Full wwPDB EM Validation Report (i)

Dec 18, 2022 – 09:42 pm GMT

PDB ID	:	7OUI
EMDB ID	:	EMD-13078
Title	:	Structure of C2S2M2-type Photosystem supercomplex from Arabidopsis thaliana (digitonin-extracted)
Authors	:	Graca, A.T.; Hall, M.; Persson, K.; Schroder, W.P.
Deposited on	:	2021-06-11
Resolution	:	2.79 Å(reported)

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:

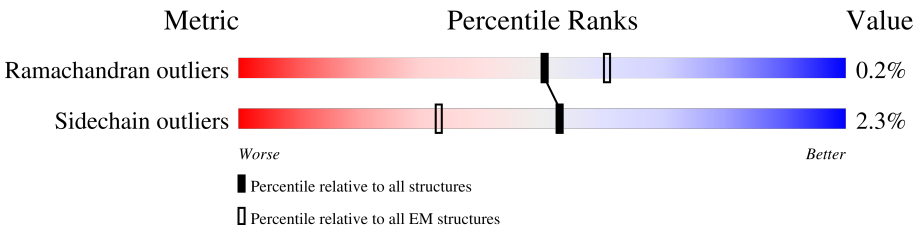
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.79 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	1	266	76% 71% 5% 24%
1	3	266	76% 71% 5% 24%
1	5	266	76% 71% 5% 24%
1	7	266	76% 71% 5% 24%
2	2	243	84% 84% • 16%
2	6	243	84% 84% • 16%
3	4	212	92% 95% • •
3	8	212	92% 95% • •
4	A	352	• 92% 7%

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Mol	Chain	Length	Quality of chain
4	a	352	92% 7%
5	B	508	95%
5	b	508	95%
6	C	459	94% 6%
6	c	459	94% 6%
7	D	352	97%
7	d	352	97%
8	E	83	5% 80% 20%
8	e	83	5% 80% 20%
9	F	39	5% 74% 26%
9	f	39	74% 26%
10	H	72	6% 83% 17%
10	h	72	83% 17%
11	I	36	6% 97%
11	i	36	6% 97%
12	K	37	100%
12	k	37	100%
13	L	38	8% 95% 5%
13	l	38	8% 95% 5%
14	M	34	91% 6%
14	m	34	91% 6%
15	O	247	6% 79% 20%
15	o	247	5% 79% 20%
16	T	33	88% 12%
16	t	33	88% 12%

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Mol	Chain	Length	Quality of chain
17	W	54	100%
17	w	54	100%
18	X	42	10% 86% 14%
18	x	42	10% 86% 14%
19	Z	62	98%
19	z	62	98%
20	S	232	5% 93% 7%
20	s	232	6% 93% 7%
21	G	232	29% 83% 6% 11%
21	N	232	8% 81% 6% 13%
21	Y	232	86% 6% 8%
21	g	232	29% 83% 6% 11%
21	n	232	8% 81% 6% 13%
21	y	232	86% 6% 8%
22	R	250	20% 94% 6%
22	r	250	20% 94% 6%
23	U	28	57% 89% 11%
23	u	28	57% 89% 11%

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
24	CHL	1	301	X	-	-	-
24	CHL	1	302	X	-	-	-
24	CHL	2	601	X	-	-	-
24	CHL	2	603	X	-	-	-
24	CHL	5	301	X	-	-	-
24	CHL	5	302	X	-	-	-
24	CHL	6	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	6	603	X	-	-	-
24	CHL	G	601	X	-	-	-
24	CHL	G	605	X	-	-	-
24	CHL	G	606	X	-	-	-
24	CHL	G	607	X	-	-	-
24	CHL	G	608	X	-	-	-
24	CHL	G	609	X	-	-	-
24	CHL	N	601	X	-	-	-
24	CHL	N	605	X	-	-	-
24	CHL	N	606	X	-	-	-
24	CHL	N	607	X	-	-	-
24	CHL	N	608	X	-	-	-
24	CHL	N	609	X	-	-	-
24	CHL	R	605	X	-	-	-
24	CHL	R	606	X	-	-	-
24	CHL	R	607	X	-	-	-
24	CHL	R	613	X	-	-	-
24	CHL	S	302	X	-	-	-
24	CHL	S	306	X	-	-	-
24	CHL	S	307	X	-	-	-
24	CHL	S	308	X	-	-	-
24	CHL	Y	302	X	-	-	-
24	CHL	Y	306	X	-	-	-
24	CHL	Y	307	X	-	-	-
24	CHL	Y	308	X	-	-	-
24	CHL	Y	309	X	-	-	-
24	CHL	Y	310	X	-	-	-
24	CHL	g	601	X	-	-	-
24	CHL	g	605	X	-	-	-
24	CHL	g	606	X	-	-	-
24	CHL	g	607	X	-	-	-
24	CHL	g	608	X	-	-	-
24	CHL	g	609	X	-	-	-
24	CHL	n	601	X	-	-	-
24	CHL	n	605	X	-	-	-
24	CHL	n	606	X	-	-	-
24	CHL	n	607	X	-	-	-
24	CHL	n	608	X	-	-	-
24	CHL	n	609	X	-	-	-
24	CHL	r	605	X	-	-	-
24	CHL	r	606	X	-	-	-
24	CHL	r	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	r	613	X	-	-	-
24	CHL	s	302	X	-	-	-
24	CHL	s	306	X	-	-	-
24	CHL	s	307	X	-	-	-
24	CHL	s	308	X	-	-	-
24	CHL	y	302	X	-	-	-
24	CHL	y	306	X	-	-	-
24	CHL	y	307	X	-	-	-
24	CHL	y	308	X	-	-	-
24	CHL	y	309	X	-	-	-
24	CHL	y	310	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	605	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	605	X	-	-	-
25	CLA	A	401	X	-	-	-
25	CLA	A	402	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	G	602	X	-	-	-
25	CLA	G	603	X	-	-	-
25	CLA	G	604	X	-	-	-
25	CLA	G	610	X	-	-	-
25	CLA	G	611	X	-	-	-
25	CLA	G	612	X	-	-	-
25	CLA	G	613	X	-	-	-
25	CLA	G	614	X	-	-	-
25	CLA	N	602	X	-	-	-
25	CLA	N	603	X	-	-	-
25	CLA	N	604	X	-	-	-
25	CLA	N	610	X	-	-	-
25	CLA	N	611	X	-	-	-
25	CLA	N	612	X	-	-	-
25	CLA	N	613	X	-	-	-
25	CLA	N	614	X	-	-	-
25	CLA	R	601	X	-	-	-
25	CLA	R	602	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	608	X	-	-	-
25	CLA	R	609	X	-	-	-
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	612	X	-	-	-
25	CLA	R	614	X	-	-	-
25	CLA	S	303	X	-	-	-
25	CLA	S	304	X	-	-	-
25	CLA	S	305	X	-	-	-
25	CLA	S	309	X	-	-	-
25	CLA	S	310	X	-	-	-
25	CLA	S	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	S	312	X	-	-	-
25	CLA	S	313	X	-	-	-
25	CLA	S	314	X	-	-	-
25	CLA	Y	303	X	-	-	-
25	CLA	Y	304	X	-	-	-
25	CLA	Y	305	X	-	-	-
25	CLA	Y	311	X	-	-	-
25	CLA	Y	312	X	-	-	-
25	CLA	Y	313	X	-	-	-
25	CLA	Y	314	X	-	-	-
25	CLA	Y	315	X	-	-	-
25	CLA	a	402	X	-	-	-
25	CLA	a	403	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	g	602	X	-	-	-
25	CLA	g	603	X	-	-	-
25	CLA	g	604	X	-	-	-
25	CLA	g	610	X	-	-	-
25	CLA	g	611	X	-	-	-
25	CLA	g	612	X	-	-	-
25	CLA	g	613	X	-	-	-
25	CLA	g	614	X	-	-	-
25	CLA	n	602	X	-	-	-
25	CLA	n	603	X	-	-	-
25	CLA	n	604	X	-	-	-
25	CLA	n	610	X	-	-	-
25	CLA	n	611	X	-	-	-
25	CLA	n	612	X	-	-	-
25	CLA	n	613	X	-	-	-
25	CLA	n	614	X	-	-	-
25	CLA	r	601	X	-	-	-
25	CLA	r	602	X	-	-	-
25	CLA	r	603	X	-	-	-
25	CLA	r	604	X	-	-	-
25	CLA	r	608	X	-	-	-
25	CLA	r	609	X	-	-	-
25	CLA	r	610	X	-	-	-
25	CLA	r	611	X	-	-	-
25	CLA	r	612	X	-	-	-
25	CLA	r	614	X	-	-	-
25	CLA	s	303	X	-	-	-
25	CLA	s	304	X	-	-	-
25	CLA	s	305	X	-	-	-
25	CLA	s	309	X	-	-	-
25	CLA	s	310	X	-	-	-
25	CLA	s	311	X	-	-	-
25	CLA	s	312	X	-	-	-
25	CLA	s	313	X	-	-	-
25	CLA	s	314	X	-	-	-
25	CLA	y	303	X	-	-	-
25	CLA	y	304	X	-	-	-
25	CLA	y	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	y	311	X	-	-	-
25	CLA	y	312	X	-	-	-
25	CLA	y	313	X	-	-	-
25	CLA	y	314	X	-	-	-
25	CLA	y	315	X	-	-	-

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 85897 atoms, of which 1470 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 Lhcb1.4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	202	1537	996	250	286	5	0	0
1	3	202	1537	996	250	286	5	0	0
1	5	202	1537	996	250	286	5	0	0
1	7	202	1537	996	250	286	5	0	0

- Molecule 2 is a protein called Lhcb3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	205	1593	1040	258	290	5	0	0
2	6	205	1593	1040	258	290	5	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	204	1597	1048	262	283	4	0	0
3	8	204	1597	1048	262	283	4	0	0

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	326	2548	1664	419	452	13	0	0
4	a	326	2548	1664	419	452	13	0	0

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	487	3810	2495	644	659	12	0	0
5	b	487	3810	2495	644	659	12	0	0

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	433	3373	2221	563	578	11	0	0
6	c	433	3373	2221	563	578	11	0	0

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	342	2722	1800	445	465	12	0	0
7	d	342	2722	1800	445	465	12	0	0

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	E	66	543	357	88	98	0	0
8	e	66	543	357	88	98	0	0

- Molecule 9 is a protein called Cytochrome b559 subunit beta (PsbF).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	29	224	147	40	36	1	0	0
9	f	29	224	147	40	36	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H	60	446	293	70	81	2	0	0
10	h	60	446	293	70	81	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	I	35	286	195	44	46	1	0	0
11	i	35	286	195	44	46	1	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	37	301	211	44	45	1	0	0
12	k	37	301	211	44	45	1	0	0

- Molecule 13 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	L	36	302	200	47	55	0	0
13	l	36	302	200	47	55	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	32	250	173	35	41	1	0	0
14	m	32	250	173	35	41	1	0	0

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	197	1516	969	241	302	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	o	197	1516	969	241	302	4	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	T	29	239	168	33	37	1	0	0
			Total	C	N	O	S		
16	t	29	239	168	33	37	1	0	0

- Molecule 17 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	W	54	427	282	61	83	1	0	0
			Total	C	N	O	S		
17	w	54	427	282	61	83	1	0	0

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	X	36	248	162	39	47	0	0
			Total	C	N	O		
18	x	36	248	162	39	47	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	62	464	313	69	81	1	0	0
			Total	C	N	O	S		
19	z	62	464	313	69	81	1	0	0

- Molecule 20 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	216	1670	1091	272	303	4	0	0
			Total	C	N	O	S		
20	s	216	1670	1091	272	303	4	0	0

- Molecule 21 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	G	206	1562	1010	255	292	5	0	0
21	N	202	1536	994	251	286	5	0	0
21	Y	213	1621	1048	266	302	5	0	0
21	g	206	1562	1010	255	292	5	0	0
21	n	202	1536	994	251	286	5	0	0
21	y	213	1621	1048	266	302	5	0	0

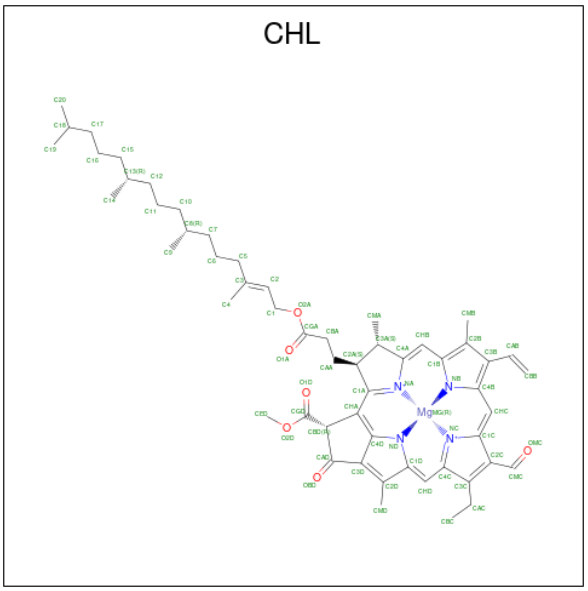
- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	235	1827	1183	298	343	3	0	0
22	r	235	1827	1183	298	343	3	0	0

- Molecule 23 is a protein called PsbTn.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	U	25	194	122	36	33	3	0	0
23	u	25	194	122	36	33	3	0	0

- Molecule 24 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	1	1	92	70	2	8	12	0
			Total	C	Mg	N	O	
24	1	1	92	70	2	8	12	0
			Total	C	Mg	N	O	
24	2	1	110	88	2	8	12	0
			Total	C	Mg	N	O	
24	2	1	110	88	2	8	12	0
			Total	C	Mg	N	O	
24	S	1	184	140	4	16	24	0
			Total	C	Mg	N	O	
24	S	1	184	140	4	16	24	0
			Total	C	Mg	N	O	
24	S	1	184	140	4	16	24	0
			Total	C	Mg	N	O	
24	S	1	184	140	4	16	24	0
			Total	C	Mg	N	O	
24	G	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	G	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	G	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	G	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	G	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	G	1	335	269	6	24	36	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	N	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	N	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	N	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	N	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	N	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	N	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	Y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	Y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	Y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	Y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	Y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	Y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	R	1	195	153	4	16	22	0
			Total	C	Mg	N	O	
24	R	1	195	153	4	16	22	0
			Total	C	Mg	N	O	
24	R	1	195	153	4	16	22	0
			Total	C	Mg	N	O	
24	R	1	195	153	4	16	22	0
			Total	C	Mg	N	O	
24	5	1	92	70	2	8	12	0
			Total	C	Mg	N	O	
24	5	1	92	70	2	8	12	0
			Total	C	Mg	N	O	
24	6	1	110	88	2	8	12	0
			Total	C	Mg	N	O	
24	6	1	110	88	2	8	12	0
			Total	C	Mg	N	O	
24	s	1	184	140	4	16	24	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	s	1	184	140	4	16	24	0
			Total	C	Mg	N	O	
24	s	1	184	140	4	16	24	0
			Total	C	Mg	N	O	
24	s	1	184	140	4	16	24	0
			Total	C	Mg	N	O	
24	g	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	g	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	g	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	g	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	g	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	g	1	335	269	6	24	36	0
			Total	C	Mg	N	O	
24	n	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	n	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	n	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	n	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	n	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	n	1	348	282	6	24	36	0
			Total	C	Mg	N	O	
24	y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	y	1	344	278	6	24	36	0
			Total	C	Mg	N	O	
24	y	1	344	278	6	24	36	0

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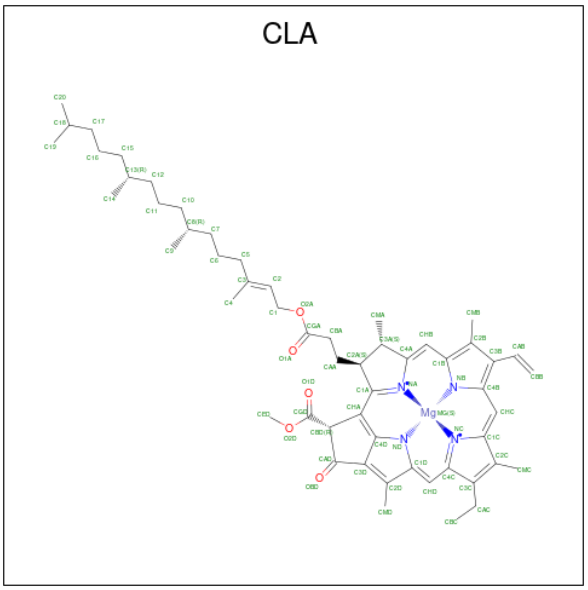
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	r	1	195	153	4	16	22	0
			Total	C	Mg	N	O	
24	r	1	195	153	4	16	22	0
			Total	C	Mg	N	O	
24	r	1	195	153	4	16	22	0
			Total	C	Mg	N	O	
24	r	1	195	153	4	16	22	0

- Molecule 25 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	
25	2	1	163	133	3	12	15	0
			Total	C	Mg	N	O	
25	2	1	163	133	3	12	15	0
			Total	C	Mg	N	O	
25	2	1	163	133	3	12	15	0
			Total	C	Mg	N	O	
25	A	1	190	160	3	12	15	0
			Total	C	Mg	N	O	
25	A	1	190	160	3	12	15	0
			Total	C	Mg	N	O	
25	A	1	190	160	3	12	15	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	B	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	C	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	D	1	180	150	3	12	15	0
			Total	C	Mg	N	O	
25	D	1	180	150	3	12	15	0
			Total	C	Mg	N	O	
25	D	1	180	150	3	12	15	0
			Total	C	Mg	N	O	
25	S	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	S	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	S	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	S	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	S	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	S	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	S	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	S	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	S	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	G	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	G	1	472	392	8	32	40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	G	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	G	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	G	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	G	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	G	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	G	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	N	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	N	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	N	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	N	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	N	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	N	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	N	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	N	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	Y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	Y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	Y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	Y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	Y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	Y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	Y	1	470	390	8	32	40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	Y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	R	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	R	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	R	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	R	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	R	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	R	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	R	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	R	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	R	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	R	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	6	1	163	133	3	12	15	0
			Total	C	Mg	N	O	
25	6	1	163	133	3	12	15	0
			Total	C	Mg	N	O	
25	6	1	163	133	3	12	15	0
			Total	C	Mg	N	O	
25	a	1	190	160	3	12	15	0
			Total	C	Mg	N	O	
25	a	1	190	160	3	12	15	0
			Total	C	Mg	N	O	
25	a	1	190	160	3	12	15	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	b	1	1040	880	16	64	80	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	c	1	840	710	13	52	65	0
			Total	C	Mg	N	O	
25	d	1	180	150	3	12	15	0
			Total	C	Mg	N	O	
25	d	1	180	150	3	12	15	0
			Total	C	Mg	N	O	
25	d	1	180	150	3	12	15	0
			Total	C	Mg	N	O	
25	s	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	s	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	s	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	s	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	s	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	s	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	s	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	s	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	s	1	465	375	9	36	45	0
			Total	C	Mg	N	O	
25	g	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	g	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	g	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	g	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	g	1	472	392	8	32	40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	g	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	g	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	g	1	472	392	8	32	40	0
			Total	C	Mg	N	O	
25	n	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	n	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	n	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	n	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	n	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	n	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	n	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	n	1	473	393	8	32	40	0
			Total	C	Mg	N	O	
25	y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	y	1	470	390	8	32	40	0
			Total	C	Mg	N	O	
25	r	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	r	1	543	443	10	40	50	0

