	311	A86	O1-C15-C14	2.11	117.44	113.21
37	11	303	CLA	CHA-C1A-NA	-2.11	121.58	126.40
37	37	303	CLA	O2A-CGA-CBA	2.11	118.52	111.91
47	15	302	KC1	CBB-CAB-C3B	-2.11	117.14	127.62
39	K	101	BCR	C29-C30-C25	2.11	113.72	110.48
41	31	317	LMG	O3-C3-C2	-2.11	105.48	110.35
39	A	410	BCR	C33-C5-C6	-2.11	122.16	124.53
48	40	213	A86	O1-C15-C14	2.10	117.43	113.21
37	33	303	CLA	C1-O2A-CGA	2.10	121.97	116.44
44	C	517	DGD	C5B-C4B-C3B	-2.10	103.74	114.42
47	35	304	KC1	O1D-CGD-CBD	-2.10	120.18	124.48
37	37	303	CLA	CHA-C1A-NA	-2.10	121.58	126.40
37	31	304	CLA	CHA-C1A-NA	-2.10	121.58	126.40
37	18	202	CLA	CHC-C1C-NC	2.10	127.39	124.20
37	18	204	CLA	O2A-CGA-CBA	2.10	118.51	111.91
37	b	515	CLA	C11-C10-C8	-2.10	109.12	115.92
47	13	306	KC1	O2D-CGD-O1D	-2.10	119.73	123.84
37	32	204	CLA	CHA-C1A-NA	-2.10	121.58	126.40
48	33	312	A86	C41-C32-C31	-2.10	108.59	110.47
37	34	301	CLA	CMB-C2B-C3B	2.10	128.61	124.68
39	h	101	BCR	C11-C10-C9	-2.10	124.31	127.31
37	38	201	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
47	33	306	KC1	O2D-CGD-O1D	-2.10	119.73	123.84
43	d	408	LHG	O8-C6-C5	-2.10	102.32	108.43
47	17	308	KC1	CHB-C1B-C2B	-2.10	121.07	125.48
37	W	101	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
48	32	217	A86	C23-C16-C22	-2.10	104.27	107.37
47	33	309	KC1	O1D-CGD-CBD	-2.10	120.19	124.48
48	31	313	A86	C-C1-C24	2.10	121.39	118.08
44	J	101	DGD	C8B-C7B-C6B	-2.10	103.77	114.42
47	36	304	KC1	CMC-C2C-C1C	2.10	128.24	125.04
48	33	313	A86	O4-C34-C33	2.10	112.82	107.59
48	16	310	A86	C8-C6-C5	-2.10	115.72	118.94
41	a	410	LMG	O3-C3-C2	-2.10	105.50	110.35
48	17	310	A86	C12-C11-C13	2.10	119.55	116.02
39	c	514	BCR	C16-C15-C14	-2.10	119.18	123.47
45	d	406	PL9	C8-C7-C3	2.10	117.91	111.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	B	522	SQD	O47-C7-O49	-2.10	118.63	123.70
37	19	303	CLA	CHB-C4A-NA	2.10	127.41	124.51
50	21	212	DD6	C22-C16-C15	2.10	115.71	110.05
37	a	403	CLA	C11-C12-C13	-2.10	109.14	115.92
39	c	519	BCR	C15-C14-C13	-2.10	124.32	127.31
44	c	517	DGD	C5B-C4B-C3B	-2.10	103.78	114.42
44	j	101	DGD	C8B-C7B-C6B	-2.10	103.78	114.42
47	15	309	KC1	CHB-C1B-C2B	-2.10	121.08	125.48
48	38	214	A86	C34-O4-C38	-2.10	113.99	117.90
50	36	312	DD6	C10-C9-C8	-2.10	116.67	123.22
44	C	516	DGD	O2D-C2D-C1D	-2.10	104.95	110.05
50	19	312	DD6	C41-C32-C31	-2.10	107.14	110.47
37	17	309	CLA	C4-C3-C5	2.10	118.80	115.27
37	40	209	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
48	34	316	A86	C26-C25-C24	-2.10	116.68	123.22
37	31	306	CLA	CMC-C2C-C1C	2.10	128.23	125.04
43	a	412	LHG	C29-C28-C27	-2.10	103.79	114.42
37	39	301	CLA	CBA-CAA-C2A	2.09	120.05	113.86
50	20	310	DD6	C9-C8-C6	-2.09	120.53	126.42
48	33	314	A86	C28-C27-C26	-2.09	119.99	122.92
37	36	306	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
48	16	311	A86	C23-C16-C22	-2.09	104.28	107.37
37	33	308	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
48	34	311	A86	C36-C31-C32	-2.09	117.62	119.70
46	F	101	HEM	CMA-C3A-C4A	-2.09	125.25	128.46
47	37	307	KC1	CHB-C1B-NB	-2.09	122.53	124.45
37	b	503	CLA	CHB-C4A-NA	2.09	127.41	124.51
43	D	411	LHG	C29-C28-C27	-2.09	103.80	114.42
37	17	304	CLA	CAA-C2A-C1A	2.09	118.83	111.97
37	B	515	CLA	C11-C10-C8	-2.09	109.15	115.92
48	17	314	A86	C41-C32-C31	-2.09	108.60	110.47
47	20	304	KC1	O1D-CGD-CBD	-2.09	120.20	124.48
37	w	101	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
37	32	202	CLA	CED-O2D-CGD	2.09	120.67	115.94
47	13	302	KC1	CMC-C2C-C1C	2.09	128.22	125.04
39	a	413	BCR	C33-C5-C6	-2.09	122.18	124.53
37	16	309	CLA	CMC-C2C-C1C	2.09	128.22	125.04
43	D	409	LHG	O8-C23-O10	-2.09	118.32	123.59
47	39	308	KC1	CHC-C4B-NB	-2.09	122.53	124.45
37	c	502	CLA	CMB-C2B-C1B	2.09	131.67	128.46
37	11	303	CLA	CMC-C2C-C1C	2.09	128.22	125.04
37	31	304	CLA	CMC-C2C-C1C	2.09	128.22	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	c	514	BCR	C20-C21-C22	-2.09	124.33	127.31
44	c	516	DGD	O2D-C2D-C1D	-2.09	104.97	110.05
37	41	202	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
37	C	505	CLA	C1-O2A-CGA	2.09	121.92	116.44
50	20	312	DD6	C23-C16-C17	-2.09	105.36	108.98
37	39	303	CLA	CHB-C4A-NA	2.09	127.40	124.51
37	B	502	CLA	C1B-CHB-C4A	-2.09	125.99	130.12
37	C	511	CLA	CMC-C2C-C1C	2.09	128.22	125.04
37	11	308	CLA	CED-O2D-CGD	2.09	120.65	115.94
37	32	206	CLA	C7-C6-C5	-2.09	107.69	113.36
37	13	308	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
44	C	517	DGD	C1D-C2D-C3D	-2.09	105.65	110.00
45	D	408	PL9	C8-C7-C3	2.09	117.87	111.98
37	D	405	CLA	CHB-C4A-NA	2.08	127.39	124.51
50	41	212	DD6	C22-C16-C15	2.08	115.67	110.05
37	21	202	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
37	39	306	CLA	CHA-C1A-NA	-2.08	121.63	126.40
37	11	305	CLA	CMC-C2C-C1C	2.08	128.21	125.04
37	c	501	CLA	CHB-C4A-NA	2.08	127.39	124.51
39	y	101	BCR	C29-C30-C25	2.08	113.69	110.48
37	35	301	CLA	CAC-C3C-C4C	2.08	127.51	124.81
50	40	212	DD6	C9-C8-C6	-2.08	120.57	126.42
37	33	308	CLA	CHD-C4C-NC	2.08	127.48	124.20
37	B	513	CLA	CHB-C4A-NA	2.08	127.39	124.51
37	34	301	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
43	d	407	LHG	O8-C23-O10	-2.08	118.34	123.59
48	34	311	A86	C28-C27-C26	-2.08	120.01	122.92
40	b	521	SQD	O47-C7-O49	-2.08	118.67	123.70
37	c	511	CLA	CMC-C2C-C1C	2.08	128.21	125.04
47	31	305	KC1	CAA-C2A-C1A	-2.08	115.18	124.75
37	34	303	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
48	13	313	A86	C8-C6-C5	2.08	122.13	118.94
37	33	308	CLA	CED-O2D-CGD	2.08	120.64	115.94
48	35	314	A86	C9-C8-C6	-2.08	120.57	126.42
37	C	505	CLA	C4-C3-C5	2.08	118.77	115.27
37	B	516	CLA	CHA-C1A-NA	-2.08	121.64	126.40
48	13	312	A86	C-C1-C24	2.08	121.35	118.08
37	19	301	CLA	CBA-CAA-C2A	2.08	120.00	113.86
37	19	306	CLA	CHA-C1A-NA	-2.08	121.64	126.40
37	15	307	CLA	O2A-CGA-CBA	2.08	118.43	111.91
37	20	307	CLA	O2A-CGA-CBA	2.08	120.71	114.03
47	17	305	KC1	O2A-CGA-O1A	-2.08	118.35	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	38	202	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
39	A	410	BCR	C27-C26-C25	2.08	125.75	122.73
44	c	517	DGD	C1D-C2D-C3D	-2.08	105.67	110.00
47	15	309	KC1	O1D-CGD-CBD	-2.08	120.23	124.48
47	40	206	KC1	O1D-CGD-CBD	-2.08	120.23	124.48
48	15	314	A86	C9-C8-C6	-2.08	120.58	126.42
39	y	101	BCR	C33-C5-C6	-2.08	122.20	124.53
37	13	310	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
38	a	405	PHO	CBA-CAA-C2A	-2.08	107.75	113.81
37	39	306	CLA	CMB-C2B-C3B	2.08	128.56	124.68
37	40	208	CLA	CHA-C1A-NA	-2.08	121.64	126.40
48	12	216	A86	C23-C16-C22	-2.08	104.31	107.37
37	c	512	CLA	CBC-CAC-C3C	-2.08	106.71	112.43
37	33	303	CLA	CMC-C2C-C1C	2.08	128.20	125.04
37	14	301	CLA	C6-C7-C8	-2.07	109.21	115.92
48	18	214	A86	C25-C24-C1	-2.07	120.59	126.42
47	32	212	KC1	CHB-C1B-C2B	-2.07	121.13	125.48
46	f	101	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
44	j	101	DGD	O5E-C6E-C5E	-2.07	104.17	111.29
37	32	213	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
47	31	309	KC1	CMC-C2C-C1C	2.07	128.20	125.04
37	31	301	CLA	CHA-C1A-NA	-2.07	121.65	126.40
38	D	403	PHO	CBA-CAA-C2A	-2.07	107.75	113.81
38	D	403	PHO	C1-C2-C3	-2.07	122.46	126.04
47	16	308	KC1	O2A-CGA-O1A	-2.07	118.36	122.67
43	D	409	LHG	C27-C26-C25	-2.07	103.90	114.42
37	W	102	CLA	CHA-C1A-NA	-2.07	121.65	126.40
37	14	308	CLA	C6-C7-C8	-2.07	109.22	115.92
47	16	304	KC1	O1D-CGD-CBD	-2.07	120.24	124.48
37	a	404	CLA	C1-O2A-CGA	2.07	121.88	116.44
39	C	514	BCR	C20-C21-C22	-2.07	124.35	127.31
37	18	201	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
43	d	407	LHG	C27-C26-C25	-2.07	103.91	114.42
39	A	406	BCR	C7-C8-C9	-2.07	123.11	126.23
47	32	209	KC1	O1D-CGD-CBD	-2.07	120.25	124.48
48	19	311	A86	C23-C16-C22	-2.07	104.31	107.37
37	36	309	CLA	CMC-C2C-C1C	2.07	128.19	125.04
39	K	101	BCR	C33-C5-C6	-2.07	122.20	124.53
41	17	317	LMG	C6-C5-C4	-2.07	108.16	113.00
37	39	301	CLA	O2A-CGA-CBA	2.07	118.40	111.91
37	C	506	CLA	CHB-C4A-NA	2.07	127.37	124.51
37	c	505	CLA	CHB-C4A-NA	2.07	127.37	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	503	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
37	34	305	CLA	CMC-C2C-C1C	2.07	128.19	125.04
37	40	209	CLA	O2A-CGA-CBA	2.07	120.68	114.03
48	21	214	A86	C7-C6-C8	2.07	121.33	118.08
37	33	310	CLA	CHB-C4A-NA	2.07	127.37	124.51
37	b	516	CLA	C6-C7-C8	-2.07	109.24	115.92
37	34	301	CLA	C6-C7-C8	-2.07	109.24	115.92
48	33	313	A86	C10-C9-C8	-2.07	116.77	123.22
47	12	208	KC1	O1D-CGD-CBD	-2.07	120.25	124.48
48	18	215	A86	C9-C8-C6	-2.07	120.61	126.42
44	C	516	DGD	CAB-C9B-C8B	-2.07	103.93	114.42
37	19	301	CLA	O2A-CGA-CBA	2.07	118.39	111.91
48	33	312	A86	C-C1-C24	2.07	121.33	118.08
37	Z	101	CLA	C6-C7-C8	-2.07	109.24	115.92
37	17	309	CLA	CAC-C3C-C4C	2.07	127.49	124.81
37	12	205	CLA	C7-C6-C5	-2.07	107.75	113.36
46	F	101	HEM	C4D-ND-C1D	2.07	107.21	105.07
48	38	213	A86	C10-C9-C8	-2.07	116.77	123.22
37	C	506	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
47	34	306	KC1	CMC-C2C-C1C	2.07	128.18	125.04
37	b	516	CLA	CHA-C1A-NA	-2.06	121.67	126.40
37	c	503	CLA	CHA-C1A-NA	-2.06	121.67	126.40
37	b	513	CLA	CHB-C4A-NA	2.06	127.37	124.51
37	13	303	CLA	CMC-C2C-C1C	2.06	128.18	125.04
41	31	317	LMG	O2-C2-C1	-2.06	105.03	110.05
45	D	408	PL9	C31-C32-C33	-2.06	105.10	111.88
39	a	413	BCR	C27-C26-C25	2.06	125.73	122.73
44	H	102	DGD	O3E-C3E-C2E	-2.06	105.58	110.35
48	36	310	A86	C19-C18-C17	-2.06	106.79	110.77
47	16	304	KC1	CMC-C2C-C1C	2.06	128.18	125.04
37	13	308	CLA	CED-O2D-CGD	2.06	120.60	115.94
50	40	214	DD6	C23-C16-C17	-2.06	105.40	108.98
37	C	505	CLA	CHB-C4A-NA	2.06	127.36	124.51
37	C	503	CLA	CHA-C1A-NA	-2.06	121.67	126.40
37	B	516	CLA	C6-C7-C8	-2.06	109.25	115.92
47	37	307	KC1	CHB-C1B-C2B	-2.06	121.15	125.48
37	34	308	CLA	C6-C7-C8	-2.06	109.25	115.92
37	14	301	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
48	17	312	A86	C-C1-C24	2.06	121.33	118.08
47	17	308	KC1	CHB-C1B-NB	-2.06	122.56	124.45
37	c	506	CLA	CHB-C4A-NA	2.06	127.36	124.51
45	d	406	PL9	C31-C32-C33	-2.06	105.11	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	35	319	A86	O1-C15-C14	-2.06	109.07	113.21
47	37	304	KC1	O2A-CGA-O1A	-2.06	118.39	122.67
48	13	313	A86	C10-C9-C8	-2.06	116.79	123.22
48	33	313	A86	C8-C6-C5	2.06	122.10	118.94
37	41	204	CLA	C1-O2A-CGA	2.06	121.85	116.44
47	36	304	KC1	O1D-CGD-CBD	-2.06	120.27	124.48
41	11	317	LMG	C6-C5-C4	-2.06	108.18	113.00
41	16	316	LMG	O1-C1-C2	-2.06	105.09	108.30
50	40	214	DD6	C34-C35-C36	2.06	115.96	111.85
48	38	213	A86	C12-C11-C13	2.06	119.48	116.02
37	19	306	CLA	CMB-C2B-C3B	2.06	128.53	124.68
48	37	312	A86	C8-C6-C5	-2.06	115.78	118.94
37	c	511	CLA	CHA-C1A-NA	-2.06	121.68	126.40
37	b	509	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
44	H	102	DGD	C5B-C4B-C3B	-2.06	103.97	114.42
47	13	309	KC1	O1D-CGD-CBD	-2.06	120.27	124.48
47	18	205	KC1	O1D-CGD-CBD	-2.06	120.27	124.48
37	c	505	CLA	C1-O2A-CGA	2.06	121.85	116.44
37	b	502	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
37	D	401	CLA	C1-O2A-CGA	2.06	121.84	116.44
44	J	101	DGD	O5E-C6E-C5E	-2.06	104.23	111.29
37	C	512	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
37	z	101	CLA	C6-C7-C8	-2.06	109.27	115.92
37	12	212	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
47	11	304	KC1	CHB-C4A-NA	2.06	127.45	124.20
44	c	516	DGD	CAB-C9B-C8B	-2.06	103.98	114.42
37	C	503	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
47	15	304	KC1	CMC-C2C-C1C	2.06	128.17	125.04
48	14	312	A86	C19-C18-C17	2.06	114.75	110.77
41	36	314	LMG	O1-C1-C2	-2.06	105.09	108.30
48	18	212	A86	C3-C2-C1	-2.06	124.38	127.31
47	15	304	KC1	CED-O2D-CGD	2.06	120.59	115.94
47	36	308	KC1	O2A-CGA-O1A	-2.06	118.40	122.67
37	b	515	CLA	CHA-C1A-NA	-2.06	121.69	126.40
37	14	301	CLA	CMB-C2B-C3B	2.06	128.52	124.68
41	B	521	LMG	O2-C2-C1	-2.06	105.05	110.05
37	C	502	CLA	CMB-C2B-C1B	2.06	131.62	128.46
48	15	314	A86	C-C1-C2	-2.06	120.04	122.92
48	17	320	A86	C-C1-C24	2.06	121.31	118.08
37	15	310	CLA	O2A-CGA-CBA	2.05	120.63	114.03
37	19	304	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
47	11	306	KC1	CBD-CHA-C1A	2.05	132.71	128.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	b	521	SQD	O5-C5-C4	2.05	113.42	109.69
38	a	406	PHO	C1B-NB-C4B	2.05	111.31	107.09
41	B	520	LMG	O2-C2-C1	-2.05	105.06	110.05
44	h	102	DGD	C5B-C4B-C3B	-2.05	104.00	114.42
44	h	102	DGD	O3E-C3E-C2E	-2.05	105.60	110.35
37	31	310	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
38	a	406	PHO	O2A-CGA-O1A	-2.05	118.41	123.59
47	37	307	KC1	CHC-C1C-NC	2.05	127.44	124.20
37	D	402	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
37	C	511	CLA	CHA-C1A-NA	-2.05	121.70	126.40
37	31	301	CLA	CHB-C4A-NA	2.05	127.35	124.51
48	14	311	A86	C28-C27-C26	-2.05	120.05	122.92
37	34	308	CLA	CHB-C4A-NA	2.05	127.35	124.51
48	15	319	A86	O1-C15-C14	-2.05	109.10	113.21
47	17	308	KC1	CHC-C1C-NC	2.05	127.43	124.20
37	c	505	CLA	CMB-C2B-C3B	2.05	128.51	124.68
47	19	308	KC1	CHC-C4B-NB	-2.05	122.57	124.45
48	35	316	A86	C19-C18-C17	-2.05	106.82	110.77
41	a	410	LMG	O1-C1-C2	-2.05	105.10	108.30
41	36	314	LMG	O7-C10-O9	-2.05	118.75	123.70
37	a	403	CLA	CMA-C3A-C2A	-2.05	105.57	113.83
38	A	404	PHO	O2A-CGA-O1A	-2.05	118.42	123.59
48	21	211	A86	C35-C34-C33	2.05	113.45	109.88
37	35	310	CLA	O2A-CGA-CBA	2.05	120.61	114.03
37	B	507	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
37	15	305	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
37	34	303	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
47	11	309	KC1	CMC-C2C-C1C	2.05	128.16	125.04
37	d	401	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
37	38	201	CLA	CHA-C1A-NA	-2.05	121.71	126.40
48	37	311	A86	C10-C9-C8	-2.05	116.83	123.22
48	41	214	A86	C7-C6-C8	2.05	121.30	118.08
37	B	514	CLA	CMB-C2B-C3B	2.05	128.50	124.68
37	B	512	CLA	CMA-C3A-C4A	-2.05	106.28	111.77
37	b	512	CLA	CMA-C3A-C4A	-2.05	106.28	111.77
41	b	520	LMG	O2-C2-C1	-2.05	105.08	110.05
37	d	403	CLA	CHB-C4A-NA	2.05	127.34	124.51
45	D	404	PL9	C27-C28-C29	-2.04	122.74	127.66
37	38	203	CLA	CED-O2D-CGD	2.04	120.56	115.94
48	32	214	A86	C35-C34-C33	2.04	113.44	109.88
50	20	312	DD6	C34-C35-C36	2.04	115.93	111.85
48	15	312	A86	C4-C5-C6	-2.04	124.39	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	31	317	LMG	C6-C5-C4	-2.04	108.22	113.00
47	11	304	KC1	CAA-C2A-C1A	-2.04	115.35	124.75
38	a	405	PHO	C1-C2-C3	-2.04	122.51	126.04
37	39	304	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
48	19	313	A86	C10-C9-C8	2.04	129.59	123.22
48	15	316	A86	C19-C18-C17	-2.04	106.83	110.77
37	18	202	CLA	CHA-C1A-NA	-2.04	121.72	126.40
37	A	403	CLA	CMA-C3A-C2A	-2.04	105.59	113.83
45	d	406	PL9	C36-C34-C33	-2.04	116.98	121.12
48	15	313	A86	C7-C6-C5	-2.04	120.06	122.92
48	34	312	A86	C19-C18-C17	2.04	114.72	110.77
39	a	408	BCR	C7-C8-C9	-2.04	123.15	126.23
37	c	512	CLA	C11-C12-C13	-2.04	109.32	115.92
48	13	315	A86	O4-C38-O5	-2.04	118.91	122.96
37	13	308	CLA	CHD-C4C-NC	2.04	127.42	124.20
47	35	304	KC1	CMC-C2C-C1C	2.04	128.15	125.04
40	B	522	SQD	O5-C5-C4	2.04	113.40	109.69
37	b	516	CLA	CMB-C2B-C3B	2.04	128.49	124.68
37	B	515	CLA	CHA-C1A-NA	-2.04	121.73	126.40
37	37	301	CLA	CHA-C1A-NA	-2.04	121.73	126.40
37	41	210	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
37	31	301	CLA	C1-C2-C3	-2.04	122.52	126.04
48	16	310	A86	C19-C18-C17	-2.04	106.84	110.77
37	21	210	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
44	C	516	DGD	O6E-C5E-C6E	-2.04	101.37	106.44
47	15	309	KC1	CBD-CHA-C1A	2.04	132.68	128.88
37	38	203	CLA	CGD-CBD-CAD	-2.04	104.13	110.73
38	A	404	PHO	C1B-NB-C4B	2.04	111.28	107.09
44	C	517	DGD	C8B-C7B-C6B	-2.04	104.08	114.42
41	b	519	LMG	O2-C2-C1	-2.04	105.10	110.05
44	c	516	DGD	O6E-C5E-C6E	-2.04	101.37	106.44
41	A	408	LMG	O1-C1-C2	-2.04	105.12	108.30
44	J	101	DGD	O2D-C2D-C1D	-2.04	105.10	110.05
37	21	204	CLA	C1-O2A-CGA	2.04	121.79	116.44
37	b	516	CLA	CHB-C4A-NA	2.04	127.33	124.51
37	11	310	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
48	19	313	A86	O4-C38-O5	-2.04	118.92	122.96
37	b	514	CLA	CMB-C2B-C3B	2.04	128.49	124.68
37	C	512	CLA	C11-C12-C13	-2.04	109.34	115.92
37	B	509	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
48	21	215	A86	C22-C16-C17	-2.04	105.44	108.98
39	H	101	BCR	C11-C10-C9	-2.04	124.40	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	j	101	DGD	O2D-C2D-C1D	-2.04	105.10	110.05
37	41	205	CLA	O2A-CGA-CBA	2.04	120.57	114.03
48	41	215	A86	C22-C16-C17	-2.04	105.45	108.98
37	B	508	CLA	CMC-C2C-C1C	2.04	128.14	125.04
37	14	303	CLA	CHA-C1A-NA	-2.04	121.74	126.40
48	33	313	A86	C28-C27-C26	-2.03	120.07	122.92
48	35	313	A86	C23-C16-C22	-2.03	104.37	107.37
44	c	517	DGD	C8B-C7B-C6B	-2.03	104.10	114.42
37	11	310	CLA	CED-O2D-CGD	2.03	120.54	115.94
47	38	205	KC1	O1D-CGD-CBD	-2.03	120.32	124.48
48	32	215	A86	C9-C10-C11	-2.03	120.63	126.61
37	33	303	CLA	CHA-C1A-NA	-2.03	121.74	126.40
37	B	516	CLA	CMB-C2B-C3B	2.03	128.48	124.68
37	C	505	CLA	CMB-C2B-C3B	2.03	128.48	124.68
47	31	307	KC1	CBD-CHA-C1A	2.03	132.67	128.88
48	13	312	A86	C10-C9-C8	-2.03	116.87	123.22
48	33	312	A86	C10-C9-C8	-2.03	116.87	123.22
48	15	316	A86	C-C1-C24	2.03	121.28	118.08
37	21	205	CLA	O2A-CGA-CBA	2.03	120.56	114.03
47	31	305	KC1	CHB-C4A-NA	2.03	127.41	124.20
41	11	317	LMG	O2-C2-C1	-2.03	105.11	110.05
44	c	516	DGD	O6E-C1E-O5D	-2.03	105.16	109.97
37	15	301	CLA	CHA-C1A-NA	-2.03	121.74	126.40
37	13	303	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
37	35	301	CLA	CHA-C1A-NA	-2.03	121.74	126.40
47	35	309	KC1	CBD-CHA-C1A	2.03	132.67	128.88
40	40	202	SQD	O48-C23-O10	-2.03	118.46	123.59
48	13	313	A86	C28-C27-C26	-2.03	120.08	122.92
48	41	211	A86	C35-C34-C33	2.03	113.42	109.88
44	C	516	DGD	C5B-C4B-C3B	-2.03	104.11	114.42
37	W	102	CLA	CHB-C4A-NA	2.03	127.32	124.51
47	11	309	KC1	CHB-C1B-C2B	-2.03	121.22	125.48
37	14	305	CLA	CMC-C2C-C1C	2.03	128.13	125.04
37	b	513	CLA	CAC-C3C-C4C	2.03	127.44	124.81
37	c	506	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
47	36	302	KC1	CHB-C1B-NB	-2.03	122.59	124.45
37	c	513	CLA	C4-C3-C5	2.03	118.69	115.27
37	18	204	CLA	C1-C2-C3	-2.03	122.53	126.04
37	40	203	CLA	CHA-C1A-NA	-2.03	121.75	126.40
41	D	412	LMG	O1-C7-C8	-2.03	106.00	110.90
37	b	513	CLA	CHA-C1A-NA	-2.03	121.75	126.40
37	18	201	CLA	C1-C2-C3	-2.03	122.53	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B	513	CLA	CAC-C3C-C4C	2.03	127.44	124.81
37	B	516	CLA	CHB-C4A-NA	2.03	127.32	124.51
48	14	313	A86	C23-C16-C22	-2.03	104.38	107.37
37	41	206	CLA	CHA-C1A-NA	-2.03	121.75	126.40
45	d	402	PL9	C27-C28-C29	-2.03	122.78	127.66
48	31	312	A86	C8-C6-C5	-2.03	115.83	118.94
48	31	313	A86	C19-C18-C17	-2.03	106.86	110.77
37	36	306	CLA	CBA-CAA-C2A	2.03	119.85	113.86
37	34	308	CLA	CMA-C3A-C2A	-2.03	105.65	113.83
37	19	301	CLA	C6-C7-C8	-2.03	109.37	115.92
37	B	513	CLA	CHA-C1A-NA	-2.03	121.76	126.40
44	c	516	DGD	C5B-C4B-C3B	-2.03	104.14	114.42
45	D	408	PL9	C36-C34-C33	-2.03	117.02	121.12
44	C	516	DGD	O6E-C1E-O5D	-2.03	105.18	109.97
37	18	203	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
48	12	214	A86	C9-C10-C11	-2.03	120.65	126.61
48	17	311	A86	C40-C32-C31	-2.03	108.66	110.47
37	z	101	CLA	CHA-C1A-NA	-2.03	121.76	126.40
37	20	301	CLA	CHA-C1A-NA	-2.03	121.76	126.40
37	12	209	CLA	CBC-CAC-C3C	-2.03	106.85	112.43
37	36	303	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
37	35	308	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
39	C	515	BCR	C2-C1-C6	2.02	113.60	110.48
48	12	202	A86	C25-C24-C1	-2.02	120.73	126.42
37	14	307	CLA	CBA-CAA-C2A	-2.02	107.89	113.86
47	35	309	KC1	O1D-CGD-CBD	-2.02	120.34	124.48
37	17	302	CLA	CED-O2D-CGD	2.02	120.52	115.94
37	16	306	CLA	CBA-CAA-C2A	2.02	119.84	113.86
37	b	509	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
48	34	313	A86	C23-C16-C22	-2.02	104.39	107.37
48	19	313	A86	C35-C34-C33	2.02	113.41	109.88
47	18	207	KC1	CAB-C3B-C4B	2.02	129.78	124.90
48	11	313	A86	C19-C18-C17	-2.02	106.87	110.77
47	14	306	KC1	CBC-CAC-C3C	-2.02	106.86	112.43
37	c	505	CLA	CMC-C2C-C1C	2.02	128.12	125.04
43	a	412	LHG	O8-C23-C24	2.02	118.25	111.91
37	41	202	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
44	c	516	DGD	C7A-C6A-C5A	-2.02	104.16	114.42
41	16	316	LMG	O7-C10-O9	-2.02	118.81	123.70
47	13	309	KC1	CHC-C1C-NC	2.02	127.39	124.20
47	33	309	KC1	CHC-C1C-NC	2.02	127.39	124.20
37	W	102	CLA	C1-C2-C3	-2.02	122.55	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	34	307	CLA	CBA-CAA-C2A	-2.02	107.89	113.86
48	35	315	A86	C9-C8-C6	-2.02	120.74	126.42
37	19	305	CLA	C1-C2-C3	-2.02	122.55	126.04
48	35	313	A86	C7-C6-C5	-2.02	120.09	122.92
47	16	302	KC1	CHB-C1B-NB	-2.02	122.60	124.45
41	d	409	LMG	O1-C7-C8	-2.02	106.02	110.90
37	B	505	CLA	C6-C7-C8	-2.02	109.39	115.92
48	15	314	A86	C12-C11-C13	2.02	119.42	116.02
44	c	517	DGD	O6D-C5D-C6D	-2.02	102.59	106.67
37	b	515	CLA	C2A-C3A-C4A	-2.02	98.61	101.87
37	38	203	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
47	12	211	KC1	CHB-C1B-NB	-2.02	122.60	124.45
48	35	314	A86	C-C1-C2	-2.02	120.09	122.92
50	40	214	DD6	C41-C32-C31	-2.02	107.26	110.47
37	21	206	CLA	CHA-C1A-NA	-2.02	121.77	126.40
37	37	301	CLA	CED-O2D-CGD	2.02	120.50	115.94
44	C	516	DGD	C7A-C6A-C5A	-2.02	104.17	114.42
48	35	316	A86	C-C1-C24	2.02	121.26	118.08
37	21	202	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
37	Z	101	CLA	CHA-C1A-NA	-2.02	121.78	126.40
48	13	313	A86	C4-C3-C2	-2.02	119.34	123.47
48	33	313	A86	C4-C3-C2	-2.02	119.34	123.47
37	14	308	CLA	CHB-C4A-NA	2.02	127.30	124.51
37	35	305	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
50	20	312	DD6	C41-C32-C31	-2.02	107.26	110.47
37	b	503	CLA	CHA-C1A-NA	-2.02	121.78	126.40
47	34	306	KC1	CBC-CAC-C3C	-2.02	106.87	112.43
48	41	214	A86	C9-C10-C11	-2.02	120.68	126.61
37	b	507	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
37	B	503	CLA	CHA-C1A-NA	-2.02	121.78	126.40
37	B	509	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
37	14	303	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
39	H	101	BCR	C38-C26-C27	-2.02	109.75	113.62
37	39	305	CLA	C1-C2-C3	-2.02	122.56	126.04
48	15	315	A86	C9-C8-C6	-2.01	120.76	126.42
37	15	301	CLA	CAC-C3C-C4C	2.01	127.42	124.81
44	C	517	DGD	O6D-C5D-C6D	-2.01	102.60	106.67
48	14	311	A86	C36-C31-C32	-2.01	117.70	119.70
37	14	308	CLA	CMA-C3A-C2A	-2.01	105.70	113.83
48	11	312	A86	C8-C6-C5	-2.01	115.85	118.94
37	c	507	CLA	CHA-C1A-NA	-2.01	121.78	126.40
40	b	521	SQD	O48-C23-C24	2.01	118.23	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	A	407	SQD	C4-C3-C2	2.01	114.34	110.82
40	a	409	SQD	C4-C3-C2	2.01	114.34	110.82
37	39	301	CLA	C6-C7-C8	-2.01	109.41	115.92
45	D	404	PL9	C36-C37-C38	-2.01	105.26	111.88
37	a	403	CLA	C4-C3-C5	2.01	118.66	115.27
37	c	501	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
37	13	308	CLA	CHA-C1A-NA	-2.01	121.79	126.40
39	h	101	BCR	C15-C16-C17	-2.01	119.35	123.47
48	32	203	A86	C4-C3-C2	-2.01	119.35	123.47
48	12	214	A86	C7-C6-C8	2.01	121.25	118.08
37	34	303	CLA	CHA-C1A-NA	-2.01	121.79	126.40
40	16	315	SQD	O48-C23-O10	-2.01	118.52	123.59
37	b	508	CLA	CMC-C2C-C1C	2.01	128.10	125.04
48	36	313	A86	C25-C24-C1	-2.01	120.77	126.42
37	15	308	CLA	C1-O2A-CGA	2.01	121.72	116.44
48	18	212	A86	C23-C16-C17	-2.01	105.49	108.98
39	H	101	BCR	C15-C16-C17	-2.01	119.36	123.47
48	35	312	A86	C28-C27-C26	2.01	125.74	122.92
47	38	210	KC1	CHC-C1C-NC	2.01	127.37	124.20
48	39	313	A86	O4-C38-O5	-2.01	118.97	122.96
44	C	517	DGD	C7B-C6B-C5B	-2.01	104.22	114.42
47	31	309	KC1	CHB-C1B-C2B	-2.01	121.27	125.48
39	A	406	BCR	C27-C26-C25	2.01	125.65	122.73
37	b	505	CLA	C6-C7-C8	-2.01	109.42	115.92
37	18	211	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
37	12	204	CLA	C1-C2-C3	-2.01	122.57	126.04
51	19	315	LMU	O1'-C1'-C2'	2.01	111.44	108.30
48	31	311	A86	C19-C18-C17	-2.01	106.89	110.77
48	32	203	A86	C25-C24-C1	-2.01	120.77	126.42
37	15	307	CLA	C4-C3-C5	2.01	118.65	115.27
48	15	315	A86	C34-O4-C38	-2.01	114.15	117.90
47	21	207	KC1	CHC-C4B-NB	-2.01	122.61	124.45
47	40	207	KC1	CHC-C4B-NB	-2.01	122.61	124.45
43	37	315	LHG	O7-C7-C8	-2.01	107.17	111.50
37	a	407	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
37	18	201	CLA	CHA-C1A-NA	-2.01	121.80	126.40
37	12	204	CLA	CMC-C2C-C1C	2.01	128.09	125.04
40	B	522	SQD	O6-C1-C2	2.01	111.44	108.30
47	14	309	KC1	CHC-C4B-NB	-2.01	122.61	124.45
48	16	314	A86	C25-C24-C1	-2.01	120.78	126.42
48	37	319	A86	C-C1-C24	2.01	121.24	118.08
37	B	515	CLA	C2A-C3A-C4A	-2.01	98.63	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	15	303	CLA	O2A-CGA-CBA	2.01	118.20	111.91
40	B	522	SQD	C4-C3-C2	2.01	114.33	110.82
47	37	304	KC1	CBC-CAC-C3C	-2.01	106.90	112.43
39	B	517	BCR	C38-C26-C27	-2.01	109.76	113.62
39	K	101	BCR	C27-C26-C25	2.01	125.64	122.73
48	37	319	A86	C25-C24-C1	-2.01	120.78	126.42
45	d	402	PL9	C36-C37-C38	-2.01	105.29	111.88
37	31	310	CLA	CED-O2D-CGD	2.01	120.47	115.94
37	18	203	CLA	CBC-CAC-C3C	-2.00	106.90	112.43
37	32	205	CLA	C1-C2-C3	-2.00	122.58	126.04
37	c	507	CLA	CAC-C3C-C4C	2.00	127.41	124.81
43	D	411	LHG	O8-C23-C24	2.00	118.19	111.91
48	35	316	A86	O4-C38-O5	-2.00	118.98	122.96
37	39	305	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
47	12	208	KC1	CBD-CHA-C1A	2.00	132.62	128.88
48	32	218	A86	C26-C25-C24	-2.00	116.97	123.22
39	c	515	BCR	C2-C1-C6	2.00	113.56	110.48
37	14	310	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
37	d	404	CLA	CHA-C1A-NA	-2.00	121.81	126.40
45	d	402	PL9	C31-C32-C33	-2.00	105.30	111.88
37	38	204	CLA	CAA-C2A-C1A	2.00	118.53	111.97
48	32	215	A86	C7-C6-C8	2.00	121.23	118.08
48	14	312	A86	C9-C10-C11	-2.00	120.72	126.61
47	18	210	KC1	CHC-C1C-NC	2.00	127.36	124.20
37	14	301	CLA	O2A-CGA-CBA	2.00	118.19	111.91
37	b	502	CLA	CBC-CAC-C3C	-2.00	106.92	112.43
48	13	311	A86	C23-C16-C22	-2.00	104.42	107.37
47	18	210	KC1	CHC-C4B-NB	-2.00	122.62	124.45

All (177) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
37	A	403	CLA	ND
37	B	501	CLA	ND
37	B	502	CLA	ND
37	B	503	CLA	ND
37	B	504	CLA	ND
37	B	505	CLA	ND
37	B	506	CLA	ND
37	B	507	CLA	ND
37	B	509	CLA	ND
37	B	510	CLA	ND

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Mol	Chain	Res	Type	Atom
37	B	511	CLA	ND
37	B	512	CLA	ND
37	B	513	CLA	ND
37	B	514	CLA	ND
37	B	515	CLA	ND
37	B	516	CLA	ND
37	B	524	CLA	ND
37	C	501	CLA	ND
37	C	502	CLA	ND
37	C	503	CLA	ND
37	C	504	CLA	ND
37	C	505	CLA	ND
37	C	506	CLA	ND
37	C	507	CLA	ND
37	C	508	CLA	ND
37	C	509	CLA	ND
37	C	510	CLA	ND
37	C	511	CLA	ND
37	C	512	CLA	ND
37	C	513	CLA	ND
37	D	401	CLA	ND
37	D	405	CLA	ND
37	D	406	CLA	ND
37	Z	101	CLA	ND
37	Z	102	CLA	ND
37	W	101	CLA	ND
37	W	102	CLA	ND
37	a	403	CLA	ND
37	a	404	CLA	ND
37	b	501	CLA	ND
37	b	502	CLA	ND
37	b	503	CLA	ND
37	b	504	CLA	ND
37	b	505	CLA	ND
37	b	506	CLA	ND
37	b	507	CLA	ND
37	b	509	CLA	ND
37	b	510	CLA	ND
37	b	511	CLA	ND
37	b	512	CLA	ND
37	b	513	CLA	ND
37	b	514	CLA	ND

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Mol	Chain	Res	Type	Atom
37	b	515	CLA	ND
37	b	516	CLA	ND
37	b	523	CLA	ND
37	c	501	CLA	ND
37	c	502	CLA	ND
37	c	503	CLA	ND
37	c	504	CLA	ND
37	c	505	CLA	ND
37	c	506	CLA	ND
37	c	507	CLA	ND
37	c	508	CLA	ND
37	c	509	CLA	ND
37	c	510	CLA	ND
37	c	511	CLA	ND
37	c	512	CLA	ND
37	c	513	CLA	ND
37	d	403	CLA	ND
37	d	404	CLA	ND
37	z	101	CLA	ND
37	z	102	CLA	ND
37	w	101	CLA	ND
37	11	303	CLA	ND
37	11	305	CLA	ND
37	11	308	CLA	ND
37	11	310	CLA	ND
37	12	203	CLA	ND
37	12	204	CLA	ND
37	12	205	CLA	ND
37	12	207	CLA	ND
37	12	209	CLA	ND
37	12	212	CLA	ND
37	13	303	CLA	ND
37	13	305	CLA	ND
37	13	307	CLA	ND
37	14	302	CLA	ND
37	14	305	CLA	ND
37	14	307	CLA	ND
37	14	308	CLA	ND
37	14	310	CLA	ND
37	15	305	CLA	ND
37	15	307	CLA	ND
37	15	308	CLA	ND

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Mol	Chain	Res	Type	Atom
37	15	310	CLA	ND
37	16	303	CLA	ND
37	16	306	CLA	ND
37	16	307	CLA	ND
37	16	309	CLA	ND
37	17	304	CLA	ND
37	17	307	CLA	ND
37	17	309	CLA	ND
37	18	201	CLA	ND
37	18	203	CLA	ND
37	18	204	CLA	ND
37	18	206	CLA	ND
37	18	208	CLA	ND
37	18	209	CLA	ND
37	19	301	CLA	ND
37	19	302	CLA	ND
37	19	303	CLA	ND
37	19	304	CLA	ND
37	19	305	CLA	ND
37	19	306	CLA	ND
37	19	307	CLA	ND
37	19	309	CLA	ND
37	19	310	CLA	ND
37	20	303	CLA	ND
37	20	306	CLA	ND
37	20	307	CLA	ND
37	20	308	CLA	ND
37	21	202	CLA	ND
37	21	205	CLA	ND
37	21	206	CLA	ND
37	21	208	CLA	ND
37	21	209	CLA	ND
37	31	301	CLA	ND
37	31	304	CLA	ND
37	31	306	CLA	ND
37	31	310	CLA	ND
37	32	202	CLA	ND
37	32	204	CLA	ND
37	32	205	CLA	ND
37	32	206	CLA	ND
37	32	208	CLA	ND
37	32	210	CLA	ND

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Mol	Chain	Res	Type	Atom
37	32	213	CLA	ND
37	33	303	CLA	ND
37	33	305	CLA	ND
37	33	307	CLA	ND
37	34	302	CLA	ND
37	34	305	CLA	ND
37	34	307	CLA	ND
37	34	308	CLA	ND
37	34	310	CLA	ND
37	35	305	CLA	ND
37	35	307	CLA	ND
37	35	310	CLA	ND
37	36	303	CLA	ND
37	36	306	CLA	ND
37	36	307	CLA	ND
37	36	309	CLA	ND
37	37	303	CLA	ND
37	37	306	CLA	ND
37	37	308	CLA	ND
37	38	201	CLA	ND
37	38	203	CLA	ND
37	38	204	CLA	ND
37	38	208	CLA	ND
37	38	209	CLA	ND
37	39	301	CLA	ND
37	39	302	CLA	ND
37	39	303	CLA	ND
37	39	304	CLA	ND
37	39	305	CLA	ND
37	39	307	CLA	ND
37	39	309	CLA	ND
37	39	310	CLA	ND
37	40	205	CLA	ND
37	40	208	CLA	ND
37	40	209	CLA	ND
37	40	210	CLA	ND
37	41	202	CLA	ND
37	41	205	CLA	ND
37	41	206	CLA	ND
37	41	208	CLA	ND
37	41	209	CLA	ND

All (5070) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	B	501	CLA	CHA-CBD-CGD-O1D
37	B	501	CLA	CHA-CBD-CGD-O2D
37	B	514	CLA	CHA-CBD-CGD-O1D
37	B	514	CLA	CHA-CBD-CGD-O2D
37	B	514	CLA	CAD-CBD-CGD-O1D
37	C	501	CLA	C1A-C2A-CAA-CBA
37	C	501	CLA	C2-C3-C5-C6
37	C	501	CLA	C4-C3-C5-C6
37	C	503	CLA	C14-C13-C15-C16
37	C	504	CLA	C2-C3-C5-C6
37	C	504	CLA	C4-C3-C5-C6
37	C	506	CLA	C1A-C2A-CAA-CBA
37	C	507	CLA	C4-C3-C5-C6
37	C	508	CLA	CHA-CBD-CGD-O1D
37	C	508	CLA	CHA-CBD-CGD-O2D
37	D	401	CLA	CHA-CBD-CGD-O1D
37	D	401	CLA	CHA-CBD-CGD-O2D
37	D	402	CLA	CHA-CBD-CGD-O1D
37	D	402	CLA	CHA-CBD-CGD-O2D
37	D	405	CLA	C1A-C2A-CAA-CBA
37	D	405	CLA	C3A-C2A-CAA-CBA
37	D	406	CLA	C2-C3-C5-C6
37	D	406	CLA	C4-C3-C5-C6
37	a	404	CLA	C1A-C2A-CAA-CBA
37	a	404	CLA	CHA-CBD-CGD-O1D
37	a	404	CLA	CHA-CBD-CGD-O2D
37	b	501	CLA	CHA-CBD-CGD-O1D
37	b	501	CLA	CHA-CBD-CGD-O2D
37	b	514	CLA	CHA-CBD-CGD-O1D
37	b	514	CLA	CHA-CBD-CGD-O2D
37	b	514	CLA	CAD-CBD-CGD-O1D
37	c	501	CLA	C1A-C2A-CAA-CBA
37	c	501	CLA	C2-C3-C5-C6
37	c	501	CLA	C4-C3-C5-C6
37	c	503	CLA	C14-C13-C15-C16
37	c	504	CLA	C2-C3-C5-C6
37	c	504	CLA	C4-C3-C5-C6
37	c	506	CLA	C1A-C2A-CAA-CBA
37	c	507	CLA	C4-C3-C5-C6
37	c	508	CLA	CHA-CBD-CGD-O1D
37	c	508	CLA	CHA-CBD-CGD-O2D
37	d	401	CLA	CHA-CBD-CGD-O1D
37	d	401	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
37	d	403	CLA	C1A-C2A-CAA-CBA
37	d	403	CLA	C3A-C2A-CAA-CBA
37	d	404	CLA	C2-C3-C5-C6
37	d	404	CLA	C4-C3-C5-C6
37	11	301	CLA	C1A-C2A-CAA-CBA
37	11	301	CLA	C3A-C2A-CAA-CBA
37	11	303	CLA	C1A-C2A-CAA-CBA
37	11	308	CLA	CHA-CBD-CGD-O1D
37	11	308	CLA	CHA-CBD-CGD-O2D
37	11	310	CLA	CBD-CGD-O2D-CED
37	12	203	CLA	C3A-C2A-CAA-CBA
37	12	204	CLA	C1A-C2A-CAA-CBA
37	12	205	CLA	C1A-C2A-CAA-CBA
37	12	210	CLA	CHA-CBD-CGD-O1D
37	12	210	CLA	CHA-CBD-CGD-O2D
37	12	212	CLA	CHA-CBD-CGD-O1D
37	12	212	CLA	CHA-CBD-CGD-O2D
37	13	303	CLA	C1A-C2A-CAA-CBA
37	13	307	CLA	CHA-CBD-CGD-O1D
37	13	307	CLA	CHA-CBD-CGD-O2D
37	13	308	CLA	CHA-CBD-CGD-O1D
37	13	308	CLA	CHA-CBD-CGD-O2D
37	13	310	CLA	CHA-CBD-CGD-O1D
37	13	310	CLA	CHA-CBD-CGD-O2D
37	14	301	CLA	C1A-C2A-CAA-CBA
37	14	301	CLA	C3A-C2A-CAA-CBA
37	14	302	CLA	C6-C7-C8-C9
37	14	308	CLA	CHA-CBD-CGD-O1D
37	14	308	CLA	CHA-CBD-CGD-O2D
37	15	301	CLA	C1A-C2A-CAA-CBA
37	15	301	CLA	C3A-C2A-CAA-CBA
37	15	303	CLA	C1A-C2A-CAA-CBA
37	15	308	CLA	CHA-CBD-CGD-O1D
37	15	308	CLA	C2-C3-C5-C6
37	15	308	CLA	C4-C3-C5-C6
37	15	310	CLA	CHA-CBD-CGD-O2D
37	16	301	CLA	C1A-C2A-CAA-CBA
37	16	301	CLA	C3A-C2A-CAA-CBA
37	16	303	CLA	C1A-C2A-CAA-CBA
37	16	306	CLA	C1A-C2A-CAA-CBA
37	16	306	CLA	CHA-CBD-CGD-O1D
37	16	306	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
37	16	309	CLA	C1A-C2A-CAA-CBA
37	17	304	CLA	C1A-C2A-CAA-CBA
37	18	202	CLA	C1A-C2A-CAA-CBA
37	18	202	CLA	C3A-C2A-CAA-CBA
37	18	204	CLA	C1A-C2A-CAA-CBA
37	18	209	CLA	CHA-CBD-CGD-O1D
37	18	209	CLA	CHA-CBD-CGD-O2D
37	19	301	CLA	C3A-C2A-CAA-CBA
37	19	302	CLA	C2-C3-C5-C6
37	19	302	CLA	C4-C3-C5-C6
37	19	305	CLA	C2-C3-C5-C6
37	20	301	CLA	C1A-C2A-CAA-CBA
37	20	303	CLA	C1A-C2A-CAA-CBA
37	20	303	CLA	C2-C3-C5-C6
37	20	303	CLA	C4-C3-C5-C6
37	21	204	CLA	C1A-C2A-CAA-CBA
37	21	204	CLA	CHA-CBD-CGD-O1D
37	21	204	CLA	CHA-CBD-CGD-O2D
37	21	204	CLA	C4-C3-C5-C6
37	21	208	CLA	CHA-CBD-CGD-O1D
37	21	208	CLA	CHA-CBD-CGD-O2D
37	21	208	CLA	C2-C3-C5-C6
37	21	208	CLA	C4-C3-C5-C6
37	21	209	CLA	CHA-CBD-CGD-O2D
37	21	210	CLA	CHA-CBD-CGD-O1D
37	21	210	CLA	CHA-CBD-CGD-O2D
37	31	302	CLA	C1A-C2A-CAA-CBA
37	31	302	CLA	C3A-C2A-CAA-CBA
37	31	304	CLA	C1A-C2A-CAA-CBA
37	31	310	CLA	CBD-CGD-O2D-CED
37	32	202	CLA	CHA-CBD-CGD-O1D
37	32	202	CLA	CHA-CBD-CGD-O2D
37	32	204	CLA	C3A-C2A-CAA-CBA
37	32	205	CLA	C1A-C2A-CAA-CBA
37	32	206	CLA	C1A-C2A-CAA-CBA
37	32	211	CLA	CHA-CBD-CGD-O1D
37	32	211	CLA	CHA-CBD-CGD-O2D
37	32	213	CLA	CHA-CBD-CGD-O1D
37	32	213	CLA	CHA-CBD-CGD-O2D
37	33	303	CLA	C1A-C2A-CAA-CBA
37	33	307	CLA	CHA-CBD-CGD-O1D
37	33	307	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
37	33	308	CLA	CHA-CBD-CGD-O1D
37	33	308	CLA	CHA-CBD-CGD-O2D
37	33	310	CLA	CHA-CBD-CGD-O1D
37	33	310	CLA	CHA-CBD-CGD-O2D
37	34	301	CLA	C1A-C2A-CAA-CBA
37	34	301	CLA	C3A-C2A-CAA-CBA
37	34	302	CLA	C6-C7-C8-C9
37	34	308	CLA	CHA-CBD-CGD-O1D
37	34	308	CLA	CHA-CBD-CGD-O2D
37	35	301	CLA	C1A-C2A-CAA-CBA
37	35	301	CLA	C3A-C2A-CAA-CBA
37	35	303	CLA	C1A-C2A-CAA-CBA
37	35	308	CLA	CHA-CBD-CGD-O1D
37	35	308	CLA	C2-C3-C5-C6
37	35	308	CLA	C4-C3-C5-C6
37	35	310	CLA	CHA-CBD-CGD-O2D
37	36	301	CLA	C1A-C2A-CAA-CBA
37	36	301	CLA	C3A-C2A-CAA-CBA
37	36	303	CLA	C1A-C2A-CAA-CBA
37	36	306	CLA	C1A-C2A-CAA-CBA
37	36	306	CLA	CHA-CBD-CGD-O1D
37	36	306	CLA	CHA-CBD-CGD-O2D
37	36	309	CLA	C1A-C2A-CAA-CBA
37	37	303	CLA	C1A-C2A-CAA-CBA
37	37	308	CLA	CBD-CGD-O2D-CED
37	38	202	CLA	C1A-C2A-CAA-CBA
37	38	202	CLA	C3A-C2A-CAA-CBA
37	38	202	CLA	CBD-CGD-O2D-CED
37	38	204	CLA	C1A-C2A-CAA-CBA
37	38	209	CLA	CHA-CBD-CGD-O1D
37	38	209	CLA	CHA-CBD-CGD-O2D
37	39	301	CLA	C3A-C2A-CAA-CBA
37	39	302	CLA	C2-C3-C5-C6
37	39	302	CLA	C4-C3-C5-C6
37	39	305	CLA	C2-C3-C5-C6
37	40	203	CLA	C1A-C2A-CAA-CBA
37	40	205	CLA	C1A-C2A-CAA-CBA
37	40	205	CLA	C2-C3-C5-C6
37	40	205	CLA	C4-C3-C5-C6
37	41	204	CLA	C1A-C2A-CAA-CBA
37	41	204	CLA	CHA-CBD-CGD-O1D
37	41	204	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
37	41	204	CLA	C4-C3-C5-C6
37	41	208	CLA	CHA-CBD-CGD-O1D
37	41	208	CLA	CHA-CBD-CGD-O2D
37	41	208	CLA	C2-C3-C5-C6
37	41	208	CLA	C4-C3-C5-C6
37	41	209	CLA	CHA-CBD-CGD-O2D
37	41	210	CLA	CHA-CBD-CGD-O1D
37	41	210	CLA	CHA-CBD-CGD-O2D
39	A	406	BCR	C1-C6-C7-C8
39	A	406	BCR	C7-C8-C9-C10
39	A	406	BCR	C7-C8-C9-C34
39	A	410	BCR	C6-C7-C8-C9
39	A	410	BCR	C7-C8-C9-C10
39	B	517	BCR	C20-C21-C22-C37
39	B	517	BCR	C21-C22-C23-C24
39	B	518	BCR	C7-C8-C9-C10
39	B	525	BCR	C11-C10-C9-C8
39	B	525	BCR	C10-C11-C12-C13
39	B	525	BCR	C37-C22-C23-C24
39	C	514	BCR	C21-C22-C23-C24
39	C	514	BCR	C37-C22-C23-C24
39	C	515	BCR	C7-C8-C9-C10
39	C	515	BCR	C7-C8-C9-C34
39	C	519	BCR	C1-C6-C7-C8
39	C	519	BCR	C23-C24-C25-C30
39	D	407	BCR	C7-C8-C9-C10
39	D	407	BCR	C7-C8-C9-C34
39	D	407	BCR	C11-C10-C9-C34
39	D	407	BCR	C21-C22-C23-C24
39	D	407	BCR	C22-C23-C24-C25
39	H	101	BCR	C1-C6-C7-C8
39	H	101	BCR	C21-C22-C23-C24
39	H	101	BCR	C37-C22-C23-C24
39	K	101	BCR	C6-C7-C8-C9
39	K	101	BCR	C10-C11-C12-C13
39	K	101	BCR	C11-C12-C13-C14
39	K	101	BCR	C11-C12-C13-C35
39	K	101	BCR	C18-C19-C20-C21
39	K	101	BCR	C21-C22-C23-C24
39	0	101	BCR	C1-C6-C7-C8
39	0	101	BCR	C7-C8-C9-C10
39	a	408	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
39	a	408	BCR	C7-C8-C9-C10
39	a	408	BCR	C7-C8-C9-C34
39	a	413	BCR	C6-C7-C8-C9
39	a	413	BCR	C7-C8-C9-C10
39	b	517	BCR	C20-C21-C22-C37
39	b	517	BCR	C21-C22-C23-C24
39	b	518	BCR	C7-C8-C9-C10
39	b	524	BCR	C11-C10-C9-C8
39	b	524	BCR	C10-C11-C12-C13
39	b	524	BCR	C37-C22-C23-C24
39	c	514	BCR	C21-C22-C23-C24
39	c	514	BCR	C37-C22-C23-C24
39	c	515	BCR	C7-C8-C9-C10
39	c	515	BCR	C7-C8-C9-C34
39	c	519	BCR	C1-C6-C7-C8
39	c	519	BCR	C23-C24-C25-C30
39	d	405	BCR	C7-C8-C9-C10
39	d	405	BCR	C7-C8-C9-C34
39	d	405	BCR	C11-C10-C9-C34
39	d	405	BCR	C21-C22-C23-C24
39	d	405	BCR	C22-C23-C24-C25
39	h	101	BCR	C1-C6-C7-C8
39	h	101	BCR	C21-C22-C23-C24
39	h	101	BCR	C37-C22-C23-C24
39	y	101	BCR	C6-C7-C8-C9
39	y	101	BCR	C10-C11-C12-C13
39	y	101	BCR	C11-C12-C13-C14
39	y	101	BCR	C11-C12-C13-C35
39	y	101	BCR	C18-C19-C20-C21
39	y	101	BCR	C21-C22-C23-C24
39	5	101	BCR	C1-C6-C7-C8
39	5	101	BCR	C7-C8-C9-C10
40	A	407	SQD	C5-C6-S-O7
40	B	519	SQD	O5-C1-O6-C44
40	B	519	SQD	C8-C7-O47-C45
40	B	519	SQD	O5-C5-C6-S
40	L	101	SQD	O5-C1-O6-C44
40	L	101	SQD	C8-C7-O47-C45
40	L	101	SQD	O5-C5-C6-S
40	a	409	SQD	C5-C6-S-O7
40	16	315	SQD	C2-C1-O6-C44
40	16	315	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
40	16	315	SQD	O5-C5-C6-S
40	17	301	SQD	C2-C1-O6-C44
40	17	301	SQD	O5-C1-O6-C44
40	17	301	SQD	C8-C7-O47-C45
40	17	301	SQD	C5-C6-S-O7
40	17	301	SQD	C5-C6-S-O8
40	17	301	SQD	C5-C6-S-O9
40	36	315	SQD	C2-C1-O6-C44
40	36	315	SQD	O5-C1-O6-C44
40	36	315	SQD	C8-C7-O47-C45
40	36	315	SQD	C5-C6-S-O7
40	36	315	SQD	C5-C6-S-O8
40	36	315	SQD	C5-C6-S-O9
40	40	202	SQD	C2-C1-O6-C44
40	40	202	SQD	O5-C1-O6-C44
40	40	202	SQD	O5-C5-C6-S
41	A	408	LMG	O1-C7-C8-O7
41	L	102	LMG	O9-C10-O7-C8
41	a	410	LMG	O1-C7-C8-O7
41	l	101	LMG	O9-C10-O7-C8
41	11	316	LMG	O9-C10-O7-C8
41	11	316	LMG	C11-C10-O7-C8
41	12	201	LMG	O6-C1-O1-C7
41	17	317	LMG	O9-C10-O7-C8
41	17	317	LMG	C11-C10-O7-C8
41	31	316	LMG	O9-C10-O7-C8
41	31	316	LMG	C11-C10-O7-C8
41	32	201	LMG	O6-C1-O1-C7
41	37	316	LMG	O9-C10-O7-C8
41	37	316	LMG	C11-C10-O7-C8
43	B	523	LHG	C4-O6-P-O5
43	D	409	LHG	O1-C1-C2-C3
43	D	409	LHG	C1-C2-C3-O3
43	D	409	LHG	C4-O6-P-O3
43	D	410	LHG	O1-C1-C2-C3
43	D	410	LHG	C4-O6-P-O3
43	D	410	LHG	C4-O6-P-O4
43	D	410	LHG	C4-O6-P-O5
43	D	410	LHG	C8-C7-O7-C5
43	D	411	LHG	C4-O6-P-O3
43	D	411	LHG	C4-O6-P-O4
43	D	411	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
43	D	411	LHG	C8-C7-O7-C5
43	a	412	LHG	C4-O6-P-O3
43	a	412	LHG	C4-O6-P-O4
43	a	412	LHG	C4-O6-P-O5
43	a	412	LHG	C8-C7-O7-C5
43	b	522	LHG	C4-O6-P-O5
43	d	407	LHG	O1-C1-C2-C3
43	d	407	LHG	C1-C2-C3-O3
43	d	407	LHG	C4-O6-P-O3
43	d	408	LHG	O1-C1-C2-C3
43	d	408	LHG	C4-O6-P-O3
43	d	408	LHG	C4-O6-P-O4
43	d	408	LHG	C4-O6-P-O5
43	d	408	LHG	C8-C7-O7-C5
43	17	316	LHG	C4-O6-P-O5
43	19	314	LHG	C3-O3-P-O4
43	21	201	LHG	C3-O3-P-O4
43	21	201	LHG	C4-O6-P-O4
43	21	217	LHG	O1-C1-C2-C3
43	21	217	LHG	C3-O3-P-O5
43	21	217	LHG	C4-O6-P-O4
43	21	217	LHG	O7-C5-C6-O8
43	37	315	LHG	C4-O6-P-O5
43	37	321	LHG	O1-C1-C2-C3
43	37	321	LHG	C3-O3-P-O5
43	37	321	LHG	C4-O6-P-O4
43	37	321	LHG	O7-C5-C6-O8
43	39	314	LHG	C3-O3-P-O4
43	41	201	LHG	C3-O3-P-O4
43	41	201	LHG	C4-O6-P-O4
45	D	404	PL9	C9-C11-C12-C13
45	D	404	PL9	C32-C33-C34-C36
45	D	404	PL9	C37-C38-C39-C40
45	D	404	PL9	C44-C46-C47-C48
45	D	404	PL9	C47-C48-C49-C50
45	D	408	PL9	C39-C41-C42-C43
45	d	402	PL9	C9-C11-C12-C13
45	d	402	PL9	C32-C33-C34-C36
45	d	402	PL9	C37-C38-C39-C40
45	d	402	PL9	C44-C46-C47-C48
45	d	402	PL9	C47-C48-C49-C50
45	d	406	PL9	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
46	F	101	HEM	C1A-C2A-CAA-CBA
46	F	101	HEM	C3A-C2A-CAA-CBA
46	V	201	HEM	C2B-C3B-CAB-CBB
46	V	201	HEM	C4B-C3B-CAB-CBB
46	f	101	HEM	C1A-C2A-CAA-CBA
46	f	101	HEM	C3A-C2A-CAA-CBA
46	v	201	HEM	C2B-C3B-CAB-CBB
46	v	201	HEM	C4B-C3B-CAB-CBB
47	11	302	KC1	C3A-C2A-CAA-CBA
47	11	302	KC1	C2A-CAA-CBA-CGA
47	11	304	KC1	C2B-C3B-CAB-CBB
47	11	304	KC1	C4B-C3B-CAB-CBB
47	11	304	KC1	C2A-CAA-CBA-CGA
47	11	306	KC1	C1A-C2A-CAA-CBA
47	11	306	KC1	C3A-C2A-CAA-CBA
47	11	306	KC1	C2B-C3B-CAB-CBB
47	11	306	KC1	C4B-C3B-CAB-CBB
47	11	306	KC1	C2A-CAA-CBA-CGA
47	11	309	KC1	C3A-C2A-CAA-CBA
47	11	309	KC1	C2A-CAA-CBA-CGA
47	12	206	KC1	C1A-C2A-CAA-CBA
47	12	206	KC1	C3A-C2A-CAA-CBA
47	12	206	KC1	C2A-CAA-CBA-CGA
47	12	208	KC1	C2A-CAA-CBA-CGA
47	12	211	KC1	C3A-C2A-CAA-CBA
47	12	211	KC1	C2A-CAA-CBA-CGA
47	13	302	KC1	C3A-C2A-CAA-CBA
47	13	302	KC1	C2A-CAA-CBA-CGA
47	13	304	KC1	C1A-C2A-CAA-CBA
47	13	304	KC1	C3A-C2A-CAA-CBA
47	13	304	KC1	C2B-C3B-CAB-CBB
47	13	304	KC1	C4B-C3B-CAB-CBB
47	13	304	KC1	C2A-CAA-CBA-CGA
47	13	306	KC1	C1A-C2A-CAA-CBA
47	13	306	KC1	C3A-C2A-CAA-CBA
47	13	306	KC1	C2A-CAA-CBA-CGA
47	13	309	KC1	C3A-C2A-CAA-CBA
47	13	309	KC1	C2A-CAA-CBA-CGA
47	14	304	KC1	C2A-CAA-CBA-CGA
47	14	306	KC1	C1A-C2A-CAA-CBA
47	14	306	KC1	C3A-C2A-CAA-CBA
47	14	306	KC1	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
47	14	309	KC1	C3A-C2A-CAA-CBA
47	15	302	KC1	C3A-C2A-CAA-CBA
47	15	302	KC1	C2B-C3B-CAB-CBB
47	15	302	KC1	C4B-C3B-CAB-CBB
47	15	302	KC1	C2A-CAA-CBA-CGA
47	15	304	KC1	C3A-C2A-CAA-CBA
47	15	304	KC1	C2A-CAA-CBA-CGA
47	15	306	KC1	C3A-C2A-CAA-CBA
47	15	306	KC1	C2A-CAA-CBA-CGA
47	15	309	KC1	C3A-C2A-CAA-CBA
47	15	309	KC1	C2A-CAA-CBA-CGA
47	16	302	KC1	C3A-C2A-CAA-CBA
47	16	302	KC1	C2A-CAA-CBA-CGA
47	16	304	KC1	C3A-C2A-CAA-CBA
47	16	304	KC1	C2A-CAA-CBA-CGA
47	16	305	KC1	C2A-CAA-CBA-CGA
47	16	308	KC1	C3A-C2A-CAA-CBA
47	16	308	KC1	C2A-CAA-CBA-CGA
47	17	303	KC1	C3A-C2A-CAA-CBA
47	17	303	KC1	C2A-CAA-CBA-CGA
47	17	305	KC1	C2A-CAA-CBA-CGA
47	17	306	KC1	C1A-C2A-CAA-CBA
47	17	306	KC1	C3A-C2A-CAA-CBA
47	17	306	KC1	C2A-CAA-CBA-CGA
47	17	308	KC1	C3A-C2A-CAA-CBA
47	17	308	KC1	C2A-CAA-CBA-CGA
47	18	205	KC1	C3A-C2A-CAA-CBA
47	18	205	KC1	C2A-CAA-CBA-CGA
47	18	207	KC1	C1A-C2A-CAA-CBA
47	18	207	KC1	C3A-C2A-CAA-CBA
47	18	207	KC1	C2A-CAA-CBA-CGA
47	18	207	KC1	CHA-CBD-CGD-O1D
47	18	207	KC1	CHA-CBD-CGD-O2D
47	18	210	KC1	C3A-C2A-CAA-CBA
47	19	308	KC1	C2A-CAA-CBA-CGA
47	20	302	KC1	C3A-C2A-CAA-CBA
47	20	302	KC1	C2A-CAA-CBA-CGA
47	20	302	KC1	CBD-CGD-O2D-CED
47	20	304	KC1	C3A-C2A-CAA-CBA
47	20	304	KC1	C2A-CAA-CBA-CGA
47	20	305	KC1	C1A-C2A-CAA-CBA
47	20	305	KC1	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
47	20	305	KC1	C2A-CAA-CBA-CGA
47	21	203	KC1	C3A-C2A-CAA-CBA
47	21	203	KC1	C2A-CAA-CBA-CGA
47	21	207	KC1	C2B-C3B-CAB-CBB
47	21	207	KC1	C4B-C3B-CAB-CBB
47	31	303	KC1	C3A-C2A-CAA-CBA
47	31	303	KC1	C2A-CAA-CBA-CGA
47	31	305	KC1	C2B-C3B-CAB-CBB
47	31	305	KC1	C4B-C3B-CAB-CBB
47	31	305	KC1	C2A-CAA-CBA-CGA
47	31	307	KC1	C1A-C2A-CAA-CBA
47	31	307	KC1	C3A-C2A-CAA-CBA
47	31	307	KC1	C2B-C3B-CAB-CBB
47	31	307	KC1	C4B-C3B-CAB-CBB
47	31	307	KC1	C2A-CAA-CBA-CGA
47	31	309	KC1	C3A-C2A-CAA-CBA
47	31	309	KC1	C2A-CAA-CBA-CGA
47	32	207	KC1	C1A-C2A-CAA-CBA
47	32	207	KC1	C3A-C2A-CAA-CBA
47	32	207	KC1	C2A-CAA-CBA-CGA
47	32	209	KC1	C2A-CAA-CBA-CGA
47	32	212	KC1	C3A-C2A-CAA-CBA
47	32	212	KC1	C2A-CAA-CBA-CGA
47	33	302	KC1	C3A-C2A-CAA-CBA
47	33	302	KC1	C2A-CAA-CBA-CGA
47	33	304	KC1	C1A-C2A-CAA-CBA
47	33	304	KC1	C3A-C2A-CAA-CBA
47	33	304	KC1	C2B-C3B-CAB-CBB
47	33	304	KC1	C4B-C3B-CAB-CBB
47	33	304	KC1	C2A-CAA-CBA-CGA
47	33	306	KC1	C1A-C2A-CAA-CBA
47	33	306	KC1	C3A-C2A-CAA-CBA
47	33	306	KC1	C2A-CAA-CBA-CGA
47	33	309	KC1	C3A-C2A-CAA-CBA
47	33	309	KC1	C2A-CAA-CBA-CGA
47	34	304	KC1	C2A-CAA-CBA-CGA
47	34	306	KC1	C1A-C2A-CAA-CBA
47	34	306	KC1	C3A-C2A-CAA-CBA
47	34	306	KC1	C2A-CAA-CBA-CGA
47	34	309	KC1	C3A-C2A-CAA-CBA
47	35	302	KC1	C3A-C2A-CAA-CBA
47	35	302	KC1	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
47	35	304	KC1	C3A-C2A-CAA-CBA
47	35	304	KC1	C2B-C3B-CAB-CBB
47	35	304	KC1	C2A-CAA-CBA-CGA
47	35	306	KC1	C3A-C2A-CAA-CBA
47	35	306	KC1	C2A-CAA-CBA-CGA
47	35	309	KC1	C3A-C2A-CAA-CBA
47	35	309	KC1	C2A-CAA-CBA-CGA
47	36	302	KC1	C3A-C2A-CAA-CBA
47	36	302	KC1	C2A-CAA-CBA-CGA
47	36	304	KC1	C3A-C2A-CAA-CBA
47	36	304	KC1	C2A-CAA-CBA-CGA
47	36	305	KC1	C2A-CAA-CBA-CGA
47	36	308	KC1	C3A-C2A-CAA-CBA
47	36	308	KC1	C2A-CAA-CBA-CGA
47	37	302	KC1	C3A-C2A-CAA-CBA
47	37	302	KC1	C2A-CAA-CBA-CGA
47	37	304	KC1	C2A-CAA-CBA-CGA
47	37	305	KC1	C1A-C2A-CAA-CBA
47	37	305	KC1	C3A-C2A-CAA-CBA
47	37	305	KC1	C2A-CAA-CBA-CGA
47	37	307	KC1	C3A-C2A-CAA-CBA
47	37	307	KC1	C2A-CAA-CBA-CGA
47	38	205	KC1	C3A-C2A-CAA-CBA
47	38	205	KC1	C2A-CAA-CBA-CGA
47	38	207	KC1	C1A-C2A-CAA-CBA
47	38	207	KC1	C3A-C2A-CAA-CBA
47	38	207	KC1	C2A-CAA-CBA-CGA
47	38	207	KC1	CHA-CBD-CGD-O1D
47	38	207	KC1	CHA-CBD-CGD-O2D
47	38	210	KC1	C3A-C2A-CAA-CBA
47	39	308	KC1	C2A-CAA-CBA-CGA
47	40	204	KC1	C3A-C2A-CAA-CBA
47	40	204	KC1	C2A-CAA-CBA-CGA
47	40	204	KC1	CBD-CGD-O2D-CED
47	40	206	KC1	C3A-C2A-CAA-CBA
47	40	206	KC1	C2A-CAA-CBA-CGA
47	40	207	KC1	C1A-C2A-CAA-CBA
47	40	207	KC1	C3A-C2A-CAA-CBA
47	40	207	KC1	C2A-CAA-CBA-CGA
47	41	203	KC1	C3A-C2A-CAA-CBA
47	41	203	KC1	C2A-CAA-CBA-CGA
47	41	207	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
47	41	207	KC1	C4B-C3B-CAB-CBB
48	11	311	A86	C24-C25-C26-C27
48	11	312	A86	C24-C25-C26-C27
48	11	313	A86	C39-C38-O4-C34
48	11	313	A86	O5-C38-O4-C34
48	11	314	A86	C-C1-C24-C25
48	11	314	A86	C2-C1-C24-C25
48	11	314	A86	C12-C11-C13-O
48	11	314	A86	C39-C38-O4-C34
48	11	315	A86	C39-C38-O4-C34
48	11	315	A86	O5-C38-O4-C34
48	12	202	A86	C11-C10-C9-C8
48	12	202	A86	C10-C11-C13-O
48	12	202	A86	C12-C11-C13-O
48	12	202	A86	C13-C14-C15-C16
48	12	202	A86	C39-C38-O4-C34
48	12	202	A86	O5-C38-O4-C34
48	12	202	A86	C5-C6-C8-C9
48	12	202	A86	C7-C6-C8-C9
48	12	213	A86	C-C1-C24-C25
48	12	213	A86	C2-C1-C24-C25
48	12	215	A86	C26-C27-C29-C30
48	12	215	A86	C35-C34-O4-C38
48	12	216	A86	C-C1-C24-C25
48	12	216	A86	C2-C1-C24-C25
48	12	216	A86	C5-C6-C8-C9
48	12	216	A86	C7-C6-C8-C9
48	12	217	A86	C-C1-C24-C25
48	12	217	A86	O-C13-C14-C15
48	12	217	A86	C11-C13-C14-C15
48	12	217	A86	C13-C14-C15-C16
48	12	217	A86	O5-C38-O4-C34
48	12	220	A86	C-C1-C24-C25
48	12	220	A86	C2-C1-C24-C25
48	12	220	A86	C11-C10-C9-C8
48	12	220	A86	O5-C38-O4-C34
48	12	220	A86	C3-C4-C5-C6
48	13	311	A86	C-C1-C24-C25
48	13	311	A86	C2-C1-C24-C25
48	13	312	A86	C5-C6-C8-C9
48	13	312	A86	C7-C6-C8-C9
48	13	313	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
48	13	313	A86	O-C13-C14-C15
48	13	313	A86	C11-C13-C14-C15
48	13	313	A86	C13-C14-C15-C16
48	13	313	A86	C33-C34-O4-C38
48	13	313	A86	C39-C38-O4-C34
48	13	313	A86	C5-C6-C8-C9
48	13	313	A86	C7-C6-C8-C9
48	13	314	A86	C11-C10-C9-C8
48	13	314	A86	C13-C14-C15-C16
48	13	314	A86	C24-C25-C26-C27
48	13	314	A86	C39-C38-O4-C34
48	13	314	A86	O5-C38-O4-C34
48	13	315	A86	C11-C10-C9-C8
48	13	315	A86	C13-C14-C15-C16
48	13	315	A86	O5-C38-O4-C34
48	13	315	A86	C5-C6-C8-C9
48	13	315	A86	C7-C6-C8-C9
48	14	311	A86	C39-C38-O4-C34
48	14	313	A86	C-C1-C24-C25
48	14	313	A86	C2-C1-C24-C25
48	14	313	A86	C24-C25-C26-C27
48	14	313	A86	C26-C27-C29-C30
48	14	313	A86	C33-C34-O4-C38
48	14	313	A86	C39-C38-O4-C34
48	14	313	A86	C5-C6-C8-C9
48	14	313	A86	C7-C6-C8-C9
48	14	314	A86	C-C1-C24-C25
48	14	314	A86	C2-C1-C24-C25
48	14	314	A86	C5-C6-C8-C9
48	14	314	A86	C7-C6-C8-C9
48	14	316	A86	C11-C13-C14-C15
48	14	316	A86	C13-C14-C15-C16
48	15	311	A86	C24-C25-C26-C27
48	15	311	A86	O5-C38-O4-C34
48	15	312	A86	C-C1-C24-C25
48	15	312	A86	C2-C1-C24-C25
48	15	312	A86	C39-C38-O4-C34
48	15	312	A86	O5-C38-O4-C34
48	15	312	A86	C5-C6-C8-C9
48	15	312	A86	C7-C6-C8-C9
48	15	313	A86	C-C1-C24-C25
48	15	313	A86	C26-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
48	15	313	A86	C35-C34-O4-C38
48	15	314	A86	C2-C1-C24-C25
48	15	314	A86	C11-C10-C9-C8
48	15	314	A86	C39-C38-O4-C34
48	15	315	A86	C-C1-C24-C25
48	15	315	A86	C2-C1-C24-C25
48	15	315	A86	C39-C38-O4-C34
48	15	315	A86	O5-C38-O4-C34
48	15	315	A86	C5-C6-C8-C9
48	15	315	A86	C7-C6-C8-C9
48	15	316	A86	O-C13-C14-C15
48	15	316	A86	C11-C13-C14-C15
48	15	316	A86	C13-C14-C15-C16
48	15	316	A86	O5-C38-O4-C34
48	15	319	A86	C5-C6-C8-C9
48	15	319	A86	C7-C6-C8-C9
48	16	311	A86	C24-C25-C26-C27
48	16	313	A86	C12-C11-C13-C14
48	16	314	A86	C10-C11-C13-O
48	16	314	A86	C12-C11-C13-O
48	16	314	A86	O5-C38-O4-C34
48	17	310	A86	C12-C11-C13-C14
48	17	310	A86	C7-C6-C8-C9
48	17	311	A86	C39-C38-O4-C34
48	17	311	A86	C5-C6-C8-C9
48	17	311	A86	C7-C6-C8-C9
48	17	312	A86	C24-C25-C26-C27
48	17	312	A86	C33-C34-O4-C38
48	17	313	A86	C-C1-C24-C25
48	17	313	A86	C2-C1-C24-C25
48	17	314	A86	C-C1-C24-C25
48	17	314	A86	C2-C1-C24-C25
48	17	314	A86	C11-C13-C14-C15
48	17	314	A86	C5-C6-C8-C9
48	17	314	A86	C7-C6-C8-C9
48	17	315	A86	C11-C10-C9-C8
48	17	315	A86	C10-C11-C13-O
48	17	315	A86	C12-C11-C13-O
48	17	315	A86	C11-C13-C14-C15
48	17	315	A86	C13-C14-C15-C16
48	17	320	A86	C-C1-C24-C25
48	17	320	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
48	17	320	A86	C39-C38-O4-C34
48	17	320	A86	C5-C6-C8-C9
48	17	320	A86	C7-C6-C8-C9
48	18	212	A86	C24-C25-C26-C27
48	18	212	A86	C39-C38-O4-C34
48	18	212	A86	O5-C38-O4-C34
48	18	213	A86	C5-C6-C8-C9
48	18	213	A86	C7-C6-C8-C9
48	18	214	A86	C-C1-C24-C25
48	18	214	A86	C2-C1-C24-C25
48	18	214	A86	C11-C10-C9-C8
48	18	215	A86	C10-C11-C13-O
48	18	215	A86	C12-C11-C13-O
48	18	215	A86	O-C13-C14-C15
48	18	215	A86	C11-C13-C14-C15
48	18	215	A86	C13-C14-C15-C16
48	18	215	A86	C39-C38-O4-C34
48	18	215	A86	O5-C38-O4-C34
48	19	313	A86	C-C1-C24-C25
48	19	313	A86	C2-C1-C24-C25
48	20	309	A86	C11-C10-C9-C8
48	20	311	A86	C-C1-C24-C25
48	20	311	A86	C10-C11-C13-O
48	20	311	A86	C11-C13-C14-C15
48	20	311	A86	C26-C27-C29-C30
48	21	211	A86	C-C1-C24-C25
48	21	211	A86	C2-C1-C24-C25
48	21	211	A86	O5-C38-O4-C34
48	21	213	A86	C35-C34-O4-C38
48	21	214	A86	C-C1-C24-C25
48	21	214	A86	C2-C1-C24-C25
48	21	215	A86	C-C1-C24-C25
48	21	215	A86	C2-C1-C24-C25
48	21	215	A86	C39-C38-O4-C34
48	31	311	A86	C24-C25-C26-C27
48	31	312	A86	C24-C25-C26-C27
48	31	313	A86	O5-C38-O4-C34
48	31	314	A86	C-C1-C24-C25
48	31	314	A86	C2-C1-C24-C25
48	31	314	A86	C12-C11-C13-O
48	31	314	A86	C39-C38-O4-C34
48	31	315	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
48	31	315	A86	O5-C38-O4-C34
48	32	203	A86	C11-C10-C9-C8
48	32	203	A86	C10-C11-C13-O
48	32	203	A86	C12-C11-C13-O
48	32	203	A86	C13-C14-C15-C16
48	32	203	A86	C39-C38-O4-C34
48	32	203	A86	O5-C38-O4-C34
48	32	203	A86	C5-C6-C8-C9
48	32	203	A86	C7-C6-C8-C9
48	32	214	A86	C-C1-C24-C25
48	32	214	A86	C2-C1-C24-C25
48	32	216	A86	C26-C27-C29-C30
48	32	216	A86	C35-C34-O4-C38
48	32	217	A86	C-C1-C24-C25
48	32	217	A86	C2-C1-C24-C25
48	32	217	A86	C5-C6-C8-C9
48	32	217	A86	C7-C6-C8-C9
48	32	218	A86	C-C1-C24-C25
48	32	218	A86	O-C13-C14-C15
48	32	218	A86	C11-C13-C14-C15
48	32	218	A86	C13-C14-C15-C16
48	32	218	A86	O5-C38-O4-C34
48	32	221	A86	C-C1-C24-C25
48	32	221	A86	C2-C1-C24-C25
48	32	221	A86	C11-C10-C9-C8
48	32	221	A86	O5-C38-O4-C34
48	32	221	A86	C3-C4-C5-C6
48	33	311	A86	C-C1-C24-C25
48	33	311	A86	C2-C1-C24-C25
48	33	312	A86	C5-C6-C8-C9
48	33	312	A86	C7-C6-C8-C9
48	33	313	A86	C12-C11-C13-C14
48	33	313	A86	O-C13-C14-C15
48	33	313	A86	C11-C13-C14-C15
48	33	313	A86	C13-C14-C15-C16
48	33	313	A86	C33-C34-O4-C38
48	33	313	A86	C39-C38-O4-C34
48	33	313	A86	C5-C6-C8-C9
48	33	313	A86	C7-C6-C8-C9
48	33	314	A86	C11-C10-C9-C8
48	33	314	A86	C13-C14-C15-C16
48	33	314	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
48	33	314	A86	C24-C25-C26-C27
48	33	314	A86	C39-C38-O4-C34
48	33	314	A86	O5-C38-O4-C34
48	33	315	A86	C11-C10-C9-C8
48	33	315	A86	C13-C14-C15-C16
48	33	315	A86	O5-C38-O4-C34
48	33	315	A86	C5-C6-C8-C9
48	33	315	A86	C7-C6-C8-C9
48	34	311	A86	C39-C38-O4-C34
48	34	313	A86	C-C1-C24-C25
48	34	313	A86	C2-C1-C24-C25
48	34	313	A86	C24-C25-C26-C27
48	34	313	A86	C26-C27-C29-C30
48	34	313	A86	C33-C34-O4-C38
48	34	313	A86	C39-C38-O4-C34
48	34	313	A86	C5-C6-C8-C9
48	34	313	A86	C7-C6-C8-C9
48	34	314	A86	C-C1-C24-C25
48	34	314	A86	C2-C1-C24-C25
48	34	314	A86	C5-C6-C8-C9
48	34	314	A86	C7-C6-C8-C9
48	34	316	A86	C11-C13-C14-C15
48	34	316	A86	C13-C14-C15-C16
48	35	311	A86	C24-C25-C26-C27
48	35	312	A86	C-C1-C24-C25
48	35	312	A86	C2-C1-C24-C25
48	35	312	A86	C39-C38-O4-C34
48	35	312	A86	O5-C38-O4-C34
48	35	312	A86	C5-C6-C8-C9
48	35	312	A86	C7-C6-C8-C9
48	35	313	A86	C-C1-C24-C25
48	35	313	A86	C26-C27-C29-C30
48	35	313	A86	C35-C34-O4-C38
48	35	314	A86	C2-C1-C24-C25
48	35	314	A86	C11-C10-C9-C8
48	35	314	A86	C39-C38-O4-C34
48	35	315	A86	C-C1-C24-C25
48	35	315	A86	C2-C1-C24-C25
48	35	315	A86	C39-C38-O4-C34
48	35	315	A86	O5-C38-O4-C34
48	35	315	A86	C5-C6-C8-C9
48	35	315	A86	C7-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
48	35	316	A86	O-C13-C14-C15
48	35	316	A86	C11-C13-C14-C15
48	35	316	A86	C13-C14-C15-C16
48	35	316	A86	O5-C38-O4-C34
48	35	319	A86	C5-C6-C8-C9
48	35	319	A86	C7-C6-C8-C9
48	36	311	A86	C24-C25-C26-C27
48	36	313	A86	C10-C11-C13-O
48	36	313	A86	C12-C11-C13-O
48	36	313	A86	O5-C38-O4-C34
48	37	309	A86	C12-C11-C13-C14
48	37	309	A86	C7-C6-C8-C9
48	37	310	A86	C39-C38-O4-C34
48	37	310	A86	C5-C6-C8-C9
48	37	310	A86	C7-C6-C8-C9
48	37	311	A86	C24-C25-C26-C27
48	37	311	A86	C33-C34-O4-C38
48	37	312	A86	C-C1-C24-C25
48	37	312	A86	C2-C1-C24-C25
48	37	313	A86	C-C1-C24-C25
48	37	313	A86	C2-C1-C24-C25
48	37	313	A86	C11-C13-C14-C15
48	37	313	A86	C5-C6-C8-C9
48	37	313	A86	C7-C6-C8-C9
48	37	314	A86	C11-C10-C9-C8
48	37	314	A86	C10-C11-C13-O
48	37	314	A86	C12-C11-C13-O
48	37	314	A86	C11-C13-C14-C15
48	37	314	A86	C13-C14-C15-C16
48	37	319	A86	C-C1-C24-C25
48	37	319	A86	C2-C1-C24-C25
48	37	319	A86	C39-C38-O4-C34
48	37	319	A86	C5-C6-C8-C9
48	37	319	A86	C7-C6-C8-C9
48	38	212	A86	C24-C25-C26-C27
48	38	212	A86	C39-C38-O4-C34
48	38	212	A86	O5-C38-O4-C34
48	38	213	A86	C5-C6-C8-C9
48	38	213	A86	C7-C6-C8-C9
48	38	214	A86	C-C1-C24-C25
48	38	214	A86	C2-C1-C24-C25
48	38	214	A86	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
48	38	215	A86	C11-C13-C14-C15
48	38	215	A86	C13-C14-C15-C16
48	38	215	A86	C39-C38-O4-C34
48	38	215	A86	O5-C38-O4-C34
48	39	313	A86	C-C1-C24-C25
48	39	313	A86	C2-C1-C24-C25
48	40	201	A86	C12-C11-C13-C14
48	40	211	A86	C11-C10-C9-C8
48	40	213	A86	C-C1-C24-C25
48	40	213	A86	C10-C11-C13-O
48	40	213	A86	C11-C13-C14-C15
48	40	213	A86	C26-C27-C29-C30
48	41	211	A86	C-C1-C24-C25
48	41	211	A86	C2-C1-C24-C25
48	41	211	A86	O5-C38-O4-C34
48	41	213	A86	C35-C34-O4-C38
48	41	214	A86	C-C1-C24-C25
48	41	214	A86	C2-C1-C24-C25
48	41	215	A86	C-C1-C24-C25
48	41	215	A86	C2-C1-C24-C25
48	41	215	A86	C39-C38-O4-C34
50	16	312	DD6	C-C1-C2-C3
50	16	312	DD6	C-C1-C24-C25
50	16	312	DD6	C2-C1-C24-C25
50	16	312	DD6	C9-C10-C11-C13
50	16	312	DD6	C10-C11-C13-C14
50	16	312	DD6	C12-C11-C13-C14
50	16	312	DD6	C4-C5-C6-C7
50	16	312	DD6	C7-C6-C8-C9
50	19	312	DD6	C-C1-C2-C3
50	19	312	DD6	C-C1-C24-C25
50	19	312	DD6	C9-C10-C11-C12
50	19	312	DD6	C4-C5-C6-C7
50	19	312	DD6	C5-C6-C8-C9
50	19	312	DD6	C7-C6-C8-C9
50	20	310	DD6	C-C1-C2-C3
50	20	310	DD6	C-C1-C24-C25
50	20	310	DD6	C2-C1-C24-C25
50	20	310	DD6	C9-C10-C11-C12
50	20	310	DD6	C9-C10-C11-C13
50	20	310	DD6	C10-C11-C13-C14
50	20	310	DD6	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
50	20	310	DD6	C3-C4-C5-C6
50	20	310	DD6	C4-C5-C6-C7
50	20	310	DD6	C4-C5-C6-C8
50	20	312	DD6	C-C1-C2-C3
50	20	312	DD6	C2-C1-C24-C25
50	20	312	DD6	C9-C10-C11-C12
50	20	312	DD6	C13-C14-C15-C16
50	20	312	DD6	C4-C5-C6-C7
50	20	312	DD6	C7-C6-C8-C9
50	21	212	DD6	C-C1-C2-C3
50	21	212	DD6	C24-C1-C2-C3
50	21	212	DD6	C9-C10-C11-C12
50	21	212	DD6	C12-C11-C13-C14
50	21	212	DD6	C4-C5-C6-C8
50	21	212	DD6	C7-C6-C8-C9
50	21	216	DD6	C-C1-C2-C3
50	21	216	DD6	C2-C1-C24-C25
50	21	216	DD6	C9-C10-C11-C12
50	21	216	DD6	C10-C11-C13-C14
50	21	216	DD6	C4-C5-C6-C7
50	21	216	DD6	C4-C5-C6-C8
50	21	216	DD6	C5-C6-C8-C9
50	36	312	DD6	C-C1-C2-C3
50	36	312	DD6	C-C1-C24-C25
50	36	312	DD6	C2-C1-C24-C25
50	36	312	DD6	C9-C10-C11-C13
50	36	312	DD6	C10-C11-C13-C14
50	36	312	DD6	C12-C11-C13-C14
50	36	312	DD6	C4-C5-C6-C7
50	36	312	DD6	C7-C6-C8-C9
50	39	312	DD6	C-C1-C2-C3
50	39	312	DD6	C-C1-C24-C25
50	39	312	DD6	C9-C10-C11-C12
50	39	312	DD6	C4-C5-C6-C7
50	39	312	DD6	C5-C6-C8-C9
50	39	312	DD6	C7-C6-C8-C9
50	40	212	DD6	C-C1-C2-C3
50	40	212	DD6	C-C1-C24-C25
50	40	212	DD6	C2-C1-C24-C25
50	40	212	DD6	C9-C10-C11-C12
50	40	212	DD6	C9-C10-C11-C13
50	40	212	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
50	40	212	DD6	C1-C2-C3-C4
50	40	212	DD6	C3-C4-C5-C6
50	40	212	DD6	C4-C5-C6-C7
50	40	212	DD6	C4-C5-C6-C8
50	40	214	DD6	C-C1-C2-C3
50	40	214	DD6	C2-C1-C24-C25
50	40	214	DD6	C9-C10-C11-C12
50	40	214	DD6	C13-C14-C15-C16
50	40	214	DD6	C4-C5-C6-C7
50	40	214	DD6	C7-C6-C8-C9
50	41	212	DD6	C-C1-C2-C3
50	41	212	DD6	C24-C1-C2-C3
50	41	212	DD6	C9-C10-C11-C12
50	41	212	DD6	C12-C11-C13-C14
50	41	212	DD6	C4-C5-C6-C8
50	41	212	DD6	C7-C6-C8-C9
50	41	216	DD6	C-C1-C2-C3
50	41	216	DD6	C2-C1-C24-C25
50	41	216	DD6	C9-C10-C11-C12
50	41	216	DD6	C10-C11-C13-C14
50	41	216	DD6	C4-C5-C6-C7
50	41	216	DD6	C4-C5-C6-C8
50	41	216	DD6	C5-C6-C8-C9
48	11	311	A86	O5-C38-O4-C34
48	12	215	A86	C39-C38-O4-C34
48	12	216	A86	C39-C38-O4-C34
48	12	220	A86	C39-C38-O4-C34
48	13	312	A86	C39-C38-O4-C34
48	14	314	A86	C39-C38-O4-C34
48	14	314	A86	O5-C38-O4-C34
48	15	313	A86	C39-C38-O4-C34
48	15	314	A86	O5-C38-O4-C34
48	15	316	A86	C39-C38-O4-C34
48	15	319	A86	C39-C38-O4-C34
48	16	310	A86	C39-C38-O4-C34
48	16	314	A86	C39-C38-O4-C34
48	17	312	A86	C39-C38-O4-C34
48	17	315	A86	C39-C38-O4-C34
48	18	214	A86	C39-C38-O4-C34
48	21	211	A86	C39-C38-O4-C34
48	21	213	A86	C39-C38-O4-C34
48	31	311	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
48	31	313	A86	C39-C38-O4-C34
48	32	216	A86	C39-C38-O4-C34
48	32	217	A86	C39-C38-O4-C34
48	32	221	A86	C39-C38-O4-C34
48	33	312	A86	C39-C38-O4-C34
48	34	314	A86	C39-C38-O4-C34
48	34	314	A86	O5-C38-O4-C34
48	35	313	A86	C39-C38-O4-C34
48	35	314	A86	O5-C38-O4-C34
48	35	319	A86	C39-C38-O4-C34
48	36	310	A86	C39-C38-O4-C34
48	36	313	A86	C39-C38-O4-C34
48	37	311	A86	C39-C38-O4-C34
48	37	314	A86	C39-C38-O4-C34
48	38	214	A86	C39-C38-O4-C34
48	41	211	A86	C39-C38-O4-C34
48	41	213	A86	C39-C38-O4-C34
37	17	309	CLA	O1D-CGD-O2D-CED
37	37	308	CLA	O1D-CGD-O2D-CED
48	11	311	A86	C39-C38-O4-C34
48	12	217	A86	C39-C38-O4-C34
48	13	312	A86	O5-C38-O4-C34
48	13	313	A86	O5-C38-O4-C34
48	13	315	A86	C39-C38-O4-C34
48	14	311	A86	O5-C38-O4-C34
48	14	312	A86	C39-C38-O4-C34
48	14	313	A86	O5-C38-O4-C34
48	15	311	A86	C39-C38-O4-C34
48	16	311	A86	C39-C38-O4-C34
48	17	320	A86	O5-C38-O4-C34
48	31	311	A86	C39-C38-O4-C34
48	32	218	A86	C39-C38-O4-C34
48	33	312	A86	O5-C38-O4-C34
48	33	313	A86	O5-C38-O4-C34
48	33	315	A86	C39-C38-O4-C34
48	34	311	A86	O5-C38-O4-C34
48	34	312	A86	C39-C38-O4-C34
48	34	313	A86	O5-C38-O4-C34
48	35	311	A86	C39-C38-O4-C34
48	35	316	A86	C39-C38-O4-C34
48	36	311	A86	C39-C38-O4-C34
48	37	319	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
37	14	301	CLA	CBD-CGD-O2D-CED
37	16	307	CLA	CBD-CGD-O2D-CED
37	17	309	CLA	CBD-CGD-O2D-CED
37	18	201	CLA	CBD-CGD-O2D-CED
37	18	202	CLA	CBD-CGD-O2D-CED
37	21	206	CLA	CBD-CGD-O2D-CED
37	32	213	CLA	CBD-CGD-O2D-CED
37	34	301	CLA	CBD-CGD-O2D-CED
37	36	307	CLA	CBD-CGD-O2D-CED
37	38	201	CLA	CBD-CGD-O2D-CED
37	41	206	CLA	CBD-CGD-O2D-CED
37	C	513	CLA	O1A-CGA-O2A-C1
37	c	513	CLA	O1A-CGA-O2A-C1
48	12	216	A86	O5-C38-O4-C34
48	17	312	A86	O5-C38-O4-C34
48	32	217	A86	O5-C38-O4-C34
48	37	311	A86	O5-C38-O4-C34
37	21	206	CLA	O1D-CGD-O2D-CED
37	41	206	CLA	O1D-CGD-O2D-CED
47	12	206	KC1	C4C-C3C-CAC-CBC
47	32	207	KC1	C4C-C3C-CAC-CBC
48	17	313	A86	C39-C38-O4-C34
48	19	313	A86	C39-C38-O4-C34
48	35	311	A86	O5-C38-O4-C34
48	39	313	A86	C39-C38-O4-C34
37	18	202	CLA	O1D-CGD-O2D-CED
47	20	302	KC1	O1D-CGD-O2D-CED
47	40	204	KC1	O1D-CGD-O2D-CED
45	D	404	PL9	C47-C48-C49-C51
45	d	402	PL9	C47-C48-C49-C51
37	C	501	CLA	CBD-CGD-O2D-CED
37	C	502	CLA	CBD-CGD-O2D-CED
37	c	501	CLA	CBD-CGD-O2D-CED
37	c	502	CLA	CBD-CGD-O2D-CED
37	11	301	CLA	CBD-CGD-O2D-CED
37	12	212	CLA	CBD-CGD-O2D-CED
37	16	306	CLA	CBD-CGD-O2D-CED
37	17	302	CLA	CBD-CGD-O2D-CED
37	19	301	CLA	CBD-CGD-O2D-CED
37	31	302	CLA	CBD-CGD-O2D-CED
37	36	306	CLA	CBD-CGD-O2D-CED
37	37	301	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
37	39	301	CLA	CBD-CGD-O2D-CED
48	12	215	A86	O5-C38-O4-C34
48	15	319	A86	O5-C38-O4-C34
48	17	315	A86	O5-C38-O4-C34
48	19	313	A86	O5-C38-O4-C34
48	32	216	A86	O5-C38-O4-C34
48	35	319	A86	O5-C38-O4-C34
48	37	312	A86	C39-C38-O4-C34
48	37	314	A86	O5-C38-O4-C34
48	39	313	A86	O5-C38-O4-C34
37	C	512	CLA	O1A-CGA-O2A-C1
37	c	512	CLA	O1A-CGA-O2A-C1
37	13	308	CLA	O1A-CGA-O2A-C1
37	18	203	CLA	O1A-CGA-O2A-C1
37	33	308	CLA	O1A-CGA-O2A-C1
37	38	203	CLA	O1A-CGA-O2A-C1
41	17	317	LMG	O10-C28-O8-C9
41	37	316	LMG	O10-C28-O8-C9
37	38	202	CLA	O1D-CGD-O2D-CED
48	11	312	A86	C39-C38-O4-C34
48	15	313	A86	O5-C38-O4-C34
48	16	310	A86	O5-C38-O4-C34
48	18	214	A86	O5-C38-O4-C34
48	21	213	A86	O5-C38-O4-C34
48	31	312	A86	C39-C38-O4-C34
48	35	313	A86	O5-C38-O4-C34
48	36	310	A86	O5-C38-O4-C34
48	38	214	A86	O5-C38-O4-C34
48	41	213	A86	O5-C38-O4-C34
37	11	310	CLA	O1D-CGD-O2D-CED
37	31	310	CLA	O1D-CGD-O2D-CED
48	14	316	A86	C39-C38-O4-C34
48	34	316	A86	C39-C38-O4-C34
37	13	307	CLA	CBD-CGD-O2D-CED
37	33	307	CLA	CBD-CGD-O2D-CED
40	B	519	SQD	O49-C7-O47-C45
40	L	101	SQD	O49-C7-O47-C45
43	D	411	LHG	O9-C7-O7-C5
43	a	412	LHG	O9-C7-O7-C5
43	21	201	LHG	O9-C7-O7-C5
43	41	201	LHG	O9-C7-O7-C5
47	12	206	KC1	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
47	32	207	KC1	C2C-C3C-CAC-CBC
48	31	314	A86	O5-C38-O4-C34
37	B	507	CLA	C3-C5-C6-C7
37	B	514	CLA	C3-C5-C6-C7
37	C	511	CLA	C3-C5-C6-C7
37	C	512	CLA	C3-C5-C6-C7
37	b	507	CLA	C3-C5-C6-C7
37	b	514	CLA	C3-C5-C6-C7
37	c	511	CLA	C3-C5-C6-C7
37	c	512	CLA	C3-C5-C6-C7
37	13	301	CLA	C3-C5-C6-C7
37	15	308	CLA	C3-C5-C6-C7
37	17	302	CLA	C3-C5-C6-C7
37	21	202	CLA	C3-C5-C6-C7
37	21	206	CLA	C3-C5-C6-C7
37	33	301	CLA	C3-C5-C6-C7
37	35	308	CLA	C3-C5-C6-C7
37	37	301	CLA	C3-C5-C6-C7
37	38	208	CLA	C3-C5-C6-C7
37	41	202	CLA	C3-C5-C6-C7
37	41	206	CLA	C3-C5-C6-C7
38	A	404	PHO	C3-C5-C6-C7
38	a	406	PHO	C3-C5-C6-C7
37	C	513	CLA	CBA-CGA-O2A-C1
37	c	513	CLA	CBA-CGA-O2A-C1
37	18	203	CLA	CBA-CGA-O2A-C1
41	17	317	LMG	C29-C28-O8-C9
41	37	316	LMG	C29-C28-O8-C9
48	11	314	A86	O5-C38-O4-C34
48	14	315	A86	C39-C38-O4-C34
48	14	316	A86	O5-C38-O4-C34
48	34	315	A86	C39-C38-O4-C34
48	34	316	A86	O5-C38-O4-C34
41	B	521	LMG	C11-C10-O7-C8
41	L	102	LMG	C11-C10-O7-C8
41	b	520	LMG	C11-C10-O7-C8
41	l	101	LMG	C11-C10-O7-C8
37	W	102	CLA	CBD-CGD-O2D-CED
37	31	301	CLA	CBD-CGD-O2D-CED
48	11	319	A86	C39-C38-O4-C34
48	31	319	A86	C39-C38-O4-C34
48	37	309	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
41	11	316	LMG	O6-C5-C6-O5
41	17	317	LMG	O6-C5-C6-O5
41	31	316	LMG	O6-C5-C6-O5
41	37	316	LMG	O6-C5-C6-O5
48	17	311	A86	O5-C38-O4-C34
48	21	215	A86	O5-C38-O4-C34
48	37	310	A86	O5-C38-O4-C34
48	41	215	A86	O5-C38-O4-C34
47	11	306	KC1	CAA-CBA-CGA-O1A
47	11	306	KC1	CAA-CBA-CGA-O2A
47	31	307	KC1	CAA-CBA-CGA-O1A
47	31	307	KC1	CAA-CBA-CGA-O2A
37	11	307	CLA	C3-C5-C6-C7
37	12	209	CLA	C3-C5-C6-C7
37	13	307	CLA	C3-C5-C6-C7
37	14	307	CLA	C3-C5-C6-C7
37	15	307	CLA	C3-C5-C6-C7
37	17	307	CLA	C3-C5-C6-C7
37	31	308	CLA	C3-C5-C6-C7
37	32	210	CLA	C3-C5-C6-C7
37	33	307	CLA	C3-C5-C6-C7
37	34	307	CLA	C3-C5-C6-C7
37	35	307	CLA	C3-C5-C6-C7
37	37	306	CLA	C3-C5-C6-C7
48	11	319	A86	O5-C38-O4-C34
48	31	319	A86	O5-C38-O4-C34
48	37	309	A86	O5-C38-O4-C34
37	B	514	CLA	C4-C3-C5-C6
37	b	514	CLA	C4-C3-C5-C6
37	19	310	CLA	C4-C3-C5-C6
37	39	310	CLA	C4-C3-C5-C6
37	B	514	CLA	C2-C3-C5-C6
37	C	507	CLA	C2-C3-C5-C6
37	b	514	CLA	C2-C3-C5-C6
37	c	507	CLA	C2-C3-C5-C6
37	21	204	CLA	C2-C3-C5-C6
37	39	310	CLA	C2-C3-C5-C6
37	41	204	CLA	C2-C3-C5-C6
37	21	205	CLA	CBD-CGD-O2D-CED
37	38	203	CLA	CBD-CGD-O2D-CED
37	41	205	CLA	CBD-CGD-O2D-CED
37	B	501	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
37	B	506	CLA	C2A-CAA-CBA-CGA
37	b	501	CLA	C2A-CAA-CBA-CGA
37	b	506	CLA	C2A-CAA-CBA-CGA
37	11	301	CLA	C2A-CAA-CBA-CGA
37	12	204	CLA	C2A-CAA-CBA-CGA
37	14	302	CLA	C2A-CAA-CBA-CGA
37	17	302	CLA	C2A-CAA-CBA-CGA
37	19	309	CLA	C2A-CAA-CBA-CGA
37	31	302	CLA	C2A-CAA-CBA-CGA
37	32	205	CLA	C2A-CAA-CBA-CGA
37	34	302	CLA	C2A-CAA-CBA-CGA
37	37	301	CLA	C2A-CAA-CBA-CGA
37	39	309	CLA	C2A-CAA-CBA-CGA
48	17	310	A86	C39-C38-O4-C34
37	11	301	CLA	C3-C5-C6-C7
37	12	204	CLA	C3-C5-C6-C7
37	18	208	CLA	C3-C5-C6-C7
37	31	302	CLA	C3-C5-C6-C7
37	32	205	CLA	C3-C5-C6-C7
37	C	512	CLA	CBA-CGA-O2A-C1
37	c	512	CLA	CBA-CGA-O2A-C1
37	13	308	CLA	CBA-CGA-O2A-C1
37	33	308	CLA	CBA-CGA-O2A-C1
37	38	203	CLA	CBA-CGA-O2A-C1
37	18	203	CLA	CBD-CGD-O2D-CED
48	14	312	A86	O5-C38-O4-C34
48	34	312	A86	O5-C38-O4-C34
41	16	316	LMG	O9-C10-O7-C8
41	36	314	LMG	O9-C10-O7-C8
45	D	404	PL9	C37-C38-C39-C41
45	d	402	PL9	C37-C38-C39-C41
48	16	311	A86	O5-C38-O4-C34
48	36	311	A86	O5-C38-O4-C34
39	B	525	BCR	C13-C14-C15-C16
39	b	524	BCR	C13-C14-C15-C16
48	11	313	A86	C24-C25-C26-C27
48	11	315	A86	C24-C25-C26-C27
48	11	319	A86	C24-C25-C26-C27
48	12	214	A86	C24-C25-C26-C27
48	12	215	A86	C24-C25-C26-C27
48	12	217	A86	C11-C10-C9-C8
48	12	220	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
48	13	312	A86	C24-C25-C26-C27
48	13	313	A86	C24-C25-C26-C27
48	14	311	A86	C24-C25-C26-C27
48	14	315	A86	C24-C25-C26-C27
48	15	313	A86	C24-C25-C26-C27
48	16	310	A86	C24-C25-C26-C27
48	17	310	A86	C11-C10-C9-C8
48	17	310	A86	C24-C25-C26-C27
48	18	212	A86	C11-C10-C9-C8
48	18	213	A86	C11-C10-C9-C8
48	18	215	A86	C11-C10-C9-C8
48	20	311	A86	C11-C10-C9-C8
48	21	211	A86	C11-C10-C9-C8
48	21	214	A86	C24-C25-C26-C27
48	31	315	A86	C24-C25-C26-C27
48	31	319	A86	C24-C25-C26-C27
48	32	215	A86	C24-C25-C26-C27
48	32	216	A86	C24-C25-C26-C27
48	32	218	A86	C11-C10-C9-C8
48	32	221	A86	C24-C25-C26-C27
48	33	312	A86	C24-C25-C26-C27
48	33	313	A86	C24-C25-C26-C27
48	34	311	A86	C24-C25-C26-C27
48	34	315	A86	C24-C25-C26-C27
48	35	313	A86	C24-C25-C26-C27
48	36	310	A86	C24-C25-C26-C27
48	37	309	A86	C11-C10-C9-C8
48	37	309	A86	C24-C25-C26-C27
48	37	312	A86	C24-C25-C26-C27
48	38	212	A86	C11-C10-C9-C8
48	38	213	A86	C11-C10-C9-C8
48	38	215	A86	C11-C10-C9-C8
48	40	213	A86	C11-C10-C9-C8
48	41	211	A86	C11-C10-C9-C8
48	41	214	A86	C24-C25-C26-C27
50	16	312	DD6	C24-C25-C26-C27
50	20	312	DD6	C24-C25-C26-C27
50	21	212	DD6	C24-C25-C26-C27
50	21	212	DD6	C3-C4-C5-C6
50	21	216	DD6	C1-C2-C3-C4
50	36	312	DD6	C24-C25-C26-C27
50	40	214	DD6	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
50	41	212	DD6	C24-C25-C26-C27
50	41	212	DD6	C3-C4-C5-C6
50	41	216	DD6	C1-C2-C3-C4
48	17	310	A86	O5-C38-O4-C34
48	19	311	A86	C39-C38-O4-C34
48	39	311	A86	C39-C38-O4-C34
37	B	516	CLA	CBD-CGD-O2D-CED
37	D	406	CLA	CBD-CGD-O2D-CED
37	b	516	CLA	CBD-CGD-O2D-CED
37	d	404	CLA	CBD-CGD-O2D-CED
37	12	209	CLA	CBD-CGD-O2D-CED
37	32	210	CLA	CBD-CGD-O2D-CED
37	14	301	CLA	O1D-CGD-O2D-CED
37	34	301	CLA	O1D-CGD-O2D-CED
43	D	409	LHG	O2-C2-C3-O3
43	d	407	LHG	O2-C2-C3-O3
43	17	316	LHG	O2-C2-C3-O3
43	37	315	LHG	O2-C2-C3-O3
37	B	502	CLA	C3-C5-C6-C7
37	b	502	CLA	C3-C5-C6-C7
37	19	307	CLA	C3-C5-C6-C7
37	19	310	CLA	C3-C5-C6-C7
37	39	307	CLA	C3-C5-C6-C7
37	39	310	CLA	C3-C5-C6-C7
37	C	511	CLA	CBA-CGA-O2A-C1
37	c	511	CLA	CBA-CGA-O2A-C1
41	16	316	LMG	C29-C28-O8-C9
41	36	314	LMG	C29-C28-O8-C9
48	19	311	A86	O5-C38-O4-C34
48	20	311	A86	C39-C38-O4-C34
48	39	311	A86	O5-C38-O4-C34
48	40	213	A86	C39-C38-O4-C34
40	17	301	SQD	O10-C23-O48-C46
40	36	315	SQD	O10-C23-O48-C46
44	C	516	DGD	O6E-C5E-C6E-O5E
44	c	516	DGD	O6E-C5E-C6E-O5E
43	21	201	LHG	C8-C7-O7-C5
43	41	201	LHG	C8-C7-O7-C5
37	21	209	CLA	CBD-CGD-O2D-CED
37	41	209	CLA	CBD-CGD-O2D-CED
43	19	314	LHG	C27-C28-C29-C30
43	39	314	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
37	D	406	CLA	C3-C5-C6-C7
37	W	101	CLA	C3-C5-C6-C7
37	d	404	CLA	C3-C5-C6-C7
37	w	101	CLA	C3-C5-C6-C7
37	14	302	CLA	C3-C5-C6-C7
37	34	302	CLA	C3-C5-C6-C7
37	Z	101	CLA	CBA-CGA-O2A-C1
37	z	101	CLA	CBA-CGA-O2A-C1
41	11	317	LMG	O6-C5-C6-O5
41	31	317	LMG	O6-C5-C6-O5
43	17	316	LHG	O9-C7-O7-C5
43	37	315	LHG	O9-C7-O7-C5
47	11	309	KC1	CAA-CBA-CGA-O2A
47	14	309	KC1	CAA-CBA-CGA-O2A
47	15	306	KC1	CAA-CBA-CGA-O2A
47	21	207	KC1	CAA-CBA-CGA-O2A
47	31	309	KC1	CAA-CBA-CGA-O2A
47	34	309	KC1	CAA-CBA-CGA-O2A
47	35	304	KC1	CAA-CBA-CGA-O1A
47	35	306	KC1	CAA-CBA-CGA-O2A
47	41	207	KC1	CAA-CBA-CGA-O2A
41	11	316	LMG	C4-C5-C6-O5
41	31	316	LMG	C4-C5-C6-O5
37	B	502	CLA	C4-C3-C5-C6
37	B	503	CLA	C4-C3-C5-C6
37	B	505	CLA	C4-C3-C5-C6
37	C	503	CLA	C4-C3-C5-C6
37	b	502	CLA	C4-C3-C5-C6
37	b	503	CLA	C4-C3-C5-C6
37	b	505	CLA	C4-C3-C5-C6
37	c	503	CLA	C4-C3-C5-C6
37	20	301	CLA	C4-C3-C5-C6
37	40	203	CLA	C4-C3-C5-C6
41	17	317	LMG	C4-C5-C6-O5
41	37	316	LMG	C4-C5-C6-O5
37	B	502	CLA	C2-C3-C5-C6
37	B	503	CLA	C2-C3-C5-C6
37	B	505	CLA	C2-C3-C5-C6
37	C	503	CLA	C2-C3-C5-C6
37	b	502	CLA	C2-C3-C5-C6
37	b	503	CLA	C2-C3-C5-C6
37	b	505	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
37	c	503	CLA	C2-C3-C5-C6
37	20	301	CLA	C2-C3-C5-C6
37	40	203	CLA	C2-C3-C5-C6
37	W	101	CLA	CBD-CGD-O2D-CED
37	w	101	CLA	CBD-CGD-O2D-CED
37	W	102	CLA	C2A-CAA-CBA-CGA
37	13	301	CLA	C2A-CAA-CBA-CGA
37	31	301	CLA	C2A-CAA-CBA-CGA
37	33	301	CLA	C2A-CAA-CBA-CGA
37	C	511	CLA	O1A-CGA-O2A-C1
37	c	511	CLA	O1A-CGA-O2A-C1
37	39	307	CLA	O1A-CGA-O2A-C1
41	A	408	LMG	O6-C1-O1-C7
41	a	410	LMG	O6-C1-O1-C7
45	D	404	PL9	C24-C26-C27-C28
45	D	404	PL9	C29-C31-C32-C33
45	D	404	PL9	C34-C36-C37-C38
45	d	402	PL9	C24-C26-C27-C28
45	d	402	PL9	C29-C31-C32-C33
45	d	402	PL9	C34-C36-C37-C38
37	b	523	CLA	C3-C5-C6-C7
37	C	505	CLA	CBA-CGA-O2A-C1
37	W	102	CLA	CBA-CGA-O2A-C1
37	19	307	CLA	CBA-CGA-O2A-C1
37	31	301	CLA	CBA-CGA-O2A-C1
37	39	307	CLA	CBA-CGA-O2A-C1
37	B	510	CLA	CBD-CGD-O2D-CED
37	b	510	CLA	CBD-CGD-O2D-CED
37	18	201	CLA	O1D-CGD-O2D-CED
37	38	201	CLA	O1D-CGD-O2D-CED
37	C	505	CLA	O1A-CGA-O2A-C1
37	c	505	CLA	O1A-CGA-O2A-C1
37	19	307	CLA	O1A-CGA-O2A-C1
41	16	316	LMG	C11-C10-O7-C8
41	36	314	LMG	C11-C10-O7-C8
47	11	309	KC1	CAA-CBA-CGA-O1A
47	13	304	KC1	CAA-CBA-CGA-O1A
47	13	304	KC1	CAA-CBA-CGA-O2A
47	15	304	KC1	CAA-CBA-CGA-O1A
47	31	309	KC1	CAA-CBA-CGA-O1A
47	33	304	KC1	CAA-CBA-CGA-O1A
47	33	304	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
41	C	518	LMG	O6-C5-C6-O5
41	c	518	LMG	O6-C5-C6-O5
45	D	408	PL9	C42-C43-C44-C45
45	d	406	PL9	C42-C43-C44-C45
37	12	212	CLA	O1D-CGD-O2D-CED
37	32	213	CLA	O1D-CGD-O2D-CED
37	13	301	CLA	CBD-CGD-O2D-CED
37	16	309	CLA	CBD-CGD-O2D-CED
37	33	301	CLA	CBD-CGD-O2D-CED
37	36	309	CLA	CBD-CGD-O2D-CED
37	Z	101	CLA	O1A-CGA-O2A-C1
37	z	101	CLA	O1A-CGA-O2A-C1
37	B	524	CLA	C3-C5-C6-C7
37	C	508	CLA	C3-C5-C6-C7
37	c	508	CLA	C3-C5-C6-C7
37	16	307	CLA	O1D-CGD-O2D-CED
37	36	307	CLA	O1D-CGD-O2D-CED
37	C	506	CLA	CBA-CGA-O2A-C1
37	C	510	CLA	CBA-CGA-O2A-C1
37	c	505	CLA	CBA-CGA-O2A-C1
37	c	506	CLA	CBA-CGA-O2A-C1
37	c	510	CLA	CBA-CGA-O2A-C1
37	19	305	CLA	CBA-CGA-O2A-C1
37	39	305	CLA	CBA-CGA-O2A-C1
40	17	301	SQD	C24-C23-O48-C46
40	36	315	SQD	C24-C23-O48-C46
41	11	317	LMG	C29-C28-O8-C9
41	31	317	LMG	C29-C28-O8-C9
48	11	314	A86	C24-C25-C26-C27
48	14	316	A86	C11-C10-C9-C8
48	15	314	A86	C24-C25-C26-C27
48	16	313	A86	C1-C2-C3-C4
48	17	313	A86	C24-C25-C26-C27
48	21	211	A86	C24-C25-C26-C27
48	31	314	A86	C24-C25-C26-C27
48	34	316	A86	C11-C10-C9-C8
48	35	314	A86	C24-C25-C26-C27
48	40	201	A86	C1-C2-C3-C4
48	41	211	A86	C24-C25-C26-C27
50	21	216	DD6	C24-C25-C26-C27
50	41	216	DD6	C24-C25-C26-C27
43	D	411	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
43	a	412	LHG	C7-C8-C9-C10
43	21	217	LHG	C23-C24-C25-C26
41	11	317	LMG	C4-C5-C6-O5
41	31	317	LMG	C4-C5-C6-O5
47	13	302	KC1	CAA-CBA-CGA-O2A
47	14	309	KC1	CAA-CBA-CGA-O1A
47	15	302	KC1	CAA-CBA-CGA-O1A
47	15	302	KC1	CAA-CBA-CGA-O2A
47	15	306	KC1	CAA-CBA-CGA-O1A
47	16	304	KC1	CAA-CBA-CGA-O1A
47	16	304	KC1	CAA-CBA-CGA-O2A
47	18	205	KC1	CAA-CBA-CGA-O2A
47	19	308	KC1	CAA-CBA-CGA-O1A
47	21	207	KC1	CAA-CBA-CGA-O1A
47	33	302	KC1	CAA-CBA-CGA-O2A
47	34	309	KC1	CAA-CBA-CGA-O1A
47	35	302	KC1	CAA-CBA-CGA-O1A
47	35	302	KC1	CAA-CBA-CGA-O2A
47	35	306	KC1	CAA-CBA-CGA-O1A
47	36	304	KC1	CAA-CBA-CGA-O1A
47	36	304	KC1	CAA-CBA-CGA-O2A
47	38	205	KC1	CAA-CBA-CGA-O2A
47	39	308	KC1	CAA-CBA-CGA-O1A
47	41	207	KC1	CAA-CBA-CGA-O1A
37	B	513	CLA	C8-C10-C11-C12
37	C	508	CLA	C8-C10-C11-C12
37	W	101	CLA	C8-C10-C11-C12
37	b	501	CLA	C8-C10-C11-C12
37	b	513	CLA	C8-C10-C11-C12
37	c	503	CLA	C8-C10-C11-C12
37	c	508	CLA	C8-C10-C11-C12
37	w	101	CLA	C8-C10-C11-C12
37	13	308	CLA	C10-C11-C12-C13
37	33	308	CLA	C10-C11-C12-C13
43	37	321	LHG	C23-C24-C25-C26
37	19	310	CLA	C2-C3-C5-C6
37	A	405	CLA	C11-C10-C8-C9
37	B	501	CLA	C11-C10-C8-C9
37	Z	101	CLA	C11-C12-C13-C14
37	a	407	CLA	C11-C10-C8-C9
37	b	501	CLA	C11-C10-C8-C9
37	z	101	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
37	21	206	CLA	C11-C12-C13-C14
37	41	206	CLA	C11-C12-C13-C14
37	16	306	CLA	O1D-CGD-O2D-CED
37	17	302	CLA	O1D-CGD-O2D-CED
37	33	307	CLA	O1D-CGD-O2D-CED
37	36	306	CLA	O1D-CGD-O2D-CED
37	37	301	CLA	O1D-CGD-O2D-CED
48	17	313	A86	O5-C38-O4-C34
48	37	312	A86	O5-C38-O4-C34
37	B	501	CLA	C8-C10-C11-C12
37	C	503	CLA	C8-C10-C11-C12
37	C	508	CLA	C5-C6-C7-C8
37	18	202	CLA	C2A-CAA-CBA-CGA
37	19	306	CLA	C2A-CAA-CBA-CGA
37	38	202	CLA	C2A-CAA-CBA-CGA
37	39	306	CLA	C2A-CAA-CBA-CGA
39	A	410	BCR	C7-C8-C9-C34
39	B	518	BCR	C7-C8-C9-C34
39	D	407	BCR	C37-C22-C23-C24
39	K	101	BCR	C7-C8-C9-C34
39	0	101	BCR	C37-C22-C23-C24
39	a	413	BCR	C7-C8-C9-C34
39	b	518	BCR	C7-C8-C9-C34
39	d	405	BCR	C37-C22-C23-C24
39	y	101	BCR	C7-C8-C9-C34
39	5	101	BCR	C37-C22-C23-C24
48	11	312	A86	C-C1-C24-C25
48	11	313	A86	C-C1-C24-C25
48	11	319	A86	C-C1-C24-C25
48	12	215	A86	C-C1-C24-C25
48	12	220	A86	C7-C6-C8-C9
48	13	313	A86	C-C1-C24-C25
48	13	314	A86	C-C1-C24-C25
48	13	315	A86	C-C1-C24-C25
48	14	316	A86	C-C1-C24-C25
48	15	314	A86	C-C1-C24-C25
48	15	314	A86	C7-C6-C8-C9
48	16	311	A86	C-C1-C24-C25
48	16	313	A86	C-C1-C24-C25
48	16	313	A86	C7-C6-C8-C9
48	17	311	A86	C-C1-C24-C25
48	19	311	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
48	21	211	A86	C7-C6-C8-C9
48	21	213	A86	C-C1-C24-C25
48	31	312	A86	C-C1-C24-C25
48	31	319	A86	C-C1-C24-C25
48	32	216	A86	C-C1-C24-C25
48	32	221	A86	C7-C6-C8-C9
48	33	313	A86	C-C1-C24-C25
48	33	314	A86	C-C1-C24-C25
48	33	315	A86	C-C1-C24-C25
48	34	316	A86	C-C1-C24-C25
48	35	314	A86	C-C1-C24-C25
48	35	314	A86	C7-C6-C8-C9
48	36	311	A86	C-C1-C24-C25
48	39	311	A86	C-C1-C24-C25
48	40	201	A86	C-C1-C24-C25
48	40	201	A86	C7-C6-C8-C9
48	41	211	A86	C7-C6-C8-C9
48	41	213	A86	C-C1-C24-C25
50	20	310	DD6	C7-C6-C8-C9
50	20	312	DD6	C-C1-C24-C25
50	20	312	DD6	C12-C11-C13-C14
50	21	212	DD6	C-C1-C24-C25
50	21	216	DD6	C-C1-C24-C25
50	21	216	DD6	C12-C11-C13-C14
50	21	216	DD6	C7-C6-C8-C9
50	40	212	DD6	C7-C6-C8-C9
50	40	214	DD6	C-C1-C24-C25
50	40	214	DD6	C12-C11-C13-C14
50	41	212	DD6	C-C1-C24-C25
50	41	216	DD6	C-C1-C24-C25
50	41	216	DD6	C12-C11-C13-C14
50	41	216	DD6	C7-C6-C8-C9
39	K	101	BCR	C7-C8-C9-C10
39	y	101	BCR	C7-C8-C9-C10
48	11	312	A86	C2-C1-C24-C25
48	11	313	A86	C2-C1-C24-C25
48	11	319	A86	C2-C1-C24-C25
48	12	215	A86	C2-C1-C24-C25
48	12	220	A86	C5-C6-C8-C9
48	13	313	A86	C2-C1-C24-C25
48	13	314	A86	C2-C1-C24-C25
48	16	313	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
48	16	313	A86	C5-C6-C8-C9
48	17	311	A86	C2-C1-C24-C25
48	19	311	A86	C2-C1-C24-C25
48	21	213	A86	C2-C1-C24-C25
48	31	312	A86	C2-C1-C24-C25
48	31	319	A86	C2-C1-C24-C25
48	32	216	A86	C2-C1-C24-C25
48	32	221	A86	C5-C6-C8-C9
48	33	313	A86	C2-C1-C24-C25
48	33	314	A86	C2-C1-C24-C25
48	37	310	A86	C2-C1-C24-C25
48	39	311	A86	C2-C1-C24-C25
48	40	201	A86	C2-C1-C24-C25
48	40	201	A86	C5-C6-C8-C9
48	41	213	A86	C2-C1-C24-C25
41	C	518	LMG	C4-C5-C6-O5
43	D	409	LHG	C23-C24-C25-C26
43	d	407	LHG	C23-C24-C25-C26
37	19	305	CLA	O1A-CGA-O2A-C1
37	39	305	CLA	O1A-CGA-O2A-C1
37	C	512	CLA	C15-C16-C17-C18
37	Z	101	CLA	C8-C10-C11-C12
37	c	512	CLA	C15-C16-C17-C18
37	z	101	CLA	C8-C10-C11-C12
37	39	303	CLA	C13-C15-C16-C17
37	13	307	CLA	O1D-CGD-O2D-CED
48	11	312	A86	O5-C38-O4-C34
48	31	312	A86	O5-C38-O4-C34
37	15	307	CLA	CBD-CGD-O2D-CED
41	c	518	LMG	C4-C5-C6-O5
47	15	304	KC1	CAA-CBA-CGA-O2A
47	18	205	KC1	CAA-CBA-CGA-O1A
47	19	308	KC1	CAA-CBA-CGA-O2A
47	20	302	KC1	CAA-CBA-CGA-O1A
47	35	304	KC1	CAA-CBA-CGA-O2A
47	38	205	KC1	CAA-CBA-CGA-O1A
47	39	308	KC1	CAA-CBA-CGA-O2A
47	40	204	KC1	CAA-CBA-CGA-O1A
37	12	203	CLA	C3-C5-C6-C7
37	32	204	CLA	C3-C5-C6-C7
37	D	406	CLA	CBA-CGA-O2A-C1
37	d	404	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	19	306	CLA	CBA-CGA-O2A-C1
37	39	306	CLA	CBA-CGA-O2A-C1
37	B	501	CLA	C13-C15-C16-C17
37	B	507	CLA	C13-C15-C16-C17
37	b	501	CLA	C13-C15-C16-C17
37	b	507	CLA	C13-C15-C16-C17
37	19	303	CLA	C13-C15-C16-C17
37	19	307	CLA	C10-C11-C12-C13
37	32	211	CLA	C10-C11-C12-C13
37	39	307	CLA	C10-C11-C12-C13
41	B	521	LMG	C10-C11-C12-C13
41	b	520	LMG	C10-C11-C12-C13
43	B	523	LHG	C23-C24-C25-C26
43	b	522	LHG	C23-C24-C25-C26
44	C	517	DGD	O6E-C5E-C6E-O5E
44	c	517	DGD	O6E-C5E-C6E-O5E
37	B	502	CLA	C5-C6-C7-C8
37	B	506	CLA	C10-C11-C12-C13
37	B	507	CLA	C15-C16-C17-C18
37	B	511	CLA	C15-C16-C17-C18
37	B	524	CLA	C15-C16-C17-C18
37	C	506	CLA	C10-C11-C12-C13
37	W	101	CLA	C13-C15-C16-C17
37	b	502	CLA	C5-C6-C7-C8
37	b	506	CLA	C10-C11-C12-C13
37	b	507	CLA	C15-C16-C17-C18
37	b	511	CLA	C15-C16-C17-C18
37	b	523	CLA	C15-C16-C17-C18
37	c	506	CLA	C10-C11-C12-C13
37	c	508	CLA	C5-C6-C7-C8
37	w	101	CLA	C13-C15-C16-C17
37	12	210	CLA	C10-C11-C12-C13
37	13	301	CLA	C15-C16-C17-C18
37	33	301	CLA	C15-C16-C17-C18
37	39	303	CLA	C8-C10-C11-C12
37	c	502	CLA	O1D-CGD-O2D-CED
41	L	102	LMG	O10-C28-O8-C9
41	l	101	LMG	O10-C28-O8-C9
41	11	317	LMG	C10-C11-C12-C13
41	31	317	LMG	C10-C11-C12-C13
41	32	201	LMG	C10-C11-C12-C13
44	J	101	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
44	j	101	DGD	C1A-C2A-C3A-C4A
37	35	307	CLA	CBD-CGD-O2D-CED
37	C	502	CLA	O1D-CGD-O2D-CED
37	B	513	CLA	C10-C11-C12-C13
37	C	505	CLA	C13-C15-C16-C17
37	C	513	CLA	C10-C11-C12-C13
37	b	513	CLA	C10-C11-C12-C13
37	c	505	CLA	C13-C15-C16-C17
37	c	513	CLA	C10-C11-C12-C13
37	12	203	CLA	C8-C10-C11-C12
37	19	303	CLA	C8-C10-C11-C12
37	32	204	CLA	C8-C10-C11-C12
37	11	308	CLA	CBA-CGA-O2A-C1
37	32	202	CLA	CBA-CGA-O2A-C1
40	B	522	SQD	C24-C23-O48-C46
40	b	521	SQD	C24-C23-O48-C46
47	13	302	KC1	CAA-CBA-CGA-O1A
47	20	302	KC1	CAA-CBA-CGA-O2A
47	33	302	KC1	CAA-CBA-CGA-O1A
47	40	204	KC1	CAA-CBA-CGA-O2A
37	B	501	CLA	C5-C6-C7-C8
37	B	506	CLA	C15-C16-C17-C18
37	C	507	CLA	C10-C11-C12-C13
37	W	101	CLA	C10-C11-C12-C13
37	b	501	CLA	C5-C6-C7-C8
37	b	506	CLA	C15-C16-C17-C18
37	c	507	CLA	C10-C11-C12-C13
37	w	101	CLA	C10-C11-C12-C13
37	12	203	CLA	C15-C16-C17-C18
37	18	209	CLA	C10-C11-C12-C13
37	19	306	CLA	C10-C11-C12-C13
37	32	204	CLA	C15-C16-C17-C18
37	38	209	CLA	C10-C11-C12-C13
37	39	306	CLA	C10-C11-C12-C13
41	11	316	LMG	C28-C29-C30-C31
41	12	201	LMG	C10-C11-C12-C13
41	16	316	LMG	C10-C11-C12-C13
41	31	316	LMG	C28-C29-C30-C31
41	36	314	LMG	C10-C11-C12-C13
43	a	412	LHG	C23-C24-C25-C26
43	19	314	LHG	C23-C24-C25-C26
43	21	217	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
43	37	321	LHG	C7-C8-C9-C10
43	39	314	LHG	C23-C24-C25-C26
37	B	509	CLA	CBD-CGD-O2D-CED
37	b	509	CLA	CBD-CGD-O2D-CED
37	20	301	CLA	CBD-CGD-O2D-CED
37	40	203	CLA	CBD-CGD-O2D-CED
37	C	512	CLA	C10-C11-C12-C13
37	D	401	CLA	C13-C15-C16-C17
37	a	404	CLA	C13-C15-C16-C17
37	c	512	CLA	C10-C11-C12-C13
37	12	205	CLA	C6-C7-C8-C10
37	14	302	CLA	C6-C7-C8-C10
37	32	206	CLA	C6-C7-C8-C10
37	34	302	CLA	C6-C7-C8-C10
37	C	506	CLA	O1A-CGA-O2A-C1
37	11	308	CLA	O1A-CGA-O2A-C1
37	32	202	CLA	O1A-CGA-O2A-C1
39	K	101	BCR	C9-C10-C11-C12
39	y	101	BCR	C9-C10-C11-C12
48	12	216	A86	C24-C25-C26-C27
48	13	311	A86	C24-C25-C26-C27
48	13	313	A86	C11-C10-C9-C8
48	14	312	A86	C24-C25-C26-C27
48	14	314	A86	C24-C25-C26-C27
48	15	319	A86	C24-C25-C26-C27
48	15	319	A86	C3-C4-C5-C6
48	16	314	A86	C11-C10-C9-C8
48	17	314	A86	C11-C10-C9-C8
48	18	214	A86	C24-C25-C26-C27
48	21	213	A86	C3-C4-C5-C6
48	21	215	A86	C24-C25-C26-C27
48	32	217	A86	C24-C25-C26-C27
48	33	311	A86	C24-C25-C26-C27
48	33	313	A86	C11-C10-C9-C8
48	34	312	A86	C24-C25-C26-C27
48	34	314	A86	C24-C25-C26-C27
48	35	319	A86	C24-C25-C26-C27
48	35	319	A86	C3-C4-C5-C6
48	36	313	A86	C11-C10-C9-C8
48	37	313	A86	C11-C10-C9-C8
48	38	214	A86	C24-C25-C26-C27
48	41	213	A86	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
48	41	215	A86	C24-C25-C26-C27
50	20	310	DD6	C11-C10-C9-C8
50	40	212	DD6	C11-C10-C9-C8
43	D	411	LHG	C23-C24-C25-C26
37	B	516	CLA	CBA-CGA-O2A-C1
37	b	516	CLA	CBA-CGA-O2A-C1
37	C	513	CLA	C2A-CAA-CBA-CGA
37	c	513	CLA	C2A-CAA-CBA-CGA
37	11	307	CLA	C2A-CAA-CBA-CGA
37	18	208	CLA	C2A-CAA-CBA-CGA
37	31	308	CLA	C2A-CAA-CBA-CGA
37	35	307	CLA	C2A-CAA-CBA-CGA
37	38	208	CLA	C2A-CAA-CBA-CGA
37	C	501	CLA	O1D-CGD-O2D-CED
37	c	501	CLA	O1D-CGD-O2D-CED
37	31	302	CLA	O1D-CGD-O2D-CED
37	A	405	CLA	C5-C6-C7-C8
37	B	507	CLA	C8-C10-C11-C12
37	B	515	CLA	C10-C11-C12-C13
37	a	407	CLA	C5-C6-C7-C8
37	b	507	CLA	C8-C10-C11-C12
37	b	515	CLA	C10-C11-C12-C13
37	W	102	CLA	O1A-CGA-O2A-C1
37	c	506	CLA	O1A-CGA-O2A-C1
37	31	301	CLA	O1A-CGA-O2A-C1
41	C	518	LMG	O10-C28-O8-C9
41	c	518	LMG	O10-C28-O8-C9
44	C	517	DGD	O6E-C1E-O5D-C6D
44	c	517	DGD	O6E-C1E-O5D-C6D
37	11	301	CLA	O1D-CGD-O2D-CED
45	D	408	PL9	C44-C46-C47-C48
45	d	406	PL9	C44-C46-C47-C48
39	B	525	BCR	C18-C19-C20-C21
39	D	407	BCR	C10-C11-C12-C13
39	b	524	BCR	C18-C19-C20-C21
39	d	405	BCR	C10-C11-C12-C13
41	D	412	LMG	O6-C5-C6-O5
41	d	409	LMG	O6-C5-C6-O5
40	36	315	SQD	O49-C7-O47-C45
37	D	402	CLA	C3-C5-C6-C7
37	d	401	CLA	C3-C5-C6-C7
37	19	301	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
37	39	301	CLA	C3-C5-C6-C7
37	C	506	CLA	C13-C15-C16-C17
37	W	102	CLA	C13-C15-C16-C17
37	c	506	CLA	C13-C15-C16-C17
37	11	308	CLA	C10-C11-C12-C13
37	18	201	CLA	C13-C15-C16-C17
37	31	301	CLA	C13-C15-C16-C17
37	38	201	CLA	C13-C15-C16-C17
37	21	208	CLA	CBA-CGA-O2A-C1
37	40	208	CLA	CBA-CGA-O2A-C1
37	41	208	CLA	CBA-CGA-O2A-C1
41	A	408	LMG	C29-C28-O8-C9
41	a	410	LMG	C29-C28-O8-C9
37	C	510	CLA	O1A-CGA-O2A-C1
37	c	510	CLA	O1A-CGA-O2A-C1
41	16	316	LMG	O10-C28-O8-C9
41	36	314	LMG	O10-C28-O8-C9
37	B	524	CLA	C8-C10-C11-C12
37	C	503	CLA	C5-C6-C7-C8
37	C	503	CLA	C10-C11-C12-C13
37	C	510	CLA	C8-C10-C11-C12
37	b	523	CLA	C8-C10-C11-C12
37	c	503	CLA	C5-C6-C7-C8
37	c	503	CLA	C10-C11-C12-C13
37	c	510	CLA	C8-C10-C11-C12
37	14	302	CLA	C8-C10-C11-C12
37	32	202	CLA	C10-C11-C12-C13
37	34	302	CLA	C8-C10-C11-C12
48	14	315	A86	O5-C38-O4-C34
48	34	315	A86	O5-C38-O4-C34
44	C	517	DGD	C4E-C5E-C6E-O5E
44	c	517	DGD	C4E-C5E-C6E-O5E
47	18	210	KC1	CAA-CBA-CGA-O2A
37	A	405	CLA	C8-C10-C11-C12
37	B	516	CLA	C8-C10-C11-C12
37	a	407	CLA	C8-C10-C11-C12
37	b	516	CLA	C8-C10-C11-C12
37	19	307	CLA	C13-C15-C16-C17
37	39	307	CLA	C13-C15-C16-C17
43	19	314	LHG	C3-O3-P-O6
43	21	201	LHG	C3-O3-P-O6
43	21	217	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
43	37	321	LHG	C4-O6-P-O3
43	39	314	LHG	C3-O3-P-O6
43	41	201	LHG	C3-O3-P-O6
37	14	308	CLA	CBA-CGA-O2A-C1
37	20	306	CLA	CBA-CGA-O2A-C1
37	34	308	CLA	CBA-CGA-O2A-C1
37	39	310	CLA	CBA-CGA-O2A-C1
37	12	203	CLA	C13-C15-C16-C17
37	14	302	CLA	C10-C11-C12-C13
37	18	201	CLA	C10-C11-C12-C13
37	18	209	CLA	C13-C15-C16-C17
37	32	204	CLA	C13-C15-C16-C17
37	34	302	CLA	C10-C11-C12-C13
37	38	201	CLA	C10-C11-C12-C13
37	38	209	CLA	C13-C15-C16-C17
37	D	406	CLA	O1A-CGA-O2A-C1
43	17	316	LHG	C1-C2-C3-O3
43	37	315	LHG	C1-C2-C3-O3
40	17	301	SQD	O49-C7-O47-C45
37	37	306	CLA	C4-C3-C5-C6
44	C	516	DGD	C4E-C5E-C6E-O5E
44	c	516	DGD	C4E-C5E-C6E-O5E
37	B	510	CLA	C15-C16-C17-C18
37	C	506	CLA	C8-C10-C11-C12
37	C	509	CLA	C13-C15-C16-C17
37	b	510	CLA	C15-C16-C17-C18
37	c	506	CLA	C8-C10-C11-C12
37	c	509	CLA	C13-C15-C16-C17
37	d	404	CLA	O1A-CGA-O2A-C1
37	C	503	CLA	C3-C5-C6-C7
37	c	503	CLA	C3-C5-C6-C7
37	18	204	CLA	C3-C5-C6-C7
37	38	204	CLA	C3-C5-C6-C7
47	12	208	KC1	CAA-CBA-CGA-O2A
47	32	209	KC1	CAA-CBA-CGA-O2A
47	38	210	KC1	CAA-CBA-CGA-O2A
37	19	310	CLA	CBA-CGA-O2A-C1
40	B	519	SQD	C24-C23-O48-C46
40	L	101	SQD	C24-C23-O48-C46
44	H	102	DGD	O6E-C5E-C6E-O5E
37	C	503	CLA	C13-C15-C16-C17
37	c	503	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
44	h	102	DGD	O6E-C5E-C6E-O5E
39	B	525	BCR	C15-C16-C17-C18
39	b	524	BCR	C15-C16-C17-C18
48	12	213	A86	C24-C25-C26-C27
48	15	315	A86	C24-C25-C26-C27
48	15	316	A86	C11-C10-C9-C8
48	16	313	A86	C3-C4-C5-C6
48	17	320	A86	C3-C4-C5-C6
48	20	311	A86	C24-C25-C26-C27
48	32	214	A86	C24-C25-C26-C27
48	35	315	A86	C11-C10-C9-C8
48	35	315	A86	C24-C25-C26-C27
48	35	316	A86	C11-C10-C9-C8
48	40	201	A86	C3-C4-C5-C6
48	40	213	A86	C24-C25-C26-C27
50	20	310	DD6	C24-C25-C26-C27
50	40	212	DD6	C24-C25-C26-C27
44	H	102	DGD	C1A-C2A-C3A-C4A
44	h	102	DGD	C1A-C2A-C3A-C4A
40	B	519	SQD	C32-C33-C34-C35
41	C	518	LMG	C19-C20-C21-C22
41	c	518	LMG	C19-C20-C21-C22
43	D	410	LHG	C33-C34-C35-C36
43	D	411	LHG	C16-C17-C18-C19
43	d	408	LHG	C33-C34-C35-C36
43	17	316	LHG	C11-C10-C9-C8
43	19	314	LHG	C18-C19-C20-C21
48	18	213	A86	C39-C38-O4-C34
43	21	217	LHG	C8-C7-O7-C5
43	37	321	LHG	C8-C7-O7-C5
39	B	525	BCR	C11-C10-C9-C34
39	C	515	BCR	C20-C21-C22-C37
39	0	101	BCR	C20-C21-C22-C37
39	b	524	BCR	C11-C10-C9-C34
39	c	515	BCR	C20-C21-C22-C37
39	5	101	BCR	C20-C21-C22-C37
37	20	301	CLA	C3-C5-C6-C7
37	40	203	CLA	C3-C5-C6-C7
40	A	407	SQD	C16-C17-C18-C19
40	L	101	SQD	C32-C33-C34-C35
40	a	409	SQD	C16-C17-C18-C19
40	16	315	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
41	B	521	LMG	C18-C19-C20-C21
41	b	520	LMG	C18-C19-C20-C21
43	D	410	LHG	C32-C33-C34-C35
43	a	412	LHG	C16-C17-C18-C19
43	d	408	LHG	C32-C33-C34-C35
43	21	201	LHG	C11-C10-C9-C8
43	37	315	LHG	C11-C10-C9-C8
43	39	314	LHG	C18-C19-C20-C21
44	H	102	DGD	C3A-C4A-C5A-C6A
44	h	102	DGD	C3A-C4A-C5A-C6A
48	38	213	A86	C39-C38-O4-C34
47	14	309	KC1	C2A-CAA-CBA-CGA
47	18	210	KC1	C2A-CAA-CBA-CGA
47	34	309	KC1	C2A-CAA-CBA-CGA
47	38	210	KC1	C2A-CAA-CBA-CGA
37	D	402	CLA	C16-C17-C18-C19
37	d	401	CLA	C16-C17-C18-C19
37	11	308	CLA	C16-C17-C18-C20
37	32	202	CLA	C16-C17-C18-C20
40	A	407	SQD	C14-C15-C16-C17
40	A	407	SQD	C18-C19-C20-C21
40	a	409	SQD	C14-C15-C16-C17
40	a	409	SQD	C18-C19-C20-C21
40	40	202	SQD	C14-C15-C16-C17
41	A	408	LMG	C32-C33-C34-C35
41	a	410	LMG	C32-C33-C34-C35
44	H	102	DGD	CBA-CCA-CDA-CEA
44	h	102	DGD	CBA-CCA-CDA-CEA
40	B	519	SQD	C46-C45-O47-C7
40	L	101	SQD	C46-C45-O47-C7
37	19	301	CLA	O1D-CGD-O2D-CED
37	39	301	CLA	O1D-CGD-O2D-CED
47	15	309	KC1	CAA-CBA-CGA-O2A
47	17	303	KC1	CAA-CBA-CGA-O1A
47	35	309	KC1	CAA-CBA-CGA-O2A
47	37	302	KC1	CAA-CBA-CGA-O1A
37	C	507	CLA	C13-C15-C16-C17
37	c	507	CLA	C13-C15-C16-C17
41	B	521	LMG	C19-C20-C21-C22
41	b	520	LMG	C19-C20-C21-C22
43	39	314	LHG	C31-C32-C33-C34
43	41	201	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
37	B	516	CLA	O1A-CGA-O2A-C1
40	A	407	SQD	C10-C11-C12-C13
41	L	102	LMG	C14-C15-C16-C17
41	l	101	LMG	C14-C15-C16-C17
43	39	314	LHG	C34-C35-C36-C37
41	A	408	LMG	C4-C5-C6-O5
41	a	410	LMG	C4-C5-C6-O5
37	41	205	CLA	O1D-CGD-O2D-CED
40	a	409	SQD	C10-C11-C12-C13
40	17	301	SQD	C9-C10-C11-C12
40	36	315	SQD	C9-C10-C11-C12
43	B	523	LHG	C13-C14-C15-C16
43	B	523	LHG	C27-C28-C29-C30
43	B	523	LHG	C28-C29-C30-C31
43	b	522	LHG	C27-C28-C29-C30
43	b	522	LHG	C28-C29-C30-C31
43	19	314	LHG	C31-C32-C33-C34
43	41	201	LHG	C10-C11-C12-C13
37	21	205	CLA	O1D-CGD-O2D-CED
39	A	406	BCR	C20-C21-C22-C23
39	B	525	BCR	C16-C17-C18-C19
39	B	525	BCR	C20-C21-C22-C23
39	a	408	BCR	C20-C21-C22-C23
39	b	524	BCR	C16-C17-C18-C19
39	b	524	BCR	C20-C21-C22-C23
40	B	519	SQD	C2-C1-O6-C44
40	L	101	SQD	C2-C1-O6-C44
41	12	201	LMG	C2-C1-O1-C7
41	32	201	LMG	C2-C1-O1-C7
44	C	517	DGD	C2E-C1E-O5D-C6D
44	c	517	DGD	C2E-C1E-O5D-C6D
50	16	312	DD6	C24-C1-C2-C3
50	19	312	DD6	C4-C5-C6-C8
50	21	216	DD6	C24-C1-C2-C3
50	36	312	DD6	C24-C1-C2-C3
50	39	312	DD6	C4-C5-C6-C8
50	41	216	DD6	C24-C1-C2-C3
37	B	502	CLA	CBA-CGA-O2A-C1
37	b	502	CLA	CBA-CGA-O2A-C1
40	B	519	SQD	C10-C11-C12-C13
40	L	101	SQD	C10-C11-C12-C13
40	17	301	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
43	B	523	LHG	C16-C17-C18-C19
43	b	522	LHG	C13-C14-C15-C16
43	b	522	LHG	C16-C17-C18-C19
43	19	314	LHG	C34-C35-C36-C37
44	H	102	DGD	C7A-C8A-C9A-CAA
44	H	102	DGD	C3B-C4B-C5B-C6B
44	h	102	DGD	C7A-C8A-C9A-CAA
44	h	102	DGD	C3B-C4B-C5B-C6B
37	b	501	CLA	C10-C11-C12-C13
37	15	308	CLA	C5-C6-C7-C8
37	16	301	CLA	C8-C10-C11-C12
37	16	306	CLA	C8-C10-C11-C12
37	36	301	CLA	C8-C10-C11-C12
37	36	306	CLA	C8-C10-C11-C12
37	19	306	CLA	O1A-CGA-O2A-C1
37	39	306	CLA	O1A-CGA-O2A-C1
37	16	306	CLA	C16-C17-C18-C20
37	36	306	CLA	C16-C17-C18-C20
37	13	308	CLA	C4-C3-C5-C6
37	15	307	CLA	C4-C3-C5-C6
37	17	307	CLA	C4-C3-C5-C6
37	33	308	CLA	C4-C3-C5-C6
40	A	407	SQD	C17-C18-C19-C20
40	a	409	SQD	C17-C18-C19-C20
40	36	315	SQD	C27-C28-C29-C30
41	C	518	LMG	C18-C19-C20-C21
41	c	518	LMG	C18-C19-C20-C21
43	D	411	LHG	C11-C10-C9-C8
43	a	412	LHG	C11-C10-C9-C8
43	21	201	LHG	C10-C11-C12-C13
37	17	307	CLA	C2-C3-C5-C6
37	37	306	CLA	C2-C3-C5-C6
37	D	402	CLA	C6-C7-C8-C9
37	W	102	CLA	C6-C7-C8-C9
37	d	401	CLA	C6-C7-C8-C9
37	14	302	CLA	C11-C12-C13-C14
37	31	301	CLA	C6-C7-C8-C9
37	34	302	CLA	C11-C12-C13-C14
37	18	203	CLA	O1D-CGD-O2D-CED
40	B	522	SQD	C7-C8-C9-C10
40	b	521	SQD	C7-C8-C9-C10
37	11	307	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
41	D	412	LMG	C37-C38-C39-C40
41	L	102	LMG	C15-C16-C17-C18
41	d	409	LMG	C37-C38-C39-C40
43	D	410	LHG	C13-C14-C15-C16
43	D	410	LHG	C34-C35-C36-C37
43	d	408	LHG	C13-C14-C15-C16
43	d	408	LHG	C34-C35-C36-C37
43	21	201	LHG	C24-C25-C26-C27
43	21	217	LHG	C30-C31-C32-C33
43	37	321	LHG	C30-C31-C32-C33
43	41	201	LHG	C24-C25-C26-C27
37	B	501	CLA	C10-C11-C12-C13
47	12	208	KC1	CAA-CBA-CGA-O1A
47	15	309	KC1	CAA-CBA-CGA-O1A
47	16	305	KC1	CAA-CBA-CGA-O1A
47	18	210	KC1	CAA-CBA-CGA-O1A
47	32	209	KC1	CAA-CBA-CGA-O1A
47	35	309	KC1	CAA-CBA-CGA-O1A
47	36	305	KC1	CAA-CBA-CGA-O1A
47	38	210	KC1	CAA-CBA-CGA-O1A
37	B	510	CLA	C2A-CAA-CBA-CGA
37	C	506	CLA	C2A-CAA-CBA-CGA
37	C	507	CLA	C2A-CAA-CBA-CGA
37	b	510	CLA	C2A-CAA-CBA-CGA
37	c	506	CLA	C2A-CAA-CBA-CGA
37	c	507	CLA	C2A-CAA-CBA-CGA
37	12	212	CLA	C2A-CAA-CBA-CGA
37	15	307	CLA	C2A-CAA-CBA-CGA
37	32	213	CLA	C2A-CAA-CBA-CGA
37	W	102	CLA	O1D-CGD-O2D-CED
37	b	516	CLA	O1A-CGA-O2A-C1
37	14	308	CLA	O1A-CGA-O2A-C1
39	K	101	BCR	C37-C22-C23-C24
39	y	101	BCR	C37-C22-C23-C24
48	13	312	A86	C-C1-C24-C25
48	15	316	A86	C7-C6-C8-C9
48	33	312	A86	C-C1-C24-C25
48	35	316	A86	C7-C6-C8-C9
50	19	312	DD6	C12-C11-C13-C14
50	39	312	DD6	C12-C11-C13-C14
37	31	308	CLA	C2C-C3C-CAC-CBC
41	A	408	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
41	b	519	LMG	C12-C13-C14-C15
41	l	101	LMG	C15-C16-C17-C18
43	D	410	LHG	C24-C25-C26-C27
43	D	411	LHG	C14-C15-C16-C17
43	a	412	LHG	C14-C15-C16-C17
43	d	408	LHG	C24-C25-C26-C27
43	D	411	LHG	O1-C1-C2-C3
43	a	412	LHG	O1-C1-C2-C3
39	B	525	BCR	C21-C22-C23-C24
39	b	524	BCR	C21-C22-C23-C24
48	12	217	A86	C2-C1-C24-C25
48	13	312	A86	C2-C1-C24-C25
48	15	314	A86	C5-C6-C8-C9
48	15	316	A86	C5-C6-C8-C9
48	20	311	A86	C2-C1-C24-C25
48	21	211	A86	C5-C6-C8-C9
48	32	218	A86	C2-C1-C24-C25
48	33	312	A86	C2-C1-C24-C25
48	35	314	A86	C5-C6-C8-C9
48	35	316	A86	C5-C6-C8-C9
48	40	213	A86	C2-C1-C24-C25
48	41	211	A86	C5-C6-C8-C9
37	B	501	CLA	C3-C5-C6-C7
37	C	509	CLA	C3-C5-C6-C7
37	c	509	CLA	C3-C5-C6-C7
37	17	309	CLA	C3-C5-C6-C7
37	C	507	CLA	C8-C10-C11-C12
37	c	507	CLA	C8-C10-C11-C12
37	35	308	CLA	C5-C6-C7-C8
40	B	519	SQD	C33-C34-C35-C36
40	L	101	SQD	C33-C34-C35-C36
40	17	301	SQD	C29-C30-C31-C32
40	36	315	SQD	C29-C30-C31-C32
41	B	520	LMG	C12-C13-C14-C15
41	a	410	LMG	C18-C19-C20-C21
41	11	316	LMG	C13-C14-C15-C16
41	31	316	LMG	C13-C14-C15-C16
43	D	409	LHG	C32-C33-C34-C35
43	D	411	LHG	C15-C16-C17-C18
43	a	412	LHG	C15-C16-C17-C18
43	d	407	LHG	C32-C33-C34-C35
40	A	407	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
40	a	409	SQD	C7-C8-C9-C10
37	31	301	CLA	O1D-CGD-O2D-CED
37	38	203	CLA	O1D-CGD-O2D-CED
40	A	407	SQD	C11-C12-C13-C14
40	a	409	SQD	C11-C12-C13-C14
40	17	301	SQD	C11-C12-C13-C14
40	40	202	SQD	C18-C19-C20-C21
41	A	408	LMG	C17-C18-C19-C20
41	B	520	LMG	C13-C14-C15-C16
41	B	520	LMG	C31-C32-C33-C34
41	D	412	LMG	C30-C31-C32-C33
41	L	102	LMG	C33-C34-C35-C36
41	a	410	LMG	C17-C18-C19-C20
41	b	519	LMG	C13-C14-C15-C16
41	b	519	LMG	C31-C32-C33-C34
41	d	409	LMG	C30-C31-C32-C33
41	l	101	LMG	C33-C34-C35-C36
41	11	316	LMG	C30-C31-C32-C33
41	31	316	LMG	C30-C31-C32-C33
43	B	523	LHG	C30-C31-C32-C33
43	b	522	LHG	C30-C31-C32-C33
43	19	314	LHG	C25-C26-C27-C28
43	39	314	LHG	C25-C26-C27-C28
41	16	316	LMG	O6-C5-C6-O5
41	36	314	LMG	O6-C5-C6-O5
37	34	308	CLA	O1A-CGA-O2A-C1
37	Z	101	CLA	C16-C17-C18-C20
37	z	101	CLA	C16-C17-C18-C20
37	11	308	CLA	C16-C17-C18-C19
37	16	306	CLA	C16-C17-C18-C19
37	32	202	CLA	C16-C17-C18-C19
37	36	306	CLA	C16-C17-C18-C19
41	C	518	LMG	O6-C1-O1-C7
41	c	518	LMG	O6-C1-O1-C7
41	16	316	LMG	O6-C1-O1-C7
41	36	314	LMG	O6-C1-O1-C7
44	C	517	DGD	O6D-C1D-O3G-C3G
44	c	517	DGD	O6D-C1D-O3G-C3G
37	W	101	CLA	C5-C6-C7-C8
37	b	508	CLA	C8-C10-C11-C12
37	w	101	CLA	C5-C6-C7-C8
37	21	208	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	41	208	CLA	C13-C15-C16-C17
40	16	315	SQD	C18-C19-C20-C21
40	36	315	SQD	C11-C12-C13-C14
41	C	518	LMG	C17-C18-C19-C20
41	c	518	LMG	C17-C18-C19-C20
37	Z	102	CLA	CBD-CGD-O2D-CED
41	A	408	LMG	C35-C36-C37-C38
41	B	520	LMG	C30-C31-C32-C33
41	a	410	LMG	C35-C36-C37-C38
41	b	519	LMG	C30-C31-C32-C33
43	a	412	LHG	C12-C13-C14-C15
43	b	522	LHG	C32-C33-C34-C35
44	C	516	DGD	C4B-C5B-C6B-C7B
44	J	101	DGD	C3A-C4A-C5A-C6A
44	c	516	DGD	C4B-C5B-C6B-C7B
44	j	101	DGD	C3A-C4A-C5A-C6A
41	C	518	LMG	C10-C11-C12-C13
41	c	518	LMG	C10-C11-C12-C13
37	B	508	CLA	C8-C10-C11-C12
47	16	305	KC1	CAA-CBA-CGA-O2A
47	17	303	KC1	CAA-CBA-CGA-O2A
47	17	306	KC1	CAA-CBA-CGA-O1A
47	36	305	KC1	CAA-CBA-CGA-O2A
47	37	305	KC1	CAA-CBA-CGA-O1A
37	20	306	CLA	O1A-CGA-O2A-C1
37	40	208	CLA	O1A-CGA-O2A-C1
40	B	519	SQD	C17-C18-C19-C20
40	L	101	SQD	C17-C18-C19-C20
41	A	408	LMG	C15-C16-C17-C18
41	A	408	LMG	C20-C21-C22-C23
41	B	520	LMG	C17-C18-C19-C20
41	L	102	LMG	C29-C30-C31-C32
41	a	410	LMG	C15-C16-C17-C18
41	a	410	LMG	C20-C21-C22-C23
41	b	519	LMG	C17-C18-C19-C20
41	l	101	LMG	C29-C30-C31-C32
43	B	523	LHG	C32-C33-C34-C35
43	D	411	LHG	C12-C13-C14-C15
43	D	411	LHG	C27-C28-C29-C30
43	a	412	LHG	C27-C28-C29-C30
43	19	314	LHG	C13-C14-C15-C16
43	39	314	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
37	b	501	CLA	C3-C5-C6-C7
37	11	303	CLA	C3-C5-C6-C7
37	31	304	CLA	C3-C5-C6-C7
37	12	210	CLA	CBA-CGA-O2A-C1
37	32	211	CLA	CBA-CGA-O2A-C1
41	D	412	LMG	C35-C36-C37-C38
41	d	409	LMG	C35-C36-C37-C38
43	37	315	LHG	C16-C17-C18-C19
44	c	517	DGD	C5A-C6A-C7A-C8A
37	D	406	CLA	O1D-CGD-O2D-CED
37	d	404	CLA	O1D-CGD-O2D-CED
37	B	524	CLA	C3A-C2A-CAA-CBA
37	C	506	CLA	C3A-C2A-CAA-CBA
37	Z	101	CLA	C3A-C2A-CAA-CBA
37	W	102	CLA	C3A-C2A-CAA-CBA
37	b	523	CLA	C3A-C2A-CAA-CBA
37	c	506	CLA	C3A-C2A-CAA-CBA
37	z	101	CLA	C3A-C2A-CAA-CBA
37	11	303	CLA	C3A-C2A-CAA-CBA
37	12	205	CLA	C3A-C2A-CAA-CBA
37	13	303	CLA	C3A-C2A-CAA-CBA
37	15	303	CLA	C3A-C2A-CAA-CBA
37	16	303	CLA	C3A-C2A-CAA-CBA
37	16	306	CLA	C3A-C2A-CAA-CBA
37	17	304	CLA	C3A-C2A-CAA-CBA
37	17	309	CLA	C3A-C2A-CAA-CBA
37	18	203	CLA	C3A-C2A-CAA-CBA
37	18	204	CLA	C3A-C2A-CAA-CBA
37	19	303	CLA	C3A-C2A-CAA-CBA
37	20	301	CLA	C3A-C2A-CAA-CBA
37	20	303	CLA	C3A-C2A-CAA-CBA
37	20	308	CLA	C3A-C2A-CAA-CBA
37	21	204	CLA	C3A-C2A-CAA-CBA
37	21	205	CLA	C3A-C2A-CAA-CBA
37	31	301	CLA	C3A-C2A-CAA-CBA
37	31	304	CLA	C3A-C2A-CAA-CBA
37	32	206	CLA	C3A-C2A-CAA-CBA
37	33	303	CLA	C3A-C2A-CAA-CBA
37	35	303	CLA	C3A-C2A-CAA-CBA
37	36	303	CLA	C3A-C2A-CAA-CBA
37	36	306	CLA	C3A-C2A-CAA-CBA
37	37	303	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	37	308	CLA	C3A-C2A-CAA-CBA
37	38	203	CLA	C3A-C2A-CAA-CBA
37	38	204	CLA	C3A-C2A-CAA-CBA
37	39	303	CLA	C3A-C2A-CAA-CBA
37	40	203	CLA	C3A-C2A-CAA-CBA
37	40	205	CLA	C3A-C2A-CAA-CBA
37	40	210	CLA	C3A-C2A-CAA-CBA
37	41	204	CLA	C3A-C2A-CAA-CBA
37	41	205	CLA	C3A-C2A-CAA-CBA
38	D	403	PHO	C3A-C2A-CAA-CBA
38	a	405	PHO	C3A-C2A-CAA-CBA
37	C	503	CLA	C15-C16-C17-C18
37	c	503	CLA	C15-C16-C17-C18
48	14	316	A86	C3-C4-C5-C6
48	34	316	A86	C3-C4-C5-C6
48	37	310	A86	C11-C10-C9-C8
41	B	521	LMG	C16-C17-C18-C19
41	b	520	LMG	C16-C17-C18-C19
43	17	316	LHG	C16-C17-C18-C19
44	C	516	DGD	C7B-C8B-C9B-CAB
44	C	517	DGD	C5A-C6A-C7A-C8A
44	c	516	DGD	C7B-C8B-C9B-CAB
37	21	208	CLA	O1A-CGA-O2A-C1
37	39	310	CLA	O1A-CGA-O2A-C1
37	41	208	CLA	O1A-CGA-O2A-C1
41	C	518	LMG	C16-C17-C18-C19
41	c	518	LMG	C16-C17-C18-C19
43	D	409	LHG	C28-C29-C30-C31
43	d	407	LHG	C28-C29-C30-C31
43	17	316	LHG	C13-C14-C15-C16
43	21	217	LHG	C29-C30-C31-C32
41	A	408	LMG	C7-C8-C9-O8
41	a	410	LMG	C7-C8-C9-O8
37	z	102	CLA	CBD-CGD-O2D-CED
37	32	211	CLA	CBD-CGD-O2D-CED
43	37	315	LHG	C13-C14-C15-C16
43	37	321	LHG	C29-C30-C31-C32
48	20	311	A86	O5-C38-O4-C34
37	C	503	CLA	O2A-C1-C2-C3
37	c	503	CLA	O2A-C1-C2-C3
39	A	406	BCR	C14-C15-C16-C17
39	a	408	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	37	308	CLA	C3-C5-C6-C7
43	D	411	LHG	C31-C32-C33-C34
43	a	412	LHG	C31-C32-C33-C34
37	19	310	CLA	O1A-CGA-O2A-C1
37	B	511	CLA	C4-C3-C5-C6
37	b	511	CLA	C4-C3-C5-C6
37	18	208	CLA	C4-C3-C5-C6
45	D	404	PL9	C30-C29-C31-C32
45	d	402	PL9	C30-C29-C31-C32
37	b	511	CLA	C2-C3-C5-C6
37	18	208	CLA	C2-C3-C5-C6
37	38	208	CLA	C2-C3-C5-C6
45	D	404	PL9	C12-C11-C9-C8
45	D	408	PL9	C13-C14-C16-C17
45	d	402	PL9	C12-C11-C9-C8
45	d	406	PL9	C13-C14-C16-C17
40	B	522	SQD	C8-C7-O47-C45
40	b	521	SQD	C8-C7-O47-C45
41	A	408	LMG	C11-C10-O7-C8
41	a	410	LMG	C11-C10-O7-C8
37	C	513	CLA	CBD-CGD-O2D-CED
37	14	307	CLA	CBD-CGD-O2D-CED
48	40	213	A86	O5-C38-O4-C34
44	H	102	DGD	C4E-C5E-C6E-O5E
44	h	102	DGD	C4E-C5E-C6E-O5E
43	D	409	LHG	O1-C1-C2-O2
43	d	407	LHG	O1-C1-C2-O2
41	A	408	LMG	C19-C20-C21-C22
41	a	410	LMG	C19-C20-C21-C22
41	12	201	LMG	C33-C34-C35-C36
43	D	411	LHG	C28-C29-C30-C31
43	a	412	LHG	C28-C29-C30-C31
43	17	316	LHG	C27-C28-C29-C30
43	37	315	LHG	C27-C28-C29-C30
37	B	514	CLA	C13-C15-C16-C17
37	b	514	CLA	C13-C15-C16-C17
41	32	201	LMG	C33-C34-C35-C36
37	c	513	CLA	CBD-CGD-O2D-CED
37	33	303	CLA	C3-C5-C6-C7
44	J	101	DGD	C5B-C6B-C7B-C8B
44	j	101	DGD	C5B-C6B-C7B-C8B
37	B	502	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	b	502	CLA	O1A-CGA-O2A-C1
37	34	307	CLA	CBD-CGD-O2D-CED
47	17	306	KC1	CAA-CBA-CGA-O2A
47	37	302	KC1	CAA-CBA-CGA-O2A
47	37	305	KC1	CAA-CBA-CGA-O2A
37	C	509	CLA	C2-C1-O2A-CGA
37	c	509	CLA	C2-C1-O2A-CGA
44	H	102	DGD	CCB-CDB-CEB-CFB
44	h	102	DGD	CCB-CDB-CEB-CFB
37	B	506	CLA	C13-C15-C16-C17
37	b	506	CLA	C13-C15-C16-C17
37	19	303	CLA	C10-C11-C12-C13
37	39	303	CLA	C10-C11-C12-C13
51	39	315	LMU	C1-C2-C3-C4
44	C	516	DGD	C8A-C9A-CAA-CBA
44	c	516	DGD	C8A-C9A-CAA-CBA
40	17	301	SQD	C7-C8-C9-C10
40	36	315	SQD	C7-C8-C9-C10
43	D	410	LHG	C23-C24-C25-C26
43	d	408	LHG	C23-C24-C25-C26
37	13	303	CLA	C3-C5-C6-C7
37	39	303	CLA	C3-C5-C6-C7
39	A	406	BCR	C5-C6-C7-C8
39	A	410	BCR	C1-C6-C7-C8
39	A	410	BCR	C5-C6-C7-C8
39	B	517	BCR	C1-C6-C7-C8
39	B	517	BCR	C5-C6-C7-C8
39	B	518	BCR	C1-C6-C7-C8
39	B	518	BCR	C5-C6-C7-C8
39	B	525	BCR	C1-C6-C7-C8
39	B	525	BCR	C5-C6-C7-C8
39	C	514	BCR	C5-C6-C7-C8
39	C	519	BCR	C5-C6-C7-C8
39	C	519	BCR	C23-C24-C25-C26
39	D	407	BCR	C1-C6-C7-C8
39	D	407	BCR	C5-C6-C7-C8
39	H	101	BCR	C5-C6-C7-C8
39	K	101	BCR	C1-C6-C7-C8
39	K	101	BCR	C5-C6-C7-C8
39	0	101	BCR	C5-C6-C7-C8
39	0	101	BCR	C23-C24-C25-C26
39	a	408	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
39	a	413	BCR	C1-C6-C7-C8
39	a	413	BCR	C5-C6-C7-C8
39	b	517	BCR	C1-C6-C7-C8
39	b	517	BCR	C5-C6-C7-C8
39	b	518	BCR	C1-C6-C7-C8
39	b	518	BCR	C5-C6-C7-C8
39	b	524	BCR	C1-C6-C7-C8
39	b	524	BCR	C5-C6-C7-C8
39	c	519	BCR	C5-C6-C7-C8
39	c	519	BCR	C23-C24-C25-C26
39	d	405	BCR	C1-C6-C7-C8
39	d	405	BCR	C5-C6-C7-C8
39	h	101	BCR	C5-C6-C7-C8
39	y	101	BCR	C1-C6-C7-C8
39	y	101	BCR	C5-C6-C7-C8
39	5	101	BCR	C5-C6-C7-C8
40	B	522	SQD	C11-C10-C9-C8
40	b	521	SQD	C11-C10-C9-C8
43	D	409	LHG	C25-C26-C27-C28
43	d	407	LHG	C25-C26-C27-C28
37	W	101	CLA	CBA-CGA-O2A-C1
37	w	101	CLA	CBA-CGA-O2A-C1
40	16	315	SQD	C24-C23-O48-C46
40	40	202	SQD	C24-C23-O48-C46
41	B	521	LMG	C29-C28-O8-C9
41	C	518	LMG	C29-C28-O8-C9
41	b	520	LMG	C29-C28-O8-C9
41	c	518	LMG	C29-C28-O8-C9
37	B	524	CLA	C10-C11-C12-C13
37	W	102	CLA	C15-C16-C17-C18
37	b	523	CLA	C10-C11-C12-C13
37	31	301	CLA	C15-C16-C17-C18
51	19	315	LMU	C1-C2-C3-C4
43	19	314	LHG	C11-C12-C13-C14
43	39	314	LHG	C11-C12-C13-C14
44	H	102	DGD	CBB-CCB-CDB-CEB
44	h	102	DGD	CBB-CCB-CDB-CEB
37	12	210	CLA	O1A-CGA-O2A-C1
37	32	211	CLA	O1A-CGA-O2A-C1
37	C	502	CLA	C13-C15-C16-C17
37	c	502	CLA	C13-C15-C16-C17
38	D	403	PHO	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	B	509	CLA	C4-C3-C5-C6
37	b	509	CLA	C4-C3-C5-C6
37	13	303	CLA	C4-C3-C5-C6
37	33	303	CLA	C4-C3-C5-C6
37	B	509	CLA	C2-C3-C5-C6
37	B	510	CLA	C12-C13-C15-C16
37	B	511	CLA	C2-C3-C5-C6
37	D	402	CLA	C6-C7-C8-C10
37	W	102	CLA	C6-C7-C8-C10
37	b	509	CLA	C2-C3-C5-C6
37	b	510	CLA	C12-C13-C15-C16
37	d	401	CLA	C6-C7-C8-C10
37	13	308	CLA	C2-C3-C5-C6
37	14	302	CLA	C11-C12-C13-C15
37	15	307	CLA	C2-C3-C5-C6
37	19	306	CLA	C11-C12-C13-C15
37	31	301	CLA	C6-C7-C8-C10
37	33	308	CLA	C2-C3-C5-C6
37	34	302	CLA	C11-C12-C13-C15
37	39	306	CLA	C11-C12-C13-C15
37	19	303	CLA	C3-C5-C6-C7
37	B	512	CLA	C10-C11-C12-C13
37	b	512	CLA	C10-C11-C12-C13
37	12	203	CLA	C10-C11-C12-C13
37	32	204	CLA	C10-C11-C12-C13
38	a	405	PHO	C13-C15-C16-C17
48	15	315	A86	C11-C10-C9-C8
48	17	311	A86	C11-C10-C9-C8
48	18	213	A86	C24-C25-C26-C27
48	20	311	A86	C3-C4-C5-C6
48	38	213	A86	C24-C25-C26-C27
48	40	213	A86	C3-C4-C5-C6
50	21	216	DD6	C3-C4-C5-C6
50	41	216	DD6	C3-C4-C5-C6
41	B	521	LMG	O9-C10-O7-C8
41	b	520	LMG	O9-C10-O7-C8
43	21	217	LHG	O9-C7-O7-C5
41	17	317	LMG	C28-C29-C30-C31
41	37	316	LMG	C28-C29-C30-C31
37	11	310	CLA	CBA-CGA-O2A-C1
37	31	310	CLA	CBA-CGA-O2A-C1
41	L	102	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
41	l	101	LMG	C29-C28-O8-C9
44	J	101	DGD	C2A-C1A-O1G-C1G
44	j	101	DGD	C2A-C1A-O1G-C1G
47	20	305	KC1	C2C-C3C-CAC-CBC
47	40	207	KC1	C2C-C3C-CAC-CBC
37	B	503	CLA	C2A-CAA-CBA-CGA
37	b	503	CLA	C2A-CAA-CBA-CGA
37	B	508	CLA	C13-C15-C16-C17
37	b	508	CLA	C13-C15-C16-C17
37	13	308	CLA	C5-C6-C7-C8
37	33	308	CLA	C5-C6-C7-C8
41	A	408	LMG	C13-C14-C15-C16
43	B	523	LHG	C11-C12-C13-C14
43	b	522	LHG	C11-C12-C13-C14
41	a	410	LMG	C13-C14-C15-C16
43	D	409	LHG	C9-C10-C11-C12
43	D	409	LHG	C14-C15-C16-C17
43	d	407	LHG	C9-C10-C11-C12
43	d	407	LHG	C14-C15-C16-C17
40	16	315	SQD	C23-C24-C25-C26
40	40	202	SQD	C23-C24-C25-C26
41	11	316	LMG	C10-C11-C12-C13
41	31	316	LMG	C10-C11-C12-C13
37	C	510	CLA	C13-C15-C16-C17
37	c	510	CLA	C13-C15-C16-C17
41	12	201	LMG	C32-C33-C34-C35
41	32	201	LMG	C32-C33-C34-C35
43	D	409	LHG	C11-C10-C9-C8
43	d	407	LHG	C11-C10-C9-C8
51	19	315	LMU	C11-C10-C9-C8
51	39	315	LMU	C11-C10-C9-C8
47	11	309	KC1	C2B-C3B-CAB-CBB
47	13	306	KC1	C2B-C3B-CAB-CBB
47	14	304	KC1	C2B-C3B-CAB-CBB
47	14	306	KC1	C2B-C3B-CAB-CBB
47	14	309	KC1	C2B-C3B-CAB-CBB
47	15	304	KC1	C2B-C3B-CAB-CBB
47	15	306	KC1	C2B-C3B-CAB-CBB
47	15	309	KC1	C2B-C3B-CAB-CBB
47	16	304	KC1	C2B-C3B-CAB-CBB
47	16	305	KC1	C2B-C3B-CAB-CBB
47	16	308	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
47	17	305	KC1	C2B-C3B-CAB-CBB
47	17	308	KC1	C2B-C3B-CAB-CBB
47	18	205	KC1	C2B-C3B-CAB-CBB
47	18	210	KC1	C2B-C3B-CAB-CBB
47	20	304	KC1	C2B-C3B-CAB-CBB
47	20	305	KC1	C2B-C3B-CAB-CBB
47	31	309	KC1	C2B-C3B-CAB-CBB
47	33	306	KC1	C2B-C3B-CAB-CBB
47	34	304	KC1	C2B-C3B-CAB-CBB
47	34	306	KC1	C2B-C3B-CAB-CBB
47	34	309	KC1	C2B-C3B-CAB-CBB
47	35	302	KC1	C2B-C3B-CAB-CBB
47	35	306	KC1	C2B-C3B-CAB-CBB
47	35	309	KC1	C2B-C3B-CAB-CBB
47	36	304	KC1	C2B-C3B-CAB-CBB
47	36	305	KC1	C2B-C3B-CAB-CBB
47	36	308	KC1	C2B-C3B-CAB-CBB
47	37	304	KC1	C2B-C3B-CAB-CBB
47	37	307	KC1	C2B-C3B-CAB-CBB
47	38	205	KC1	C2B-C3B-CAB-CBB
47	38	210	KC1	C2B-C3B-CAB-CBB
47	40	206	KC1	C2B-C3B-CAB-CBB
47	40	207	KC1	C2B-C3B-CAB-CBB
47	20	305	KC1	CAA-CBA-CGA-O1A
47	40	207	KC1	CAA-CBA-CGA-O1A
44	C	516	DGD	CCA-CDA-CEA-CFA
44	c	516	DGD	CCA-CDA-CEA-CFA
39	H	101	BCR	C22-C23-C24-C25
39	h	101	BCR	C22-C23-C24-C25
37	19	302	CLA	CBD-CGD-O2D-CED
40	B	519	SQD	C31-C32-C33-C34
40	L	101	SQD	C31-C32-C33-C34
41	A	408	LMG	C36-C37-C38-C39
41	B	520	LMG	C29-C30-C31-C32
41	B	521	LMG	C31-C32-C33-C34
41	a	410	LMG	C36-C37-C38-C39
41	b	519	LMG	C29-C30-C31-C32
41	b	520	LMG	C31-C32-C33-C34
43	19	314	LHG	C10-C11-C12-C13
43	39	314	LHG	C10-C11-C12-C13
44	C	517	DGD	CBA-CCA-CDA-CEA
44	c	517	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
47	11	309	KC1	C4B-C3B-CAB-CBB
47	13	306	KC1	C4B-C3B-CAB-CBB
47	14	304	KC1	C4B-C3B-CAB-CBB
47	14	306	KC1	C4B-C3B-CAB-CBB
47	14	309	KC1	C4B-C3B-CAB-CBB
47	15	304	KC1	C4B-C3B-CAB-CBB
47	15	306	KC1	C4B-C3B-CAB-CBB
47	15	309	KC1	C4B-C3B-CAB-CBB
47	16	304	KC1	C4B-C3B-CAB-CBB
47	16	305	KC1	C4B-C3B-CAB-CBB
47	17	305	KC1	C4B-C3B-CAB-CBB
47	17	308	KC1	C4B-C3B-CAB-CBB
47	18	205	KC1	C4B-C3B-CAB-CBB
47	20	304	KC1	C4B-C3B-CAB-CBB
47	31	309	KC1	C4B-C3B-CAB-CBB
47	33	306	KC1	C4B-C3B-CAB-CBB
47	34	304	KC1	C4B-C3B-CAB-CBB
47	34	306	KC1	C4B-C3B-CAB-CBB
47	34	309	KC1	C4B-C3B-CAB-CBB
47	35	302	KC1	C4B-C3B-CAB-CBB
47	35	304	KC1	C4B-C3B-CAB-CBB
47	35	306	KC1	C4B-C3B-CAB-CBB
47	35	309	KC1	C4B-C3B-CAB-CBB
47	36	304	KC1	C4B-C3B-CAB-CBB
47	36	305	KC1	C4B-C3B-CAB-CBB
47	37	304	KC1	C4B-C3B-CAB-CBB
47	37	307	KC1	C4B-C3B-CAB-CBB
47	38	205	KC1	C4B-C3B-CAB-CBB
47	40	206	KC1	C4B-C3B-CAB-CBB
37	16	303	CLA	CBD-CGD-O2D-CED
37	36	303	CLA	CBD-CGD-O2D-CED
43	37	321	LHG	O9-C7-O7-C5
37	13	308	CLA	C3-C5-C6-C7
37	33	308	CLA	C3-C5-C6-C7
41	A	408	LMG	C38-C39-C40-C41
41	D	412	LMG	C36-C37-C38-C39
41	a	410	LMG	C38-C39-C40-C41
41	d	409	LMG	C36-C37-C38-C39
37	b	516	CLA	O1D-CGD-O2D-CED
41	11	316	LMG	C2-C1-O1-C7
41	16	316	LMG	C2-C1-O1-C7
41	31	316	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
41	36	314	LMG	C2-C1-O1-C7
41	C	518	LMG	O7-C8-C9-O8
41	c	518	LMG	O7-C8-C9-O8
37	D	402	CLA	C16-C17-C18-C20
37	d	401	CLA	C16-C17-C18-C20
43	B	523	LHG	C14-C15-C16-C17
43	b	522	LHG	C14-C15-C16-C17
37	38	208	CLA	C4-C3-C5-C6
45	D	404	PL9	C12-C11-C9-C10
45	d	402	PL9	C12-C11-C9-C10
43	17	316	LHG	C7-C8-C9-C10
43	37	315	LHG	C7-C8-C9-C10
37	21	206	CLA	C2-C3-C5-C6
37	35	307	CLA	C2-C3-C5-C6
37	41	206	CLA	C2-C3-C5-C6
37	B	508	CLA	C14-C13-C15-C16
37	B	510	CLA	C14-C13-C15-C16
37	B	511	CLA	C14-C13-C15-C16
37	b	508	CLA	C14-C13-C15-C16
37	b	510	CLA	C14-C13-C15-C16
37	b	511	CLA	C14-C13-C15-C16
37	12	205	CLA	C6-C7-C8-C9
37	14	301	CLA	C6-C7-C8-C9
37	18	202	CLA	C14-C13-C15-C16
37	32	206	CLA	C6-C7-C8-C9
37	34	301	CLA	C6-C7-C8-C9
37	38	202	CLA	C14-C13-C15-C16
37	41	209	CLA	O1D-CGD-O2D-CED
37	39	302	CLA	CBD-CGD-O2D-CED
47	40	207	KC1	CBD-CGD-O2D-CED
41	17	317	LMG	C16-C17-C18-C19
41	37	316	LMG	C16-C17-C18-C19
37	16	306	CLA	C3-C5-C6-C7
37	36	306	CLA	C3-C5-C6-C7
37	B	516	CLA	O1D-CGD-O2D-CED
37	D	401	CLA	C2A-CAA-CBA-CGA
37	a	404	CLA	C2A-CAA-CBA-CGA
43	D	411	LHG	C9-C10-C11-C12
39	0	101	BCR	C7-C8-C9-C34
39	5	101	BCR	C7-C8-C9-C34
48	37	310	A86	C-C1-C24-C25
37	21	209	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
37	12	205	CLA	C10-C11-C12-C13
37	32	206	CLA	C10-C11-C12-C13
47	20	305	KC1	CBD-CGD-O2D-CED
41	A	408	LMG	C37-C38-C39-C40
41	a	410	LMG	C37-C38-C39-C40
43	B	523	LHG	C33-C34-C35-C36
43	a	412	LHG	C9-C10-C11-C12
43	b	522	LHG	C33-C34-C35-C36
39	K	101	BCR	C17-C18-C19-C20
39	y	101	BCR	C17-C18-C19-C20
48	16	310	A86	C2-C1-C24-C25
48	17	310	A86	C5-C6-C8-C9
48	36	310	A86	C2-C1-C24-C25
48	37	309	A86	C5-C6-C8-C9
50	20	310	DD6	C5-C6-C8-C9
50	40	212	DD6	C5-C6-C8-C9
37	W	101	CLA	O1A-CGA-O2A-C1
37	w	101	CLA	O1A-CGA-O2A-C1
41	B	521	LMG	O10-C28-O8-C9
41	b	520	LMG	O10-C28-O8-C9
41	11	317	LMG	O10-C28-O8-C9
41	31	317	LMG	O10-C28-O8-C9
37	A	405	CLA	C1A-C2A-CAA-CBA
37	B	503	CLA	C1A-C2A-CAA-CBA
37	B	524	CLA	C1A-C2A-CAA-CBA
37	C	502	CLA	C1A-C2A-CAA-CBA
37	C	503	CLA	C1A-C2A-CAA-CBA
37	C	508	CLA	C1A-C2A-CAA-CBA
37	C	511	CLA	C1A-C2A-CAA-CBA
37	D	401	CLA	C1A-C2A-CAA-CBA
37	D	402	CLA	C1A-C2A-CAA-CBA
37	D	406	CLA	C1A-C2A-CAA-CBA
37	W	102	CLA	C1A-C2A-CAA-CBA
37	a	407	CLA	C1A-C2A-CAA-CBA
37	b	503	CLA	C1A-C2A-CAA-CBA
37	b	523	CLA	C1A-C2A-CAA-CBA
37	c	502	CLA	C1A-C2A-CAA-CBA
37	c	503	CLA	C1A-C2A-CAA-CBA
37	c	508	CLA	C1A-C2A-CAA-CBA
37	c	511	CLA	C1A-C2A-CAA-CBA
37	d	401	CLA	C1A-C2A-CAA-CBA
37	d	404	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	11	305	CLA	C1A-C2A-CAA-CBA
37	11	308	CLA	C1A-C2A-CAA-CBA
37	11	310	CLA	C1A-C2A-CAA-CBA
37	12	203	CLA	C1A-C2A-CAA-CBA
37	12	210	CLA	C1A-C2A-CAA-CBA
37	13	308	CLA	C1A-C2A-CAA-CBA
37	14	305	CLA	C1A-C2A-CAA-CBA
37	16	307	CLA	C1A-C2A-CAA-CBA
37	17	309	CLA	C1A-C2A-CAA-CBA
37	18	201	CLA	C1A-C2A-CAA-CBA
37	18	203	CLA	C1A-C2A-CAA-CBA
37	19	301	CLA	C1A-C2A-CAA-CBA
37	19	303	CLA	C1A-C2A-CAA-CBA
37	19	305	CLA	C1A-C2A-CAA-CBA
37	19	306	CLA	C1A-C2A-CAA-CBA
37	19	307	CLA	C1A-C2A-CAA-CBA
37	20	308	CLA	C1A-C2A-CAA-CBA
37	21	205	CLA	C1A-C2A-CAA-CBA
37	21	206	CLA	C1A-C2A-CAA-CBA
37	21	208	CLA	C1A-C2A-CAA-CBA
37	31	301	CLA	C1A-C2A-CAA-CBA
37	31	306	CLA	C1A-C2A-CAA-CBA
37	31	310	CLA	C1A-C2A-CAA-CBA
37	32	202	CLA	C1A-C2A-CAA-CBA
37	32	204	CLA	C1A-C2A-CAA-CBA
37	32	211	CLA	C1A-C2A-CAA-CBA
37	33	308	CLA	C1A-C2A-CAA-CBA
37	34	305	CLA	C1A-C2A-CAA-CBA
37	36	307	CLA	C1A-C2A-CAA-CBA
37	37	308	CLA	C1A-C2A-CAA-CBA
37	38	201	CLA	C1A-C2A-CAA-CBA
37	38	203	CLA	C1A-C2A-CAA-CBA
37	39	301	CLA	C1A-C2A-CAA-CBA
37	39	303	CLA	C1A-C2A-CAA-CBA
37	39	305	CLA	C1A-C2A-CAA-CBA
37	39	306	CLA	C1A-C2A-CAA-CBA
37	39	307	CLA	C1A-C2A-CAA-CBA
37	40	210	CLA	C1A-C2A-CAA-CBA
37	41	205	CLA	C1A-C2A-CAA-CBA
37	41	206	CLA	C1A-C2A-CAA-CBA
37	41	208	CLA	C1A-C2A-CAA-CBA
43	D	410	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
43	d	408	LHG	O9-C7-O7-C5
44	J	101	DGD	C5A-C6A-C7A-C8A
44	j	101	DGD	C5A-C6A-C7A-C8A
48	11	319	A86	C3-C4-C5-C6
48	14	314	A86	C3-C4-C5-C6
48	31	319	A86	C3-C4-C5-C6
48	34	314	A86	C3-C4-C5-C6
48	35	314	A86	C3-C4-C5-C6
50	19	312	DD6	C3-C4-C5-C6
50	39	312	DD6	C3-C4-C5-C6
37	C	509	CLA	C15-C16-C17-C18
37	c	509	CLA	C15-C16-C17-C18
37	21	206	CLA	C10-C11-C12-C13
37	41	206	CLA	C10-C11-C12-C13
43	21	201	LHG	C4-O6-P-O3
37	11	307	CLA	C4C-C3C-CAC-CBC
37	B	504	CLA	CBD-CGD-O2D-CED
37	b	504	CLA	CBD-CGD-O2D-CED
40	16	315	SQD	C13-C14-C15-C16
40	40	202	SQD	C13-C14-C15-C16
41	A	408	LMG	C30-C31-C32-C33
37	13	301	CLA	C5-C6-C7-C8
37	16	307	CLA	CBA-CGA-O2A-C1
37	36	307	CLA	CBA-CGA-O2A-C1
43	17	316	LHG	C24-C23-O8-C6
43	37	315	LHG	C24-C23-O8-C6
41	l	101	LMG	O6-C5-C6-O5
37	31	308	CLA	C4C-C3C-CAC-CBC
41	a	410	LMG	C30-C31-C32-C33
43	21	217	LHG	C26-C27-C28-C29
43	37	321	LHG	C26-C27-C28-C29
43	17	316	LHG	C23-C24-C25-C26
43	37	315	LHG	C23-C24-C25-C26
43	39	314	LHG	C32-C33-C34-C35
44	H	102	DGD	CCA-CDA-CEA-CFA
44	h	102	DGD	CCA-CDA-CEA-CFA
51	39	315	LMU	C7-C8-C9-C10
37	33	301	CLA	C5-C6-C7-C8
37	B	515	CLA	C16-C17-C18-C19
37	b	515	CLA	C16-C17-C18-C19
51	19	315	LMU	C7-C8-C9-C10
47	20	304	KC1	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
47	20	305	KC1	CAA-CBA-CGA-O2A
47	40	206	KC1	CAA-CBA-CGA-O1A
47	40	207	KC1	CAA-CBA-CGA-O2A
41	L	102	LMG	O6-C5-C6-O5
41	B	520	LMG	C37-C38-C39-C40
41	b	519	LMG	C37-C38-C39-C40
37	A	403	CLA	C5-C6-C7-C8
37	a	403	CLA	C5-C6-C7-C8
41	D	412	LMG	C20-C21-C22-C23
37	21	206	CLA	CBA-CGA-O2A-C1
37	41	206	CLA	CBA-CGA-O2A-C1
37	21	206	CLA	C4-C3-C5-C6
37	41	206	CLA	C4-C3-C5-C6
41	B	520	LMG	C4-C5-C6-O5
41	b	519	LMG	C4-C5-C6-O5
40	16	315	SQD	C12-C13-C14-C15
40	40	202	SQD	C12-C13-C14-C15
41	B	521	LMG	C34-C35-C36-C37
41	b	520	LMG	C34-C35-C36-C37
41	d	409	LMG	C20-C21-C22-C23
37	b	514	CLA	C8-C10-C11-C12
37	16	307	CLA	C10-C11-C12-C13
37	36	307	CLA	C10-C11-C12-C13
40	B	522	SQD	C12-C13-C14-C15
40	b	521	SQD	C12-C13-C14-C15
43	19	314	LHG	C32-C33-C34-C35
37	B	514	CLA	C8-C10-C11-C12
37	32	210	CLA	O1D-CGD-O2D-CED
40	A	407	SQD	O6-C44-C45-C46
40	B	519	SQD	C18-C19-C20-C21
40	L	101	SQD	C18-C19-C20-C21
40	a	409	SQD	O6-C44-C45-C46
40	16	315	SQD	O6-C44-C45-C46
40	40	202	SQD	O6-C44-C45-C46
41	A	408	LMG	O1-C7-C8-C9
41	C	518	LMG	C7-C8-C9-O8
41	a	410	LMG	O1-C7-C8-C9
41	c	518	LMG	C7-C8-C9-O8
41	11	316	LMG	C7-C8-C9-O8
41	11	317	LMG	C7-C8-C9-O8
41	31	316	LMG	C7-C8-C9-O8
41	31	317	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
43	21	201	LHG	C4-C5-C6-O8
43	37	315	LHG	C9-C10-C11-C12
43	41	201	LHG	C4-C5-C6-O8
47	32	212	KC1	CAA-CBA-CGA-O1A
37	39	310	CLA	C5-C6-C7-C8
41	D	412	LMG	C32-C33-C34-C35
43	17	316	LHG	C9-C10-C11-C12
37	11	310	CLA	O1A-CGA-O2A-C1
39	B	525	BCR	C14-C15-C16-C17
41	L	102	LMG	C16-C17-C18-C19
41	d	409	LMG	C32-C33-C34-C35
41	l	101	LMG	C16-C17-C18-C19
43	B	523	LHG	C29-C30-C31-C32
43	b	522	LHG	C29-C30-C31-C32
44	C	516	DGD	CBA-CCA-CDA-CEA
44	H	102	DGD	C2B-C3B-C4B-C5B
44	c	516	DGD	CBA-CCA-CDA-CEA
44	h	102	DGD	C2B-C3B-C4B-C5B
37	12	210	CLA	CBD-CGD-O2D-CED
41	11	317	LMG	C32-C33-C34-C35
41	31	317	LMG	C32-C33-C34-C35
43	D	410	LHG	C7-C8-C9-C10
43	d	408	LHG	C7-C8-C9-C10
37	31	310	CLA	O1A-CGA-O2A-C1
40	17	301	SQD	C35-C36-C37-C38
40	36	315	SQD	C35-C36-C37-C38
43	21	217	LHG	C11-C10-C9-C8
43	37	321	LHG	C11-C10-C9-C8
37	16	301	CLA	C3-C5-C6-C7
37	36	301	CLA	C3-C5-C6-C7
37	W	102	CLA	C8-C10-C11-C12
37	31	301	CLA	C8-C10-C11-C12
37	17	309	CLA	C2C-C3C-CAC-CBC
40	B	519	SQD	C27-C28-C29-C30
40	L	101	SQD	C27-C28-C29-C30
43	D	411	LHG	O1-C1-C2-O2
43	a	412	LHG	O1-C1-C2-O2
43	21	217	LHG	O1-C1-C2-O2
43	37	321	LHG	O1-C1-C2-O2
40	36	315	SQD	C12-C13-C14-C15
47	12	211	KC1	CAA-CBA-CGA-O1A
41	A	408	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
41	a	410	LMG	O6-C5-C6-O5
40	17	301	SQD	C12-C13-C14-C15
41	17	317	LMG	C15-C16-C17-C18
41	37	316	LMG	C15-C16-C17-C18
44	j	101	DGD	CCA-CDA-CEA-CFA
37	12	209	CLA	O1D-CGD-O2D-CED
37	W	101	CLA	C15-C16-C17-C18
37	w	101	CLA	C15-C16-C17-C18
39	A	410	BCR	C11-C10-C9-C34
39	a	413	BCR	C11-C10-C9-C34
37	14	307	CLA	C4-C3-C5-C6
37	18	209	CLA	C4-C3-C5-C6
37	34	307	CLA	C4-C3-C5-C6
37	35	307	CLA	C4-C3-C5-C6
44	J	101	DGD	CCA-CDA-CEA-CFA
37	B	512	CLA	CBA-CGA-O2A-C1
37	b	512	CLA	CBA-CGA-O2A-C1
38	D	403	PHO	CBA-CGA-O2A-C1
38	a	405	PHO	CBA-CGA-O2A-C1
41	12	201	LMG	C16-C17-C18-C19
41	32	201	LMG	C16-C17-C18-C19
43	D	411	LHG	C13-C14-C15-C16
43	39	314	LHG	C19-C20-C21-C22
43	17	316	LHG	C4-C5-O7-C7
43	37	315	LHG	C4-C5-O7-C7
37	13	307	CLA	C2A-CAA-CBA-CGA
37	33	307	CLA	C2A-CAA-CBA-CGA
37	19	310	CLA	C5-C6-C7-C8
37	16	301	CLA	C2-C1-O2A-CGA
37	18	209	CLA	C2-C1-O2A-CGA
37	36	301	CLA	C2-C1-O2A-CGA
43	a	412	LHG	C13-C14-C15-C16
43	19	314	LHG	C19-C20-C21-C22
37	C	504	CLA	C3-C5-C6-C7
37	c	504	CLA	C3-C5-C6-C7
41	C	518	LMG	C37-C38-C39-C40
41	c	518	LMG	C37-C38-C39-C40
43	17	316	LHG	C29-C30-C31-C32
43	21	217	LHG	C32-C33-C34-C35
43	37	315	LHG	C29-C30-C31-C32
43	37	321	LHG	C32-C33-C34-C35
37	16	309	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
37	36	309	CLA	O1D-CGD-O2D-CED
37	B	511	CLA	C10-C11-C12-C13
37	B	524	CLA	C13-C15-C16-C17
37	C	504	CLA	C15-C16-C17-C18
37	b	511	CLA	C10-C11-C12-C13
37	c	504	CLA	C15-C16-C17-C18
41	B	521	LMG	C17-C18-C19-C20
41	b	520	LMG	C17-C18-C19-C20
37	B	505	CLA	CBA-CGA-O2A-C1
37	B	509	CLA	CBA-CGA-O2A-C1
37	b	505	CLA	CBA-CGA-O2A-C1
37	b	509	CLA	CBA-CGA-O2A-C1
37	15	307	CLA	CBA-CGA-O2A-C1
37	35	307	CLA	CBA-CGA-O2A-C1
43	D	411	LHG	O6-C4-C5-O7
43	a	412	LHG	O6-C4-C5-O7
43	19	314	LHG	C15-C16-C17-C18
37	Z	101	CLA	C13-C15-C16-C17
37	z	101	CLA	C13-C15-C16-C17
41	B	521	LMG	C22-C23-C24-C25
41	b	520	LMG	C22-C23-C24-C25
37	16	307	CLA	O1A-CGA-O2A-C1
37	36	307	CLA	O1A-CGA-O2A-C1
41	11	316	LMG	O10-C28-O8-C9
41	31	316	LMG	O10-C28-O8-C9
44	C	516	DGD	O1A-C1A-O1G-C1G
44	c	516	DGD	O1A-C1A-O1G-C1G
43	39	314	LHG	C15-C16-C17-C18
37	16	307	CLA	C3-C5-C6-C7
37	C	510	CLA	C10-C11-C12-C13
37	c	510	CLA	C10-C11-C12-C13
41	C	518	LMG	C2-C1-O1-C7
41	c	518	LMG	C2-C1-O1-C7
50	16	312	DD6	C4-C5-C6-C8
50	20	312	DD6	C9-C10-C11-C13
50	36	312	DD6	C4-C5-C6-C8
50	40	214	DD6	C9-C10-C11-C13
40	16	315	SQD	C9-C10-C11-C12
40	40	202	SQD	C9-C10-C11-C12
41	C	518	LMG	C33-C34-C35-C36
41	c	518	LMG	C33-C34-C35-C36
40	A	407	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
40	B	519	SQD	O47-C45-C46-O48
40	B	522	SQD	O47-C45-C46-O48
40	L	101	SQD	O47-C45-C46-O48
40	a	409	SQD	O6-C44-C45-O47
40	b	521	SQD	O47-C45-C46-O48
37	B	509	CLA	O1A-CGA-O2A-C1
37	b	509	CLA	O1A-CGA-O2A-C1
37	B	515	CLA	C16-C17-C18-C20
37	b	515	CLA	C16-C17-C18-C20
37	11	307	CLA	C4-C3-C5-C6
37	12	209	CLA	C4-C3-C5-C6
37	32	210	CLA	C4-C3-C5-C6
41	37	316	LMG	C31-C32-C33-C34
37	b	523	CLA	C13-C15-C16-C17
37	A	405	CLA	C11-C10-C8-C7
37	B	502	CLA	C12-C13-C15-C16
37	B	506	CLA	C11-C10-C8-C7
37	B	507	CLA	C12-C13-C15-C16
37	B	508	CLA	C12-C13-C15-C16
37	B	511	CLA	C12-C13-C15-C16
37	B	524	CLA	C6-C7-C8-C10
37	B	524	CLA	C11-C10-C8-C7
37	C	510	CLA	C12-C13-C15-C16
37	Z	101	CLA	C6-C7-C8-C10
37	Z	101	CLA	C11-C12-C13-C15
37	a	407	CLA	C11-C10-C8-C7
37	b	501	CLA	C11-C10-C8-C7
37	b	502	CLA	C12-C13-C15-C16
37	b	506	CLA	C11-C10-C8-C7
37	b	507	CLA	C12-C13-C15-C16
37	b	508	CLA	C12-C13-C15-C16
37	b	511	CLA	C12-C13-C15-C16
37	b	523	CLA	C6-C7-C8-C10
37	b	523	CLA	C11-C10-C8-C7
37	c	510	CLA	C12-C13-C15-C16
37	z	101	CLA	C6-C7-C8-C10
37	z	101	CLA	C11-C12-C13-C15
37	14	301	CLA	C6-C7-C8-C10
37	14	301	CLA	C12-C13-C15-C16
37	18	202	CLA	C11-C10-C8-C7
37	18	202	CLA	C12-C13-C15-C16
37	19	302	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
37	21	204	CLA	C6-C7-C8-C10
37	34	301	CLA	C6-C7-C8-C10
37	34	301	CLA	C12-C13-C15-C16
37	35	308	CLA	C12-C13-C15-C16
37	38	202	CLA	C11-C10-C8-C7
37	38	202	CLA	C12-C13-C15-C16
37	39	302	CLA	C6-C7-C8-C10
37	41	204	CLA	C6-C7-C8-C10
37	36	307	CLA	C3-C5-C6-C7
37	B	506	CLA	C11-C10-C8-C9
37	B	507	CLA	C14-C13-C15-C16
37	B	510	CLA	C11-C12-C13-C14
37	B	524	CLA	C11-C10-C8-C9
37	C	509	CLA	C14-C13-C15-C16
37	C	510	CLA	C14-C13-C15-C16
37	Z	101	CLA	C6-C7-C8-C9
37	b	506	CLA	C11-C10-C8-C9
37	b	507	CLA	C14-C13-C15-C16
37	b	510	CLA	C11-C12-C13-C14
37	b	523	CLA	C11-C10-C8-C9
37	c	509	CLA	C14-C13-C15-C16
37	c	510	CLA	C14-C13-C15-C16
37	z	101	CLA	C6-C7-C8-C9
37	11	308	CLA	C14-C13-C15-C16
37	14	301	CLA	C14-C13-C15-C16
37	19	307	CLA	C14-C13-C15-C16
37	32	202	CLA	C14-C13-C15-C16
37	34	301	CLA	C14-C13-C15-C16
37	39	307	CLA	C14-C13-C15-C16
39	b	524	BCR	C14-C15-C16-C17
37	B	503	CLA	CBA-CGA-O2A-C1
37	b	503	CLA	CBA-CGA-O2A-C1
37	B	510	CLA	O1D-CGD-O2D-CED
37	B	512	CLA	O1A-CGA-O2A-C1
37	b	505	CLA	O1A-CGA-O2A-C1
37	b	512	CLA	O1A-CGA-O2A-C1
39	H	101	BCR	C7-C8-C9-C34
39	h	101	BCR	C7-C8-C9-C34
48	12	217	A86	C7-C6-C8-C9
48	16	310	A86	C-C1-C24-C25
48	17	315	A86	C-C1-C24-C25
48	18	215	A86	C7-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
48	32	218	A86	C7-C6-C8-C9
48	36	310	A86	C-C1-C24-C25
48	38	215	A86	C7-C6-C8-C9
41	16	316	LMG	C15-C16-C17-C18
41	17	317	LMG	C31-C32-C33-C34
41	36	314	LMG	C15-C16-C17-C18
48	11	315	A86	C2-C1-C24-C25
48	12	217	A86	C5-C6-C8-C9
48	14	315	A86	C2-C1-C24-C25
48	14	316	A86	C2-C1-C24-C25
48	14	316	A86	C5-C6-C8-C9
48	15	313	A86	C2-C1-C24-C25
48	18	215	A86	C5-C6-C8-C9
48	31	315	A86	C2-C1-C24-C25
48	32	218	A86	C5-C6-C8-C9
48	34	315	A86	C2-C1-C24-C25
48	34	316	A86	C2-C1-C24-C25
48	34	316	A86	C5-C6-C8-C9
48	35	313	A86	C2-C1-C24-C25
48	38	215	A86	C5-C6-C8-C9
50	20	312	DD6	C10-C11-C13-C14
50	40	214	DD6	C10-C11-C13-C14
40	17	301	SQD	C14-C15-C16-C17
40	36	315	SQD	C14-C15-C16-C17
37	b	510	CLA	O1D-CGD-O2D-CED
41	11	317	LMG	O9-C10-O7-C8
41	31	317	LMG	O9-C10-O7-C8
37	14	301	CLA	C8-C10-C11-C12
37	34	301	CLA	C8-C10-C11-C12
37	B	505	CLA	O1A-CGA-O2A-C1
37	38	208	CLA	CBA-CGA-O2A-C1
47	12	211	KC1	CAA-CBA-CGA-O2A
47	32	212	KC1	CAA-CBA-CGA-O2A
37	D	405	CLA	C15-C16-C17-C18
37	d	403	CLA	C15-C16-C17-C18
37	11	301	CLA	C8-C10-C11-C12
37	31	302	CLA	C8-C10-C11-C12
37	B	516	CLA	C3-C5-C6-C7
37	b	516	CLA	C3-C5-C6-C7
44	C	517	DGD	C5B-C6B-C7B-C8B
44	c	517	DGD	C5B-C6B-C7B-C8B
37	38	201	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	21	208	CLA	C10-C11-C12-C13
37	41	208	CLA	C10-C11-C12-C13
37	z	102	CLA	O1D-CGD-O2D-CED
41	A	408	LMG	C39-C40-C41-C42
48	12	214	A86	C39-C38-O4-C34
48	18	213	A86	O5-C38-O4-C34
37	31	308	CLA	C4-C3-C5-C6
37	38	209	CLA	C4-C3-C5-C6
37	11	307	CLA	C2-C3-C5-C6
37	12	209	CLA	C2-C3-C5-C6
37	13	303	CLA	C2-C3-C5-C6
37	14	307	CLA	C2-C3-C5-C6
37	32	210	CLA	C2-C3-C5-C6
37	34	307	CLA	C2-C3-C5-C6
41	a	410	LMG	C39-C40-C41-C42
37	Z	102	CLA	O1D-CGD-O2D-CED
37	13	301	CLA	O1D-CGD-O2D-CED
37	33	301	CLA	O1D-CGD-O2D-CED
43	D	409	LHG	C34-C35-C36-C37
43	D	411	LHG	C18-C19-C20-C21
43	d	407	LHG	C34-C35-C36-C37
40	B	522	SQD	C9-C10-C11-C12
43	D	409	LHG	C33-C34-C35-C36
43	a	412	LHG	C18-C19-C20-C21
43	d	407	LHG	C33-C34-C35-C36
47	20	305	KC1	C4C-C3C-CAC-CBC
47	40	207	KC1	C4C-C3C-CAC-CBC
48	32	215	A86	C39-C38-O4-C34
37	12	209	CLA	C2A-CAA-CBA-CGA
37	32	210	CLA	C2A-CAA-CBA-CGA
37	18	201	CLA	CBA-CGA-O2A-C1
37	18	208	CLA	CBA-CGA-O2A-C1
37	B	501	CLA	C3A-C2A-CAA-CBA
37	b	501	CLA	C3A-C2A-CAA-CBA
37	16	309	CLA	C3A-C2A-CAA-CBA
37	21	202	CLA	C3A-C2A-CAA-CBA
37	36	309	CLA	C3A-C2A-CAA-CBA
37	41	202	CLA	C3A-C2A-CAA-CBA
46	F	101	HEM	C2A-CAA-CBA-CGA
46	f	101	HEM	C2A-CAA-CBA-CGA
37	14	302	CLA	C5-C6-C7-C8
37	34	302	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
40	b	521	SQD	C9-C10-C11-C12
48	15	314	A86	C3-C4-C5-C6
48	15	316	A86	C3-C4-C5-C6
48	35	316	A86	C3-C4-C5-C6
48	12	215	A86	O-C13-C14-C15
48	12	216	A86	O-C13-C14-C15
48	13	311	A86	O-C13-C14-C15
48	13	314	A86	O-C13-C14-C15
48	14	311	A86	O-C13-C14-C15
48	14	313	A86	O-C13-C14-C15
48	14	314	A86	O-C13-C14-C15
48	15	311	A86	O-C13-C14-C15
48	15	313	A86	O-C13-C14-C15
48	15	314	A86	O-C13-C14-C15
48	16	313	A86	O-C13-C14-C15
48	17	310	A86	O-C13-C14-C15
48	17	313	A86	O-C13-C14-C15
48	18	212	A86	O-C13-C14-C15
48	19	311	A86	O-C13-C14-C15
48	19	313	A86	O-C13-C14-C15
48	20	311	A86	O-C13-C14-C15
48	21	211	A86	O-C13-C14-C15
48	21	213	A86	O-C13-C14-C15
48	21	214	A86	O-C13-C14-C15
48	32	216	A86	O-C13-C14-C15
48	32	217	A86	O-C13-C14-C15
48	33	311	A86	O-C13-C14-C15
48	34	311	A86	O-C13-C14-C15
48	34	313	A86	O-C13-C14-C15
48	34	314	A86	O-C13-C14-C15
48	35	311	A86	O-C13-C14-C15
48	35	313	A86	O-C13-C14-C15
48	35	314	A86	O-C13-C14-C15
48	37	309	A86	O-C13-C14-C15
48	37	312	A86	O-C13-C14-C15
48	38	212	A86	O-C13-C14-C15
48	39	311	A86	O-C13-C14-C15
48	39	313	A86	O-C13-C14-C15
48	40	201	A86	O-C13-C14-C15
48	40	213	A86	O-C13-C14-C15
48	41	211	A86	O-C13-C14-C15
48	41	213	A86	O-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
48	41	214	A86	O-C13-C14-C15
41	D	412	LMG	C17-C18-C19-C20
41	d	409	LMG	C17-C18-C19-C20
48	38	213	A86	O5-C38-O4-C34
47	20	304	KC1	CAA-CBA-CGA-O2A
47	40	206	KC1	CAA-CBA-CGA-O2A
37	21	202	CLA	CBA-CGA-O2A-C1
37	41	202	CLA	CBA-CGA-O2A-C1
37	11	303	CLA	C10-C11-C12-C13
37	12	203	CLA	C5-C6-C7-C8
37	31	304	CLA	C10-C11-C12-C13
37	32	204	CLA	C5-C6-C7-C8
40	B	522	SQD	C44-C45-C46-O48
40	b	521	SQD	C44-C45-C46-O48
41	C	518	LMG	O1-C7-C8-C9
41	c	518	LMG	O1-C7-C8-C9
41	11	317	LMG	O1-C7-C8-C9
41	12	201	LMG	O1-C7-C8-C9
41	31	317	LMG	O1-C7-C8-C9
41	32	201	LMG	O1-C7-C8-C9
44	H	102	DGD	C9B-CAB-CBB-CCB
37	31	308	CLA	C2-C3-C5-C6
43	39	314	LHG	C16-C17-C18-C19
44	h	102	DGD	C9B-CAB-CBB-CCB
43	41	201	LHG	C4-O6-P-O3
37	21	206	CLA	O1A-CGA-O2A-C1
37	35	307	CLA	O1A-CGA-O2A-C1
37	41	206	CLA	O1A-CGA-O2A-C1
40	A	407	SQD	C28-C29-C30-C31
40	a	409	SQD	C28-C29-C30-C31
43	19	314	LHG	C30-C31-C32-C33
37	12	205	CLA	C3-C5-C6-C7
43	D	410	LHG	C12-C13-C14-C15
43	d	408	LHG	C12-C13-C14-C15
43	d	408	LHG	C26-C27-C28-C29
43	17	316	LHG	C12-C13-C14-C15
43	17	316	LHG	C30-C31-C32-C33
43	37	315	LHG	C30-C31-C32-C33
51	19	315	LMU	C3-C4-C5-C6
51	39	315	LMU	C3-C4-C5-C6
37	19	301	CLA	CBA-CGA-O2A-C1
37	39	301	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
43	D	410	LHG	C26-C27-C28-C29
37	15	307	CLA	O1A-CGA-O2A-C1
38	D	403	PHO	O1A-CGA-O2A-C1
38	a	405	PHO	O1A-CGA-O2A-C1
43	39	314	LHG	C30-C31-C32-C33
37	B	501	CLA	CAA-CBA-CGA-O2A
37	b	501	CLA	CAA-CBA-CGA-O2A
43	19	314	LHG	C16-C17-C18-C19
43	37	315	LHG	C12-C13-C14-C15
44	C	516	DGD	C4A-C5A-C6A-C7A
44	c	516	DGD	C4A-C5A-C6A-C7A
40	L	101	SQD	C29-C30-C31-C32
40	17	301	SQD	C26-C27-C28-C29
40	36	315	SQD	C26-C27-C28-C29
41	11	316	LMG	C29-C30-C31-C32
41	31	316	LMG	C29-C30-C31-C32
43	19	314	LHG	C35-C36-C37-C38
43	39	314	LHG	C35-C36-C37-C38
44	C	516	DGD	C3A-C4A-C5A-C6A
37	32	206	CLA	C3-C5-C6-C7
43	21	201	LHG	C2-C3-O3-P
43	41	201	LHG	C2-C3-O3-P
44	c	516	DGD	C3A-C4A-C5A-C6A
40	16	315	SQD	O47-C45-C46-O48
40	40	202	SQD	O47-C45-C46-O48
41	11	316	LMG	O7-C8-C9-O8
41	11	317	LMG	O1-C7-C8-O7
41	17	317	LMG	O1-C7-C8-O7
41	31	316	LMG	O7-C8-C9-O8
41	31	317	LMG	O1-C7-C8-O7
41	37	316	LMG	O1-C7-C8-O7
43	D	411	LHG	O7-C5-C6-O8
43	a	412	LHG	O7-C5-C6-O8
43	21	201	LHG	O7-C5-C6-O8
43	41	201	LHG	O7-C5-C6-O8
37	b	509	CLA	O1D-CGD-O2D-CED
48	17	311	A86	C24-C25-C26-C27
48	19	311	A86	C24-C25-C26-C27
48	19	313	A86	C11-C10-C9-C8
48	31	313	A86	C24-C25-C26-C27
48	37	310	A86	C24-C25-C26-C27
48	39	311	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
48	39	313	A86	C11-C10-C9-C8
40	B	519	SQD	C29-C30-C31-C32
37	W	102	CLA	C10-C11-C12-C13
37	31	301	CLA	C10-C11-C12-C13
48	11	314	A86	C10-C11-C13-C14
48	12	202	A86	C10-C11-C13-C14
48	14	314	A86	C10-C11-C13-C14
48	16	314	A86	C10-C11-C13-C14
48	17	315	A86	C10-C11-C13-C14
48	20	311	A86	C10-C11-C13-C14
48	31	314	A86	C10-C11-C13-C14
48	32	203	A86	C10-C11-C13-C14
48	34	314	A86	C10-C11-C13-C14
48	36	313	A86	C10-C11-C13-C14
48	37	314	A86	C10-C11-C13-C14
48	40	213	A86	C10-C11-C13-C14
41	C	518	LMG	C32-C33-C34-C35
41	c	518	LMG	C32-C33-C34-C35
41	A	408	LMG	O9-C10-O7-C8
41	a	410	LMG	O9-C10-O7-C8
37	C	505	CLA	C2-C1-O2A-CGA
37	Z	101	CLA	C2-C1-O2A-CGA
37	c	505	CLA	C2-C1-O2A-CGA
37	z	101	CLA	C2-C1-O2A-CGA
37	11	308	CLA	C2-C1-O2A-CGA
37	12	210	CLA	C2-C1-O2A-CGA
37	14	308	CLA	C2-C1-O2A-CGA
37	32	202	CLA	C2-C1-O2A-CGA
37	32	211	CLA	C2-C1-O2A-CGA
37	34	308	CLA	C2-C1-O2A-CGA
37	38	209	CLA	C2-C1-O2A-CGA
37	B	509	CLA	O1D-CGD-O2D-CED
44	C	516	DGD	C9A-CAA-CBA-CCA
44	c	516	DGD	C9A-CAA-CBA-CCA
37	a	407	CLA	C13-C15-C16-C17
37	B	524	CLA	C11-C12-C13-C14
37	b	523	CLA	C11-C12-C13-C14
37	13	303	CLA	C6-C7-C8-C9
37	16	306	CLA	C14-C13-C15-C16
37	18	202	CLA	C11-C10-C8-C9
37	18	204	CLA	C6-C7-C8-C9
37	21	204	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	33	303	CLA	C6-C7-C8-C9
37	36	306	CLA	C14-C13-C15-C16
37	38	202	CLA	C11-C10-C8-C9
37	38	204	CLA	C6-C7-C8-C9
37	41	204	CLA	C6-C7-C8-C9
40	B	522	SQD	C10-C11-C12-C13
40	b	521	SQD	C10-C11-C12-C13
43	19	314	LHG	C24-C25-C26-C27
43	39	314	LHG	C24-C25-C26-C27
37	A	405	CLA	C13-C15-C16-C17
37	35	308	CLA	C13-C15-C16-C17
37	11	310	CLA	C4-C3-C5-C6
37	19	305	CLA	C4-C3-C5-C6
37	31	310	CLA	C4-C3-C5-C6
37	39	305	CLA	C4-C3-C5-C6
38	D	403	PHO	C1A-C2A-CAA-CBA
38	a	405	PHO	C1A-C2A-CAA-CBA
43	17	316	LHG	C2-C3-O3-P
43	21	201	LHG	C5-C4-O6-P
43	37	315	LHG	C2-C3-O3-P
43	41	201	LHG	C5-C4-O6-P
47	18	205	KC1	C1A-C2A-CAA-CBA
47	38	205	KC1	C1A-C2A-CAA-CBA
44	C	517	DGD	C8B-C9B-CAB-CBB
44	c	517	DGD	C8B-C9B-CAB-CBB
37	14	303	CLA	C2A-CAA-CBA-CGA
37	34	303	CLA	C2A-CAA-CBA-CGA
37	C	503	CLA	C16-C17-C18-C20
37	c	503	CLA	C16-C17-C18-C20
39	A	406	BCR	C23-C24-C25-C26
39	A	406	BCR	C23-C24-C25-C30
39	A	410	BCR	C23-C24-C25-C26
39	B	517	BCR	C23-C24-C25-C26
39	B	517	BCR	C23-C24-C25-C30
39	B	518	BCR	C23-C24-C25-C26
39	B	525	BCR	C23-C24-C25-C26
39	B	525	BCR	C23-C24-C25-C30
39	C	514	BCR	C23-C24-C25-C26
39	C	514	BCR	C23-C24-C25-C30
39	C	515	BCR	C5-C6-C7-C8
39	C	515	BCR	C23-C24-C25-C26
39	C	515	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
39	D	407	BCR	C23-C24-C25-C26
39	D	407	BCR	C23-C24-C25-C30
39	K	101	BCR	C23-C24-C25-C26
39	0	101	BCR	C23-C24-C25-C30
39	a	408	BCR	C23-C24-C25-C26
39	a	408	BCR	C23-C24-C25-C30
39	a	413	BCR	C23-C24-C25-C26
39	b	517	BCR	C23-C24-C25-C26
39	b	517	BCR	C23-C24-C25-C30
39	b	518	BCR	C23-C24-C25-C26
39	b	524	BCR	C23-C24-C25-C26
39	b	524	BCR	C23-C24-C25-C30
39	c	514	BCR	C5-C6-C7-C8
39	c	514	BCR	C23-C24-C25-C26
39	c	514	BCR	C23-C24-C25-C30
39	c	515	BCR	C5-C6-C7-C8
39	c	515	BCR	C23-C24-C25-C26
39	c	515	BCR	C23-C24-C25-C30
39	d	405	BCR	C23-C24-C25-C26
39	d	405	BCR	C23-C24-C25-C30
39	y	101	BCR	C23-C24-C25-C26
39	5	101	BCR	C23-C24-C25-C26
39	5	101	BCR	C23-C24-C25-C30
41	A	408	LMG	C16-C17-C18-C19
41	a	410	LMG	C16-C17-C18-C19
39	C	519	BCR	C37-C22-C23-C24
39	c	519	BCR	C37-C22-C23-C24
48	11	315	A86	C-C1-C24-C25
48	14	316	A86	C7-C6-C8-C9
48	18	212	A86	C-C1-C24-C25
48	31	315	A86	C-C1-C24-C25
48	34	316	A86	C7-C6-C8-C9
48	37	314	A86	C-C1-C24-C25
48	13	315	A86	C2-C1-C24-C25
48	18	212	A86	C2-C1-C24-C25
48	33	315	A86	C2-C1-C24-C25
48	38	212	A86	C2-C1-C24-C25
40	40	202	SQD	C11-C10-C9-C8
43	17	316	LHG	C8-C7-O7-C5
43	37	315	LHG	C8-C7-O7-C5
40	B	519	SQD	C12-C13-C14-C15
40	L	101	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
40	16	315	SQD	C11-C10-C9-C8
37	Z	101	CLA	C16-C17-C18-C19
37	z	101	CLA	C16-C17-C18-C19
37	D	402	CLA	C13-C15-C16-C17
37	d	401	CLA	C13-C15-C16-C17
43	D	409	LHG	O6-C4-C5-C6
43	d	407	LHG	O6-C4-C5-C6
37	37	303	CLA	C4-C3-C5-C6
45	d	406	PL9	C15-C14-C16-C17
43	19	314	LHG	O2-C2-C3-O3
43	39	314	LHG	O2-C2-C3-O3
41	B	521	LMG	C11-C12-C13-C14
41	b	520	LMG	C11-C12-C13-C14
41	b	520	LMG	C13-C14-C15-C16
43	41	201	LHG	C25-C26-C27-C28
37	B	501	CLA	C11-C10-C8-C7
37	B	514	CLA	C12-C13-C15-C16
37	C	502	CLA	C11-C12-C13-C15
37	C	503	CLA	C12-C13-C15-C16
37	C	509	CLA	C12-C13-C15-C16
37	C	511	CLA	C6-C7-C8-C10
37	D	406	CLA	C11-C12-C13-C15
37	D	406	CLA	C12-C13-C15-C16
37	W	101	CLA	C6-C7-C8-C10
37	W	102	CLA	C11-C12-C13-C15
37	b	514	CLA	C12-C13-C15-C16
37	c	502	CLA	C11-C12-C13-C15
37	c	503	CLA	C12-C13-C15-C16
37	c	509	CLA	C12-C13-C15-C16
37	c	511	CLA	C6-C7-C8-C10
37	d	404	CLA	C11-C12-C13-C15
37	d	404	CLA	C12-C13-C15-C16
37	w	101	CLA	C6-C7-C8-C10
37	11	308	CLA	C12-C13-C15-C16
37	14	308	CLA	C12-C13-C15-C16
37	15	308	CLA	C12-C13-C15-C16
37	16	306	CLA	C12-C13-C15-C16
37	19	307	CLA	C12-C13-C15-C16
37	31	301	CLA	C11-C12-C13-C15
37	32	202	CLA	C12-C13-C15-C16
37	33	303	CLA	C6-C7-C8-C10
37	34	308	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
37	34	308	CLA	C12-C13-C15-C16
37	36	306	CLA	C12-C13-C15-C16
37	39	307	CLA	C12-C13-C15-C16
41	B	521	LMG	C13-C14-C15-C16
37	B	513	CLA	C13-C15-C16-C17
37	b	513	CLA	C13-C15-C16-C17
48	11	315	A86	C3-C4-C5-C6
48	13	311	A86	C11-C10-C9-C8
48	15	312	A86	C24-C25-C26-C27
48	16	311	A86	C1-C2-C3-C4
48	21	214	A86	C3-C4-C5-C6
48	31	315	A86	C3-C4-C5-C6
48	33	311	A86	C11-C10-C9-C8
48	35	312	A86	C24-C25-C26-C27
48	36	311	A86	C1-C2-C3-C4
48	38	213	A86	C3-C4-C5-C6
48	41	214	A86	C3-C4-C5-C6
43	B	523	LHG	C31-C32-C33-C34
44	c	517	DGD	C1B-C2B-C3B-C4B
37	17	309	CLA	C4C-C3C-CAC-CBC
41	B	521	LMG	C35-C36-C37-C38
43	D	409	LHG	C30-C31-C32-C33
43	b	522	LHG	C31-C32-C33-C34
43	d	407	LHG	C30-C31-C32-C33
44	j	101	DGD	CDA-CEA-CFA-CGA
40	17	301	SQD	C30-C31-C32-C33
40	36	315	SQD	C30-C31-C32-C33
41	b	520	LMG	C35-C36-C37-C38
44	J	101	DGD	CDA-CEA-CFA-CGA
39	B	525	BCR	C16-C17-C18-C36
43	21	201	LHG	C25-C26-C27-C28
44	C	516	DGD	C9B-CAB-CBB-CCB
44	c	516	DGD	C9B-CAB-CBB-CCB
44	C	517	DGD	C1B-C2B-C3B-C4B
43	D	409	LHG	C17-C18-C19-C20
43	d	407	LHG	C17-C18-C19-C20
44	C	516	DGD	CAB-CBB-CCB-CDB
44	c	516	DGD	CAB-CBB-CCB-CDB
37	16	303	CLA	CBA-CGA-O2A-C1
37	36	303	CLA	CBA-CGA-O2A-C1
40	16	315	SQD	C26-C27-C28-C29
40	40	202	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
37	20	301	CLA	O1D-CGD-O2D-CED
43	D	409	LHG	C11-C12-C13-C14
43	d	407	LHG	C11-C12-C13-C14
43	21	217	LHG	C31-C32-C33-C34
43	37	321	LHG	C31-C32-C33-C34
37	B	504	CLA	CAD-CBD-CGD-O2D
37	B	510	CLA	CAD-CBD-CGD-O2D
37	B	514	CLA	CAD-CBD-CGD-O2D
37	C	501	CLA	CAD-CBD-CGD-O2D
37	C	503	CLA	CAD-CBD-CGD-O2D
37	C	513	CLA	CAD-CBD-CGD-O2D
37	W	102	CLA	CAD-CBD-CGD-O2D
37	b	504	CLA	CAD-CBD-CGD-O2D
37	b	510	CLA	CAD-CBD-CGD-O2D
37	b	514	CLA	CAD-CBD-CGD-O2D
37	c	501	CLA	CAD-CBD-CGD-O2D
37	c	503	CLA	CAD-CBD-CGD-O2D
37	c	513	CLA	CAD-CBD-CGD-O2D
37	11	305	CLA	CAD-CBD-CGD-O2D
37	12	205	CLA	CAD-CBD-CGD-O2D
37	19	304	CLA	CAD-CBD-CGD-O2D
37	20	303	CLA	CAD-CBD-CGD-O2D
37	31	301	CLA	CAD-CBD-CGD-O2D
37	31	306	CLA	CAD-CBD-CGD-O2D
37	32	206	CLA	CAD-CBD-CGD-O2D
37	39	304	CLA	CAD-CBD-CGD-O2D
37	40	205	CLA	CAD-CBD-CGD-O2D
41	16	316	LMG	C9-C8-O7-C10
41	36	314	LMG	C9-C8-O7-C10
47	11	306	KC1	CAD-CBD-CGD-O2D
47	12	206	KC1	C2B-C3B-CAB-CBB
47	12	211	KC1	CAD-CBD-CGD-O2D
47	13	302	KC1	C2B-C3B-CAB-CBB
47	14	306	KC1	CAD-CBD-CGD-O2D
47	17	303	KC1	C2B-C3B-CAB-CBB
47	17	306	KC1	C2B-C3B-CAB-CBB
47	18	207	KC1	C2B-C3B-CAB-CBB
47	20	302	KC1	C2B-C3B-CAB-CBB
47	31	307	KC1	CAD-CBD-CGD-O2D
47	32	212	KC1	CAD-CBD-CGD-O2D
47	33	302	KC1	C2B-C3B-CAB-CBB
47	34	306	KC1	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
47	37	302	KC1	C2B-C3B-CAB-CBB
47	37	305	KC1	C2B-C3B-CAB-CBB
47	40	204	KC1	C2B-C3B-CAB-CBB
48	12	215	A86	C28-C27-C29-C30
48	15	313	A86	C28-C27-C29-C30
48	16	311	A86	C28-C27-C29-C30
48	20	311	A86	C28-C27-C29-C30
48	32	216	A86	C28-C27-C29-C30
48	35	313	A86	C28-C27-C29-C30
48	36	311	A86	C28-C27-C29-C30
48	40	213	A86	C28-C27-C29-C30
44	J	101	DGD	O1B-C1B-O2G-C2G
43	D	409	LHG	C13-C14-C15-C16
43	d	407	LHG	C13-C14-C15-C16
37	37	301	CLA	C8-C10-C11-C12
37	18	209	CLA	CBA-CGA-O2A-C1
37	19	303	CLA	CBA-CGA-O2A-C1
37	39	303	CLA	CBA-CGA-O2A-C1
37	40	203	CLA	O1D-CGD-O2D-CED
37	C	506	CLA	C4-C3-C5-C6
37	c	506	CLA	C4-C3-C5-C6
37	12	203	CLA	C4-C3-C5-C6
37	32	204	CLA	C4-C3-C5-C6
45	D	408	PL9	C15-C14-C16-C17
37	33	303	CLA	C2-C3-C5-C6
40	16	315	SQD	C19-C20-C21-C22
41	11	317	LMG	C28-C29-C30-C31
41	31	317	LMG	C28-C29-C30-C31
40	17	301	SQD	C44-C45-C46-O48
40	36	315	SQD	C44-C45-C46-O48
41	B	521	LMG	O1-C7-C8-C9
41	b	520	LMG	O1-C7-C8-C9
43	d	407	LHG	C4-C5-C6-O8
43	21	217	LHG	C4-C5-C6-O8
43	37	321	LHG	C4-C5-C6-O8
48	14	314	A86	C12-C11-C13-O
48	14	316	A86	C12-C11-C13-O
48	15	314	A86	C12-C11-C13-O
48	15	316	A86	C12-C11-C13-O
48	16	313	A86	C12-C11-C13-O
48	18	214	A86	C12-C11-C13-O
48	20	311	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
48	34	314	A86	C12-C11-C13-O
48	34	316	A86	C12-C11-C13-O
48	35	314	A86	C12-C11-C13-O
48	35	316	A86	C12-C11-C13-O
48	38	214	A86	C12-C11-C13-O
48	38	215	A86	C12-C11-C13-O
48	40	201	A86	C12-C11-C13-O
48	40	213	A86	C12-C11-C13-O
41	A	408	LMG	O10-C28-O8-C9
41	a	410	LMG	O10-C28-O8-C9
40	40	202	SQD	C19-C20-C21-C22
43	B	523	LHG	O6-C4-C5-O7
43	D	409	LHG	O6-C4-C5-O7
43	b	522	LHG	O6-C4-C5-O7
43	d	407	LHG	O6-C4-C5-O7
37	B	514	CLA	C2A-CAA-CBA-CGA
37	b	514	CLA	C2A-CAA-CBA-CGA
44	J	101	DGD	C6A-C7A-C8A-C9A
44	j	101	DGD	C6A-C7A-C8A-C9A
44	j	101	DGD	O1B-C1B-O2G-C2G
37	B	503	CLA	CHA-CBD-CGD-O1D
37	B	503	CLA	CHA-CBD-CGD-O2D
37	C	505	CLA	CHA-CBD-CGD-O1D
37	C	510	CLA	CHA-CBD-CGD-O1D
37	b	503	CLA	CHA-CBD-CGD-O1D
37	b	503	CLA	CHA-CBD-CGD-O2D
37	c	505	CLA	CHA-CBD-CGD-O1D
37	c	510	CLA	CHA-CBD-CGD-O1D
37	12	204	CLA	CHA-CBD-CGD-O1D
37	12	204	CLA	CHA-CBD-CGD-O2D
37	14	302	CLA	CHA-CBD-CGD-O1D
37	15	308	CLA	CHA-CBD-CGD-O2D
37	15	310	CLA	CHA-CBD-CGD-O1D
37	18	211	CLA	CHA-CBD-CGD-O1D
37	19	302	CLA	CHA-CBD-CGD-O1D
37	19	302	CLA	CHA-CBD-CGD-O2D
37	19	303	CLA	CHA-CBD-CGD-O1D
37	19	303	CLA	CHA-CBD-CGD-O2D
37	20	306	CLA	CHA-CBD-CGD-O1D
37	20	307	CLA	CHA-CBD-CGD-O1D
37	20	307	CLA	CHA-CBD-CGD-O2D
37	21	209	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
37	32	205	CLA	CHA-CBD-CGD-O1D
37	32	205	CLA	CHA-CBD-CGD-O2D
37	34	302	CLA	CHA-CBD-CGD-O1D
37	35	308	CLA	CHA-CBD-CGD-O2D
37	35	310	CLA	CHA-CBD-CGD-O1D
37	38	211	CLA	CHA-CBD-CGD-O1D
37	39	302	CLA	CHA-CBD-CGD-O1D
37	39	302	CLA	CHA-CBD-CGD-O2D
37	39	303	CLA	CHA-CBD-CGD-O1D
37	39	303	CLA	CHA-CBD-CGD-O2D
37	40	208	CLA	CHA-CBD-CGD-O1D
37	40	209	CLA	CHA-CBD-CGD-O1D
37	40	209	CLA	CHA-CBD-CGD-O2D
37	41	209	CLA	CHA-CBD-CGD-O1D
47	11	309	KC1	CHA-CBD-CGD-O1D
47	31	309	KC1	CHA-CBD-CGD-O1D
37	B	503	CLA	O1A-CGA-O2A-C1
37	b	503	CLA	O1A-CGA-O2A-C1
37	38	208	CLA	O1A-CGA-O2A-C1
40	40	202	SQD	C11-C12-C13-C14
37	C	513	CLA	O1D-CGD-O2D-CED
37	c	513	CLA	O1D-CGD-O2D-CED
50	19	312	DD6	C24-C1-C2-C3
50	39	312	DD6	C24-C1-C2-C3
40	16	315	SQD	C11-C12-C13-C14
41	A	408	LMG	C34-C35-C36-C37
41	a	410	LMG	C34-C35-C36-C37
41	B	521	LMG	O1-C7-C8-O7
41	C	518	LMG	O1-C7-C8-O7
41	b	520	LMG	O1-C7-C8-O7
41	c	518	LMG	O1-C7-C8-O7
41	11	317	LMG	O7-C8-C9-O8
41	12	201	LMG	O1-C7-C8-O7
41	31	317	LMG	O7-C8-C9-O8
41	32	201	LMG	O1-C7-C8-O7
40	B	519	SQD	C26-C27-C28-C29
40	L	101	SQD	C26-C27-C28-C29
37	17	302	CLA	C8-C10-C11-C12
37	16	303	CLA	O1A-CGA-O2A-C1
37	18	201	CLA	O1A-CGA-O2A-C1
37	18	208	CLA	O1A-CGA-O2A-C1
37	21	202	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	36	303	CLA	O1A-CGA-O2A-C1
37	38	201	CLA	O1A-CGA-O2A-C1
43	D	410	LHG	O1-C1-C2-O2
43	d	408	LHG	O1-C1-C2-O2
43	21	201	LHG	O2-C2-C3-O3
43	41	201	LHG	O2-C2-C3-O3
48	11	314	A86	C10-C11-C13-O
48	12	202	A86	C13-C14-C15-O1
48	12	215	A86	C10-C11-C13-O
48	12	217	A86	C13-C14-C15-O1
48	13	313	A86	C13-C14-C15-O1
48	13	314	A86	C13-C14-C15-O1
48	13	315	A86	C13-C14-C15-O1
48	14	314	A86	C10-C11-C13-O
48	14	316	A86	C13-C14-C15-O1
48	15	314	A86	C10-C11-C13-O
48	15	316	A86	C10-C11-C13-O
48	15	316	A86	C13-C14-C15-O1
48	16	313	A86	C10-C11-C13-O
48	16	314	A86	C13-C14-C15-O1
48	17	310	A86	C10-C11-C13-O
48	17	315	A86	C13-C14-C15-O1
48	18	214	A86	C10-C11-C13-O
48	18	215	A86	C13-C14-C15-O1
48	31	314	A86	C10-C11-C13-O
48	32	203	A86	C13-C14-C15-O1
48	32	216	A86	C10-C11-C13-O
48	32	218	A86	C13-C14-C15-O1
48	33	313	A86	C13-C14-C15-O1
48	33	315	A86	C13-C14-C15-O1
48	34	314	A86	C10-C11-C13-O
48	34	316	A86	C13-C14-C15-O1
48	35	314	A86	C10-C11-C13-O
48	35	316	A86	C10-C11-C13-O
48	35	316	A86	C13-C14-C15-O1
48	36	313	A86	C13-C14-C15-O1
48	37	309	A86	C10-C11-C13-O
48	37	314	A86	C13-C14-C15-O1
48	38	214	A86	C10-C11-C13-O
48	38	215	A86	C10-C11-C13-O
48	38	215	A86	C13-C14-C15-O1
48	40	201	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
37	32	211	CLA	O1D-CGD-O2D-CED
41	B	520	LMG	C15-C16-C17-C18
41	b	519	LMG	C15-C16-C17-C18
43	17	316	LHG	C11-C12-C13-C14
43	37	315	LHG	C11-C12-C13-C14
37	13	307	CLA	C4-C3-C5-C6
37	33	307	CLA	C4-C3-C5-C6
37	41	202	CLA	O1A-CGA-O2A-C1
37	18	209	CLA	C2-C3-C5-C6
45	D	408	PL9	C4-C3-C7-C8
45	d	406	PL9	C4-C3-C7-C8
40	B	519	SQD	C19-C20-C21-C22
40	L	101	SQD	C19-C20-C21-C22
37	15	307	CLA	O1D-CGD-O2D-CED
43	41	201	LHG	C15-C16-C17-C18
44	j	101	DGD	C7B-C8B-C9B-CAB
37	40	205	CLA	CBD-CGD-O2D-CED
37	18	209	CLA	O1A-CGA-O2A-C1
37	19	303	CLA	O1A-CGA-O2A-C1
37	39	303	CLA	O1A-CGA-O2A-C1
44	J	101	DGD	C7B-C8B-C9B-CAB
37	13	301	CLA	C10-C11-C12-C13
37	33	301	CLA	C10-C11-C12-C13
40	A	407	SQD	C5-C6-S-O8
40	a	409	SQD	C5-C6-S-O8
37	B	513	CLA	C16-C17-C18-C20
37	b	513	CLA	C16-C17-C18-C20
37	W	101	CLA	O1D-CGD-O2D-CED
37	w	101	CLA	O1D-CGD-O2D-CED
41	11	316	LMG	C20-C21-C22-C23
37	20	303	CLA	CBD-CGD-O2D-CED
41	A	408	LMG	C14-C15-C16-C17
41	a	410	LMG	C14-C15-C16-C17
41	31	316	LMG	C20-C21-C22-C23
48	11	311	A86	C-C1-C24-C25
48	14	315	A86	C-C1-C24-C25
48	15	311	A86	C-C1-C24-C25
48	15	319	A86	C-C1-C24-C25
48	17	312	A86	C-C1-C24-C25
48	18	214	A86	C7-C6-C8-C9
48	20	309	A86	C7-C6-C8-C9
48	31	311	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
48	34	315	A86	C-C1-C24-C25
48	35	311	A86	C-C1-C24-C25
48	35	319	A86	C-C1-C24-C25
48	37	311	A86	C-C1-C24-C25
48	38	212	A86	C-C1-C24-C25
48	38	214	A86	C7-C6-C8-C9
48	40	211	A86	C7-C6-C8-C9
48	11	311	A86	C2-C1-C24-C25
48	15	311	A86	C2-C1-C24-C25
48	15	319	A86	C2-C1-C24-C25
48	17	312	A86	C2-C1-C24-C25
48	18	214	A86	C5-C6-C8-C9
48	20	309	A86	C5-C6-C8-C9
48	31	311	A86	C2-C1-C24-C25
48	35	311	A86	C2-C1-C24-C25
48	35	319	A86	C2-C1-C24-C25
48	37	311	A86	C2-C1-C24-C25
48	38	214	A86	C5-C6-C8-C9
48	40	211	A86	C5-C6-C8-C9
44	c	517	DGD	C8A-C9A-CAA-CBA
37	35	307	CLA	O1D-CGD-O2D-CED
37	Z	101	CLA	C1A-C2A-CAA-CBA
37	z	101	CLA	C1A-C2A-CAA-CBA
37	13	301	CLA	C1A-C2A-CAA-CBA
37	19	310	CLA	C1A-C2A-CAA-CBA
37	33	301	CLA	C1A-C2A-CAA-CBA
37	39	310	CLA	C1A-C2A-CAA-CBA
38	A	404	PHO	C16-C17-C18-C20
44	C	517	DGD	C8A-C9A-CAA-CBA
41	37	316	LMG	C11-C12-C13-C14
48	13	315	A86	C3-C4-C5-C6
48	18	213	A86	C3-C4-C5-C6
48	18	214	A86	C3-C4-C5-C6
48	33	315	A86	C3-C4-C5-C6
43	D	410	LHG	C3-O3-P-O6
43	d	408	LHG	C3-O3-P-O6
43	21	217	LHG	C3-O3-P-O6
43	37	321	LHG	C3-O3-P-O6
41	17	317	LMG	C11-C12-C13-C14
43	D	409	LHG	C18-C19-C20-C21
43	d	407	LHG	C18-C19-C20-C21
37	C	506	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
37	c	506	CLA	C2-C3-C5-C6
37	38	209	CLA	C2-C3-C5-C6
37	C	504	CLA	O1A-CGA-O2A-C1
37	c	504	CLA	O1A-CGA-O2A-C1
43	D	409	LHG	C4-O6-P-O5
43	D	410	LHG	C3-O3-P-O4
43	d	407	LHG	C4-O6-P-O5
43	d	408	LHG	C3-O3-P-O4
43	19	314	LHG	C3-O3-P-O5
43	21	217	LHG	C4-O6-P-O5
43	37	321	LHG	C4-O6-P-O5
43	39	314	LHG	C3-O3-P-O5
38	a	406	PHO	C16-C17-C18-C20
37	37	308	CLA	C2C-C3C-CAC-CBC
41	B	520	LMG	O6-C1-O1-C7
41	b	519	LMG	O6-C1-O1-C7
37	21	204	CLA	C5-C6-C7-C8
37	41	204	CLA	C5-C6-C7-C8
37	13	307	CLA	CBA-CGA-O2A-C1
37	20	301	CLA	CBA-CGA-O2A-C1
37	33	307	CLA	CBA-CGA-O2A-C1
37	40	203	CLA	CBA-CGA-O2A-C1
41	B	520	LMG	O6-C5-C6-O5
43	D	410	LHG	O6-C4-C5-C6
43	d	408	LHG	O6-C4-C5-C6
37	15	305	CLA	C2A-CAA-CBA-CGA
37	35	305	CLA	C2A-CAA-CBA-CGA
41	c	518	LMG	C14-C15-C16-C17
37	16	303	CLA	O1D-CGD-O2D-CED
41	C	518	LMG	C14-C15-C16-C17
44	C	517	DGD	CBB-CCB-CDB-CEB
44	c	517	DGD	CBB-CCB-CDB-CEB
37	35	303	CLA	O1A-CGA-O2A-C1
41	11	316	LMG	C14-C15-C16-C17
41	31	316	LMG	C14-C15-C16-C17
44	J	101	DGD	C8A-C9A-CAA-CBA
37	B	501	CLA	CAD-CBD-CGD-O1D
37	B	503	CLA	CAD-CBD-CGD-O1D
37	B	507	CLA	CAD-CBD-CGD-O1D
37	b	501	CLA	CAD-CBD-CGD-O1D
37	b	503	CLA	CAD-CBD-CGD-O1D
37	b	507	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
37	12	204	CLA	CAD-CBD-CGD-O1D
37	13	303	CLA	CAD-CBD-CGD-O1D
37	14	302	CLA	CAD-CBD-CGD-O1D
37	15	303	CLA	CAD-CBD-CGD-O1D
37	18	211	CLA	CAD-CBD-CGD-O1D
37	19	303	CLA	CAD-CBD-CGD-O1D
37	32	205	CLA	CAD-CBD-CGD-O1D
37	33	303	CLA	CAD-CBD-CGD-O1D
37	34	302	CLA	CAD-CBD-CGD-O1D
37	35	303	CLA	CAD-CBD-CGD-O1D
37	38	206	CLA	CAD-CBD-CGD-O1D
37	38	211	CLA	CAD-CBD-CGD-O1D
37	39	303	CLA	CAD-CBD-CGD-O1D
48	16	311	A86	C26-C27-C29-C30
48	36	311	A86	C26-C27-C29-C30
44	c	517	DGD	C1A-C2A-C3A-C4A
37	14	308	CLA	C13-C15-C16-C17
37	34	308	CLA	C13-C15-C16-C17
44	j	101	DGD	C8A-C9A-CAA-CBA
37	19	301	CLA	O1A-CGA-O2A-C1
37	39	301	CLA	O1A-CGA-O2A-C1
44	C	517	DGD	C1A-C2A-C3A-C4A
44	C	516	DGD	C4D-C5D-C6D-O5D
44	c	516	DGD	C4D-C5D-C6D-O5D
37	C	504	CLA	CBA-CGA-O2A-C1
37	c	504	CLA	CBA-CGA-O2A-C1
37	D	406	CLA	C16-C17-C18-C19
37	32	206	CLA	C4-C3-C5-C6
37	38	204	CLA	C4-C3-C5-C6
37	B	516	CLA	C6-C7-C8-C10
37	B	516	CLA	C11-C10-C8-C7
37	C	503	CLA	C11-C12-C13-C15
37	C	508	CLA	C6-C7-C8-C10
37	D	402	CLA	C12-C13-C15-C16
37	Z	101	CLA	C12-C13-C15-C16
37	W	101	CLA	C11-C10-C8-C7
37	b	516	CLA	C6-C7-C8-C10
37	b	516	CLA	C11-C10-C8-C7
37	c	503	CLA	C11-C12-C13-C15
37	c	508	CLA	C6-C7-C8-C10
37	d	401	CLA	C12-C13-C15-C16
37	z	101	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
37	w	101	CLA	C11-C10-C8-C7
37	12	203	CLA	C2-C3-C5-C6
37	13	303	CLA	C6-C7-C8-C10
37	14	308	CLA	C6-C7-C8-C10
37	21	206	CLA	C11-C12-C13-C15
37	32	204	CLA	C2-C3-C5-C6
37	41	206	CLA	C11-C12-C13-C15
38	A	404	PHO	C6-C7-C8-C10
38	a	406	PHO	C6-C7-C8-C10
41	C	518	LMG	C28-C29-C30-C31
41	c	518	LMG	C28-C29-C30-C31
43	21	217	LHG	O6-C4-C5-O7
43	37	321	LHG	O6-C4-C5-O7
41	b	519	LMG	O6-C5-C6-O5
37	15	303	CLA	O1A-CGA-O2A-C1
41	36	314	LMG	C13-C14-C15-C16
44	j	101	DGD	CBB-CCB-CDB-CEB
48	13	312	A86	C11-C10-C9-C8
48	33	312	A86	C11-C10-C9-C8
48	37	319	A86	C3-C4-C5-C6
48	38	214	A86	C3-C4-C5-C6
41	16	316	LMG	C13-C14-C15-C16
43	17	316	LHG	C10-C11-C12-C13
44	J	101	DGD	CBB-CCB-CDB-CEB
37	15	308	CLA	C13-C15-C16-C17
37	36	303	CLA	O1D-CGD-O2D-CED
43	D	409	LHG	C26-C27-C28-C29
43	d	407	LHG	C26-C27-C28-C29
43	37	315	LHG	C10-C11-C12-C13
44	C	517	DGD	C6B-C7B-C8B-C9B
37	20	301	CLA	O1A-CGA-O2A-C1
37	40	203	CLA	O1A-CGA-O2A-C1
37	19	302	CLA	O1D-CGD-O2D-CED
41	11	316	LMG	C31-C32-C33-C34
43	D	410	LHG	C31-C32-C33-C34
43	d	408	LHG	C31-C32-C33-C34
44	c	517	DGD	C6B-C7B-C8B-C9B
37	A	403	CLA	C2A-CAA-CBA-CGA
37	C	506	CLA	C16-C17-C18-C19
37	c	506	CLA	C16-C17-C18-C19
37	d	404	CLA	C16-C17-C18-C19
40	B	519	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
41	31	316	LMG	C31-C32-C33-C34
37	17	302	CLA	CAA-CBA-CGA-O2A
37	37	301	CLA	CAA-CBA-CGA-O2A
40	L	101	SQD	C16-C17-C18-C19
41	32	201	LMG	O6-C5-C6-O5
43	D	409	LHG	C4-C5-C6-O8
43	D	411	LHG	C4-C5-C6-O8
43	a	412	LHG	C4-C5-C6-O8
44	J	101	DGD	C4B-C5B-C6B-C7B
44	j	101	DGD	C4B-C5B-C6B-C7B
47	33	309	KC1	CAA-CBA-CGA-O2A
40	36	315	SQD	O6-C44-C45-O47
41	A	408	LMG	O7-C8-C9-O8
41	a	410	LMG	O7-C8-C9-O8
43	39	314	LHG	C14-C15-C16-C17
37	12	210	CLA	O1D-CGD-O2D-CED
37	14	301	CLA	C4-C3-C5-C6
37	18	202	CLA	C4-C3-C5-C6
37	18	204	CLA	C4-C3-C5-C6
37	34	301	CLA	C4-C3-C5-C6
37	38	202	CLA	C4-C3-C5-C6
40	A	407	SQD	C25-C26-C27-C28
40	a	409	SQD	C25-C26-C27-C28
41	L	102	LMG	C35-C36-C37-C38
41	l	101	LMG	C35-C36-C37-C38
37	13	307	CLA	C2-C3-C5-C6
37	33	307	CLA	C2-C3-C5-C6
47	13	309	KC1	CAA-CBA-CGA-O1A
47	33	309	KC1	CAA-CBA-CGA-O1A
47	20	305	KC1	O1D-CGD-O2D-CED
41	C	518	LMG	C36-C37-C38-C39
41	c	518	LMG	C36-C37-C38-C39
37	B	505	CLA	C11-C12-C13-C14
37	B	514	CLA	C14-C13-C15-C16
37	B	516	CLA	C6-C7-C8-C9
37	C	509	CLA	C6-C7-C8-C9
37	D	406	CLA	C11-C12-C13-C14
37	D	406	CLA	C14-C13-C15-C16
37	W	101	CLA	C6-C7-C8-C9
37	W	102	CLA	C11-C12-C13-C14
37	b	505	CLA	C11-C12-C13-C14
37	b	514	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
37	b	516	CLA	C6-C7-C8-C9
37	c	509	CLA	C6-C7-C8-C9
37	d	404	CLA	C11-C12-C13-C14
37	d	404	CLA	C14-C13-C15-C16
37	w	101	CLA	C6-C7-C8-C9
37	14	308	CLA	C14-C13-C15-C16
37	15	308	CLA	C14-C13-C15-C16
37	31	301	CLA	C11-C12-C13-C14
37	34	308	CLA	C14-C13-C15-C16
39	B	525	BCR	C22-C23-C24-C25
39	D	407	BCR	C6-C7-C8-C9
39	b	524	BCR	C22-C23-C24-C25
39	d	405	BCR	C6-C7-C8-C9
37	33	307	CLA	O1A-CGA-O2A-C1
37	38	208	CLA	CBD-CGD-O2D-CED
40	16	315	SQD	C32-C33-C34-C35
40	40	202	SQD	C32-C33-C34-C35
37	C	503	CLA	C16-C17-C18-C19
37	c	503	CLA	C16-C17-C18-C19
44	C	516	DGD	O6D-C5D-C6D-O5D
44	c	516	DGD	O6D-C5D-C6D-O5D
41	12	201	LMG	C14-C15-C16-C17
37	13	307	CLA	O1A-CGA-O2A-C1
37	38	209	CLA	O1A-CGA-O2A-C1
47	40	207	KC1	O1D-CGD-O2D-CED
37	39	303	CLA	C5-C6-C7-C8
41	b	520	LMG	C8-C9-O8-C28
50	21	212	DD6	C1-C24-C25-C26
50	41	212	DD6	C1-C24-C25-C26
41	D	412	LMG	C13-C14-C15-C16
47	13	309	KC1	CAA-CBA-CGA-O2A
48	14	311	A86	C-C1-C24-C25
48	34	311	A86	C-C1-C24-C25
37	19	303	CLA	C5-C6-C7-C8
41	d	409	LMG	C13-C14-C15-C16
43	21	201	LHG	C15-C16-C17-C18
51	19	315	LMU	C4-C5-C6-C7
51	39	315	LMU	C4-C5-C6-C7
41	B	521	LMG	C8-C9-O8-C28
41	c	518	LMG	C39-C40-C41-C42
37	Z	101	CLA	C5-C6-C7-C8
37	z	101	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
41	C	518	LMG	C39-C40-C41-C42
45	D	404	PL9	C20-C19-C21-C22
45	d	402	PL9	C20-C19-C21-C22
40	B	519	SQD	O10-C23-O48-C46
40	16	315	SQD	C17-C18-C19-C20
40	40	202	SQD	C17-C18-C19-C20
41	32	201	LMG	C14-C15-C16-C17
41	36	314	LMG	C16-C17-C18-C19
41	16	316	LMG	C16-C17-C18-C19
37	16	301	CLA	C15-C16-C17-C18
37	36	301	CLA	C15-C16-C17-C18
40	L	101	SQD	O10-C23-O48-C46
43	B	523	LHG	C18-C19-C20-C21
40	16	315	SQD	C10-C11-C12-C13
40	40	202	SQD	C10-C11-C12-C13
43	B	523	LHG	O6-C4-C5-C6
43	D	411	LHG	O6-C4-C5-C6
43	a	412	LHG	O6-C4-C5-C6
43	b	522	LHG	O6-C4-C5-C6
37	a	403	CLA	C2A-CAA-CBA-CGA
37	B	509	CLA	C2-C1-O2A-CGA
37	b	509	CLA	C2-C1-O2A-CGA
37	16	307	CLA	C2-C1-O2A-CGA
37	17	309	CLA	C2-C1-O2A-CGA
37	36	307	CLA	C2-C1-O2A-CGA
37	37	308	CLA	C2-C1-O2A-CGA
40	L	101	SQD	C9-C10-C11-C12
41	C	518	LMG	C35-C36-C37-C38
41	c	518	LMG	C35-C36-C37-C38
43	b	522	LHG	C18-C19-C20-C21
40	B	519	SQD	C9-C10-C11-C12
44	H	102	DGD	C4A-C5A-C6A-C7A
48	32	215	A86	O5-C38-O4-C34
37	33	301	CLA	CAA-CBA-CGA-O2A
37	B	511	CLA	O1A-CGA-O2A-C1
37	b	511	CLA	O1A-CGA-O2A-C1
44	h	102	DGD	C4A-C5A-C6A-C7A
48	12	214	A86	O5-C38-O4-C34
41	32	201	LMG	C11-C12-C13-C14
48	11	314	A86	C12-C11-C13-C14
48	12	202	A86	C12-C11-C13-C14
48	12	215	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
48	14	314	A86	C12-C11-C13-C14
48	15	314	A86	C12-C11-C13-C14
48	17	315	A86	C12-C11-C13-C14
48	20	311	A86	C12-C11-C13-C14
48	31	314	A86	C12-C11-C13-C14
48	32	203	A86	C12-C11-C13-C14
48	32	216	A86	C12-C11-C13-C14
48	34	314	A86	C12-C11-C13-C14
48	35	314	A86	C12-C11-C13-C14
48	37	314	A86	C12-C11-C13-C14
48	40	213	A86	C12-C11-C13-C14
41	12	201	LMG	C11-C12-C13-C14
37	34	307	CLA	O1D-CGD-O2D-CED
37	39	302	CLA	O1D-CGD-O2D-CED
37	15	303	CLA	CBA-CGA-O2A-C1
37	35	303	CLA	CBA-CGA-O2A-C1
43	19	314	LHG	O6-C4-C5-O7
43	39	314	LHG	O6-C4-C5-O7
37	14	307	CLA	O1D-CGD-O2D-CED
37	12	205	CLA	C4-C3-C5-C6
37	17	304	CLA	C4-C3-C5-C6
37	17	302	CLA	C2C-C3C-CAC-CBC
39	B	518	BCR	C23-C24-C25-C30
39	C	514	BCR	C1-C6-C7-C8
39	C	515	BCR	C1-C6-C7-C8
39	H	101	BCR	C23-C24-C25-C26
39	b	518	BCR	C23-C24-C25-C30
39	c	514	BCR	C1-C6-C7-C8
39	c	515	BCR	C1-C6-C7-C8
39	h	101	BCR	C23-C24-C25-C26
43	d	408	LHG	C25-C26-C27-C28
43	D	410	LHG	C25-C26-C27-C28
41	b	519	LMG	C28-C29-C30-C31
37	13	301	CLA	CAA-CBA-CGA-O2A
43	19	314	LHG	C14-C15-C16-C17
37	32	202	CLA	C8-C10-C11-C12
37	11	308	CLA	C8-C10-C11-C12
37	D	402	CLA	C2A-CAA-CBA-CGA
37	d	401	CLA	C2A-CAA-CBA-CGA
44	C	517	DGD	C2D-C1D-O3G-C3G
44	c	517	DGD	C2D-C1D-O3G-C3G
50	20	312	DD6	C24-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
50	40	214	DD6	C24-C1-C2-C3
40	17	301	SQD	O6-C44-C45-O47
43	B	523	LHG	C4-O6-P-O3
43	b	522	LHG	C4-O6-P-O3
43	17	316	LHG	C3-O3-P-O6
43	17	316	LHG	C4-O6-P-O3
43	37	315	LHG	C3-O3-P-O6
43	37	315	LHG	C4-O6-P-O3
41	B	520	LMG	C28-C29-C30-C31
41	11	316	LMG	C12-C13-C14-C15
41	16	316	LMG	C29-C30-C31-C32
41	36	314	LMG	C29-C30-C31-C32
37	37	308	CLA	C4C-C3C-CAC-CBC
40	B	519	SQD	C15-C16-C17-C18
40	L	101	SQD	C15-C16-C17-C18
41	B	521	LMG	C21-C22-C23-C24
41	31	316	LMG	C12-C13-C14-C15
38	a	406	PHO	C8-C10-C11-C12
37	B	505	CLA	C11-C12-C13-C15
37	B	512	CLA	C11-C10-C8-C7
37	b	505	CLA	C11-C12-C13-C15
37	b	512	CLA	C11-C10-C8-C7
37	b	523	CLA	C11-C12-C13-C15
37	12	204	CLA	C6-C7-C8-C10
37	18	204	CLA	C6-C7-C8-C10
37	32	205	CLA	C6-C7-C8-C10
37	38	204	CLA	C6-C7-C8-C10
41	b	520	LMG	C21-C22-C23-C24
40	40	202	SQD	O10-C23-O48-C46
37	B	502	CLA	C14-C13-C15-C16
37	B	512	CLA	C11-C10-C8-C9
37	B	516	CLA	C11-C10-C8-C9
37	C	502	CLA	C11-C12-C13-C14
37	C	508	CLA	C6-C7-C8-C9
37	C	511	CLA	C6-C7-C8-C9
37	b	502	CLA	C14-C13-C15-C16
37	b	512	CLA	C11-C10-C8-C9
37	b	516	CLA	C11-C10-C8-C9
37	c	502	CLA	C11-C12-C13-C14
37	c	508	CLA	C6-C7-C8-C9
37	c	511	CLA	C6-C7-C8-C9
37	14	308	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	19	302	CLA	C6-C7-C8-C9
37	34	308	CLA	C6-C7-C8-C9
37	35	308	CLA	C14-C13-C15-C16
37	39	302	CLA	C6-C7-C8-C9
38	A	404	PHO	C8-C10-C11-C12
48	11	319	A86	C1-C2-C3-C4
48	20	309	A86	C24-C25-C26-C27
48	21	213	A86	C11-C10-C9-C8
48	31	311	A86	C1-C2-C3-C4
48	31	319	A86	C1-C2-C3-C4
48	40	211	A86	C24-C25-C26-C27
48	41	213	A86	C11-C10-C9-C8
47	21	203	KC1	CAA-CBA-CGA-O1A
47	41	203	KC1	CAA-CBA-CGA-O1A
40	16	315	SQD	O10-C23-O48-C46
37	17	302	CLA	C4C-C3C-CAC-CBC
41	b	519	LMG	C21-C22-C23-C24
41	B	520	LMG	C21-C22-C23-C24
48	12	202	A86	C-C1-C24-C25
48	32	203	A86	C-C1-C24-C25
48	35	316	A86	C-C1-C24-C25
44	J	101	DGD	C2B-C3B-C4B-C5B
37	38	209	CLA	CBA-CGA-O2A-C1
43	39	314	LHG	O1-C1-C2-C3
43	D	411	LHG	C2-C3-O3-P
43	a	412	LHG	C2-C3-O3-P
48	17	315	A86	C2-C1-C24-C25
44	j	101	DGD	C2B-C3B-C4B-C5B
37	a	404	CLA	C3-C5-C6-C7
37	16	307	CLA	C12-C13-C15-C16
37	36	307	CLA	C12-C13-C15-C16
43	19	314	LHG	C1-C2-C3-O3
43	39	314	LHG	C1-C2-C3-O3
43	37	321	LHG	C25-C26-C27-C28
37	39	302	CLA	O1A-CGA-O2A-C1
37	C	510	CLA	CBD-CGD-O2D-CED
37	B	513	CLA	C16-C17-C18-C19
37	b	513	CLA	C16-C17-C18-C19
37	B	511	CLA	CBA-CGA-O2A-C1
37	b	511	CLA	CBA-CGA-O2A-C1
37	39	302	CLA	CBA-CGA-O2A-C1
43	D	409	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
43	d	407	LHG	C24-C23-O8-C6
43	21	217	LHG	C25-C26-C27-C28
47	32	207	KC1	C2B-C3B-CAB-CBB
37	c	510	CLA	CBD-CGD-O2D-CED
41	12	201	LMG	O6-C5-C6-O5
47	41	203	KC1	CAA-CBA-CGA-O2A
37	11	308	CLA	C13-C15-C16-C17
37	32	202	CLA	C13-C15-C16-C17
37	19	301	CLA	C2A-CAA-CBA-CGA
37	32	204	CLA	C2A-CAA-CBA-CGA
37	38	206	CLA	C2A-CAA-CBA-CGA
37	39	301	CLA	C2A-CAA-CBA-CGA
37	d	404	CLA	C10-C11-C12-C13
48	11	311	A86	C1-C2-C3-C4
48	12	202	A86	C3-C4-C5-C6
48	12	216	A86	C3-C4-C5-C6
48	14	313	A86	C11-C10-C9-C8
48	32	203	A86	C3-C4-C5-C6
48	32	217	A86	C3-C4-C5-C6
48	34	313	A86	C11-C10-C9-C8
48	37	319	A86	C24-C25-C26-C27
50	21	216	DD6	C11-C10-C9-C8
50	41	216	DD6	C11-C10-C9-C8
40	A	407	SQD	C9-C10-C11-C12
43	B	523	LHG	C10-C11-C12-C13
43	b	522	LHG	C10-C11-C12-C13
43	41	201	LHG	O6-C4-C5-C6
37	D	401	CLA	C3-C5-C6-C7
37	C	503	CLA	O1A-CGA-O2A-C1
37	D	406	CLA	C10-C11-C12-C13
40	a	409	SQD	C9-C10-C11-C12
44	c	517	DGD	C7B-C8B-C9B-CAB
47	21	203	KC1	CAA-CBA-CGA-O2A
43	21	201	LHG	O6-C4-C5-O7
43	21	217	LHG	C12-C13-C14-C15
44	C	517	DGD	C7B-C8B-C9B-CAB
37	c	503	CLA	O1A-CGA-O2A-C1
37	13	303	CLA	O1A-CGA-O2A-C1
37	19	302	CLA	O1A-CGA-O2A-C1
43	37	321	LHG	C12-C13-C14-C15
47	16	308	KC1	C4B-C3B-CAB-CBB
47	18	210	KC1	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
47	20	305	KC1	C4B-C3B-CAB-CBB
47	36	308	KC1	C4B-C3B-CAB-CBB
47	38	210	KC1	C4B-C3B-CAB-CBB
47	40	207	KC1	C4B-C3B-CAB-CBB
40	A	407	SQD	C19-C20-C21-C22
45	D	404	PL9	C28-C29-C31-C32
45	d	402	PL9	C28-C29-C31-C32
37	37	301	CLA	C2C-C3C-CAC-CBC
40	a	409	SQD	C19-C20-C21-C22
38	D	403	PHO	C15-C16-C17-C18
38	a	405	PHO	C15-C16-C17-C18
37	15	308	CLA	C2-C1-O2A-CGA
48	38	215	A86	C33-C34-O4-C38
37	16	301	CLA	C16-C17-C18-C19
37	36	301	CLA	C16-C17-C18-C19
37	12	203	CLA	C2A-CAA-CBA-CGA
37	18	206	CLA	C2A-CAA-CBA-CGA
37	21	205	CLA	C2A-CAA-CBA-CGA
37	41	205	CLA	C2A-CAA-CBA-CGA
41	17	317	LMG	O7-C8-C9-O8
41	37	316	LMG	O7-C8-C9-O8
43	D	409	LHG	O7-C5-C6-O8
43	d	407	LHG	O7-C5-C6-O8
37	19	302	CLA	CBA-CGA-O2A-C1
37	B	509	CLA	C3A-C2A-CAA-CBA
37	C	501	CLA	C3A-C2A-CAA-CBA
37	b	509	CLA	C3A-C2A-CAA-CBA
37	c	501	CLA	C3A-C2A-CAA-CBA
37	12	204	CLA	C3A-C2A-CAA-CBA
37	13	301	CLA	C3A-C2A-CAA-CBA
37	32	205	CLA	C3A-C2A-CAA-CBA
37	33	301	CLA	C3A-C2A-CAA-CBA
37	21	205	CLA	CAA-CBA-CGA-O1A
37	41	205	CLA	CAA-CBA-CGA-O1A
37	18	208	CLA	CBD-CGD-O2D-CED
37	14	303	CLA	CAA-CBA-CGA-O2A
37	34	303	CLA	CAA-CBA-CGA-O2A
37	37	301	CLA	C4C-C3C-CAC-CBC
48	14	315	A86	C3-C4-C5-C6
48	17	320	A86	C24-C25-C26-C27
48	34	315	A86	C3-C4-C5-C6
48	11	313	A86	O-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
48	12	213	A86	O-C13-C14-C15
48	14	316	A86	O-C13-C14-C15
48	17	312	A86	O-C13-C14-C15
48	17	314	A86	O-C13-C14-C15
48	18	213	A86	O-C13-C14-C15
48	18	214	A86	O-C13-C14-C15
48	20	309	A86	O-C13-C14-C15
48	31	313	A86	O-C13-C14-C15
48	32	214	A86	O-C13-C14-C15
48	33	314	A86	O-C13-C14-C15
48	34	316	A86	O-C13-C14-C15
48	37	313	A86	O-C13-C14-C15
48	38	213	A86	O-C13-C14-C15
48	38	214	A86	O-C13-C14-C15
48	38	215	A86	O-C13-C14-C15
48	40	211	A86	O-C13-C14-C15
43	37	321	LHG	C10-C11-C12-C13
37	14	302	CLA	C4-C3-C5-C6
37	34	302	CLA	C4-C3-C5-C6
44	J	101	DGD	O6E-C5E-C6E-O5E
40	L	101	SQD	C11-C10-C9-C8
43	21	217	LHG	C10-C11-C12-C13
45	D	404	PL9	C4-C3-C7-C8
45	d	402	PL9	C4-C3-C7-C8
40	B	519	SQD	C11-C10-C9-C8
44	j	101	DGD	O6E-C5E-C6E-O5E
37	C	504	CLA	C11-C10-C8-C9
37	Z	101	CLA	C14-C13-C15-C16
37	c	504	CLA	C11-C10-C8-C9
37	z	101	CLA	C14-C13-C15-C16
37	11	308	CLA	C11-C12-C13-C14
37	32	202	CLA	C11-C12-C13-C14
46	F	101	HEM	C3D-CAD-CBD-CGD
46	f	101	HEM	C3D-CAD-CBD-CGD
46	F	101	HEM	CAA-CBA-CGA-O1A
46	f	101	HEM	CAA-CBA-CGA-O1A
41	11	316	LMG	C29-C28-O8-C9
41	31	316	LMG	C29-C28-O8-C9
41	a	410	LMG	C40-C41-C42-C43
39	b	524	BCR	C16-C17-C18-C36
40	16	315	SQD	C44-C45-C46-O48
40	40	202	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
41	17	317	LMG	C7-C8-C9-O8
41	37	316	LMG	C7-C8-C9-O8
48	16	313	A86	C25-C26-C27-C28
48	40	201	A86	C25-C26-C27-C28
50	21	212	DD6	C4-C5-C6-C7
50	41	212	DD6	C4-C5-C6-C7
37	20	303	CLA	C3-C5-C6-C7
37	40	205	CLA	C3-C5-C6-C7
41	A	408	LMG	C40-C41-C42-C43
37	14	307	CLA	C2A-CAA-CBA-CGA
37	34	307	CLA	C2A-CAA-CBA-CGA
37	37	306	CLA	C2A-CAA-CBA-CGA
38	D	403	PHO	C2A-CAA-CBA-CGA
38	a	405	PHO	C2A-CAA-CBA-CGA
37	b	511	CLA	O1D-CGD-O2D-CED
37	D	406	CLA	C16-C17-C18-C20
37	d	404	CLA	C16-C17-C18-C20
48	18	215	A86	C33-C34-O4-C38
37	C	503	CLA	CBA-CGA-O2A-C1
37	c	503	CLA	CBA-CGA-O2A-C1
48	15	316	A86	C-C1-C24-C25
37	C	510	CLA	O1D-CGD-O2D-CED
43	37	315	LHG	C26-C27-C28-C29
47	11	306	KC1	CBD-CGD-O2D-CED
43	17	316	LHG	C26-C27-C28-C29
48	37	314	A86	C2-C1-C24-C25
37	C	510	CLA	C4-C3-C5-C6
37	c	510	CLA	C4-C3-C5-C6
37	13	301	CLA	C4-C3-C5-C6
37	33	301	CLA	C4-C3-C5-C6
37	B	501	CLA	C1A-C2A-CAA-CBA
37	B	506	CLA	C1A-C2A-CAA-CBA
37	B	511	CLA	C1A-C2A-CAA-CBA
37	b	501	CLA	C1A-C2A-CAA-CBA
37	b	506	CLA	C1A-C2A-CAA-CBA
37	b	511	CLA	C1A-C2A-CAA-CBA
37	14	308	CLA	C1A-C2A-CAA-CBA
37	17	302	CLA	C1A-C2A-CAA-CBA
37	17	307	CLA	C1A-C2A-CAA-CBA
37	18	209	CLA	C1A-C2A-CAA-CBA
37	19	304	CLA	C1A-C2A-CAA-CBA
37	21	202	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	34	308	CLA	C1A-C2A-CAA-CBA
37	37	301	CLA	C1A-C2A-CAA-CBA
37	39	304	CLA	C1A-C2A-CAA-CBA
37	41	202	CLA	C1A-C2A-CAA-CBA
43	19	314	LHG	C12-C13-C14-C15
37	17	309	CLA	CAA-CBA-CGA-O2A
37	B	524	CLA	C11-C12-C13-C15
37	11	308	CLA	C11-C10-C8-C7
37	21	208	CLA	C12-C13-C15-C16
37	32	202	CLA	C11-C10-C8-C7
37	37	303	CLA	C2-C3-C5-C6
37	41	208	CLA	C12-C13-C15-C16
47	37	304	KC1	CAA-CBA-CGA-O2A
37	c	510	CLA	O1D-CGD-O2D-CED
41	11	316	LMG	C19-C20-C21-C22
41	31	316	LMG	C19-C20-C21-C22
37	33	303	CLA	O1A-CGA-O2A-C1
46	F	101	HEM	CAD-CBD-CGD-O1D
46	f	101	HEM	CAD-CBD-CGD-O1D
37	B	501	CLA	C16-C17-C18-C20
37	b	501	CLA	C16-C17-C18-C20
37	B	511	CLA	O1D-CGD-O2D-CED
47	37	304	KC1	CAA-CBA-CGA-O1A
37	b	512	CLA	C13-C15-C16-C17
37	20	303	CLA	O1D-CGD-O2D-CED
43	41	201	LHG	O6-C4-C5-O7
46	F	101	HEM	CAD-CBD-CGD-O2D
46	f	101	HEM	CAD-CBD-CGD-O2D
37	40	205	CLA	O1D-CGD-O2D-CED
37	B	512	CLA	C13-C15-C16-C17
37	A	403	CLA	CBA-CGA-O2A-C1
37	a	403	CLA	CBA-CGA-O2A-C1
43	41	201	LHG	C27-C28-C29-C30
43	19	314	LHG	O6-C4-C5-C6
43	21	201	LHG	O6-C4-C5-C6
43	21	217	LHG	O6-C4-C5-C6
43	37	321	LHG	O6-C4-C5-C6
43	39	314	LHG	O6-C4-C5-C6
47	11	304	KC1	C3A-C2A-CAA-CBA
47	12	208	KC1	C3A-C2A-CAA-CBA
47	14	304	KC1	C3A-C2A-CAA-CBA
47	16	305	KC1	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
47	17	305	KC1	C3A-C2A-CAA-CBA
47	21	207	KC1	C3A-C2A-CAA-CBA
47	31	305	KC1	C3A-C2A-CAA-CBA
47	32	209	KC1	C3A-C2A-CAA-CBA
47	34	304	KC1	C3A-C2A-CAA-CBA
47	36	305	KC1	C3A-C2A-CAA-CBA
47	37	304	KC1	C3A-C2A-CAA-CBA
47	41	207	KC1	C3A-C2A-CAA-CBA
43	21	201	LHG	C27-C28-C29-C30
37	16	307	CLA	C14-C13-C15-C16
37	36	307	CLA	C14-C13-C15-C16
37	20	307	CLA	CAA-CBA-CGA-O2A
37	21	205	CLA	CAA-CBA-CGA-O2A
37	40	209	CLA	CAA-CBA-CGA-O2A
37	41	205	CLA	CAA-CBA-CGA-O2A
37	37	308	CLA	CAA-CBA-CGA-O2A
44	H	102	DGD	C5A-C6A-C7A-C8A
44	h	102	DGD	C5A-C6A-C7A-C8A
41	B	521	LMG	C28-C29-C30-C31
41	b	520	LMG	C28-C29-C30-C31
37	20	307	CLA	CAA-CBA-CGA-O1A
37	40	209	CLA	CAA-CBA-CGA-O1A
37	a	403	CLA	O1A-CGA-O2A-C1
44	j	101	DGD	C4A-C5A-C6A-C7A
37	B	511	CLA	CBD-CGD-O2D-CED
47	31	307	KC1	CBD-CGD-O2D-CED
48	11	313	A86	C13-C14-C15-C16
48	11	314	A86	C13-C14-C15-C16
48	12	213	A86	C13-C14-C15-C16
48	12	215	A86	C13-C14-C15-C16
48	12	216	A86	C13-C14-C15-C16
48	13	311	A86	C13-C14-C15-C16
48	14	311	A86	C13-C14-C15-C16
48	14	314	A86	C13-C14-C15-C16
48	16	310	A86	C13-C14-C15-C16
48	16	313	A86	C25-C26-C27-C29
48	16	314	A86	C13-C14-C15-C16
48	17	313	A86	C13-C14-C15-C16
48	18	212	A86	C13-C14-C15-C16
48	18	213	A86	C13-C14-C15-C16
48	18	214	A86	C13-C14-C15-C16
48	19	311	A86	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
48	20	309	A86	C13-C14-C15-C16
48	21	214	A86	C13-C14-C15-C16
48	31	313	A86	C13-C14-C15-C16
48	31	314	A86	C13-C14-C15-C16
48	32	214	A86	C13-C14-C15-C16
48	32	216	A86	C13-C14-C15-C16
48	32	217	A86	C13-C14-C15-C16
48	33	311	A86	C13-C14-C15-C16
48	34	311	A86	C13-C14-C15-C16
48	34	314	A86	C13-C14-C15-C16
48	36	310	A86	C13-C14-C15-C16
48	36	313	A86	C13-C14-C15-C16
48	37	312	A86	C13-C14-C15-C16
48	38	212	A86	C13-C14-C15-C16
48	38	213	A86	C13-C14-C15-C16
48	38	214	A86	C13-C14-C15-C16
48	39	311	A86	C13-C14-C15-C16
48	40	201	A86	C25-C26-C27-C29
48	40	211	A86	C13-C14-C15-C16
48	41	214	A86	C13-C14-C15-C16
44	J	101	DGD	C4A-C5A-C6A-C7A
41	D	412	LMG	C4-C5-C6-O5
41	d	409	LMG	C4-C5-C6-O5
40	16	315	SQD	O6-C44-C45-O47
40	40	202	SQD	O6-C44-C45-O47
43	17	316	LHG	O7-C5-C6-O8
43	37	315	LHG	O7-C5-C6-O8
37	b	511	CLA	CBD-CGD-O2D-CED
47	17	305	KC1	CAA-CBA-CGA-O2A
41	L	102	LMG	C30-C31-C32-C33
41	l	101	LMG	C30-C31-C32-C33
39	C	519	BCR	C19-C20-C21-C22
39	c	519	BCR	C19-C20-C21-C22
48	12	217	A86	C3-C4-C5-C6
48	15	316	A86	C24-C25-C26-C27
48	16	311	A86	C3-C4-C5-C6
48	17	313	A86	C3-C4-C5-C6
48	32	218	A86	C3-C4-C5-C6
48	35	316	A86	C24-C25-C26-C27
48	36	311	A86	C3-C4-C5-C6
37	32	213	CLA	CAA-CBA-CGA-O2A
37	A	403	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
43	39	314	LHG	C12-C13-C14-C15
37	D	405	CLA	C13-C15-C16-C17
37	d	403	CLA	C13-C15-C16-C17
48	12	217	A86	C10-C11-C13-C14
48	14	316	A86	C10-C11-C13-C14
48	15	314	A86	C10-C11-C13-C14
48	16	313	A86	C10-C11-C13-C14
48	17	310	A86	C10-C11-C13-C14
48	19	313	A86	C10-C11-C13-C14
48	32	218	A86	C10-C11-C13-C14
48	34	316	A86	C10-C11-C13-C14
48	35	314	A86	C10-C11-C13-C14
48	37	309	A86	C10-C11-C13-C14
48	40	201	A86	C10-C11-C13-C14
37	12	212	CLA	CAA-CBA-CGA-O2A
46	F	101	HEM	CAA-CBA-CGA-O2A
46	f	101	HEM	CAA-CBA-CGA-O2A
41	B	521	LMG	C20-C21-C22-C23
41	b	520	LMG	C20-C21-C22-C23
47	17	305	KC1	CAA-CBA-CGA-O1A
37	B	516	CLA	C2-C1-O2A-CGA
37	C	502	CLA	C2-C1-O2A-CGA
37	C	503	CLA	C2-C1-O2A-CGA
37	D	405	CLA	C2-C1-O2A-CGA
37	D	406	CLA	C2-C1-O2A-CGA
37	b	516	CLA	C2-C1-O2A-CGA
37	c	502	CLA	C2-C1-O2A-CGA
37	c	503	CLA	C2-C1-O2A-CGA
37	d	403	CLA	C2-C1-O2A-CGA
37	d	404	CLA	C2-C1-O2A-CGA
37	12	203	CLA	C2-C1-O2A-CGA
37	32	204	CLA	C2-C1-O2A-CGA
37	35	308	CLA	C2-C1-O2A-CGA
37	14	302	CLA	C2-C3-C5-C6
37	34	301	CLA	C2-C3-C5-C6
37	34	302	CLA	C2-C3-C5-C6
37	D	401	CLA	C2C-C3C-CAC-CBC
37	11	301	CLA	C6-C7-C8-C9
37	37	303	CLA	C6-C7-C8-C9
37	a	404	CLA	C2C-C3C-CAC-CBC
43	d	407	LHG	C19-C20-C21-C22
47	14	309	KC1	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
47	15	306	KC1	C1A-C2A-CAA-CBA
47	20	304	KC1	C1A-C2A-CAA-CBA
47	34	309	KC1	C1A-C2A-CAA-CBA
47	35	306	KC1	C1A-C2A-CAA-CBA
47	40	206	KC1	C1A-C2A-CAA-CBA
38	A	404	PHO	CAA-CBA-CGA-O2A
38	a	406	PHO	CAA-CBA-CGA-O2A
43	D	409	LHG	C19-C20-C21-C22
41	D	412	LMG	C34-C35-C36-C37
41	d	409	LMG	C34-C35-C36-C37
37	17	307	CLA	C2A-CAA-CBA-CGA
39	A	410	BCR	C23-C24-C25-C30
39	H	101	BCR	C23-C24-C25-C30
39	K	101	BCR	C23-C24-C25-C30
39	a	413	BCR	C23-C24-C25-C30
39	h	101	BCR	C23-C24-C25-C30
39	y	101	BCR	C23-C24-C25-C30
44	H	102	DGD	O2G-C1B-C2B-C3B
44	h	102	DGD	O2G-C1B-C2B-C3B
43	d	408	LHG	C4-C5-C6-O8
43	19	314	LHG	O1-C1-C2-C3
48	14	312	A86	C11-C10-C9-C8
48	17	312	A86	C3-C4-C5-C6
48	18	215	A86	C3-C4-C5-C6
48	34	312	A86	C11-C10-C9-C8
48	38	215	A86	C3-C4-C5-C6
50	16	312	DD6	C3-C4-C5-C6
50	36	312	DD6	C3-C4-C5-C6
37	C	505	CLA	C4-C3-C5-C6
37	c	505	CLA	C4-C3-C5-C6
48	14	311	A86	C2-C1-C24-C25
48	34	311	A86	C2-C1-C24-C25
37	c	506	CLA	C16-C17-C18-C20
37	14	301	CLA	C2-C3-C5-C6
37	18	202	CLA	C2-C3-C5-C6
37	38	202	CLA	C2-C3-C5-C6
44	C	517	DGD	O1A-C1A-O1G-C1G
44	c	517	DGD	O1A-C1A-O1G-C1G
44	C	517	DGD	C5D-C6D-O5D-C1E
44	c	517	DGD	C5D-C6D-O5D-C1E
37	C	506	CLA	C16-C17-C18-C20
37	14	310	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
37	35	305	CLA	CAA-CBA-CGA-O2A
37	C	505	CLA	C2A-CAA-CBA-CGA
37	c	505	CLA	C2A-CAA-CBA-CGA
37	35	301	CLA	C13-C15-C16-C17
37	14	307	CLA	CBA-CGA-O2A-C1
37	34	307	CLA	CBA-CGA-O2A-C1
40	40	202	SQD	C30-C31-C32-C33
37	B	513	CLA	C3-C5-C6-C7
37	b	513	CLA	C3-C5-C6-C7
37	z	102	CLA	CAA-CBA-CGA-O2A
37	15	305	CLA	CAA-CBA-CGA-O2A
40	16	315	SQD	C30-C31-C32-C33
41	11	317	LMG	C31-C32-C33-C34
41	31	317	LMG	C31-C32-C33-C34
37	11	303	CLA	C4-C3-C5-C6
37	31	304	CLA	C4-C3-C5-C6
37	b	504	CLA	O1D-CGD-O2D-CED
37	37	303	CLA	C6-C7-C8-C10
37	Z	102	CLA	CAA-CBA-CGA-O2A
37	12	212	CLA	CAA-CBA-CGA-O1A
37	21	210	CLA	CAA-CBA-CGA-O2A
37	32	213	CLA	CAA-CBA-CGA-O1A
37	34	310	CLA	CAA-CBA-CGA-O2A
37	C	506	CLA	C15-C16-C17-C18
37	c	506	CLA	C15-C16-C17-C18
40	17	301	SQD	C11-C10-C9-C8
40	36	315	SQD	C11-C10-C9-C8
43	D	410	LHG	O7-C7-C8-C9
44	c	516	DGD	O2G-C1B-C2B-C3B
40	b	521	SQD	O10-C23-O48-C46
37	B	504	CLA	O1D-CGD-O2D-CED
37	C	501	CLA	C5-C6-C7-C8
37	c	501	CLA	C5-C6-C7-C8
41	12	201	LMG	C11-C10-O7-C8
37	18	206	CLA	CAA-CBA-CGA-O2A
37	38	206	CLA	CAA-CBA-CGA-O2A
37	41	210	CLA	CAA-CBA-CGA-O2A
46	V	201	HEM	CAD-CBD-CGD-O2D
46	v	201	HEM	CAD-CBD-CGD-O2D
37	12	209	CLA	CBA-CGA-O2A-C1
37	13	303	CLA	CBA-CGA-O2A-C1
37	32	210	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	C	505	CLA	C15-C16-C17-C18
39	K	101	BCR	C11-C10-C9-C34
39	y	101	BCR	C11-C10-C9-C34
37	14	307	CLA	CAA-CBA-CGA-O2A
37	34	307	CLA	CAA-CBA-CGA-O2A
43	d	408	LHG	O7-C7-C8-C9
44	C	516	DGD	O2G-C1B-C2B-C3B
37	B	504	CLA	C4-C3-C5-C6
37	b	504	CLA	C4-C3-C5-C6
37	c	505	CLA	C15-C16-C17-C18
41	d	409	LMG	C14-C15-C16-C17
37	12	205	CLA	C2-C3-C5-C6
37	13	301	CLA	C2-C3-C5-C6
37	17	304	CLA	C2-C3-C5-C6
37	32	206	CLA	C2-C3-C5-C6
37	33	301	CLA	C2-C3-C5-C6
45	D	404	PL9	C18-C19-C21-C22
45	d	402	PL9	C18-C19-C21-C22
37	B	501	CLA	CAA-CBA-CGA-O1A
37	18	208	CLA	CAA-CBA-CGA-O2A
37	D	402	CLA	C14-C13-C15-C16
37	W	101	CLA	C11-C10-C8-C9
37	d	401	CLA	C14-C13-C15-C16
37	w	101	CLA	C11-C10-C8-C9
37	12	204	CLA	C11-C12-C13-C14
37	17	302	CLA	C11-C12-C13-C14
37	21	208	CLA	C14-C13-C15-C16
37	31	302	CLA	C6-C7-C8-C9
37	37	301	CLA	C11-C12-C13-C14
37	41	208	CLA	C14-C13-C15-C16
38	A	404	PHO	C6-C7-C8-C9
38	a	406	PHO	C6-C7-C8-C9
40	B	522	SQD	O10-C23-O48-C46
41	D	412	LMG	C14-C15-C16-C17
37	20	307	CLA	C3A-C2A-CAA-CBA
37	40	209	CLA	C3A-C2A-CAA-CBA
41	a	410	LMG	C33-C34-C35-C36
47	34	304	KC1	C2C-C3C-CAC-CBC
37	13	305	CLA	CAA-CBA-CGA-O2A
37	16	309	CLA	CAA-CBA-CGA-O2A
37	33	305	CLA	CAA-CBA-CGA-O2A
37	36	309	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
37	39	304	CLA	CAA-CBA-CGA-O2A
37	B	505	CLA	CAD-CBD-CGD-O2D
37	B	506	CLA	CAD-CBD-CGD-O2D
37	C	509	CLA	CAD-CBD-CGD-O2D
37	C	510	CLA	CAD-CBD-CGD-O2D
37	C	512	CLA	CAD-CBD-CGD-O2D
37	W	101	CLA	CAD-CBD-CGD-O2D
37	b	505	CLA	CAD-CBD-CGD-O2D
37	b	506	CLA	CAD-CBD-CGD-O2D
37	c	509	CLA	CAD-CBD-CGD-O2D
37	c	510	CLA	CAD-CBD-CGD-O2D
37	c	512	CLA	CAD-CBD-CGD-O2D
37	w	101	CLA	CAD-CBD-CGD-O2D
37	11	303	CLA	CAD-CBD-CGD-O2D
37	11	307	CLA	CAD-CBD-CGD-O2D
37	12	209	CLA	CAD-CBD-CGD-O2D
37	15	305	CLA	CAD-CBD-CGD-O2D
37	15	307	CLA	CAD-CBD-CGD-O2D
37	18	203	CLA	CAD-CBD-CGD-O2D
37	18	204	CLA	CAD-CBD-CGD-O2D
37	19	302	CLA	CAD-CBD-CGD-O2D
37	20	306	CLA	CAD-CBD-CGD-O2D
37	31	304	CLA	CAD-CBD-CGD-O2D
37	31	308	CLA	CAD-CBD-CGD-O2D
37	32	210	CLA	CAD-CBD-CGD-O2D
37	35	305	CLA	CAD-CBD-CGD-O2D
37	35	307	CLA	CAD-CBD-CGD-O2D
37	38	203	CLA	CAD-CBD-CGD-O2D
37	38	204	CLA	CAD-CBD-CGD-O2D
37	39	302	CLA	CAD-CBD-CGD-O2D
37	40	208	CLA	CAD-CBD-CGD-O2D
38	D	403	PHO	CAD-CBD-CGD-O2D
38	a	405	PHO	CAD-CBD-CGD-O2D
47	13	309	KC1	CAD-CBD-CGD-O2D
47	14	309	KC1	CAD-CBD-CGD-O2D
47	17	308	KC1	CAD-CBD-CGD-O2D
47	20	302	KC1	CAD-CBD-CGD-O2D
47	33	309	KC1	CAD-CBD-CGD-O2D
47	34	309	KC1	CAD-CBD-CGD-O2D
47	37	307	KC1	CAD-CBD-CGD-O2D
47	40	204	KC1	CAD-CBD-CGD-O2D
48	11	312	A86	C28-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
48	14	313	A86	C28-C27-C29-C30
48	31	312	A86	C28-C27-C29-C30
48	34	313	A86	C28-C27-C29-C30
37	16	301	CLA	C16-C17-C18-C20
37	36	301	CLA	C16-C17-C18-C20
37	b	501	CLA	CAA-CBA-CGA-O1A
41	A	408	LMG	C33-C34-C35-C36
43	d	408	LHG	C29-C30-C31-C32
47	14	304	KC1	C2C-C3C-CAC-CBC
51	39	315	LMU	O1'-C1-C2-C3
37	19	304	CLA	CAA-CBA-CGA-O2A
37	21	209	CLA	CAA-CBA-CGA-O2A
37	41	209	CLA	CAA-CBA-CGA-O2A
37	35	307	CLA	CAA-CBA-CGA-O2A
37	38	208	CLA	CAA-CBA-CGA-O2A
41	B	520	LMG	O8-C28-C29-C30
41	b	519	LMG	O8-C28-C29-C30
43	D	410	LHG	C29-C30-C31-C32
43	D	410	LHG	C35-C36-C37-C38
43	d	408	LHG	C35-C36-C37-C38
37	19	303	CLA	C16-C17-C18-C20
37	39	303	CLA	C16-C17-C18-C20
37	z	102	CLA	CAA-CBA-CGA-O1A
37	35	305	CLA	CAA-CBA-CGA-O1A
37	C	510	CLA	C2-C3-C5-C6
37	c	510	CLA	C2-C3-C5-C6
37	C	501	CLA	CAA-CBA-CGA-O2A
37	c	501	CLA	CAA-CBA-CGA-O2A
37	c	505	CLA	CAA-CBA-CGA-O2A
37	15	307	CLA	CAA-CBA-CGA-O2A
48	12	202	A86	C2-C1-C24-C25
48	15	316	A86	C2-C1-C24-C25
48	32	203	A86	C2-C1-C24-C25
48	35	316	A86	C2-C1-C24-C25
51	19	315	LMU	O1'-C1-C2-C3
40	B	519	SQD	C44-C45-C46-O48
40	L	101	SQD	C44-C45-C46-O48
43	D	410	LHG	C4-C5-C6-O8
44	C	516	DGD	C1G-C2G-C3G-O3G
44	H	102	DGD	C1G-C2G-C3G-O3G
44	c	516	DGD	C1G-C2G-C3G-O3G
44	h	102	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
48	12	215	A86	C12-C11-C13-O
48	12	217	A86	C12-C11-C13-O
48	13	313	A86	C12-C11-C13-O
48	17	310	A86	C12-C11-C13-O
48	19	313	A86	C12-C11-C13-O
48	32	216	A86	C12-C11-C13-O
48	32	218	A86	C12-C11-C13-O
48	33	313	A86	C12-C11-C13-O
48	37	309	A86	C12-C11-C13-O
48	39	313	A86	C12-C11-C13-O
50	19	312	DD6	C13-C14-C15-O1
50	39	312	DD6	C13-C14-C15-O1
37	Z	102	CLA	CAA-CBA-CGA-O1A
37	15	305	CLA	CAA-CBA-CGA-O1A
43	17	316	LHG	O6-C4-C5-O7
43	37	315	LHG	O6-C4-C5-O7
37	C	505	CLA	CAA-CBA-CGA-O2A
37	W	102	CLA	CAA-CBA-CGA-O2A
37	b	513	CLA	CAA-CBA-CGA-O2A
37	31	301	CLA	CAA-CBA-CGA-O2A
41	a	410	LMG	C21-C22-C23-C24
41	32	201	LMG	C31-C32-C33-C34
37	21	209	CLA	CAA-CBA-CGA-O1A
37	39	304	CLA	CAA-CBA-CGA-O1A
37	41	209	CLA	CAA-CBA-CGA-O1A
41	A	408	LMG	C21-C22-C23-C24
37	17	302	CLA	O2A-C1-C2-C3
47	17	303	KC1	C4B-C3B-CAB-CBB
47	17	306	KC1	C4B-C3B-CAB-CBB
47	37	302	KC1	C4B-C3B-CAB-CBB
47	37	305	KC1	C4B-C3B-CAB-CBB
37	33	303	CLA	CBA-CGA-O2A-C1
37	B	505	CLA	C2A-CAA-CBA-CGA
37	b	505	CLA	C2A-CAA-CBA-CGA
37	36	307	CLA	C8-C10-C11-C12
41	12	201	LMG	C31-C32-C33-C34
37	B	512	CLA	CAA-CBA-CGA-O2A
37	17	307	CLA	CAA-CBA-CGA-O2A
37	21	206	CLA	CAA-CBA-CGA-O2A
37	37	306	CLA	CAA-CBA-CGA-O2A
37	41	206	CLA	CAA-CBA-CGA-O2A
41	B	521	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
41	C	518	LMG	O7-C10-C11-C12
41	b	520	LMG	O8-C28-C29-C30
41	c	518	LMG	O7-C10-C11-C12
47	37	305	KC1	C2C-C3C-CAC-CBC
47	33	306	KC1	CBD-CGD-O2D-CED
37	B	507	CLA	CHA-CBD-CGD-O1D
37	B	507	CLA	CHA-CBD-CGD-O2D
37	B	511	CLA	CHA-CBD-CGD-O2D
37	B	516	CLA	CHA-CBD-CGD-O1D
37	B	516	CLA	CHA-CBD-CGD-O2D
37	C	504	CLA	CHA-CBD-CGD-O1D
37	C	505	CLA	CHA-CBD-CGD-O2D
37	C	507	CLA	CHA-CBD-CGD-O1D
37	b	507	CLA	CHA-CBD-CGD-O1D
37	b	507	CLA	CHA-CBD-CGD-O2D
37	b	511	CLA	CHA-CBD-CGD-O2D
37	b	516	CLA	CHA-CBD-CGD-O1D
37	b	516	CLA	CHA-CBD-CGD-O2D
37	c	504	CLA	CHA-CBD-CGD-O1D
37	c	505	CLA	CHA-CBD-CGD-O2D
37	c	507	CLA	CHA-CBD-CGD-O1D
37	13	303	CLA	CHA-CBD-CGD-O1D
37	14	302	CLA	CHA-CBD-CGD-O2D
37	15	303	CLA	CHA-CBD-CGD-O1D
37	16	309	CLA	CHA-CBD-CGD-O2D
37	17	307	CLA	CHA-CBD-CGD-O2D
37	17	309	CLA	CHA-CBD-CGD-O1D
37	17	309	CLA	CHA-CBD-CGD-O2D
37	18	208	CLA	CHA-CBD-CGD-O1D
37	18	208	CLA	CHA-CBD-CGD-O2D
37	18	211	CLA	CHA-CBD-CGD-O2D
37	19	301	CLA	CHA-CBD-CGD-O2D
37	21	206	CLA	CHA-CBD-CGD-O1D
37	21	206	CLA	CHA-CBD-CGD-O2D
37	33	303	CLA	CHA-CBD-CGD-O1D
37	34	302	CLA	CHA-CBD-CGD-O2D
37	34	307	CLA	CHA-CBD-CGD-O1D
37	36	309	CLA	CHA-CBD-CGD-O2D
37	37	306	CLA	CHA-CBD-CGD-O2D
37	37	308	CLA	CHA-CBD-CGD-O1D
37	37	308	CLA	CHA-CBD-CGD-O2D
37	38	208	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
37	38	211	CLA	CHA-CBD-CGD-O2D
37	39	301	CLA	CHA-CBD-CGD-O2D
37	41	206	CLA	CHA-CBD-CGD-O1D
37	41	206	CLA	CHA-CBD-CGD-O2D
47	11	309	KC1	CHA-CBD-CGD-O2D
47	18	210	KC1	CHA-CBD-CGD-O1D
47	18	210	KC1	CHA-CBD-CGD-O2D
47	31	309	KC1	CHA-CBD-CGD-O2D
47	38	210	KC1	CHA-CBD-CGD-O1D
47	38	210	KC1	CHA-CBD-CGD-O2D
37	18	206	CLA	CAA-CBA-CGA-O1A
37	19	304	CLA	CAA-CBA-CGA-O1A
37	38	206	CLA	CAA-CBA-CGA-O1A
37	B	513	CLA	CAA-CBA-CGA-O2A
37	b	512	CLA	CAA-CBA-CGA-O2A
37	12	209	CLA	CAA-CBA-CGA-O2A
37	32	210	CLA	CAA-CBA-CGA-O2A
43	21	217	LHG	C28-C29-C30-C31
47	34	304	KC1	C4C-C3C-CAC-CBC
37	C	505	CLA	C2-C3-C5-C6
37	c	505	CLA	C2-C3-C5-C6
43	37	321	LHG	C28-C29-C30-C31
47	17	306	KC1	C2C-C3C-CAC-CBC
37	16	307	CLA	C8-C10-C11-C12
47	14	304	KC1	C4C-C3C-CAC-CBC
43	17	316	LHG	O6-C4-C5-C6
43	37	315	LHG	O6-C4-C5-C6
37	14	310	CLA	CAA-CBA-CGA-O1A
37	34	310	CLA	CAA-CBA-CGA-O1A
37	21	202	CLA	CAA-CBA-CGA-O2A
37	41	202	CLA	CAA-CBA-CGA-O2A
48	21	215	A86	C33-C34-O4-C38
37	21	204	CLA	C10-C11-C12-C13
37	41	204	CLA	C10-C11-C12-C13
37	15	301	CLA	O1A-CGA-O2A-C1
37	35	301	CLA	O1A-CGA-O2A-C1
43	21	217	LHG	O7-C7-C8-C9
48	12	217	A86	C10-C11-C13-O
48	13	313	A86	C10-C11-C13-O
48	14	316	A86	C10-C11-C13-O
48	16	313	A86	C13-C14-C15-O1
48	20	311	A86	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
48	32	218	A86	C10-C11-C13-O
48	33	313	A86	C10-C11-C13-O
48	34	316	A86	C10-C11-C13-O
48	40	201	A86	C13-C14-C15-O1
48	40	213	A86	C13-C14-C15-O1
37	15	301	CLA	C13-C15-C16-C17
41	32	201	LMG	C11-C10-O7-C8
37	16	303	CLA	CAA-CBA-CGA-O2A
37	18	204	CLA	CAA-CBA-CGA-O2A
37	21	208	CLA	CAA-CBA-CGA-O2A
37	36	303	CLA	CAA-CBA-CGA-O2A
37	38	202	CLA	CAA-CBA-CGA-O2A
37	40	203	CLA	CAA-CBA-CGA-O2A
37	41	208	CLA	CAA-CBA-CGA-O2A
43	37	321	LHG	O7-C7-C8-C9
47	13	306	KC1	CBD-CGD-O2D-CED
41	l	101	LMG	C8-C9-O8-C28
37	13	305	CLA	CAA-CBA-CGA-O1A
48	41	215	A86	C33-C34-O4-C38
37	D	402	CLA	C11-C10-C8-C7
37	d	401	CLA	C11-C10-C8-C7
37	17	304	CLA	C6-C7-C8-C10
37	38	204	CLA	C2-C3-C5-C6
37	d	403	CLA	CAA-CBA-CGA-O2A
37	20	301	CLA	CAA-CBA-CGA-O2A
37	21	210	CLA	CAA-CBA-CGA-O1A
37	33	305	CLA	CAA-CBA-CGA-O1A
37	41	210	CLA	CAA-CBA-CGA-O1A
40	36	315	SQD	C34-C35-C36-C37
37	C	503	CLA	C11-C12-C13-C14
37	c	503	CLA	C11-C12-C13-C14
37	12	204	CLA	C6-C7-C8-C9
37	16	306	CLA	C11-C10-C8-C9
37	17	304	CLA	C6-C7-C8-C9
37	32	205	CLA	C6-C7-C8-C9
37	32	205	CLA	C11-C12-C13-C14
37	36	306	CLA	C11-C10-C8-C9
41	C	518	LMG	O9-C10-C11-C12
41	L	102	LMG	C8-C9-O8-C28
41	c	518	LMG	O9-C10-C11-C12
48	13	313	A86	C3-C4-C5-C6
48	33	313	A86	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
48	37	311	A86	C3-C4-C5-C6
48	37	313	A86	C24-C25-C26-C27
50	21	212	DD6	C11-C10-C9-C8
40	17	301	SQD	C34-C35-C36-C37
37	15	301	CLA	CBA-CGA-O2A-C1
37	35	301	CLA	CBA-CGA-O2A-C1
37	B	514	CLA	CAA-CBA-CGA-O2A
37	D	405	CLA	CAA-CBA-CGA-O2A
37	b	514	CLA	CAA-CBA-CGA-O2A
37	15	301	CLA	CAA-CBA-CGA-O2A
37	35	301	CLA	CAA-CBA-CGA-O2A
40	16	315	SQD	C4-C5-C6-S
40	40	202	SQD	C4-C5-C6-S
37	11	301	CLA	O1A-CGA-O2A-C1
37	12	209	CLA	O1A-CGA-O2A-C1
37	17	304	CLA	O1A-CGA-O2A-C1
37	34	307	CLA	O1A-CGA-O2A-C1
37	16	309	CLA	CAA-CBA-CGA-O1A
37	36	309	CLA	CAA-CBA-CGA-O1A
46	V	201	HEM	CAD-CBD-CGD-O1D
46	v	201	HEM	CAD-CBD-CGD-O1D
37	C	501	CLA	C2A-CAA-CBA-CGA
37	c	501	CLA	C2A-CAA-CBA-CGA
37	18	202	CLA	CAA-CBA-CGA-O2A
37	20	306	CLA	CAA-CBA-CGA-O2A
40	17	301	SQD	O47-C7-C8-C9
40	36	315	SQD	O47-C7-C8-C9
37	31	301	CLA	C16-C17-C18-C20
41	A	408	LMG	C22-C23-C24-C25
37	16	301	CLA	C4-C3-C5-C6
37	36	301	CLA	C4-C3-C5-C6
41	a	410	LMG	C22-C23-C24-C25
37	18	204	CLA	C2-C3-C5-C6
37	40	208	CLA	CAA-CBA-CGA-O2A
43	d	408	LHG	C16-C17-C18-C19
37	D	405	CLA	CAA-CBA-CGA-O1A
37	W	102	CLA	CAA-CBA-CGA-O1A
37	C	508	CLA	CBA-CGA-O2A-C1
37	c	508	CLA	CBA-CGA-O2A-C1
37	41	204	CLA	C3-C5-C6-C7
43	D	410	LHG	C16-C17-C18-C19
37	B	509	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	b	509	CLA	C1A-C2A-CAA-CBA
37	12	209	CLA	C1A-C2A-CAA-CBA
37	14	302	CLA	C1A-C2A-CAA-CBA
37	14	303	CLA	C1A-C2A-CAA-CBA
37	14	307	CLA	C1A-C2A-CAA-CBA
37	20	307	CLA	C1A-C2A-CAA-CBA
37	32	210	CLA	C1A-C2A-CAA-CBA
37	34	302	CLA	C1A-C2A-CAA-CBA
37	34	303	CLA	C1A-C2A-CAA-CBA
37	34	307	CLA	C1A-C2A-CAA-CBA
37	37	306	CLA	C1A-C2A-CAA-CBA
37	40	209	CLA	C1A-C2A-CAA-CBA
37	W	102	CLA	C16-C17-C18-C20
37	d	403	CLA	CAA-CBA-CGA-O1A
37	12	209	CLA	CAA-CBA-CGA-O1A
37	14	307	CLA	CAA-CBA-CGA-O1A
37	31	301	CLA	CAA-CBA-CGA-O1A
37	34	307	CLA	CAA-CBA-CGA-O1A
37	41	206	CLA	CAA-CBA-CGA-O1A
37	38	204	CLA	CAA-CBA-CGA-O2A
37	14	307	CLA	O1A-CGA-O2A-C1
37	31	302	CLA	O1A-CGA-O2A-C1
37	32	210	CLA	O1A-CGA-O2A-C1
43	B	523	LHG	C11-C10-C9-C8
37	17	307	CLA	CAA-CBA-CGA-O1A
37	21	206	CLA	CAA-CBA-CGA-O1A
37	38	208	CLA	CAA-CBA-CGA-O1A
43	D	410	LHG	C17-C18-C19-C20
43	b	522	LHG	C11-C10-C9-C8
41	17	317	LMG	O1-C7-C8-C9
41	37	316	LMG	O1-C7-C8-C9
37	31	304	CLA	O1A-CGA-O2A-C1
37	37	303	CLA	O1A-CGA-O2A-C1
37	14	302	CLA	CBD-CGD-O2D-CED
37	34	302	CLA	CBD-CGD-O2D-CED
37	C	512	CLA	C16-C17-C18-C20
37	c	512	CLA	C16-C17-C18-C20
37	15	307	CLA	CAA-CBA-CGA-O1A
37	32	210	CLA	CAA-CBA-CGA-O1A
37	37	306	CLA	CAA-CBA-CGA-O1A
40	a	409	SQD	O49-C7-C8-C9
37	14	301	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	34	301	CLA	C13-C15-C16-C17
43	d	408	LHG	C17-C18-C19-C20
43	39	314	LHG	C29-C30-C31-C32
37	11	303	CLA	O1A-CGA-O2A-C1
41	A	408	LMG	C31-C32-C33-C34
43	19	314	LHG	O9-C7-O7-C5
43	39	314	LHG	O9-C7-O7-C5
37	21	204	CLA	C3-C5-C6-C7
37	C	505	CLA	CAA-CBA-CGA-O1A
37	b	513	CLA	CAA-CBA-CGA-O1A
37	c	505	CLA	CAA-CBA-CGA-O1A
40	A	407	SQD	O49-C7-C8-C9
45	D	408	PL9	C12-C11-C9-C8
45	d	406	PL9	C12-C11-C9-C8
41	a	410	LMG	C31-C32-C33-C34
37	C	508	CLA	O1A-CGA-O2A-C1
37	c	508	CLA	O1A-CGA-O2A-C1
37	16	306	CLA	C10-C11-C12-C13
43	17	316	LHG	C3-O3-P-O5
43	21	201	LHG	C4-O6-P-O5
43	37	315	LHG	C3-O3-P-O5
43	41	201	LHG	C4-O6-P-O5
37	B	512	CLA	CAA-CBA-CGA-O1A
37	B	513	CLA	CAA-CBA-CGA-O1A
37	b	512	CLA	CAA-CBA-CGA-O1A
37	18	208	CLA	CAA-CBA-CGA-O1A
37	21	202	CLA	CAA-CBA-CGA-O1A
37	38	202	CLA	CAA-CBA-CGA-O1A
37	41	202	CLA	CAA-CBA-CGA-O1A
41	D	412	LMG	O9-C10-C11-C12
43	17	316	LHG	O9-C7-C8-C9
43	37	315	LHG	O9-C7-C8-C9
37	36	306	CLA	C10-C11-C12-C13
37	15	303	CLA	C5-C6-C7-C8
37	35	303	CLA	C5-C6-C7-C8
37	c	501	CLA	CAA-CBA-CGA-O1A
37	20	301	CLA	CAA-CBA-CGA-O1A
37	40	203	CLA	CAA-CBA-CGA-O1A
41	B	521	LMG	O10-C28-C29-C30
41	b	520	LMG	O10-C28-C29-C30
41	d	409	LMG	O9-C10-C11-C12
43	21	217	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
41	36	314	LMG	C14-C15-C16-C17
37	34	302	CLA	O1A-CGA-O2A-C1
37	Z	101	CLA	CAA-CBA-CGA-O2A
37	z	101	CLA	CAA-CBA-CGA-O2A
41	16	316	LMG	C14-C15-C16-C17
37	14	305	CLA	CAA-CBA-CGA-O2A
37	34	305	CLA	CAA-CBA-CGA-O2A
37	Z	101	CLA	C2A-CAA-CBA-CGA
37	z	101	CLA	C2A-CAA-CBA-CGA
37	C	501	CLA	CAA-CBA-CGA-O1A
37	18	202	CLA	CAA-CBA-CGA-O1A
43	37	321	LHG	O9-C7-C8-C9
37	14	302	CLA	O1A-CGA-O2A-C1
37	B	502	CLA	C8-C10-C11-C12
37	a	404	CLA	C4C-C3C-CAC-CBC
37	39	309	CLA	CAA-CBA-CGA-O1A
37	35	303	CLA	CAA-CBA-CGA-O2A
37	b	502	CLA	C8-C10-C11-C12
37	15	301	CLA	C8-C10-C11-C12
40	B	522	SQD	O10-C23-C24-C25
40	b	521	SQD	O10-C23-C24-C25
50	41	212	DD6	C11-C10-C9-C8
43	d	407	LHG	C15-C16-C17-C18
43	17	316	LHG	C19-C20-C21-C22
41	L	102	LMG	C4-C5-C6-O5
41	l	101	LMG	C4-C5-C6-O5
38	a	405	PHO	C16-C17-C18-C19
37	D	401	CLA	C4C-C3C-CAC-CBC
37	B	513	CLA	O1D-CGD-O2D-CED
37	B	505	CLA	CAD-CBD-CGD-O1D
37	B	509	CLA	CAD-CBD-CGD-O1D
37	C	502	CLA	CAD-CBD-CGD-O1D
37	C	504	CLA	CAD-CBD-CGD-O1D
37	C	505	CLA	CAD-CBD-CGD-O1D
37	C	506	CLA	CAD-CBD-CGD-O1D
37	b	505	CLA	CAD-CBD-CGD-O1D
37	b	509	CLA	CAD-CBD-CGD-O1D
37	c	502	CLA	CAD-CBD-CGD-O1D
37	c	504	CLA	CAD-CBD-CGD-O1D
37	c	505	CLA	CAD-CBD-CGD-O1D
37	c	506	CLA	CAD-CBD-CGD-O1D
37	12	209	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
37	12	212	CLA	CAD-CBD-CGD-O1D
37	13	307	CLA	CAD-CBD-CGD-O1D
37	15	307	CLA	CAD-CBD-CGD-O1D
37	18	204	CLA	CAD-CBD-CGD-O1D
37	18	206	CLA	CAD-CBD-CGD-O1D
37	32	210	CLA	CAD-CBD-CGD-O1D
37	32	213	CLA	CAD-CBD-CGD-O1D
37	33	307	CLA	CAD-CBD-CGD-O1D
37	35	307	CLA	CAD-CBD-CGD-O1D
48	31	313	A86	C26-C27-C29-C30
37	35	307	CLA	CAA-CBA-CGA-O1A
37	D	402	CLA	C11-C10-C8-C9
37	d	401	CLA	C11-C10-C8-C9
37	18	201	CLA	C14-C13-C15-C16
37	19	302	CLA	C14-C13-C15-C16
37	19	303	CLA	C14-C13-C15-C16
37	39	302	CLA	C14-C13-C15-C16
37	39	303	CLA	C14-C13-C15-C16
43	D	409	LHG	C15-C16-C17-C18
43	37	315	LHG	C19-C20-C21-C22
37	19	309	CLA	CAA-CBA-CGA-O1A
37	21	208	CLA	CAA-CBA-CGA-O1A
37	B	508	CLA	CAA-CBA-CGA-O2A
37	W	101	CLA	CAA-CBA-CGA-O2A
37	b	508	CLA	CAA-CBA-CGA-O2A
37	w	101	CLA	CAA-CBA-CGA-O2A
37	12	205	CLA	CAA-CBA-CGA-O2A
37	21	204	CLA	CAA-CBA-CGA-O2A
37	32	206	CLA	CAA-CBA-CGA-O2A
37	41	204	CLA	CAA-CBA-CGA-O2A
40	16	315	SQD	O47-C7-C8-C9
40	40	202	SQD	O47-C7-C8-C9
41	D	412	LMG	O7-C10-C11-C12
41	d	409	LMG	O7-C10-C11-C12
44	C	517	DGD	CCB-CDB-CEB-CFB
37	d	404	CLA	C5-C6-C7-C8
37	14	308	CLA	C5-C6-C7-C8
37	34	308	CLA	C5-C6-C7-C8
37	39	309	CLA	CAA-CBA-CGA-O2A
44	c	517	DGD	C9A-CAA-CBA-CCA
44	c	517	DGD	CCB-CDB-CEB-CFB
37	41	208	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
44	C	517	DGD	C9A-CAA-CBA-CCA
47	37	305	KC1	C4C-C3C-CAC-CBC
37	c	510	CLA	CAA-CBA-CGA-O2A
37	11	303	CLA	CAA-CBA-CGA-O2A
37	14	308	CLA	CAA-CBA-CGA-O2A
37	17	304	CLA	CAA-CBA-CGA-O2A
37	20	303	CLA	CAA-CBA-CGA-O2A
37	31	304	CLA	CAA-CBA-CGA-O2A
37	33	303	CLA	CAA-CBA-CGA-O2A
37	34	301	CLA	CAA-CBA-CGA-O2A
37	37	303	CLA	CAA-CBA-CGA-O2A
37	40	205	CLA	CAA-CBA-CGA-O2A
37	b	513	CLA	O1D-CGD-O2D-CED
37	D	406	CLA	C5-C6-C7-C8
37	35	301	CLA	C8-C10-C11-C12
43	D	411	LHG	C32-C33-C34-C35
43	19	314	LHG	C29-C30-C31-C32
38	D	403	PHO	C3-C5-C6-C7
38	a	405	PHO	C3-C5-C6-C7
37	16	303	CLA	CAA-CBA-CGA-O1A
43	a	412	LHG	C32-C33-C34-C35
43	21	217	LHG	C35-C36-C37-C38
37	B	507	CLA	C4-C3-C5-C6
37	W	101	CLA	C4-C3-C5-C6
37	b	507	CLA	C4-C3-C5-C6
37	w	101	CLA	C4-C3-C5-C6
37	11	301	CLA	C4-C3-C5-C6
37	31	302	CLA	C4-C3-C5-C6
37	14	303	CLA	C3A-C2A-CAA-CBA
37	19	302	CLA	C12-C13-C15-C16
37	34	303	CLA	C3A-C2A-CAA-CBA
37	39	302	CLA	C12-C13-C15-C16
45	D	408	PL9	C18-C19-C21-C22
45	d	406	PL9	C18-C19-C21-C22
37	B	514	CLA	CAA-CBA-CGA-O1A
37	b	514	CLA	CAA-CBA-CGA-O1A
37	15	301	CLA	CAA-CBA-CGA-O1A
37	18	204	CLA	CAA-CBA-CGA-O1A
37	35	301	CLA	CAA-CBA-CGA-O1A
37	36	303	CLA	CAA-CBA-CGA-O1A
37	41	204	CLA	CAA-CBA-CGA-O1A
37	C	510	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
37	15	303	CLA	CAA-CBA-CGA-O2A
37	34	308	CLA	CAA-CBA-CGA-O2A
40	17	301	SQD	O48-C23-C24-C25
40	36	315	SQD	O48-C23-C24-C25
43	37	321	LHG	C35-C36-C37-C38
39	C	519	BCR	C21-C22-C23-C24
39	c	519	BCR	C21-C22-C23-C24
48	16	311	A86	C2-C1-C24-C25
48	17	310	A86	C2-C1-C24-C25
48	36	311	A86	C2-C1-C24-C25
48	37	309	A86	C2-C1-C24-C25
50	21	212	DD6	C10-C11-C13-C14
50	41	212	DD6	C10-C11-C13-C14
37	17	304	CLA	CAA-CBA-CGA-O1A
37	21	204	CLA	CAA-CBA-CGA-O1A
37	33	303	CLA	CAA-CBA-CGA-O1A
37	37	303	CLA	CAA-CBA-CGA-O1A
37	38	204	CLA	CAA-CBA-CGA-O1A
41	B	520	LMG	O10-C28-C29-C30
41	b	519	LMG	O10-C28-C29-C30
45	D	408	PL9	C2-C3-C7-C8
45	d	406	PL9	C2-C3-C7-C8
37	19	309	CLA	CAA-CBA-CGA-O2A
48	17	314	A86	C24-C25-C26-C27
48	19	313	A86	C3-C4-C5-C6
50	19	312	DD6	C24-C25-C26-C27
50	39	312	DD6	C24-C25-C26-C27
48	11	311	A86	O-C13-C14-C15
48	17	315	A86	O-C13-C14-C15
48	31	311	A86	O-C13-C14-C15
48	37	311	A86	O-C13-C14-C15
48	37	314	A86	O-C13-C14-C15
37	C	512	CLA	CAA-CBA-CGA-O2A
37	14	301	CLA	CAA-CBA-CGA-O2A
37	19	301	CLA	CAA-CBA-CGA-O2A
37	19	303	CLA	CAA-CBA-CGA-O2A
37	39	301	CLA	CAA-CBA-CGA-O2A
37	39	303	CLA	CAA-CBA-CGA-O2A
37	B	505	CLA	C8-C10-C11-C12
37	b	505	CLA	C8-C10-C11-C12
37	18	204	CLA	O1A-CGA-O2A-C1
37	12	205	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
37	20	303	CLA	CAA-CBA-CGA-O1A
37	20	306	CLA	CAA-CBA-CGA-O1A
37	32	206	CLA	CAA-CBA-CGA-O1A
37	40	205	CLA	CAA-CBA-CGA-O1A
37	40	208	CLA	CAA-CBA-CGA-O1A
40	B	522	SQD	O49-C7-C8-C9
40	b	521	SQD	O49-C7-C8-C9
37	34	302	CLA	CBA-CGA-O2A-C1
45	D	408	PL9	C9-C11-C12-C13
45	d	406	PL9	C9-C11-C12-C13
37	B	503	CLA	C13-C15-C16-C17
37	b	503	CLA	C13-C15-C16-C17
40	A	407	SQD	C29-C30-C31-C32
47	17	306	KC1	C4C-C3C-CAC-CBC
37	c	512	CLA	CAA-CBA-CGA-O2A
37	13	303	CLA	CAA-CBA-CGA-O2A
37	38	209	CLA	CAA-CBA-CGA-O2A
37	36	309	CLA	C2A-CAA-CBA-CGA
38	D	403	PHO	C16-C17-C18-C19
41	11	317	LMG	C29-C30-C31-C32
41	31	317	LMG	C29-C30-C31-C32
43	21	201	LHG	C7-C8-C9-C10
37	C	510	CLA	CAA-CBA-CGA-O1A
37	c	510	CLA	CAA-CBA-CGA-O1A
37	13	303	CLA	CAA-CBA-CGA-O1A
41	B	521	LMG	C32-C33-C34-C35
41	b	520	LMG	C32-C33-C34-C35
37	14	305	CLA	CAA-CBA-CGA-O1A
37	34	305	CLA	CAA-CBA-CGA-O1A