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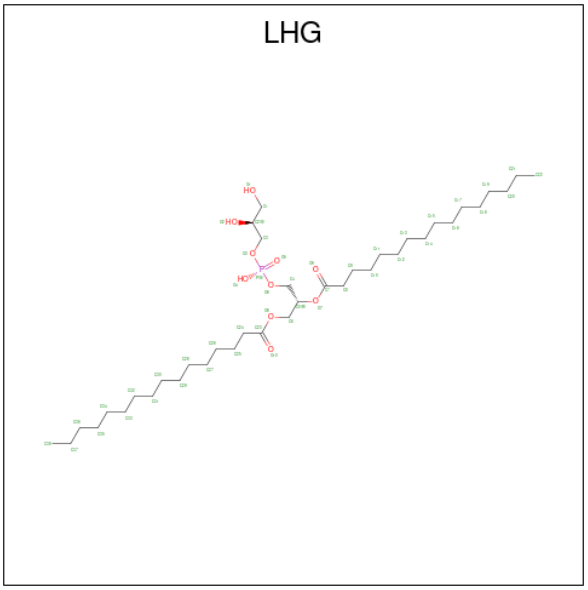
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	r	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	r	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	r	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	r	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	r	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	r	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	r	1	543	443	10	40	50	0
			Total	C	Mg	N	O	
25	r	1	543	443	10	40	50	0

- Molecule 26 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	
26	2	1	47	36	10	1	0
			Total	C	O	P	
26	B	1	142	109	30	3	0
			Total	C	O	P	
26	B	1	142	109	30	3	0

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Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C O P 142 109 30 3	0
26	C	1	Total C H O P 221 114 74 30 3	0
26	C	1	Total C H O P 221 114 74 30 3	0
26	C	1	Total C H O P 221 114 74 30 3	0
26	D	1	Total C O P 49 38 10 1	0
26	L	1	Total C O P 49 38 10 1	0
26	S	1	Total C O P 98 76 20 2	0
26	S	1	Total C O P 98 76 20 2	0
26	N	1	Total C O P 49 38 10 1	0
26	Y	1	Total C O P 98 76 20 2	0
26	Y	1	Total C O P 98 76 20 2	0
26	R	1	Total C O P 42 31 10 1	0
26	6	1	Total C O P 47 36 10 1	0
26	b	1	Total C O P 142 109 30 3	0
26	b	1	Total C O P 142 109 30 3	0
26	b	1	Total C O P 142 109 30 3	0
26	c	1	Total C H O P 221 114 74 30 3	0
26	c	1	Total C H O P 221 114 74 30 3	0
26	c	1	Total C H O P 221 114 74 30 3	0
26	d	1	Total C O P 49 38 10 1	0
26	l	1	Total C O P 49 38 10 1	0

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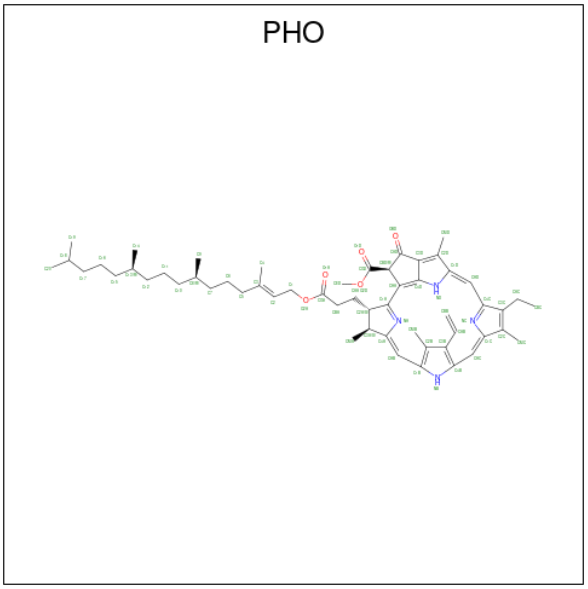
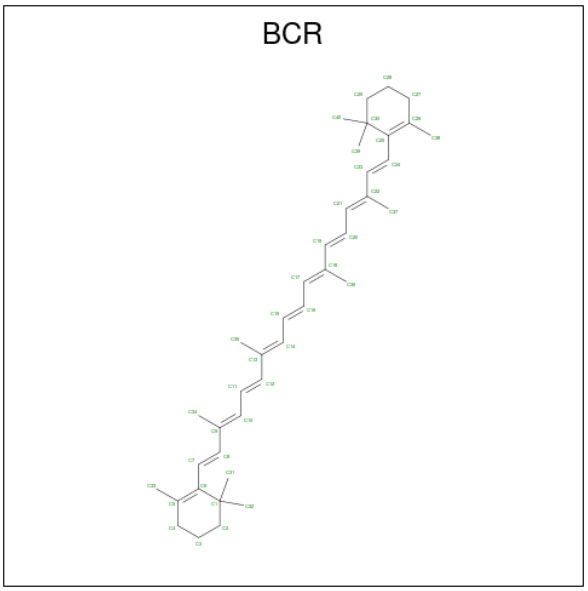
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
26	s	1	98	76	20	2	0
			Total	C	O	P	
26	s	1	98	76	20	2	0
			Total	C	O	P	
26	n	1	49	38	10	1	0
			Total	C	O	P	
26	y	1	98	76	20	2	0
			Total	C	O	P	
26	y	1	98	76	20	2	0
			Total	C	O	P	
26	r	1	42	31	10	1	0

- Molecule 27 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
27	A	1	128	110	8	10	0
			Total	C	N	O	
27	A	1	128	110	8	10	0
			Total	C	N	O	
27	a	1	128	110	8	10	0
			Total	C	N	O	
27	a	1	128	110	8	10	0

- Molecule 28 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
28	A	1	40	40	0
			Total	C	
28	B	1	120	120	0
			Total	C	
28	B	1	120	120	0
			Total	C	
28	B	1	120	120	0
			Total	C	
28	C	1	40	40	0
			Total	C	
28	D	1	40	40	0
			Total	C	
28	H	1	40	40	0
			Total	C	
28	I	1	40	40	0
			Total	C	
28	K	1	40	40	0
			Total	C	
28	T	1	40	40	0
			Total	C	
28	Z	1	40	40	0
			Total	C	
28	a	1	40	40	0
			Total	C	
28	b	1	120	120	0
			Total	C	
28	b	1	120	120	0

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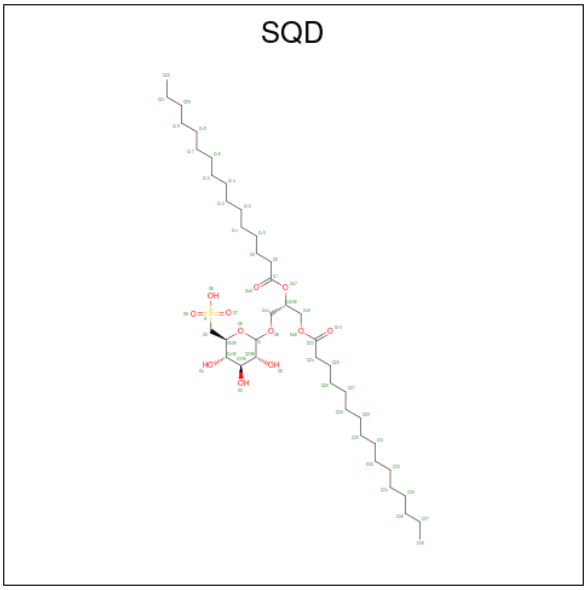
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
28	b	1	120	120	0
			Total	C	
28	c	1	40	40	0
			Total	C	
28	d	1	40	40	0
			Total	C	
28	h	1	40	40	0
			Total	C	
28	i	1	40	40	0
			Total	C	
28	k	1	40	40	0
			Total	C	
28	t	1	40	40	0
			Total	C	
28	z	1	40	40	0

- Molecule 29 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	
29	A	1	104	78	24	2	0
			Total	C	O	S	
29	A	1	104	78	24	2	0
			Total	C	O	S	
29	L	1	96	70	24	2	0

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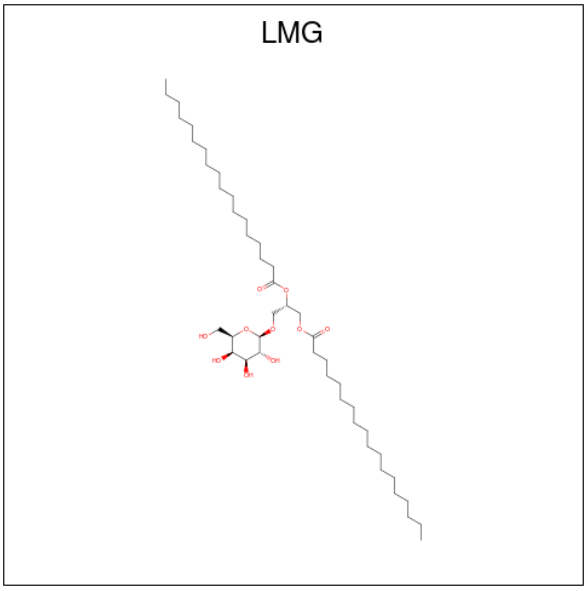
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
29	L	1	96	70	24	2	0
			Total	C	O	S	
29	a	1	104	78	24	2	0
			Total	C	O	S	
29	a	1	104	78	24	2	0
			Total	C	O	S	
29	l	1	96	70	24	2	0
			Total	C	O	S	
29	l	1	96	70	24	2	0

- Molecule 30 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	
30	A	1	88	68	20	0
			Total	C	O	
30	A	1	88	68	20	0
			Total	C	O	
30	B	1	106	86	20	0
			Total	C	O	
30	B	1	106	86	20	0
			Total	C	O	
30	C	1	51	41	10	0
			Total	C	O	
30	D	1	46	36	10	0

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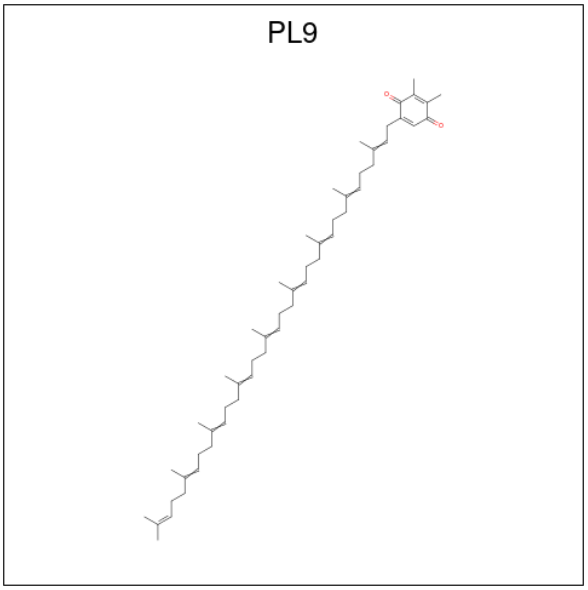
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	a	1	88	68	20	0
30	a	1	88	68	20	0
30	b	1	106	86	20	0
30	b	1	106	86	20	0
30	c	1	51	41	10	0
30	d	1	46	36	10	0

- Molecule 31 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	
31	A	1	13	11	2	0
31	D	1	55	53	2	0
31	a	1	13	11	2	0
31	d	1	55	53	2	0

- Molecule 32 is a ligand with the chemical component id AJP but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for AJP. ERROR THIS SHOULD NOT HAPPEN FOLLOWING ANNOTATION.

Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
32	A	1	177	56	92	29	0
32	B	1	177	56	92	29	0
32	S	1	95	33	53	9	0
32	G	1	95	33	53	9	0
32	N	1	190	66	106	18	0
32	N	1	190	66	106	18	0
32	Y	1	475	165	265	45	0
32	Y	1	475	165	265	45	0
32	Y	1	475	165	265	45	0
32	Y	1	475	165	265	45	0
32	Y	1	475	165	265	45	0
32	a	1	177	56	92	29	0
32	b	1	177	56	92	29	0
32	s	1	95	33	53	9	0
32	g	1	95	33	53	9	0
32	n	1	190	66	106	18	0
32	n	1	190	66	106	18	0
32	y	1	475	165	265	45	0
32	y	1	475	165	265	45	0
32	y	1	475	165	265	45	0

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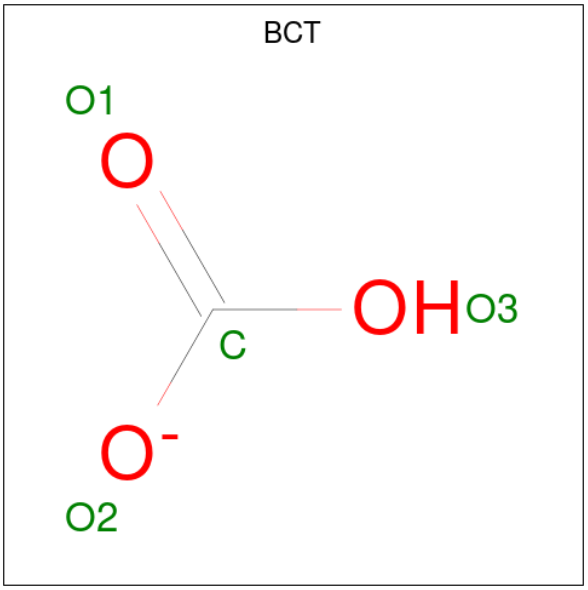
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
32	y	1	475	165	265	45	0
32	y	1	475	165	265	45	0

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

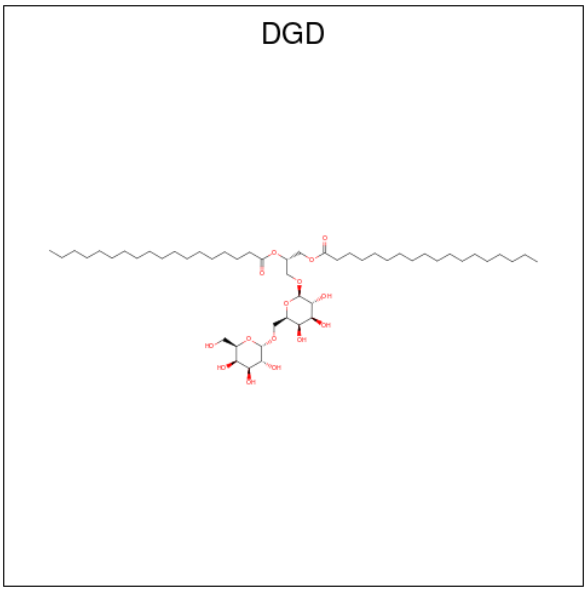


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	A	1	4	1	3	0
33	a	1	4	1	3	0

- Molecule 34 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total 59	C 44	O 15	0
35	B	1	Total 62	C 47	O 15	0
35	C	1	Total 117	C 87	O 30	0
35	C	1	Total 117	C 87	O 30	0
35	a	1	Total 59	C 44	O 15	0
35	b	1	Total 62	C 47	O 15	0
35	c	1	Total 117	C 87	O 30	0
35	c	1	Total 117	C 87	O 30	0

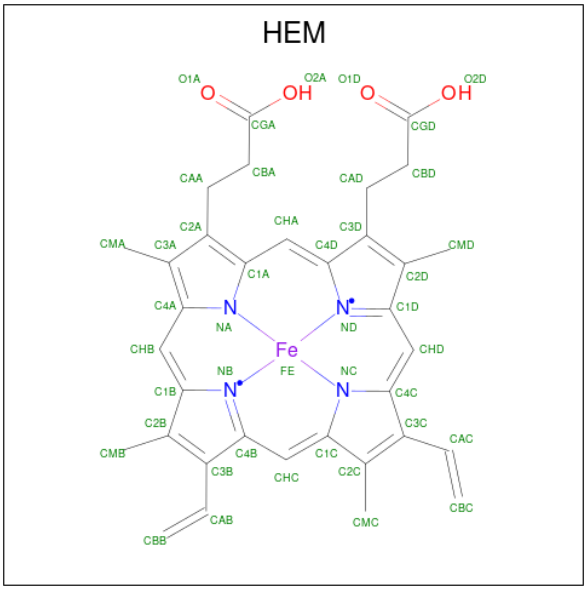
- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total 1	Ca 1	0
36	B	1	Total 1	Ca 1	0
36	a	1	Total 1	Ca 1	0
36	b	1	Total 1	Ca 1	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

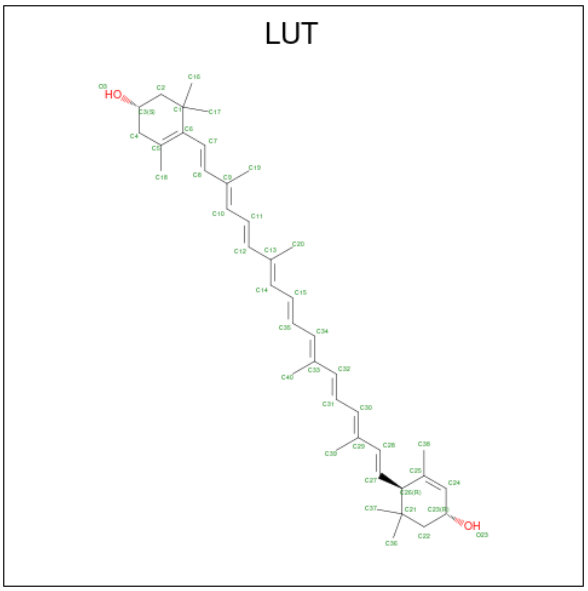
Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
37	D	1	1	1	0
37	d	1	1	1	0

- Molecule 38 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	
38	F	1	43	34	1	4	4	0
38	f	1	43	34	1	4	4	0

- Molecule 39 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	S	1	84	80	4	0
			Total	C	O	
39	S	1	84	80	4	0
			Total	C	O	
39	G	1	84	80	4	0
			Total	C	O	
39	G	1	84	80	4	0
			Total	C	O	
39	N	1	84	80	4	0
			Total	C	O	
39	N	1	84	80	4	0
			Total	C	O	
39	Y	1	84	80	4	0
			Total	C	O	
39	Y	1	84	80	4	0
			Total	C	O	
39	R	1	42	40	2	0
			Total	C	O	
39	s	1	84	80	4	0
			Total	C	O	
39	s	1	84	80	4	0
			Total	C	O	
39	g	1	84	80	4	0
			Total	C	O	
39	g	1	84	80	4	0
			Total	C	O	
39	n	1	84	80	4	0

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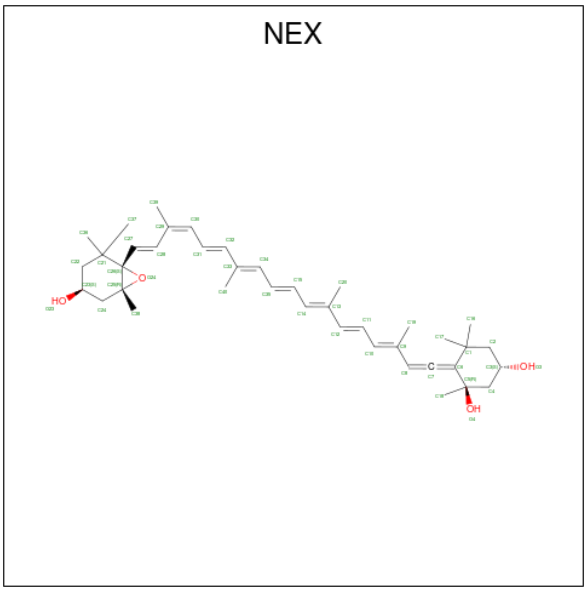
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	n	1	84	80	4	0
39	y	1	84	80	4	0
39	y	1	84	80	4	0
39	r	1	42	40	2	0

- Molecule 40 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	S	1	44	40	4	0
40	G	1	44	40	4	0
40	N	1	44	40	4	0
40	Y	1	44	40	4	0
40	R	1	44	40	4	0
40	s	1	44	40	4	0

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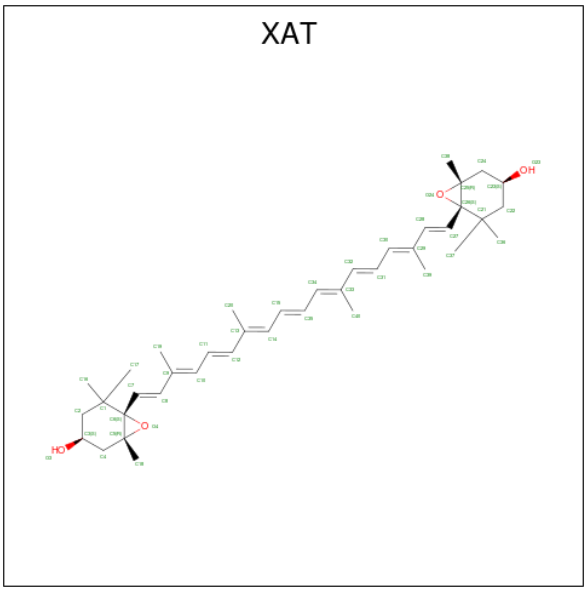
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	g	1	44	40	4	0
40	n	1	44	40	4	0
40	y	1	44	40	4	0
40	r	1	44	40	4	0

- Molecule 41 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
41	R	1	44	40	4	0
41	r	1	44	40	4	0

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
42	A	23	23	23	0
42	B	10	10	10	0
42	C	14	14	14	0

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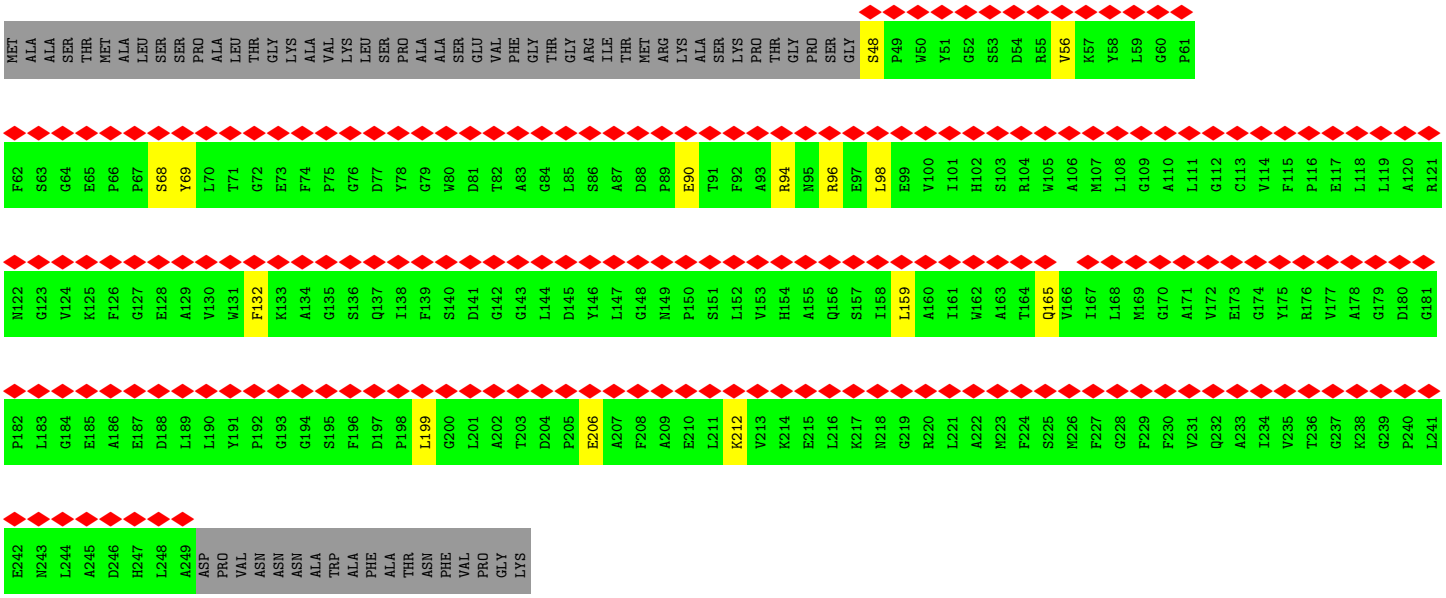
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
42	D	14	14	14	0
			Total	O	
42	H	1	1	1	0
			Total	O	
42	I	1	1	1	0
			Total	O	
42	L	3	3	3	0
			Total	O	
42	M	1	1	1	0
			Total	O	
42	T	1	1	1	0
			Total	O	
42	W	1	1	1	0
			Total	O	
42	a	23	23	23	0
			Total	O	
42	b	10	10	10	0
			Total	O	
42	c	14	14	14	0
			Total	O	
42	d	14	14	14	0
			Total	O	
42	h	1	1	1	0
			Total	O	
42	i	1	1	1	0
			Total	O	
42	l	3	3	3	0
			Total	O	
42	m	2	2	2	0
			Total	O	
42	t	1	1	1	0
			Total	O	
42	w	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.

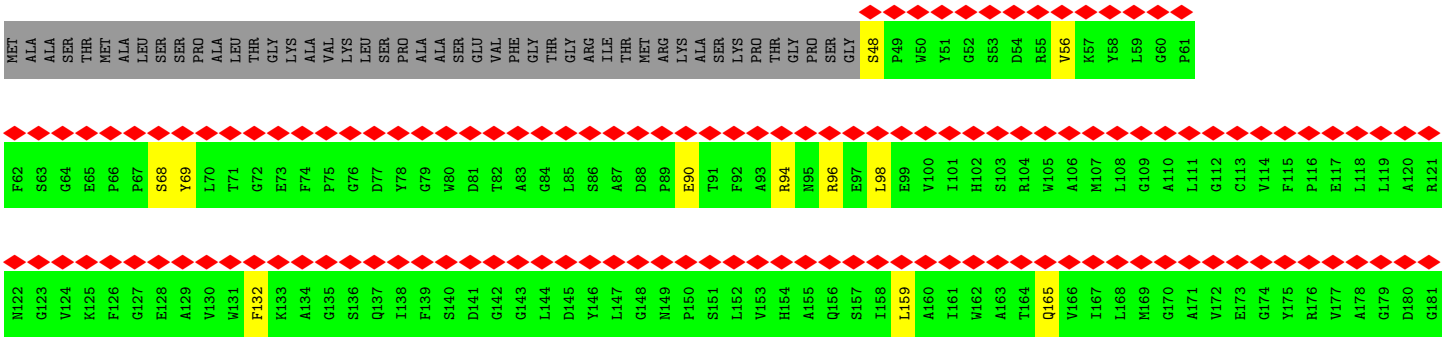
- Molecule 1: Lhcb1.4

Chain 1:



- Molecule 1: Lhcb1.4

Chain 3:



P182 L183 G184 E185 A186 E187 D188 L189 L190 Y191 P192 G193 G194 S195 F196 D197 P198 L199 G200 L201 A202 T203 D204 P205 E206 A207 F208 A209 E210 L211 K212 V213 K214 E215 L216 K217 N218 G219 R220 L221 A222 M223 F224 S225 M226 F227 G228 F229 F230 V231 Q232 A233 I234 V235 T236 G237 K238 G239 P240 L241

E242 N243 L244 A245 D246 H247 L248 A249 ASP PRO VAL ASN ASN ASN ALA TRP ALA PHE ALA THR ASN PHE VAL PRO GLY LYS

- Molecule 1: Lhcb1.4

Chain 5: 76% 71% 5% 24%

MET ALA ALA SER THR MET ALA LEU SER SER PRO ALA LEU THR GLY LYS ALA VAL LYS LEU SER PRO ALA ALA SER GLU VAL PHE GLY THR GLY ARG ILE THR MET ARG LYS ALA SER LYS PRO THR GLY PRO SER GLY S48 P49 W50 Y51 G52 S53 D54 R55 V56 K57 Y58 L59 G60 P61

F62 S63 G64 E65 P66 P67 S68 Y69 L70 T71 G72 E73 F74 P75 G76 D77 Y78 G79 W80 D81 T82 A83 G84 L85 S86 A87 D88 P89 E90 T91 F92 A93 R94 N95 R96 E97 L98 E99 V100 I101 H102 S103 R104 W105 A106 M107 L108 G109 A110 L111 G112 C113 V114 F115 P116 E117 L118 L119 A120 R121

N122 G123 V124 K125 F126 G127 E128 A129 V130 W131 F132 K133 A134 G135 S136 Q137 I138 F139 S140 D141 G142 G143 L144 D145 Y146 L147 G148 N149 P150 S151 L152 V153 H154 A155 Q156 S157 I158 L159 A160 I161 W162 A163 T164 Q165 V166 I167 L168 M169 G170 A171 V172 E173 G174 Y175 R176 V177 A178 G179 D180 G181

P182 L183 G184 E185 A186 E187 D188 L189 L190 Y191 P192 G193 G194 S195 F196 D197 P198 L199 G200 L201 A202 T203 D204 P205 E206 A207 F208 A209 E210 L211 K212 V213 K214 E215 L216 K217 N218 G219 R220 L221 A222 M223 F224 S225 M226 F227 G228 F229 F230 V231 Q232 A233 I234 V235 T236 G237 K238 G239 P240 L241

E242 N243 L244 A245 D246 H247 L248 A249 ASP PRO VAL ASN ASN ASN ALA TRP ALA PHE ALA THR ASN PHE VAL PRO GLY LYS

- Molecule 1: Lhcb1.4

Chain 7: 76% 71% 5% 24%

MET ALA ALA SER THR MET ALA LEU SER SER PRO ALA LEU THR GLY LYS ALA VAL LYS LEU SER PRO ALA ALA SER GLU VAL PHE GLY THR GLY ARG ILE THR MET ARG LYS ALA SER LYS PRO THR GLY PRO SER GLY S48 P49 W50 Y51 G52 S53 D54 R55 V56 K57 Y58 L59 G60 P61

F62 S63 G64 E65 P66 P67 S68 Y69 L70 T71 G72 E73 F74 P75 G76 D77 Y78 G79 W80 D81 T82 A83 G84 L85 S86 A87 D88 P89 E90 T91 F92 A93 R94 N95 R96 E97 L98 E99 V100 I101 H102 S103 R104 W105 A106 M107 L108 G109 A110 L111 G112 C113 V114 F115 P116 E117 L118 L119 A120 R121

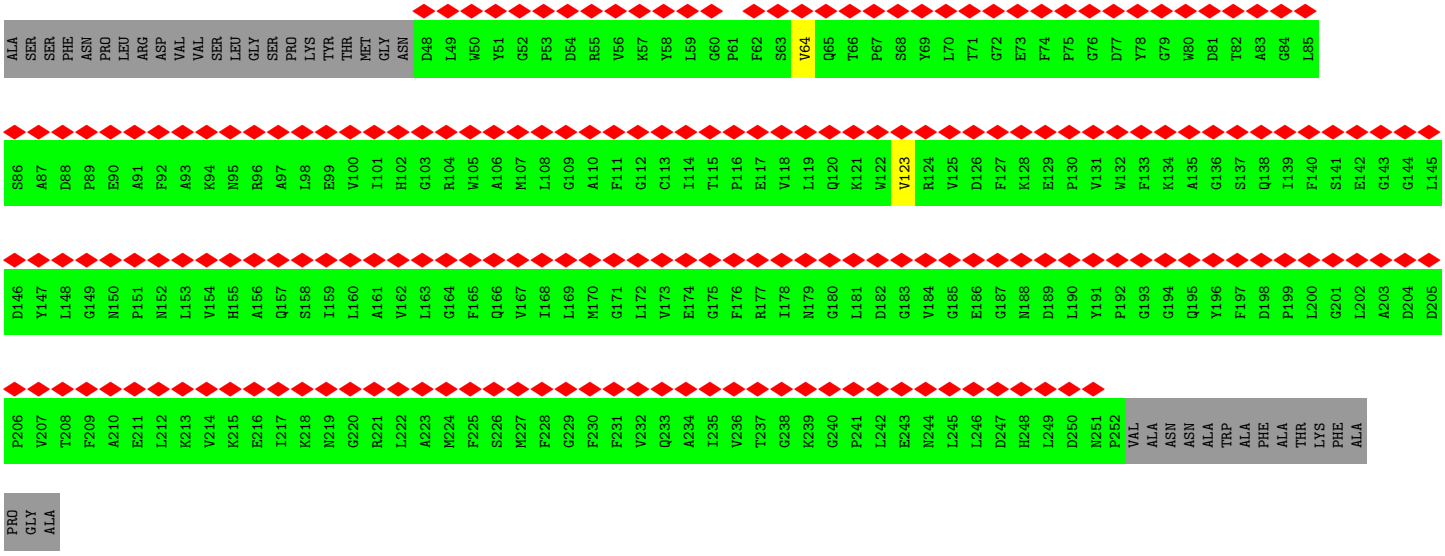
N122 G123 V124 K125 F126 G127 E128 A129 V130 W131 F132 K133 A134 G135 S136 Q137 I138 F139 S140 D141 G142 G143 L144 D145 Y146 L147 G148 N149 P150 S151 L152 V153 H154 A155 Q156 S157 I158 L159 A160 I161 W162 A163 T164 Q165 V166 I167 L168 M169 G170 A171 V172 E173 G174 Y175 R176 V177 A178 G179 D180 G181

P182 L183 G184 E185 A186 E187 D188 L189 L190 Y191 P192 G193 G194 S195 F196 D197 P198 L199 G200 L201 A202 T203 D204 P205 E206 A207 F208 A209 E210 L211 K212 V213 K214 E215 L216 K217 N218 G219 R220 L221 A222 M223 F224 S225 M226 F227 G228 F229 F230 V231 Q232 A233 I234 V235 T236 G237 K238 G239 P240 L241

E242 N243 L244 A245 D246 H247 L248 A249 ASP PRO VAL ASN ASN ASN ALA TRP ALA PHE ALA THR ASN PHE VAL PRO GLY LYS

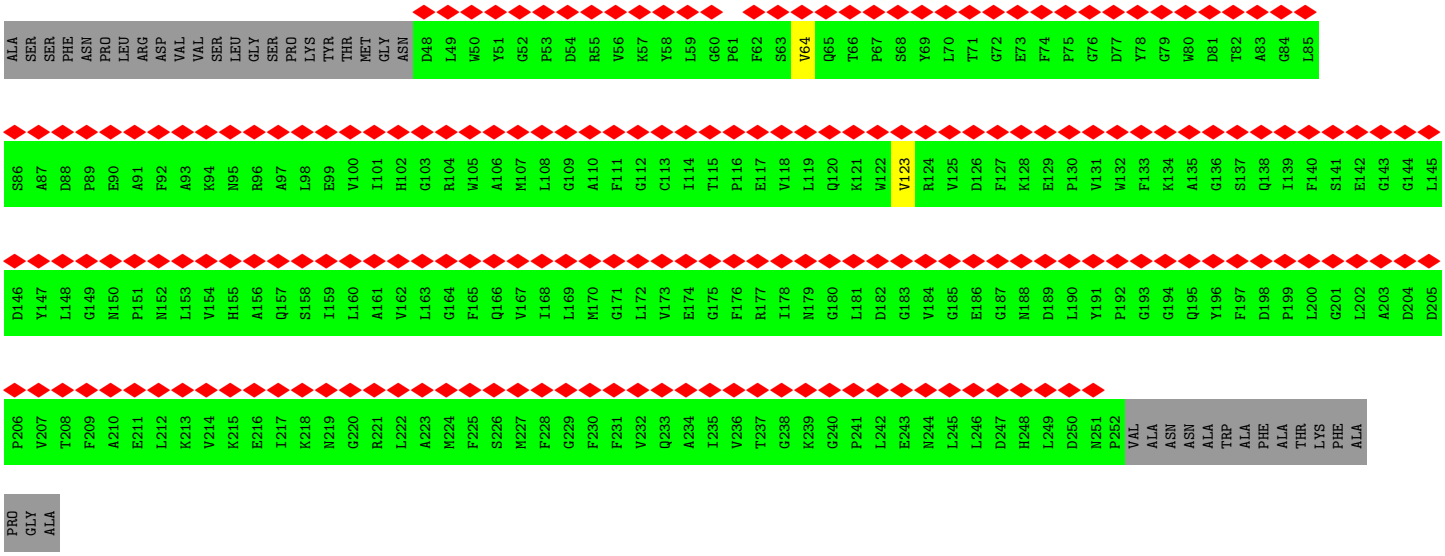
- Molecule 2: Lhcb3.1

Chain 2:



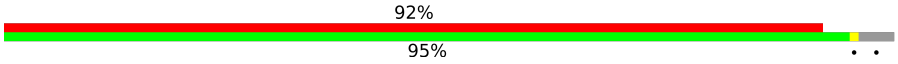
- Molecule 2: Lhcb3.1

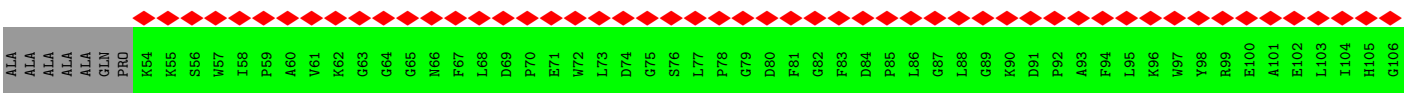
Chain 6:

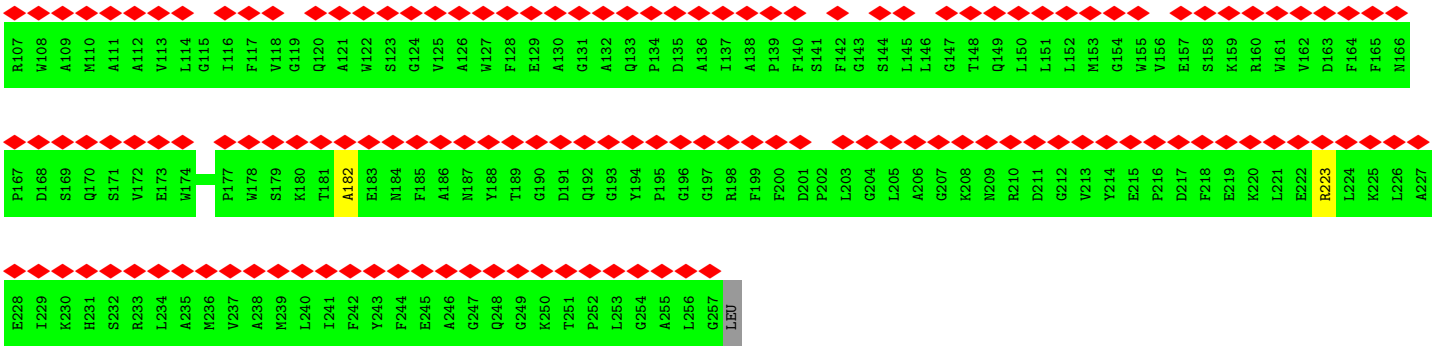


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 4:

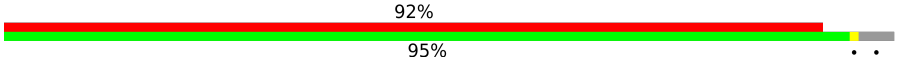


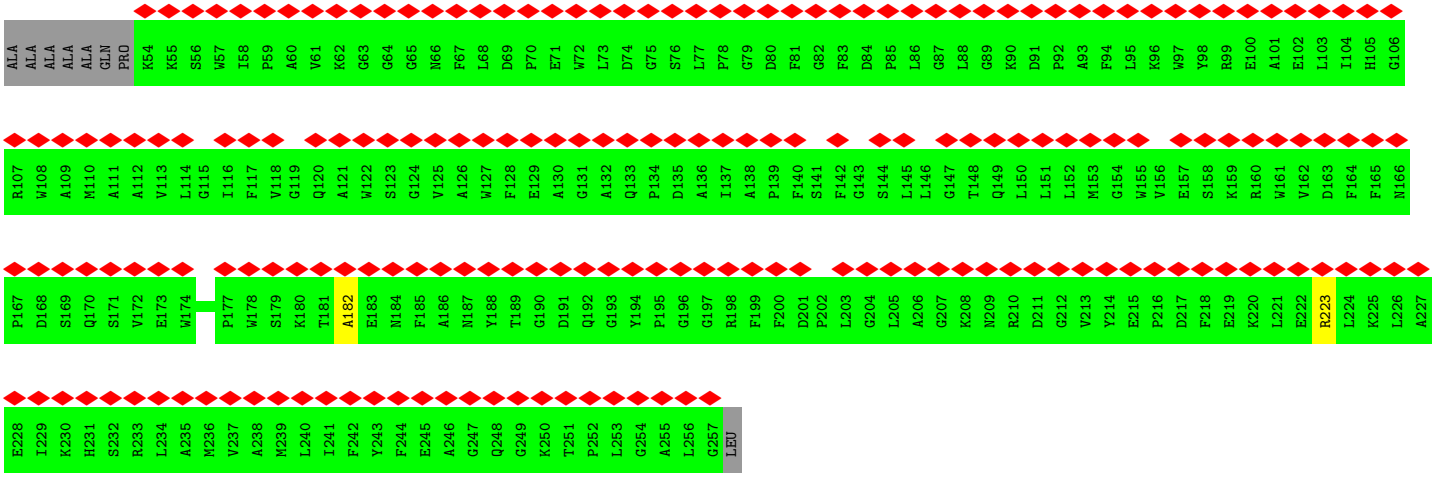




• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

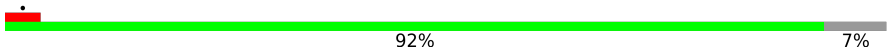
Chain 8:

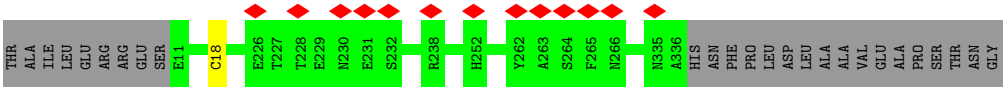




• Molecule 4: Photosystem II protein D1

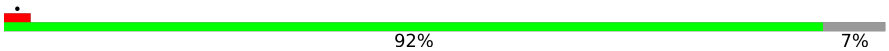
Chain A:

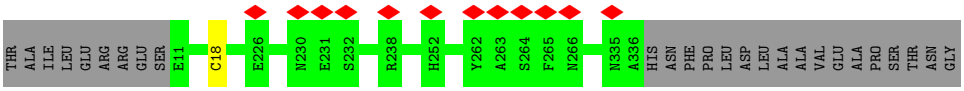




• Molecule 4: Photosystem II protein D1

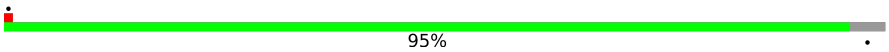
Chain a:

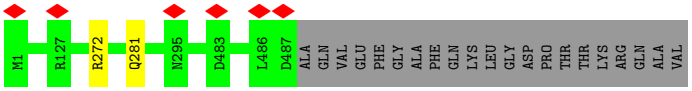




• Molecule 5: Photosystem II CP47 reaction center protein

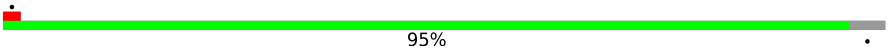
Chain B:

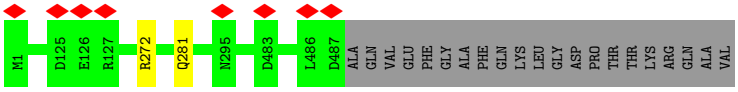




• Molecule 5: Photosystem II CP47 reaction center protein

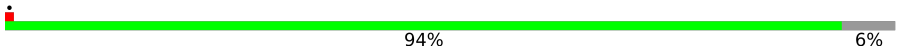
Chain b:

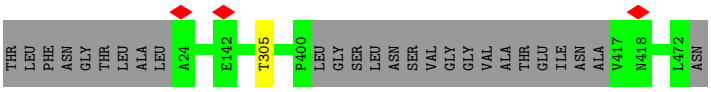




• Molecule 6: Photosystem II CP43 reaction center protein

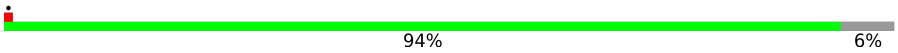
Chain C:

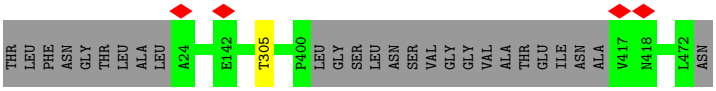




• Molecule 6: Photosystem II CP43 reaction center protein

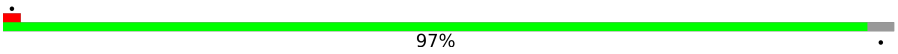
Chain c:

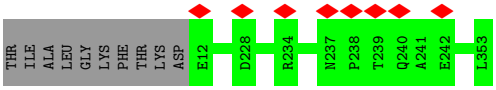




• Molecule 7: Photosystem II D2 protein

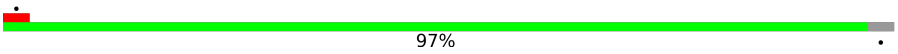
Chain D:

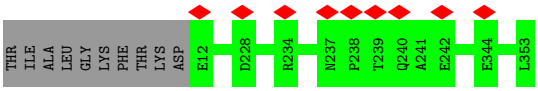




• Molecule 7: Photosystem II D2 protein

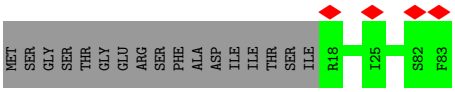
Chain d:





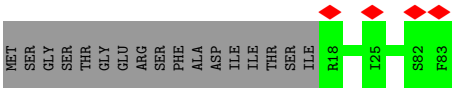
• Molecule 8: Cytochrome b559 subunit alpha

Chain E:



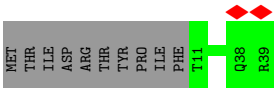
• Molecule 8: Cytochrome b559 subunit alpha

Chain e:



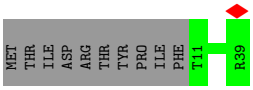
• Molecule 9: Cytochrome b559 subunit beta (PsbF)

Chain F:



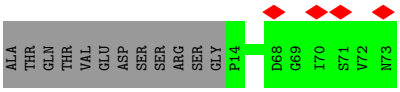
• Molecule 9: Cytochrome b559 subunit beta (PsbF)

Chain f:



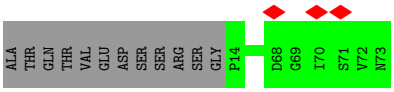
• Molecule 10: Photosystem II reaction center protein H

Chain H:



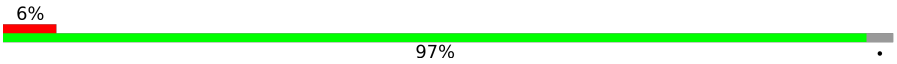
• Molecule 10: Photosystem II reaction center protein H

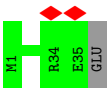
Chain h:



• Molecule 11: Photosystem II reaction center protein I

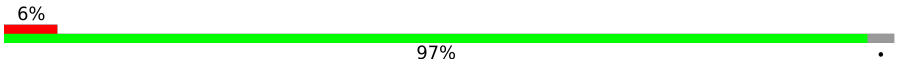
Chain I:

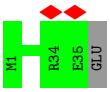




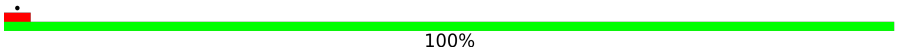
• Molecule 11: Photosystem II reaction center protein I

Chain i:

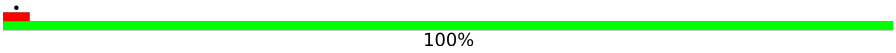




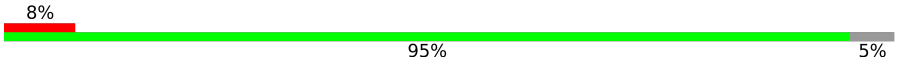
• Molecule 12: Photosystem II reaction center protein K

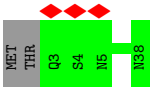
Chain K: 

• Molecule 12: Photosystem II reaction center protein K

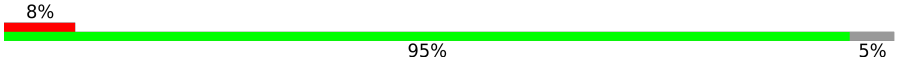
Chain k: 

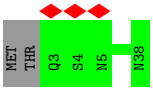
• Molecule 13: Photosystem II reaction center protein L

Chain L: 



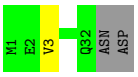
• Molecule 13: Photosystem II reaction center protein L

Chain l: 

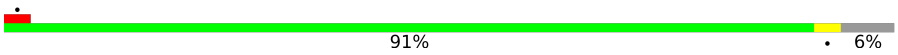


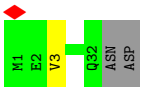
• Molecule 14: Photosystem II reaction center protein M

Chain M:



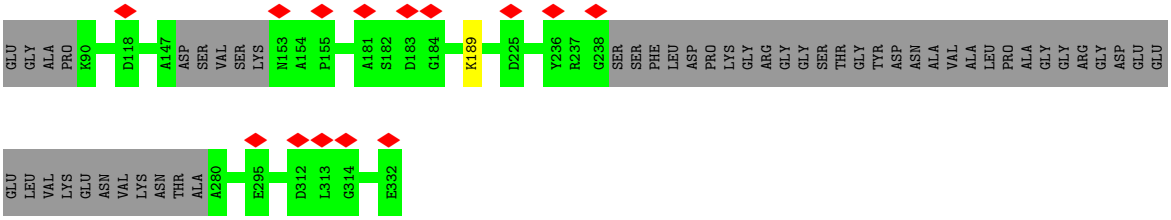
• Molecule 14: Photosystem II reaction center protein M

Chain m: 



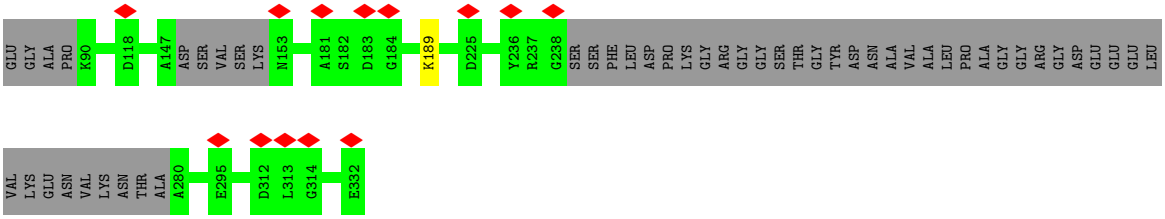
• Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain O:



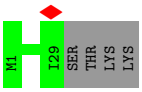
• Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain o:



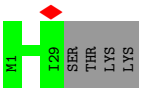
• Molecule 16: Photosystem II reaction center protein T

Chain T:



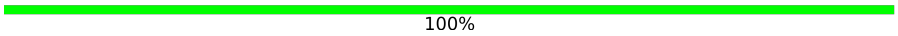
• Molecule 16: Photosystem II reaction center protein T

Chain t:



• Molecule 17: Photosystem II reaction center W protein, chloroplastic

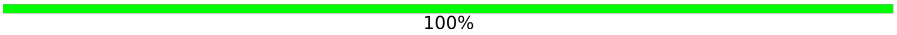
Chain W:



There are no outlier residues recorded for this chain.

• Molecule 17: Photosystem II reaction center W protein, chloroplastic

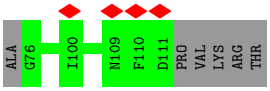
Chain w:



There are no outlier residues recorded for this chain.