All (2) ring outliers are listed below:

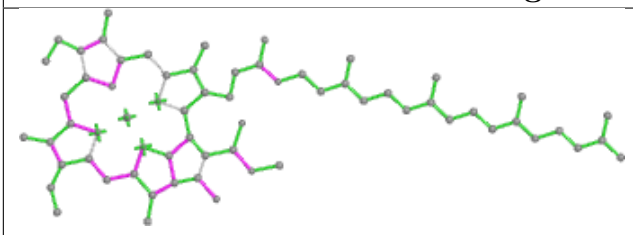
Mol	Chain	Res	Type	Atoms
48	31	313	A86	C31-C32-C33-C34-C35-C36
48	11	313	A86	C31-C32-C33-C34-C35-C36

No monomer is involved in short contacts.

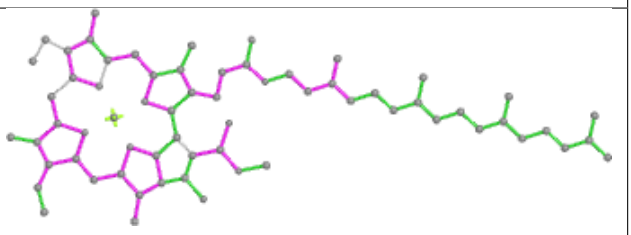
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

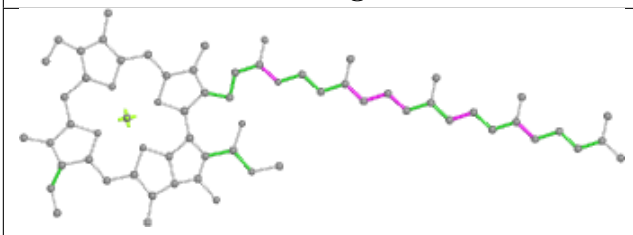
Ligand CLA B 502



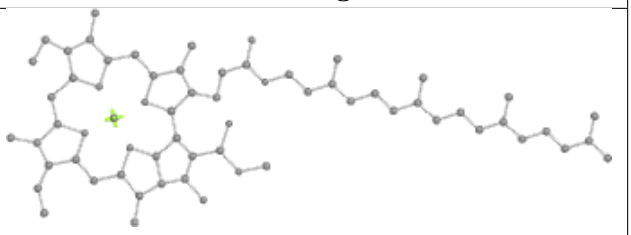
Bond lengths



Bond angles

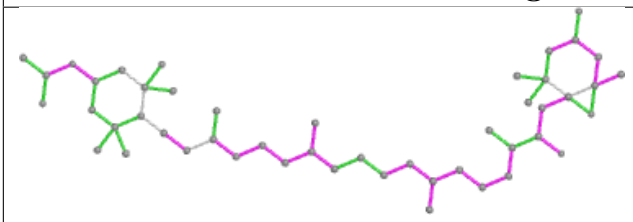


Torsions



Rings

Ligand A86 31 315



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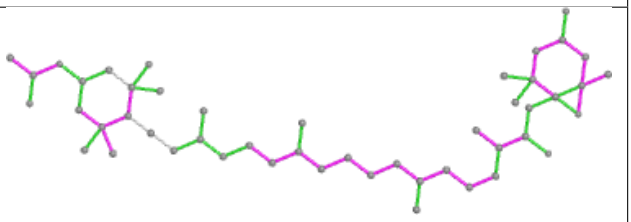
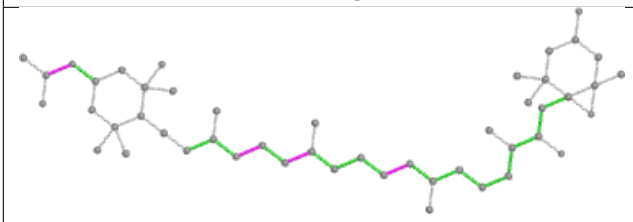
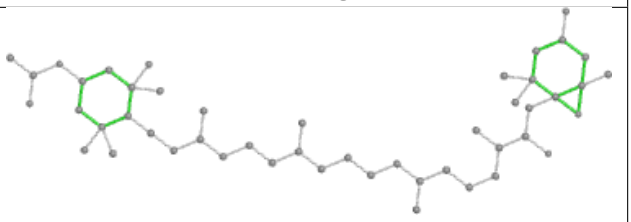


Bond angles

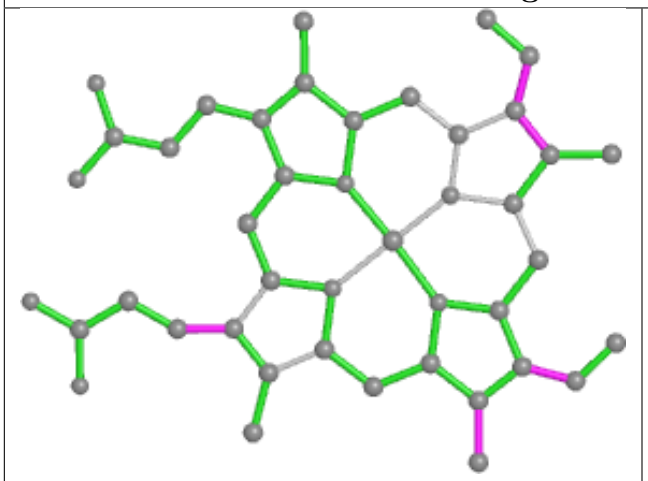


Torsions

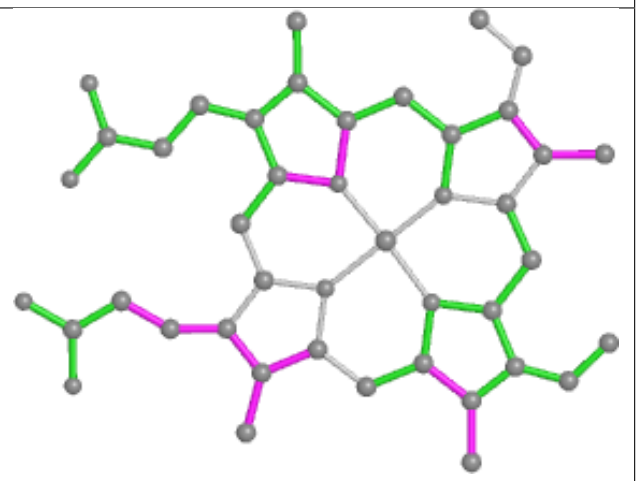


Rings

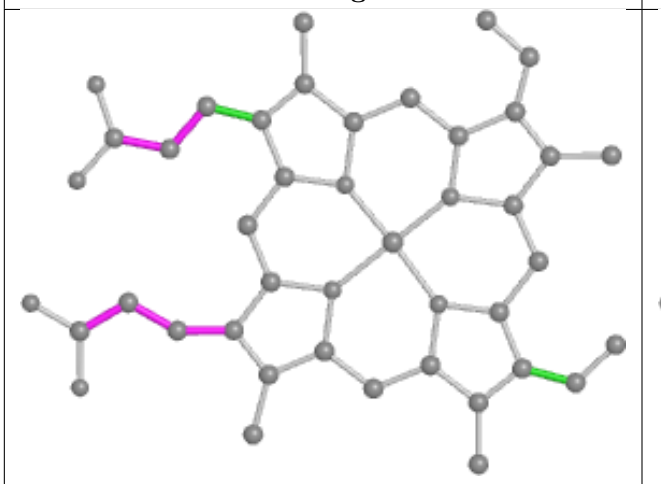
Ligand HEM F 101



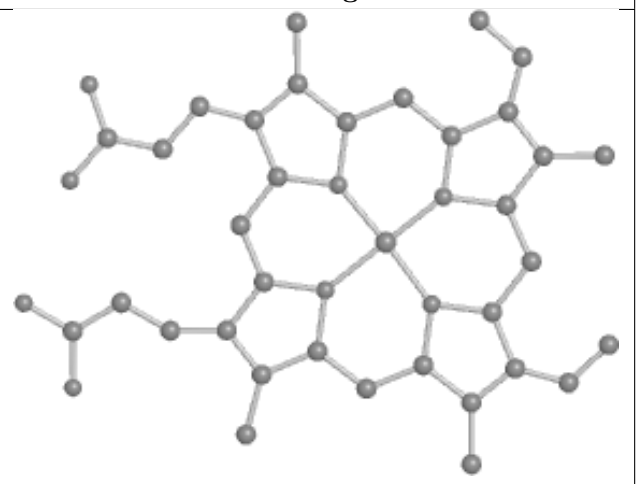
Bond lengths



Bond angles

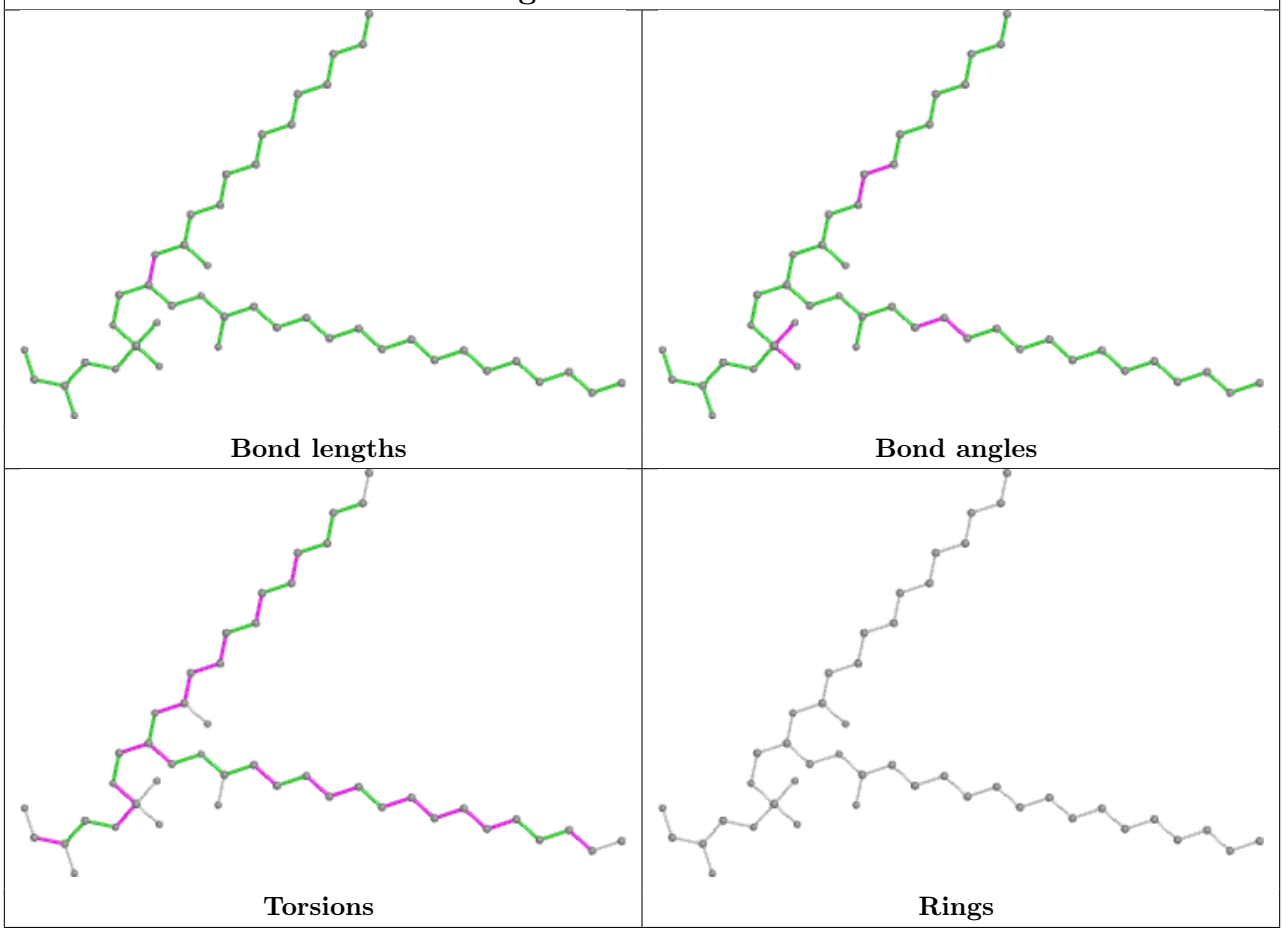


Torsions

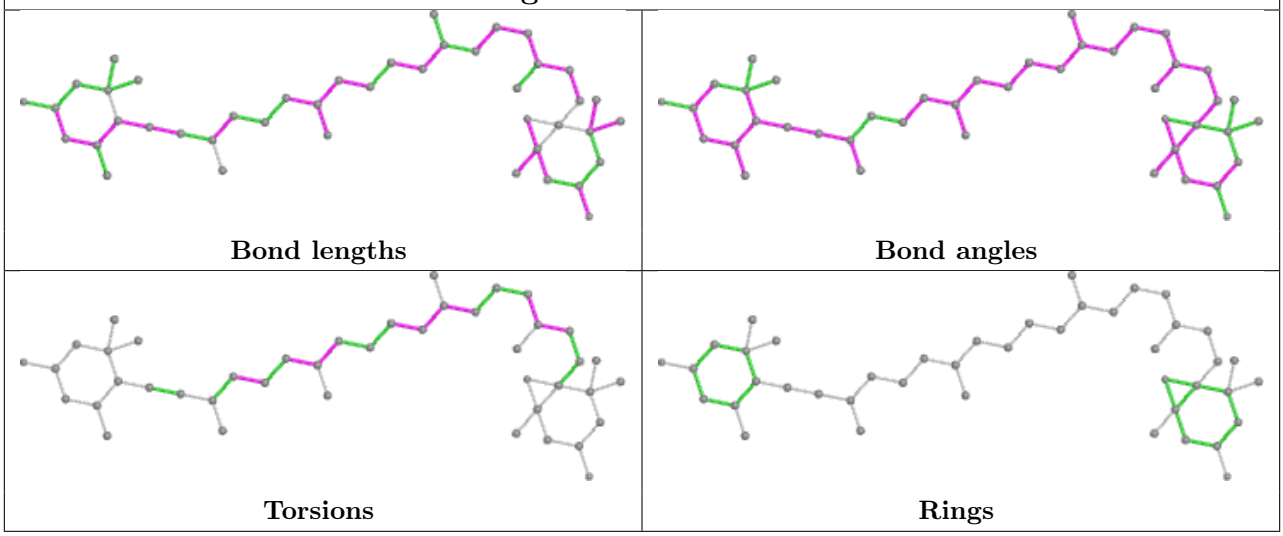


Rings

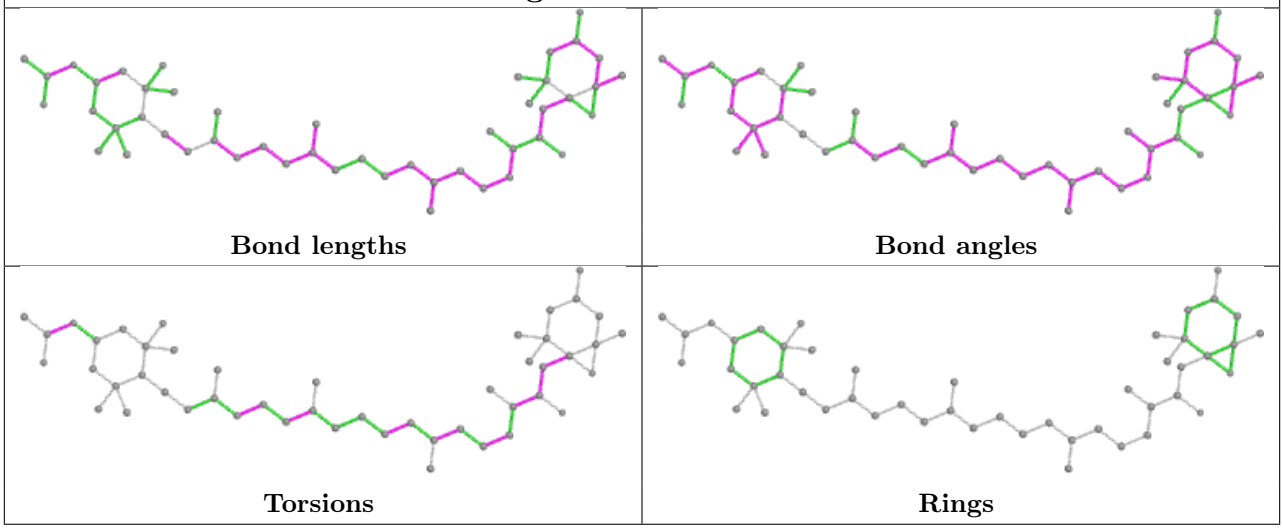
Ligand LHG 37 321



Ligand DD6 36 312



Ligand A86 15 316



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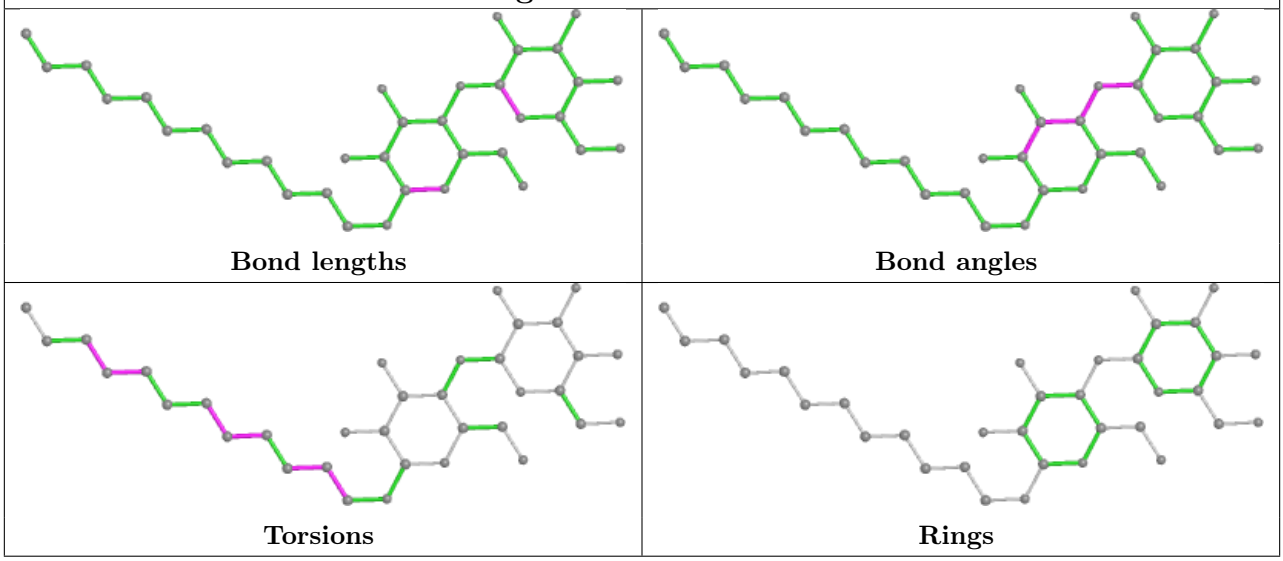
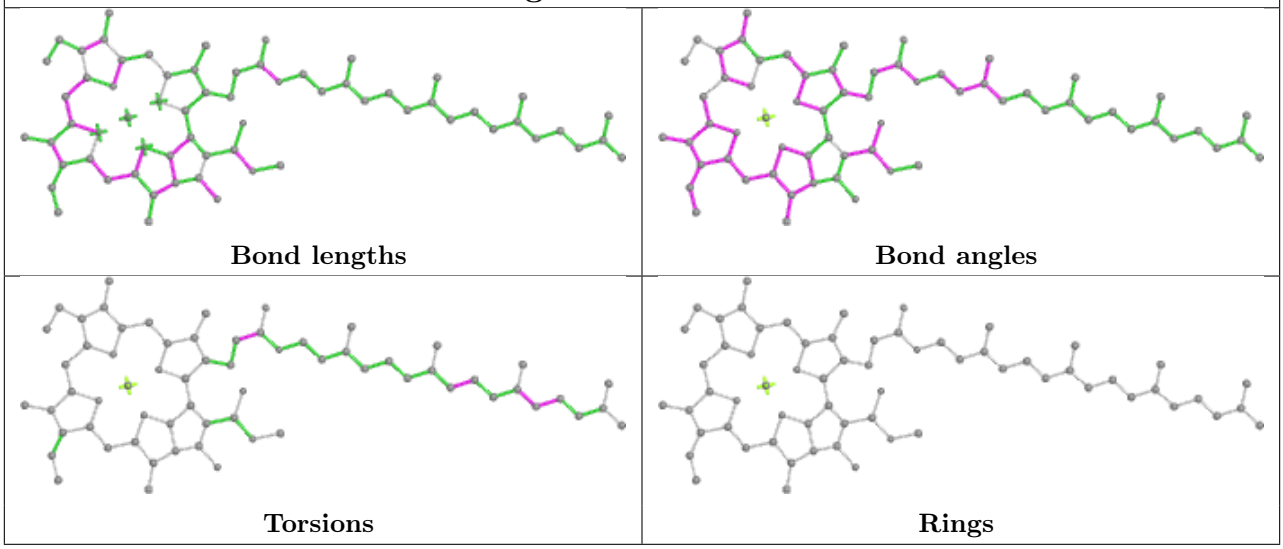


Ligand CLA B 508



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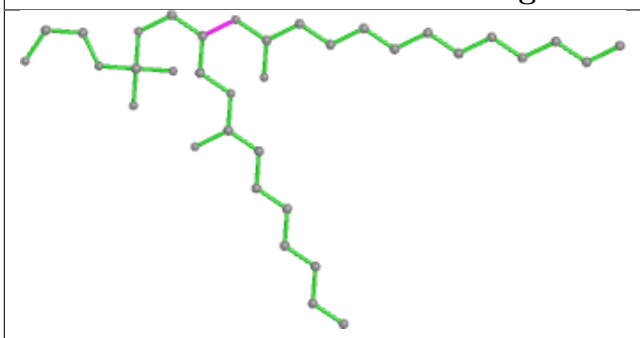
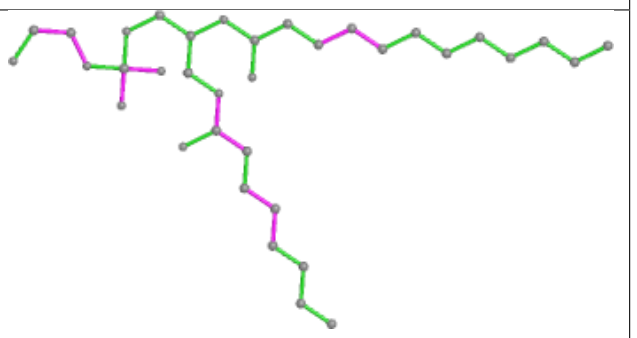
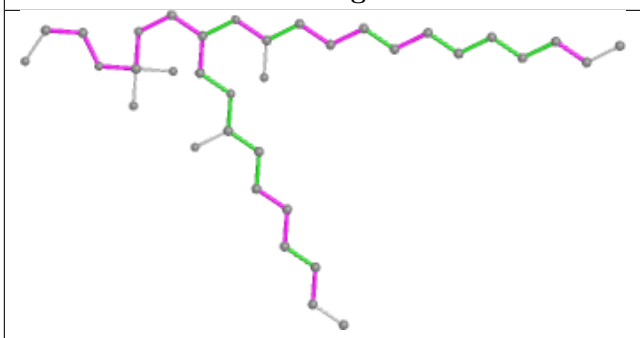
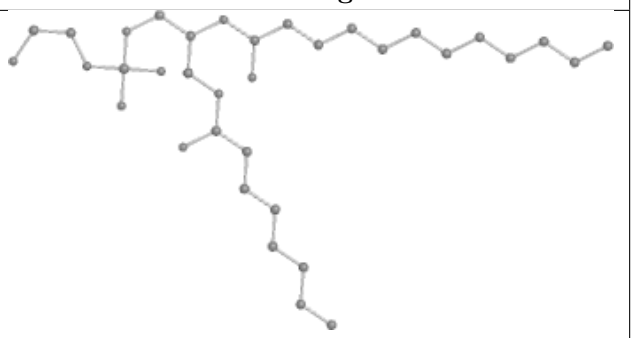
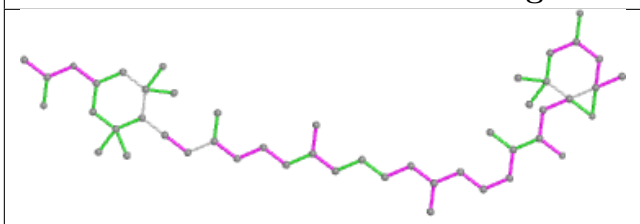
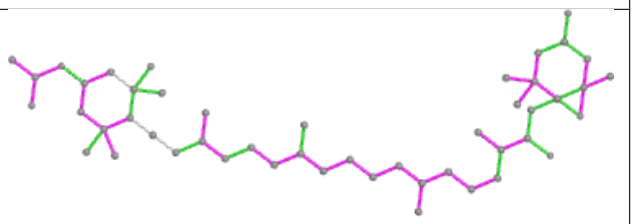
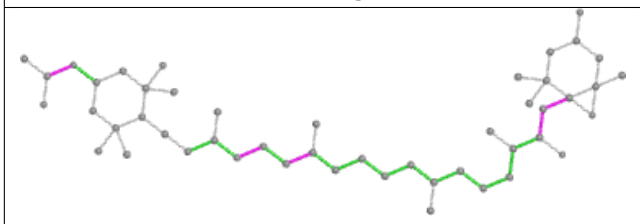
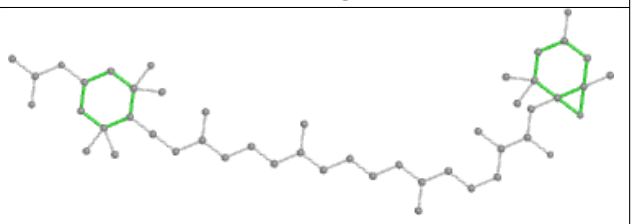
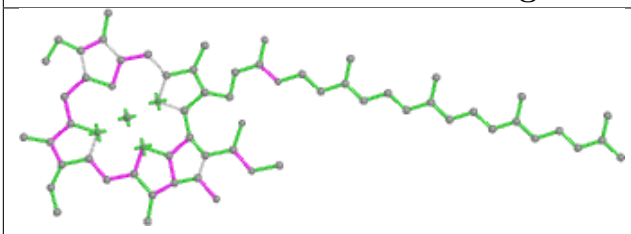
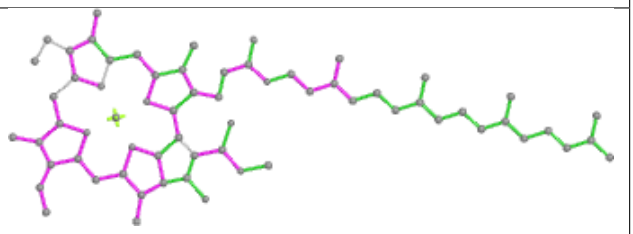
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 39 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

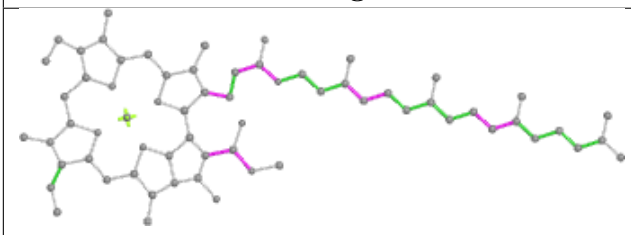
Ligand CLA 41 206



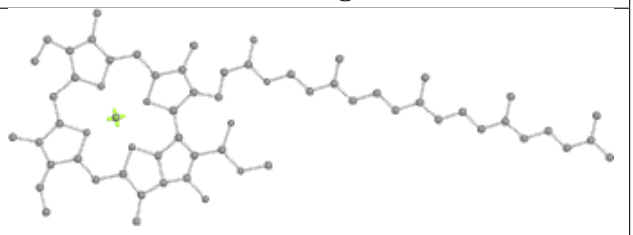
Bond lengths



Bond angles

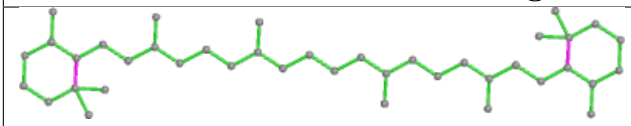


Torsions

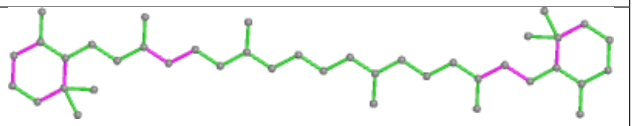


Rings

Ligand BCR 5 101



Bond lengths



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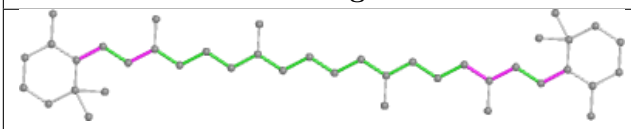

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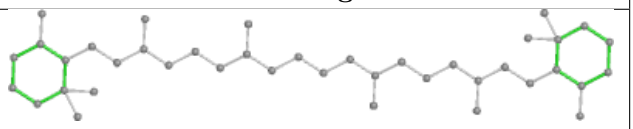
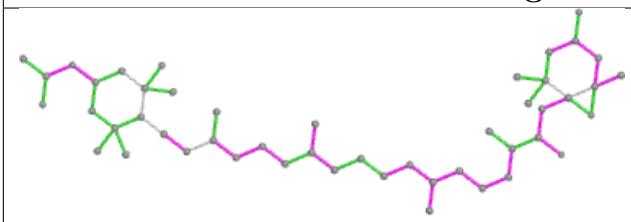


Rings

Ligand A86 14 311



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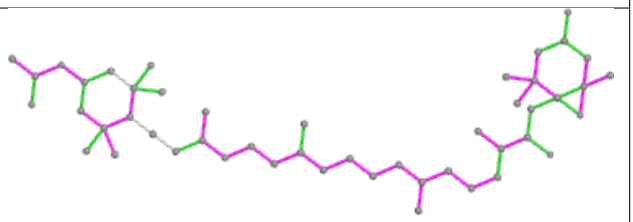

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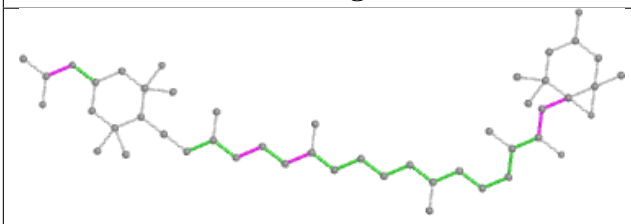

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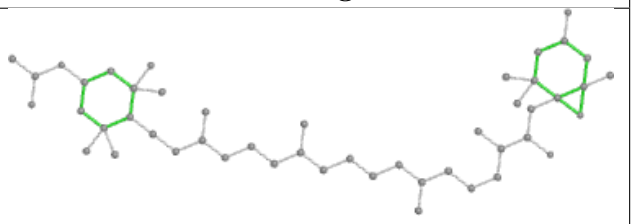

Rings

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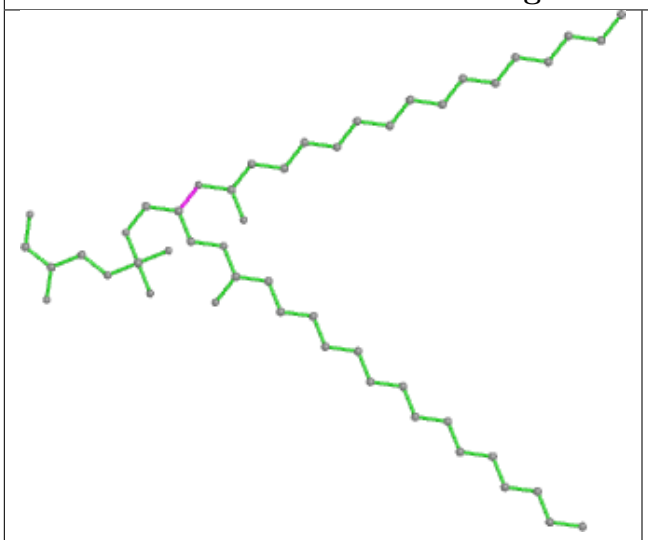

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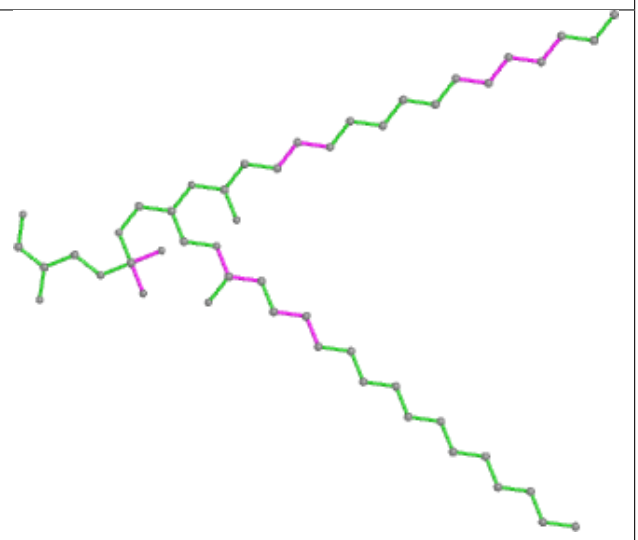

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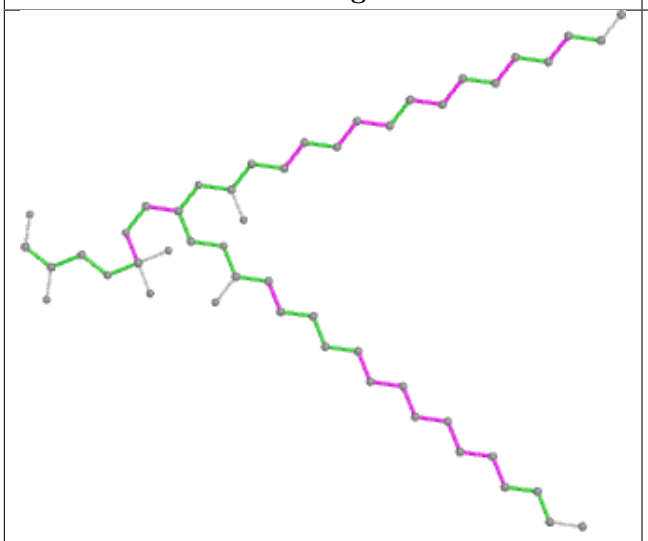

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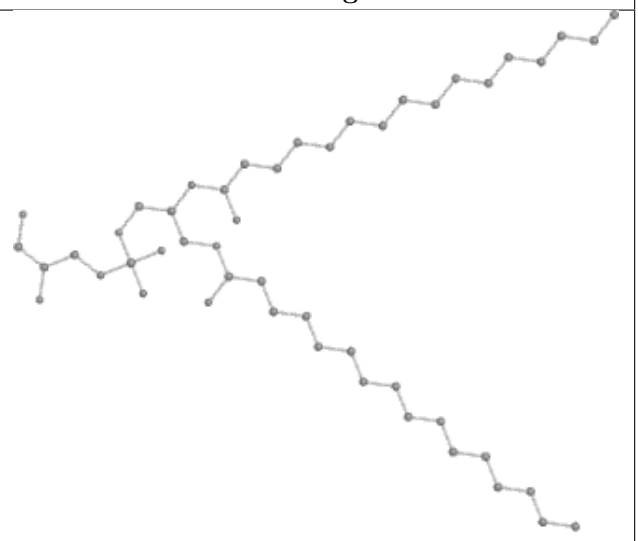

Rings

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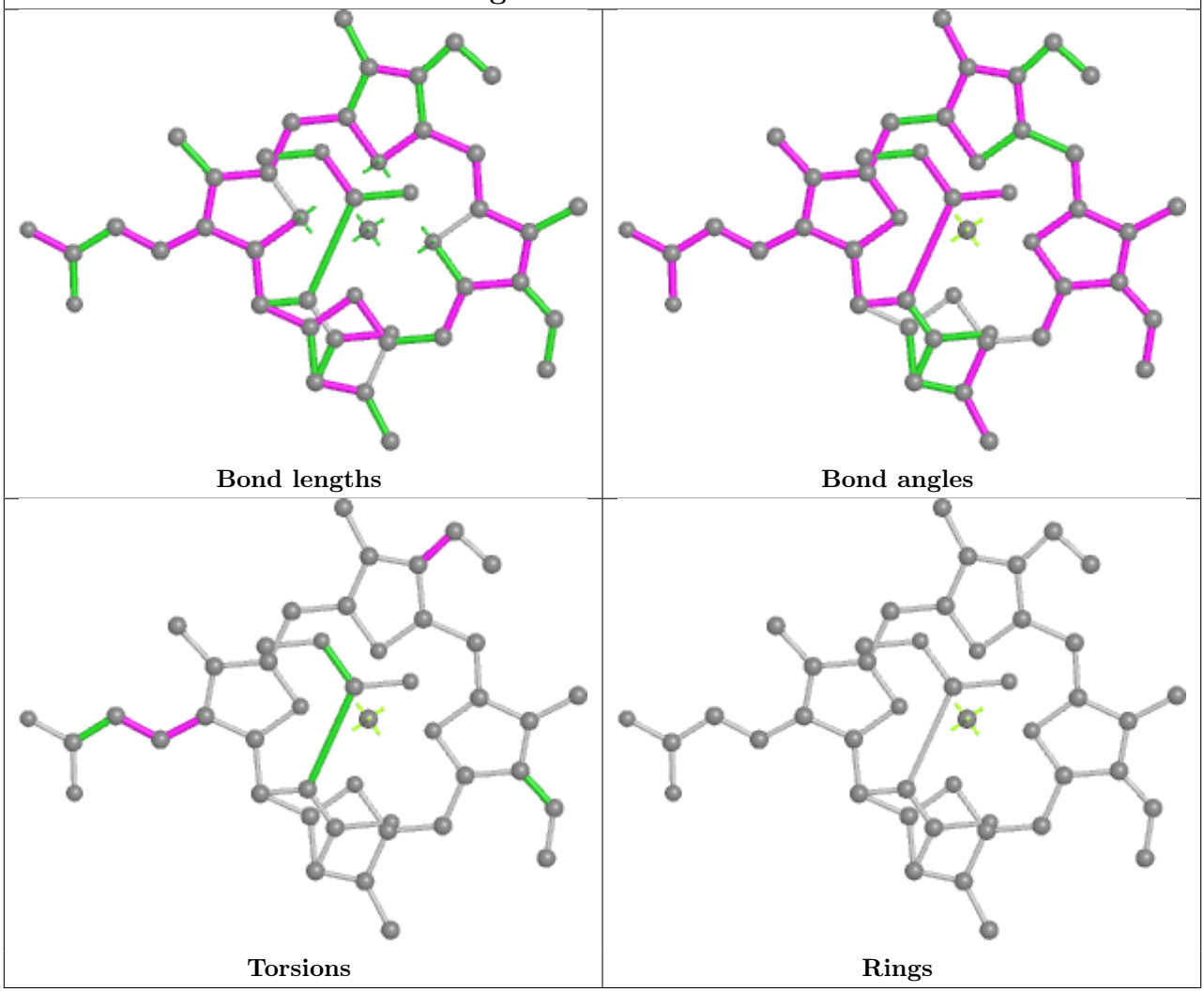

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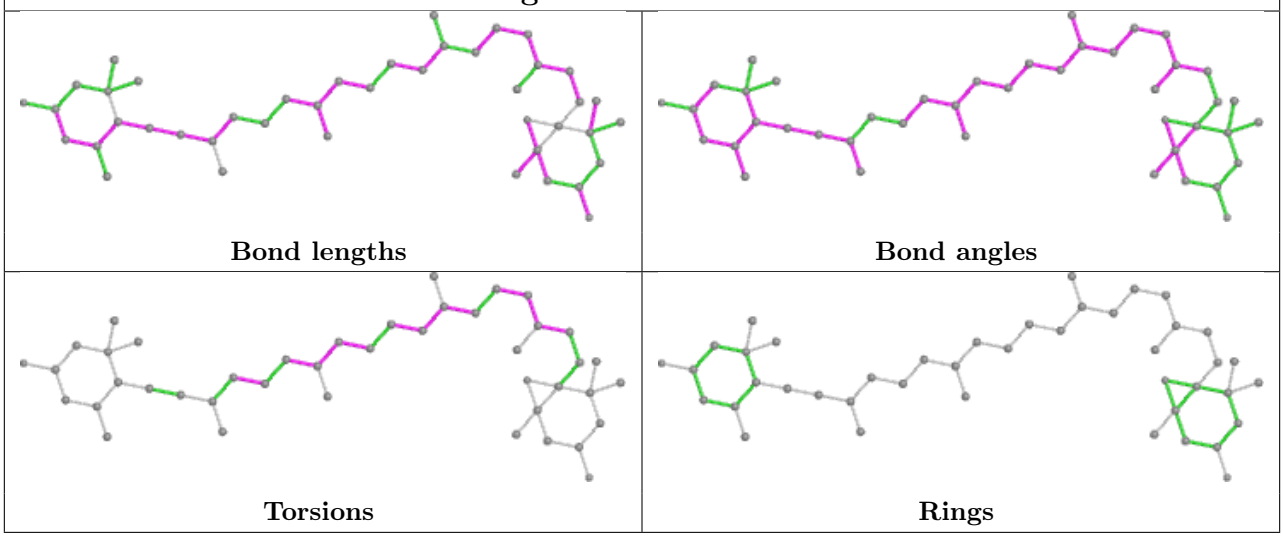

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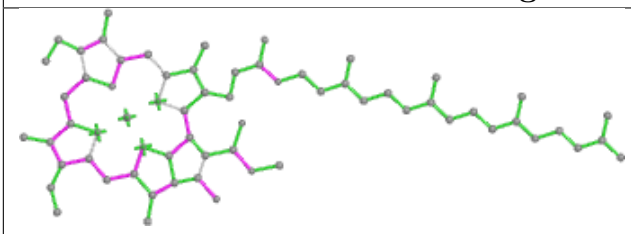
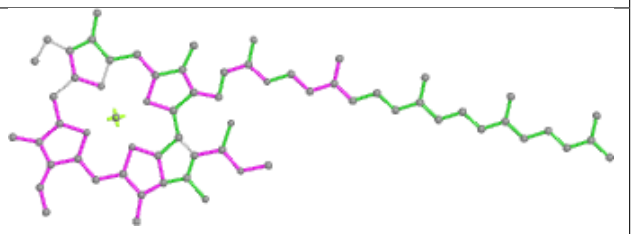
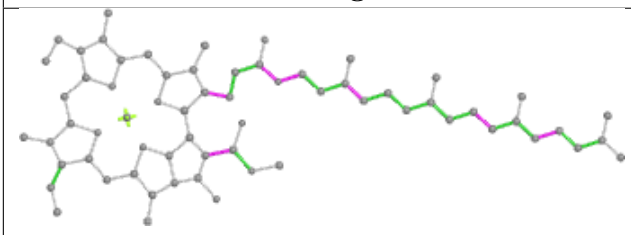
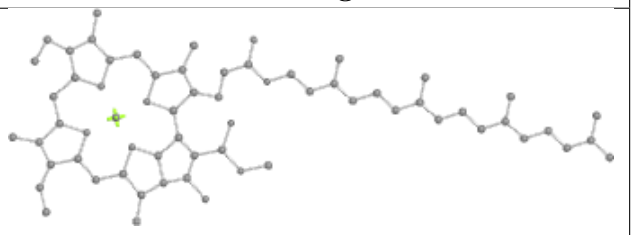
 Bond lengths	 Bond angles
 Torsions	 Rings

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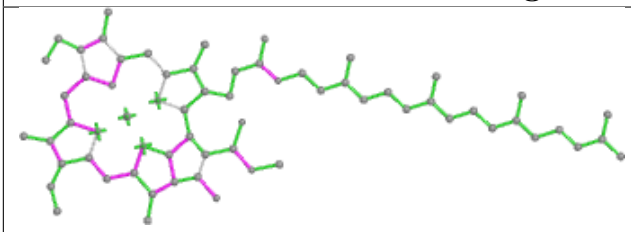
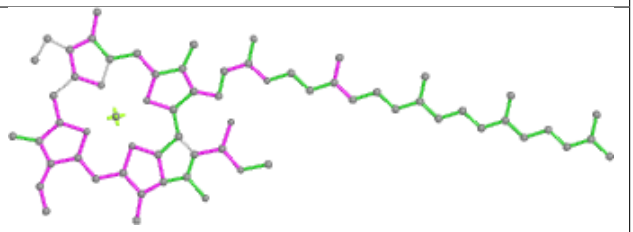
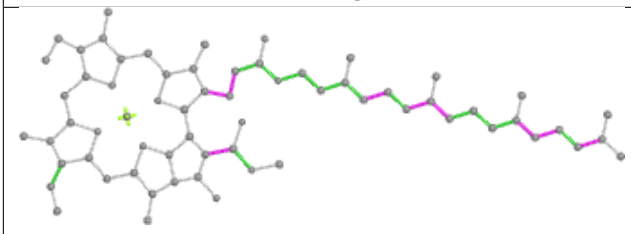
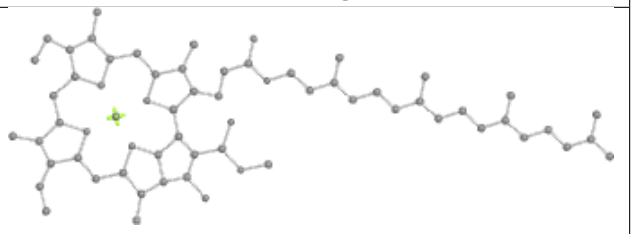
 Bond lengths	 Bond angles
 Torsions	 Rings

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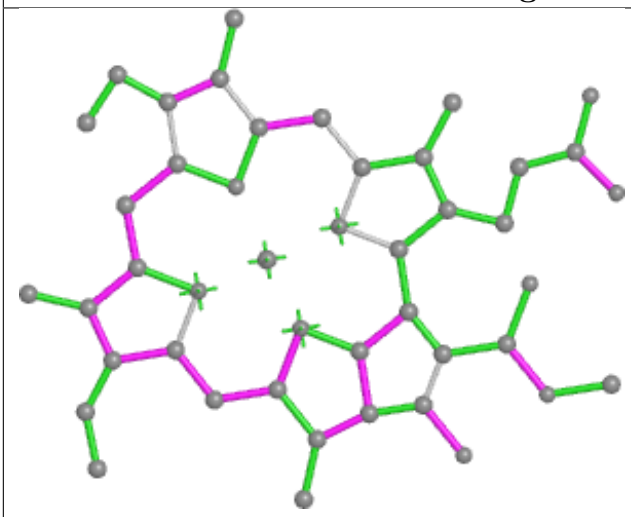

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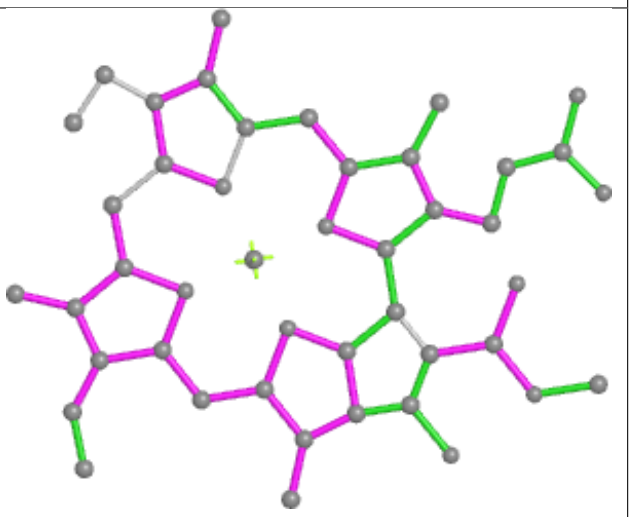

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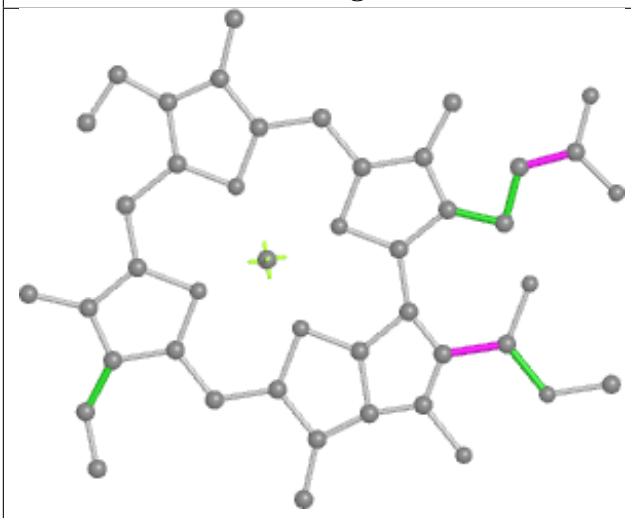

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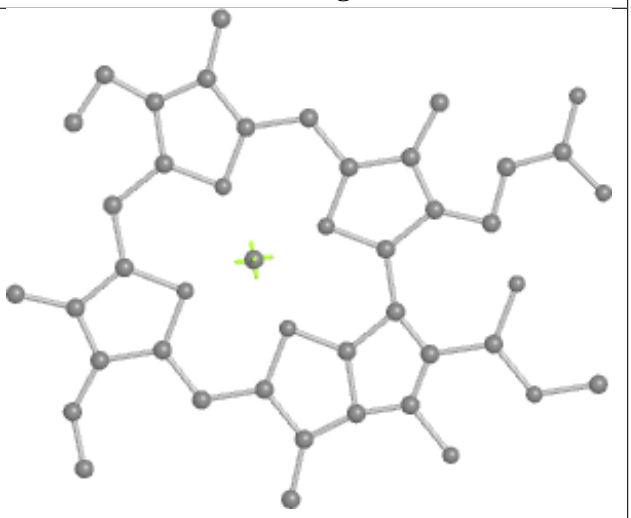

Rings

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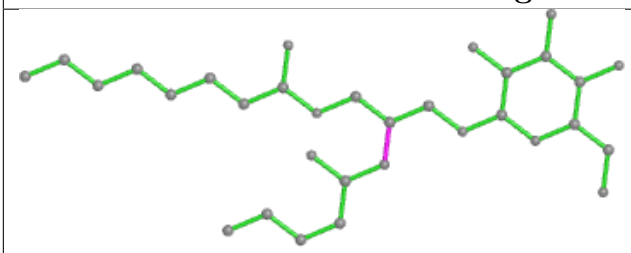

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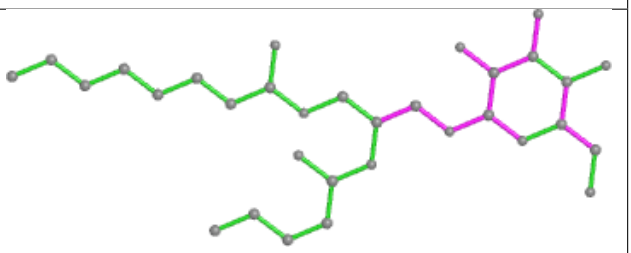

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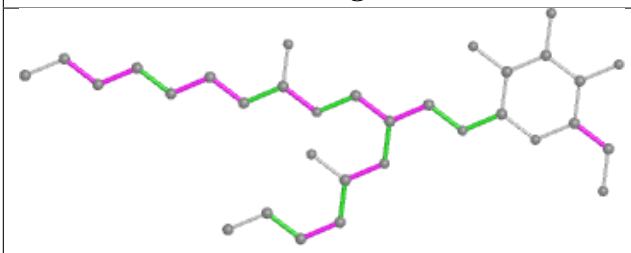

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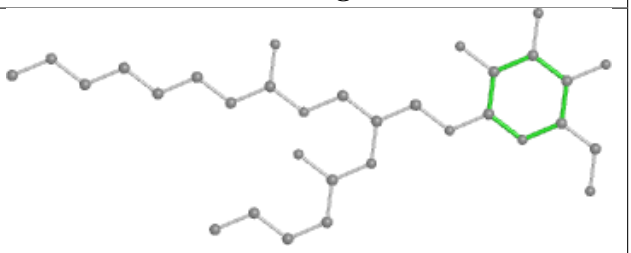
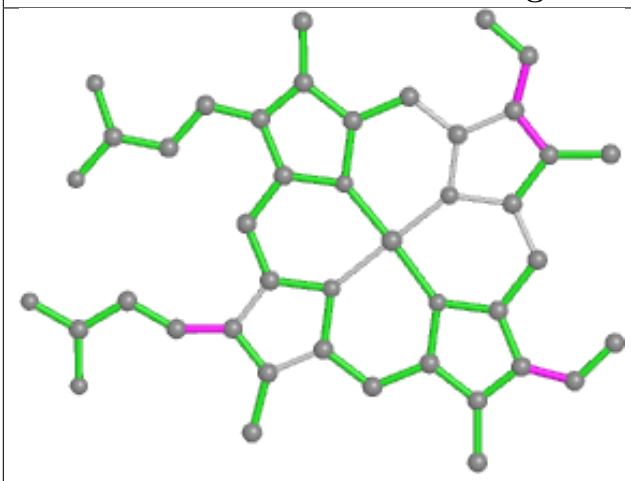


Rings

Ligand HEM f 101



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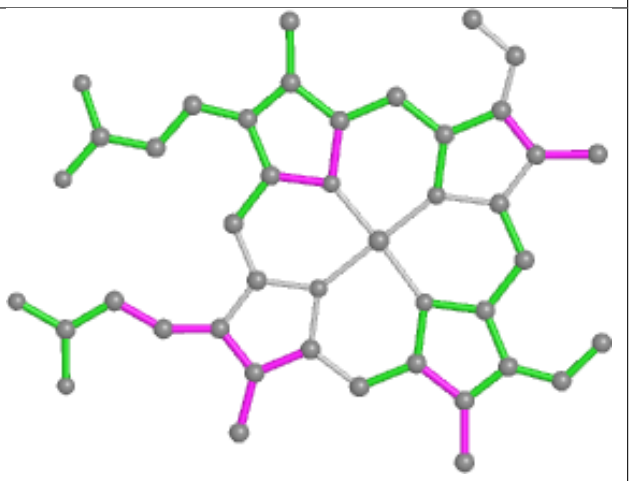

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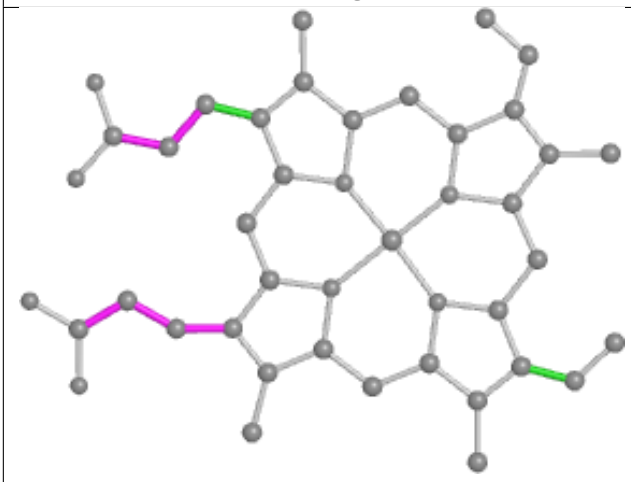

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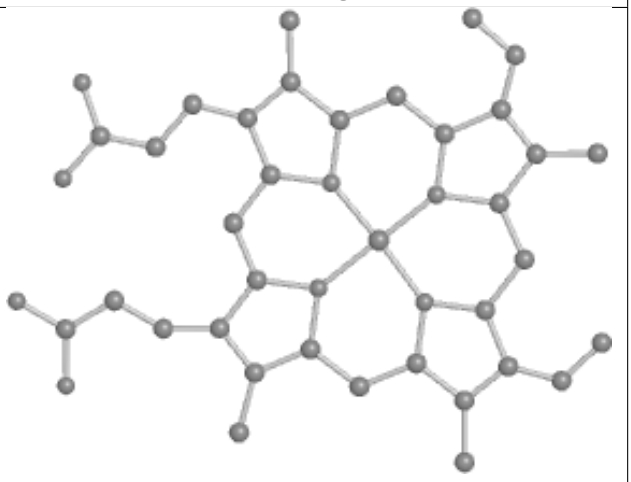
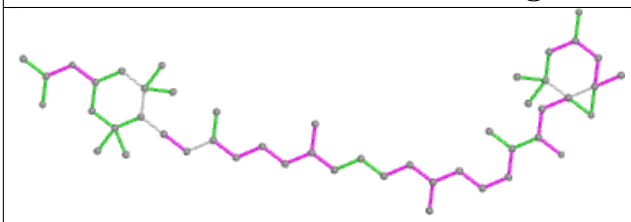


Rings

Ligand A86 21 214



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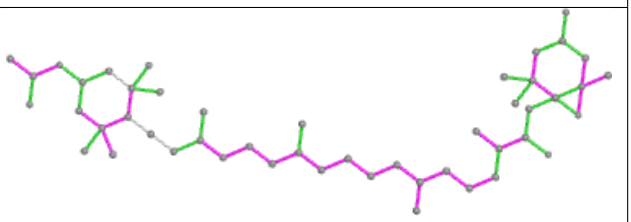

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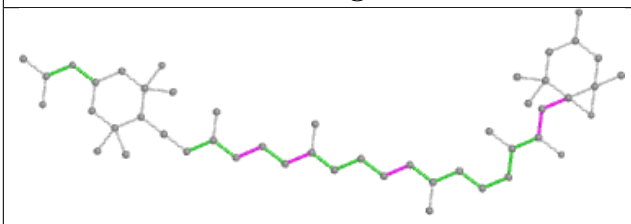

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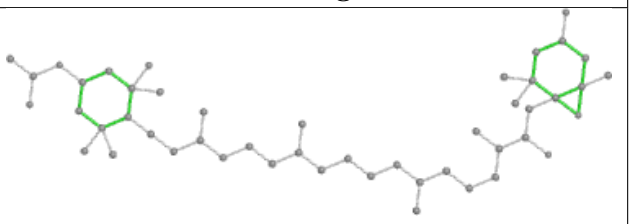

Rings

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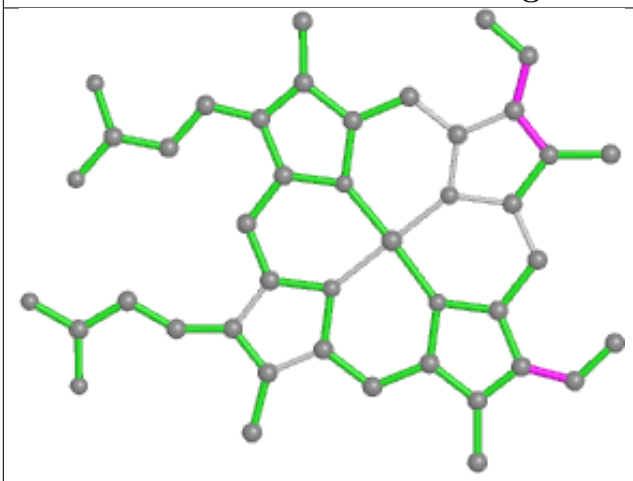

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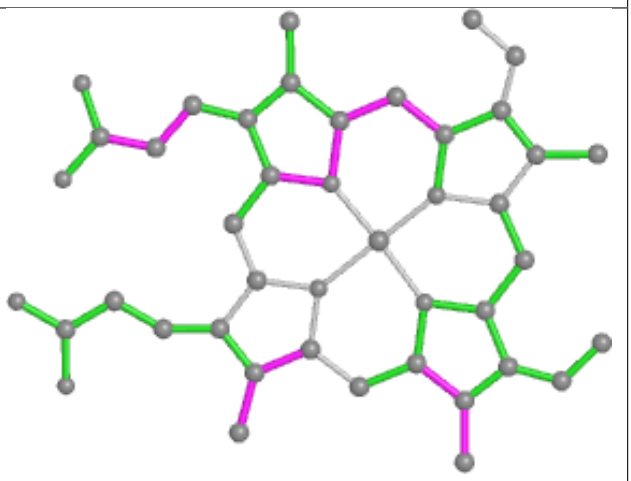

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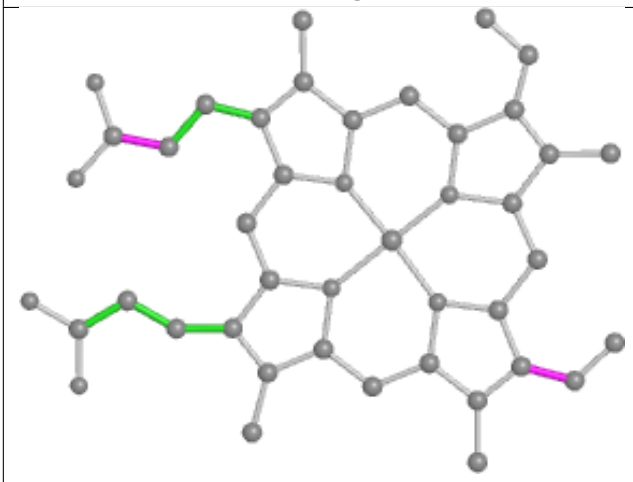

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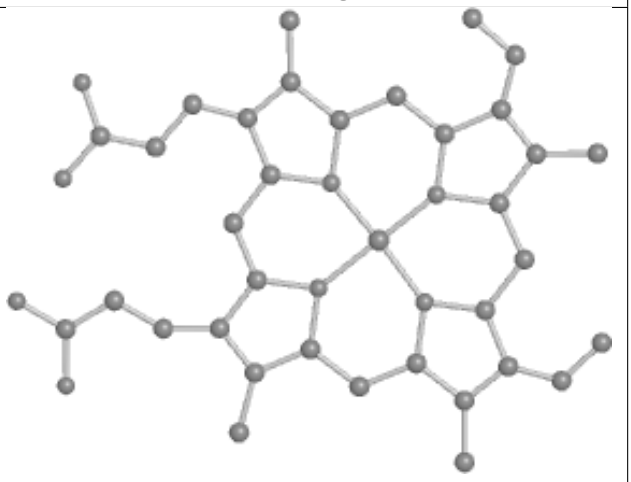
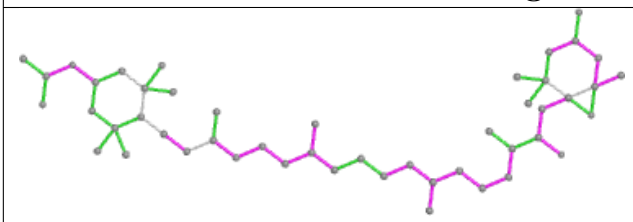


Rings

Ligand A86 37 313



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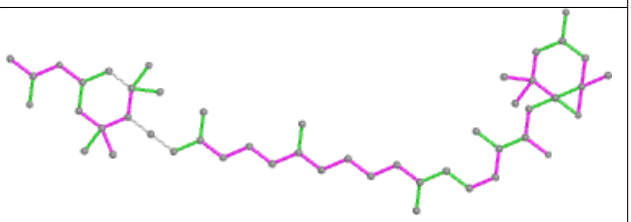
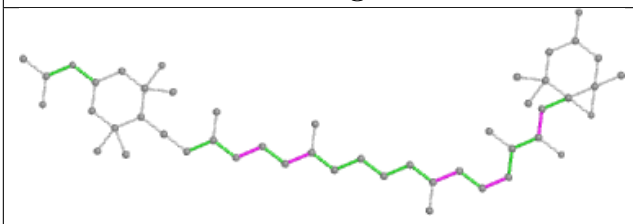


Bond angles



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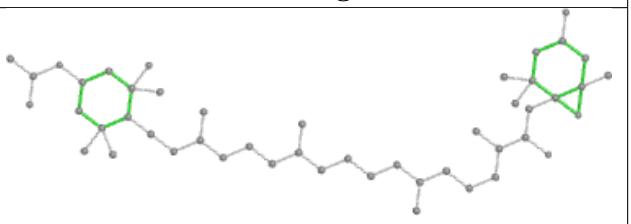

Rings

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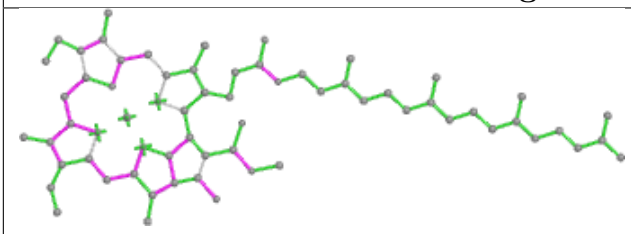
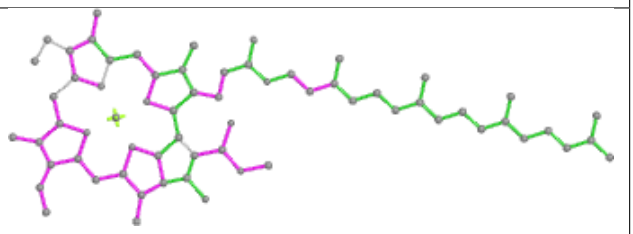
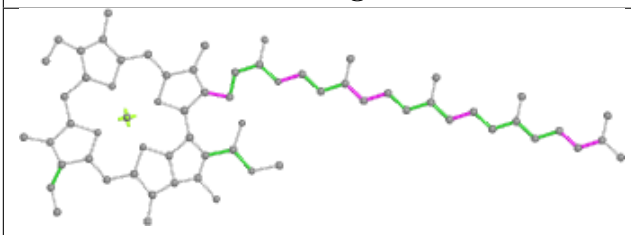
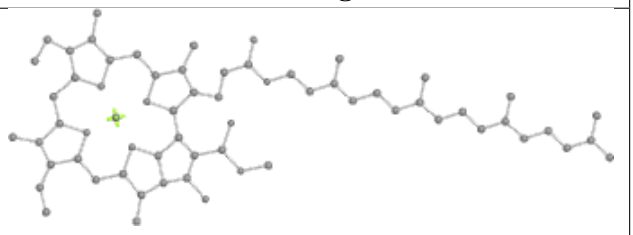
 Bond lengths	 Bond angles
 Torsions	 Rings

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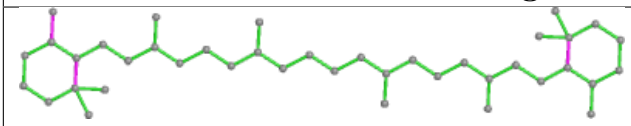
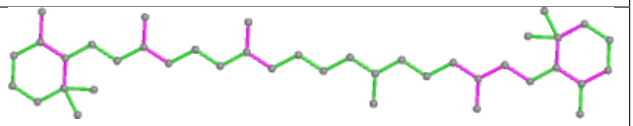
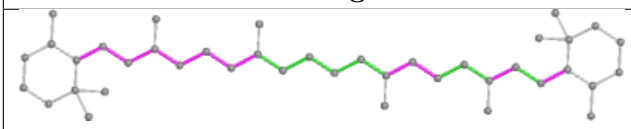
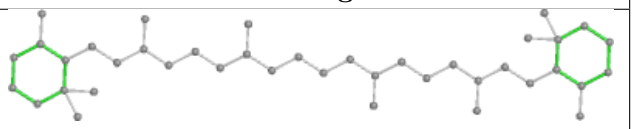
 Bond lengths	 Bond angles
 Torsions	 Rings

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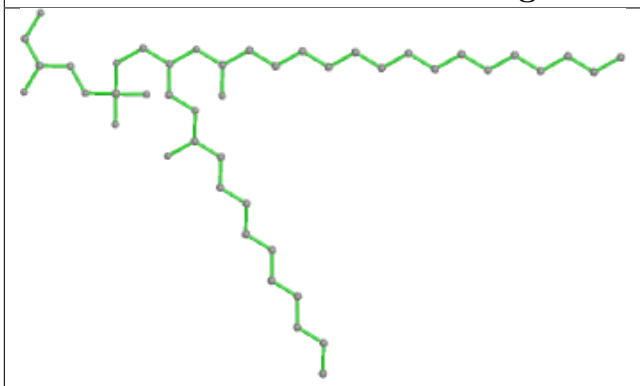	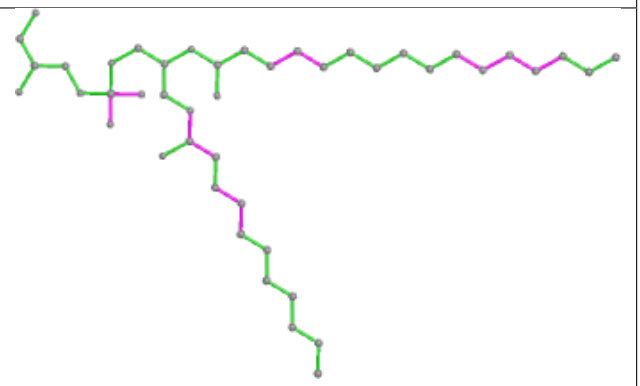
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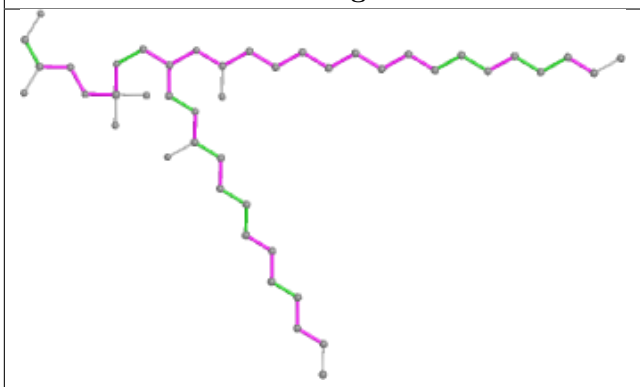	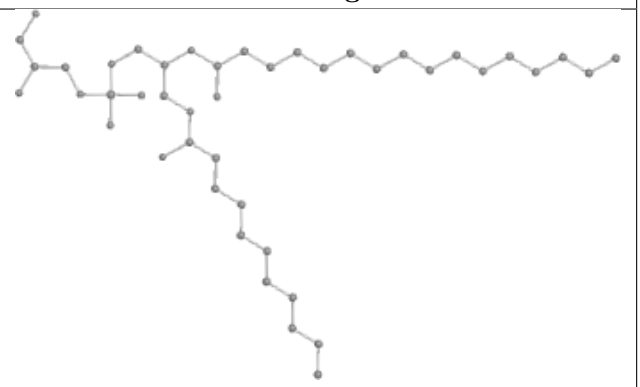
Torsions	Rings

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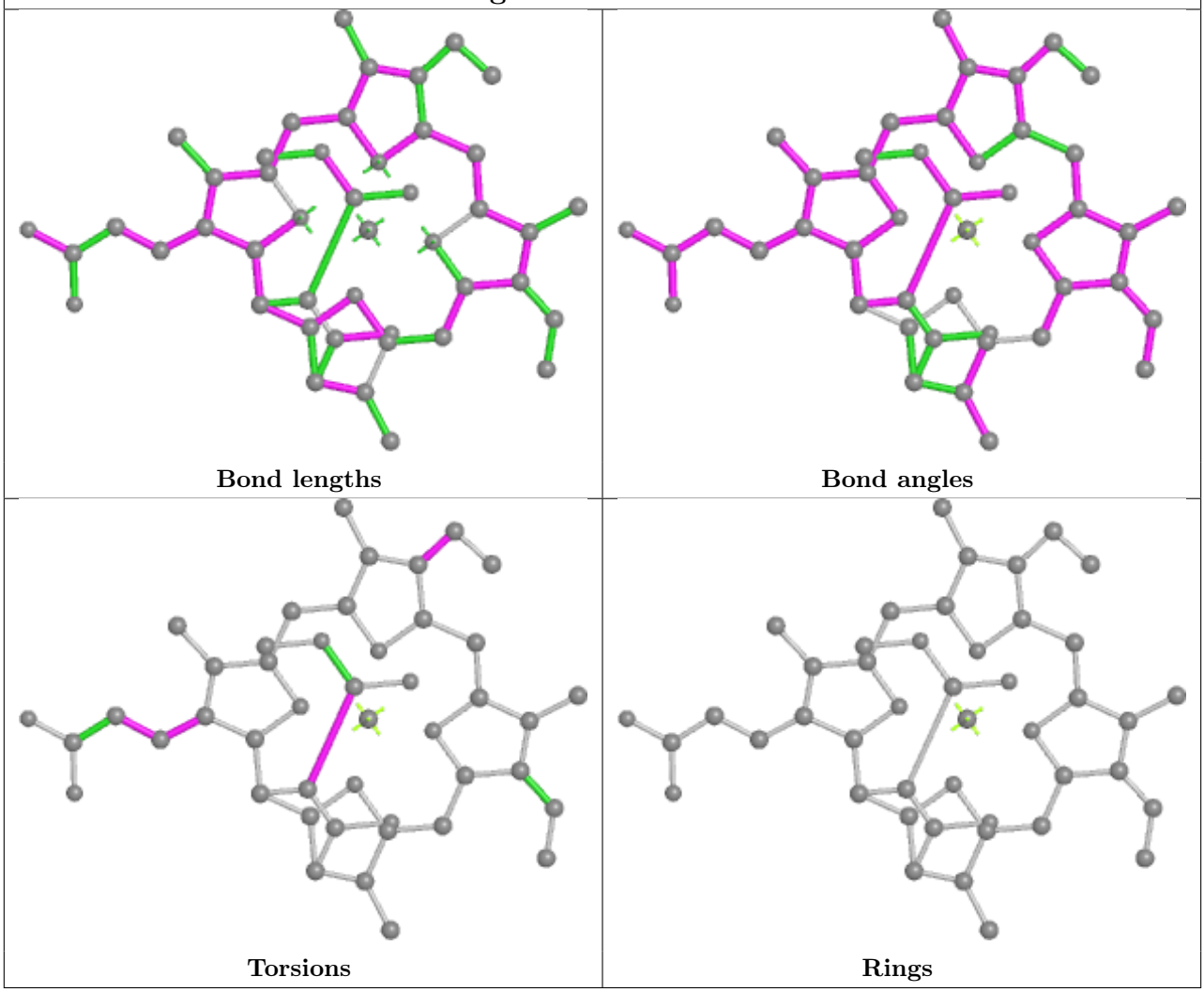

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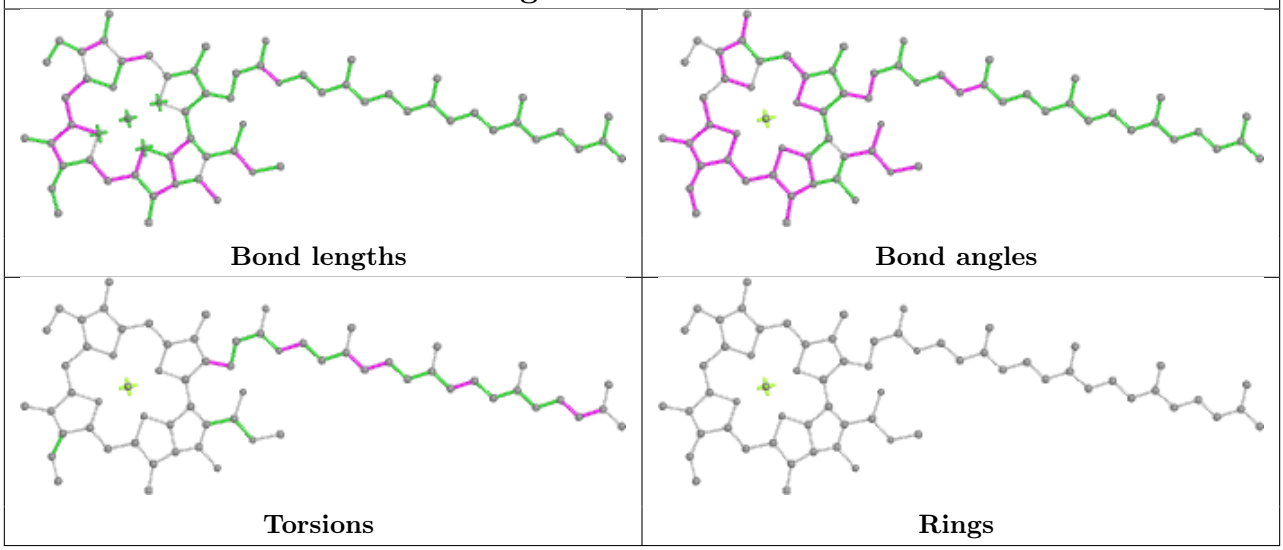

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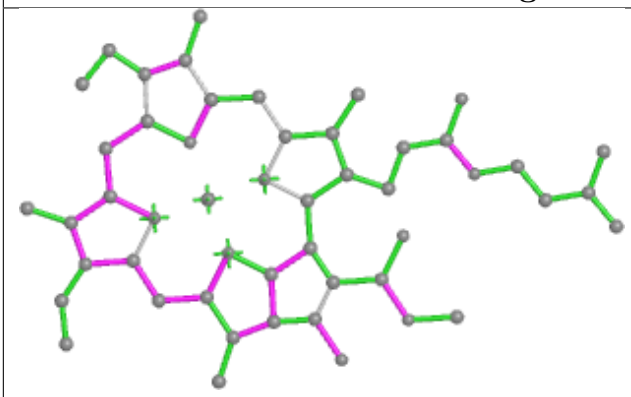

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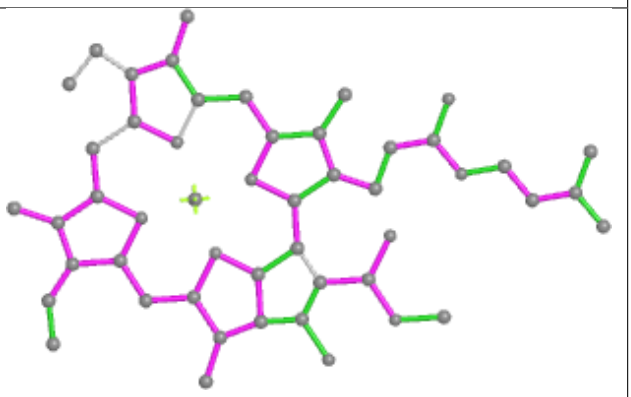

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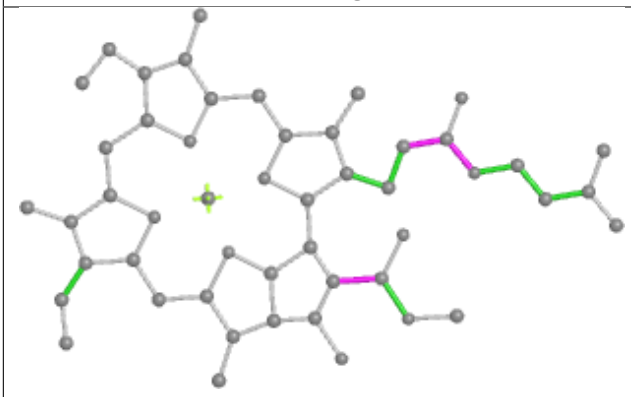

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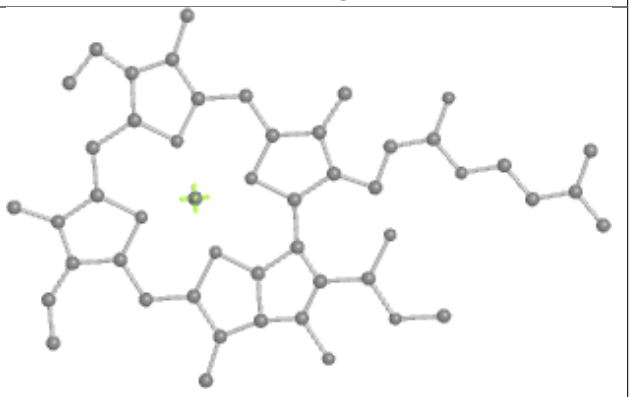
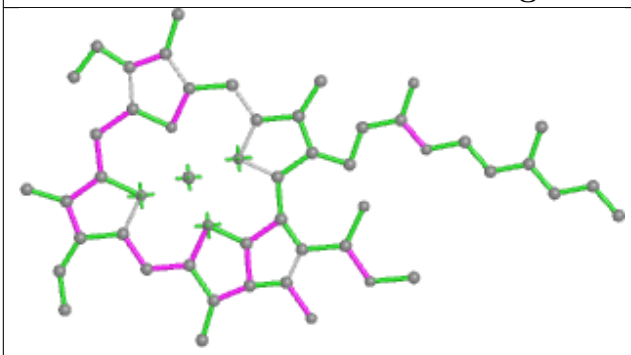


Rings

Ligand CLA 15 307



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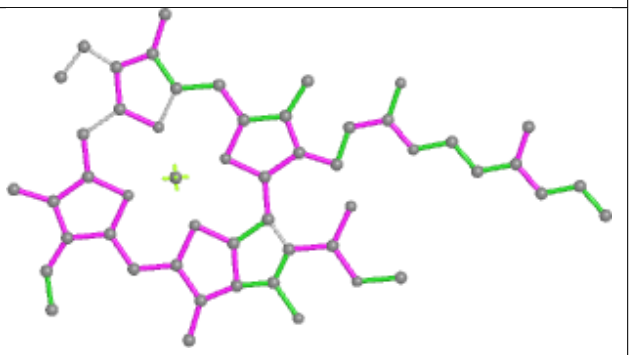

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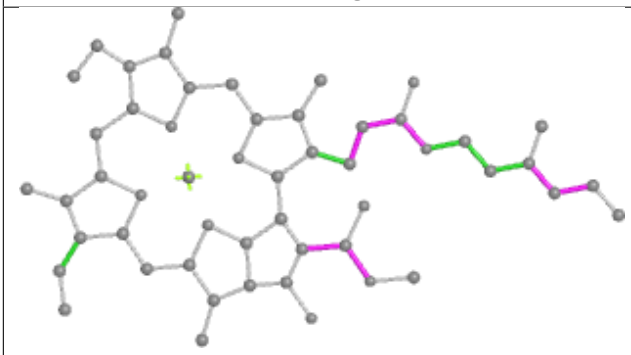

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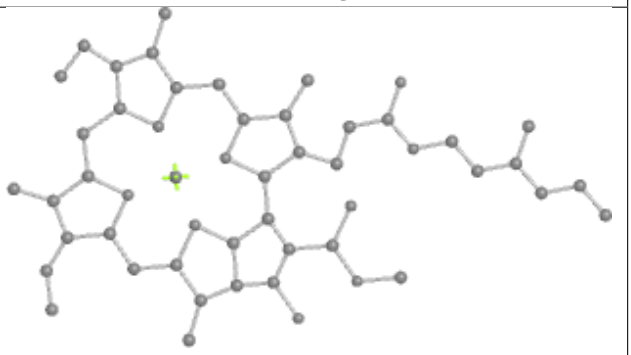
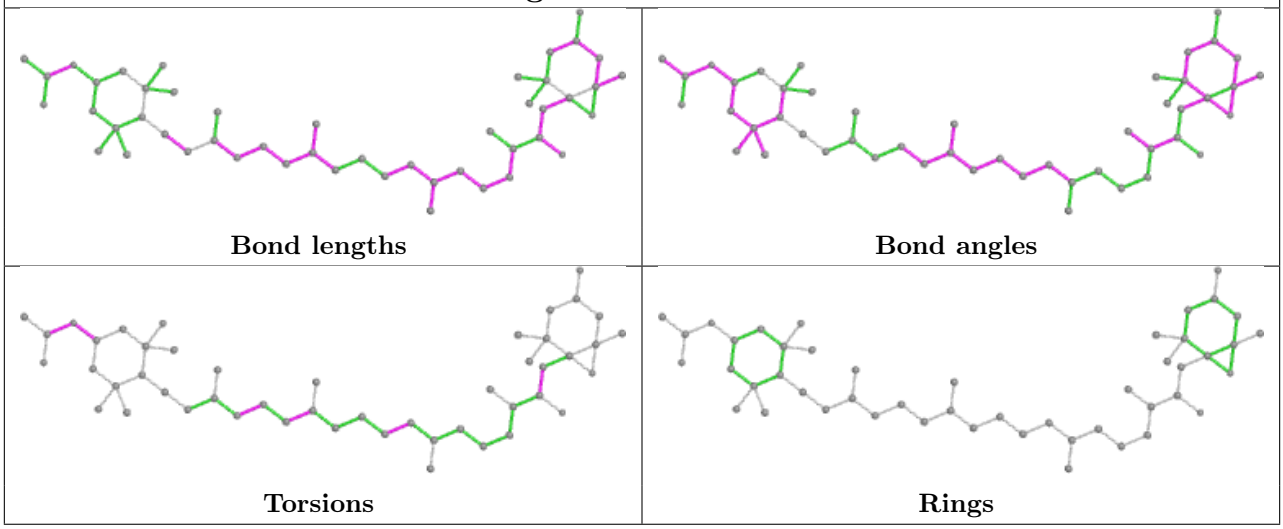


Rings

Ligand A86 17 312



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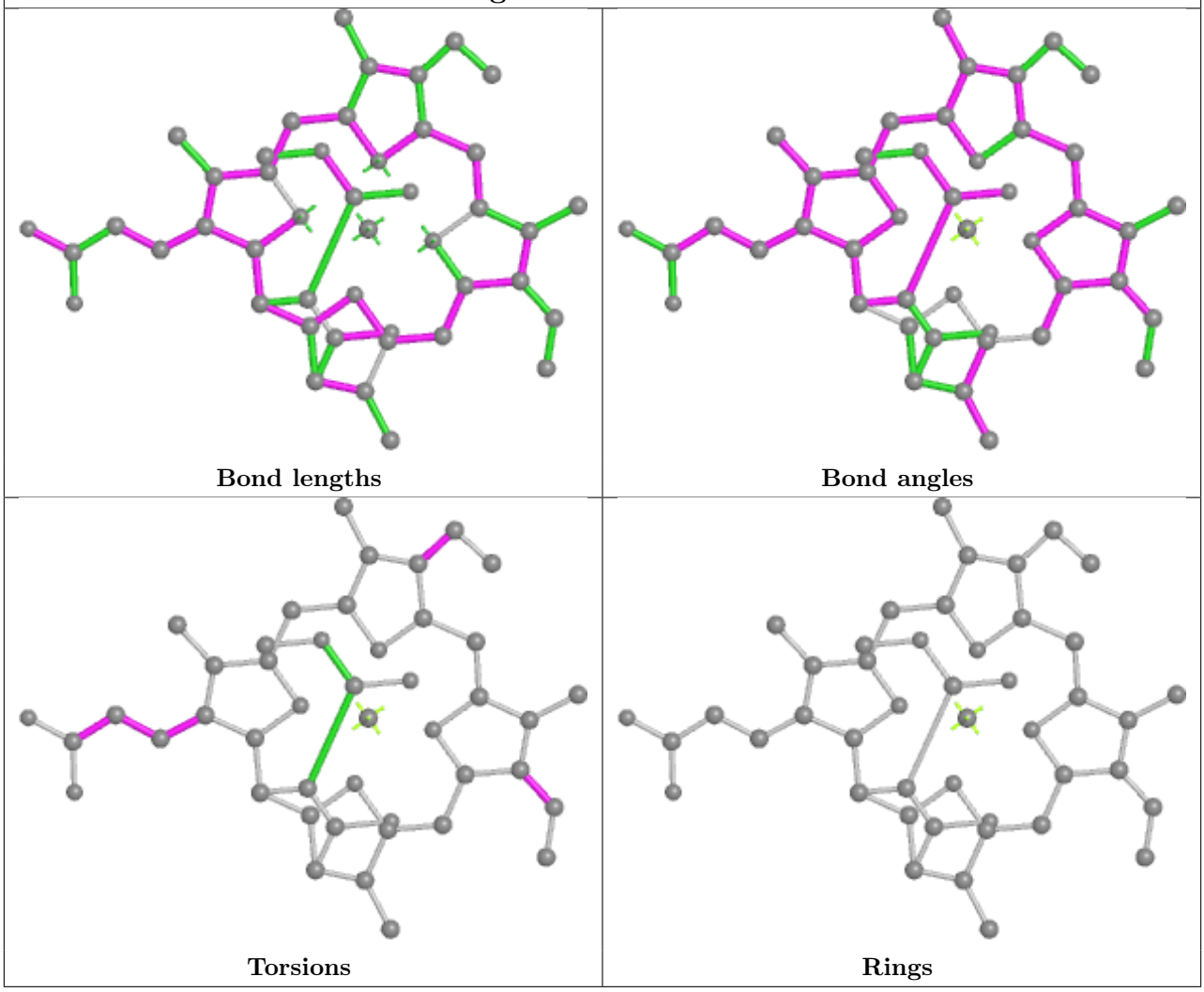

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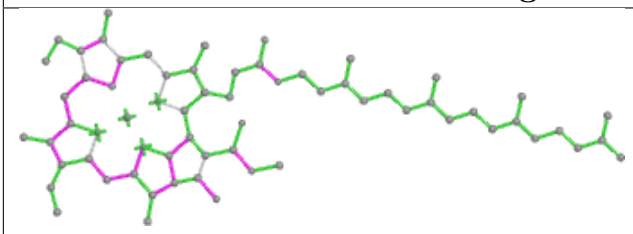