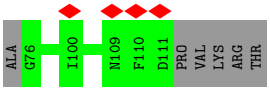
• Molecule 18: PsbX

Chain X:



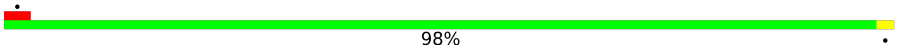
• Molecule 18: PsbX

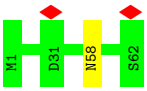
Chain x:



• Molecule 19: Photosystem II reaction center protein Z

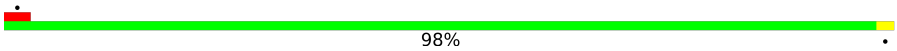
Chain Z:

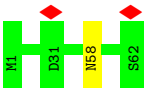




• Molecule 19: Photosystem II reaction center protein Z

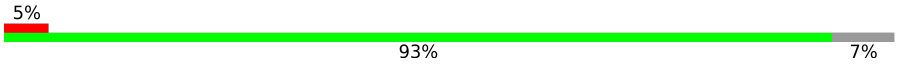
Chain z:

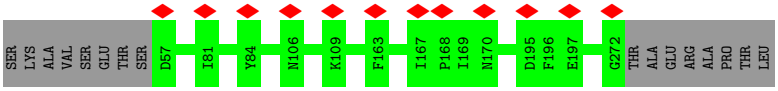




• Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic

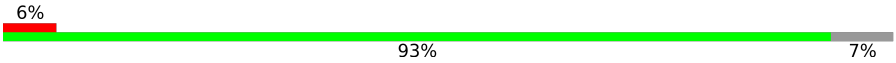
Chain S:

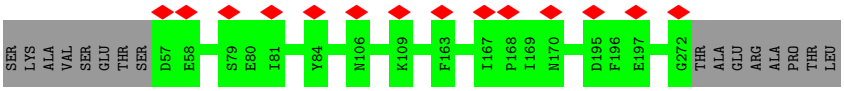




• Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic

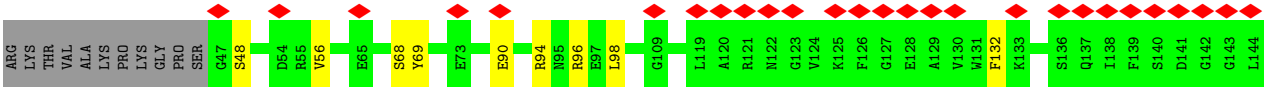
Chain s:

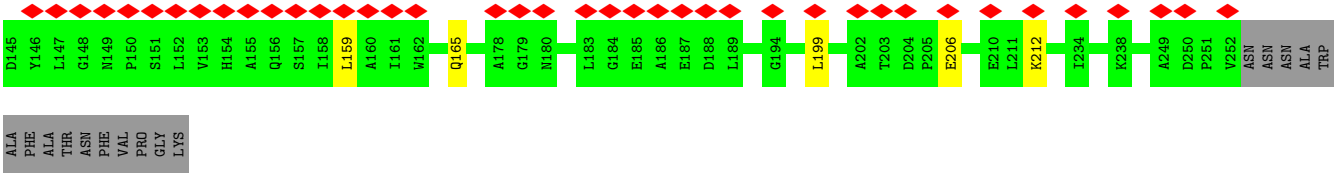




• Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

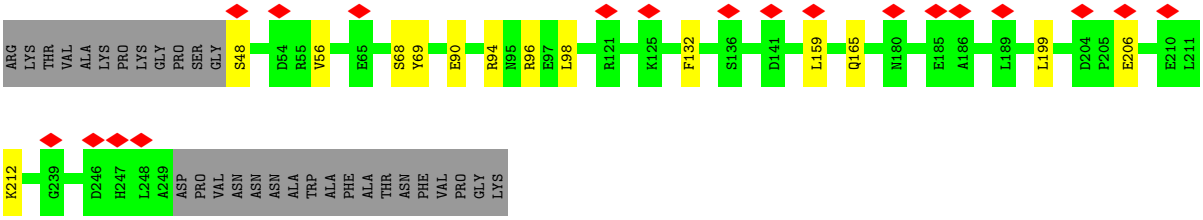
Chain G:





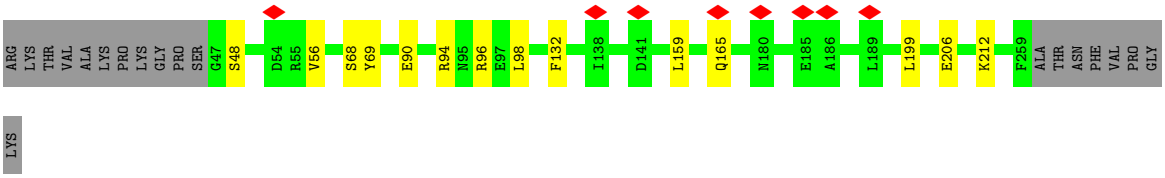
• Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

Chain N:



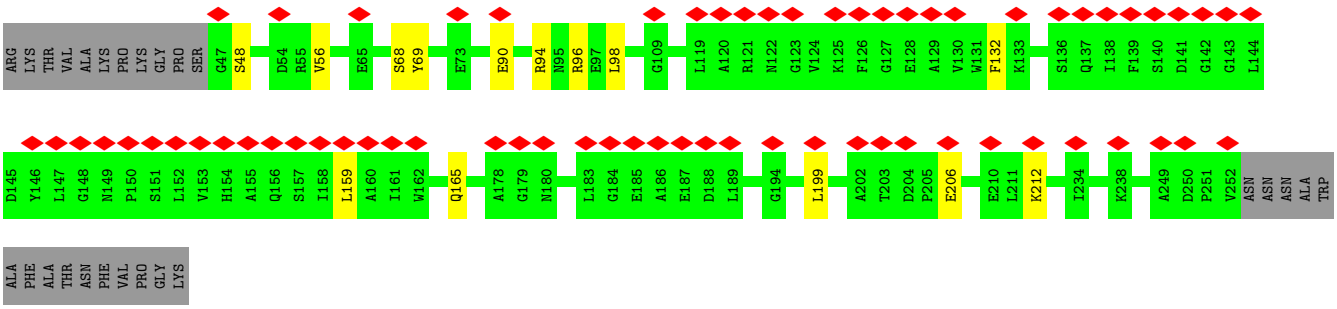
• Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

Chain Y:



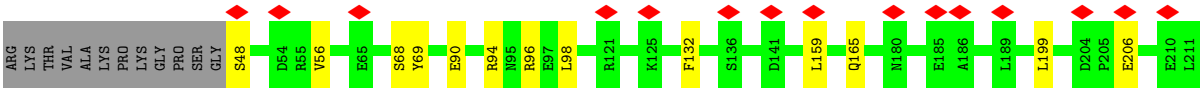
• Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

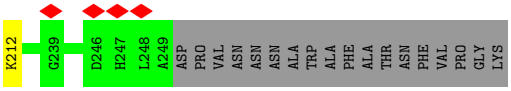
Chain g:



• Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

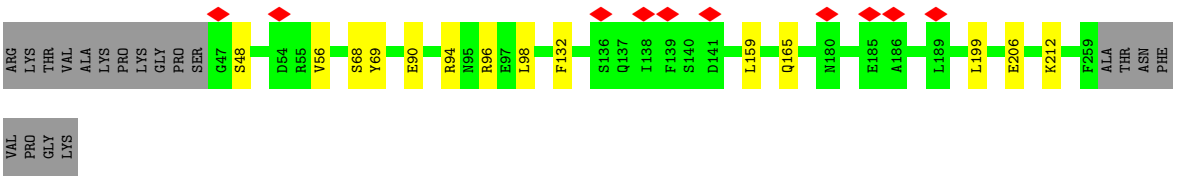
Chain n:





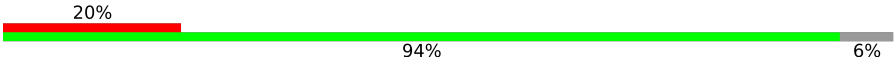
• Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

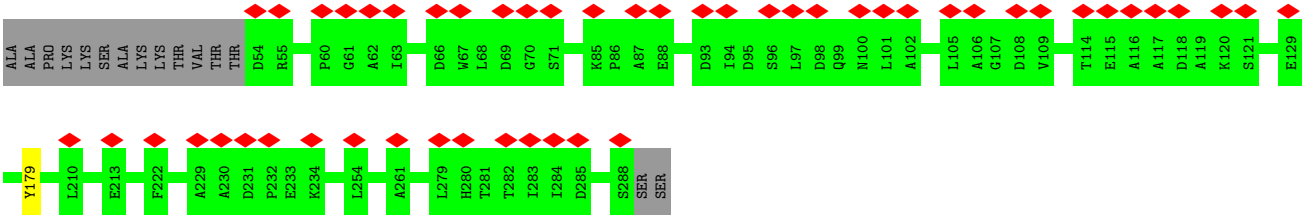
Chain y:



• Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic

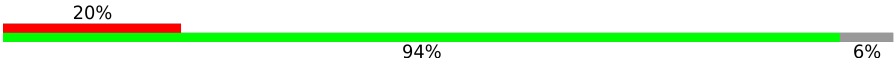
Chain R:

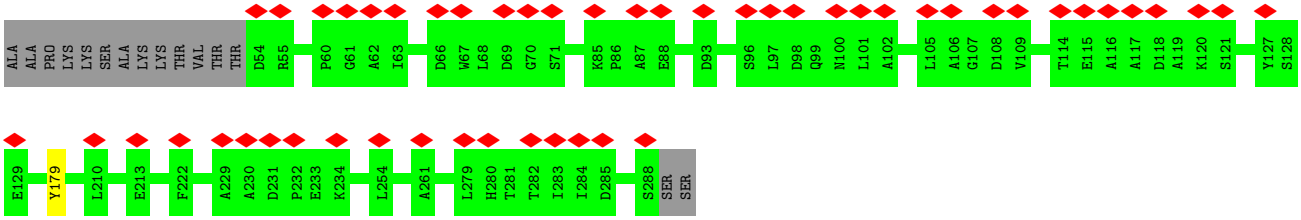




• Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic

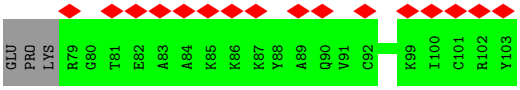
Chain r:





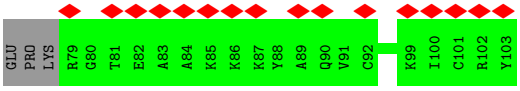
• Molecule 23: PsbTn

Chain U:



• Molecule 23: PsbTn

Chain u:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.49	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	33.682	Depositor
Minimum map value	-19.496	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.976	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	410.0, 410.0, 410.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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, PL9, AJP, CA, SQD, LHG, CHL, LUT, CLA, BCT, PHO, CL, DGD, LMG, FE2, XAT, NEX, HEM

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	1	0.31	0/1582	0.51	0/2150
1	3	0.31	0/1582	0.51	0/2150
1	5	0.31	0/1582	0.52	0/2150
1	7	0.31	0/1582	0.51	0/2150
2	2	0.27	0/1640	0.47	0/2229
2	6	0.27	0/1640	0.47	0/2229
3	4	0.28	0/1652	0.48	0/2242
3	8	0.28	0/1652	0.49	0/2242
4	A	0.25	0/2626	0.45	0/3580
4	a	0.26	0/2626	0.45	0/3580
5	B	0.25	0/3940	0.46	0/5368
5	b	0.25	0/3940	0.46	0/5368
6	C	0.25	0/3487	0.44	0/4750
6	c	0.25	0/3487	0.44	0/4750
7	D	0.26	0/2815	0.45	0/3837
7	d	0.26	0/2815	0.45	0/3837
8	E	0.25	0/561	0.47	0/763
8	e	0.25	0/561	0.47	0/763
9	F	0.24	0/229	0.45	0/311
9	f	0.24	0/229	0.45	0/311
10	H	0.24	0/455	0.45	0/619
10	h	0.24	0/455	0.45	0/619
11	I	0.26	0/294	0.48	0/397
11	i	0.26	0/294	0.49	0/397
12	K	0.26	0/312	0.39	0/428
12	k	0.26	0/312	0.39	0/428
13	L	0.24	0/310	0.37	0/421
13	l	0.24	0/310	0.37	0/421
14	M	0.25	0/254	0.38	0/347
14	m	0.25	0/254	0.38	0/347
15	O	0.26	0/1548	0.48	0/2091

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	o	0.26	0/1548	0.48	0/2091
16	T	0.27	0/246	0.39	0/333
16	t	0.27	0/246	0.39	0/333
17	W	0.25	0/438	0.41	0/594
17	w	0.25	0/438	0.41	0/594
18	X	0.25	0/250	0.43	0/339
18	x	0.25	0/250	0.43	0/339
19	Z	0.25	0/474	0.36	0/649
19	z	0.25	0/474	0.36	0/649
20	S	0.26	0/1715	0.43	0/2328
20	s	0.26	0/1715	0.43	0/2328
21	G	0.30	0/1607	0.51	0/2184
21	N	0.30	0/1580	0.52	0/2146
21	Y	0.30	0/1669	0.51	0/2270
21	g	0.30	0/1607	0.51	0/2184
21	n	0.30	0/1580	0.51	0/2146
21	y	0.30	0/1669	0.51	0/2270
22	R	0.27	0/1878	0.46	0/2561
22	r	0.27	0/1878	0.46	0/2561
23	U	0.23	0/196	0.49	0/261
23	u	0.23	0/196	0.49	0/261
All	All	0.27	0/66680	0.47	0/90696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
1	3	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
1	5	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
1	7	200/266 (75%)	188 (94%)	12 (6%)	0	100	100
2	2	203/243 (84%)	181 (89%)	20 (10%)	2 (1%)	15	44
2	6	203/243 (84%)	181 (89%)	20 (10%)	2 (1%)	15	44
3	4	202/212 (95%)	183 (91%)	18 (9%)	1 (0%)	29	61
3	8	202/212 (95%)	183 (91%)	18 (9%)	1 (0%)	29	61
4	A	324/352 (92%)	309 (95%)	14 (4%)	1 (0%)	41	72
4	a	324/352 (92%)	308 (95%)	15 (5%)	1 (0%)	41	72
5	B	485/508 (96%)	466 (96%)	18 (4%)	1 (0%)	47	78
5	b	485/508 (96%)	466 (96%)	18 (4%)	1 (0%)	47	78
6	C	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	47	78
6	c	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	47	78
7	D	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
7	d	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
8	E	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
8	e	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
9	F	27/39 (69%)	27 (100%)	0	0	100	100
9	f	27/39 (69%)	27 (100%)	0	0	100	100
10	H	58/72 (81%)	52 (90%)	6 (10%)	0	100	100
10	h	58/72 (81%)	52 (90%)	6 (10%)	0	100	100
11	I	33/36 (92%)	28 (85%)	5 (15%)	0	100	100
11	i	33/36 (92%)	28 (85%)	5 (15%)	0	100	100
12	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
13	L	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
13	l	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
14	M	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	4	13
14	m	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	4	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	191/247 (77%)	183 (96%)	8 (4%)	0	100	100
15	o	191/247 (77%)	183 (96%)	8 (4%)	0	100	100
16	T	27/33 (82%)	25 (93%)	2 (7%)	0	100	100
16	t	27/33 (82%)	25 (93%)	2 (7%)	0	100	100
17	W	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
17	w	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
18	X	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
18	x	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
20	S	214/232 (92%)	204 (95%)	10 (5%)	0	100	100
20	s	214/232 (92%)	203 (95%)	11 (5%)	0	100	100
21	G	204/232 (88%)	192 (94%)	12 (6%)	0	100	100
21	N	200/232 (86%)	189 (94%)	11 (6%)	0	100	100
21	Y	211/232 (91%)	200 (95%)	11 (5%)	0	100	100
21	g	204/232 (88%)	192 (94%)	12 (6%)	0	100	100
21	n	200/232 (86%)	189 (94%)	11 (6%)	0	100	100
21	y	211/232 (91%)	200 (95%)	11 (5%)	0	100	100
22	R	233/250 (93%)	223 (96%)	10 (4%)	0	100	100
22	r	233/250 (93%)	223 (96%)	10 (4%)	0	100	100
23	U	23/28 (82%)	19 (83%)	4 (17%)	0	100	100
23	u	23/28 (82%)	19 (83%)	4 (17%)	0	100	100
All	All	8226/9282 (89%)	7790 (95%)	422 (5%)	14 (0%)	50	78

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	123	VAL
3	4	182	ALA
4	A	18	CYS
14	M	3	VAL
2	6	123	VAL
3	8	182	ALA
4	a	18	CYS

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Mol	Chain	Res	Type
14	m	3	VAL
2	2	64	VAL
5	B	281	GLN
2	6	64	VAL
5	b	281	GLN
6	C	305	THR
6	c	305	THR

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	1	154/201 (77%)	140 (91%)	14 (9%)	9	27
1	3	154/201 (77%)	140 (91%)	14 (9%)	9	27
1	5	154/201 (77%)	140 (91%)	14 (9%)	9	27
1	7	154/201 (77%)	140 (91%)	14 (9%)	9	27
2	2	164/192 (85%)	164 (100%)	0	100	100
2	6	164/192 (85%)	164 (100%)	0	100	100
3	4	156/159 (98%)	155 (99%)	1 (1%)	86	96
3	8	156/159 (98%)	155 (99%)	1 (1%)	86	96
4	A	263/284 (93%)	263 (100%)	0	100	100
4	a	263/284 (93%)	263 (100%)	0	100	100
5	B	384/402 (96%)	383 (100%)	1 (0%)	92	98
5	b	384/402 (96%)	383 (100%)	1 (0%)	92	98
6	C	340/359 (95%)	340 (100%)	0	100	100
6	c	340/359 (95%)	340 (100%)	0	100	100
7	D	274/282 (97%)	274 (100%)	0	100	100
7	d	274/282 (97%)	274 (100%)	0	100	100
8	E	59/73 (81%)	59 (100%)	0	100	100
8	e	59/73 (81%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	F	24/34 (71%)	24 (100%)	0	100	100
9	f	24/34 (71%)	24 (100%)	0	100	100
10	H	50/60 (83%)	50 (100%)	0	100	100
10	h	50/60 (83%)	50 (100%)	0	100	100
11	I	32/33 (97%)	32 (100%)	0	100	100
11	i	32/33 (97%)	32 (100%)	0	100	100
12	K	32/32 (100%)	32 (100%)	0	100	100
12	k	32/32 (100%)	32 (100%)	0	100	100
13	L	34/36 (94%)	34 (100%)	0	100	100
13	l	34/36 (94%)	34 (100%)	0	100	100
14	M	28/30 (93%)	28 (100%)	0	100	100
14	m	28/30 (93%)	28 (100%)	0	100	100
15	O	167/204 (82%)	166 (99%)	1 (1%)	86	96
15	o	167/204 (82%)	166 (99%)	1 (1%)	86	96
16	T	26/30 (87%)	26 (100%)	0	100	100
16	t	26/30 (87%)	26 (100%)	0	100	100
17	W	47/47 (100%)	47 (100%)	0	100	100
17	w	47/47 (100%)	47 (100%)	0	100	100
18	X	29/34 (85%)	29 (100%)	0	100	100
18	x	29/34 (85%)	29 (100%)	0	100	100
19	Z	54/54 (100%)	53 (98%)	1 (2%)	57	85
19	z	54/54 (100%)	53 (98%)	1 (2%)	57	85
20	S	167/180 (93%)	167 (100%)	0	100	100
20	s	167/180 (93%)	167 (100%)	0	100	100
21	G	157/177 (89%)	143 (91%)	14 (9%)	9	28
21	N	154/177 (87%)	140 (91%)	14 (9%)	9	27
21	Y	162/177 (92%)	148 (91%)	14 (9%)	10	30
21	g	157/177 (89%)	143 (91%)	14 (9%)	9	28
21	n	154/177 (87%)	140 (91%)	14 (9%)	9	27
21	y	162/177 (92%)	148 (91%)	14 (9%)	10	30
22	R	189/201 (94%)	188 (100%)	1 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	r	189/201 (94%)	188 (100%)	1 (0%)	88 96
23	U	20/23 (87%)	20 (100%)	0	100 100
23	u	20/23 (87%)	20 (100%)	0	100 100
All	All	6640/7364 (90%)	6490 (98%)	150 (2%)	53 82

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	48	SER
1	1	56	VAL
1	1	68	SER
1	1	69	TYR
1	1	90	GLU
1	1	94	ARG
1	1	96	ARG
1	1	98	LEU
1	1	132	PHE
1	1	159	LEU
1	1	165	GLN
1	1	199	LEU
1	1	206	GLU
1	1	212	LYS
1	3	48	SER
1	3	56	VAL
1	3	68	SER
1	3	69	TYR
1	3	90	GLU
1	3	94	ARG
1	3	96	ARG
1	3	98	LEU
1	3	132	PHE
1	3	159	LEU
1	3	165	GLN
1	3	199	LEU
1	3	206	GLU
1	3	212	LYS
3	4	223	ARG
5	B	272	ARG
15	O	189	LYS
19	Z	58	ASN
21	G	48	SER