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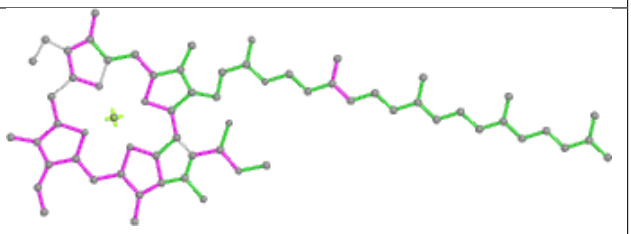

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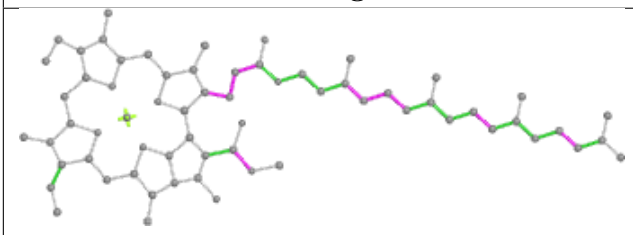

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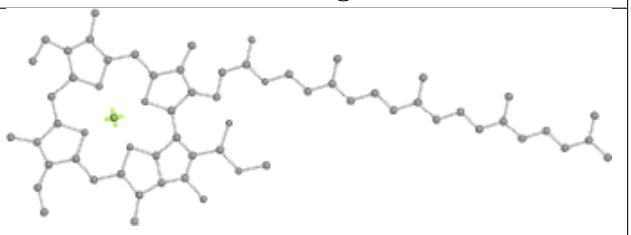

Rings

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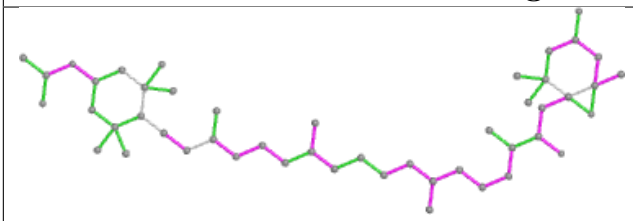

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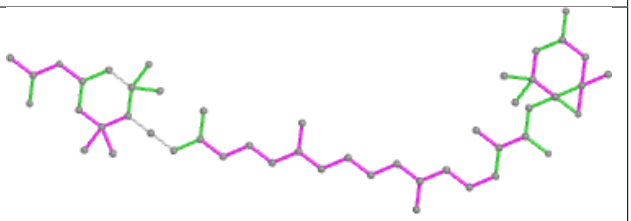

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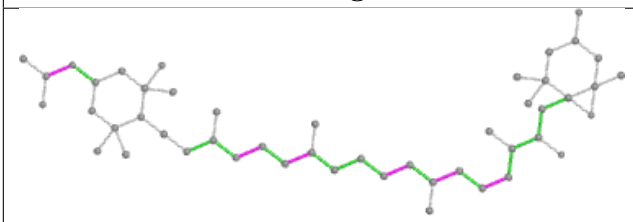

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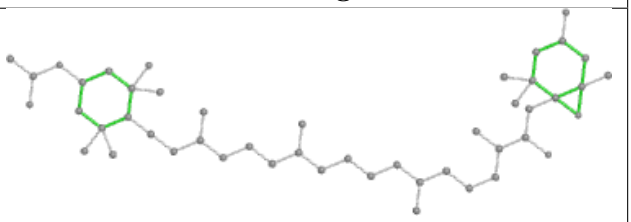

Rings

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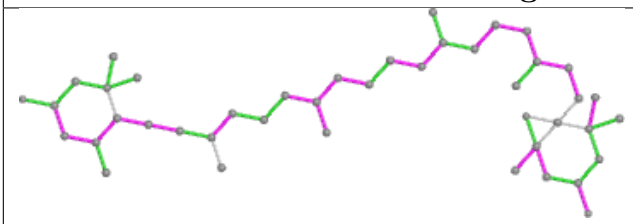

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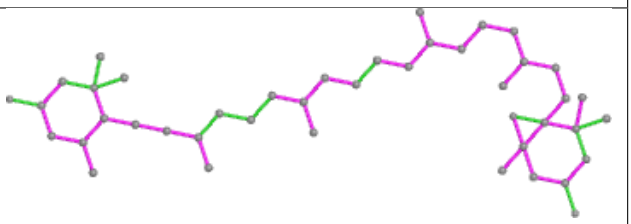

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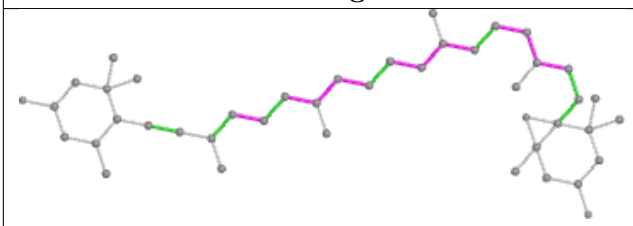

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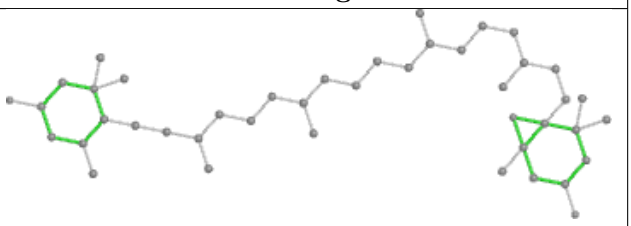
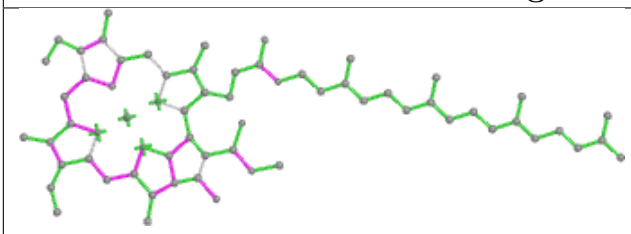
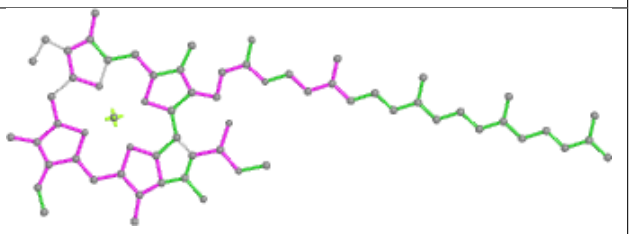
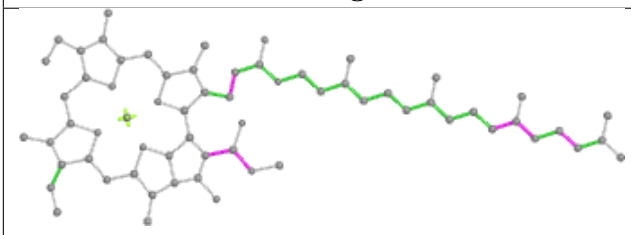
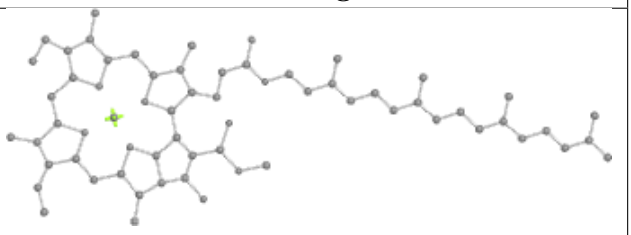


Rings

Ligand CLA b 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

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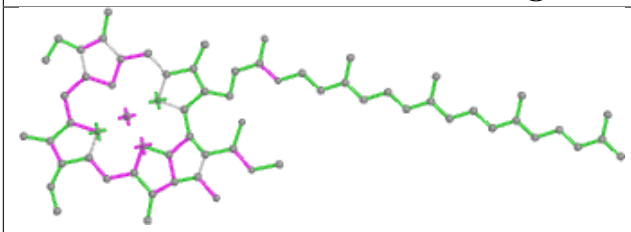
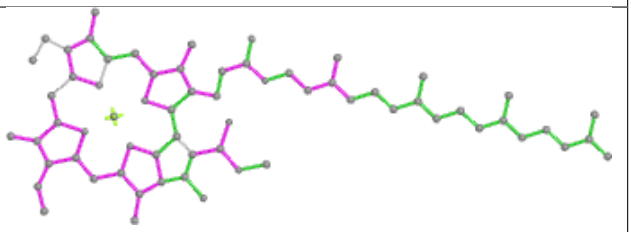
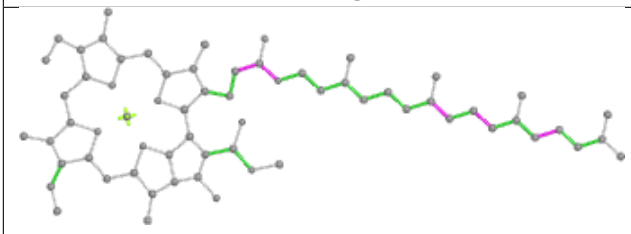
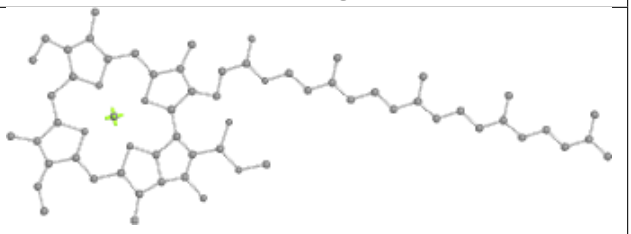
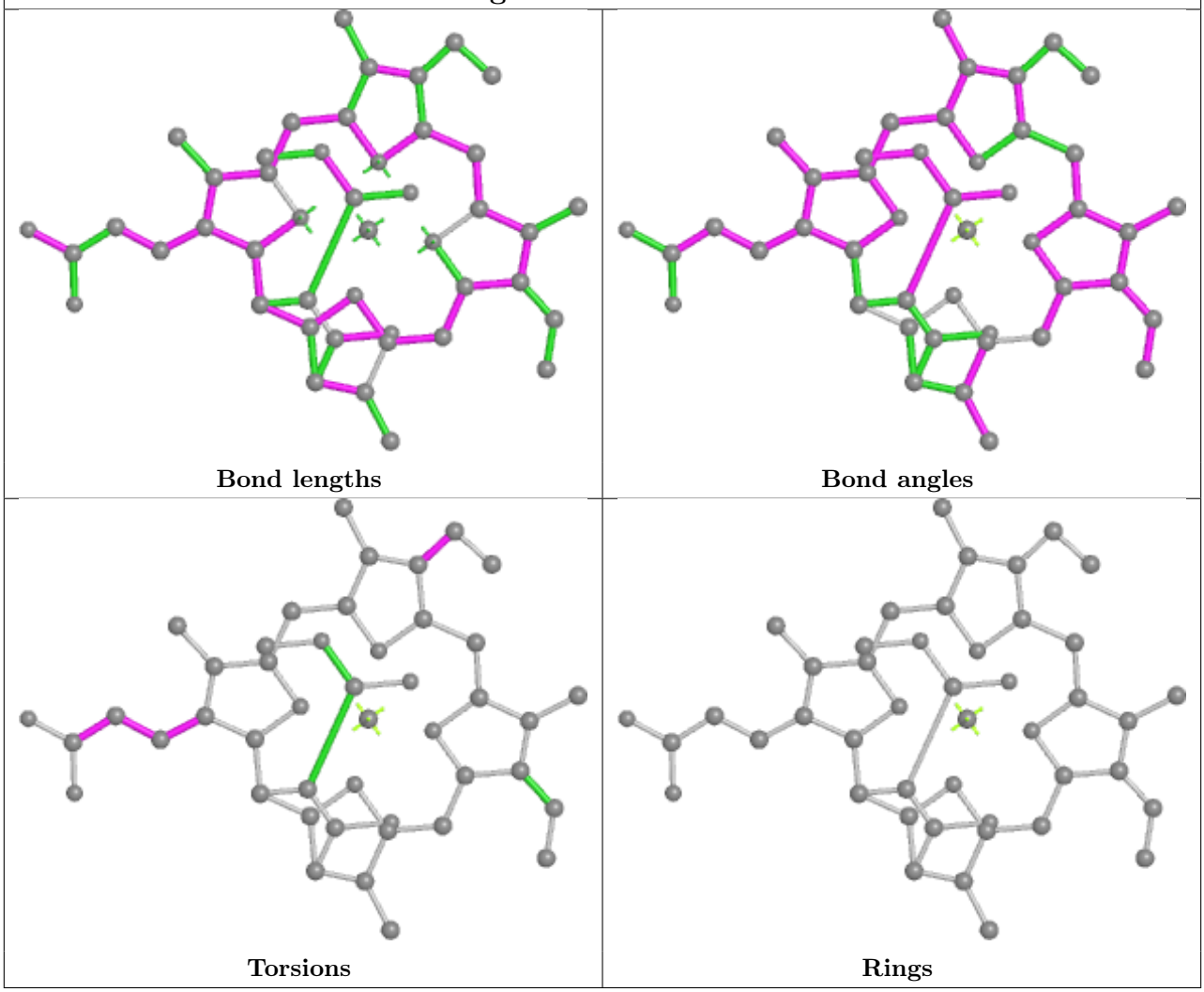
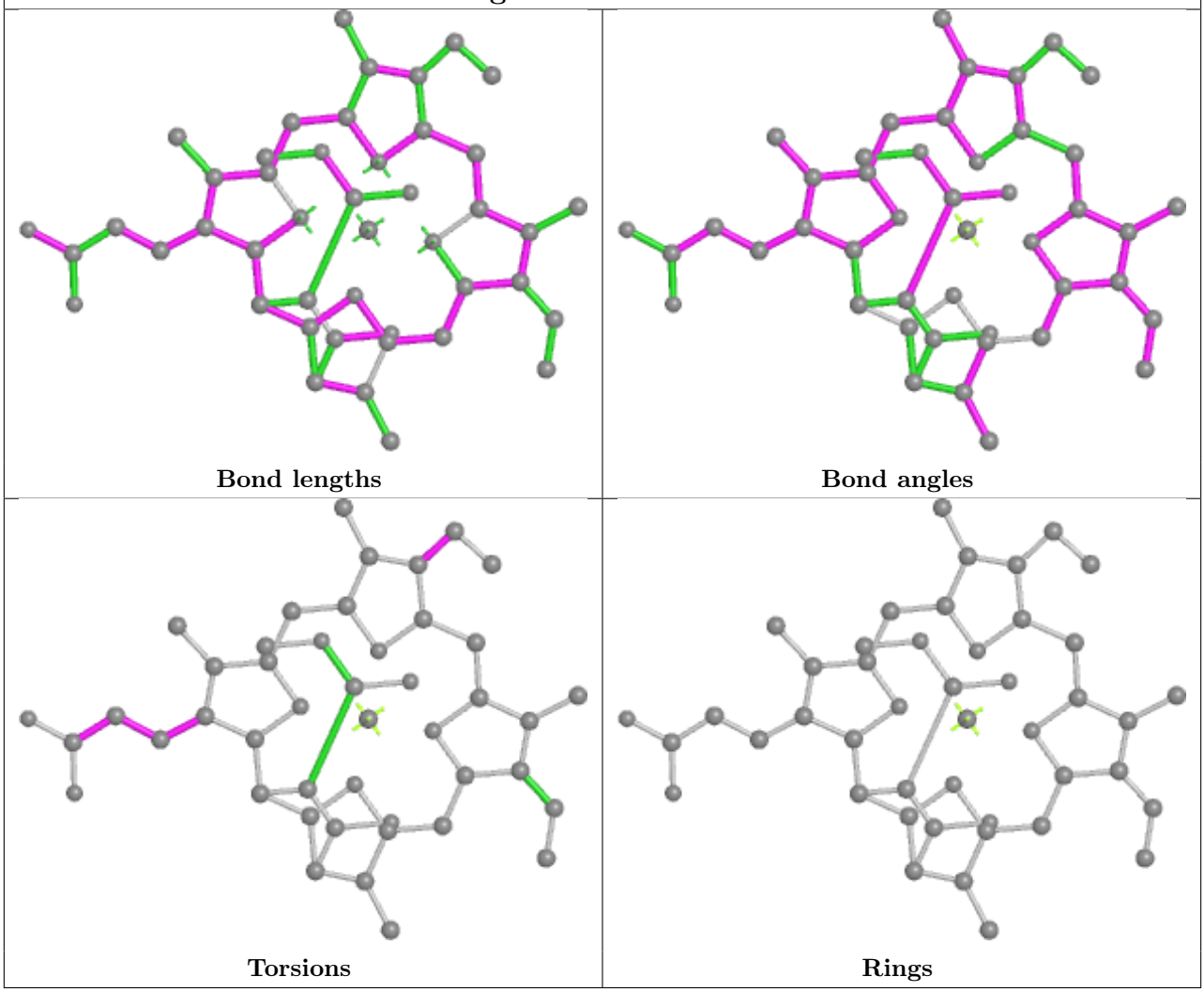
 Bond lengths	 Bond angles
 Torsions	 Rings

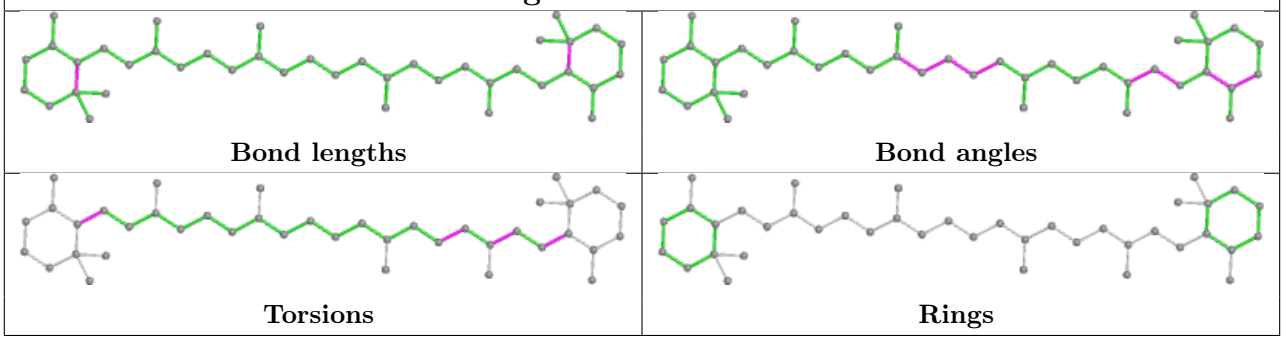
Ligand KC1 35 304



Ligand KC1 35 306



Ligand BCR C 519



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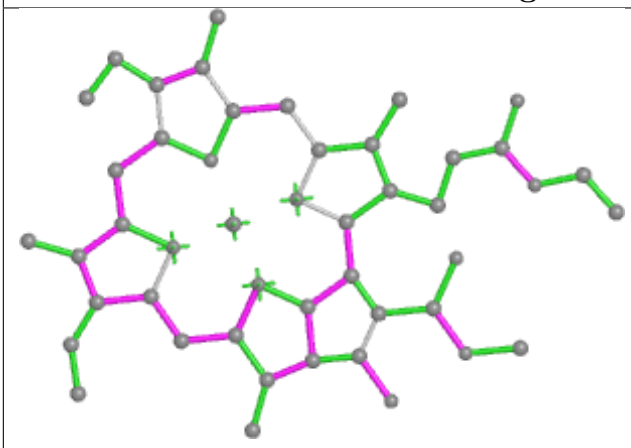
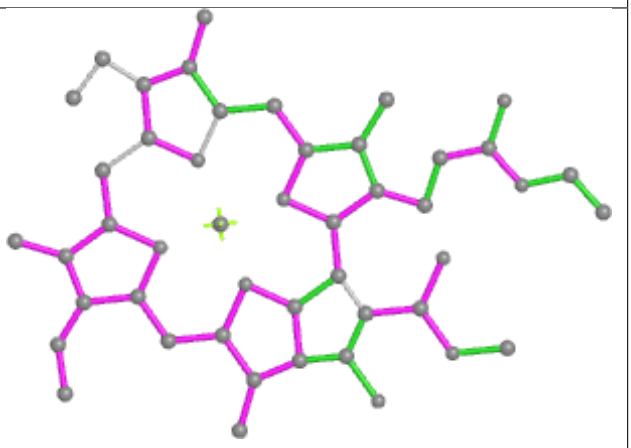
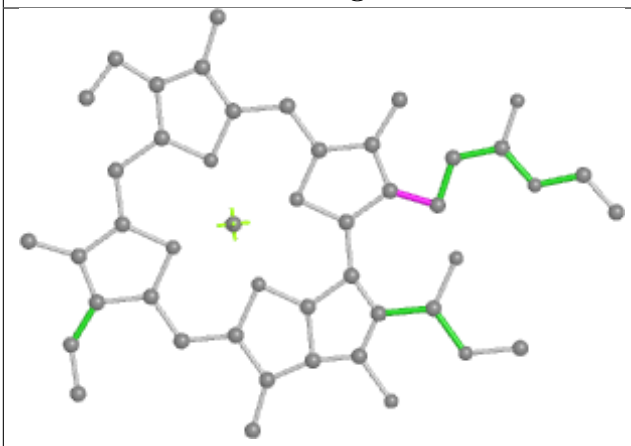
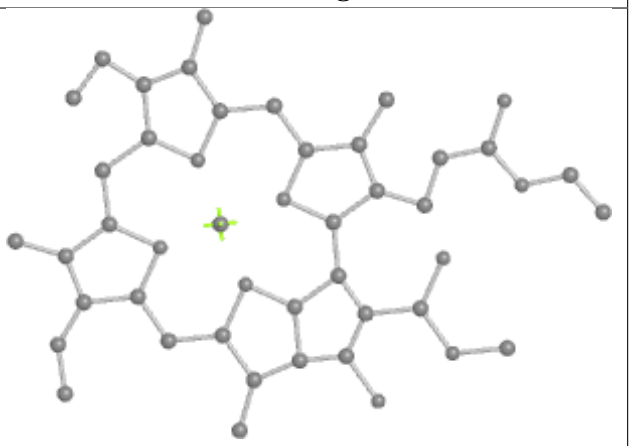
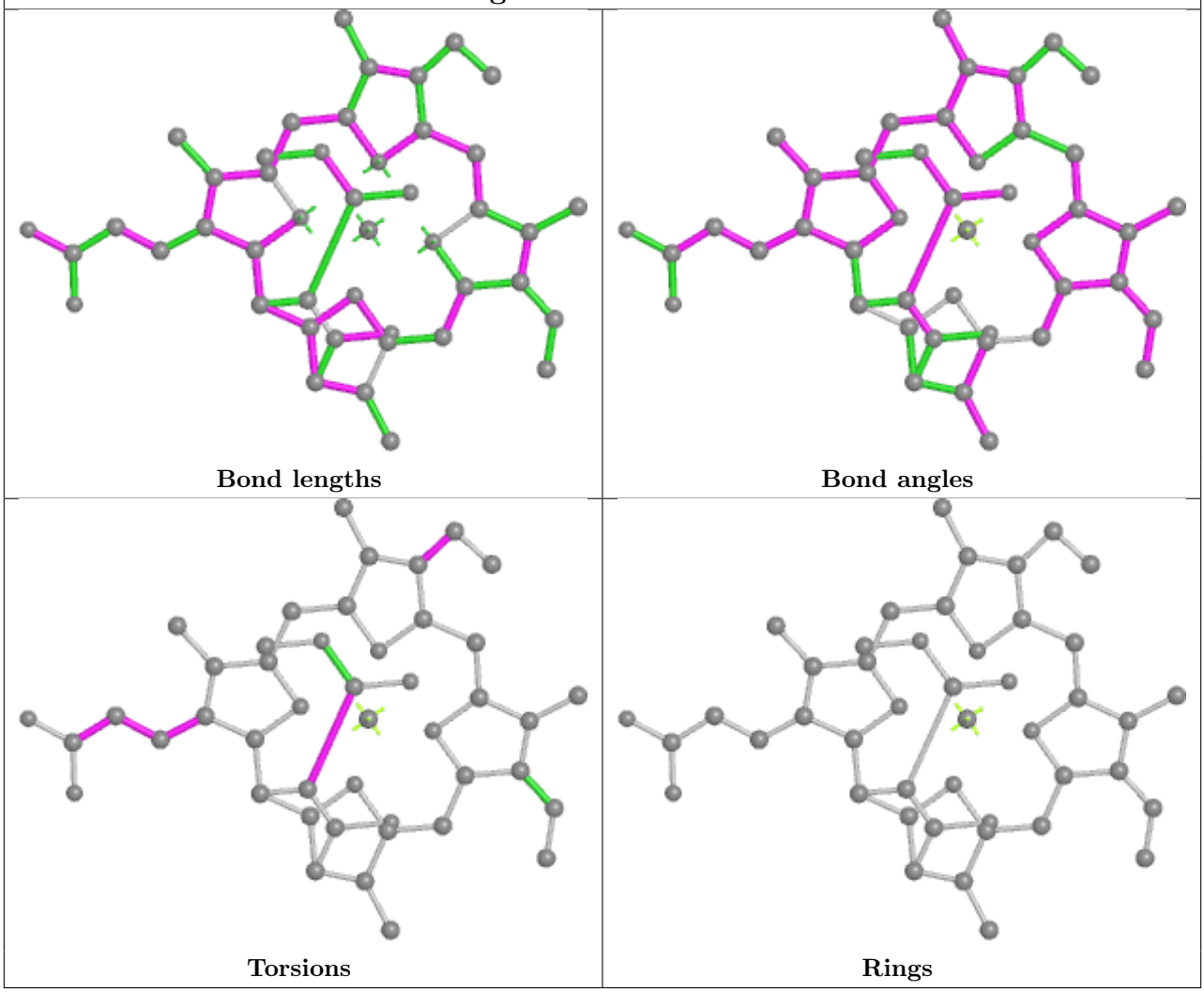
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 11 309



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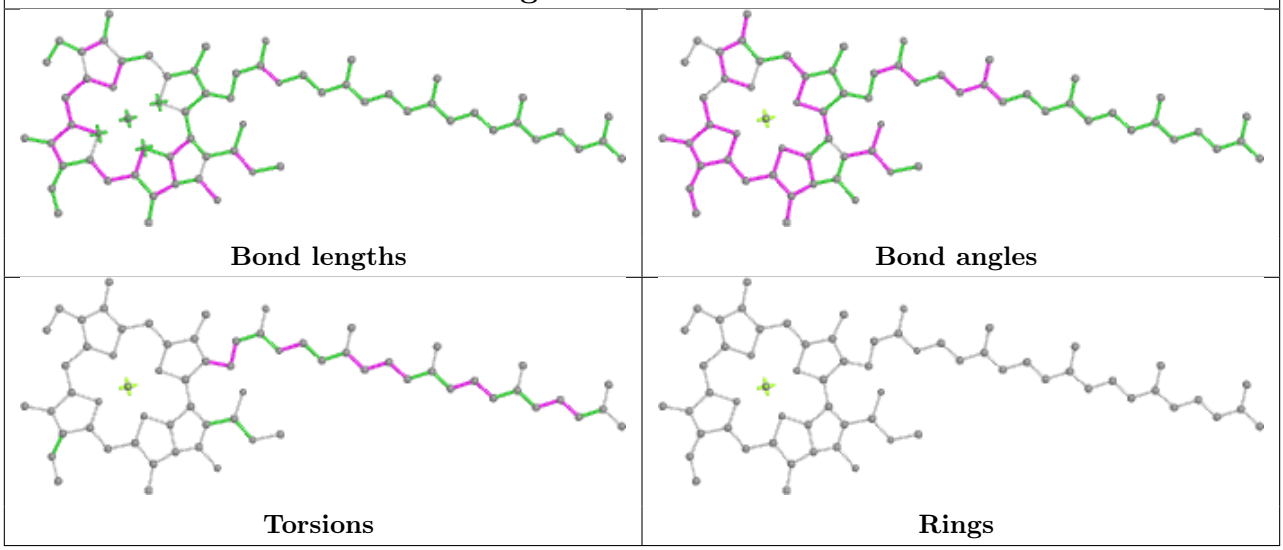

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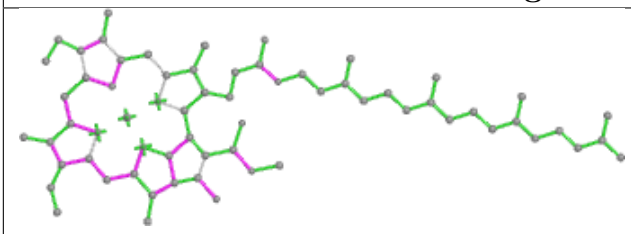
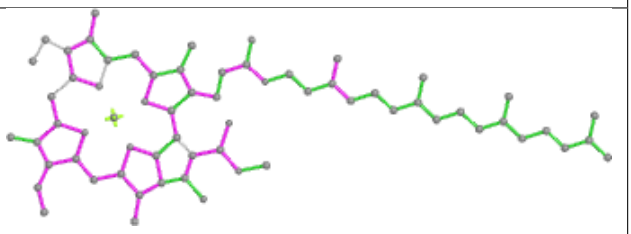
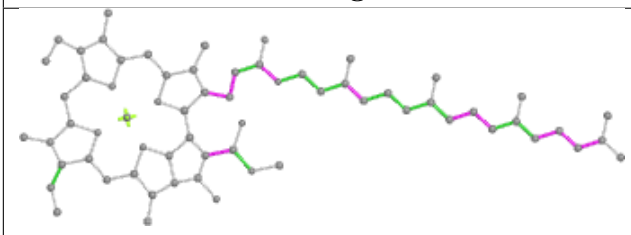
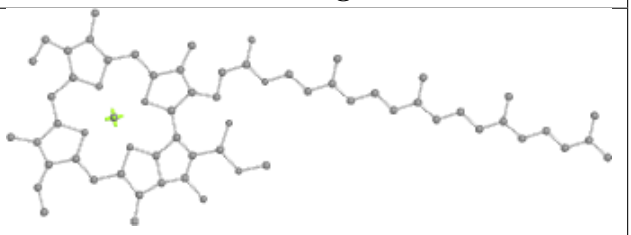
 Bond lengths	 Bond angles
 Torsions	 Rings

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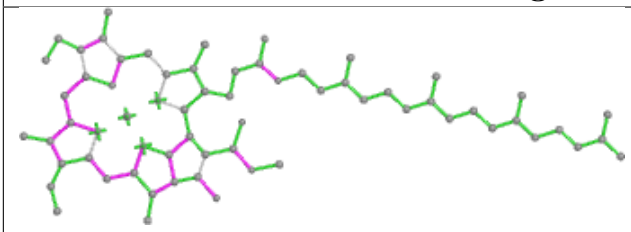
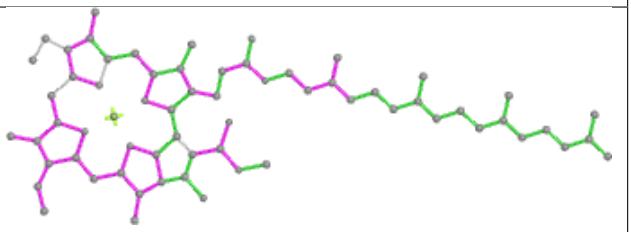
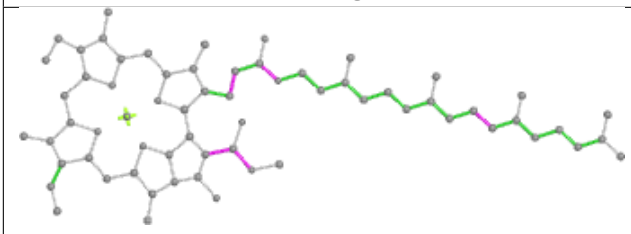
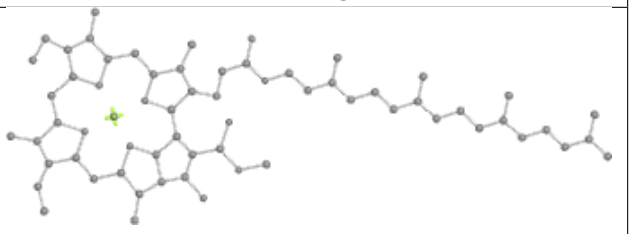
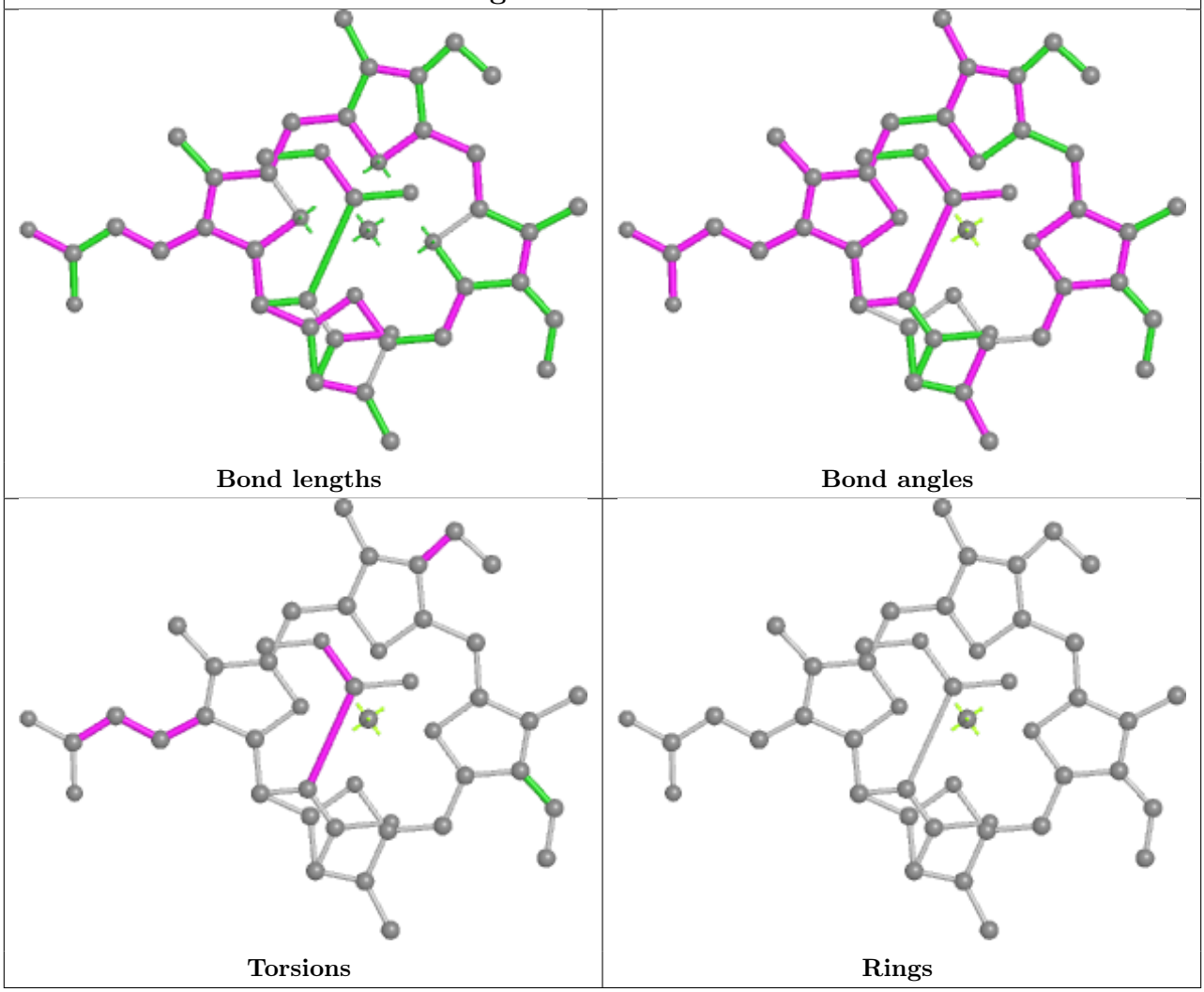
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 11 306



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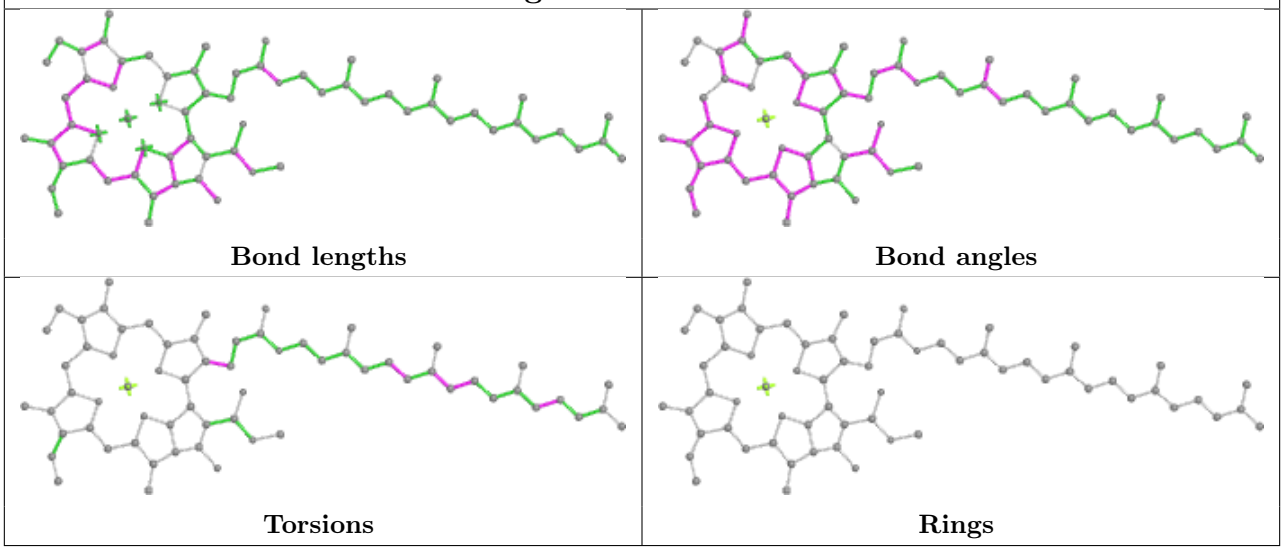

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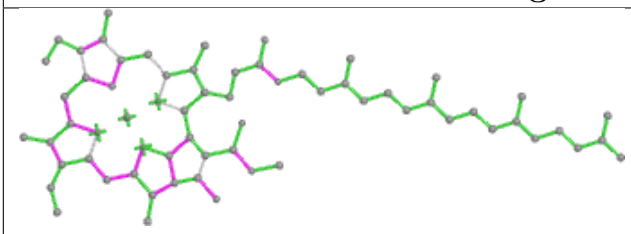

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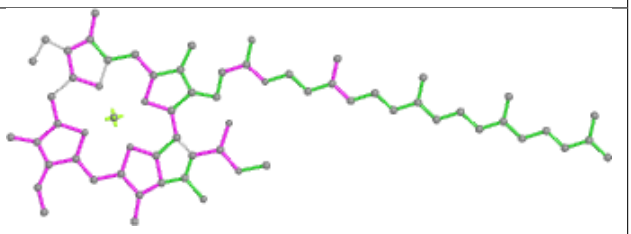

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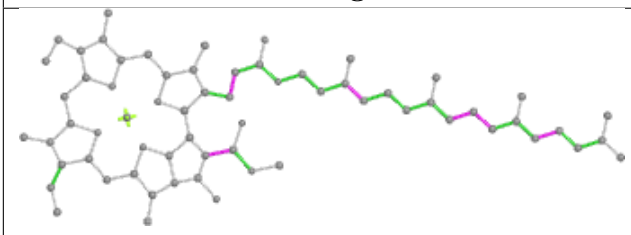
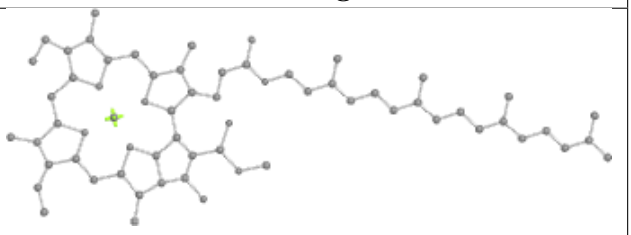


Torsions



Rings

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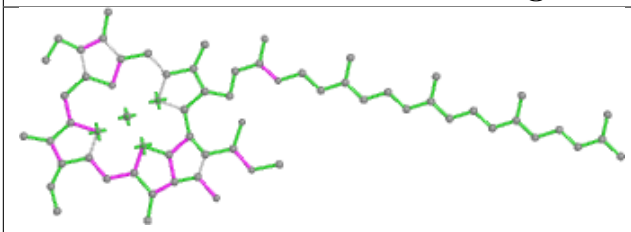

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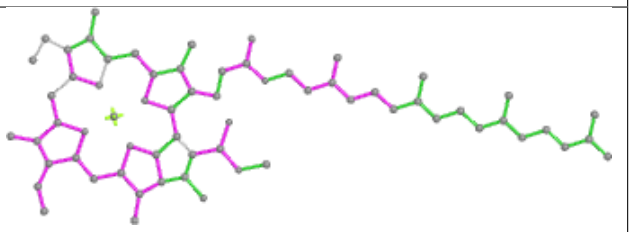

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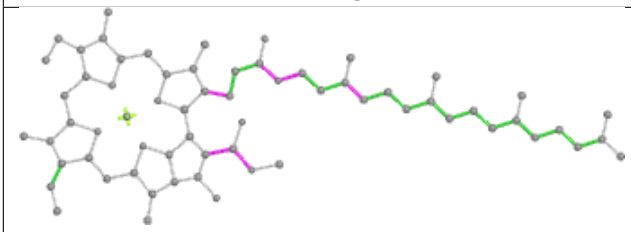

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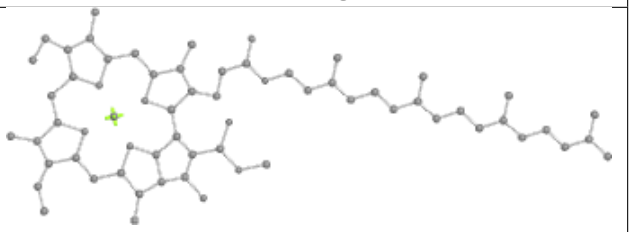

Rings

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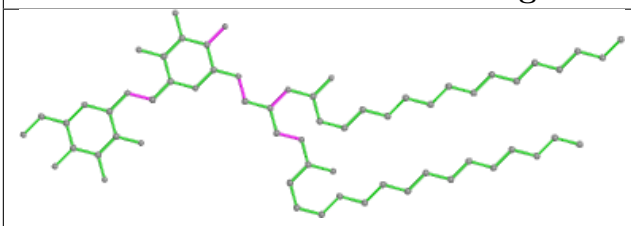

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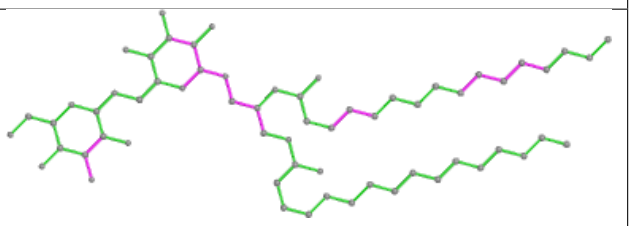

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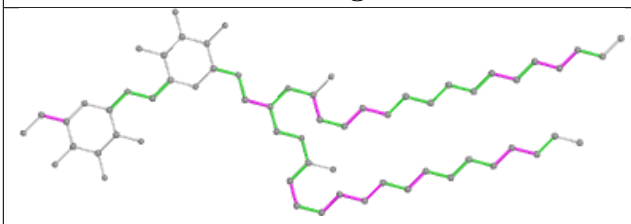

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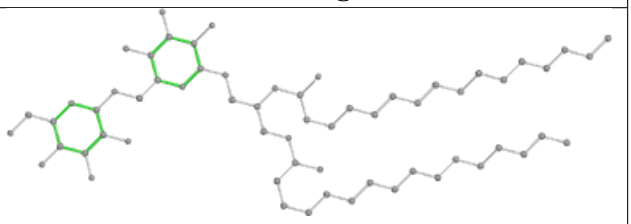
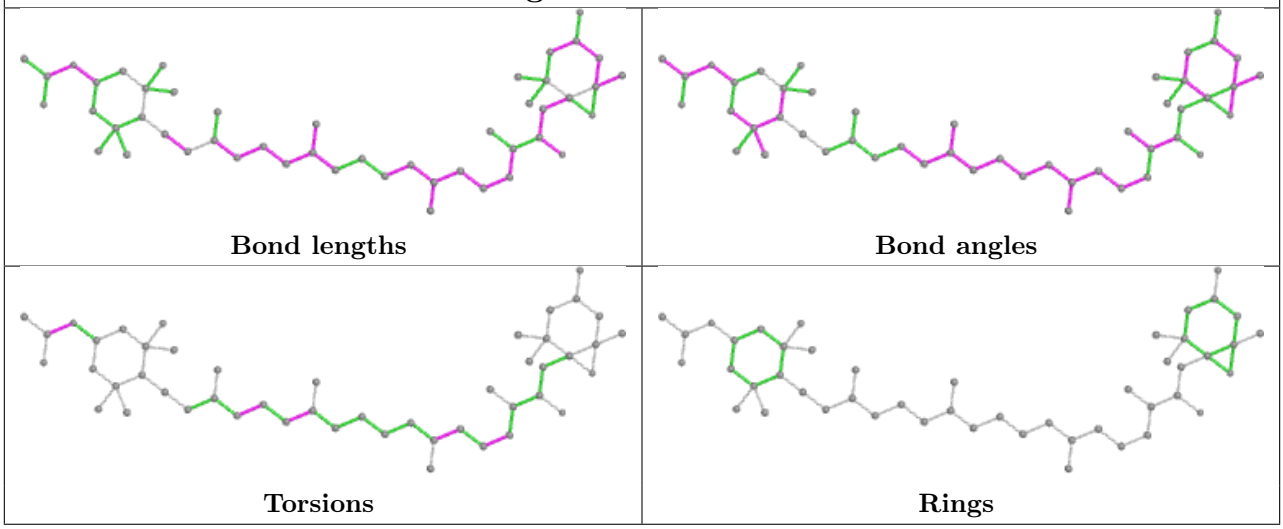


Rings

Ligand A86 33 312



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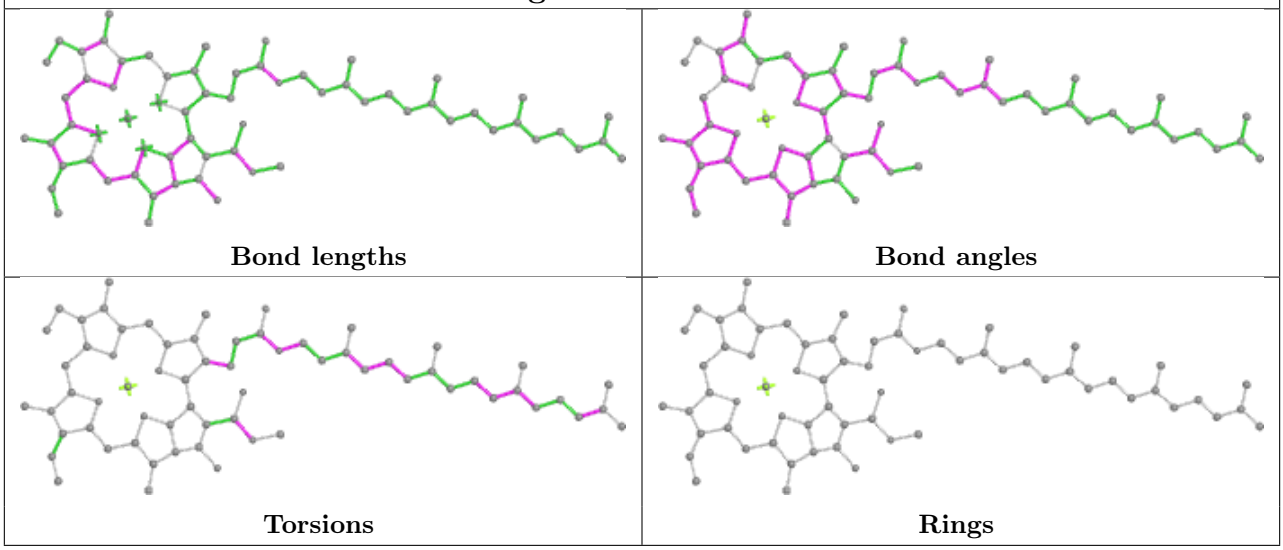

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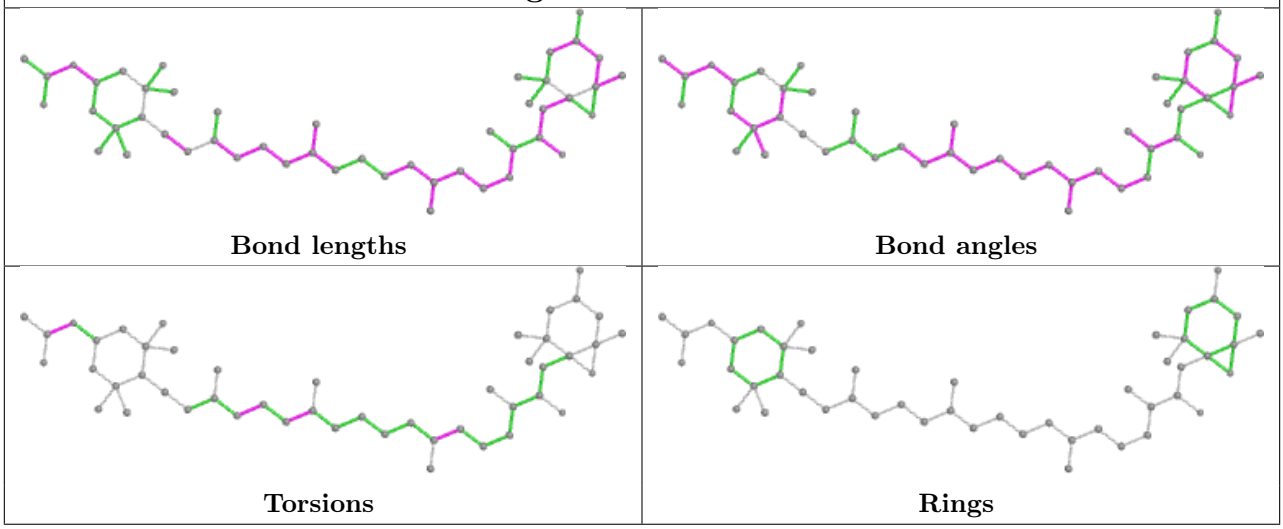

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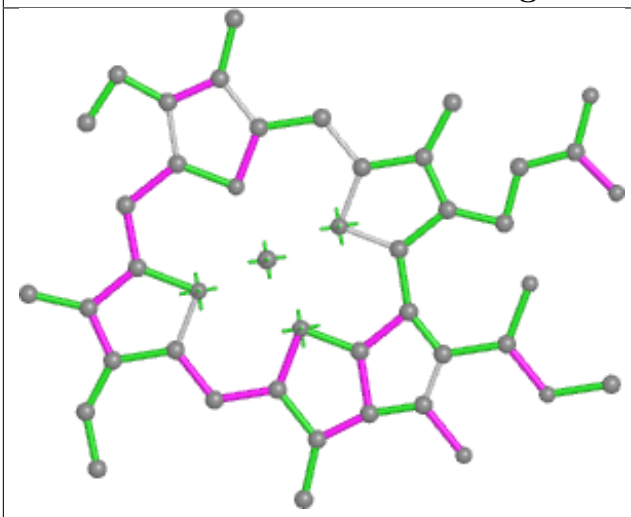

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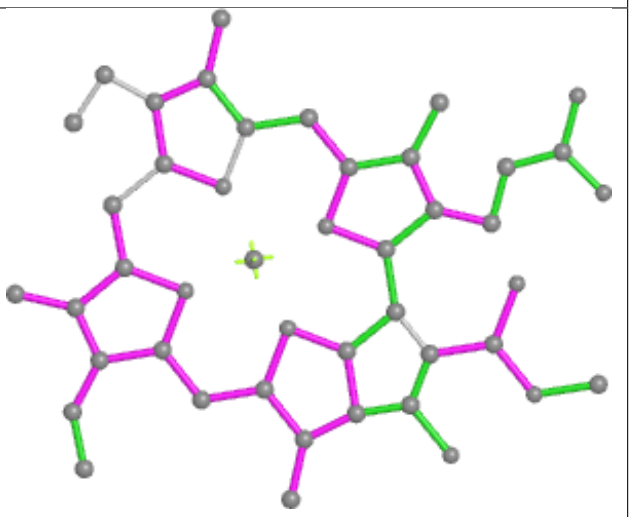

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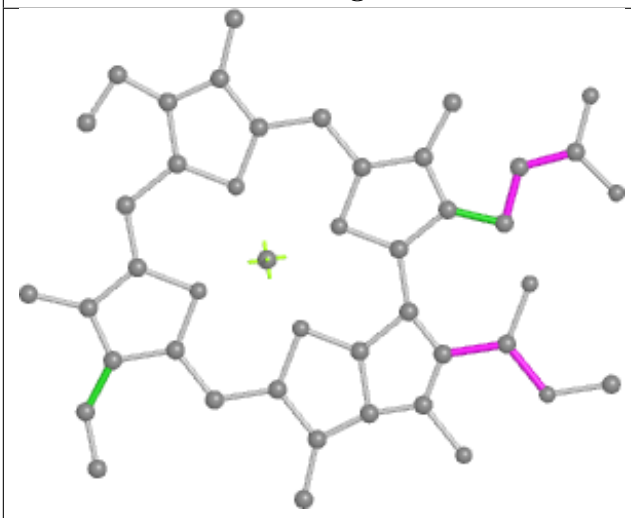

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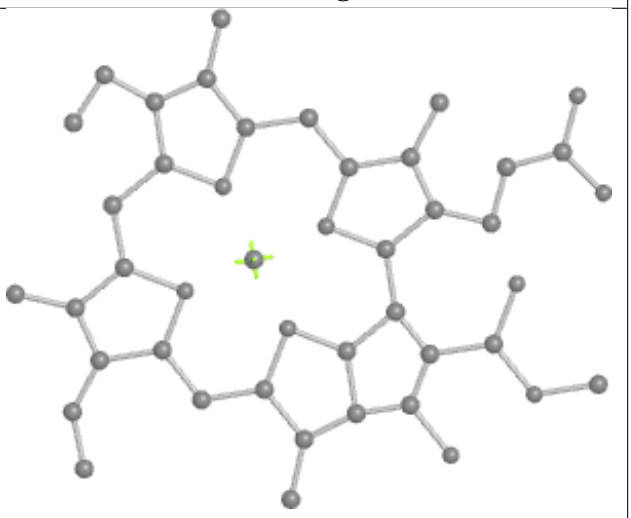

Rings

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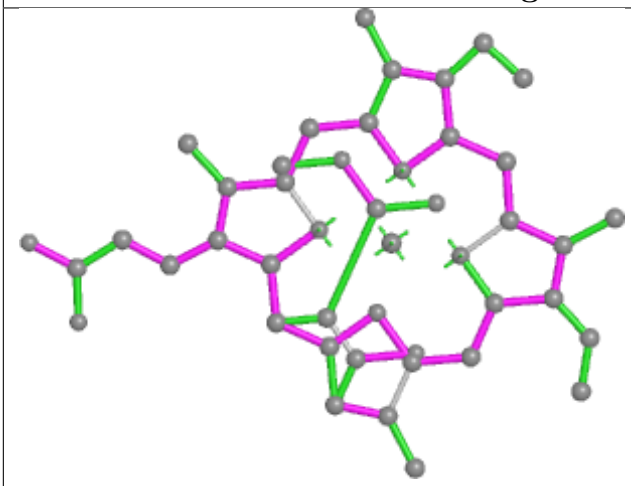

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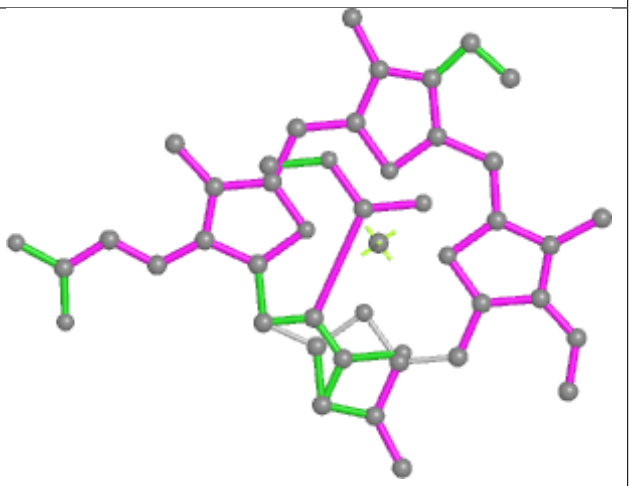

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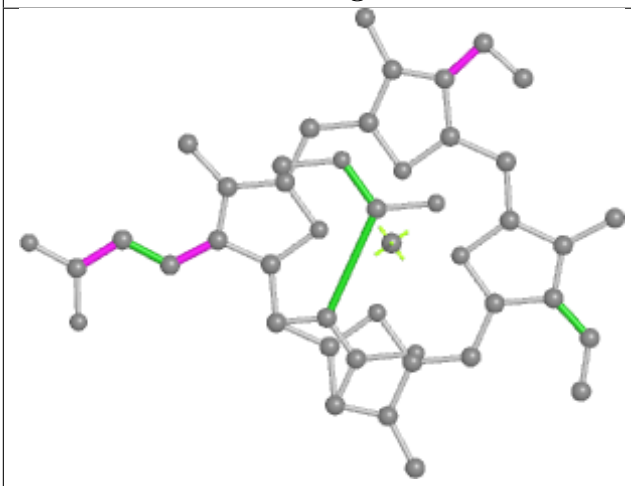

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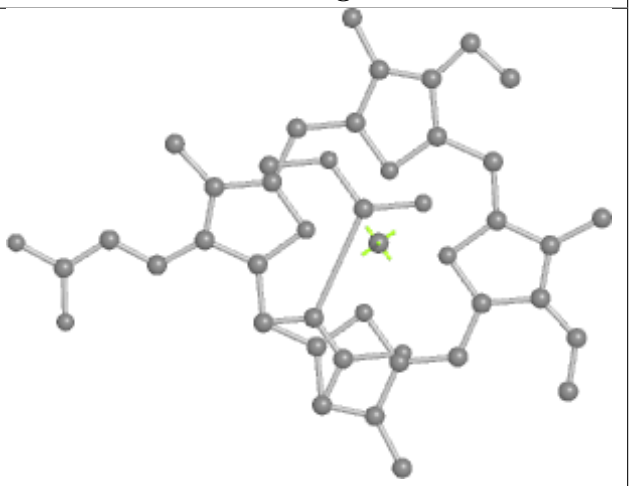

Rings

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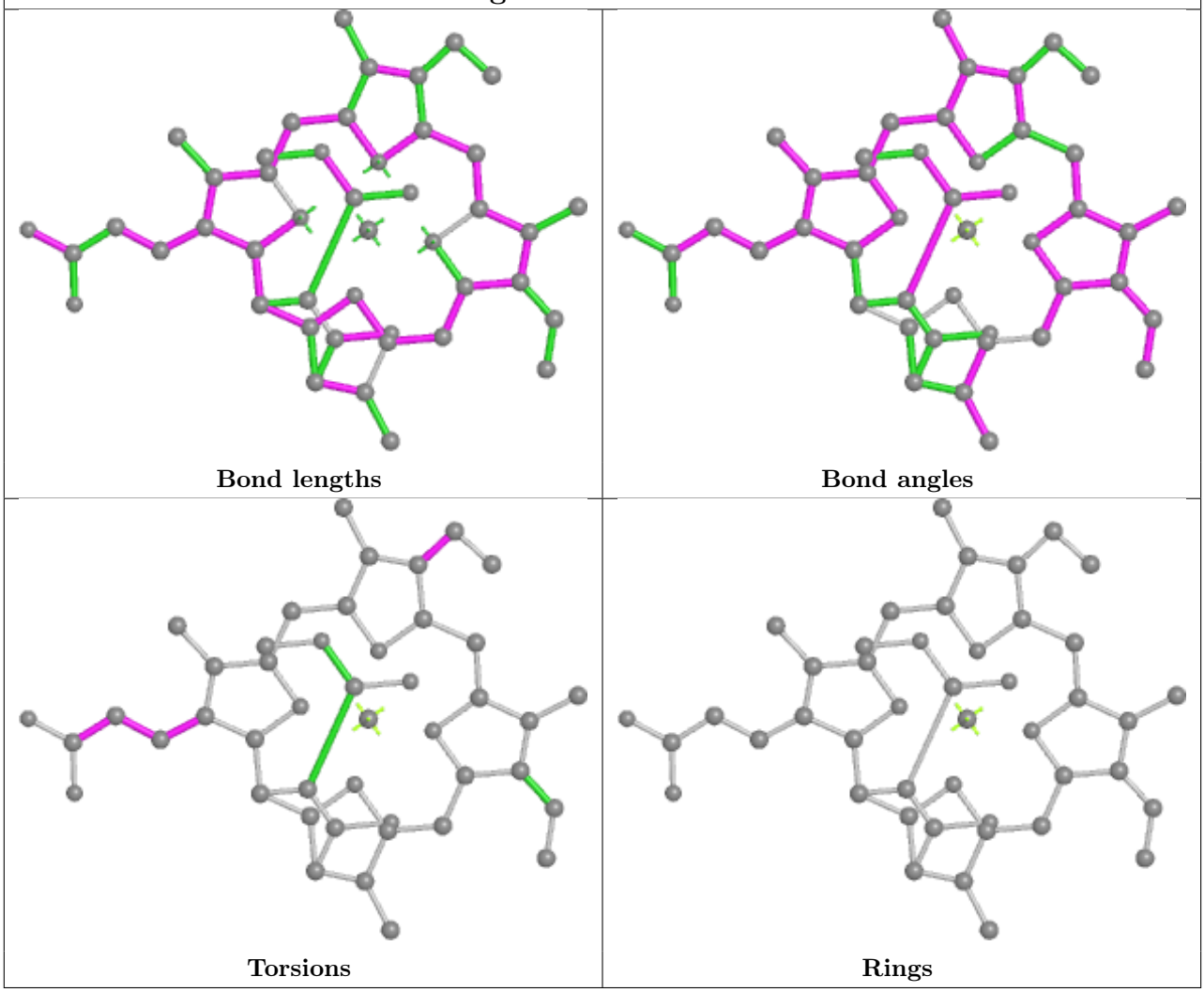

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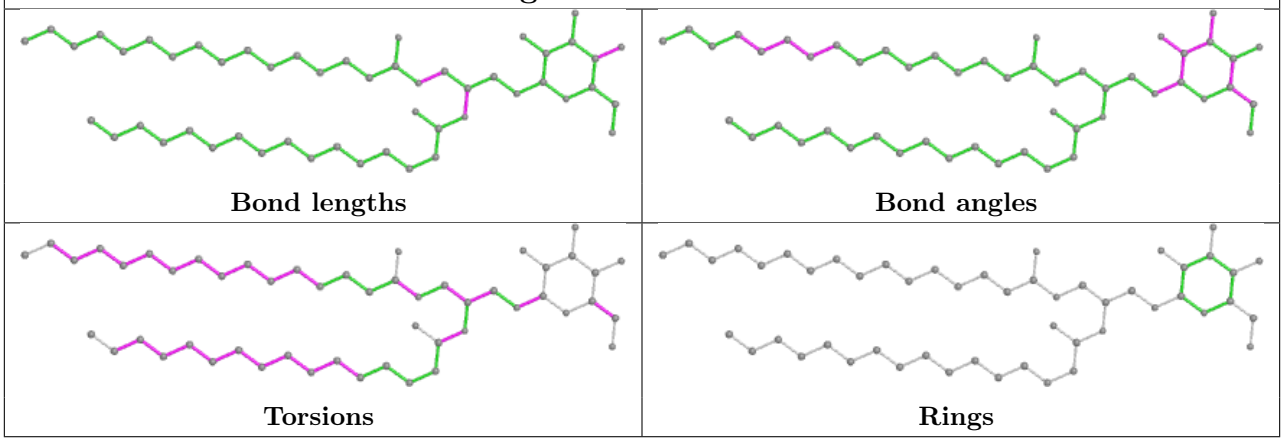
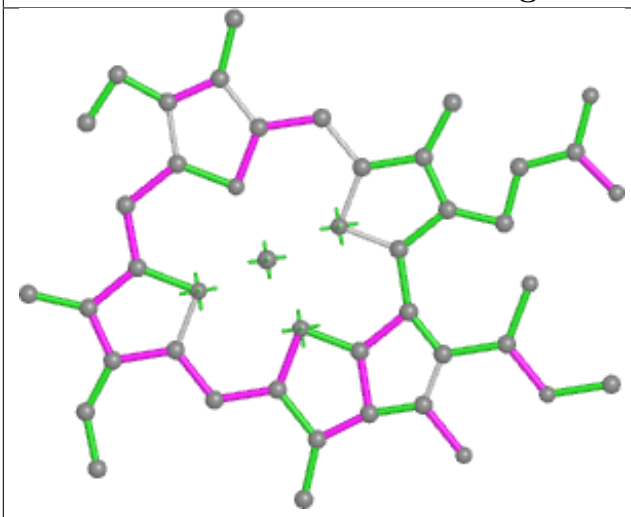


Ligand CLA 13 305



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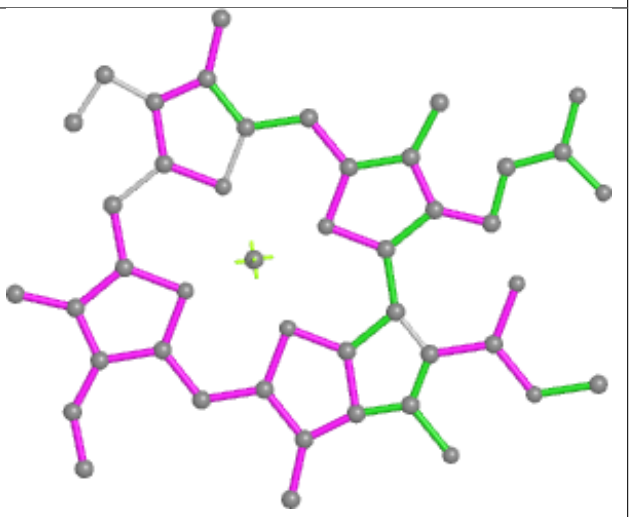
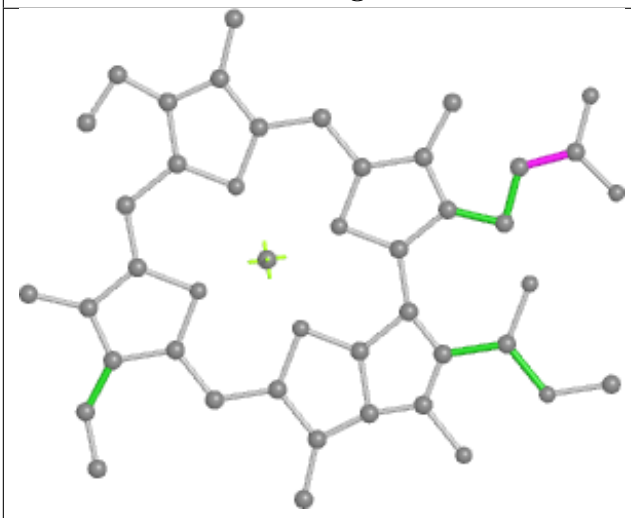


Bond angles



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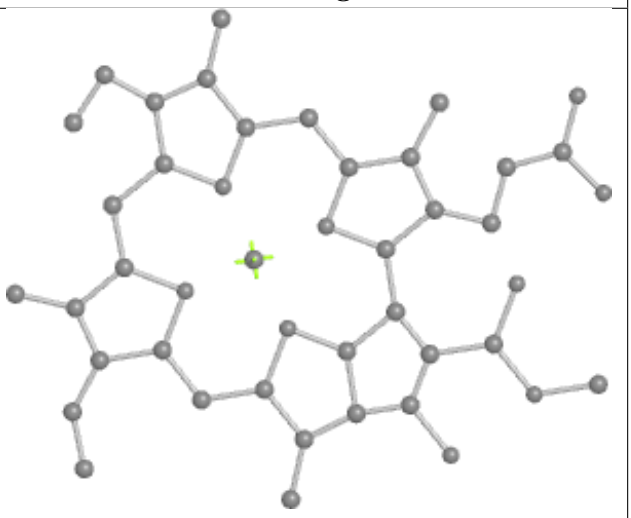
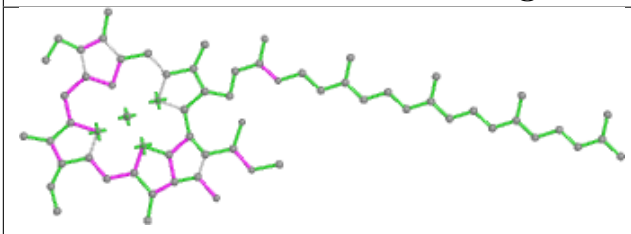


Rings

Ligand CLA W 101



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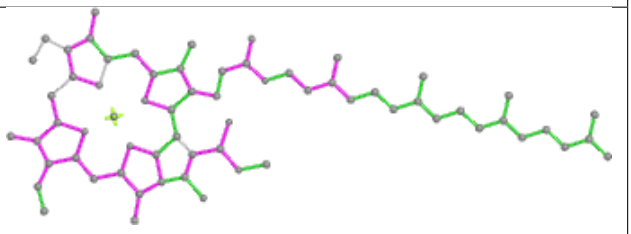

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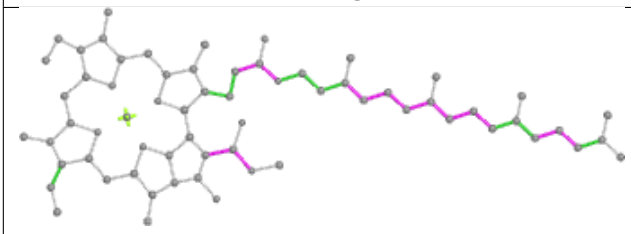

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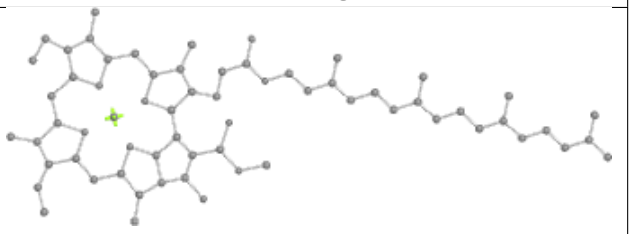
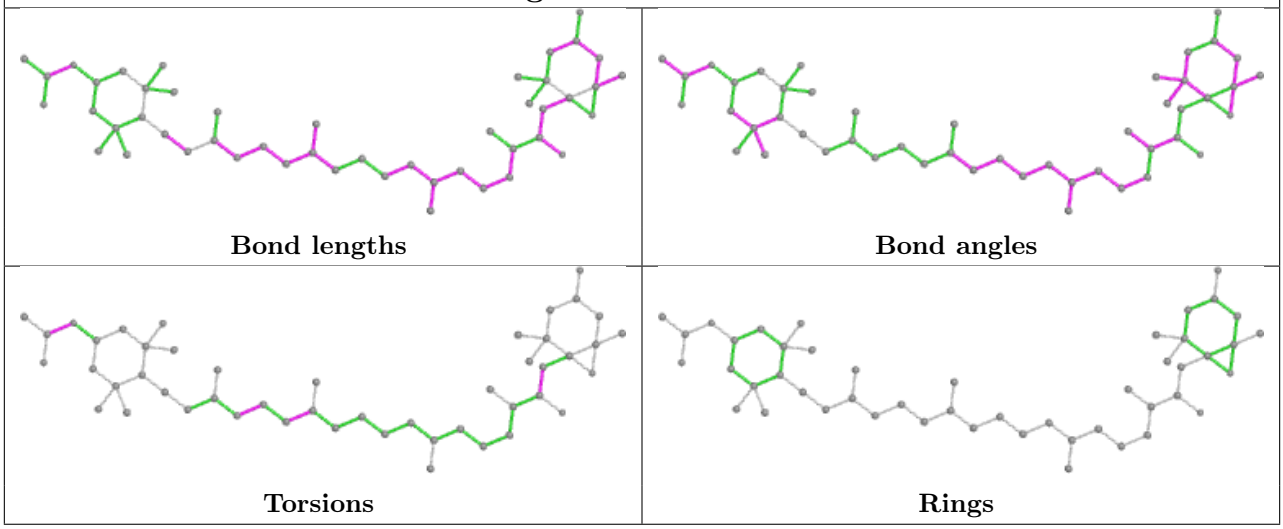


Rings

Ligand A86 15 311



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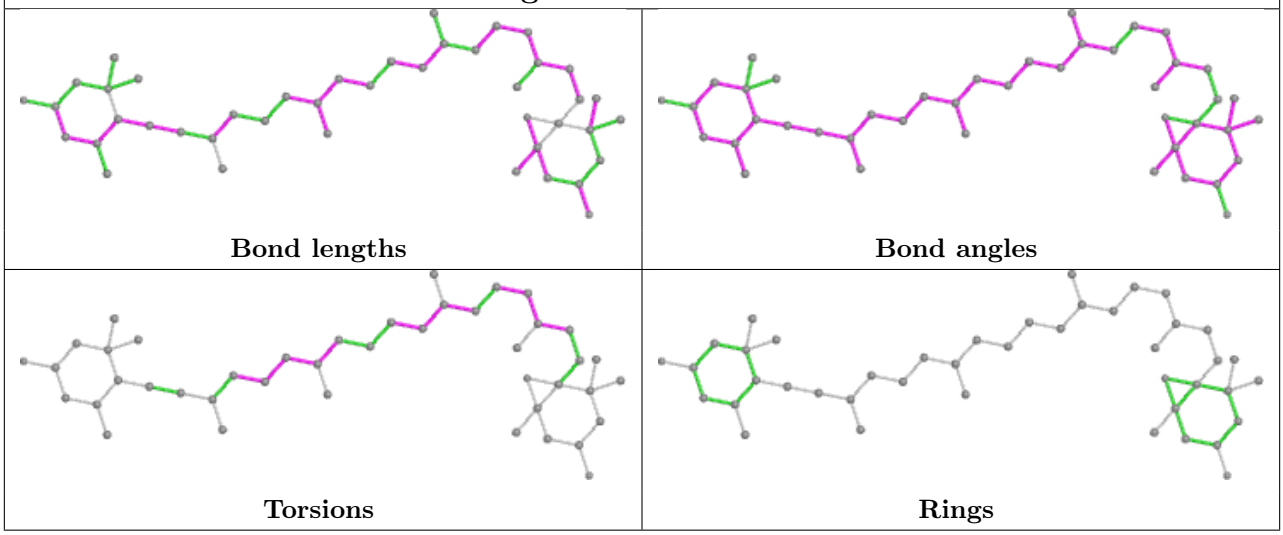

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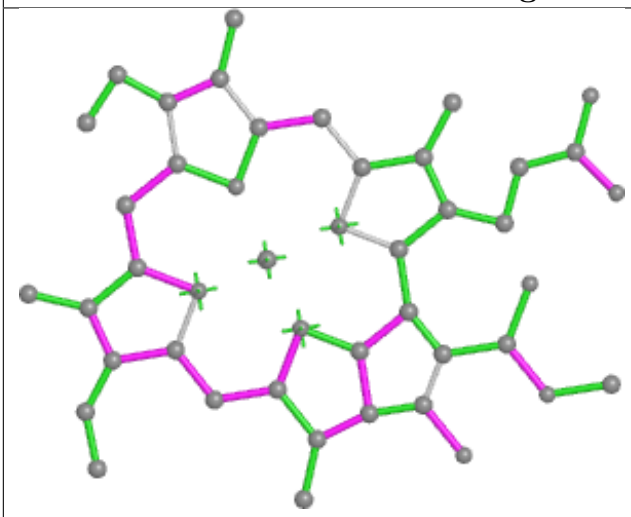

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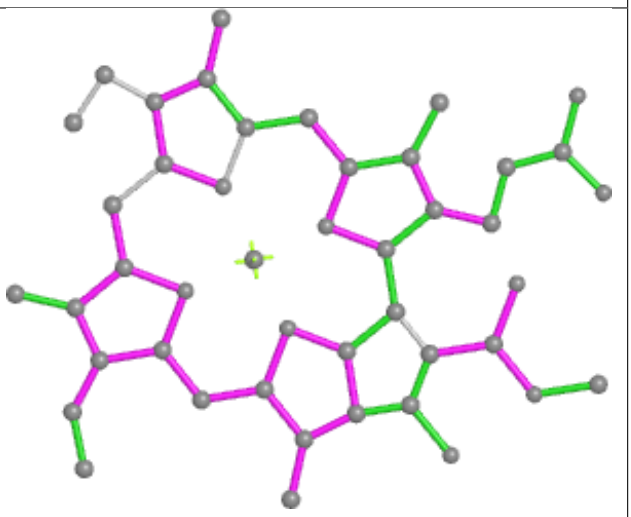

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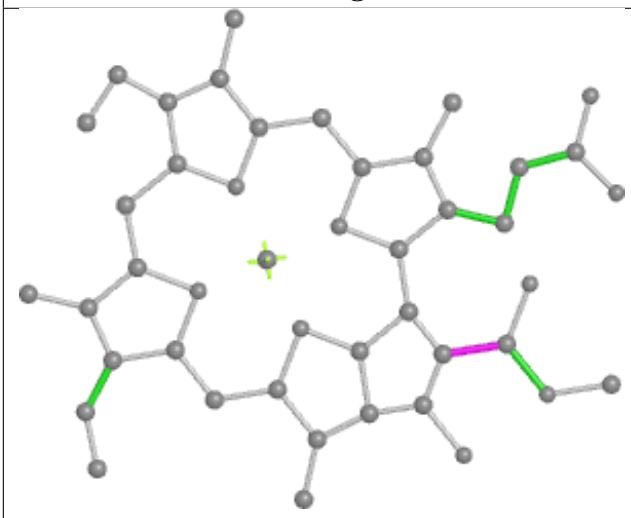

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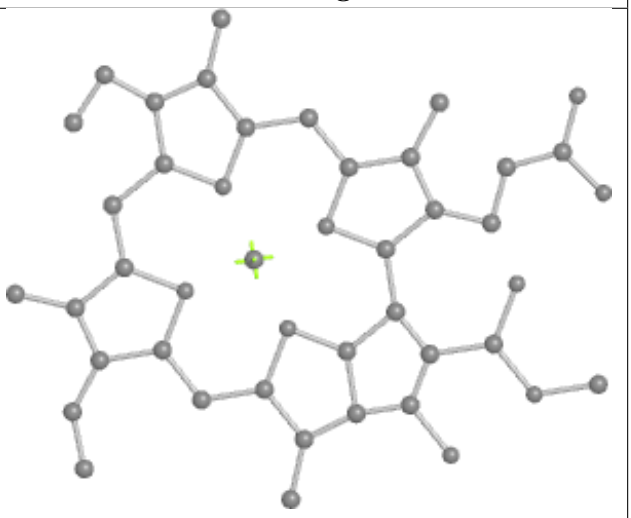

Rings

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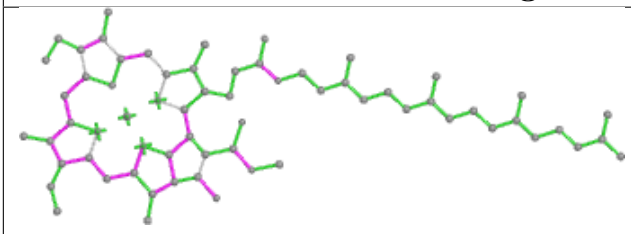

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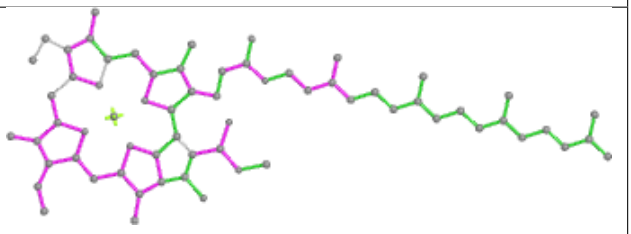

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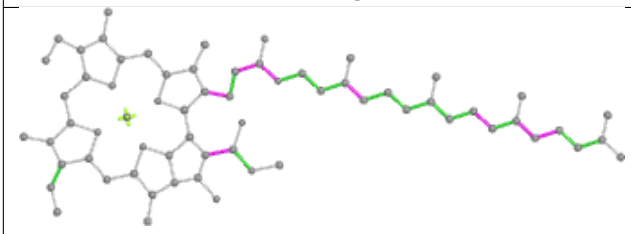

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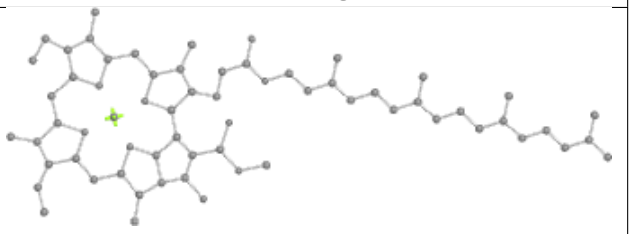
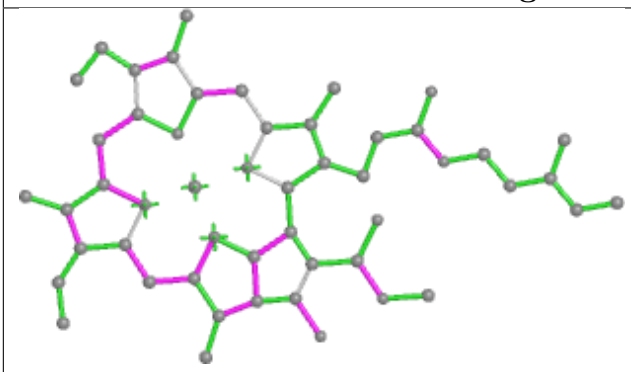


Rings

Ligand CLA 39 305



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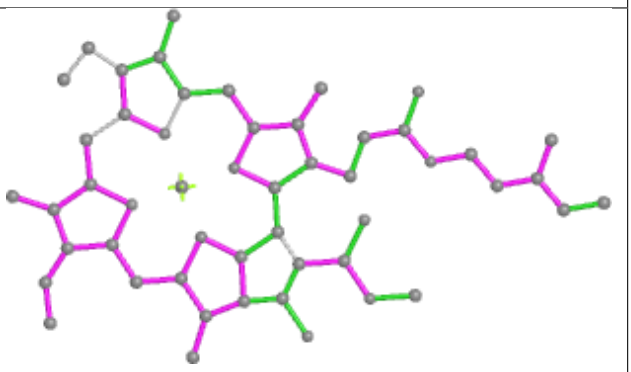

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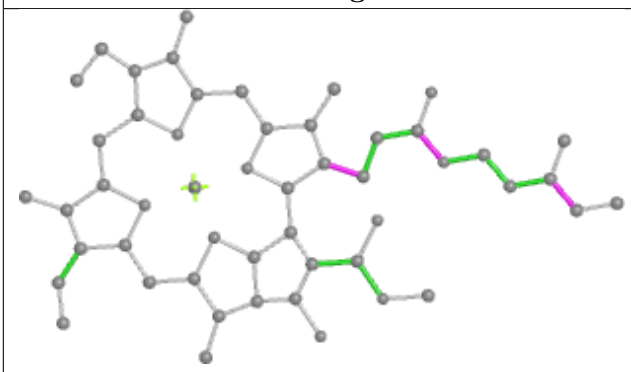

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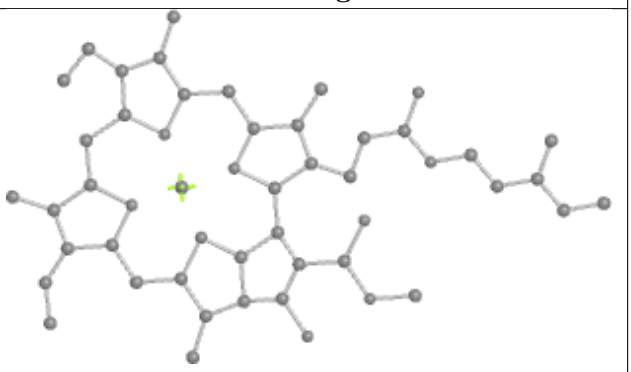
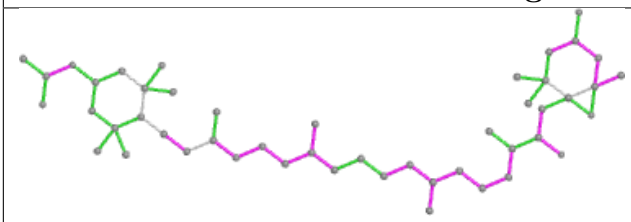
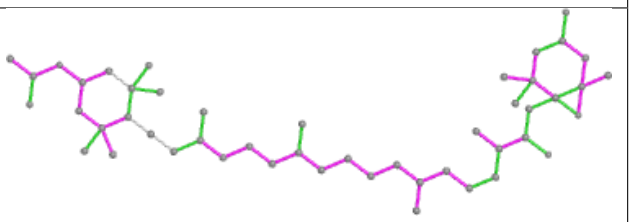


Rings

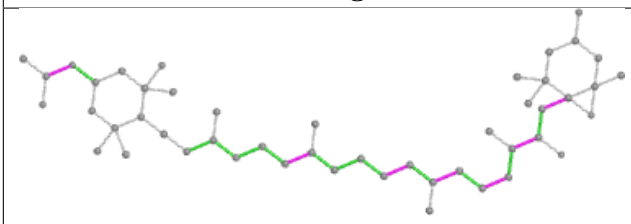
Ligand A86 12 202



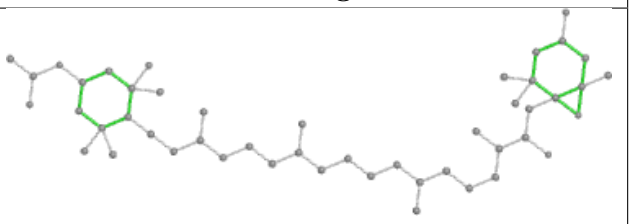
Bond lengths



Bond angles

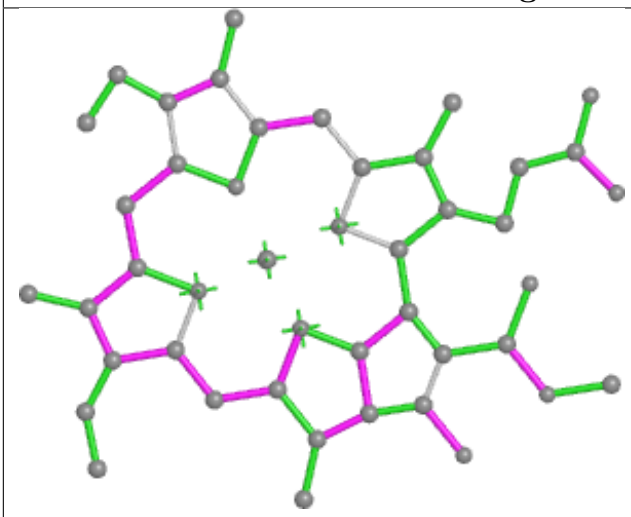


Torsions



Rings

Ligand CLA 40 209



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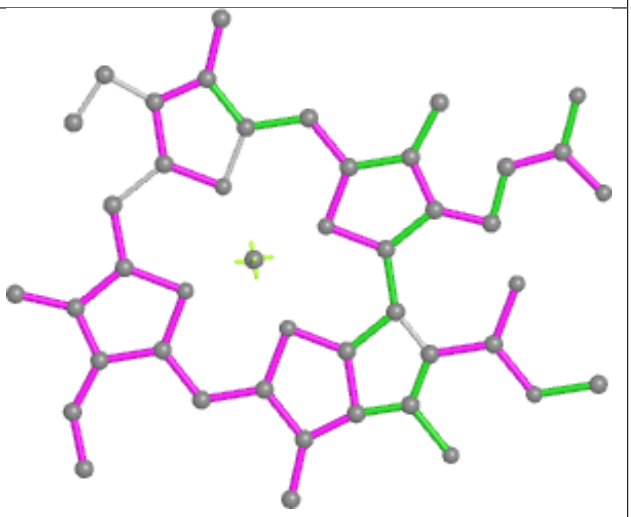

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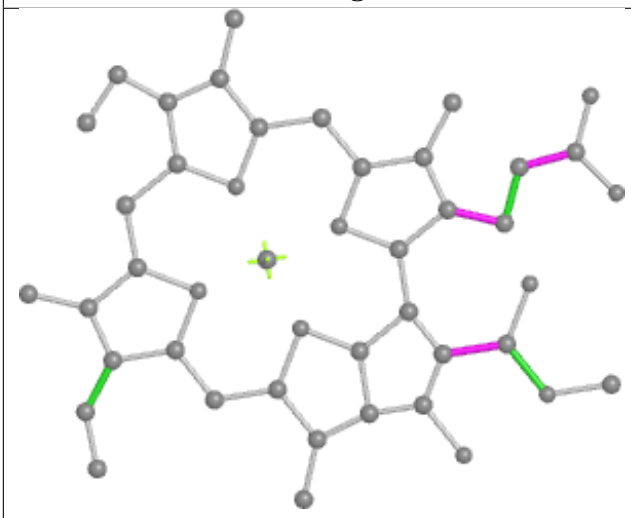

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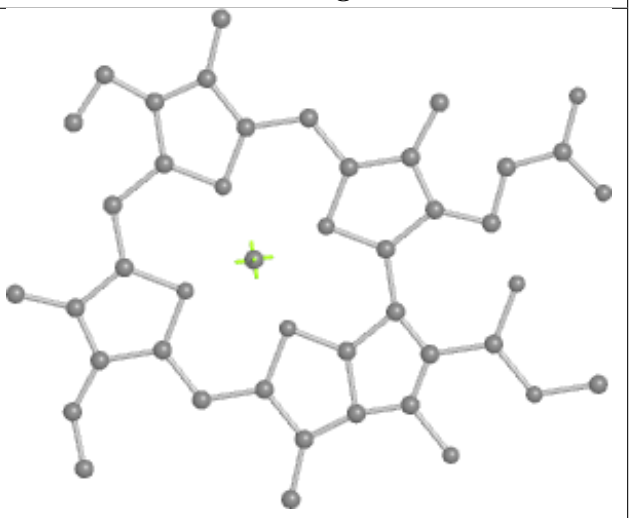

Rings

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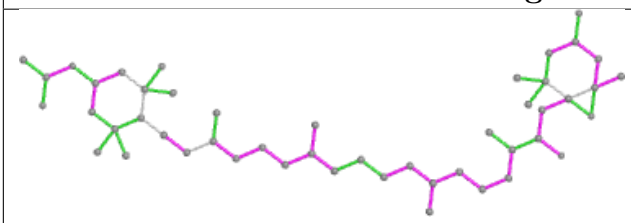

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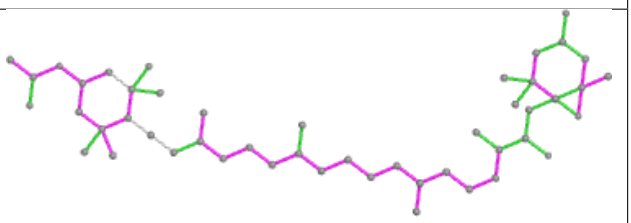

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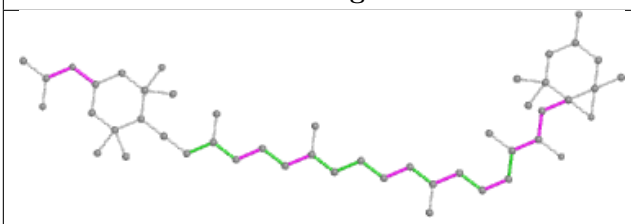

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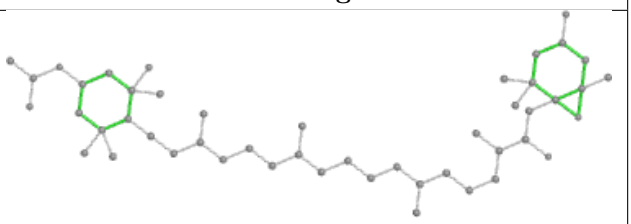

Rings

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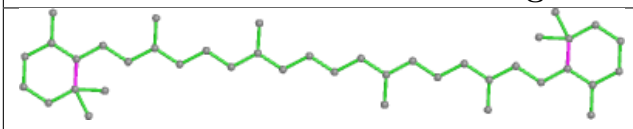

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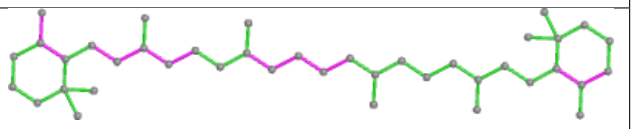

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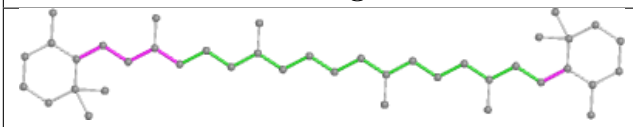

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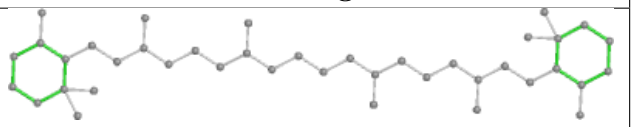

Rings

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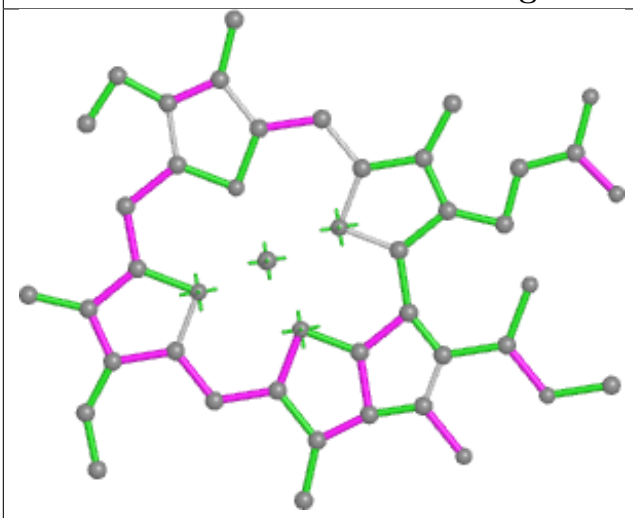

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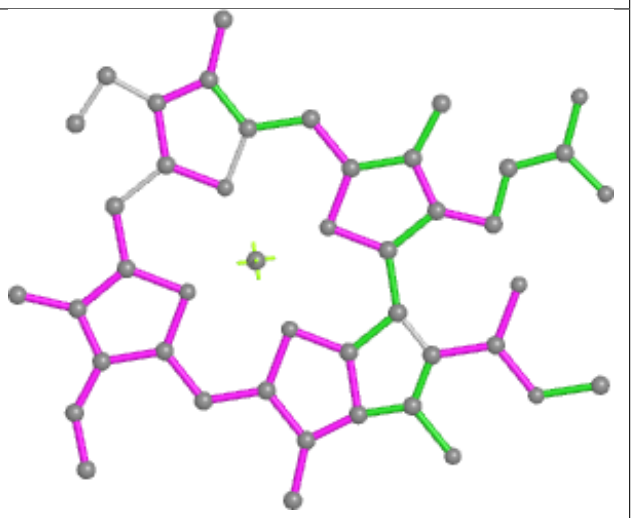

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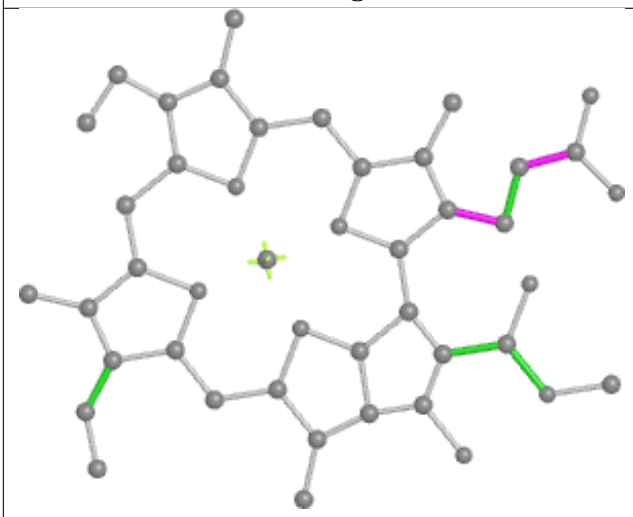

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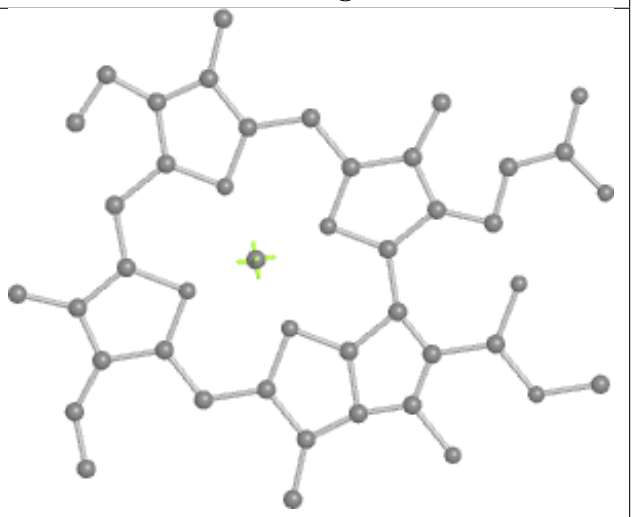

Rings

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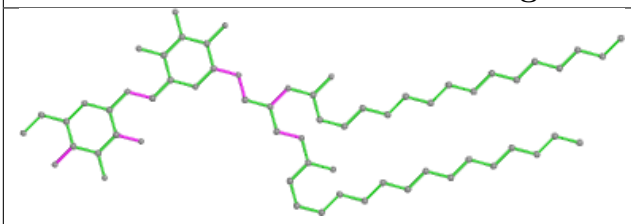

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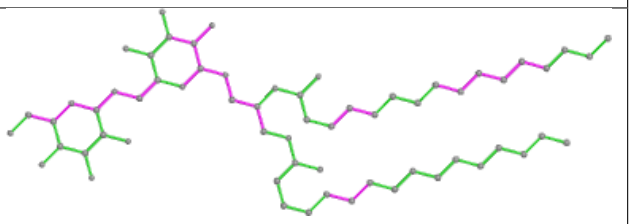

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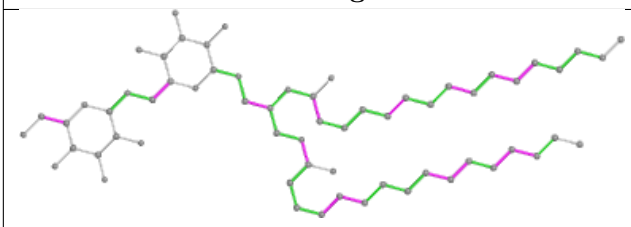

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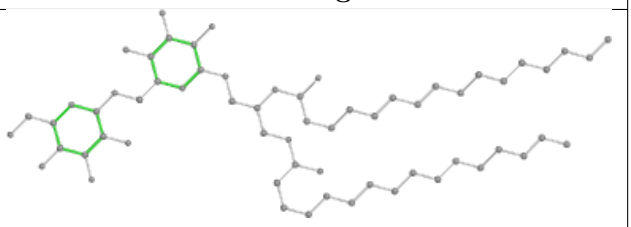

Rings

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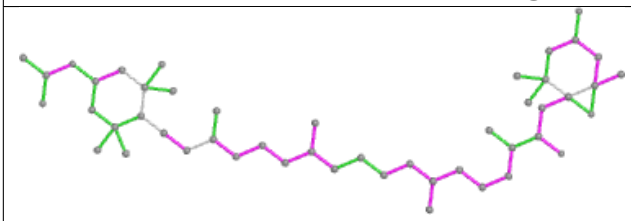

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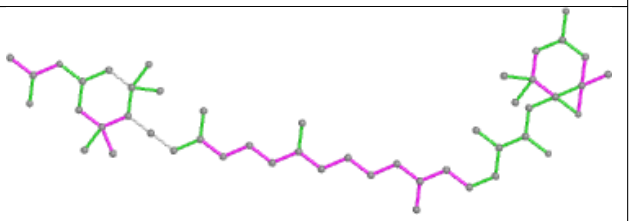

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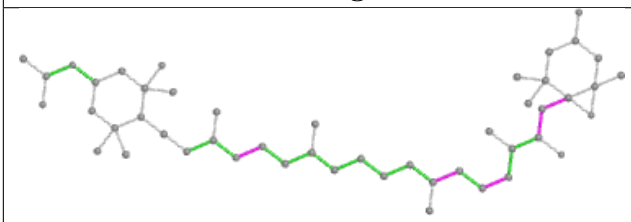

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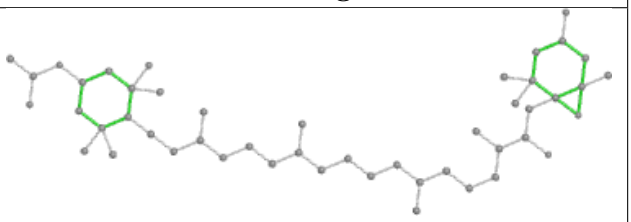

Rings

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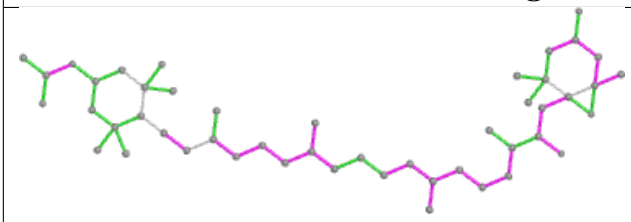

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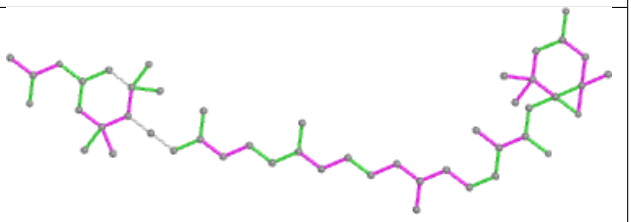

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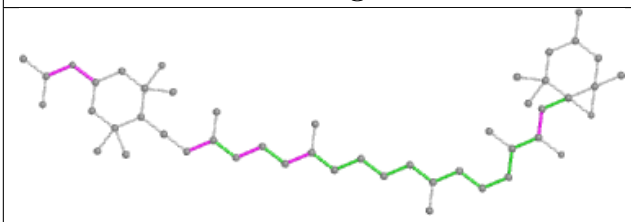

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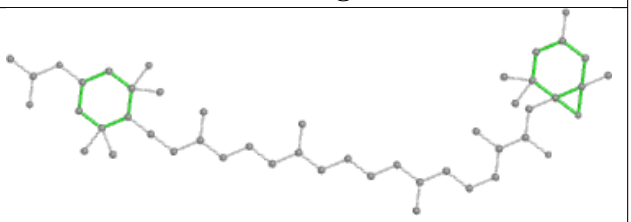

Rings

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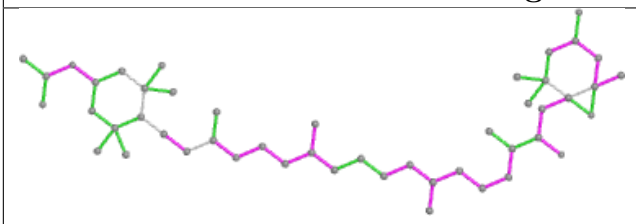
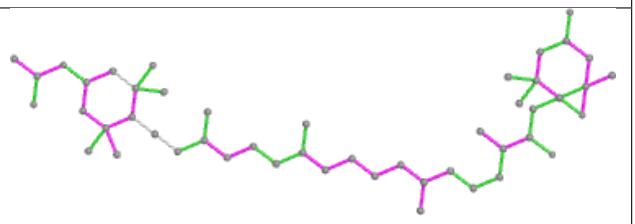
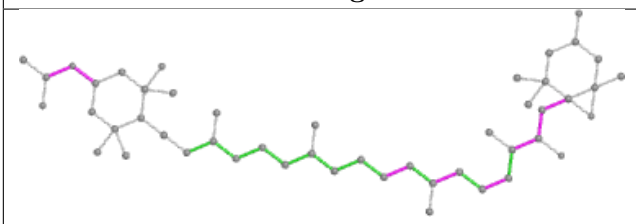
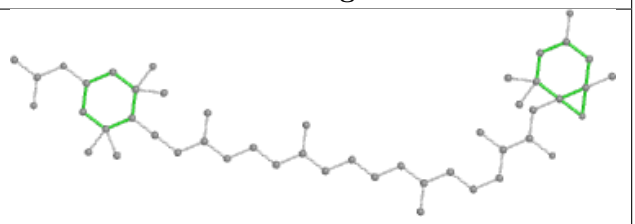
 Bond lengths	 Bond angles
 Torsions	 Rings

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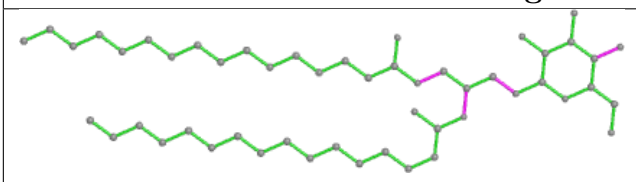
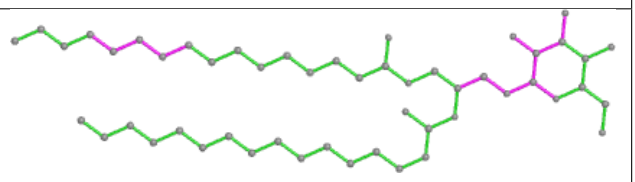
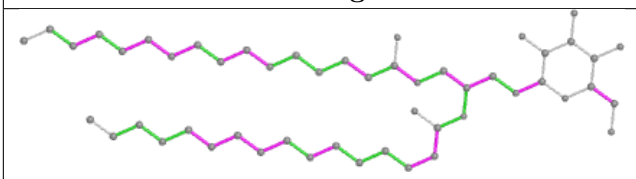
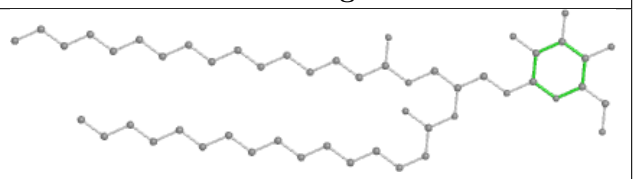
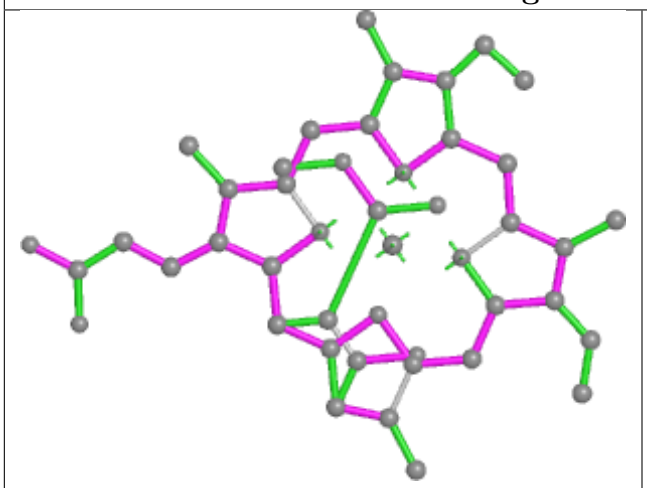
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 17 305



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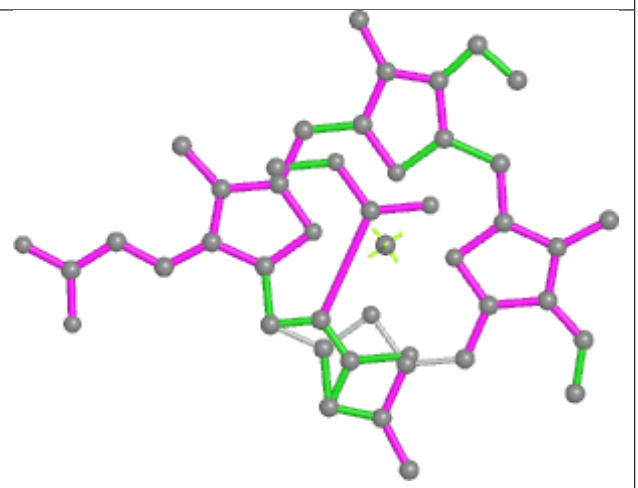

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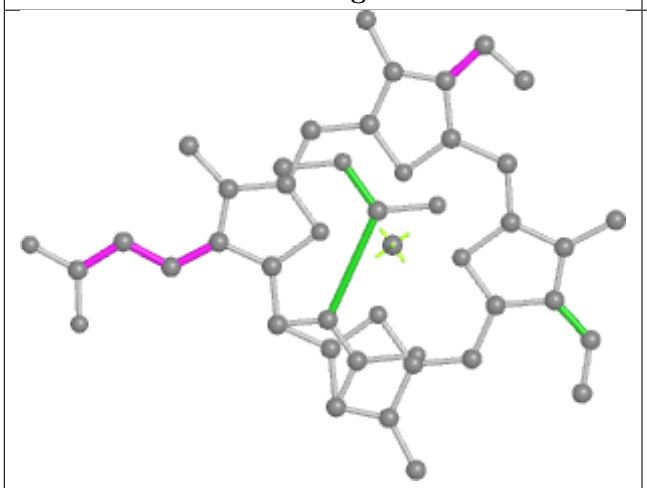

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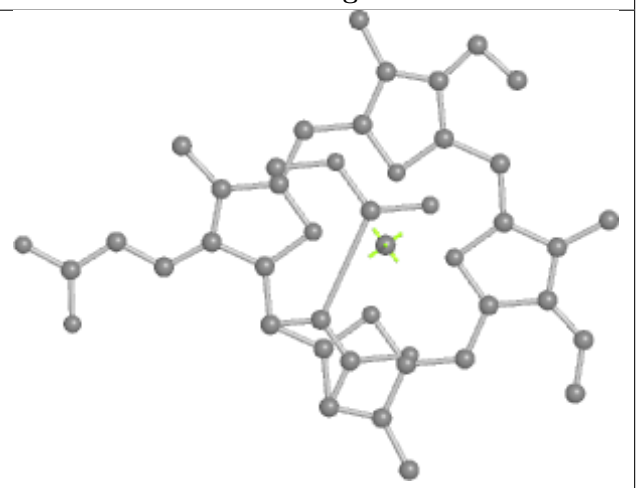
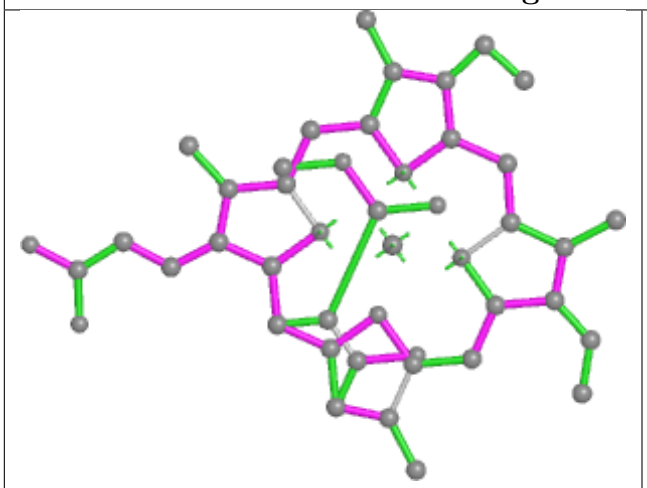


Rings

Ligand KC1 38 210



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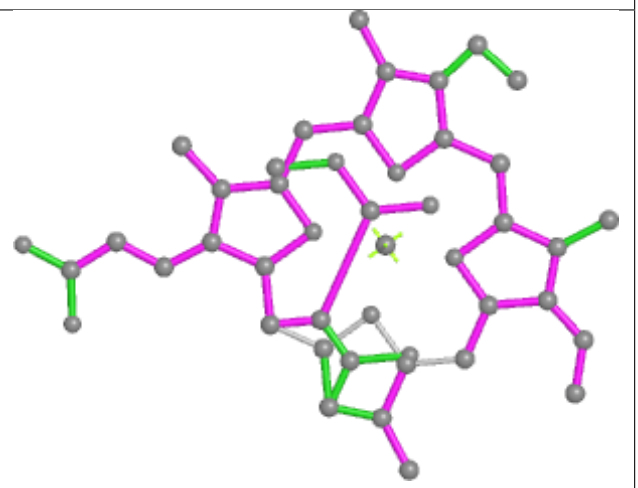

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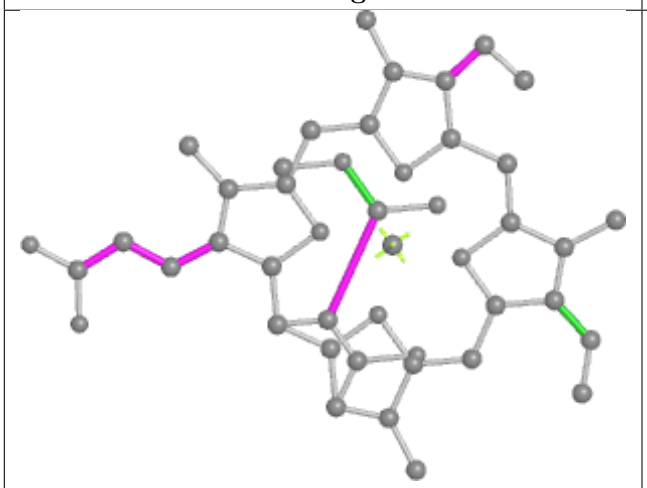

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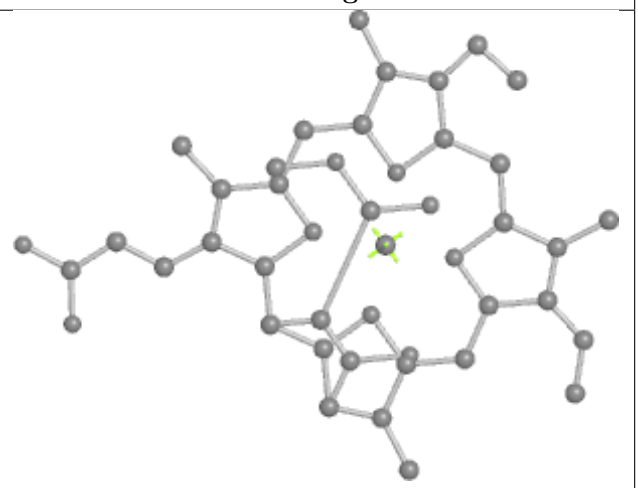

Rings

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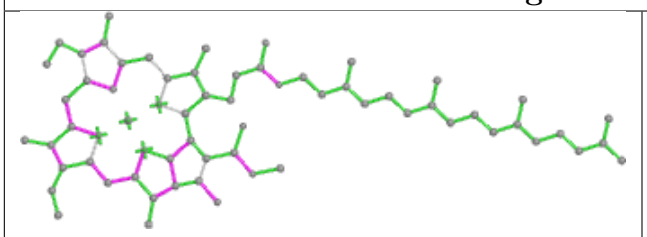

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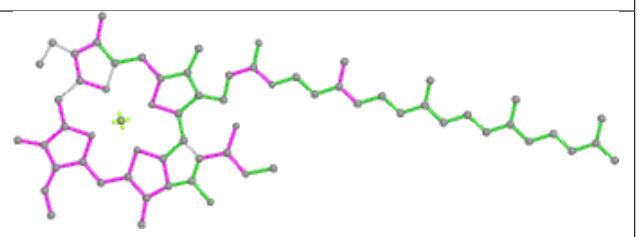
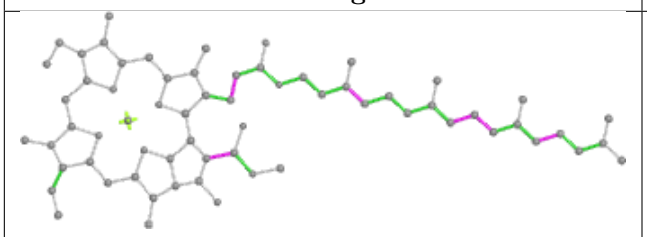


Bond angles



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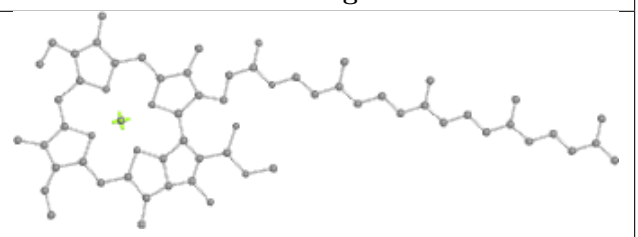
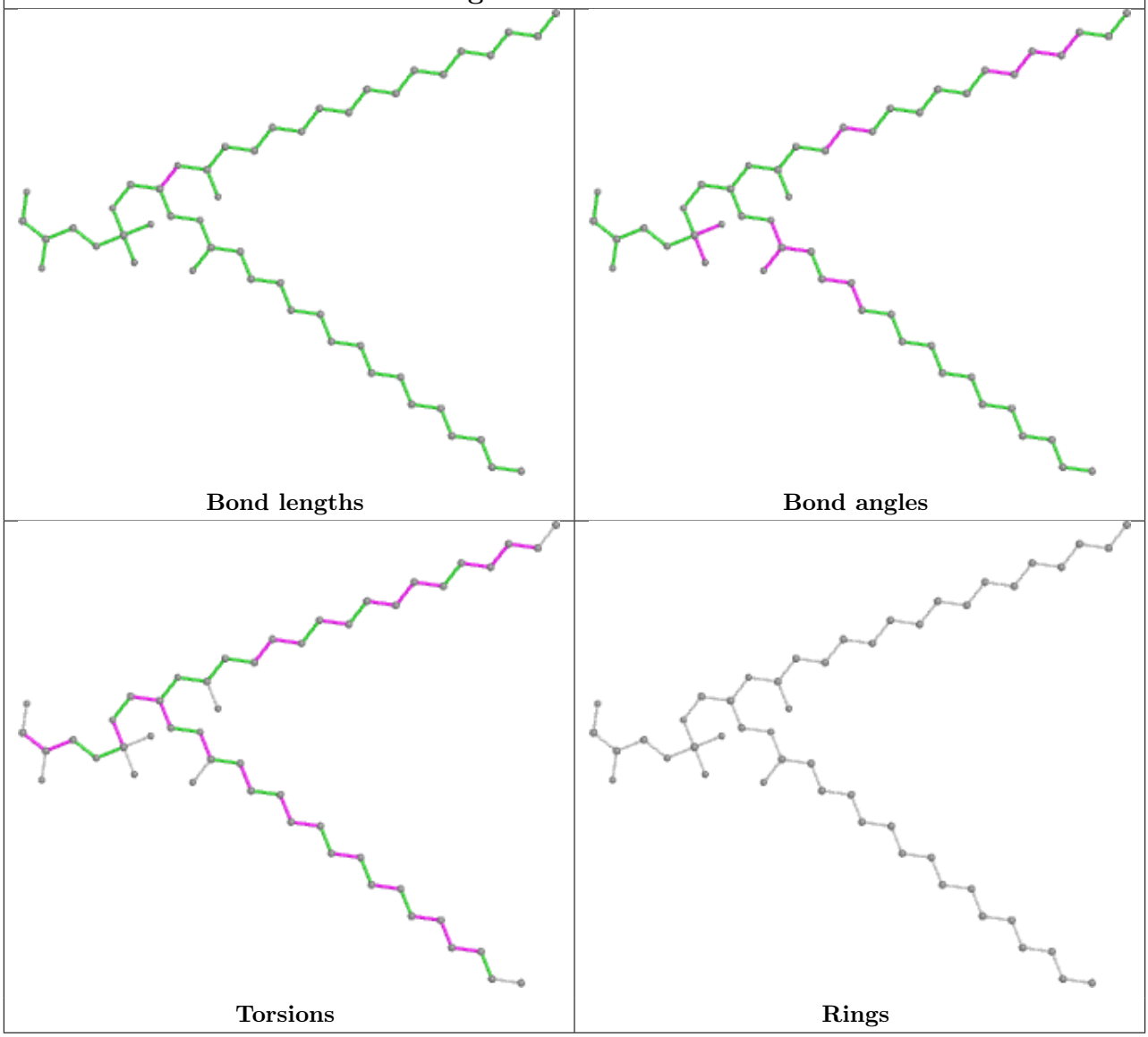
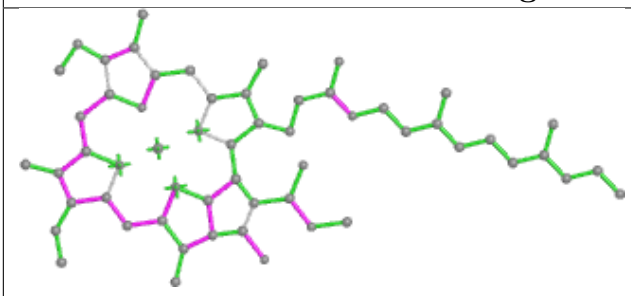
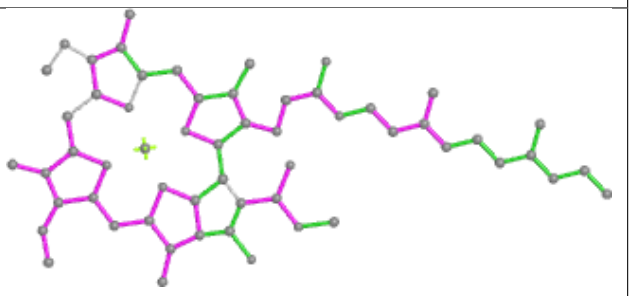
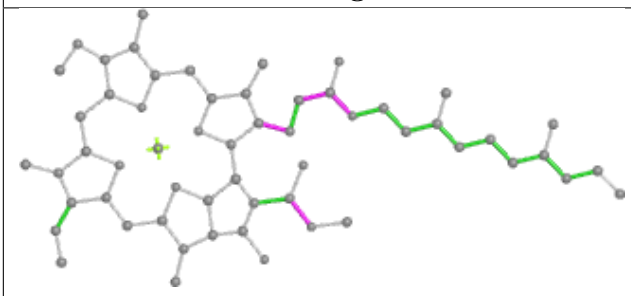
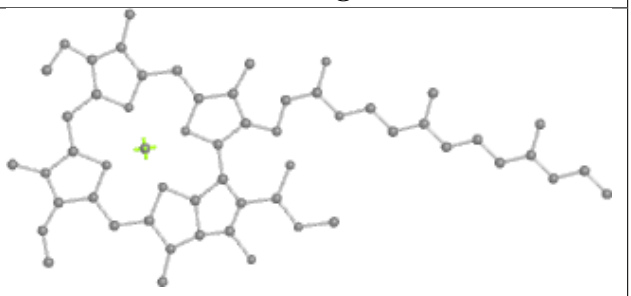


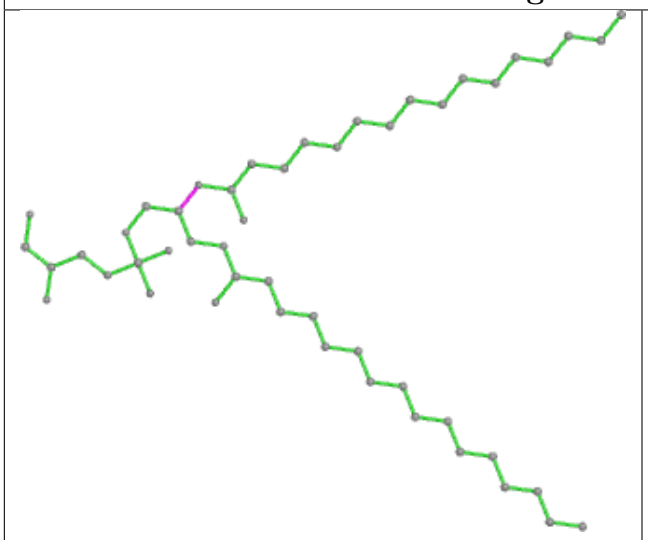
Rings

Ligand LHG D 409



Ligand CLA 16 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG b 522



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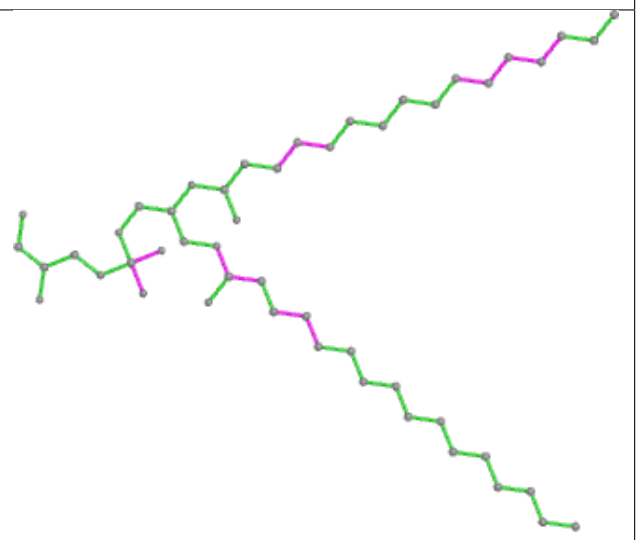

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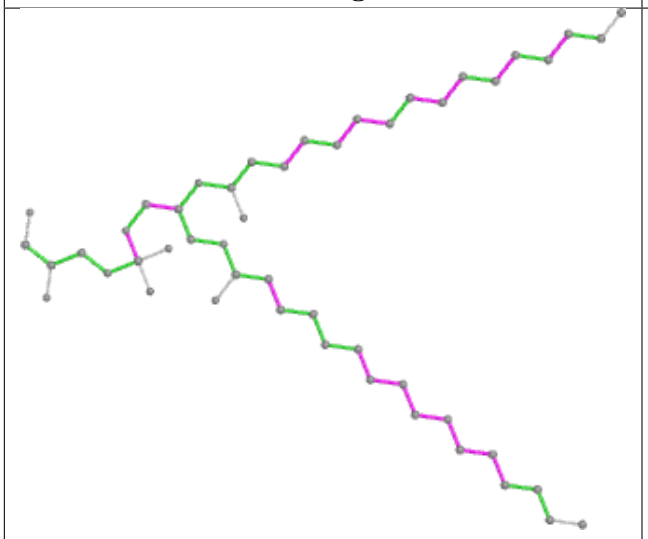

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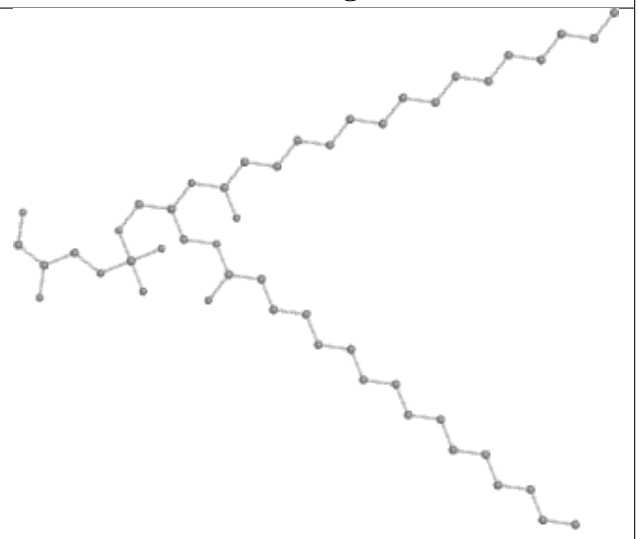
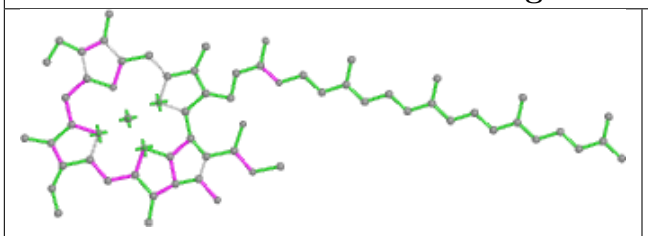


Rings

Ligand CLA B 506



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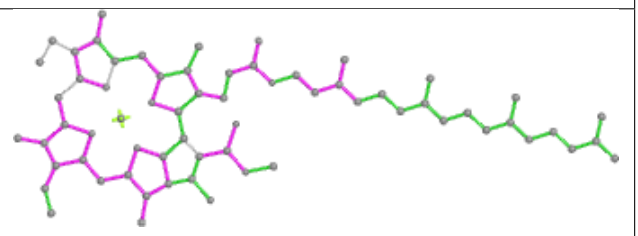

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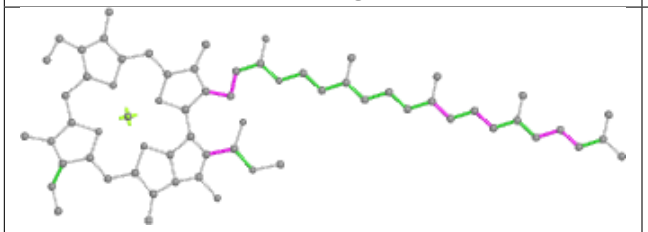

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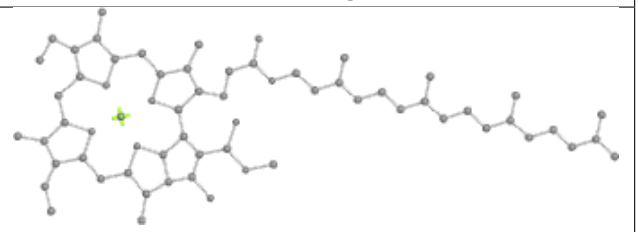

Rings

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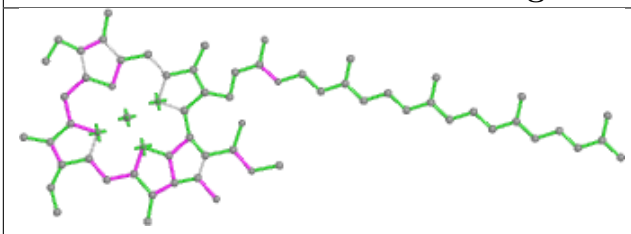
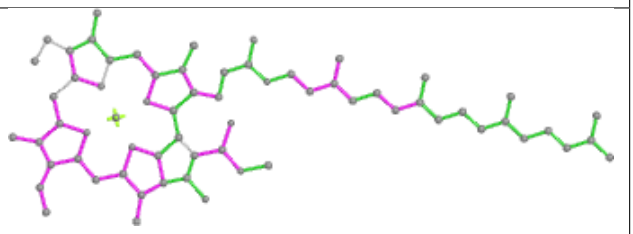
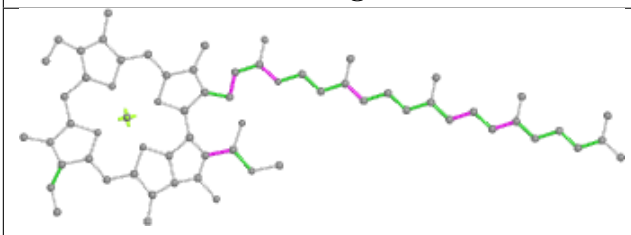
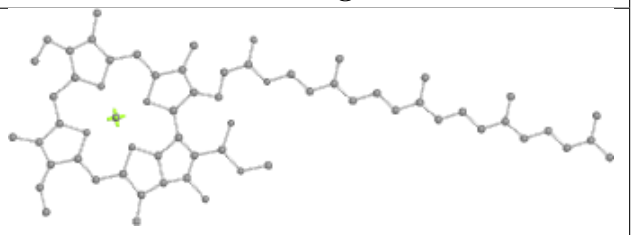
 Bond lengths	 Bond angles
 Torsions	 Rings

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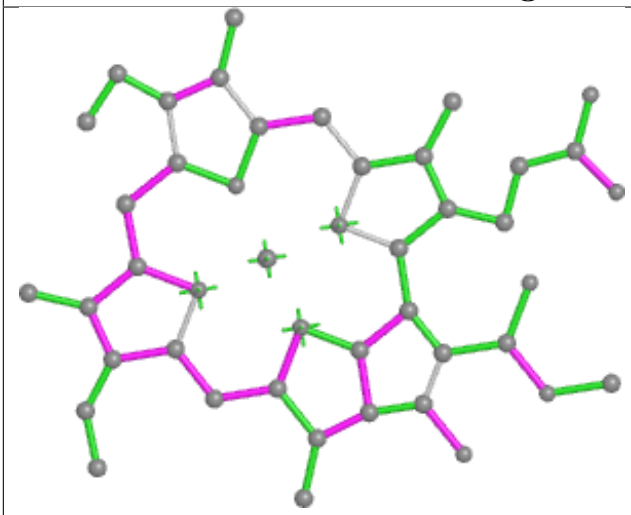
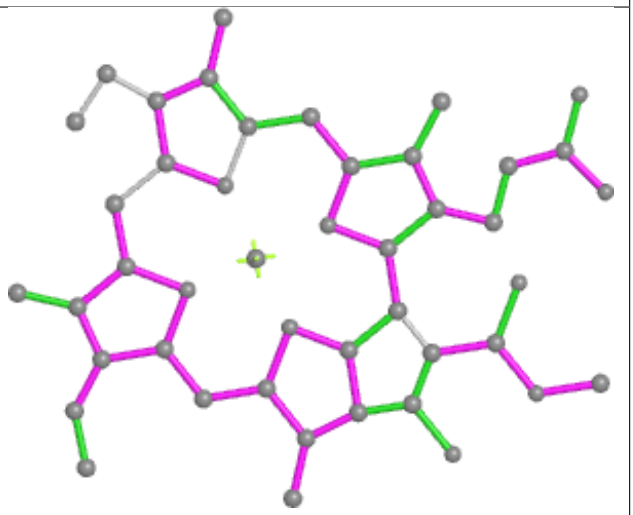
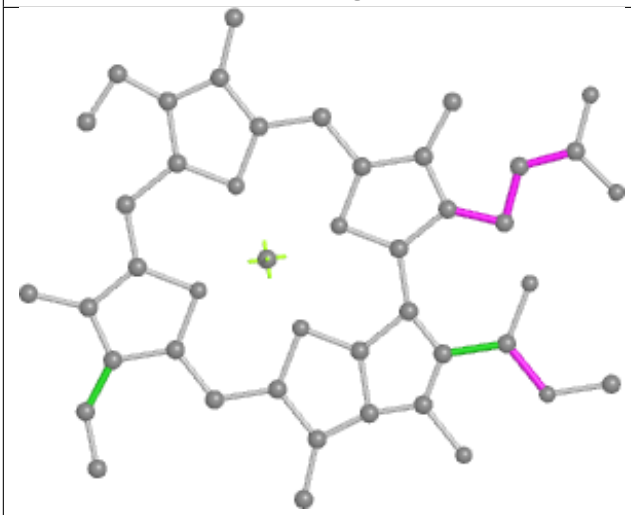
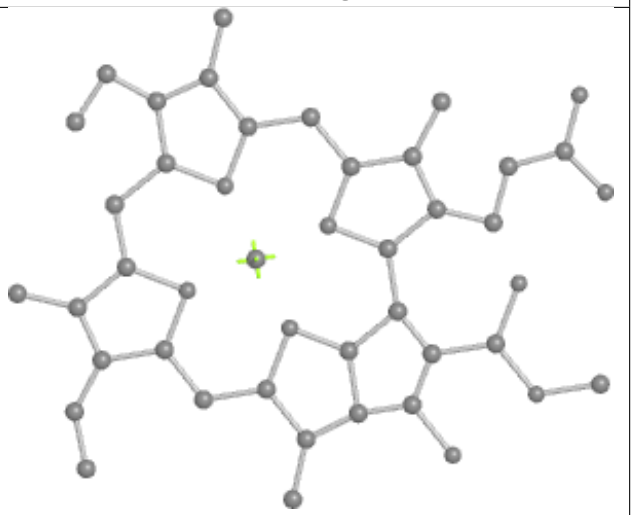
 Bond lengths	 Bond angles
 Torsions	 Rings

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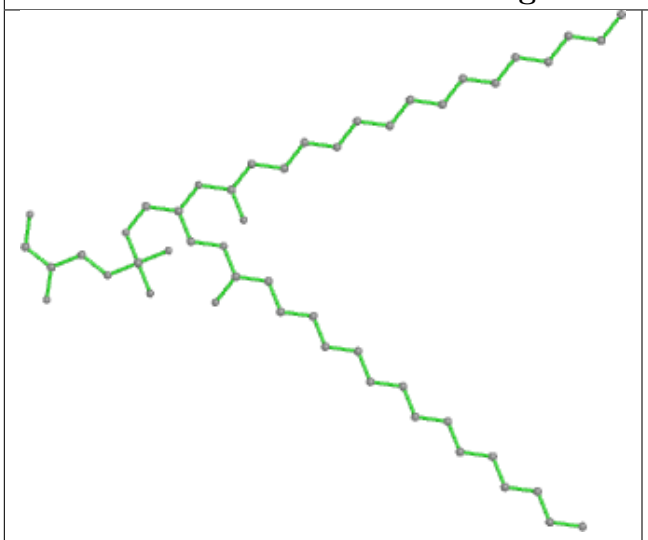

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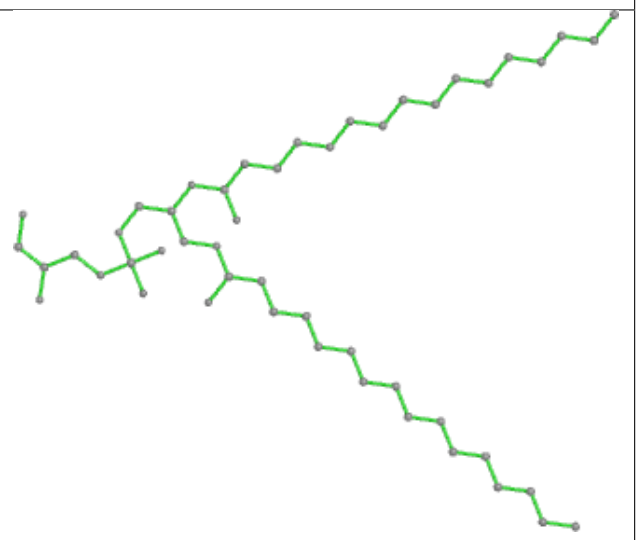

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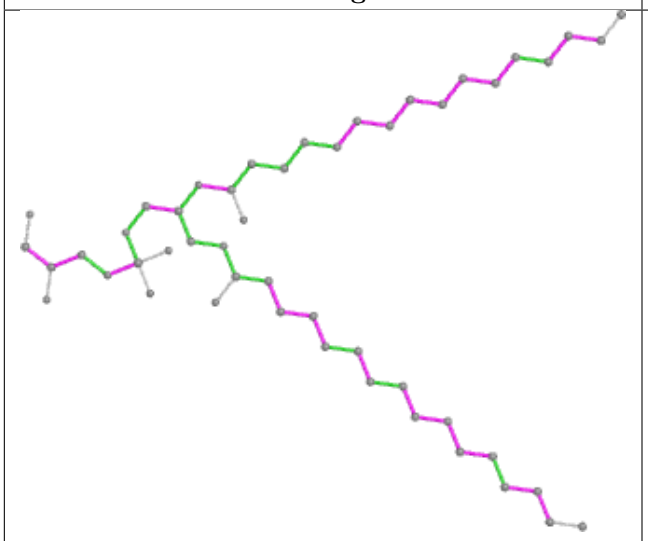

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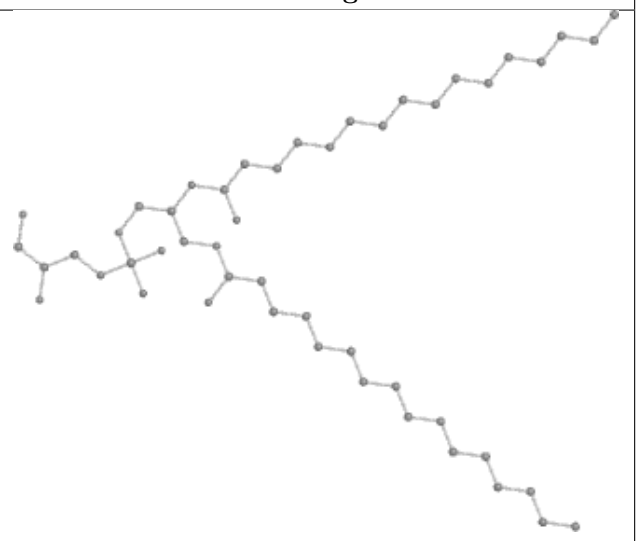

Rings

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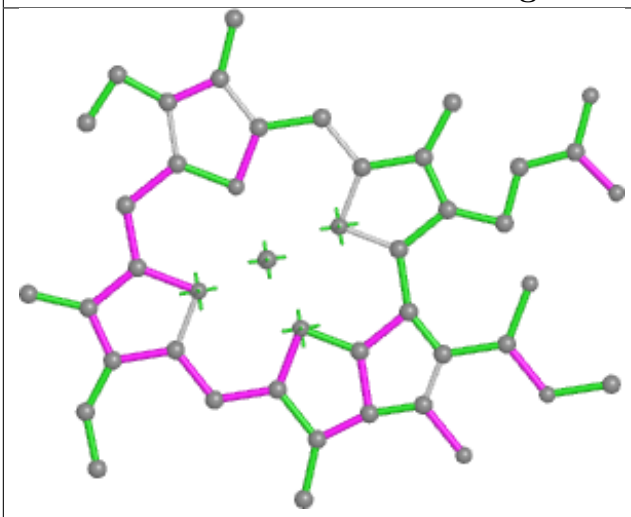

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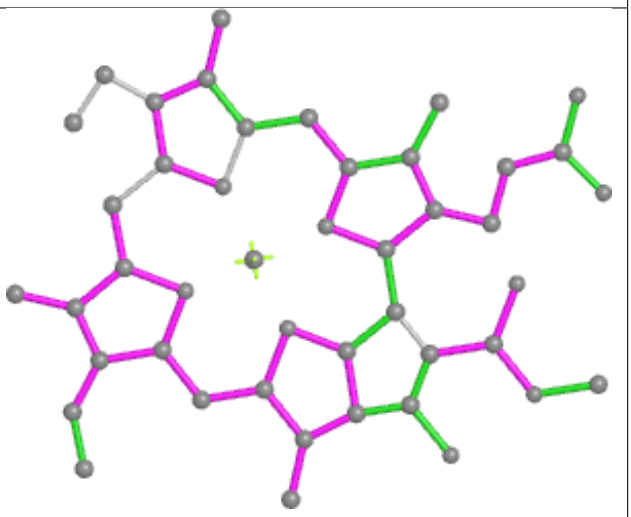

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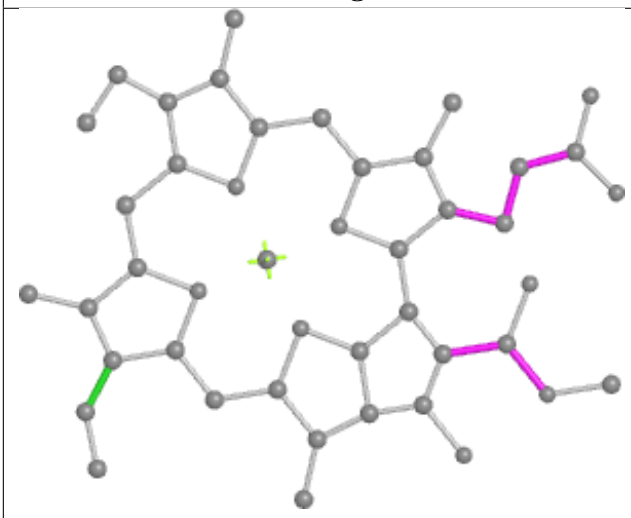

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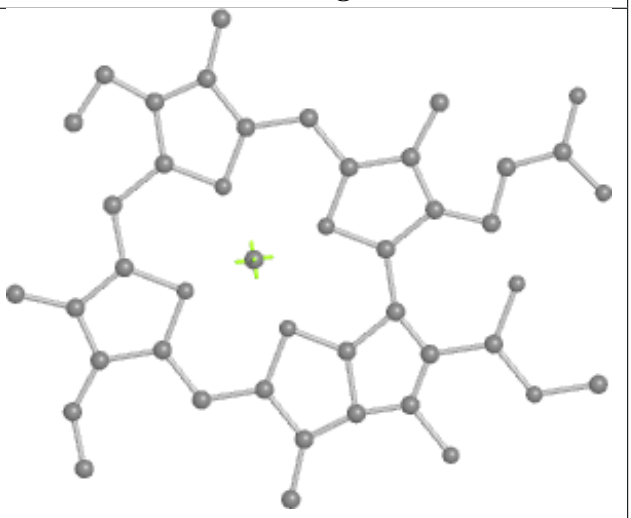

Rings

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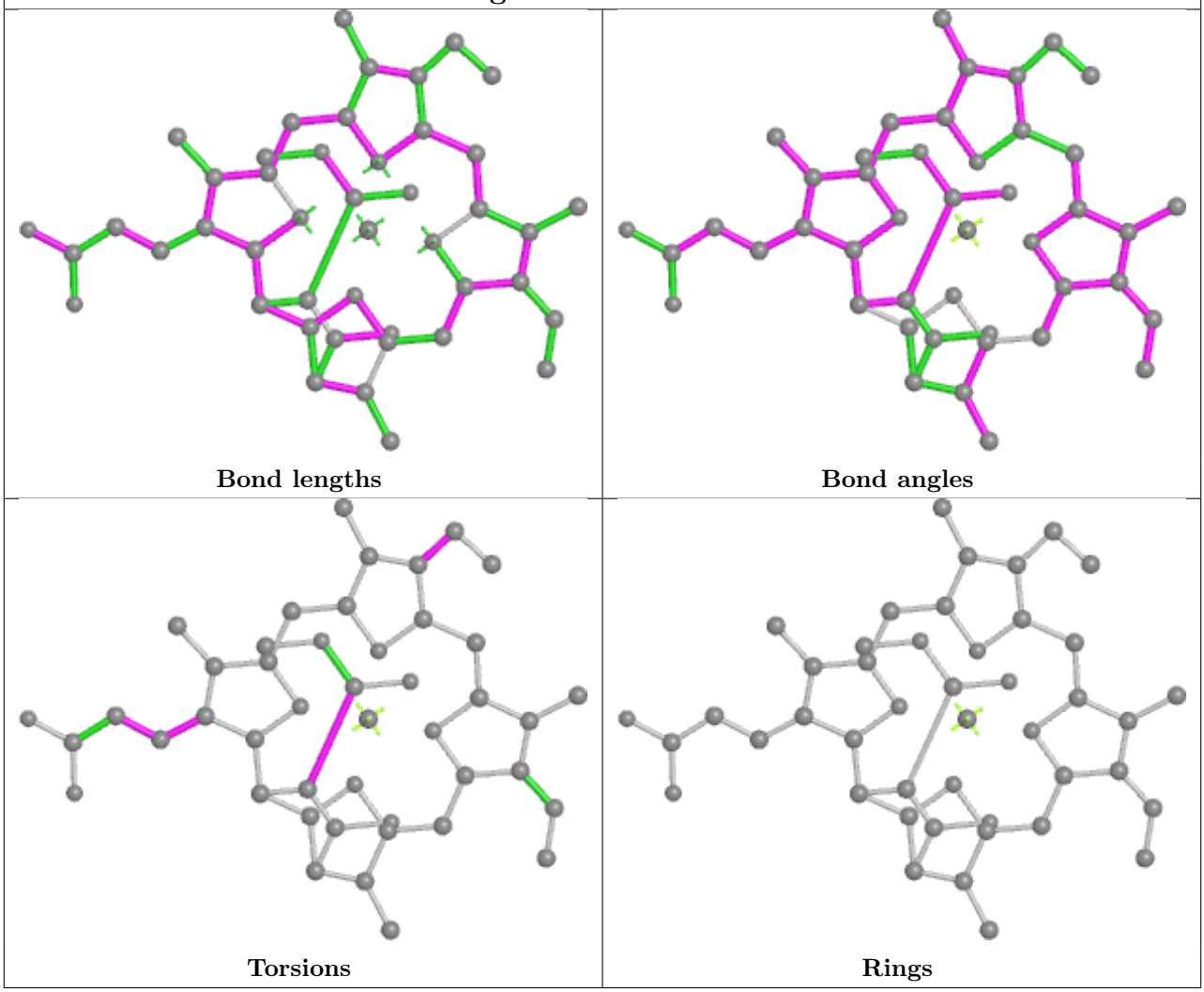

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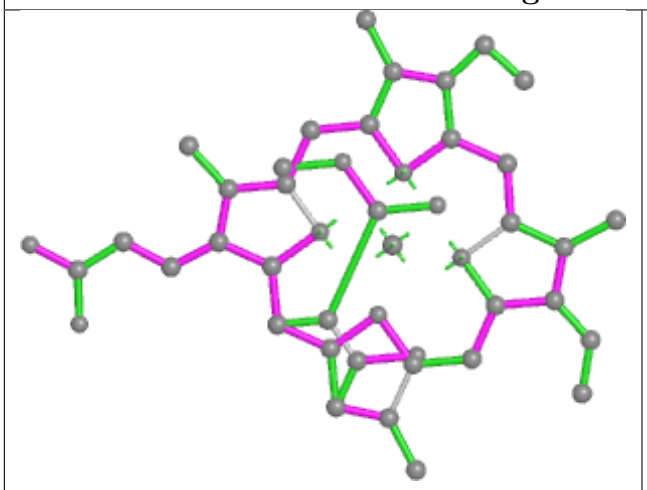

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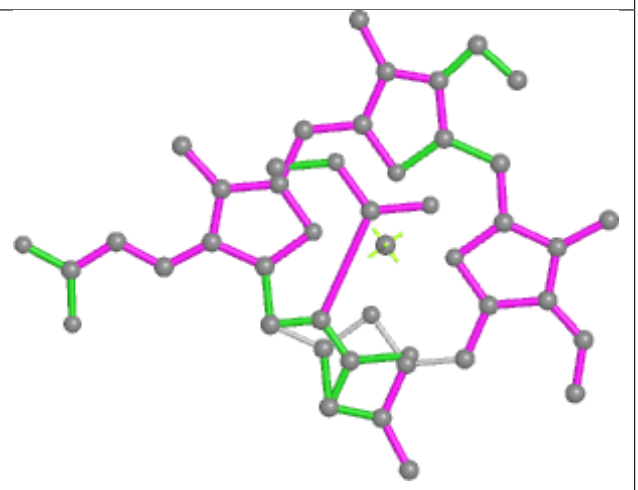

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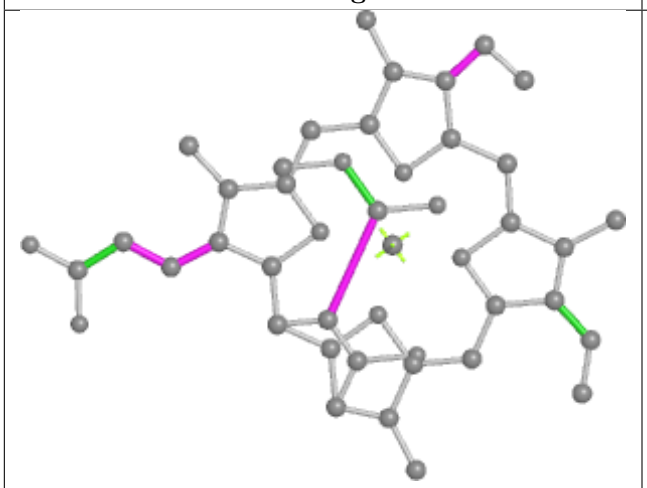

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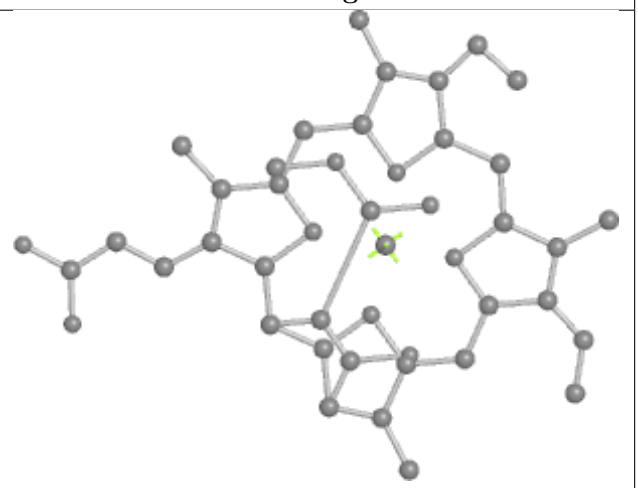
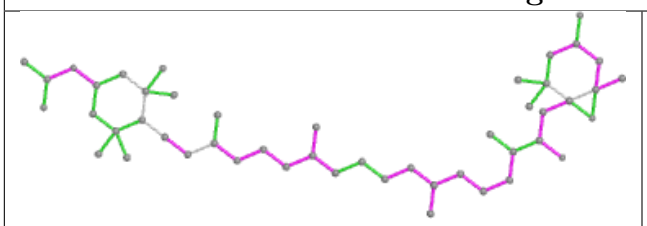


Rings

Ligand A86 37 312



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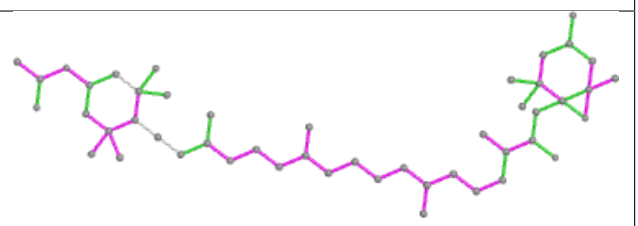

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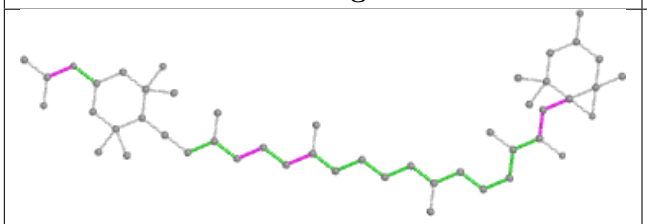

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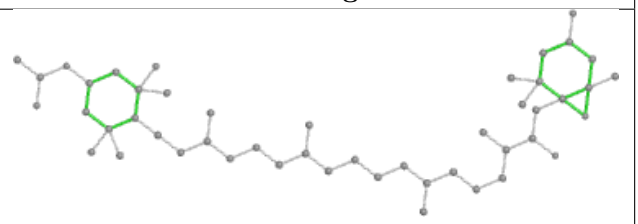
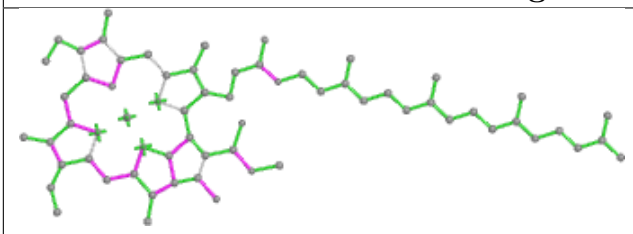


Rings

Ligand CLA a 403



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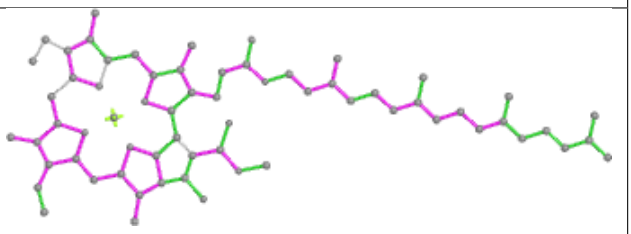

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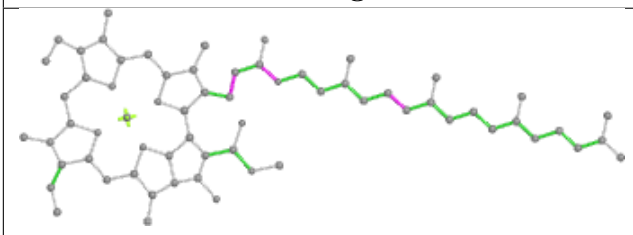

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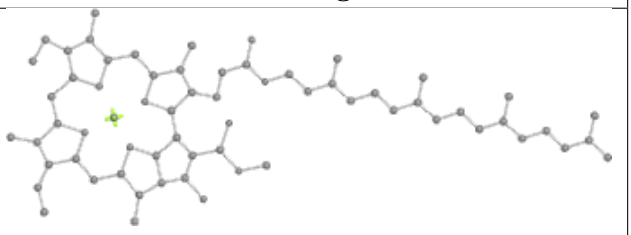
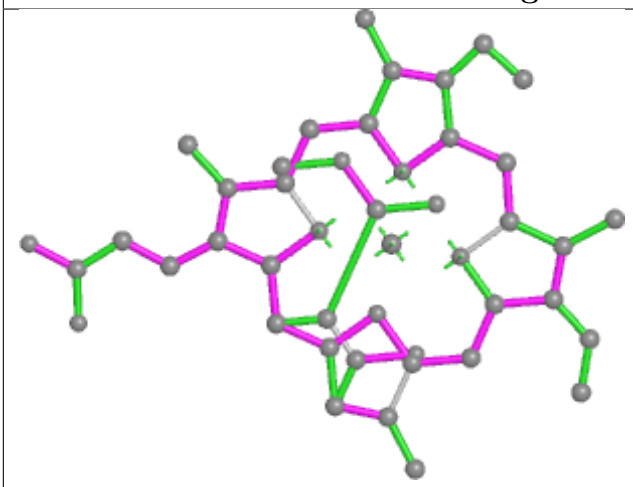


Rings

Ligand KC1 20 305



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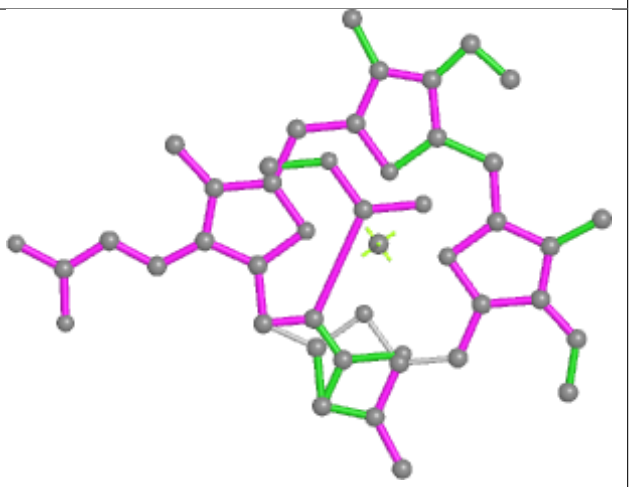

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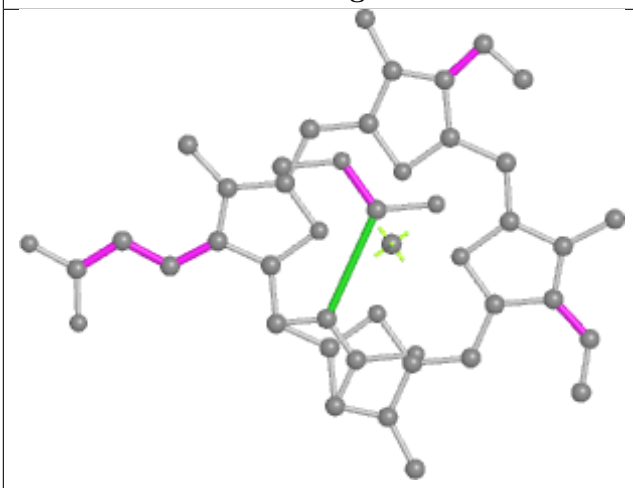

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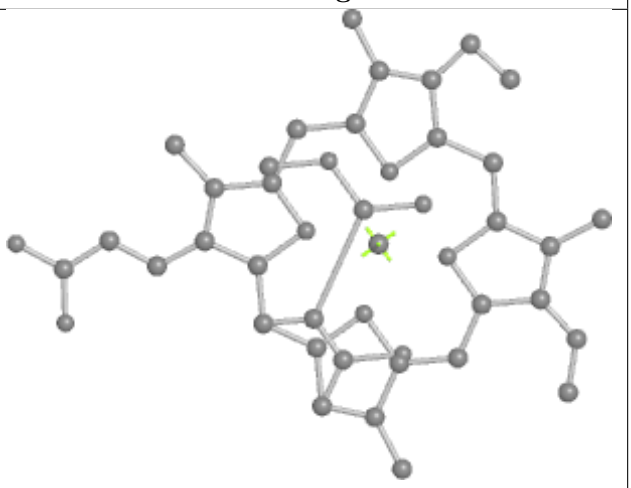

Rings

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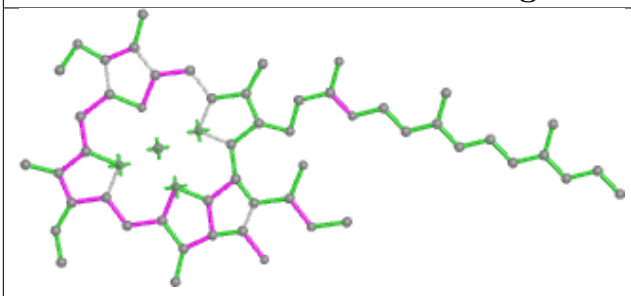
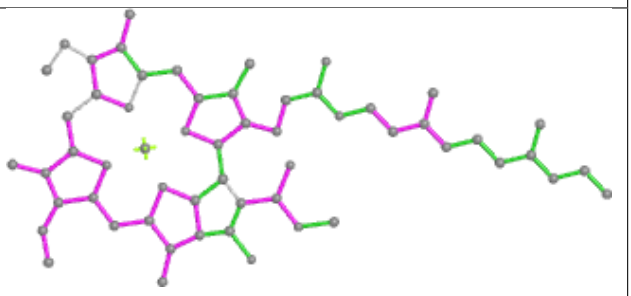
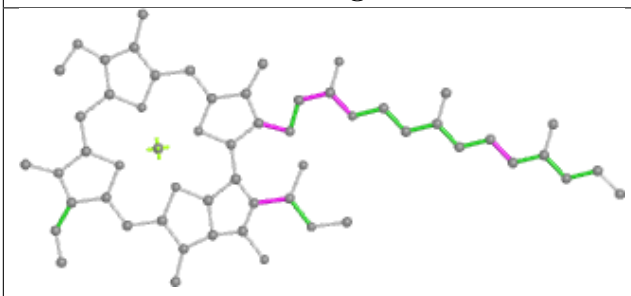
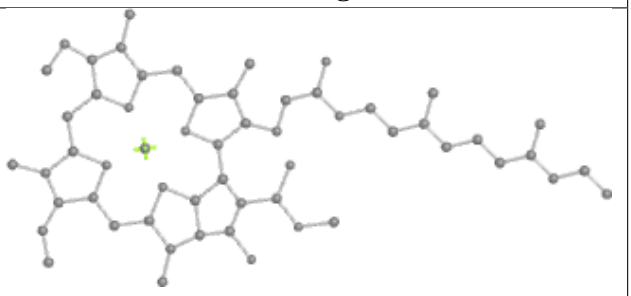
 Bond lengths	 Bond angles
 Torsions	 Rings

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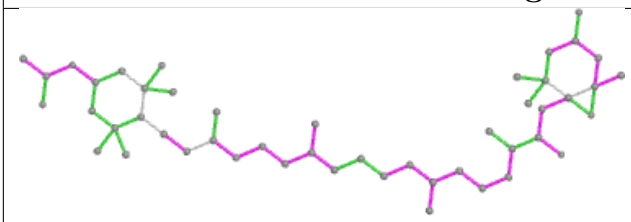
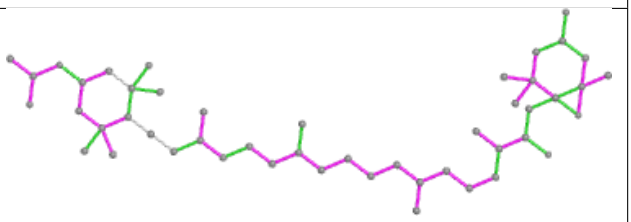
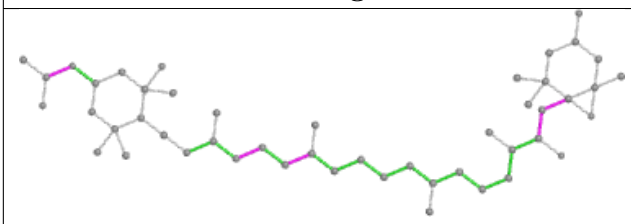
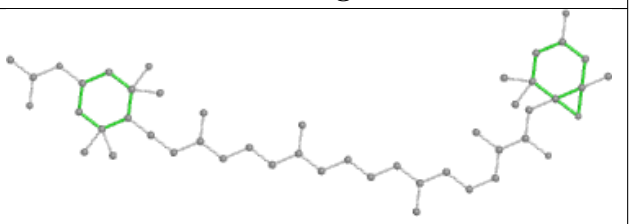
 Bond lengths	 Bond angles
 Torsions	 Rings

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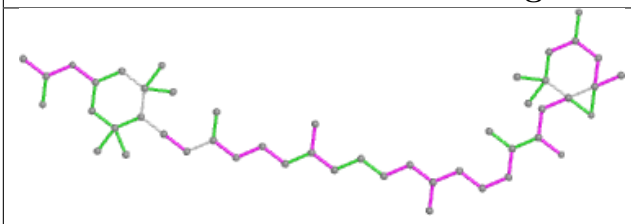

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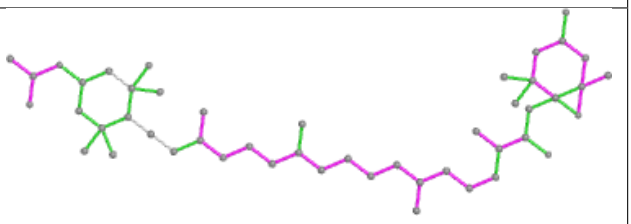

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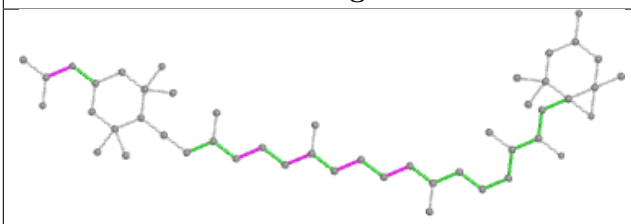

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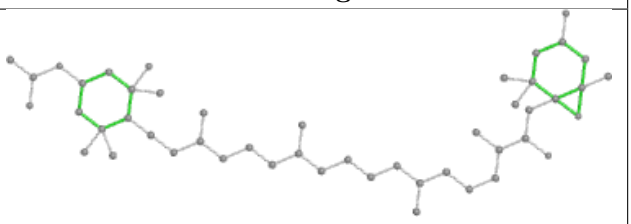

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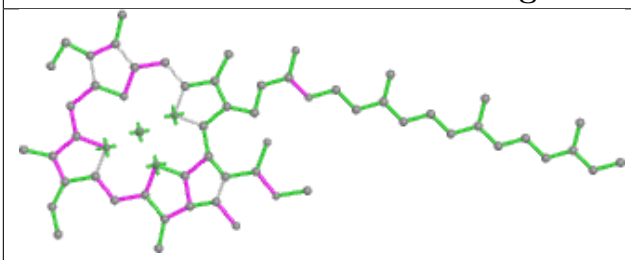

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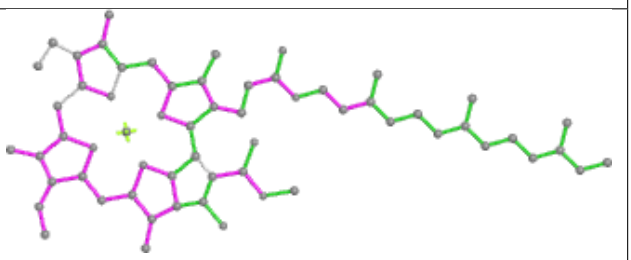

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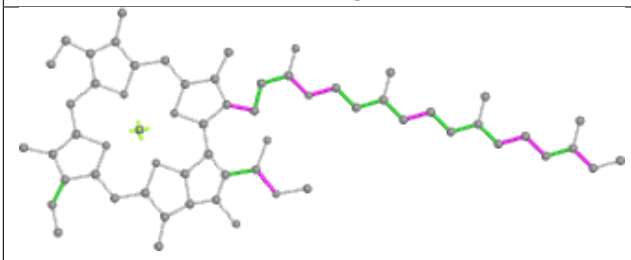

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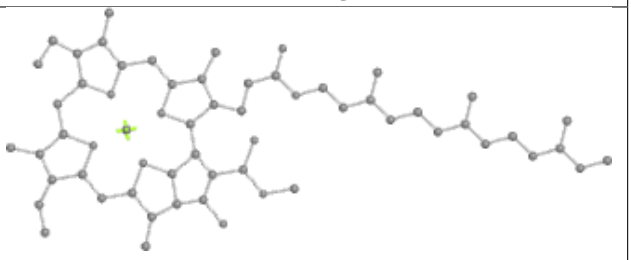

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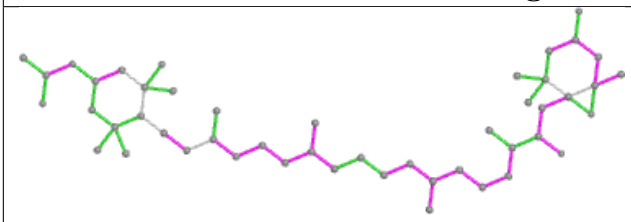

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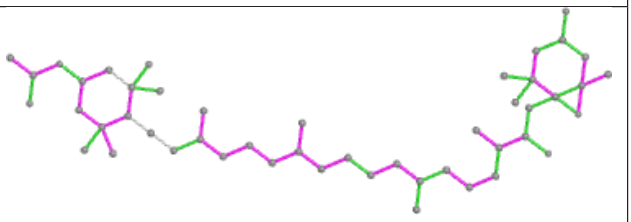

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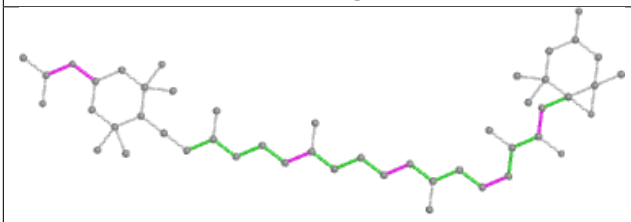

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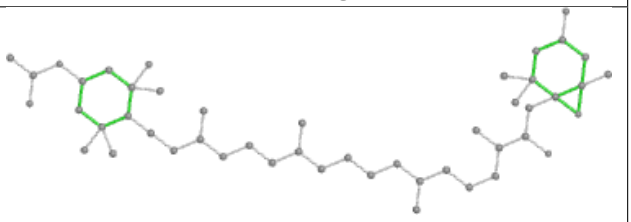

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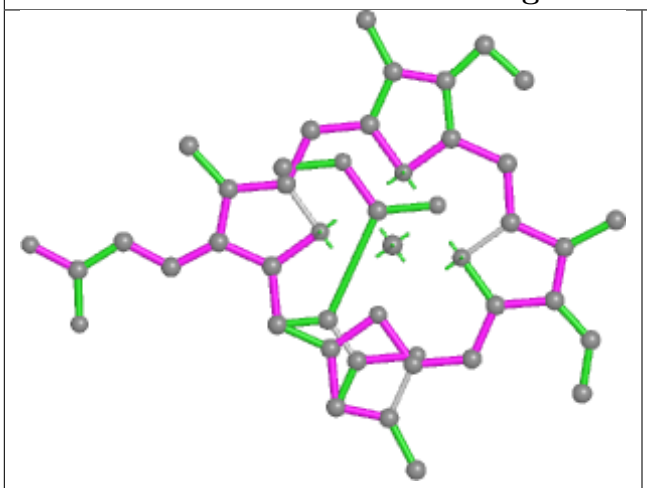

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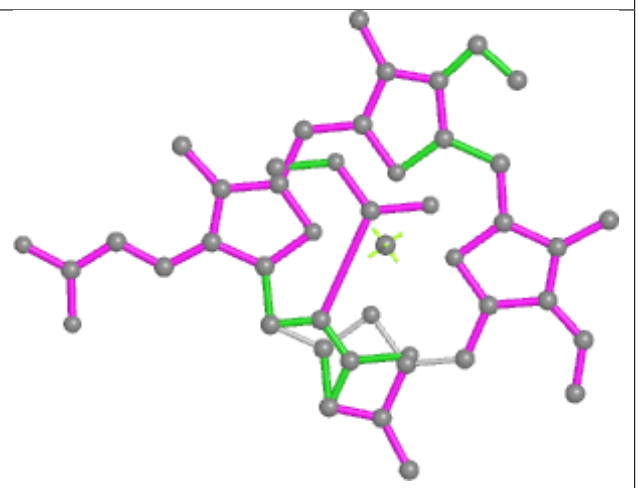

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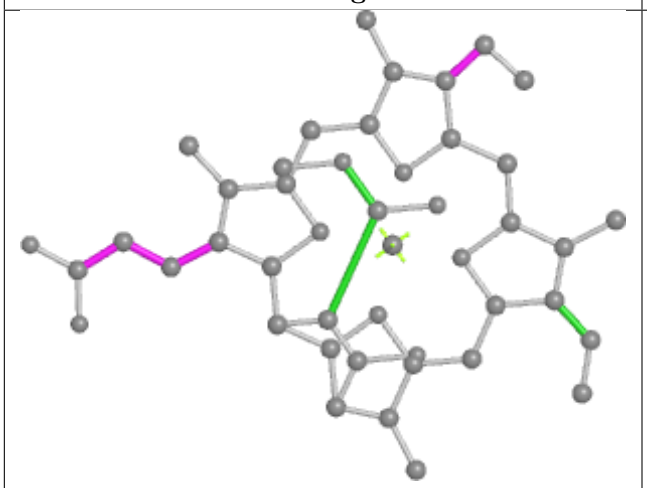

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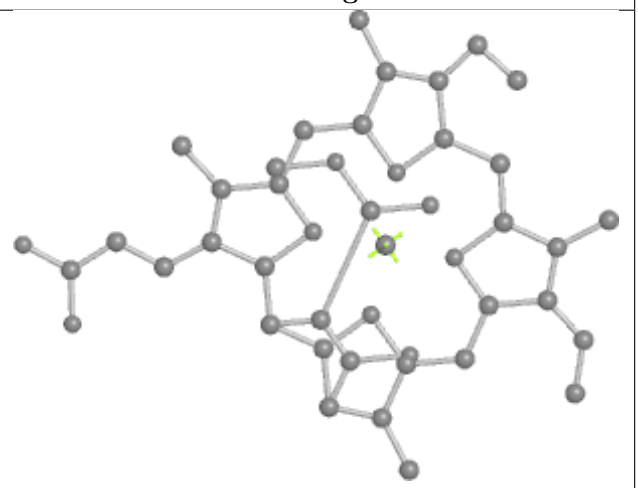

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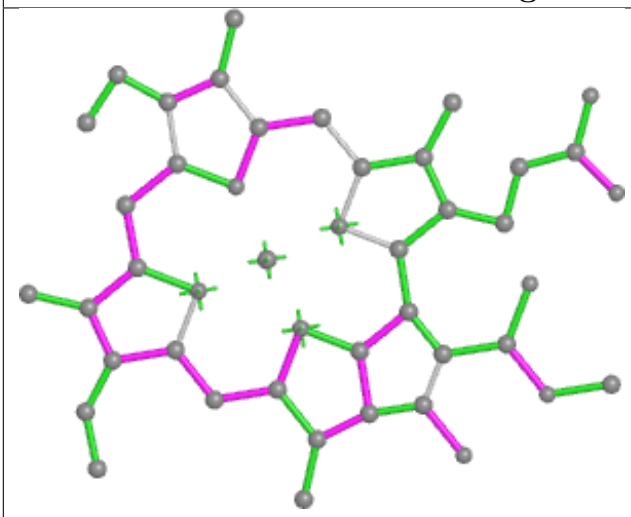

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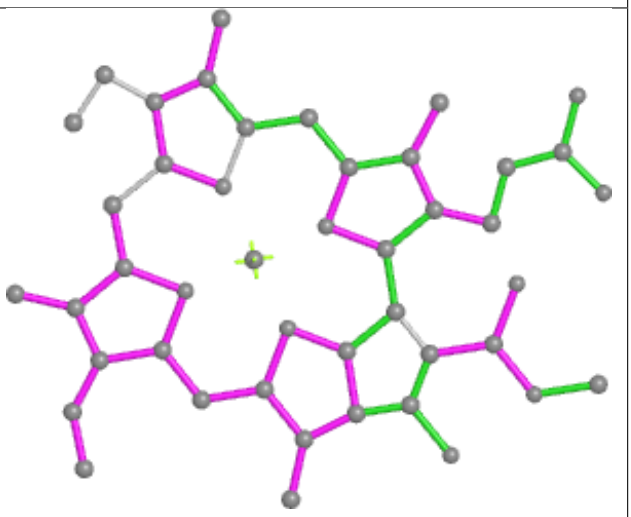

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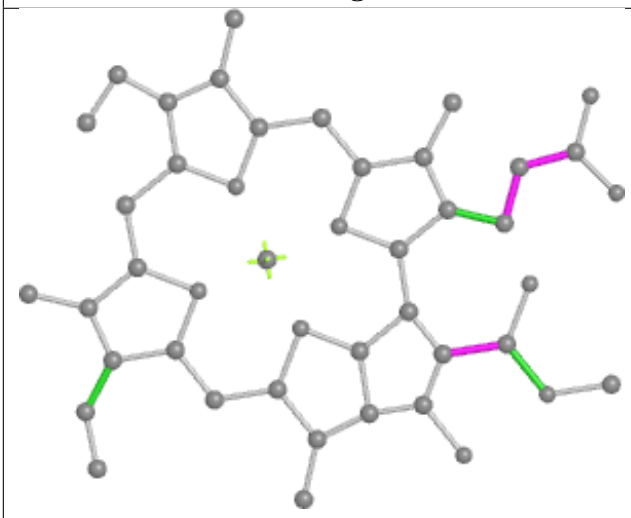

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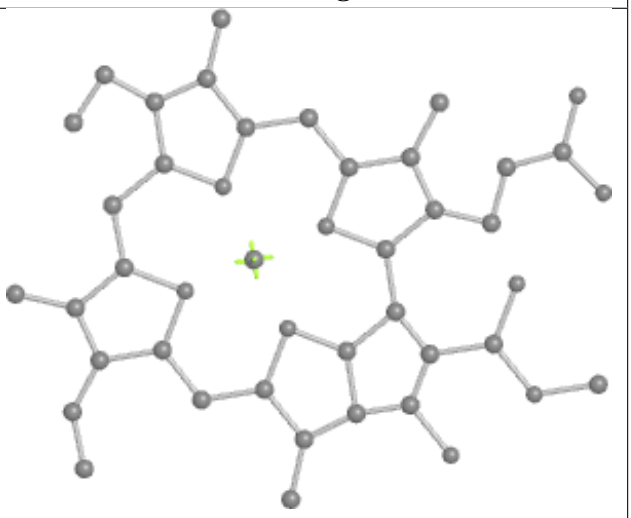

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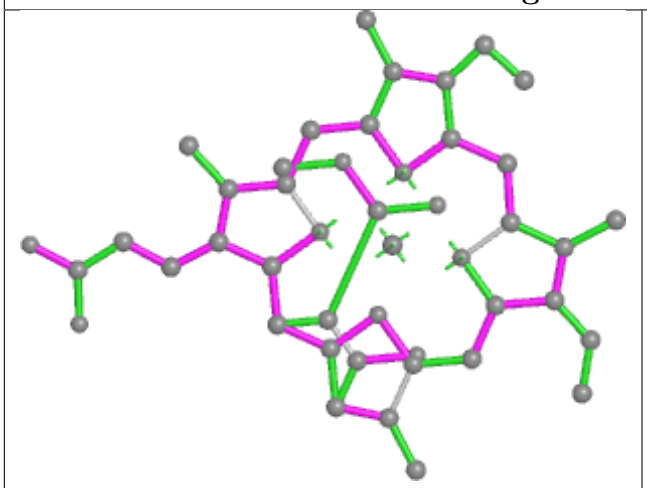

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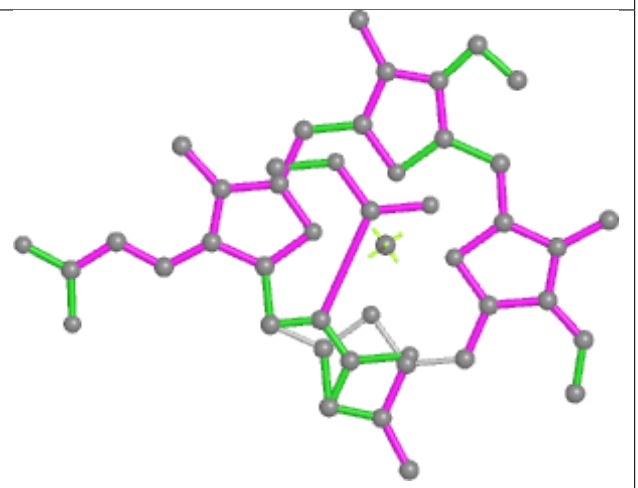

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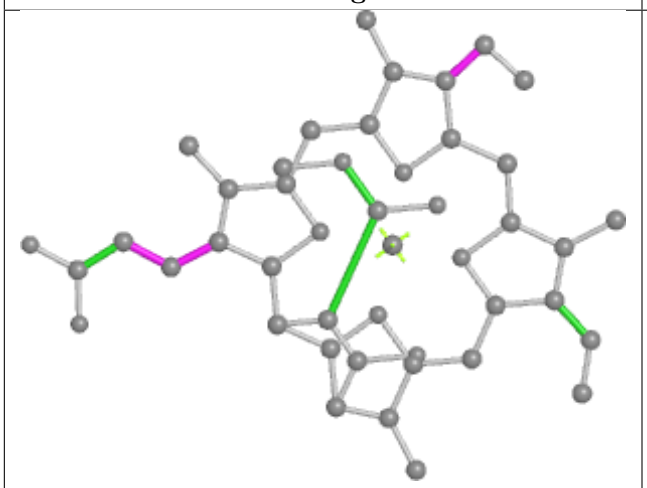

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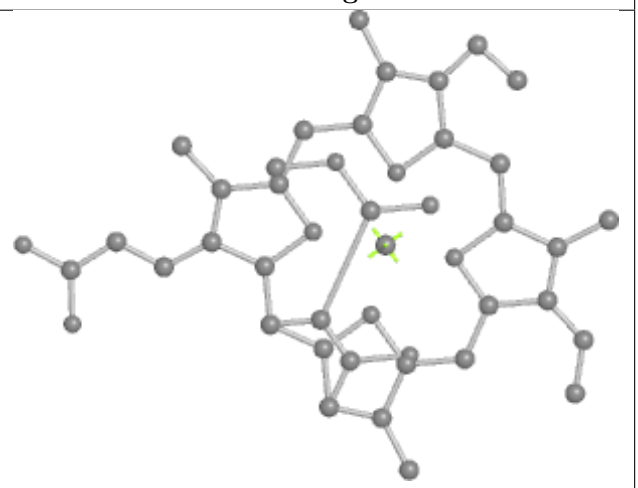

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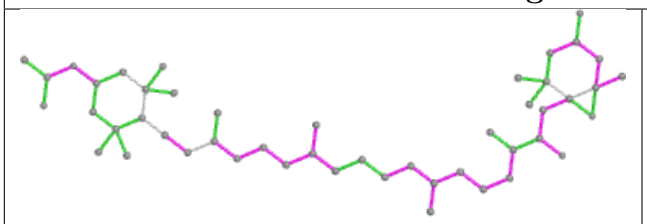

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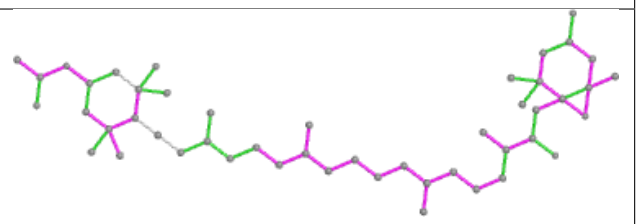

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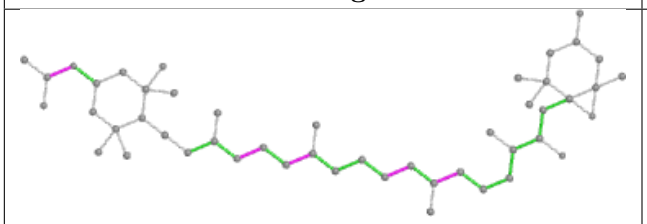

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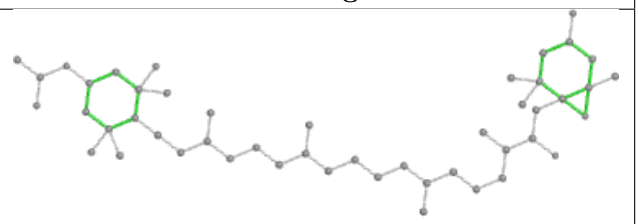

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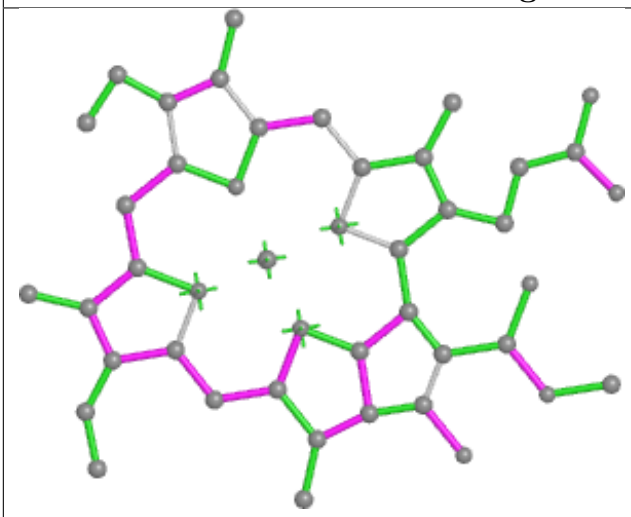

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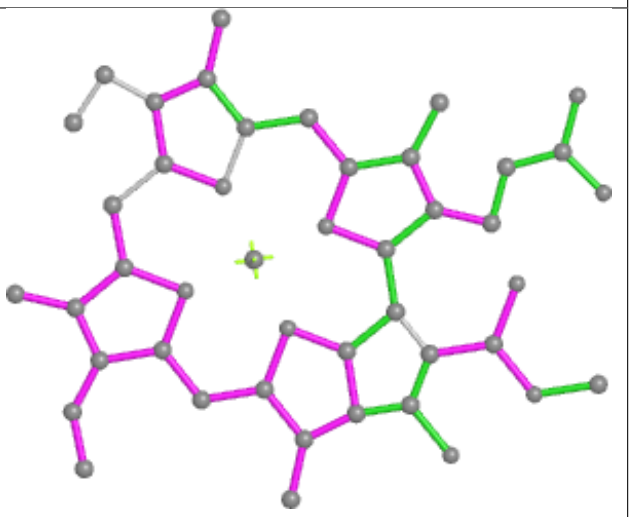

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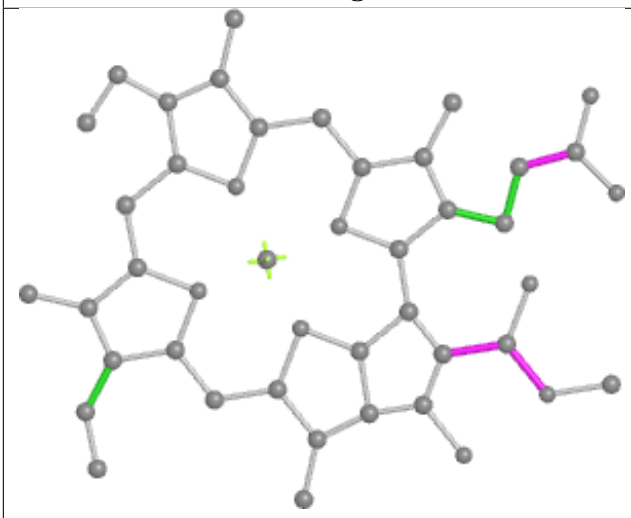

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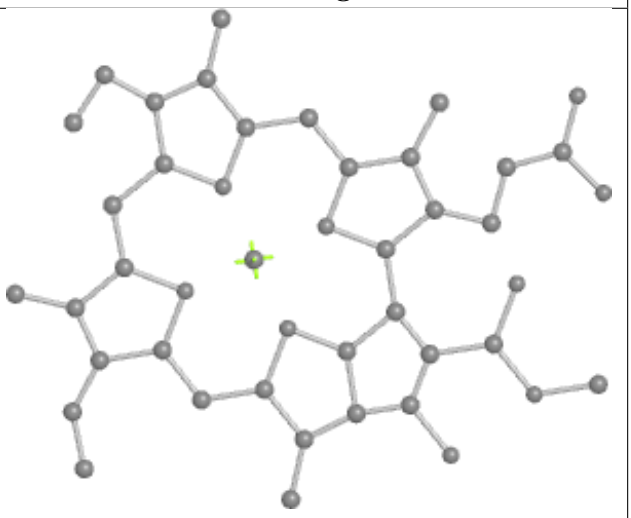

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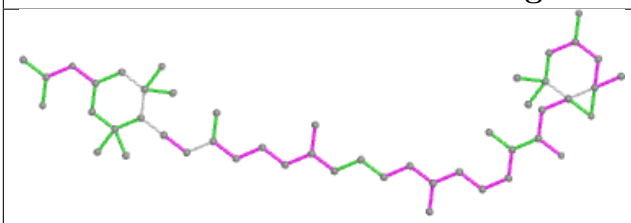

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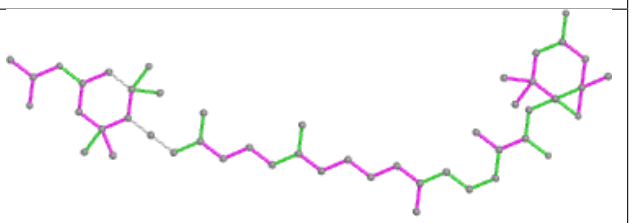

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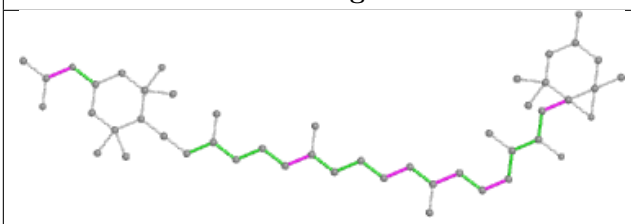

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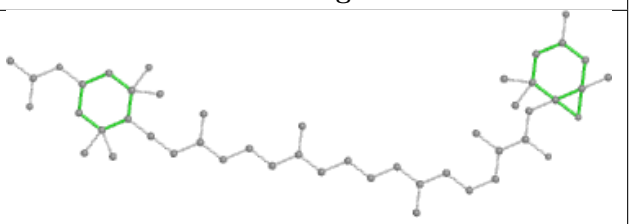

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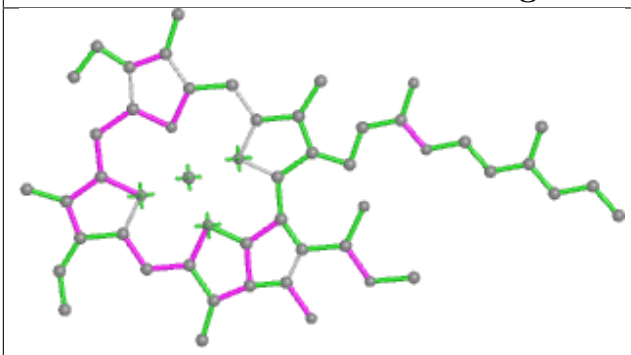
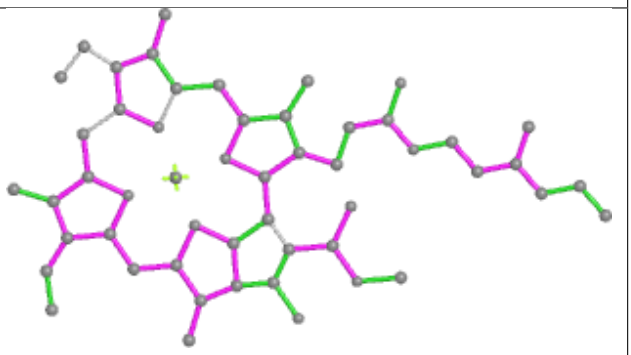
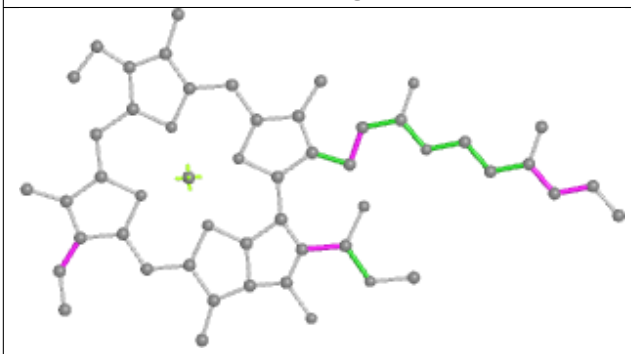
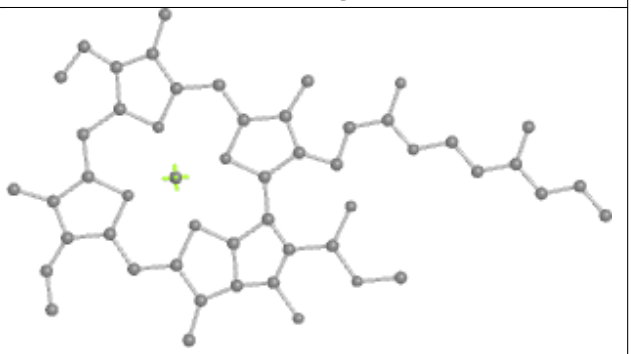
 Bond lengths	 Bond angles
 Torsions	 Rings

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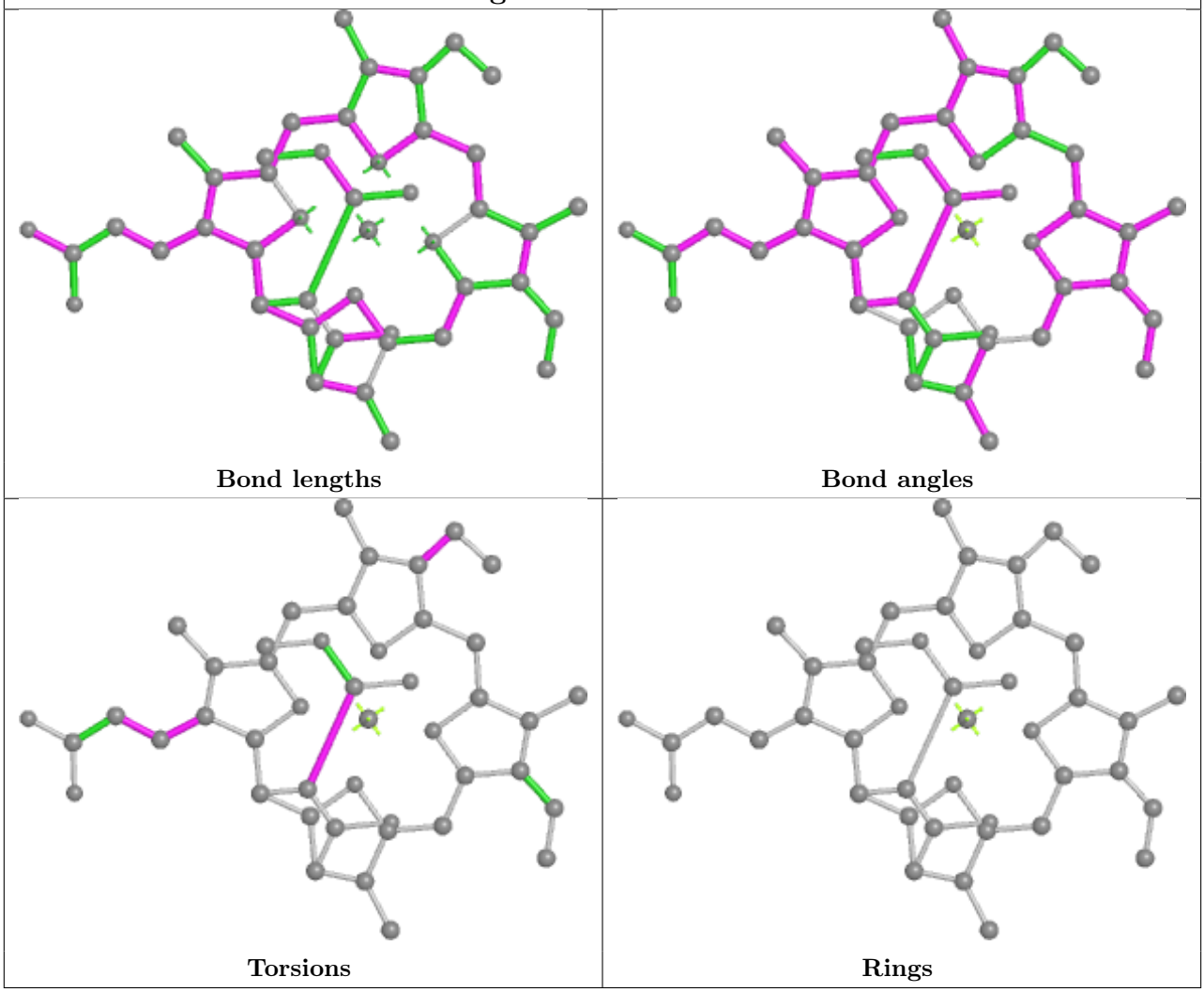

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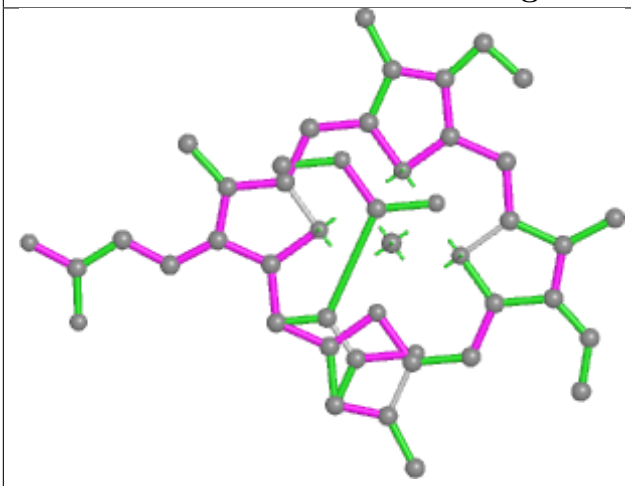

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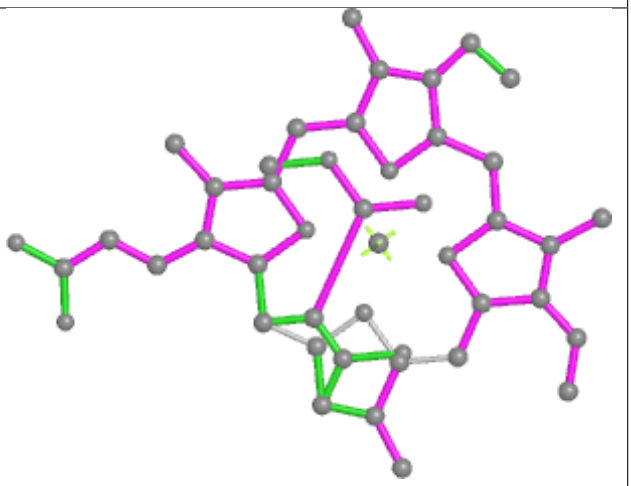

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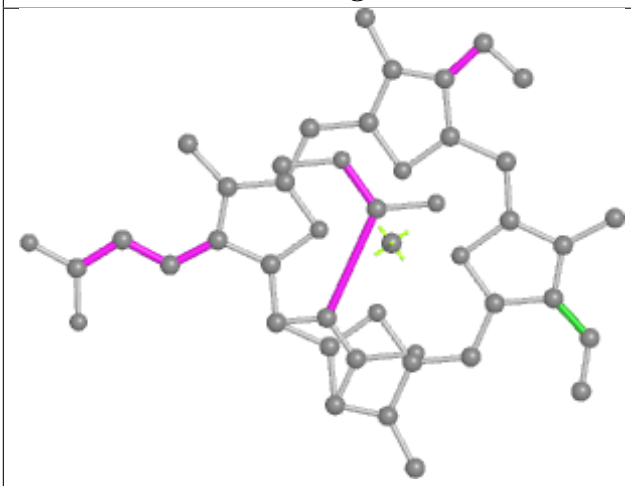

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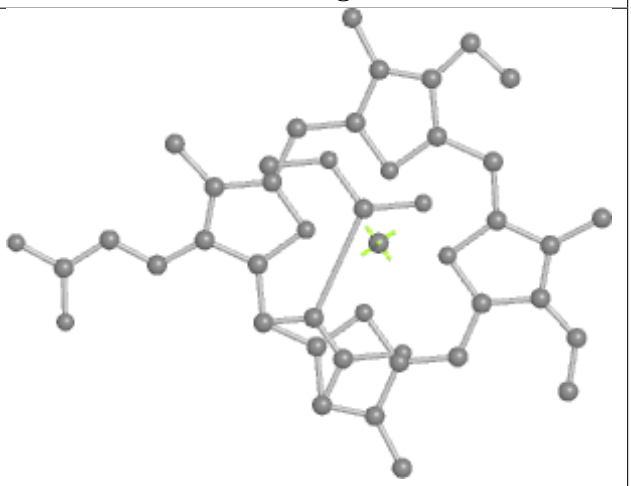

Rings

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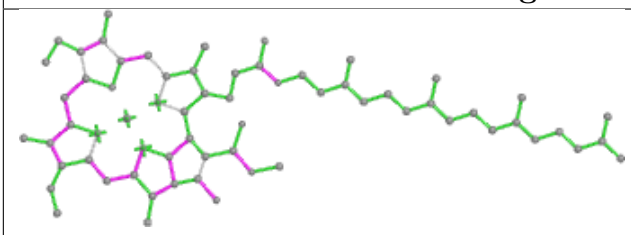

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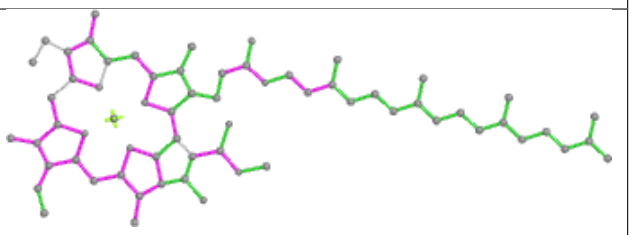

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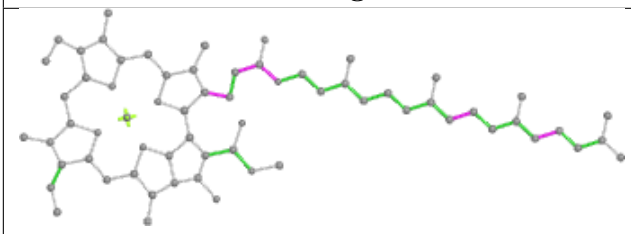

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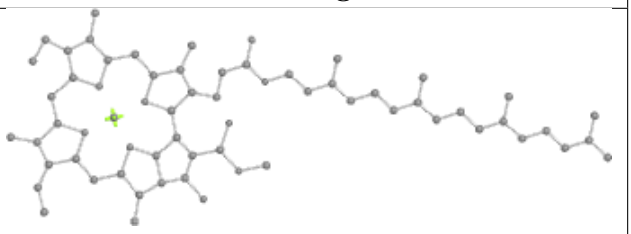

Rings

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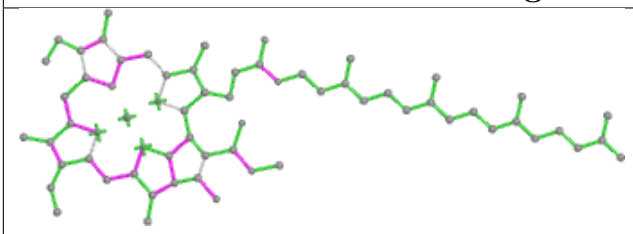

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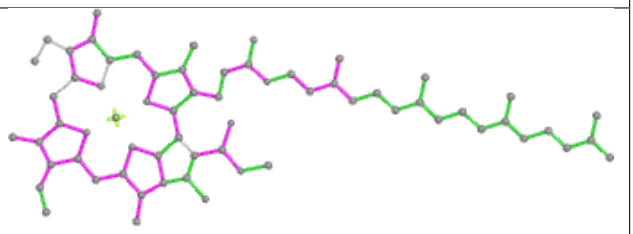

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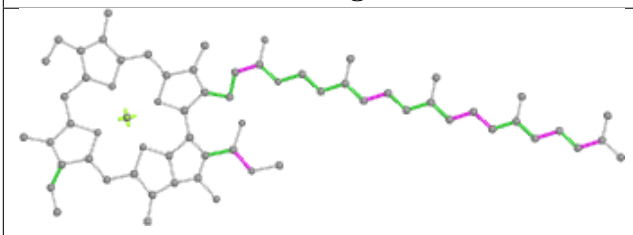
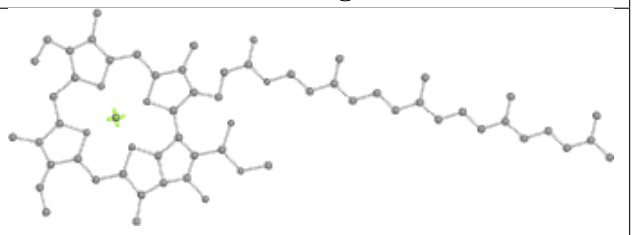
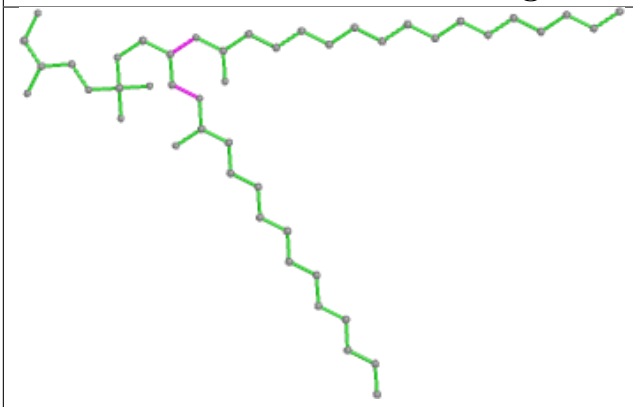


Torsions



Rings

Ligand LHG D 411



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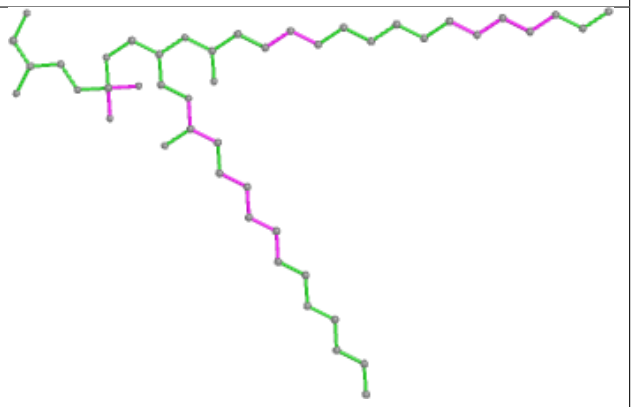
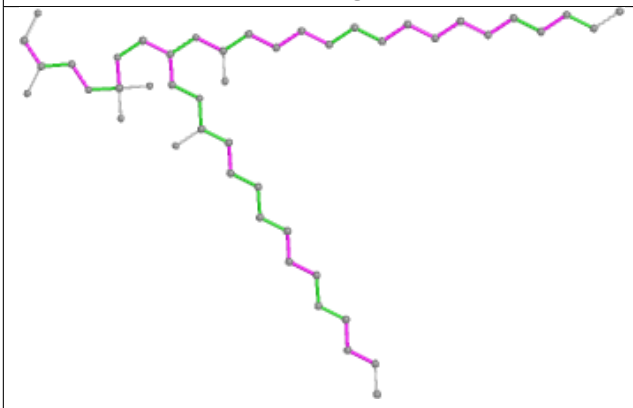


Bond angles



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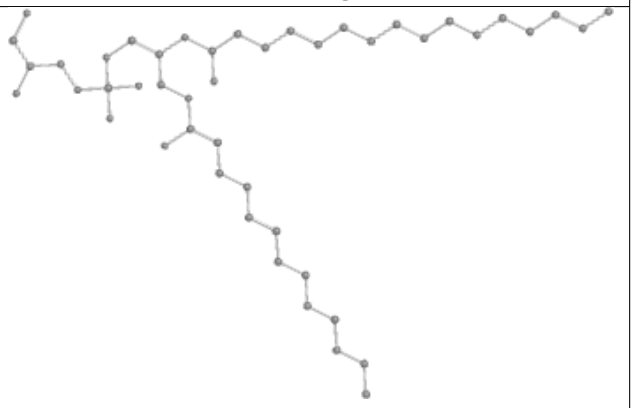

Rings

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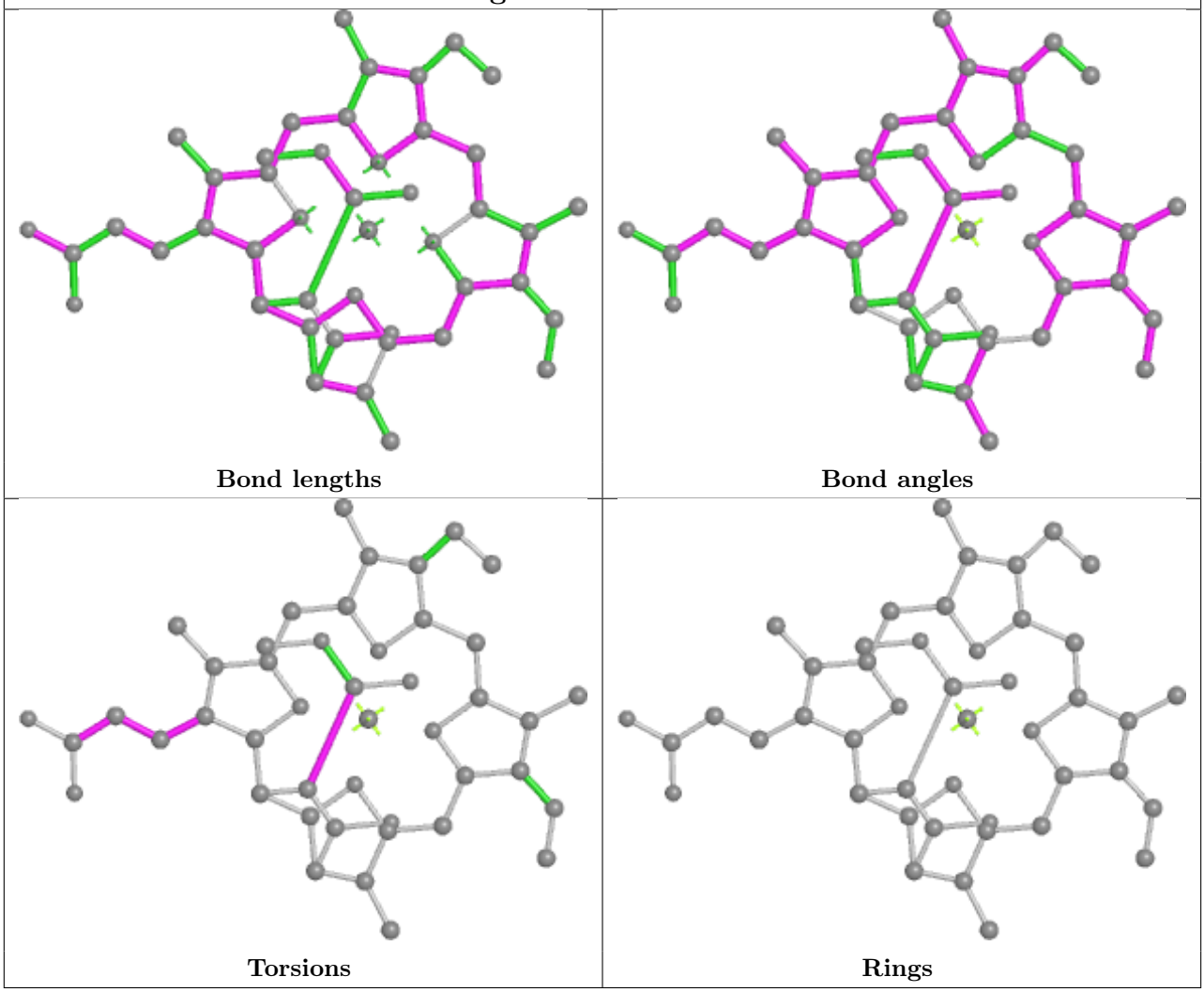
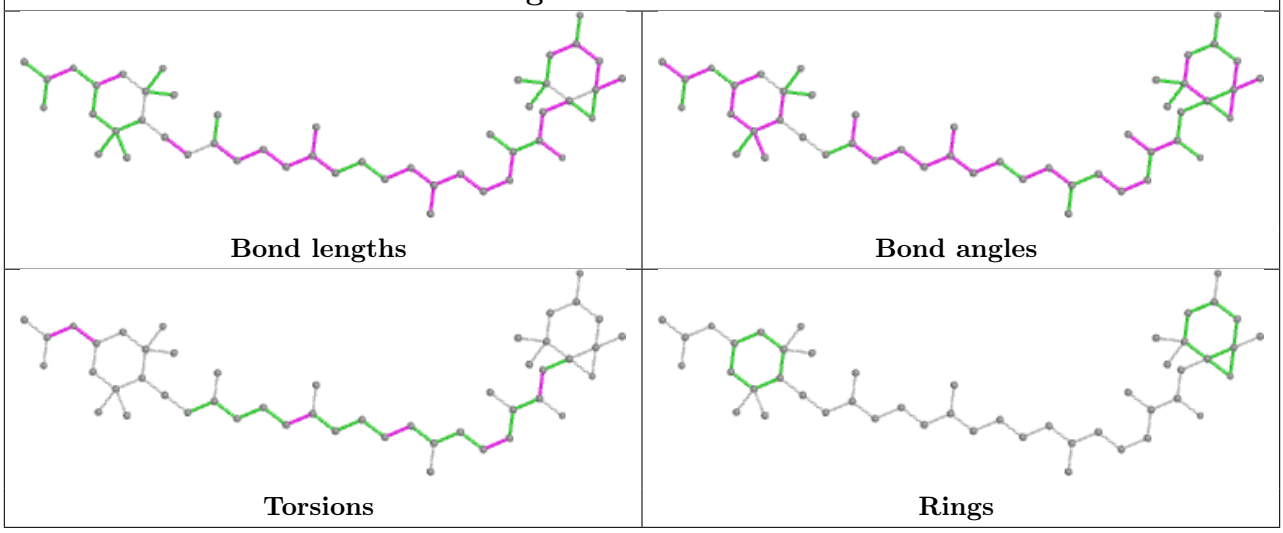


Ligand A86 21 213



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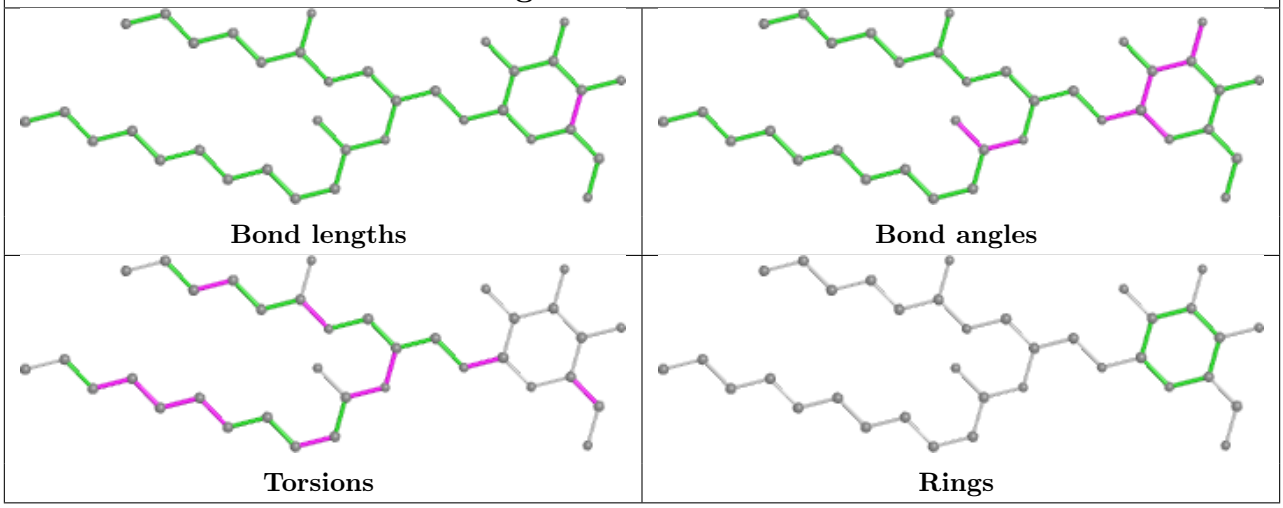

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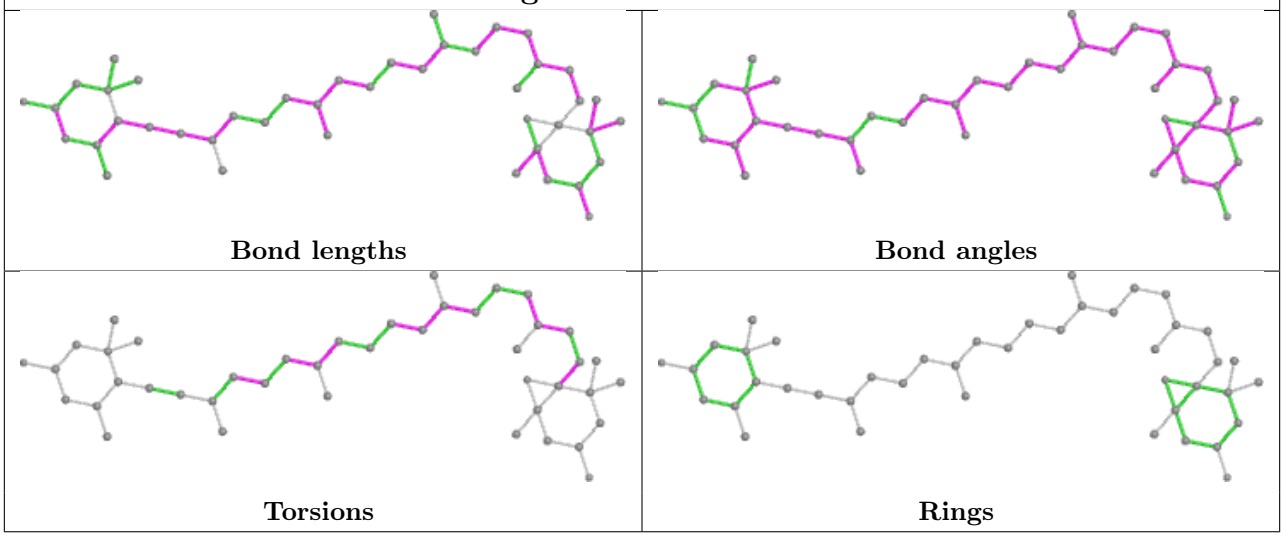

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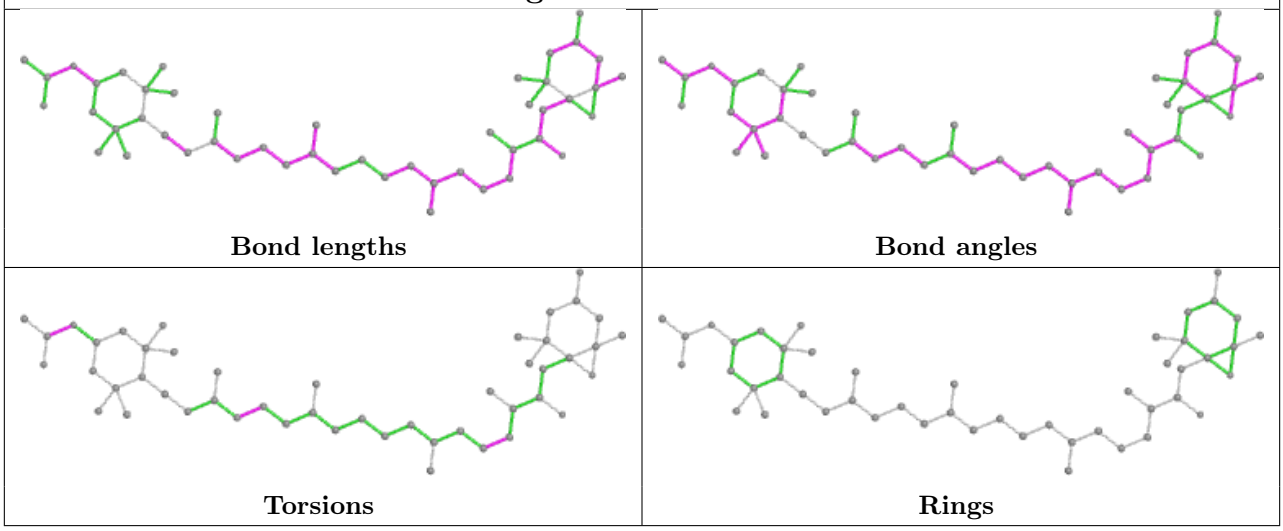
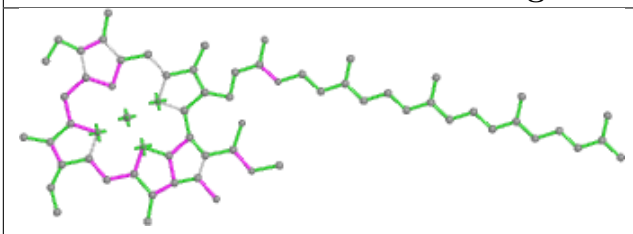
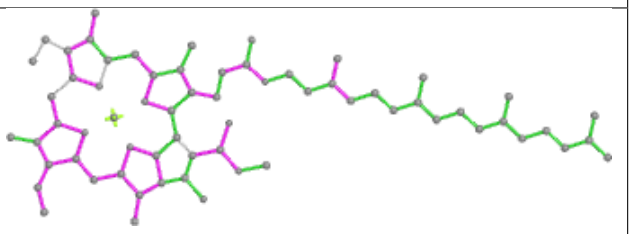


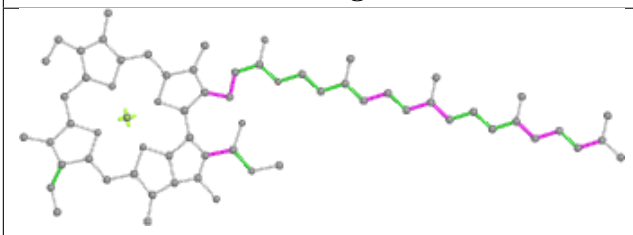
Ligand CLA d 401



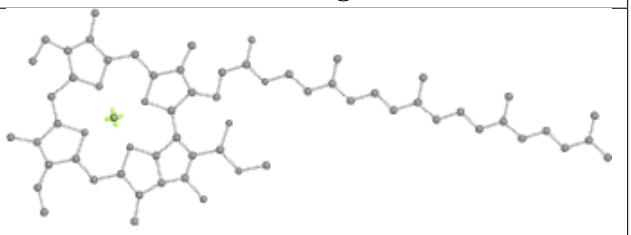
Bond lengths



Bond angles

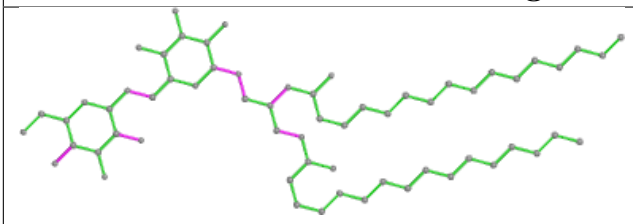


Torsions



Rings

Ligand DGD c 516



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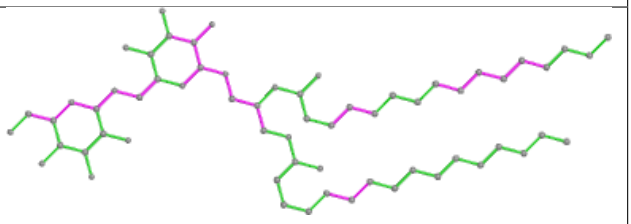
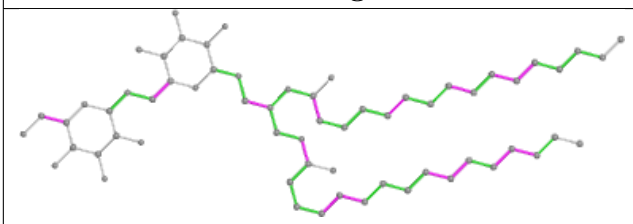


Bond angles



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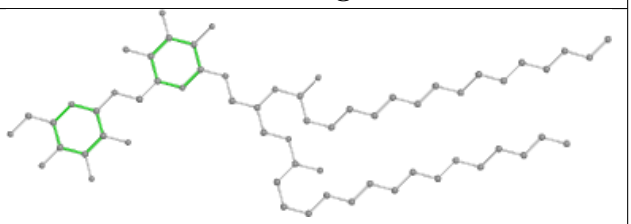

Rings

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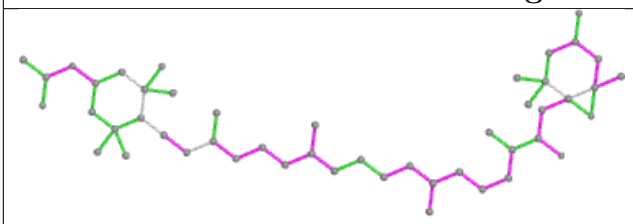

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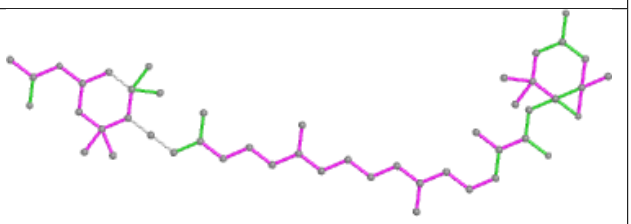
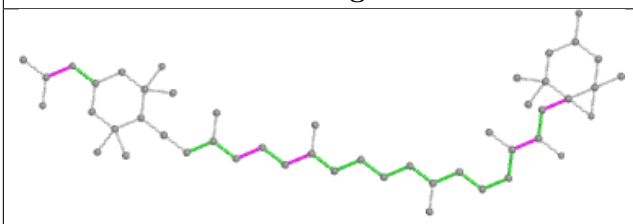


Bond angles



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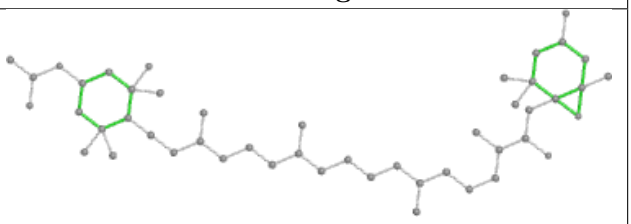

Rings

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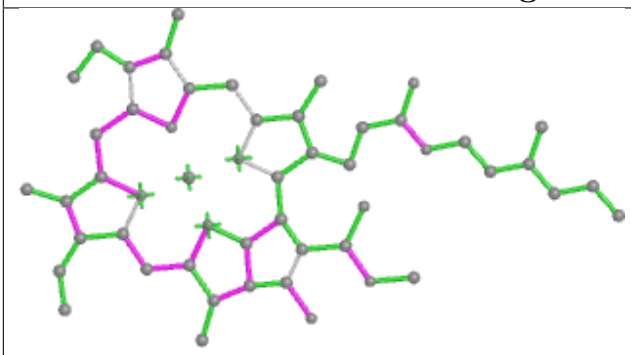
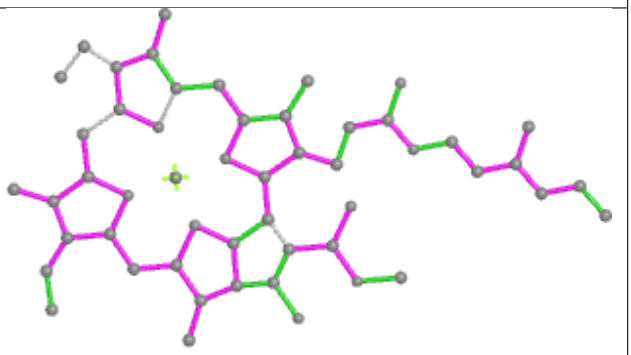
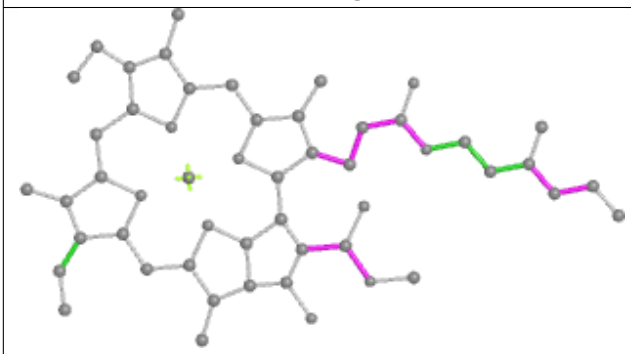
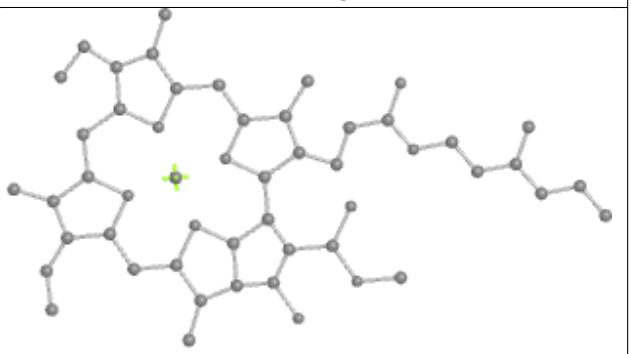
 Bond lengths	 Bond angles
 Torsions	 Rings

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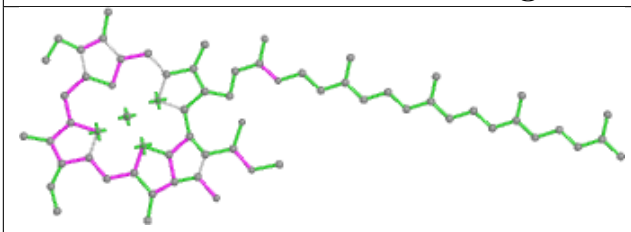
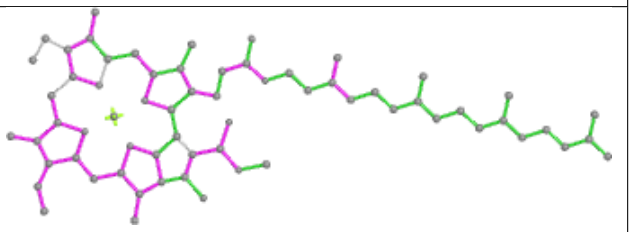
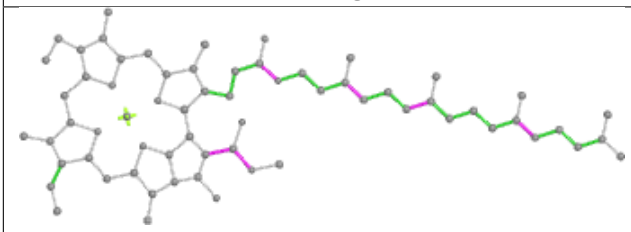
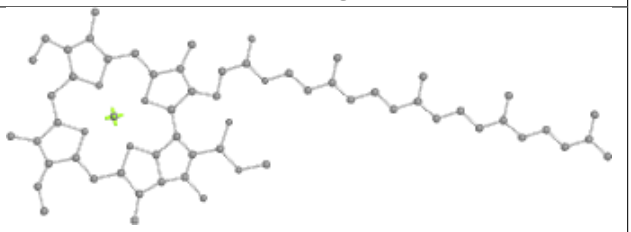
 Bond lengths	 Bond angles
 Torsions	 Rings

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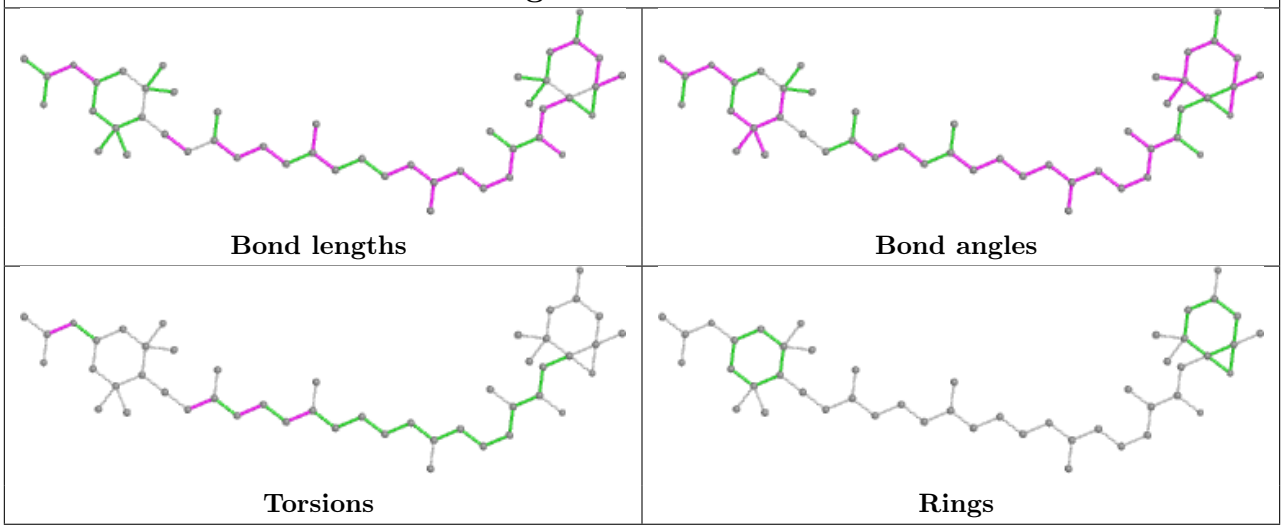

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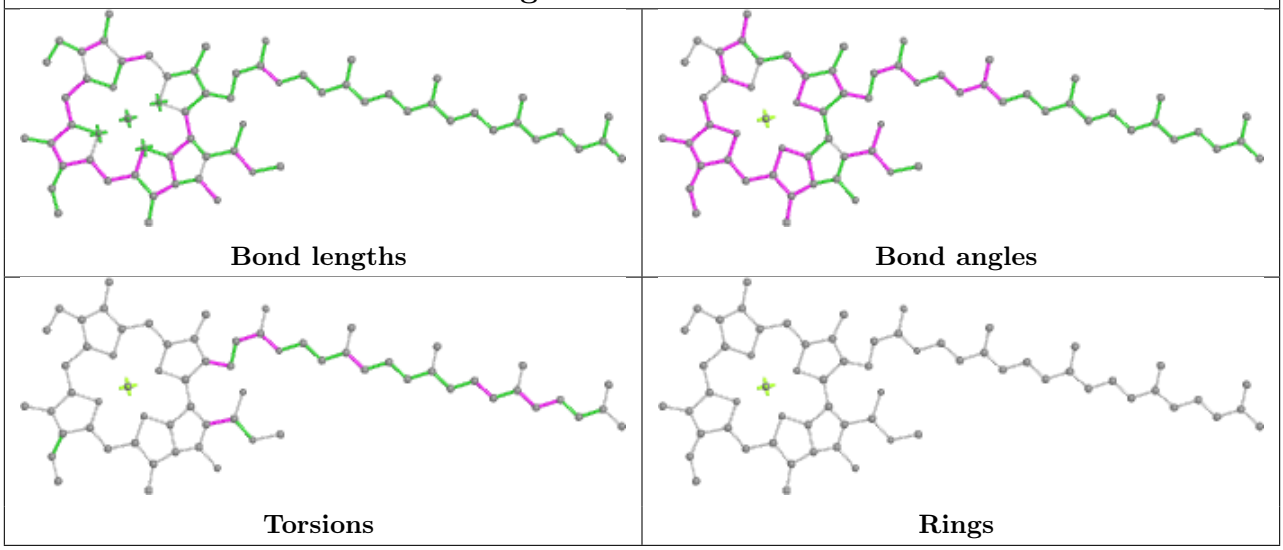

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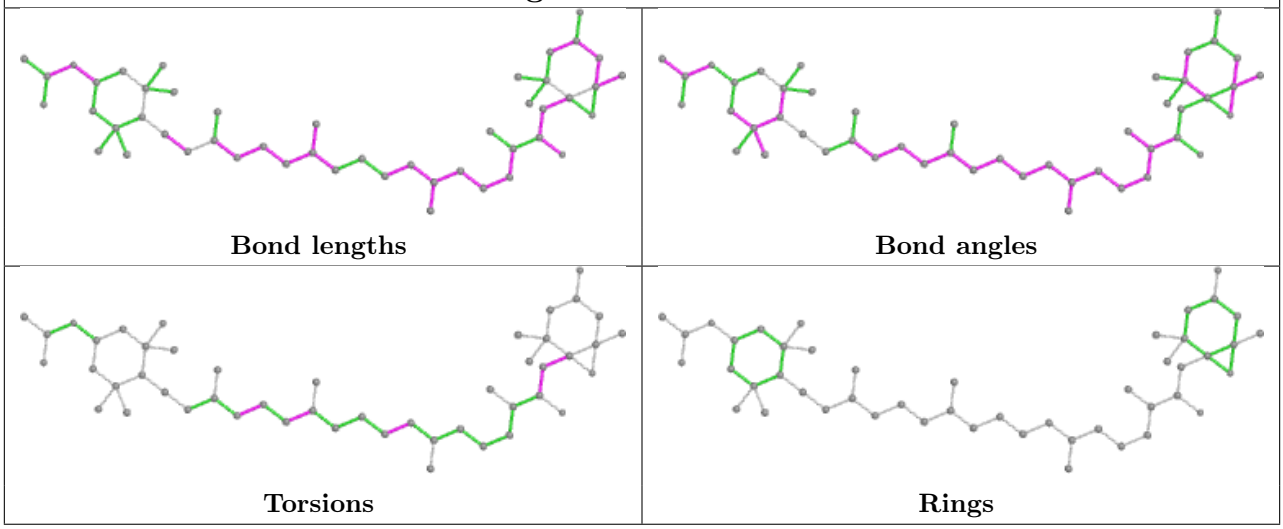
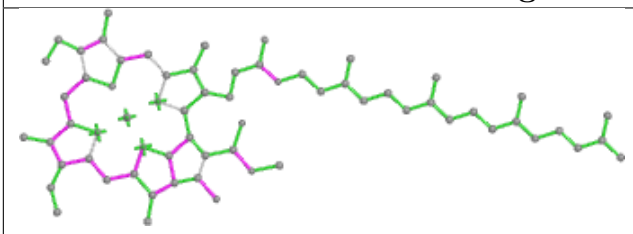


Ligand CLA W 102



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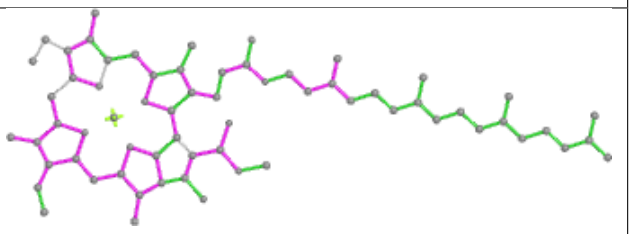
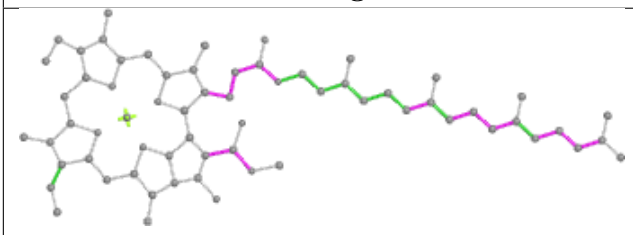
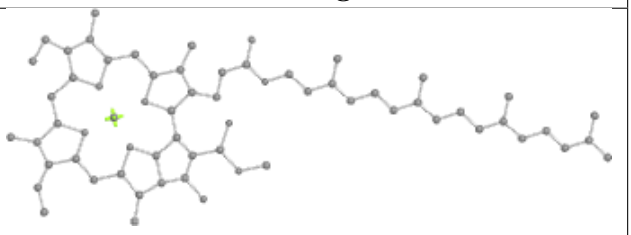


Bond angles

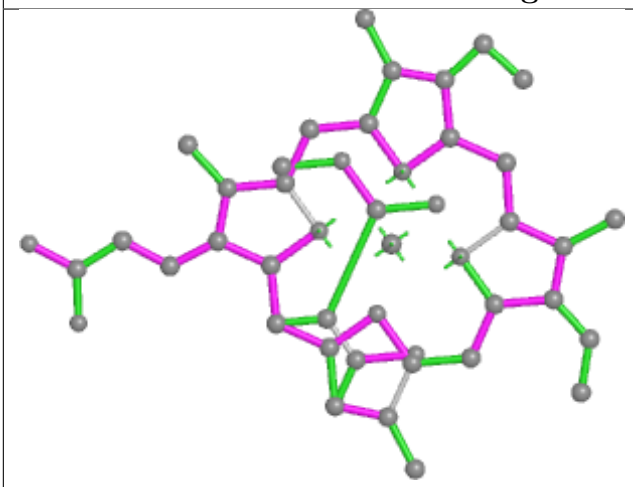


Torsions



Rings

Ligand KC1 16 304



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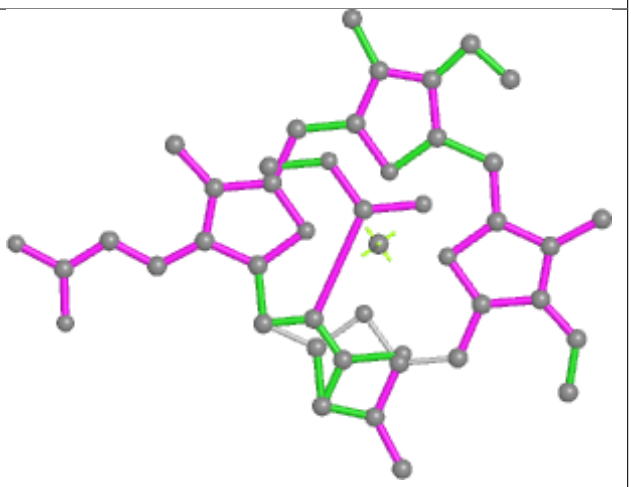
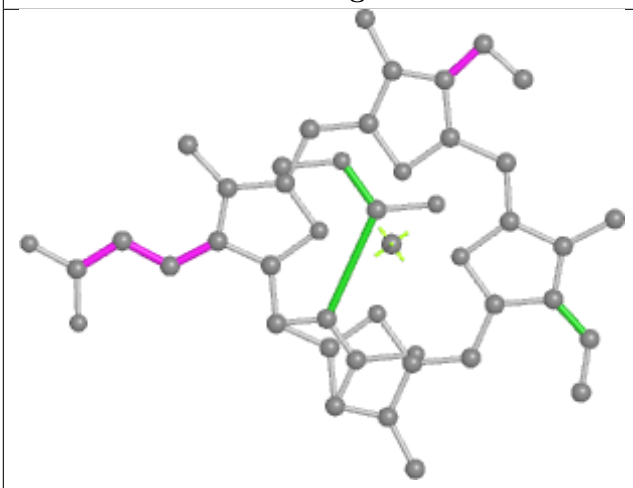


Bond angles



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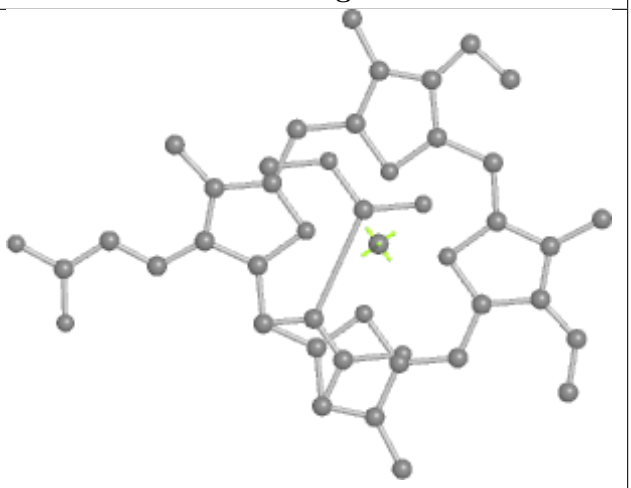
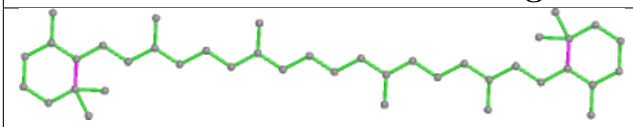


Rings

Ligand BCR b 517



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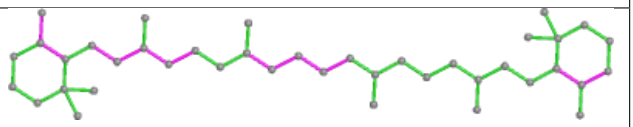
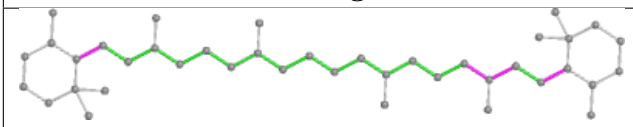


Bond angles



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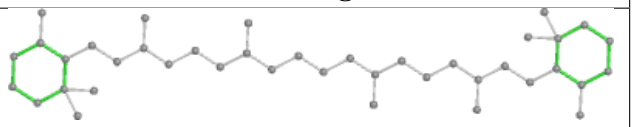
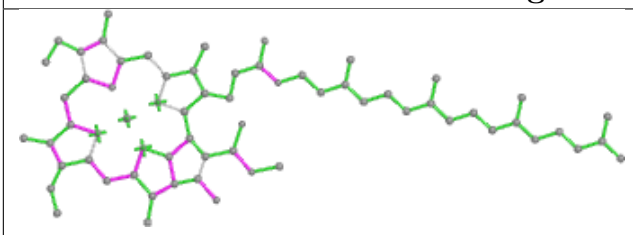


Rings

Ligand CLA b 503



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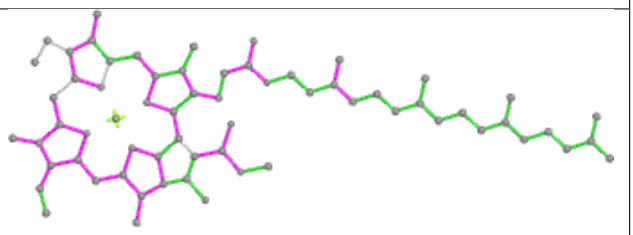
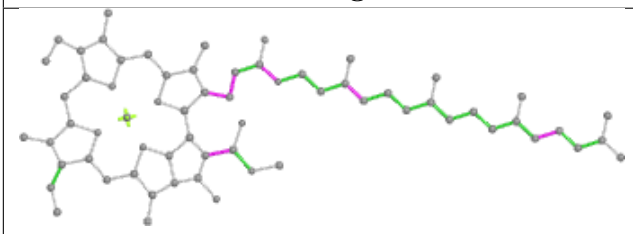


Bond angles



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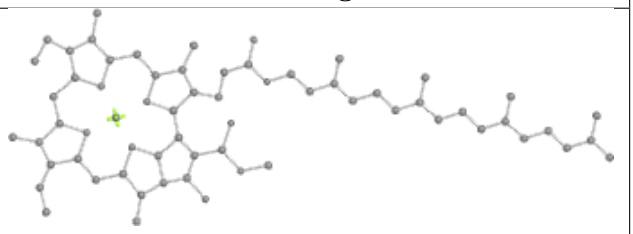
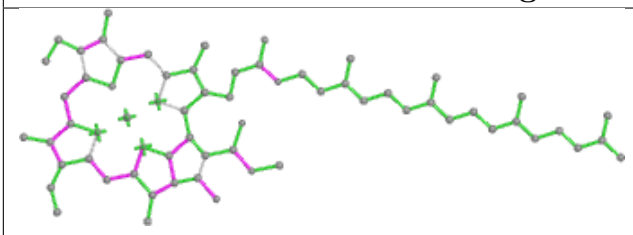


Rings

Ligand CLA 15 301



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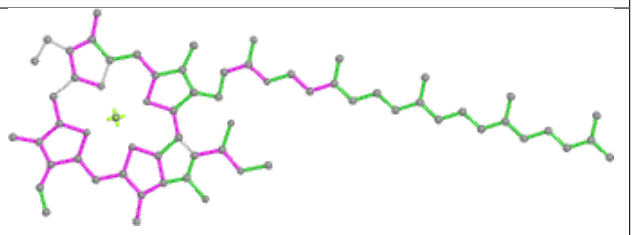
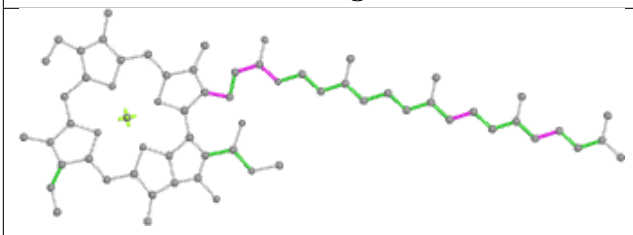


Bond angles



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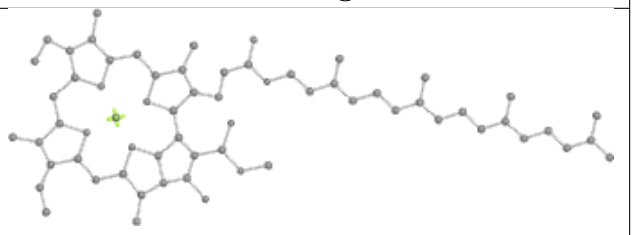
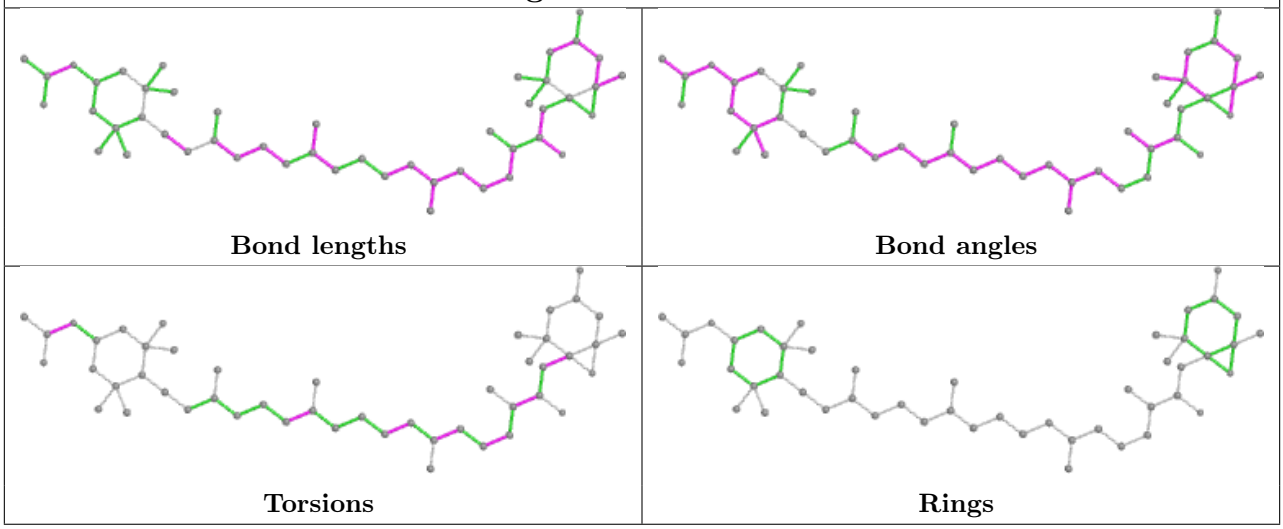
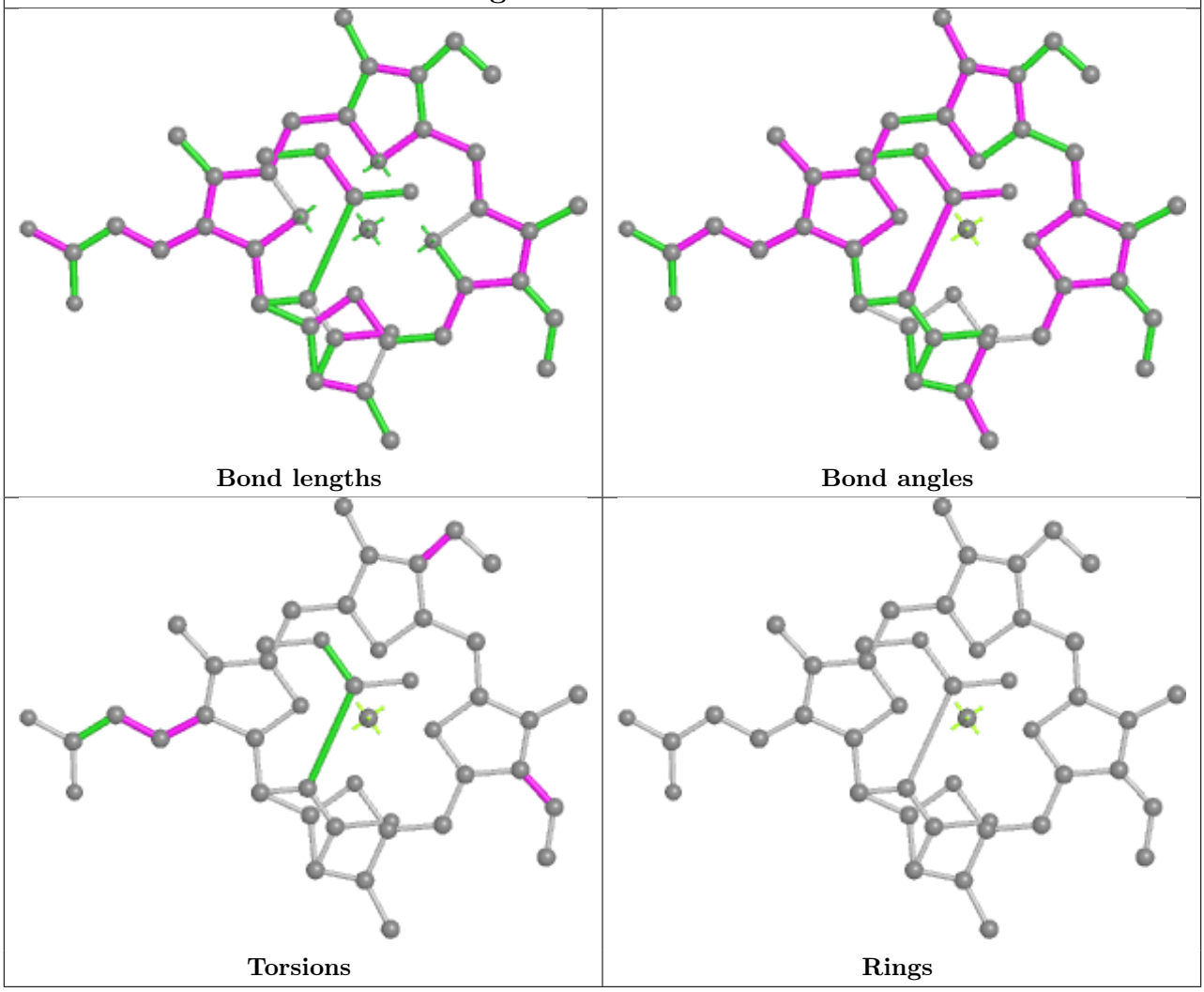


Rings

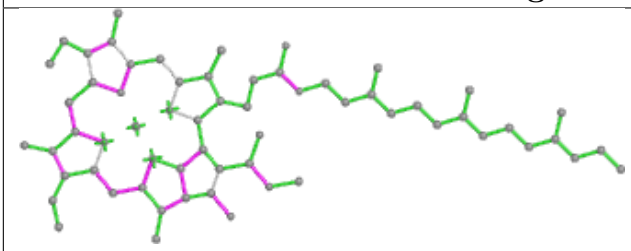
Ligand A86 32 203



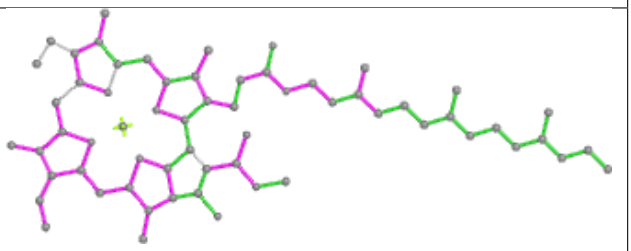
Ligand KC1 34 304



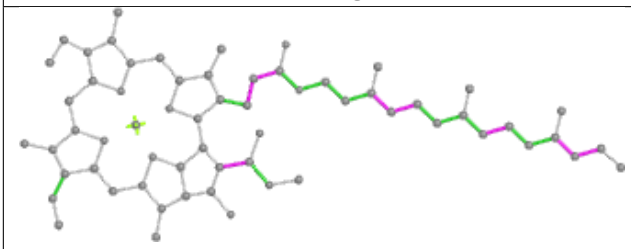
Ligand CLA b 514



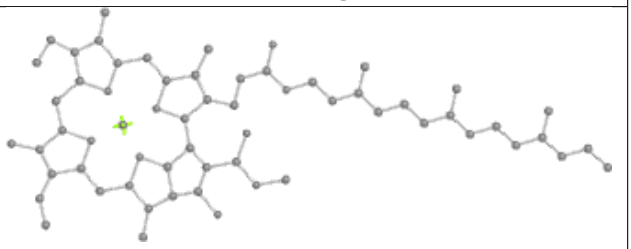
Bond lengths



Bond angles

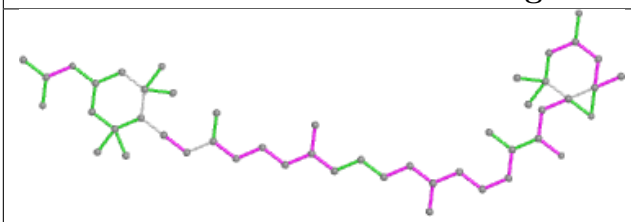


Torsions



Rings

Ligand A86 32 216



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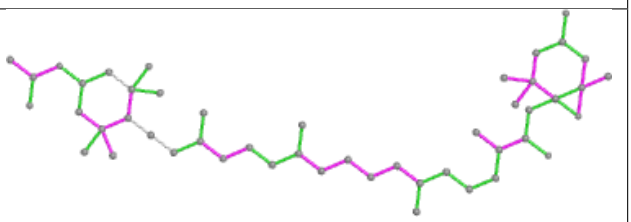

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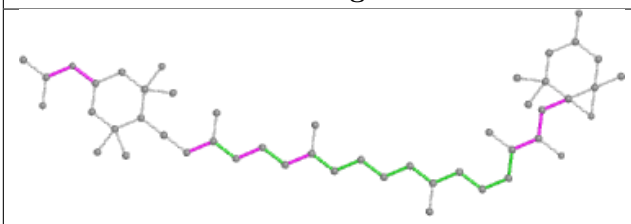

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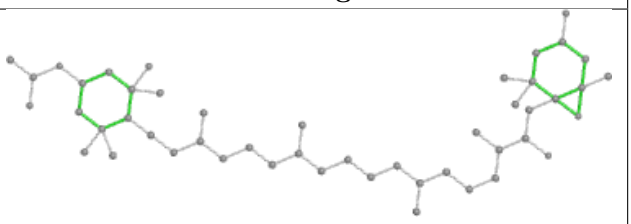
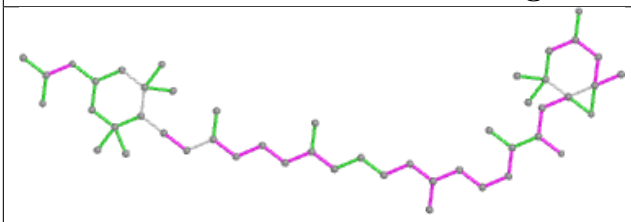


Rings

Ligand A86 40 201



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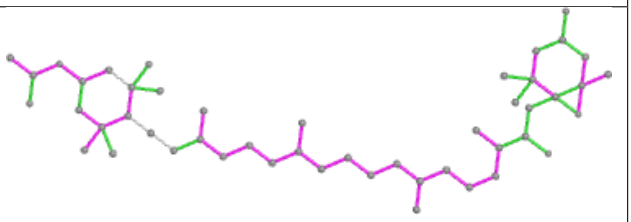

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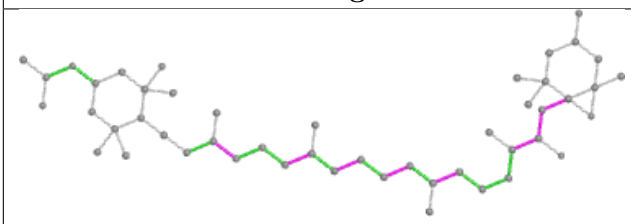

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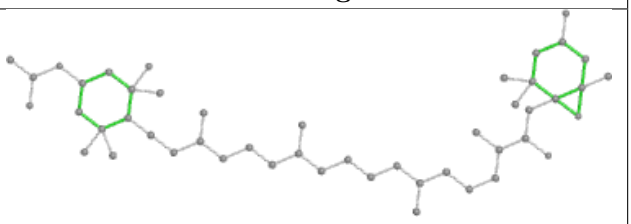
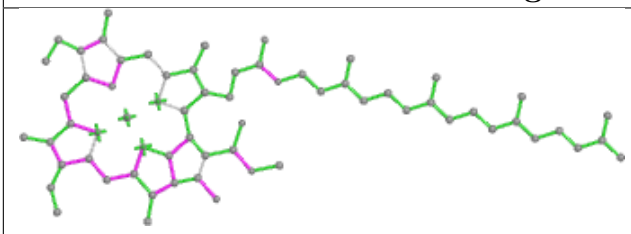


Rings

Ligand CLA B 515



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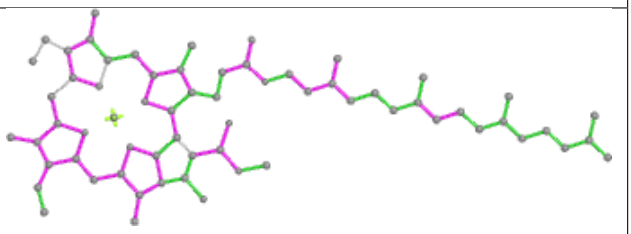

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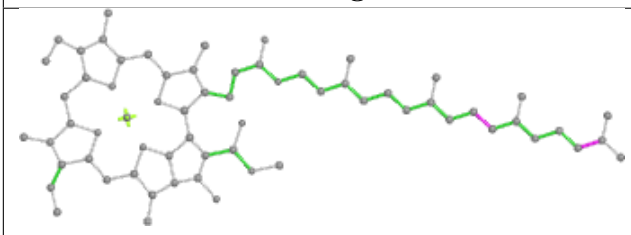

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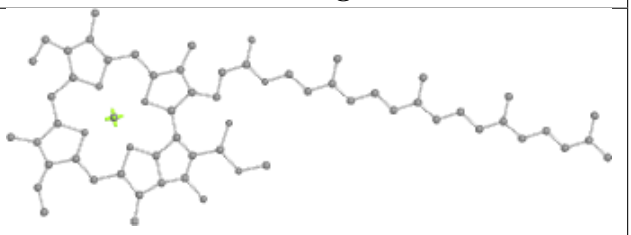
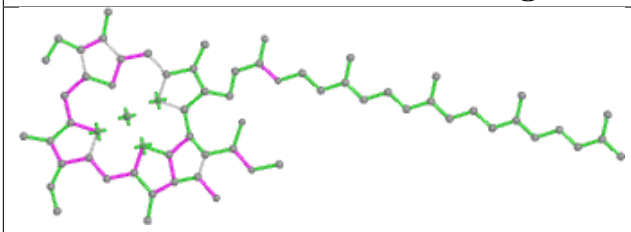


Rings

Ligand CLA 15 308



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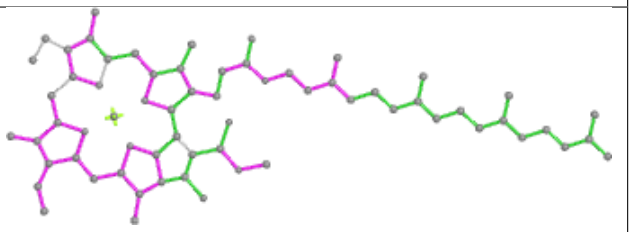

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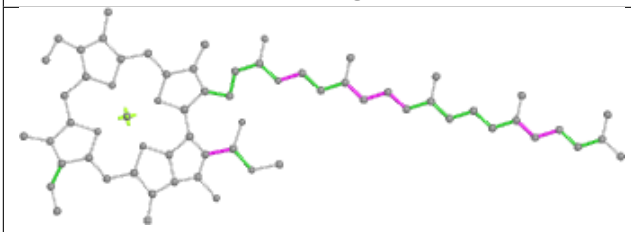

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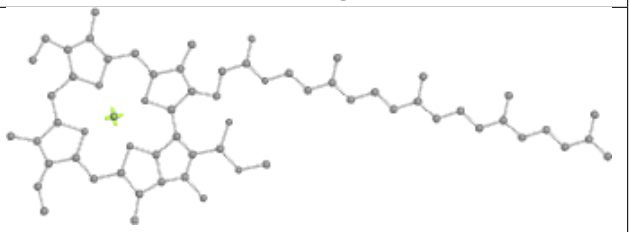
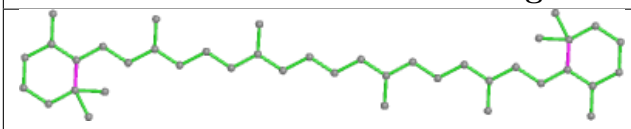


Rings

Ligand BCR b 518



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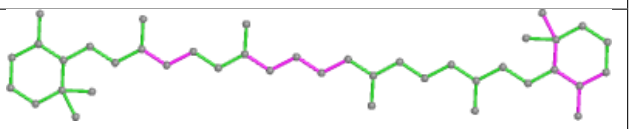

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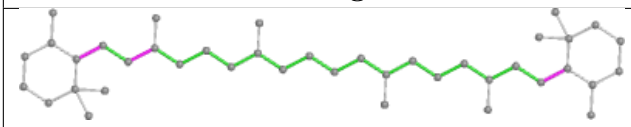
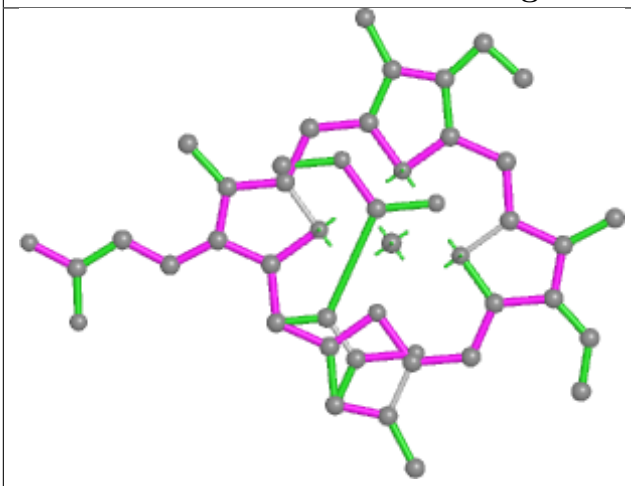


Torsions

Rings

Ligand KC1 41 203



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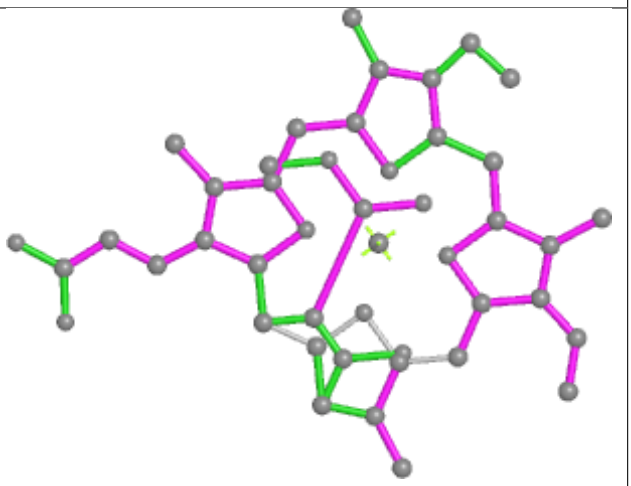

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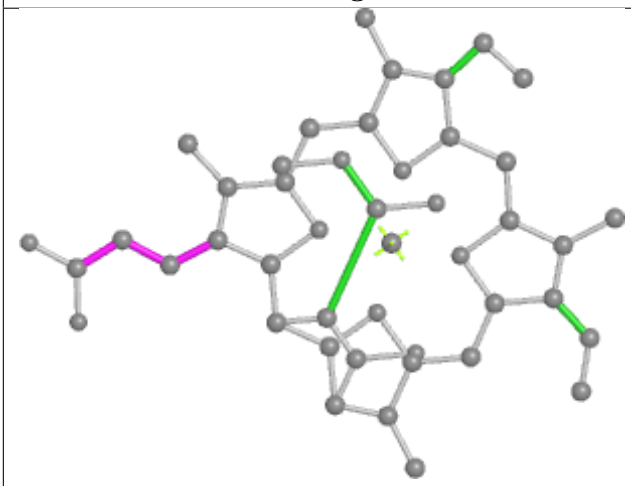

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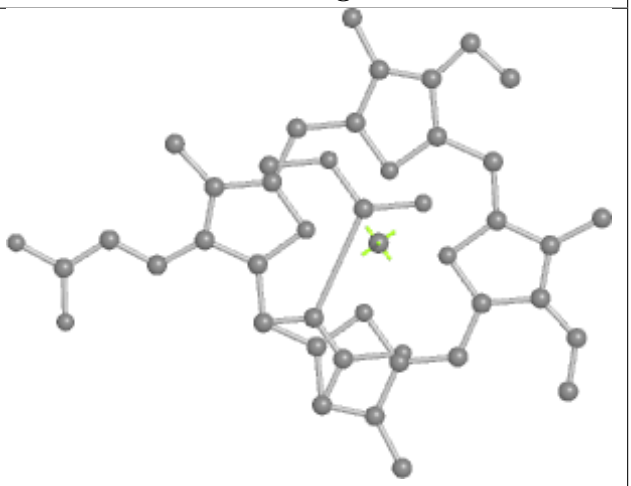
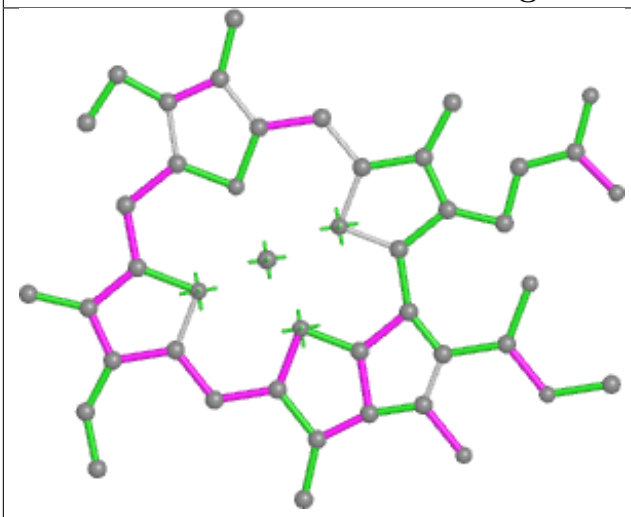


Rings

Ligand CLA 41 210



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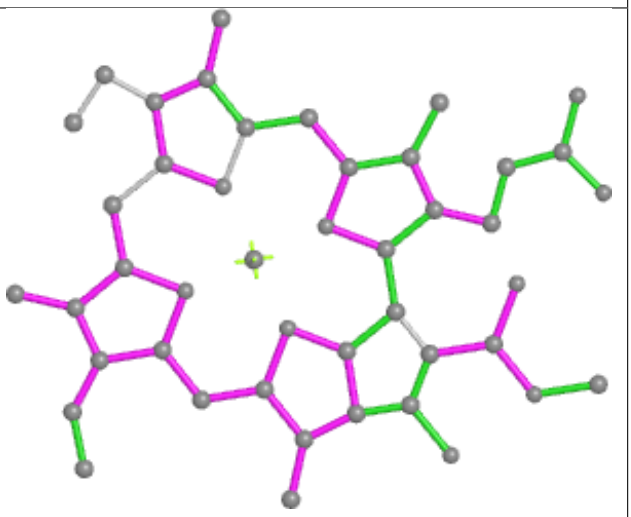

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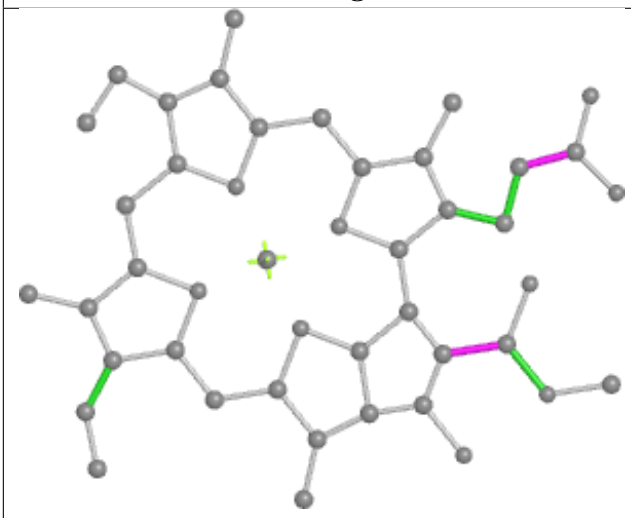

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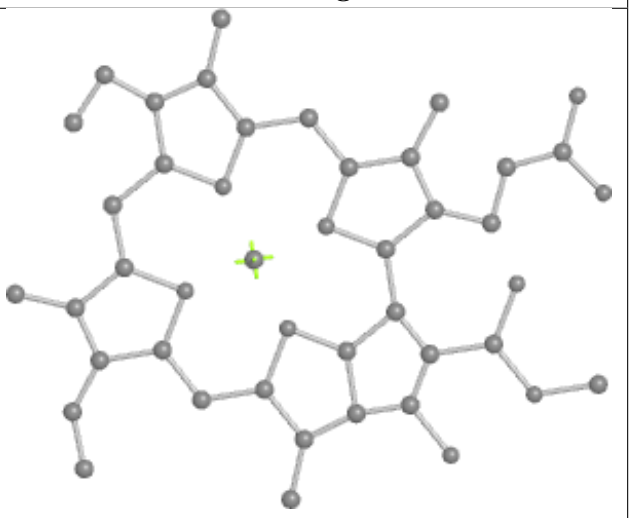
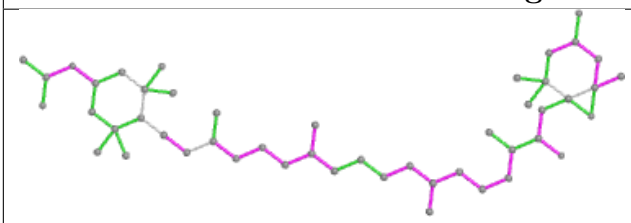


Rings

Ligand A86 31 313



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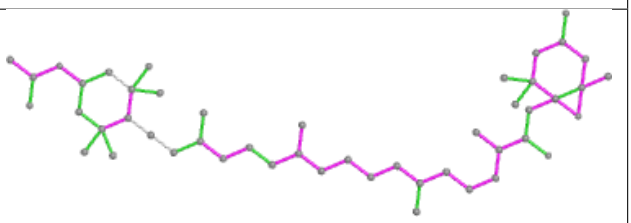

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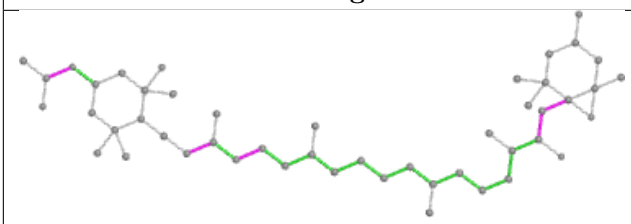

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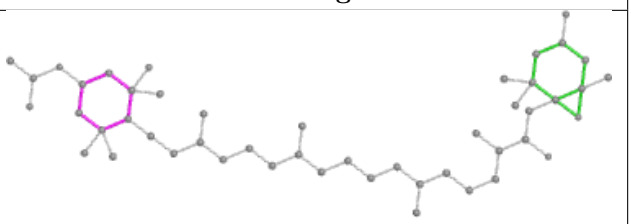

Rings

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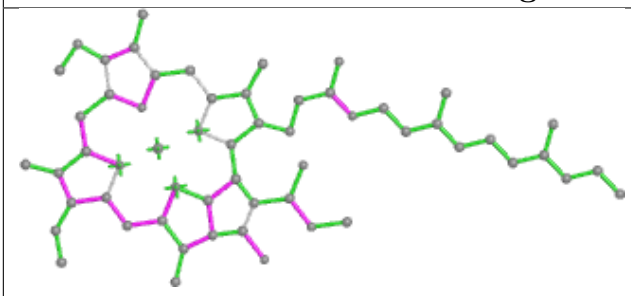

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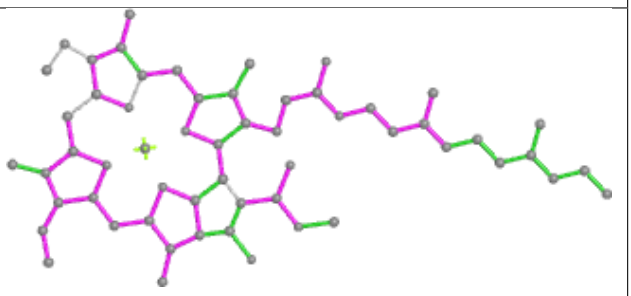
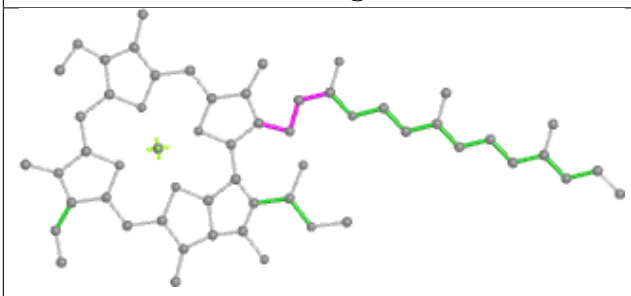


Bond angles



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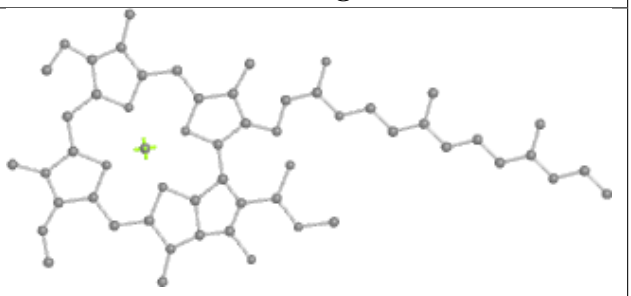
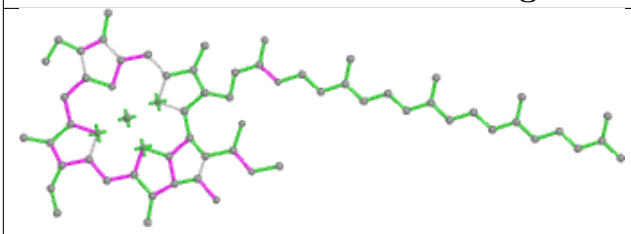


Rings

Ligand CLA 34 308



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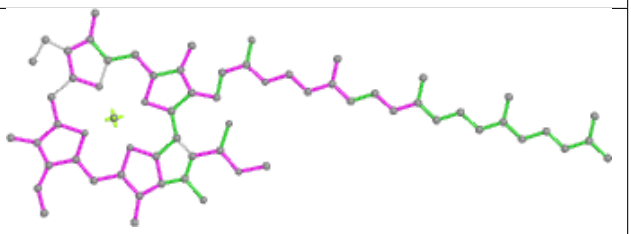

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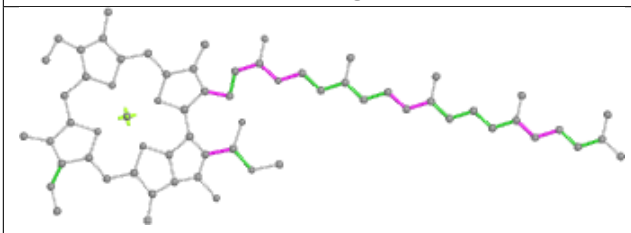

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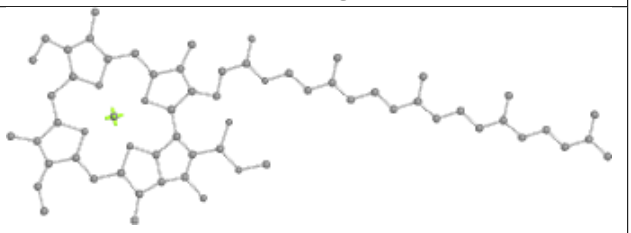
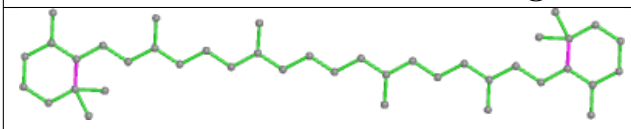


Rings

Ligand BCR c 514



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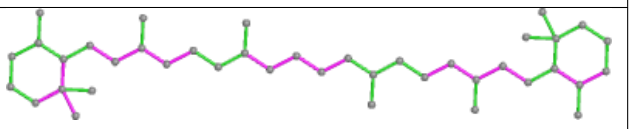

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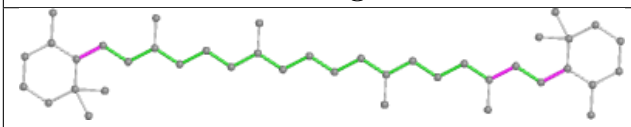

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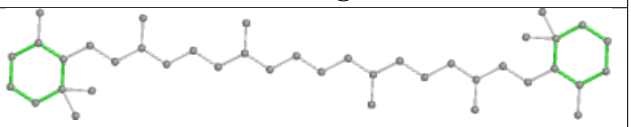

Rings

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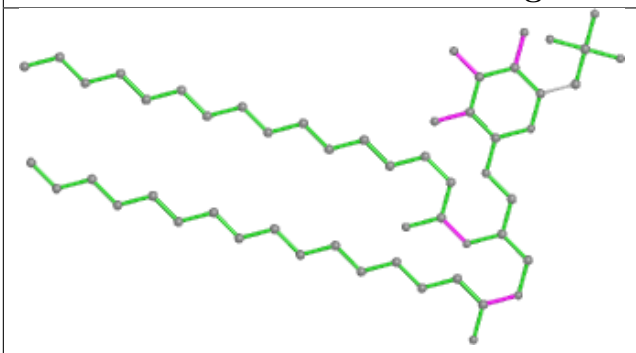
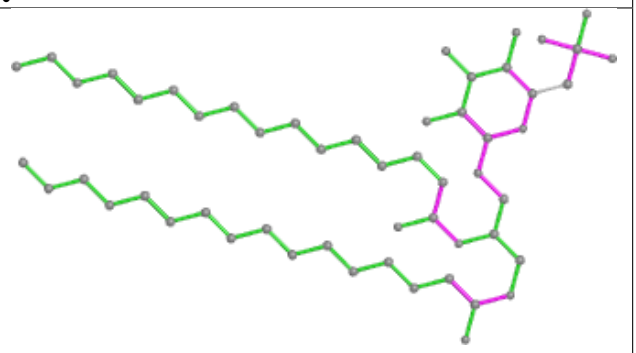
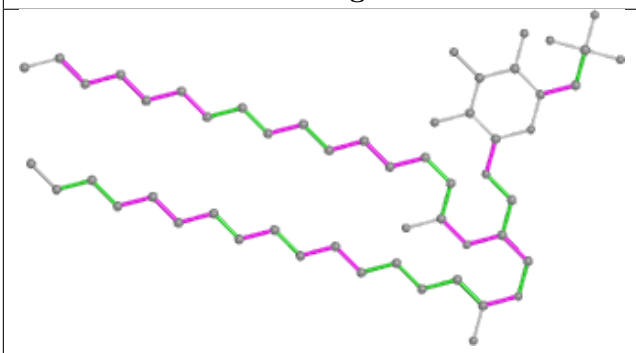
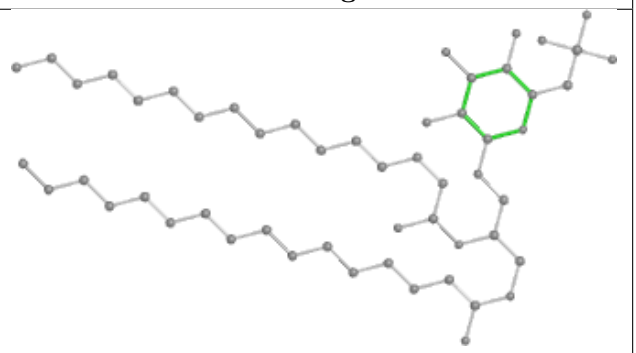
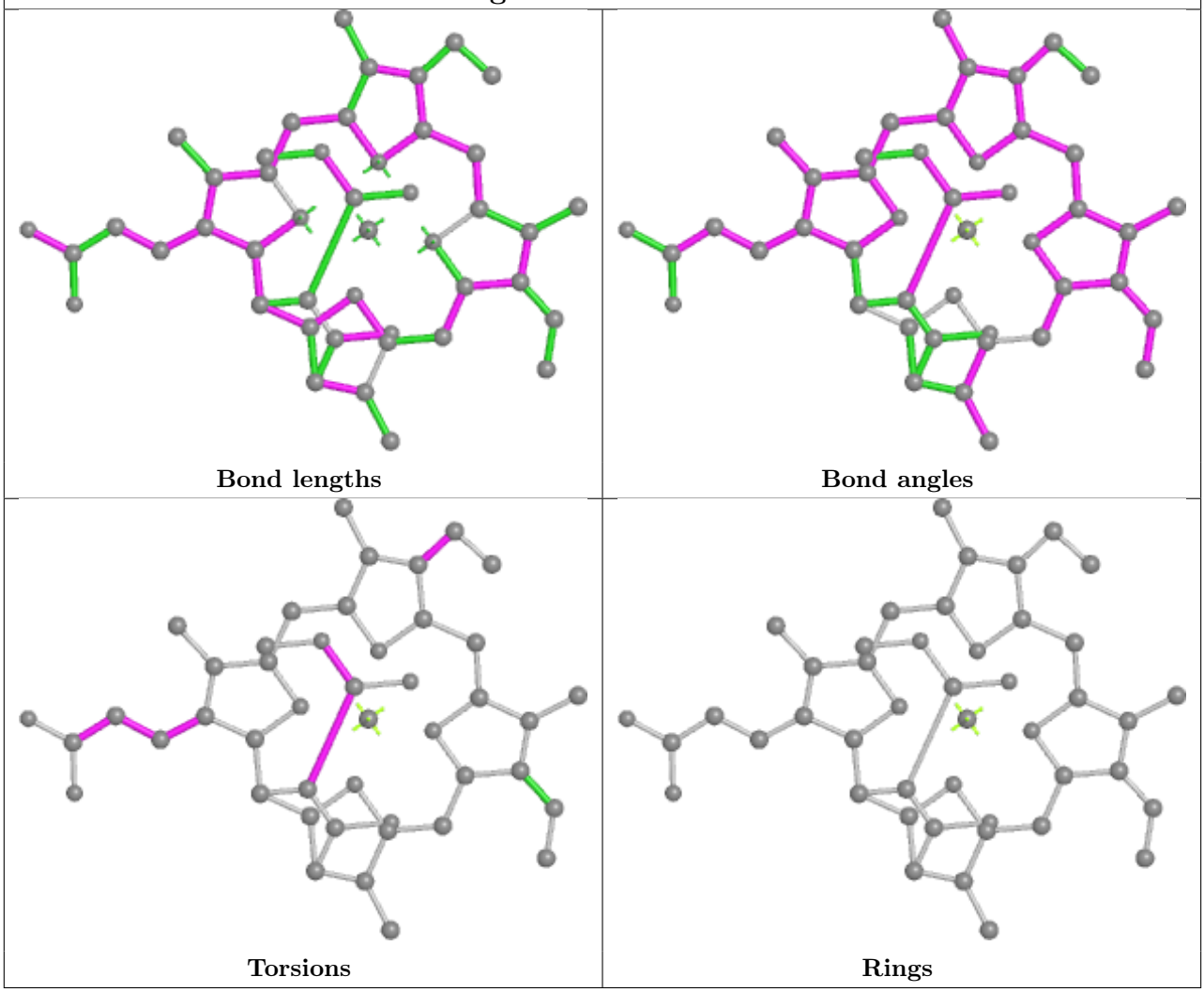
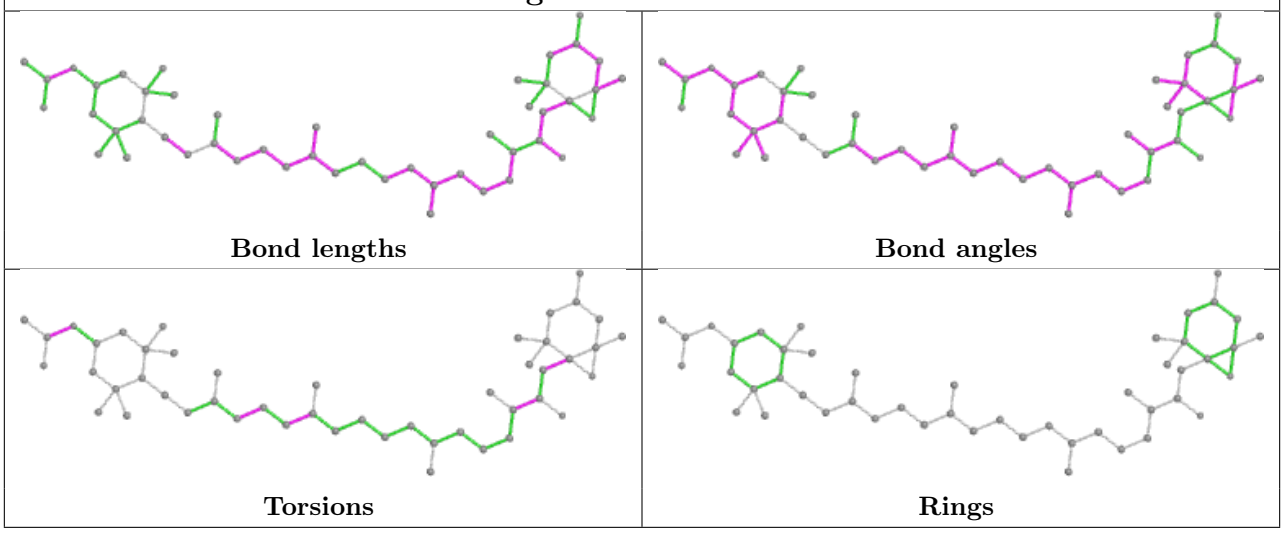
 Bond lengths	 Bond angles
 Torsions	 Rings

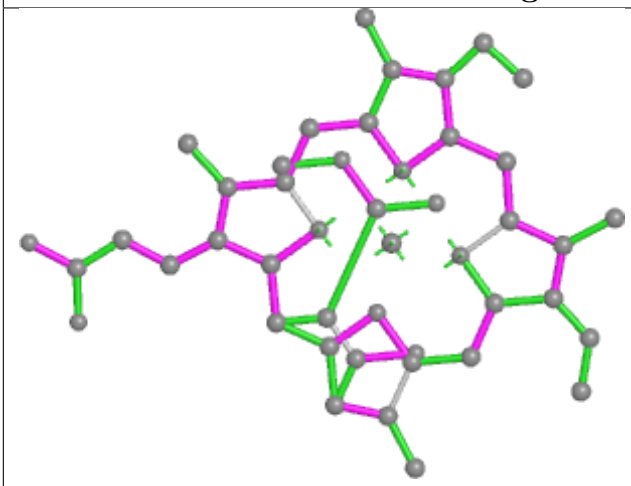
Ligand KC1 40 204



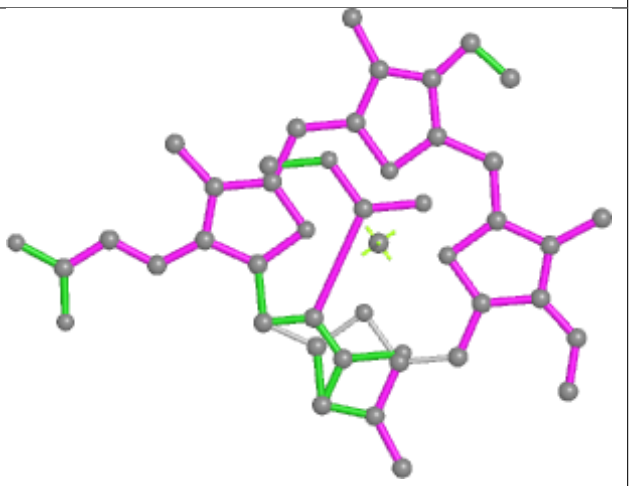
Ligand A86 11 314



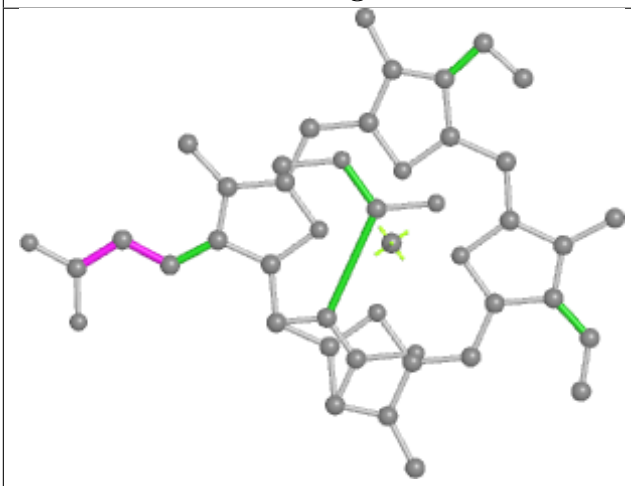
Ligand KC1 39 308



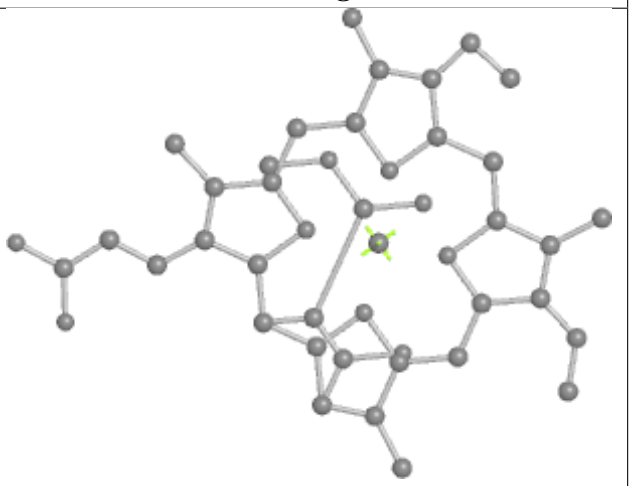
Bond lengths



Bond angles

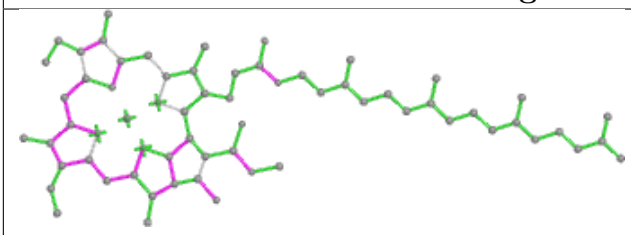


Torsions



Rings

Ligand CLA 37 308



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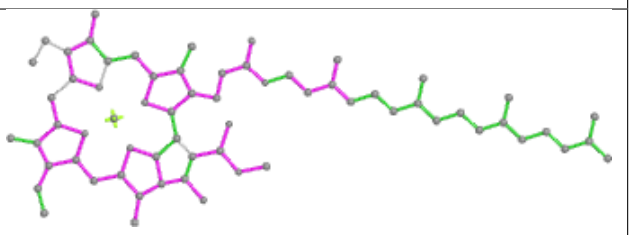

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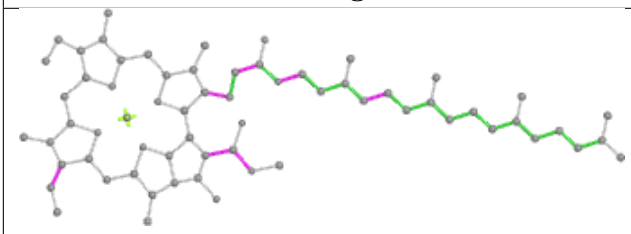

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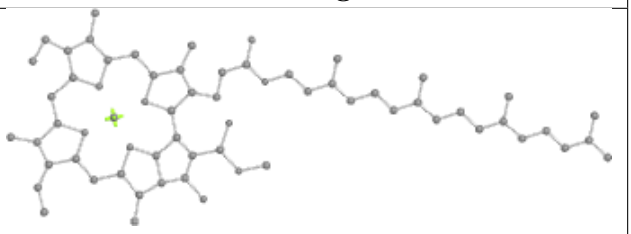
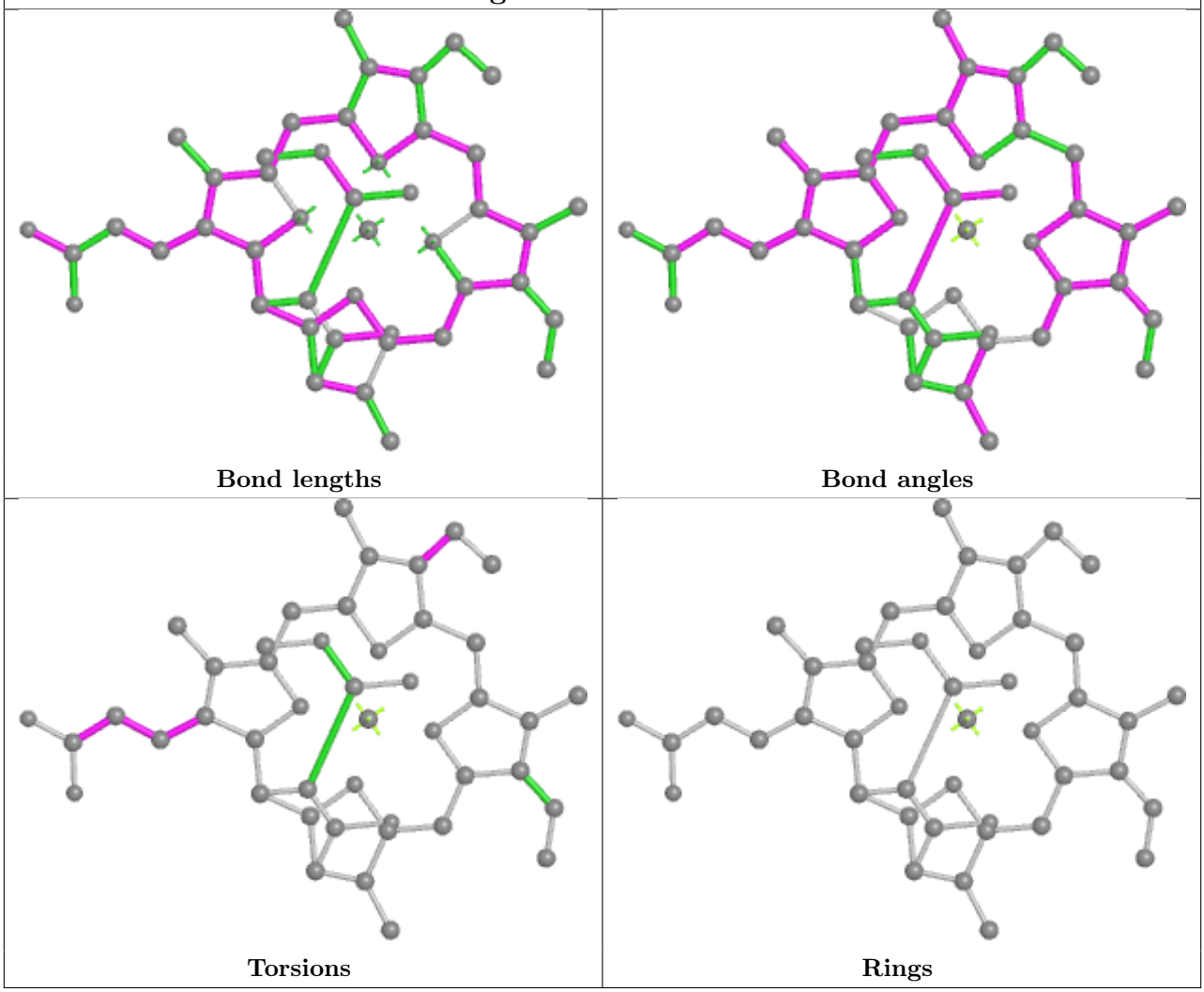
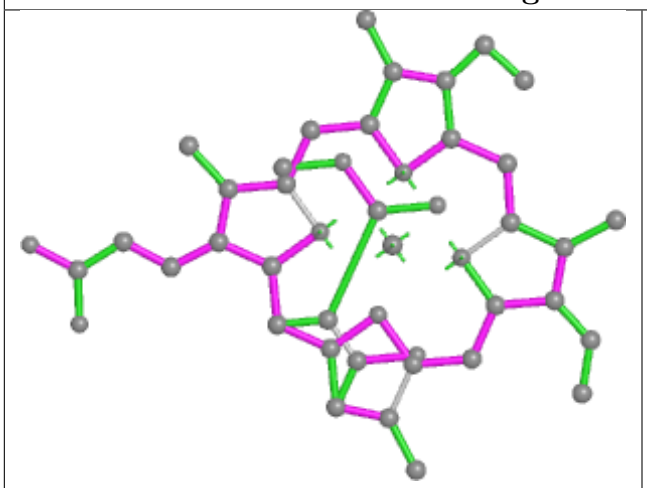


Rings

Ligand KC1 38 205



Ligand KC1 17 303



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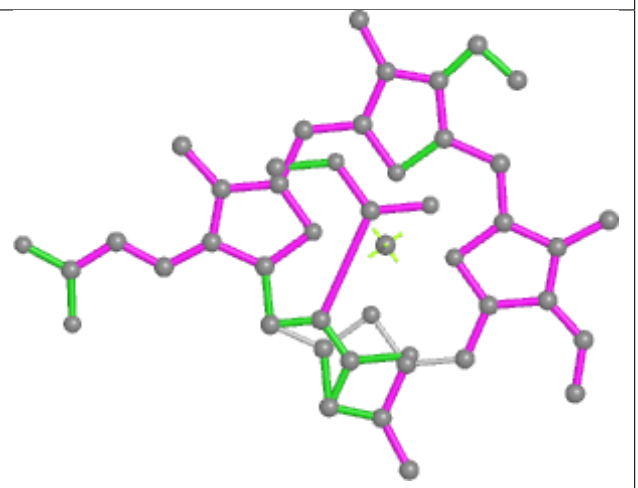
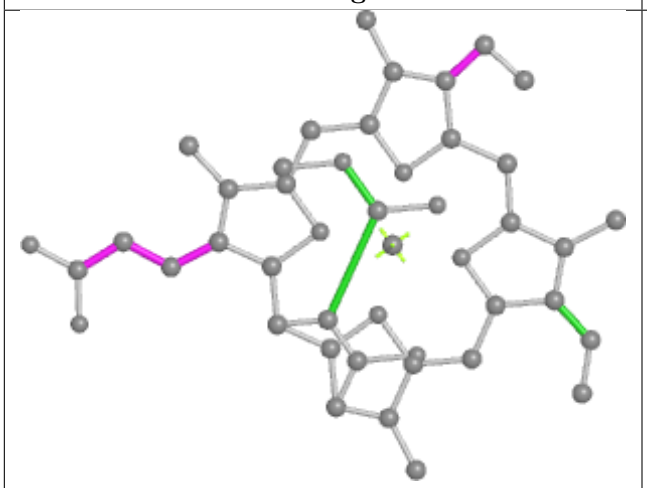


Bond angles



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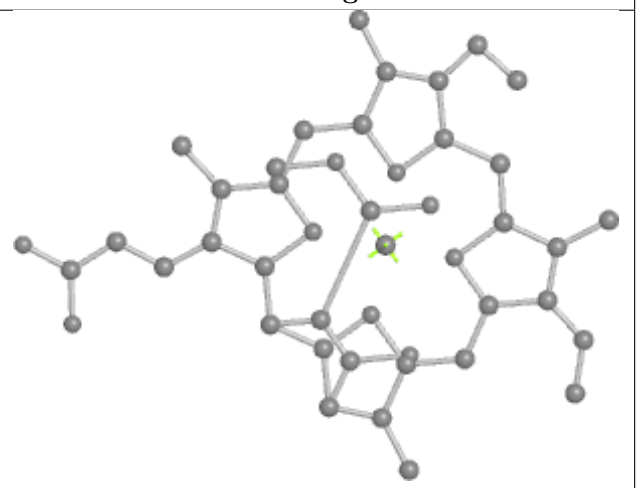
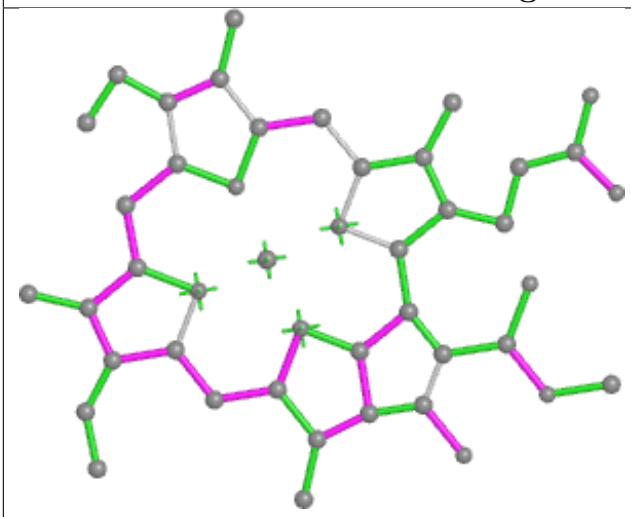


Rings

Ligand CLA 41 209



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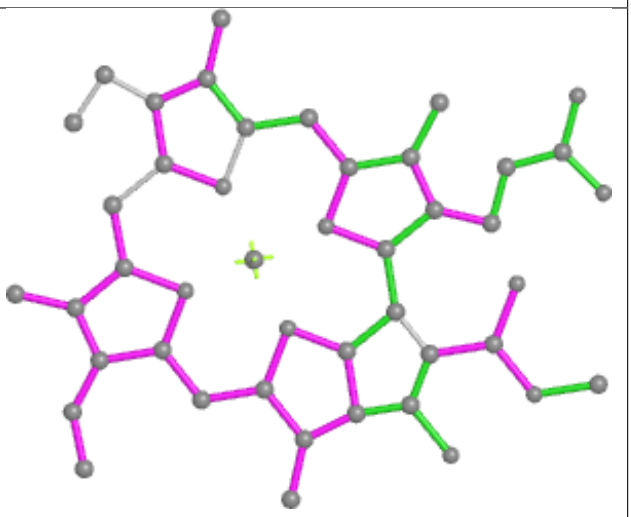
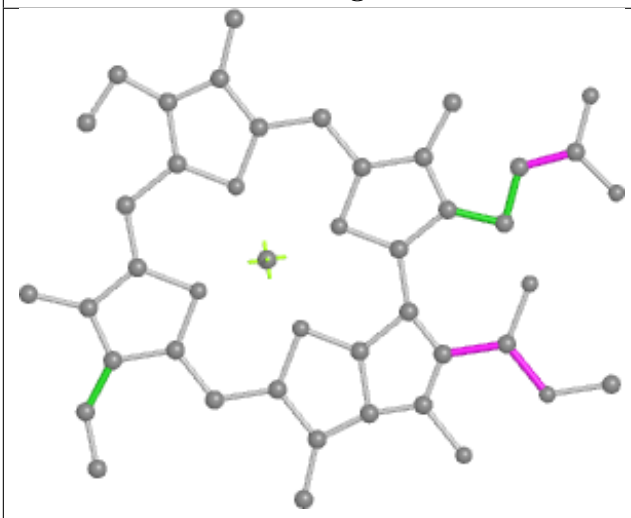
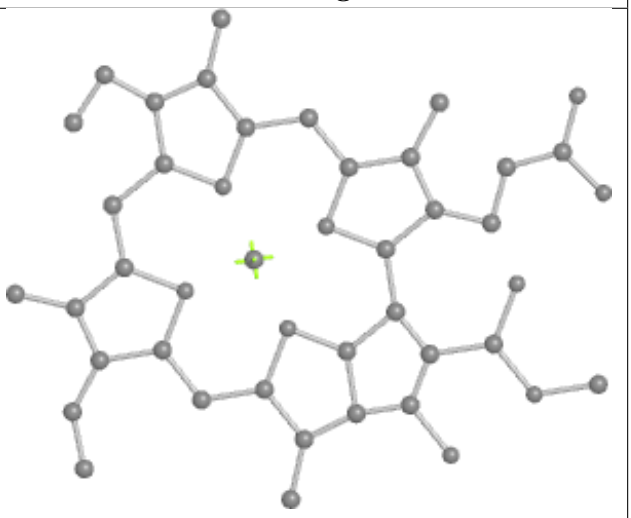


Bond angles

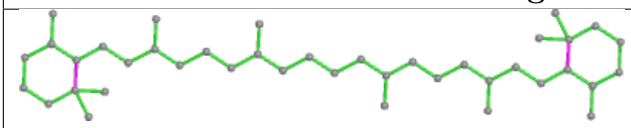


Torsions



Rings

Ligand BCR c 519



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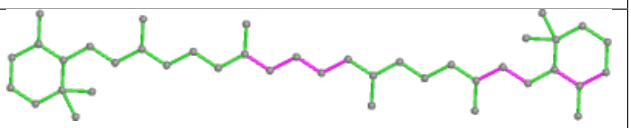
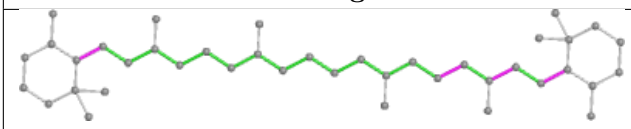


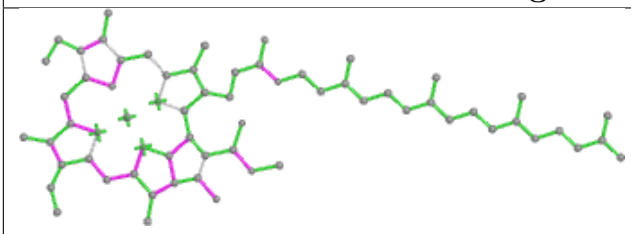
Bond angles



Torsions

Rings

Ligand CLA c 509



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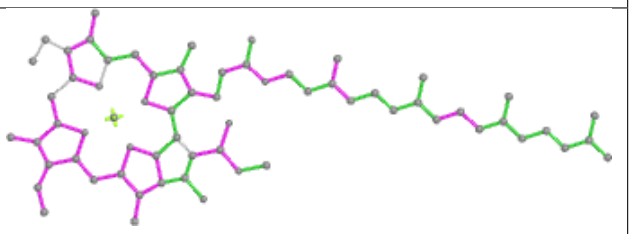
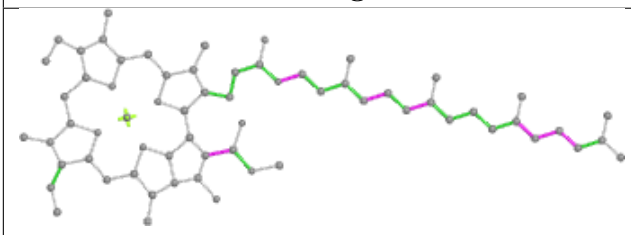


Bond angles



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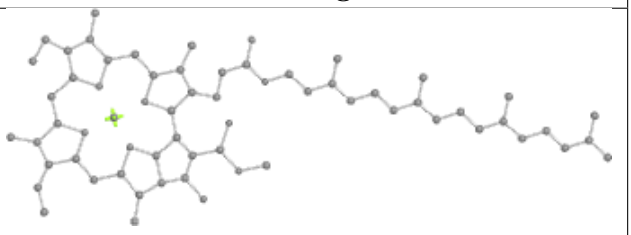
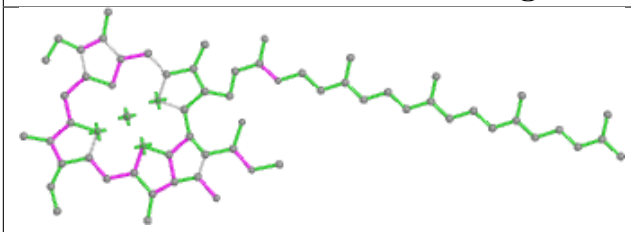


Rings

Ligand CLA 21 206



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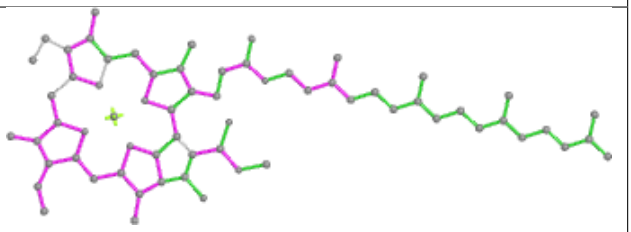
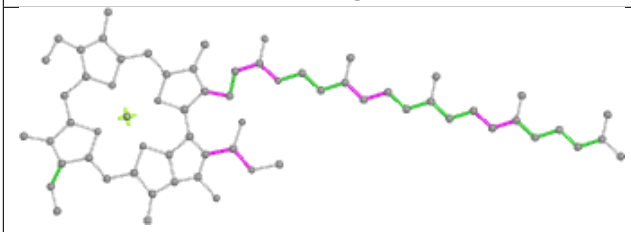


Bond angles



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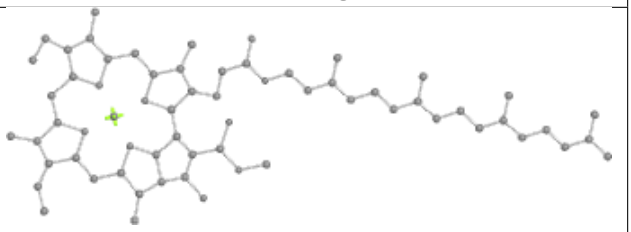
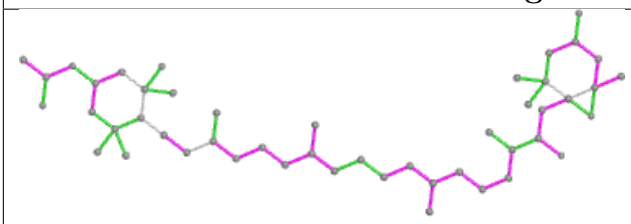


Rings

Ligand A86 14 313



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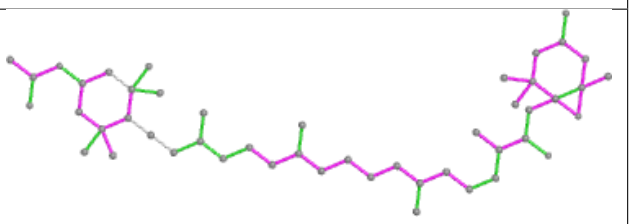
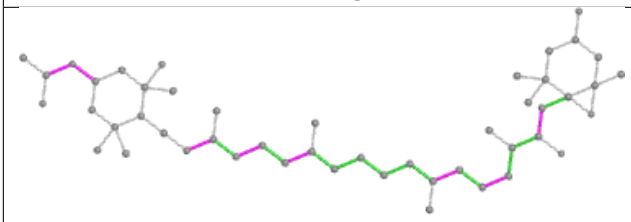
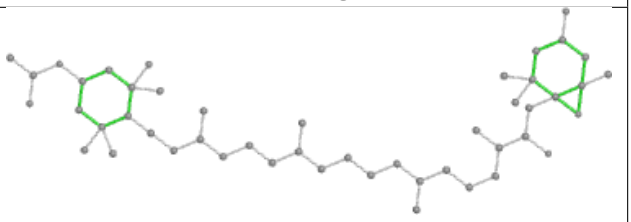


Bond angles

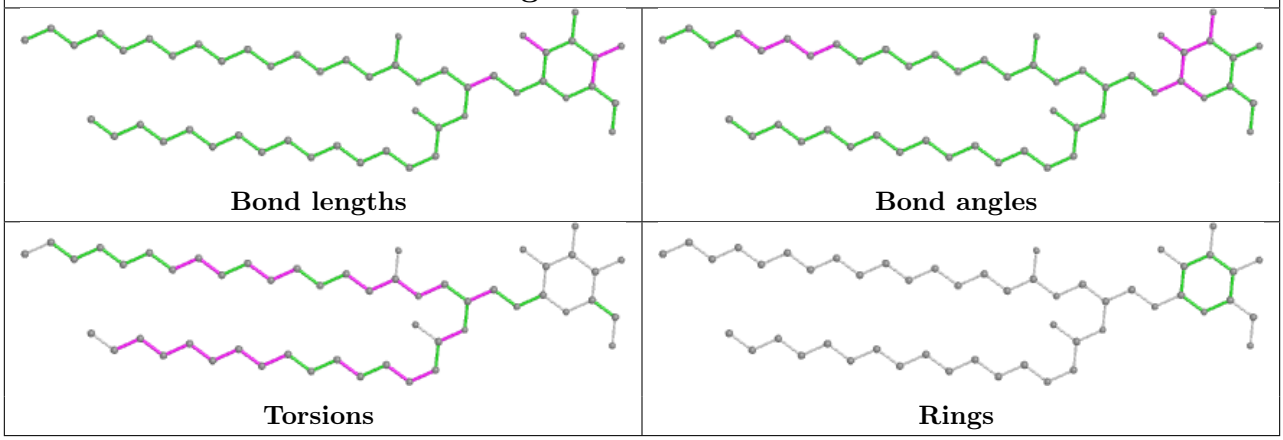


Torsions

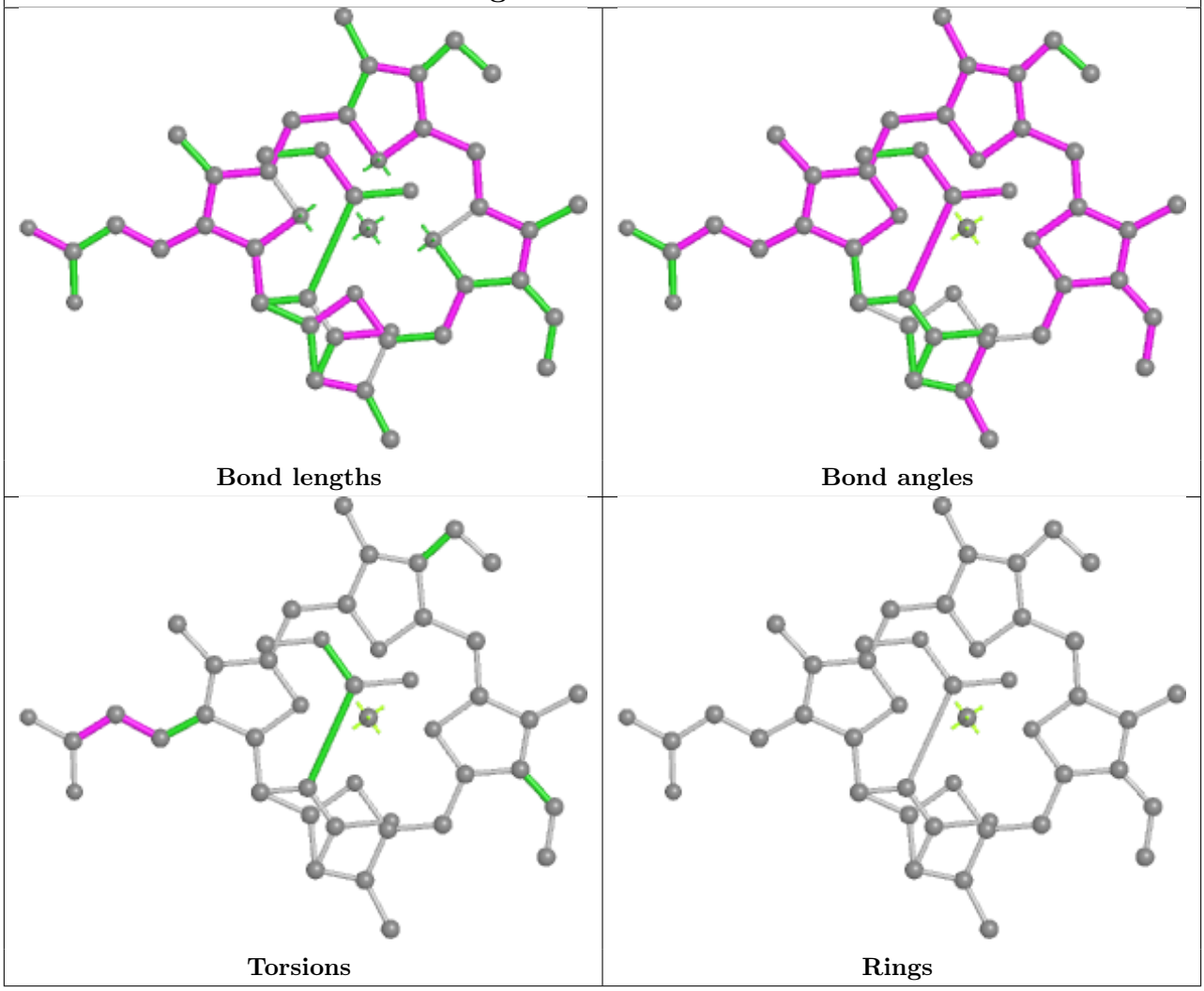


Rings

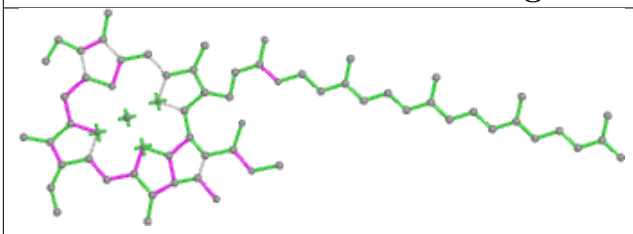
Ligand LMG B 521



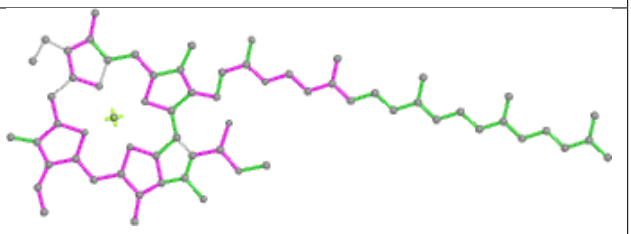
Ligand KC1 19 308



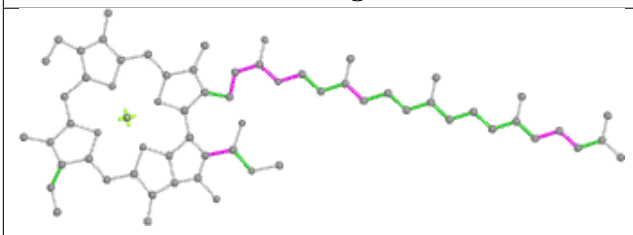
Ligand CLA C 505



Bond lengths



Bond angles



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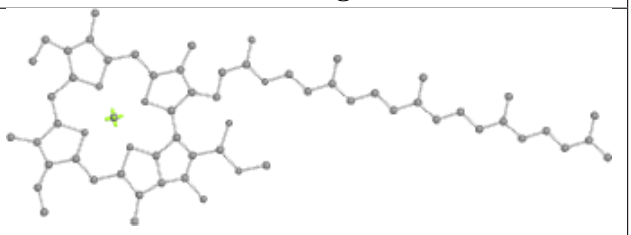
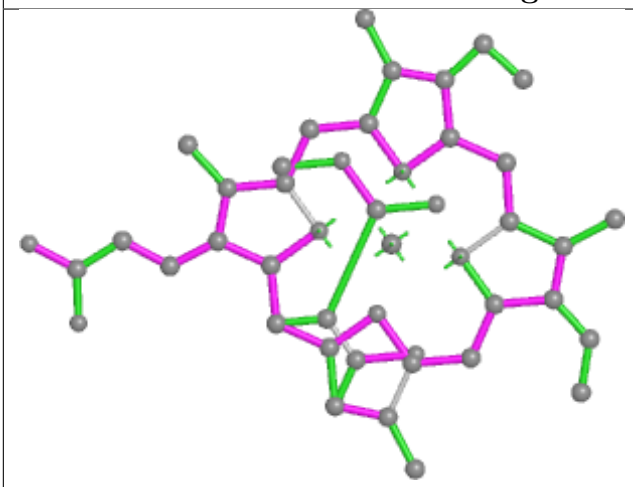


Rings

Ligand KC1 18 210



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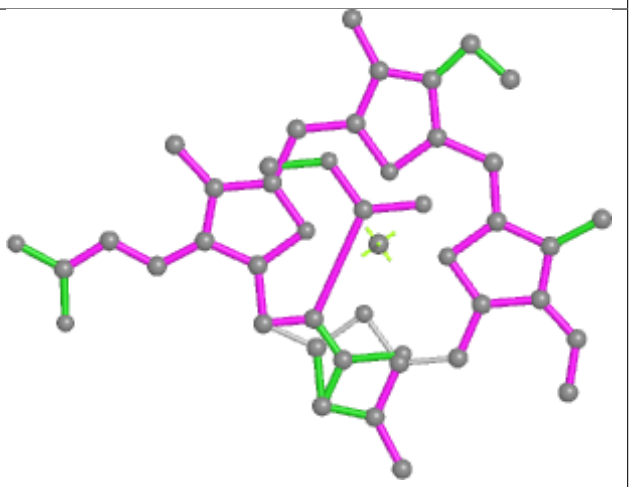
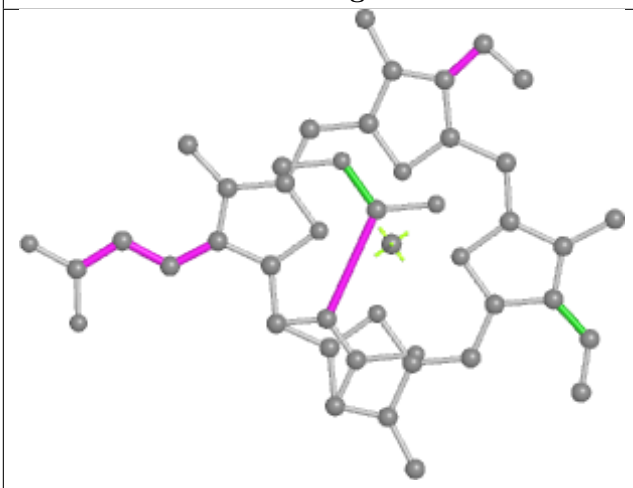


Bond angles



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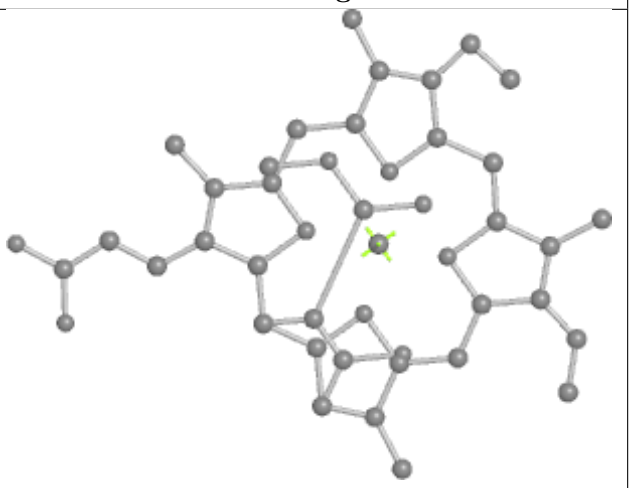

Rings

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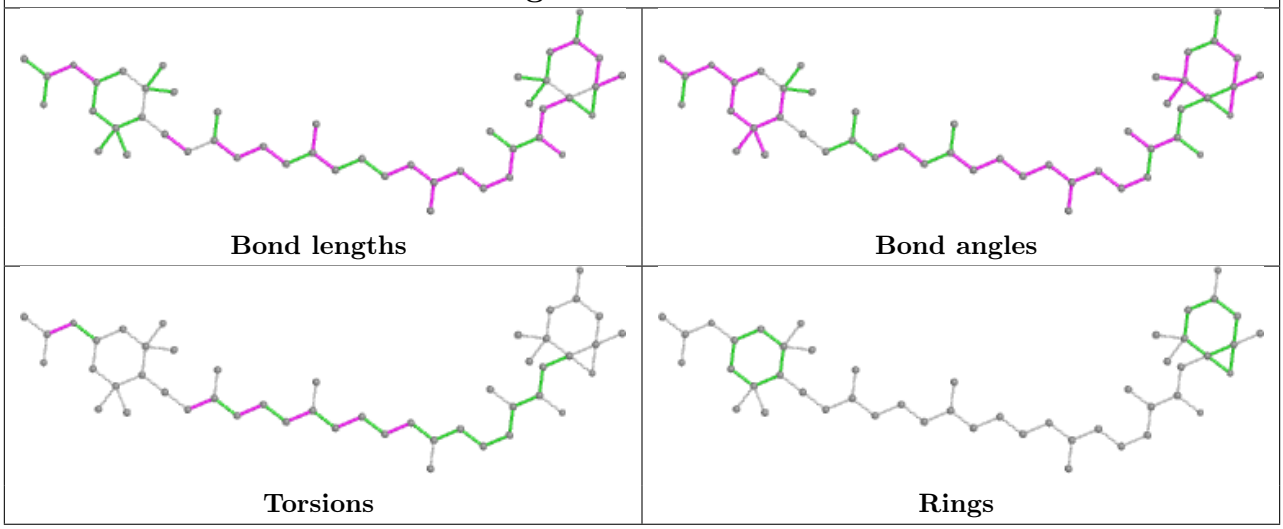
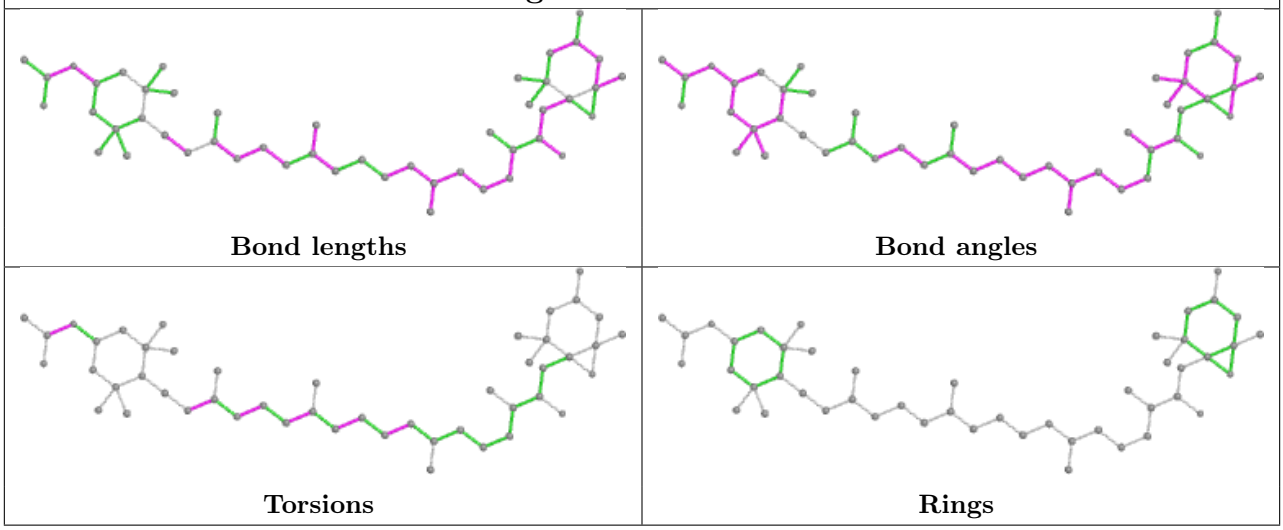
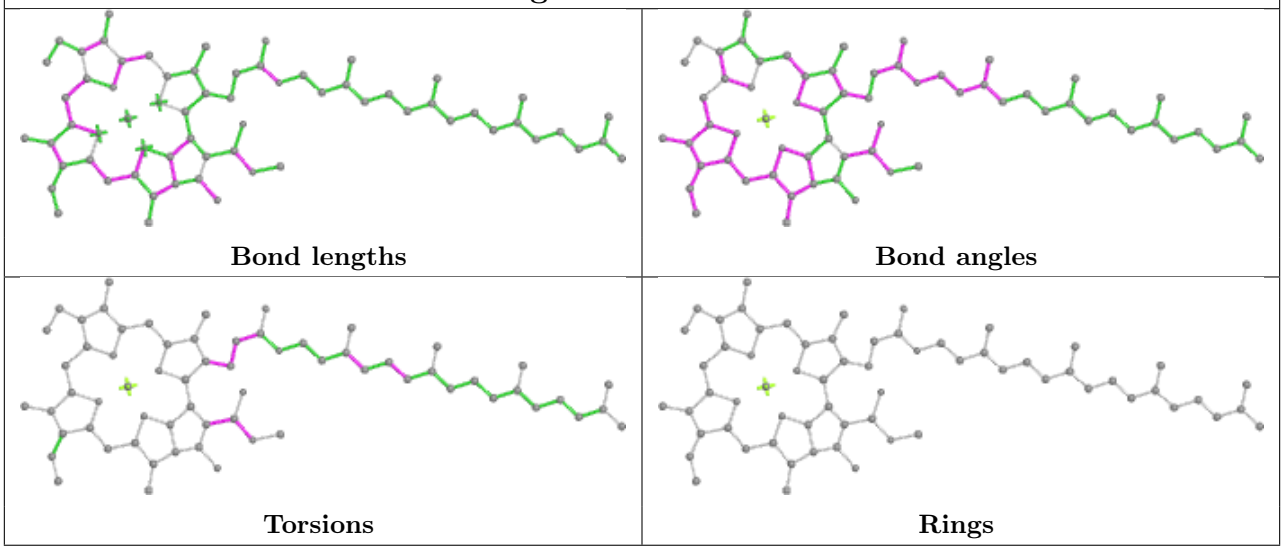


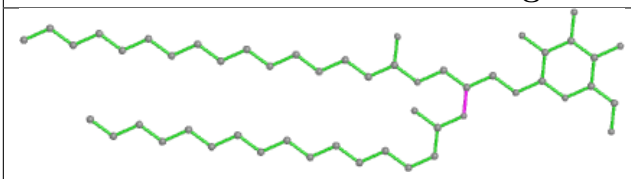
Ligand A86 36 311



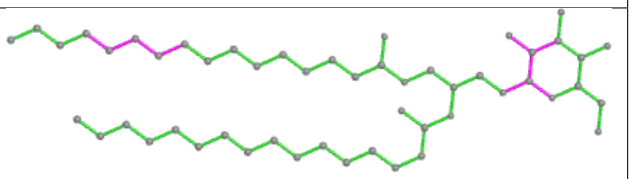
Ligand CLA c 501



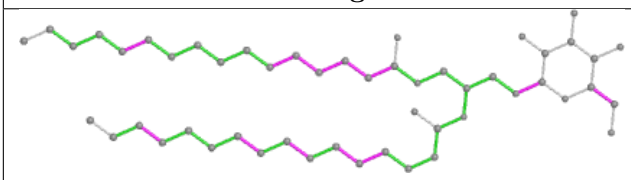
Ligand LMG b 519



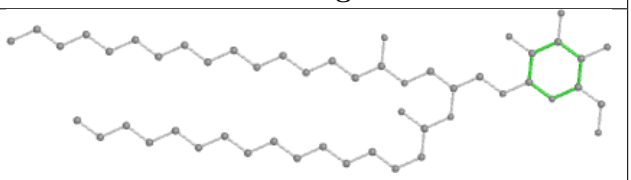
Bond lengths



Bond angles

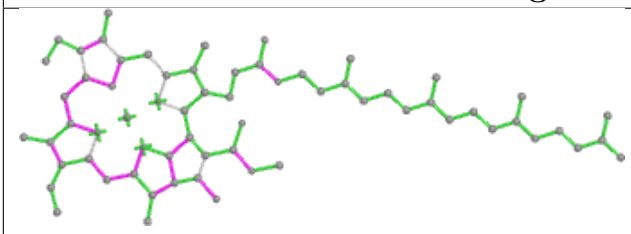


Torsions



Rings

Ligand CLA c 504



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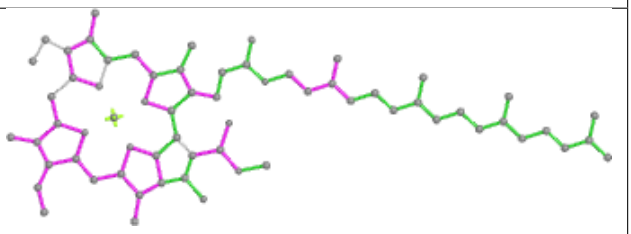
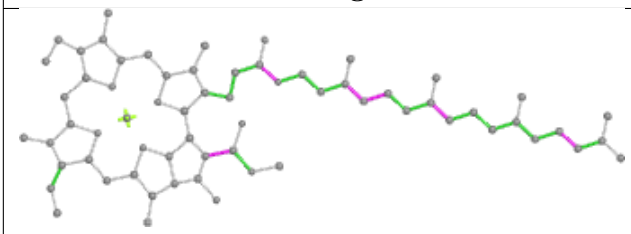
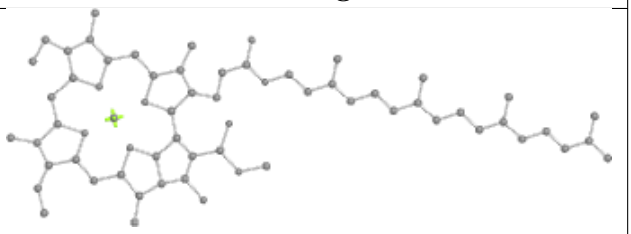


Bond angles

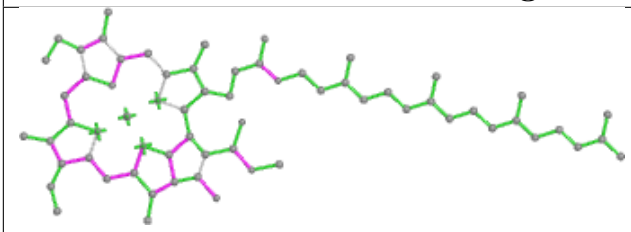


Torsions



Rings

Ligand CLA 19 310



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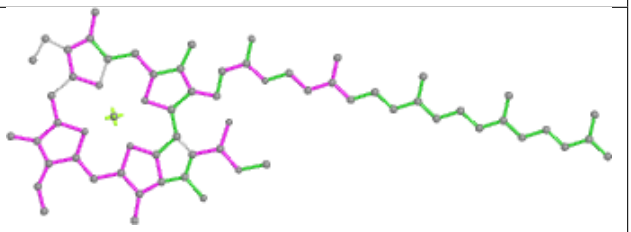

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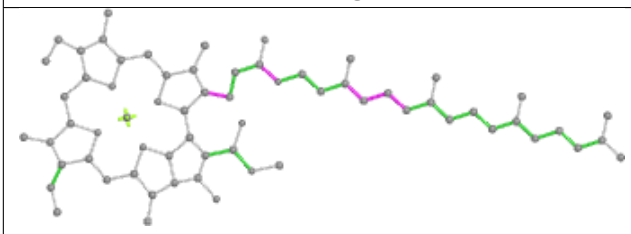

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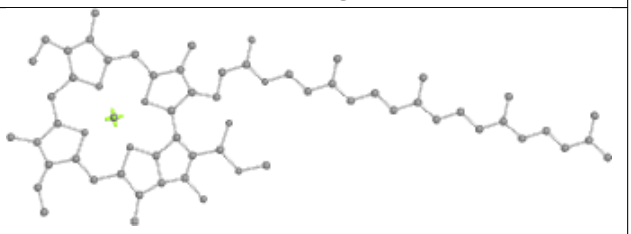
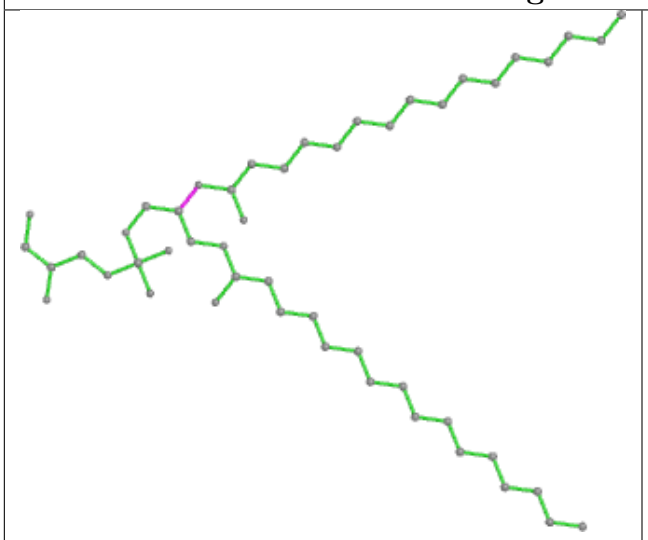


Rings

Ligand LHG d 408



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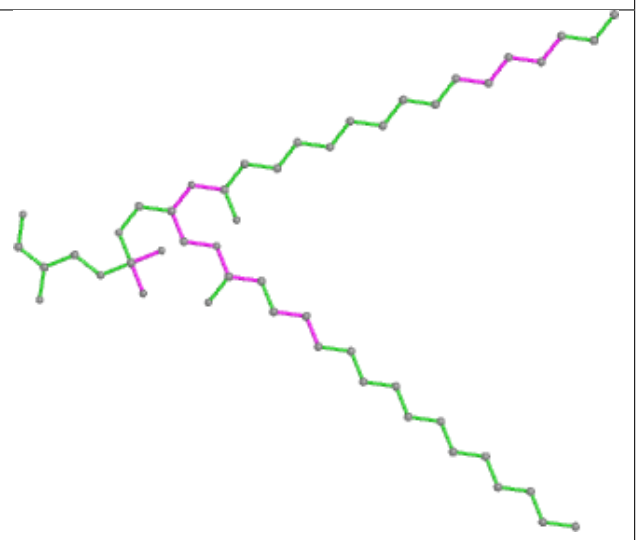

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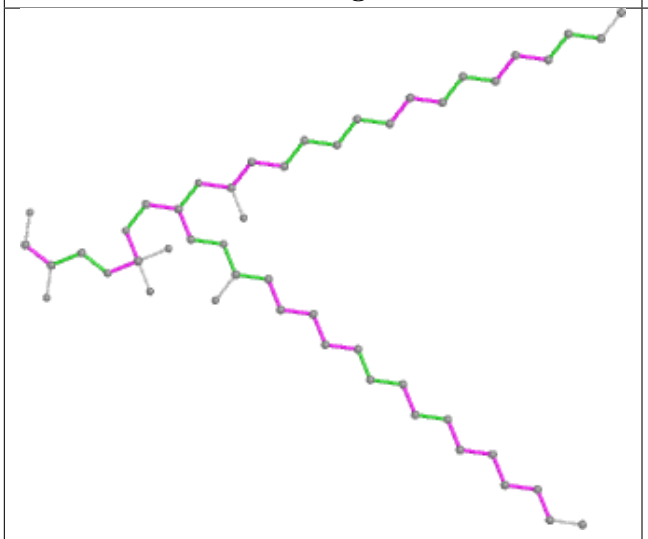

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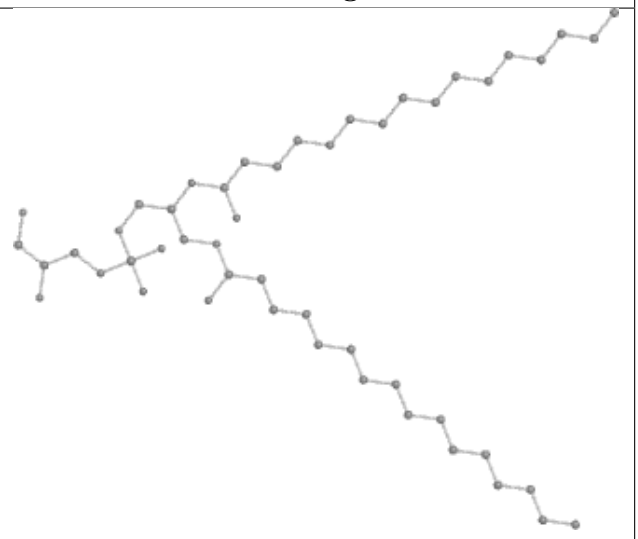

Rings

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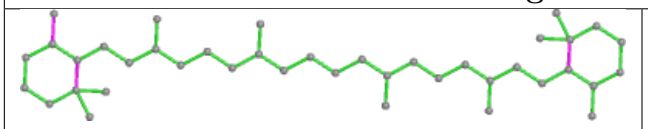

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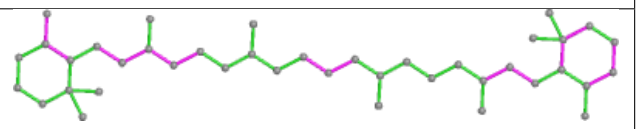

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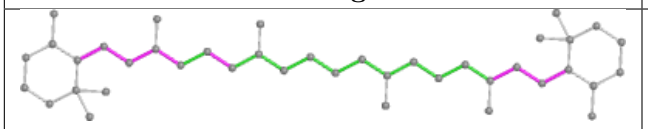

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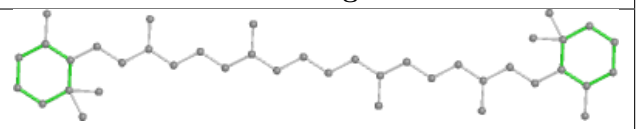

Rings

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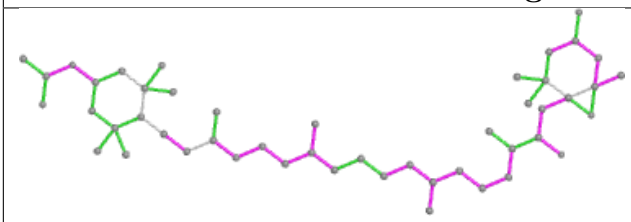
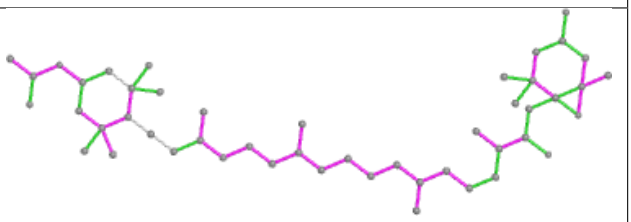
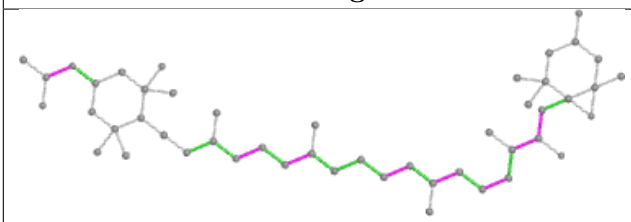
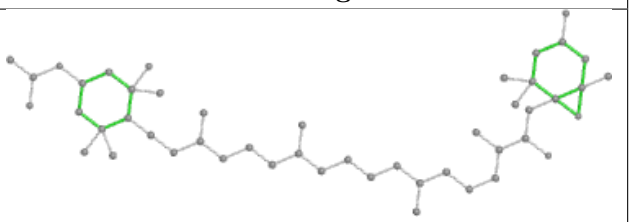
 Bond lengths	 Bond angles
 Torsions	 Rings

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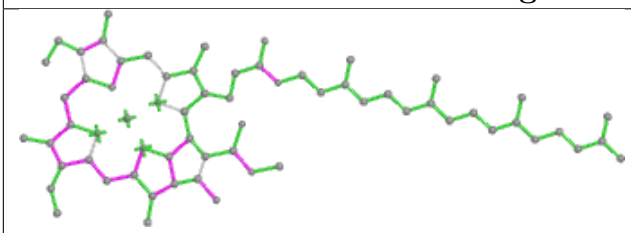
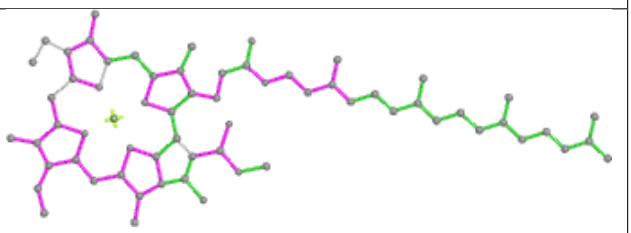
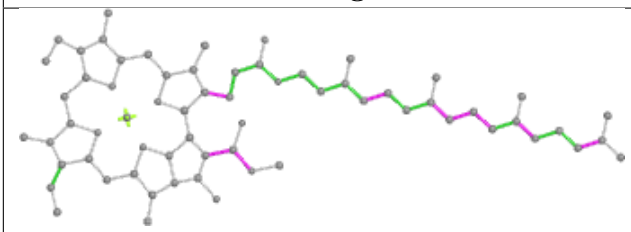
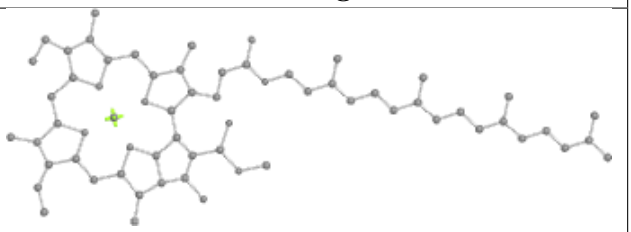
 Bond lengths	 Bond angles
 Torsions	 Rings

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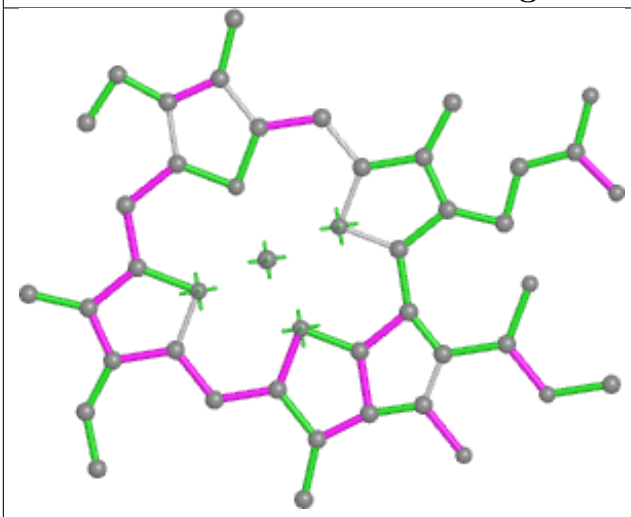

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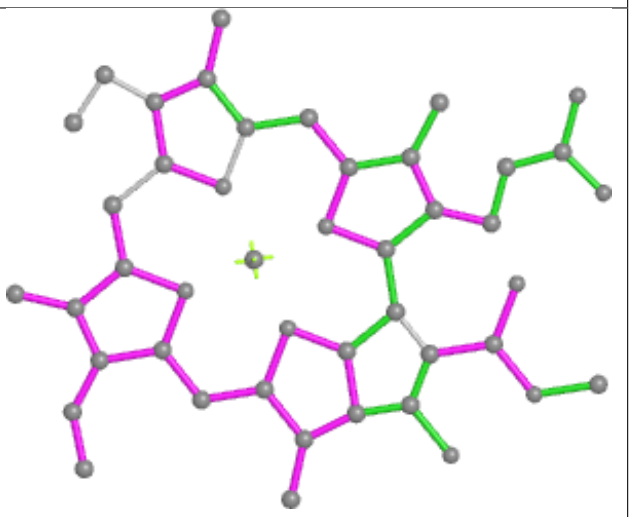

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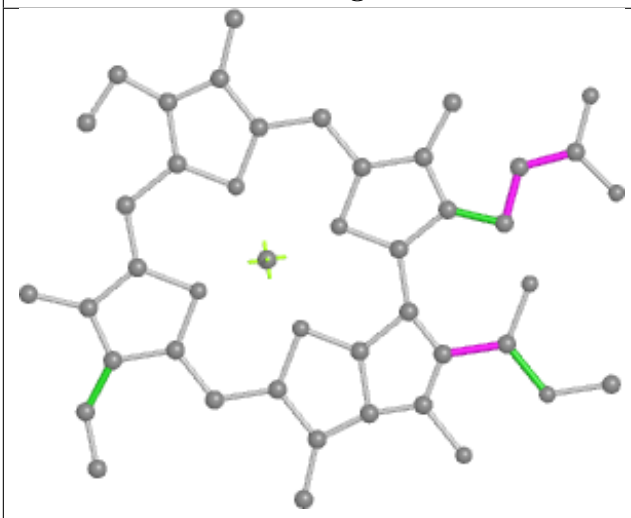

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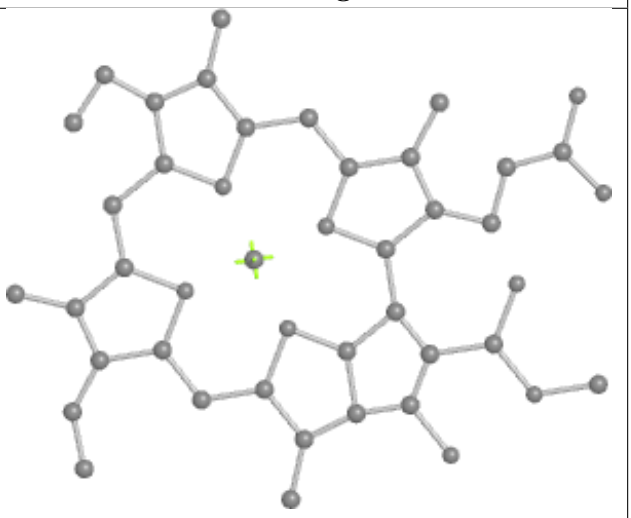
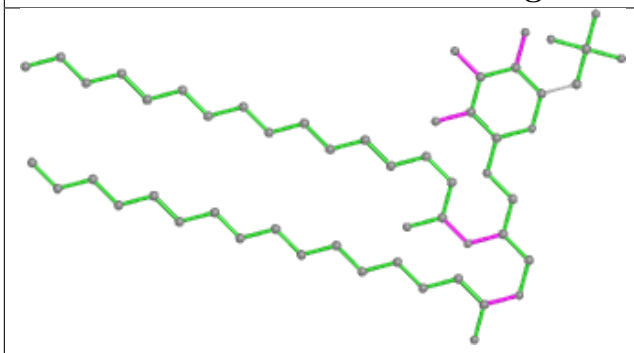


Rings

Ligand SQD A 407



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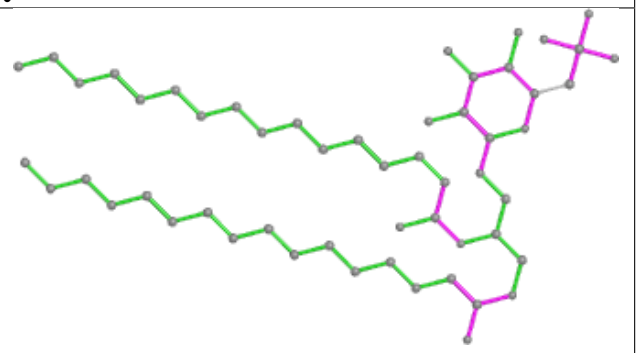

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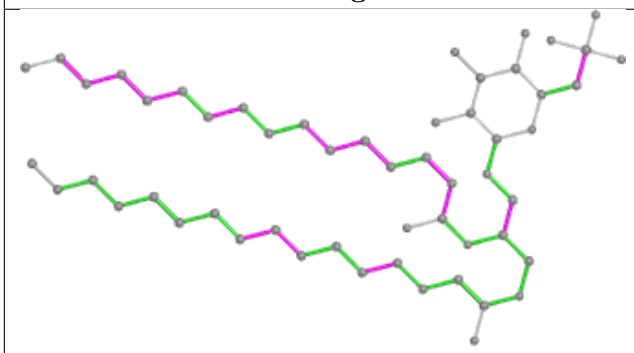

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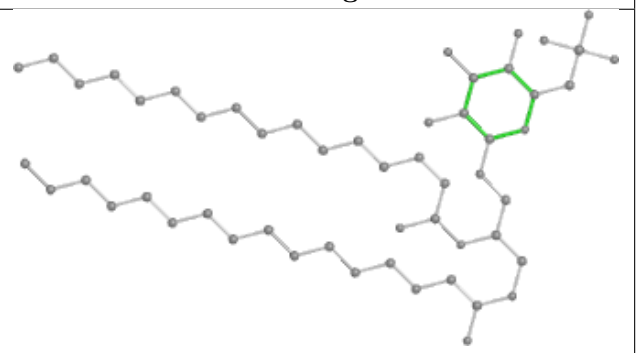
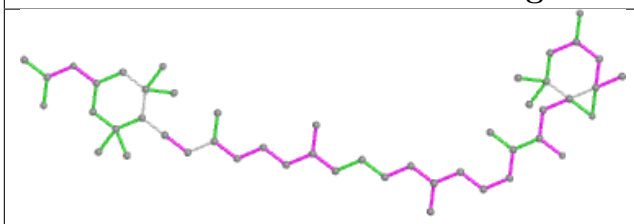


Rings

Ligand A86 38 213



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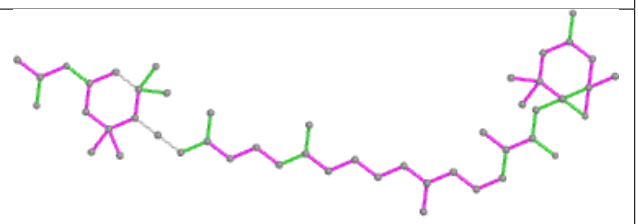
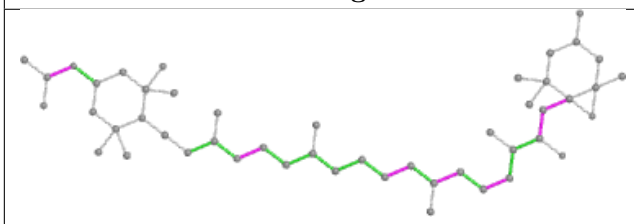


Bond angles



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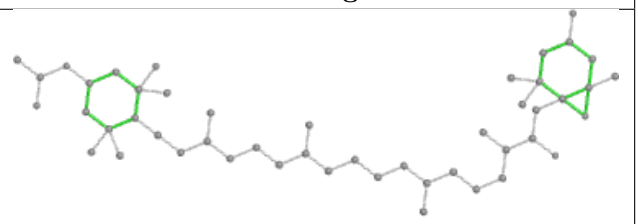

Rings

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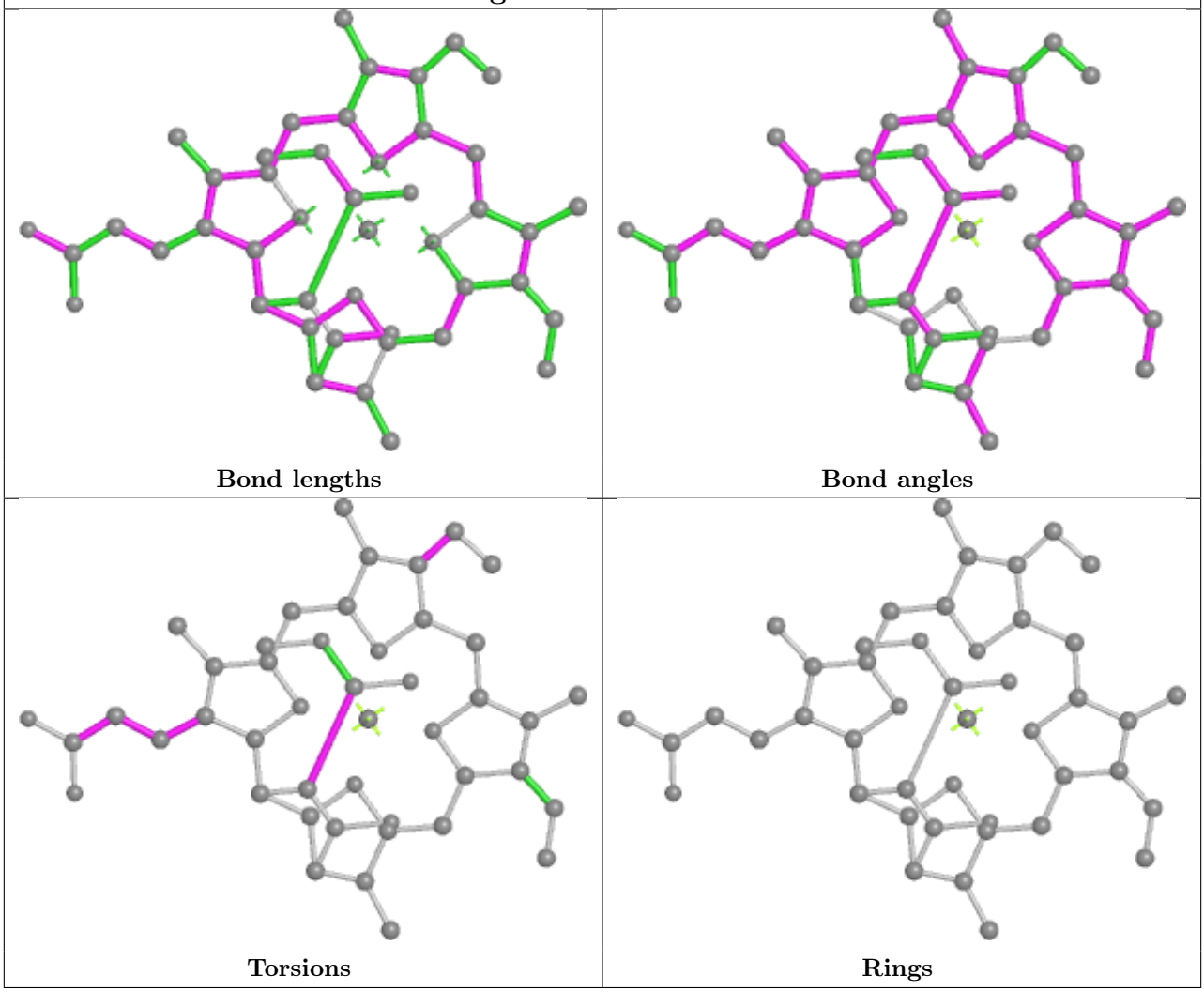
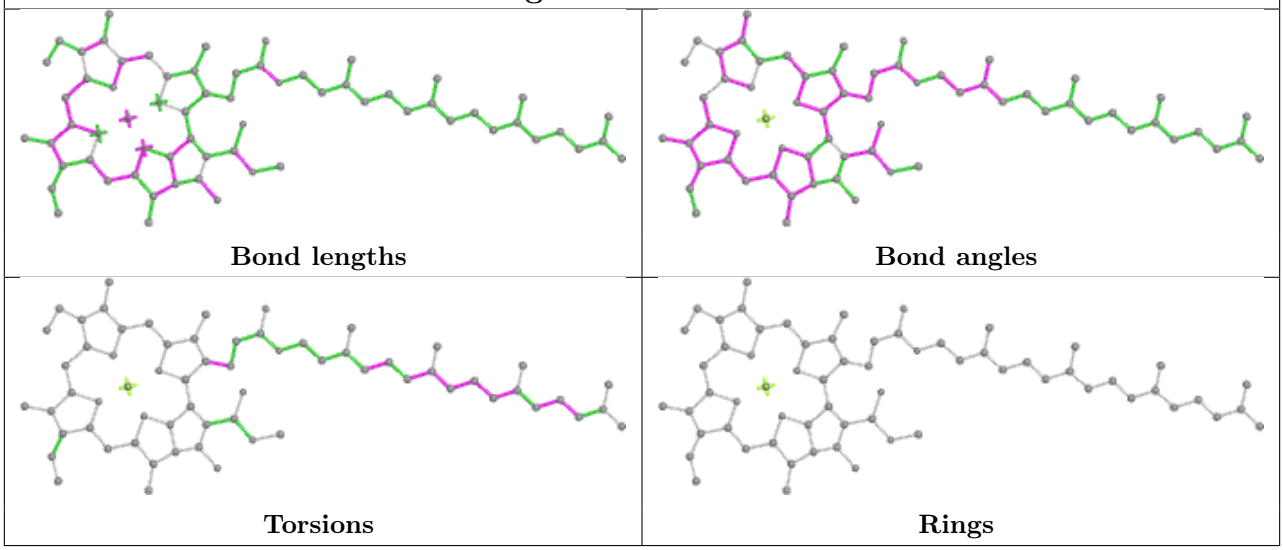


Ligand CLA B 524



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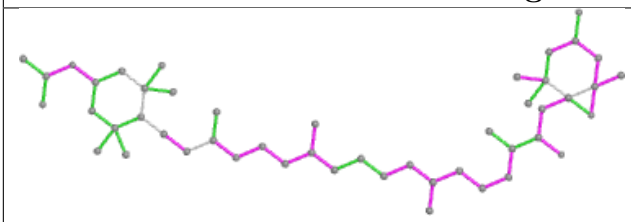
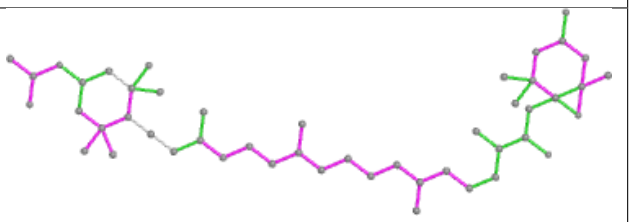
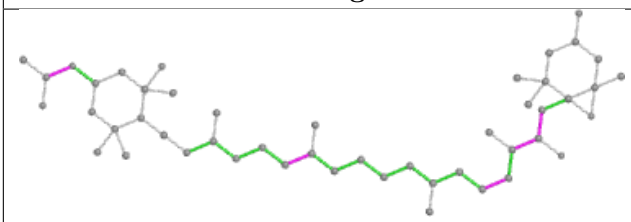
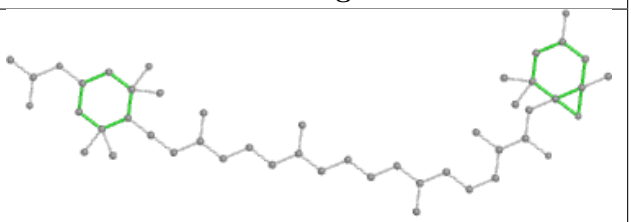
 Bond lengths	 Bond angles
 Torsions	 Rings

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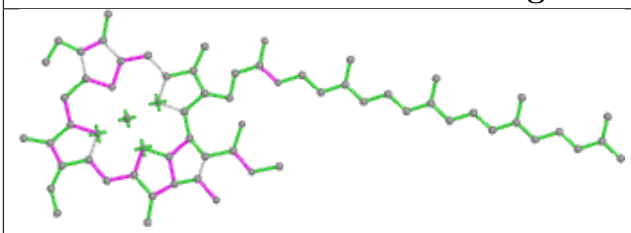
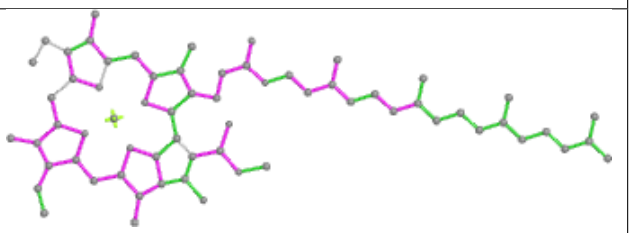
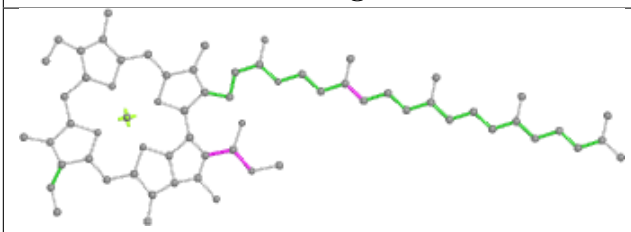
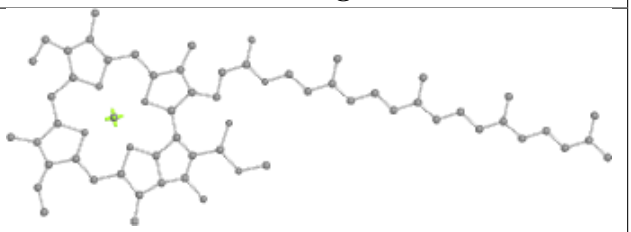
 Bond lengths	 Bond angles
 Torsions	 Rings

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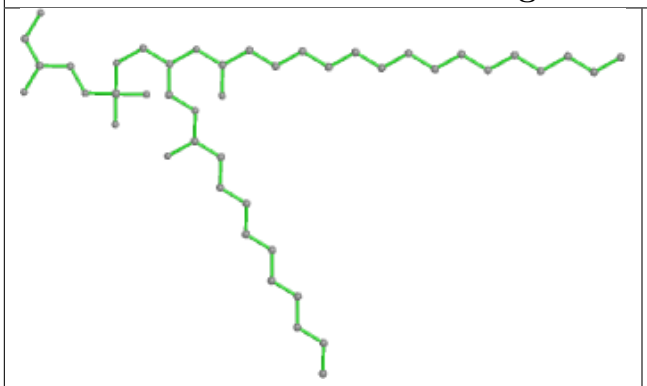
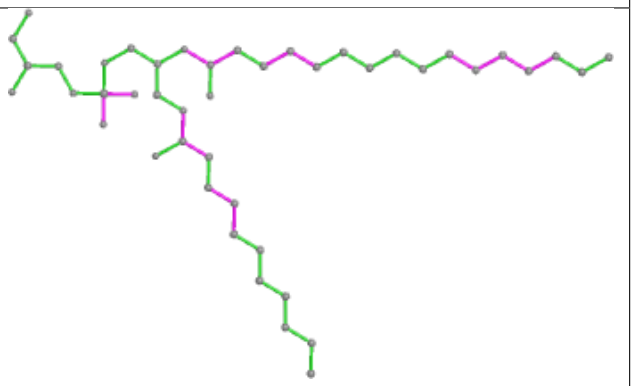
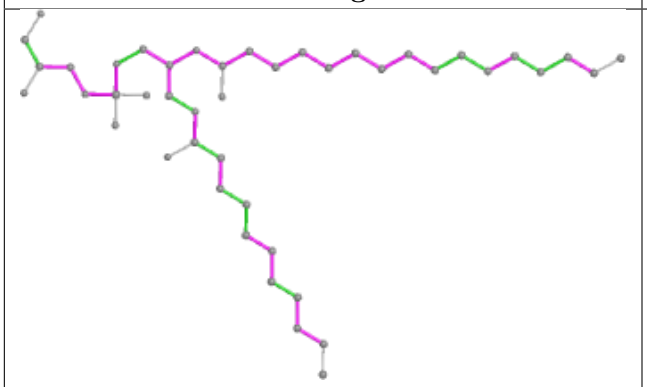
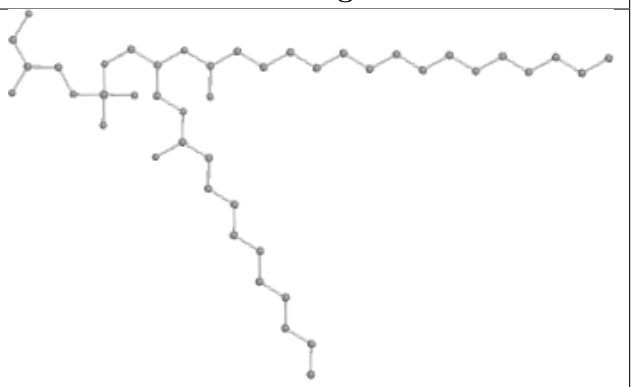
 Bond lengths	 Bond angles
 Torsions	 Rings

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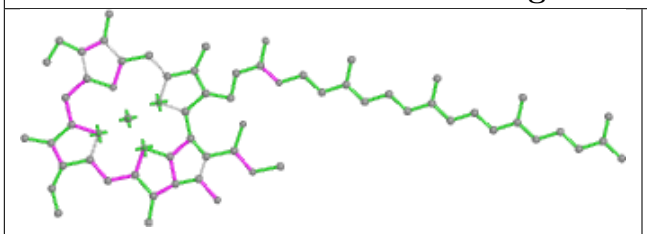
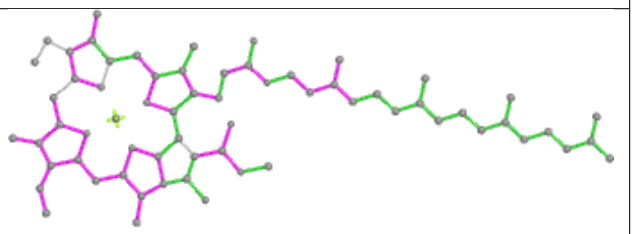
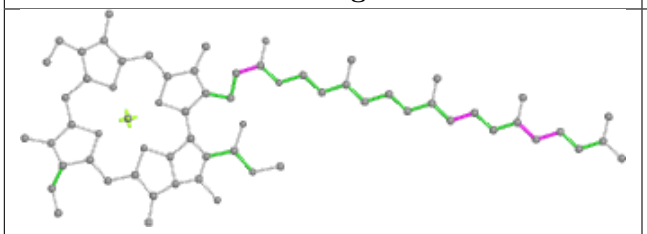
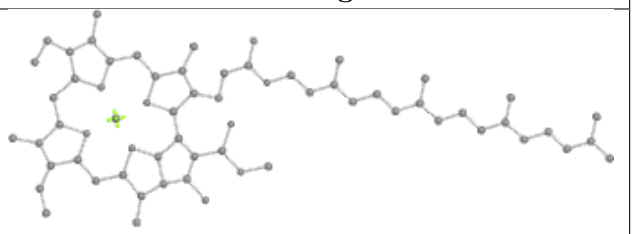
 Bond lengths	 Bond angles
 Torsions	 Rings

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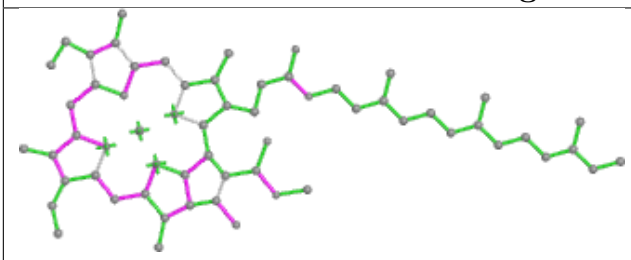
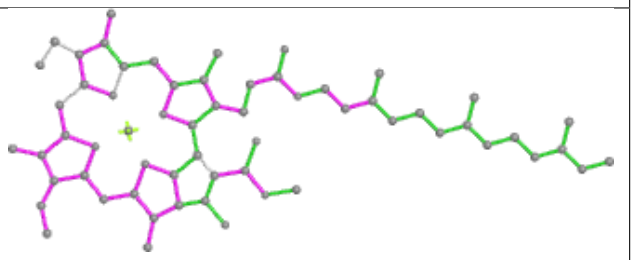
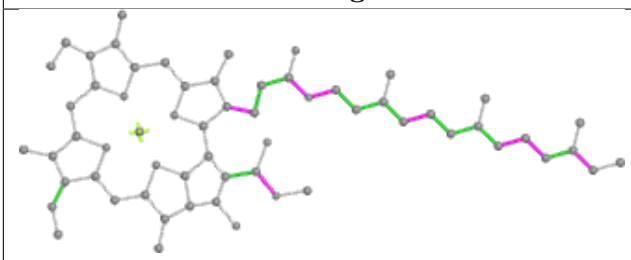
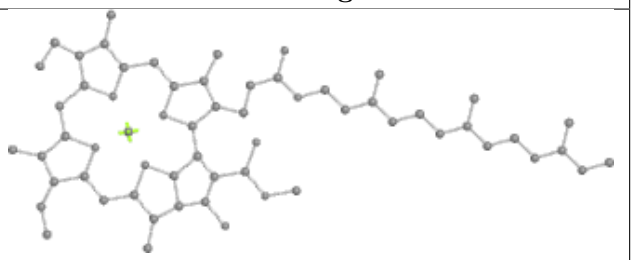
 Bond lengths	 Bond angles
 Torsions	 Rings

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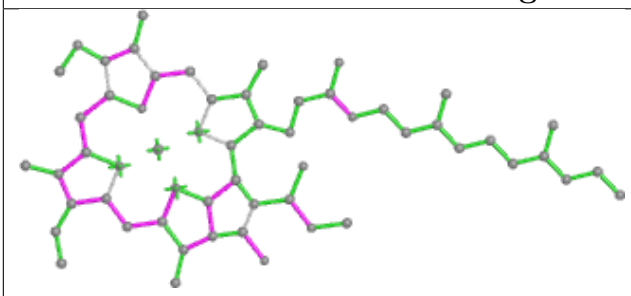
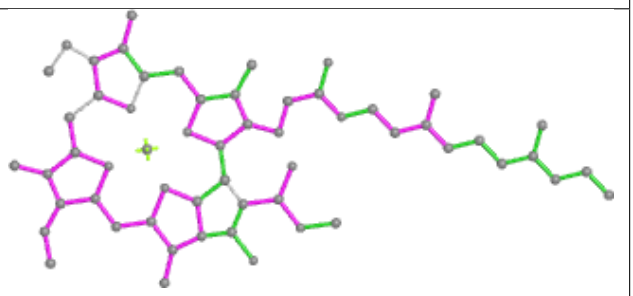
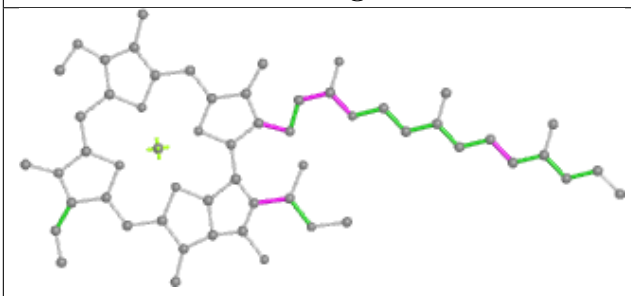
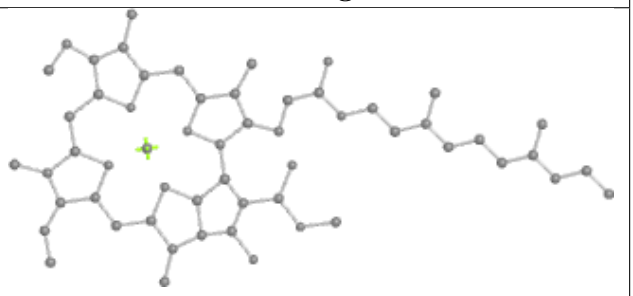
 Bond lengths	 Bond angles
 Torsions	 Rings

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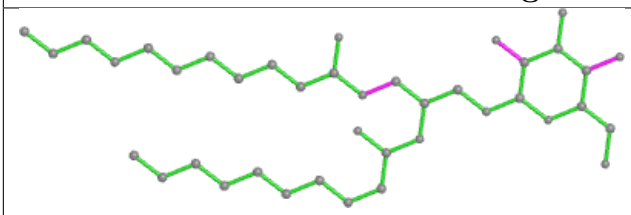

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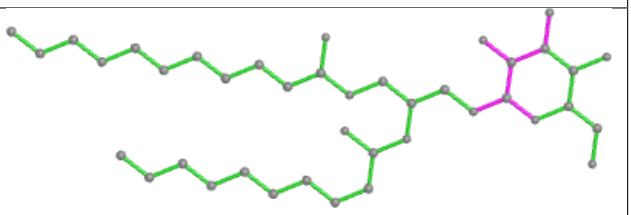

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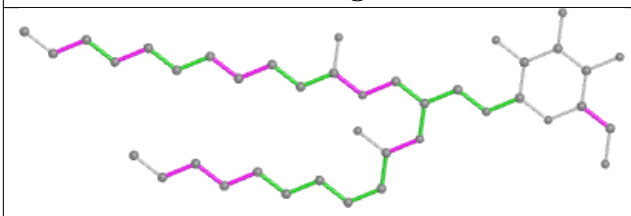

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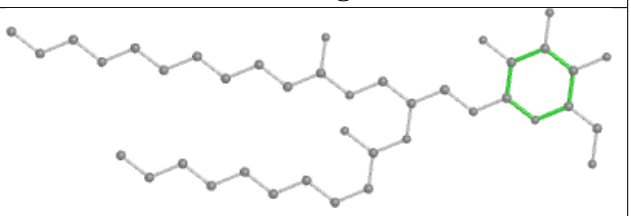

Rings

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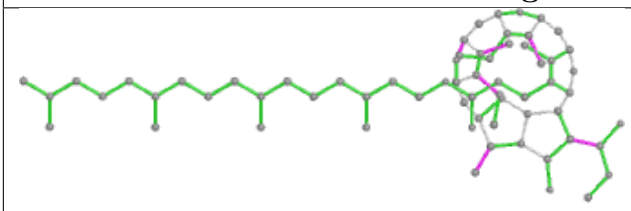

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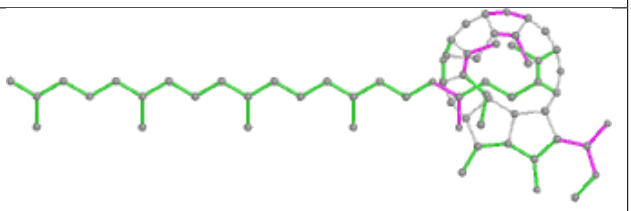

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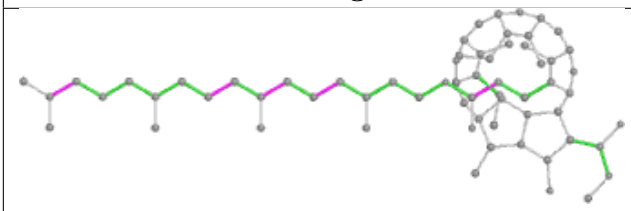

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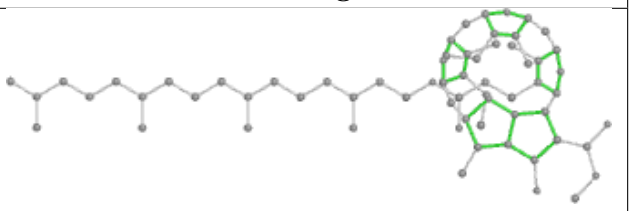
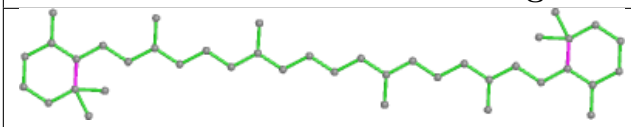


Rings

Ligand BCR a 408



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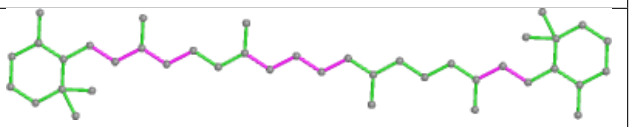

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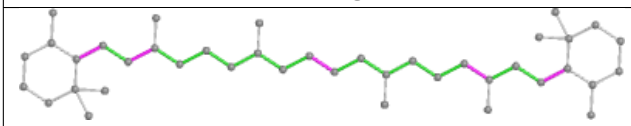

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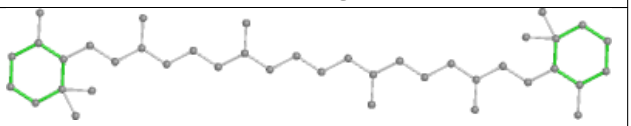

Rings

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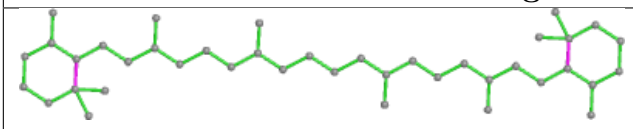

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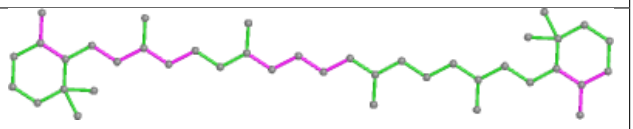

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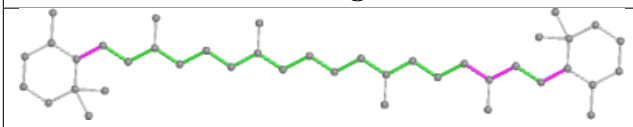

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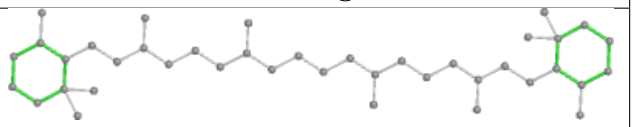
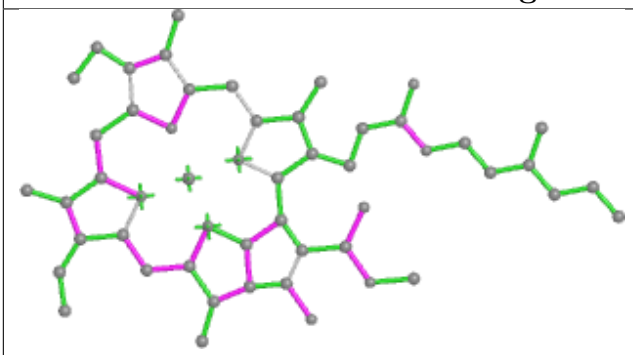


Rings

Ligand CLA 33 307



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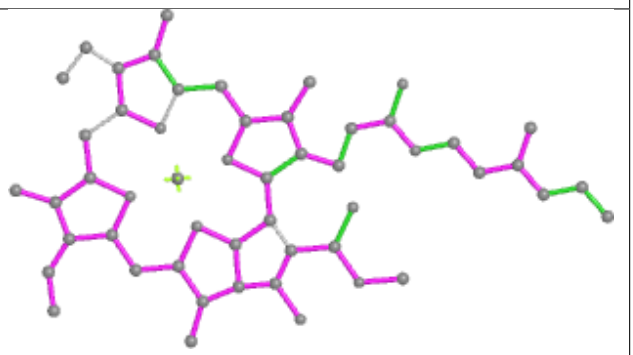

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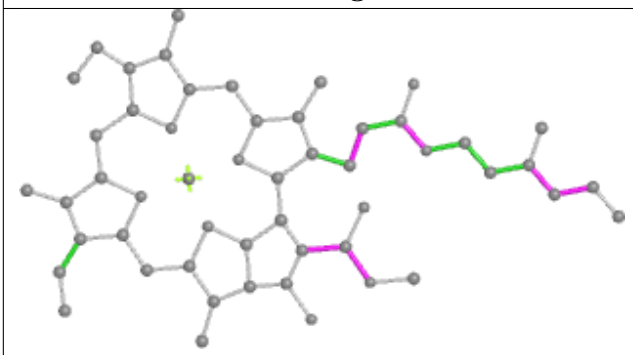

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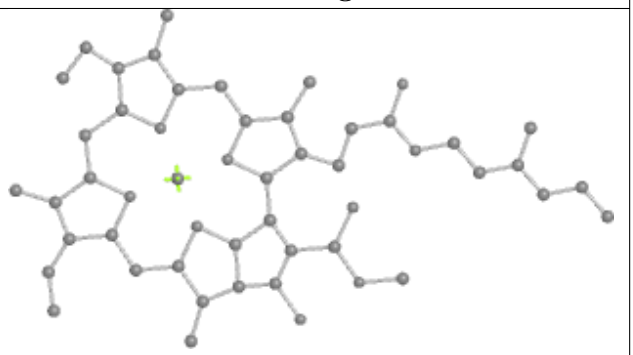

Rings

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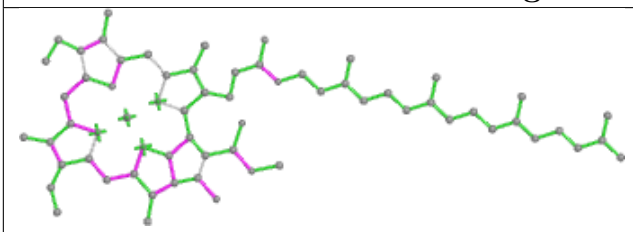

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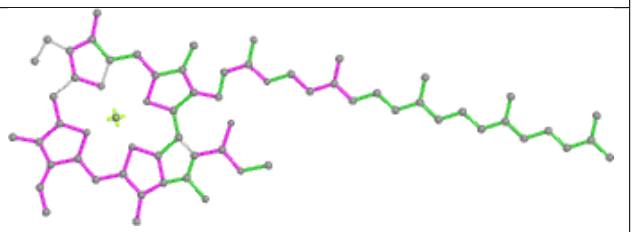

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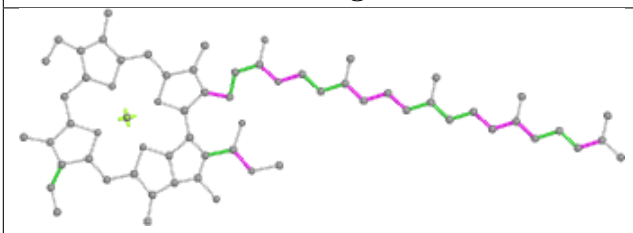

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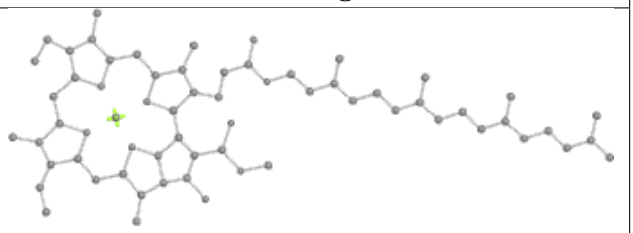

Rings

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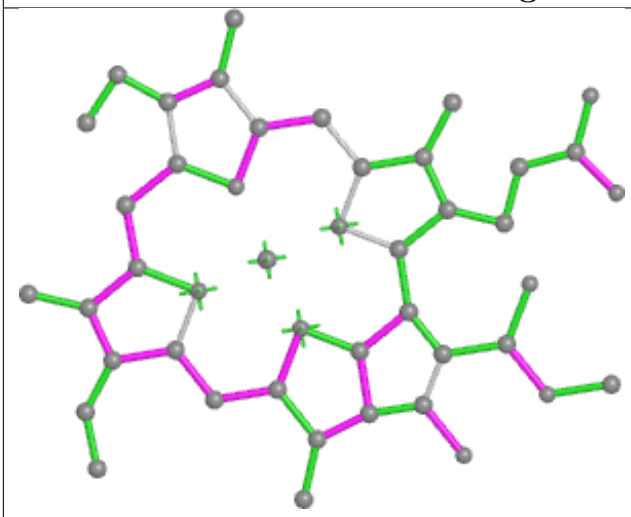

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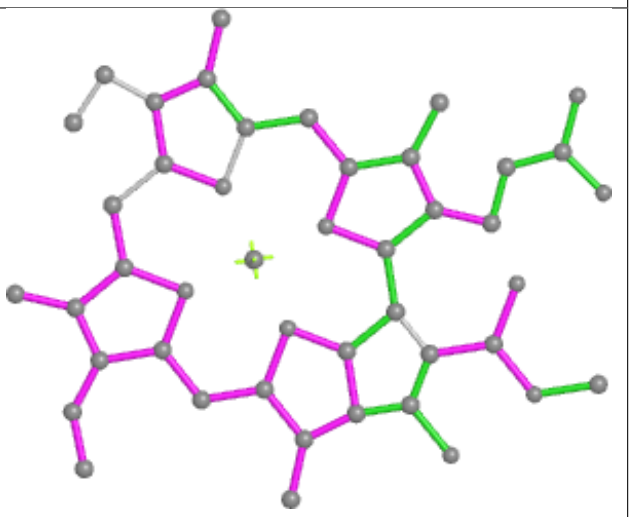

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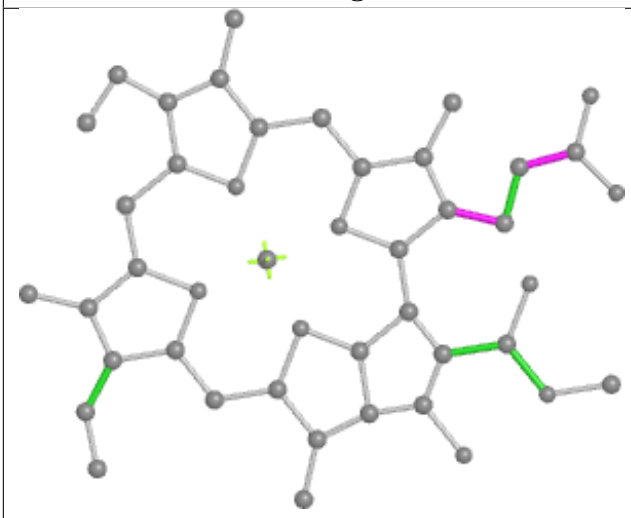

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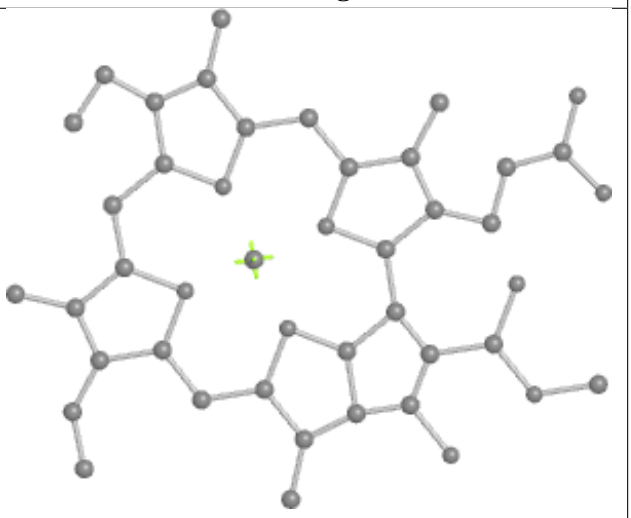

Rings

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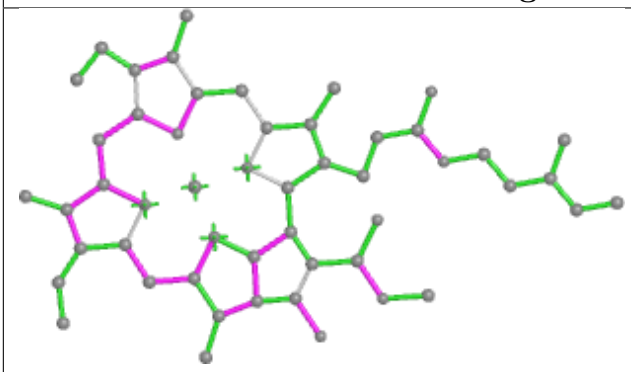

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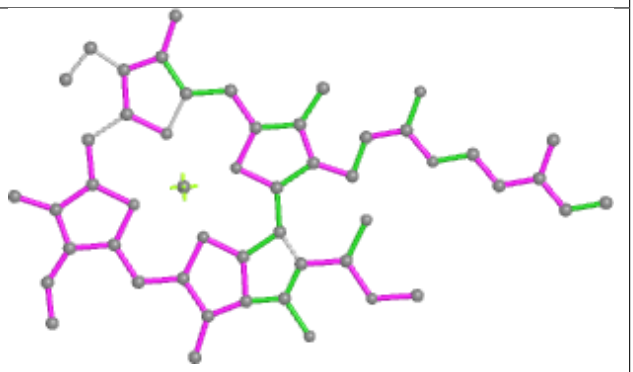

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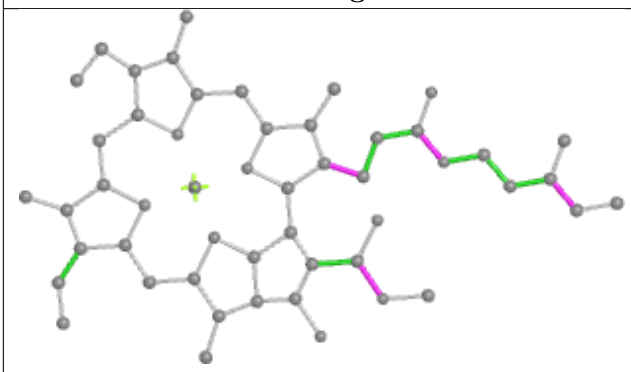

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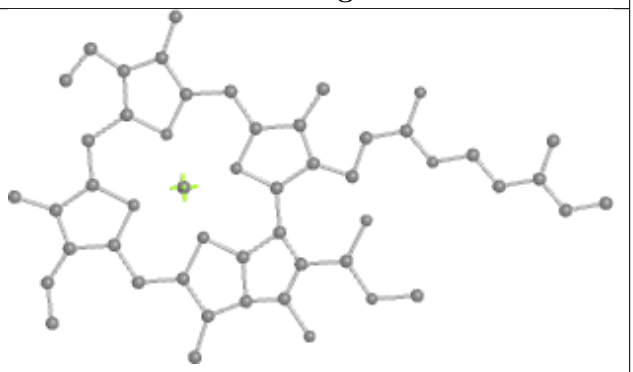

Rings

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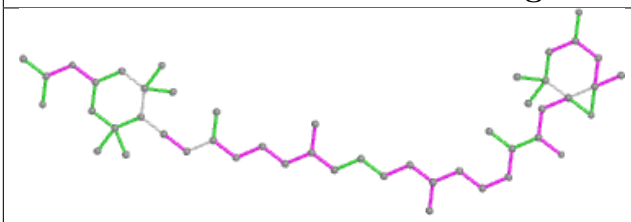

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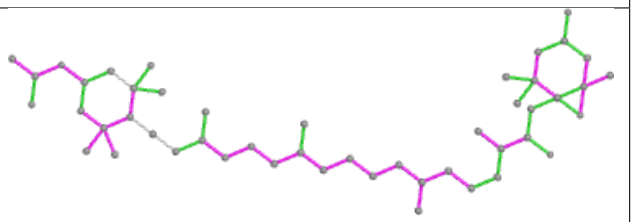

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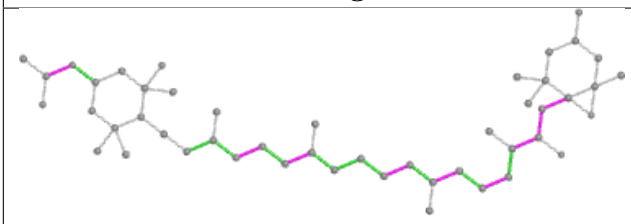

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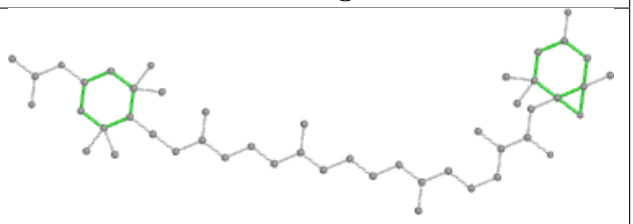

Rings

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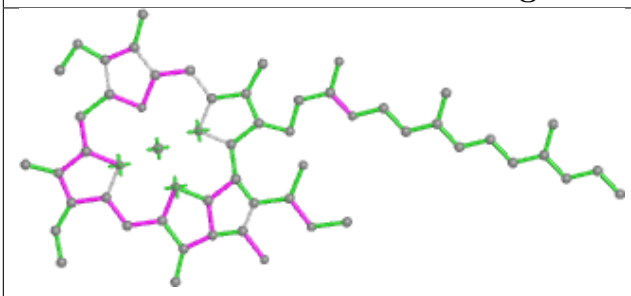

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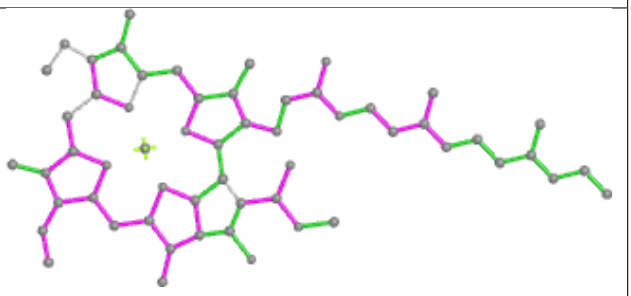

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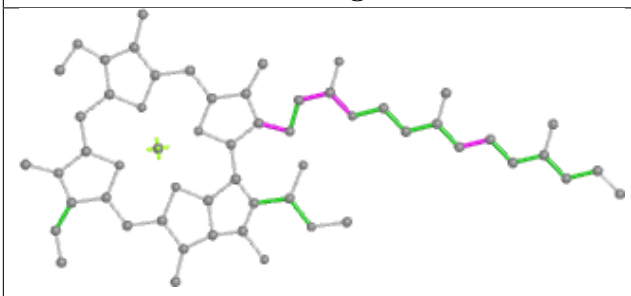

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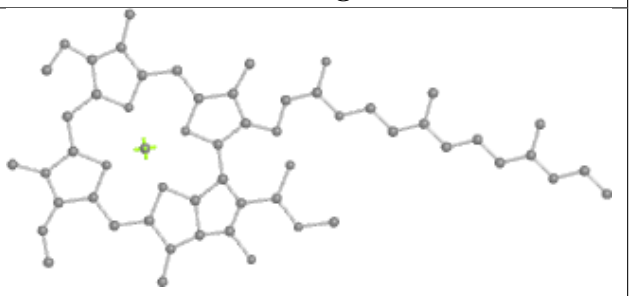
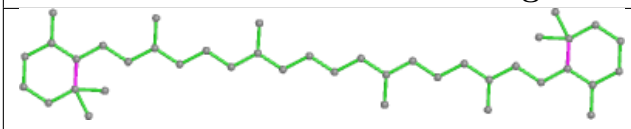


Rings

Ligand BCR A 410



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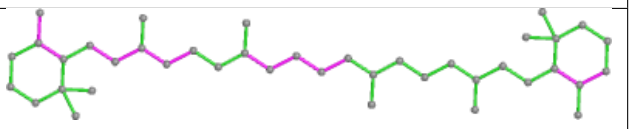

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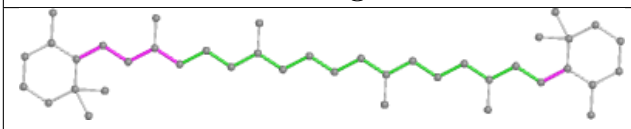

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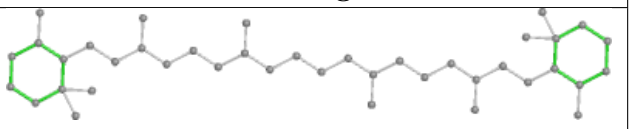

Rings

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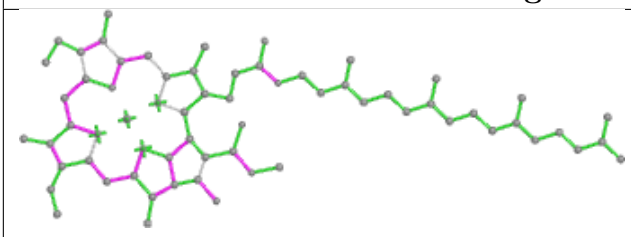

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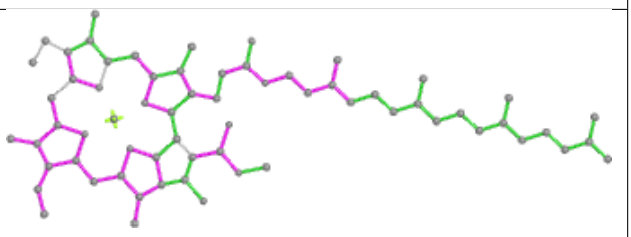
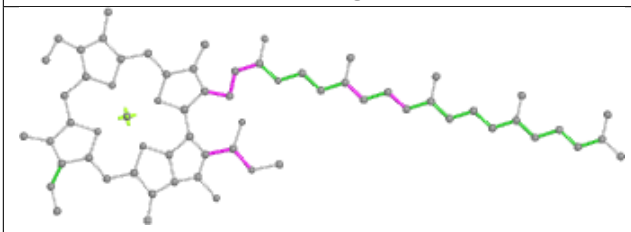
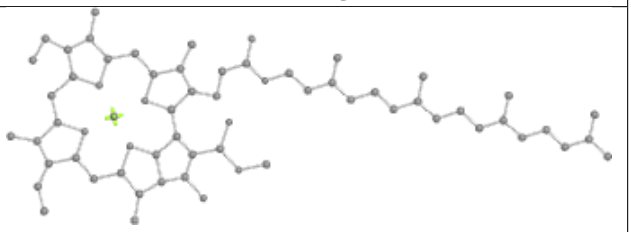


Bond angles

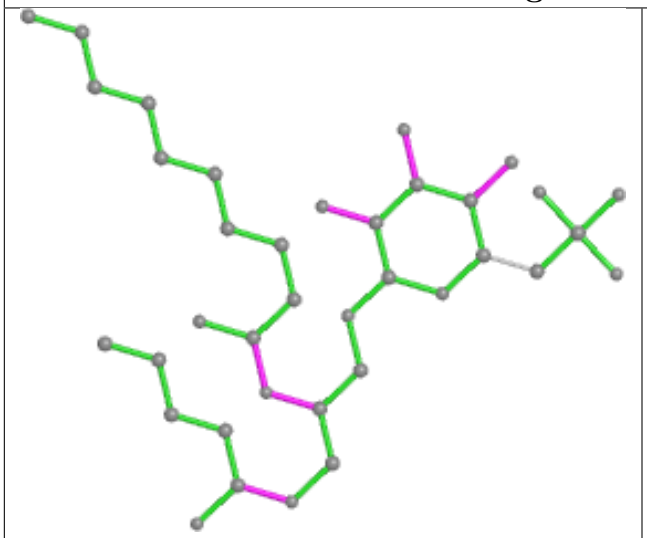


Torsions



Rings

Ligand SQD B 522



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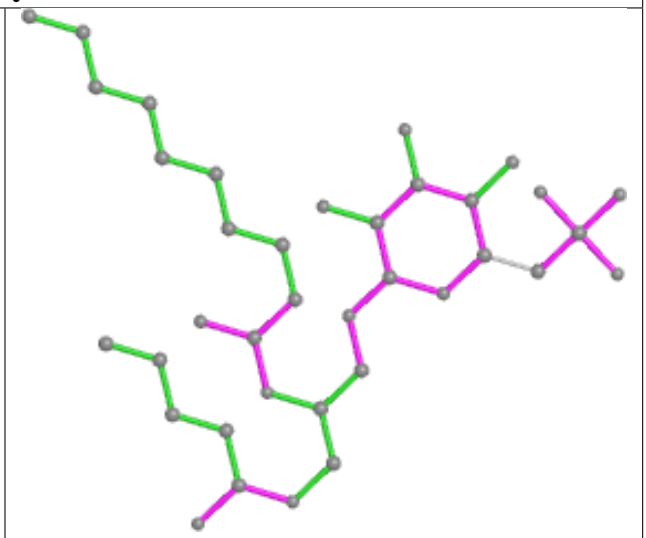

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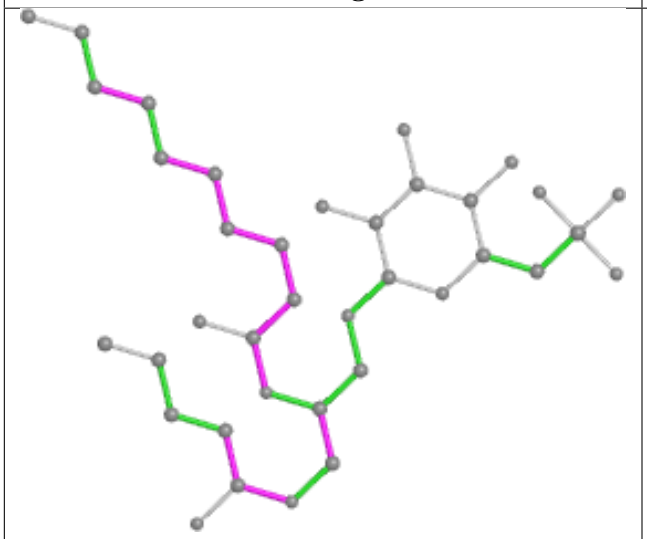