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Mol	Chain	Res	Type
21	G	56	VAL
21	G	68	SER
21	G	69	TYR
21	G	90	GLU
21	G	94	ARG
21	G	96	ARG
21	G	98	LEU
21	G	132	PHE
21	G	159	LEU
21	G	165	GLN
21	G	199	LEU
21	G	206	GLU
21	G	212	LYS
21	N	48	SER
21	N	56	VAL
21	N	68	SER
21	N	69	TYR
21	N	90	GLU
21	N	94	ARG
21	N	96	ARG
21	N	98	LEU
21	N	132	PHE
21	N	159	LEU
21	N	165	GLN
21	N	199	LEU
21	N	206	GLU
21	N	212	LYS
21	Y	48	SER
21	Y	56	VAL
21	Y	68	SER
21	Y	69	TYR
21	Y	90	GLU
21	Y	94	ARG
21	Y	96	ARG
21	Y	98	LEU
21	Y	132	PHE
21	Y	159	LEU
21	Y	165	GLN
21	Y	199	LEU
21	Y	206	GLU
21	Y	212	LYS
22	R	179	TYR

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Mol	Chain	Res	Type
1	5	48	SER
1	5	56	VAL
1	5	68	SER
1	5	69	TYR
1	5	90	GLU
1	5	94	ARG
1	5	96	ARG
1	5	98	LEU
1	5	132	PHE
1	5	159	LEU
1	5	165	GLN
1	5	199	LEU
1	5	206	GLU
1	5	212	LYS
1	7	48	SER
1	7	56	VAL
1	7	68	SER
1	7	69	TYR
1	7	90	GLU
1	7	94	ARG
1	7	96	ARG
1	7	98	LEU
1	7	132	PHE
1	7	159	LEU
1	7	165	GLN
1	7	199	LEU
1	7	206	GLU
1	7	212	LYS
3	8	223	ARG
5	b	272	ARG
15	o	189	LYS
19	z	58	ASN
21	g	48	SER
21	g	56	VAL
21	g	68	SER
21	g	69	TYR
21	g	90	GLU
21	g	94	ARG
21	g	96	ARG
21	g	98	LEU
21	g	132	PHE
21	g	159	LEU

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Mol	Chain	Res	Type
21	g	165	GLN
21	g	199	LEU
21	g	206	GLU
21	g	212	LYS
21	n	48	SER
21	n	56	VAL
21	n	68	SER
21	n	69	TYR
21	n	90	GLU
21	n	94	ARG
21	n	96	ARG
21	n	98	LEU
21	n	132	PHE
21	n	159	LEU
21	n	165	GLN
21	n	199	LEU
21	n	206	GLU
21	n	212	LYS
21	y	48	SER
21	y	56	VAL
21	y	68	SER
21	y	69	TYR
21	y	90	GLU
21	y	94	ARG
21	y	96	ARG
21	y	98	LEU
21	y	132	PHE
21	y	159	LEU
21	y	165	GLN
21	y	199	LEU
21	y	206	GLU
21	y	212	LYS
22	r	179	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	73	ASN
5	B	157	HIS
5	B	296	GLN
5	B	332	ASN
6	C	237	HIS

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Mol	Chain	Res	Type
6	C	293	ASN
6	C	311	GLN
6	C	322	GLN
6	C	327	ASN
7	D	264	ASN
7	D	351	ASN
13	L	5	ASN
13	L	34	ASN
15	O	113	GLN
15	O	202	GLN
20	S	111	GLN
20	S	135	ASN
21	N	165	GLN
22	R	245	HIS
5	b	73	ASN
5	b	157	HIS
5	b	296	GLN
5	b	332	ASN
6	c	237	HIS
6	c	293	ASN
6	c	311	GLN
6	c	322	GLN
6	c	327	ASN
7	d	264	ASN
7	d	351	ASN
13	l	5	ASN
13	l	34	ASN
15	o	113	GLN
15	o	202	GLN
20	s	111	GLN
20	s	135	ASN
21	n	165	GLN
22	r	245	HIS

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 374 ligands modelled in this entry, 22 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage and 8 are monoatomic - leaving 344 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	$\#\|Z\| > 2$
25	CLA	y	305	-	50,58,73	1.89	9 (18%)	58,95,113	1.85	14 (24%)
26	LHG	C	519	6	48,48,48	0.45	0	51,54,54	1.18	4 (7%)
25	CLA	B	614	30	65,73,73	1.62	9 (13%)	76,113,113	1.82	13 (17%)
25	CLA	y	315	-	45,53,73	2.01	10 (22%)	52,89,113	1.82	13 (25%)
24	CHL	G	607	-	46,54,74	1.71	10 (21%)	49,90,114	2.02	12 (24%)
28	BCR	T	101	16	41,41,41	1.15	3 (7%)	56,56,56	1.28	8 (14%)
25	CLA	y	313	-	60,68,73	1.79	10 (16%)	70,107,113	1.75	15 (21%)
25	CLA	c	505	-	65,73,73	1.64	9 (13%)	76,113,113	1.77	15 (19%)
28	BCR	b	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	10 (17%)
24	CHL	S	307	-	46,54,74	1.74	10 (21%)	49,90,114	2.14	10 (20%)
24	CHL	n	605	21	48,56,74	1.66	9 (18%)	51,92,114	2.06	12 (23%)
40	NEX	s	317	-	38,46,46	1.62	8 (21%)	50,70,70	2.23	11 (22%)
25	CLA	6	605	2	48,56,73	1.87	9 (18%)	55,92,113	1.94	11 (20%)
25	CLA	c	507	-	65,73,73	1.65	9 (13%)	76,113,113	1.66	14 (18%)
25	CLA	B	601	-	65,73,73	1.58	9 (13%)	76,113,113	1.92	15 (19%)
25	CLA	b	609	-	65,73,73	1.62	9 (13%)	76,113,113	1.81	17 (22%)
28	BCR	b	617	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	6 (10%)
26	LHG	2	606	25	46,46,48	0.44	0	49,52,54	1.19	4 (8%)
25	CLA	n	611	26	60,68,73	1.72	10 (16%)	70,107,113	1.69	16 (22%)
25	CLA	c	511	6	65,73,73	1.59	9 (13%)	76,113,113	2.20	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	CLA	S	309	20	45,53,73	2.05	9 (20%)	52,89,113	2.10	13 (25%)
25	CLA	b	602	-	65,73,73	1.67	9 (13%)	76,113,113	1.75	16 (21%)
35	DGD	B	626	-	63,63,67	0.49	0	77,77,81	1.29	6 (7%)
39	LUT	s	315	-	42,43,43	0.92	3 (7%)	51,60,60	1.57	8 (15%)
25	CLA	r	610	26	49,57,73	1.85	8 (16%)	55,93,113	3.07	16 (29%)
24	CHL	y	302	21	66,74,74	1.47	11 (16%)	73,114,114	1.79	15 (20%)
27	PHO	A	403	-	51,69,69	0.52	0	47,99,99	1.72	5 (10%)
25	CLA	Y	315	-	45,53,73	2.00	10 (22%)	52,89,113	1.83	13 (25%)
25	CLA	6	604	2,26	55,63,73	1.75	8 (14%)	64,101,113	2.08	19 (29%)
25	CLA	s	313	-	55,63,73	1.72	10 (18%)	64,101,113	2.40	15 (23%)
26	LHG	D	406	-	48,48,48	0.43	0	51,54,54	1.18	4 (7%)
30	LMG	A	408	-	48,48,55	0.44	0	56,56,63	1.20	5 (8%)
25	CLA	G	613	-	65,73,73	1.58	10 (15%)	76,113,113	1.92	15 (19%)
24	CHL	N	608	-	66,74,74	1.48	10 (15%)	73,114,114	1.77	9 (12%)
25	CLA	c	506	-	65,73,73	1.69	9 (13%)	76,113,113	1.70	16 (21%)
25	CLA	Y	305	-	50,58,73	1.89	9 (18%)	58,95,113	1.85	14 (24%)
25	CLA	Y	312	26	60,68,73	1.73	10 (16%)	70,107,113	1.71	16 (22%)
33	BCT	A	413	34	2,3,3	1.20	0	2,3,3	4.33	2 (100%)
24	CHL	g	609	21	61,69,74	1.55	10 (16%)	67,108,114	1.94	12 (17%)
28	BCR	H	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	9 (16%)
25	CLA	S	310	20	55,63,73	1.81	9 (16%)	64,101,113	1.76	12 (18%)
25	CLA	N	604	-	50,58,73	1.81	10 (20%)	58,95,113	2.12	15 (25%)
25	CLA	B	607	-	65,73,73	1.61	9 (13%)	76,113,113	1.77	15 (19%)
25	CLA	C	509	-	65,73,73	1.62	10 (15%)	76,113,113	1.79	13 (17%)
30	LMG	b	620	25	51,51,55	0.44	0	59,59,63	1.20	4 (6%)
25	CLA	c	509	-	65,73,73	1.63	10 (15%)	76,113,113	1.79	12 (15%)
25	CLA	B	613	-	65,73,73	1.64	9 (13%)	76,113,113	1.63	14 (18%)
25	CLA	R	612	-	60,68,73	1.64	10 (16%)	70,107,113	2.06	16 (22%)
25	CLA	b	613	-	65,73,73	1.63	9 (13%)	76,113,113	1.63	14 (18%)
24	CHL	y	310	21	56,64,74	1.62	11 (19%)	61,102,114	1.85	11 (18%)
26	LHG	R	618	25	41,41,48	0.45	0	44,47,54	1.23	4 (9%)
25	CLA	B	616	-	65,73,73	1.64	9 (13%)	76,113,113	1.69	13 (17%)
25	CLA	Y	303	21	65,73,73	1.69	10 (15%)	76,113,113	1.75	15 (19%)
25	CLA	6	602	2	60,68,73	1.71	9 (15%)	70,107,113	2.47	26 (37%)
25	CLA	c	503	-	65,73,73	1.61	9 (13%)	76,113,113	1.85	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
26	LHG	Y	319	25	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
28	BCR	c	514	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	7 (12%)
40	NEX	R	617	-	38,46,46	1.68	7 (18%)	50,70,70	3.06	17 (34%)
25	CLA	Y	304	-	65,73,73	1.63	10 (15%)	76,113,113	1.76	15 (19%)
24	CHL	N	609	21	66,74,74	1.48	9 (13%)	73,114,114	1.69	13 (17%)
26	LHG	B	625	-	45,45,48	0.44	0	48,51,54	1.19	4 (8%)
25	CLA	d	402	-	65,73,73	1.69	10 (15%)	76,113,113	1.82	17 (22%)
28	BCR	A	406	-	41,41,41	1.16	2 (4%)	56,56,56	1.34	10 (17%)
25	CLA	r	603	-	60,68,73	1.65	8 (13%)	70,107,113	2.75	19 (27%)
25	CLA	s	304	-	45,53,73	1.92	9 (20%)	52,89,113	2.10	10 (19%)
26	LHG	b	622	-	48,48,48	0.45	0	51,54,54	1.15	4 (7%)
24	CHL	S	308	-	46,54,74	1.75	12 (26%)	49,90,114	2.18	12 (24%)
39	LUT	Y	316	-	42,43,43	0.83	2 (4%)	51,60,60	1.73	9 (17%)
25	CLA	b	601	-	65,73,73	1.57	9 (13%)	76,113,113	1.92	15 (19%)
25	CLA	C	513	-	65,73,73	1.63	10 (15%)	76,113,113	1.81	17 (22%)
24	CHL	g	601	21	66,74,74	1.46	10 (15%)	73,114,114	1.74	13 (17%)
25	CLA	b	610	-	65,73,73	1.69	9 (13%)	76,113,113	1.64	13 (17%)
25	CLA	S	314	-	49,57,73	1.92	10 (20%)	55,93,113	1.82	13 (23%)
24	CHL	y	306	21	48,56,74	1.67	10 (20%)	51,92,114	2.05	11 (21%)
25	CLA	b	604	-	65,73,73	1.63	9 (13%)	76,113,113	1.79	16 (21%)
24	CHL	Y	308	-	58,66,74	1.60	10 (17%)	63,104,114	1.92	13 (20%)
24	CHL	N	601	21	56,64,74	1.60	11 (19%)	61,102,114	1.83	12 (19%)
25	CLA	Y	314	21	65,73,73	1.57	9 (13%)	76,113,113	1.89	14 (18%)
26	LHG	c	517	-	48,48,48	0.43	0	51,54,54	1.18	4 (7%)
28	BCR	B	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	10 (17%)
25	CLA	s	305	-	50,58,73	1.83	8 (16%)	58,95,113	3.36	19 (32%)
24	CHL	n	607	-	66,74,74	1.50	11 (16%)	73,114,114	1.75	12 (16%)
25	CLA	A	405	-	60,68,73	1.68	10 (16%)	70,107,113	1.83	15 (21%)
24	CHL	y	307	21	50,58,74	1.70	10 (20%)	52,94,114	1.89	14 (26%)
39	LUT	N	615	-	42,43,43	0.89	2 (4%)	51,60,60	1.73	9 (17%)
29	SQD	A	407	-	49,50,54	0.82	1 (2%)	58,61,65	0.95	3 (5%)
26	LHG	c	518	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
30	LMG	a	409	-	48,48,55	0.44	0	56,56,63	1.19	5 (8%)
35	DGD	C	516	-	63,63,67	0.52	0	77,77,81	1.23	6 (7%)
25	CLA	n	613	-	60,68,73	1.63	10 (16%)	70,107,113	1.91	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
26	LHG	S	318	25	48,48,48	0.42	0	51,54,54	1.19	4 (7%)
26	LHG	d	406	-	48,48,48	0.43	0	51,54,54	1.18	4 (7%)
25	CLA	N	603	-	65,73,73	1.61	10 (15%)	76,113,113	1.73	16 (21%)
24	CHL	1	302	-	46,54,74	1.74	11 (23%)	49,90,114	2.12	10 (20%)
25	CLA	c	502	-	65,73,73	1.63	10 (15%)	76,113,113	1.81	15 (19%)
25	CLA	R	608	22	58,66,73	1.77	9 (15%)	67,104,113	1.86	16 (23%)
25	CLA	2	605	2	48,56,73	1.87	9 (18%)	55,92,113	1.94	12 (21%)
25	CLA	D	401	42	50,58,73	1.81	10 (20%)	58,95,113	2.07	14 (24%)
30	LMG	B	623	-	55,55,55	0.43	0	63,63,63	1.23	4 (6%)
25	CLA	C	507	-	65,73,73	1.65	9 (13%)	76,113,113	1.66	14 (18%)
31	PL9	D	405	-	55,55,55	0.50	0	68,69,69	0.79	0
25	CLA	b	612	-	65,73,73	1.62	10 (15%)	76,113,113	1.78	15 (19%)
25	CLA	s	303	20	61,69,73	1.71	9 (14%)	71,108,113	1.74	15 (21%)
24	CHL	n	608	-	66,74,74	1.48	10 (15%)	73,114,114	1.77	9 (12%)
26	LHG	Y	301	21	48,48,48	0.44	0	51,54,54	1.19	4 (7%)
24	CHL	G	608	-	66,74,74	1.50	12 (18%)	73,114,114	1.77	12 (16%)
25	CLA	d	401	42	50,58,73	1.81	10 (20%)	58,95,113	2.07	14 (24%)
25	CLA	b	615	-	65,73,73	1.70	8 (12%)	76,113,113	1.70	16 (21%)
39	LUT	g	615	-	42,43,43	0.86	2 (4%)	51,60,60	1.65	8 (15%)
25	CLA	C	510	-	65,73,73	1.58	10 (15%)	76,113,113	1.75	15 (19%)
26	LHG	b	621	-	46,46,48	0.45	0	49,52,54	1.18	4 (8%)
29	SQD	L	101	-	41,42,54	0.88	1 (2%)	50,53,65	1.11	3 (6%)
25	CLA	y	311	21	60,68,73	1.77	9 (15%)	70,107,113	1.80	16 (22%)
25	CLA	b	605	-	65,73,73	1.59	9 (13%)	76,113,113	1.90	14 (18%)
25	CLA	C	512	-	65,73,73	1.60	10 (15%)	76,113,113	1.74	19 (25%)
25	CLA	n	604	-	50,58,73	1.81	10 (20%)	58,95,113	2.12	15 (25%)
25	CLA	C	511	6	65,73,73	1.60	9 (13%)	76,113,113	2.21	17 (22%)
25	CLA	G	604	40	50,58,73	1.87	9 (18%)	58,95,113	1.98	14 (24%)
40	NEX	G	617	25	38,46,46	1.52	8 (21%)	50,70,70	2.76	14 (28%)
28	BCR	d	404	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	R	603	-	60,68,73	1.66	8 (13%)	70,107,113	2.74	19 (27%)
40	NEX	S	317	-	38,46,46	1.61	8 (21%)	50,70,70	2.23	11 (22%)
25	CLA	B	610	-	65,73,73	1.70	9 (13%)	76,113,113	1.64	13 (17%)
25	CLA	B	604	-	65,73,73	1.63	10 (15%)	76,113,113	1.78	15 (19%)
25	CLA	R	604	-	48,56,73	1.80	10 (20%)	55,92,113	1.95	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
39	LUT	y	316	-	42,43,43	0.83	2 (4%)	51,60,60	1.74	8 (15%)
25	CLA	r	608	22	58,66,73	1.78	9 (15%)	67,104,113	1.86	16 (23%)
25	CLA	c	510	-	65,73,73	1.58	10 (15%)	76,113,113	1.75	15 (19%)
24	CHL	Y	309	-	66,74,74	1.49	11 (16%)	73,114,114	1.71	13 (17%)
25	CLA	s	309	20	45,53,73	2.05	9 (20%)	52,89,113	2.09	13 (25%)
25	CLA	b	614	30	65,73,73	1.62	9 (13%)	76,113,113	1.82	13 (17%)
29	SQD	a	408	-	49,50,54	0.82	1 (2%)	58,61,65	0.95	3 (5%)
28	BCR	C	514	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
41	XAT	r	616	-	39,47,47	1.16	6 (15%)	54,74,74	2.42	16 (29%)
25	CLA	B	602	-	65,73,73	1.67	9 (13%)	76,113,113	1.75	17 (22%)
31	PL9	d	405	-	55,55,55	0.50	0	68,69,69	0.78	0
28	BCR	z	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.29	8 (14%)
25	CLA	B	615	-	65,73,73	1.70	8 (12%)	76,113,113	1.71	16 (21%)
35	DGD	A	415	-	60,60,67	0.49	0	74,74,81	1.22	5 (6%)
25	CLA	r	602	22	60,68,73	1.72	9 (15%)	70,107,113	1.88	18 (25%)
39	LUT	Y	317	-	42,43,43	0.92	4 (9%)	51,60,60	1.50	6 (11%)
24	CHL	g	608	-	66,74,74	1.50	12 (18%)	73,114,114	1.76	12 (16%)
25	CLA	B	608	-	65,73,73	1.63	10 (15%)	76,113,113	1.78	15 (19%)
24	CHL	r	613	-	42,50,74	1.71	9 (21%)	44,85,114	2.27	10 (22%)
25	CLA	n	612	-	60,68,73	1.77	9 (15%)	70,107,113	1.88	15 (21%)
25	CLA	g	604	40	50,58,73	1.88	9 (18%)	58,95,113	1.97	14 (24%)
25	CLA	a	406	-	60,68,73	1.68	10 (16%)	70,107,113	1.83	15 (21%)
25	CLA	R	602	22	60,68,73	1.72	9 (15%)	70,107,113	1.89	18 (25%)
28	BCR	b	619	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	8 (14%)
24	CHL	R	613	-	42,50,74	1.72	8 (19%)	44,85,114	2.28	10 (22%)
25	CLA	b	608	-	65,73,73	1.62	10 (15%)	76,113,113	1.78	15 (19%)
24	CHL	Y	302	21	66,74,74	1.46	11 (16%)	73,114,114	1.79	15 (20%)
25	CLA	r	609	22	65,73,73	1.69	9 (13%)	76,113,113	1.73	17 (22%)
30	LMG	c	520	-	51,51,55	0.45	0	59,59,63	1.23	4 (6%)
25	CLA	R	614	22	45,53,73	2.06	8 (17%)	52,89,113	1.75	14 (26%)
30	LMG	B	620	25	51,51,55	0.44	0	59,59,63	1.21	4 (6%)
24	CHL	s	302	20	46,54,74	1.72	11 (23%)	49,90,114	2.08	11 (22%)
25	CLA	r	614	22	45,53,73	2.06	8 (17%)	52,89,113	1.75	14 (26%)
25	CLA	N	610	21	65,73,73	1.71	9 (13%)	76,113,113	1.74	16 (21%)
24	CHL	n	601	21	56,64,74	1.60	11 (19%)	61,102,114	1.82	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CHL	G	605	21	46,54,74	1.73	10 (21%)	49,90,114	2.03	9 (18%)
29	SQD	a	412	-	53,54,54	0.80	1 (1%)	62,65,65	0.97	2 (3%)
33	BCT	a	414	34	2,3,3	1.20	0	2,3,3	4.33	2 (100%)
24	CHL	s	306	-	46,54,74	1.74	12 (26%)	49,90,114	2.13	13 (26%)
25	CLA	G	602	21	65,73,73	1.70	10 (15%)	76,113,113	1.77	16 (21%)
25	CLA	N	602	21	65,73,73	1.70	10 (15%)	76,113,113	1.71	17 (22%)
25	CLA	N	614	-	48,56,73	1.81	9 (18%)	55,92,113	2.03	12 (21%)
24	CHL	6	601	2	64,72,74	1.51	11 (17%)	70,111,114	2.05	14 (20%)
25	CLA	g	602	21	65,73,73	1.70	10 (15%)	76,113,113	1.77	16 (21%)
26	LHG	C	518	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
28	BCR	B	617	-	41,41,41	1.18	2 (4%)	56,56,56	1.30	6 (10%)
26	LHG	6	606	25	46,46,48	0.44	0	49,52,54	1.19	4 (8%)
25	CLA	B	603	-	65,73,73	1.62	9 (13%)	76,113,113	1.70	15 (19%)
25	CLA	c	504	-	60,68,73	1.65	8 (13%)	70,107,113	2.68	21 (30%)
35	DGD	C	515	-	56,56,67	0.48	0	70,70,81	1.23	6 (8%)
39	LUT	S	316	-	42,43,43	0.89	4 (9%)	51,60,60	1.65	8 (15%)
39	LUT	s	316	-	42,43,43	0.89	4 (9%)	51,60,60	1.65	8 (15%)
25	CLA	r	601	-	49,57,73	1.84	9 (18%)	55,93,113	3.32	18 (32%)
25	CLA	S	313	-	55,63,73	1.72	10 (18%)	64,101,113	2.39	15 (23%)
31	PL9	A	409	-	13,13,55	0.96	0	17,17,69	0.72	0
38	HEM	F	101	9	41,50,50	1.91	8 (19%)	45,82,82	1.71	6 (13%)
25	CLA	C	505	-	65,73,73	1.64	9 (13%)	76,113,113	1.76	15 (19%)
26	LHG	y	319	25	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
25	CLA	R	610	26	49,57,73	1.85	8 (16%)	55,93,113	3.07	16 (29%)
25	CLA	g	603	-	60,68,73	1.67	9 (15%)	70,107,113	1.81	14 (20%)
24	CHL	Y	310	21	56,64,74	1.62	10 (17%)	61,102,114	1.84	11 (18%)
30	LMG	b	623	-	55,55,55	0.43	0	63,63,63	1.23	4 (6%)
25	CLA	Y	313	-	60,68,73	1.79	10 (16%)	70,107,113	1.75	15 (21%)
25	CLA	b	603	-	65,73,73	1.62	9 (13%)	76,113,113	1.71	15 (19%)
40	NEX	N	617	-	38,46,46	1.67	7 (18%)	50,70,70	2.43	18 (36%)
25	CLA	B	611	-	65,73,73	1.60	9 (13%)	76,113,113	1.80	16 (21%)
25	CLA	R	611	-	49,57,73	1.96	10 (20%)	55,93,113	3.54	22 (40%)
24	CHL	r	605	-	46,54,74	1.74	10 (21%)	49,90,114	2.19	13 (26%)
35	DGD	a	401	-	60,60,67	0.48	0	74,74,81	1.22	5 (6%)
40	NEX	y	318	-	38,46,46	1.73	9 (23%)	50,70,70	2.21	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	s	314	-	49,57,73	1.93	10 (20%)	55,93,113	1.82	13 (23%)
24	CHL	r	606	-	46,54,74	1.73	9 (19%)	49,90,114	2.00	9 (18%)
25	CLA	r	612	-	60,68,73	1.64	10 (16%)	70,107,113	2.06	16 (22%)
26	LHG	b	625	-	45,45,48	0.44	0	48,51,54	1.19	4 (8%)
26	LHG	r	618	25	41,41,48	0.46	0	44,47,54	1.22	4 (9%)
25	CLA	g	614	-	48,56,73	1.89	9 (18%)	55,92,113	1.80	13 (23%)
29	SQD	l	101	-	53,54,54	0.80	1 (1%)	62,65,65	1.01	3 (4%)
24	CHL	R	605	-	46,54,74	1.74	11 (23%)	49,90,114	2.19	13 (26%)
38	HEM	f	101	9	41,50,50	1.91	9 (21%)	45,82,82	1.71	6 (13%)
24	CHL	y	308	-	58,66,74	1.60	11 (18%)	63,104,114	1.92	13 (20%)
29	SQD	A	411	-	53,54,54	0.80	1 (1%)	62,65,65	0.97	2 (3%)
24	CHL	2	601	2	64,72,74	1.50	10 (15%)	70,111,114	2.05	14 (20%)
25	CLA	g	611	-	60,68,73	1.67	10 (16%)	70,107,113	1.79	20 (28%)
25	CLA	n	603	-	65,73,73	1.61	10 (15%)	76,113,113	1.73	16 (21%)
25	CLA	S	304	-	45,53,73	1.92	10 (22%)	52,89,113	2.09	10 (19%)
26	LHG	l	103	-	48,48,48	0.44	0	51,54,54	1.17	4 (7%)
24	CHL	s	307	-	46,54,74	1.74	11 (23%)	49,90,114	2.13	11 (22%)
26	LHG	n	618	25	48,48,48	0.43	0	51,54,54	1.15	4 (7%)
24	CHL	1	301	1	46,54,74	1.74	11 (23%)	49,90,114	2.02	11 (22%)
35	DGD	c	515	-	56,56,67	0.48	0	70,70,81	1.23	6 (8%)
24	CHL	5	302	-	46,54,74	1.74	11 (23%)	49,90,114	2.11	9 (18%)
25	CLA	y	314	21	65,73,73	1.58	9 (13%)	76,113,113	1.90	14 (18%)
24	CHL	Y	307	21	50,58,74	1.70	10 (20%)	52,94,114	1.88	14 (26%)
26	LHG	N	618	25	48,48,48	0.43	0	51,54,54	1.15	4 (7%)
28	BCR	h	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.30	9 (16%)
25	CLA	n	610	21	65,73,73	1.71	9 (13%)	76,113,113	1.75	16 (21%)
25	CLA	y	312	26	60,68,73	1.73	10 (16%)	70,107,113	1.71	16 (22%)
27	PHO	A	404	-	51,69,69	0.52	0	47,99,99	1.71	7 (14%)
25	CLA	C	501	-	65,73,73	1.58	8 (12%)	76,113,113	2.48	20 (26%)
25	CLA	C	503	-	65,73,73	1.60	9 (13%)	76,113,113	1.85	16 (21%)
24	CHL	G	609	21	61,69,74	1.55	11 (18%)	67,108,114	1.92	13 (19%)
25	CLA	N	611	26	60,68,73	1.72	10 (16%)	70,107,113	1.69	16 (22%)
25	CLA	Y	311	21	60,68,73	1.77	9 (15%)	70,107,113	1.80	16 (22%)
25	CLA	G	610	-	64,72,73	1.60	8 (12%)	74,111,113	2.00	17 (22%)
25	CLA	B	612	-	65,73,73	1.63	10 (15%)	76,113,113	1.78	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	CLA	B	609	-	65,73,73	1.62	9 (13%)	76,113,113	1.81	17 (22%)
25	CLA	G	611	-	60,68,73	1.66	8 (13%)	70,107,113	1.78	20 (28%)
28	BCR	D	404	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	g	613	-	65,73,73	1.59	10 (15%)	76,113,113	1.92	14 (18%)
24	CHL	Y	306	21	48,56,74	1.67	10 (20%)	51,92,114	2.05	11 (21%)
26	LHG	y	301	21	48,48,48	0.44	0	51,54,54	1.18	4 (7%)
31	PL9	a	410	-	13,13,55	0.96	0	17,17,69	0.72	0
28	BCR	I	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.28	9 (16%)
40	NEX	r	617	-	38,46,46	1.68	8 (21%)	50,70,70	3.05	17 (34%)
24	CHL	S	302	20	46,54,74	1.72	10 (21%)	49,90,114	2.08	11 (22%)
25	CLA	2	604	2,26	55,63,73	1.75	8 (14%)	64,101,113	2.08	19 (29%)
40	NEX	n	617	-	38,46,46	1.67	7 (18%)	50,70,70	2.43	18 (36%)
28	BCR	i	101	-	41,41,41	1.20	2 (4%)	56,56,56	1.27	9 (16%)
28	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	9 (16%)
30	LMG	a	411	-	40,40,55	0.48	0	48,48,63	1.28	4 (8%)
25	CLA	r	611	-	49,57,73	1.95	10 (20%)	55,93,113	3.54	22 (40%)
25	CLA	S	312	-	49,57,73	1.98	9 (18%)	55,93,113	1.89	14 (25%)
26	LHG	c	519	6	48,48,48	0.45	0	51,54,54	1.18	4 (7%)
24	CHL	n	606	-	46,54,74	1.73	12 (26%)	49,90,114	2.13	14 (28%)
25	CLA	R	609	22	65,73,73	1.68	9 (13%)	76,113,113	1.72	17 (22%)
24	CHL	R	607	-	61,69,74	1.55	11 (18%)	67,108,114	1.91	13 (19%)
25	CLA	g	610	-	64,72,73	1.61	8 (12%)	74,111,113	2.00	16 (21%)
24	CHL	G	601	21	66,74,74	1.46	11 (16%)	73,114,114	1.75	14 (19%)
24	CHL	N	605	21	48,56,74	1.67	10 (20%)	51,92,114	2.07	12 (23%)
24	CHL	N	606	-	46,54,74	1.73	12 (26%)	49,90,114	2.11	13 (26%)
39	LUT	R	615	-	42,43,43	0.96	3 (7%)	51,60,60	1.67	9 (17%)
39	LUT	n	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.53	6 (11%)
25	CLA	c	512	-	65,73,73	1.60	10 (15%)	76,113,113	1.74	18 (23%)
26	LHG	S	301	-	48,48,48	0.44	0	51,54,54	1.16	4 (7%)
25	CLA	G	612	21	60,68,73	1.77	9 (15%)	70,107,113	1.71	12 (17%)
25	CLA	S	303	20	61,69,73	1.71	10 (16%)	71,108,113	1.74	14 (19%)
26	LHG	L	102	-	48,48,48	0.44	0	51,54,54	1.17	4 (7%)
28	BCR	B	619	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	8 (14%)
41	XAT	R	616	-	39,47,47	1.17	6 (15%)	54,74,74	2.41	16 (29%)
25	CLA	N	612	-	60,68,73	1.76	9 (15%)	70,107,113	1.87	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	CLA	C	508	-	65,73,73	1.58	9 (13%)	76,113,113	1.88	17 (22%)
39	LUT	n	615	-	42,43,43	0.88	2 (4%)	51,60,60	1.72	9 (17%)
25	CLA	a	403	-	65,73,73	1.59	10 (15%)	76,113,113	1.80	16 (21%)
24	CHL	r	607	-	61,69,74	1.55	11 (18%)	67,108,114	1.90	13 (19%)
26	LHG	s	318	25	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
25	CLA	D	402	-	65,73,73	1.69	10 (15%)	76,113,113	1.82	17 (22%)
39	LUT	N	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.53	6 (11%)
25	CLA	c	501	-	65,73,73	1.58	8 (12%)	76,113,113	2.48	20 (26%)
24	CHL	2	603	2	46,54,74	1.86	13 (28%)	49,90,114	2.53	17 (34%)
25	CLA	S	305	-	50,58,73	1.83	8 (16%)	58,95,113	3.36	19 (32%)
26	LHG	B	622	-	48,48,48	0.45	0	51,54,54	1.15	4 (7%)
24	CHL	g	606	-	50,58,74	1.65	9 (18%)	52,94,114	2.14	11 (21%)
26	LHG	C	517	-	48,48,48	0.44	0	51,54,54	1.18	4 (7%)
25	CLA	R	601	-	49,57,73	1.84	9 (18%)	55,93,113	3.30	18 (32%)
25	CLA	G	614	-	48,56,73	1.89	9 (18%)	55,92,113	1.80	13 (23%)
25	CLA	b	616	-	65,73,73	1.64	9 (13%)	76,113,113	1.69	13 (17%)
25	CLA	D	403	-	65,73,73	1.60	8 (12%)	76,113,113	2.73	21 (27%)
25	CLA	c	508	-	65,73,73	1.58	9 (13%)	76,113,113	1.88	16 (21%)
25	CLA	g	612	21	60,68,73	1.77	8 (13%)	70,107,113	1.71	12 (17%)
39	LUT	G	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.44	4 (7%)
35	DGD	b	626	-	63,63,67	0.49	0	77,77,81	1.29	6 (7%)
39	LUT	g	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.44	4 (7%)
27	PHO	a	405	-	51,69,69	0.52	0	47,99,99	1.71	7 (14%)
29	SQD	l	102	-	41,42,54	0.88	1 (2%)	50,53,65	1.11	3 (6%)
25	CLA	2	602	2	60,68,73	1.71	9 (15%)	70,107,113	2.47	26 (37%)
25	CLA	n	602	21	65,73,73	1.70	10 (15%)	76,113,113	1.72	17 (22%)
25	CLA	n	614	-	48,56,73	1.81	9 (18%)	55,92,113	2.02	12 (21%)
40	NEX	g	617	25	38,46,46	1.61	8 (21%)	50,70,70	2.77	15 (30%)
39	LUT	G	615	-	42,43,43	0.87	3 (7%)	51,60,60	1.65	8 (15%)
25	CLA	c	513	-	65,73,73	1.63	10 (15%)	76,113,113	1.81	17 (22%)
29	SQD	L	103	-	53,54,54	0.80	1 (1%)	62,65,65	1.01	3 (4%)
25	CLA	s	310	20	55,63,73	1.80	9 (16%)	64,101,113	1.76	11 (17%)
30	LMG	A	410	-	40,40,55	0.48	0	48,48,63	1.28	4 (8%)
24	CHL	N	607	-	66,74,74	1.50	11 (16%)	73,114,114	1.75	12 (16%)
24	CHL	g	607	-	46,54,74	1.71	9 (19%)	49,90,114	2.02	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	A	402	-	65,73,73	1.59	10 (15%)	76,113,113	1.80	16 (21%)
24	CHL	G	606	-	50,58,74	1.65	9 (18%)	52,94,114	2.13	12 (23%)
25	CLA	s	311	26	56,64,73	1.71	9 (16%)	65,102,113	2.18	13 (20%)
24	CHL	S	306	-	46,54,74	1.75	12 (26%)	49,90,114	2.13	13 (26%)
24	CHL	R	606	-	46,54,74	1.74	10 (21%)	49,90,114	2.01	9 (18%)
24	CHL	y	309	-	66,74,74	1.49	11 (16%)	73,114,114	1.70	13 (17%)
25	CLA	a	402	-	65,73,73	1.60	10 (15%)	76,113,113	1.74	16 (21%)
24	CHL	6	603	2	46,54,74	1.86	13 (28%)	49,90,114	2.53	17 (34%)
25	CLA	C	504	-	60,68,73	1.66	8 (13%)	70,107,113	2.67	21 (30%)
24	CHL	s	308	-	46,54,74	1.75	12 (26%)	49,90,114	2.18	12 (24%)
30	LMG	C	520	-	51,51,55	0.45	0	59,59,63	1.23	4 (6%)
26	LHG	B	621	-	46,46,48	0.45	0	49,52,54	1.18	4 (8%)
39	LUT	r	615	-	42,43,43	0.95	3 (7%)	51,60,60	1.68	9 (17%)
25	CLA	C	502	-	65,73,73	1.63	9 (13%)	76,113,113	1.81	15 (19%)
25	CLA	N	613	-	60,68,73	1.63	10 (16%)	70,107,113	1.91	18 (25%)
28	BCR	Z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
40	NEX	Y	318	-	38,46,46	1.73	8 (21%)	50,70,70	2.21	18 (36%)
25	CLA	s	312	-	49,57,73	1.98	9 (18%)	55,93,113	1.89	14 (25%)
39	LUT	S	315	-	42,43,43	0.92	3 (7%)	51,60,60	1.57	8 (15%)
25	CLA	A	401	-	65,73,73	1.60	10 (15%)	76,113,113	1.74	16 (21%)
28	BCR	k	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.30	9 (16%)
25	CLA	y	304	-	65,73,73	1.63	10 (15%)	76,113,113	1.76	15 (19%)
25	CLA	B	606	-	65,73,73	1.57	9 (13%)	76,113,113	1.81	14 (18%)
25	CLA	r	604	-	48,56,73	1.79	9 (18%)	55,92,113	1.95	16 (29%)
30	LMG	D	407	-	46,46,55	0.44	0	54,54,63	1.21	4 (7%)
27	PHO	a	404	-	51,69,69	0.52	0	47,99,99	1.72	5 (10%)
25	CLA	S	311	26	56,64,73	1.72	9 (16%)	65,102,113	2.18	13 (20%)
25	CLA	b	611	-	65,73,73	1.60	9 (13%)	76,113,113	1.80	16 (21%)
24	CHL	n	609	21	66,74,74	1.48	10 (15%)	73,114,114	1.69	13 (17%)
26	LHG	s	301	-	48,48,48	0.44	0	51,54,54	1.16	4 (7%)
25	CLA	b	607	-	65,73,73	1.62	9 (13%)	76,113,113	1.77	15 (19%)
25	CLA	d	403	-	65,73,73	1.60	8 (12%)	76,113,113	2.73	21 (27%)
25	CLA	y	303	21	65,73,73	1.69	10 (15%)	76,113,113	1.75	15 (19%)
24	CHL	g	605	21	46,54,74	1.72	11 (23%)	49,90,114	2.04	9 (18%)
25	CLA	B	605	-	65,73,73	1.60	9 (13%)	76,113,113	1.90	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	LMG	d	407	-	46,46,55	0.44	0	54,54,63	1.21	4 (7%)
25	CLA	C	506	-	65,73,73	1.69	9 (13%)	76,113,113	1.70	16 (21%)
25	CLA	G	603	-	60,68,73	1.67	9 (15%)	70,107,113	1.81	14 (20%)
35	DGD	c	516	-	63,63,67	0.52	0	77,77,81	1.23	6 (7%)
25	CLA	b	606	-	65,73,73	1.57	9 (13%)	76,113,113	1.81	14 (18%)
24	CHL	5	301	1	46,54,74	1.74	10 (21%)	49,90,114	2.02	11 (22%)
39	LUT	y	317	-	42,43,43	0.92	3 (7%)	51,60,60	1.50	6 (11%)
28	BCR	t	101	16	41,41,41	1.15	3 (7%)	56,56,56	1.27	8 (14%)
28	BCR	a	407	-	41,41,41	1.15	2 (4%)	56,56,56	1.34	10 (17%)