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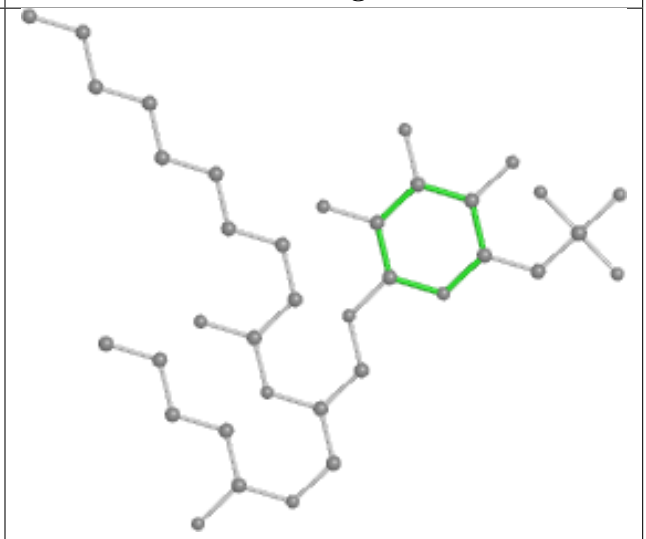

Rings

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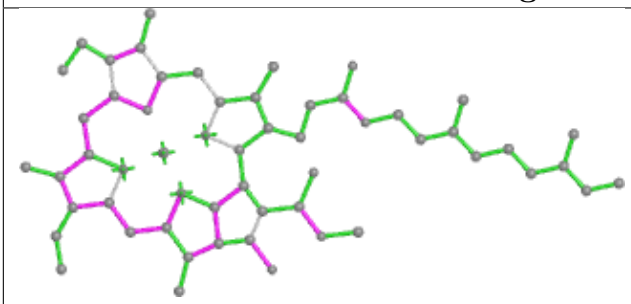
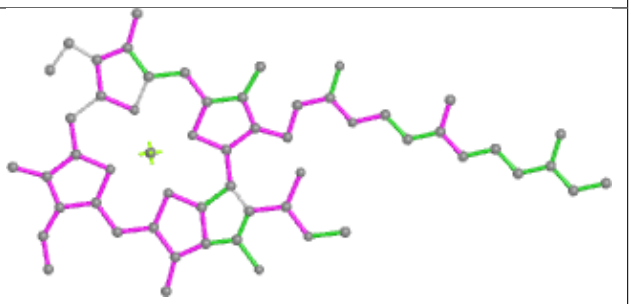
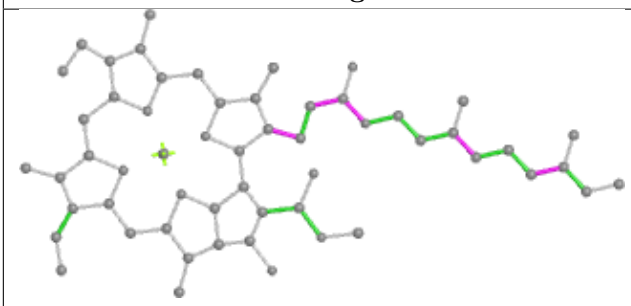
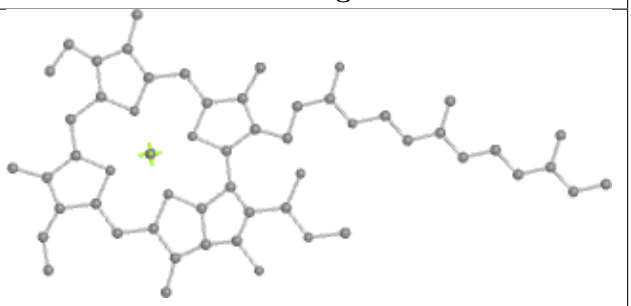
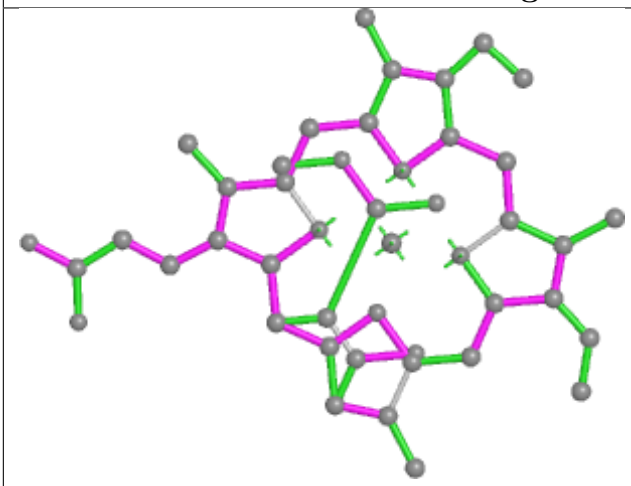
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 17 308



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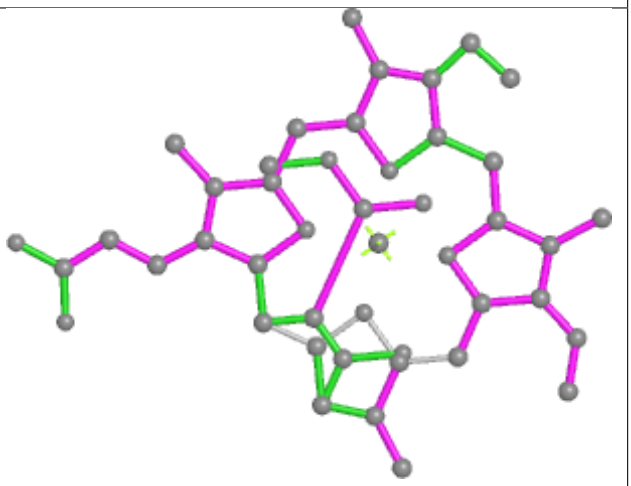

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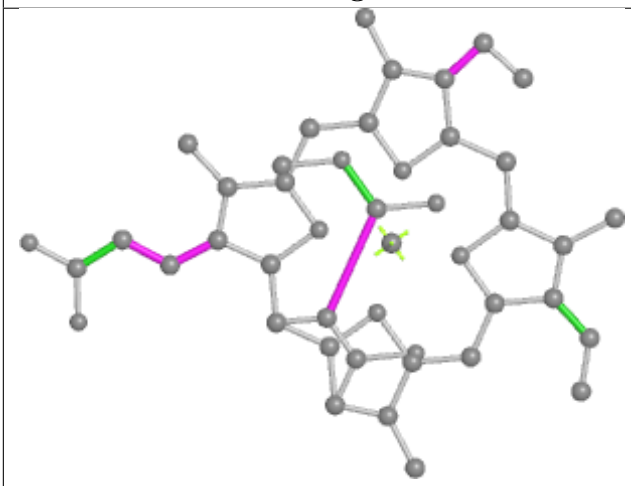

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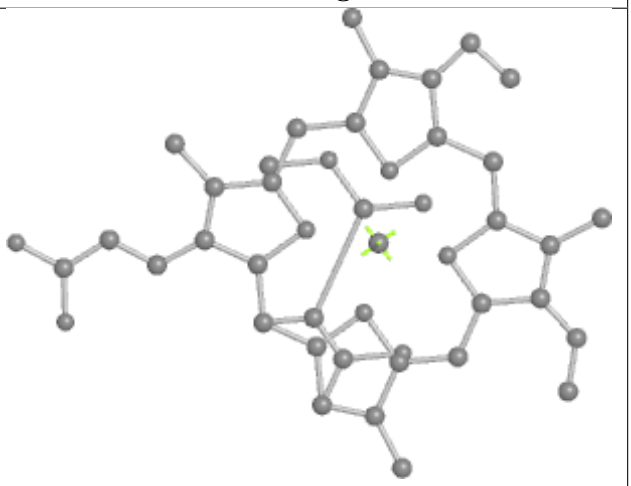
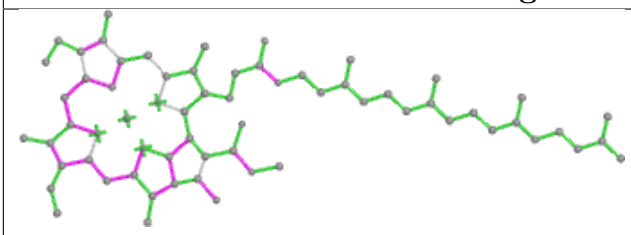


Rings

Ligand CLA 37 301



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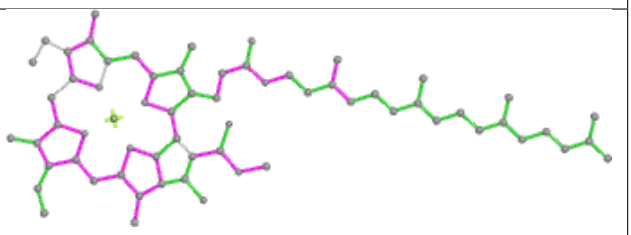

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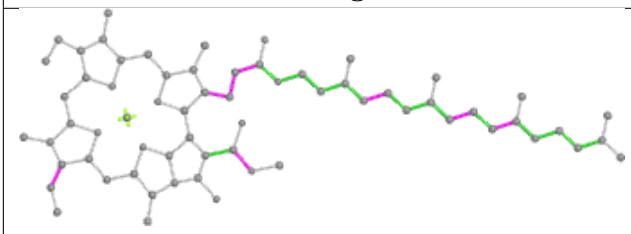

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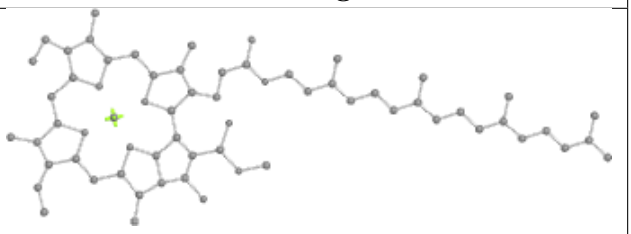

Rings

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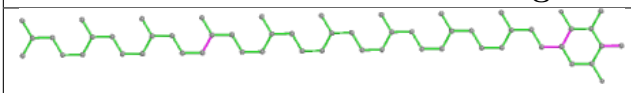

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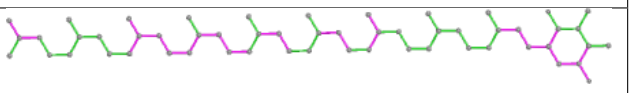

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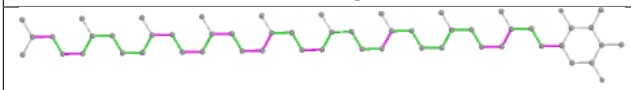

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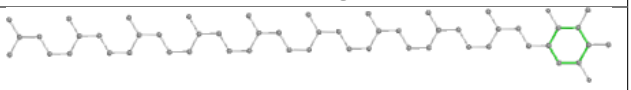

Rings

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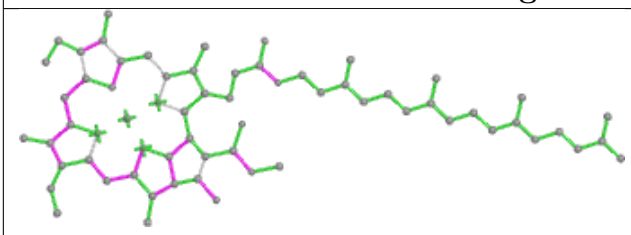

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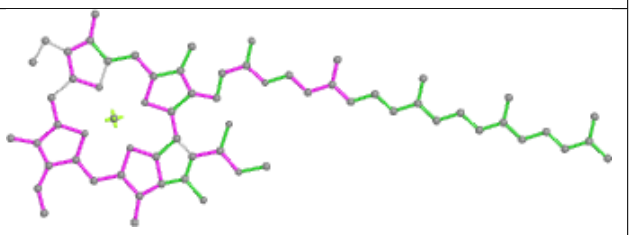

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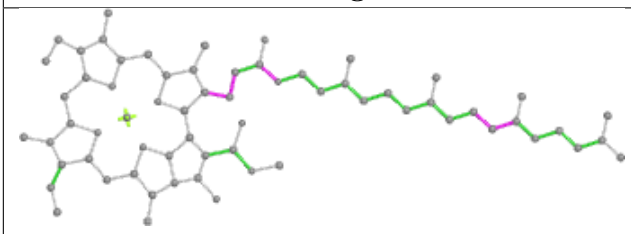

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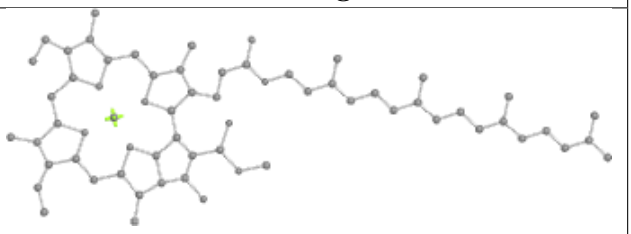

Rings

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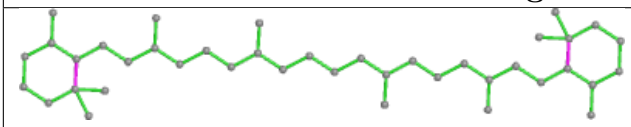

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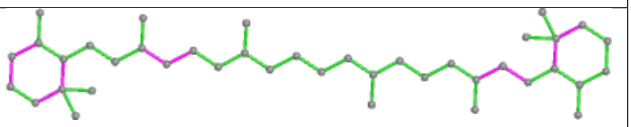

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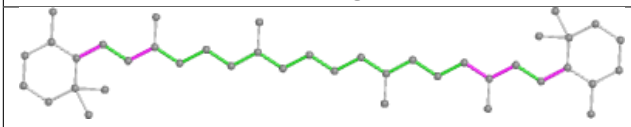

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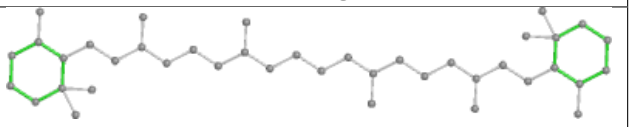

Rings

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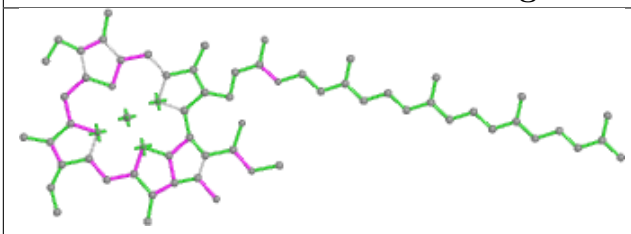

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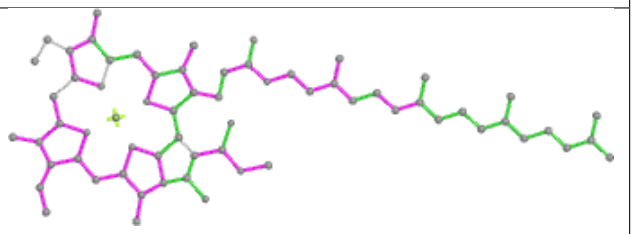

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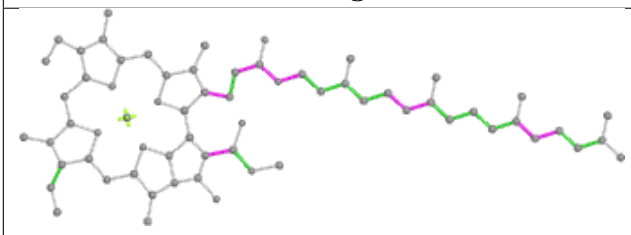

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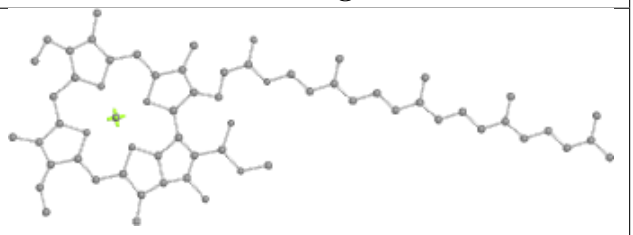
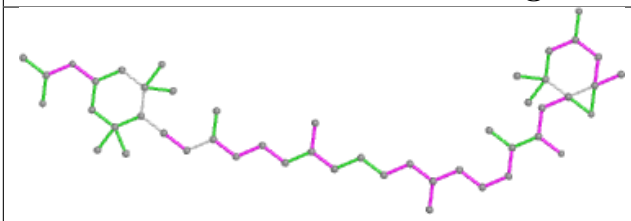


Rings

Ligand A86 31 311



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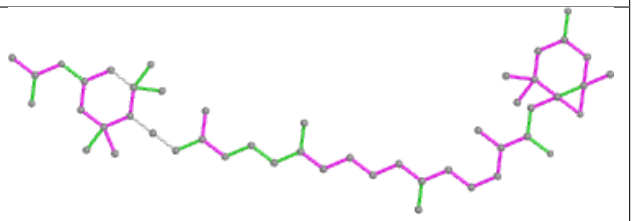

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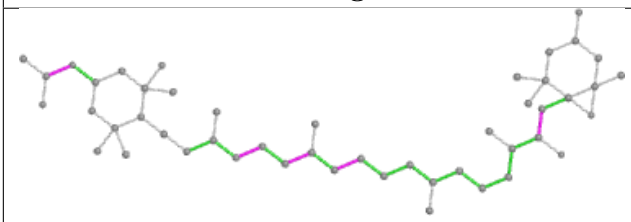

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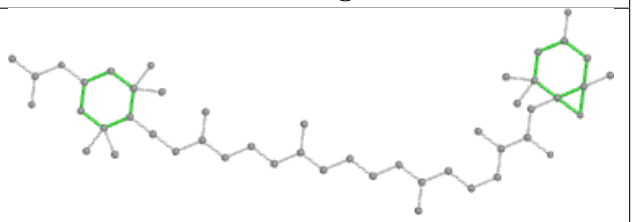
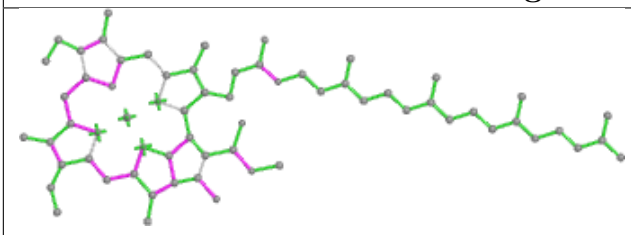


Rings

Ligand CLA B 510



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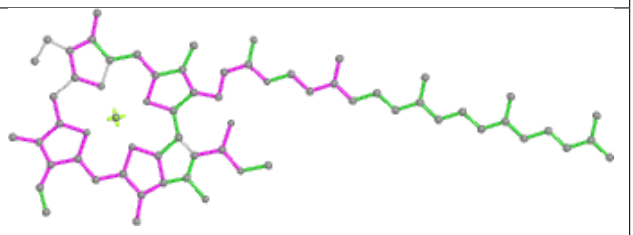

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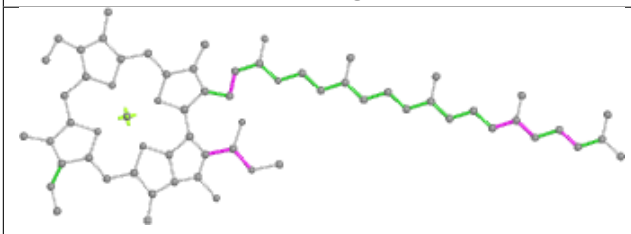

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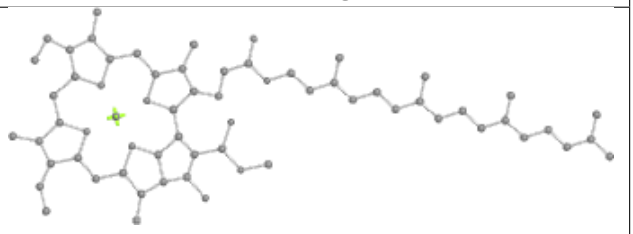

Rings

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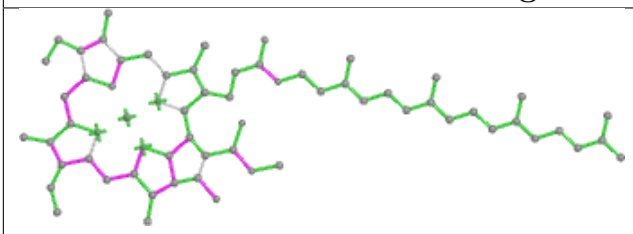

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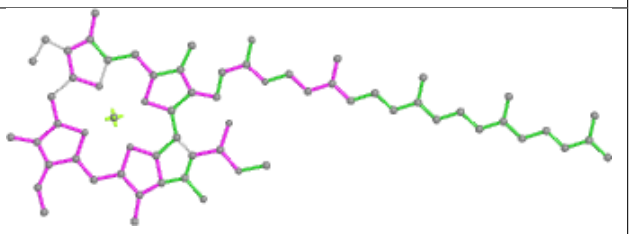

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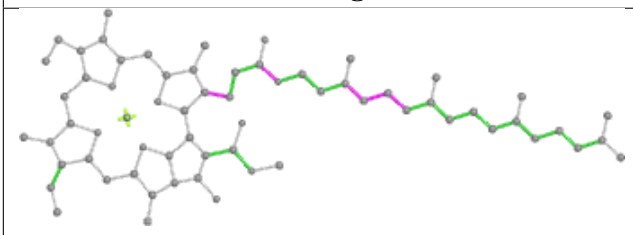

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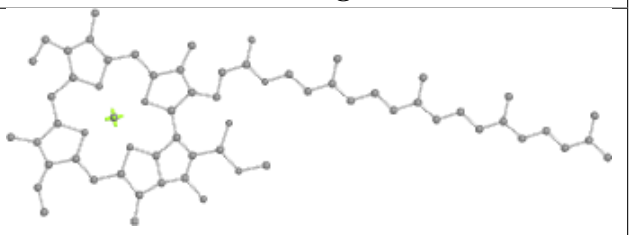

Rings

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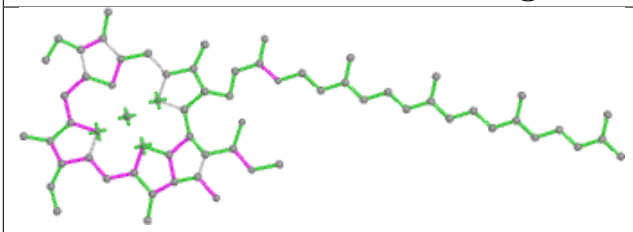

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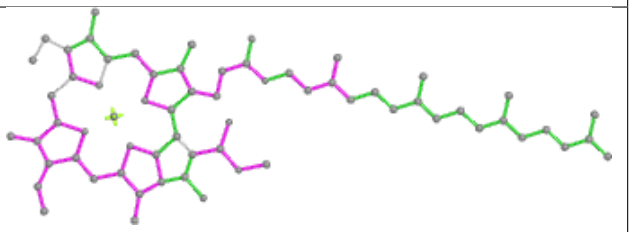

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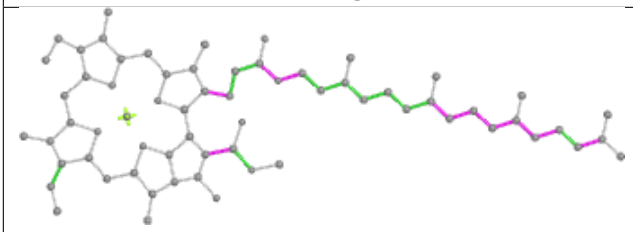

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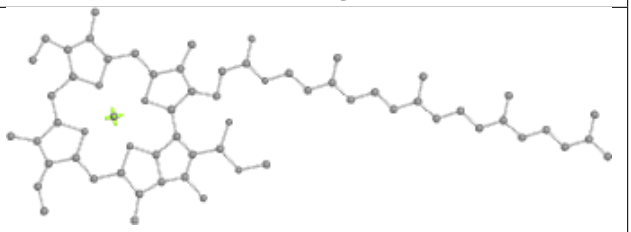
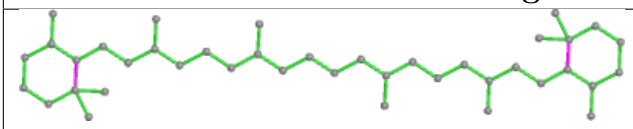


Rings

Ligand BCR C 514



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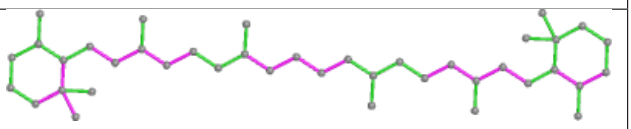

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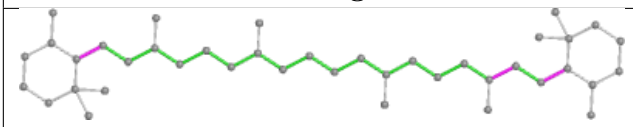
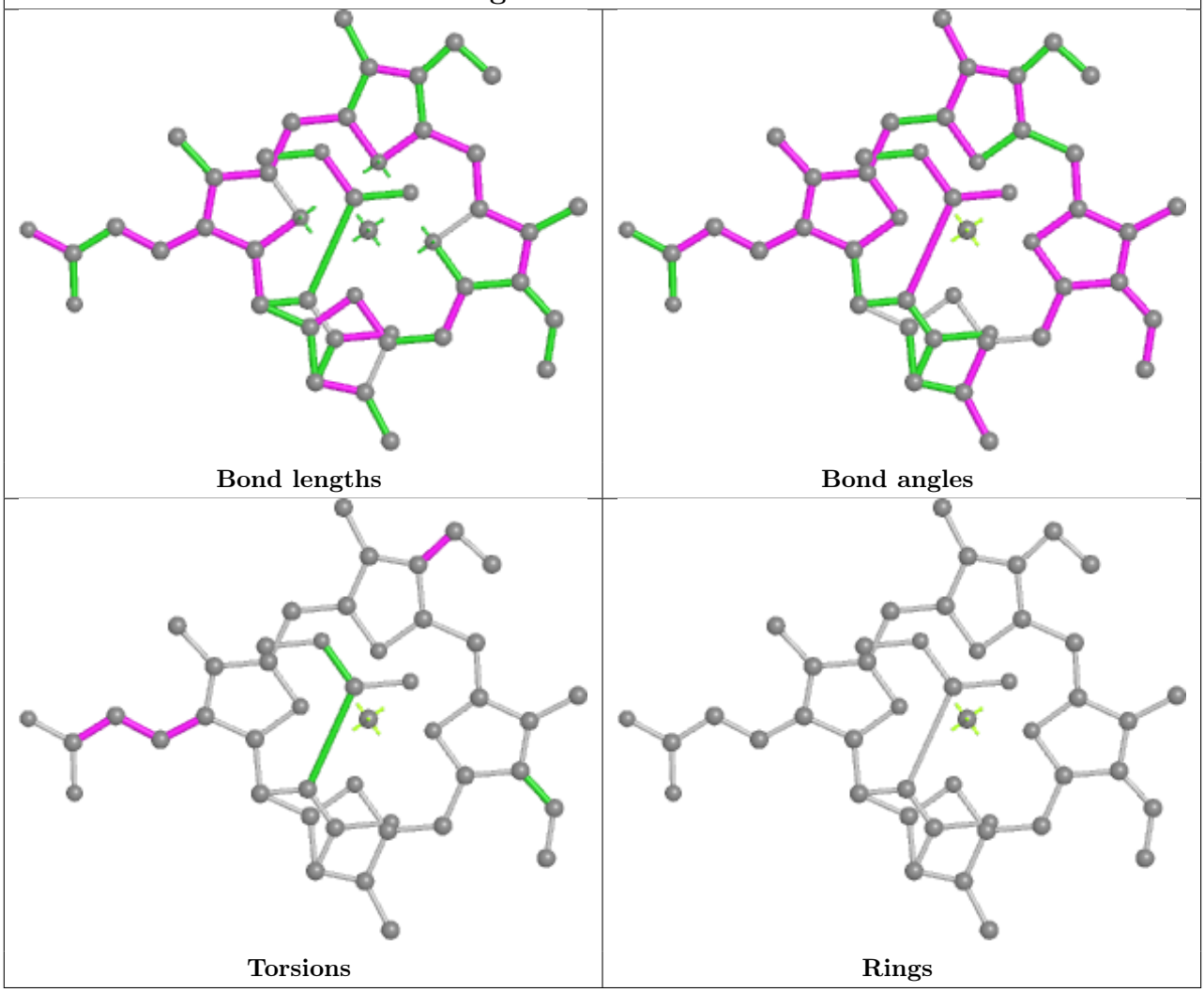


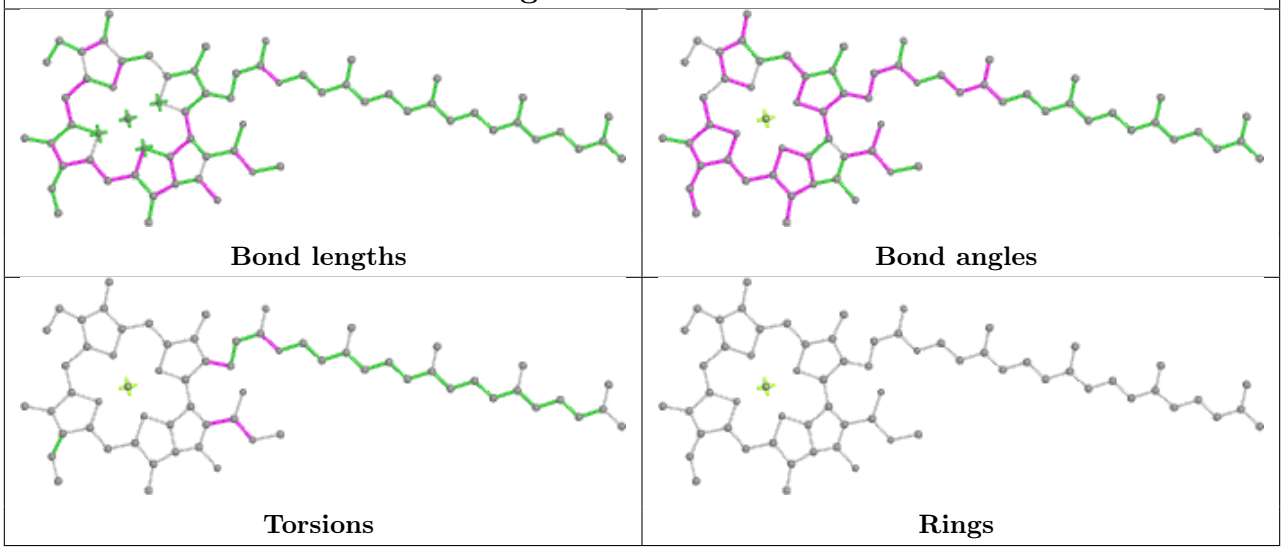
Torsions

Rings

Ligand KC1 13 304



Ligand CLA 18 203



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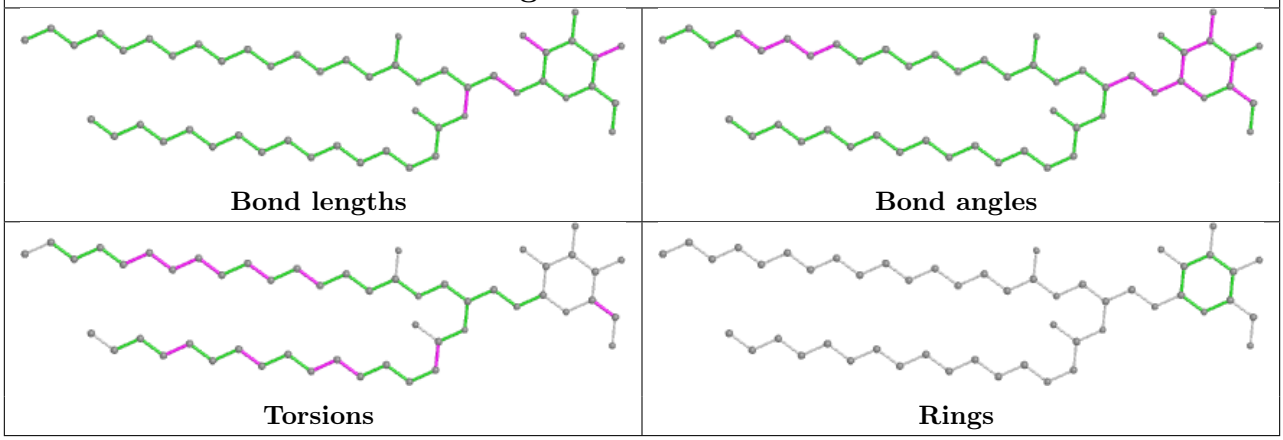
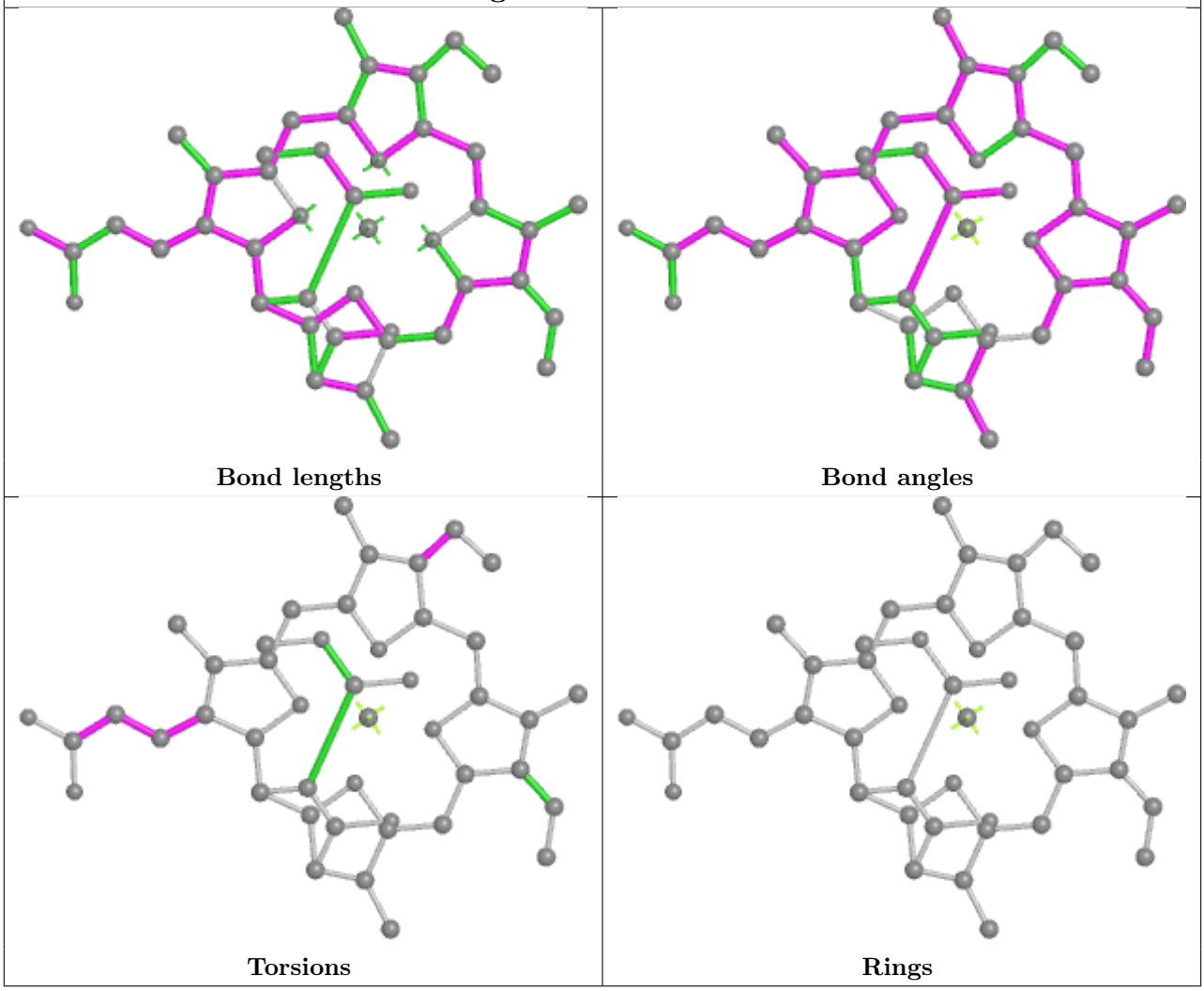


Ligand KC1 37 302



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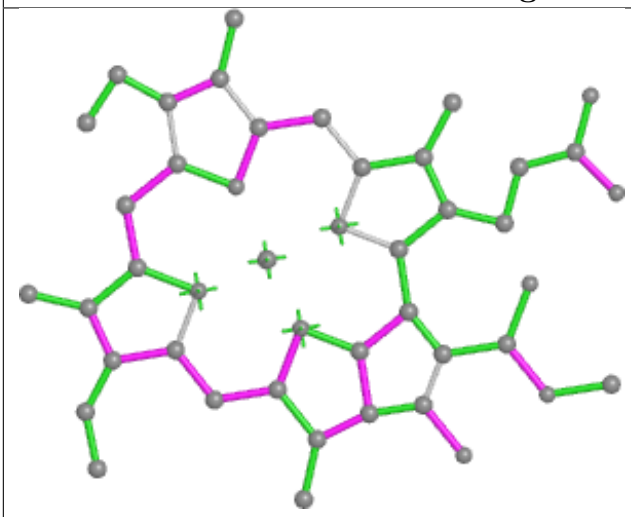
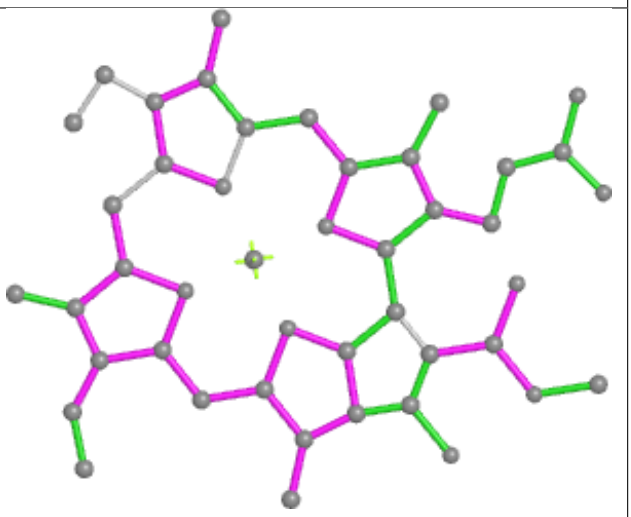
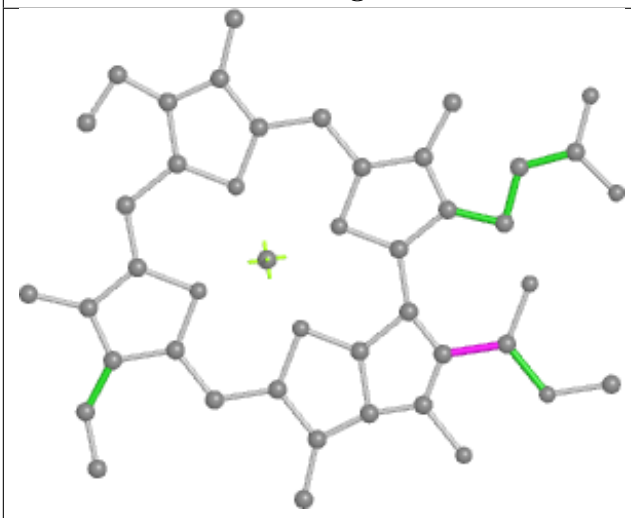


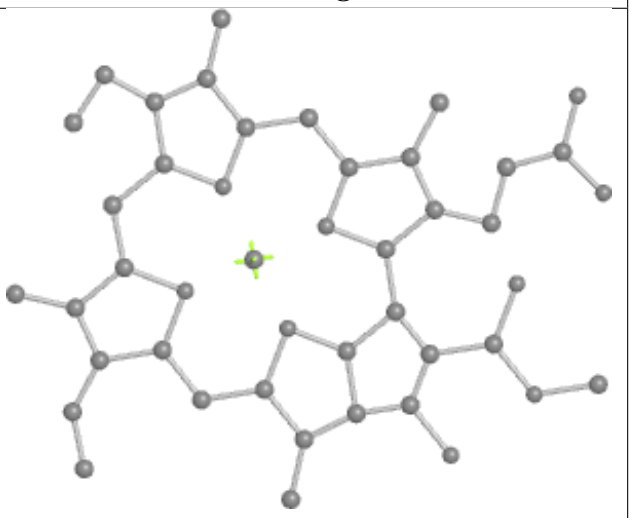
Bond lengths



Bond angles

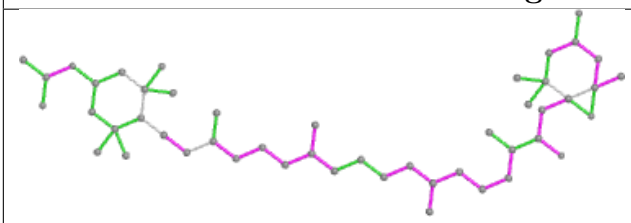


Torsions



Rings

Ligand A86 17 310



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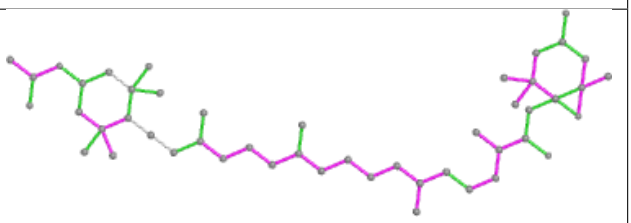

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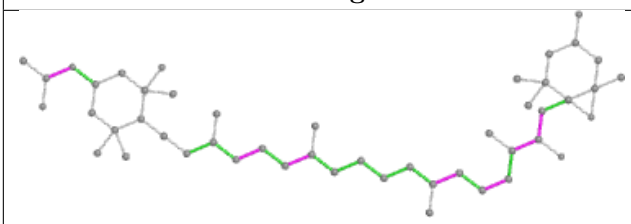

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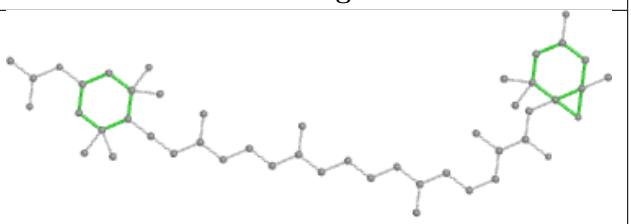
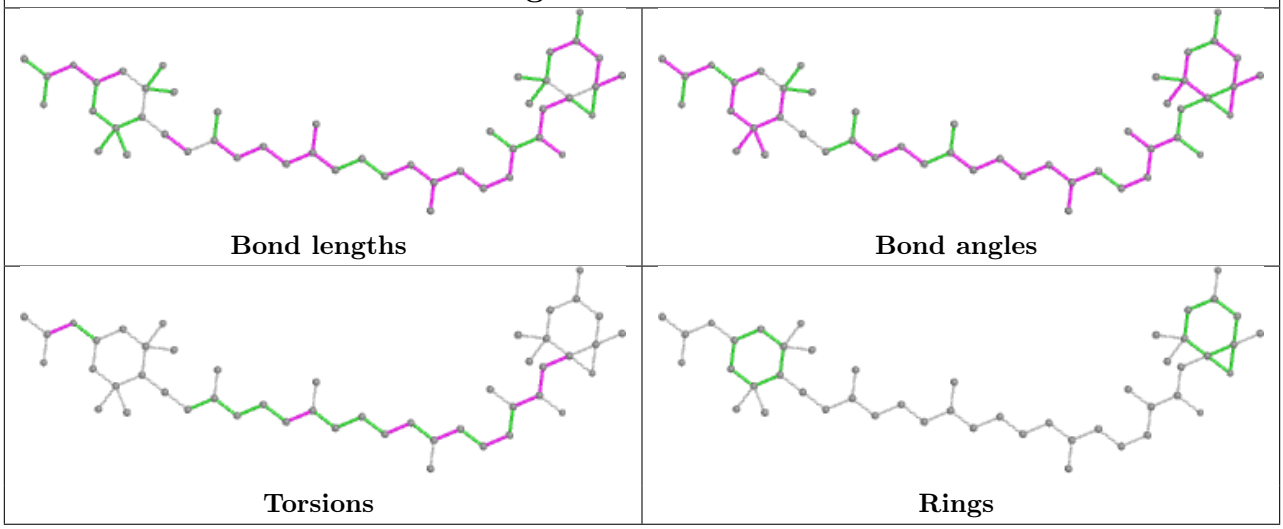


Rings

Ligand A86 14 316



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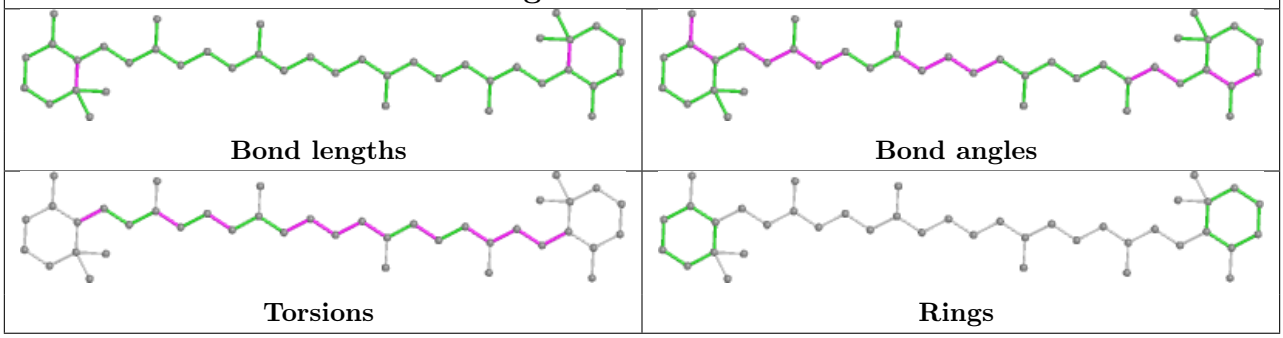
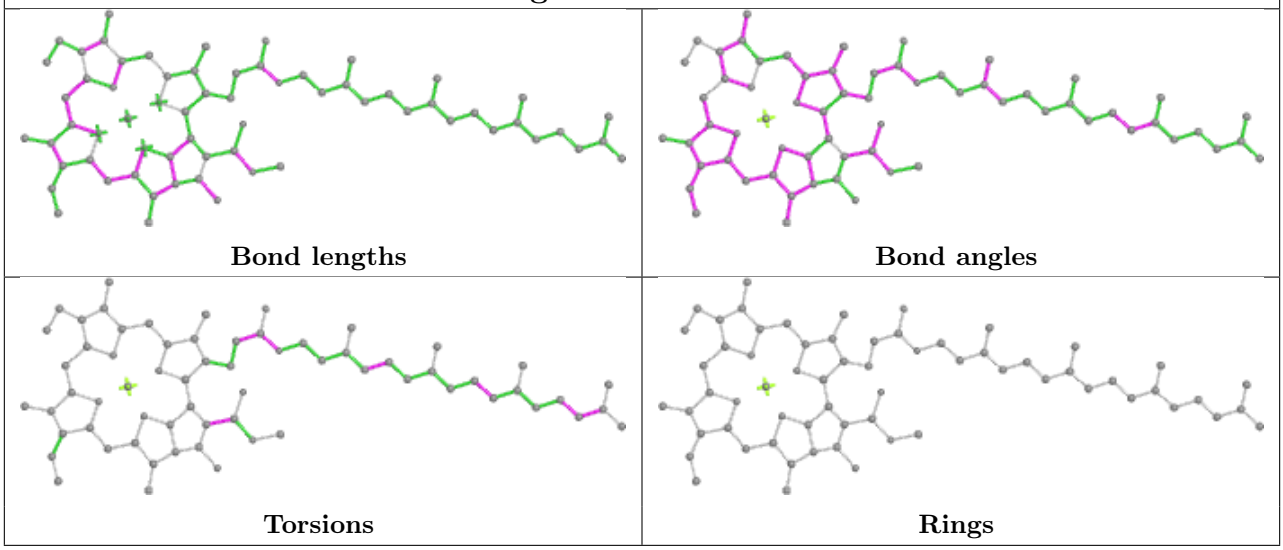
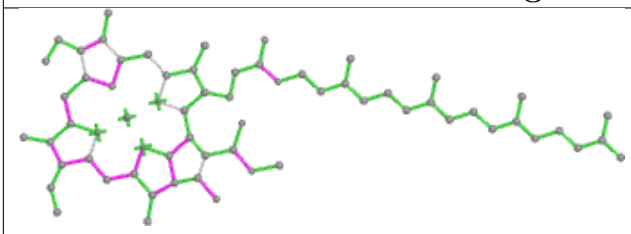
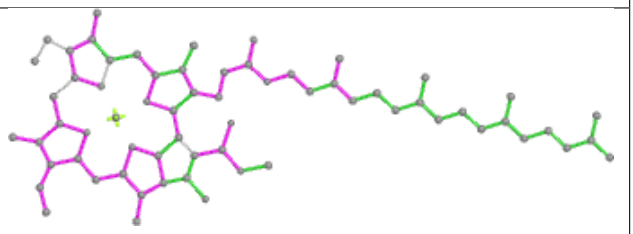
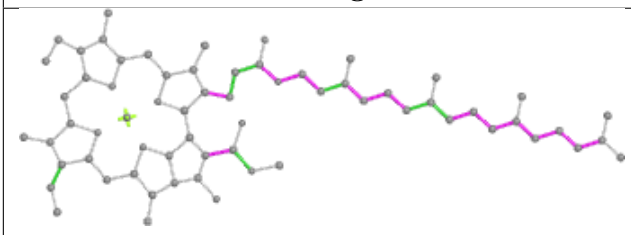
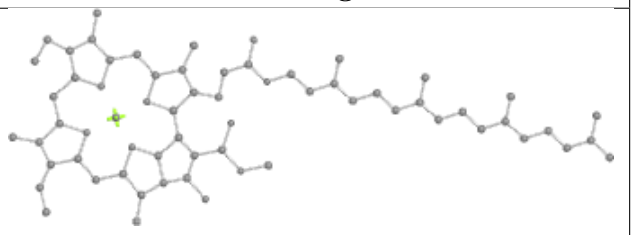


Ligand CLA c 512



Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

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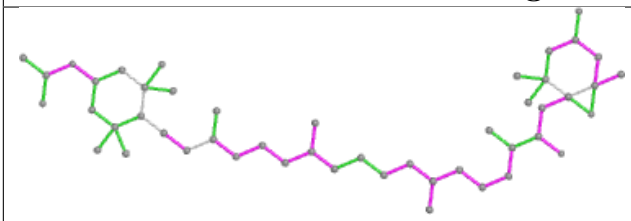
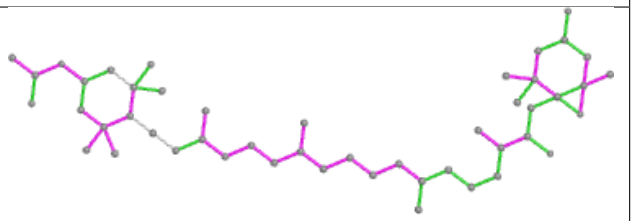
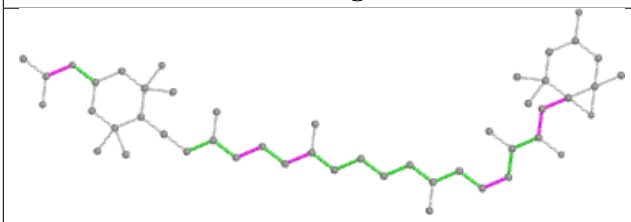
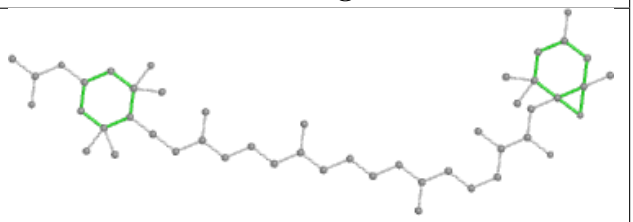
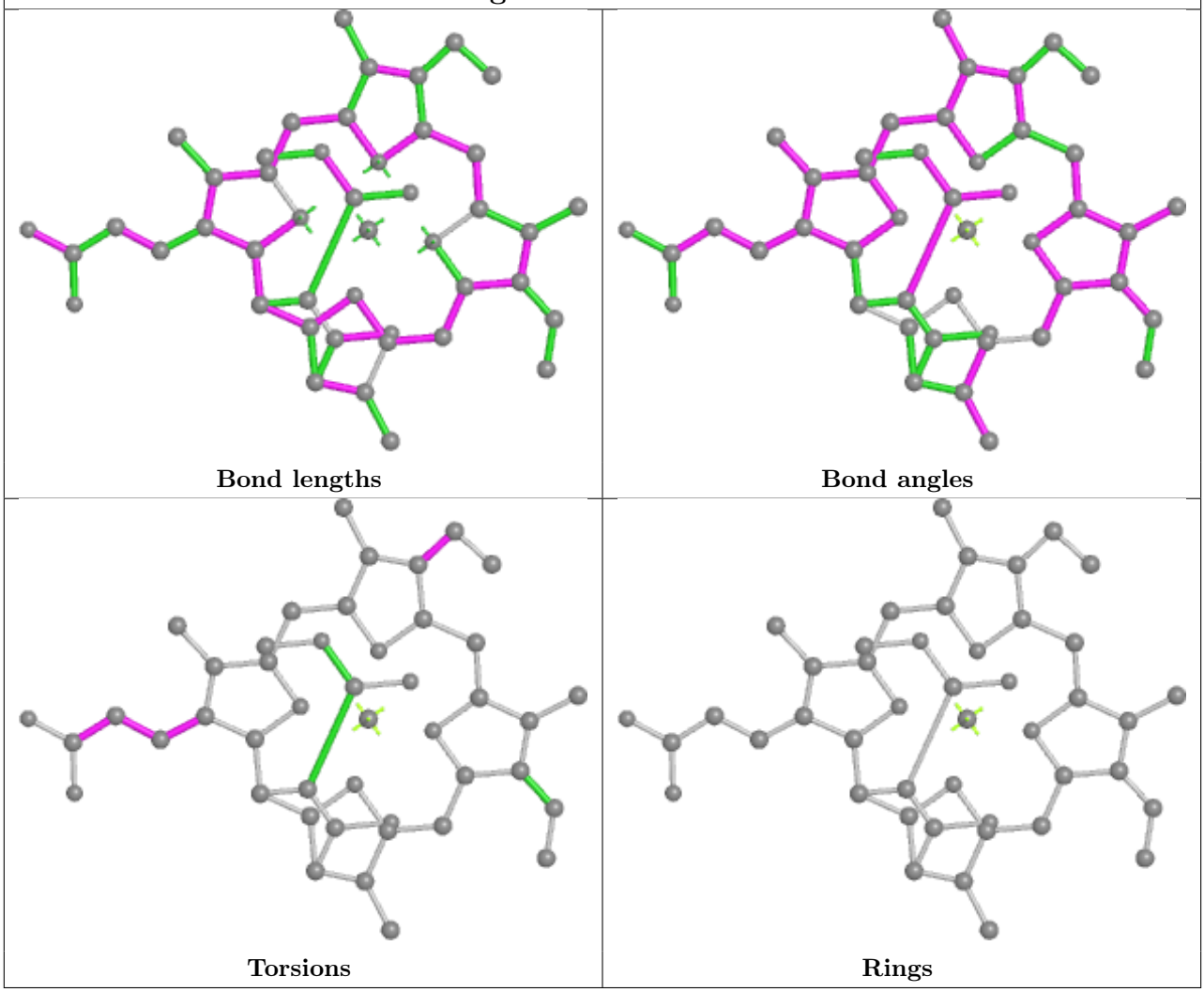
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 40 206



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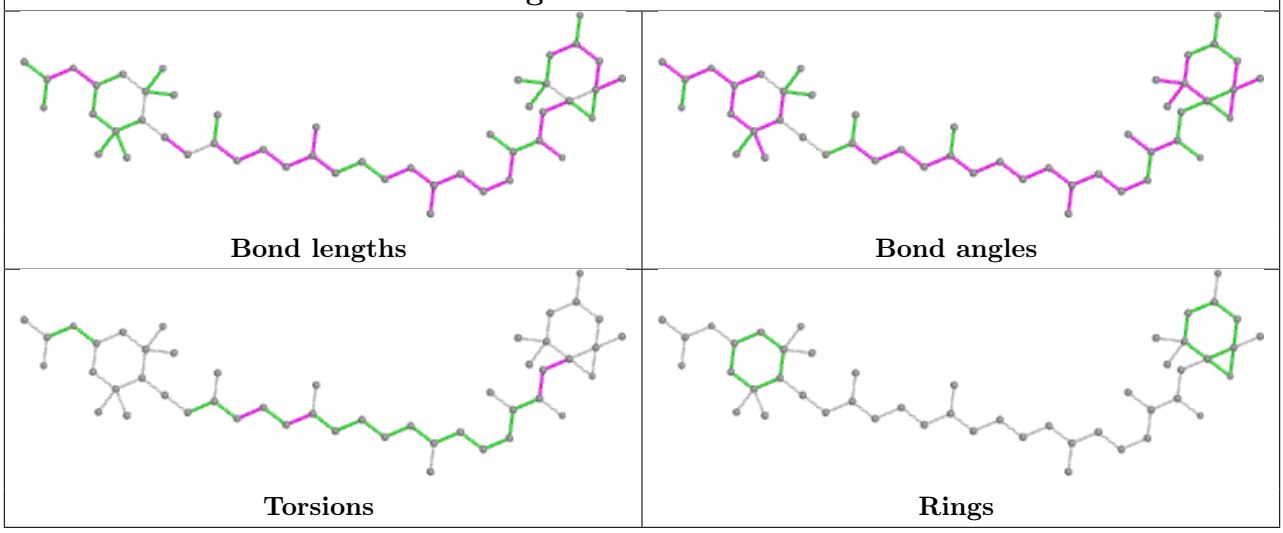

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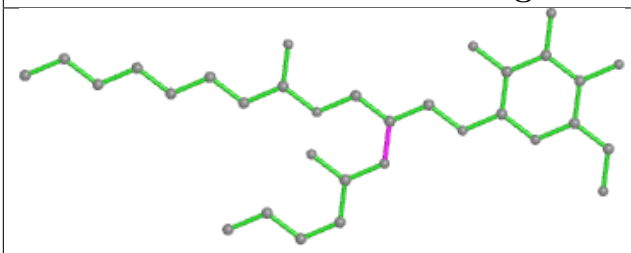
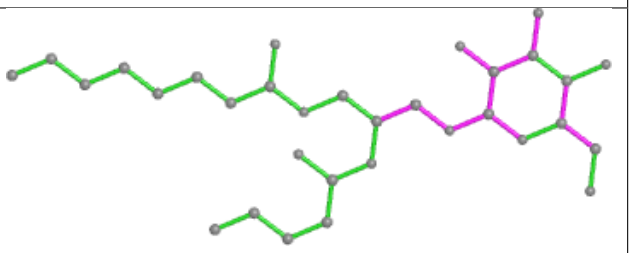
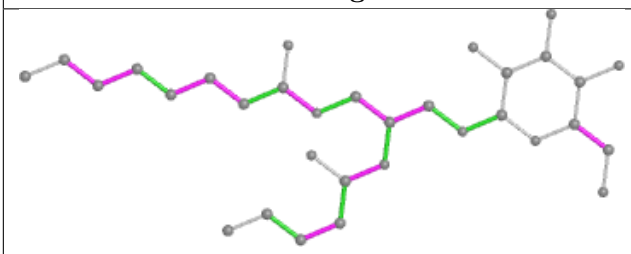
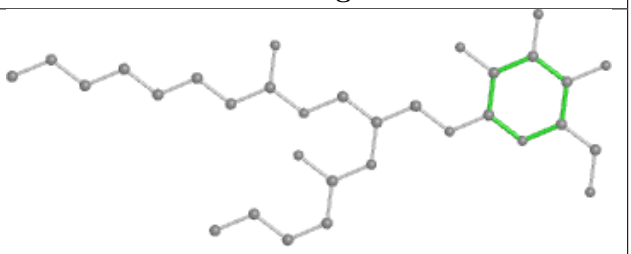
 Bond lengths	 Bond angles
 Torsions	 Rings

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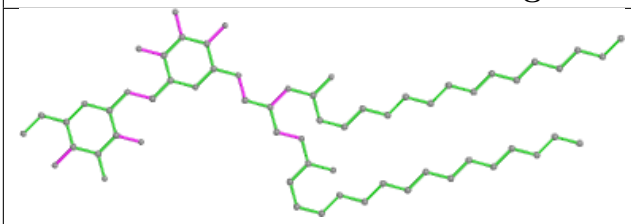
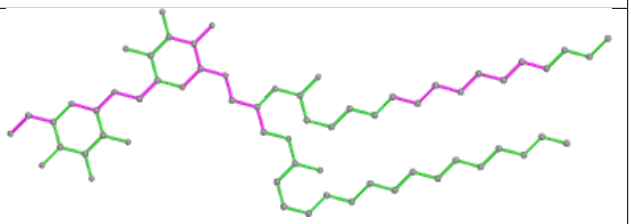
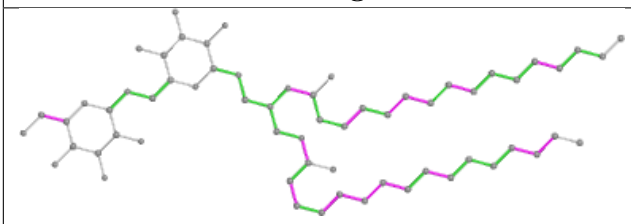
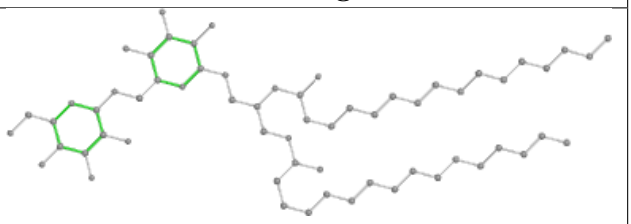
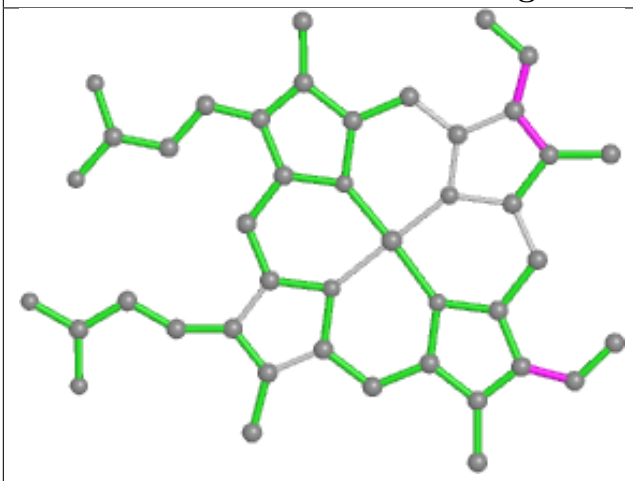
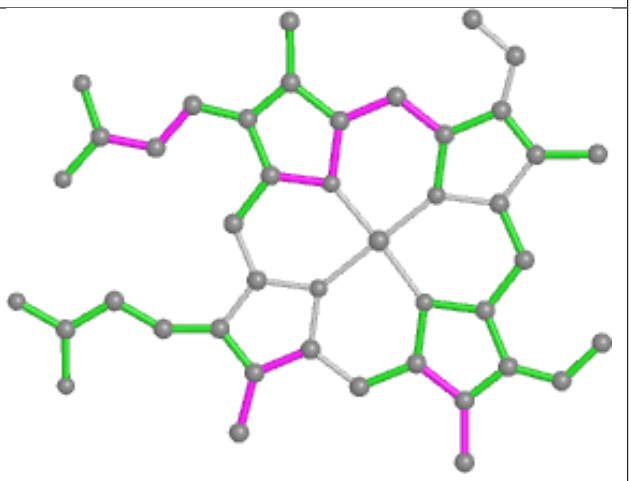
 Bond lengths	 Bond angles
 Torsions	 Rings

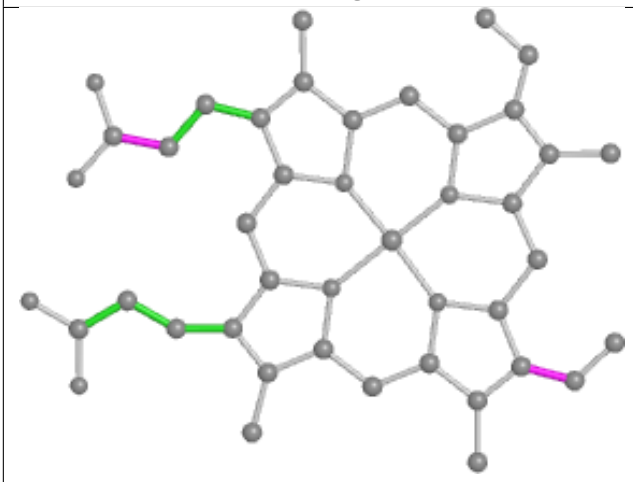
Ligand HEM V 201



Bond lengths



Bond angles



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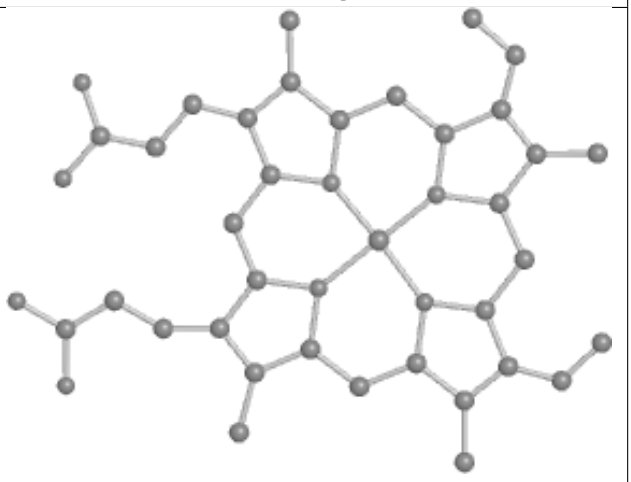
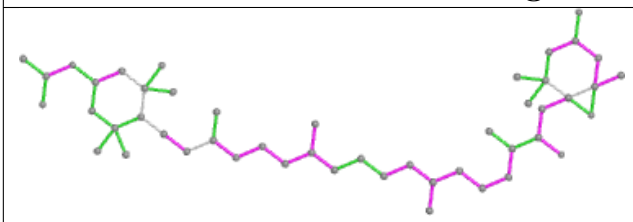


Rings

Ligand A86 21 211



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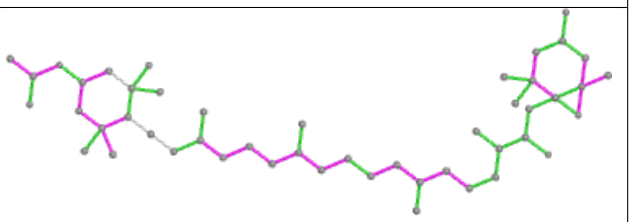
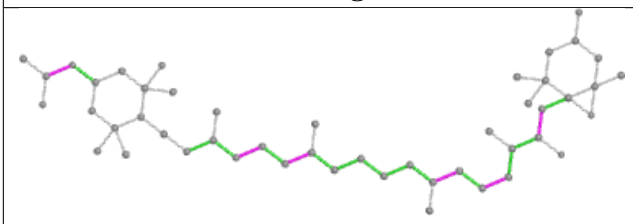


Bond angles



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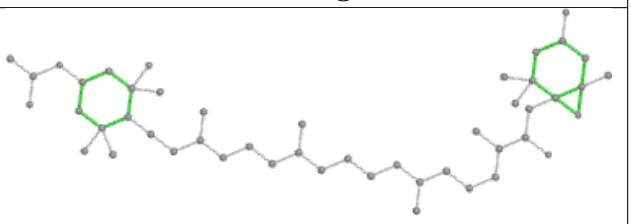
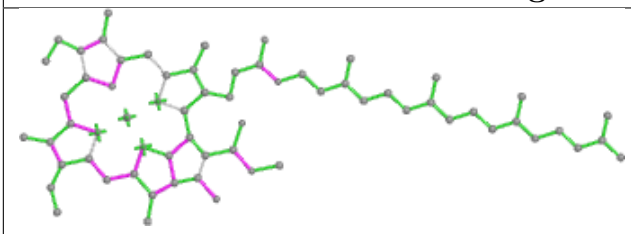


Rings

Ligand CLA a 404



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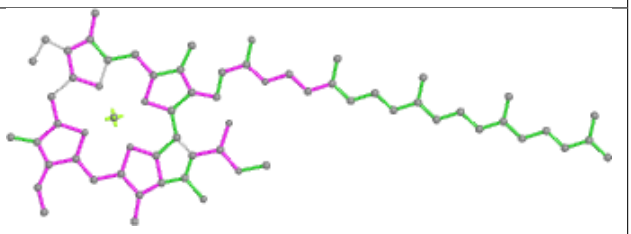
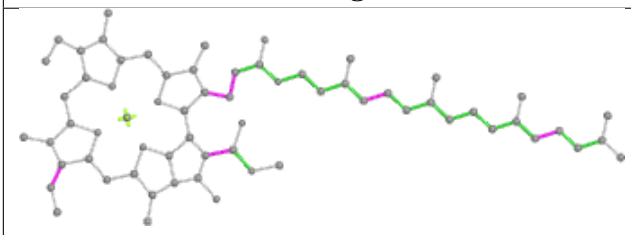


Bond angles



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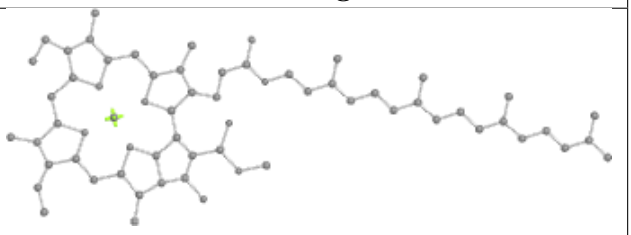
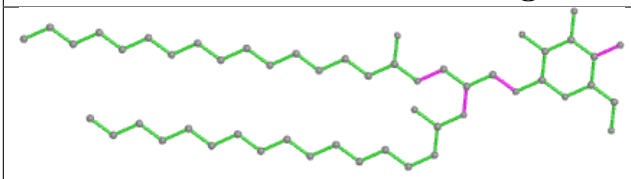


Rings

Ligand LMG C 518



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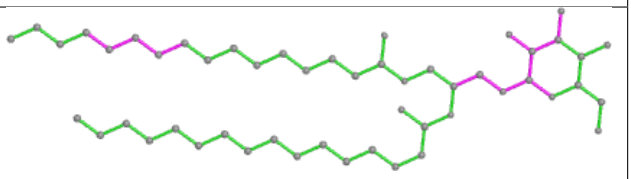
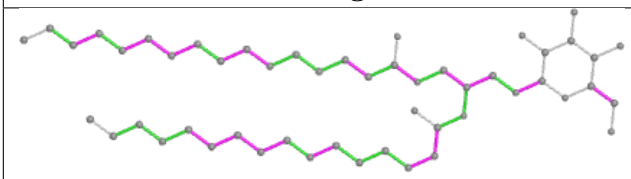


Bond angles



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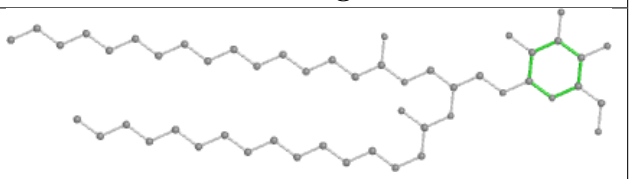
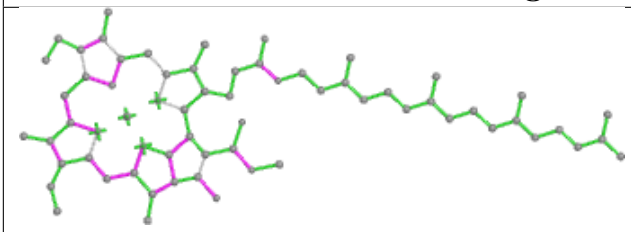


Rings

Ligand CLA B 516



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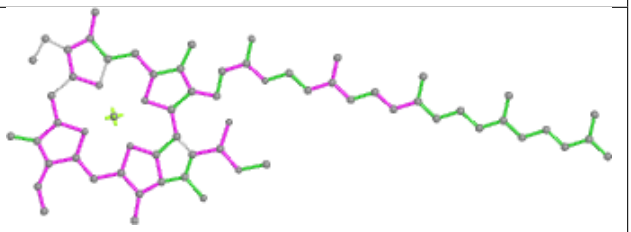
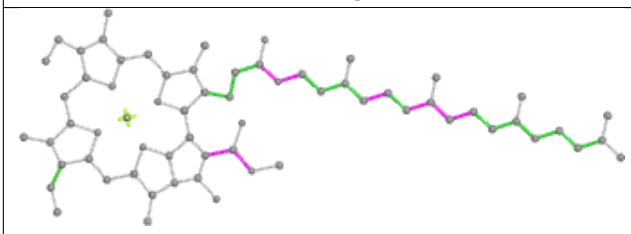


Bond angles



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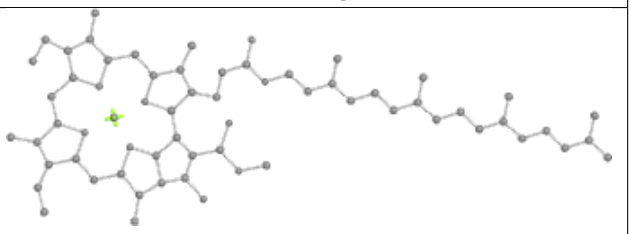
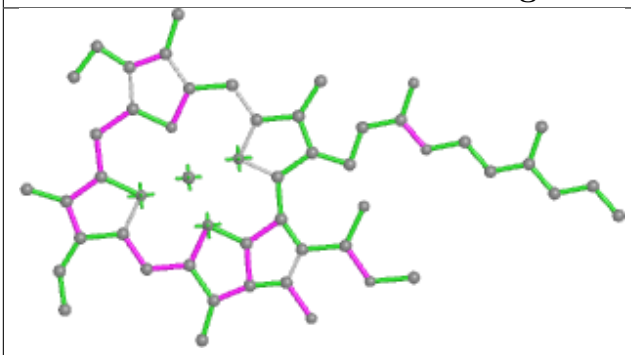
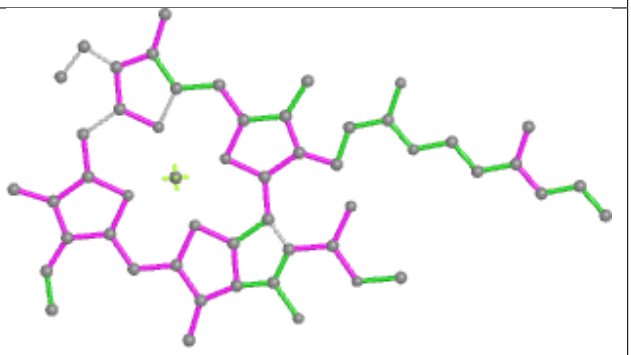


Rings

Ligand CLA 35 307



Bond lengths



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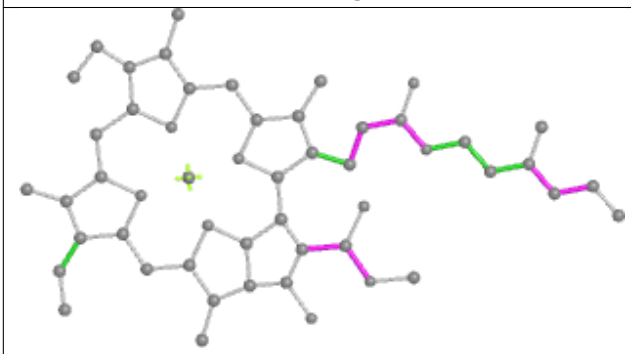
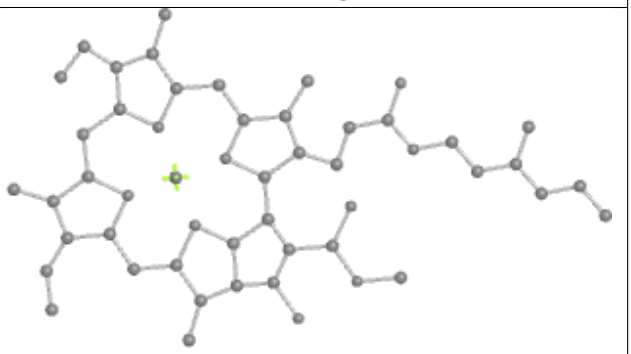
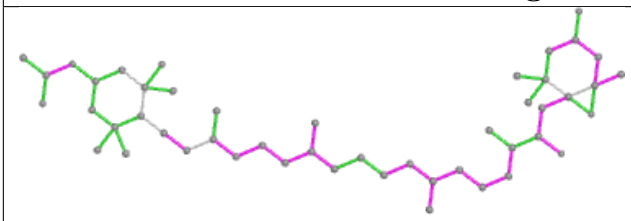


Torsions



Rings

Ligand A86 15 313



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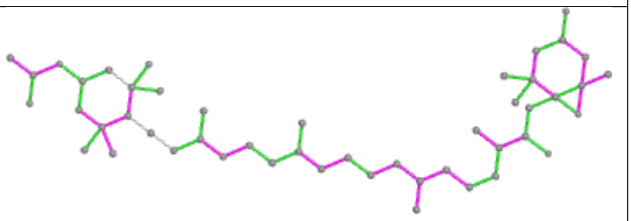

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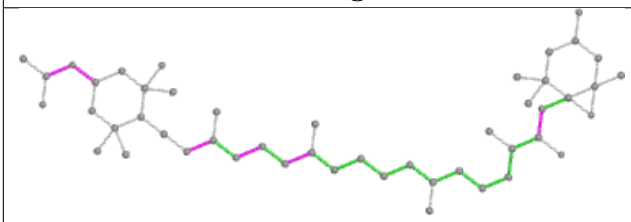

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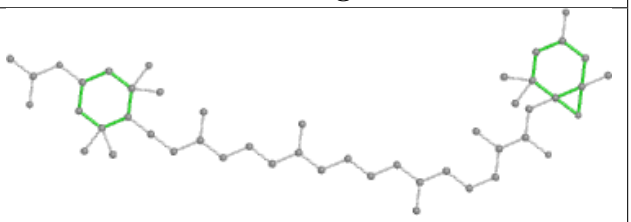
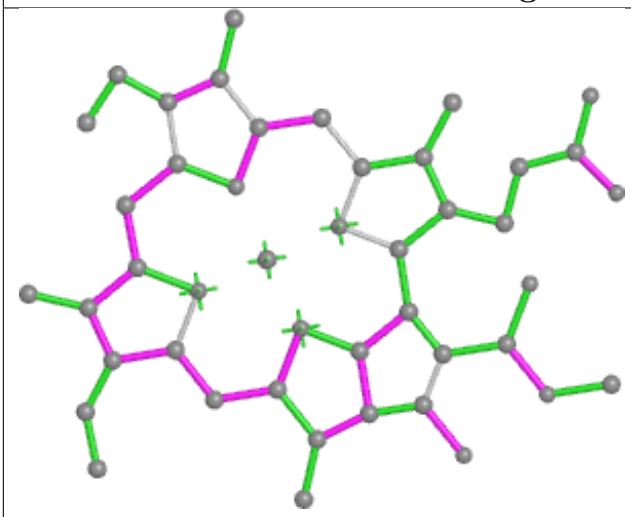


Rings

Ligand CLA 15 310



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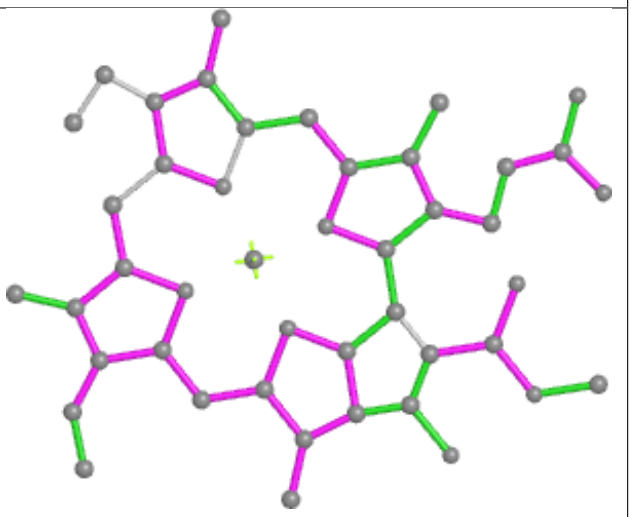

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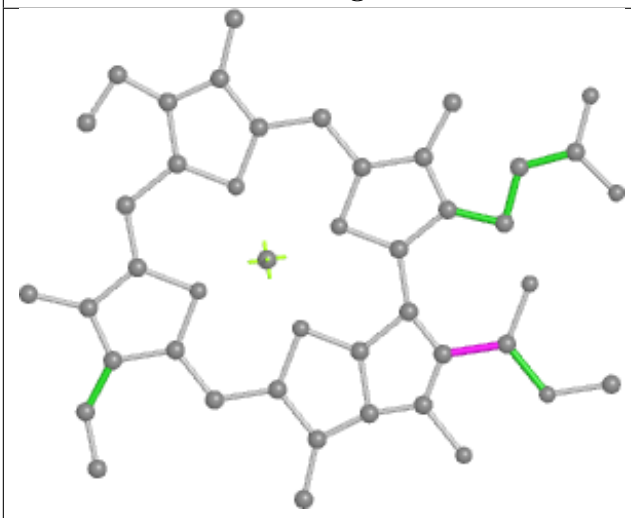

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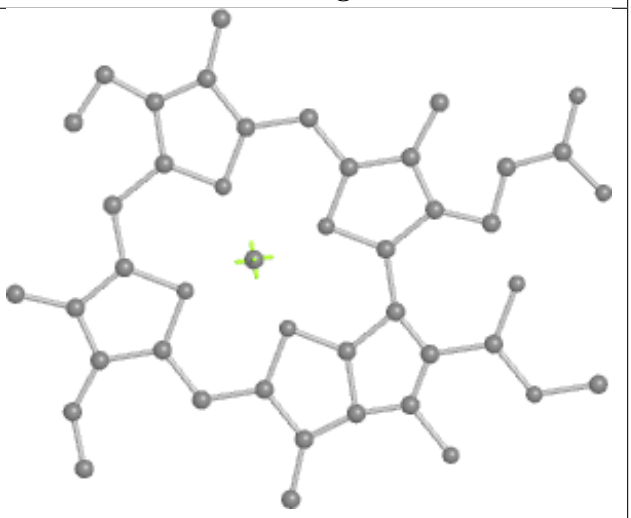
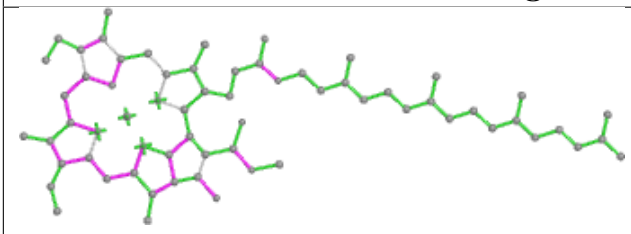


Rings

Ligand CLA B 501



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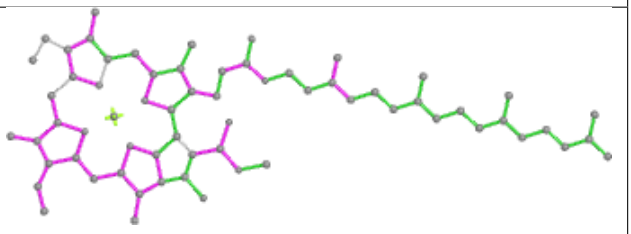

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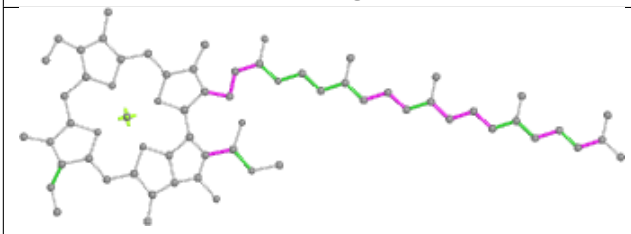

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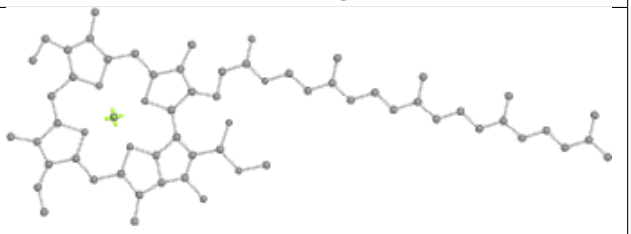
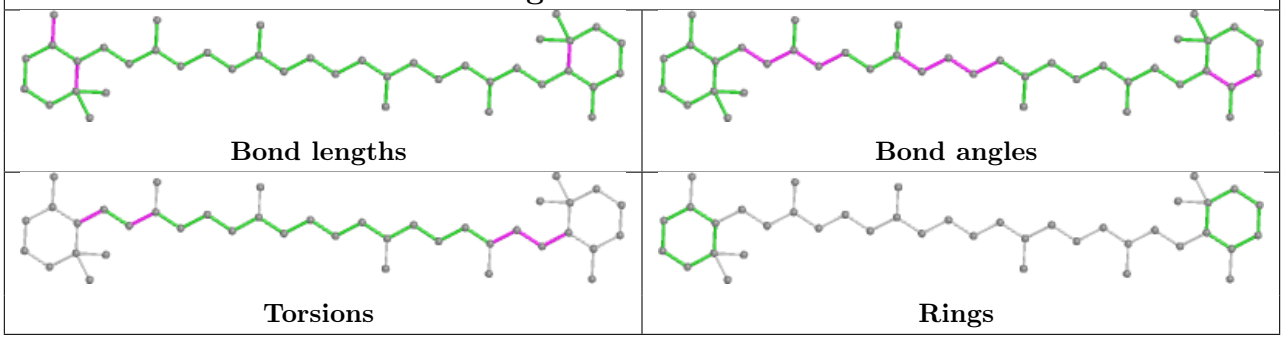


Rings

Ligand BCR h 101



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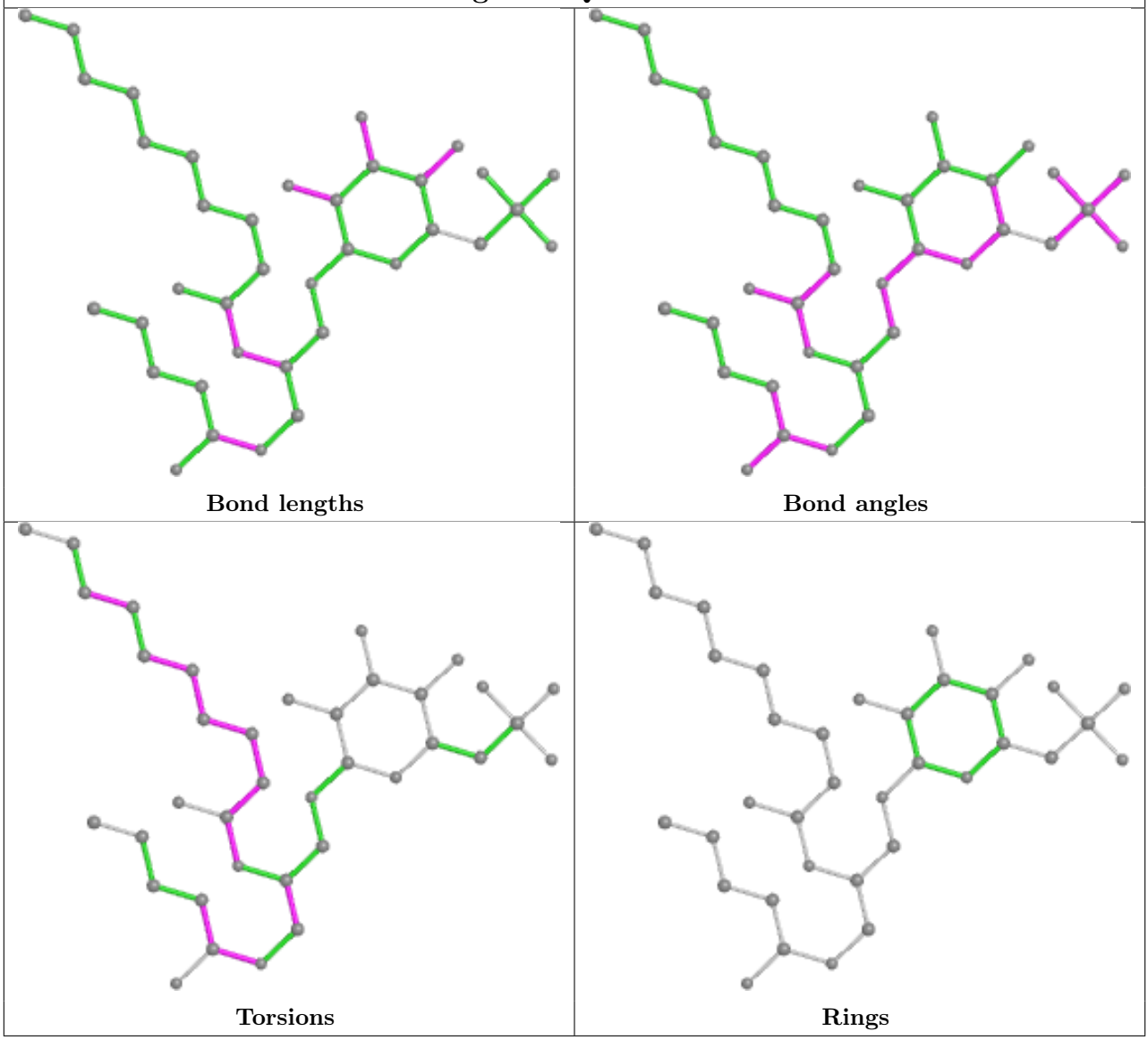
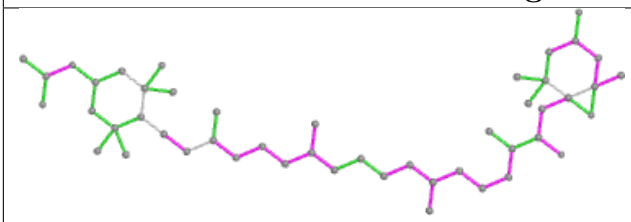
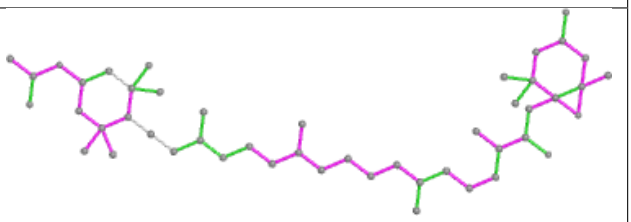
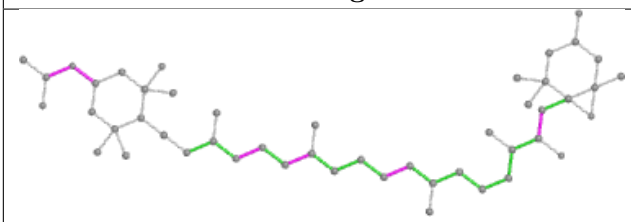
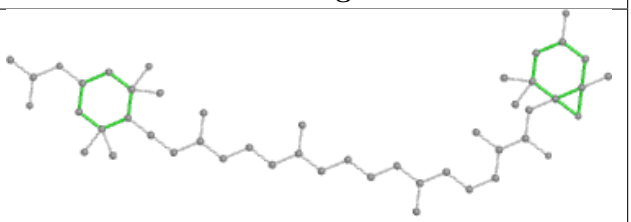


Ligand A86 37 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

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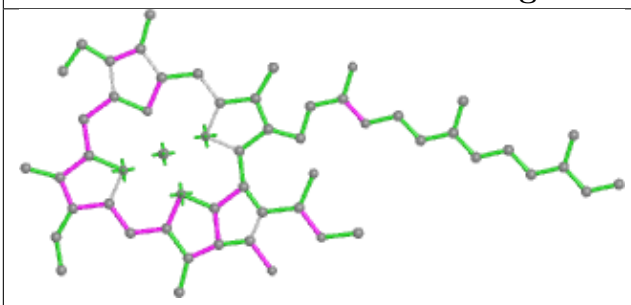
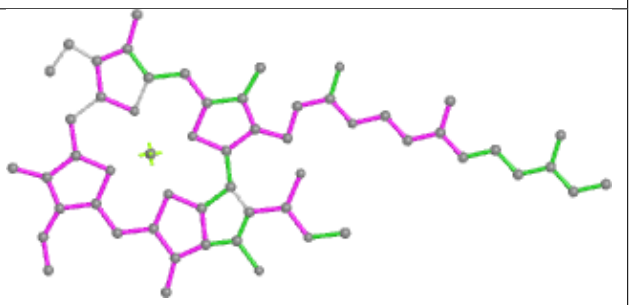
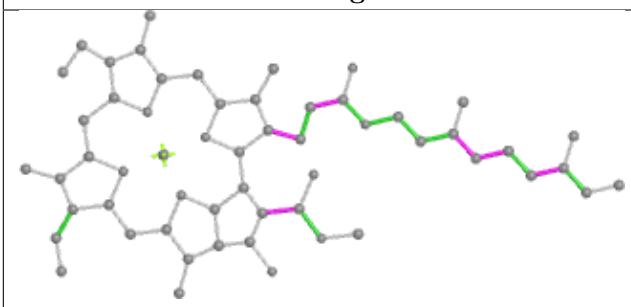
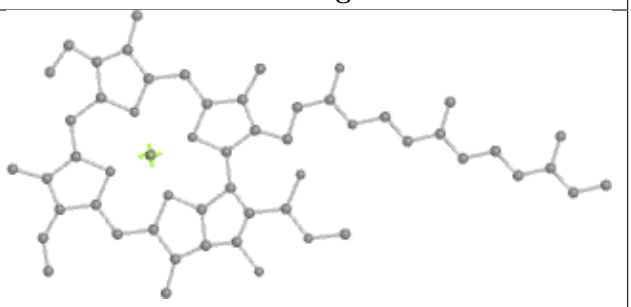
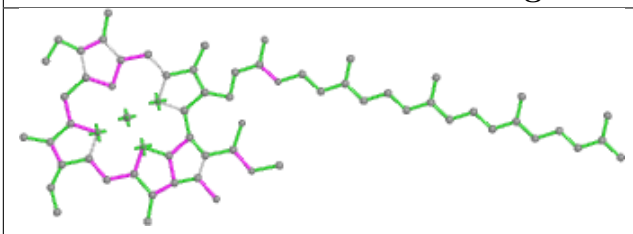
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 504



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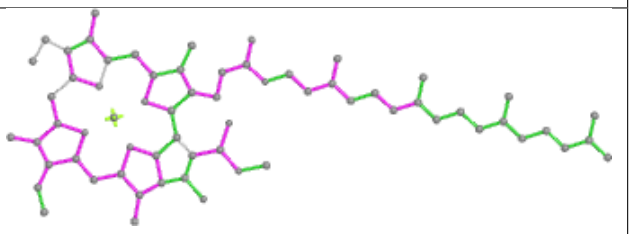

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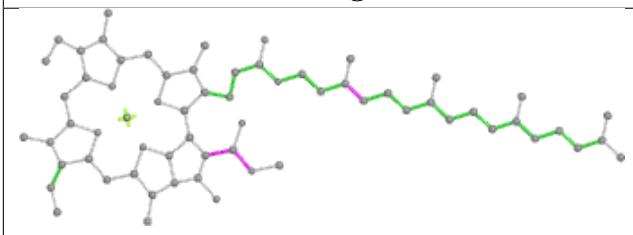

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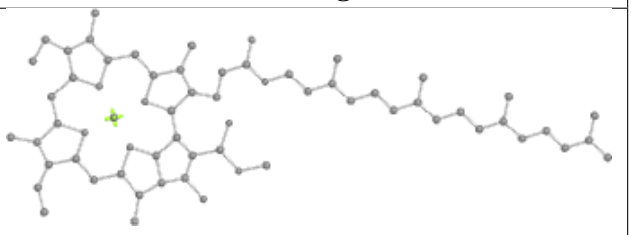
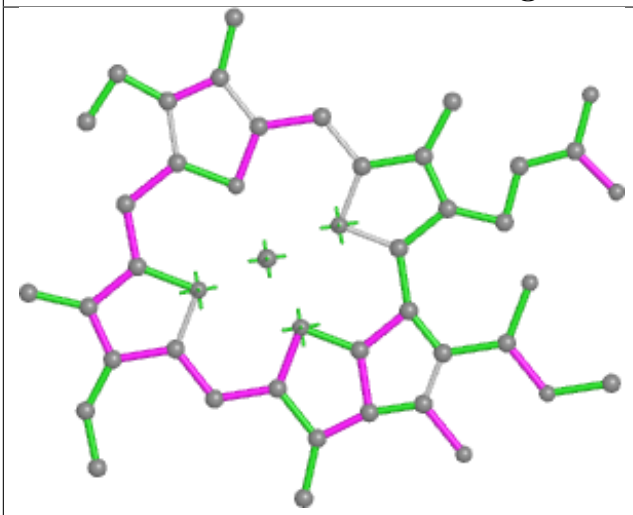


Rings

Ligand CLA 39 304



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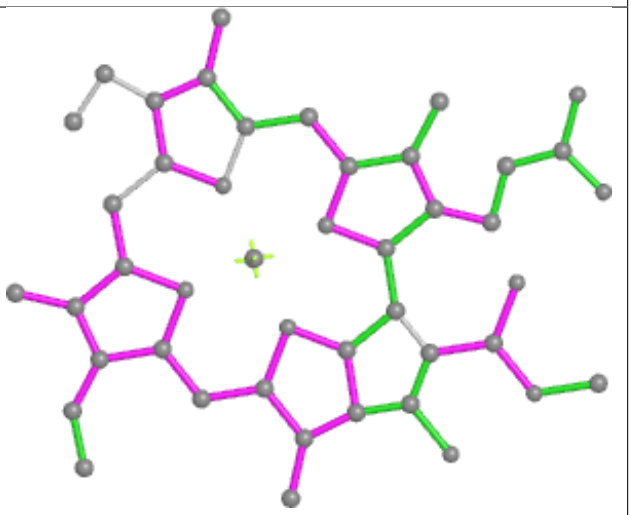

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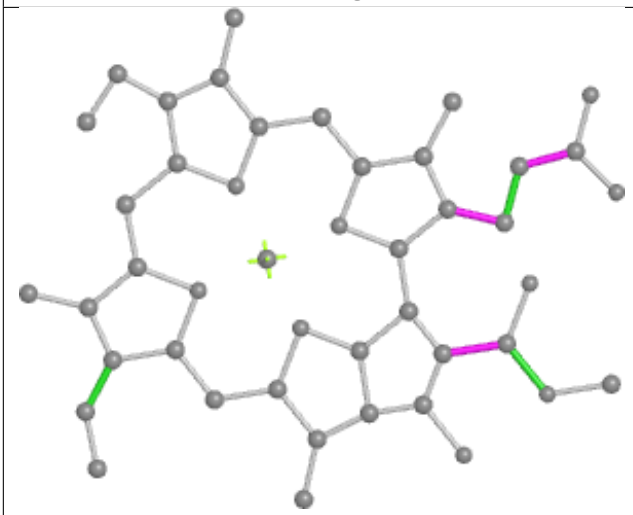

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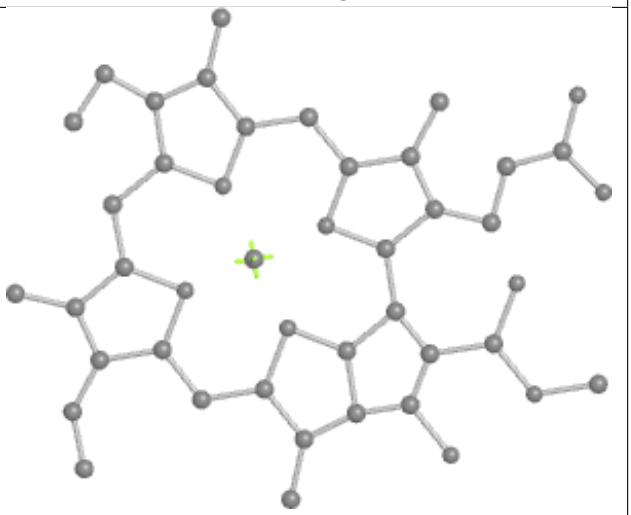
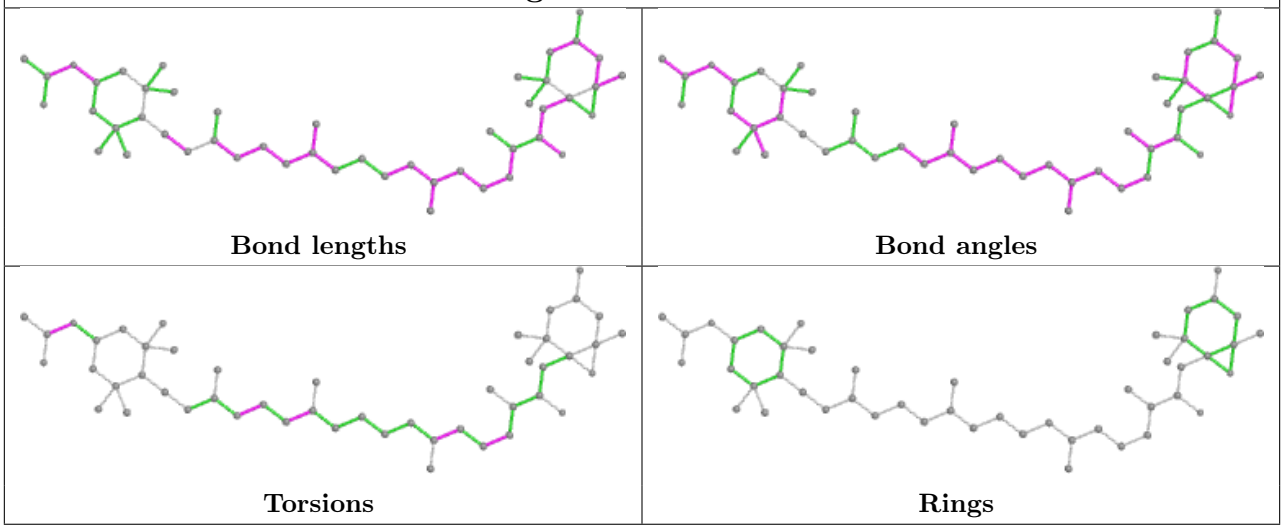


Rings

Ligand A86 13 312



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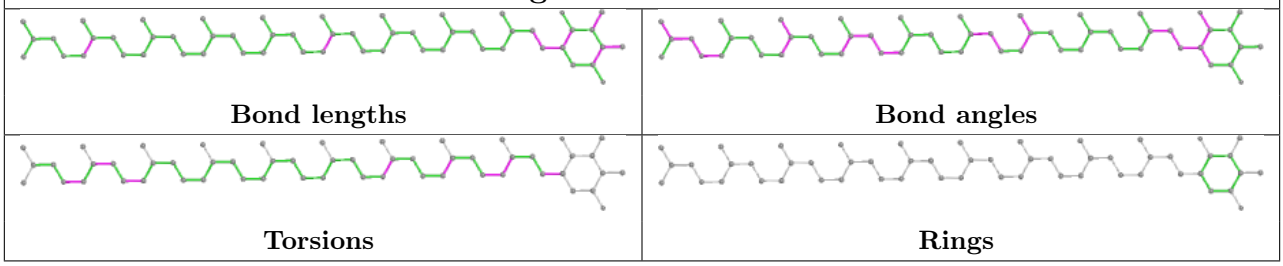

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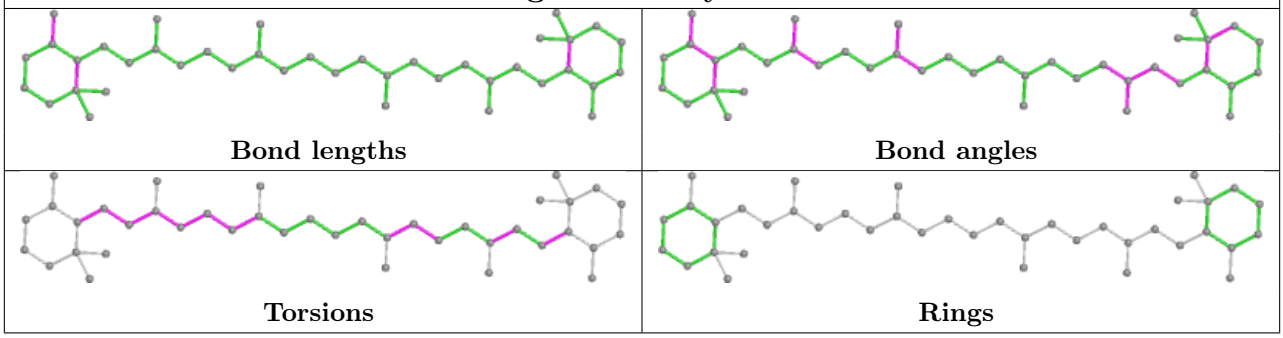

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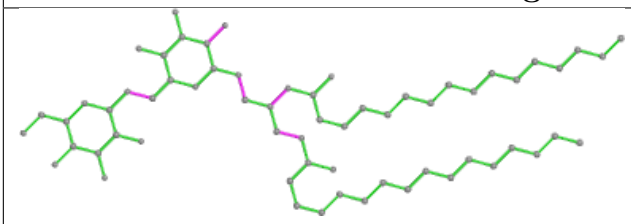
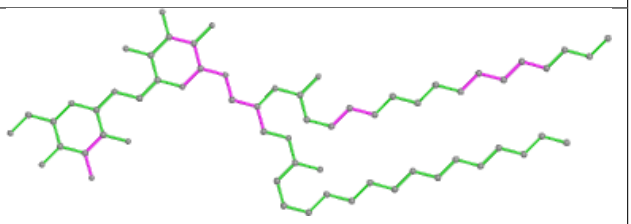
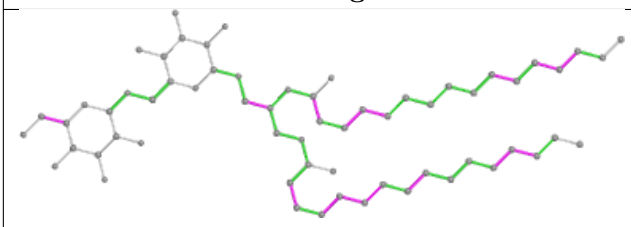


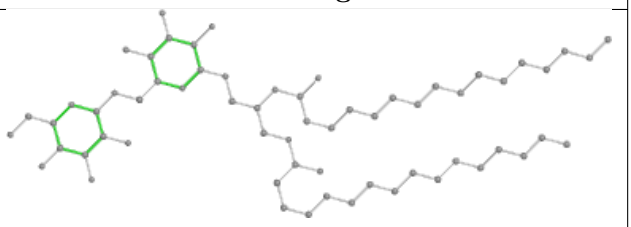
Bond lengths



Bond angles

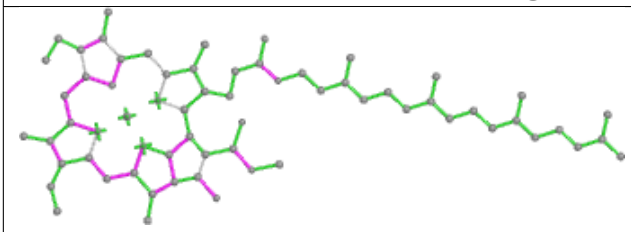


Torsions



Rings

Ligand CLA w 101



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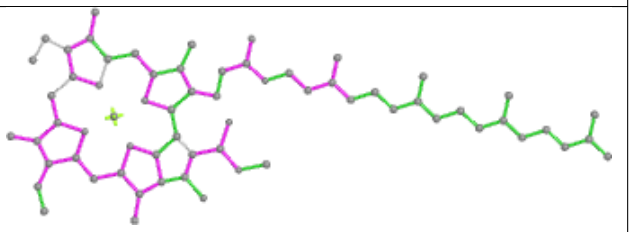

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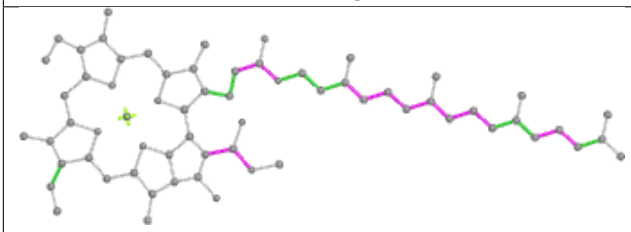

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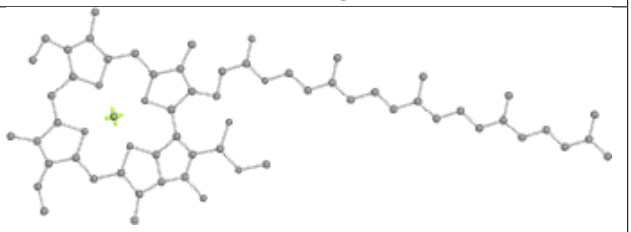
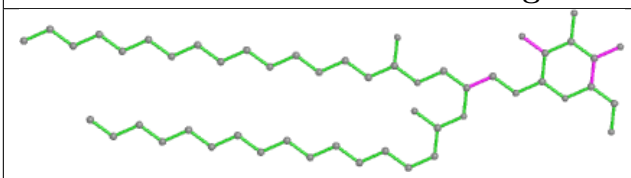


Rings

Ligand LMG b 520



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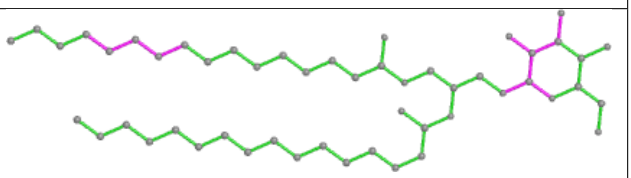

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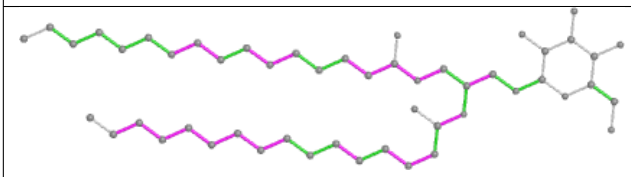

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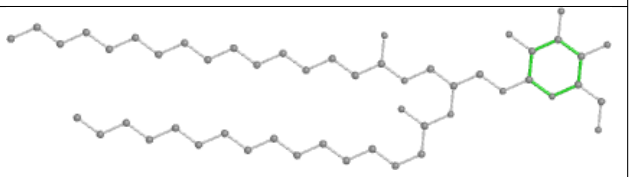
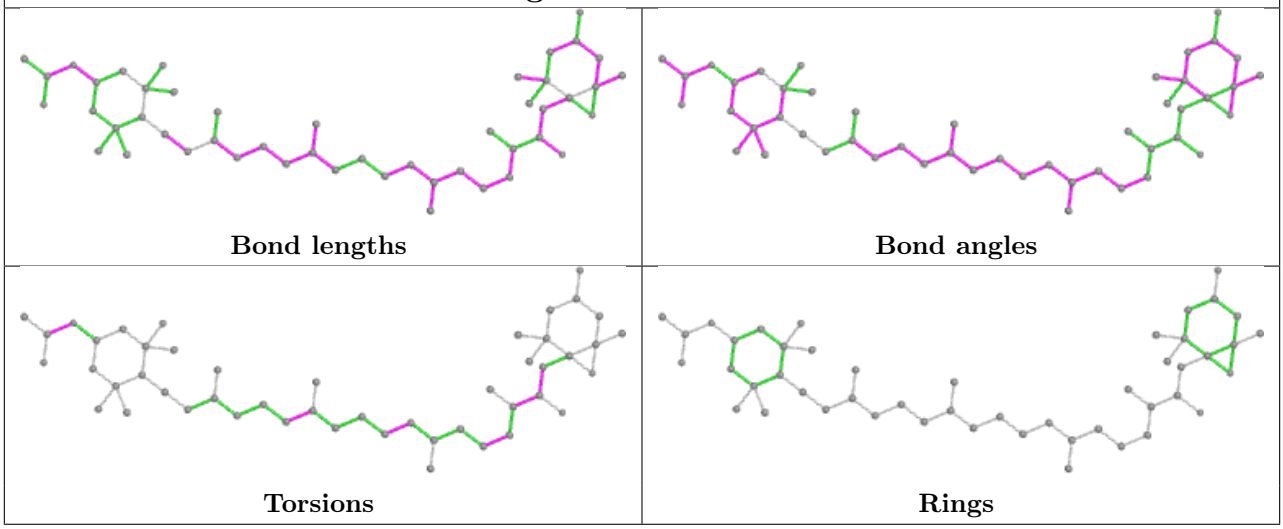
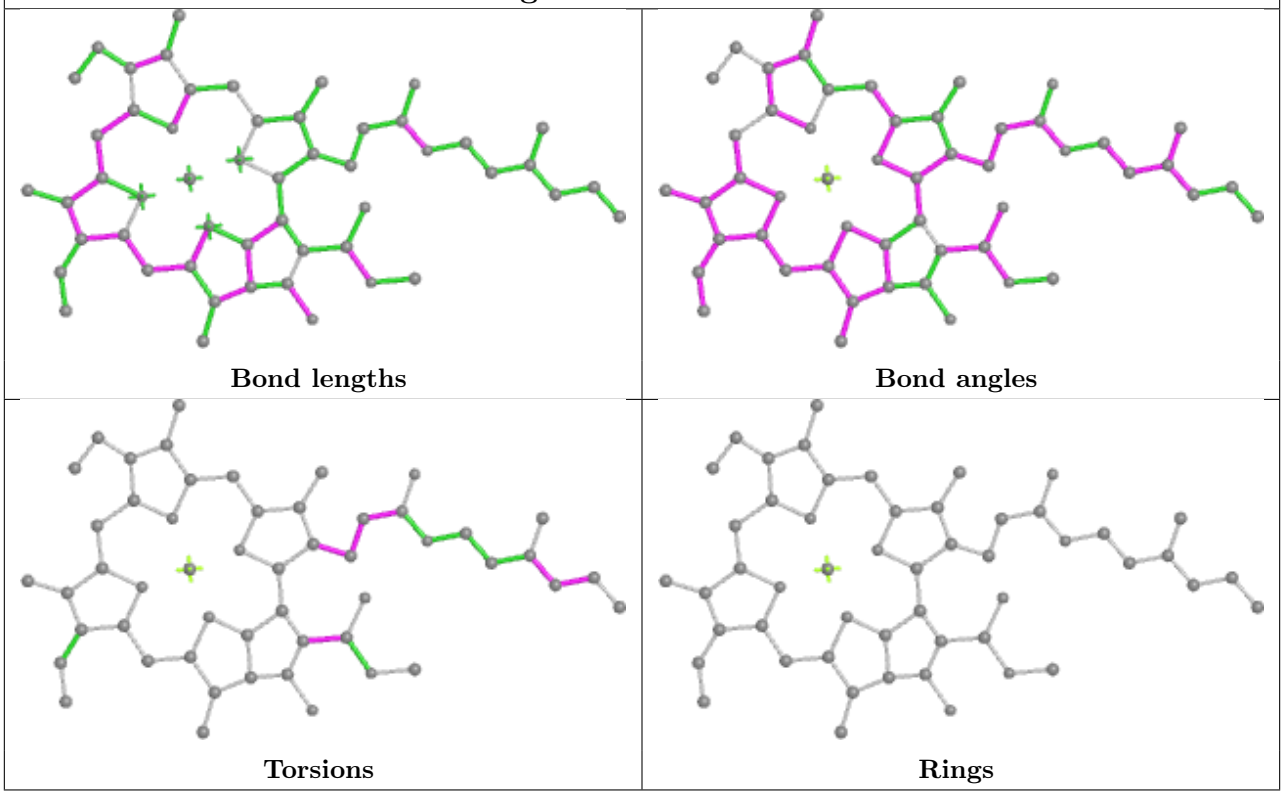


Rings

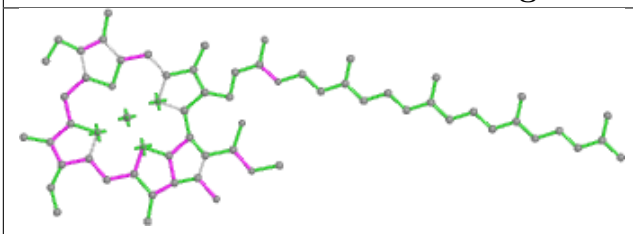
Ligand A86 19 313



Ligand CLA 37 306



Ligand CLA 31 301



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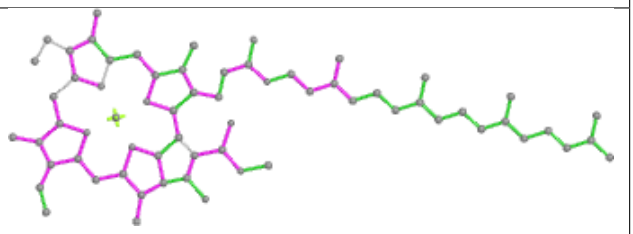
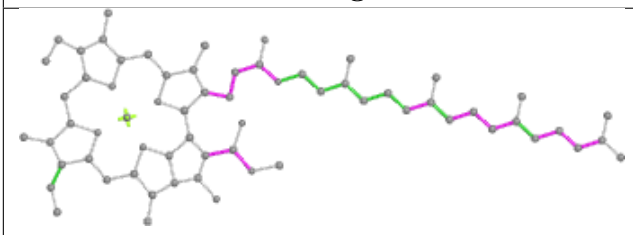
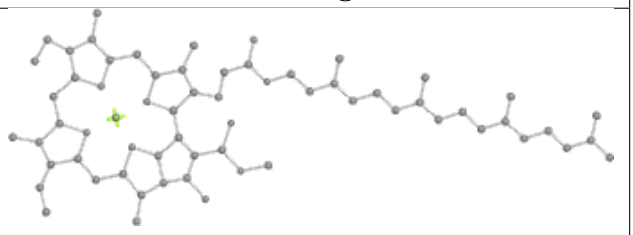


Bond angles

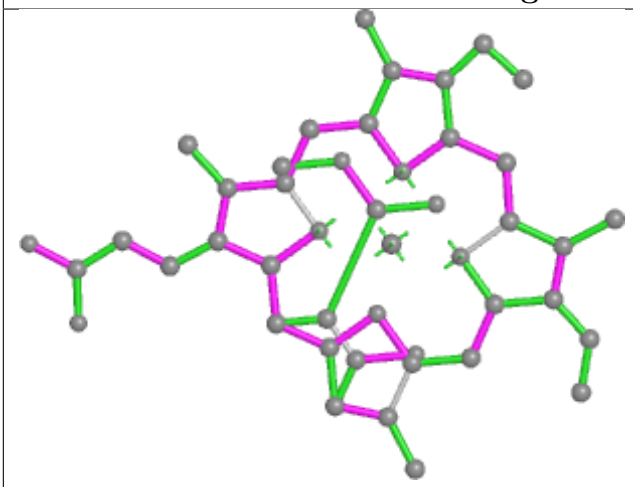


Torsions

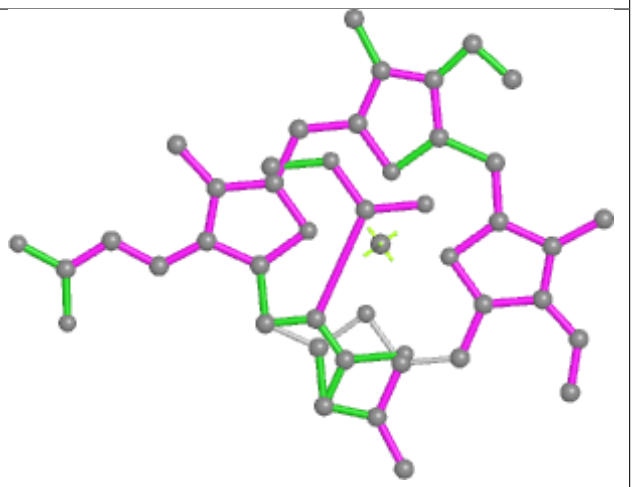


Rings

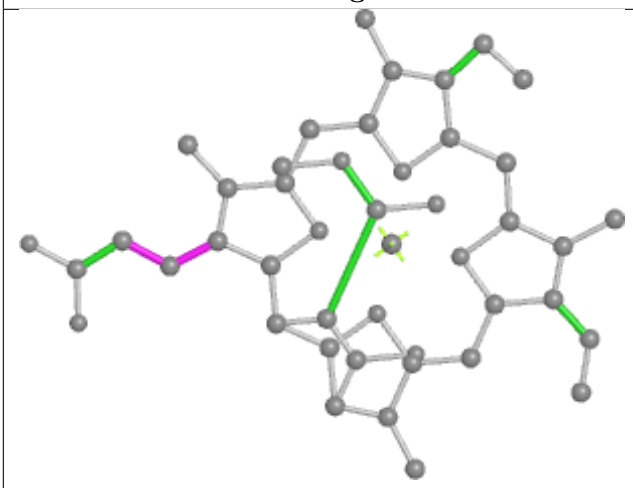
Ligand KC1 31 303



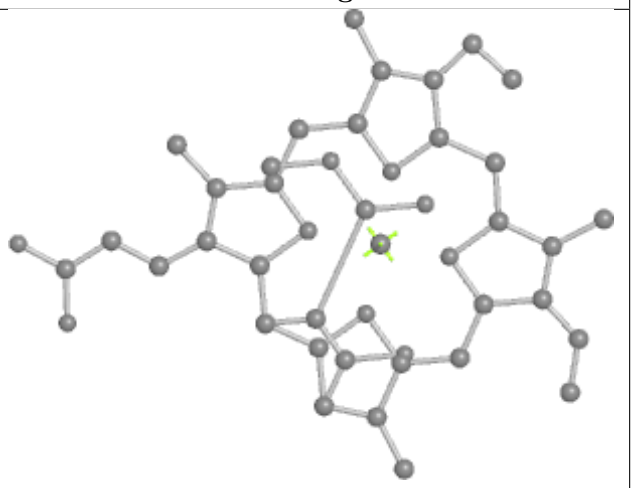
Bond lengths



Bond angles

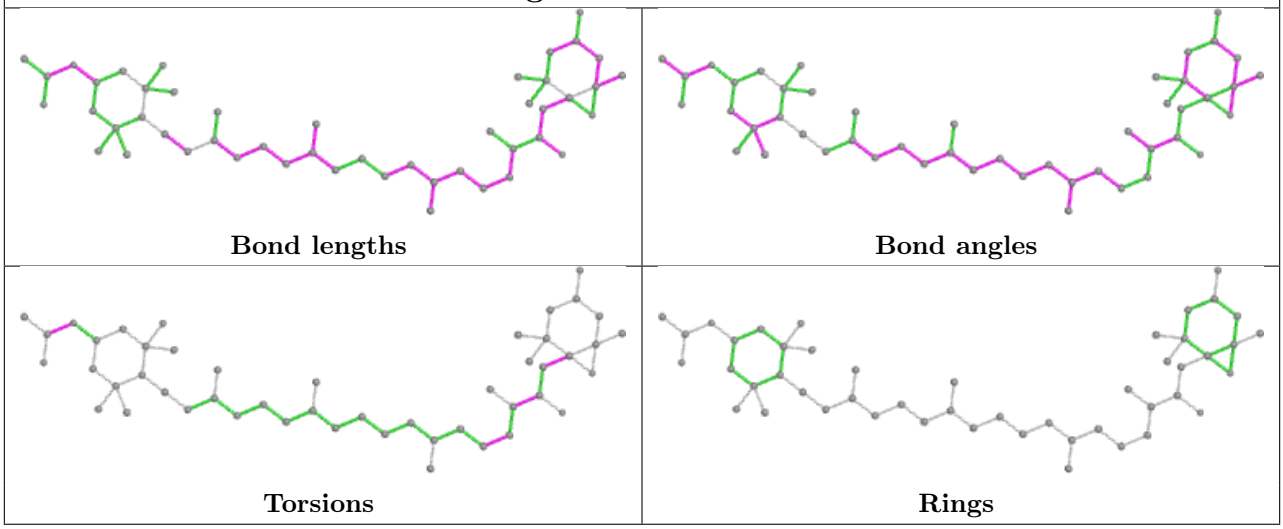


Torsions

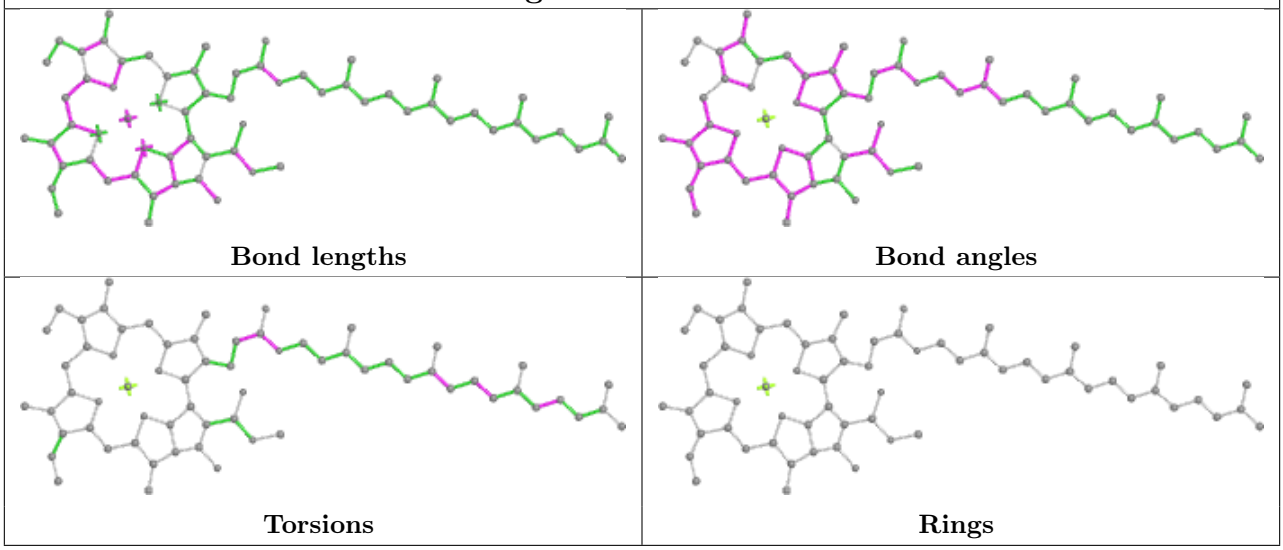


Rings

Ligand A86 16 314



Ligand CLA B 512



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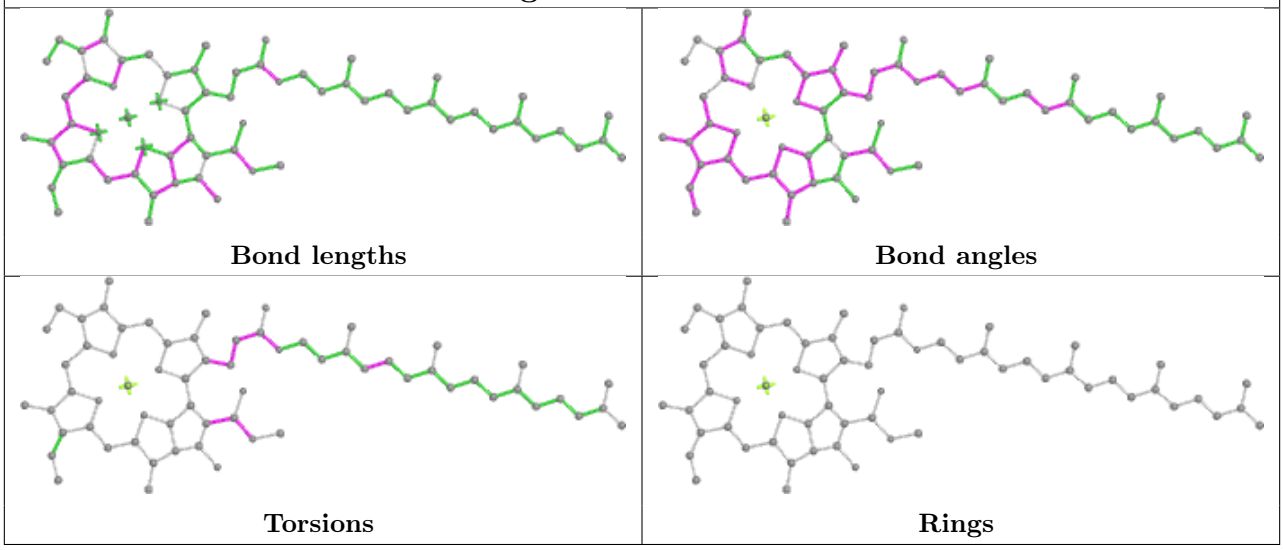

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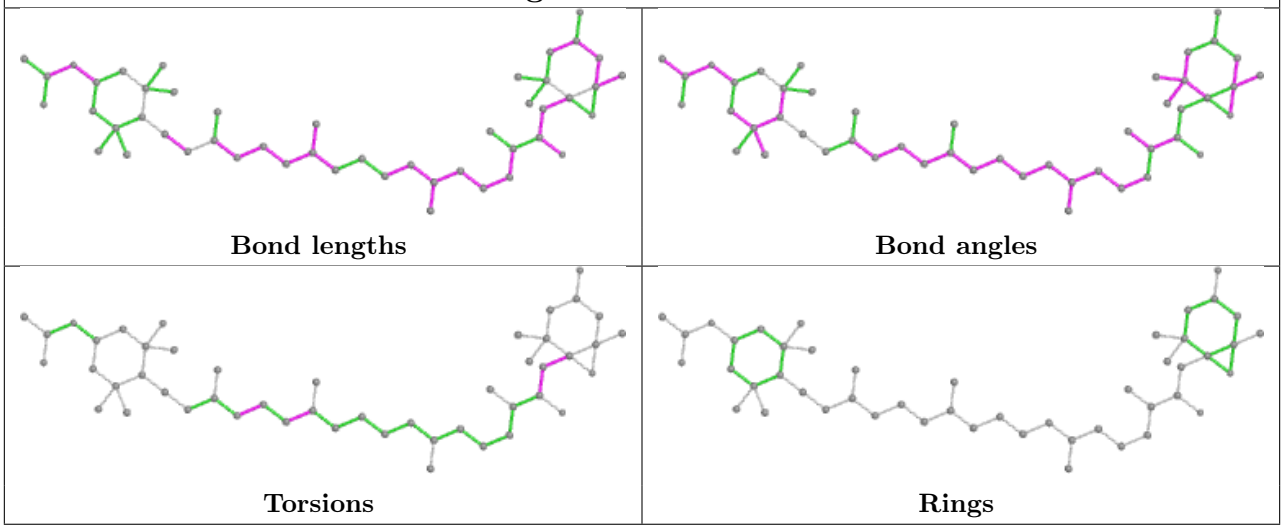

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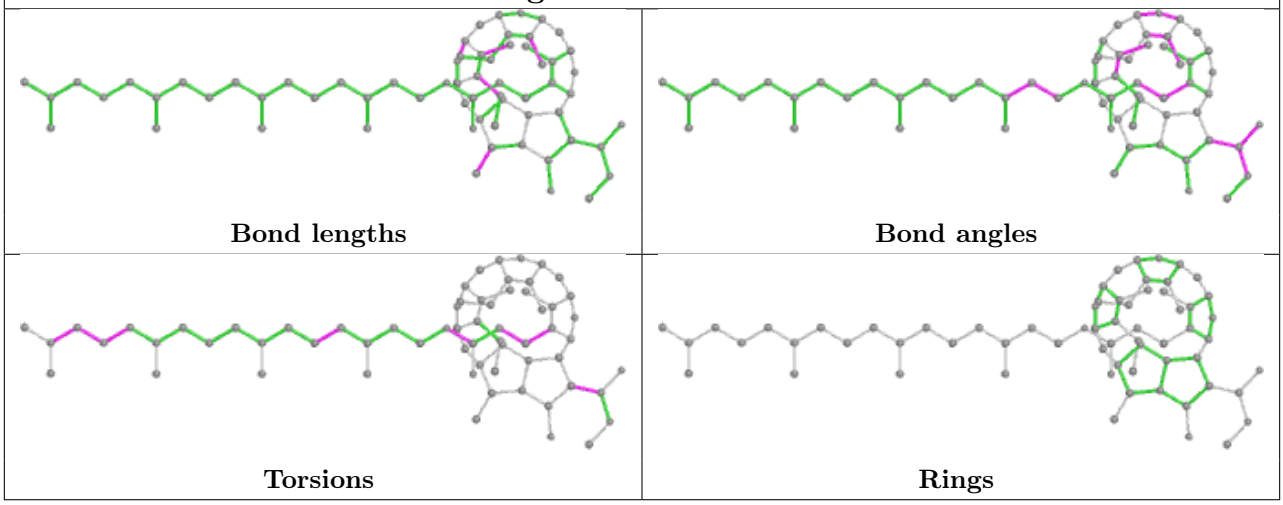

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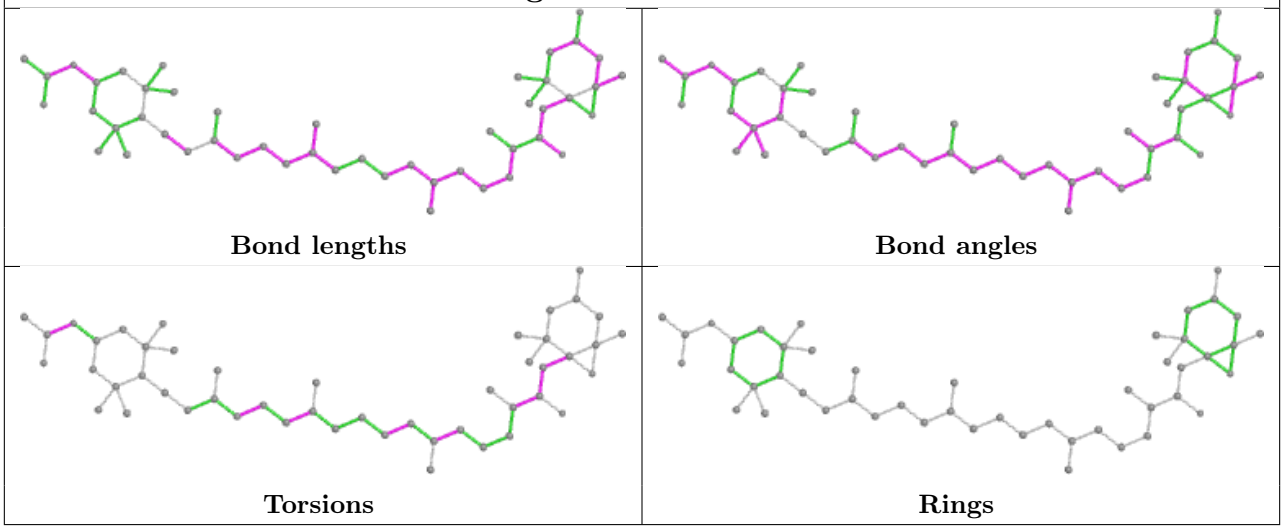

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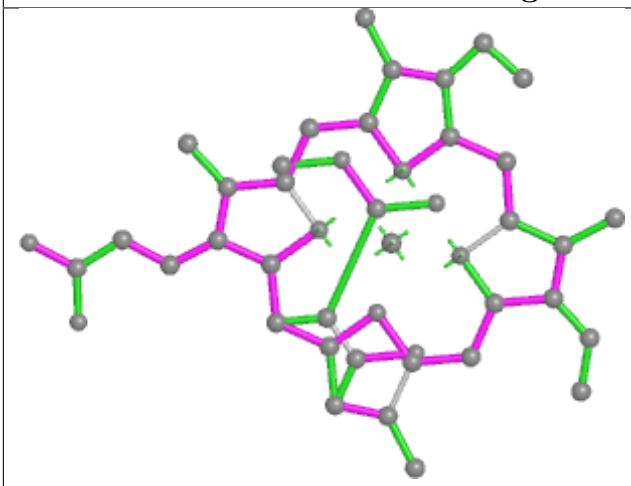

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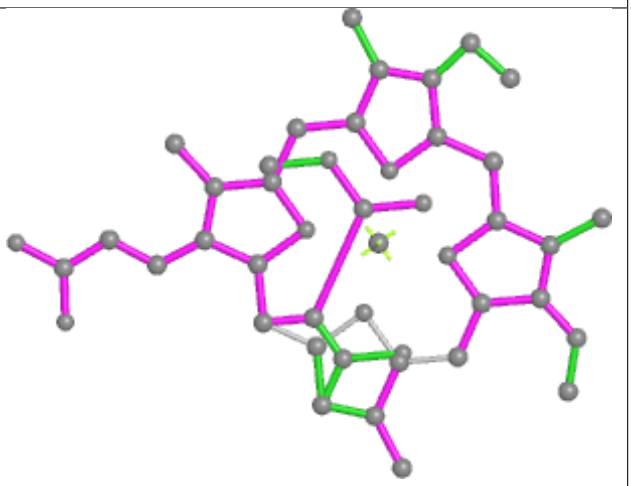
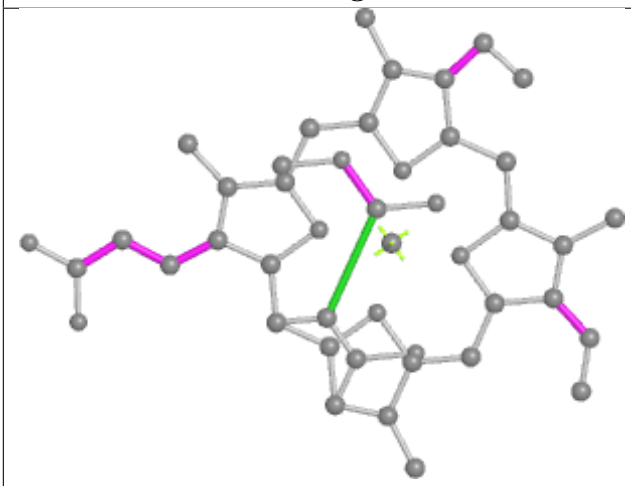
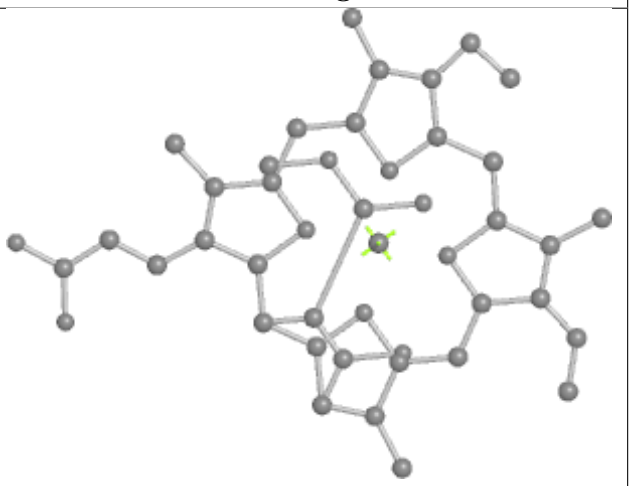


Bond angles

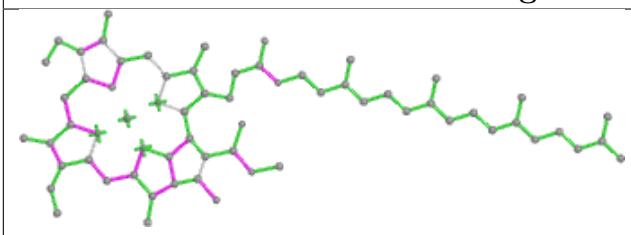


Torsions



Rings

Ligand CLA 12 205



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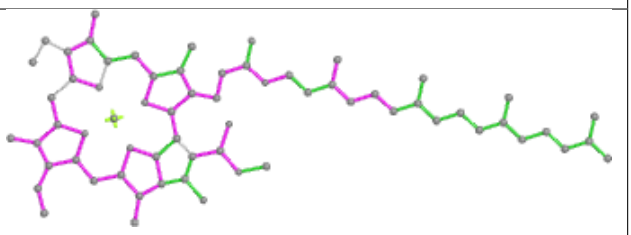

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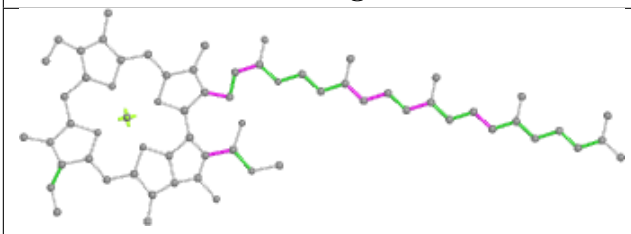

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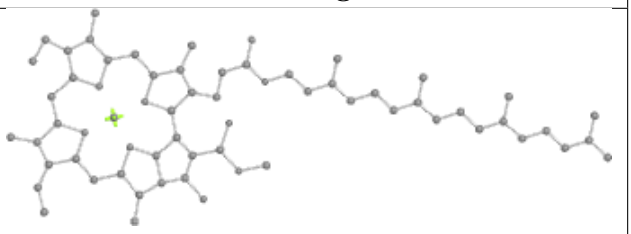

Rings

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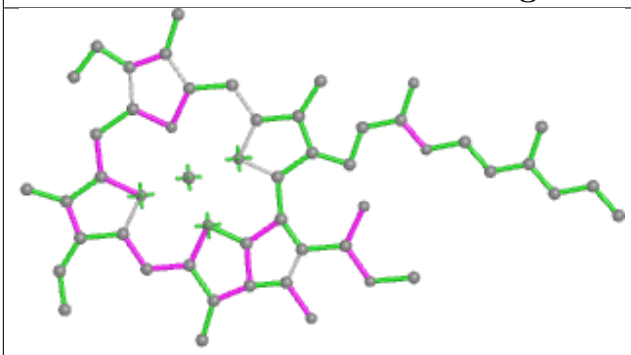
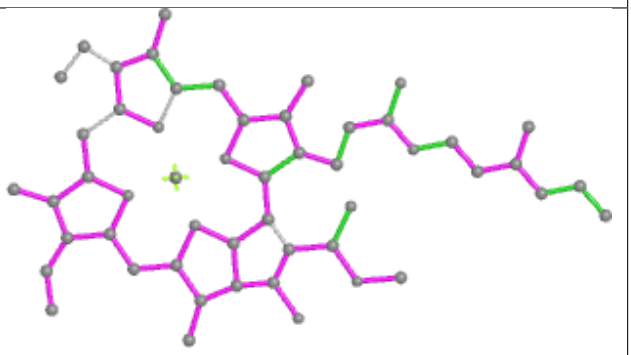
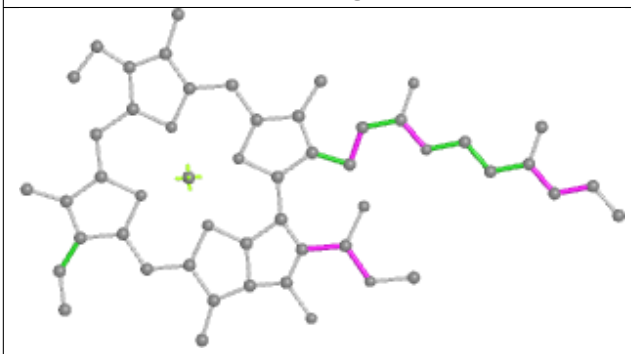
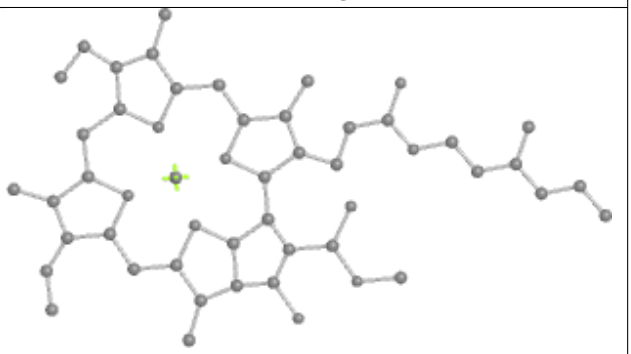
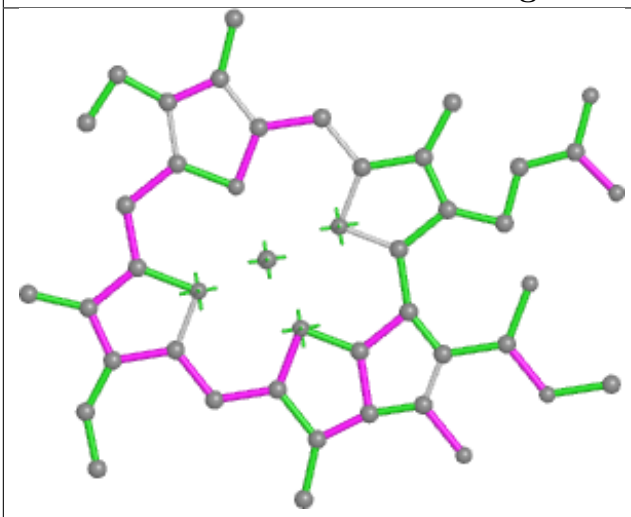
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 33 305



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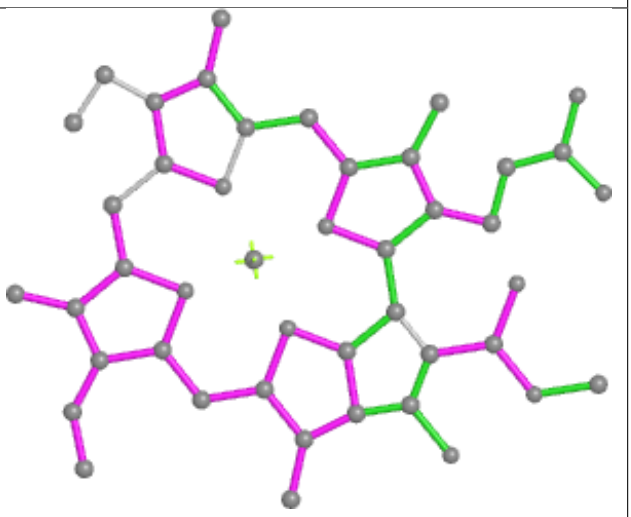
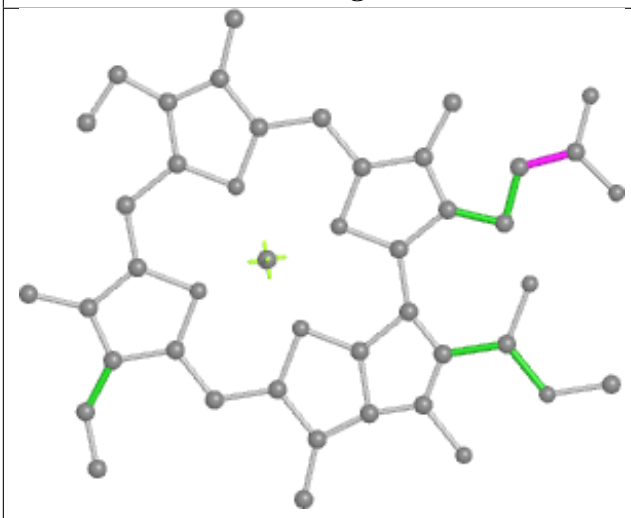


Bond angles



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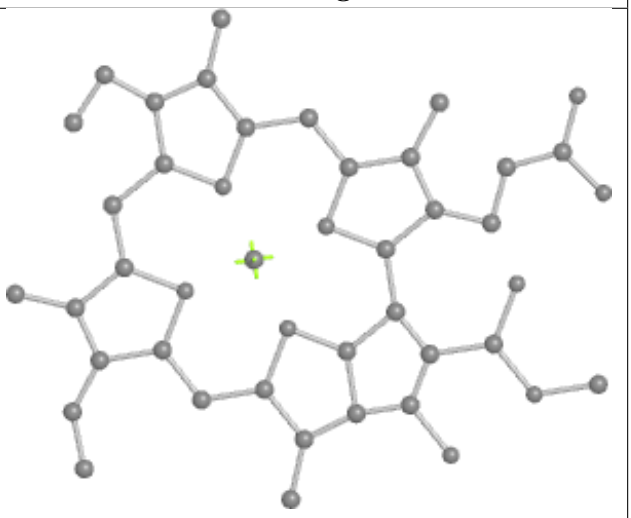
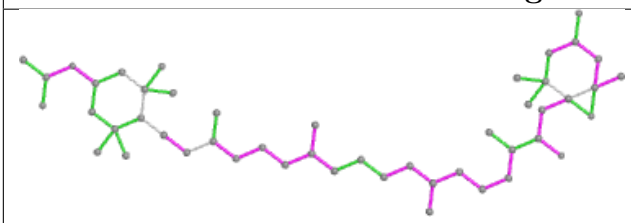


Rings

Ligand A86 38 214



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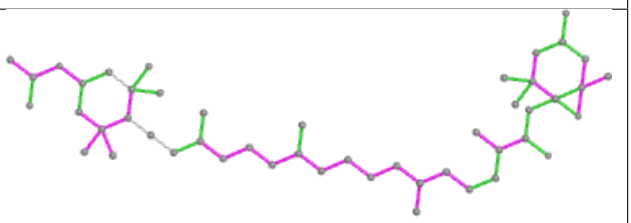

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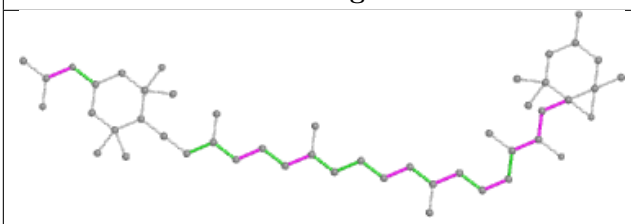

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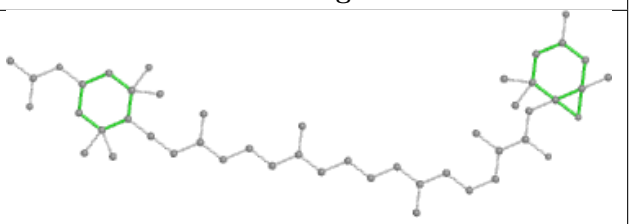

Rings

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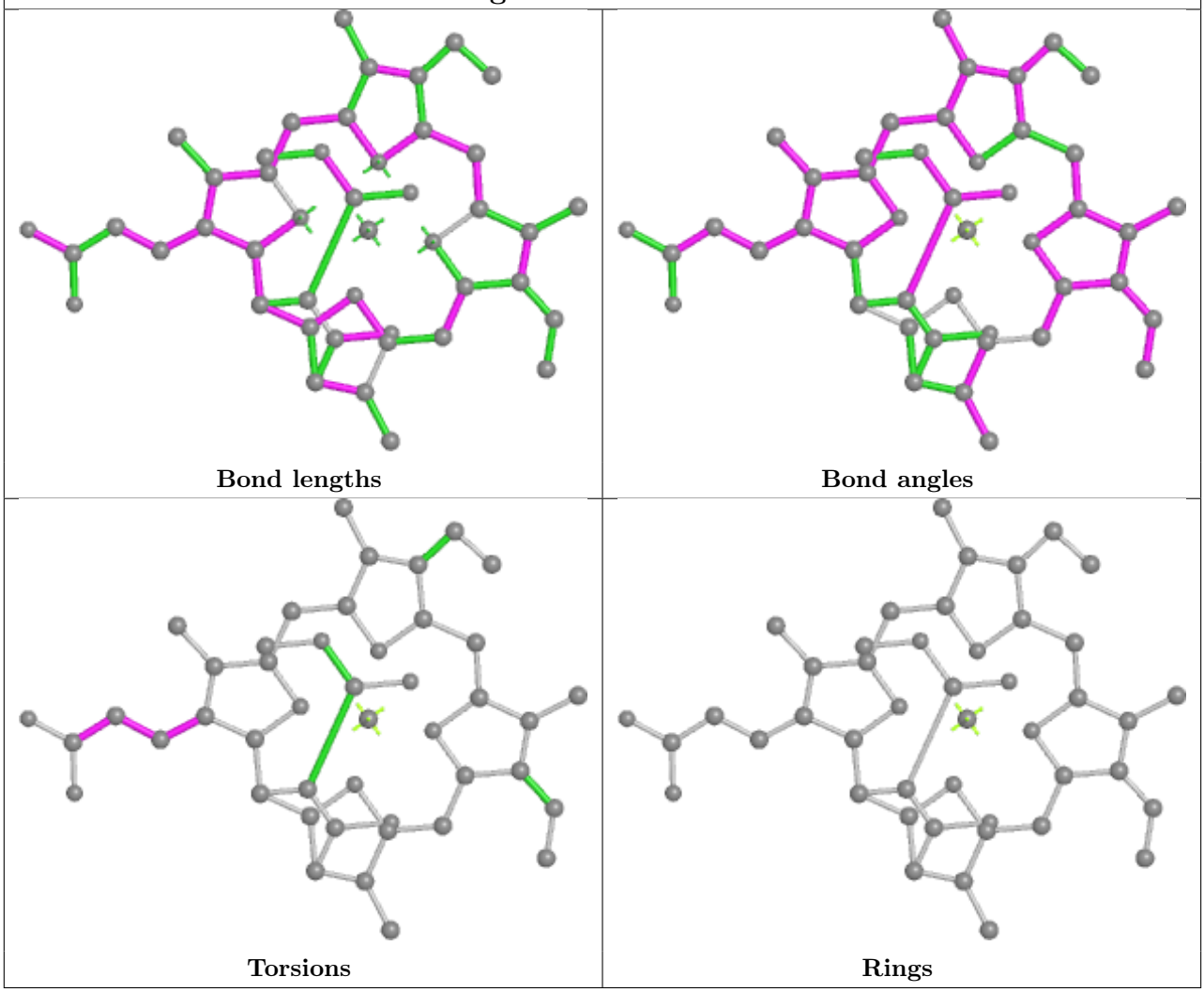

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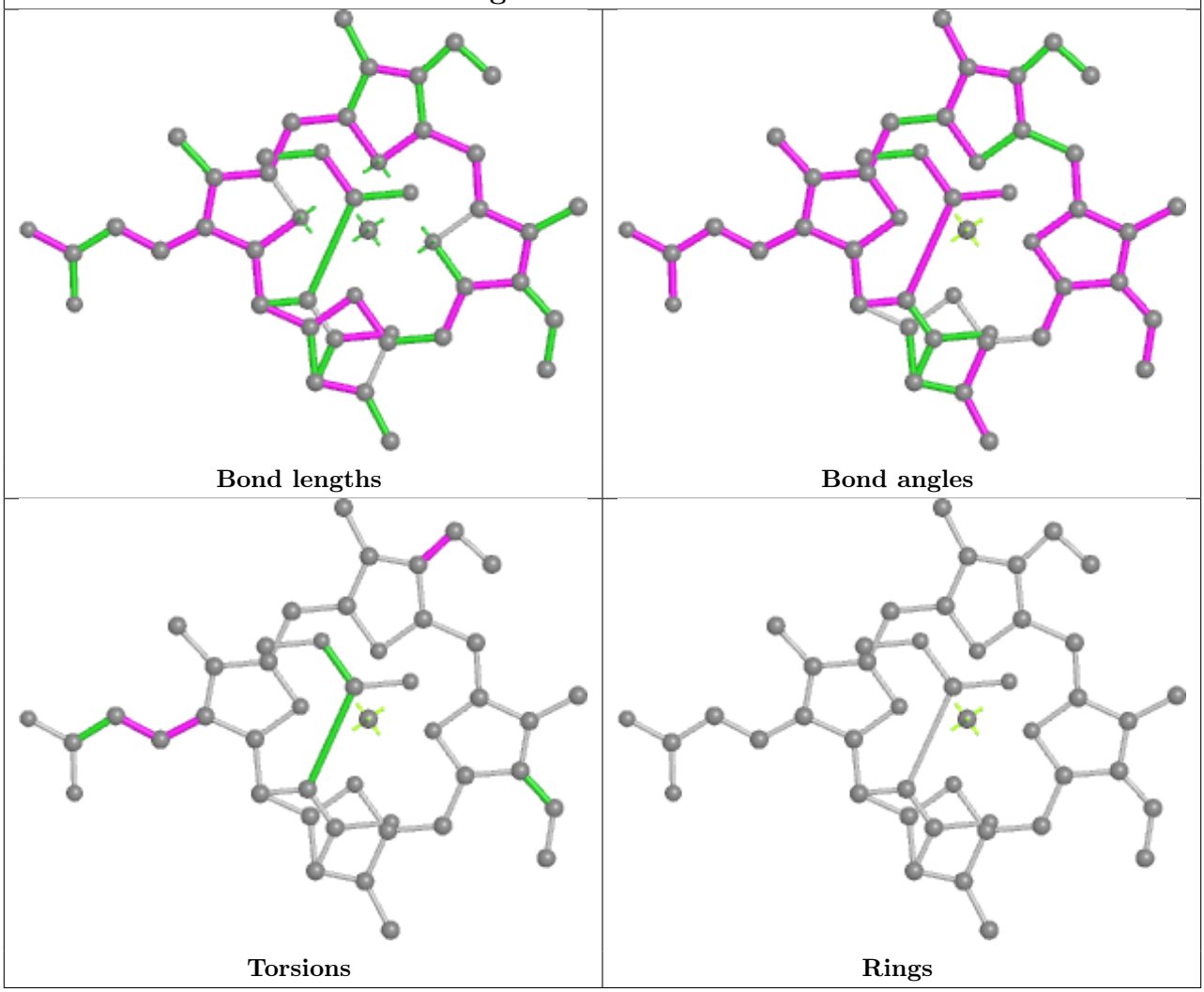

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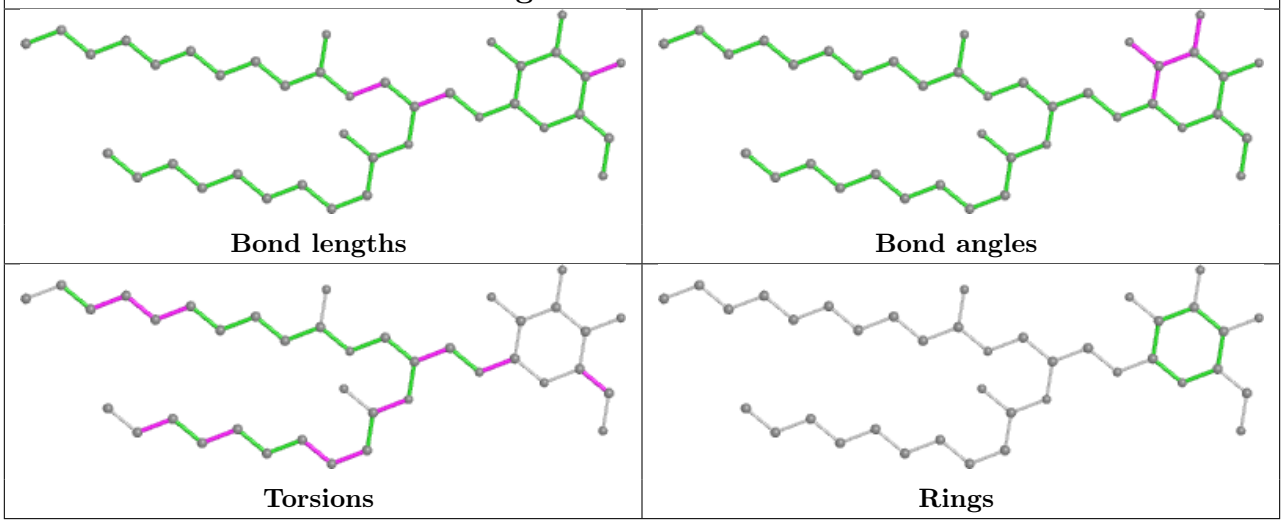

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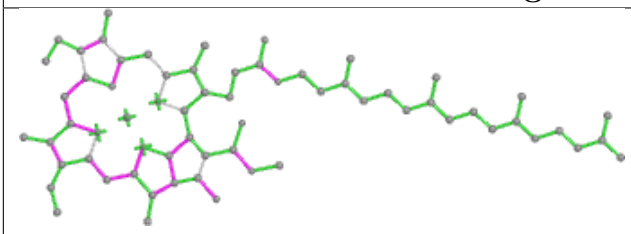
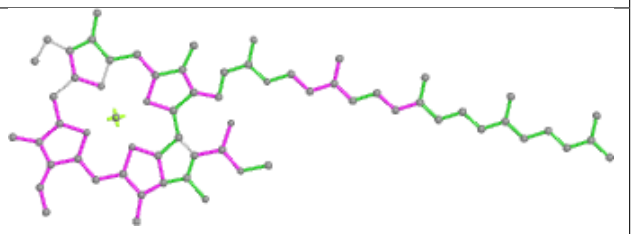
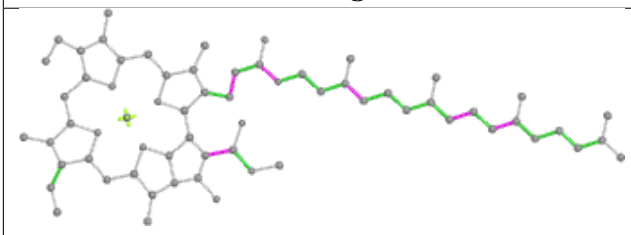
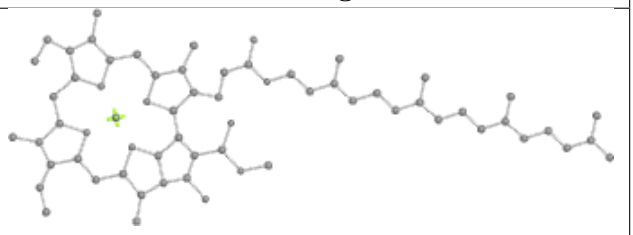
 Bond lengths	 Bond angles
 Torsions	 Rings

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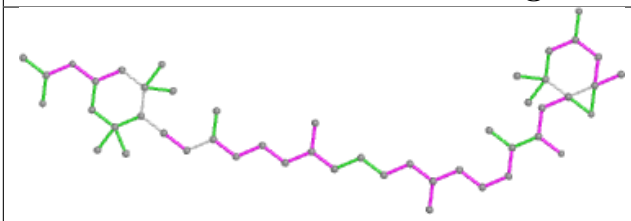
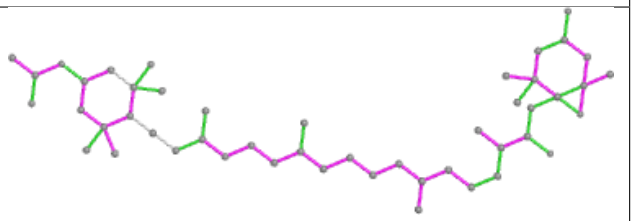
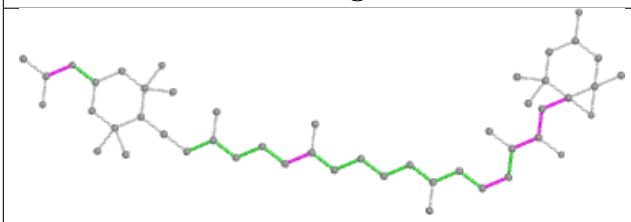
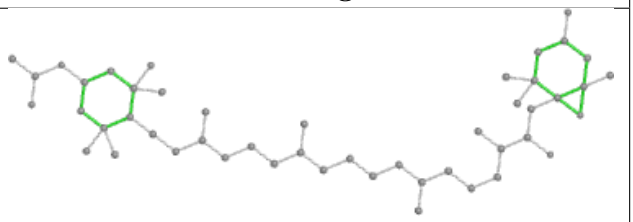
 Bond lengths	 Bond angles
 Torsions	 Rings

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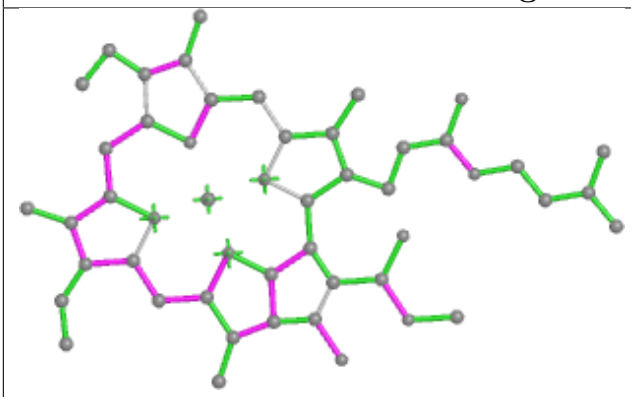
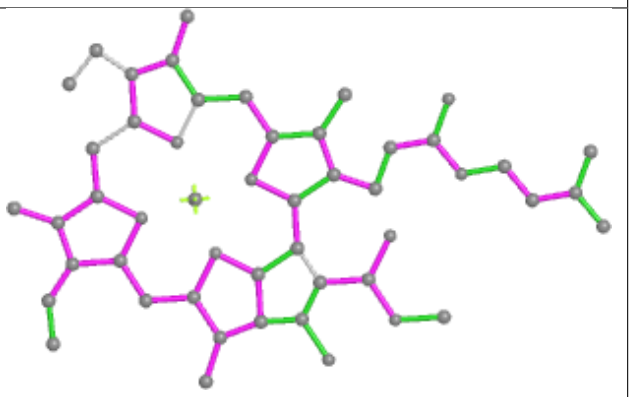
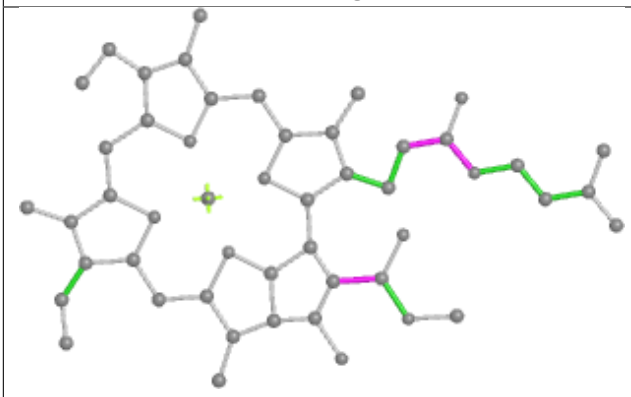
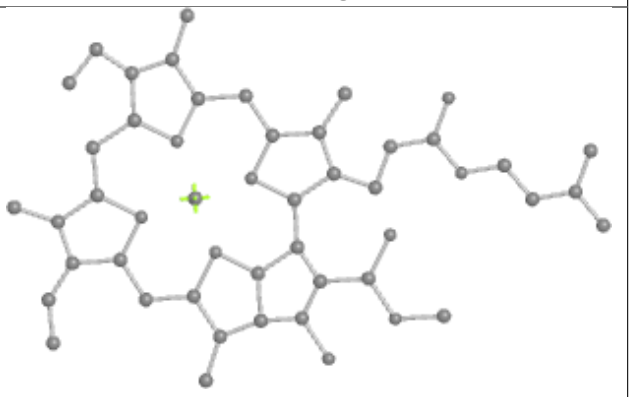
 Bond lengths	 Bond angles
 Torsions	 Rings

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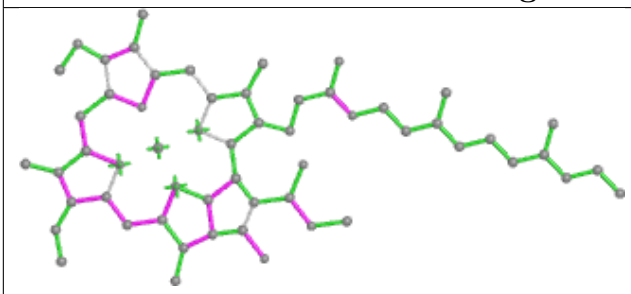
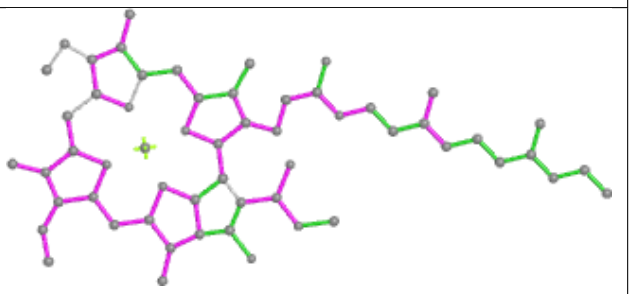
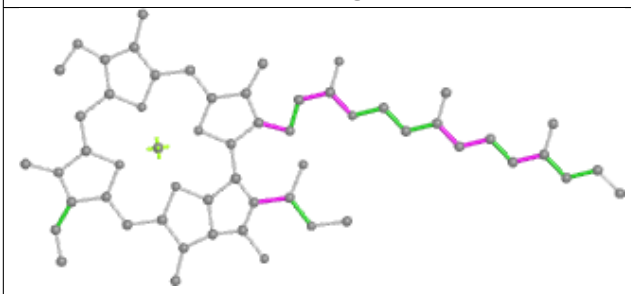
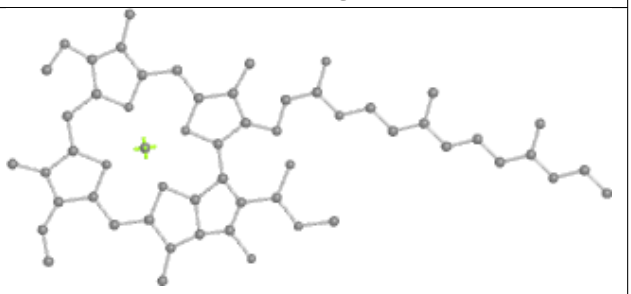
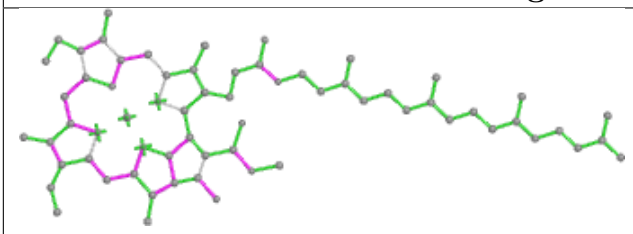
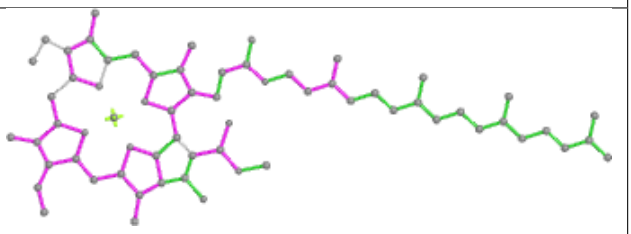
 Bond lengths	 Bond angles
 Torsions	 Rings

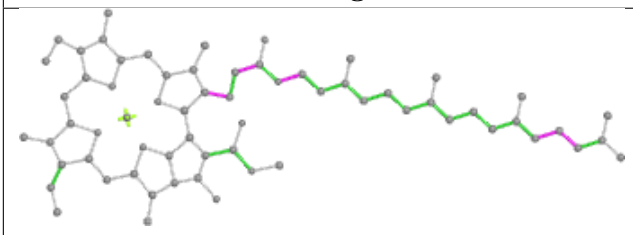
Ligand CLA d 403



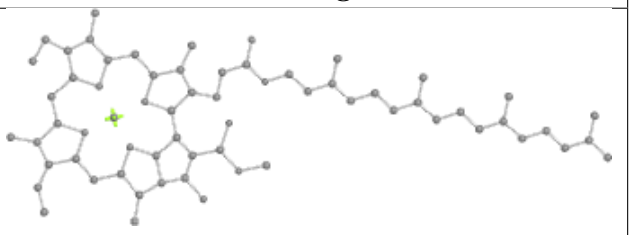
Bond lengths



Bond angles

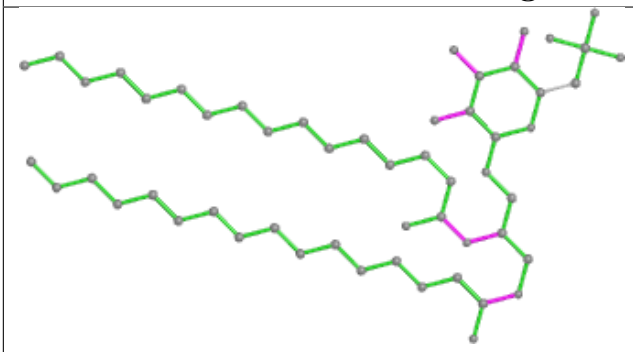


Torsions



Rings

Ligand SQD 40 202



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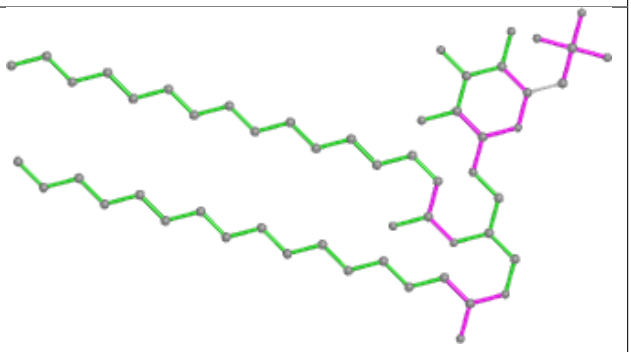

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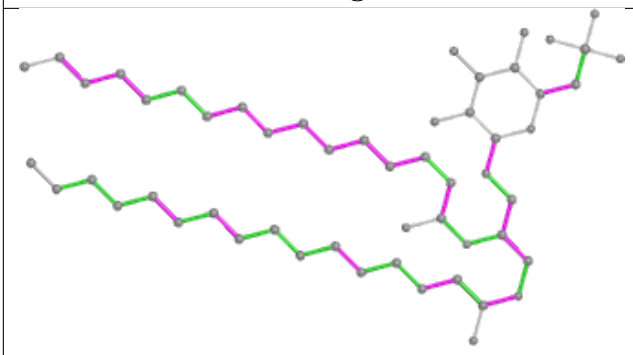

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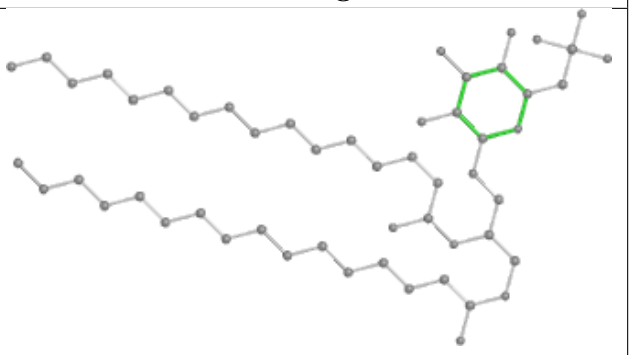
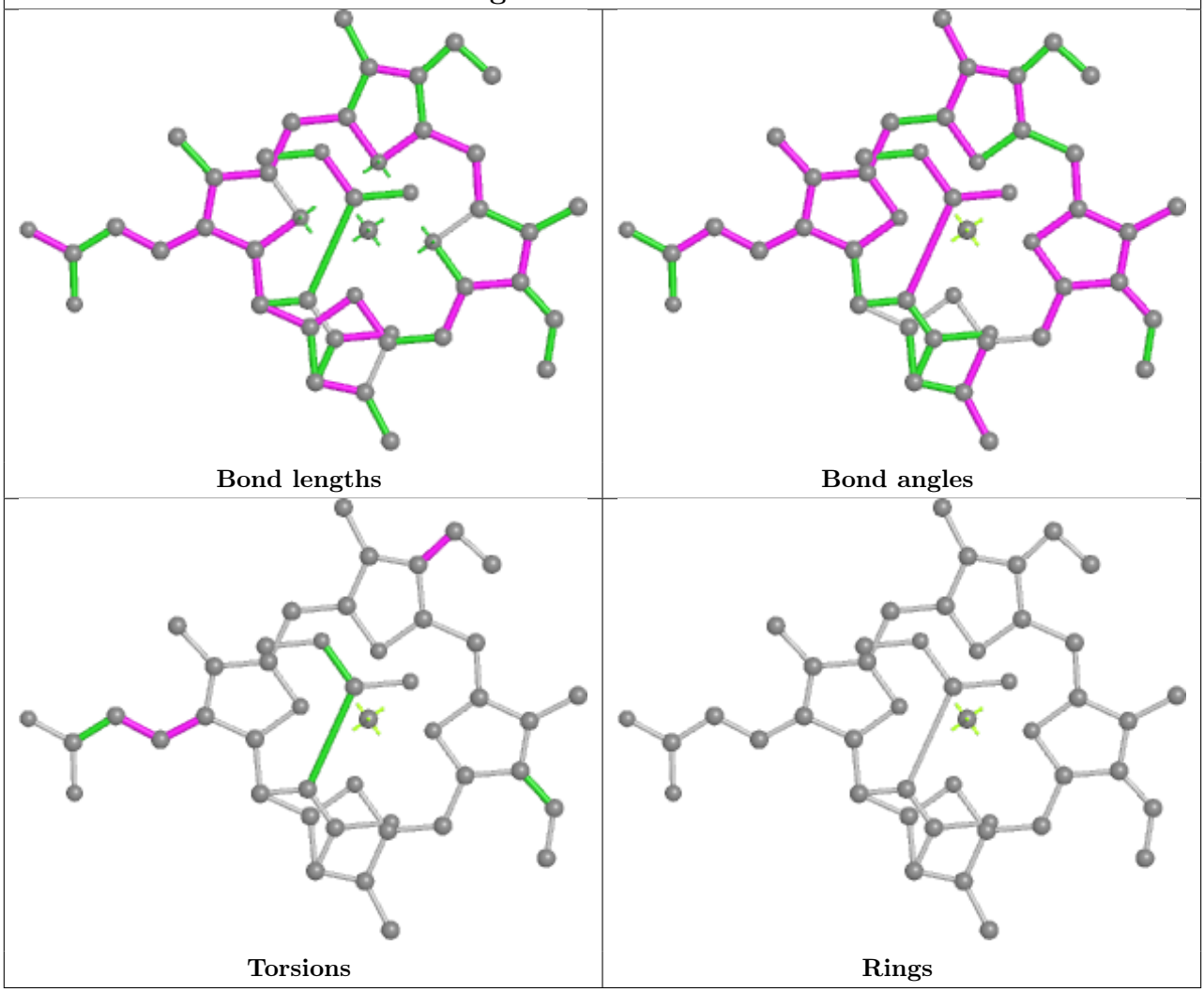


Rings

Ligand KC1 11 304



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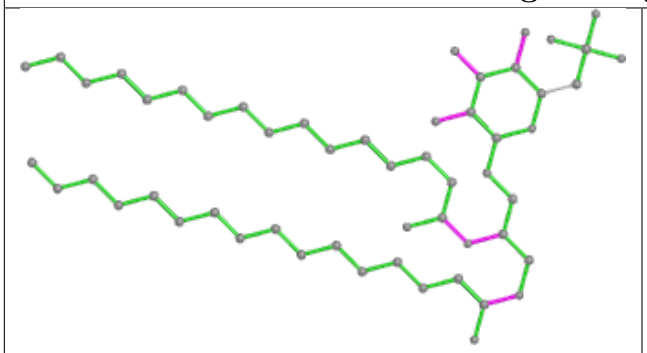

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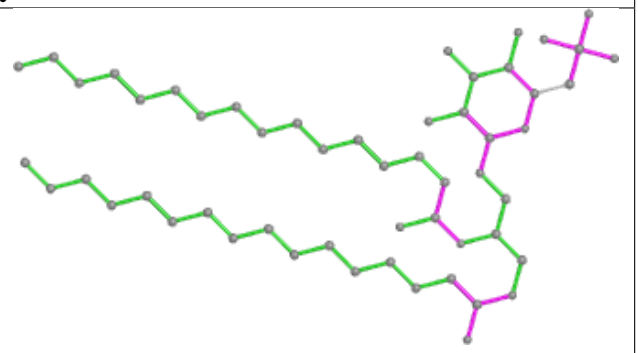

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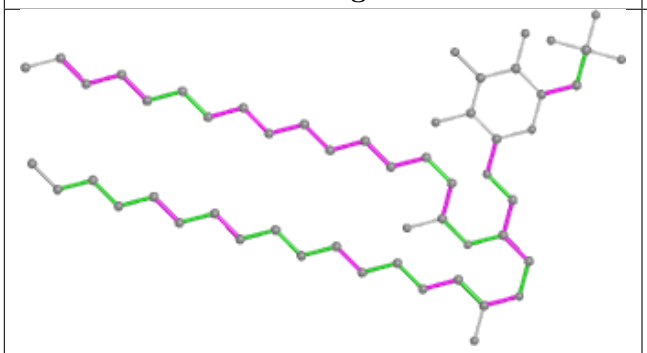

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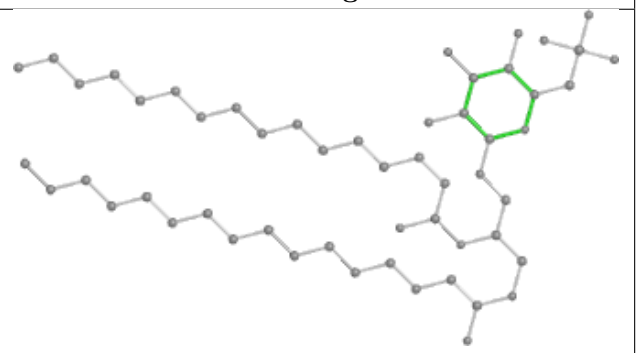

Rings

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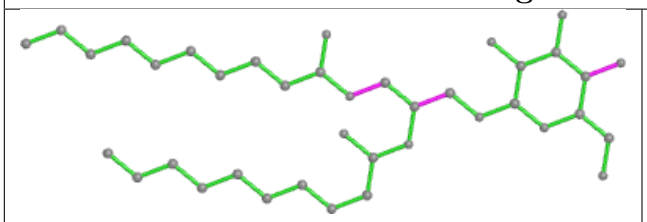

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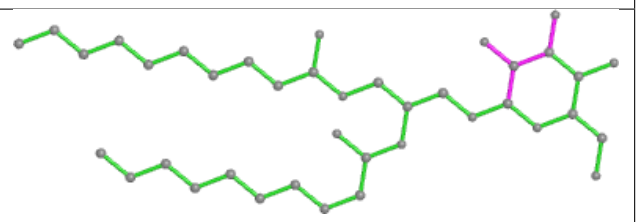

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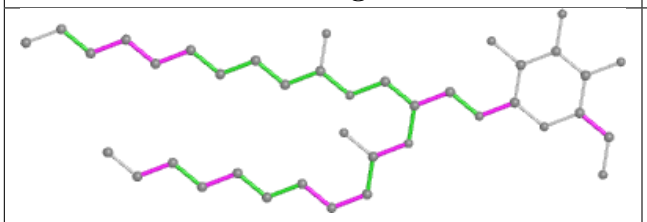

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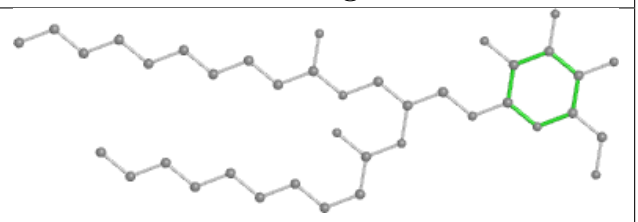

Rings

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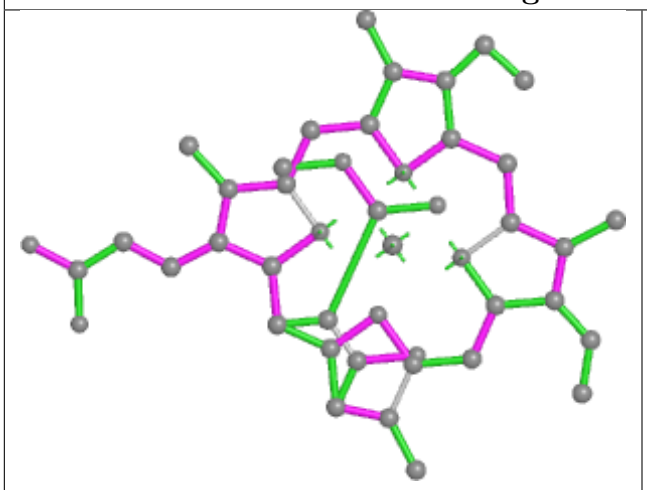

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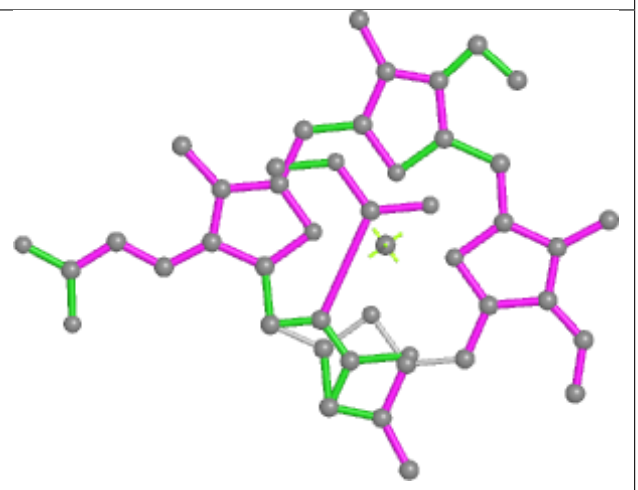

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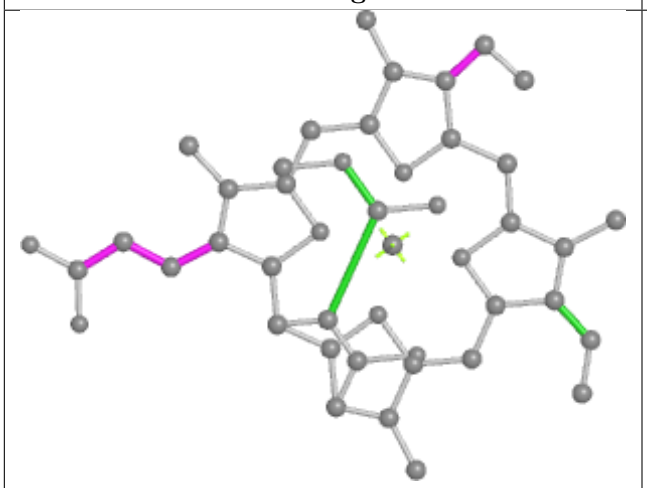

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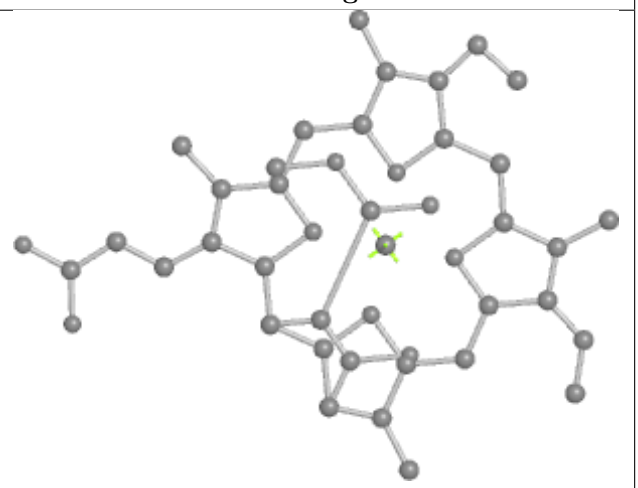
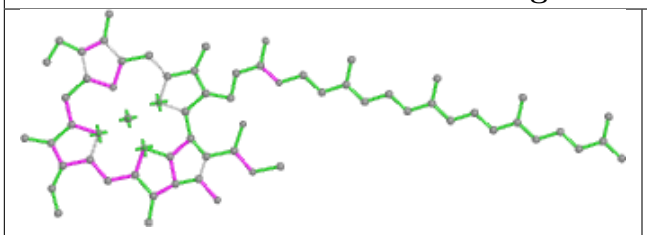


Rings

Ligand CLA c 503



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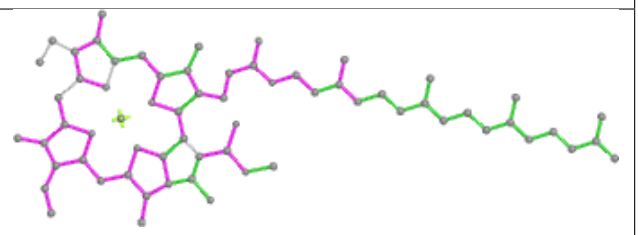

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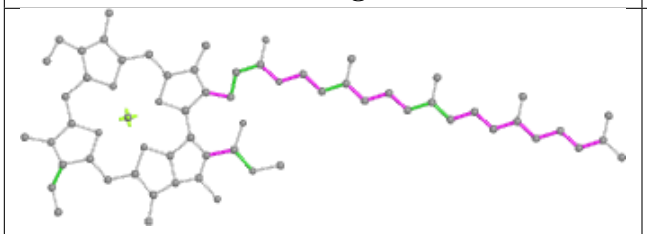

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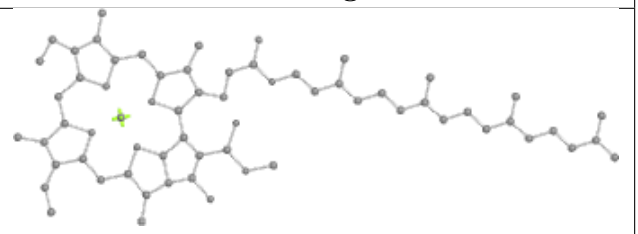

Rings

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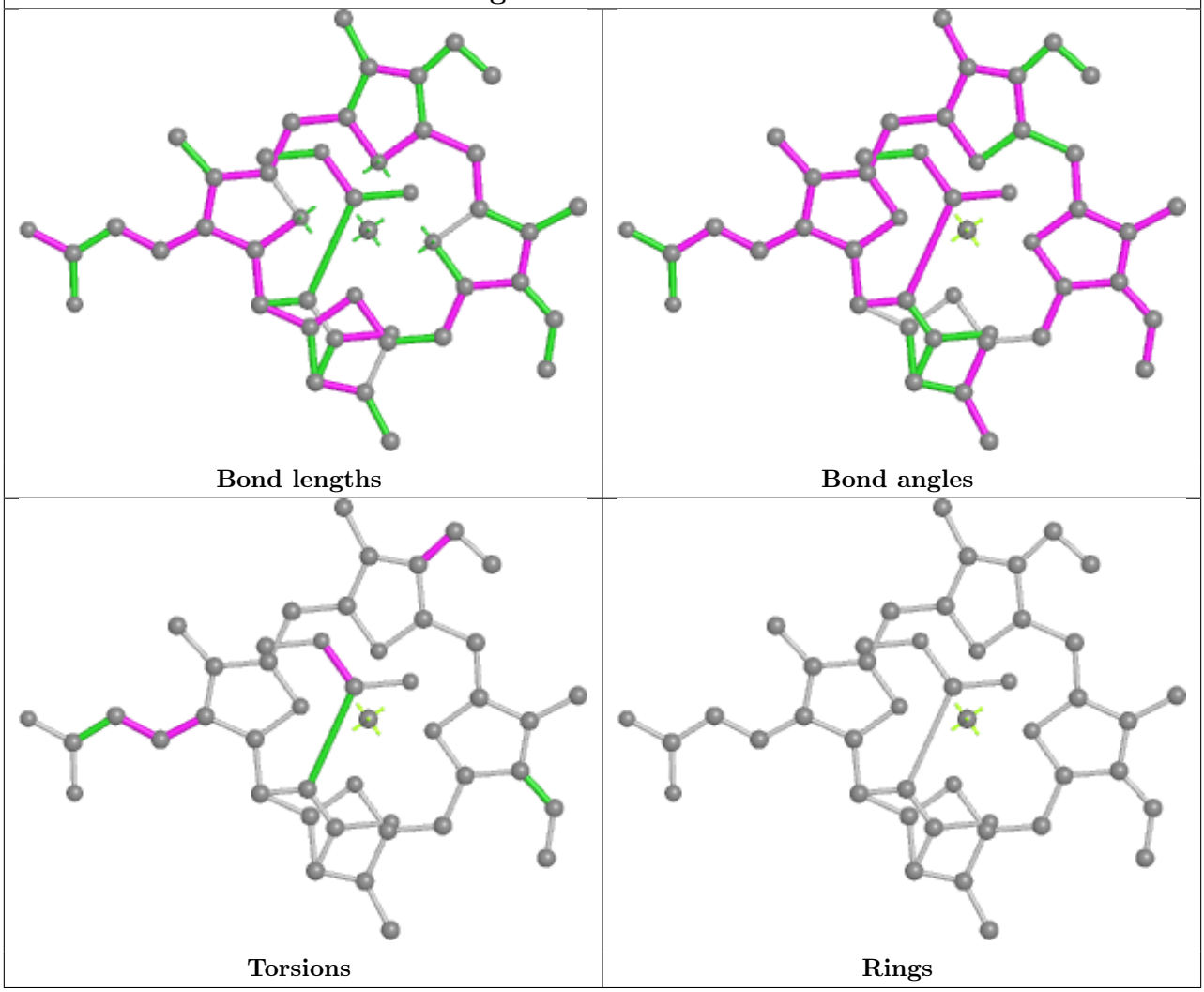

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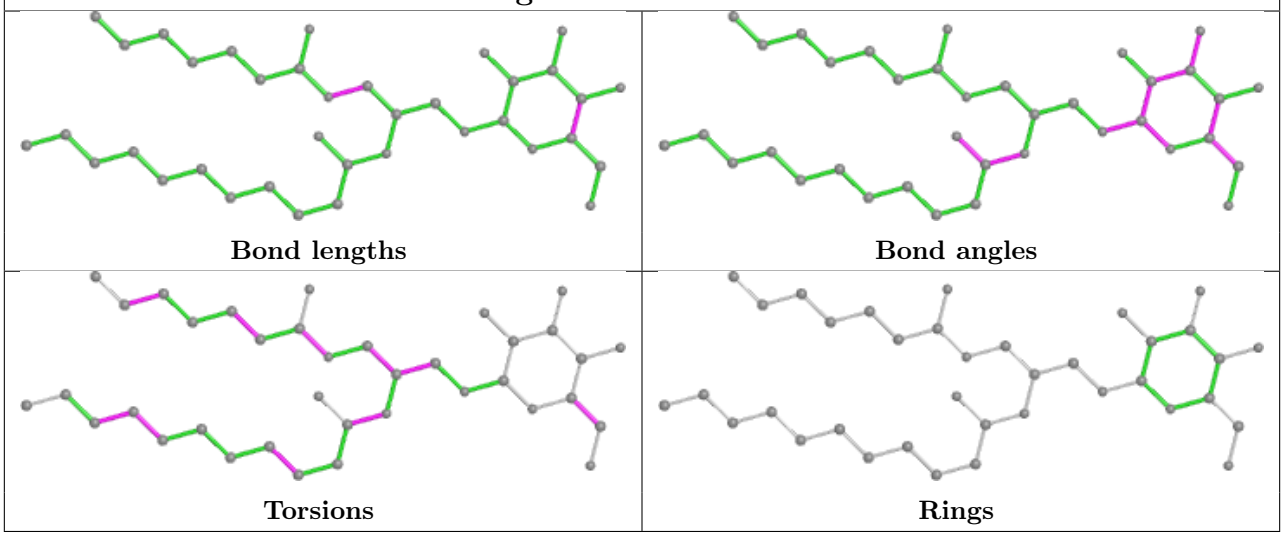

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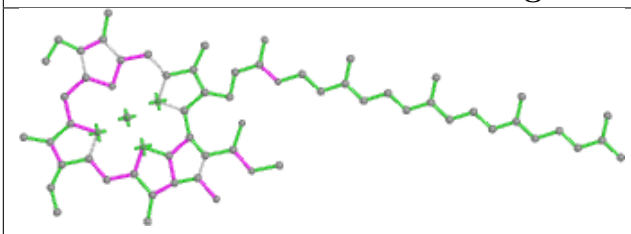

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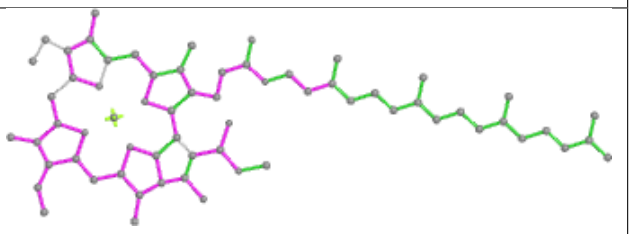

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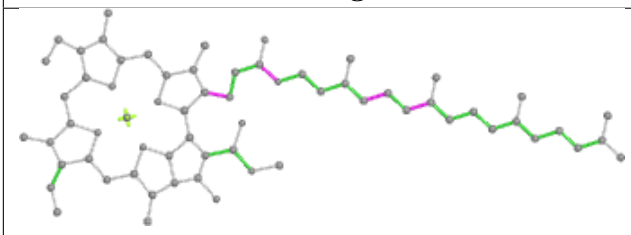

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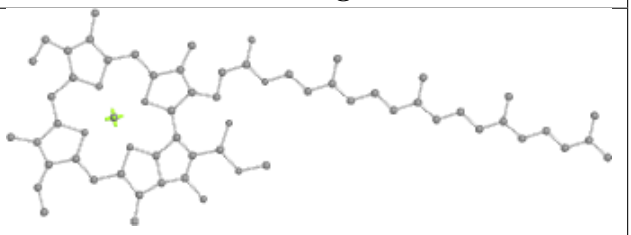

Rings

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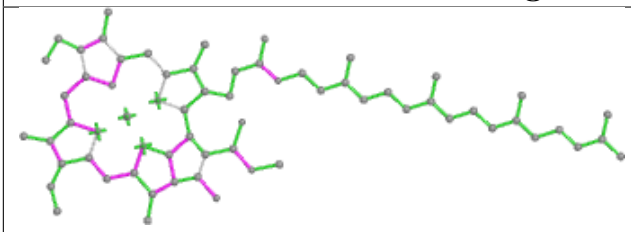

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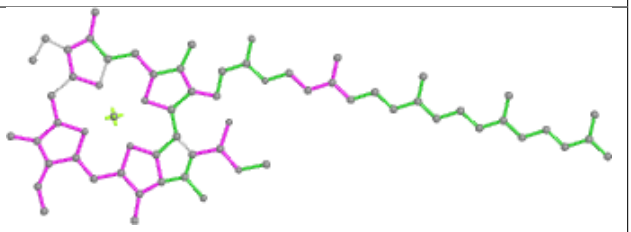
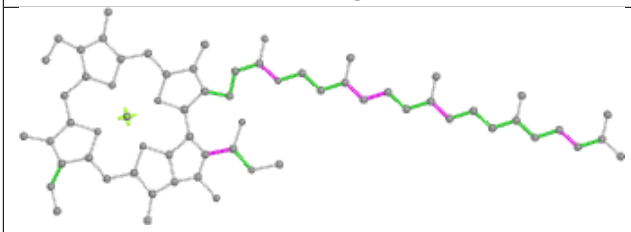


Bond angles



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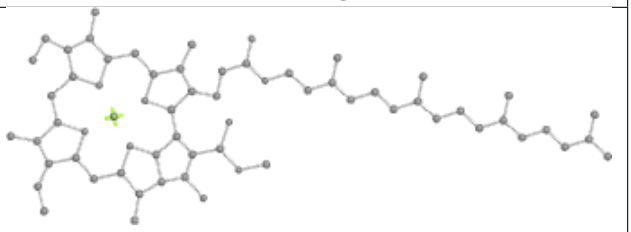

Rings

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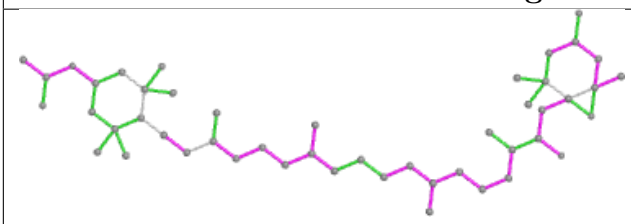

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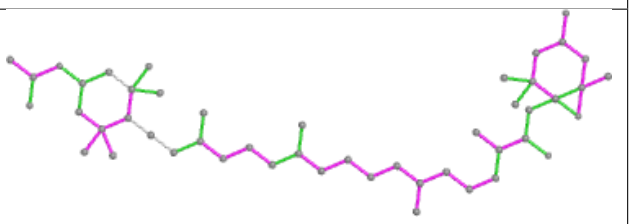

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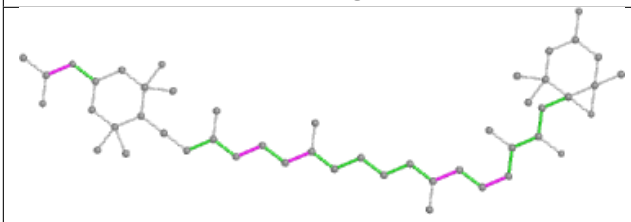

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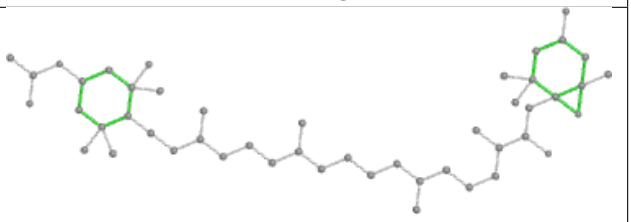

Rings

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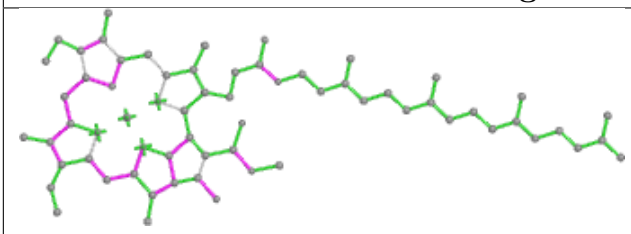
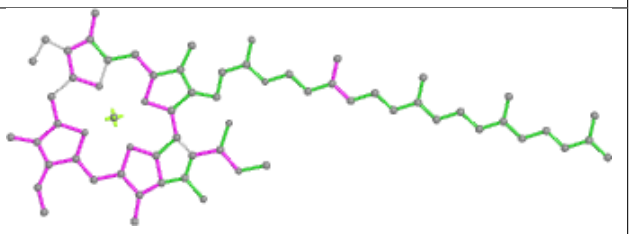
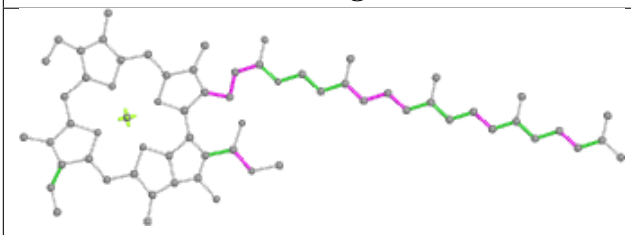
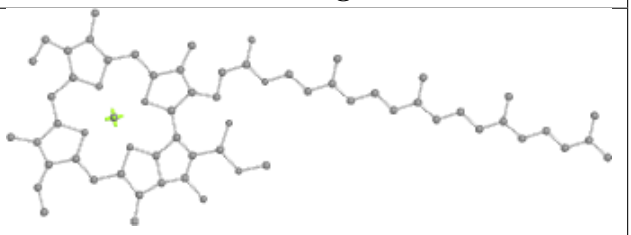
 Bond lengths	 Bond angles
 Torsions	 Rings

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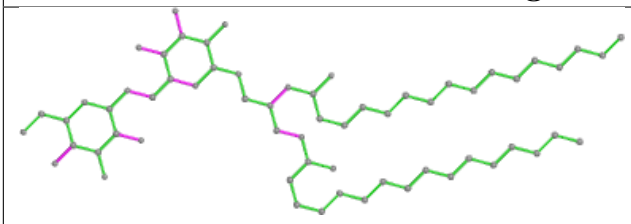
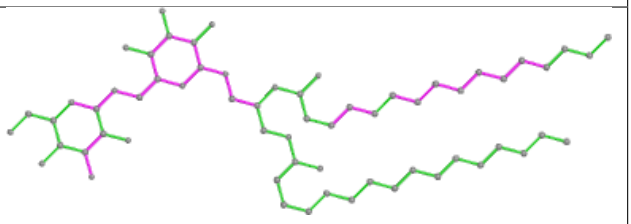
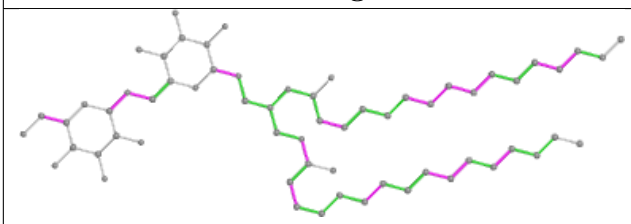
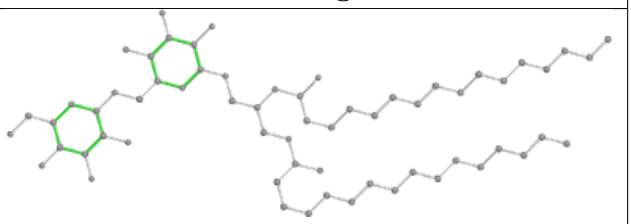
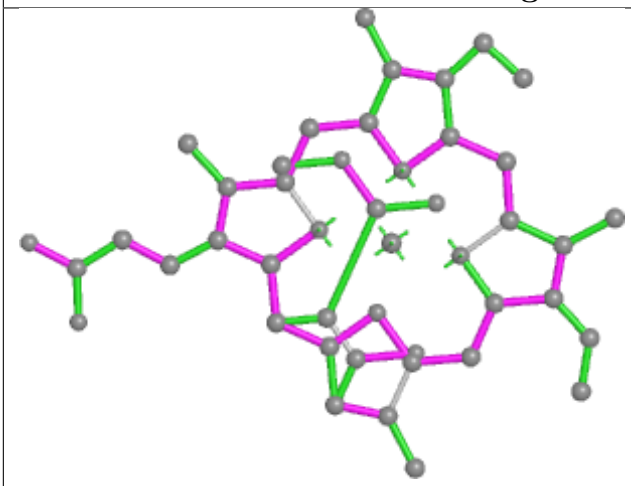
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 20 304



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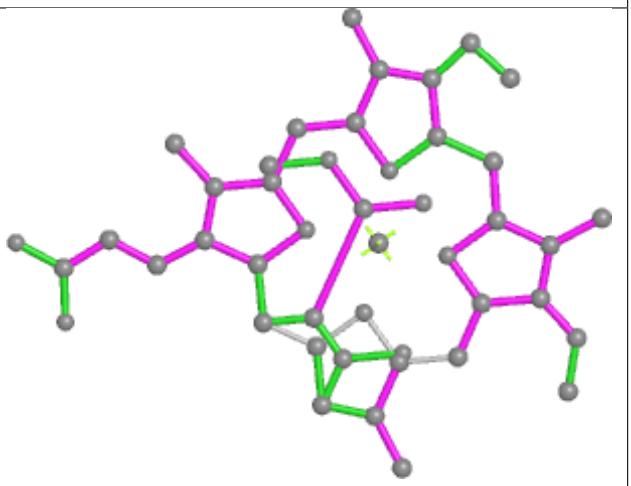

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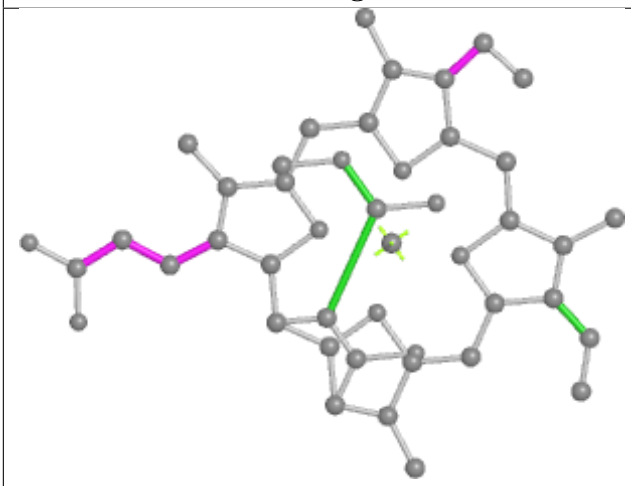

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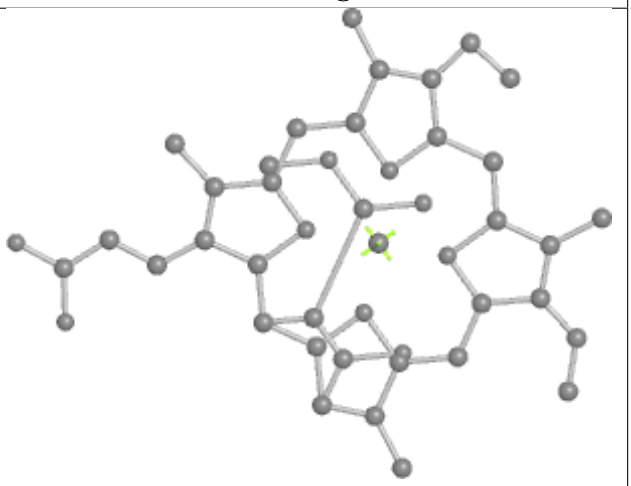
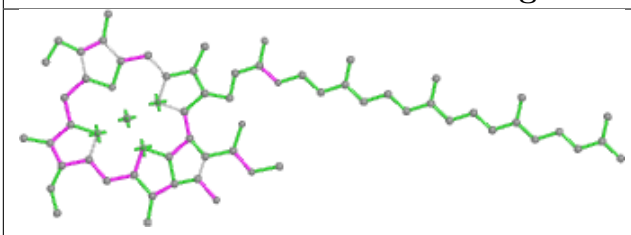


Rings

Ligand CLA 38 209



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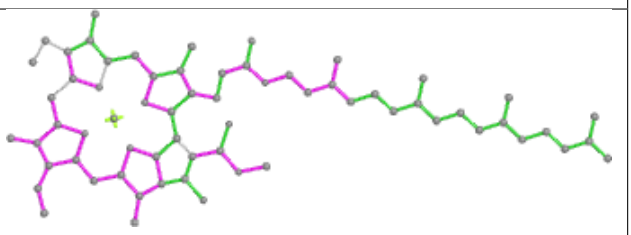
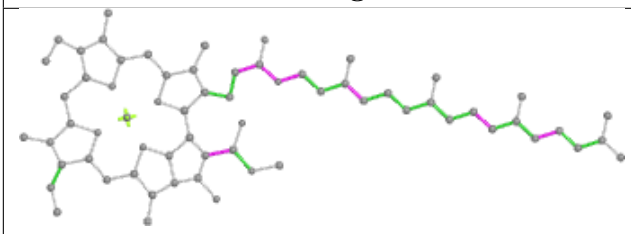


Bond angles



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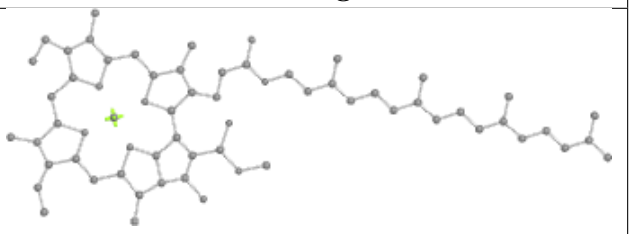

Rings

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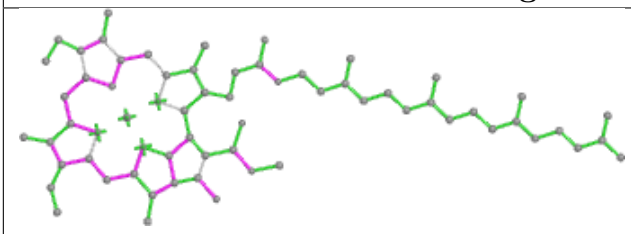
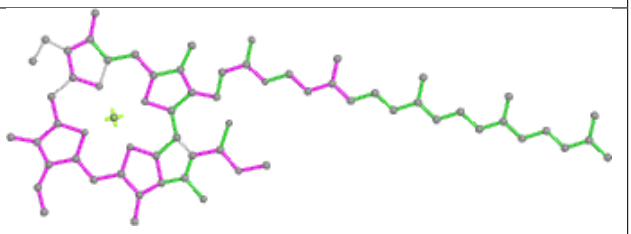
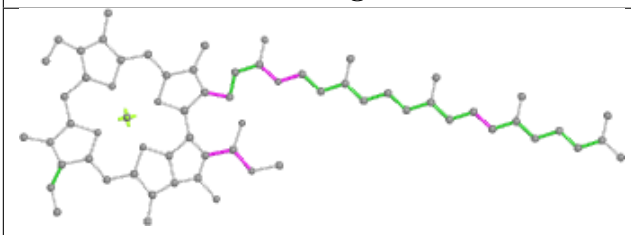


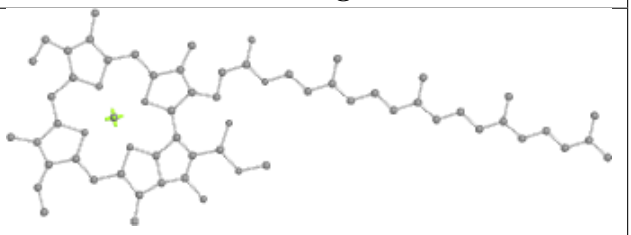
Bond lengths



Bond angles

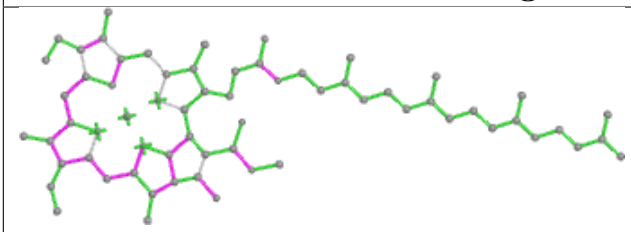


Torsions



Rings

Ligand CLA 38 201



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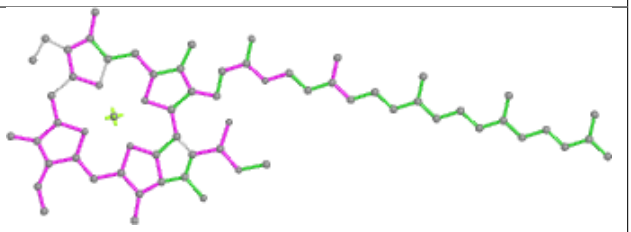

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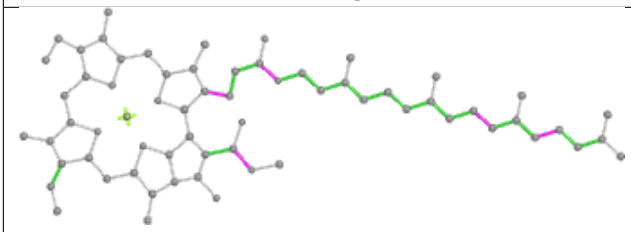

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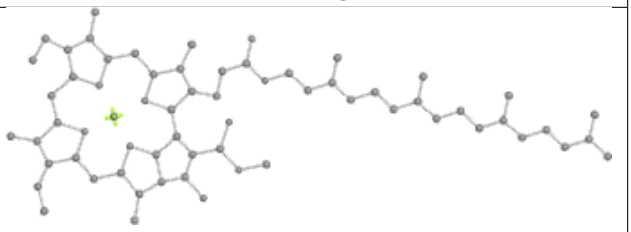
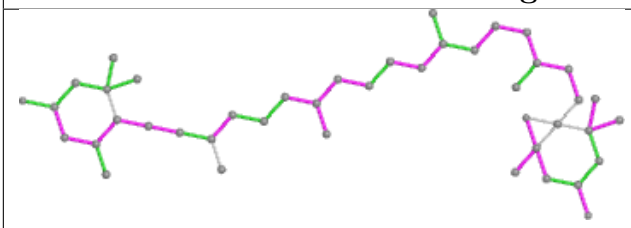


Rings

Ligand DD6 16 312



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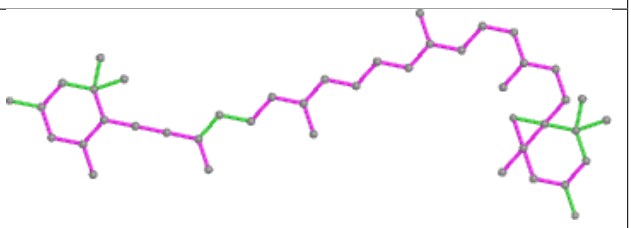

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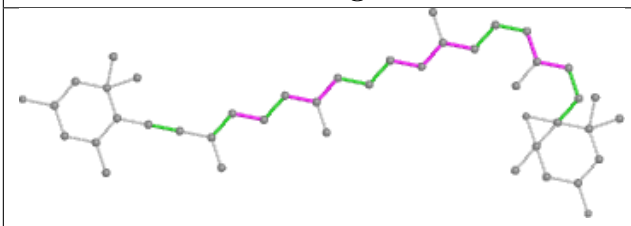

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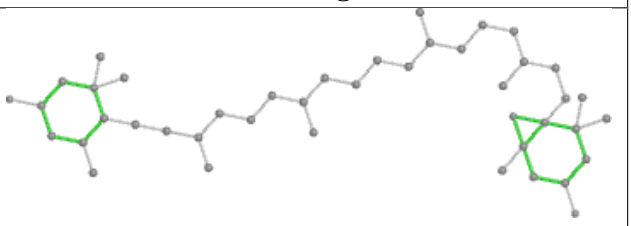
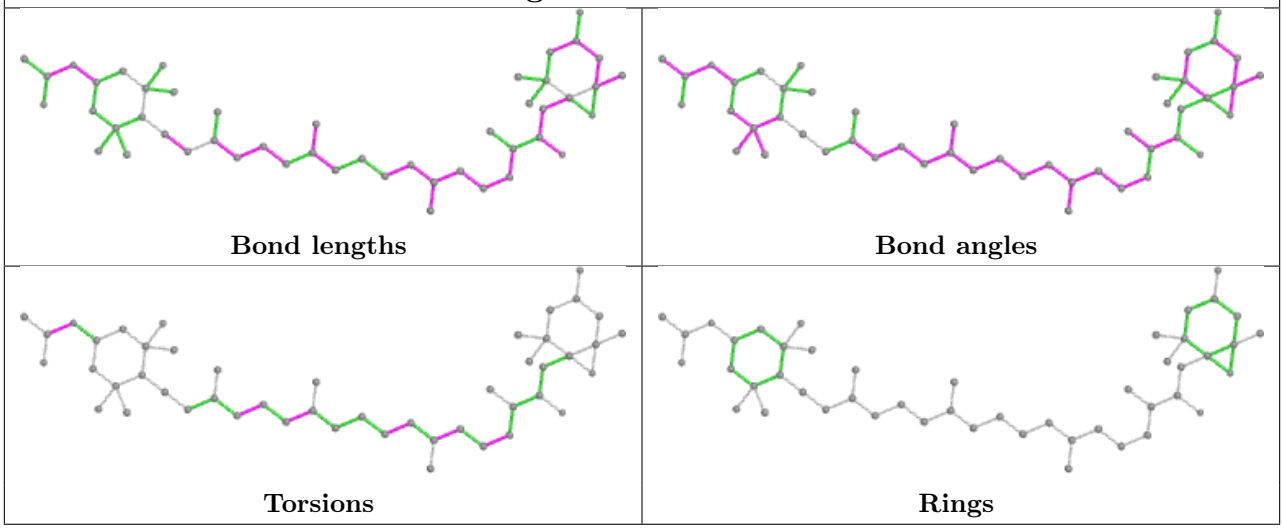
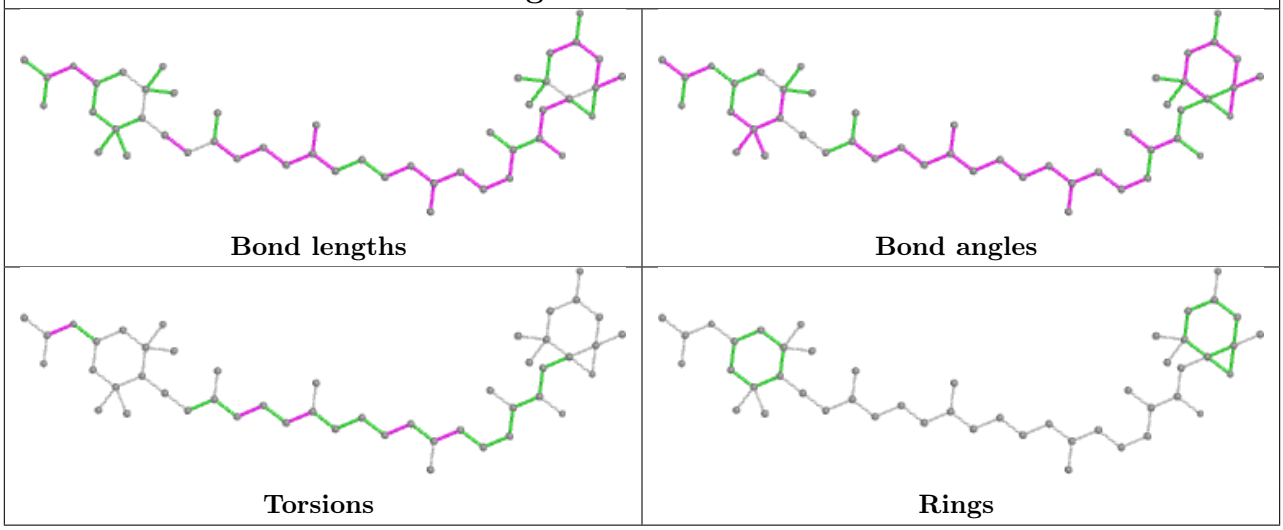


Rings

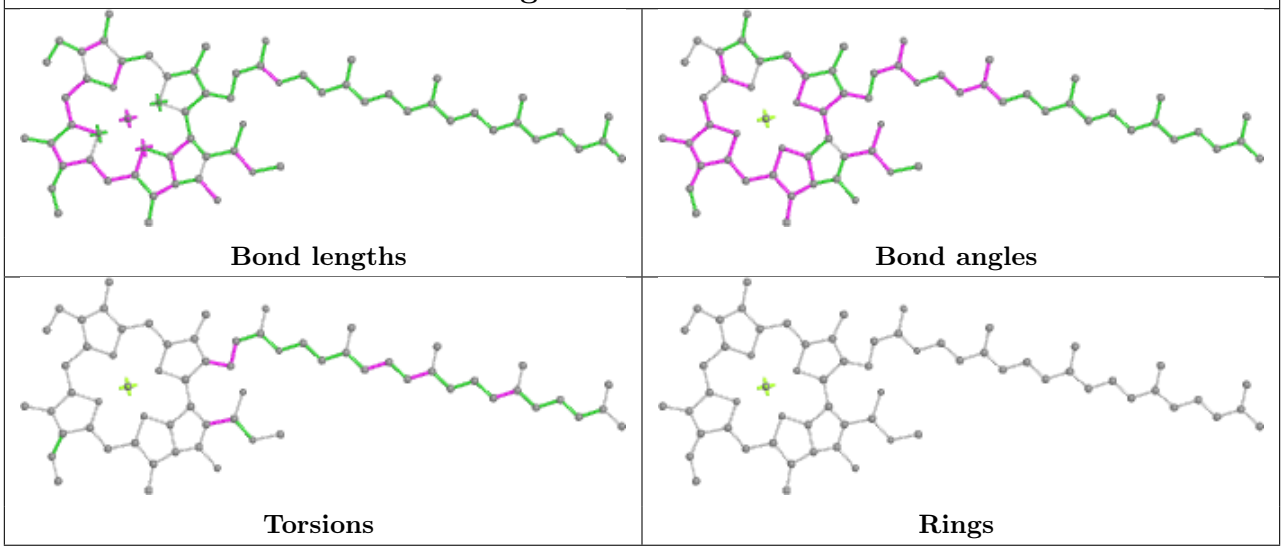
Ligand A86 12 220



Ligand A86 37 319



Ligand CLA 12 204



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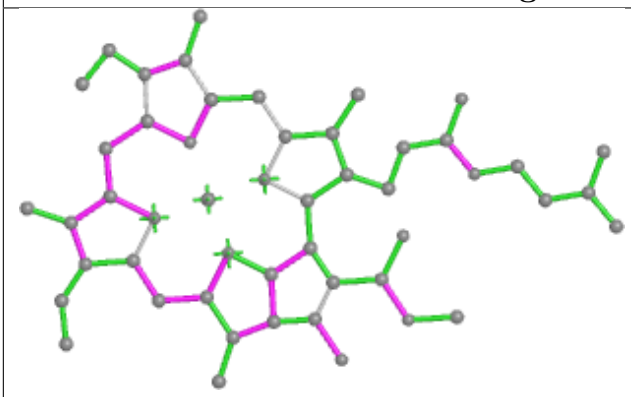
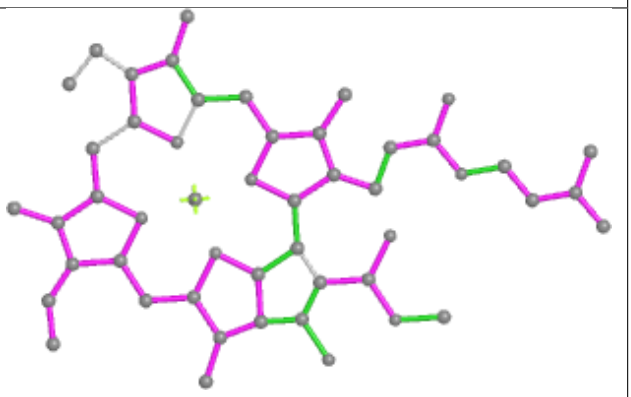
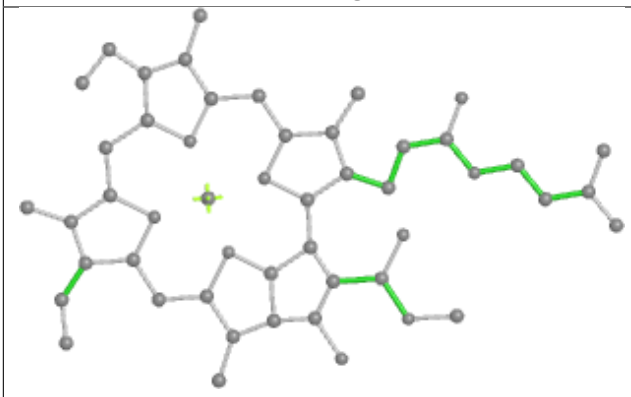
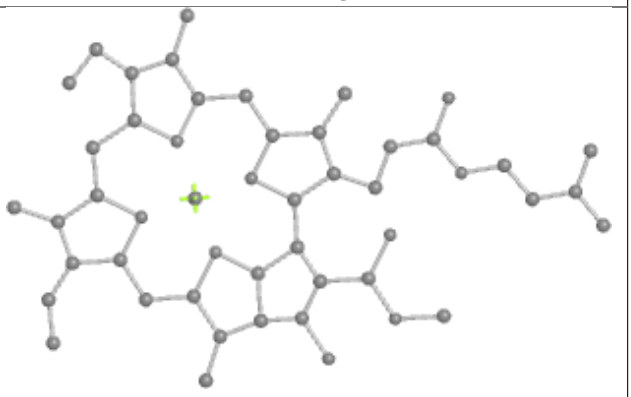
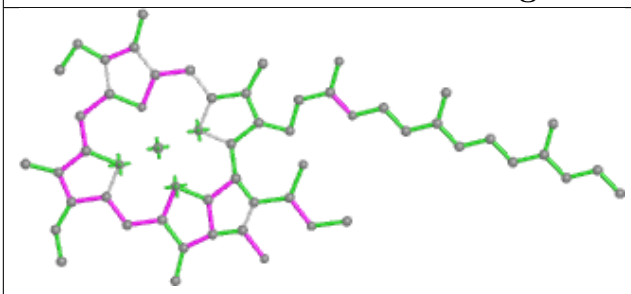
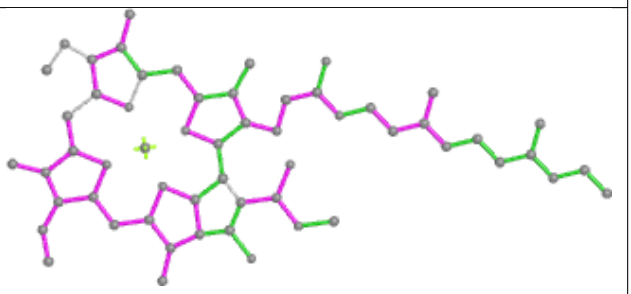
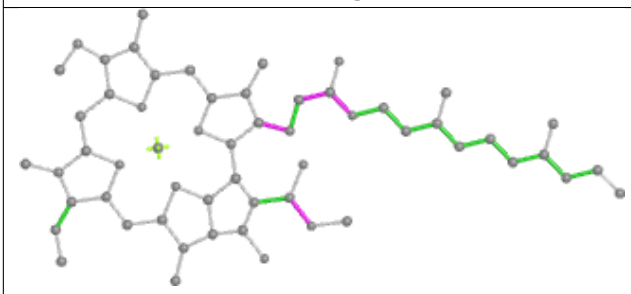
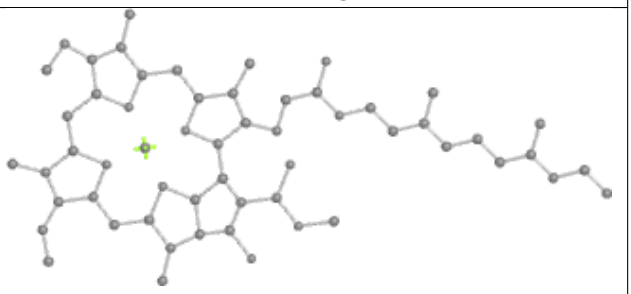
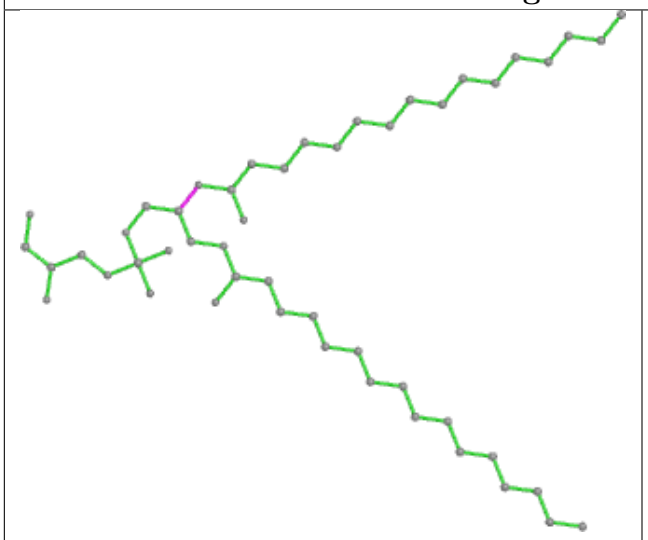
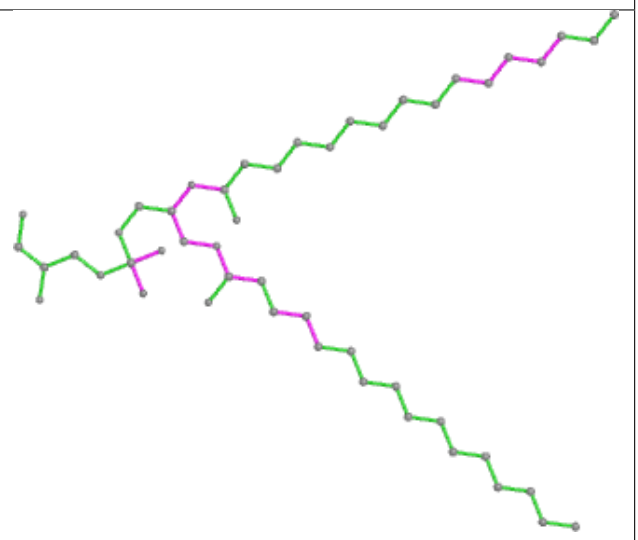
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 36 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

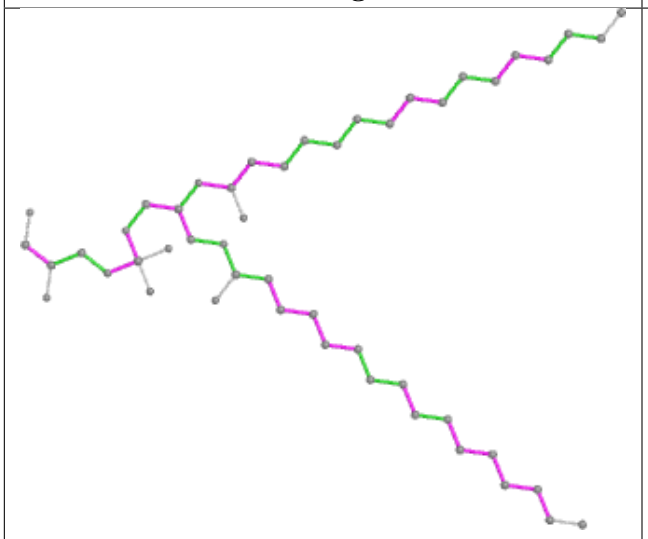
Ligand LHG D 410



Bond lengths



Bond angles



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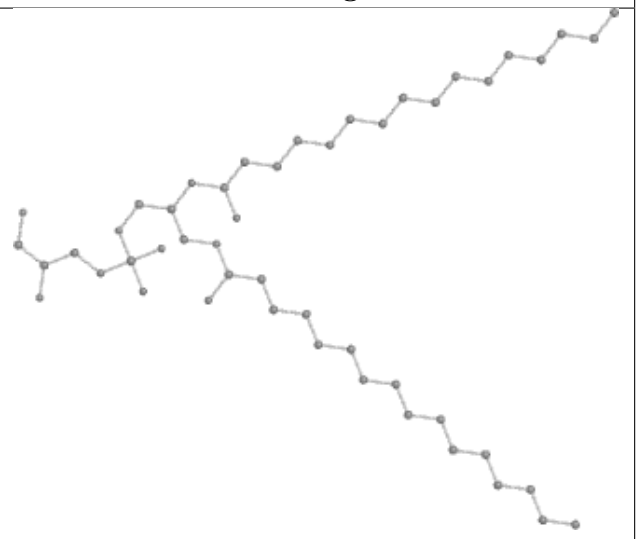
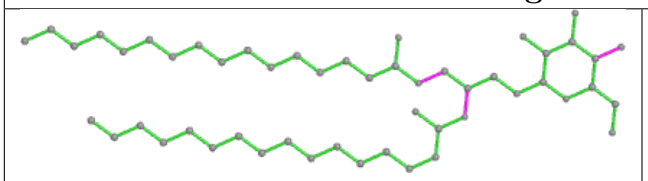


Rings

Ligand LMG a 410



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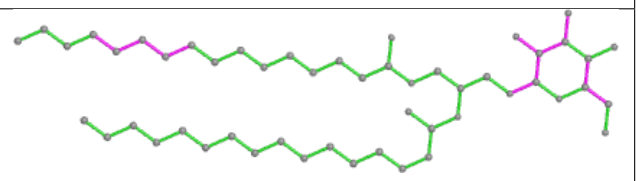
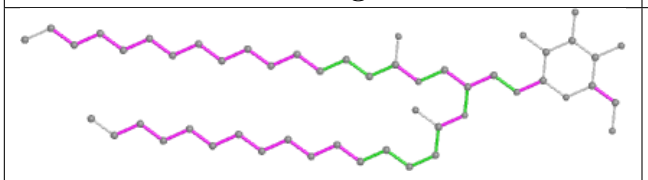


Bond angles



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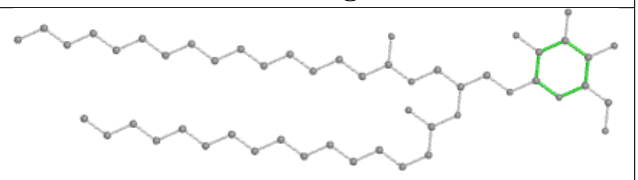
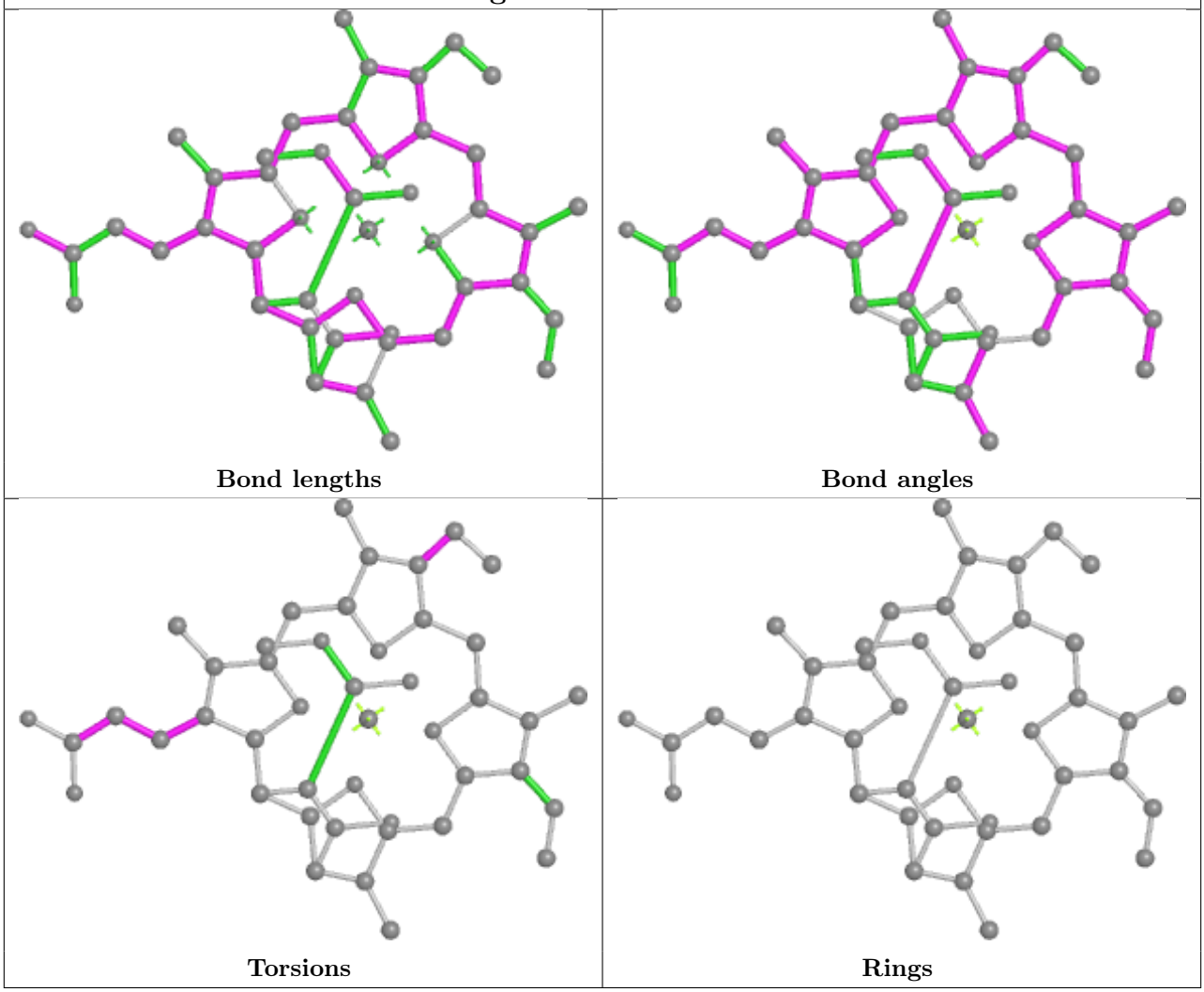
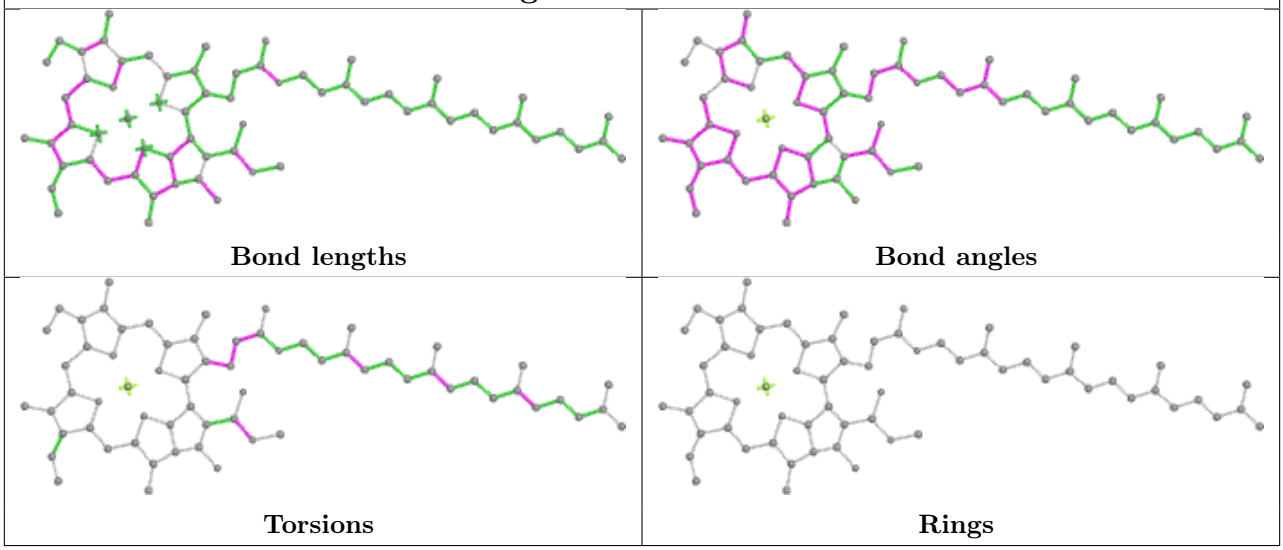


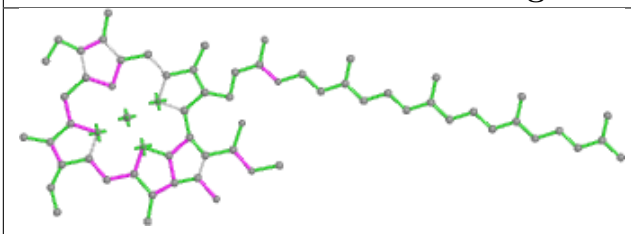
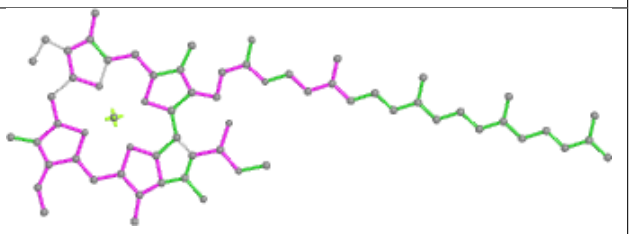
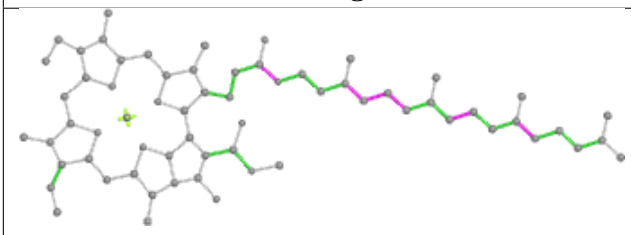
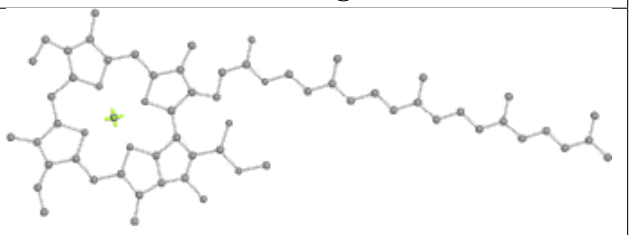
Rings

Ligand KC1 13 302



Ligand CLA 38 202



Ligand CLA b 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

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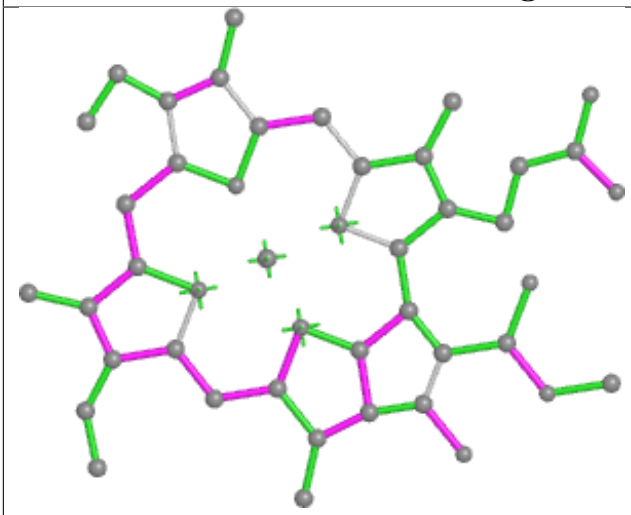
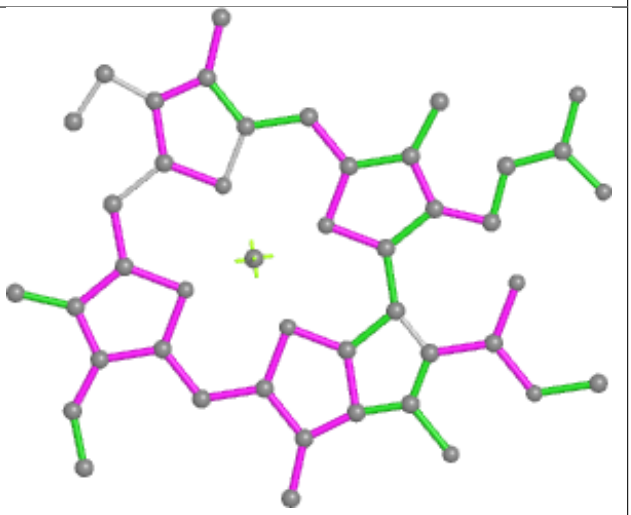
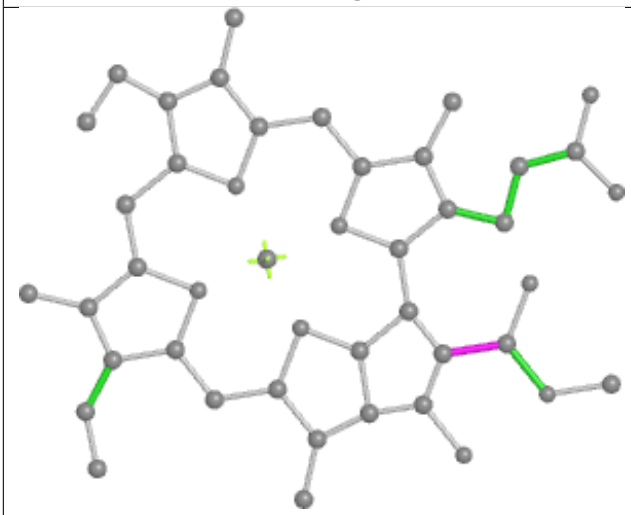
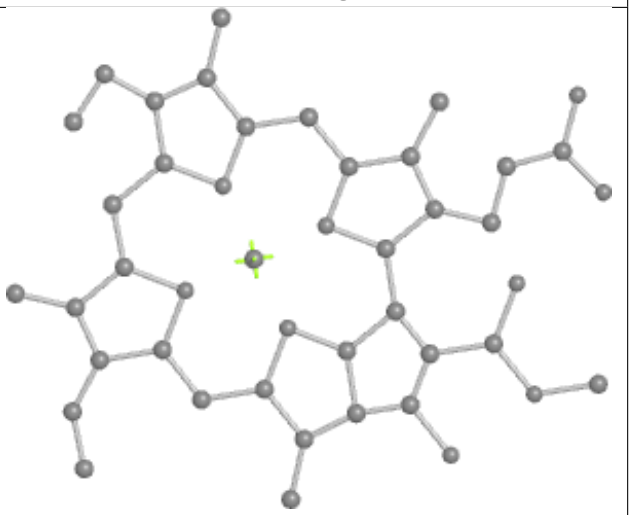
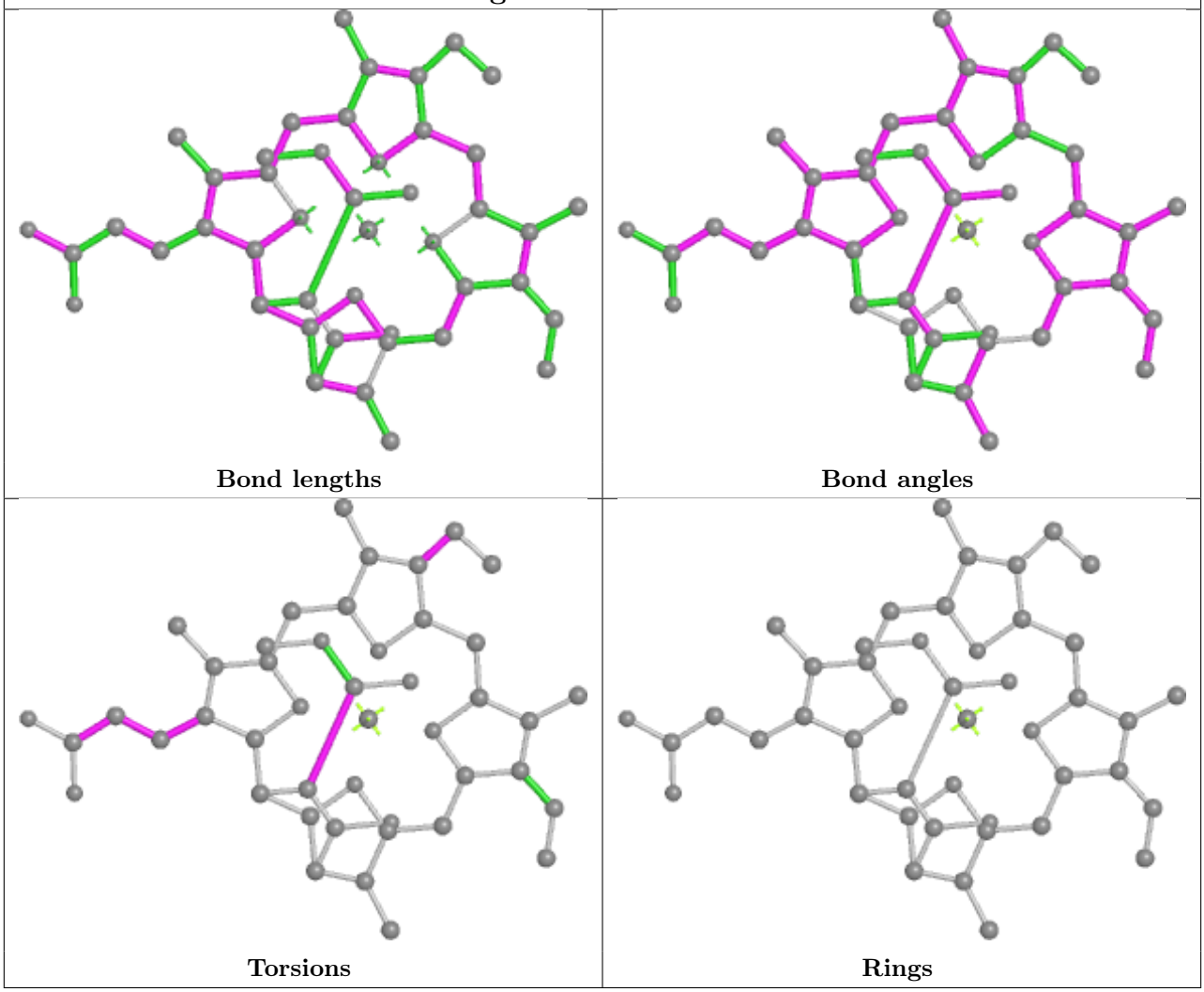
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 34 309



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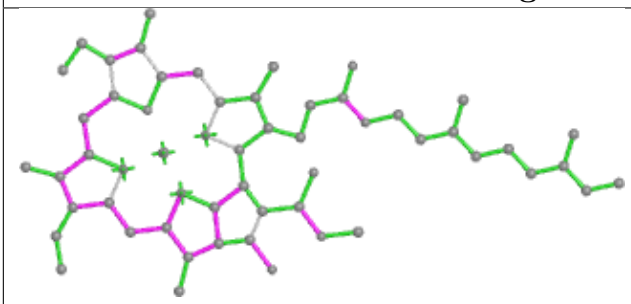
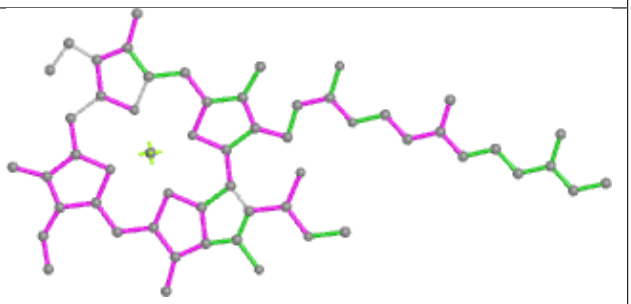
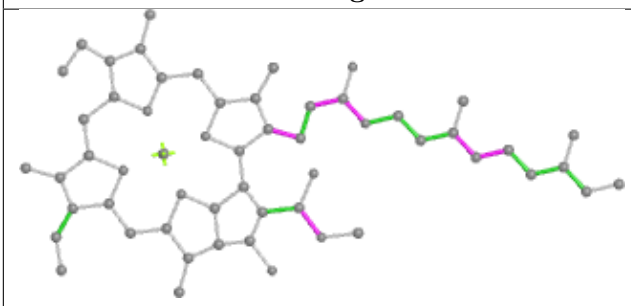
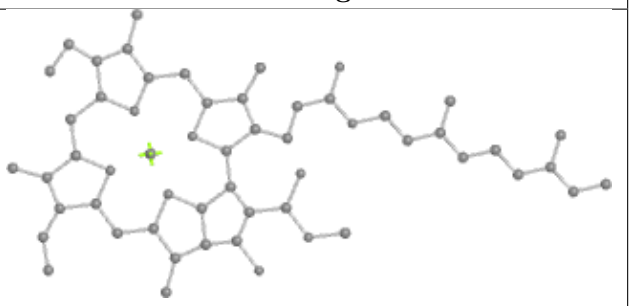
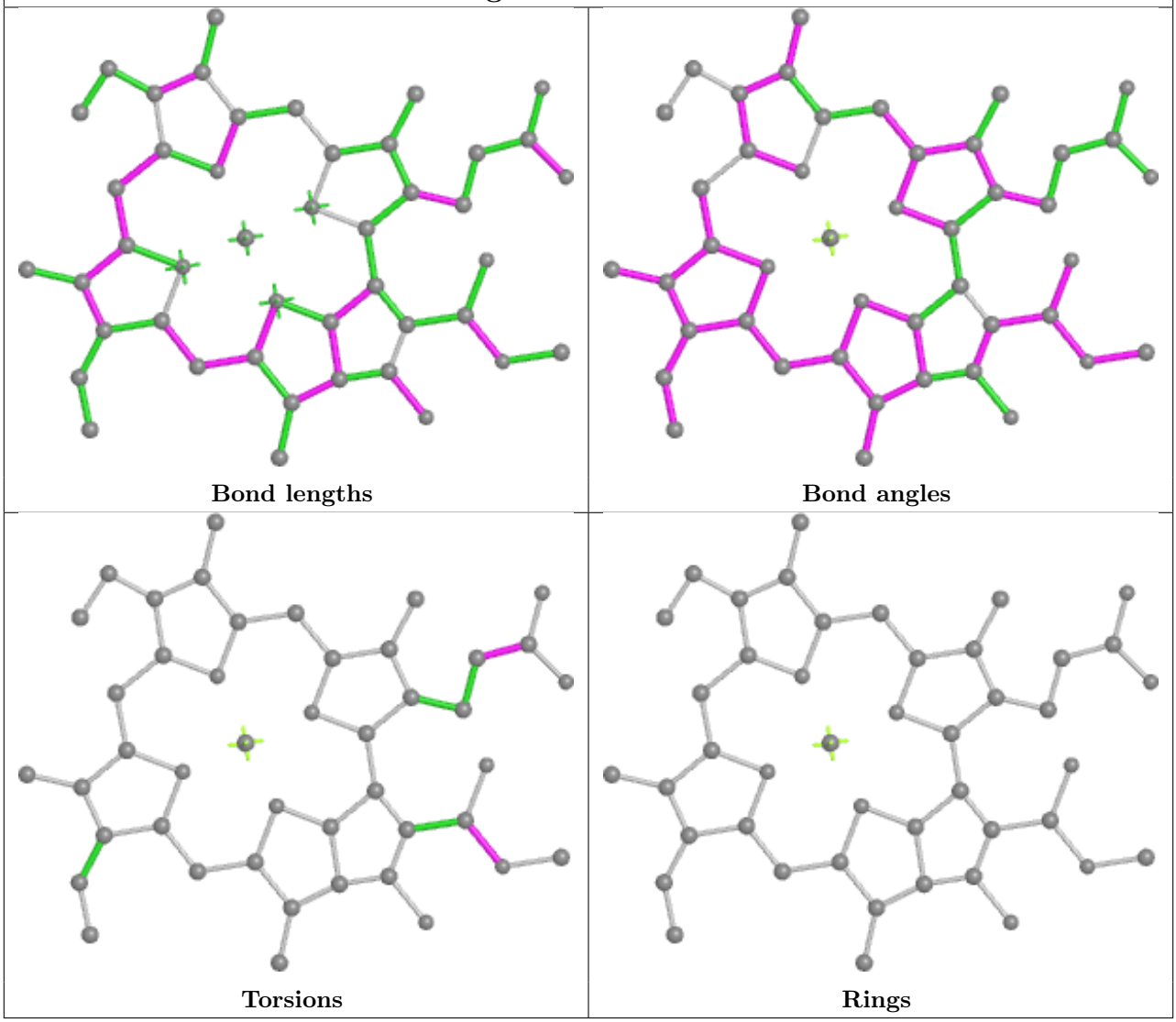
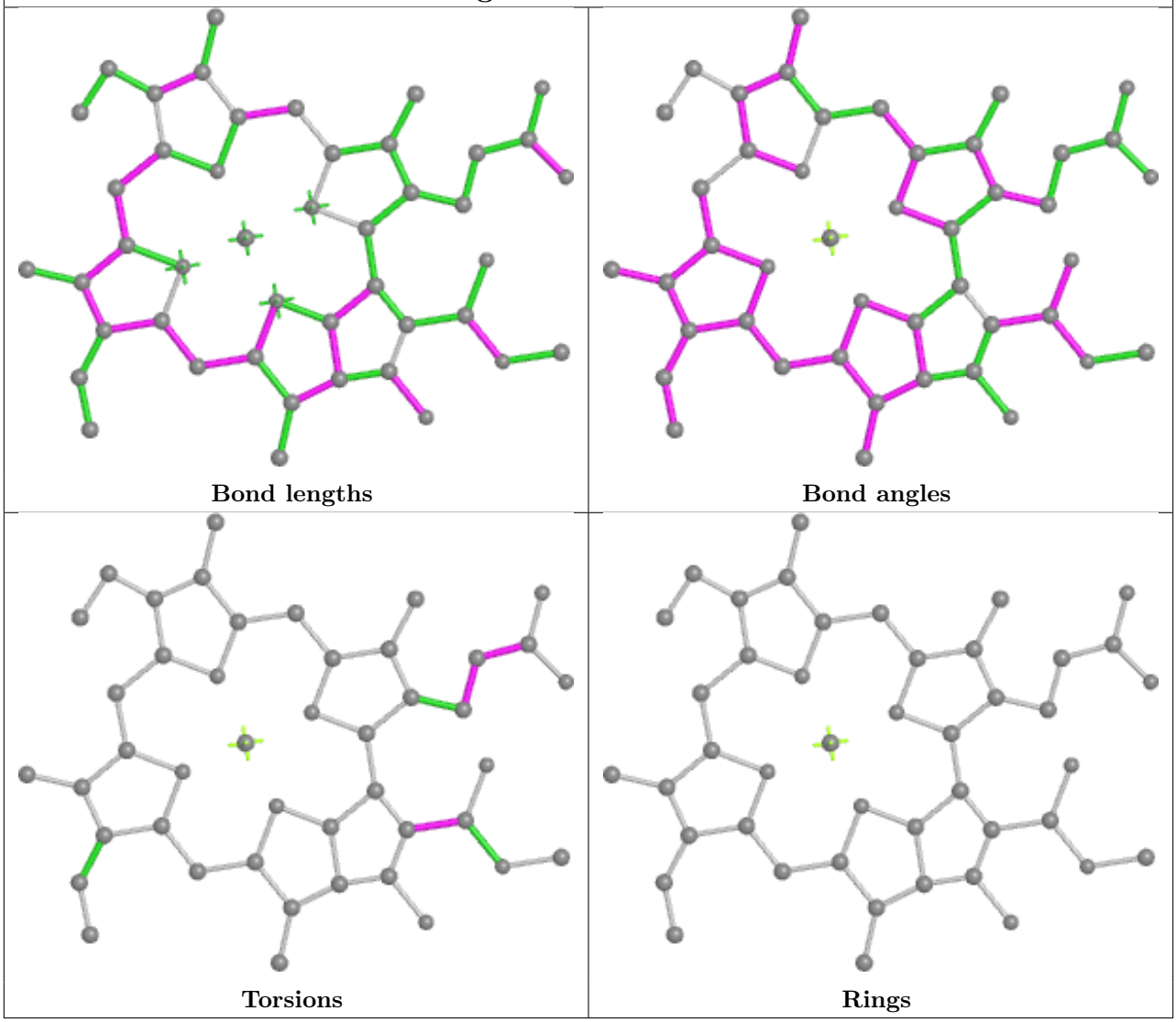
 Bond lengths	 Bond angles
 Torsions	 Rings

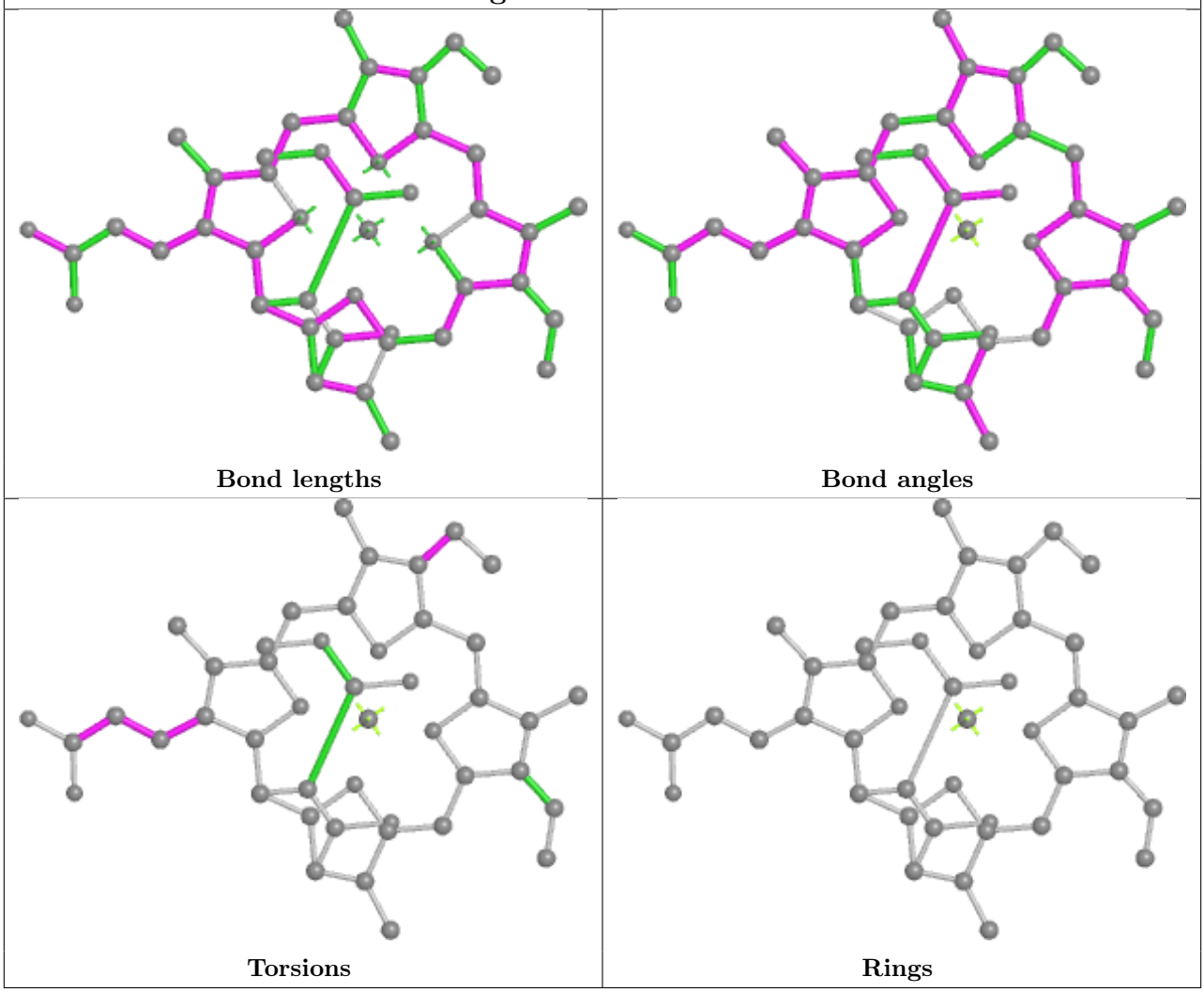
Ligand CLA z 102



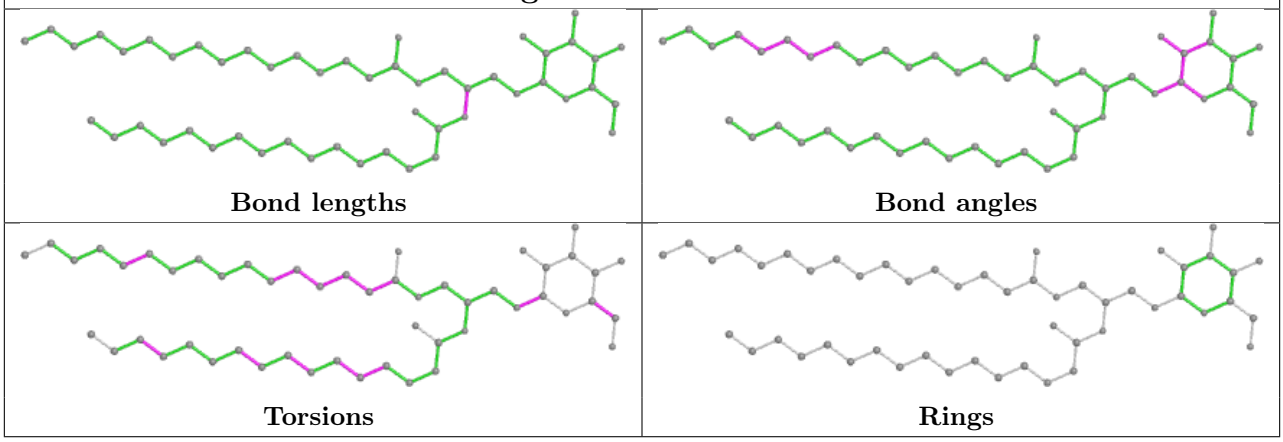
Ligand CLA 35 305



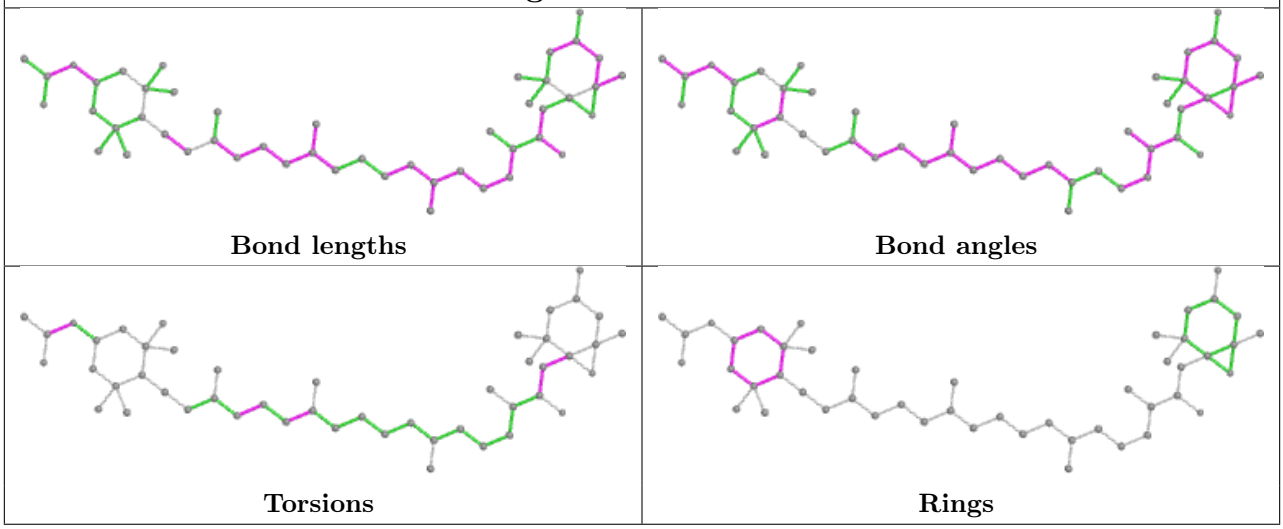
Ligand KC1 16 305



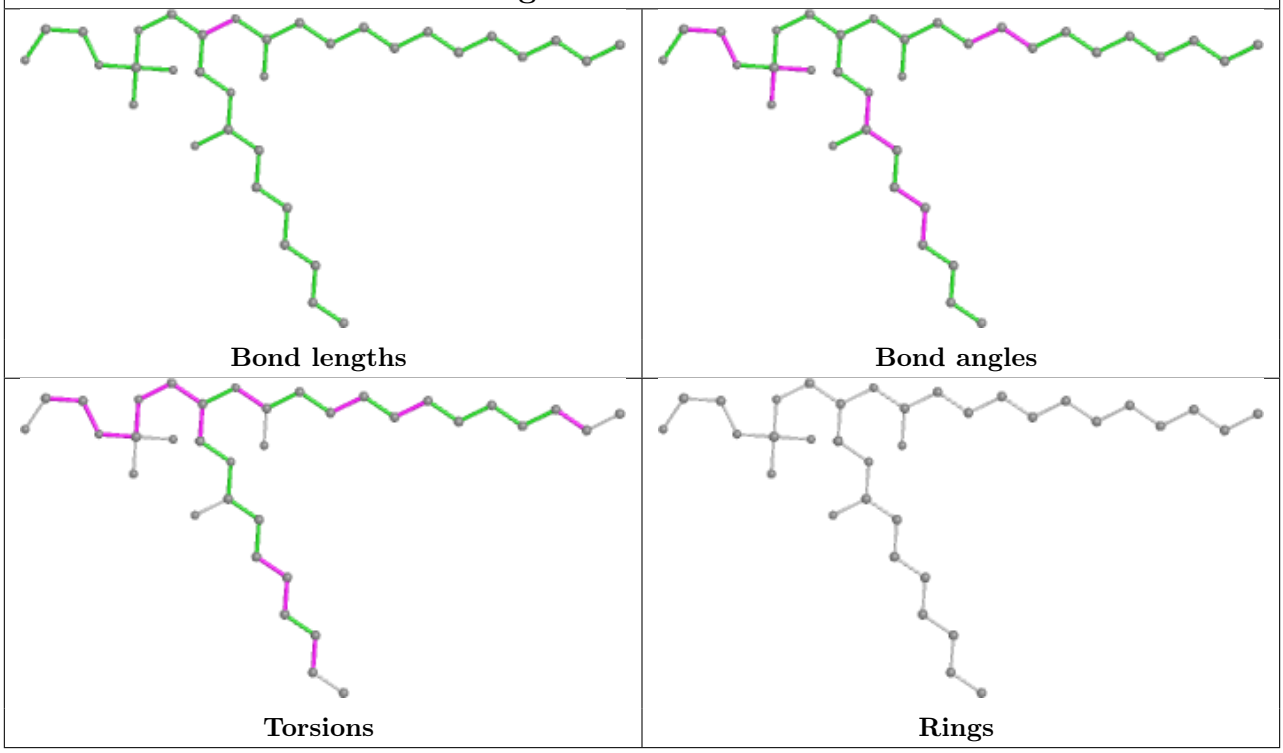
Ligand LMG B 520



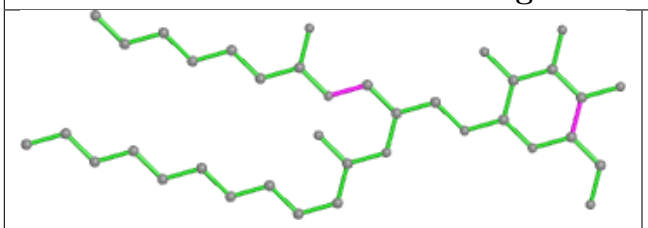
Ligand A86 11 313



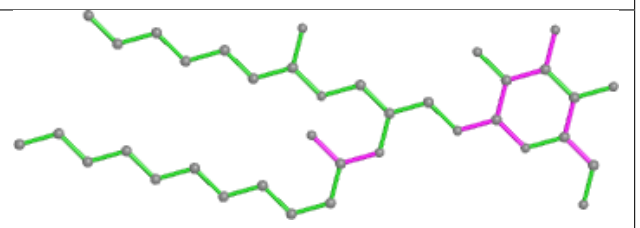
Ligand LHG 41 201



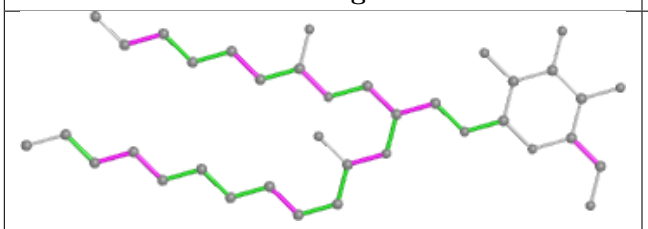
Ligand LMG 37 316



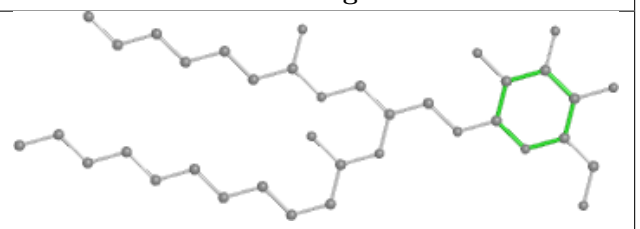
Bond lengths



Bond angles

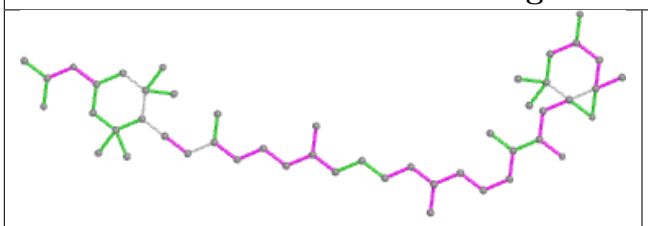


Torsions



Rings

Ligand A86 38 212



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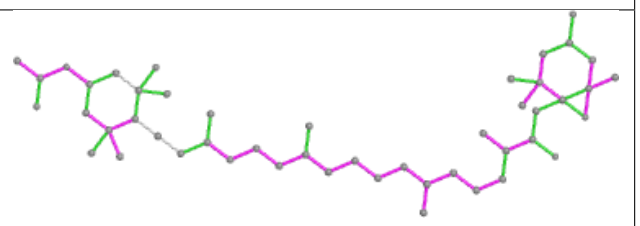

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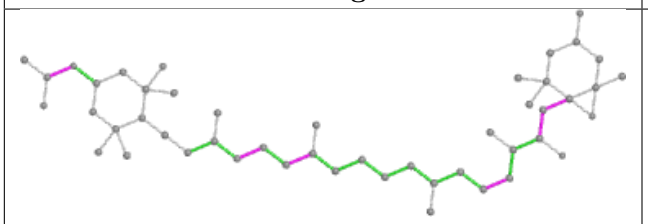

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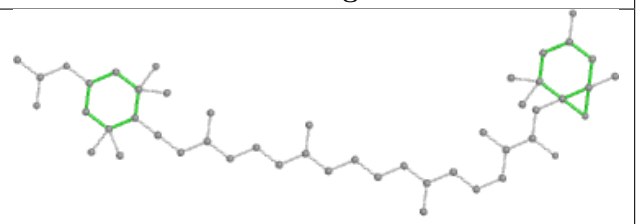
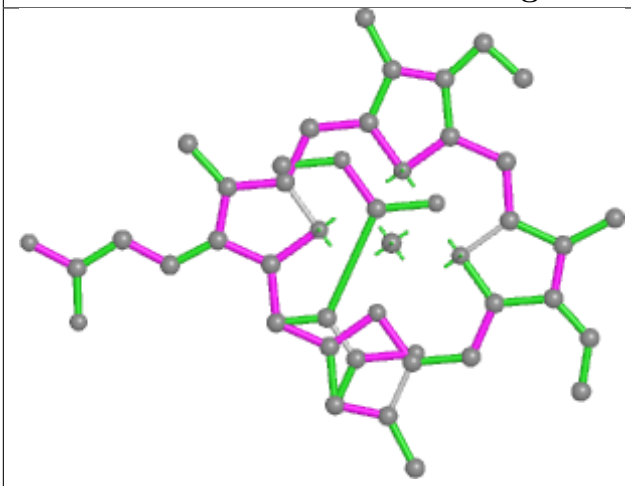


Rings

Ligand KC1 11 302



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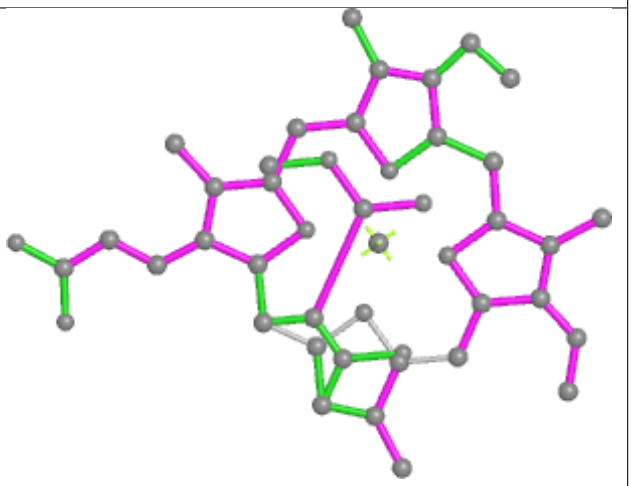

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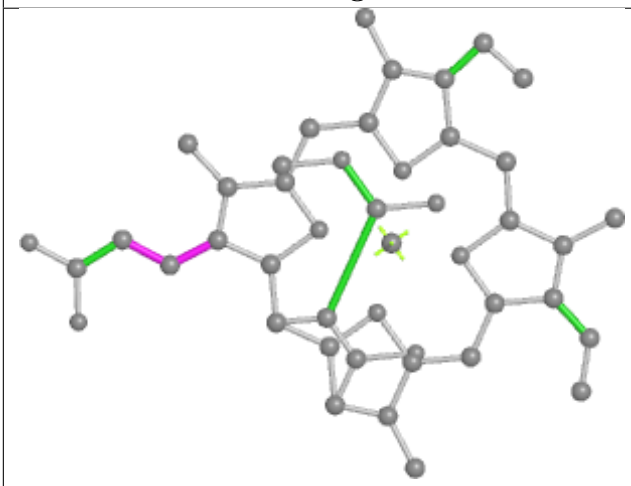

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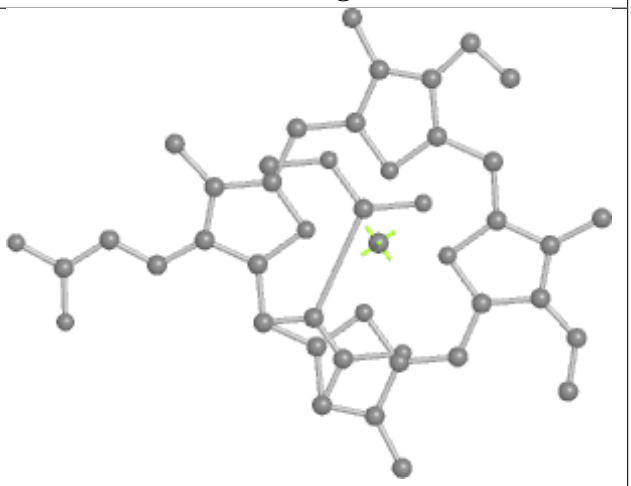
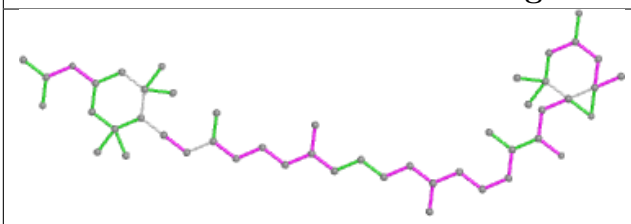


Rings

Ligand A86 33 311



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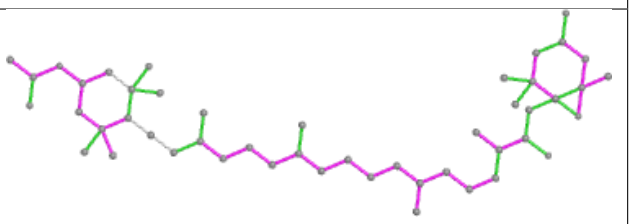

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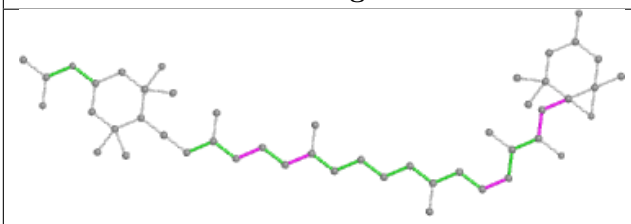

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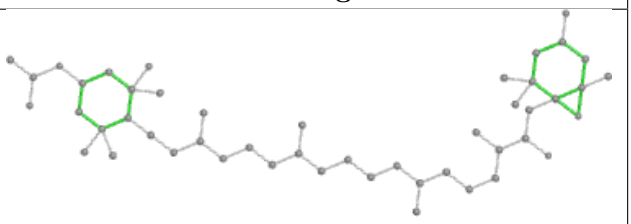
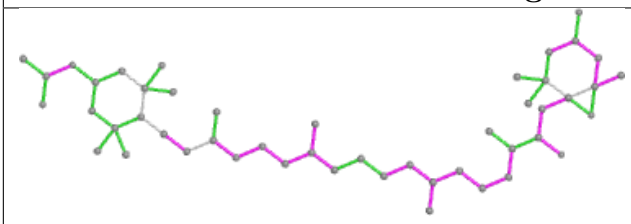
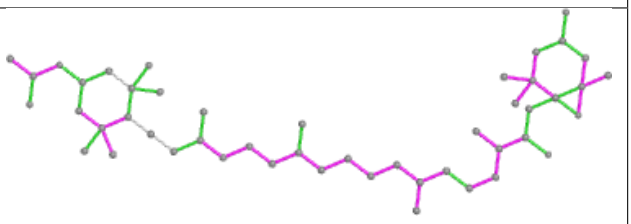
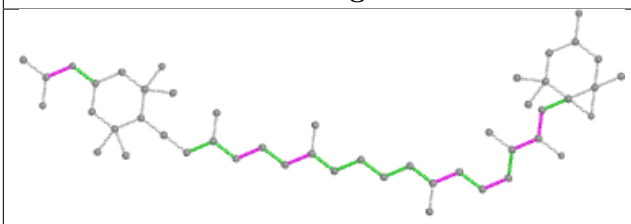
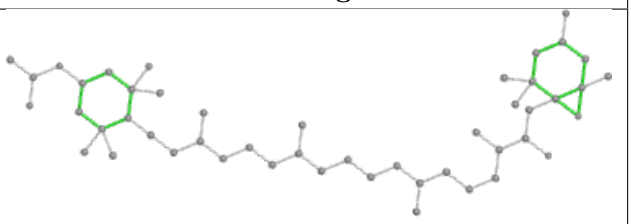
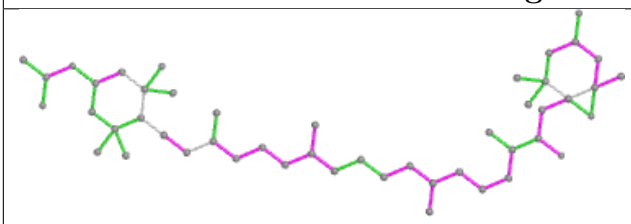
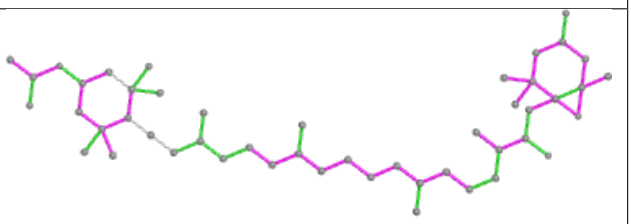
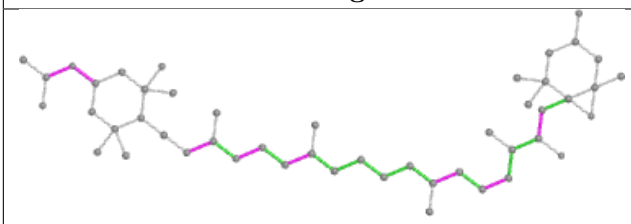
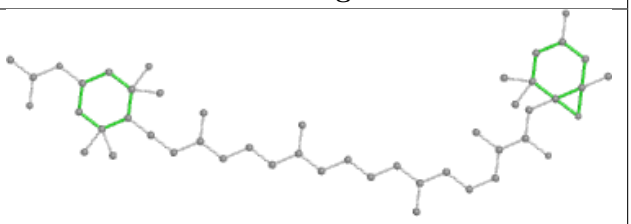
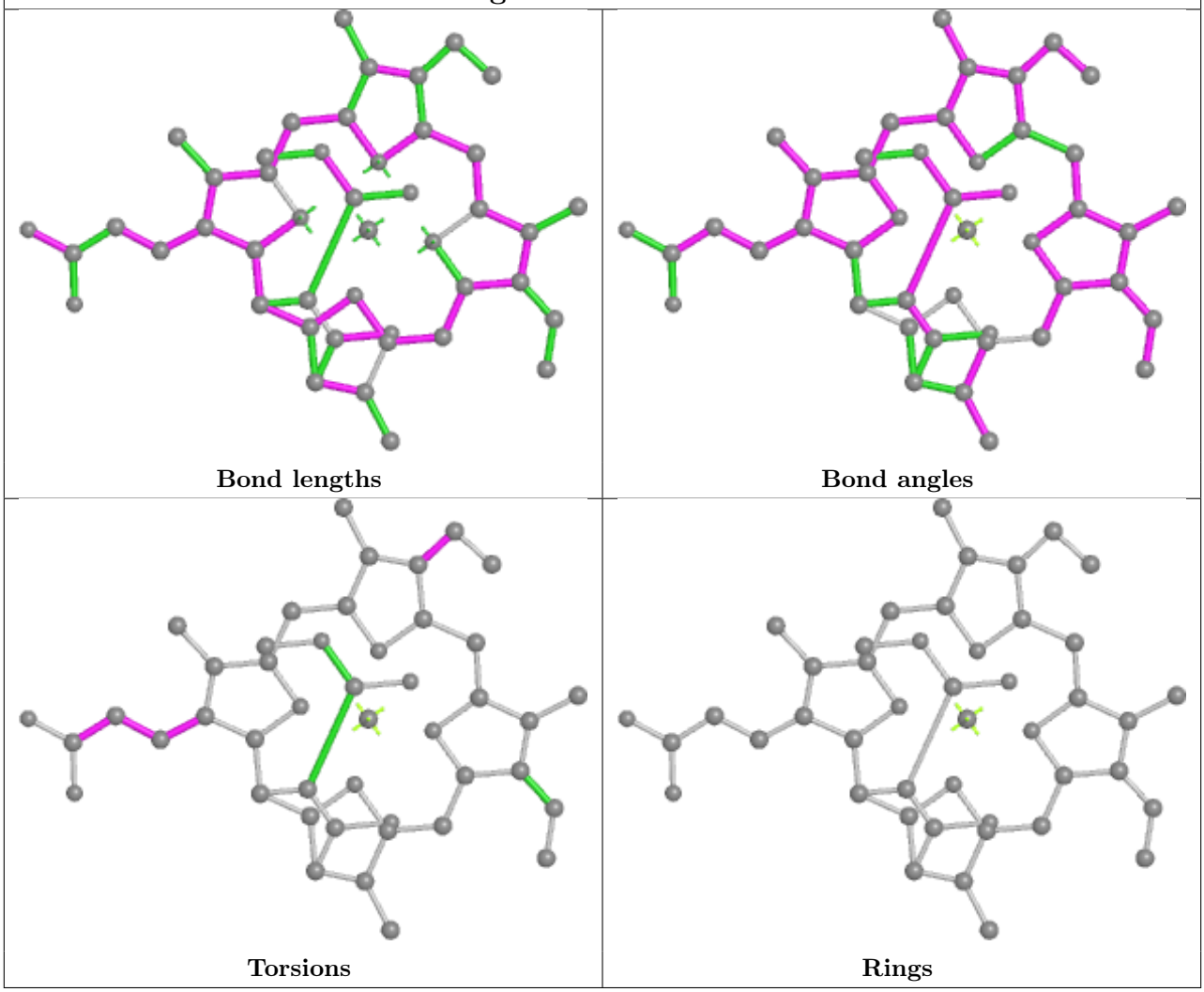


Rings

Ligand A86 37 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 34 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 15 302



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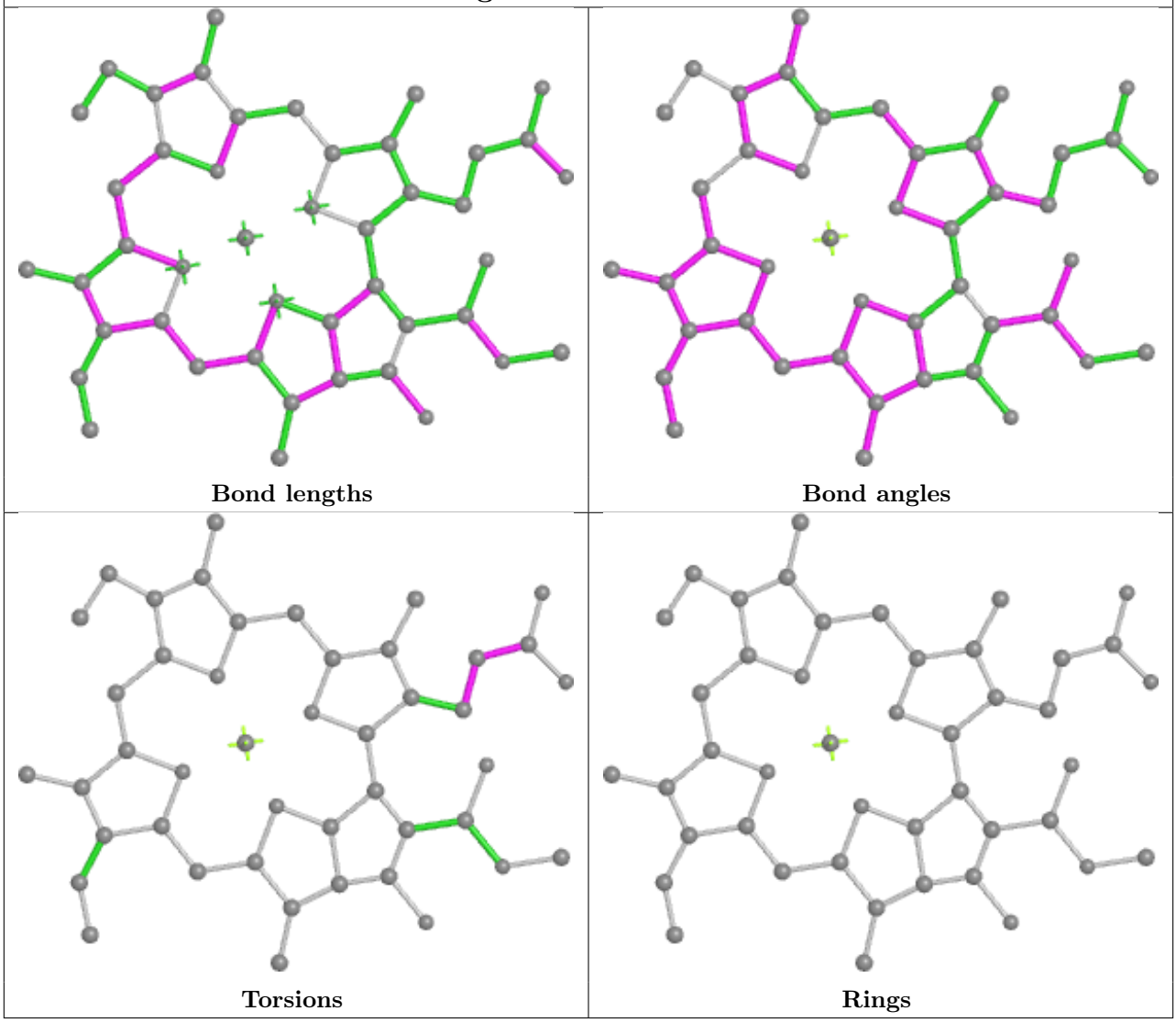

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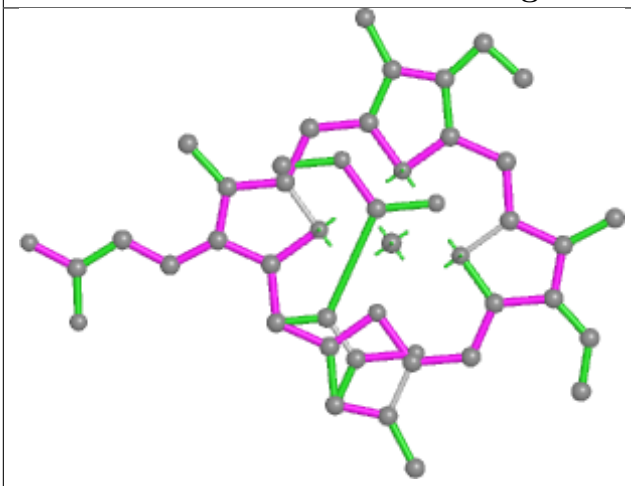
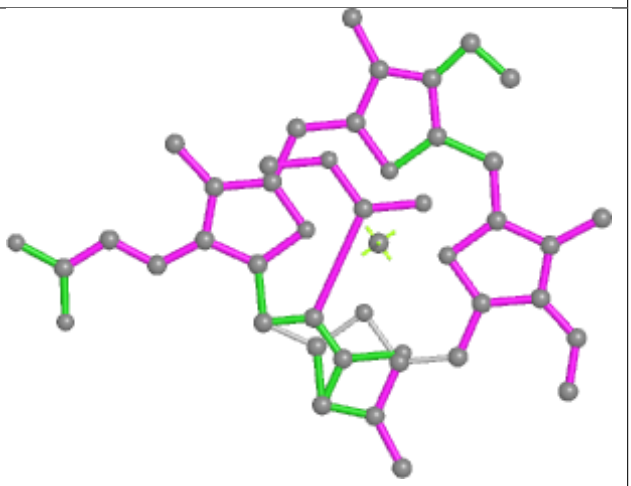
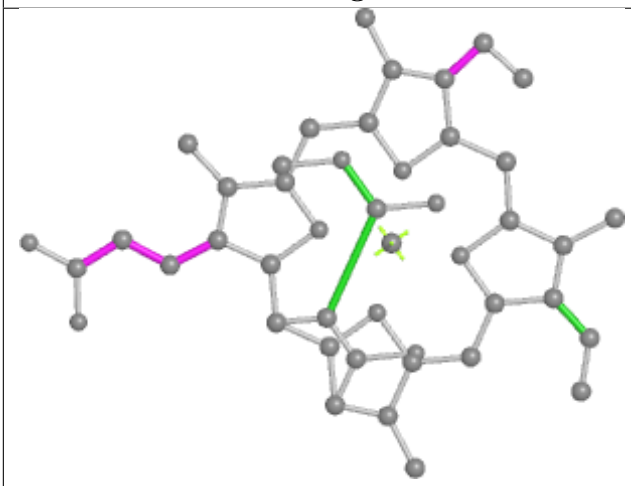


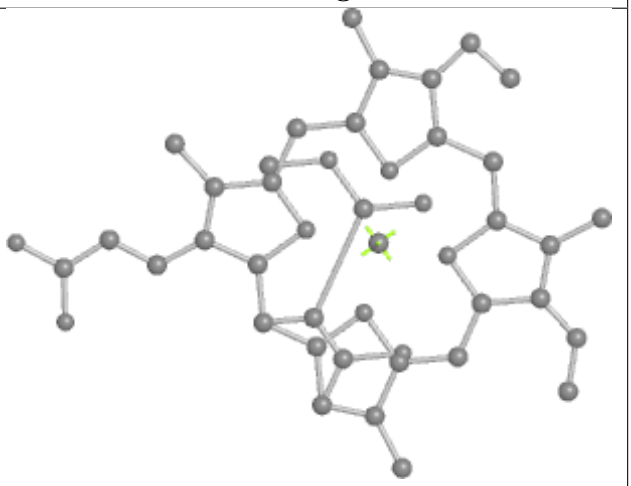
Bond lengths



Bond angles

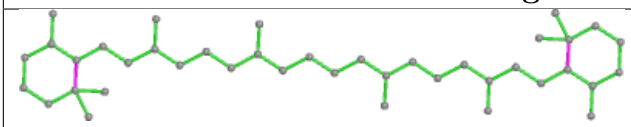


Torsions



Rings

Ligand BCR C 515



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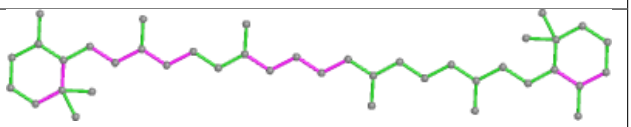
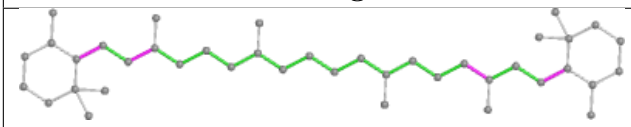


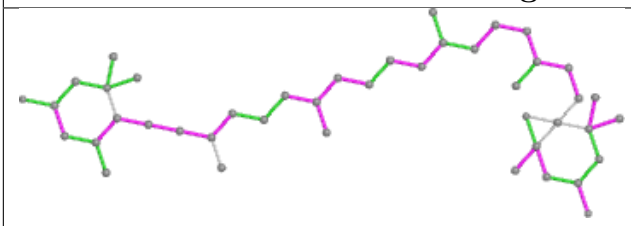
Bond angles



Torsions

Rings

Ligand DD6 39 312



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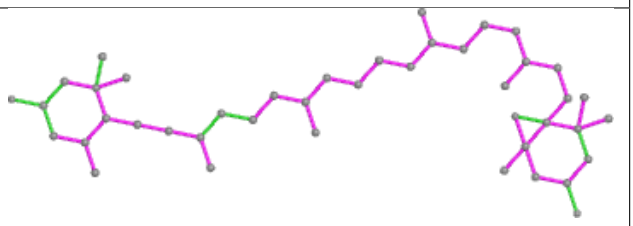
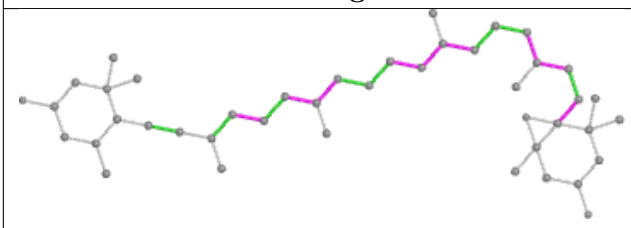


Bond angles



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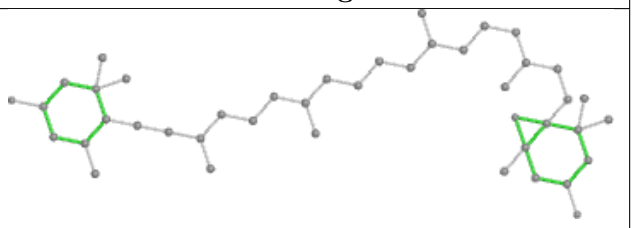
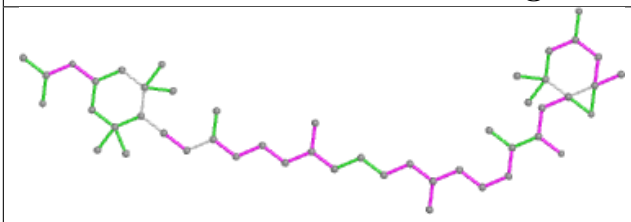


Rings

Ligand A86 13 311



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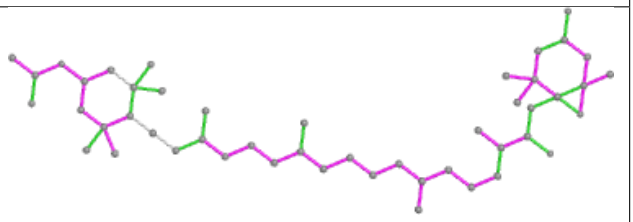
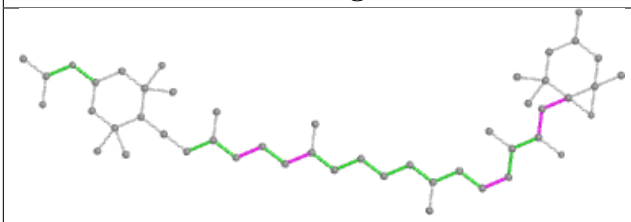


Bond angles



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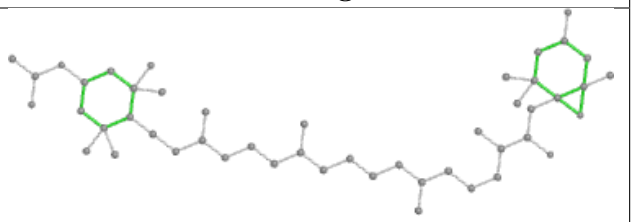
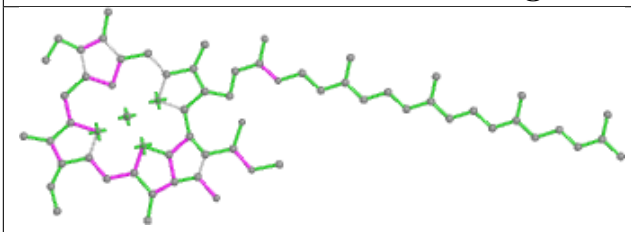


Rings

Ligand CLA C 508



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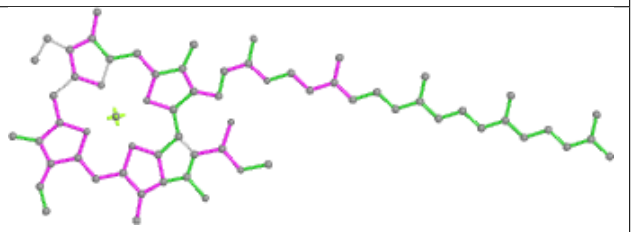
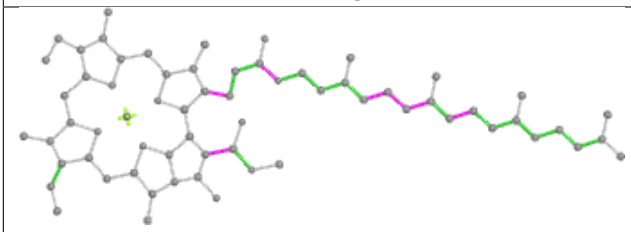


Bond angles



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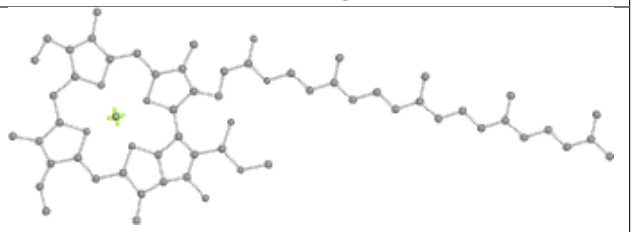
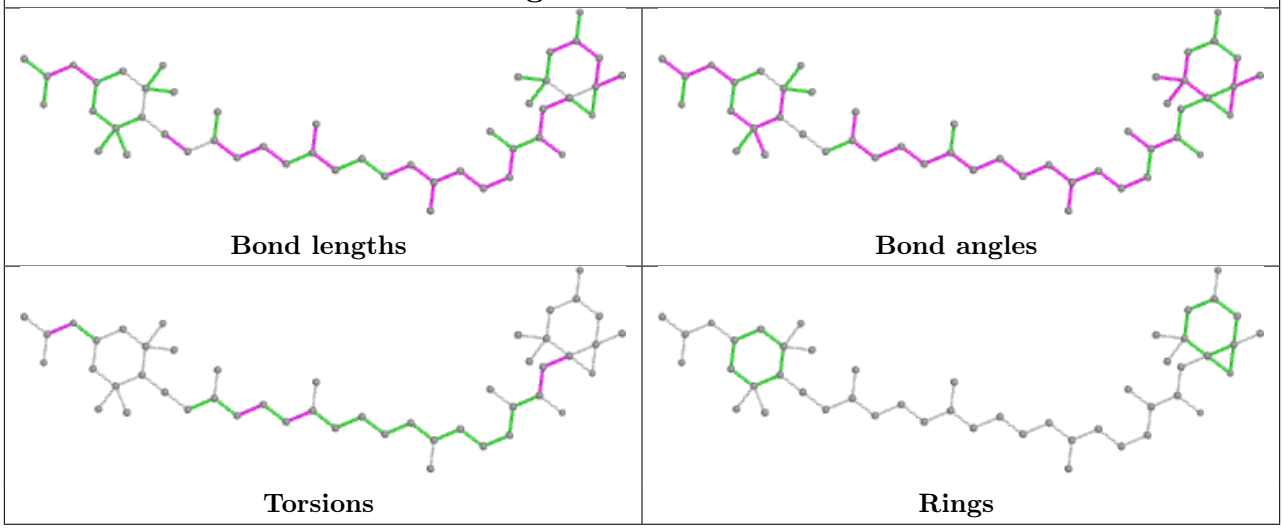
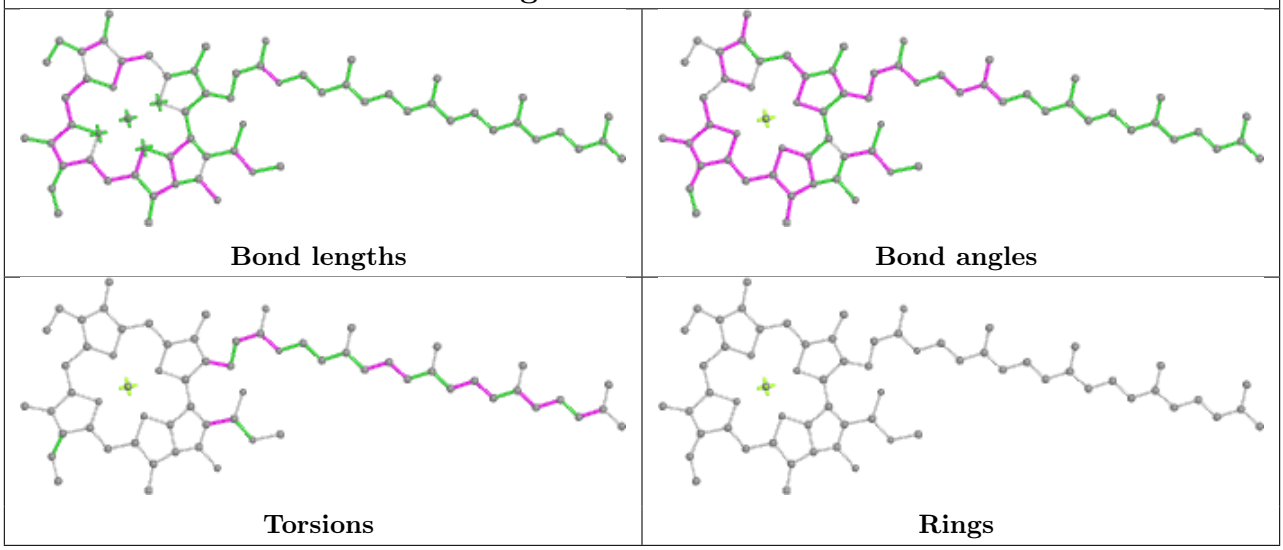


Rings

Ligand A86 34 311



Ligand CLA 39 303



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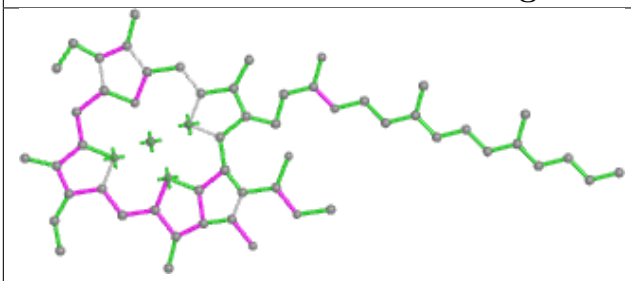
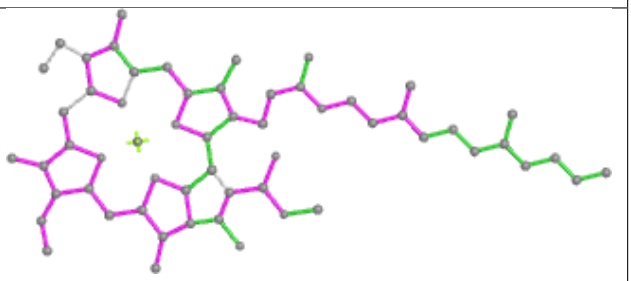
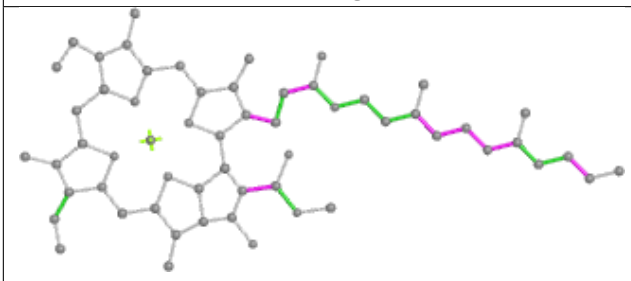
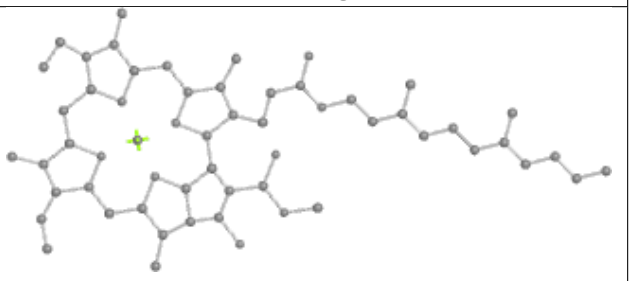
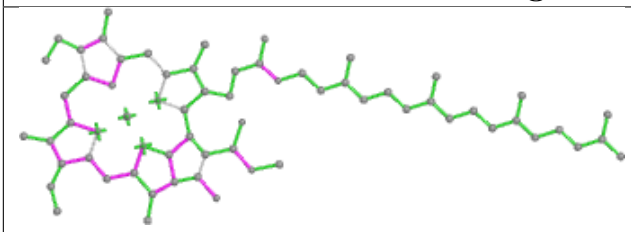
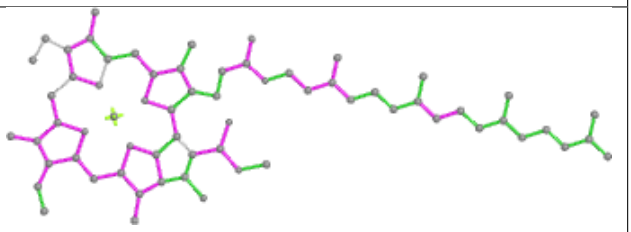
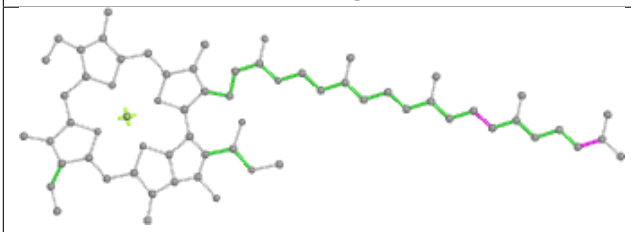
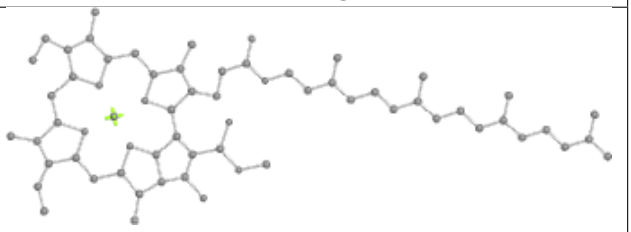
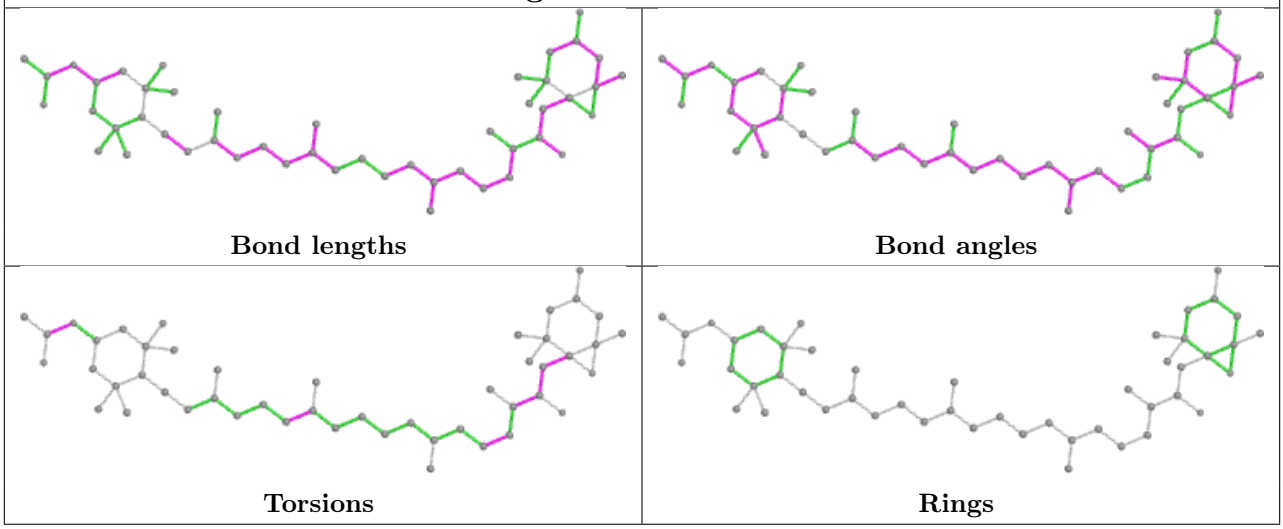
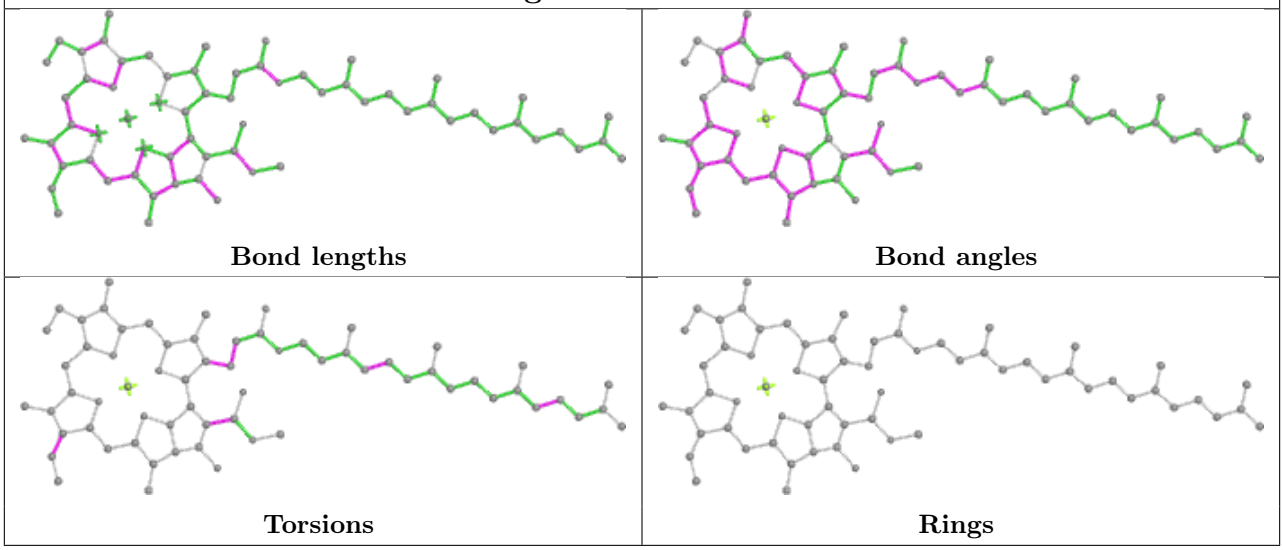
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 37 314



Ligand CLA D 401



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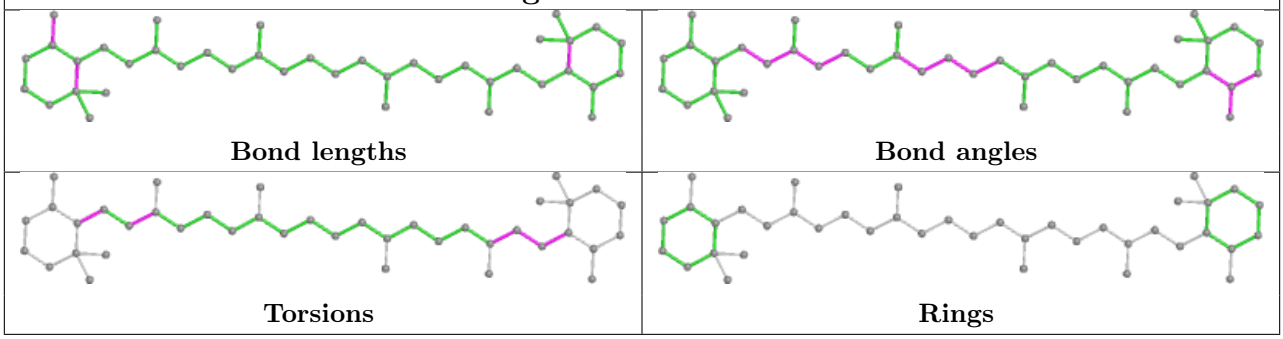

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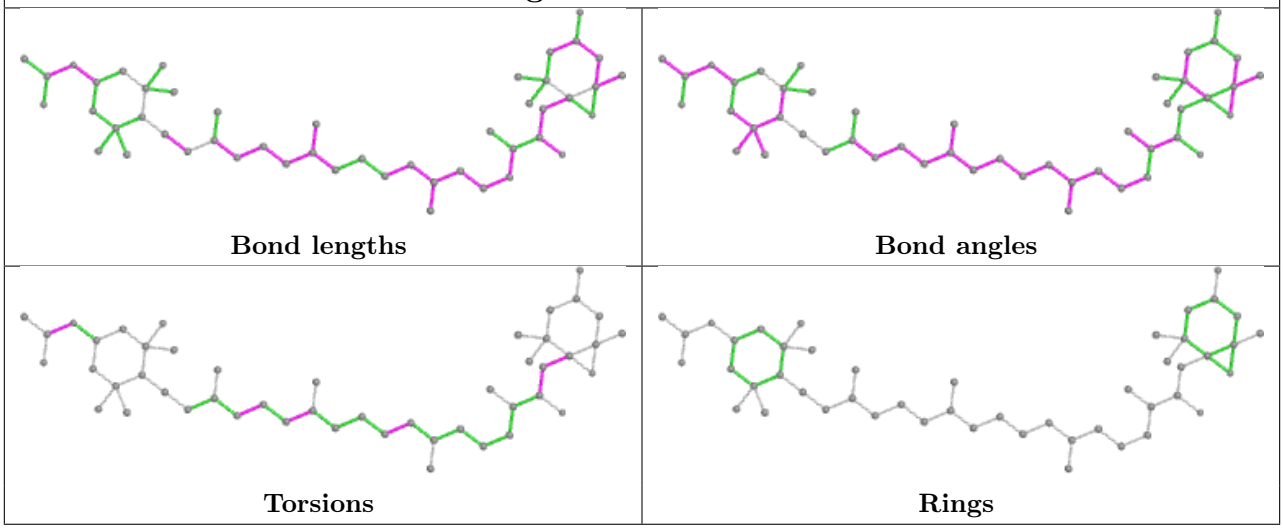

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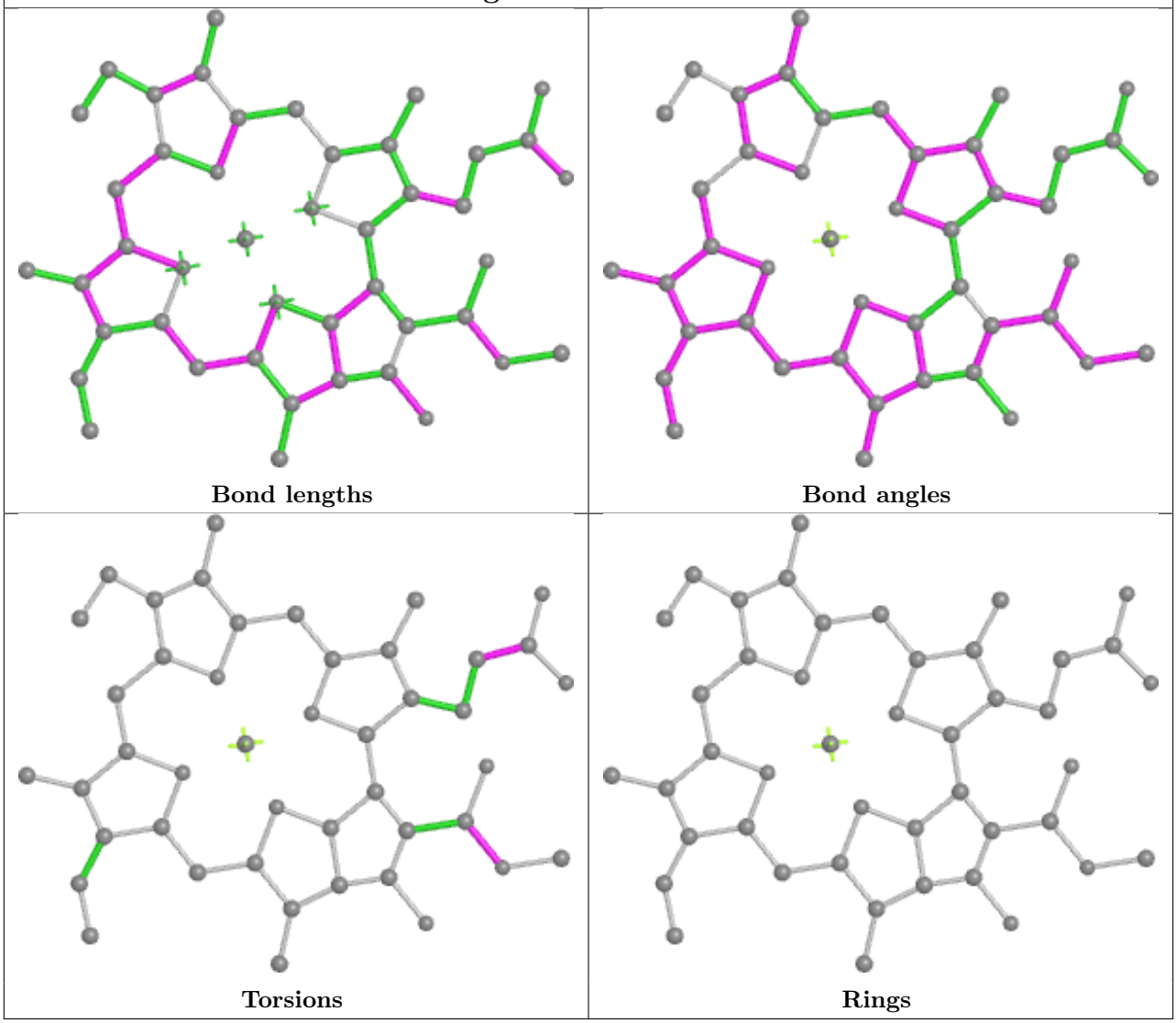

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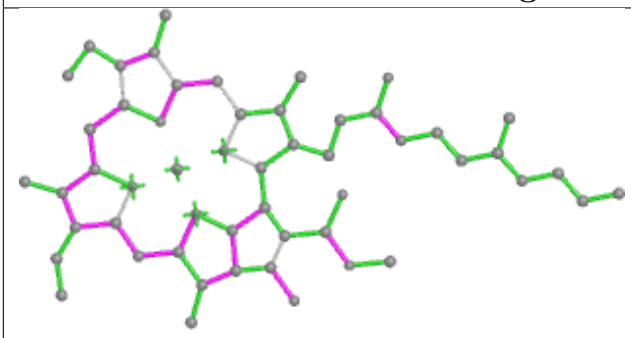
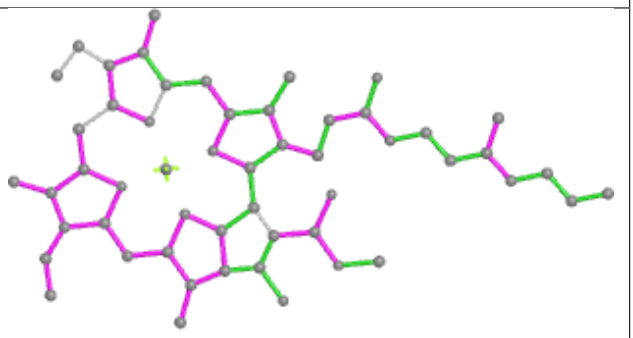
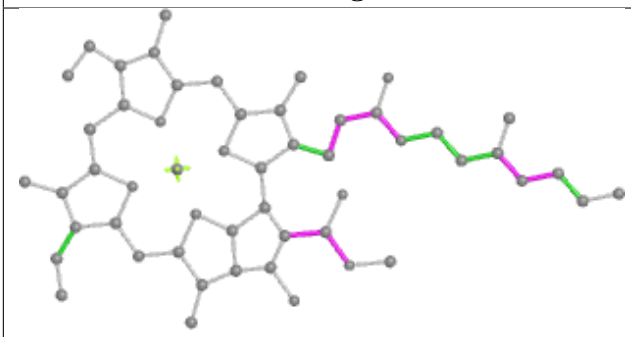
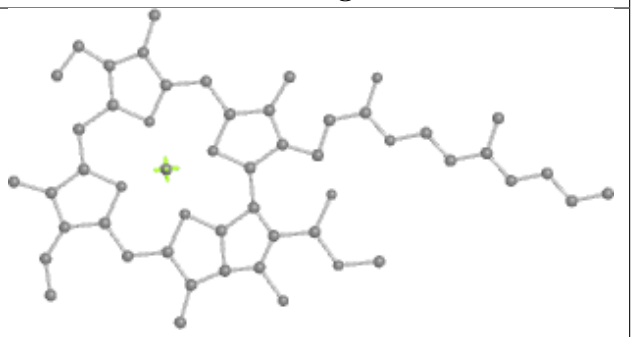
 Bond lengths	 Bond angles
 Torsions	 Rings

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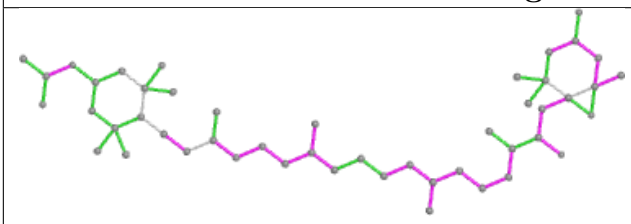
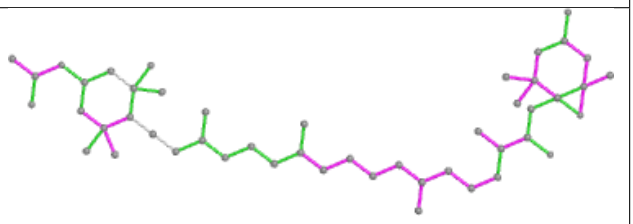
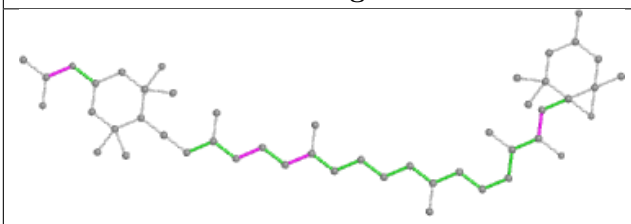
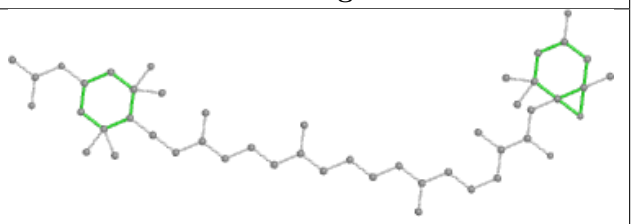
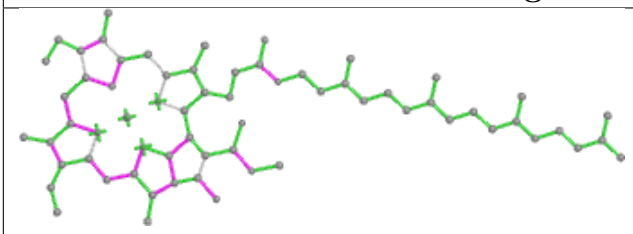
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 503



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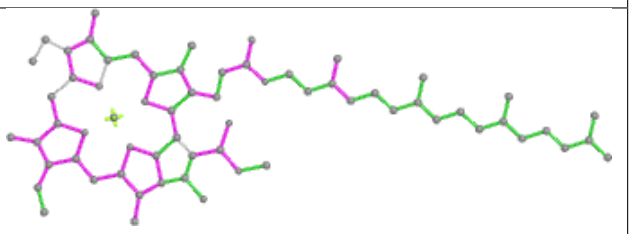

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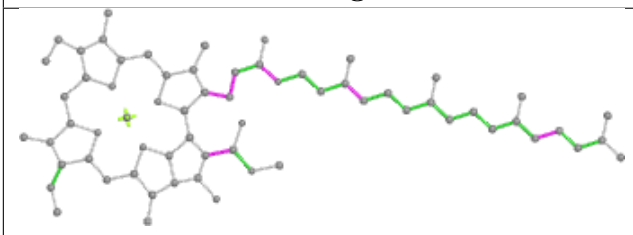

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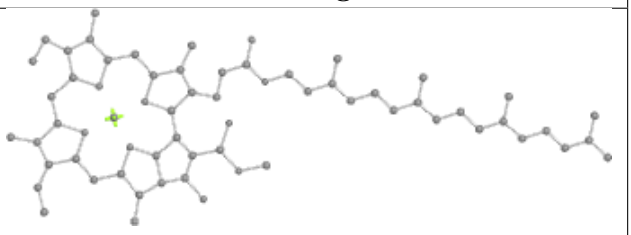
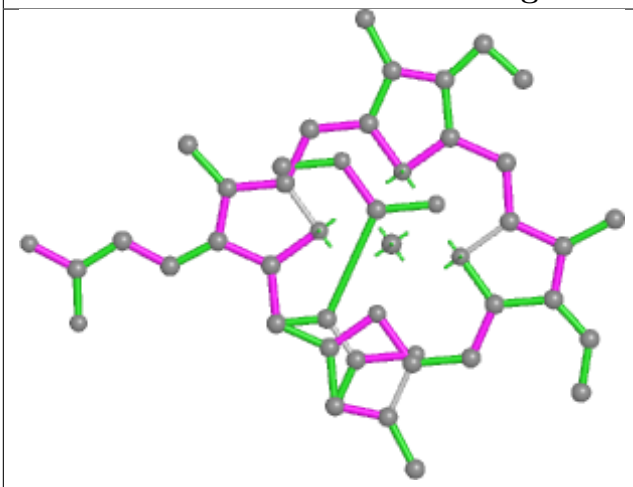


Rings

Ligand KC1 32 207



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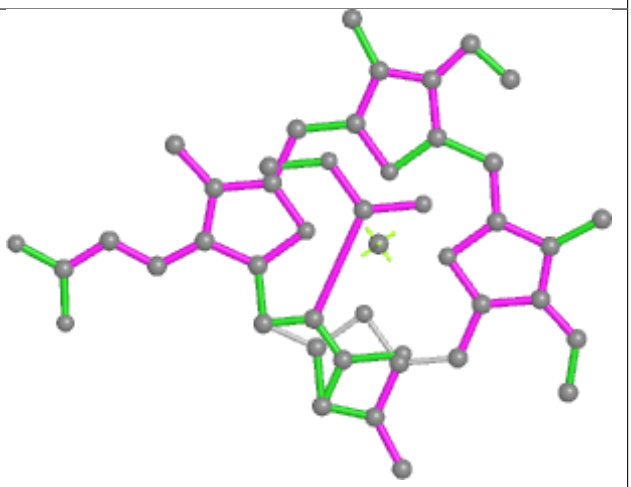

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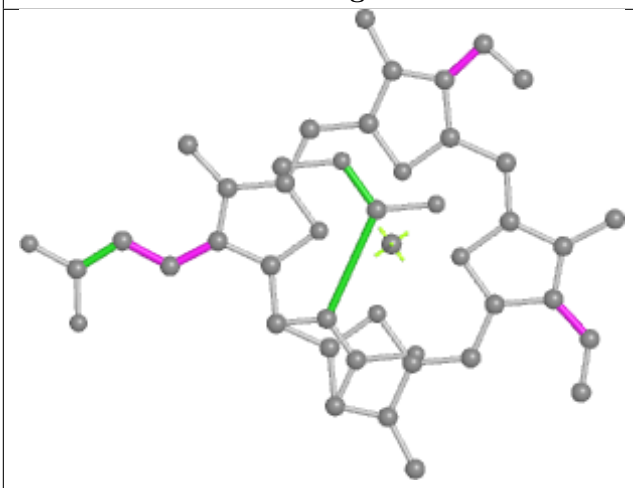

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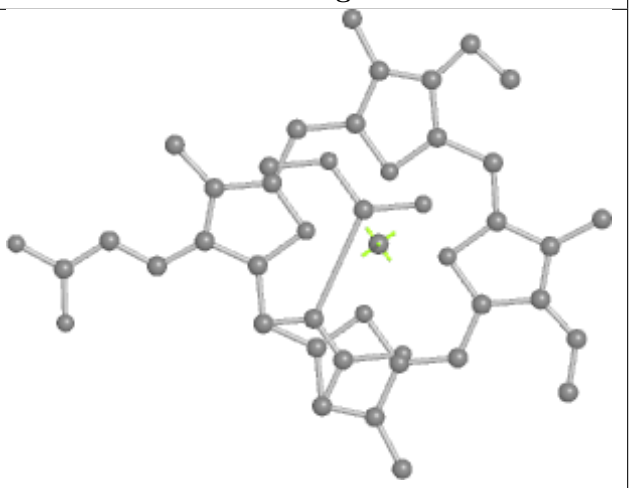

Rings

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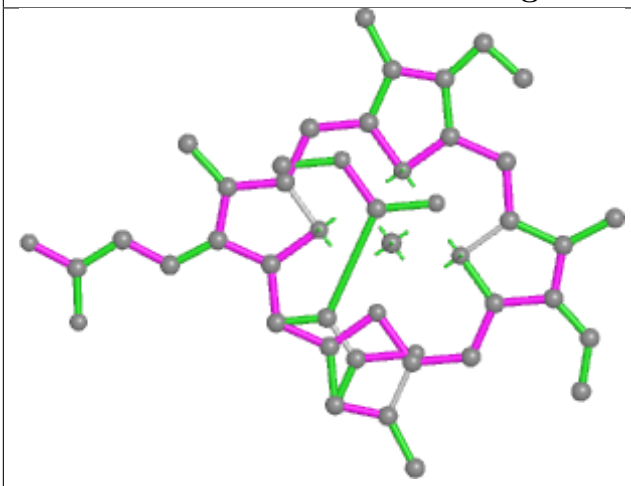

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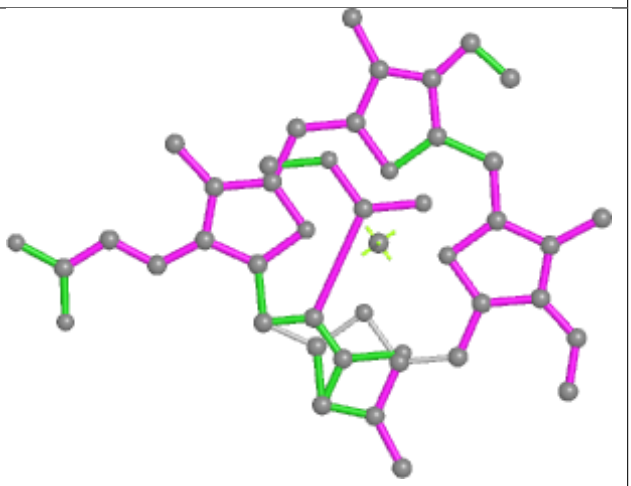

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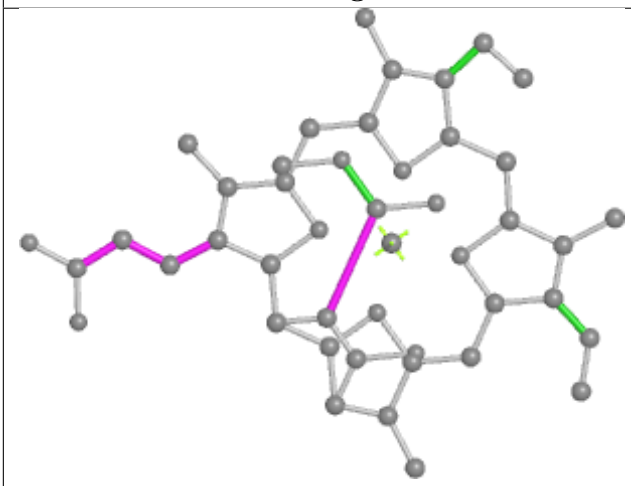

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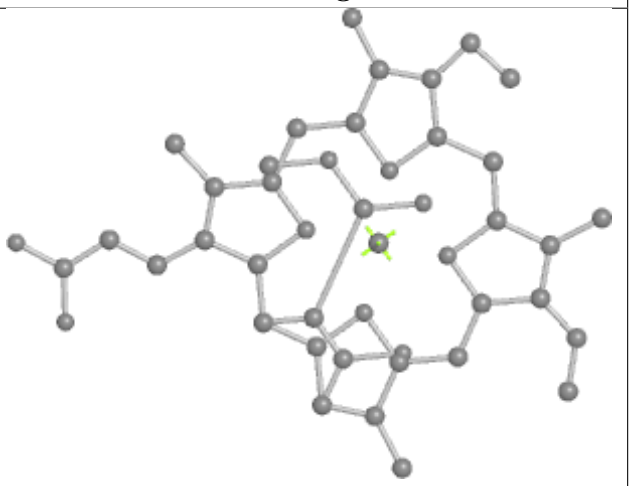
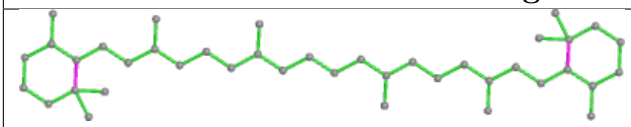


Rings

Ligand BCR B 518



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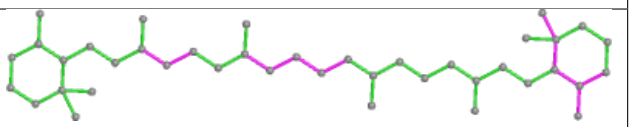

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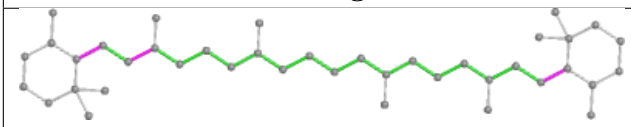
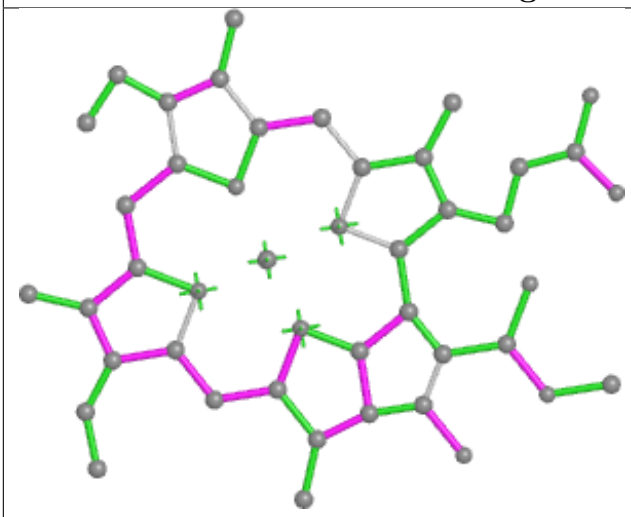


Torsions

Rings

Ligand CLA 20 307



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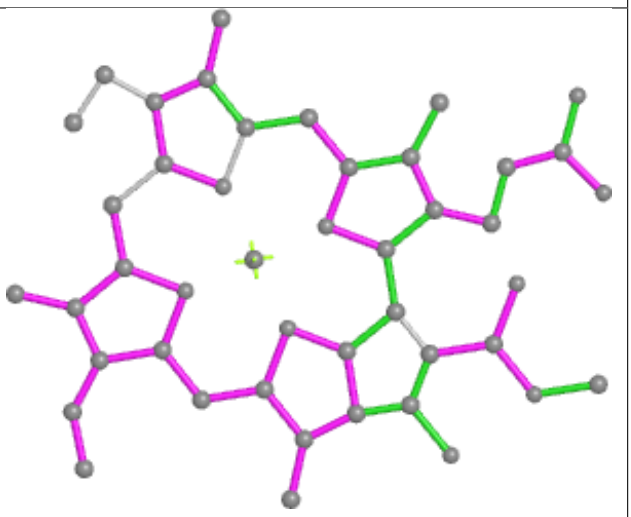

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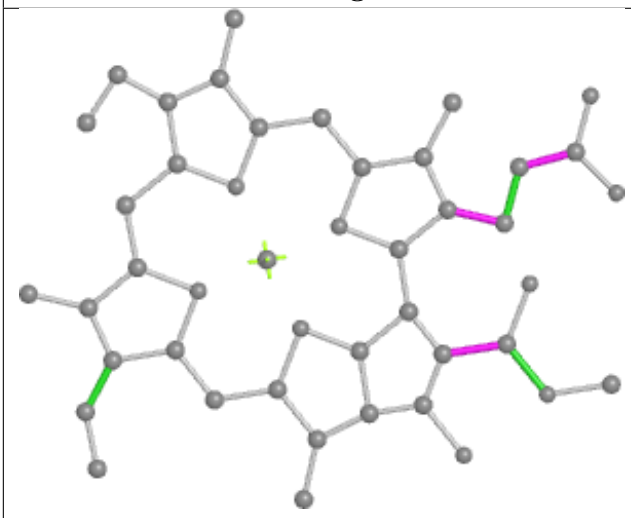

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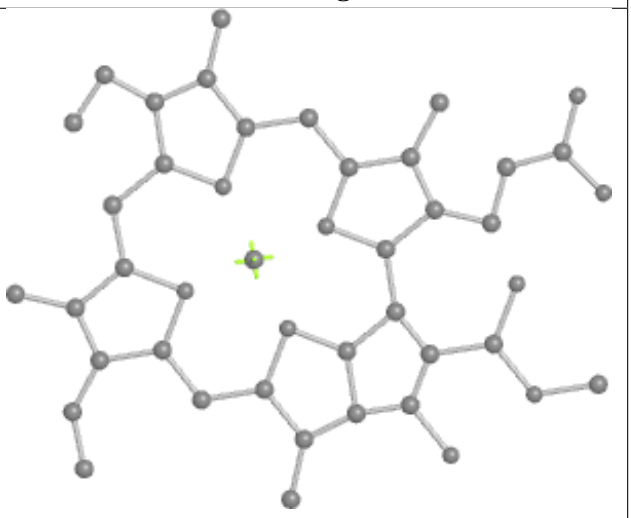

Rings

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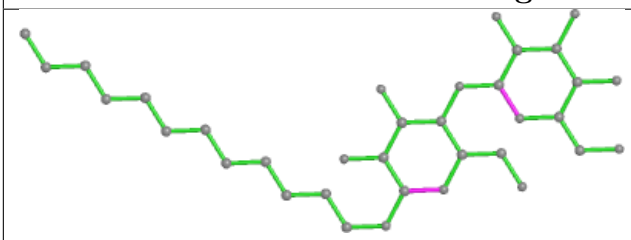

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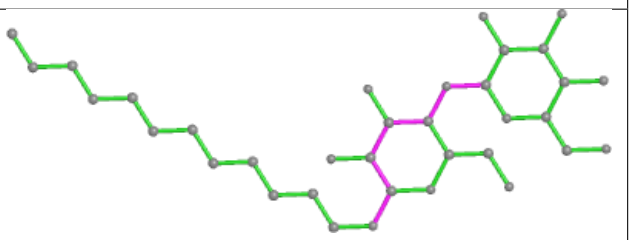

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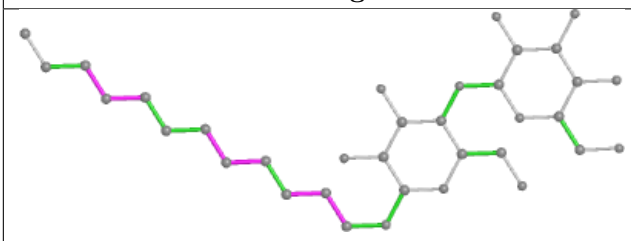

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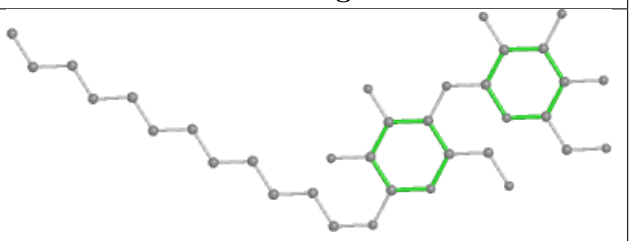
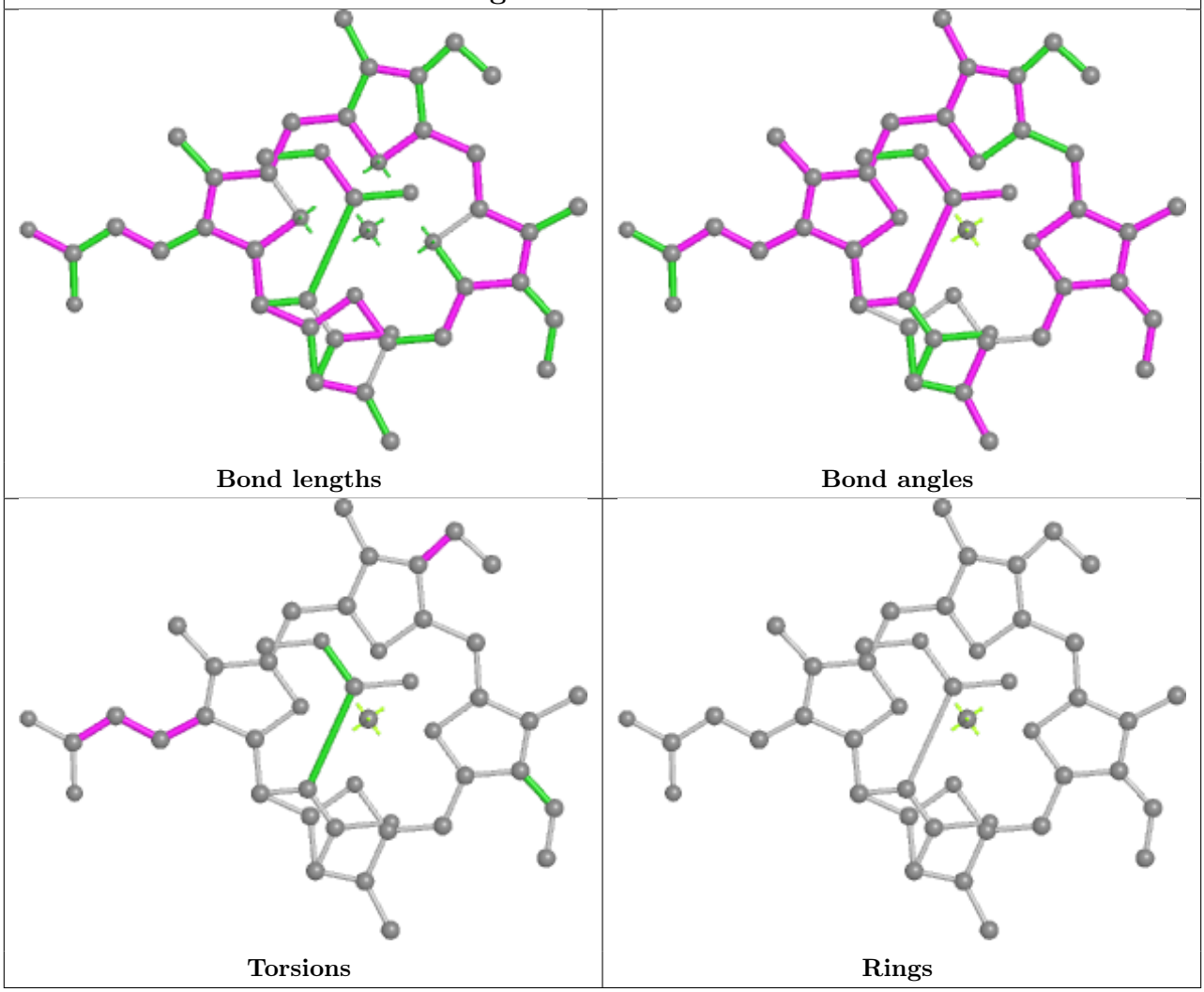


Rings

Ligand KC1 35 309



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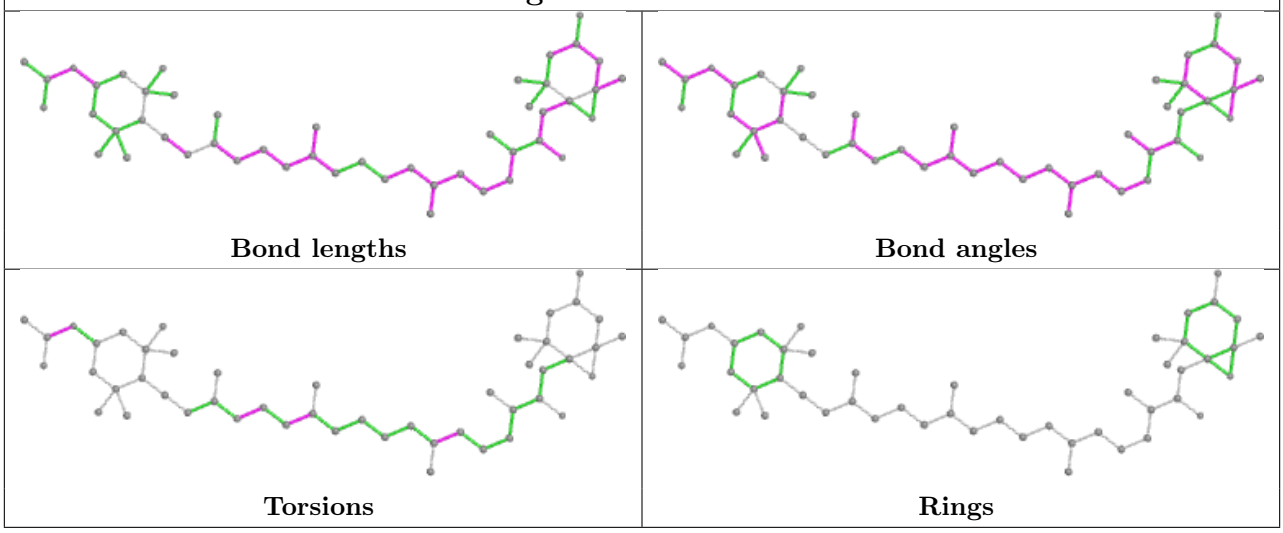

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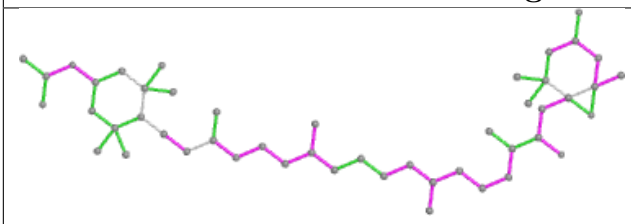
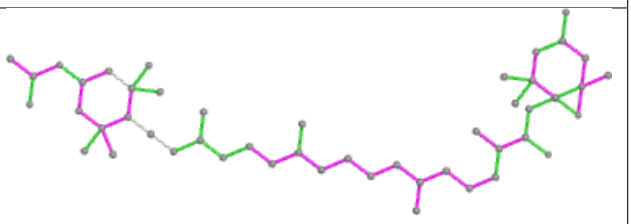
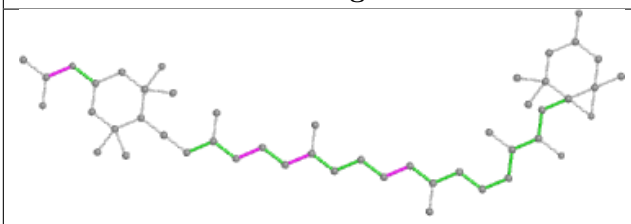
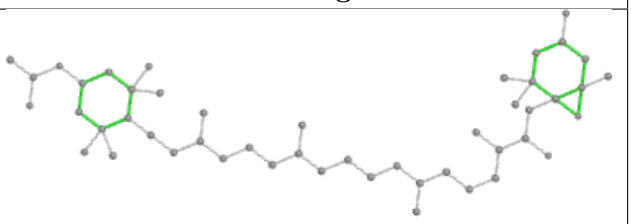
 Bond lengths	 Bond angles
 Torsions	 Rings

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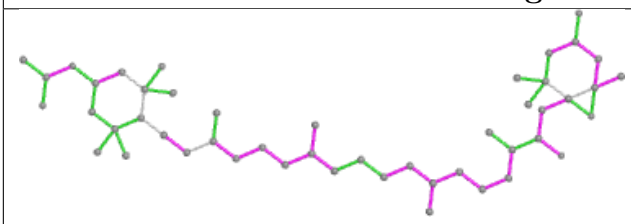
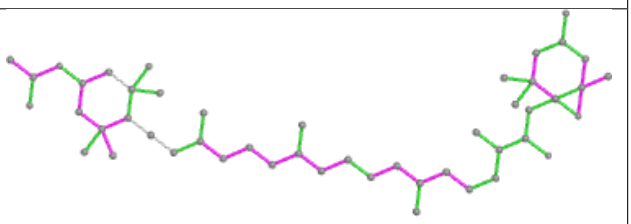
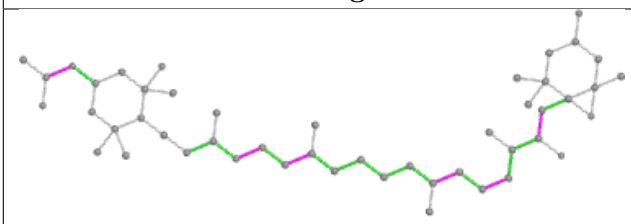
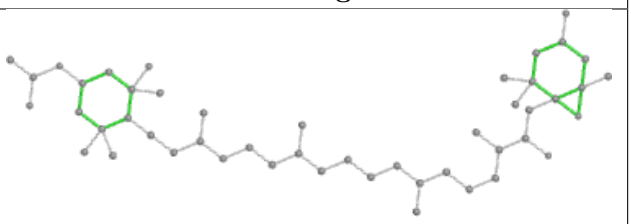
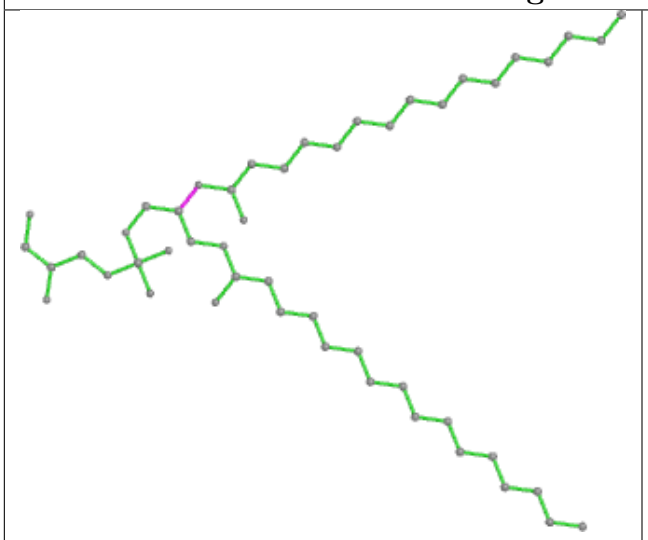
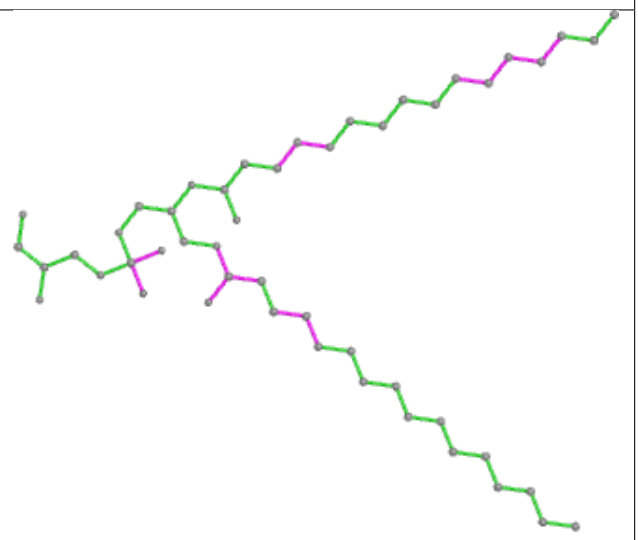
 Bond lengths	 Bond angles
 Torsions	 Rings

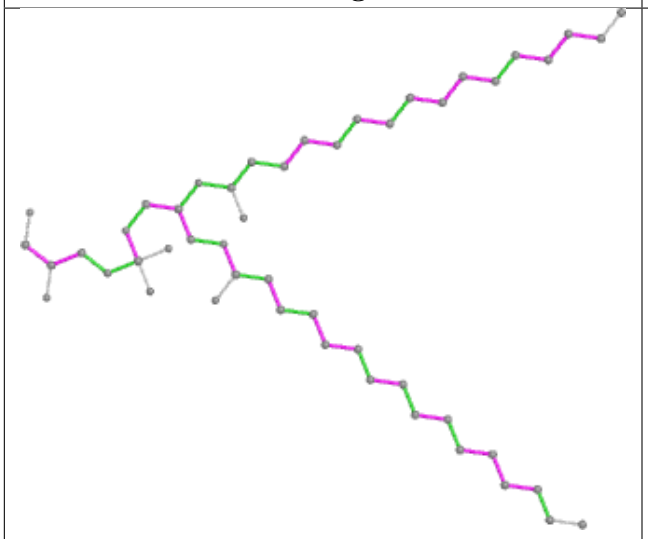
Ligand LHG d 407



Bond lengths



Bond angles



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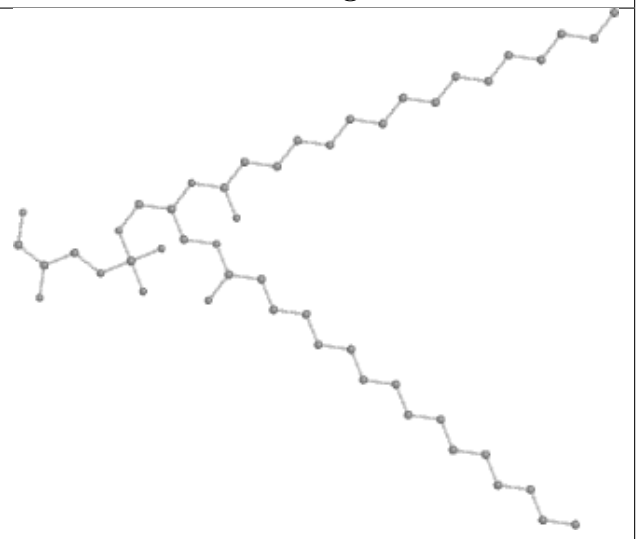
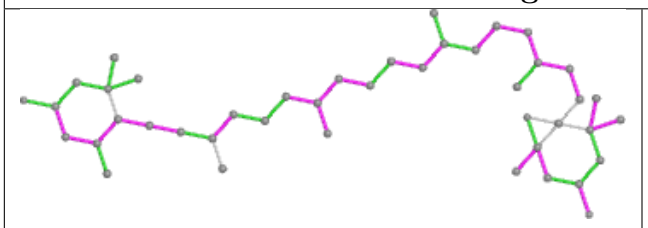


Rings

Ligand DD6 20 312



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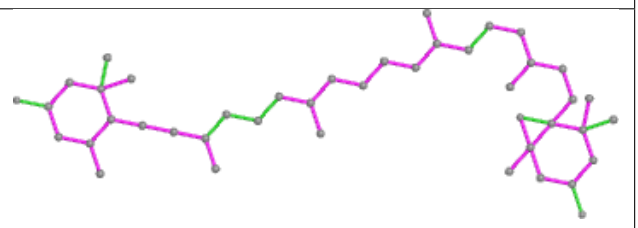
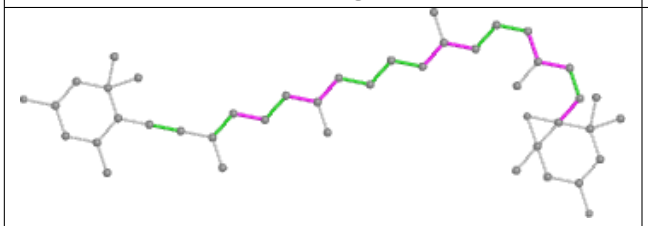
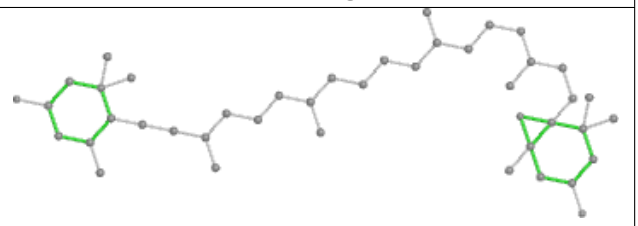


Bond angles



Torsions



Rings

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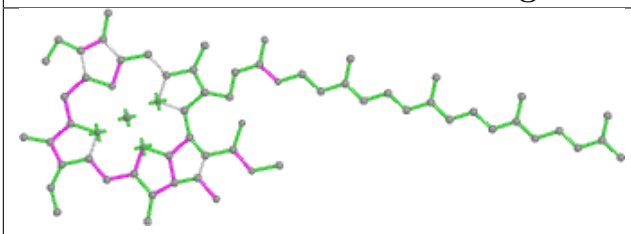
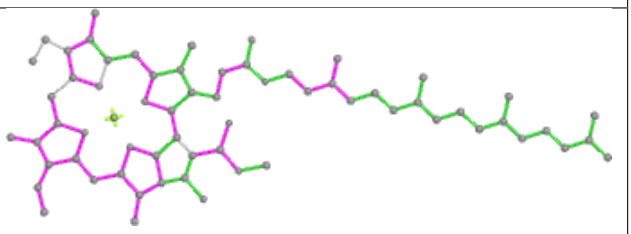
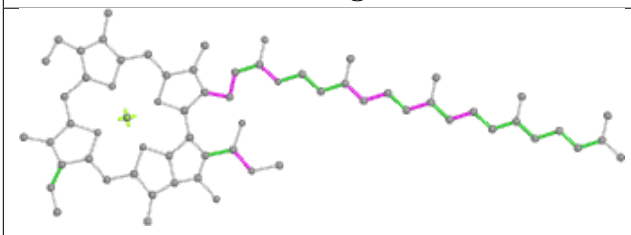
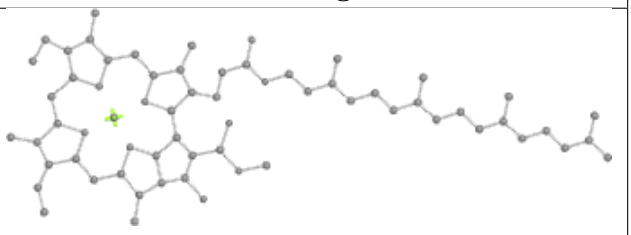
 Bond lengths	 Bond angles
 Torsions	 Rings

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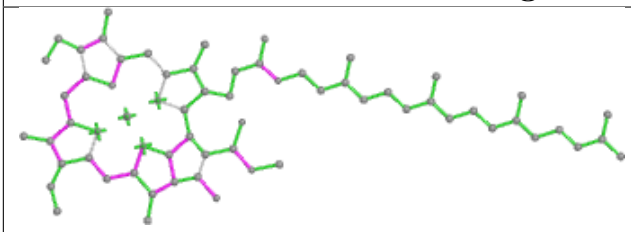
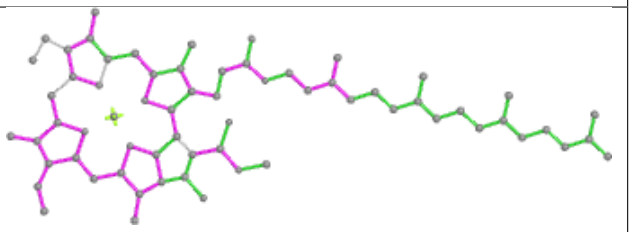
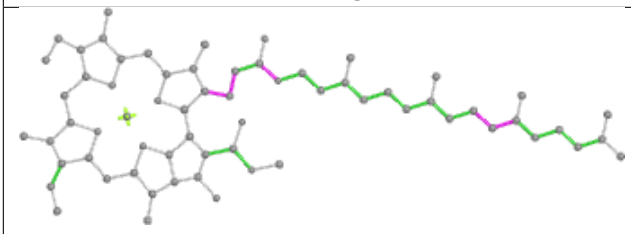
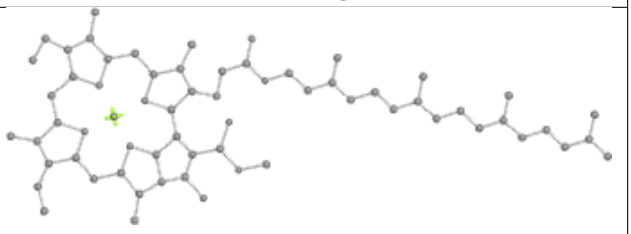
 Bond lengths	 Bond angles
 Torsions	 Rings

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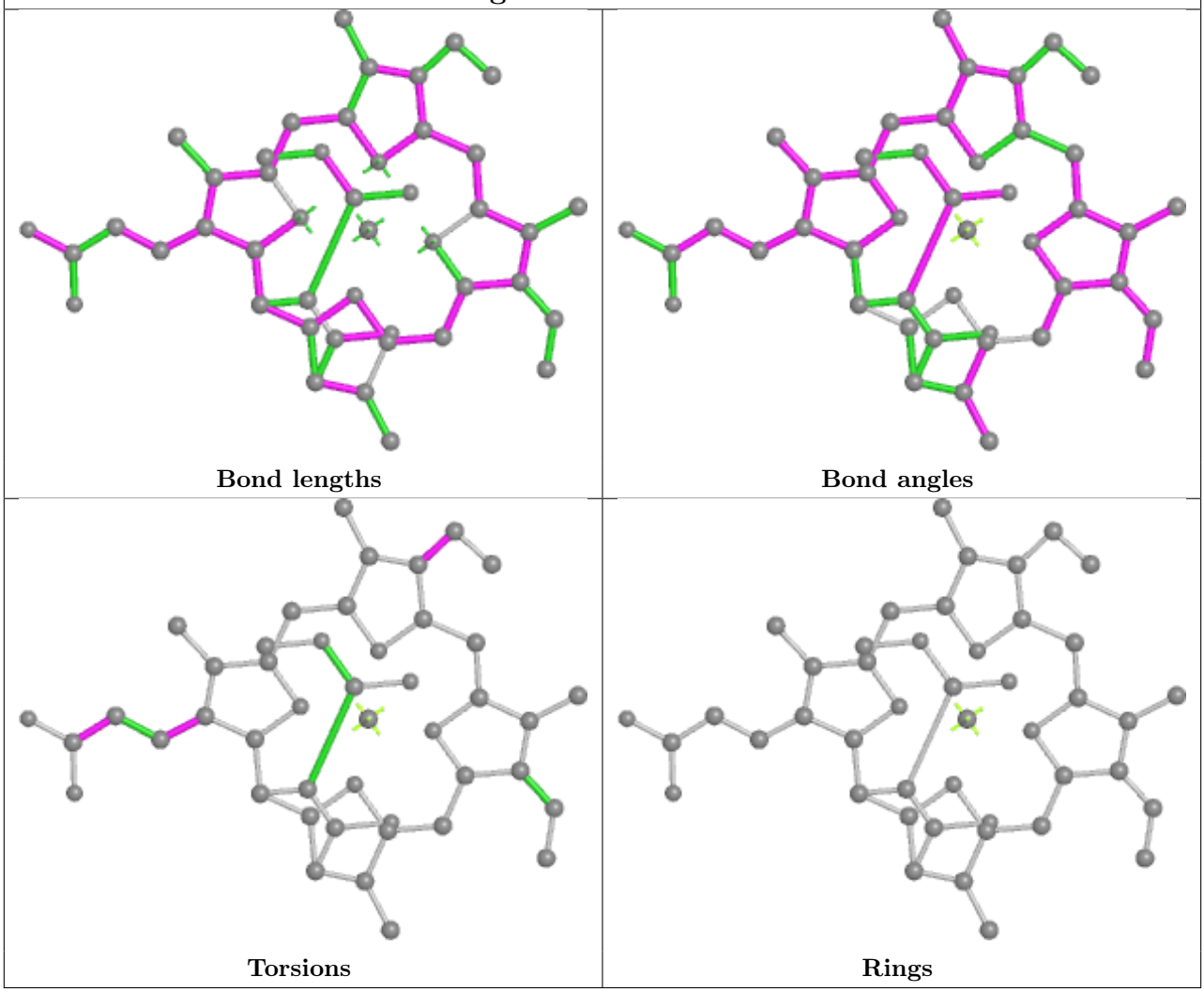

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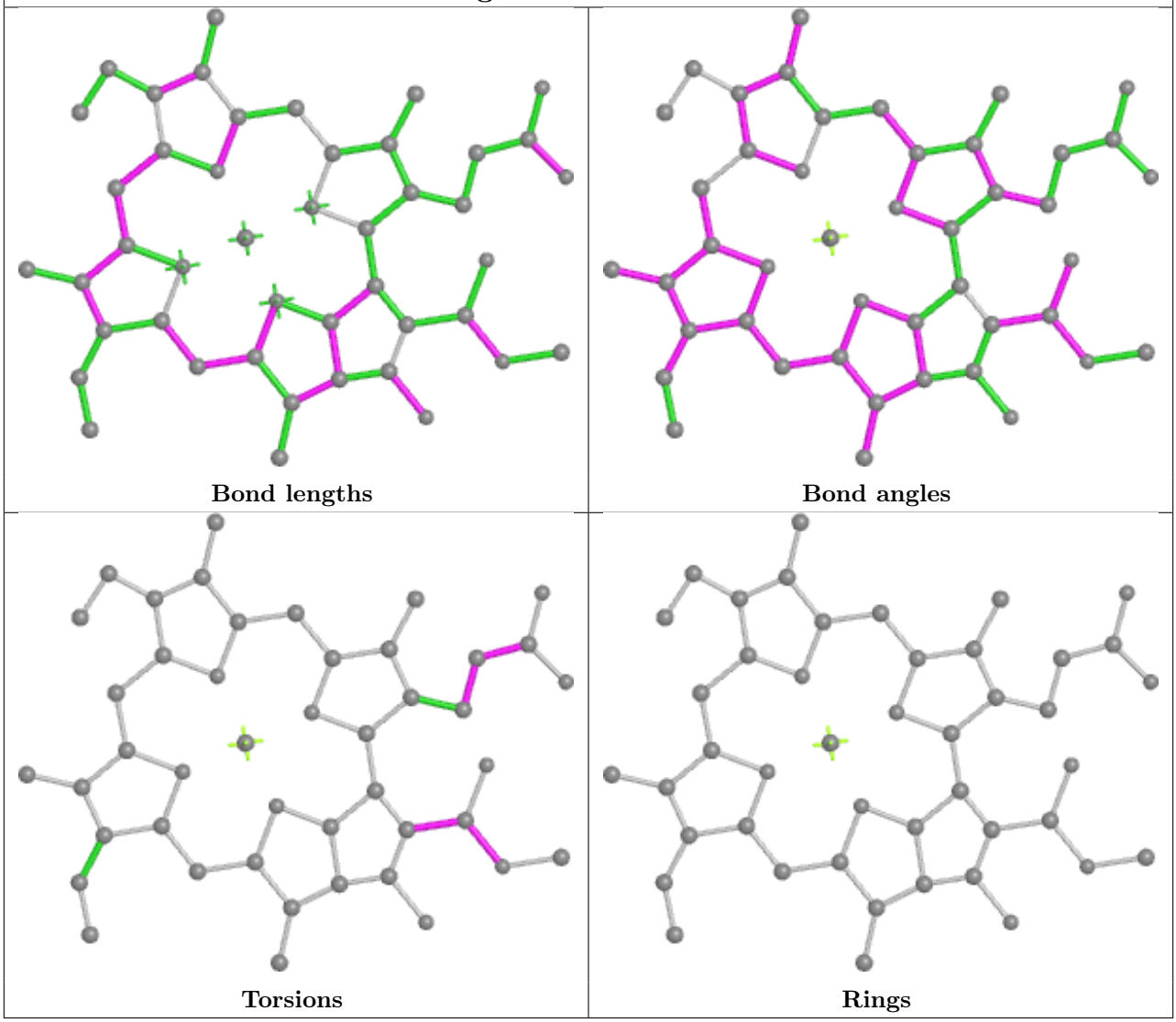

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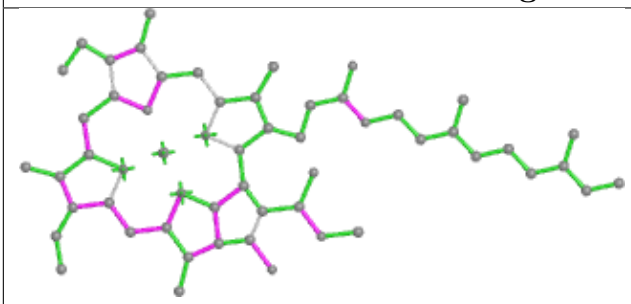
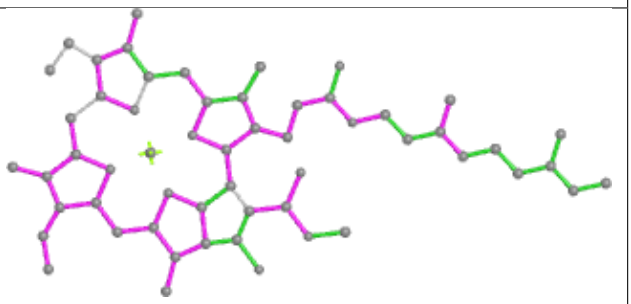
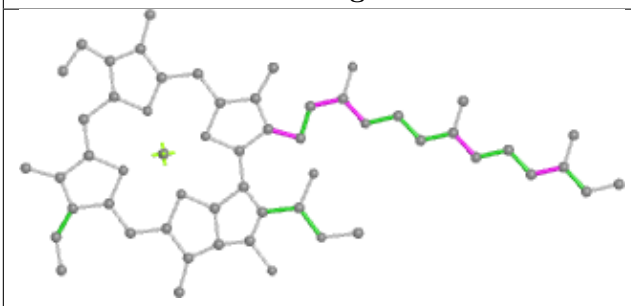
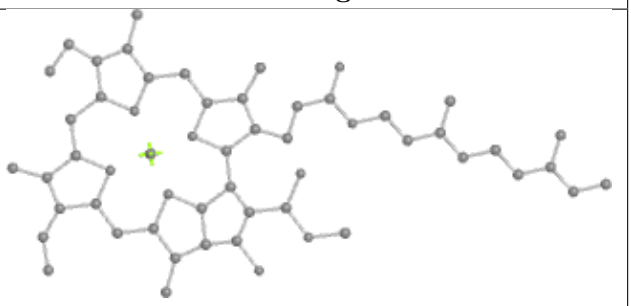
 Bond lengths	 Bond angles
 Torsions	 Rings

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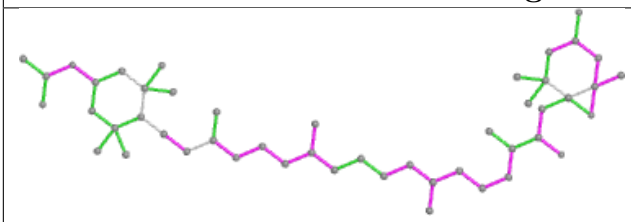
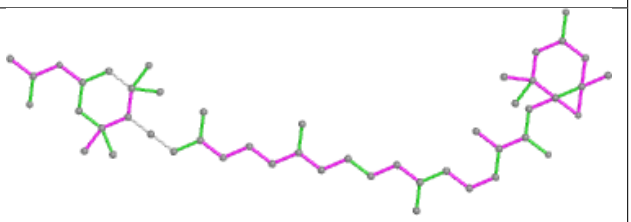
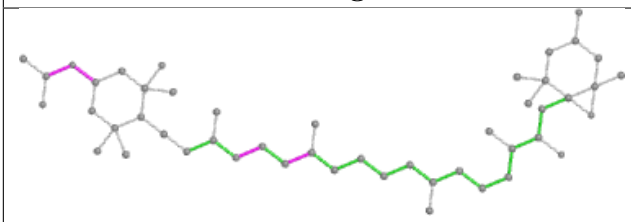
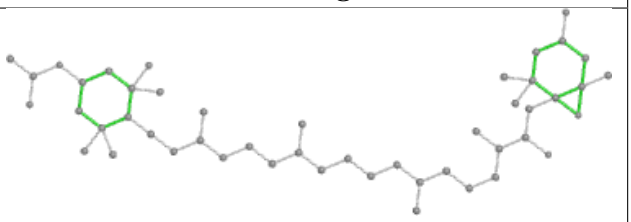
 Bond lengths	 Bond angles
 Torsions	 Rings

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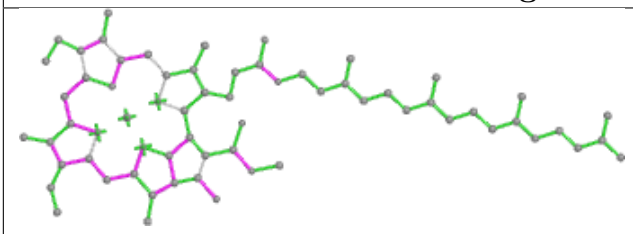

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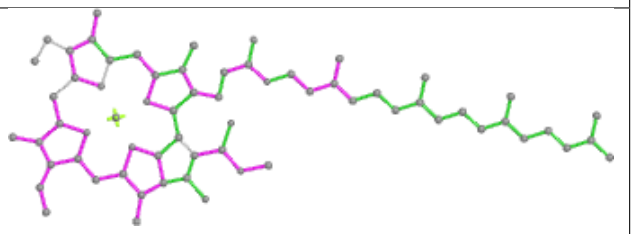

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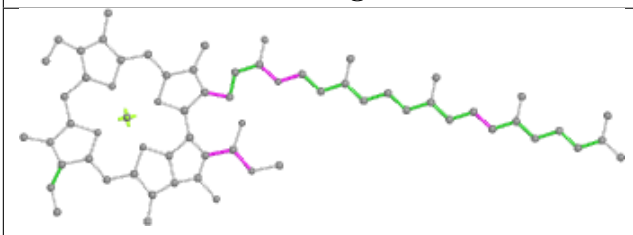

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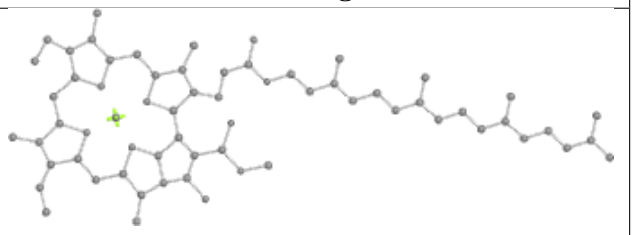
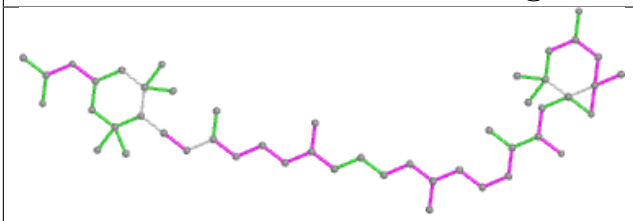


Rings

Ligand A86 21 215



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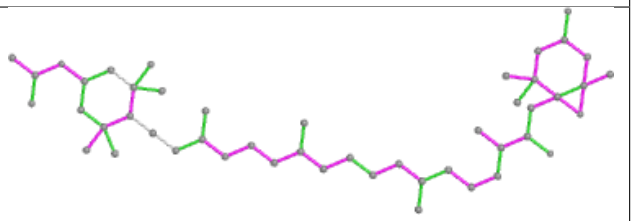

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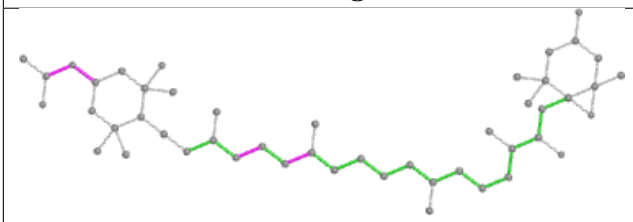

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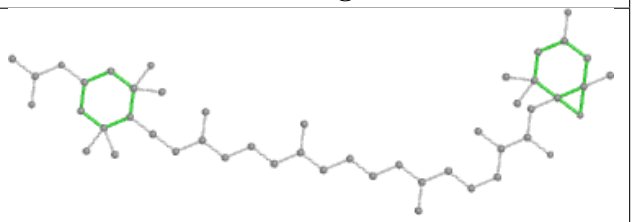
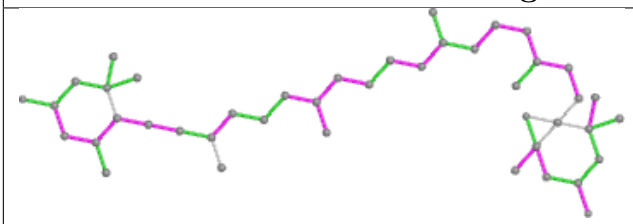


Rings

Ligand DD6 41 216



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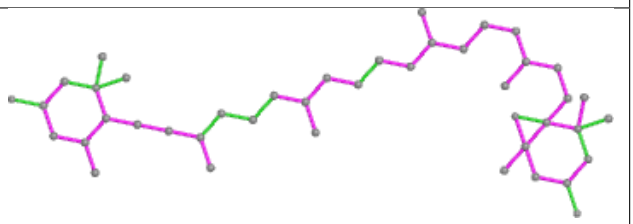

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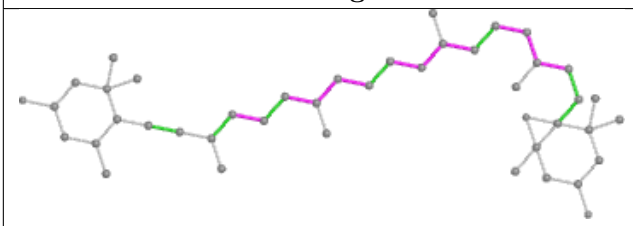

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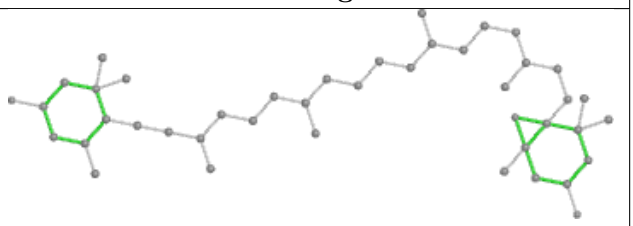

Rings

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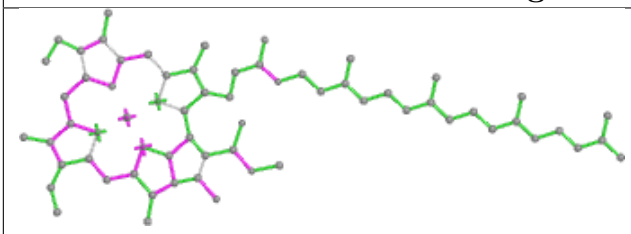
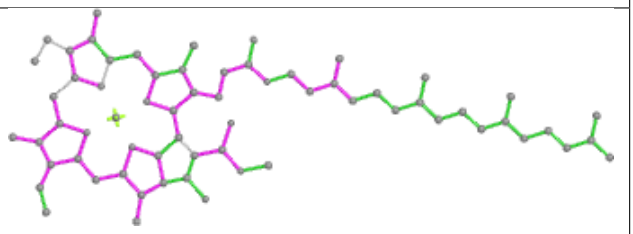
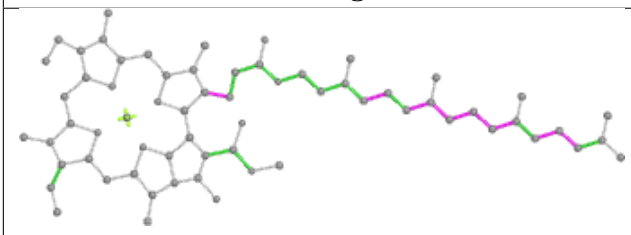
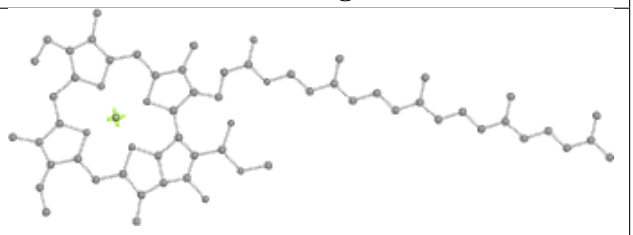
 Bond lengths	 Bond angles
 Torsions	 Rings

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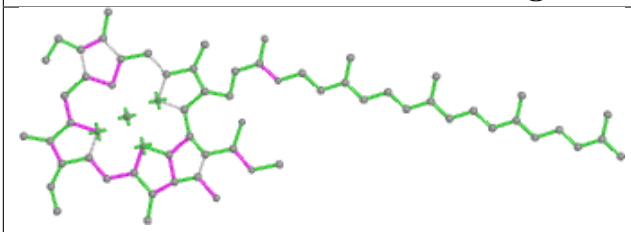
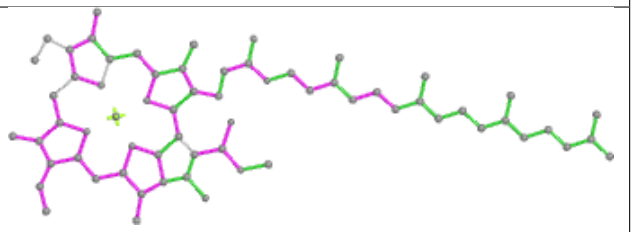
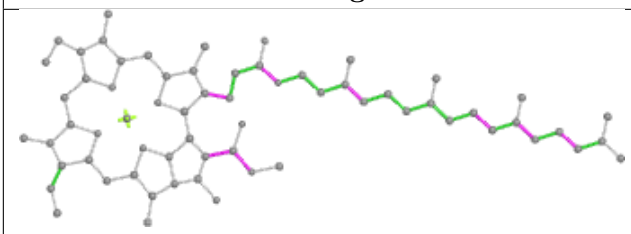
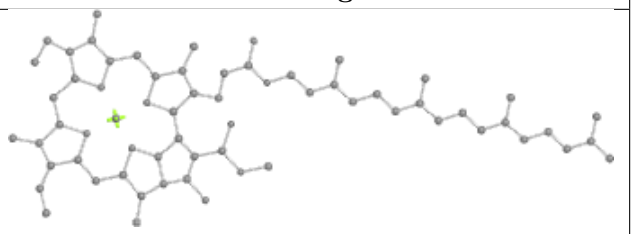
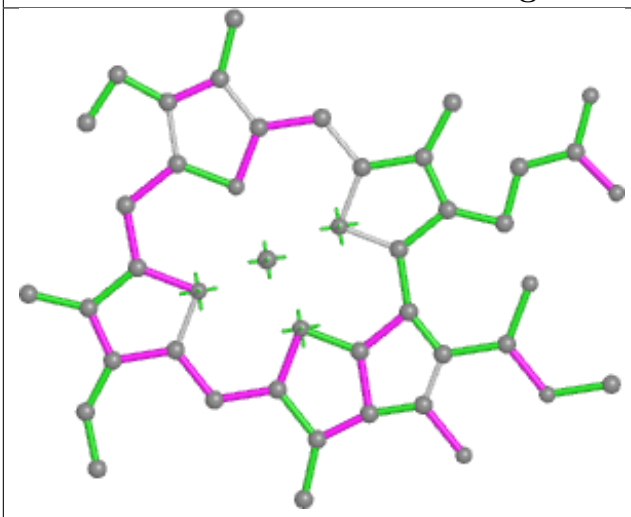
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 14 310



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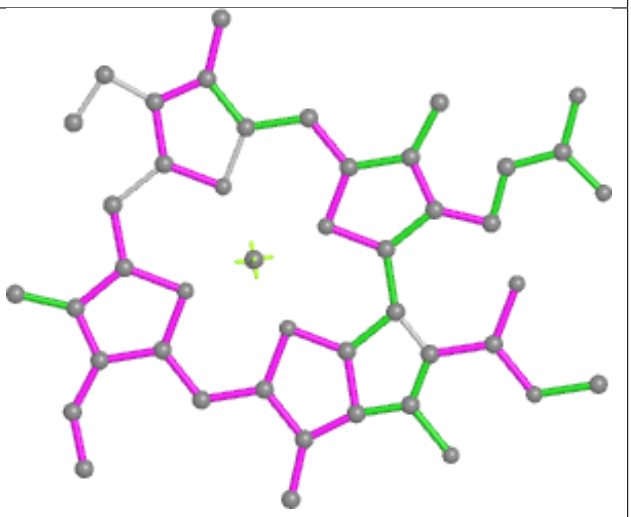
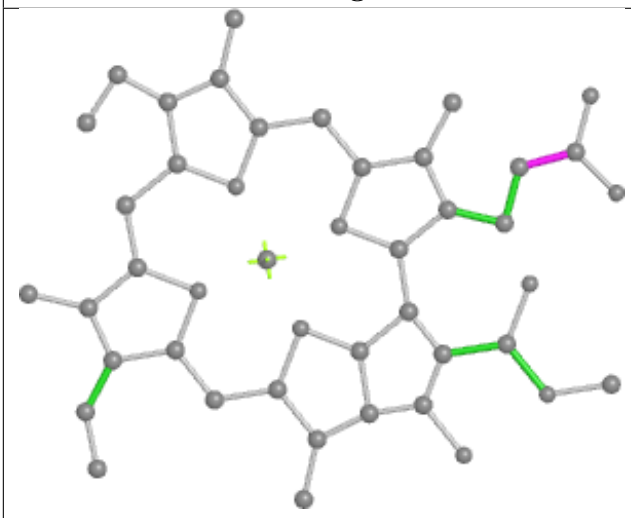


Bond angles



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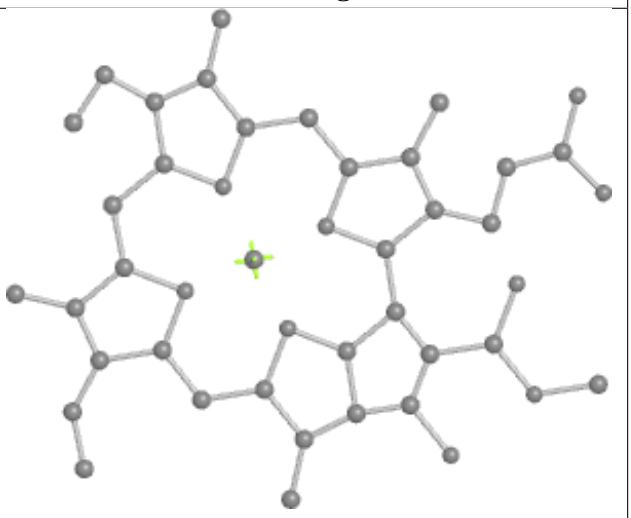

Rings

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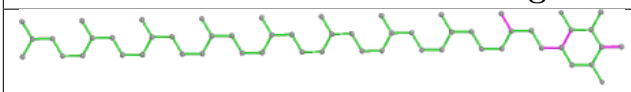

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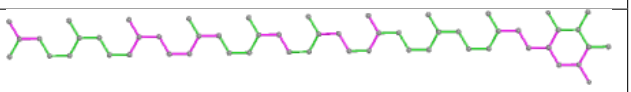

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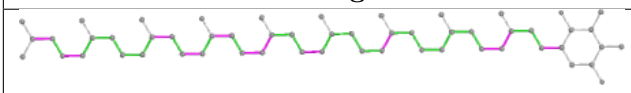

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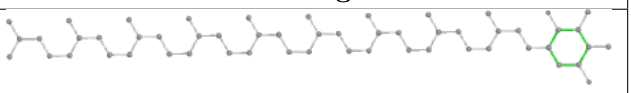

Rings

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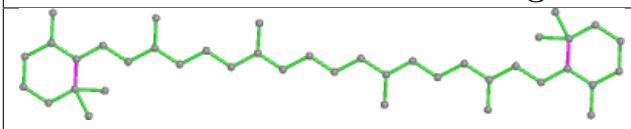
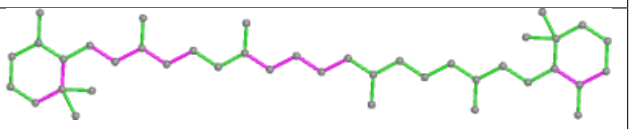
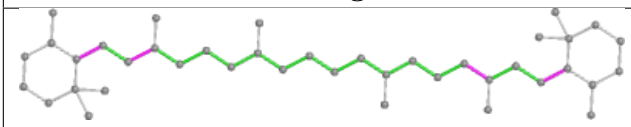
 Bond lengths	 Bond angles
 Torsions	Rings

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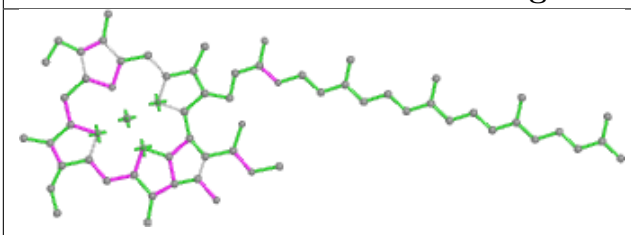
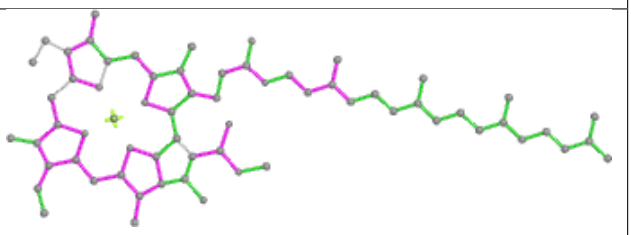
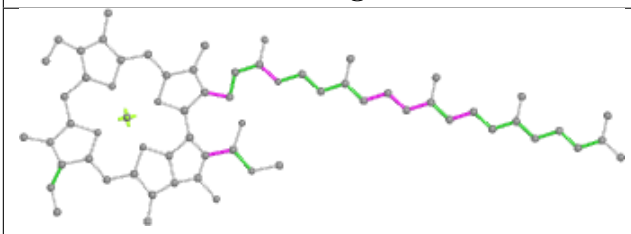
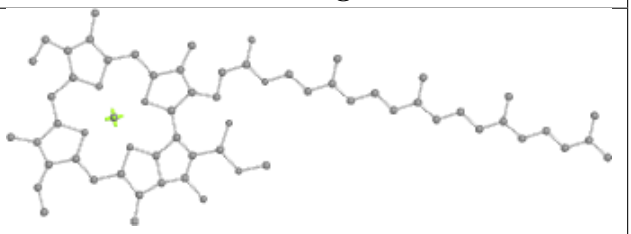
 Bond lengths	 Bond angles
 Torsions	 Rings

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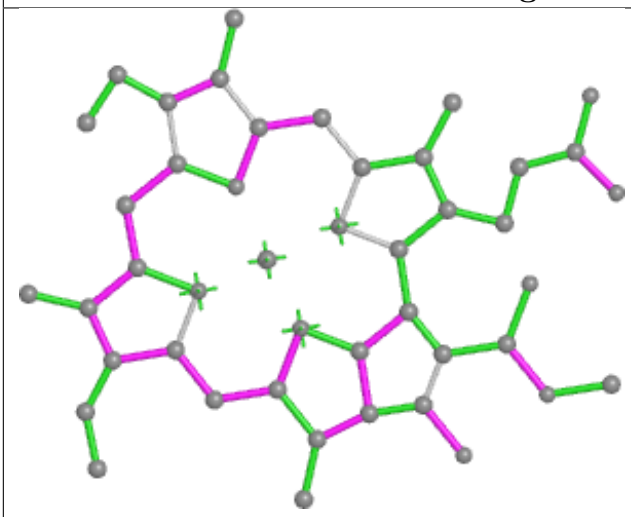

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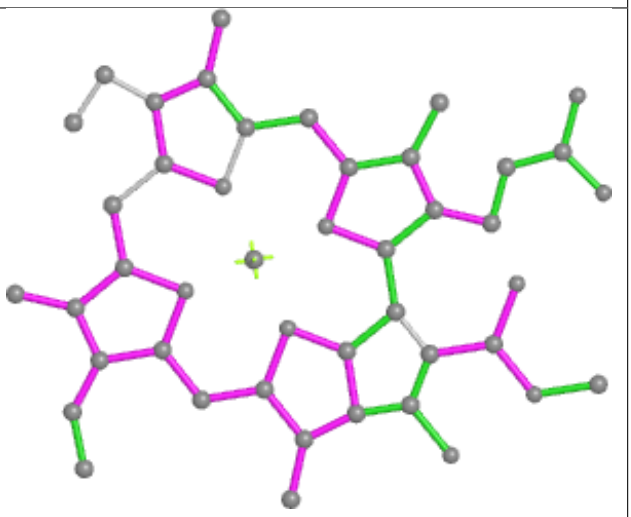

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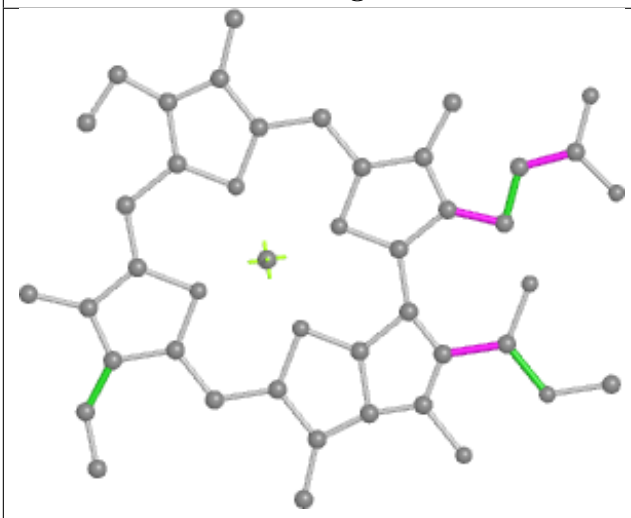

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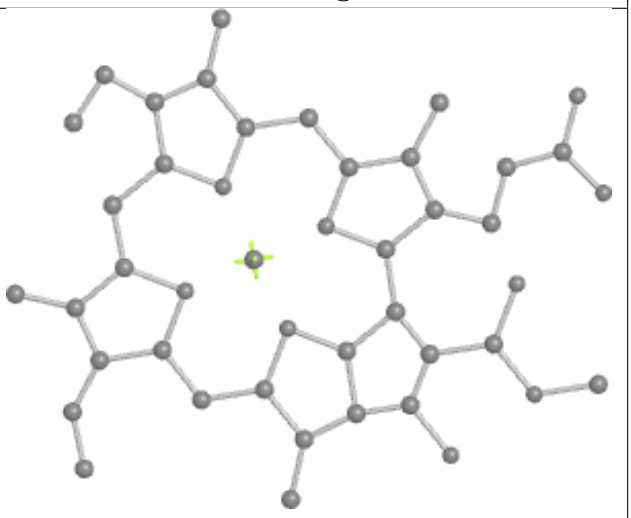

Rings

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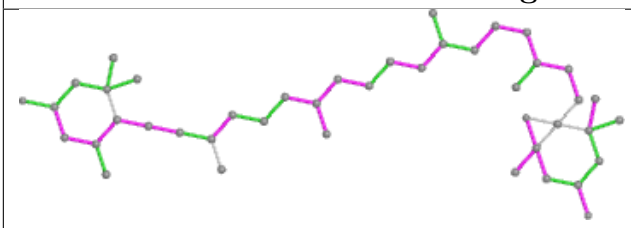

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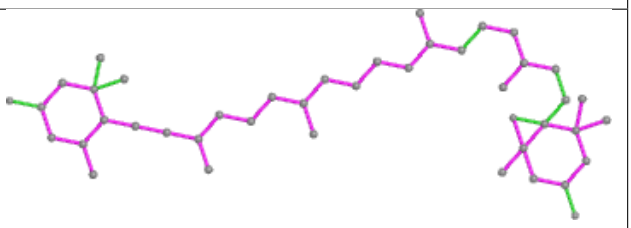

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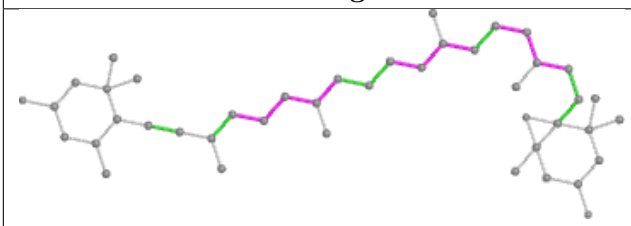

Torsions

Rings

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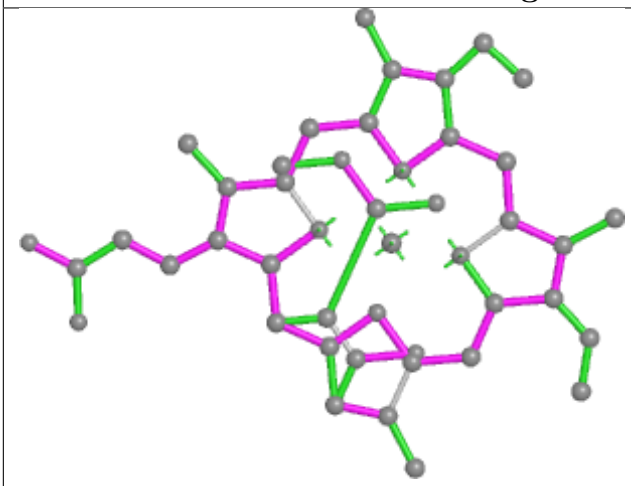

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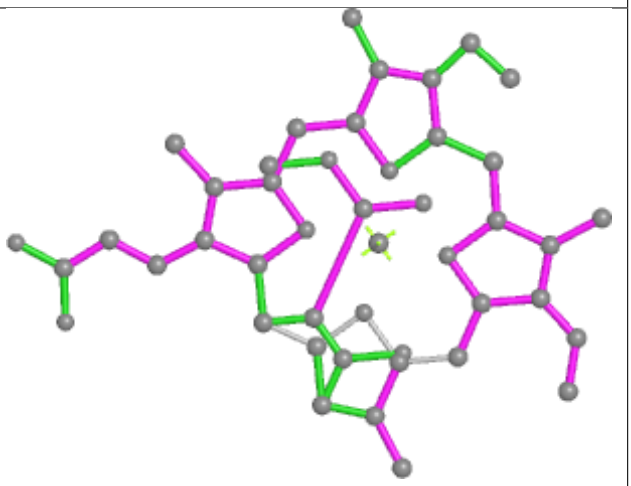

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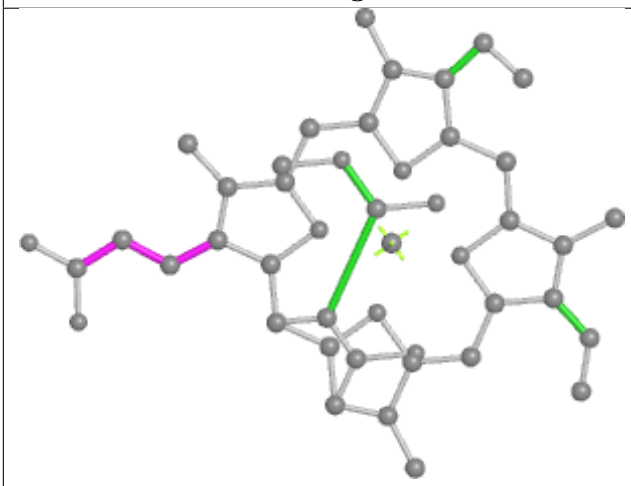

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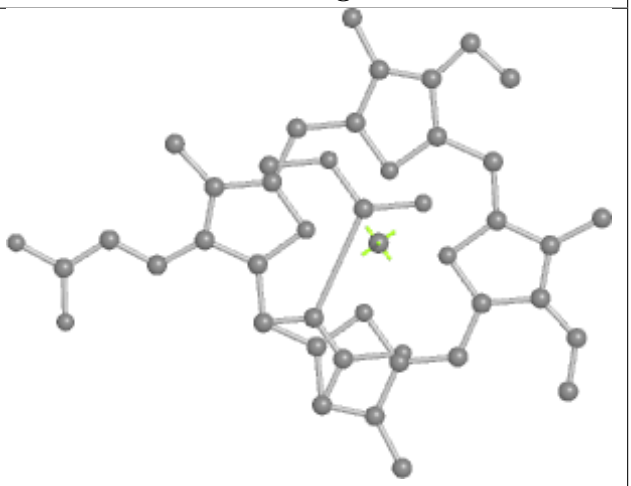

Rings

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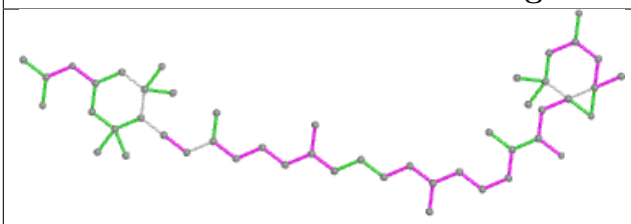

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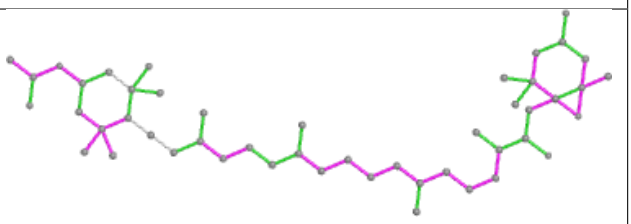

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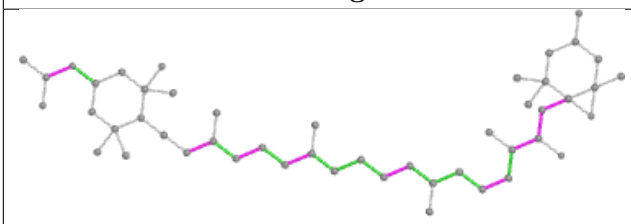

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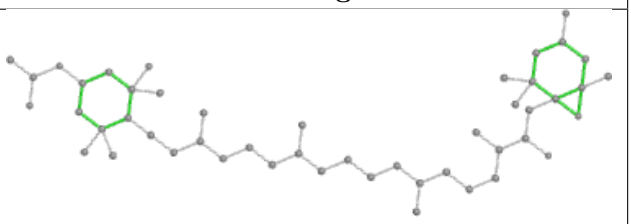

Rings

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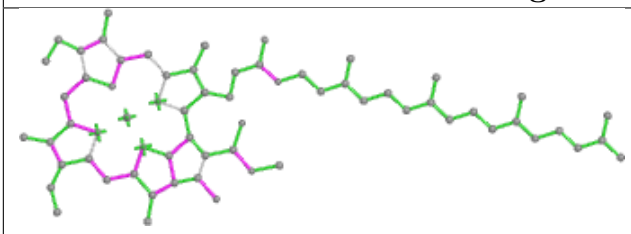
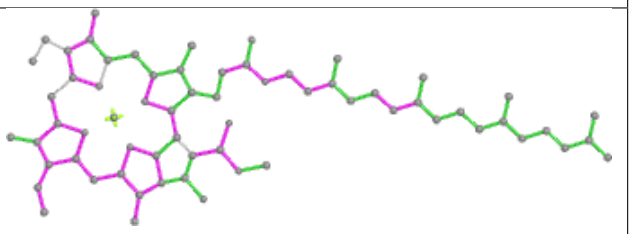
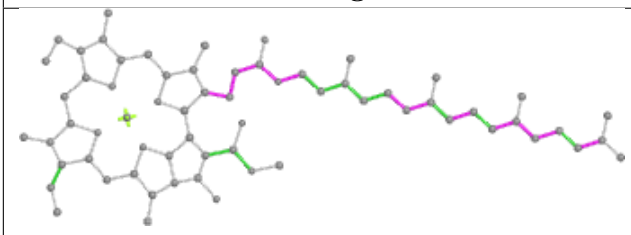
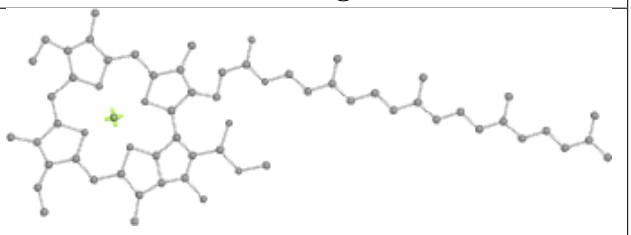
 Bond lengths	 Bond angles
 Torsions	 Rings

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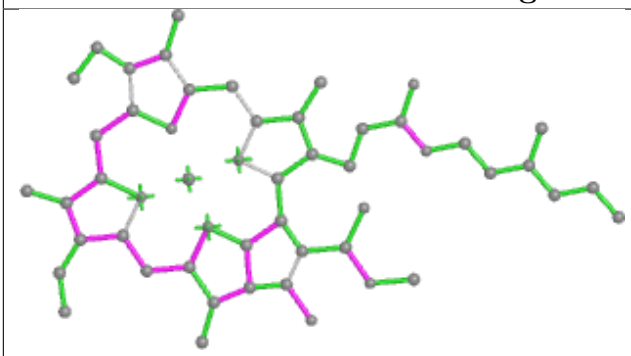
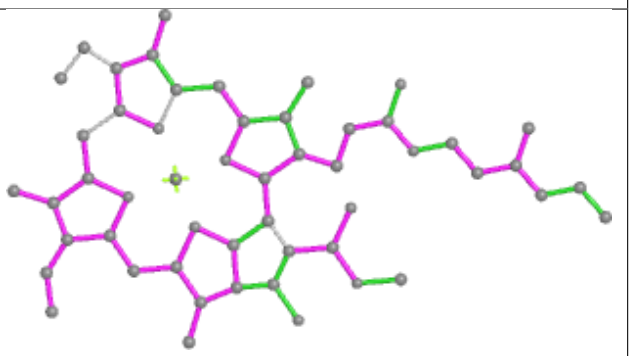
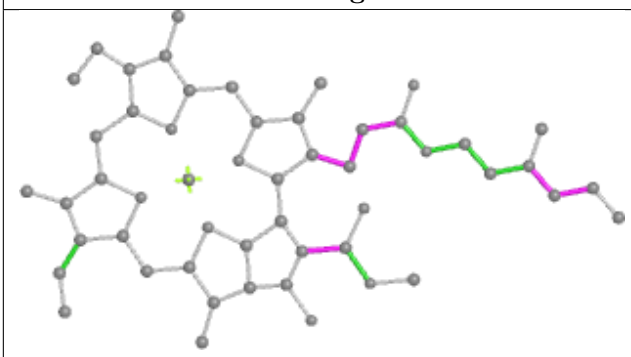
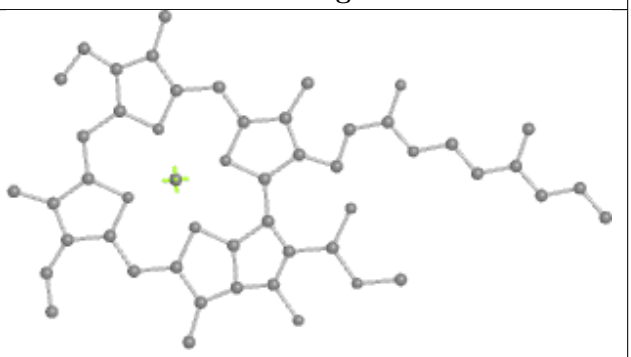
 Bond lengths	 Bond angles
 Torsions	 Rings

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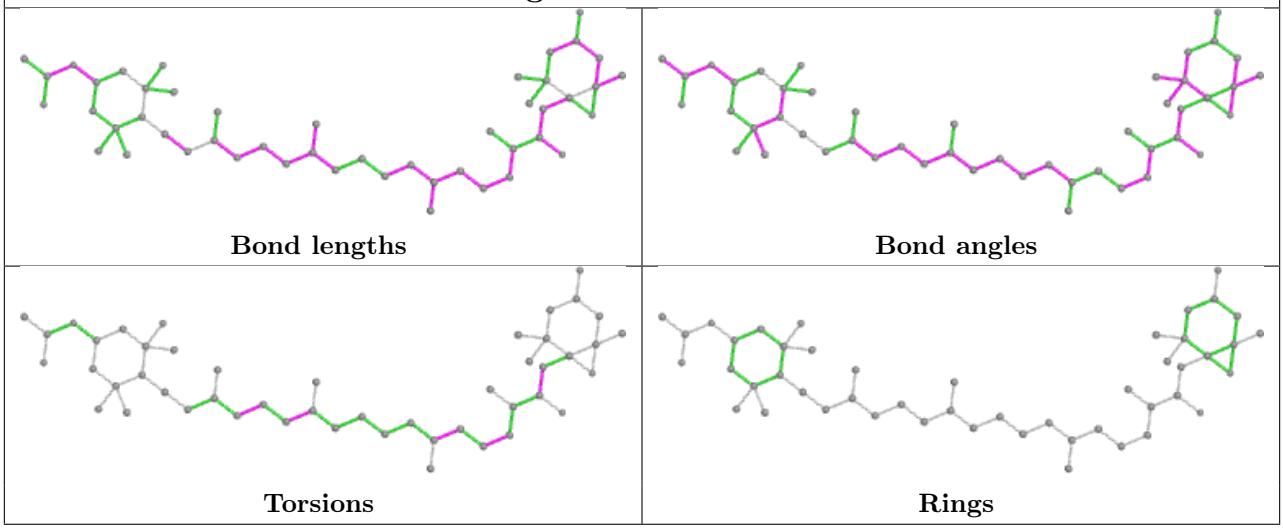

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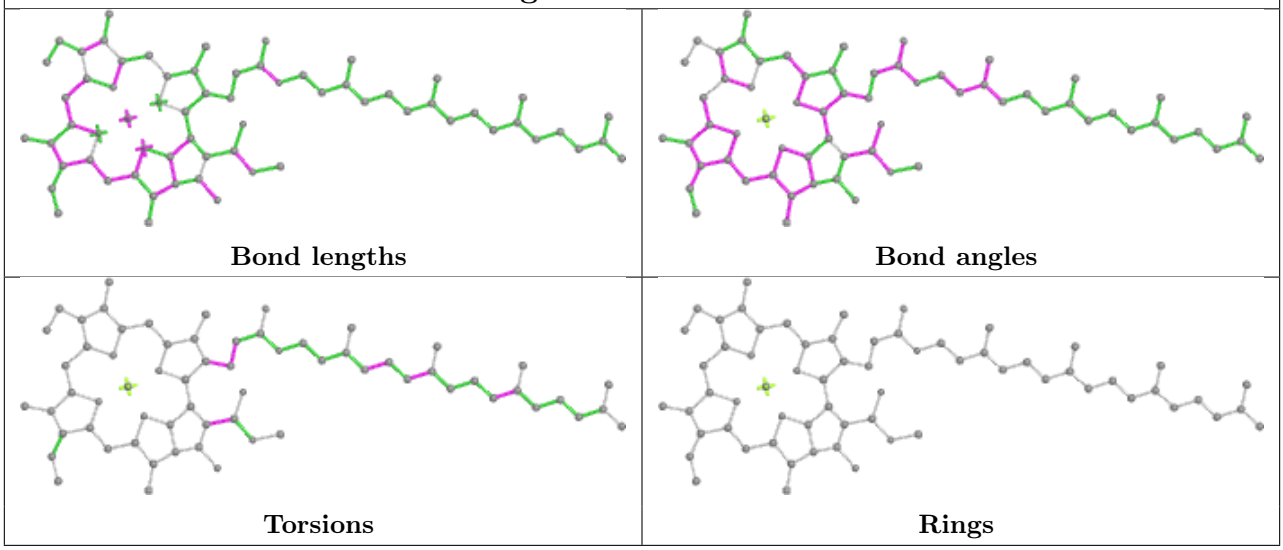

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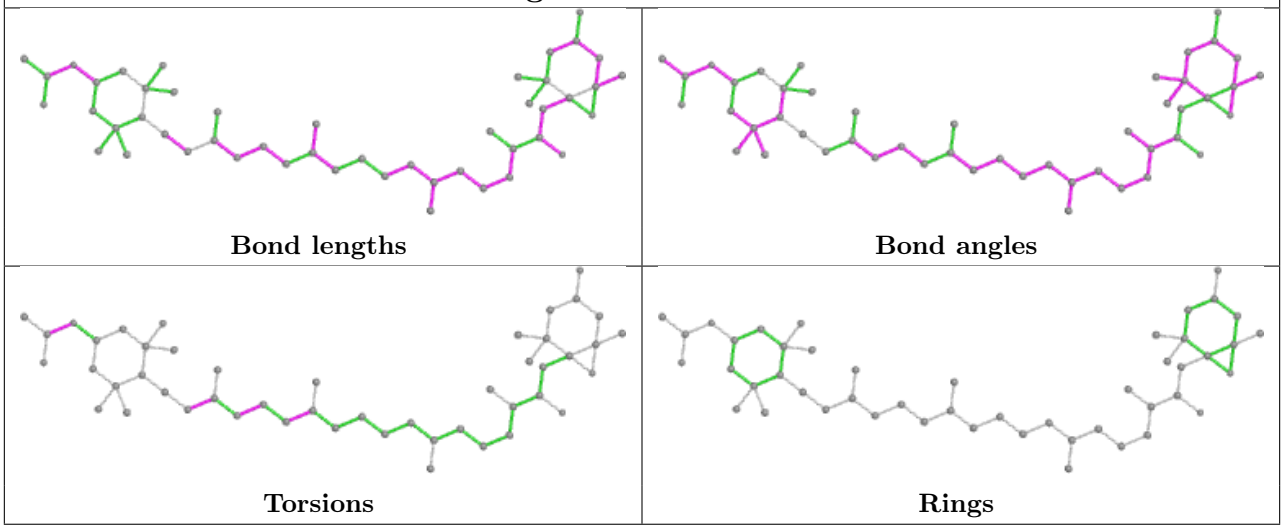

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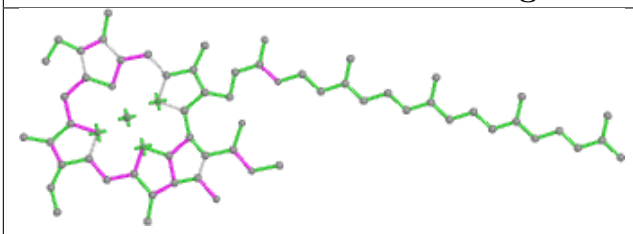

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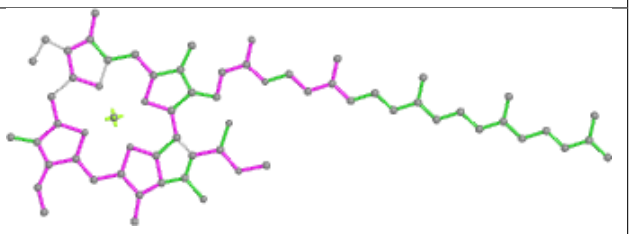
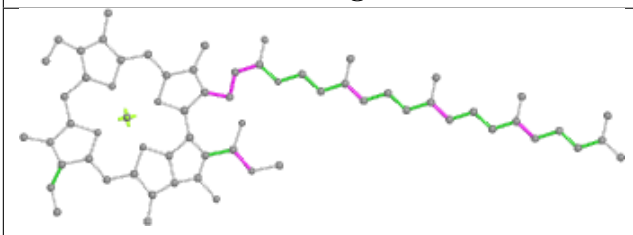
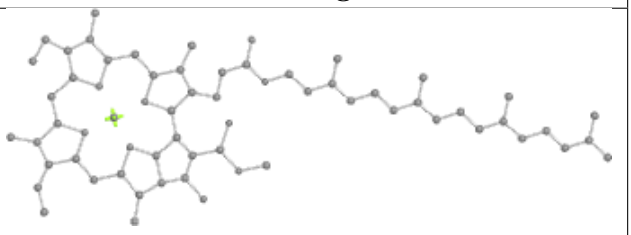


Bond angles

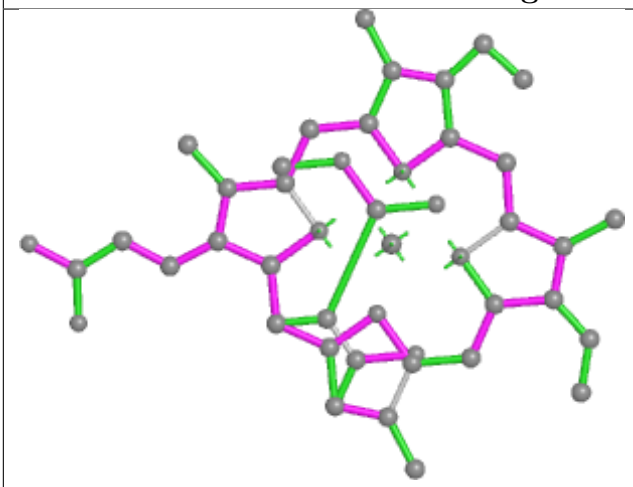


Torsions



Rings

Ligand KC1 36 305



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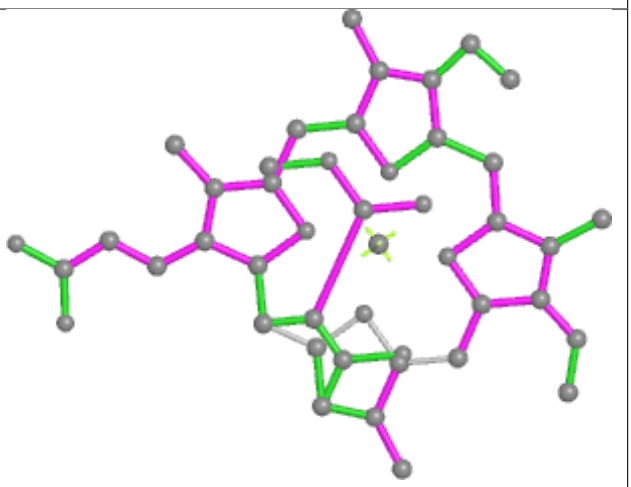

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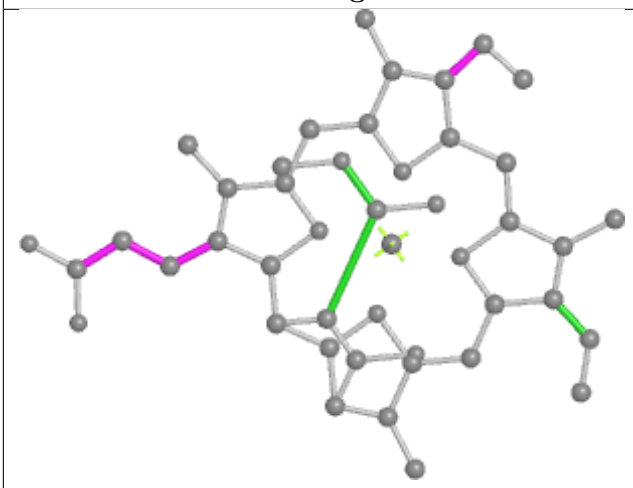

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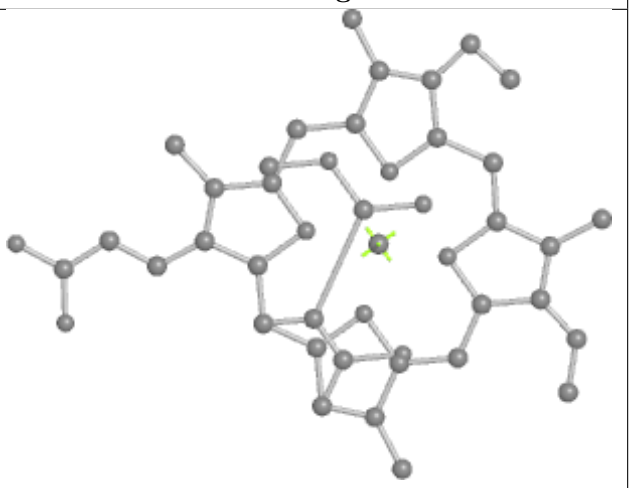

Rings

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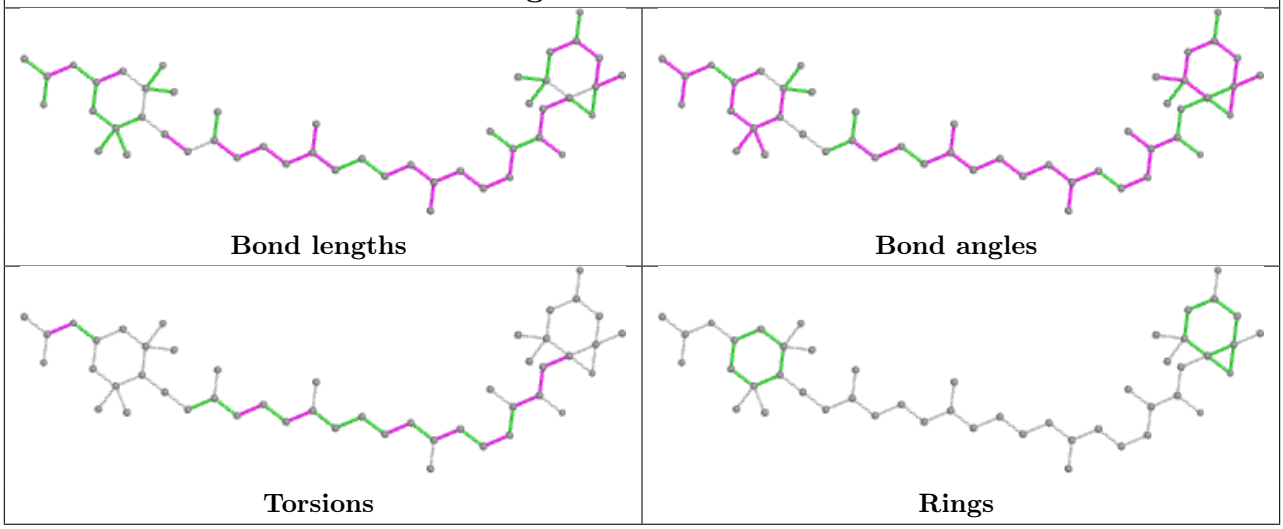

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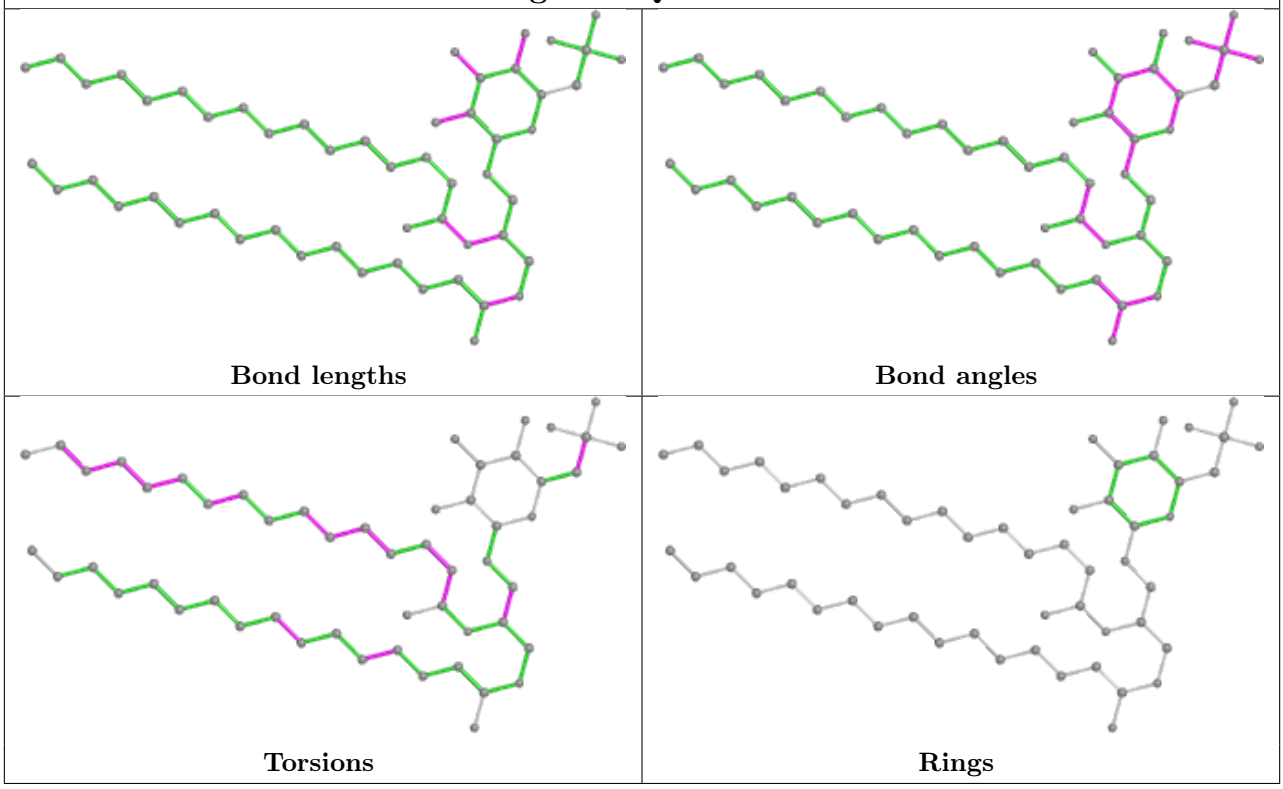

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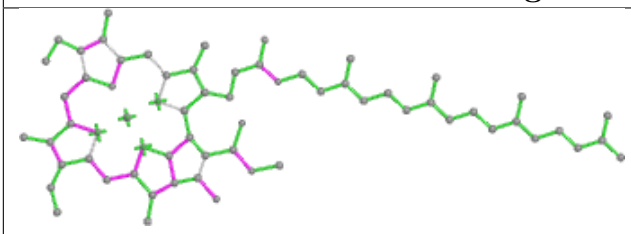
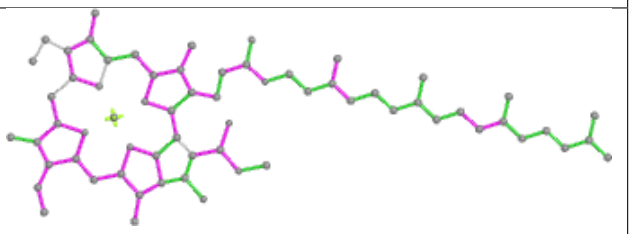
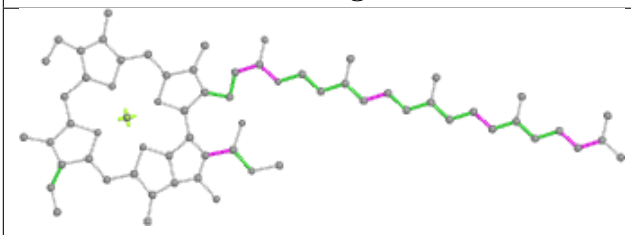


Bond lengths



Bond angles



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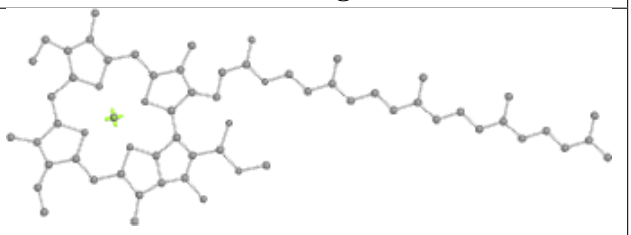
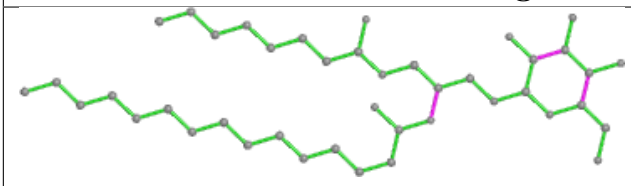


Rings

Ligand LMG 31 316



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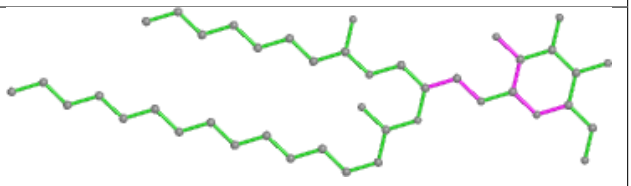

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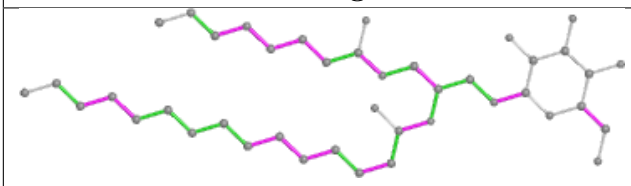

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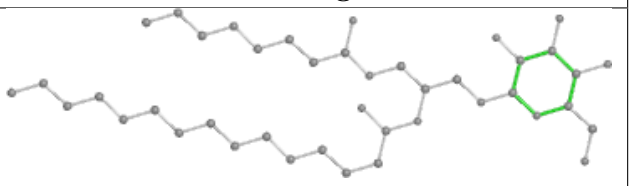
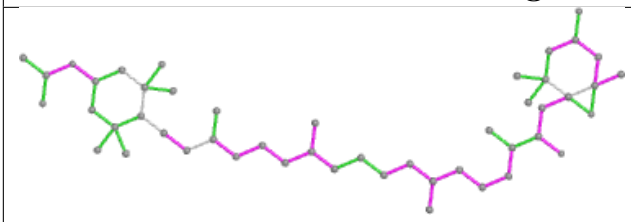


Rings

Ligand A86 18 212



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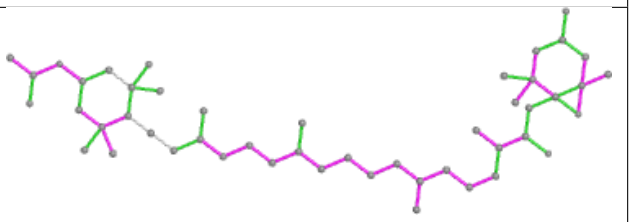

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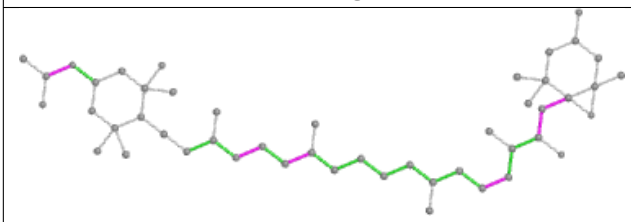

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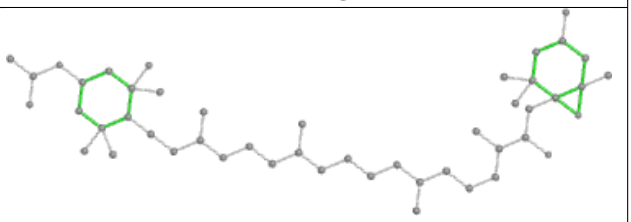

Rings

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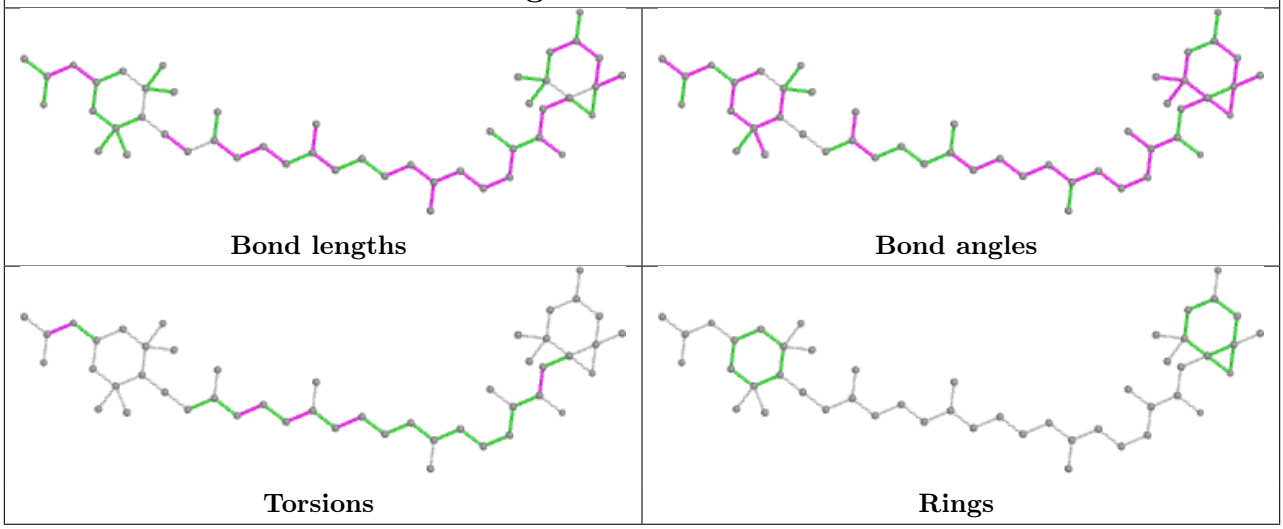
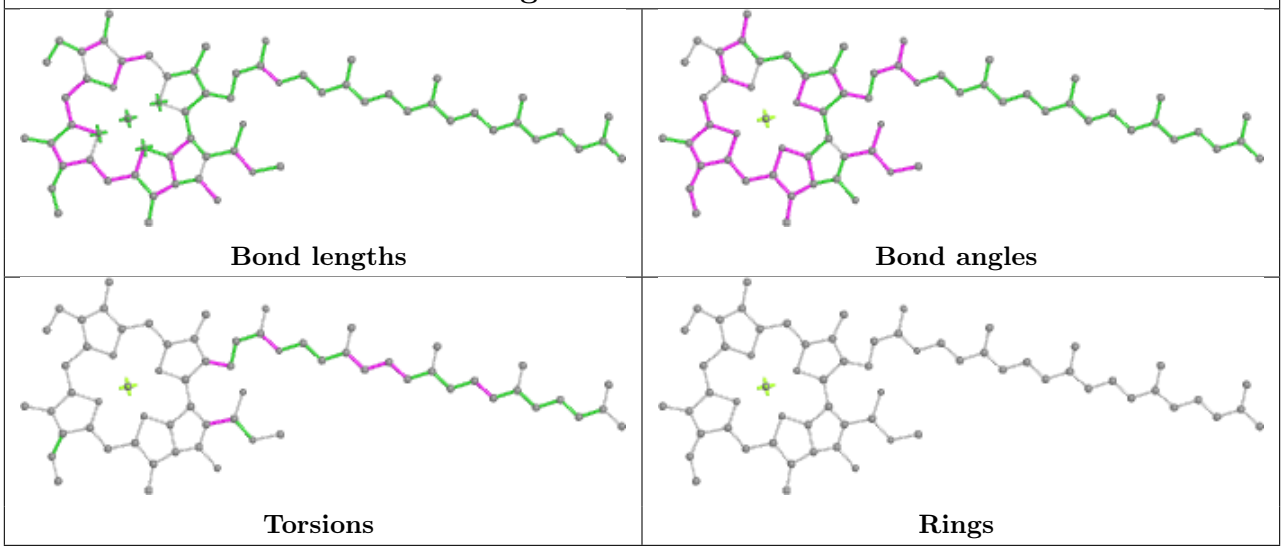
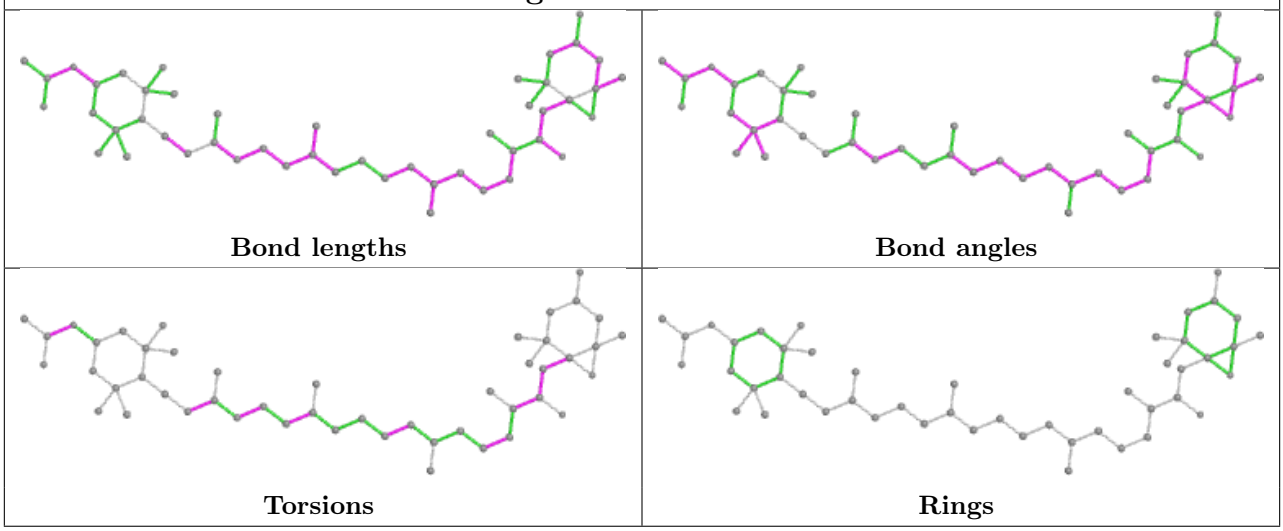


Ligand CLA 33 308



Ligand A86 20 311



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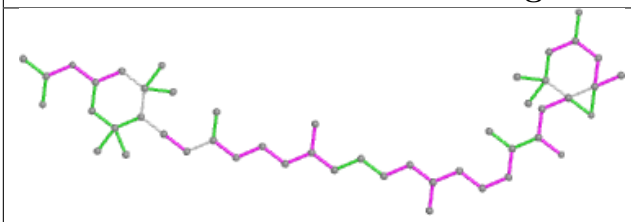
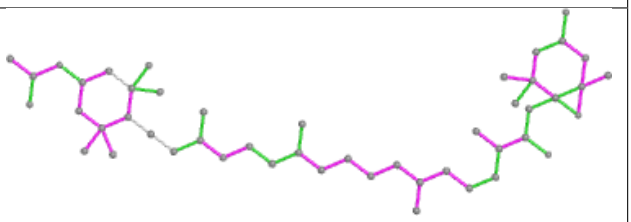
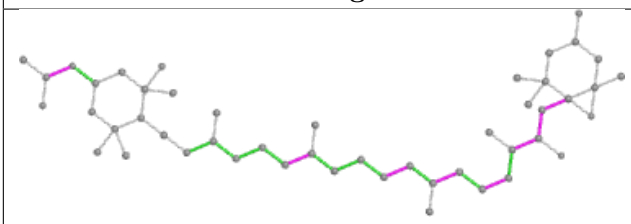
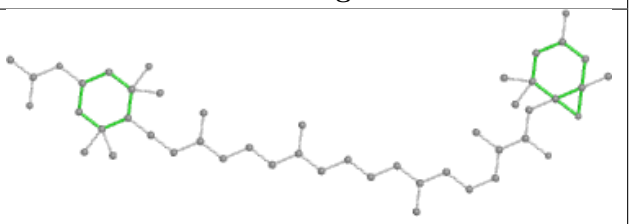
 Bond lengths	 Bond angles
 Torsions	 Rings

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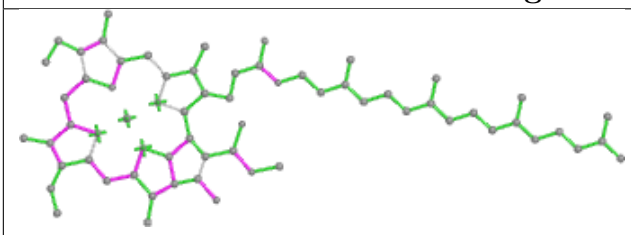
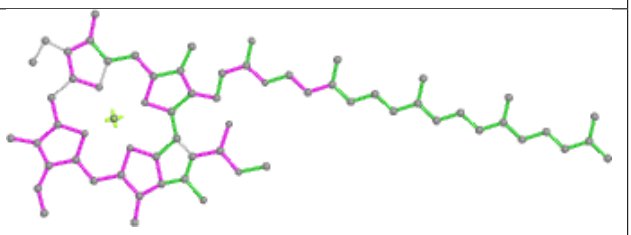
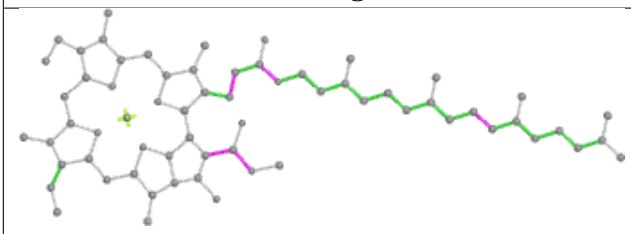
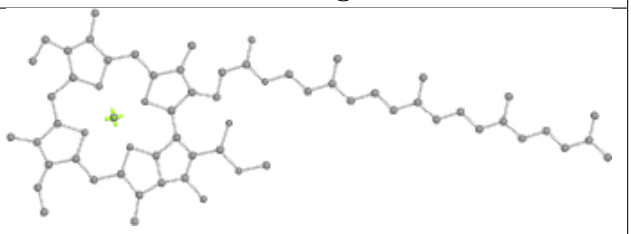
 Bond lengths	 Bond angles
 Torsions	 Rings

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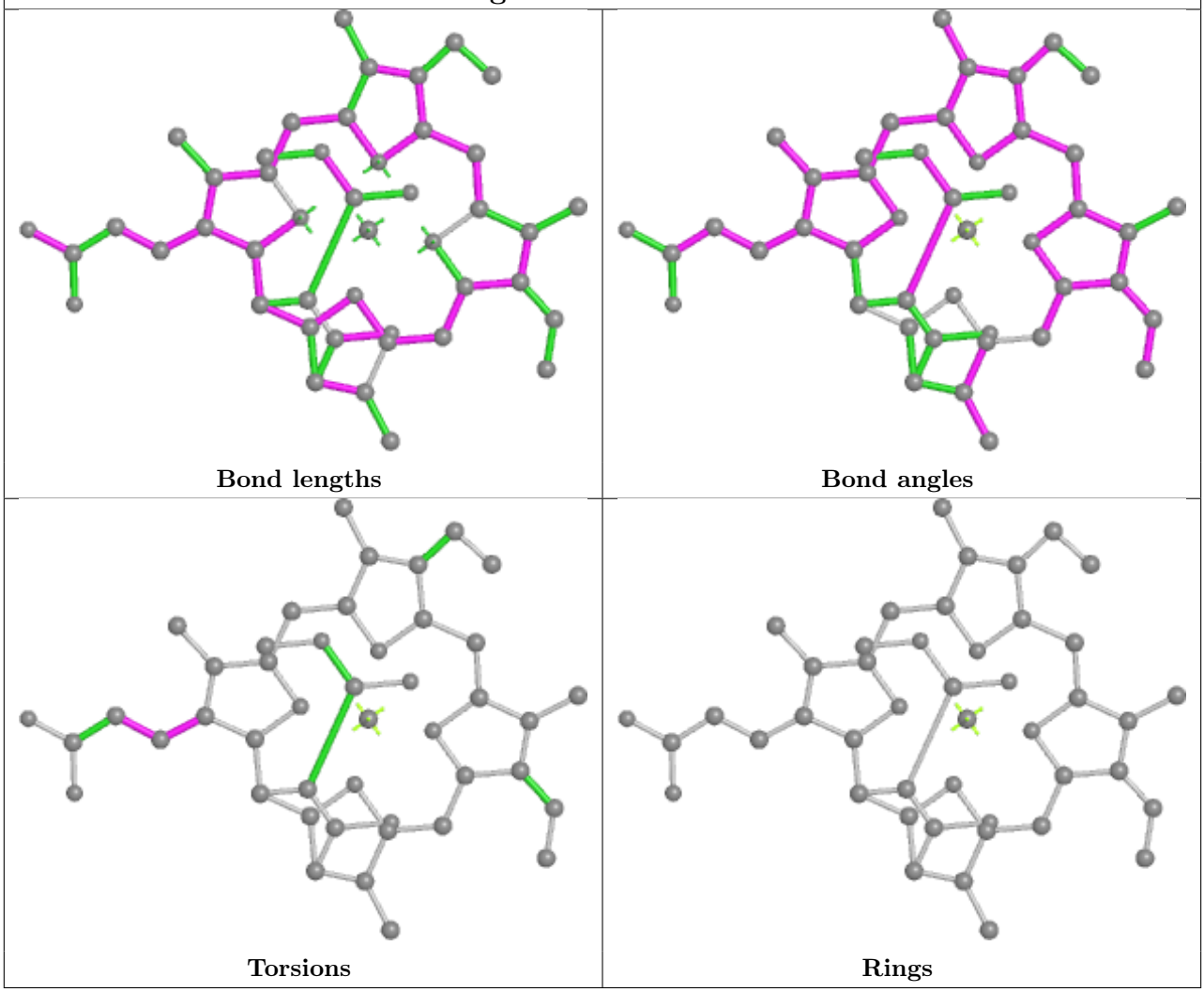

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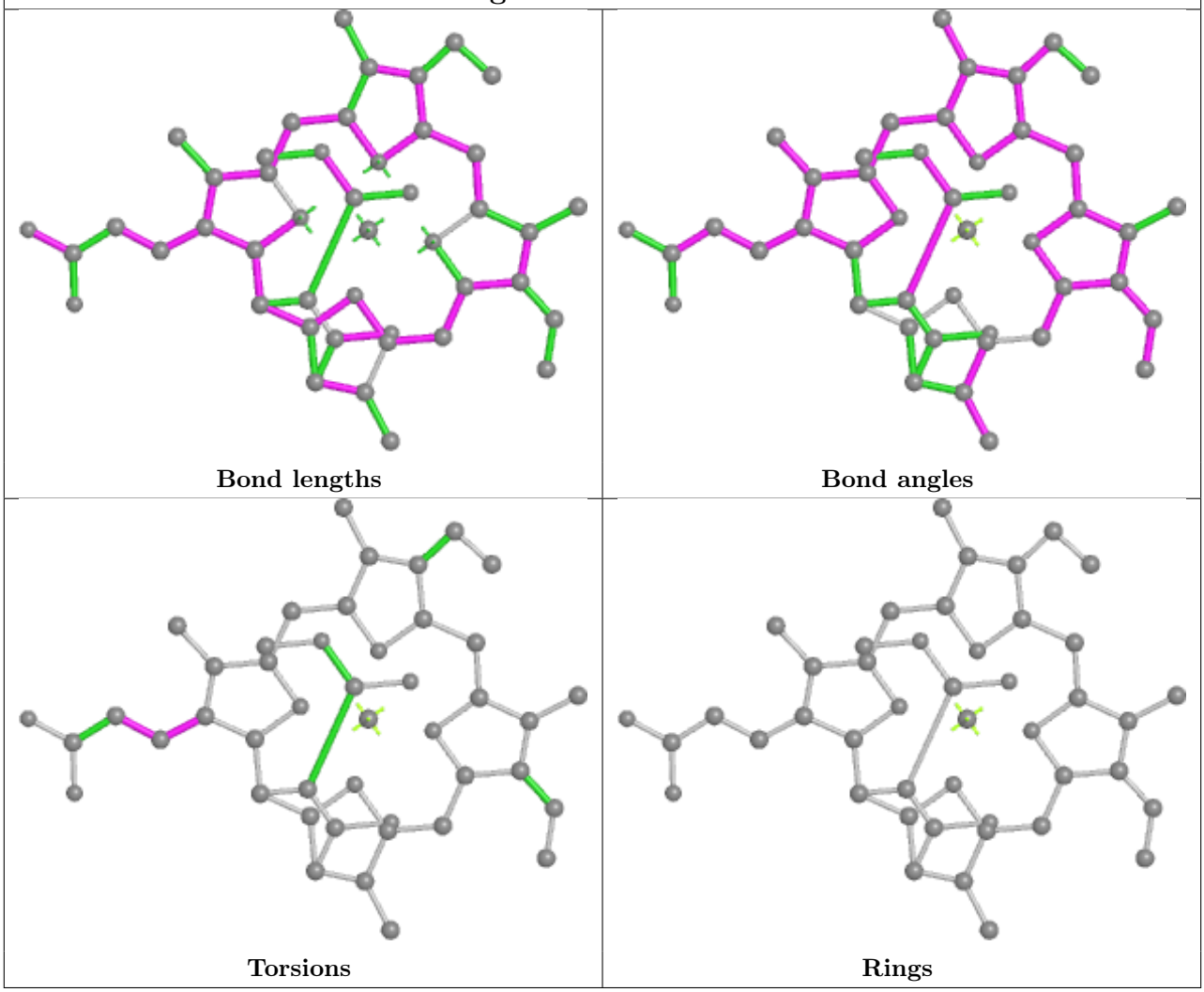

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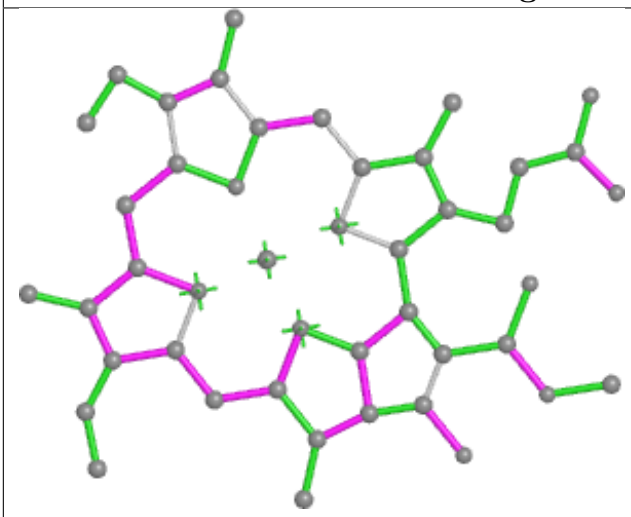

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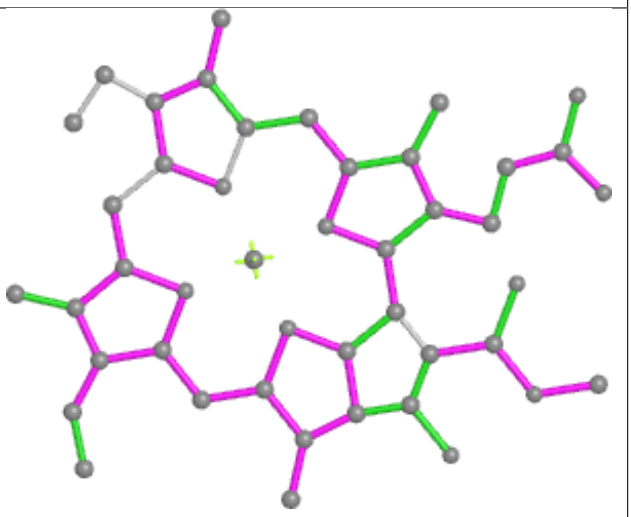

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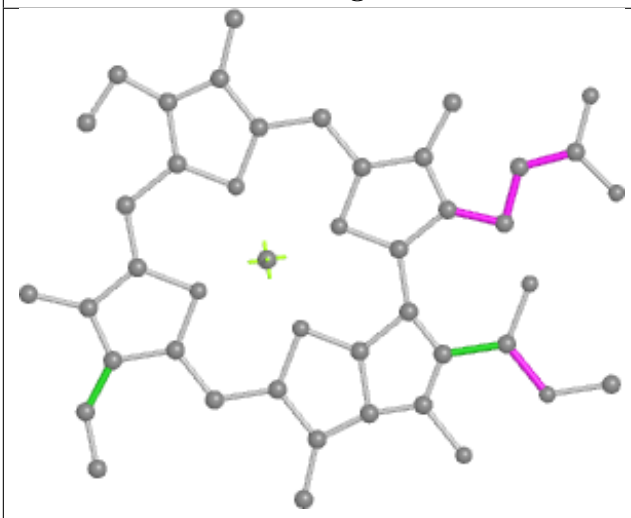

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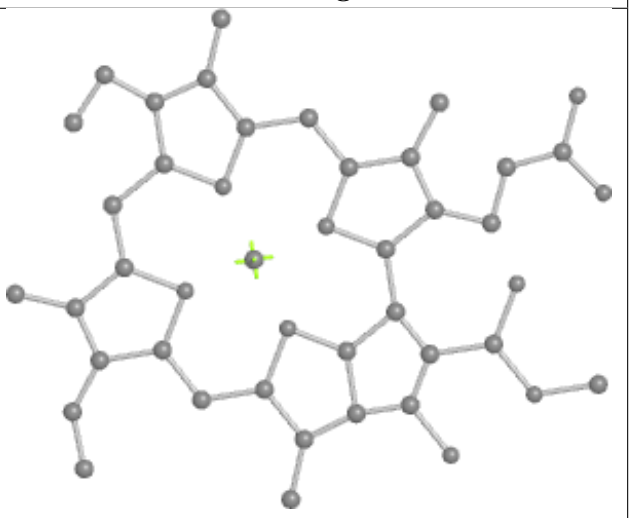

Rings

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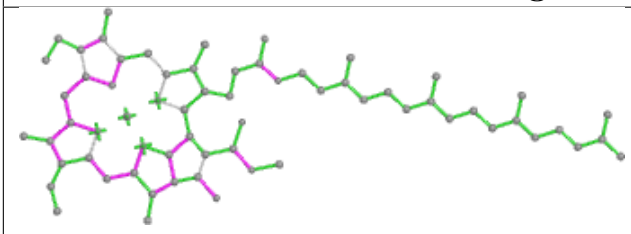

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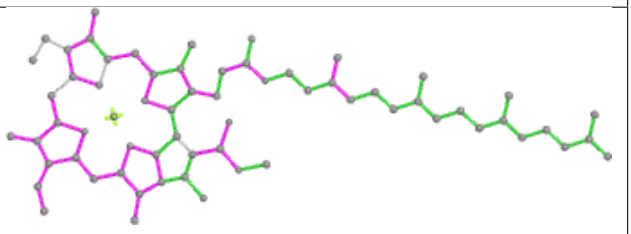

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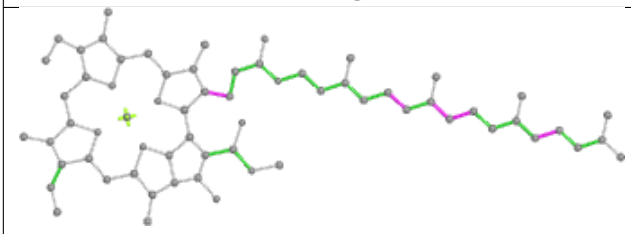

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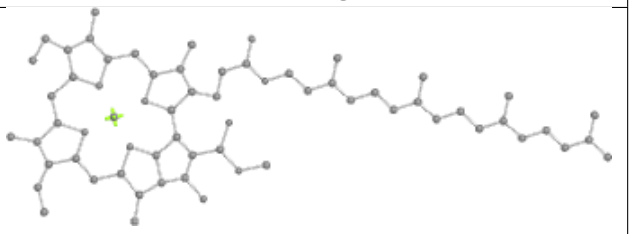

Rings

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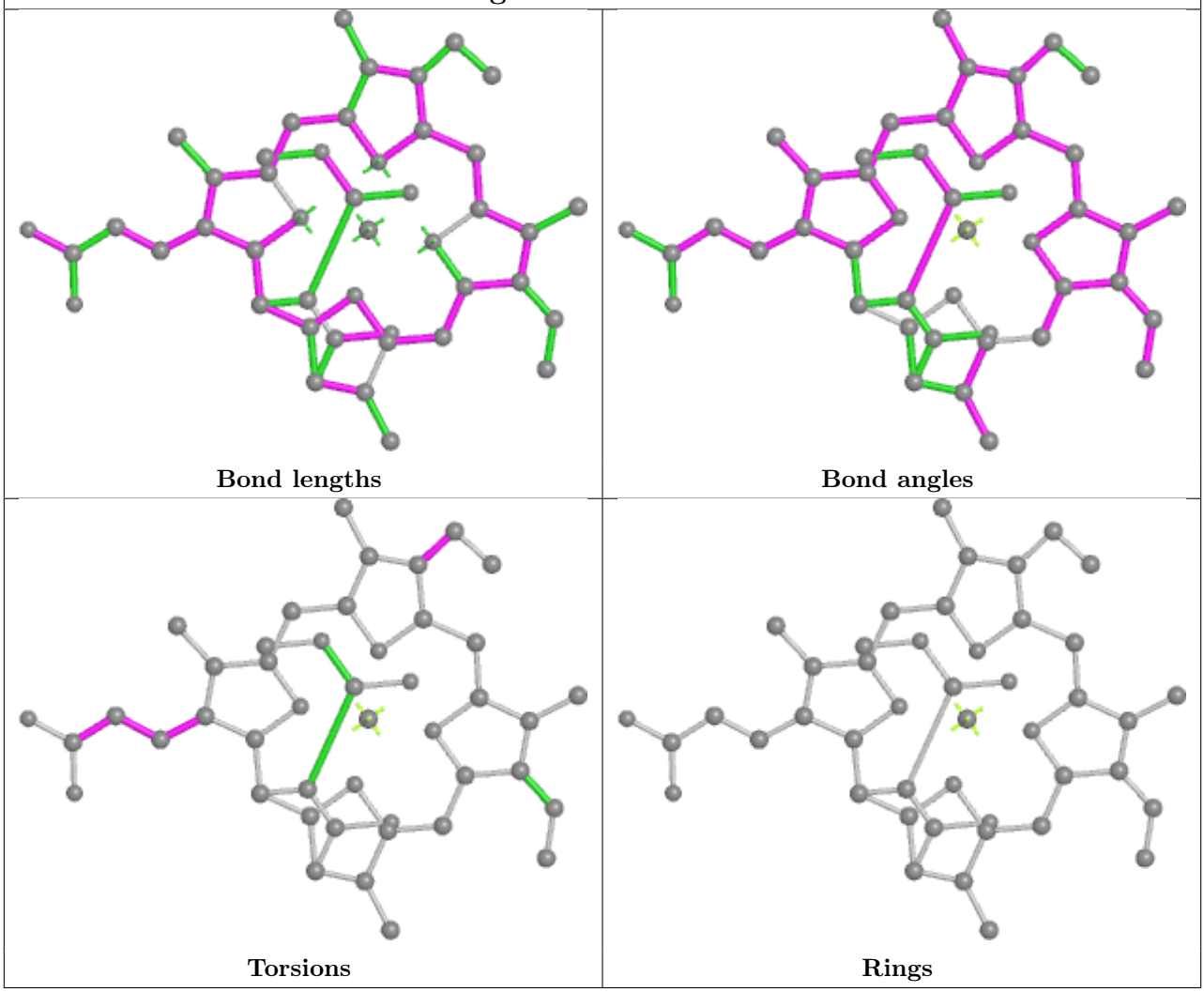

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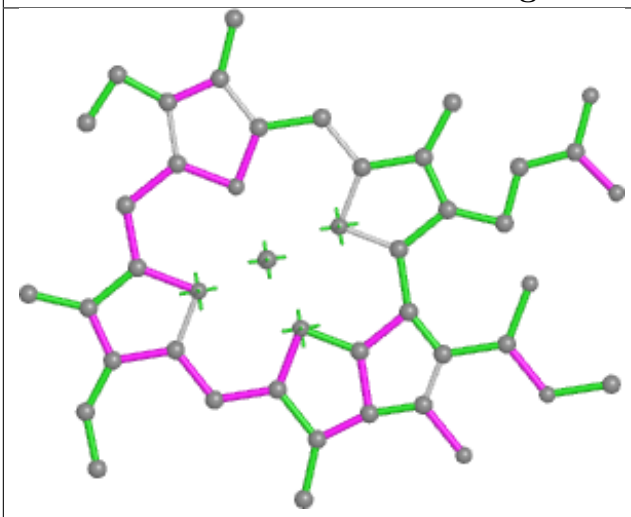

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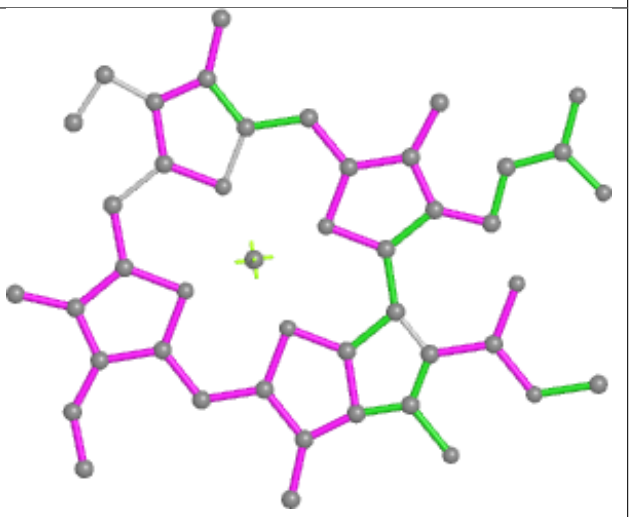

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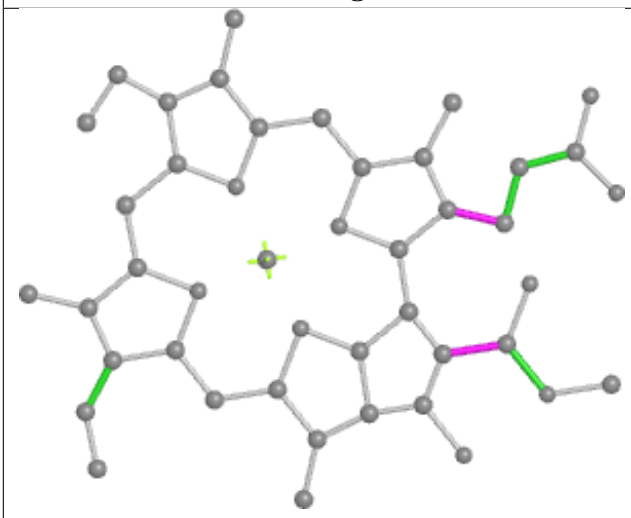

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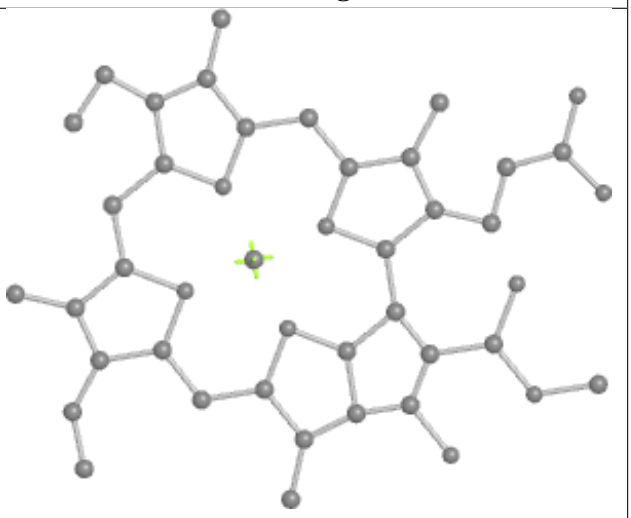

Rings

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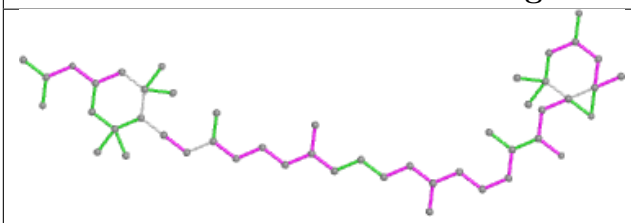

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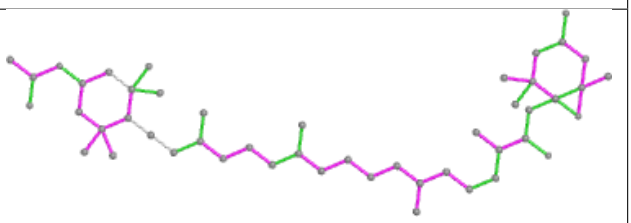

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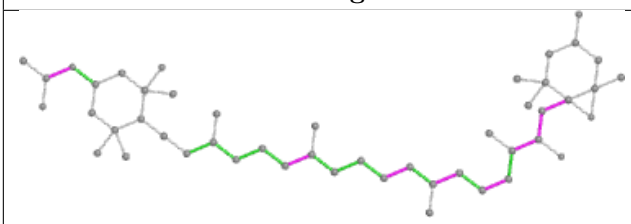

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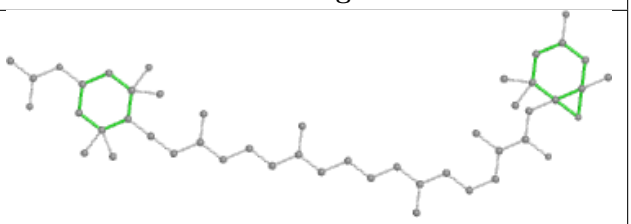

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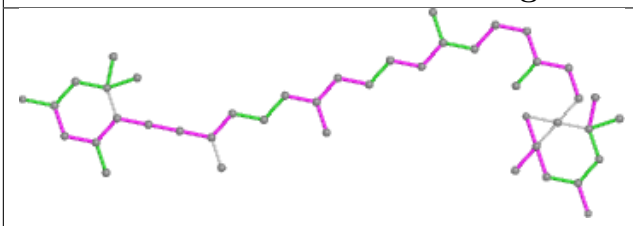

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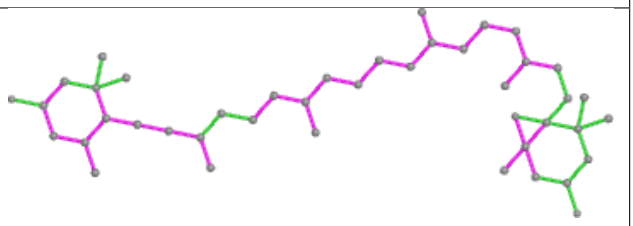

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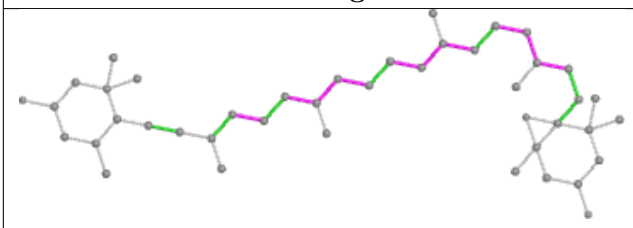

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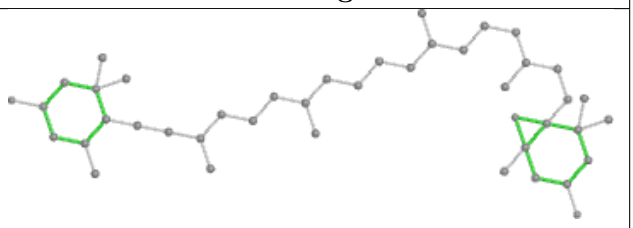

Rings

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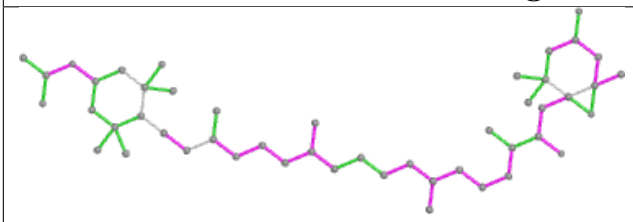

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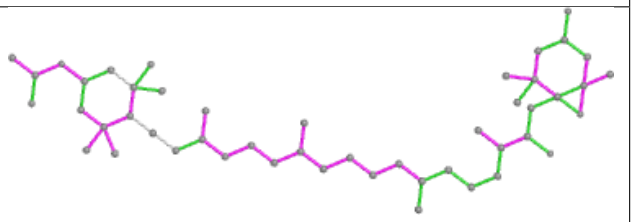

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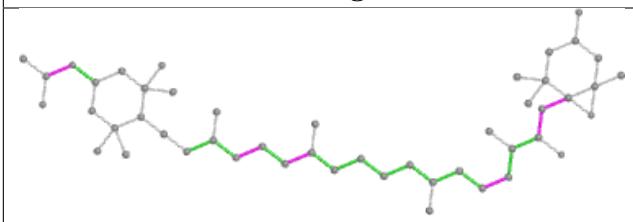

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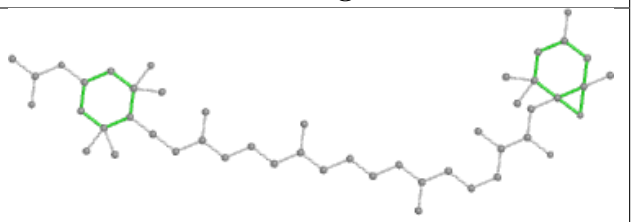

Rings

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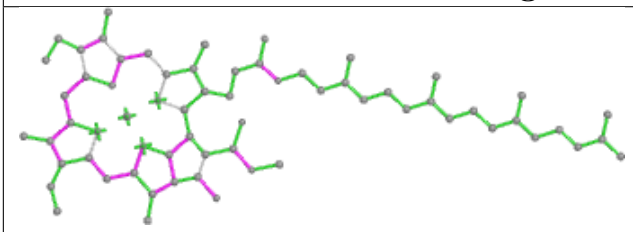

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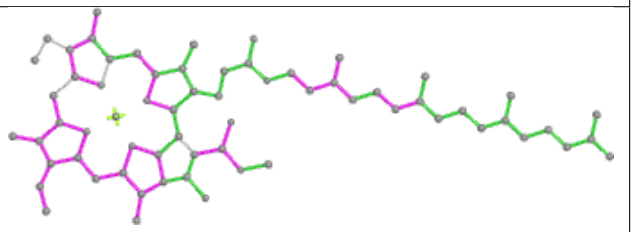

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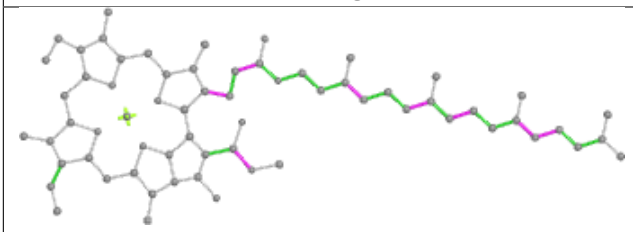

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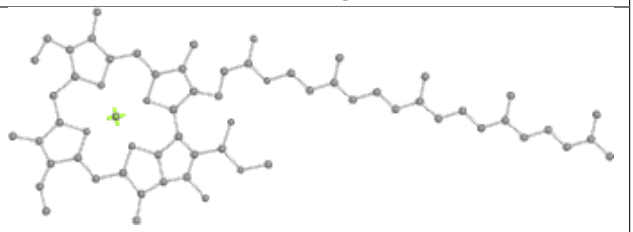

Rings

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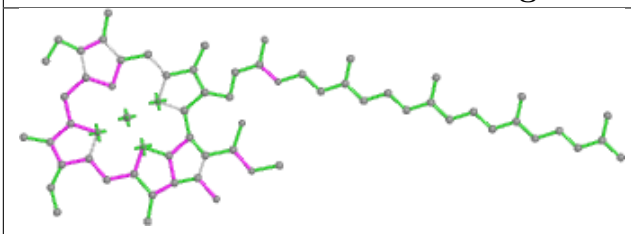

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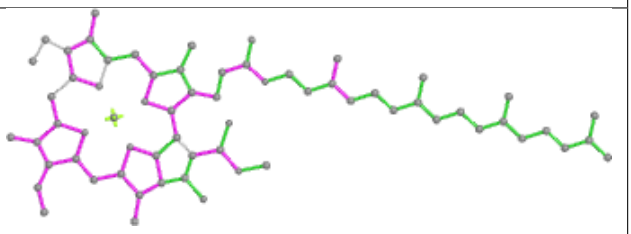

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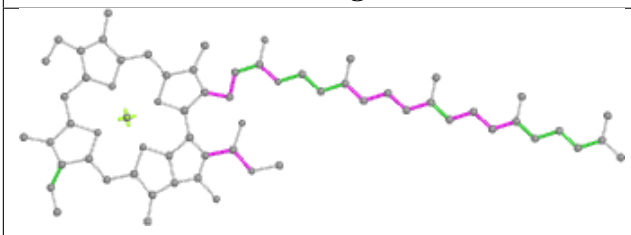

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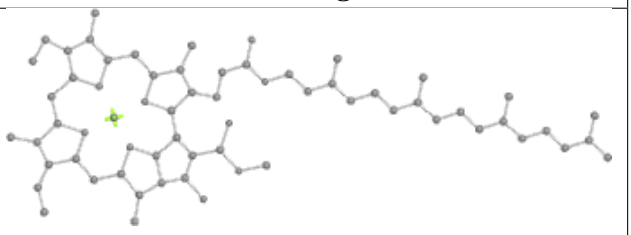

Rings

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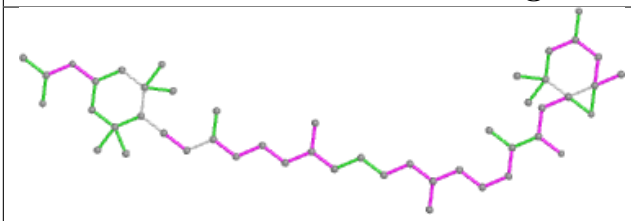

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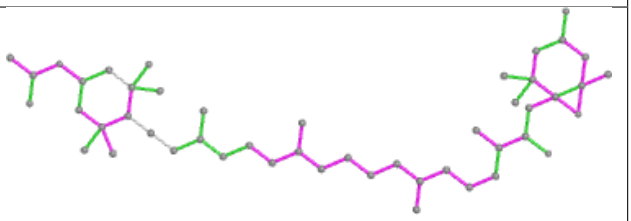

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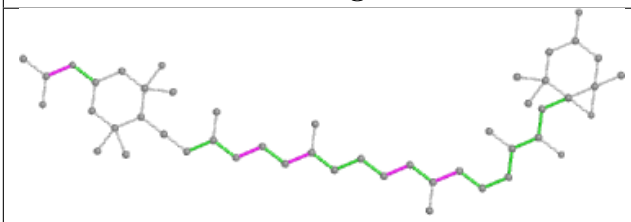

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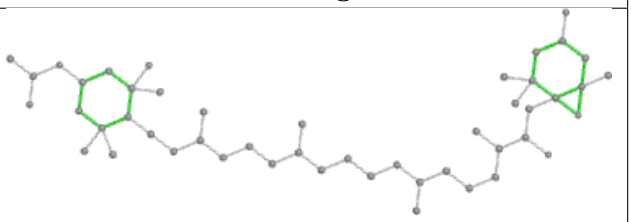

Rings

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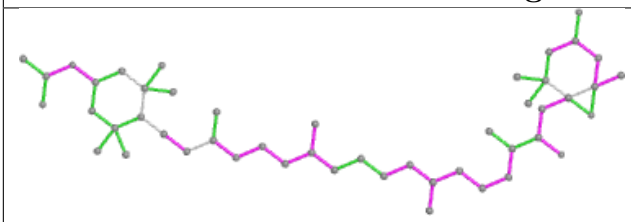

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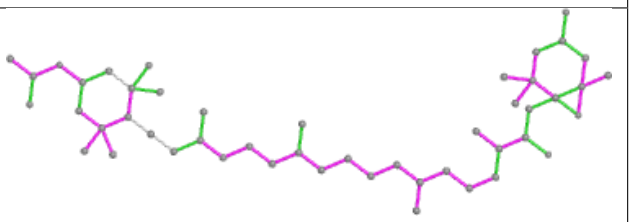

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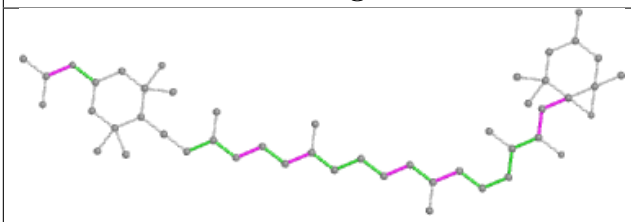

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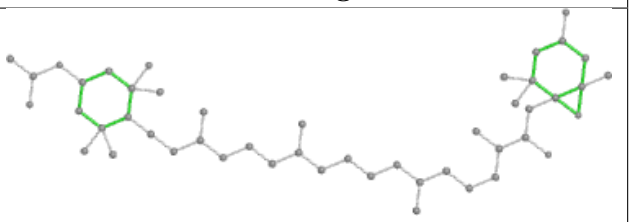

Rings

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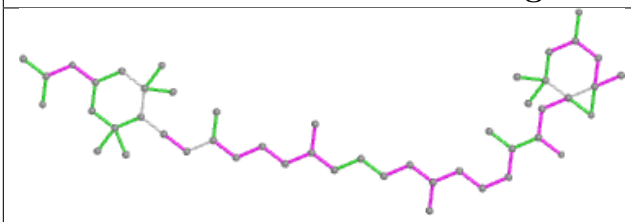
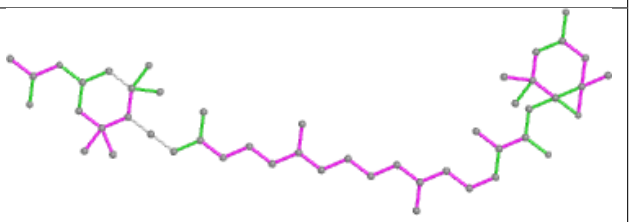
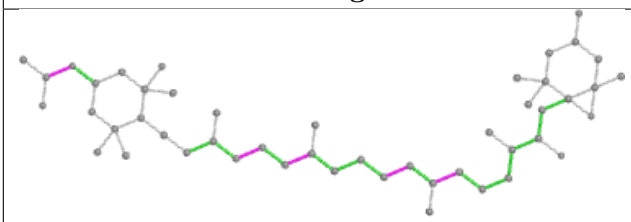
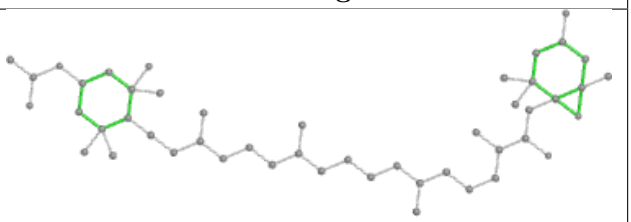
 Bond lengths	 Bond angles
 Torsions	 Rings

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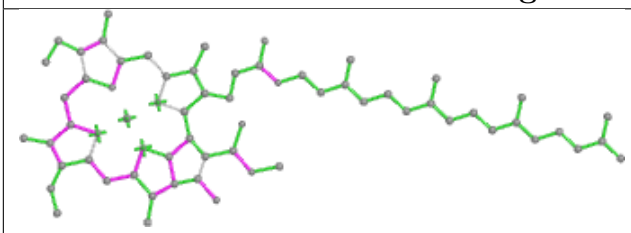
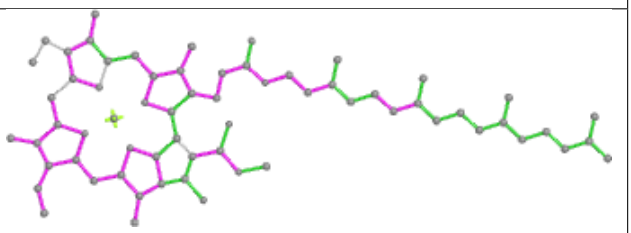
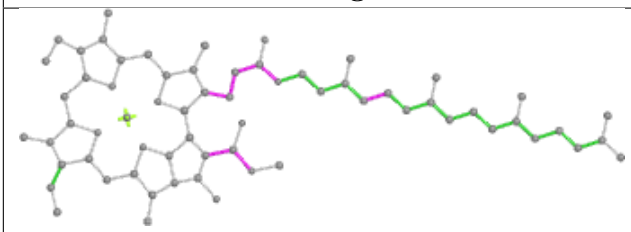
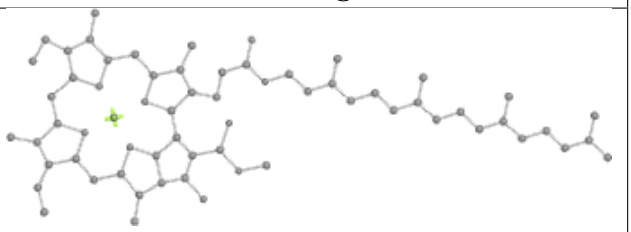
 Bond lengths	 Bond angles
 Torsions	 Rings

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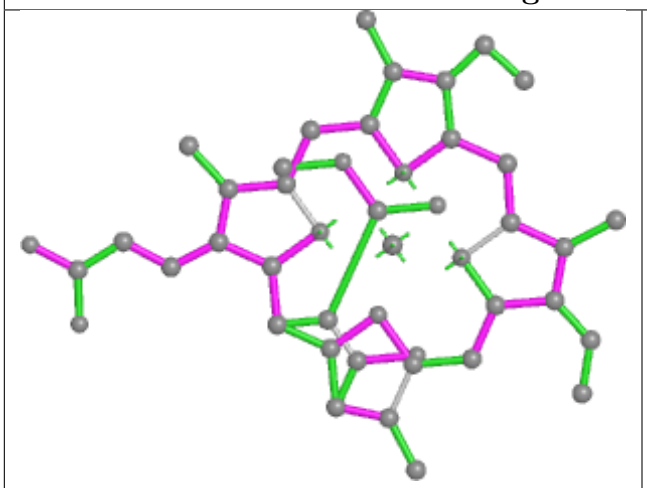

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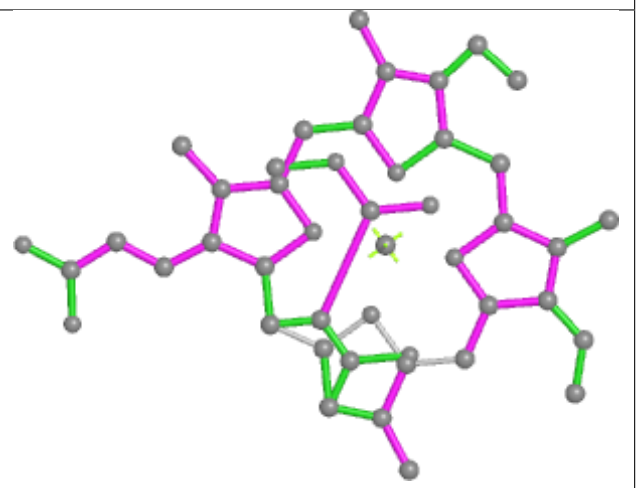

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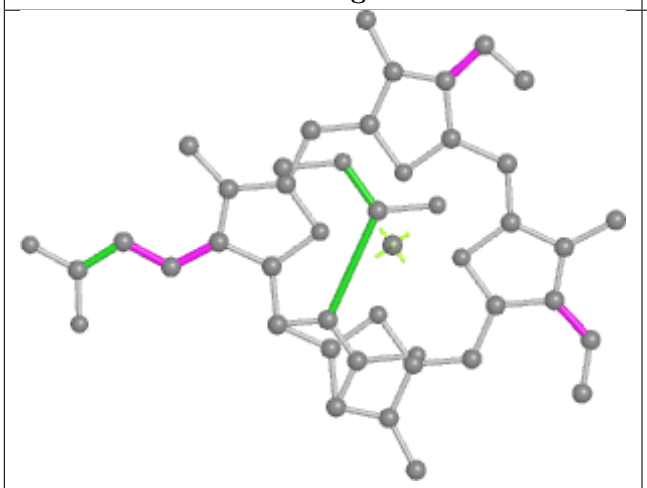

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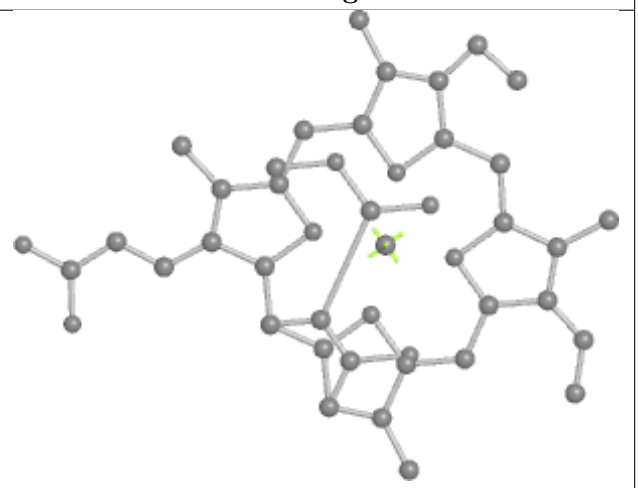

Rings

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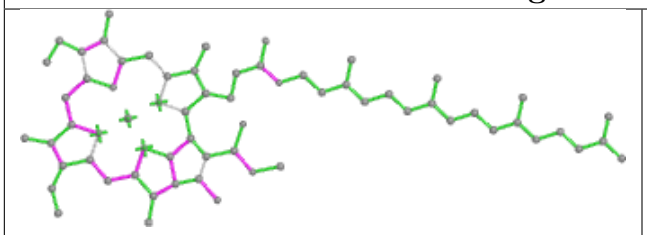

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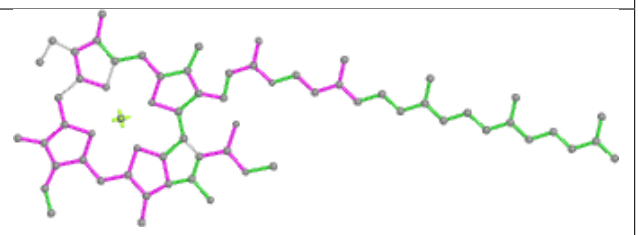

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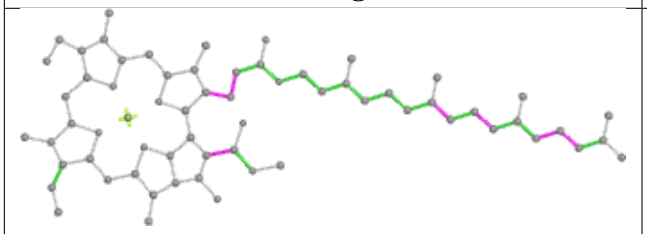

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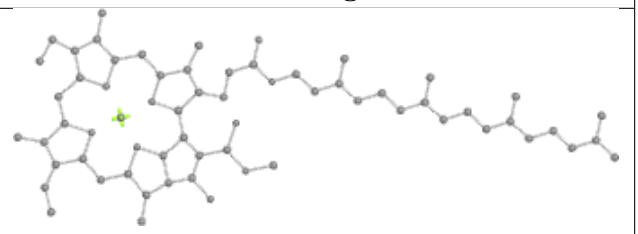

Rings

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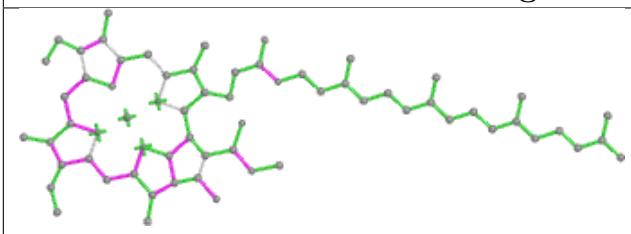
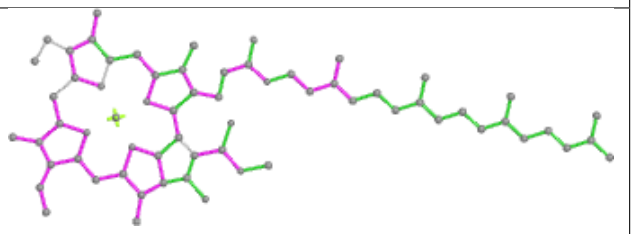
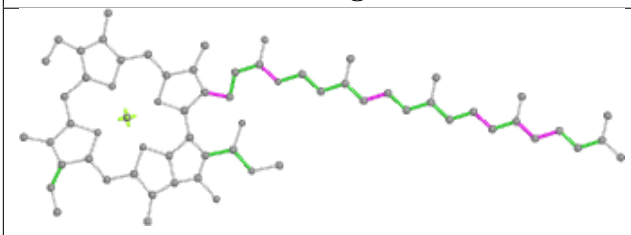
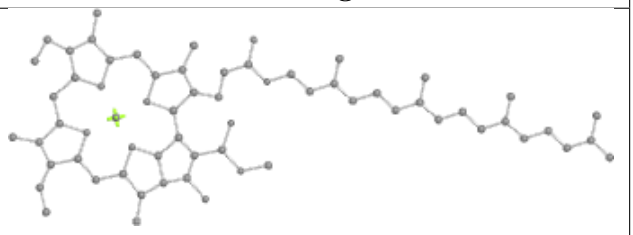
 Bond lengths	 Bond angles
 Torsions	 Rings

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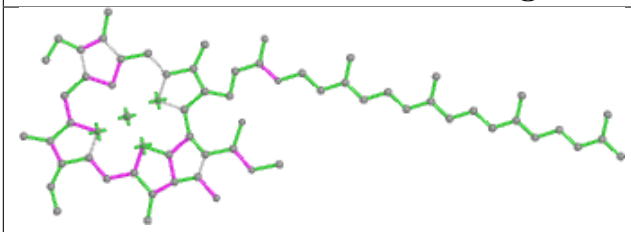
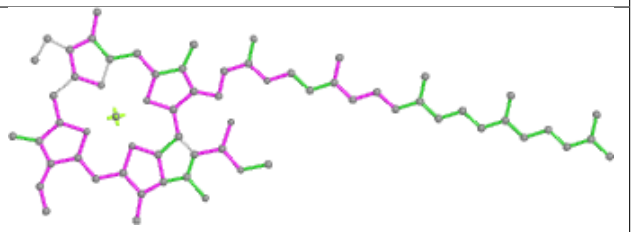
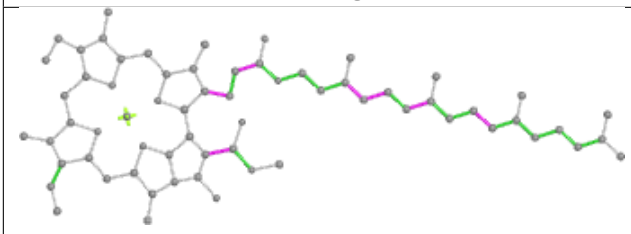
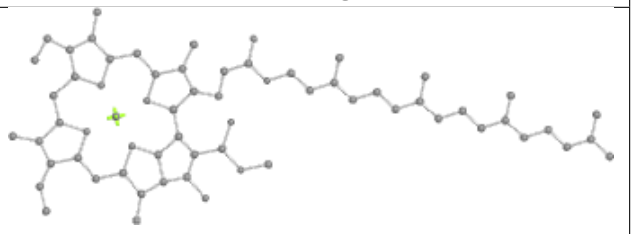
 Bond lengths	 Bond angles
 Torsions	 Rings

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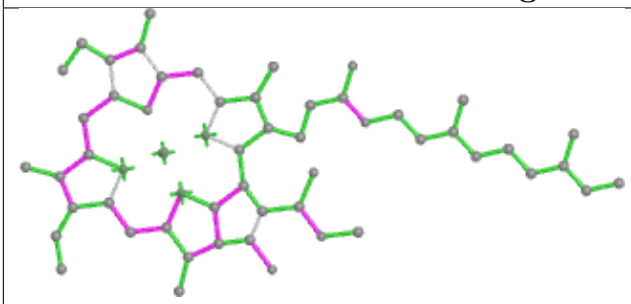
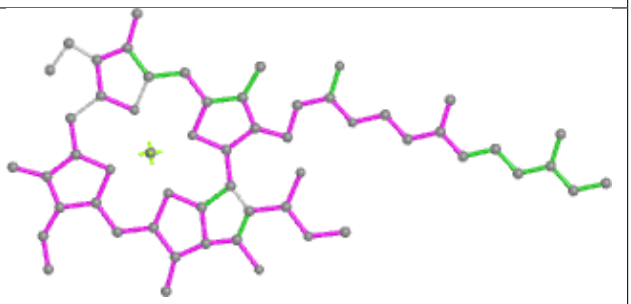
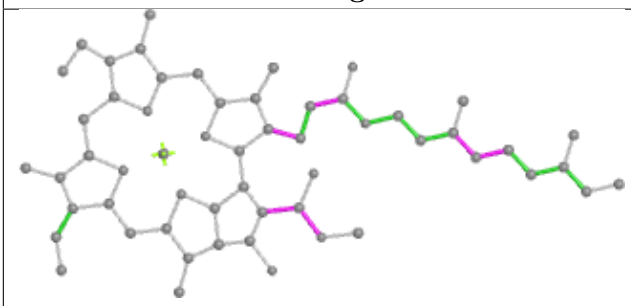
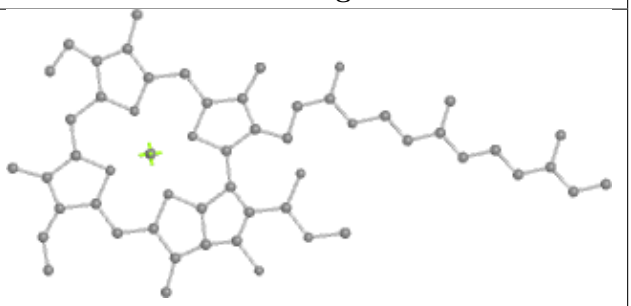
 Bond lengths	 Bond angles
 Torsions	 Rings

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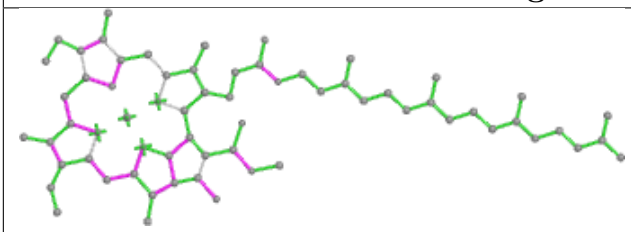
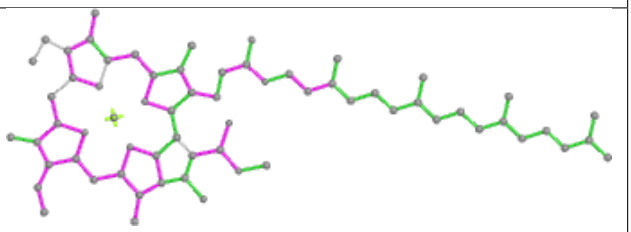
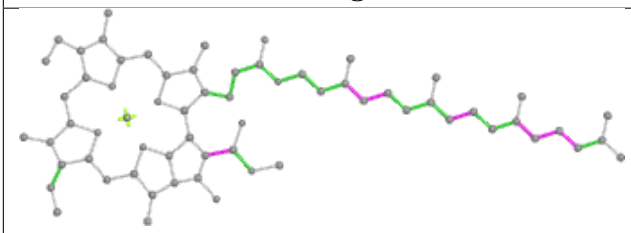
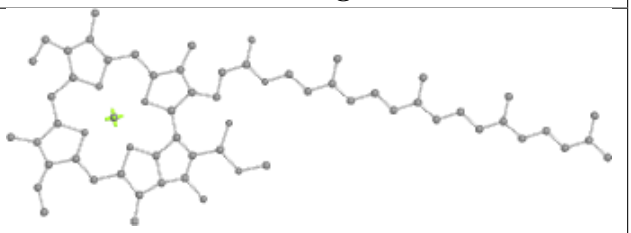
 Bond lengths	 Bond angles
 Torsions	 Rings

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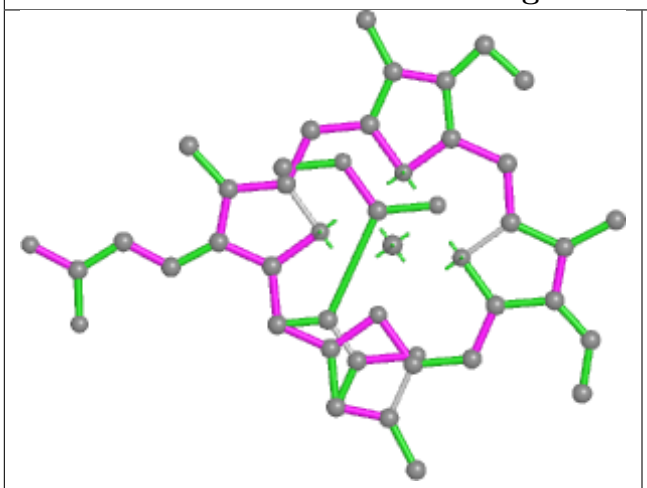

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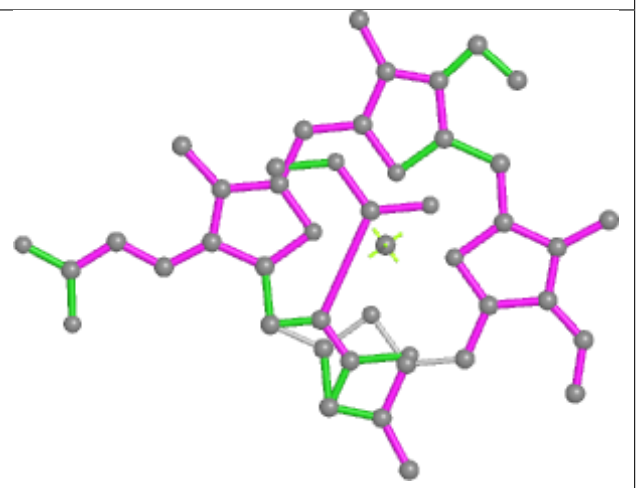

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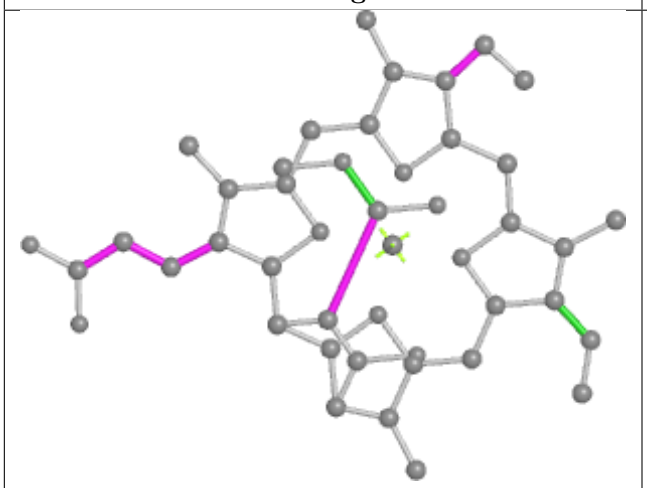

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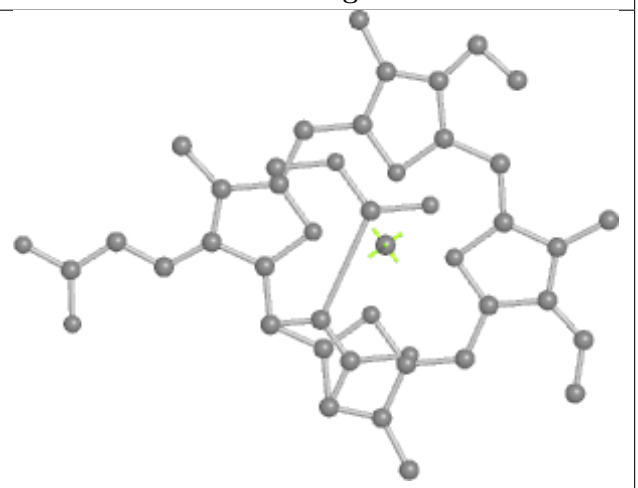

Rings

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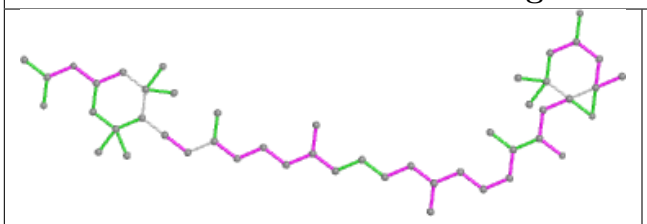

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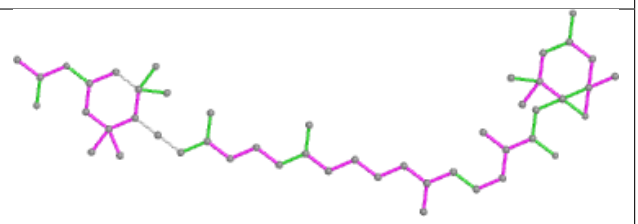

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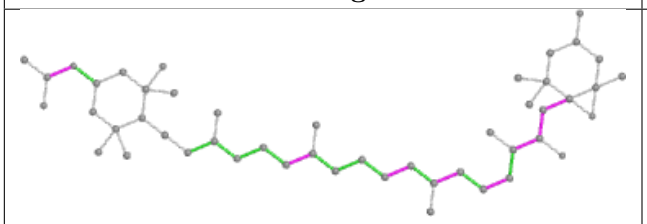

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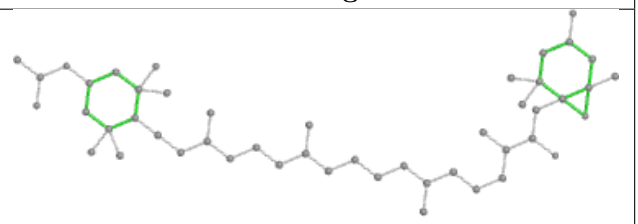

Rings

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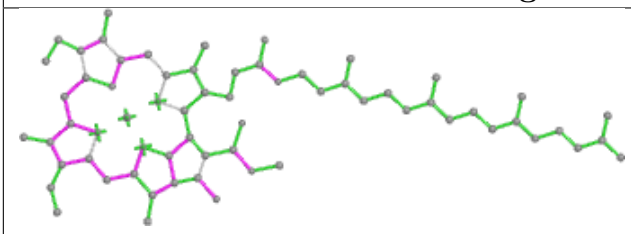
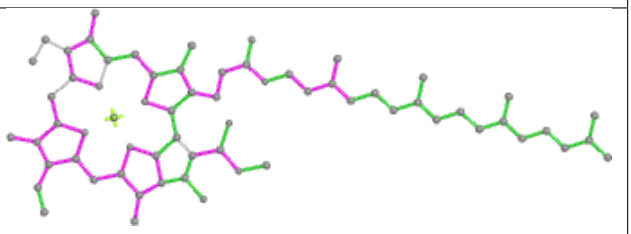
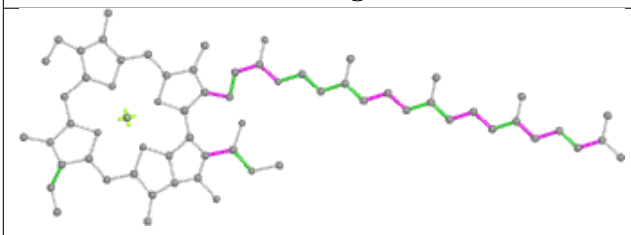
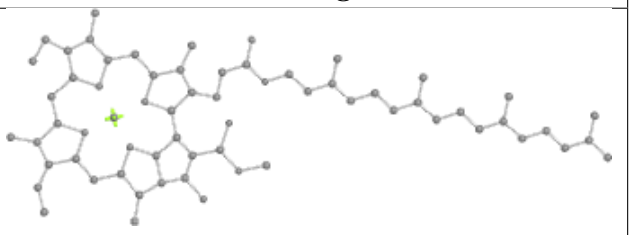
 Bond lengths	 Bond angles
 Torsions	 Rings

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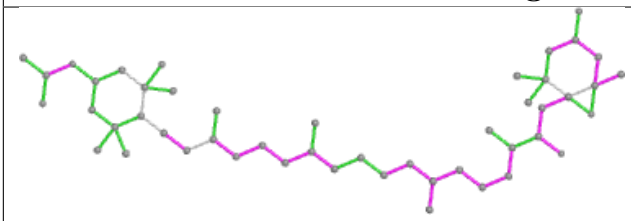
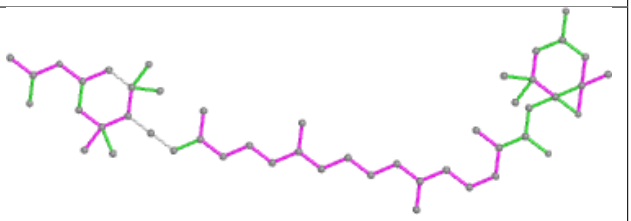
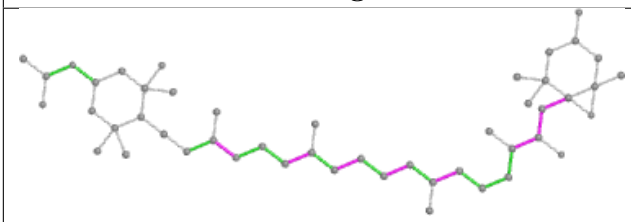
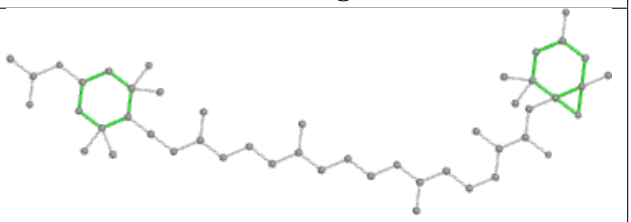
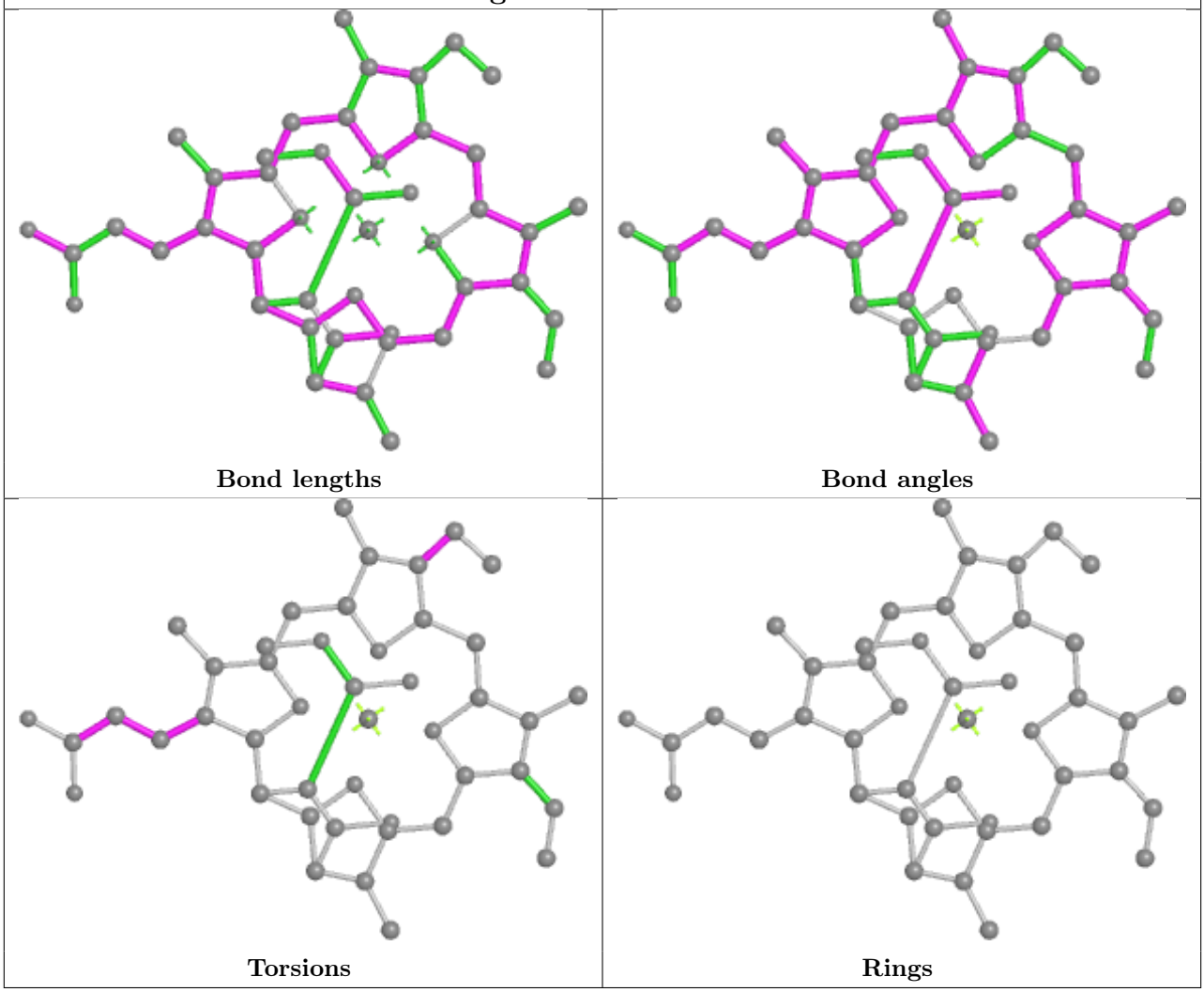
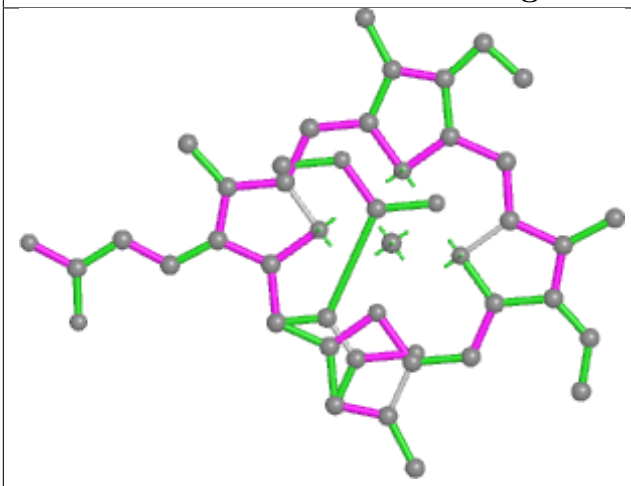
 Bond lengths	 Bond angles
 Torsions	 Rings

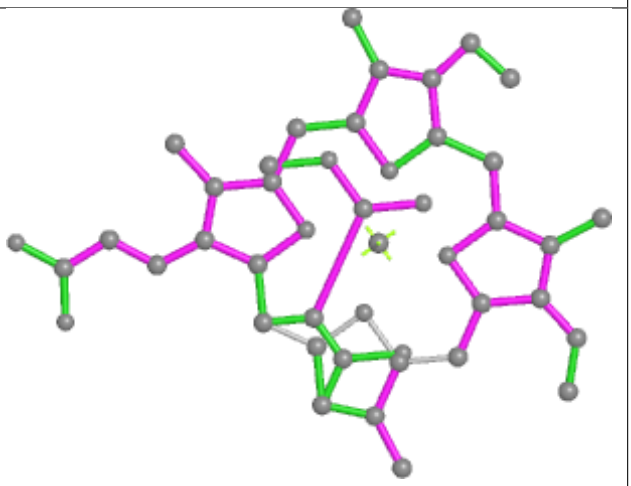
Ligand KC1 18 205



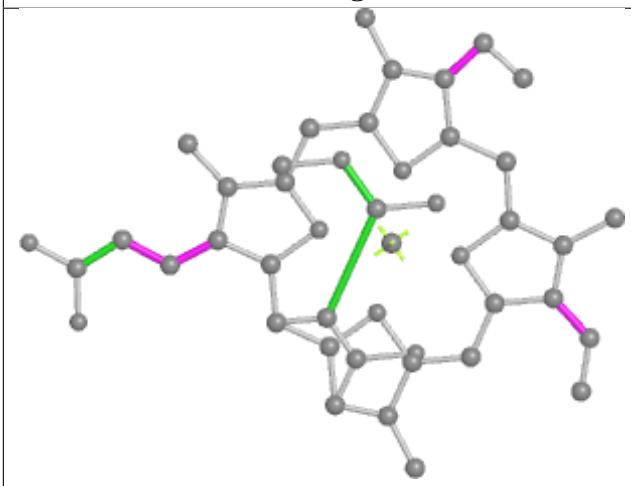
Ligand KC1 12 206



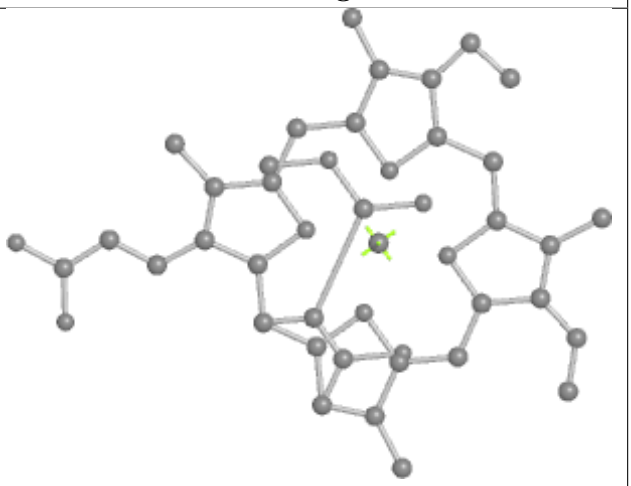
Bond lengths



Bond angles

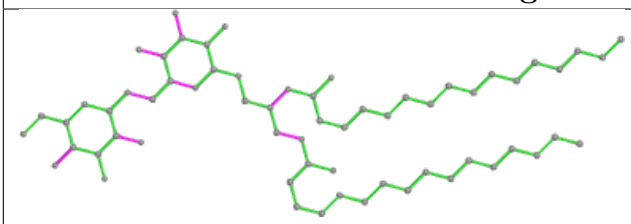


Torsions



Rings

Ligand DGD C 517



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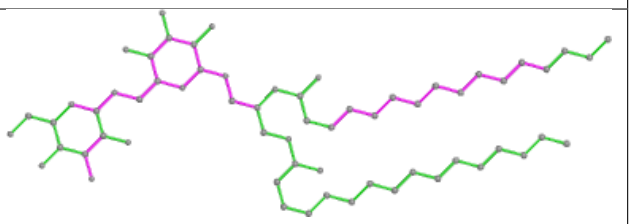
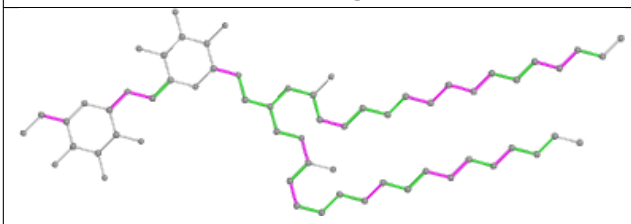
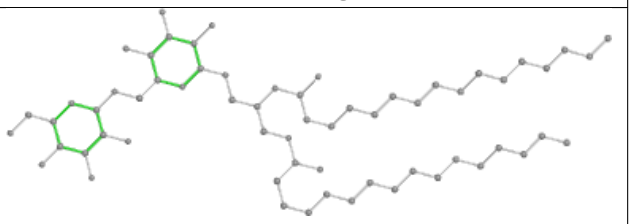


Bond angles

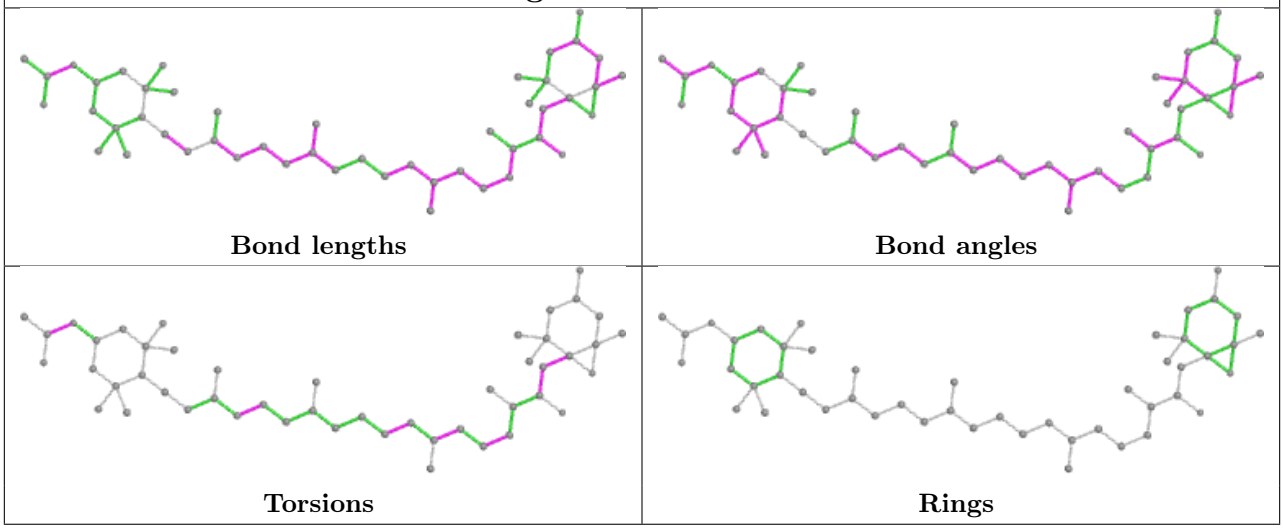


Torsions

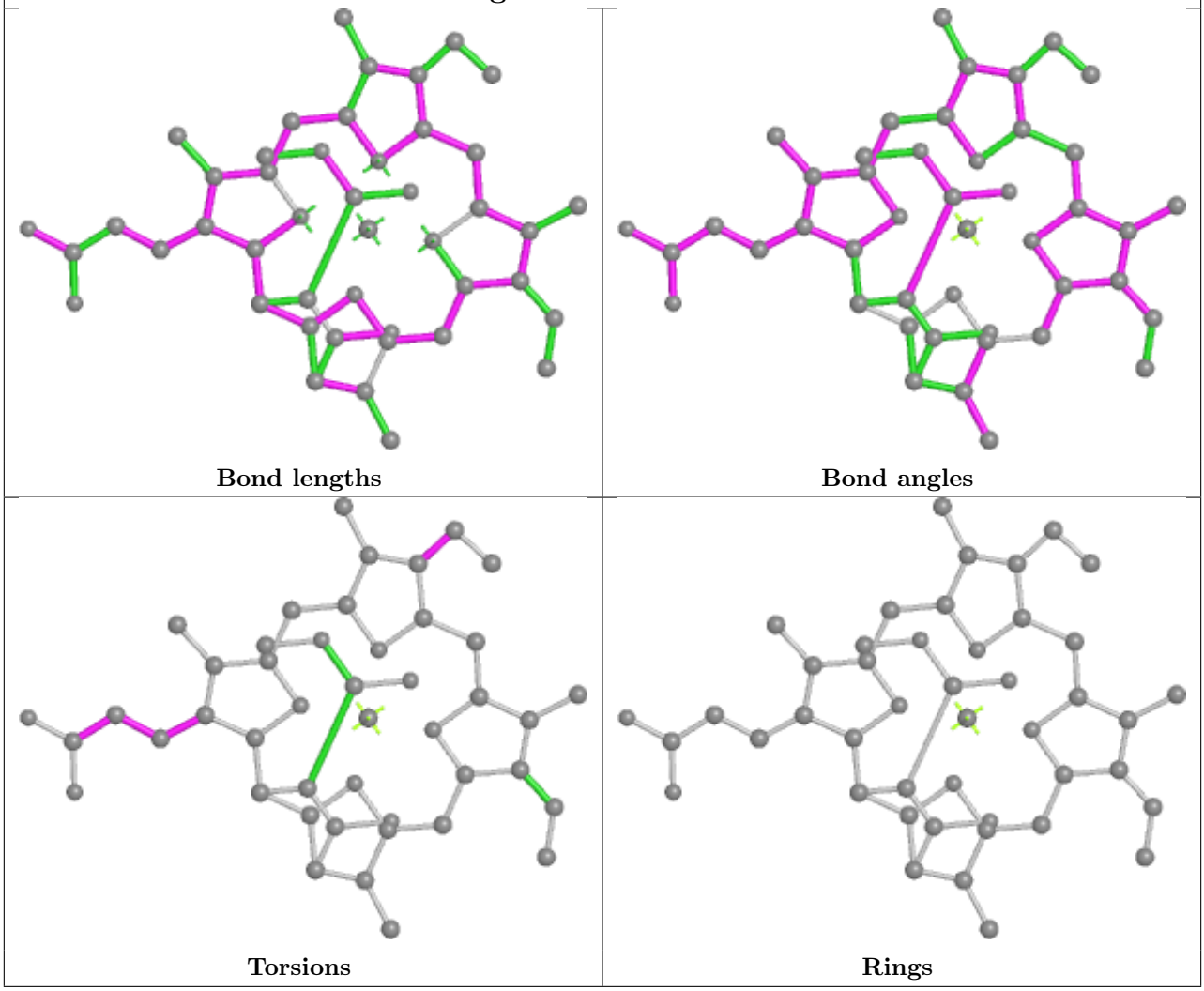


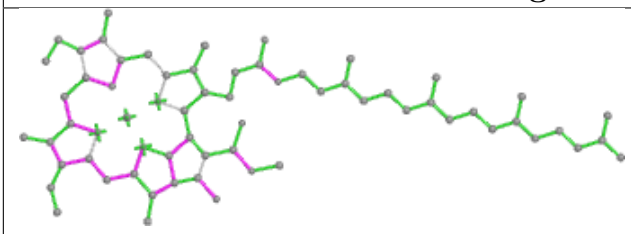
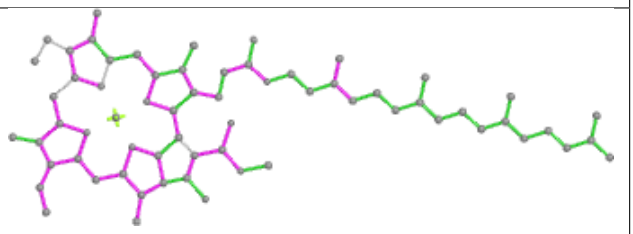
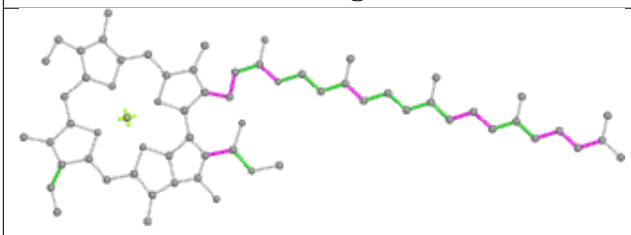
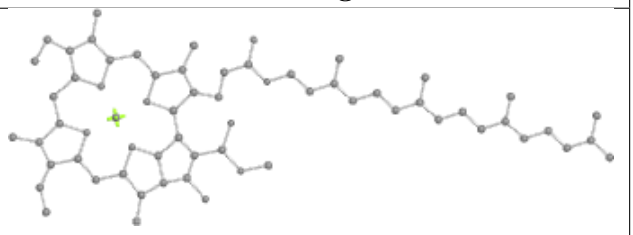
Rings

Ligand A86 18 213



Ligand KC1 36 304



Ligand CLA c 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

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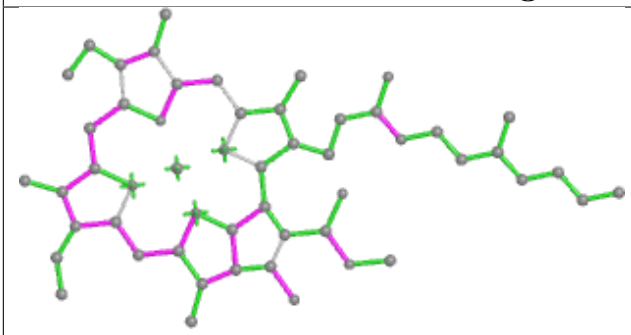
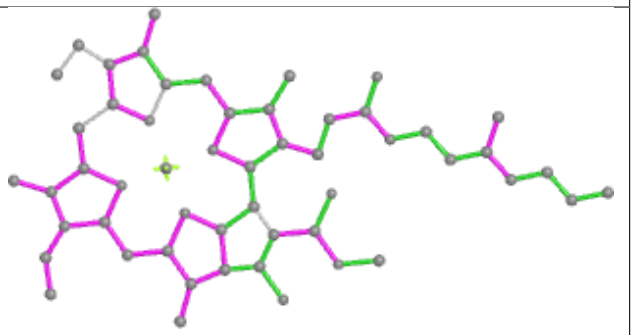
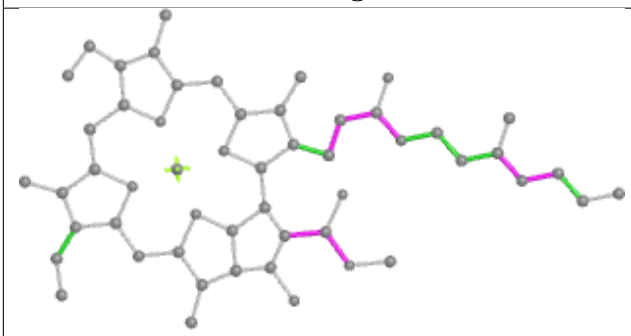
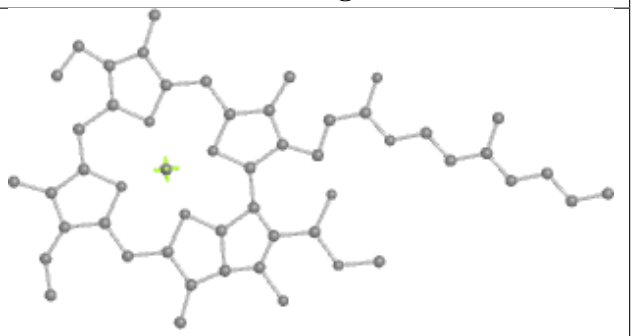
 Bond lengths	 Bond angles
 Torsions	 Rings

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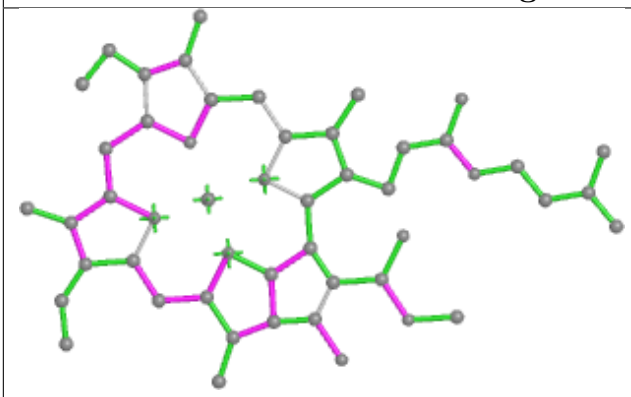
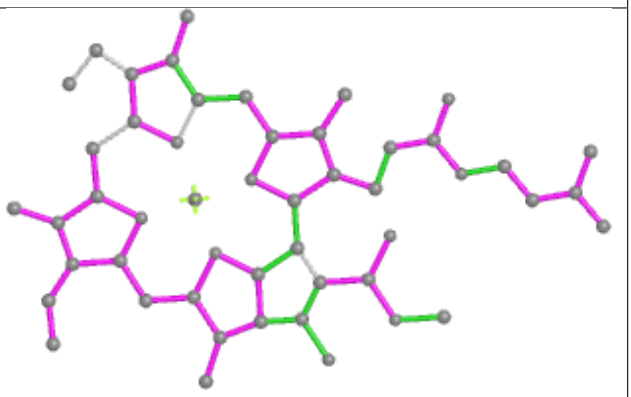
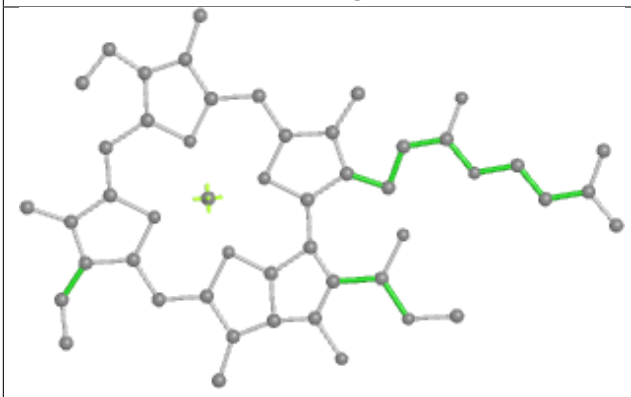
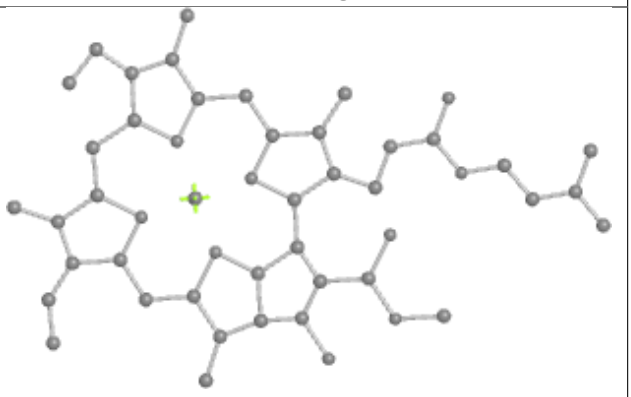
 Bond lengths	 Bond angles
 Torsions	 Rings

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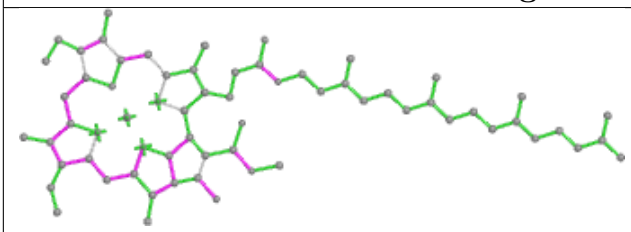
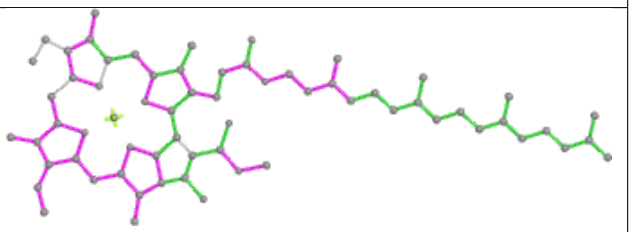
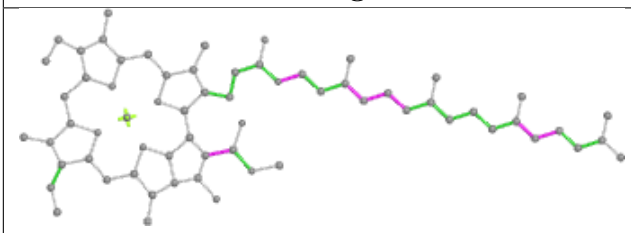
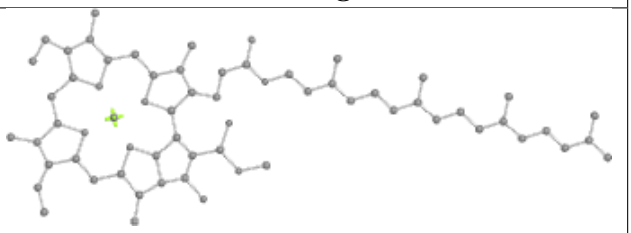
 Bond lengths	 Bond angles
 Torsions	 Rings

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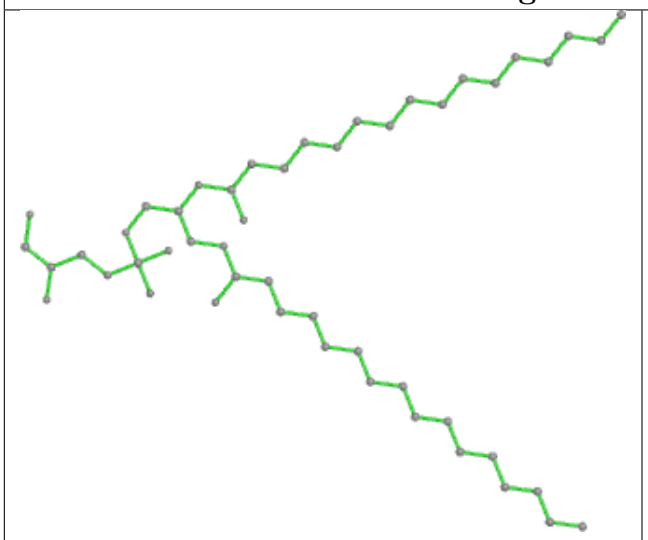

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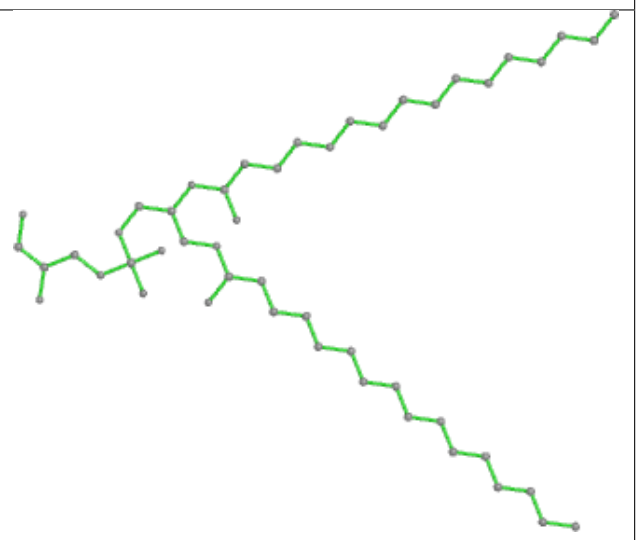
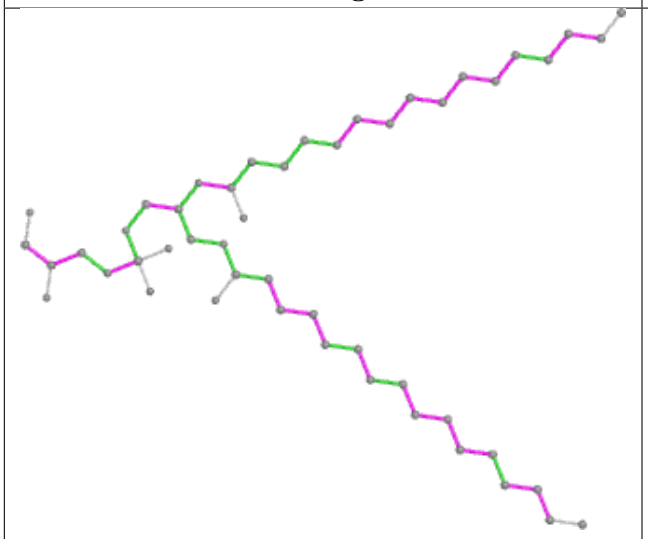


Bond angles



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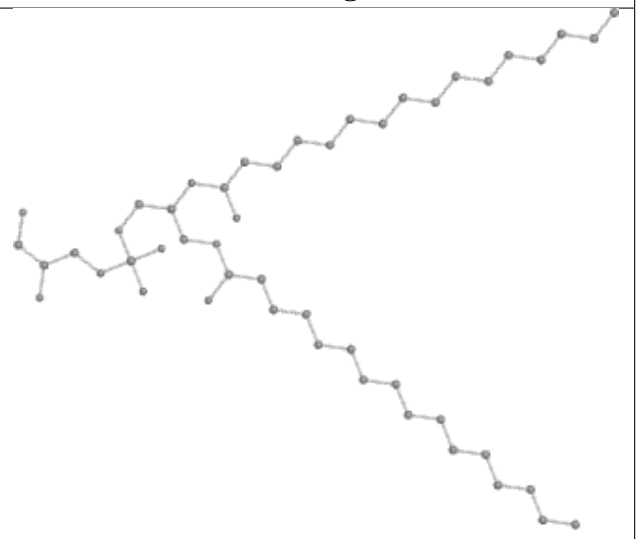
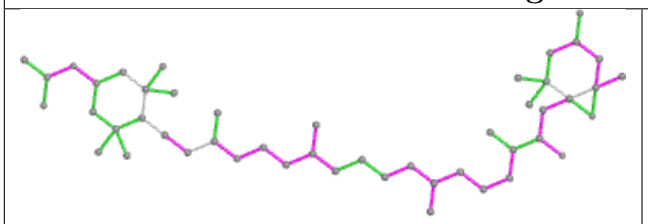


Rings

Ligand A86 12 216



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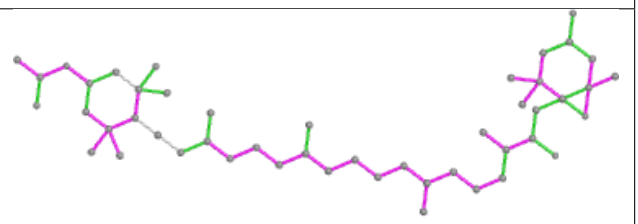

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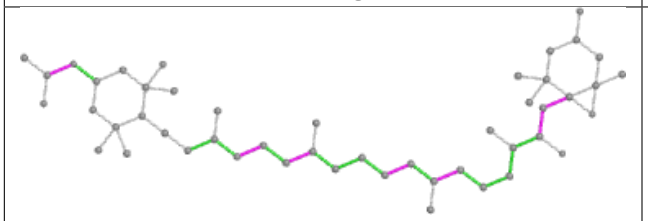

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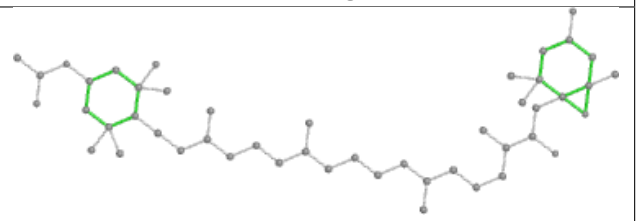

Rings

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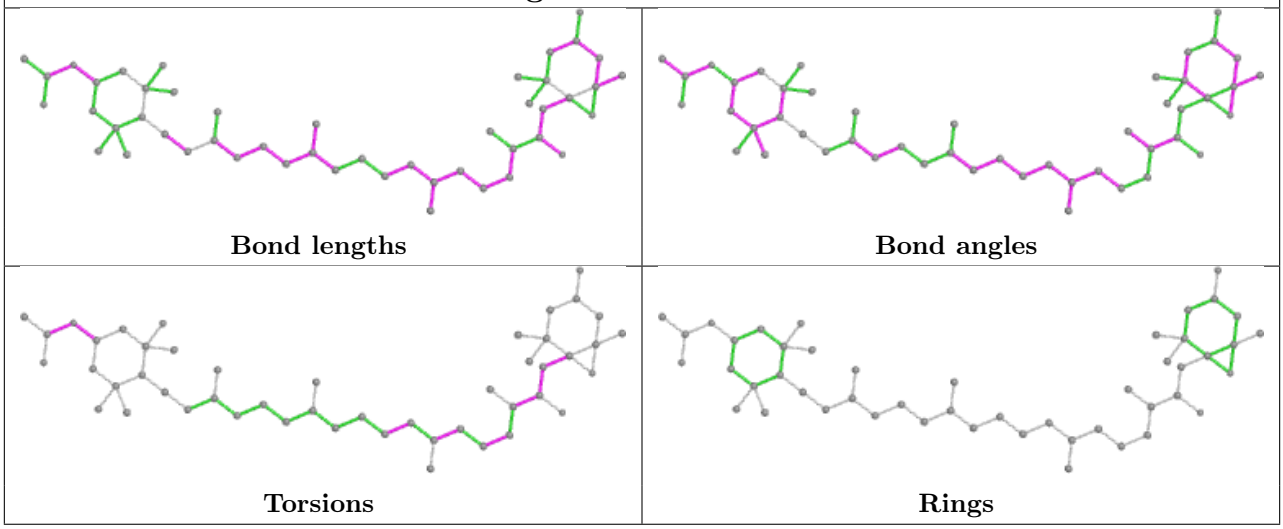
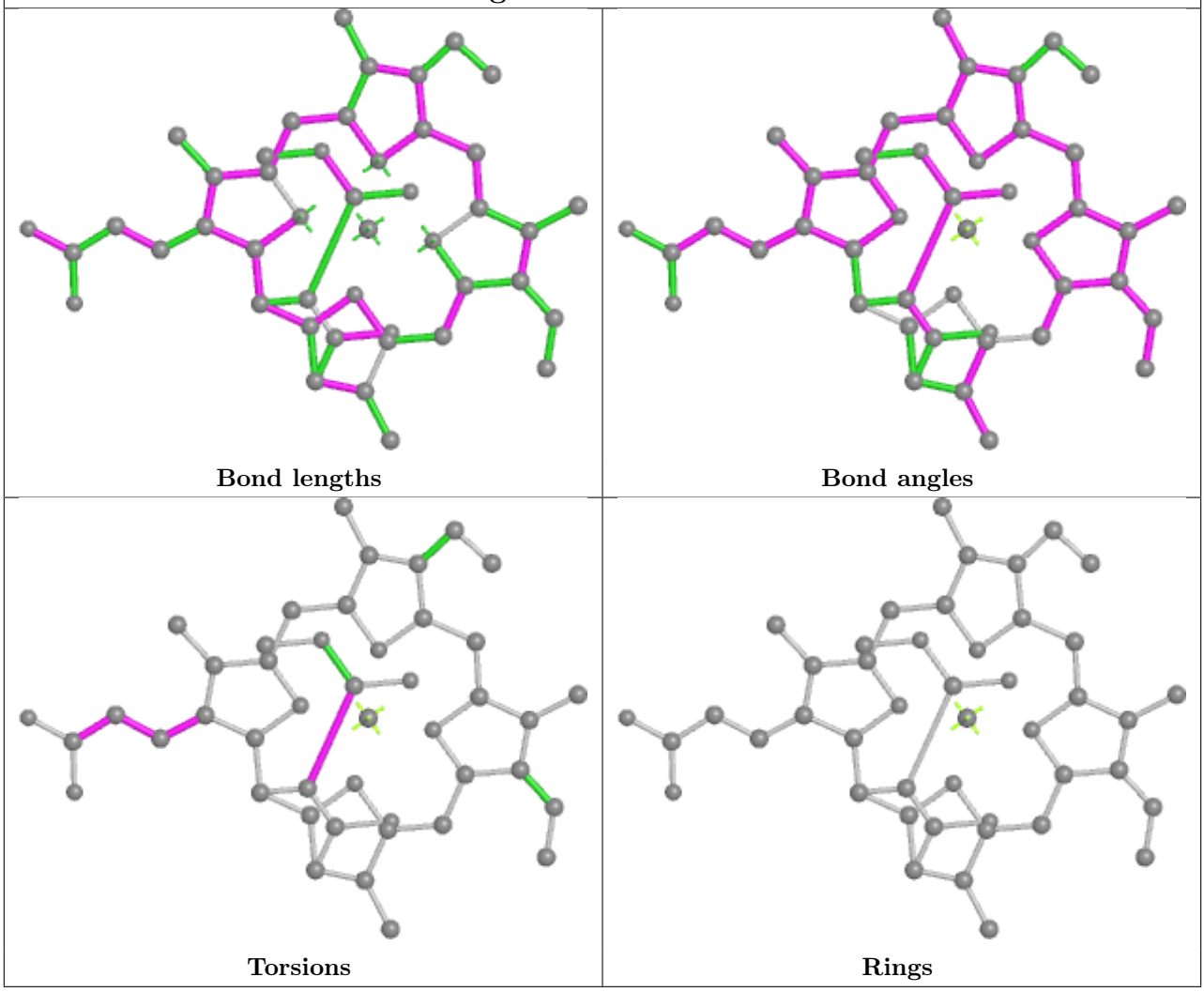


Ligand KC1 32 212



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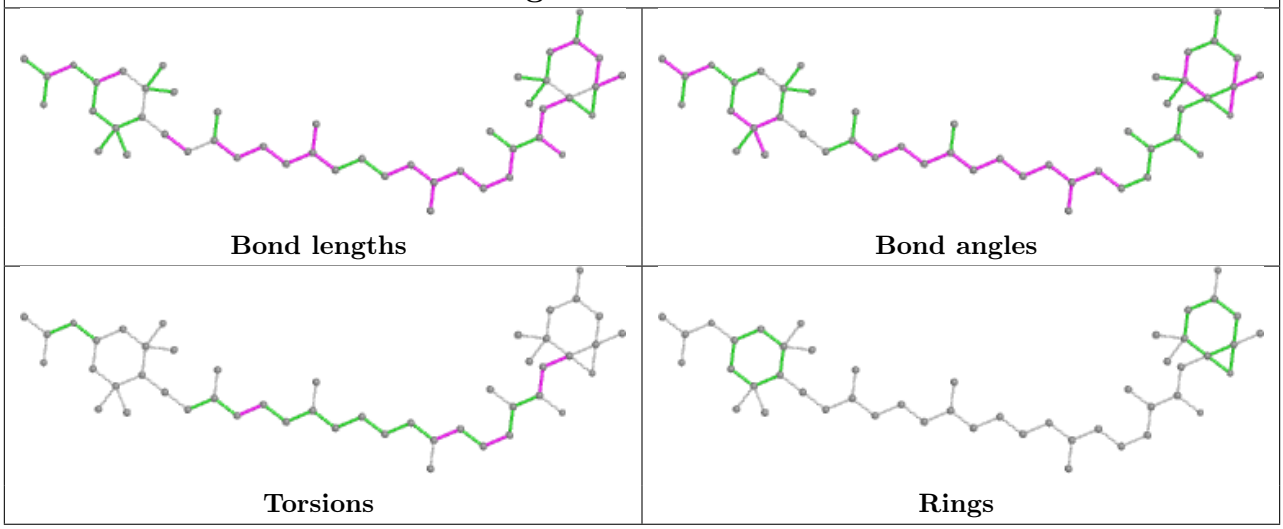

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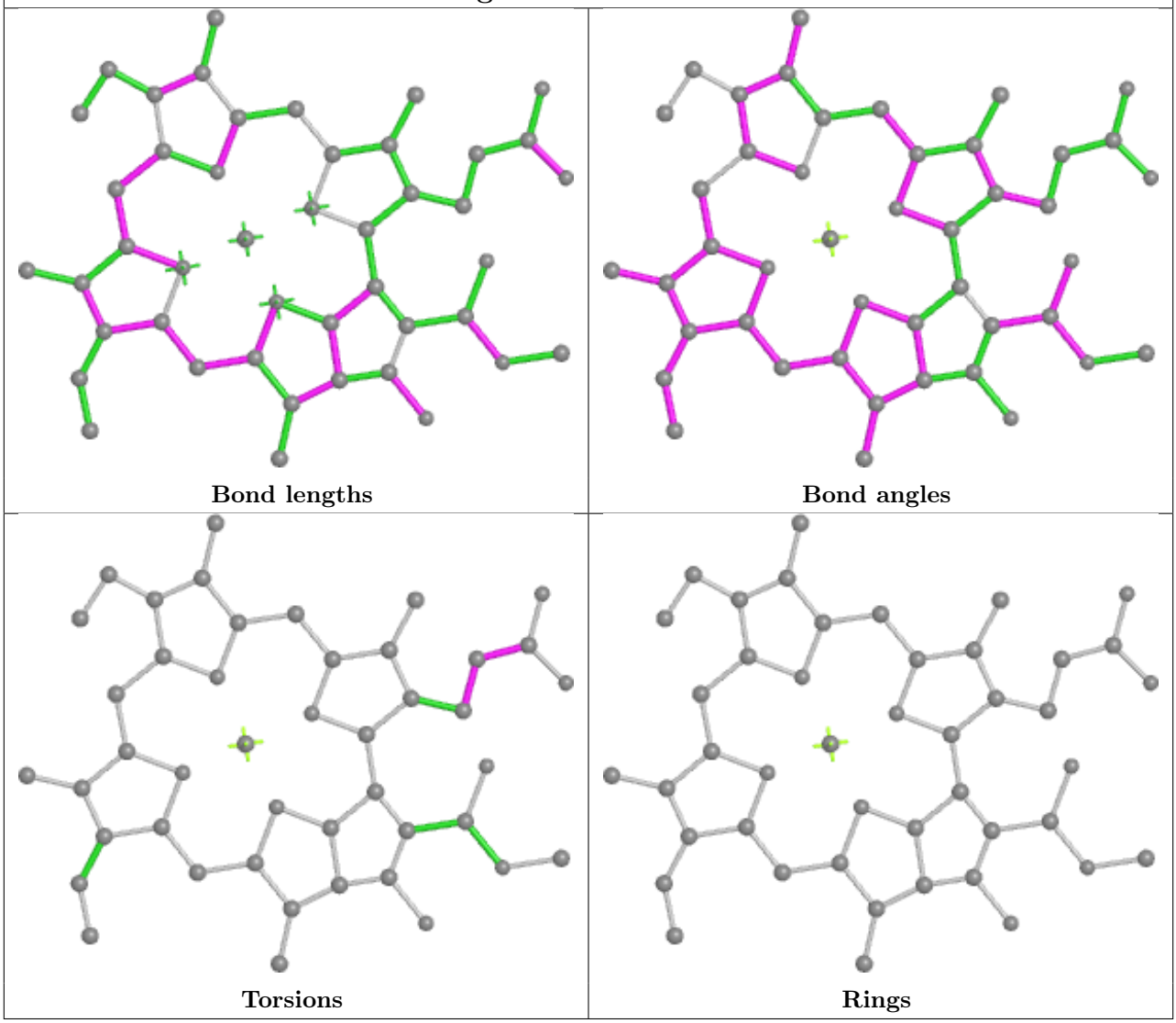

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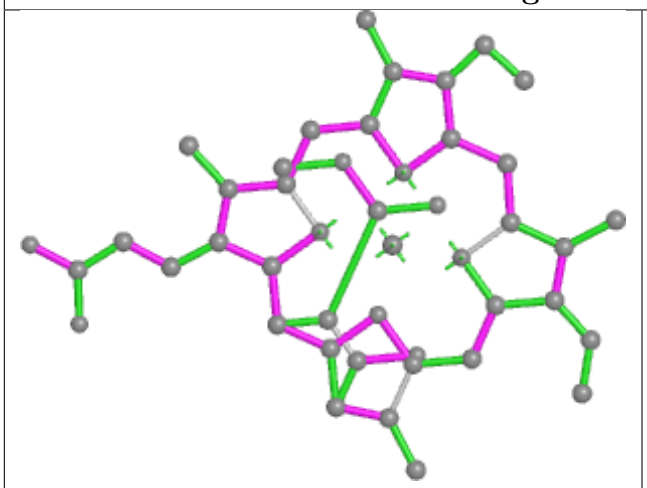

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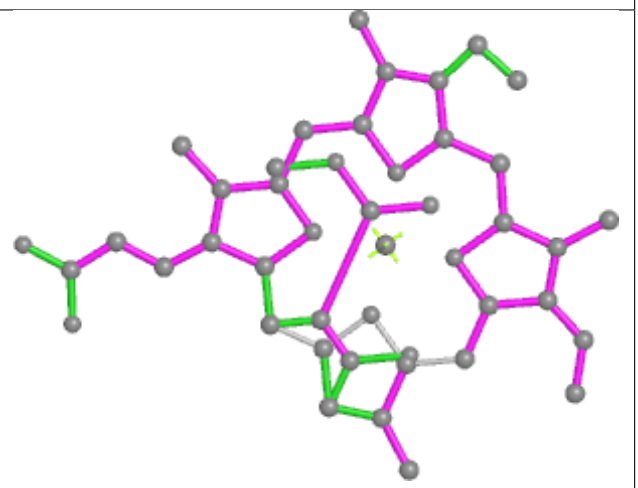

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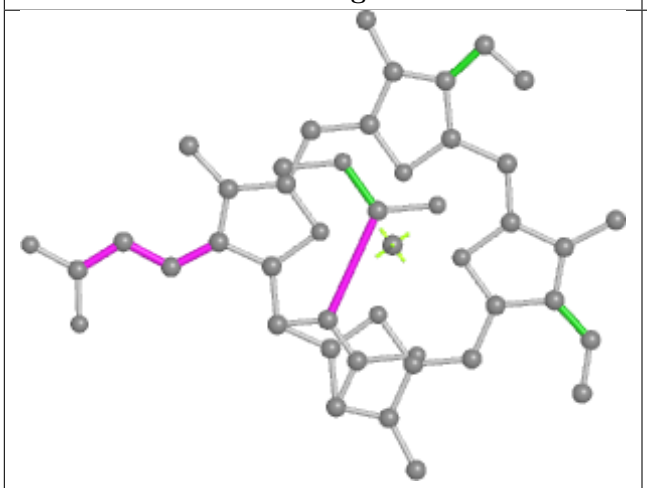

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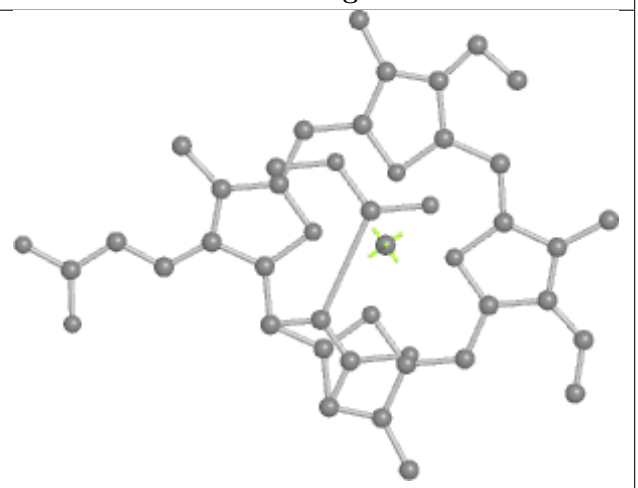

Rings

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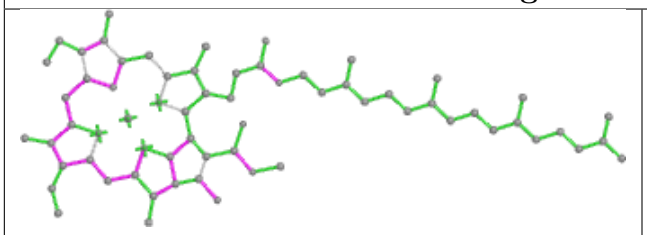

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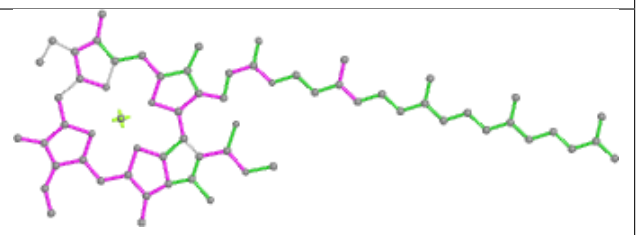

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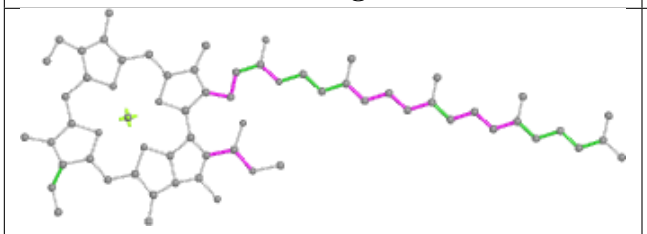

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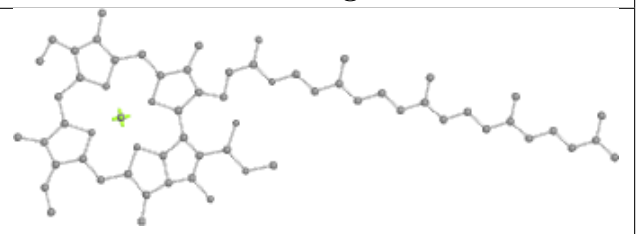

Rings

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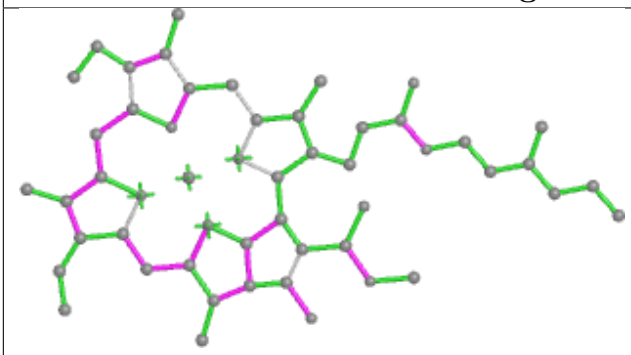
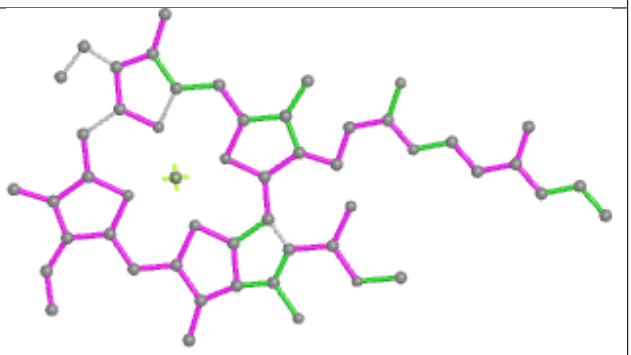
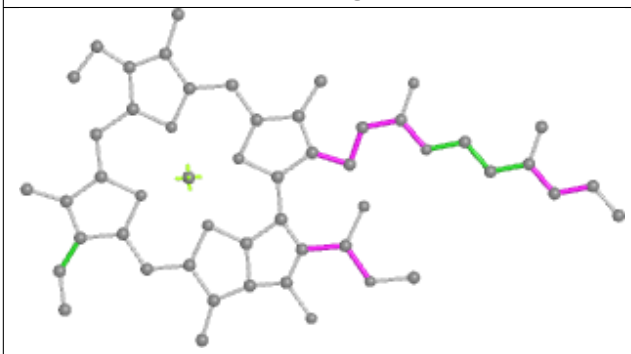
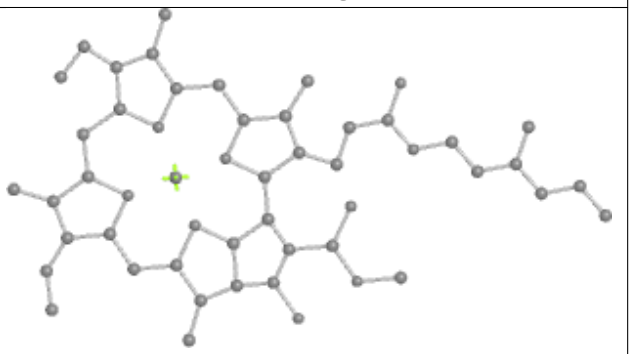
 Bond lengths	 Bond angles
 Torsions	 Rings

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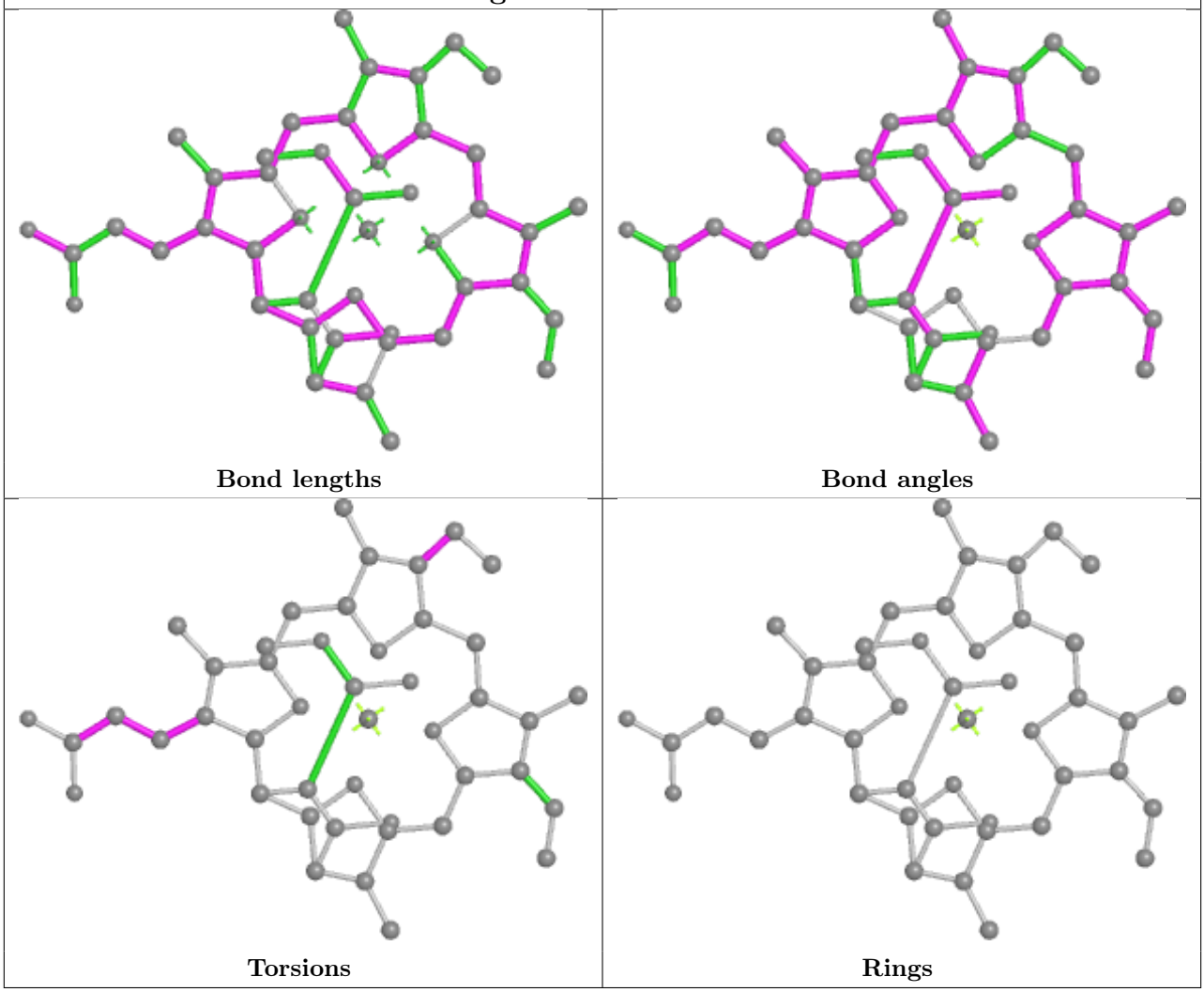
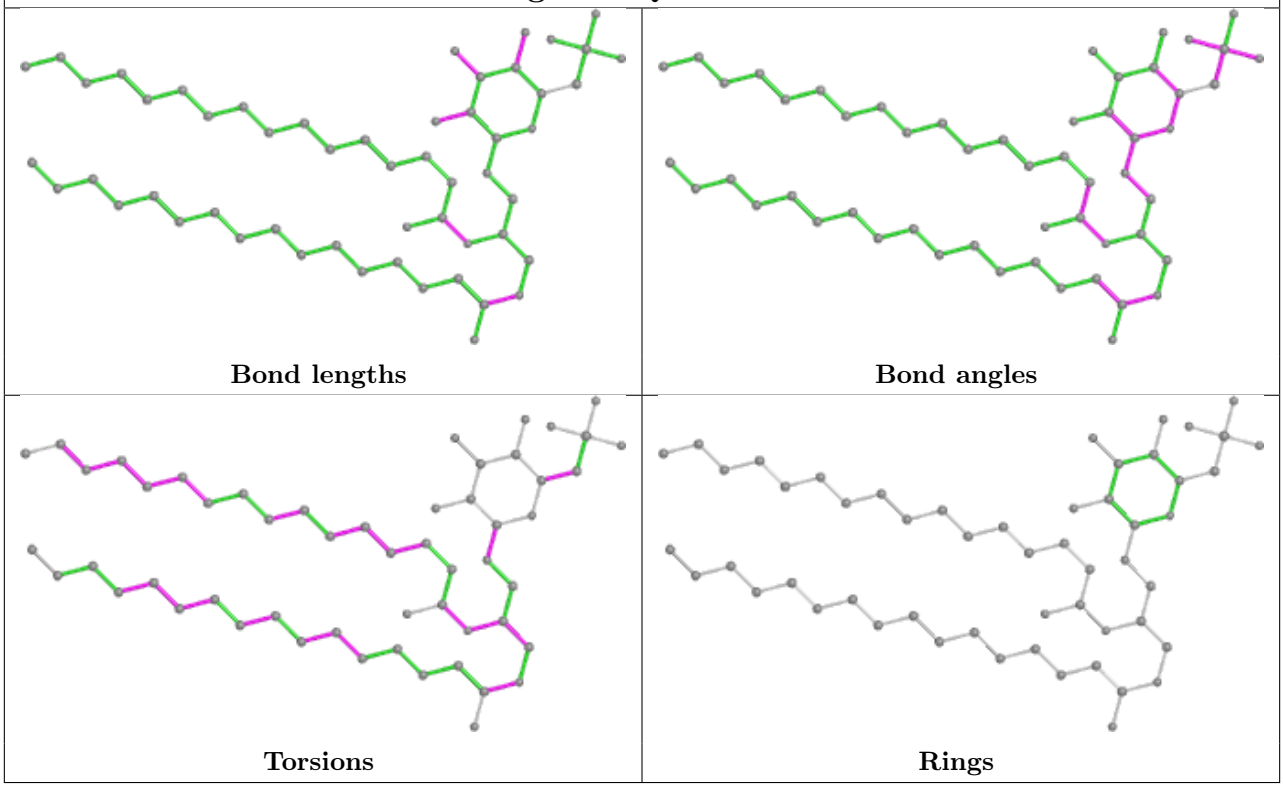


Ligand SQD L 101



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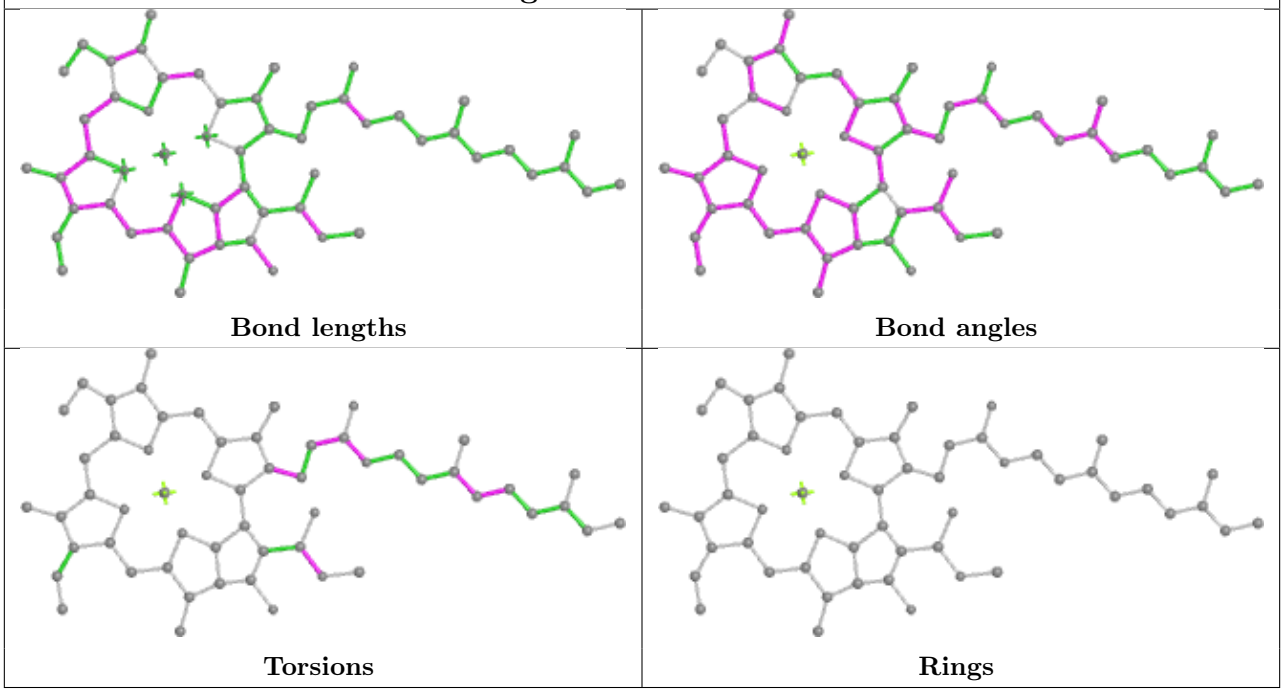
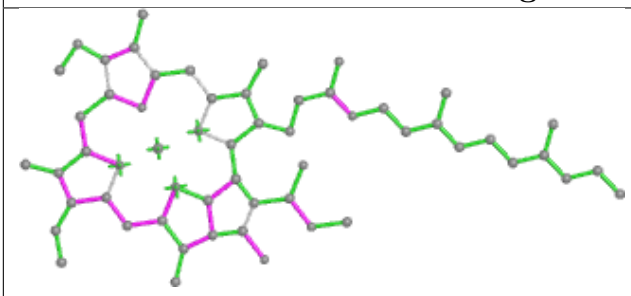
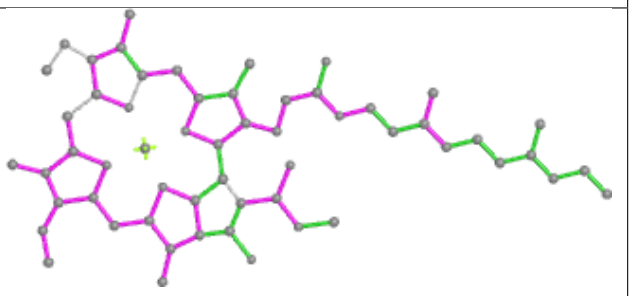


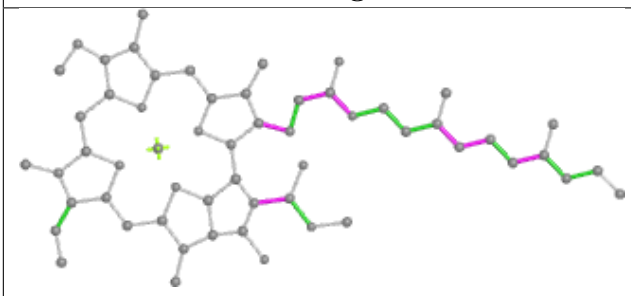
Ligand CLA 13 303



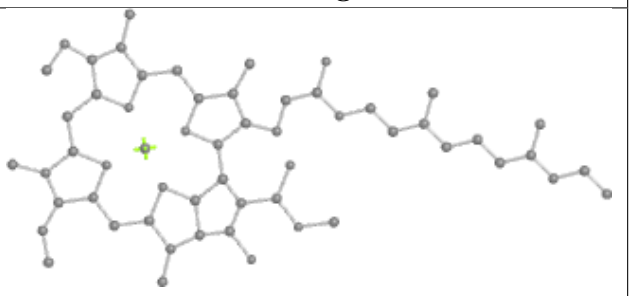
Bond lengths



Bond angles

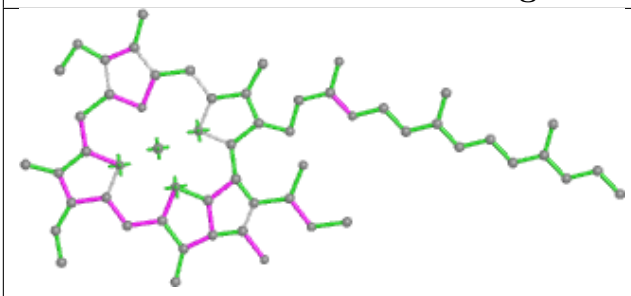


Torsions



Rings

Ligand CLA 34 303



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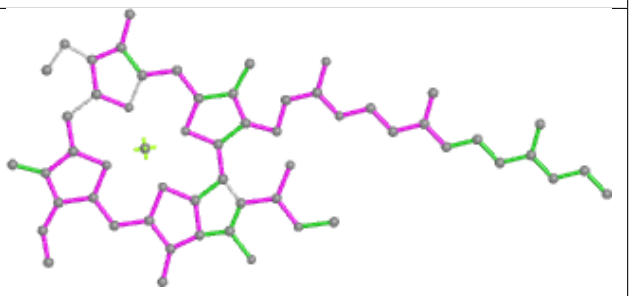
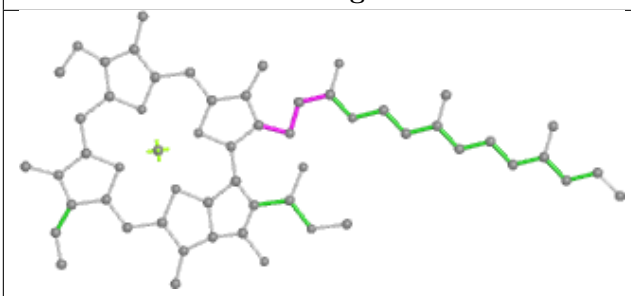


Bond angles



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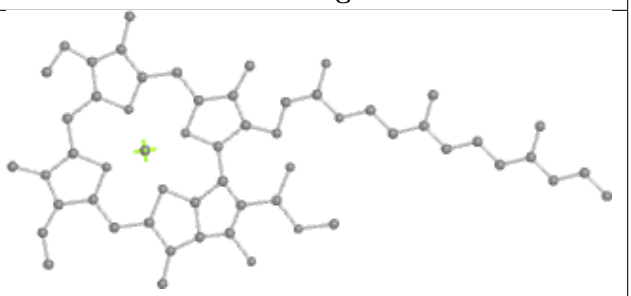

Rings

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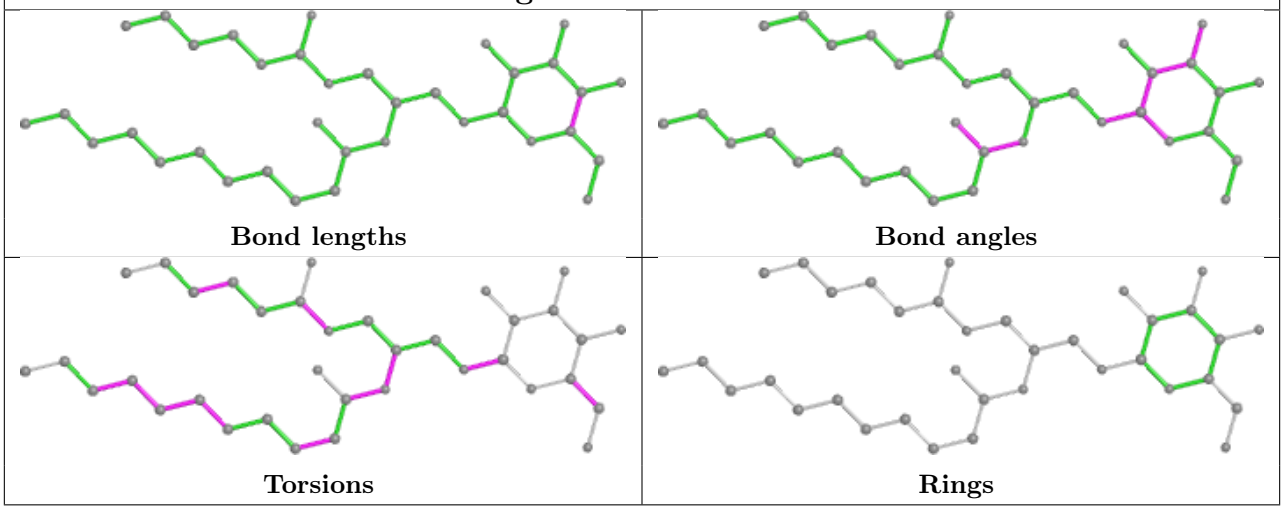
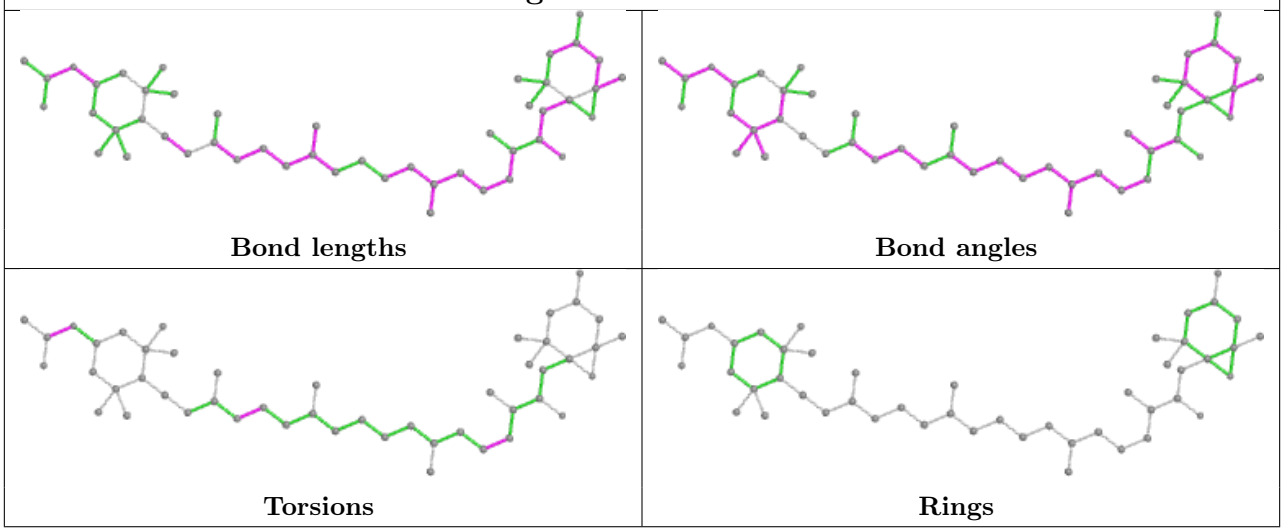


Ligand A86 34 312



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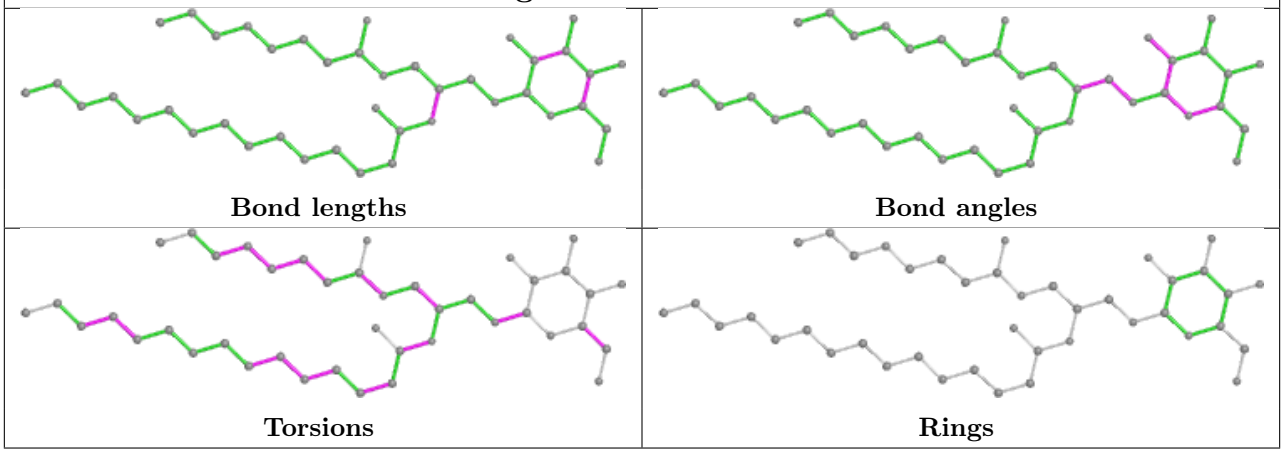

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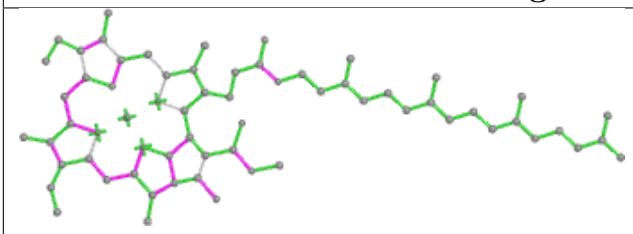

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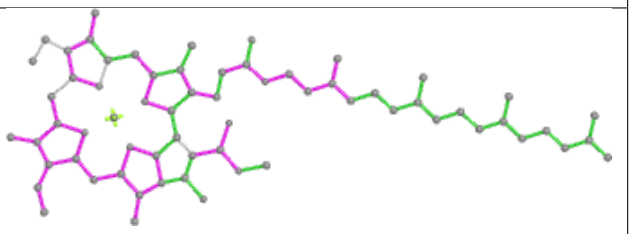

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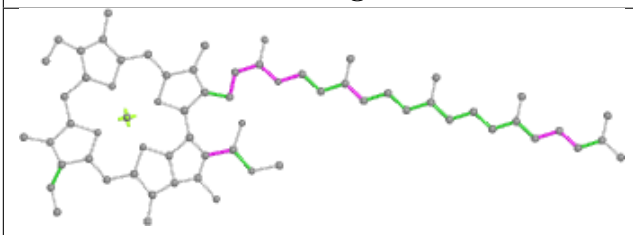

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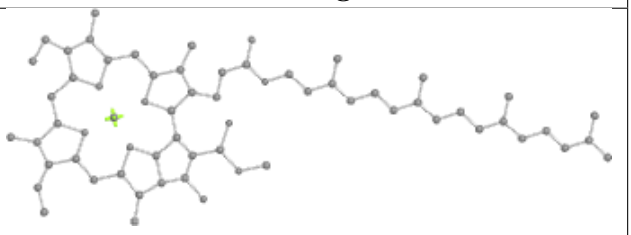
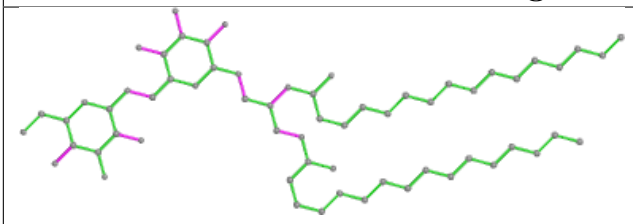


Rings

Ligand DGD j 101



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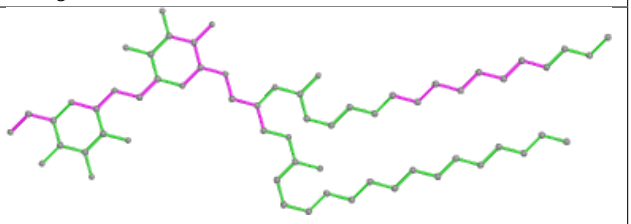

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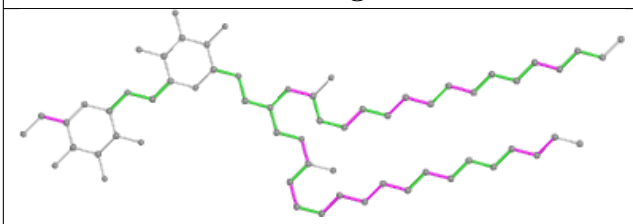

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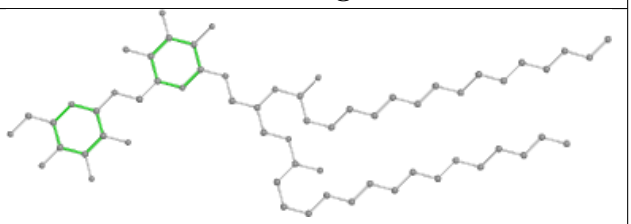
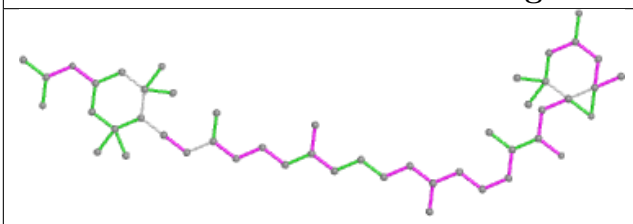


Rings

Ligand A86 16 310



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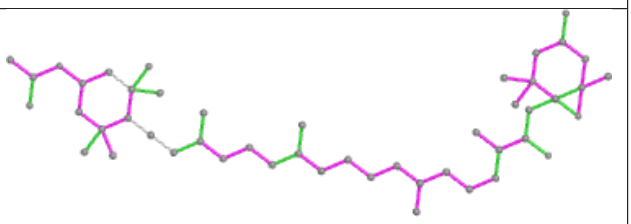

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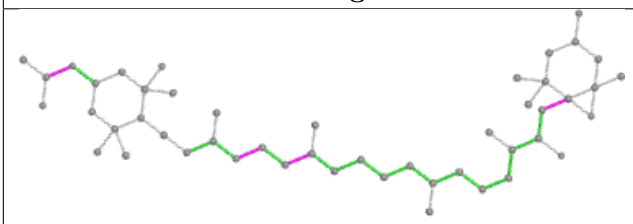

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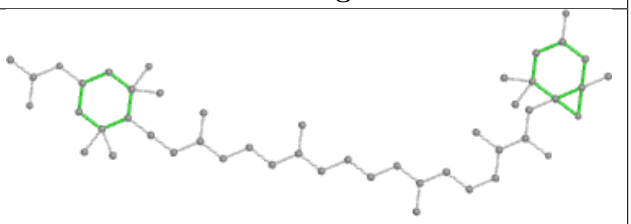

Rings

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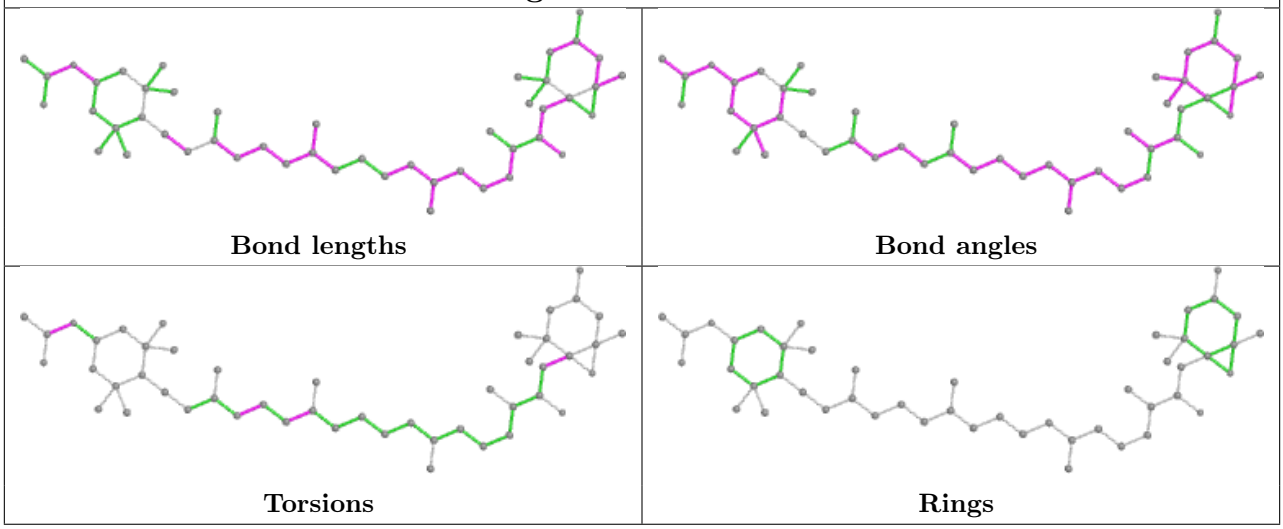

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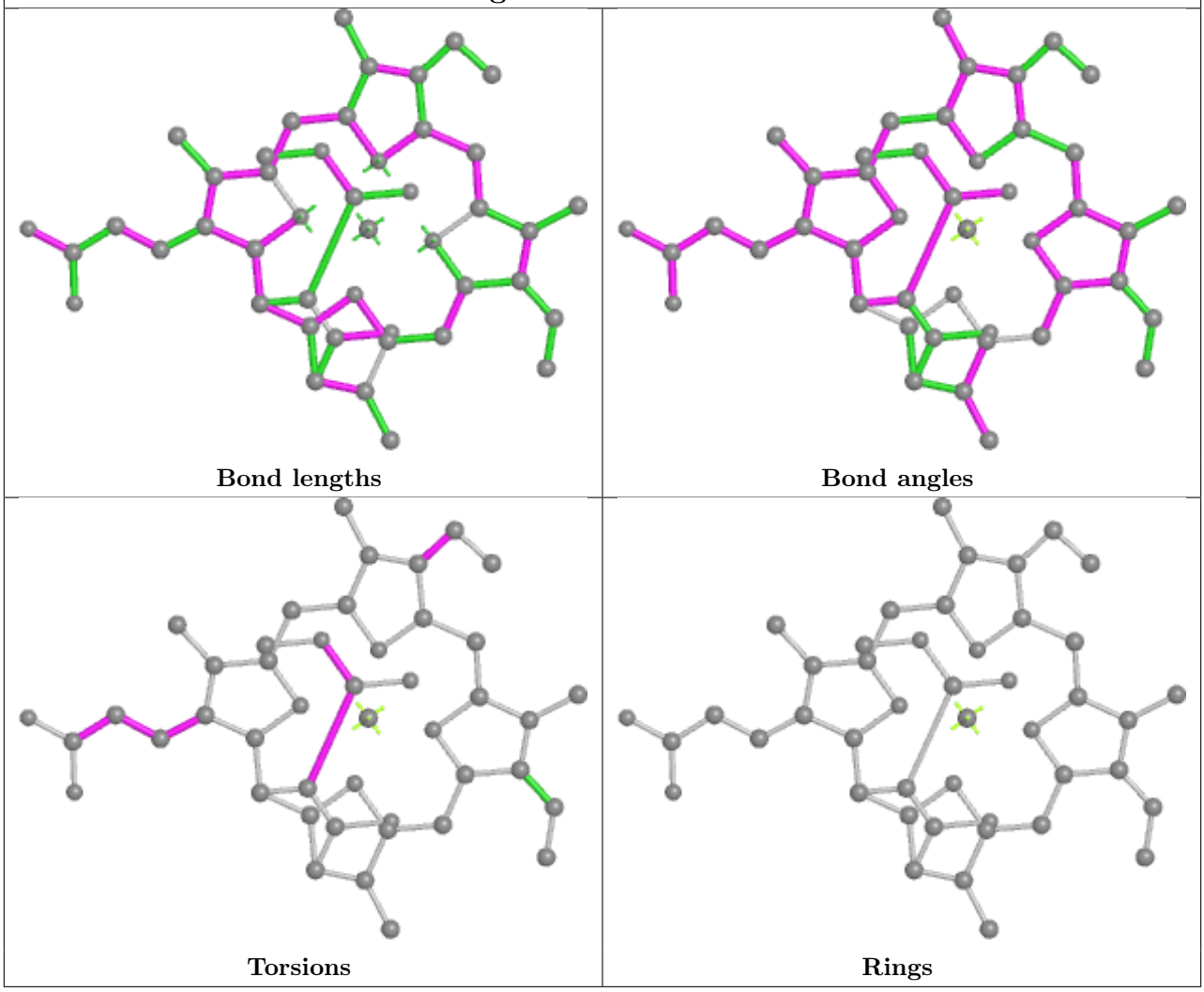

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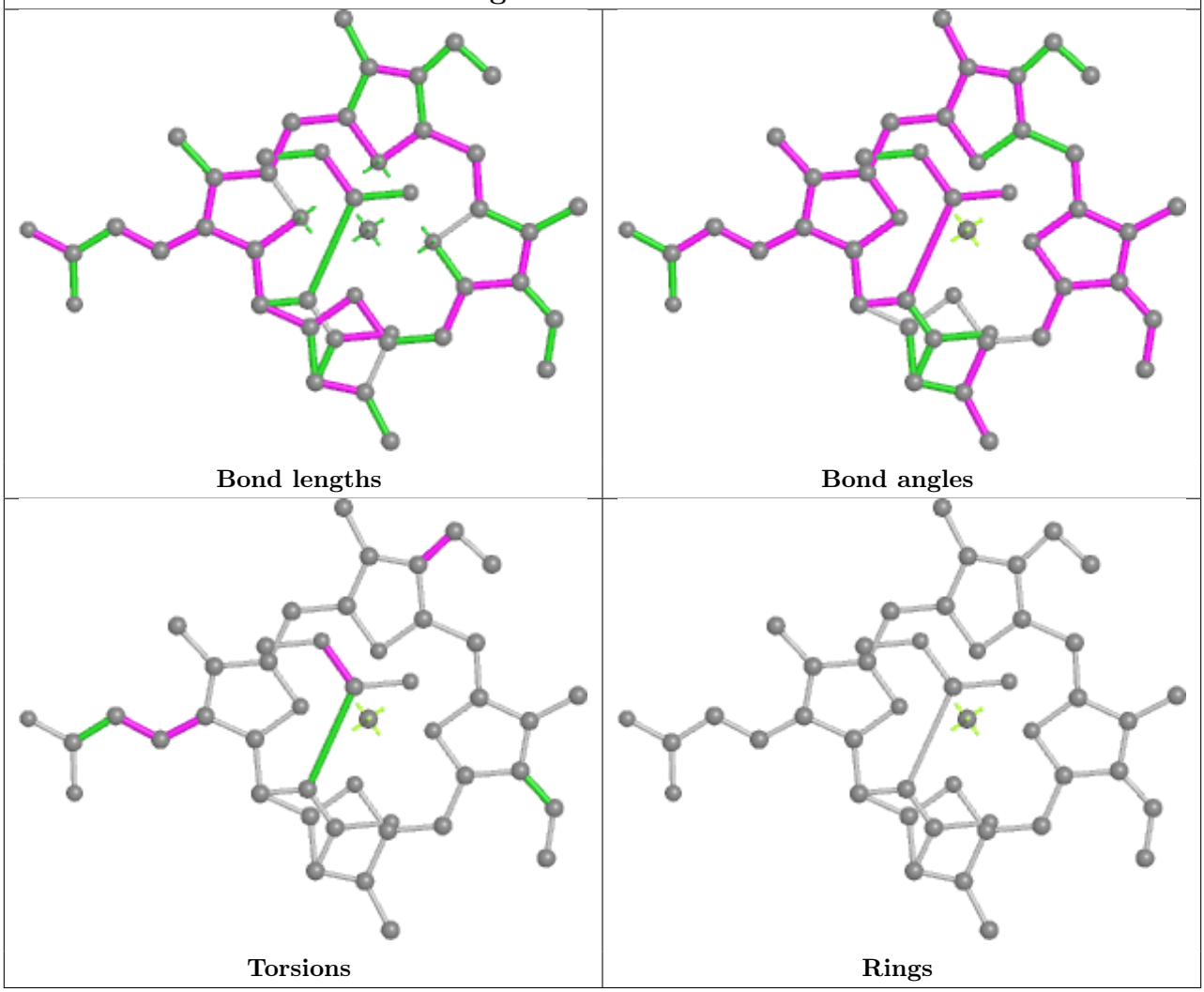

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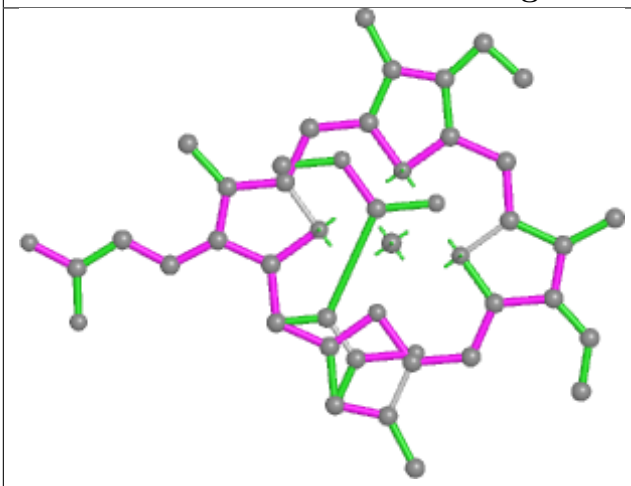

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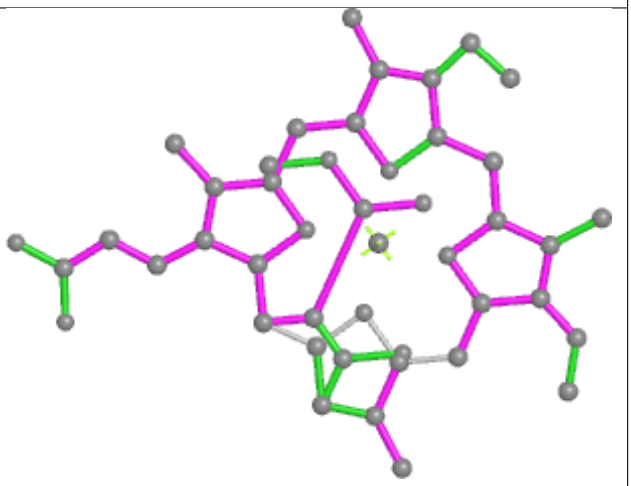
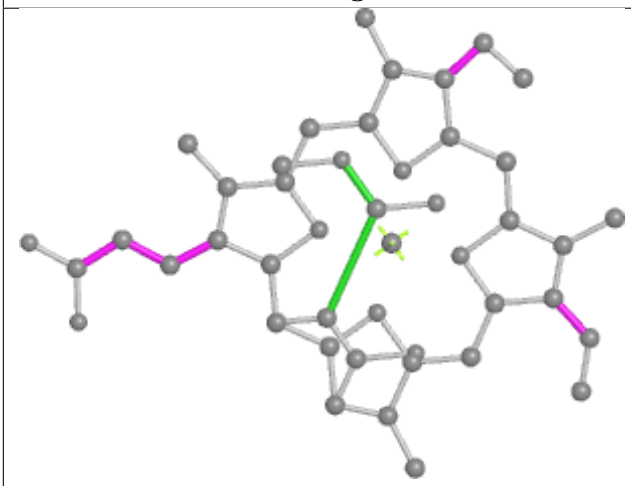
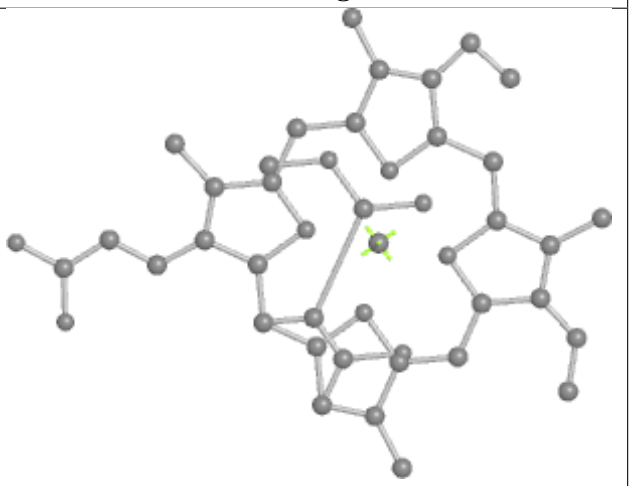


Bond angles

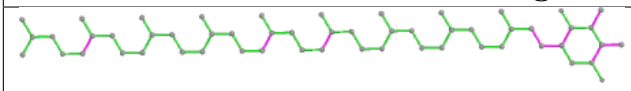


Torsions



Rings

Ligand PL9 d 406



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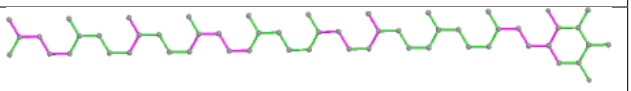

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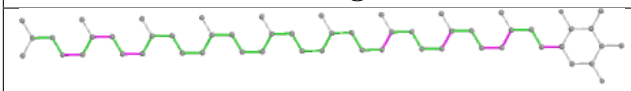

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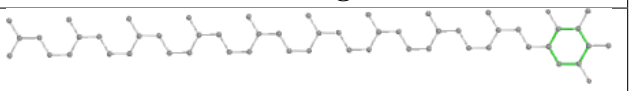

Rings

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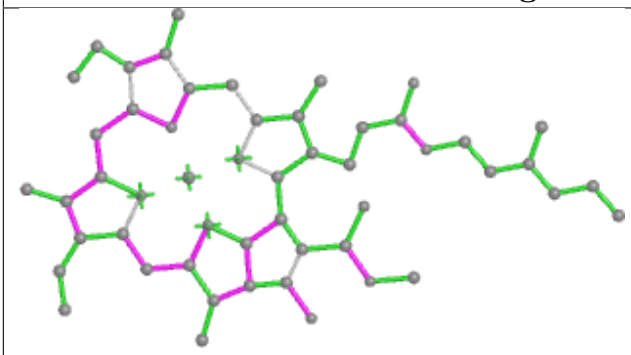
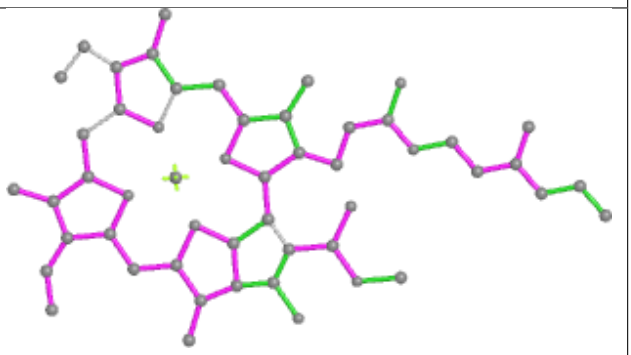
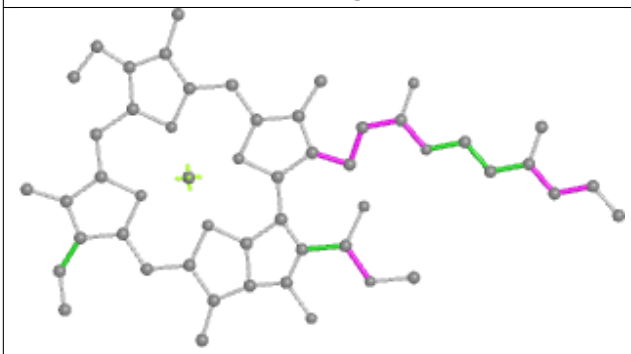
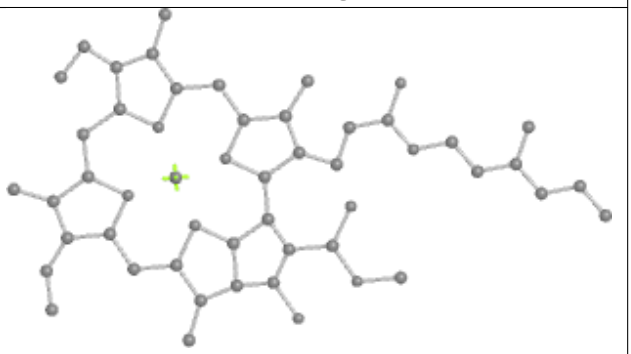
 Bond lengths	 Bond angles
 Torsions	 Rings

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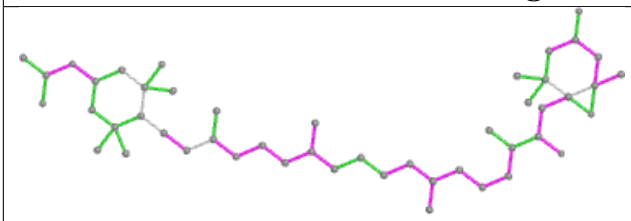
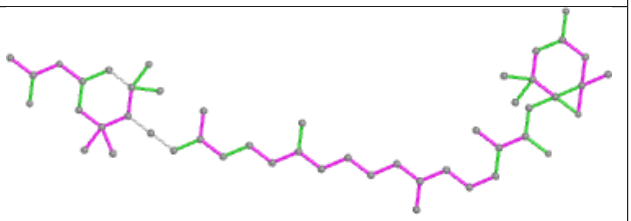
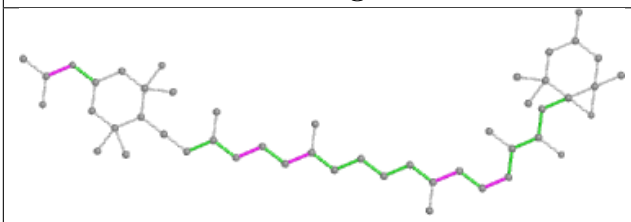
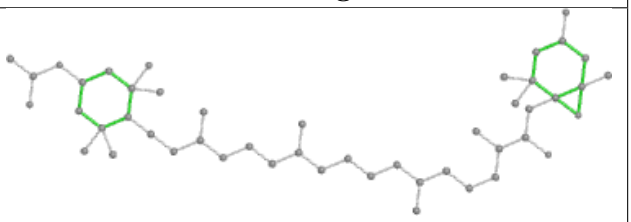
 Bond lengths	 Bond angles
 Torsions	 Rings

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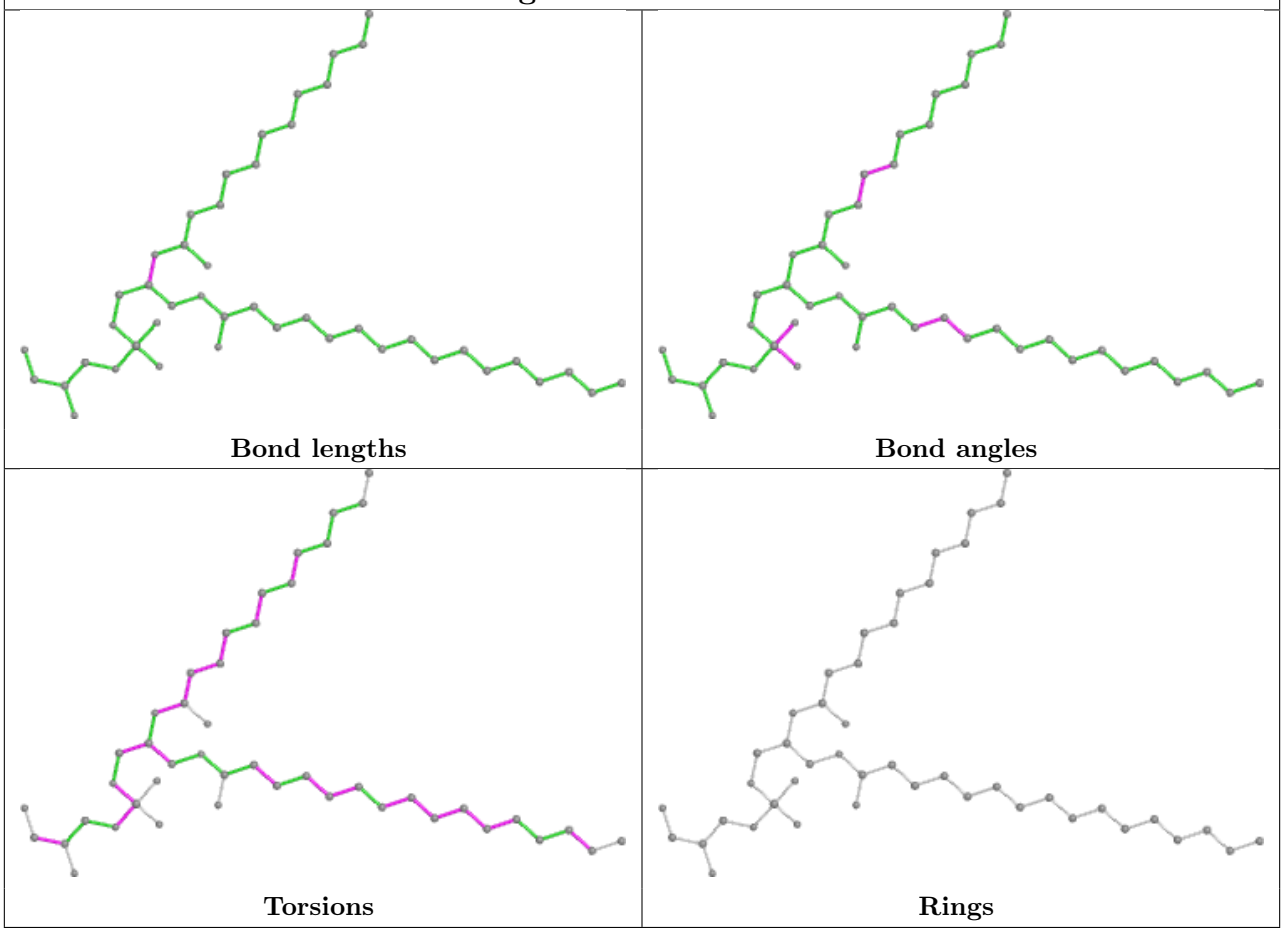

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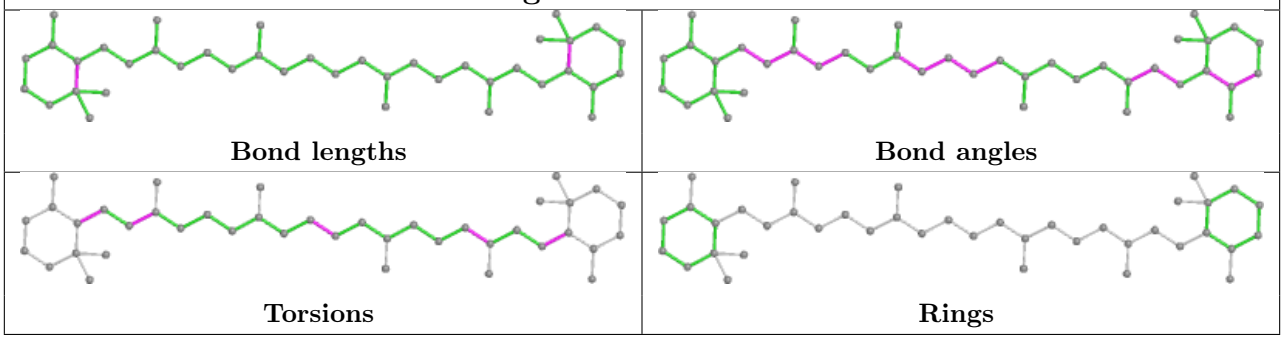

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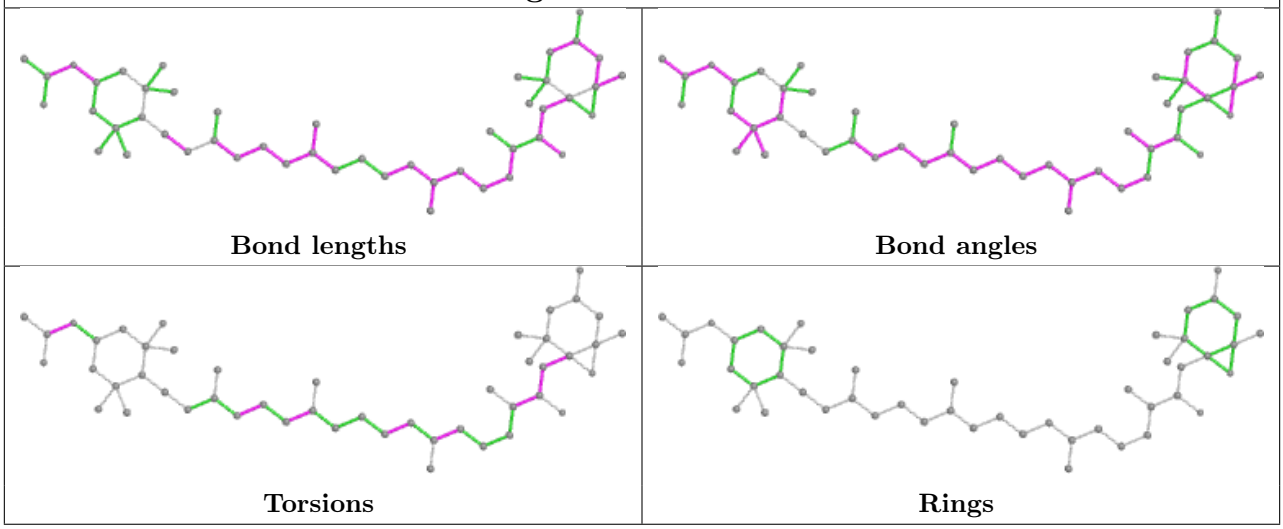

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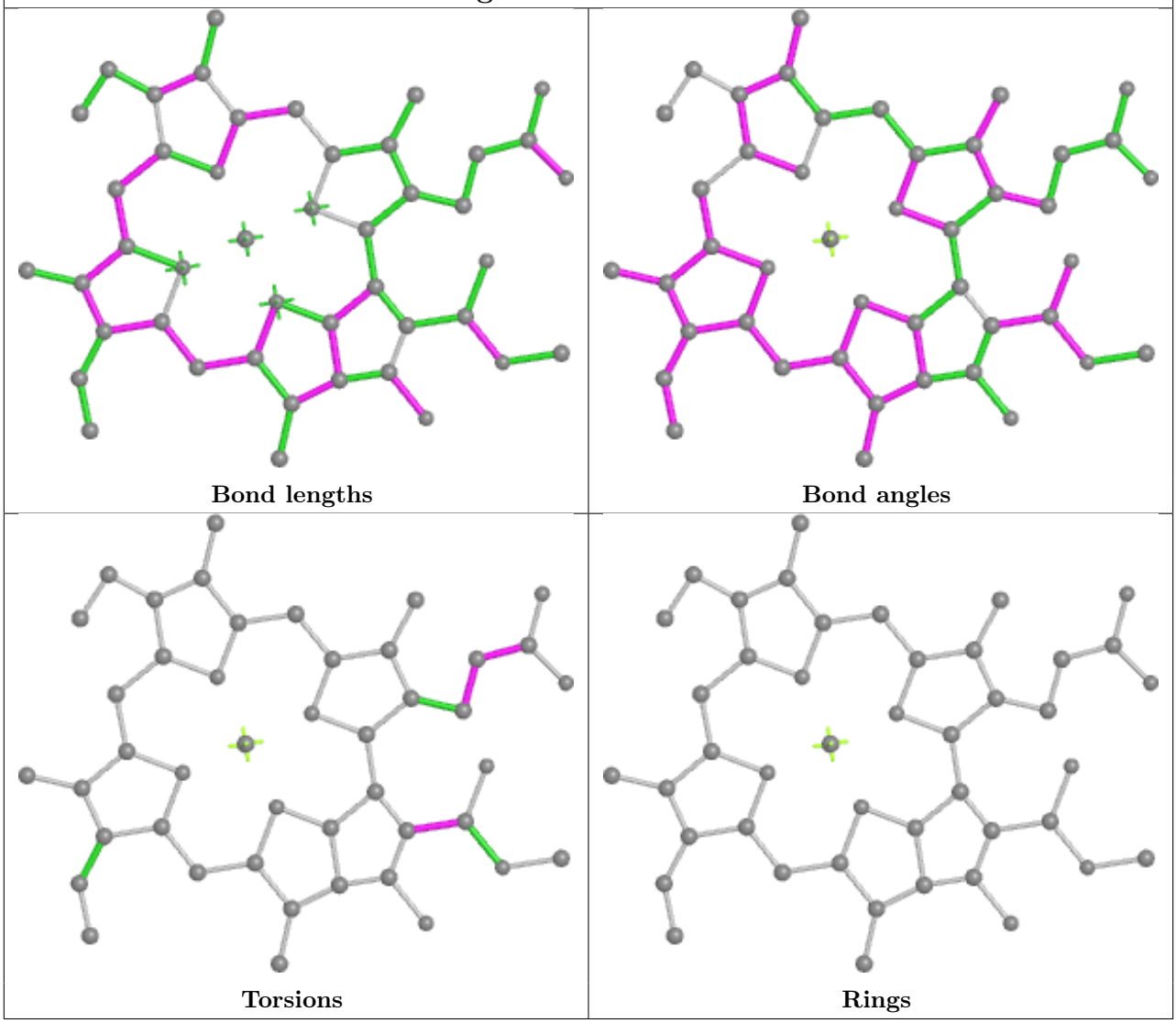

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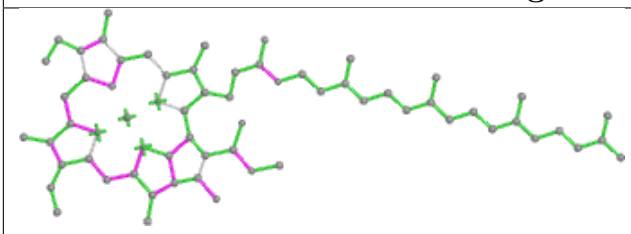
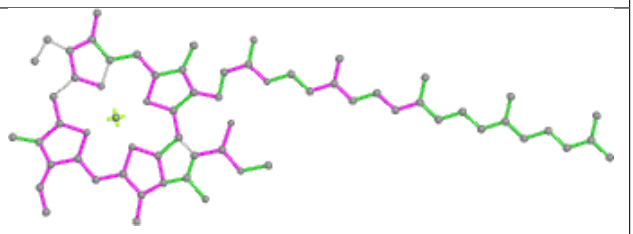
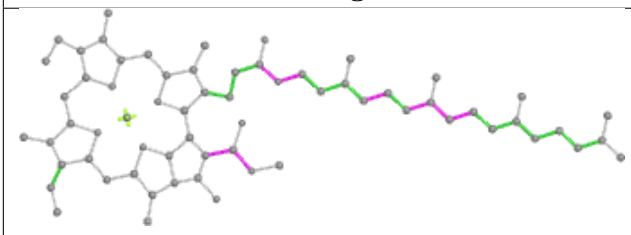
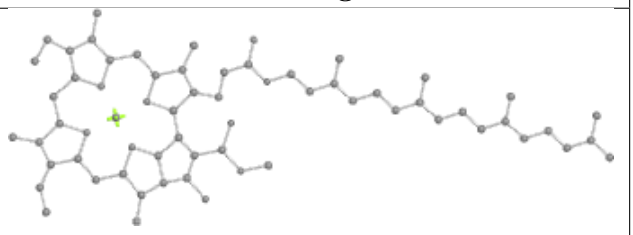
 Bond lengths	 Bond angles
 Torsions	 Rings

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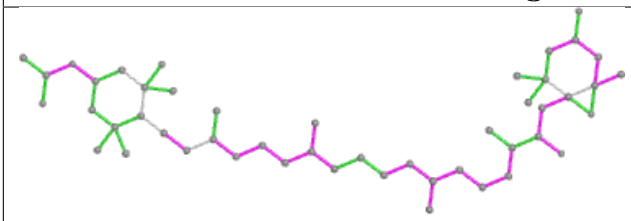
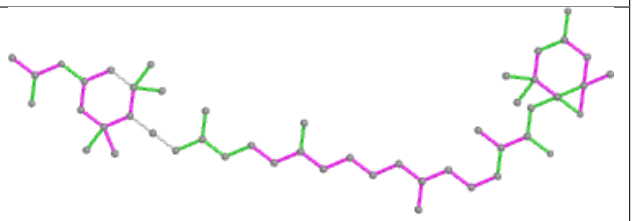
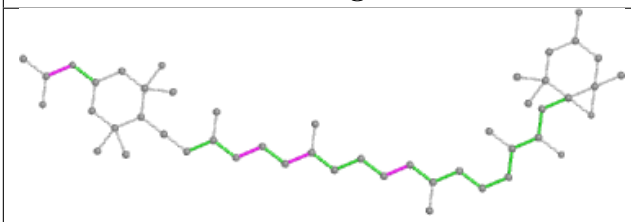
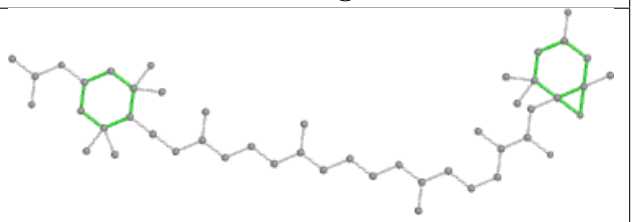
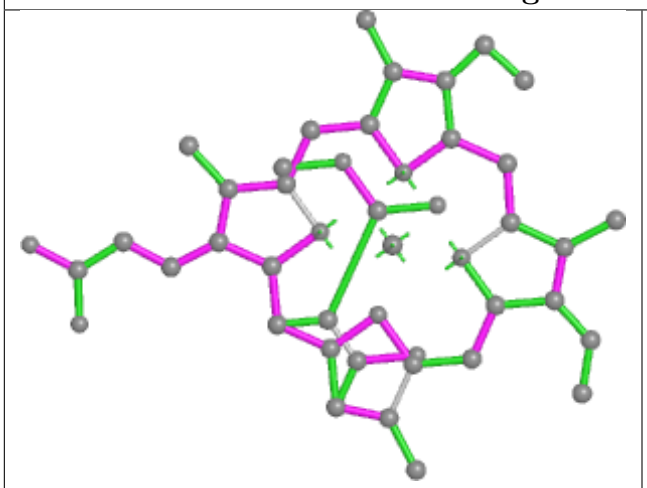
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 12 208



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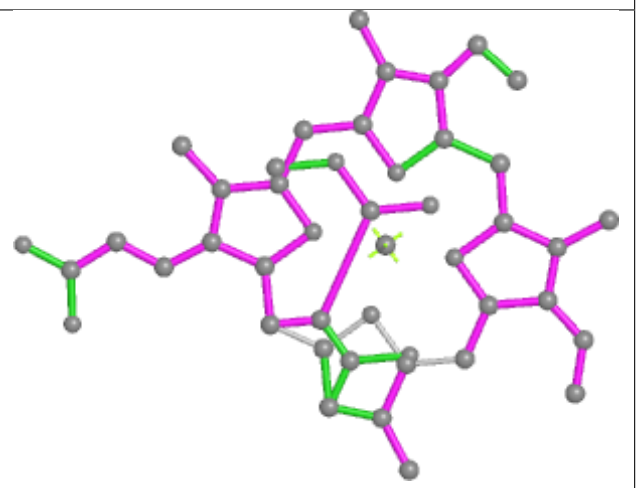
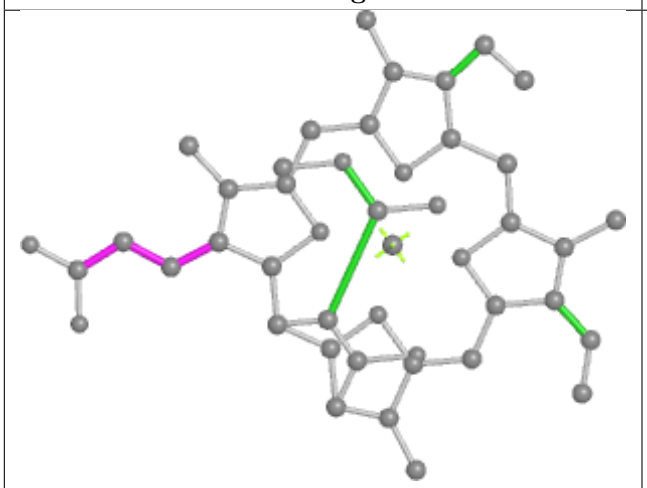


Bond angles



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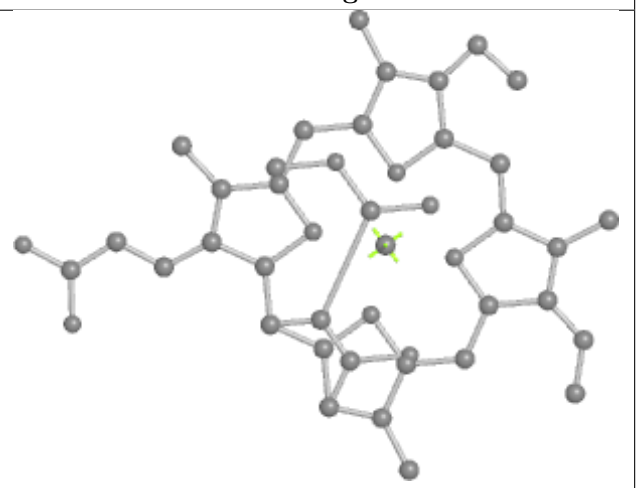
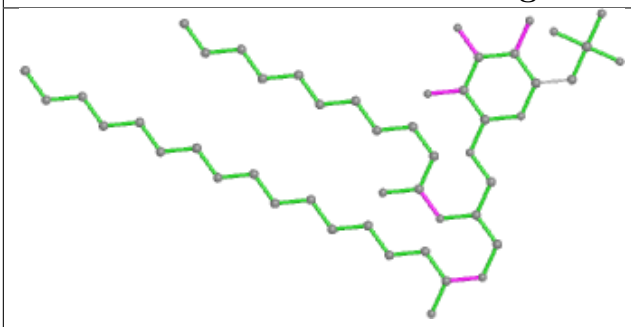
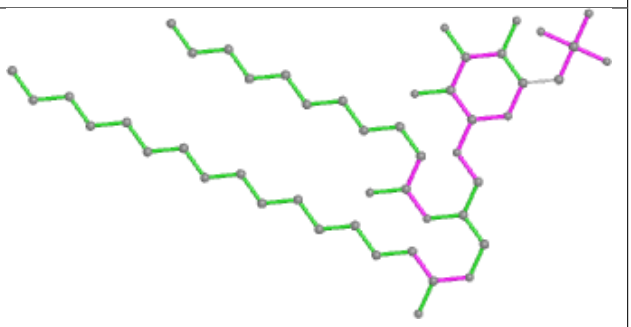
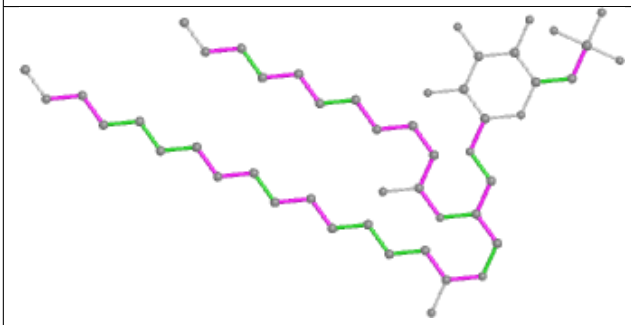
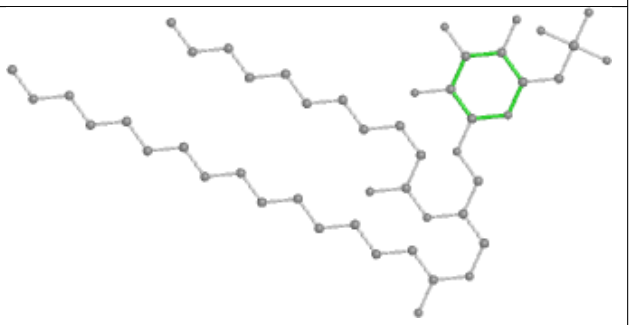
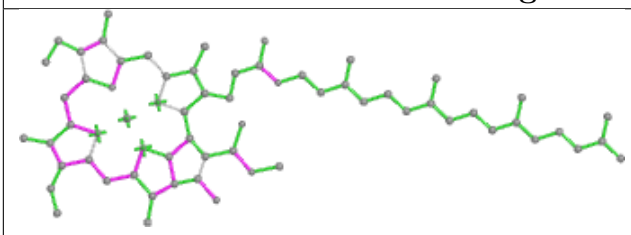
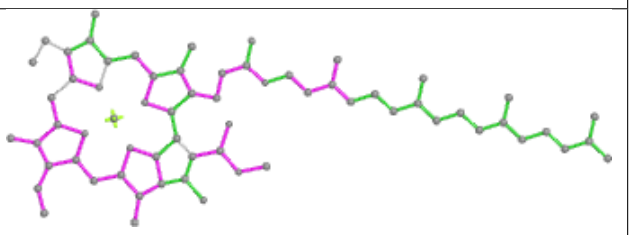
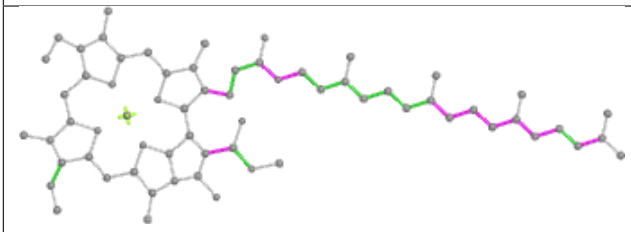
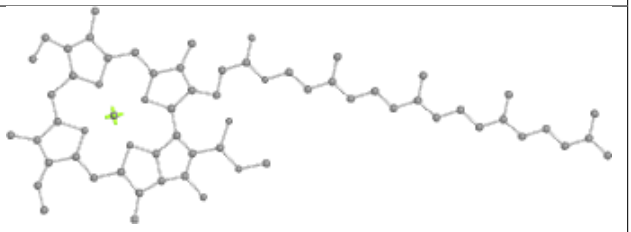
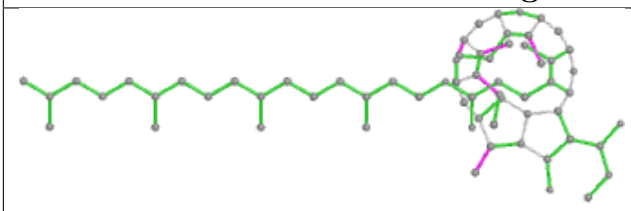


Rings

Ligand SQD 17 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 32 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO D 403



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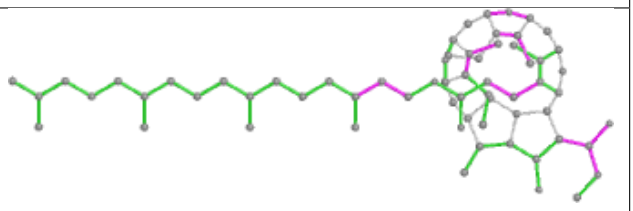

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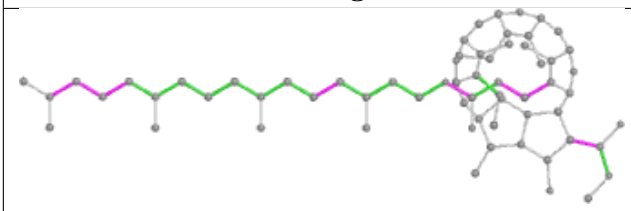

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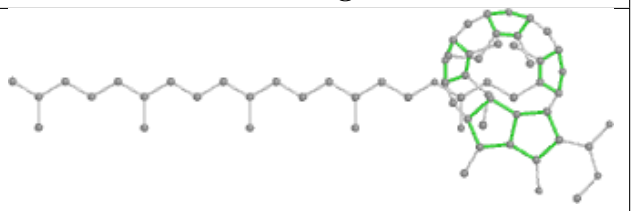
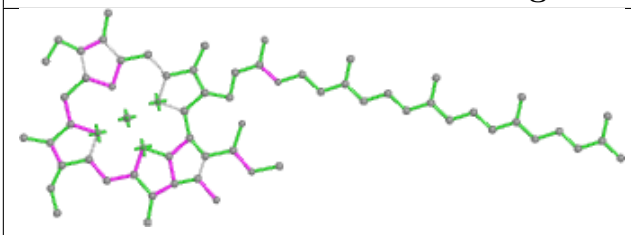


Rings

Ligand CLA c 502



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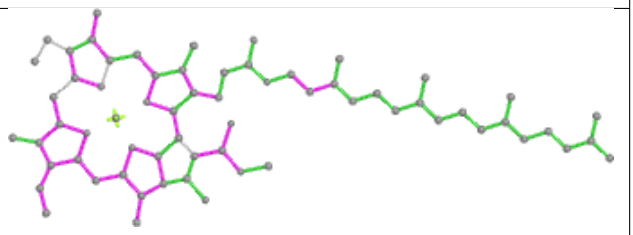

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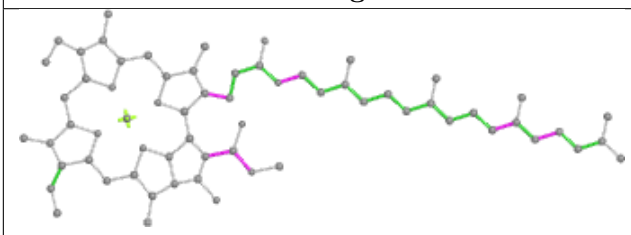

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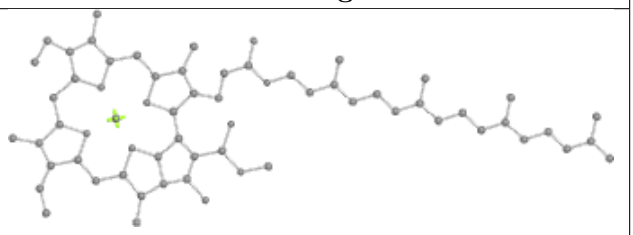
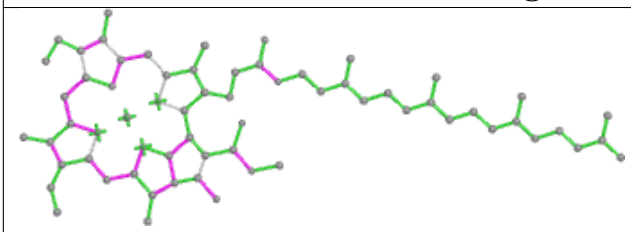


Rings

Ligand CLA D 405



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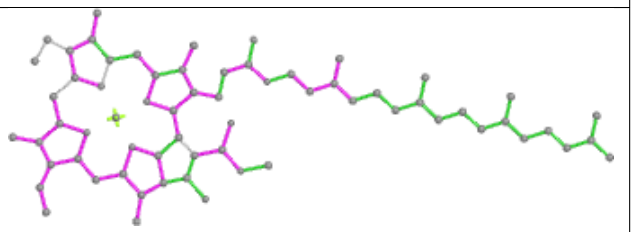

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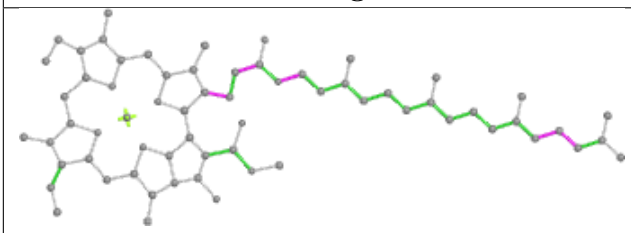

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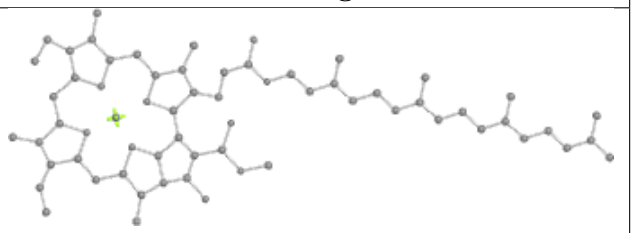

Rings

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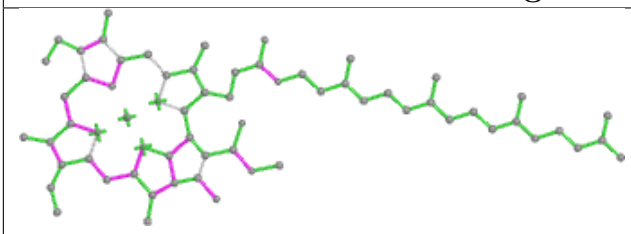
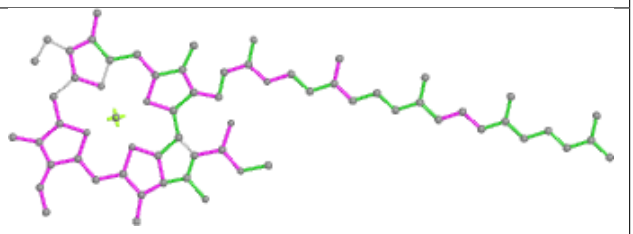
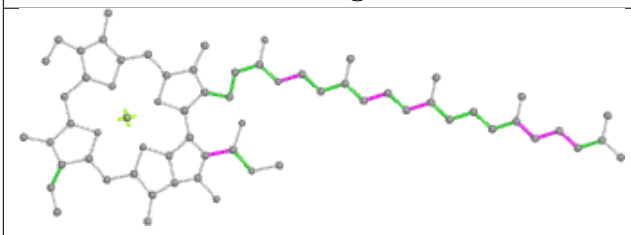
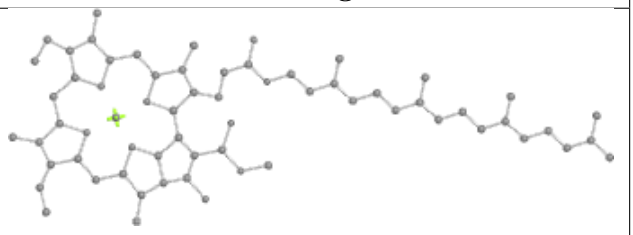
 Bond lengths	 Bond angles
 Torsions	 Rings

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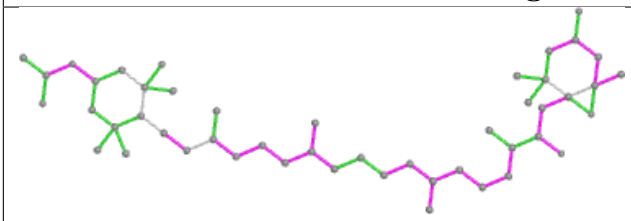
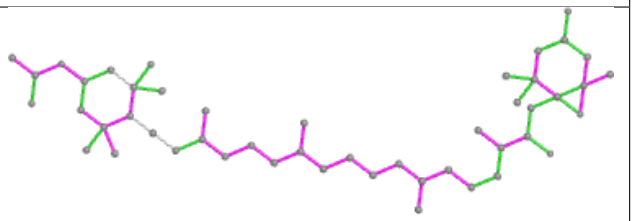
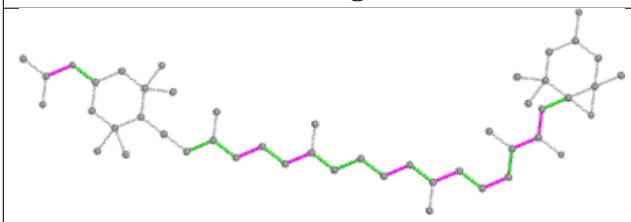
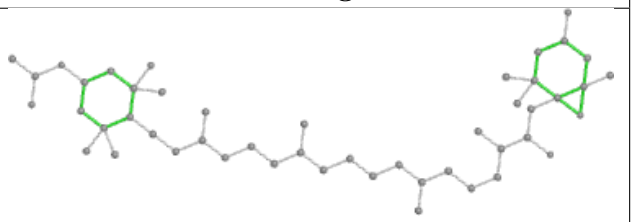
 Bond lengths	 Bond angles
 Torsions	 Rings

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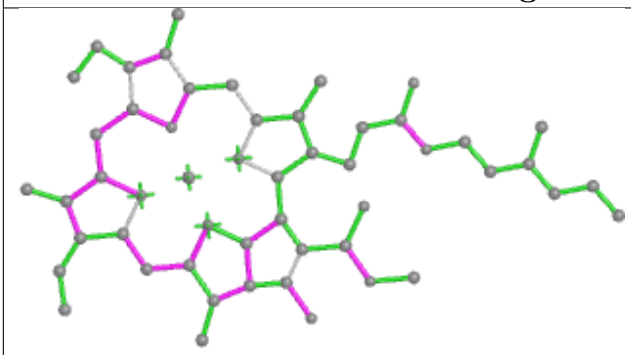
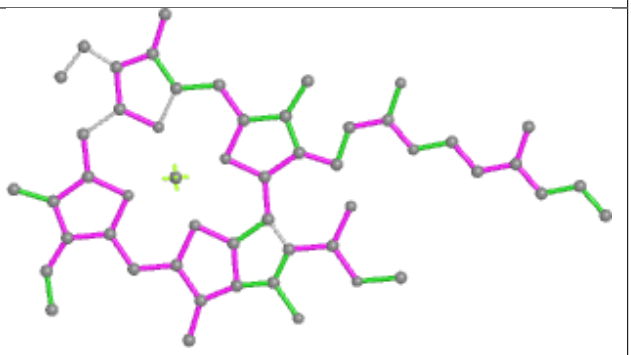
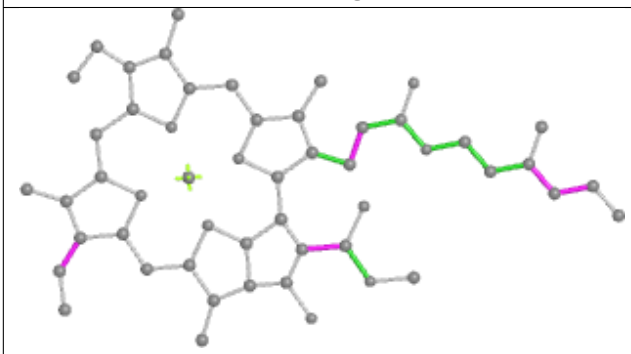
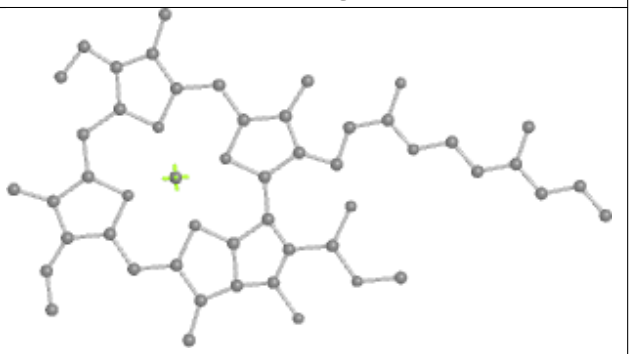
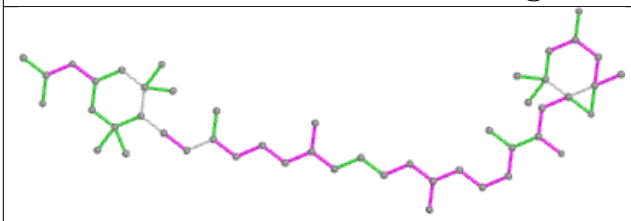
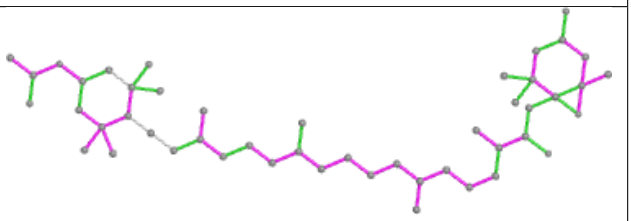
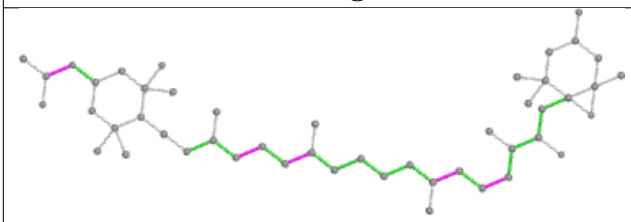
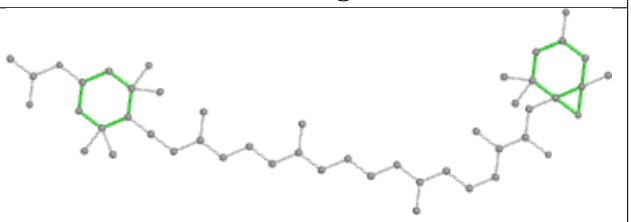
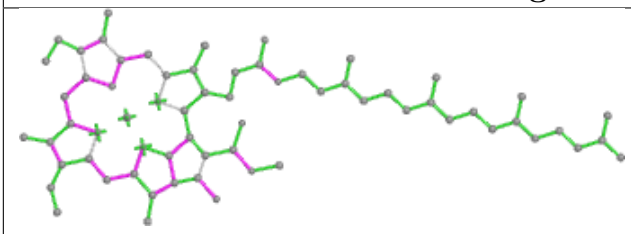
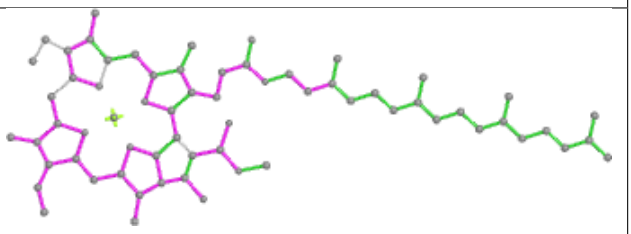
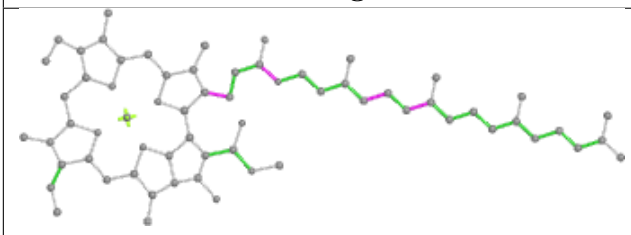
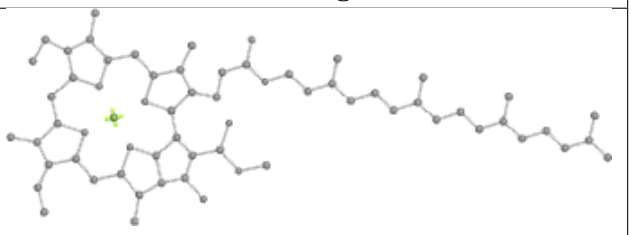
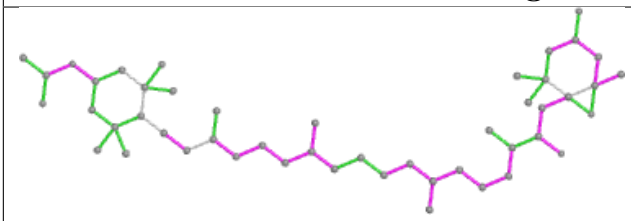
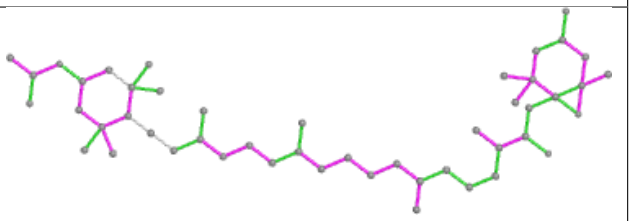
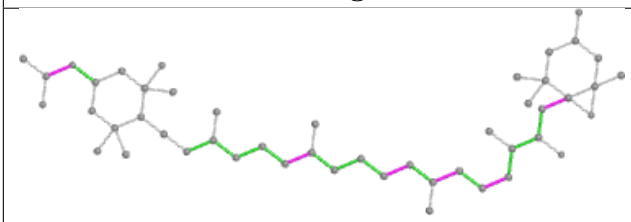
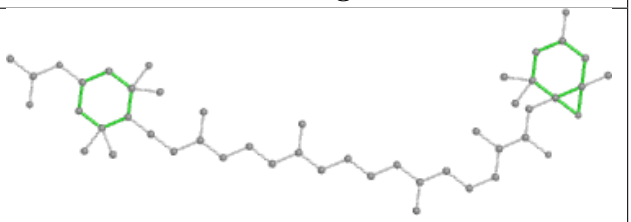
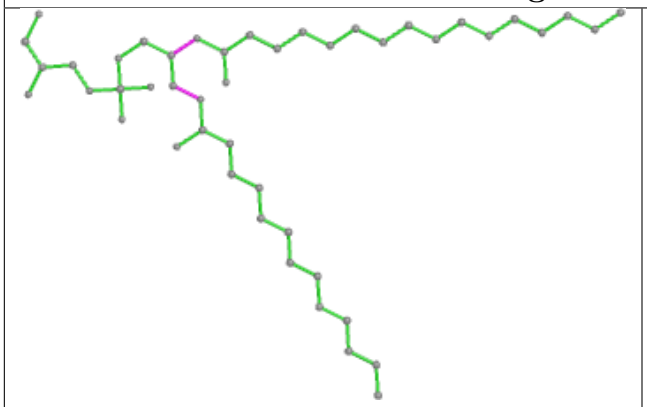
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 17 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 33 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG a 412



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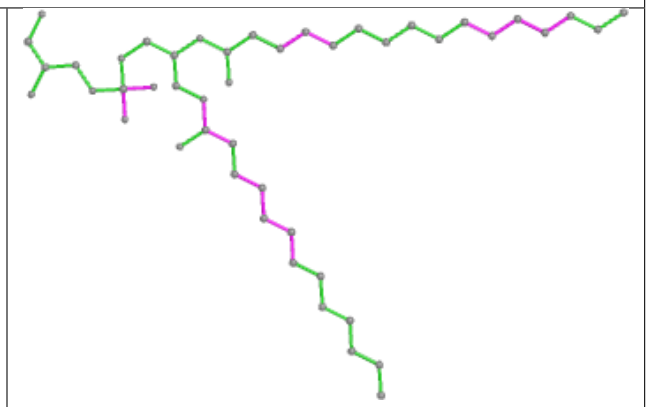
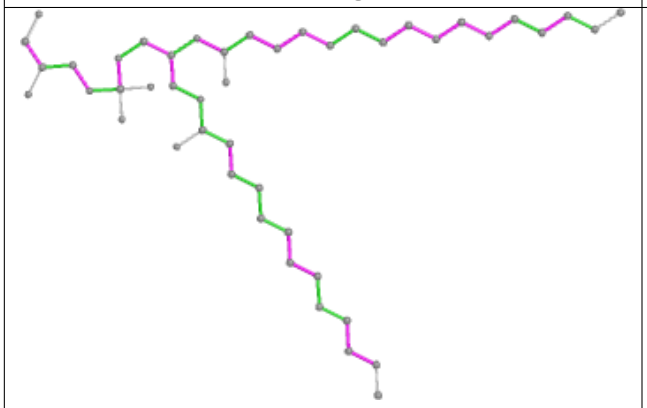
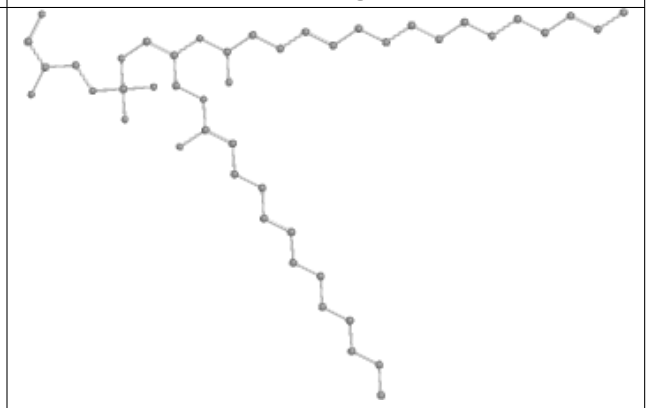


Bond angles

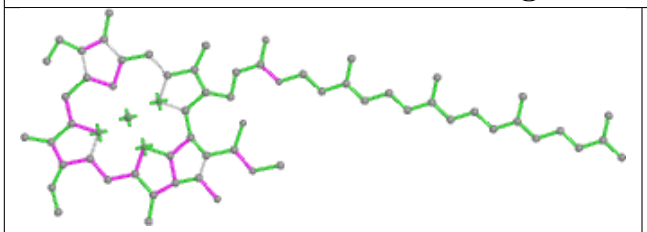


Torsions



Rings

Ligand CLA 11 303



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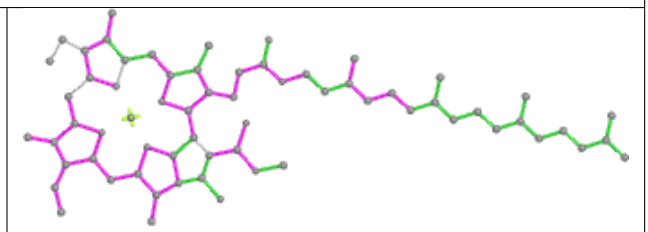
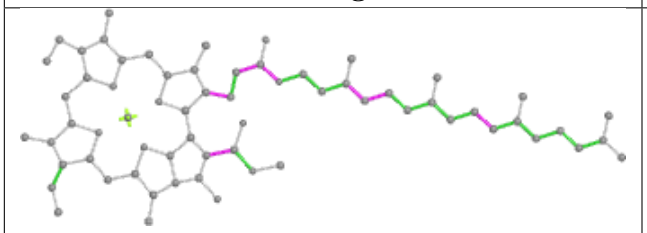


Bond angles



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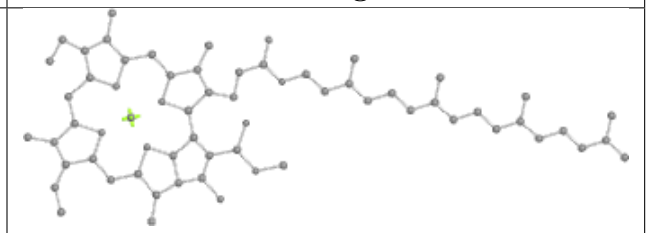
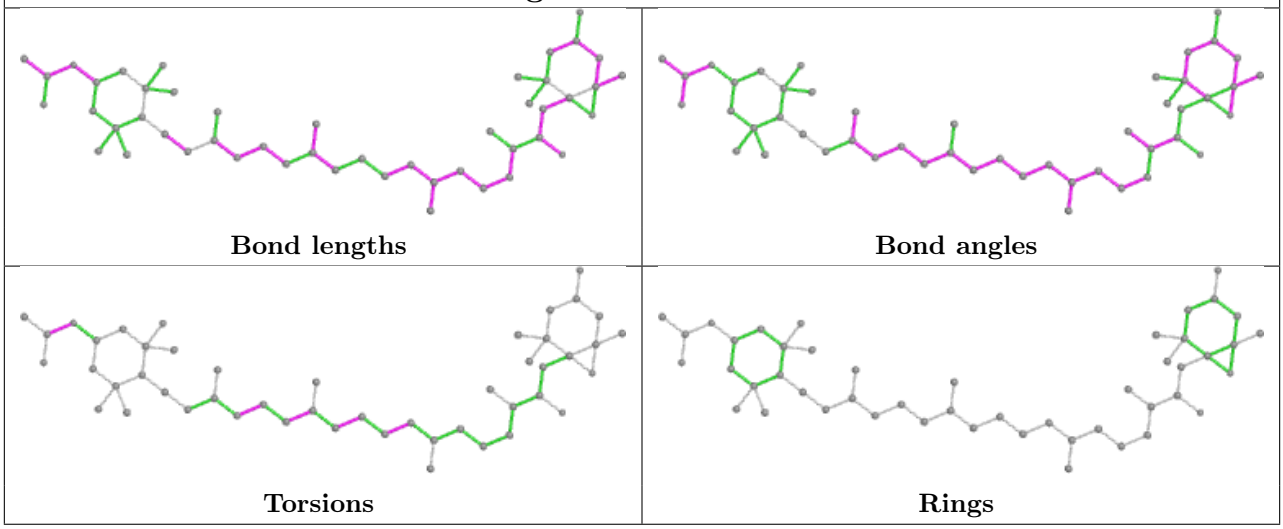
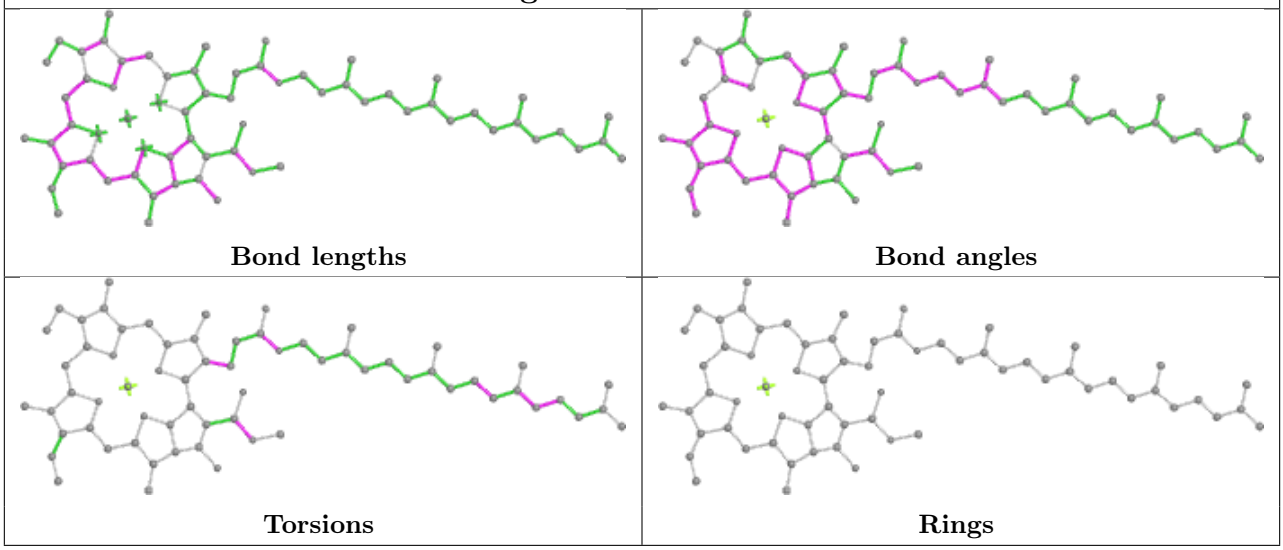


Rings

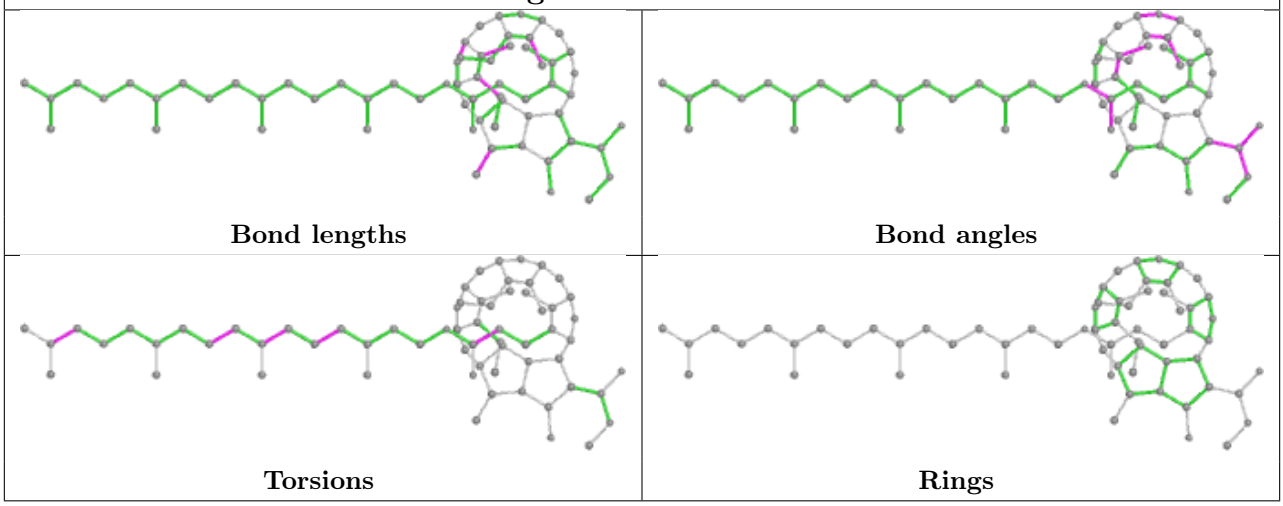
Ligand A86 31 319



Ligand CLA 18 201



Ligand PHO a 406



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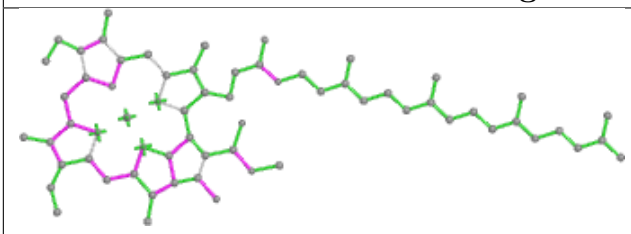
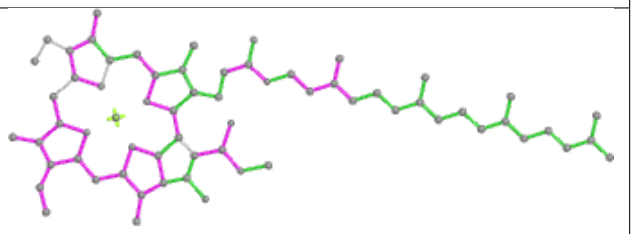
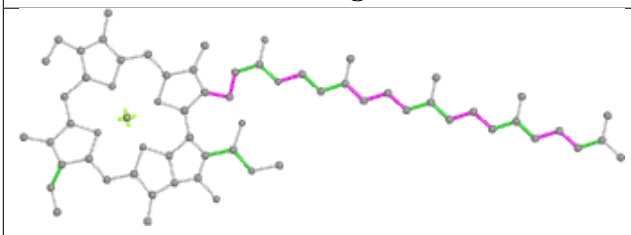
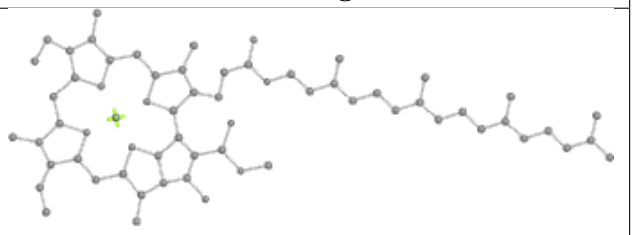
 Bond lengths	 Bond angles
 Torsions	 Rings

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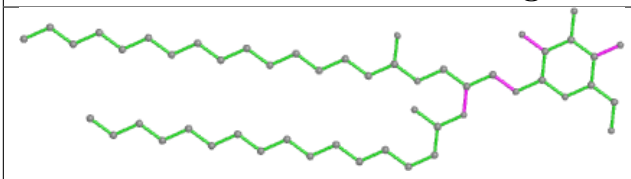
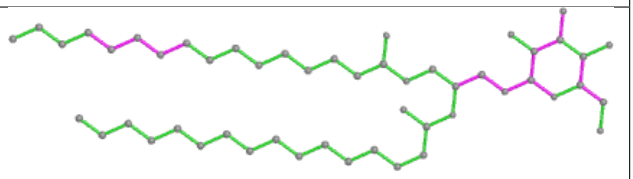
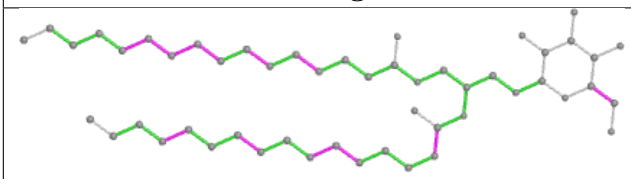
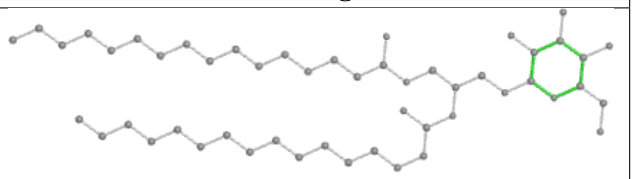
 Bond lengths	 Bond angles
 Torsions	 Rings

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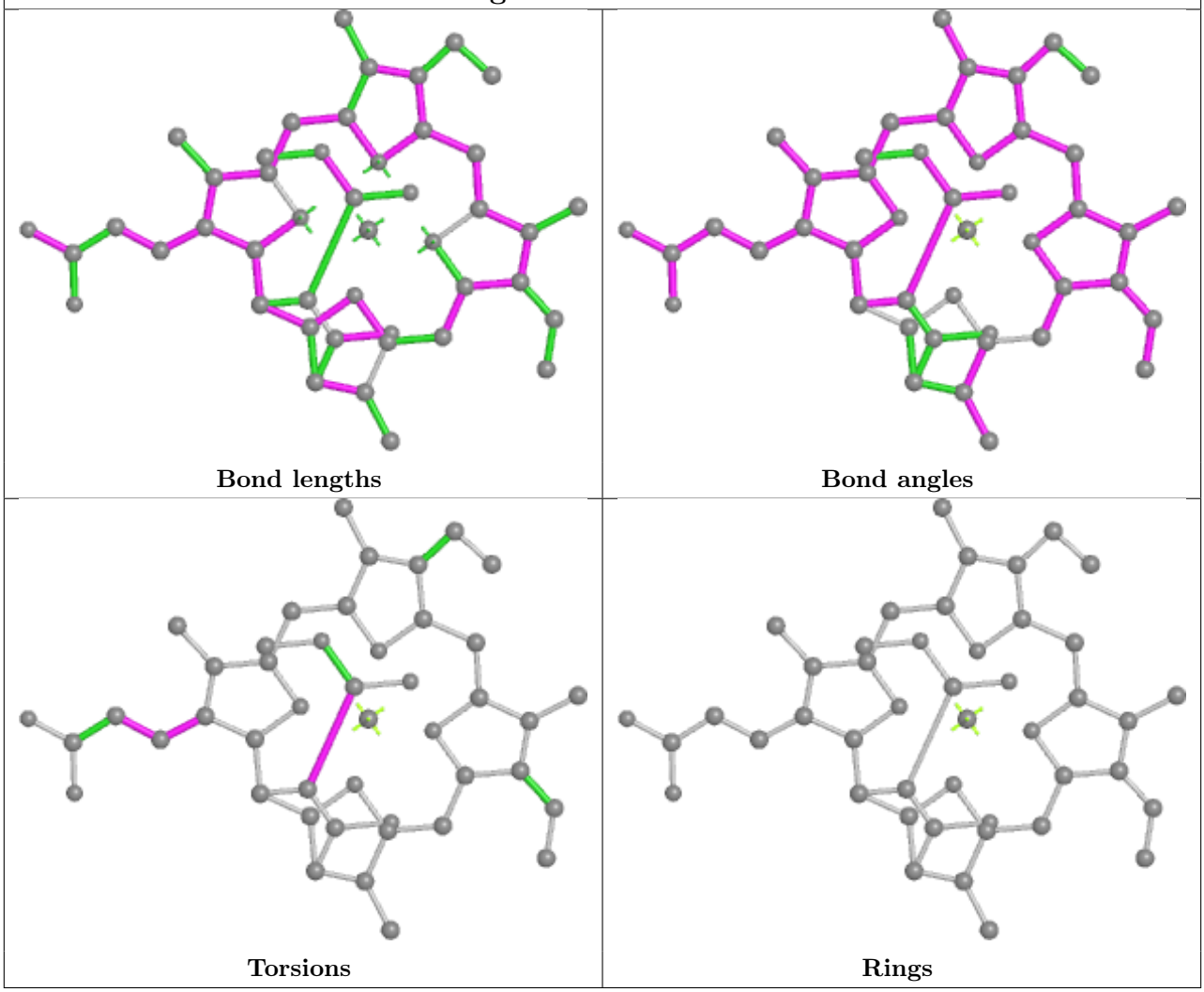

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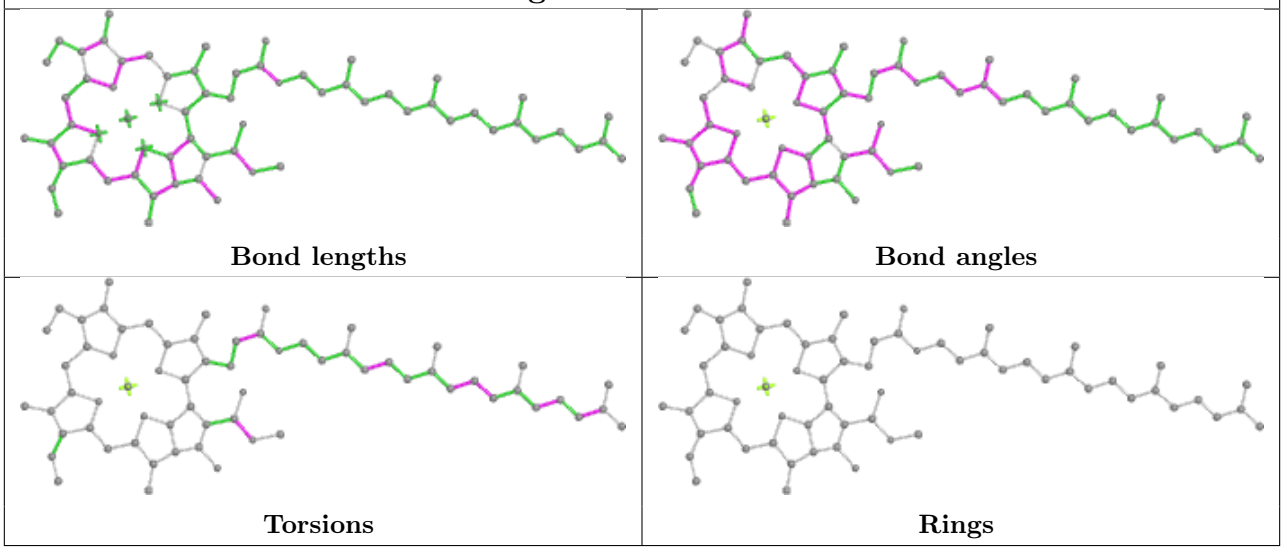

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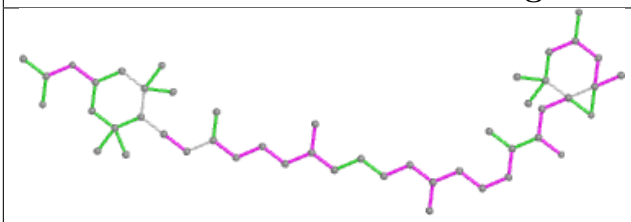
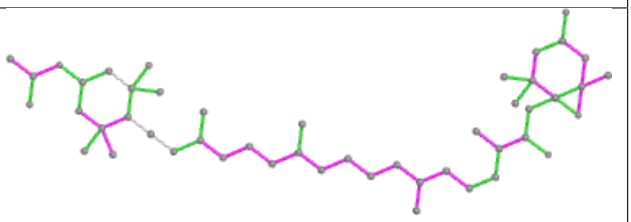
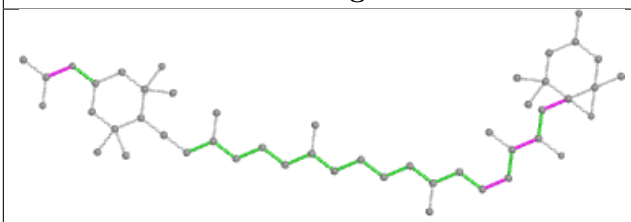
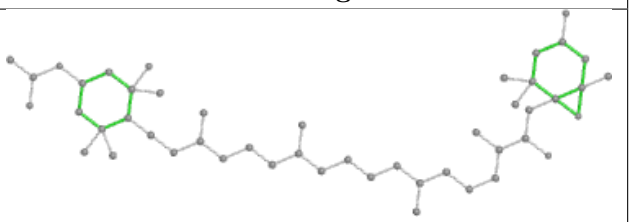
 Bond lengths	 Bond angles
 Torsions	 Rings

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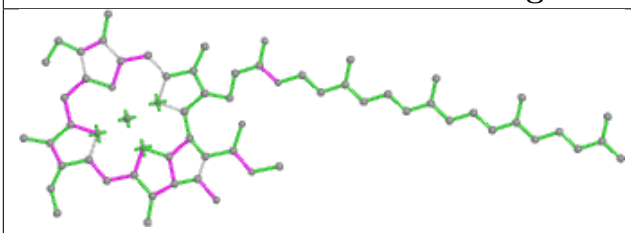
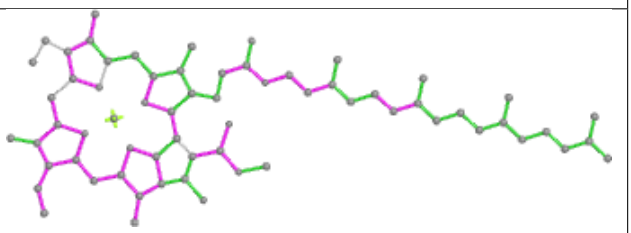
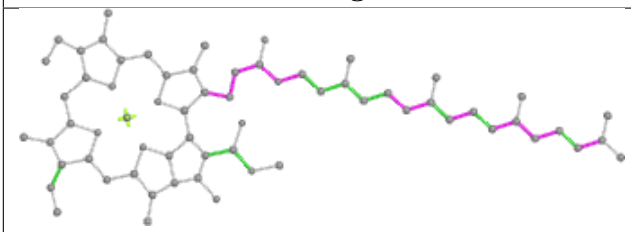
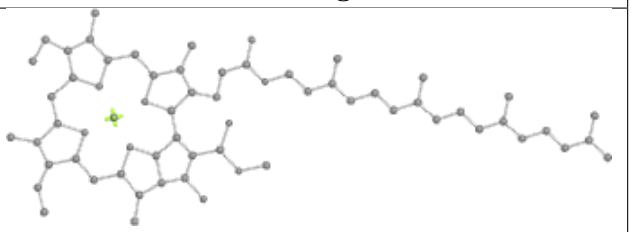
 Bond lengths	 Bond angles
 Torsions	 Rings

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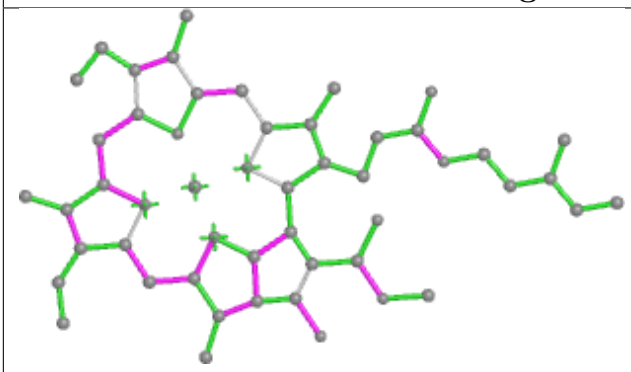
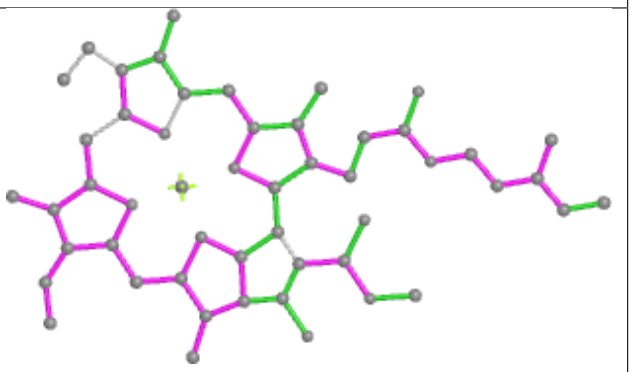
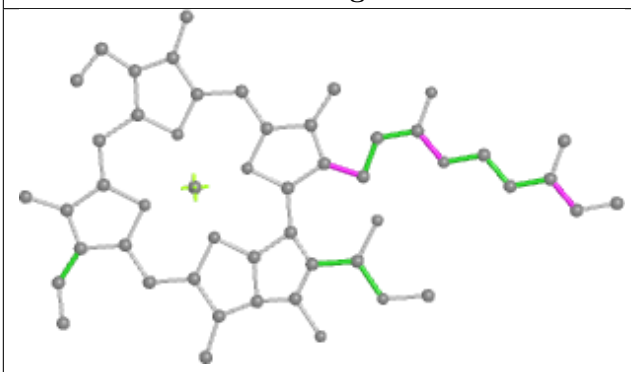
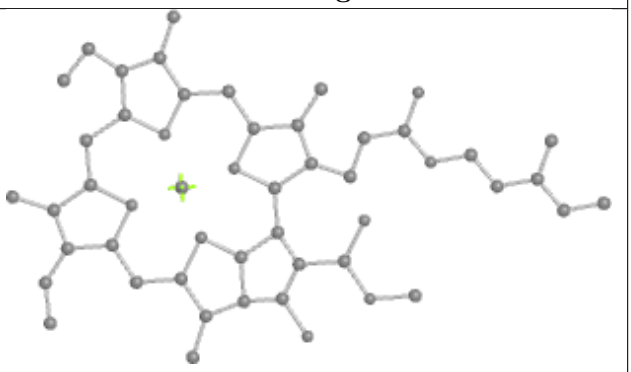
 Bond lengths	 Bond angles
 Torsions	 Rings

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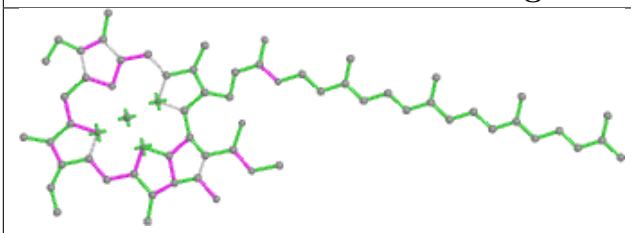
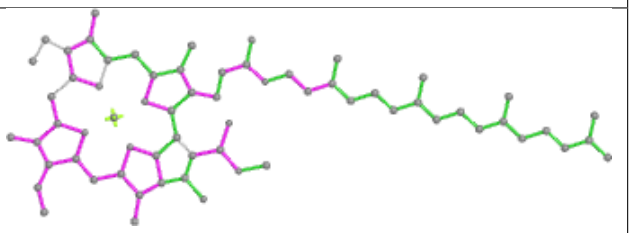
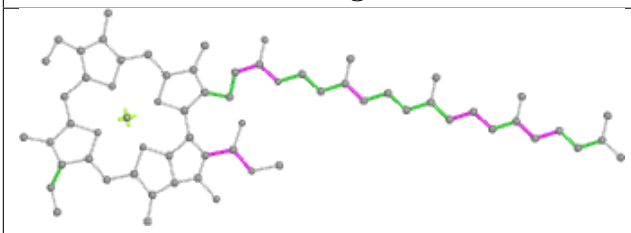
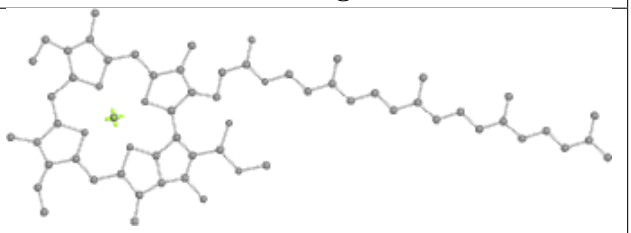
 Bond lengths	 Bond angles
 Torsions	 Rings

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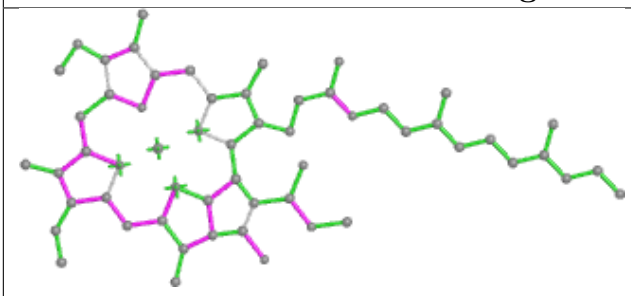

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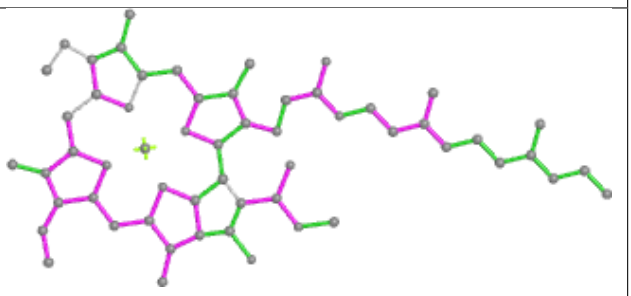

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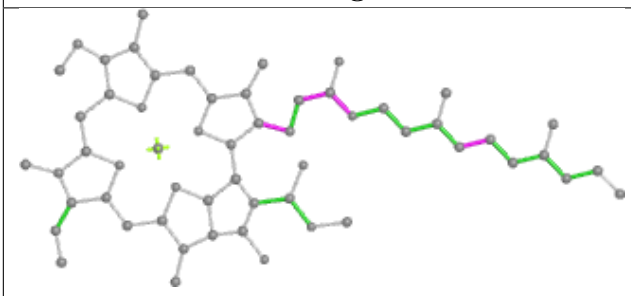

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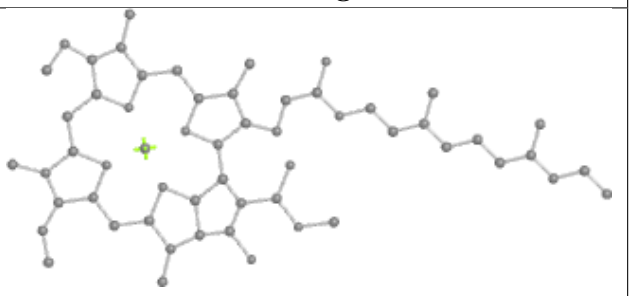

Rings

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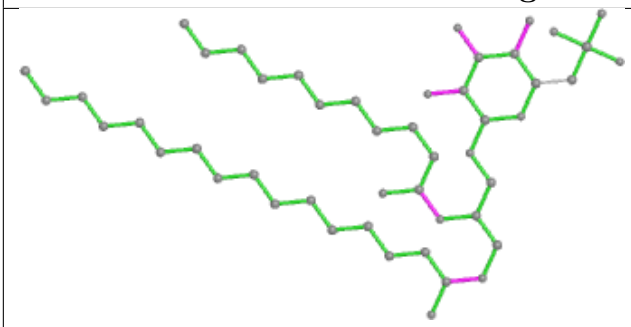

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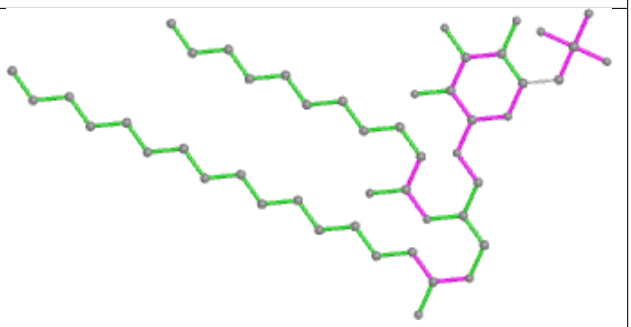

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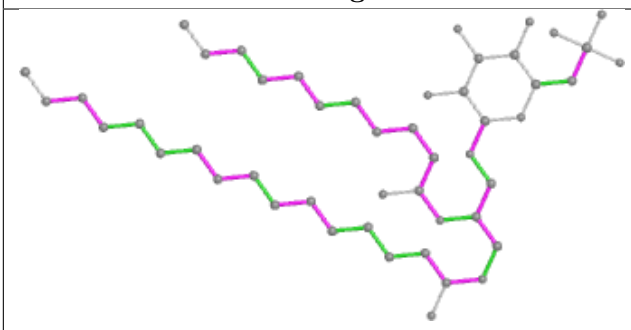

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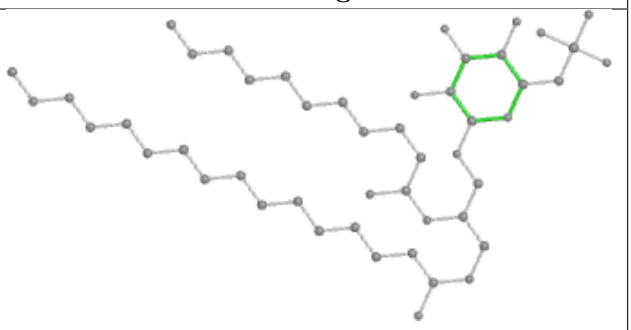

Rings

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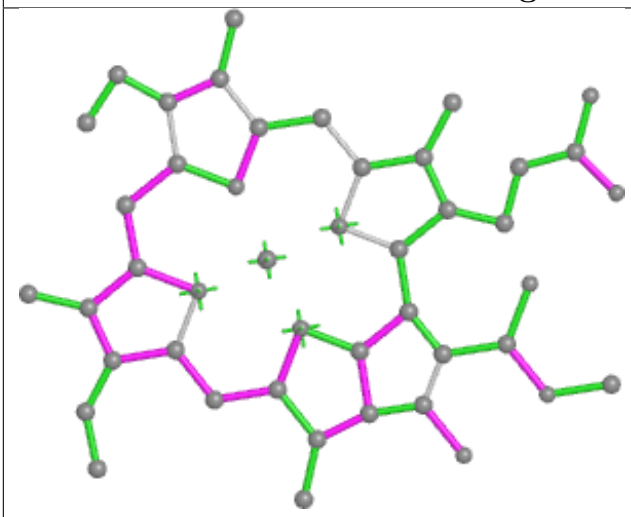

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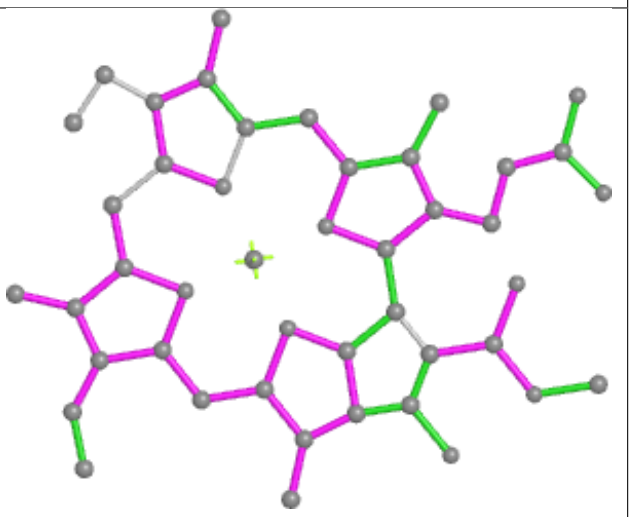

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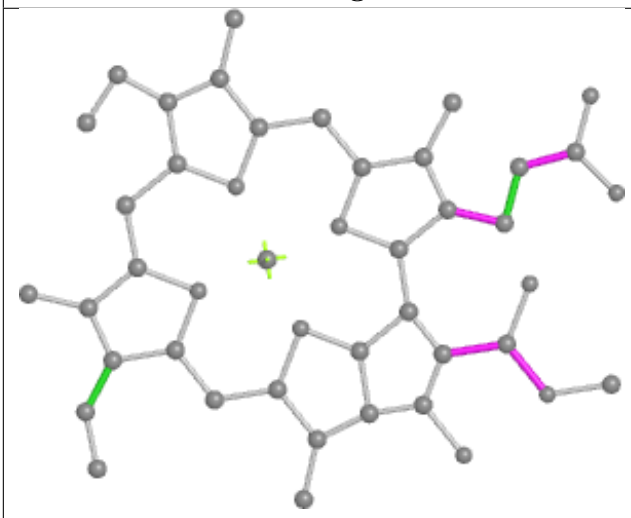

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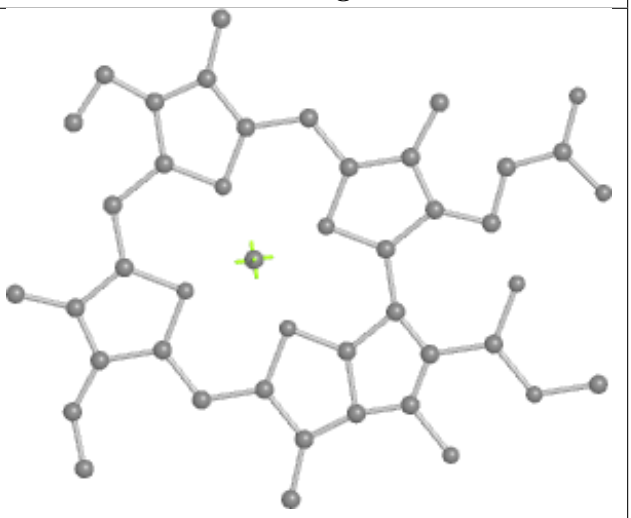

Rings

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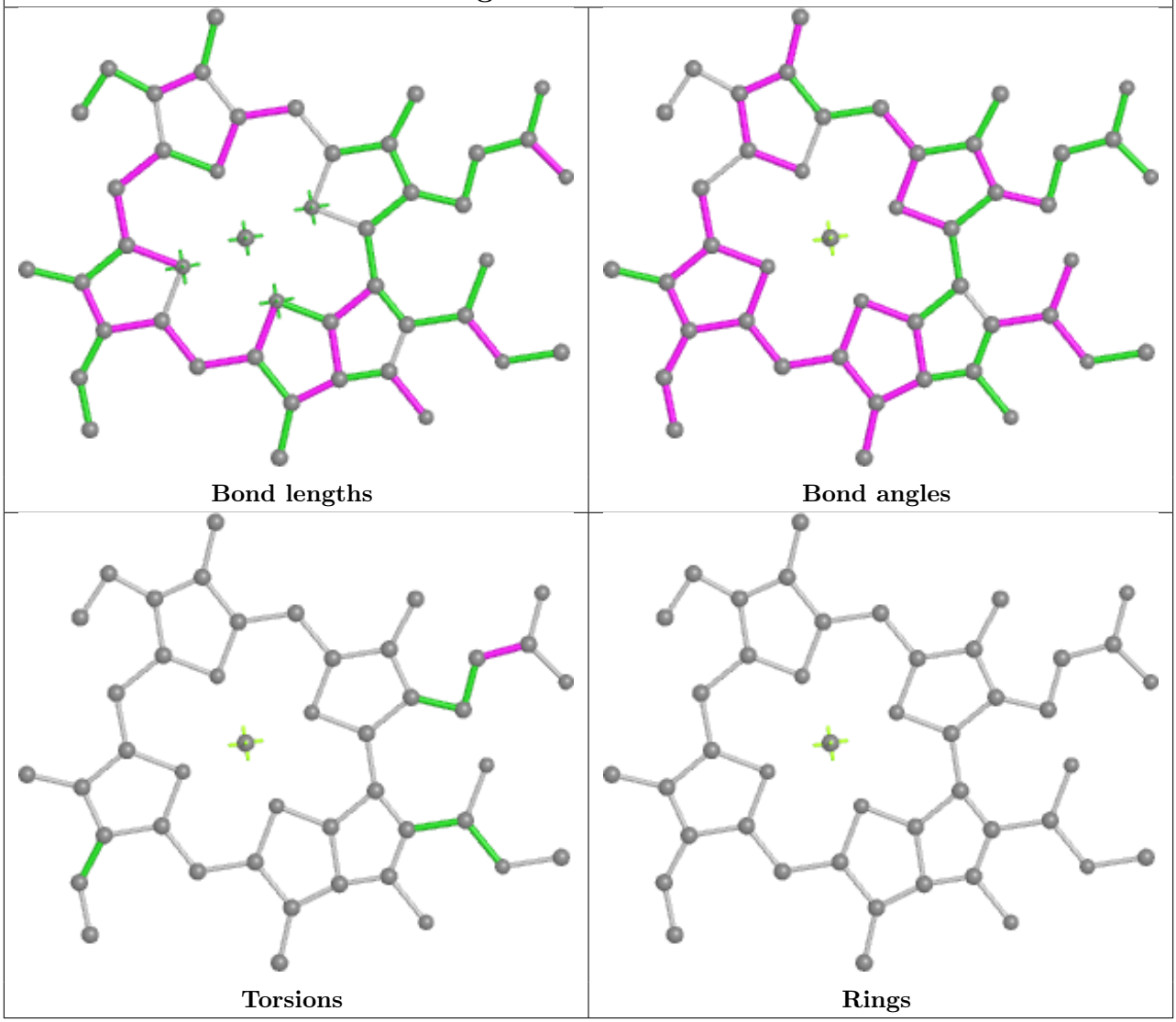

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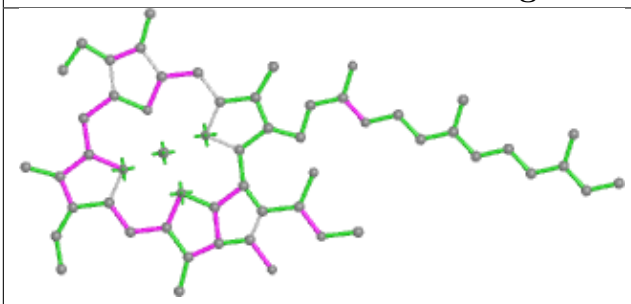
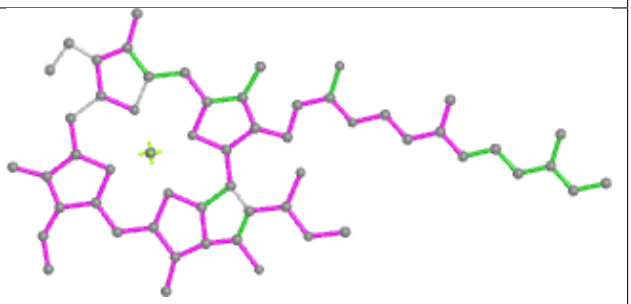
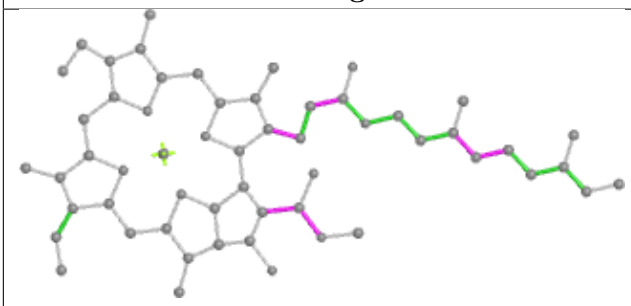
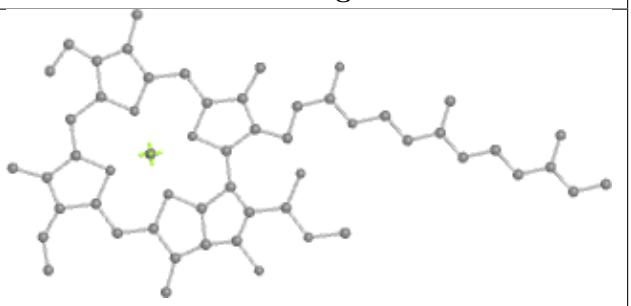
 Bond lengths	 Bond angles
 Torsions	 Rings

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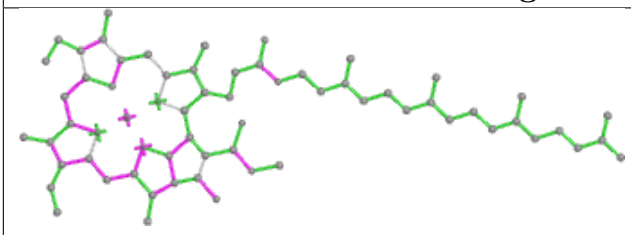
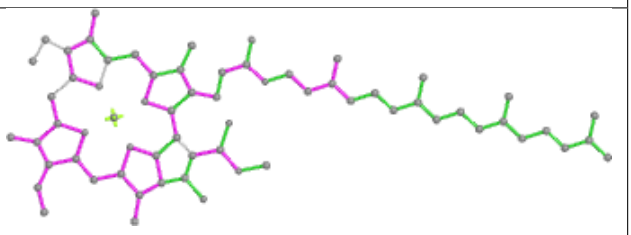
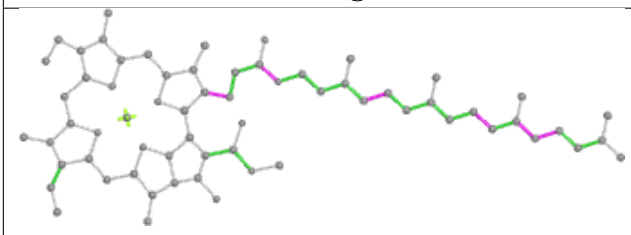
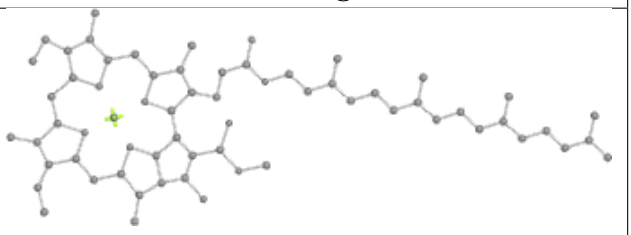
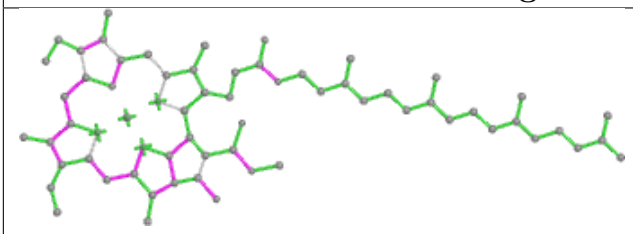
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 31 302



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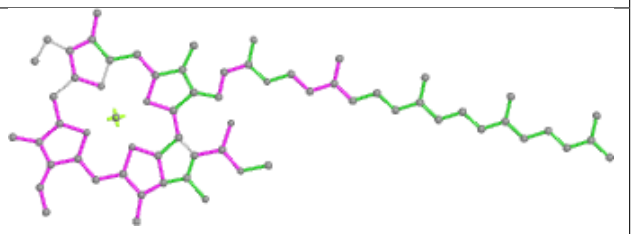
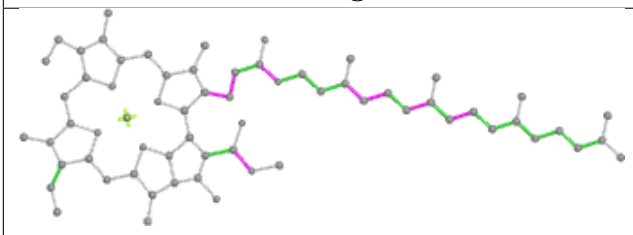


Bond angles



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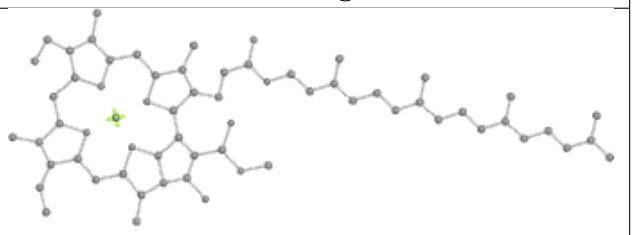

Rings

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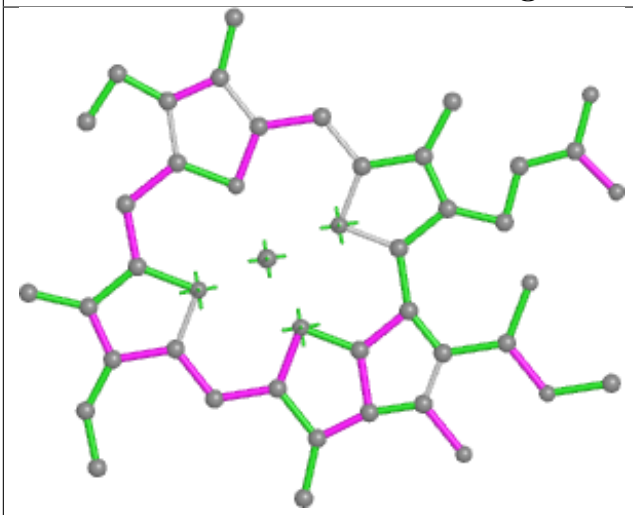

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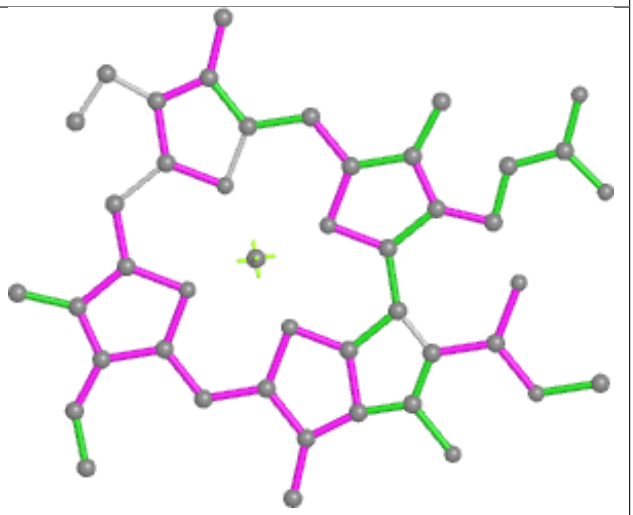
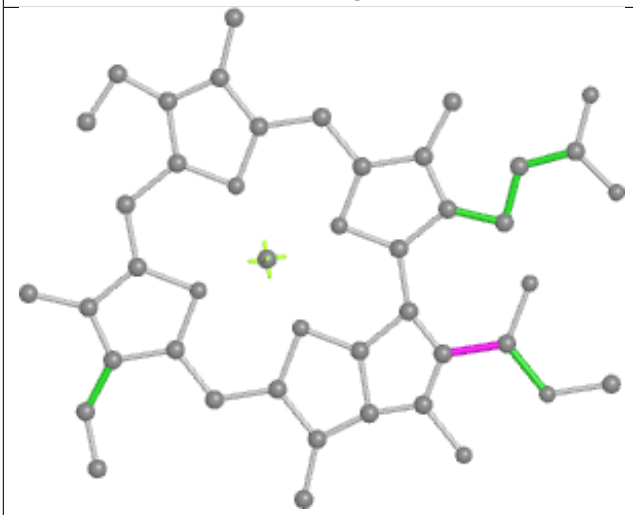
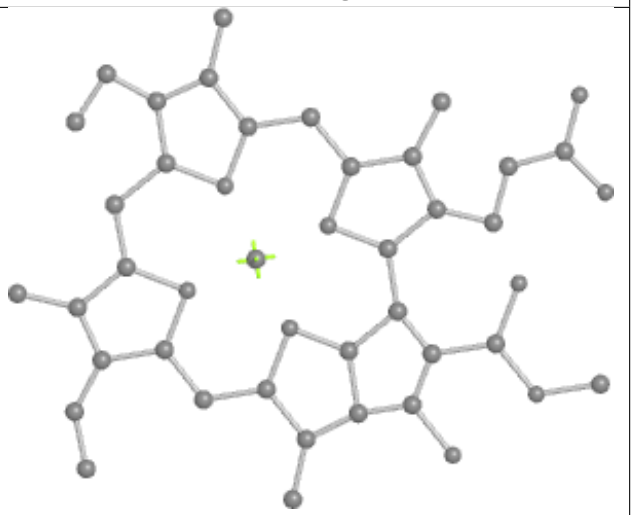


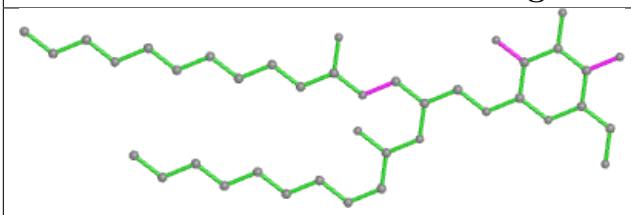
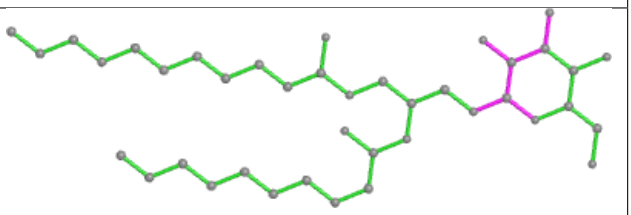
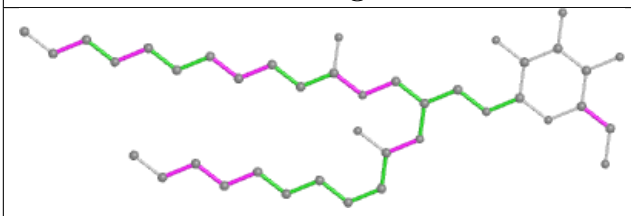
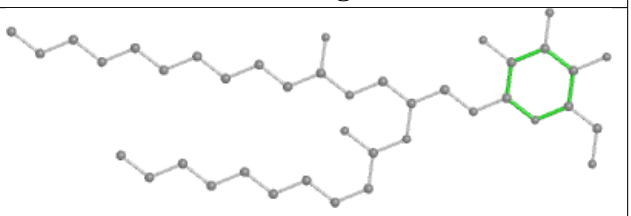
Bond angles

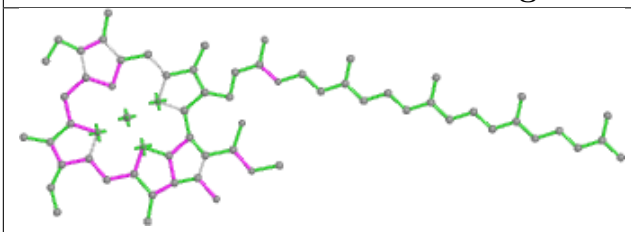
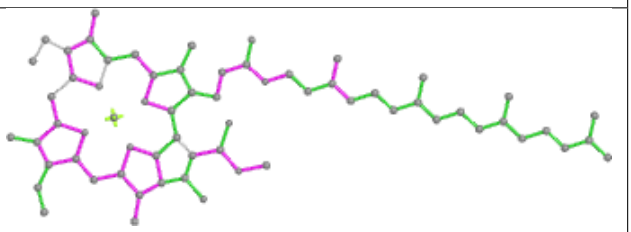
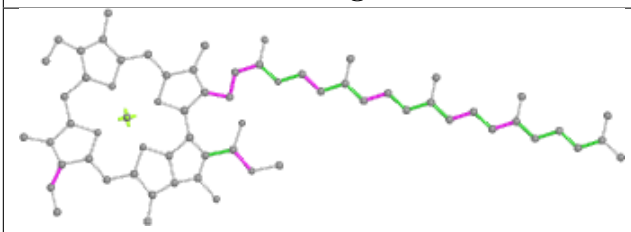
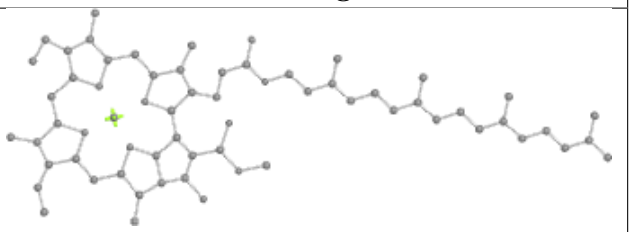


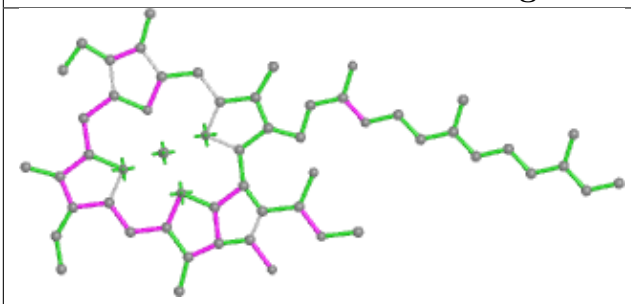
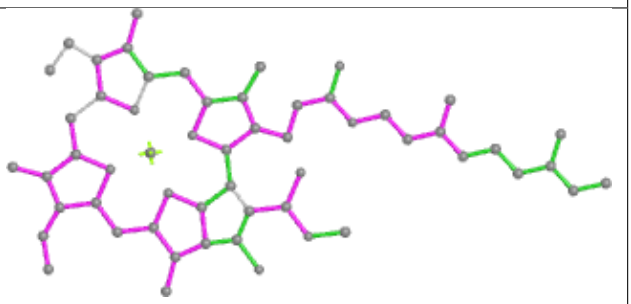
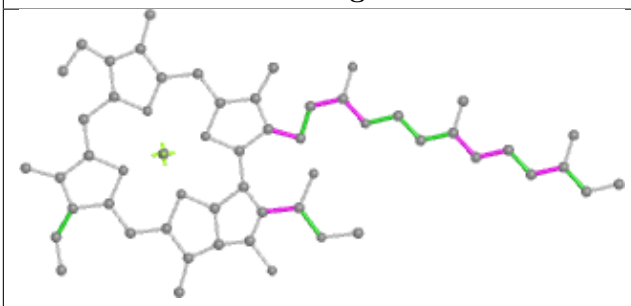
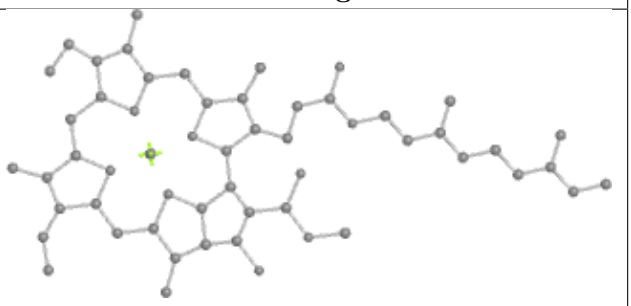
Torsions

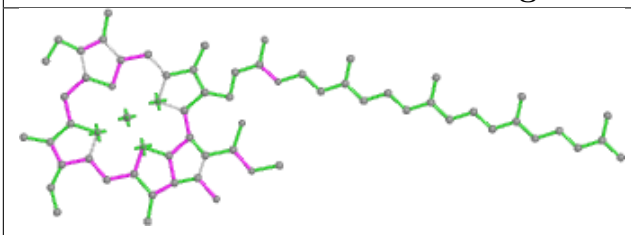
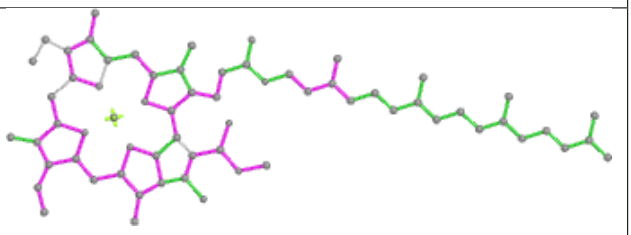
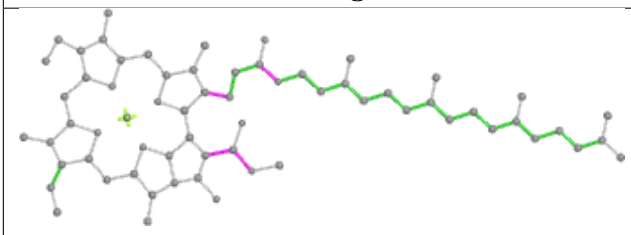
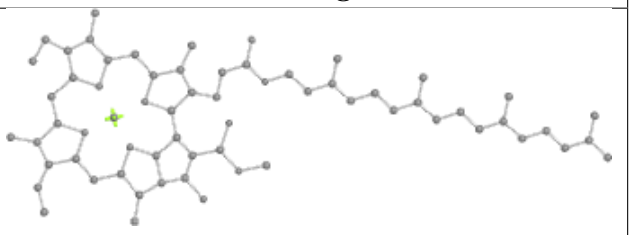


Rings

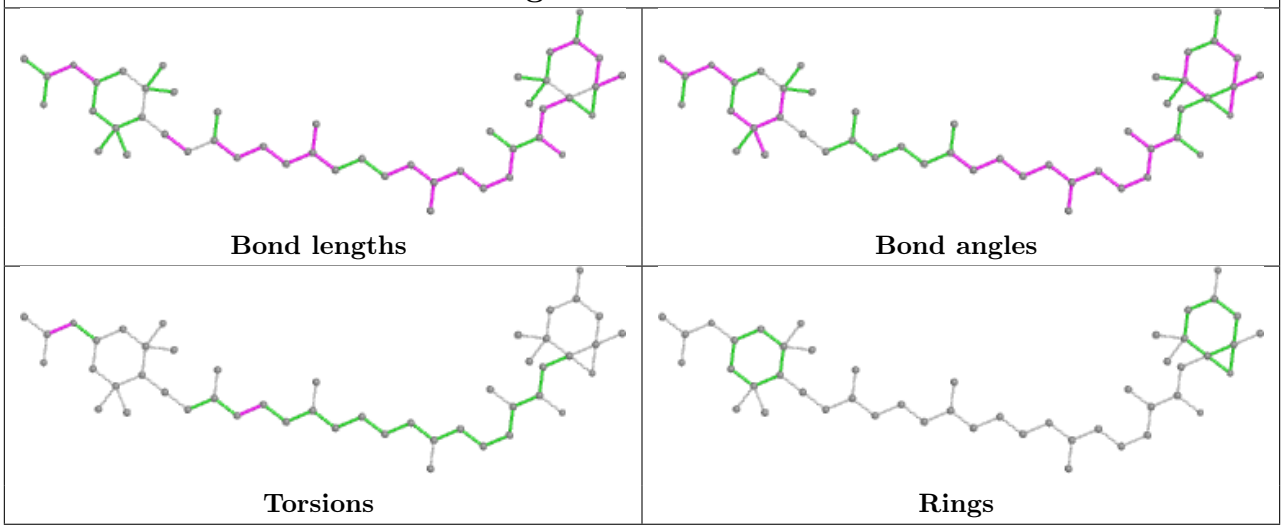
Ligand LMG l 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 17 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

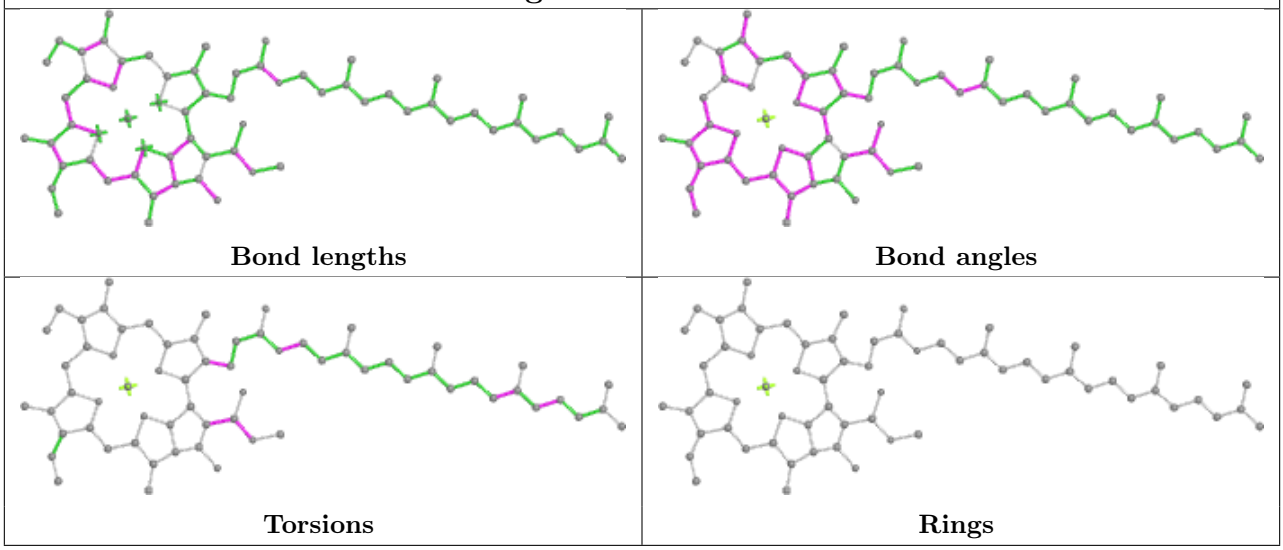
Ligand CLA 18 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 38 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 32 215



Ligand CLA C 502



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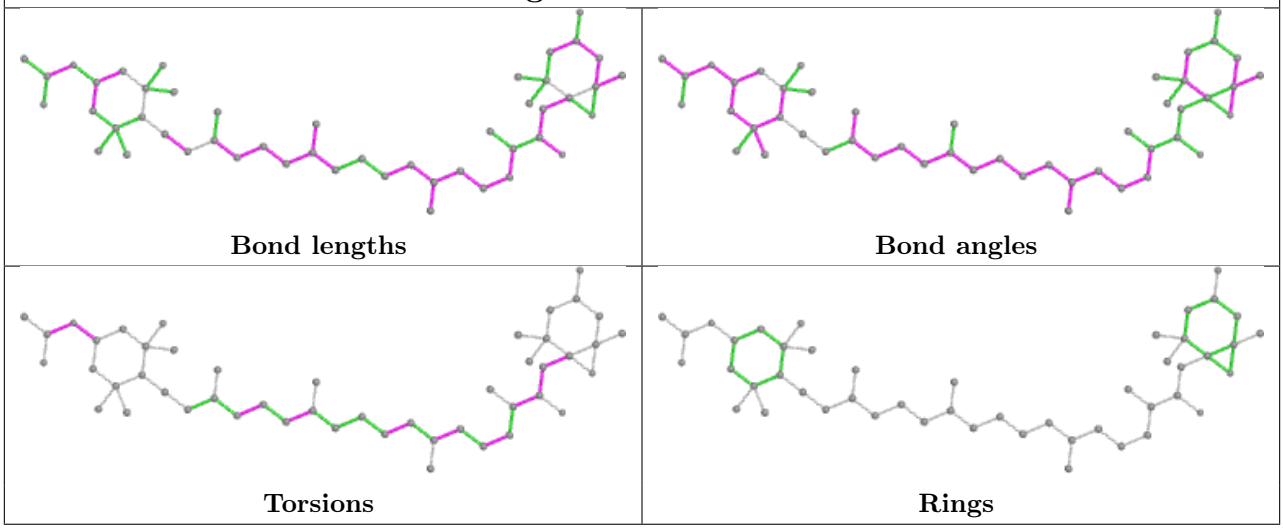
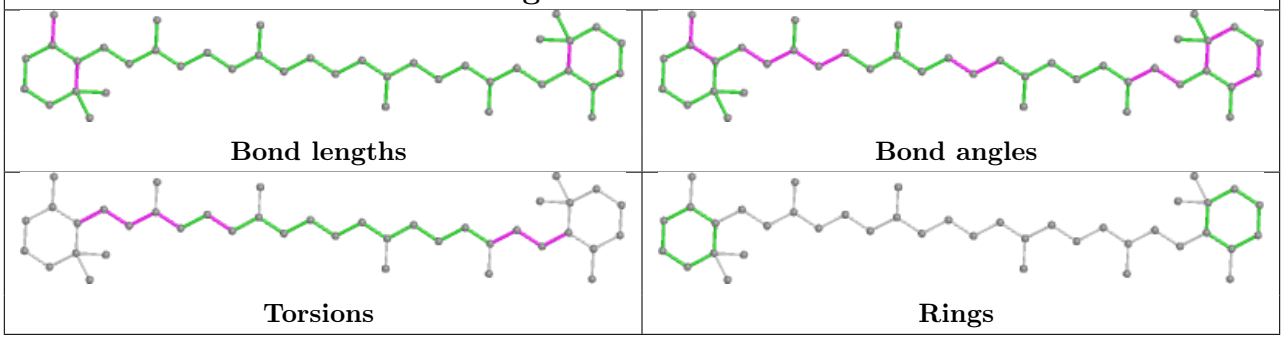


Ligand BCR D 407



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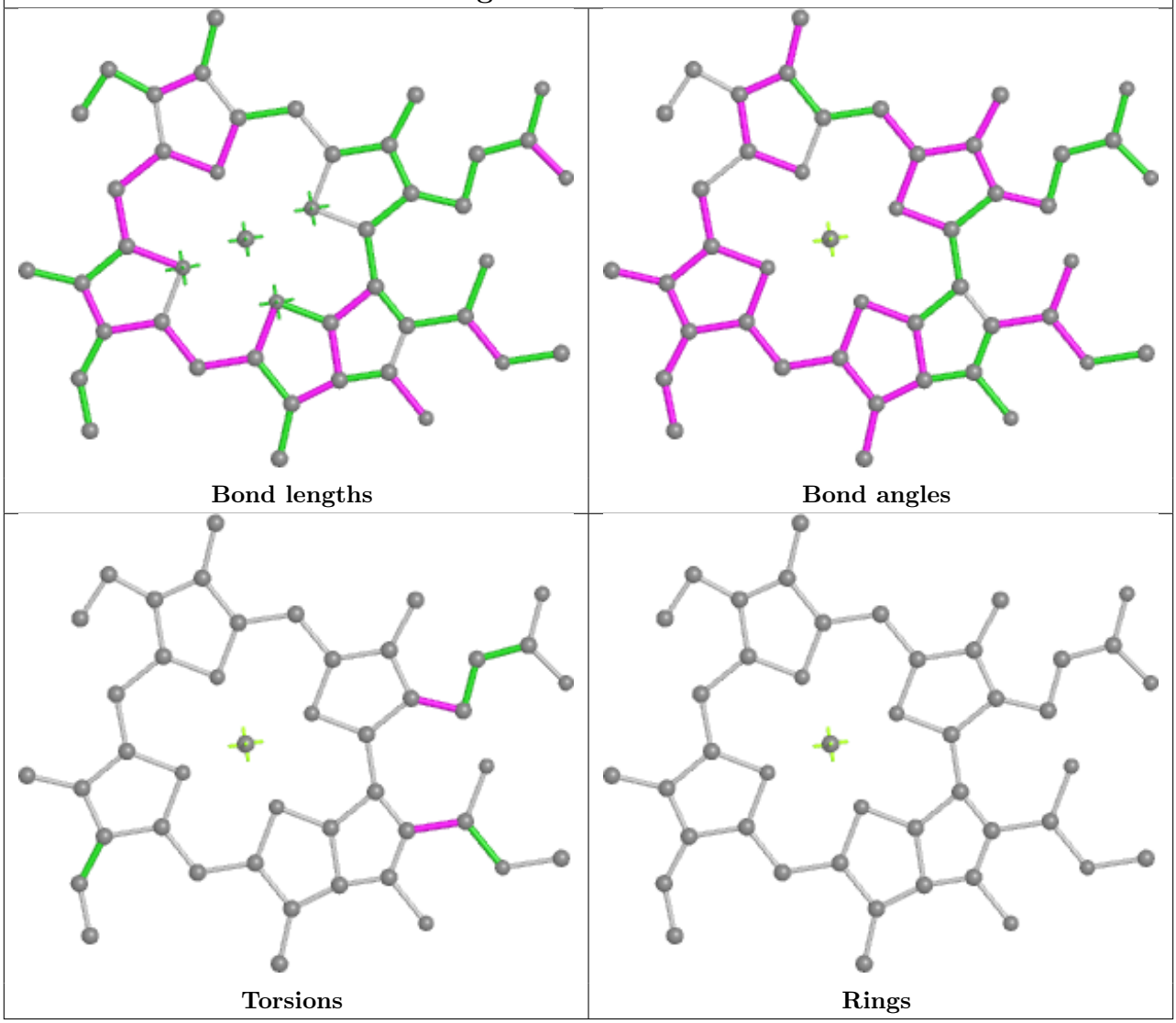

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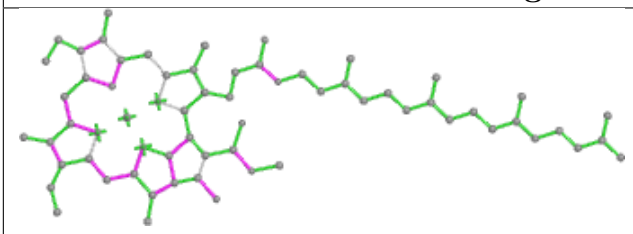
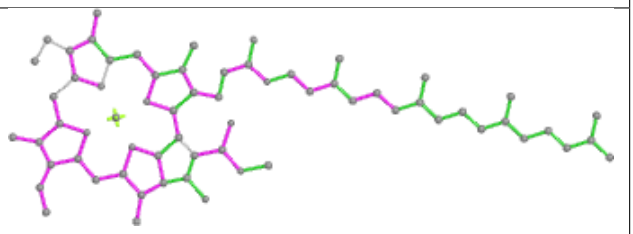
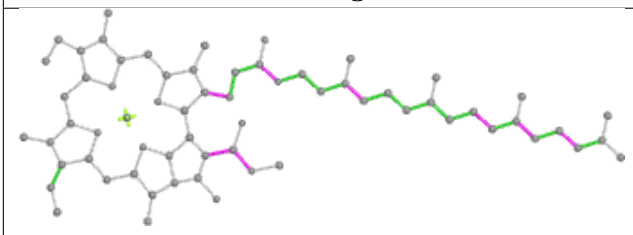


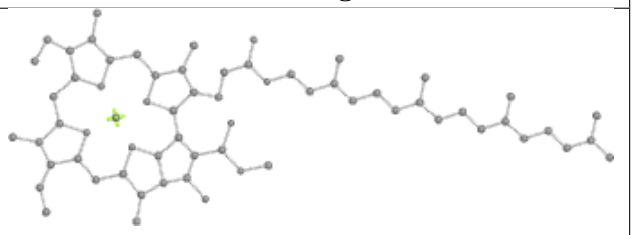
Bond lengths



Bond angles

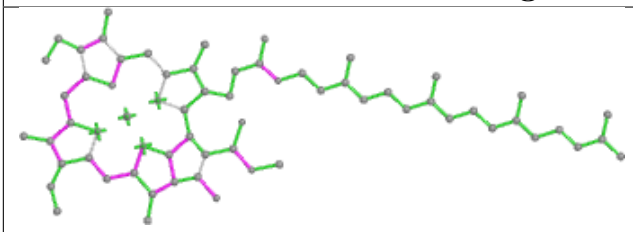


Torsions



Rings

Ligand CLA 16 306



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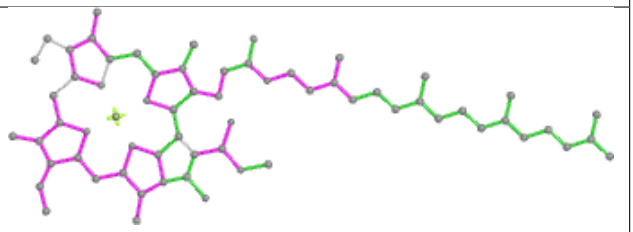
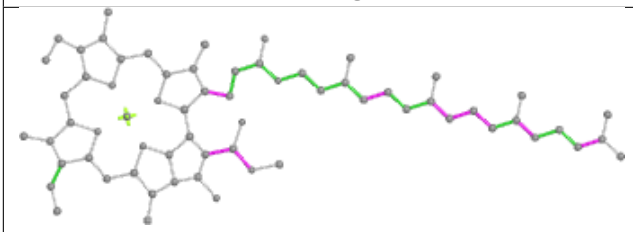


Bond angles



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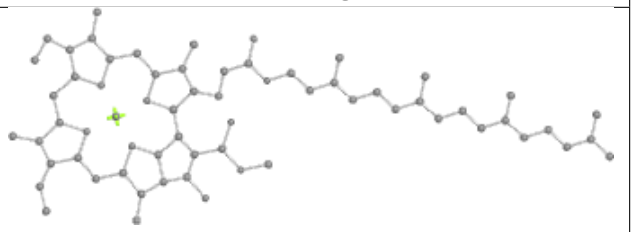
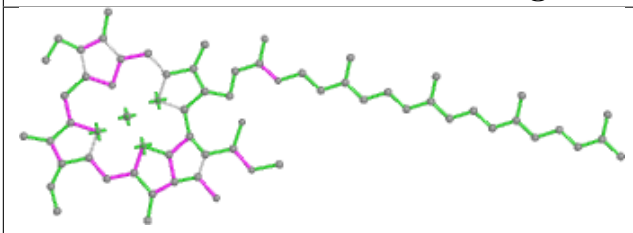
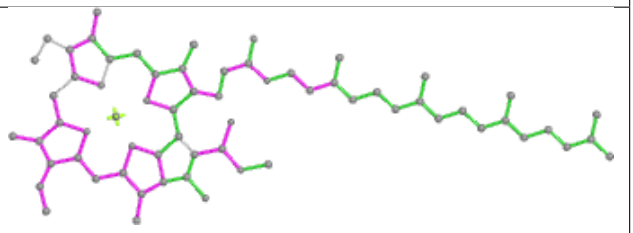


Rings

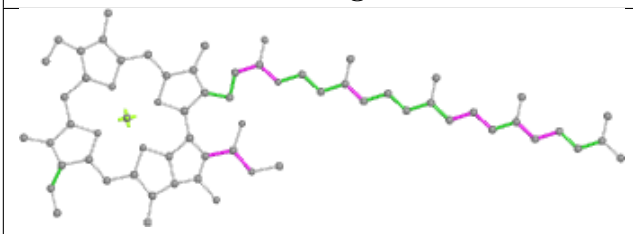
Ligand CLA c 510



Bond lengths



Bond angles



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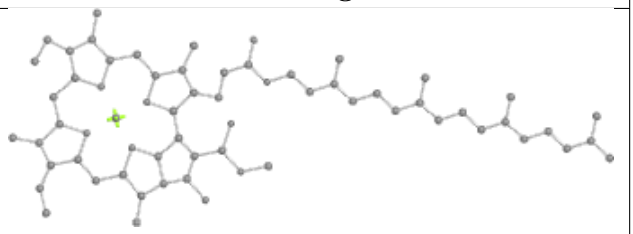
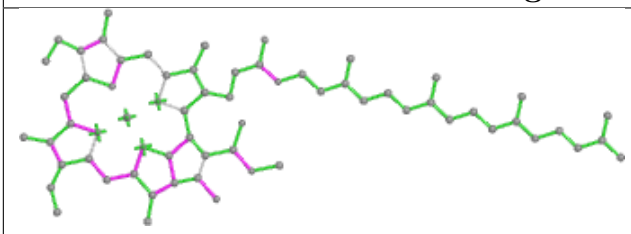
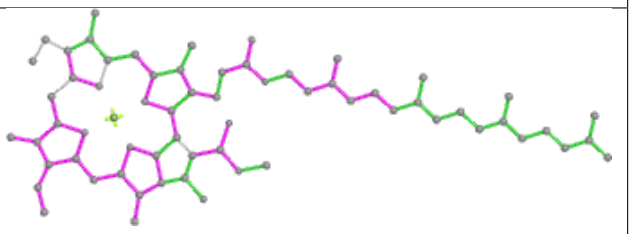
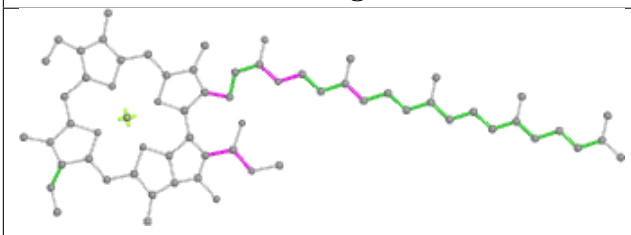
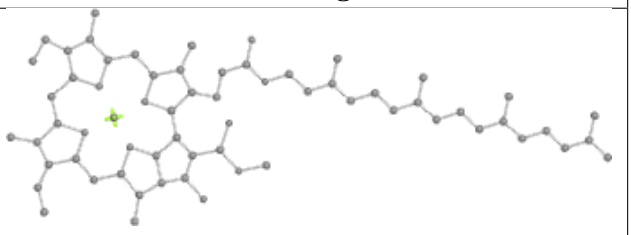
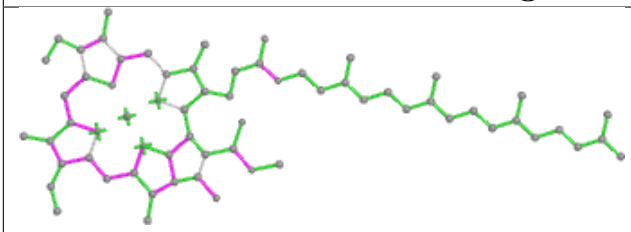
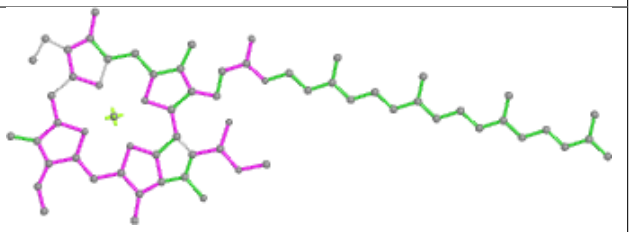
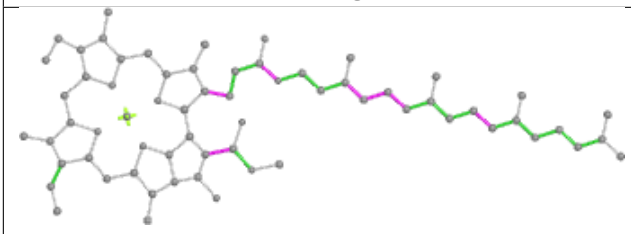
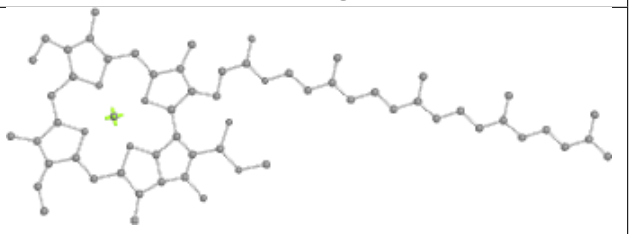
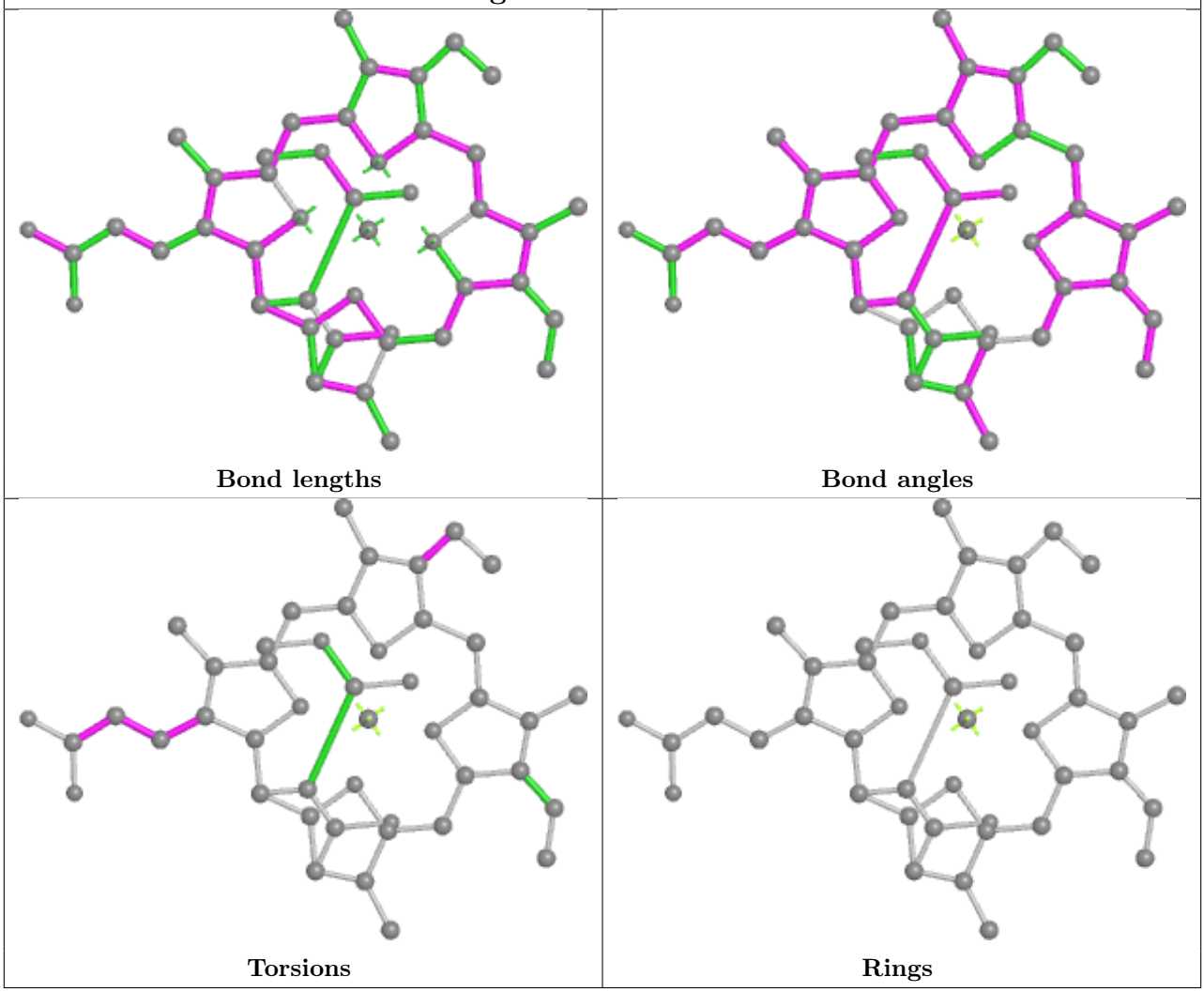


Rings

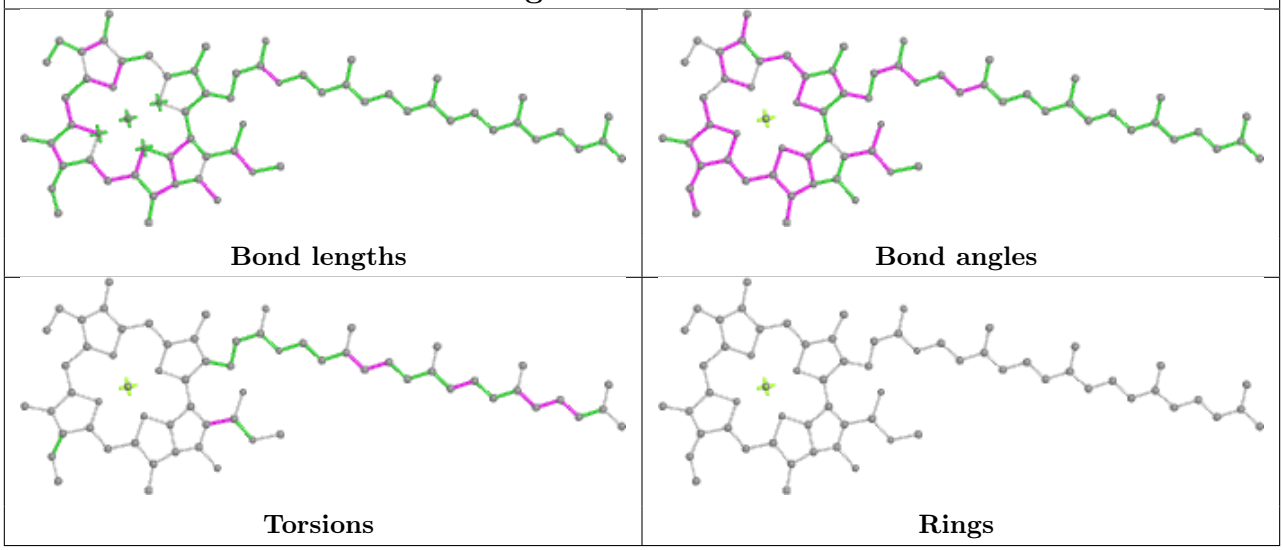
Ligand CLA B 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 13 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

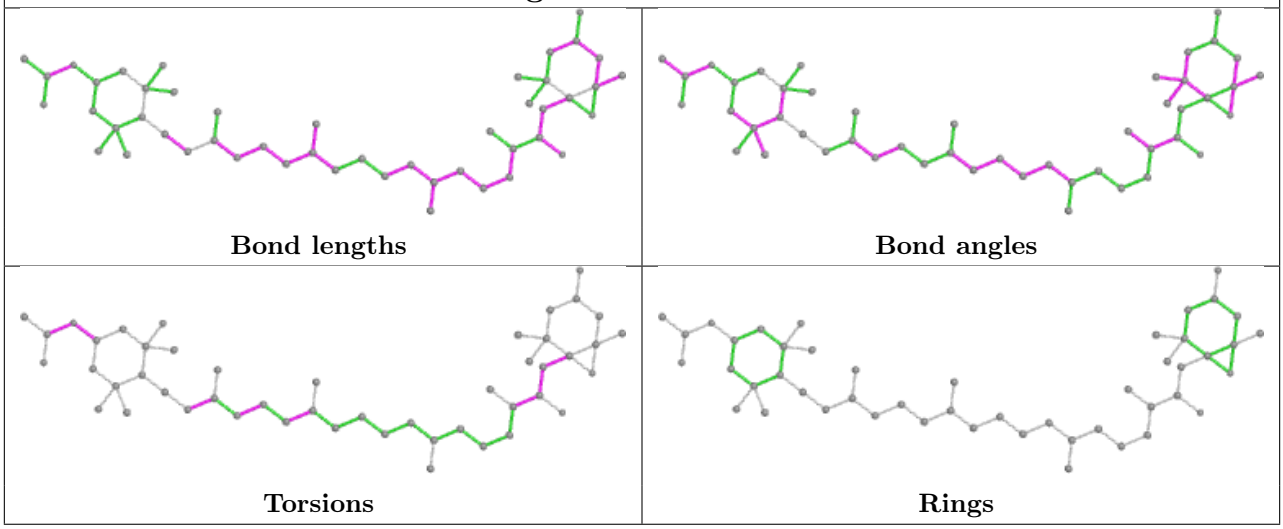
Ligand KC1 15 309



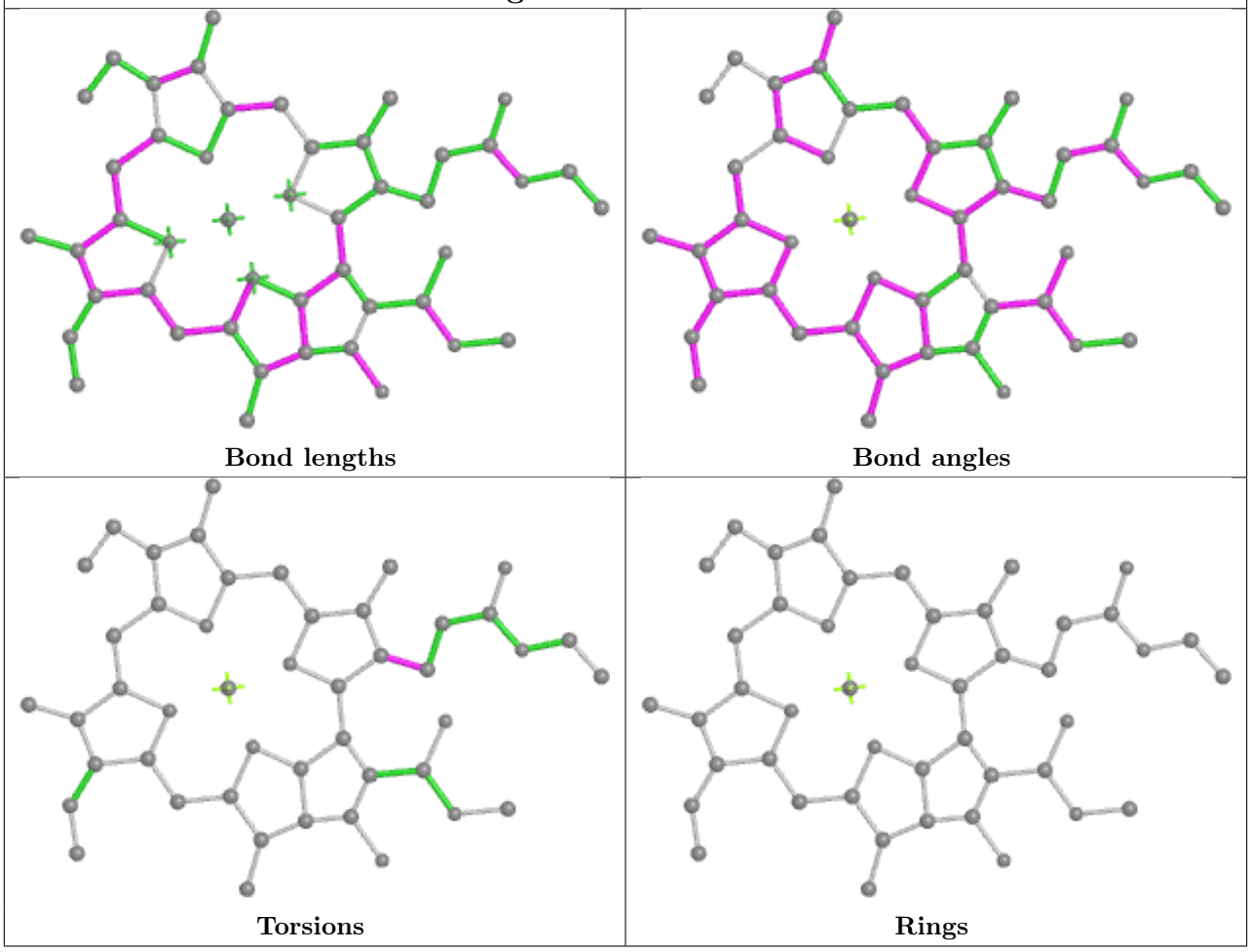
Ligand CLA B 507



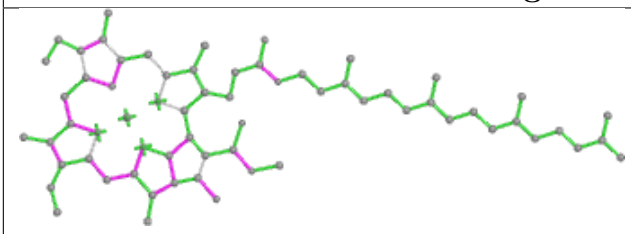
Ligand A86 12 215



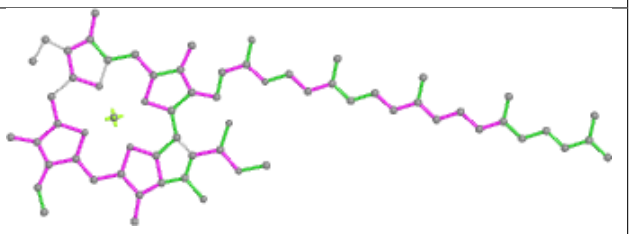
Ligand CLA 40 210



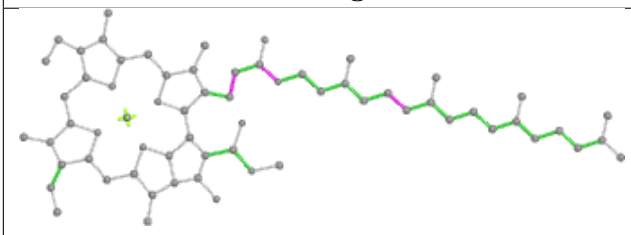
Ligand CLA A 403



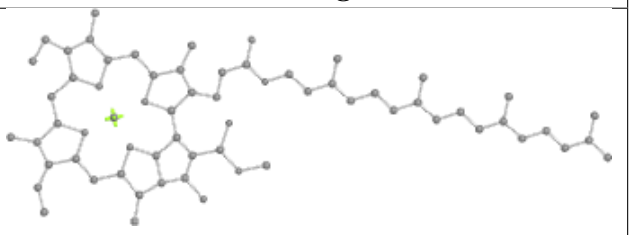
Bond lengths



Bond angles

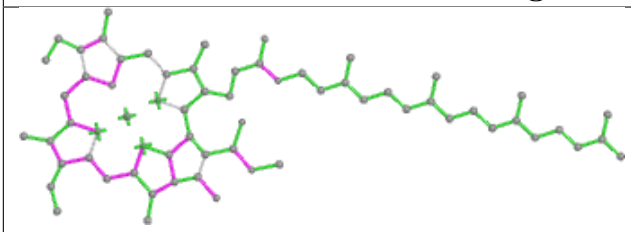


Torsions

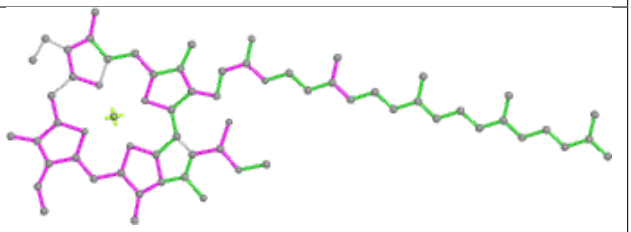


Rings

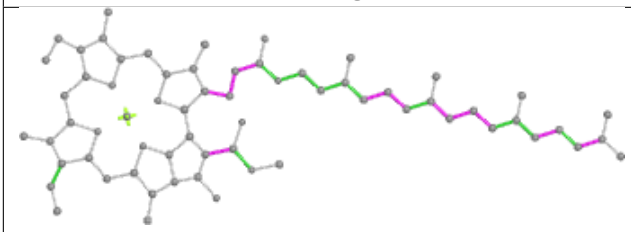
Ligand CLA b 501



Bond lengths



Bond angles



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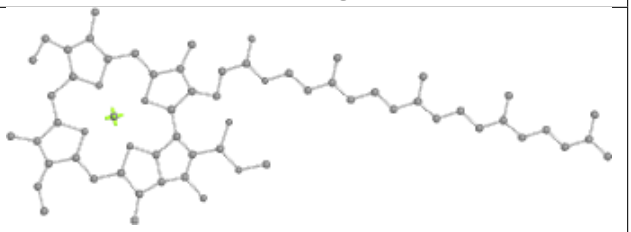
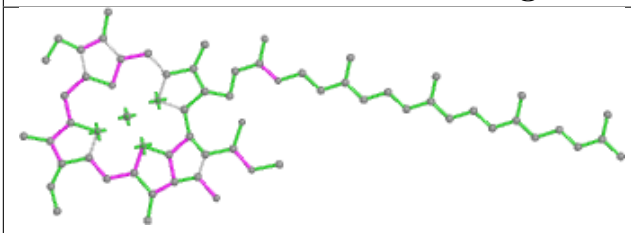


Rings

Ligand CLA 14 301



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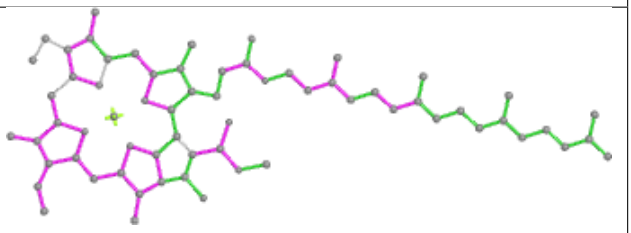

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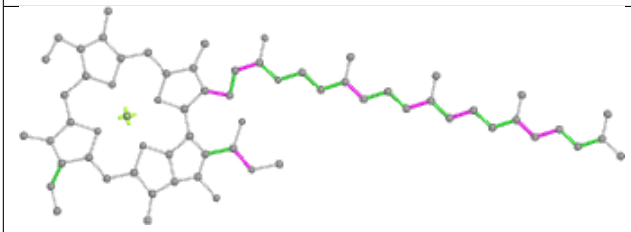

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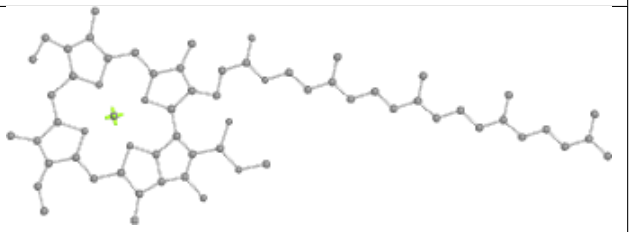
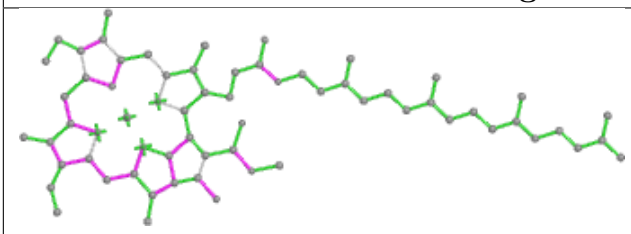


Rings

Ligand CLA 31 304



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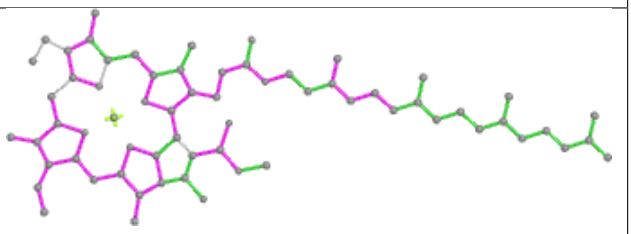

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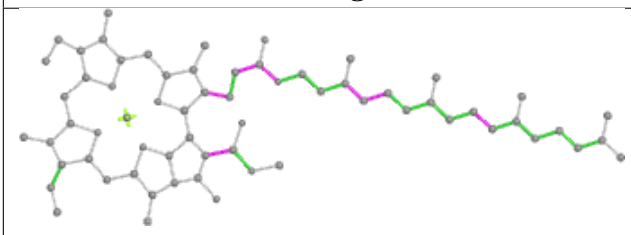

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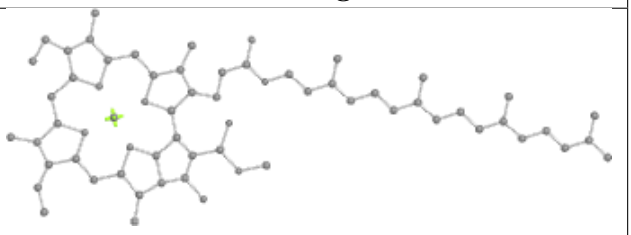
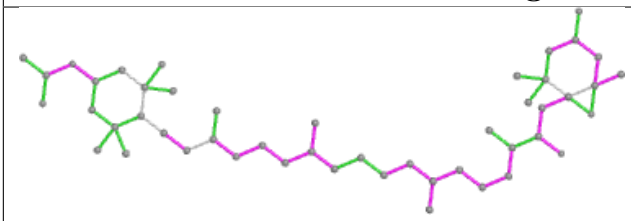


Rings

Ligand A86 11 315



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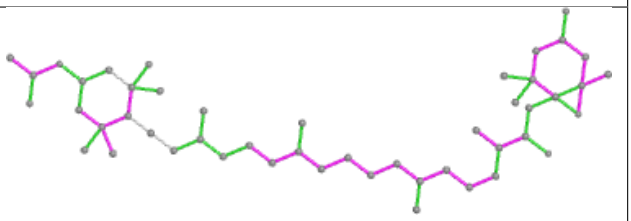
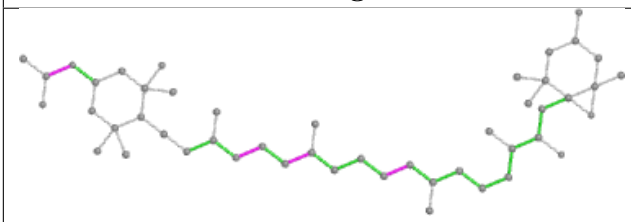


Bond angles



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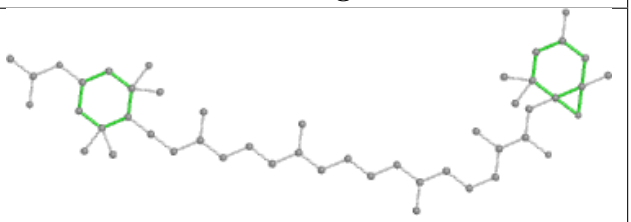
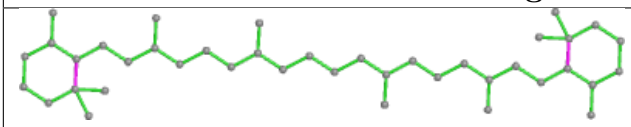


Rings

Ligand BCR b 524



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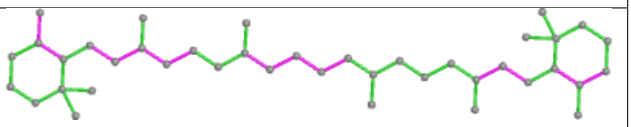
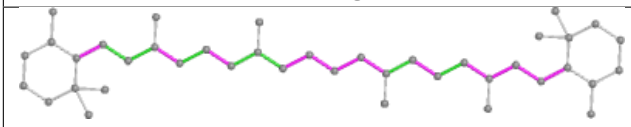
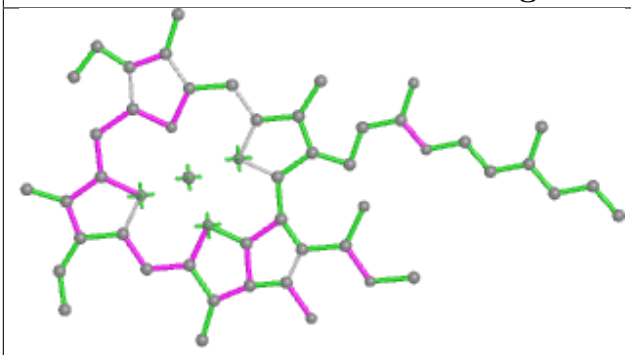
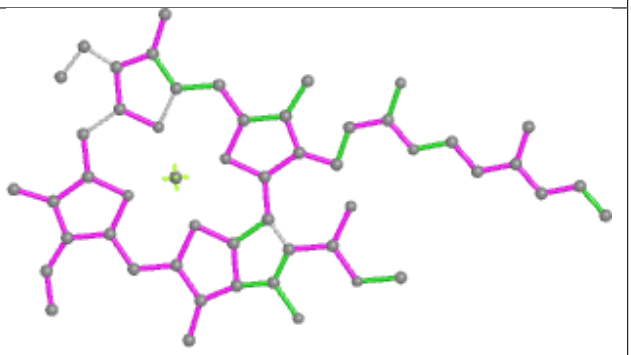
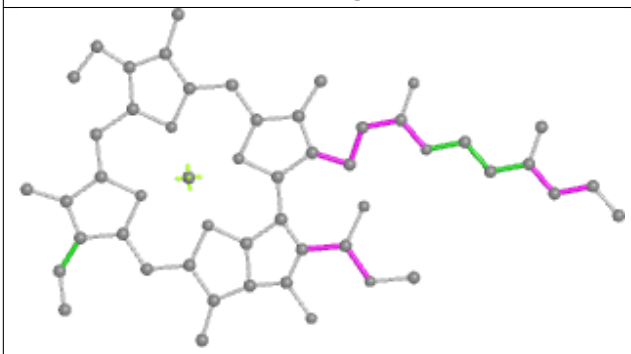
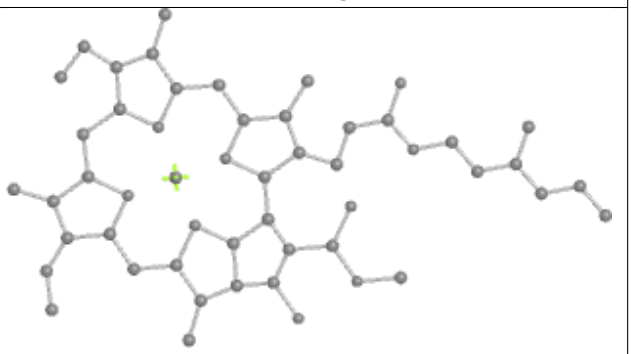


Bond angles



Torsions

Rings

Ligand CLA 12 209	
 Bond lengths	 Bond angles
 Torsions	 Rings

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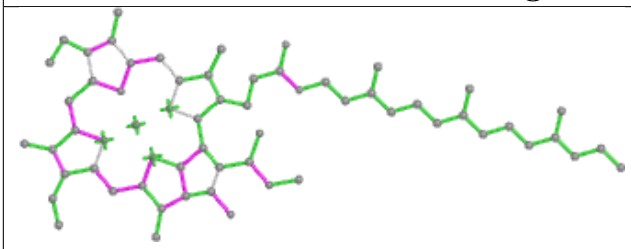
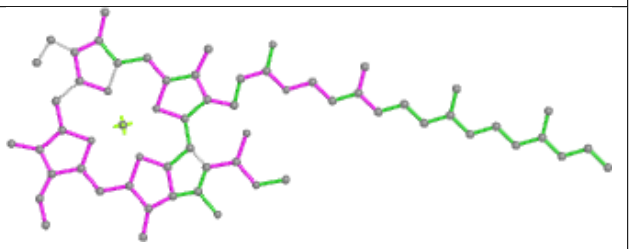
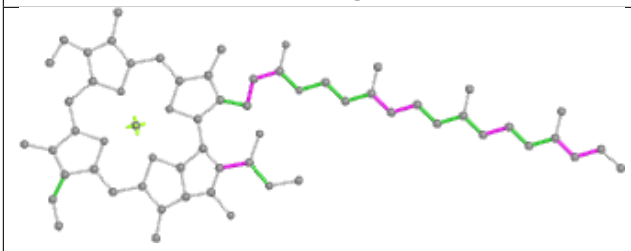
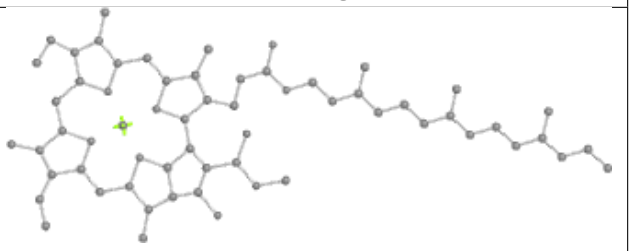
 Bond lengths	 Bond angles
 Torsions	 Rings

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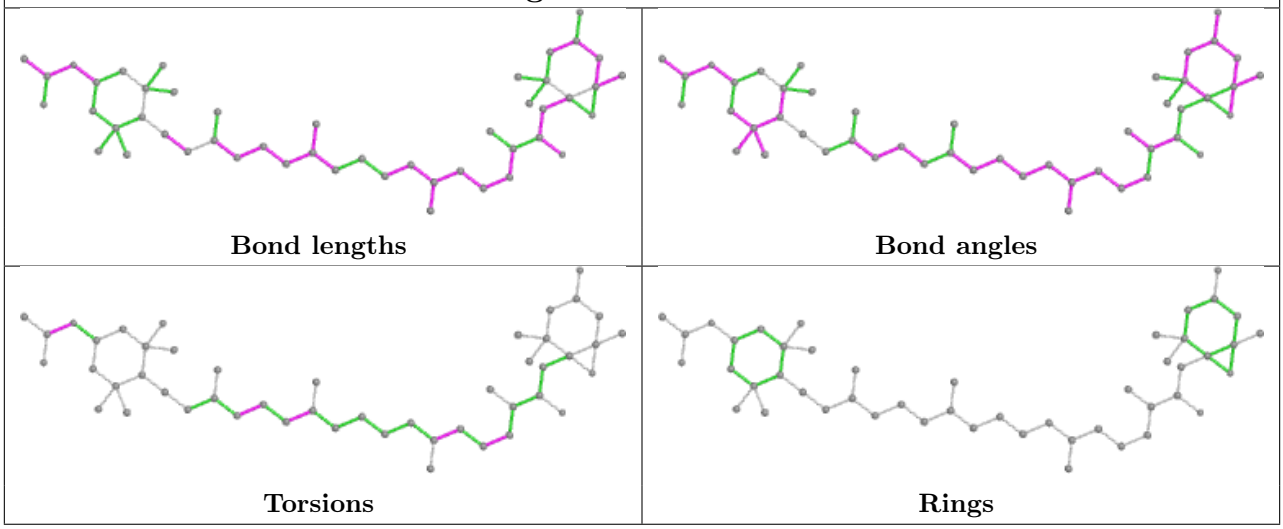
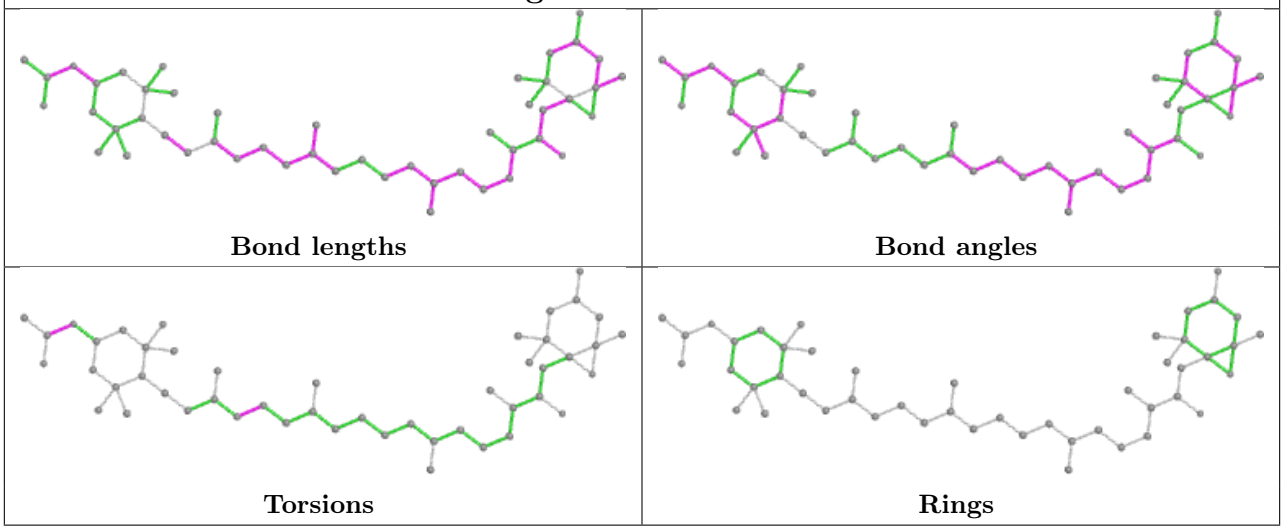
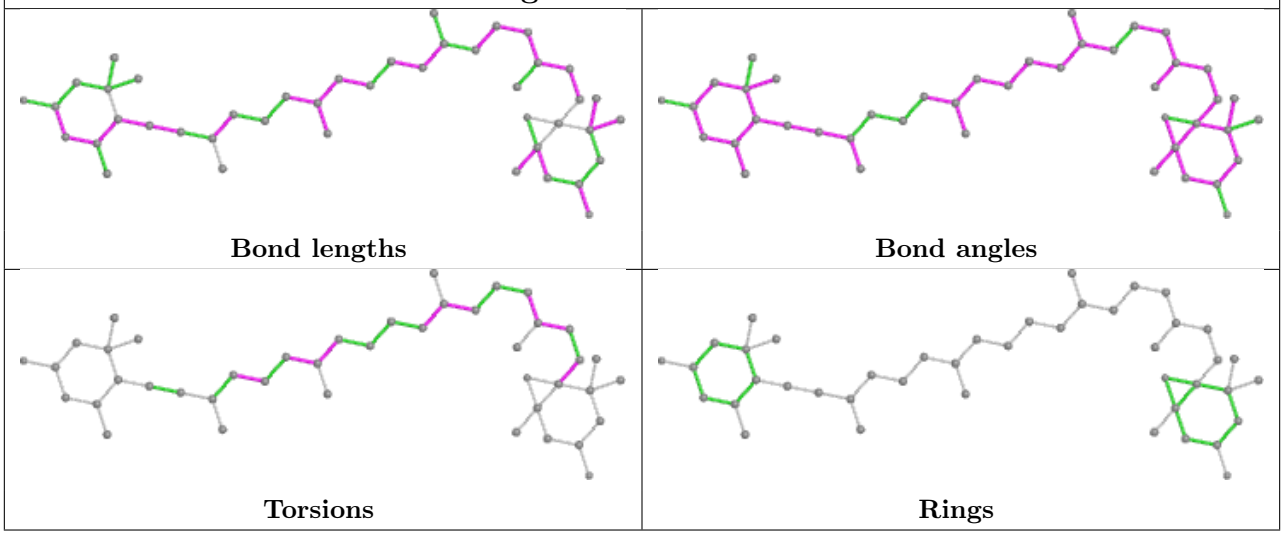


Ligand A86 12 214



Ligand DD6 40 214



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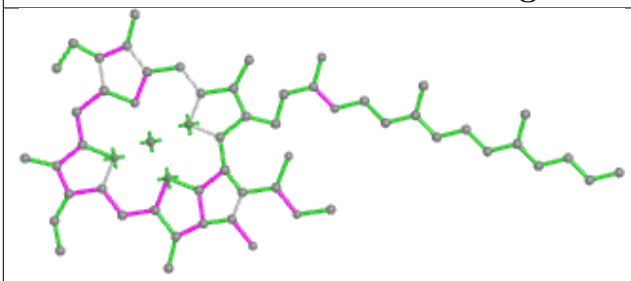
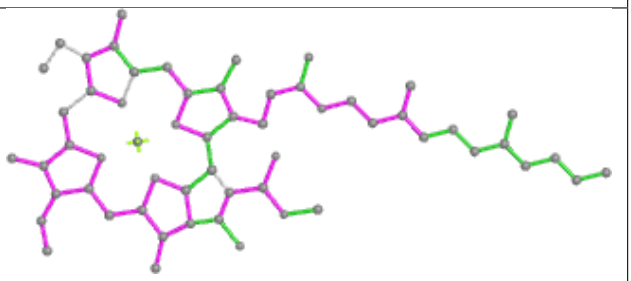
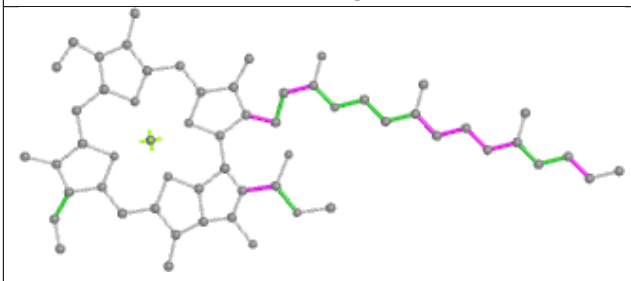
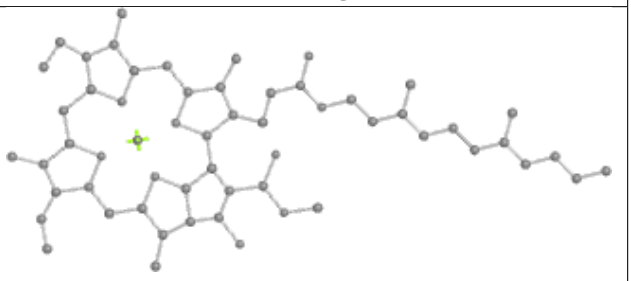
 Bond lengths	 Bond angles
 Torsions	 Rings

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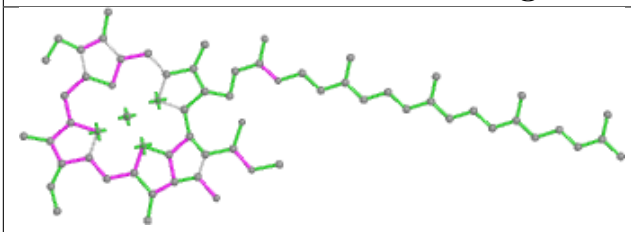
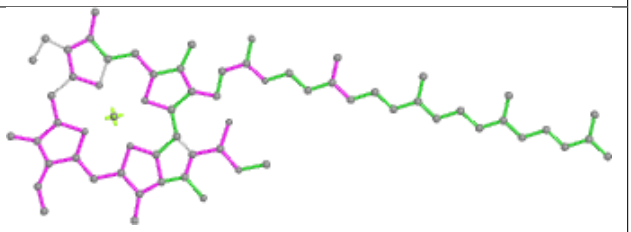
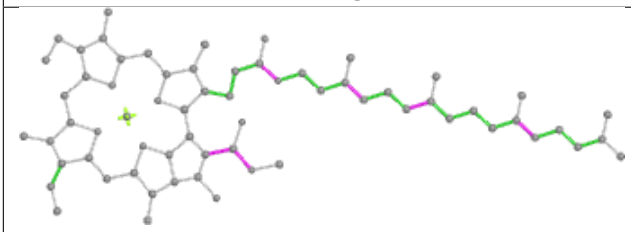
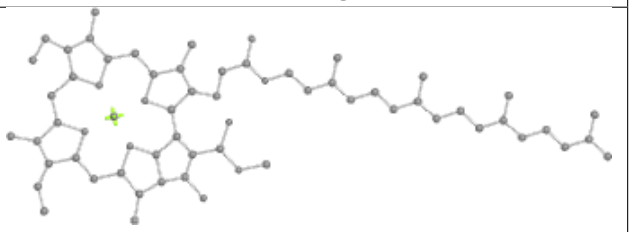
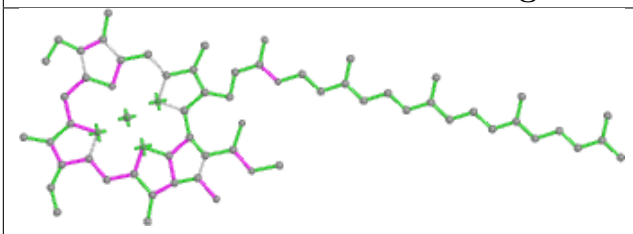
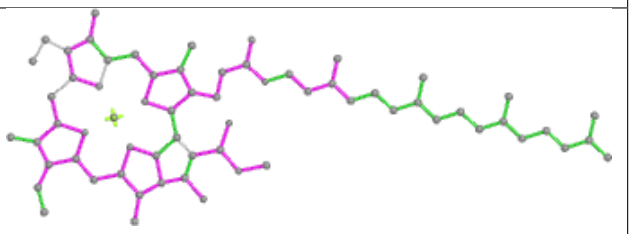
 Bond lengths	 Bond angles
 Torsions	 Rings

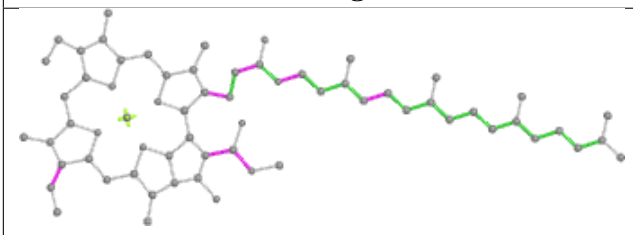
Ligand CLA 17 309



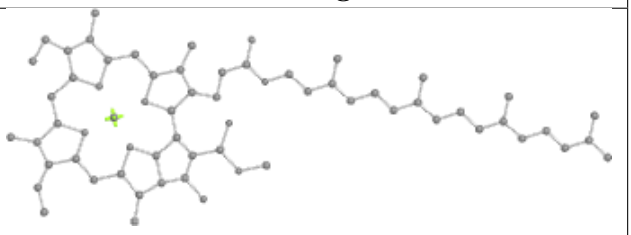
Bond lengths



Bond angles

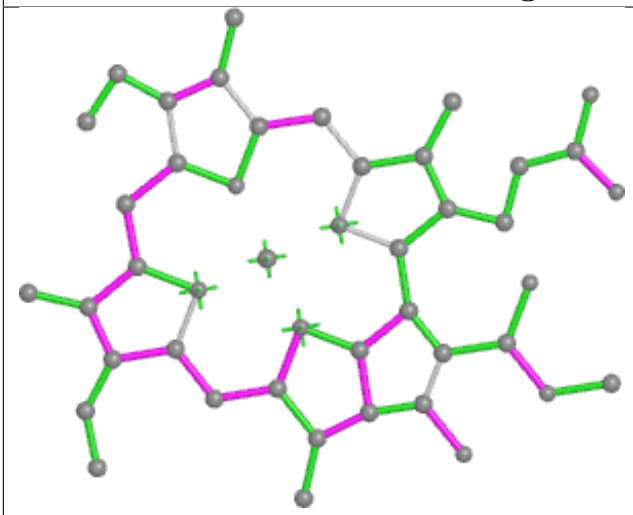


Torsions



Rings

Ligand CLA 35 310



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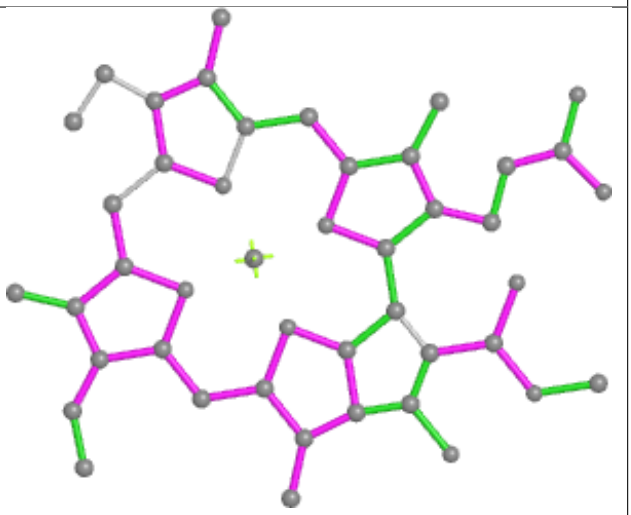
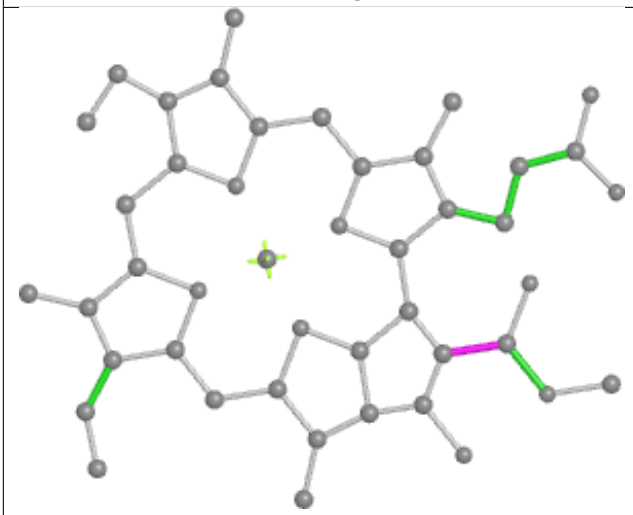
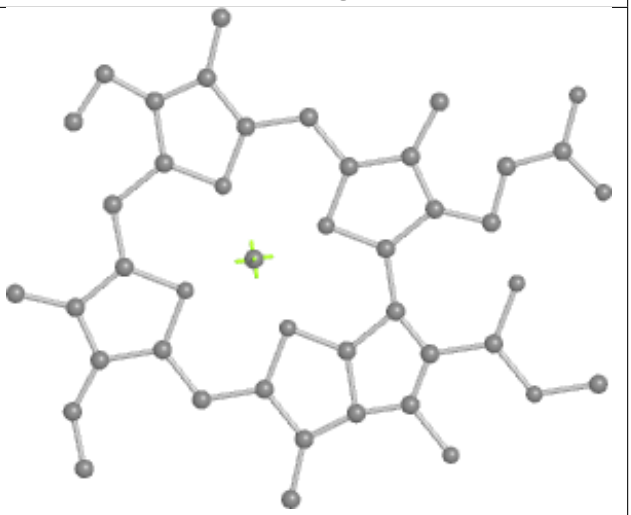


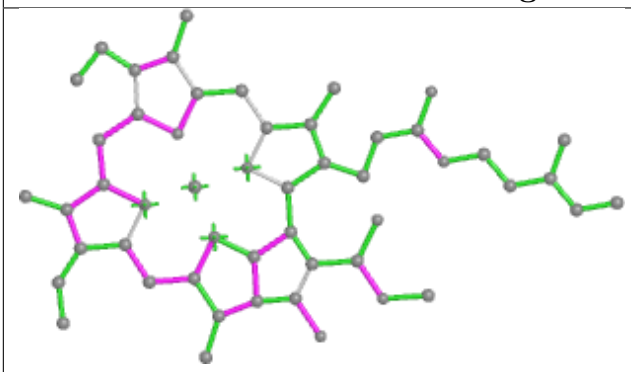
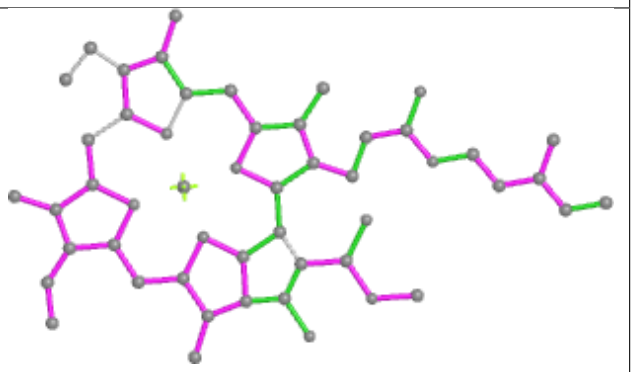
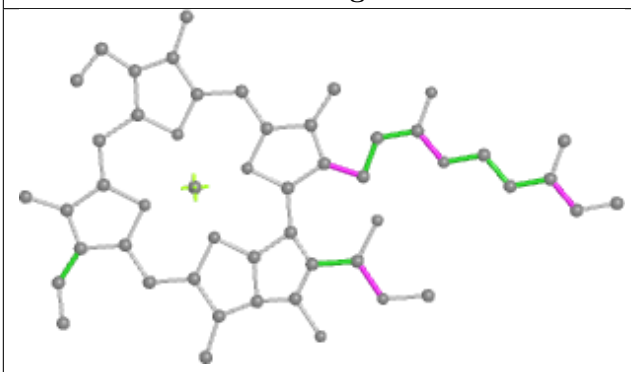
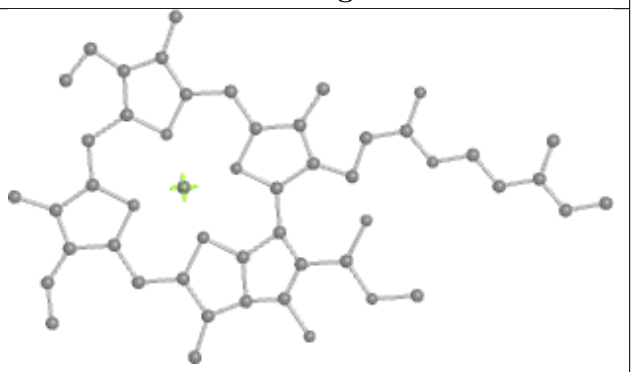
Bond angles



Torsions



Rings

Ligand CLA 31 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

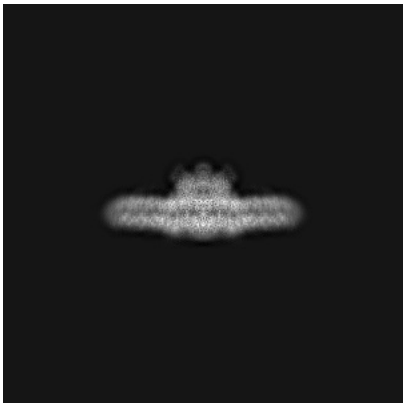
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31905. These allow visual inspection of the internal detail of the map and identification of artifacts.

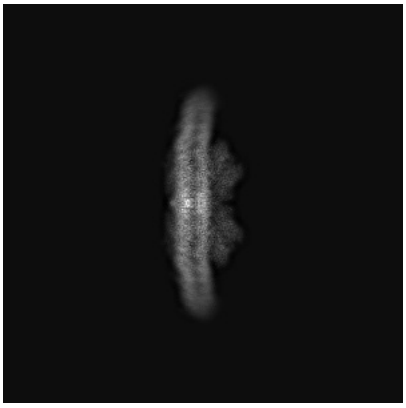
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

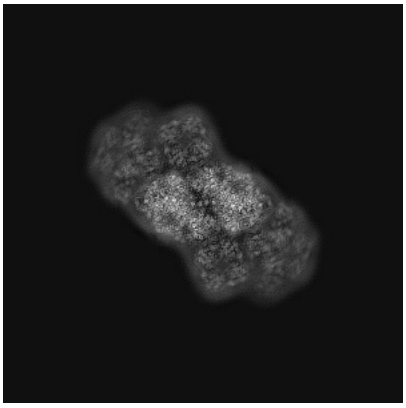
6.1.1 Primary map



X



Y

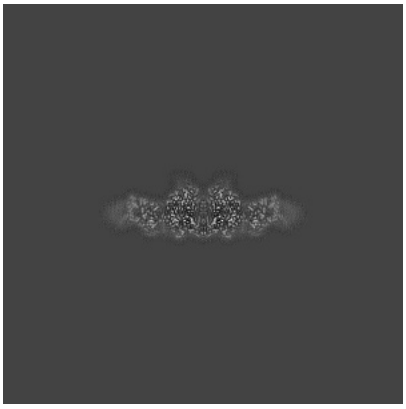


Z

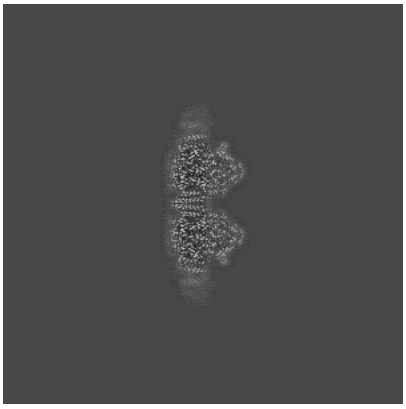
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

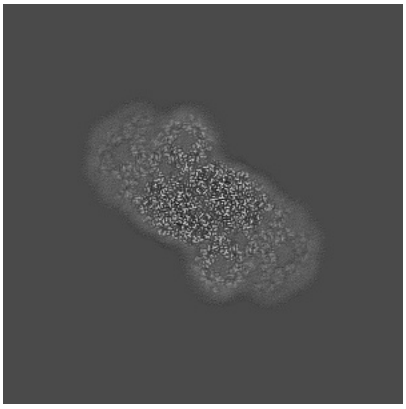
6.2.1 Primary map



X Index: 256



Y Index: 256



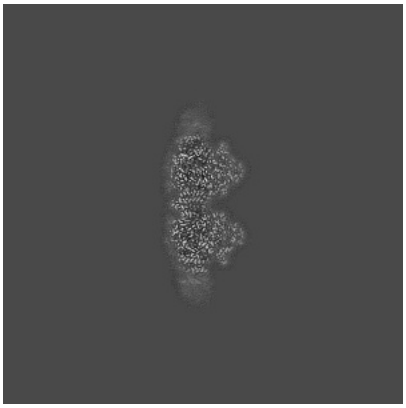
Z Index: 256

The images above show central slices of the map in three orthogonal directions.

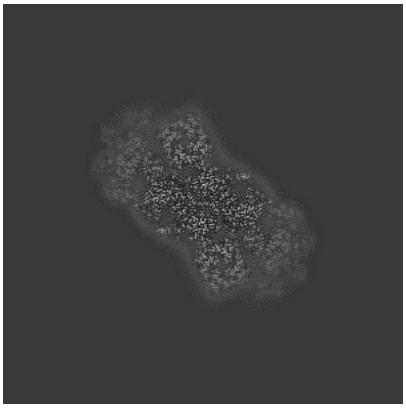
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 252



Y Index: 257



Z Index: 234

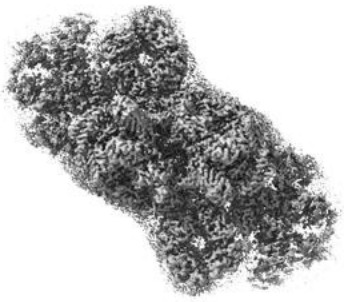
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

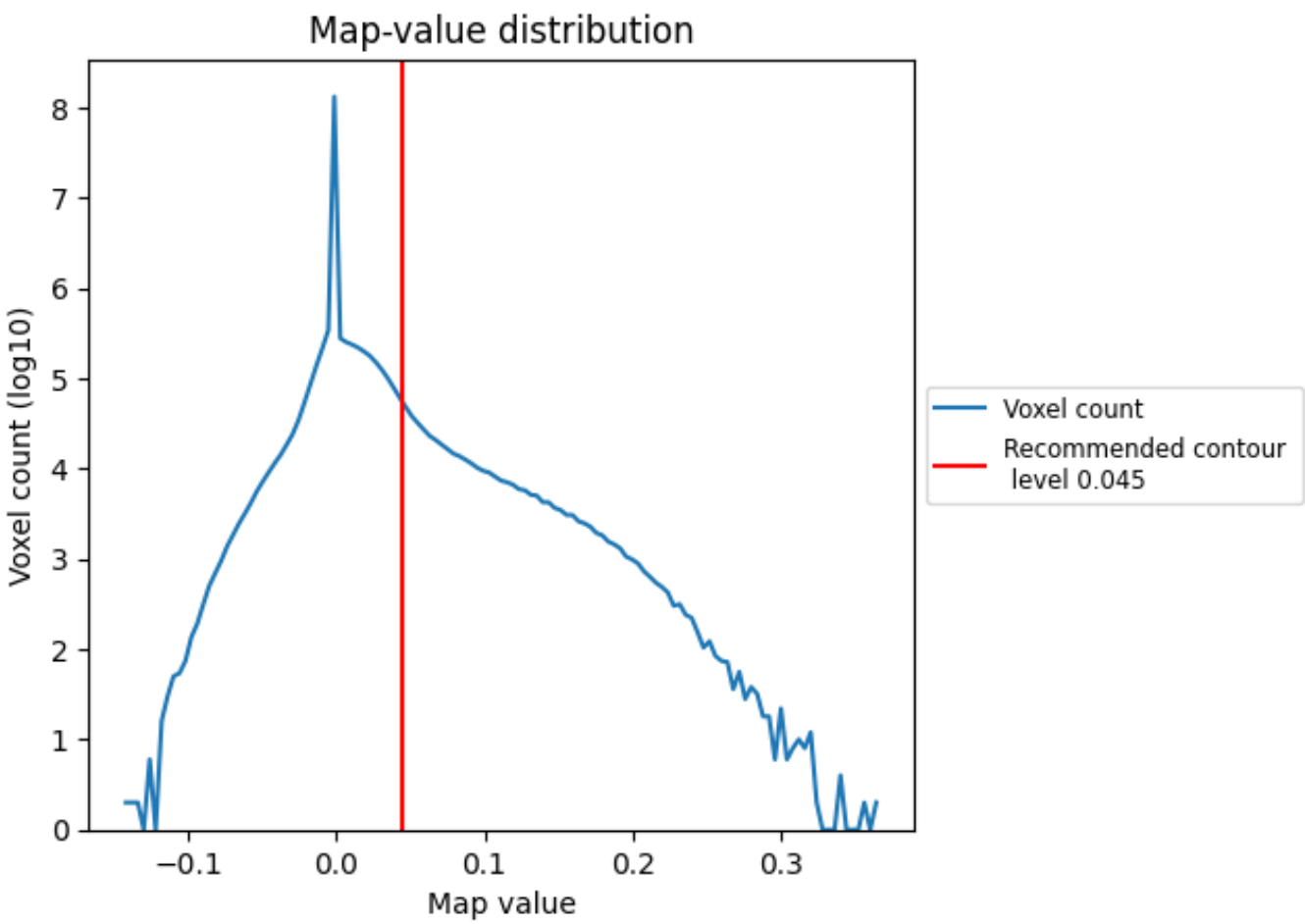
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

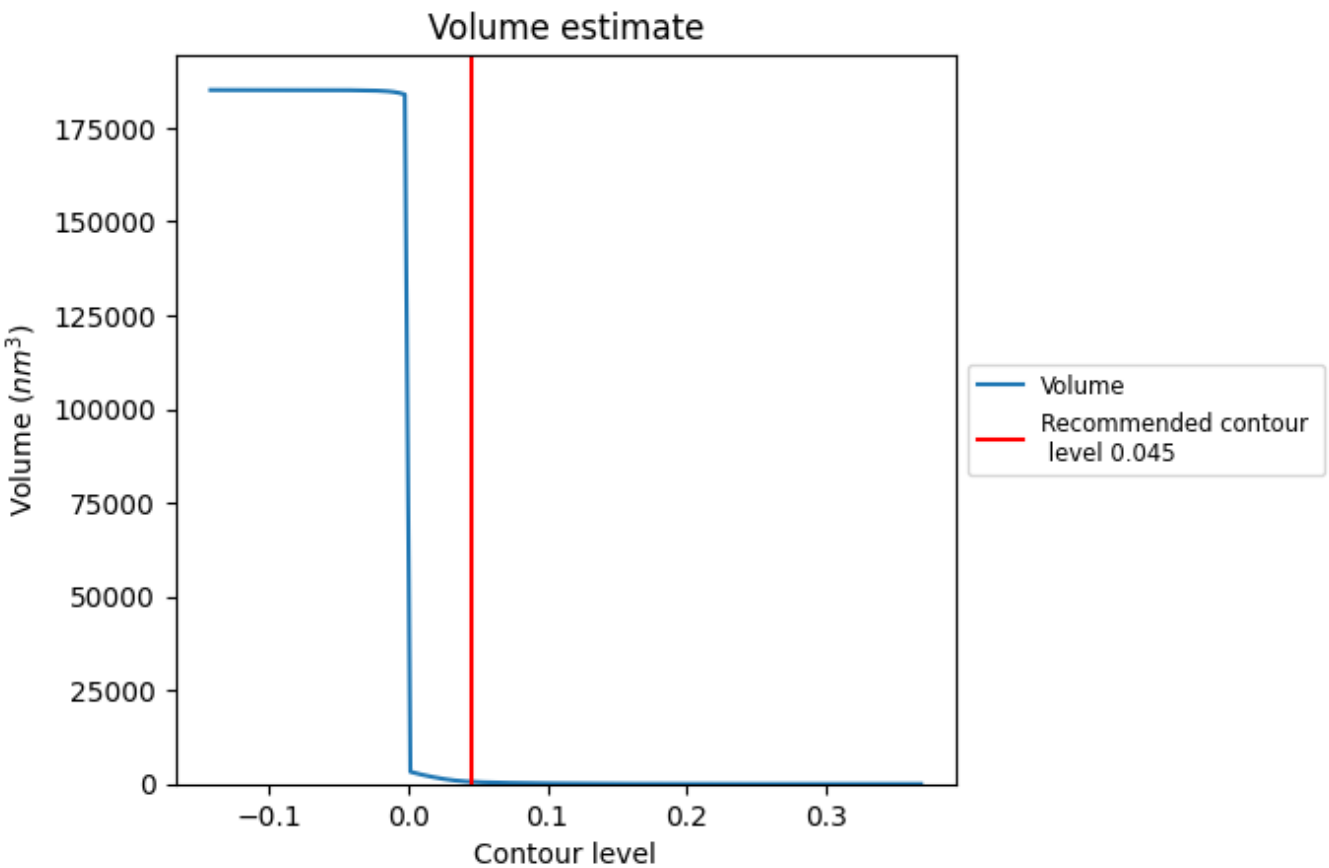
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

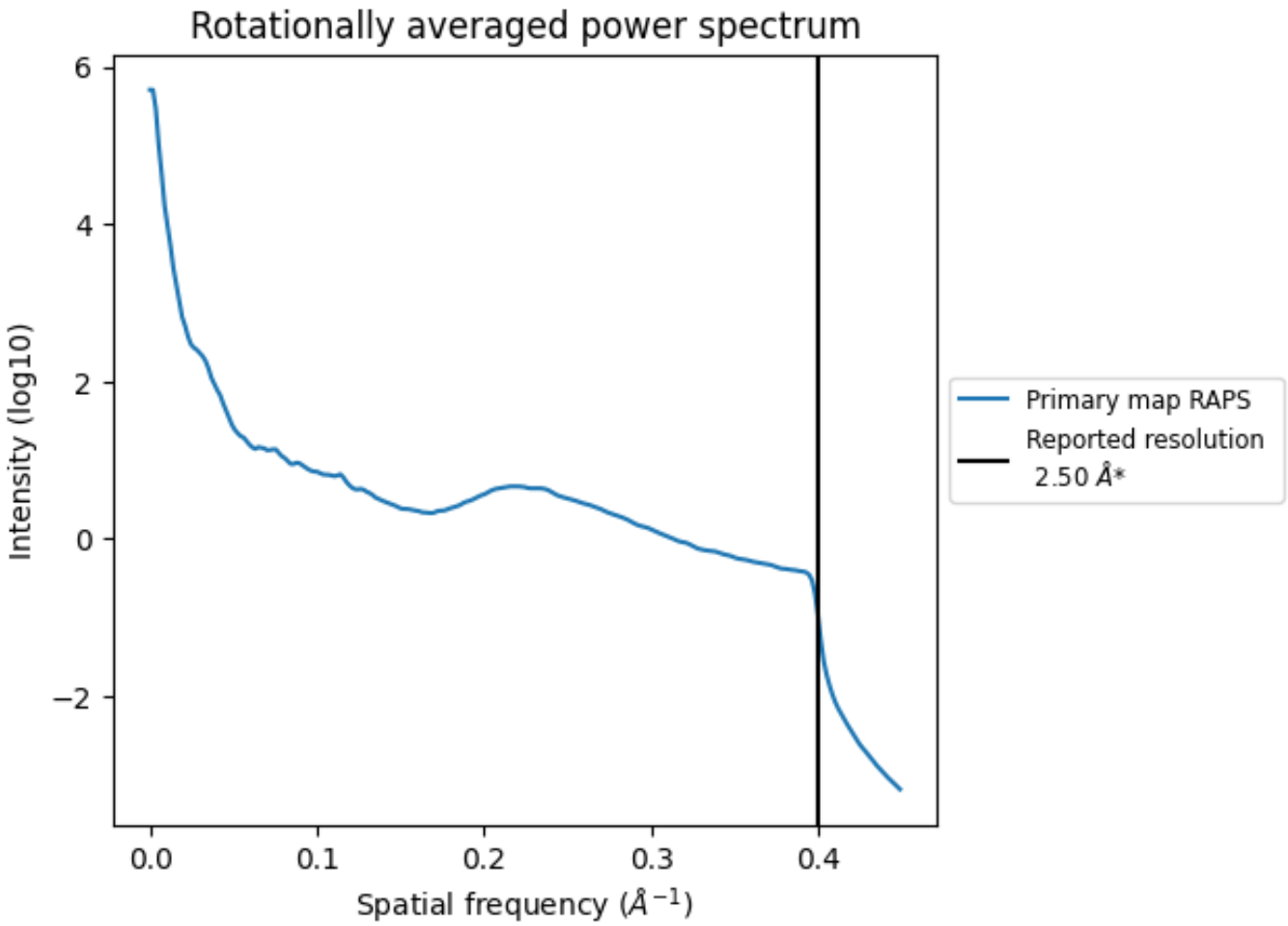
7.2 Volume estimate (i)



The volume at the recommended contour level is 588 nm^3; this corresponds to an approximate mass of 532 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

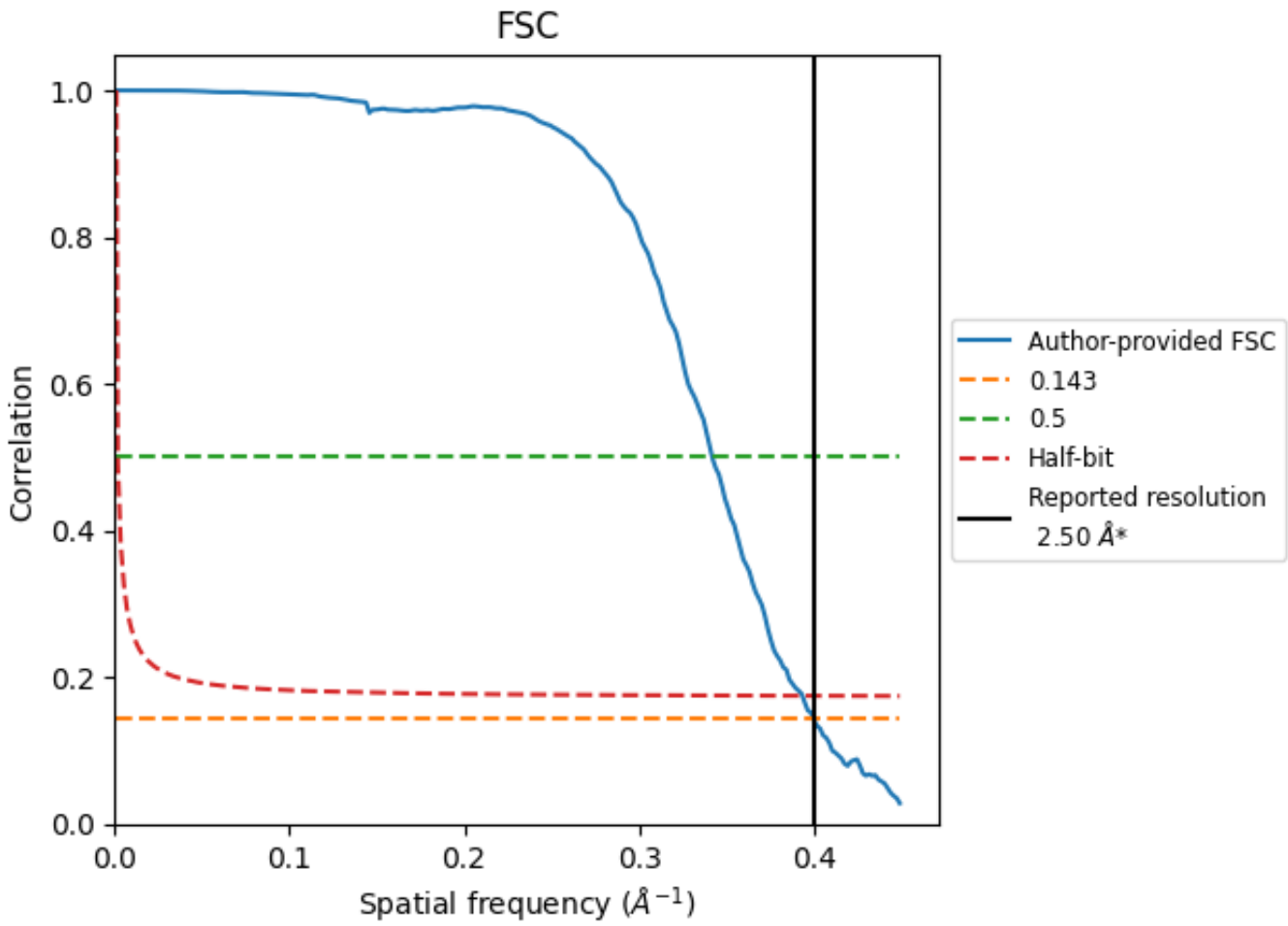


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

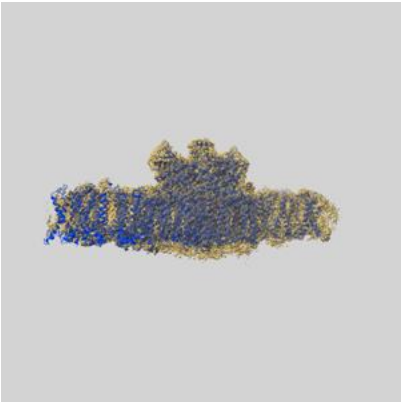
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.92	2.54
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

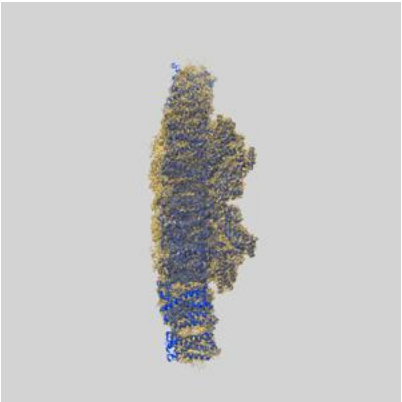
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31905 and PDB model 7VD5. Per-residue inclusion information can be found in section 3 on page 51.

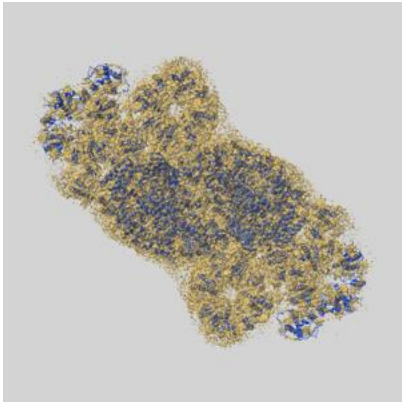
9.1 Map-model overlay (i)



X



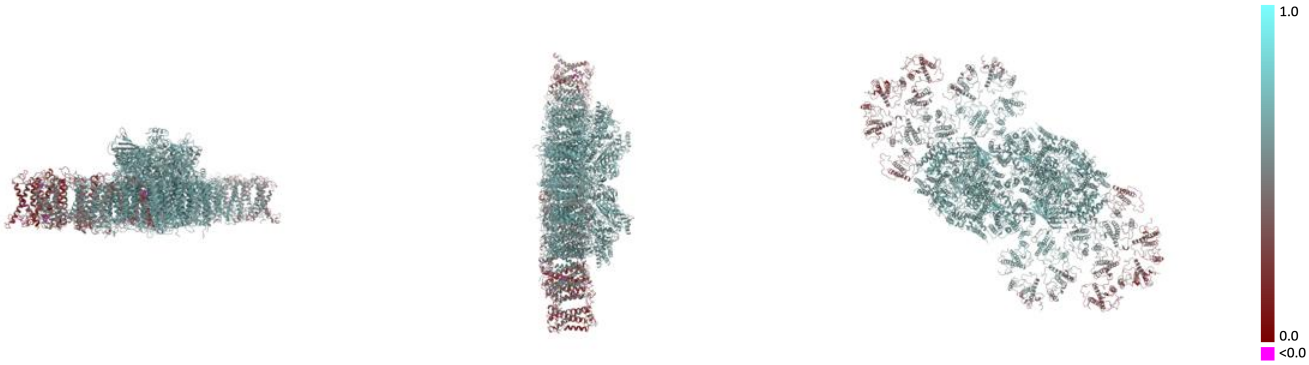
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

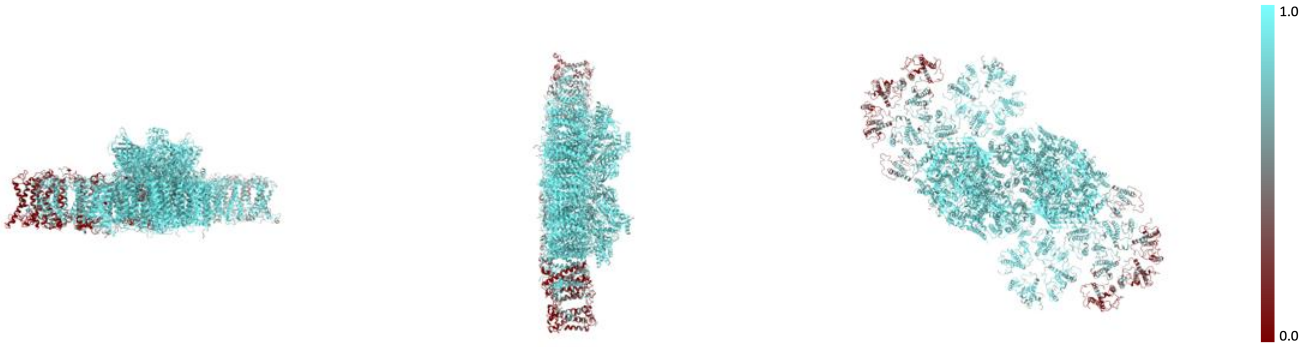
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

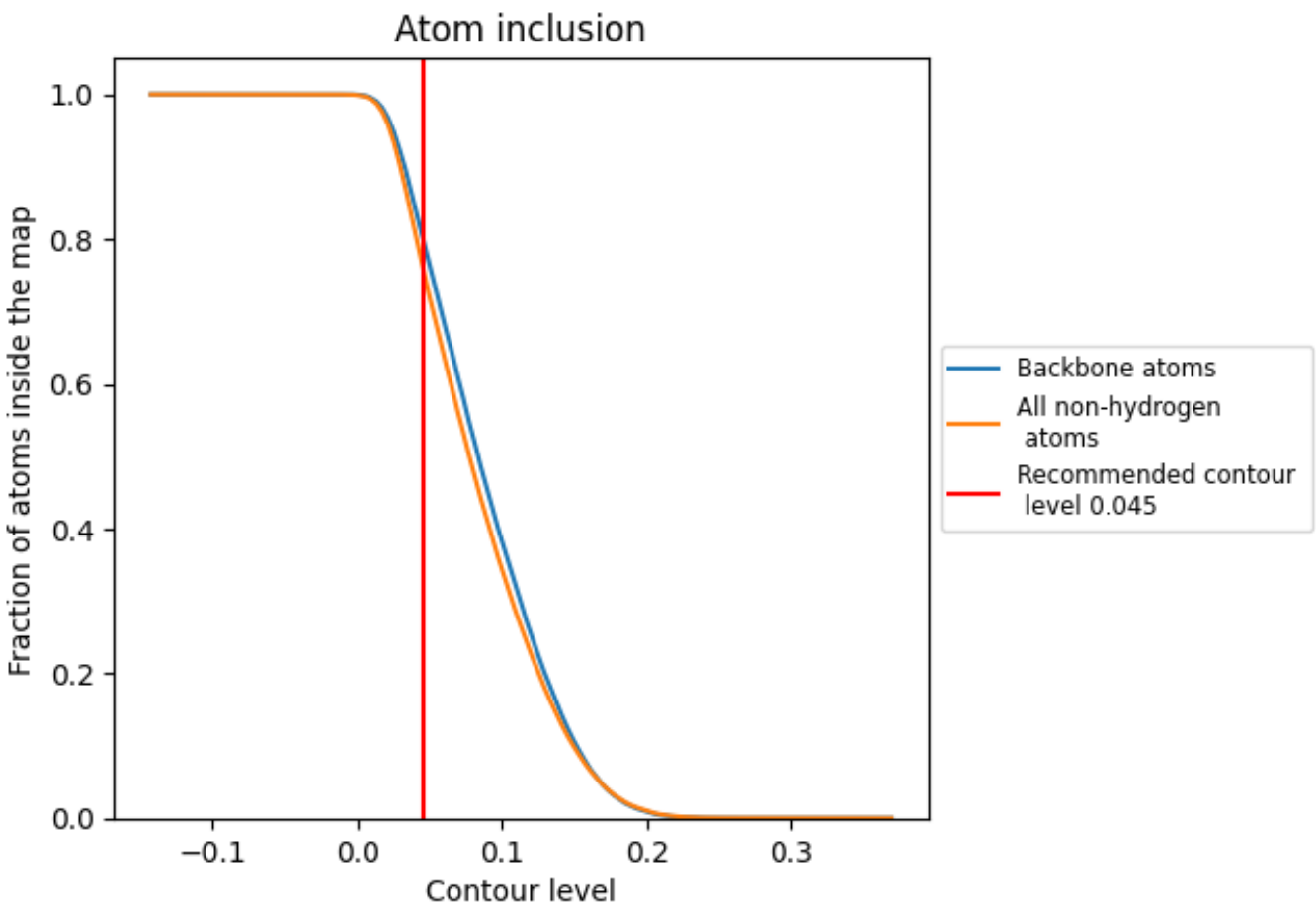
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7644	0.5430
0	0.9590	0.6360
1	0.9333	0.6130
11	0.8818	0.6000
12	0.8679	0.5780
13	0.7225	0.4570
14	0.7446	0.4800
15	0.2426	0.2840
16	0.6782	0.4740
17	0.5852	0.4350
18	0.2379	0.2830
19	0.7832	0.5510
20	0.5018	0.3420
21	0.1257	0.2530
31	0.8694	0.5900
32	0.8711	0.5790
33	0.7220	0.4550
34	0.7456	0.4770
35	0.2397	0.2850
36	0.6891	0.4790
37	0.5831	0.4360
38	0.2398	0.2860
39	0.7832	0.5490
40	0.4818	0.3370
41	0.1301	0.2520
5	0.9590	0.6400
6	0.9333	0.6080
A	0.9634	0.6690
B	0.9352	0.6540
C	0.9440	0.6550
D	0.9415	0.6620
E	0.9018	0.6110
F	0.9198	0.5950
H	0.9339	0.6390
I	0.9539	0.6560

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Chain	Atom inclusion	Q-score
J	0.8939	0.6380
K	0.9196	0.6260
L	0.8897	0.6400
M	0.8594	0.6400
O	0.8834	0.6120
Q	0.8666	0.5980
T	0.9102	0.6520
U	0.9066	0.6120
V	0.9318	0.6200
W	0.8075	0.5830
X	0.8378	0.5580
Y	0.8273	0.5920
Z	0.8642	0.5670
a	0.9625	0.6680
b	0.9369	0.6550
c	0.9431	0.6530
d	0.9387	0.6610
e	0.8918	0.6110
f	0.9198	0.5950
h	0.9388	0.6350
i	0.9539	0.6570
j	0.8875	0.6360
k	0.9358	0.6190
l	0.9478	0.6530
m	0.8626	0.6410
o	0.8872	0.6120
q	0.8726	0.6000
t	0.9102	0.6570
u	0.9066	0.6140
v	0.9299	0.6220
w	0.8523	0.6140
x	0.8224	0.5620
y	0.8408	0.6050
z	0.8716	0.5650