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
25	CLA	y	305	-	1/1/12/20	7/19/97/115	-
26	LHG	C	519	6	-	21/53/53/53	-
25	CLA	B	614	30	1/1/15/20	13/37/115/115	-
25	CLA	y	315	-	1/1/11/20	8/13/91/115	-
24	CHL	G	607	-	2/2/16/26	6/15/113/137	-
28	BCR	T	101	16	-	17/29/63/63	0/2/2/2
25	CLA	y	313	-	1/1/14/20	11/31/109/115	-
25	CLA	c	505	-	1/1/15/20	12/37/115/115	-
28	BCR	b	618	-	-	3/29/63/63	0/2/2/2
24	CHL	S	307	-	3/3/16/26	7/15/113/137	-
24	CHL	n	605	21	3/3/16/26	7/18/116/137	-
40	NEX	s	317	-	-	6/27/83/83	0/3/3/3
25	CLA	6	605	2	1/1/11/20	10/17/95/115	-
25	CLA	c	507	-	1/1/15/20	15/37/115/115	-
25	CLA	B	601	-	1/1/15/20	16/37/115/115	-
25	CLA	b	609	-	1/1/15/20	11/37/115/115	-
28	BCR	b	617	-	-	3/29/63/63	0/2/2/2
26	LHG	2	606	25	-	25/51/51/53	-
25	CLA	n	611	26	1/1/14/20	12/31/109/115	-
25	CLA	c	511	6	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	S	309	20	1/1/11/20	5/13/91/115	-
25	CLA	b	602	-	1/1/15/20	14/37/115/115	-
35	DGD	B	626	-	-	23/51/91/95	0/2/2/2
39	LUT	s	315	-	-	4/29/67/67	0/2/2/2
25	CLA	r	610	26	1/1/11/20	9/18/96/115	-
24	CHL	y	302	21	2/2/20/26	23/39/137/137	-
27	PHO	A	403	-	-	12/37/103/103	0/5/6/6
25	CLA	Y	315	-	1/1/11/20	8/13/91/115	-
25	CLA	6	604	2,26	1/1/13/20	9/25/103/115	-
25	CLA	s	313	-	1/1/13/20	10/25/103/115	-
26	LHG	D	406	-	-	18/53/53/53	-
30	LMG	A	408	-	-	18/43/63/70	0/1/1/1
25	CLA	G	613	-	1/1/15/20	16/37/115/115	-
24	CHL	N	608	-	3/3/20/26	15/39/137/137	-
25	CLA	c	506	-	1/1/15/20	11/37/115/115	-
25	CLA	Y	305	-	1/1/12/20	7/19/97/115	-
25	CLA	Y	312	26	1/1/14/20	11/31/109/115	-
24	CHL	g	609	21	3/3/19/26	10/33/131/137	-
28	BCR	H	101	-	-	6/29/63/63	0/2/2/2
25	CLA	S	310	20	1/1/13/20	9/25/103/115	-
25	CLA	N	604	-	1/1/12/20	6/19/97/115	-
25	CLA	B	607	-	1/1/15/20	16/37/115/115	-
25	CLA	C	509	-	1/1/15/20	7/37/115/115	-
30	LMG	b	620	25	-	15/46/66/70	0/1/1/1
25	CLA	c	509	-	1/1/15/20	7/37/115/115	-
25	CLA	B	613	-	1/1/15/20	15/37/115/115	-
25	CLA	R	612	-	1/1/14/20	11/31/109/115	-
25	CLA	b	613	-	1/1/15/20	15/37/115/115	-
24	CHL	y	310	21	3/3/18/26	11/27/125/137	-
26	LHG	R	618	25	-	12/46/46/53	-
25	CLA	B	616	-	1/1/15/20	17/37/115/115	-
25	CLA	Y	303	21	1/1/15/20	12/37/115/115	-
25	CLA	6	602	2	1/1/14/20	13/31/109/115	-
25	CLA	c	503	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	Y	319	25	-	23/53/53/53	-
28	BCR	c	514	-	-	2/29/63/63	0/2/2/2
40	NEX	R	617	-	-	6/27/83/83	0/3/3/3
25	CLA	Y	304	-	1/1/15/20	22/37/115/115	-
24	CHL	N	609	21	2/2/20/26	15/39/137/137	-
26	LHG	B	625	-	-	14/50/50/53	-
25	CLA	d	402	-	1/1/15/20	10/37/115/115	-
28	BCR	A	406	-	-	5/29/63/63	0/2/2/2
25	CLA	r	603	-	1/1/14/20	13/31/109/115	-
25	CLA	s	304	-	1/1/11/20	2/13/91/115	-
26	LHG	b	622	-	-	18/53/53/53	-
24	CHL	S	308	-	3/3/16/26	2/15/113/137	-
39	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
25	CLA	b	601	-	1/1/15/20	16/37/115/115	-
25	CLA	C	513	-	1/1/15/20	13/37/115/115	-
24	CHL	g	601	21	2/2/20/26	24/39/137/137	-
25	CLA	b	610	-	1/1/15/20	9/37/115/115	-
25	CLA	S	314	-	1/1/11/20	3/18/96/115	-
24	CHL	y	306	21	3/3/16/26	9/18/116/137	-
25	CLA	b	604	-	1/1/15/20	15/37/115/115	-
24	CHL	Y	308	-	2/2/18/26	8/30/128/137	-
24	CHL	N	601	21	2/2/18/26	13/27/125/137	-
25	CLA	Y	314	21	1/1/15/20	16/37/115/115	-
26	LHG	c	517	-	-	17/53/53/53	-
28	BCR	B	618	-	-	3/29/63/63	0/2/2/2
25	CLA	s	305	-	1/1/12/20	9/19/97/115	-
24	CHL	n	607	-	2/2/20/26	18/39/137/137	-
25	CLA	A	405	-	1/1/14/20	9/31/109/115	-
24	CHL	y	307	21	3/3/16/26	3/20/118/137	-
39	LUT	N	615	-	-	8/29/67/67	0/2/2/2
29	SQD	A	407	-	-	21/45/65/69	0/1/1/1
26	LHG	c	518	-	-	12/53/53/53	-
30	LMG	a	409	-	-	18/43/63/70	0/1/1/1
35	DGD	C	516	-	-	28/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	n	613	-	1/1/14/20	21/31/109/115	-
26	LHG	S	318	25	-	20/53/53/53	-
26	LHG	d	406	-	-	18/53/53/53	-
25	CLA	N	603	-	1/1/15/20	17/37/115/115	-
24	CHL	1	302	-	3/3/16/26	5/15/113/137	-
25	CLA	c	502	-	1/1/15/20	6/37/115/115	-
25	CLA	R	608	22	1/1/13/20	15/29/107/115	-
25	CLA	2	605	2	1/1/11/20	10/17/95/115	-
25	CLA	D	401	42	1/1/12/20	2/19/97/115	-
30	LMG	B	623	-	-	28/50/70/70	0/1/1/1
25	CLA	C	507	-	1/1/15/20	15/37/115/115	-
31	PL9	D	405	-	-	5/53/73/73	0/1/1/1
25	CLA	b	612	-	1/1/15/20	8/37/115/115	-
25	CLA	s	303	20	1/1/14/20	16/33/111/115	-
24	CHL	n	608	-	3/3/20/26	15/39/137/137	-
26	LHG	Y	301	21	-	16/53/53/53	-
24	CHL	G	608	-	3/3/20/26	22/39/137/137	-
25	CLA	d	401	42	1/1/12/20	2/19/97/115	-
25	CLA	b	615	-	1/1/15/20	10/37/115/115	-
39	LUT	g	615	-	-	5/29/67/67	0/2/2/2
25	CLA	C	510	-	1/1/15/20	14/37/115/115	-
26	LHG	b	621	-	-	19/51/51/53	-
29	SQD	L	101	-	-	13/37/57/69	0/1/1/1
25	CLA	y	311	21	1/1/14/20	10/31/109/115	-
25	CLA	b	605	-	1/1/15/20	7/37/115/115	-
25	CLA	C	512	-	1/1/15/20	12/37/115/115	-
25	CLA	n	604	-	1/1/12/20	6/19/97/115	-
25	CLA	C	511	6	1/1/15/20	7/37/115/115	-
25	CLA	G	604	40	1/1/12/20	11/19/97/115	-
40	NEX	G	617	25	-	11/27/83/83	0/3/3/3
28	BCR	d	404	-	-	5/29/63/63	0/2/2/2
25	CLA	R	603	-	1/1/14/20	13/31/109/115	-
40	NEX	S	317	-	-	6/27/83/83	0/3/3/3
25	CLA	B	610	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	604	-	1/1/15/20	15/37/115/115	-
25	CLA	R	604	-	1/1/11/20	4/17/95/115	-
39	LUT	y	316	-	-	3/29/67/67	0/2/2/2
25	CLA	r	608	22	1/1/13/20	15/29/107/115	-
25	CLA	c	510	-	1/1/15/20	14/37/115/115	-
24	CHL	Y	309	-	3/3/20/26	20/39/137/137	-
25	CLA	s	309	20	1/1/11/20	5/13/91/115	-
25	CLA	b	614	30	1/1/15/20	13/37/115/115	-
29	SQD	a	408	-	-	21/45/65/69	0/1/1/1
28	BCR	C	514	-	-	2/29/63/63	0/2/2/2
41	XAT	r	616	-	-	2/31/93/93	0/4/4/4
25	CLA	B	602	-	1/1/15/20	14/37/115/115	-
31	PL9	d	405	-	-	5/53/73/73	0/1/1/1
28	BCR	z	101	-	-	8/29/63/63	0/2/2/2
25	CLA	B	615	-	1/1/15/20	10/37/115/115	-
35	DGD	A	415	-	-	27/48/88/95	0/2/2/2
25	CLA	r	602	22	1/1/14/20	10/31/109/115	-
39	LUT	Y	317	-	-	3/29/67/67	0/2/2/2
24	CHL	g	608	-	3/3/20/26	22/39/137/137	-
25	CLA	B	608	-	1/1/15/20	12/37/115/115	-
24	CHL	r	613	-	3/3/15/26	6/10/108/137	-
25	CLA	n	612	-	1/1/14/20	18/31/109/115	-
25	CLA	g	604	40	1/1/12/20	11/19/97/115	-
25	CLA	a	406	-	1/1/14/20	9/31/109/115	-
25	CLA	R	602	22	1/1/14/20	10/31/109/115	-
28	BCR	b	619	-	-	3/29/63/63	0/2/2/2
24	CHL	R	613	-	3/3/15/26	6/10/108/137	-
25	CLA	b	608	-	1/1/15/20	12/37/115/115	-
24	CHL	Y	302	21	2/2/20/26	23/39/137/137	-
25	CLA	r	609	22	1/1/15/20	14/37/115/115	-
30	LMG	c	520	-	-	18/46/66/70	0/1/1/1
25	CLA	R	614	22	1/1/11/20	8/13/91/115	-
30	LMG	B	620	25	-	15/46/66/70	0/1/1/1
24	CHL	s	302	20	2/2/16/26	4/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	r	614	22	1/1/11/20	8/13/91/115	-
25	CLA	N	610	21	1/1/15/20	15/37/115/115	-
24	CHL	n	601	21	2/2/18/26	13/27/125/137	-
24	CHL	G	605	21	3/3/16/26	9/15/113/137	-
29	SQD	a	412	-	-	22/49/69/69	0/1/1/1
24	CHL	s	306	-	3/3/16/26	7/15/113/137	-
25	CLA	G	602	21	1/1/15/20	15/37/115/115	-
25	CLA	N	602	21	1/1/15/20	13/37/115/115	-
25	CLA	N	614	-	1/1/11/20	4/17/95/115	-
24	CHL	6	601	2	3/3/19/26	16/37/135/137	-
25	CLA	g	602	21	1/1/15/20	15/37/115/115	-
26	LHG	C	518	-	-	12/53/53/53	-
28	BCR	B	617	-	-	3/29/63/63	0/2/2/2
26	LHG	6	606	25	-	25/51/51/53	-
25	CLA	B	603	-	1/1/15/20	11/37/115/115	-
25	CLA	c	504	-	1/1/14/20	14/31/109/115	-
35	DGD	C	515	-	-	17/44/84/95	0/2/2/2
39	LUT	S	316	-	-	4/29/67/67	0/2/2/2
39	LUT	s	316	-	-	4/29/67/67	0/2/2/2
25	CLA	r	601	-	1/1/11/20	11/18/96/115	-
25	CLA	S	313	-	1/1/13/20	10/25/103/115	-
31	PL9	A	409	-	-	2/5/18/73	0/1/1/1
38	HEM	F	101	9	-	1/12/54/54	-
25	CLA	C	505	-	1/1/15/20	12/37/115/115	-
26	LHG	y	319	25	-	23/53/53/53	-
25	CLA	R	610	26	1/1/11/20	9/18/96/115	-
25	CLA	g	603	-	1/1/14/20	11/31/109/115	-
24	CHL	Y	310	21	3/3/18/26	11/27/125/137	-
30	LMG	b	623	-	-	28/50/70/70	0/1/1/1
25	CLA	Y	313	-	1/1/14/20	11/31/109/115	-
25	CLA	b	603	-	1/1/15/20	11/37/115/115	-
40	NEX	N	617	-	-	10/27/83/83	0/3/3/3
25	CLA	B	611	-	1/1/15/20	10/37/115/115	-
25	CLA	R	611	-	1/1/11/20	11/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	r	605	-	3/3/16/26	3/15/113/137	-
35	DGD	a	401	-	-	27/48/88/95	0/2/2/2
40	NEX	y	318	-	-	7/27/83/83	1/3/3/3
25	CLA	s	314	-	1/1/11/20	3/18/96/115	-
24	CHL	r	606	-	3/3/16/26	11/15/113/137	-
25	CLA	r	612	-	1/1/14/20	11/31/109/115	-
26	LHG	b	625	-	-	14/50/50/53	-
26	LHG	r	618	25	-	12/46/46/53	-
25	CLA	g	614	-	1/1/11/20	9/17/95/115	-
29	SQD	l	101	-	-	27/49/69/69	0/1/1/1
24	CHL	R	605	-	3/3/16/26	3/15/113/137	-
38	HEM	f	101	9	-	1/12/54/54	-
24	CHL	y	308	-	2/2/18/26	8/30/128/137	-
29	SQD	A	411	-	-	22/49/69/69	0/1/1/1
24	CHL	2	601	2	3/3/19/26	16/37/135/137	-
25	CLA	g	611	-	1/1/14/20	16/31/109/115	-
25	CLA	n	603	-	1/1/15/20	17/37/115/115	-
25	CLA	S	304	-	1/1/11/20	2/13/91/115	-
26	LHG	l	103	-	-	29/53/53/53	-
24	CHL	s	307	-	3/3/16/26	7/15/113/137	-
26	LHG	n	618	25	-	29/53/53/53	-
24	CHL	1	301	1	3/3/16/26	4/15/113/137	-
35	DGD	c	515	-	-	17/44/84/95	0/2/2/2
24	CHL	5	302	-	3/3/16/26	5/15/113/137	-
25	CLA	y	314	21	1/1/15/20	16/37/115/115	-
24	CHL	Y	307	21	3/3/16/26	3/20/118/137	-
26	LHG	N	618	25	-	29/53/53/53	-
28	BCR	h	101	-	-	6/29/63/63	0/2/2/2
25	CLA	n	610	21	1/1/15/20	15/37/115/115	-
25	CLA	y	312	26	1/1/14/20	11/31/109/115	-
27	PHO	A	404	-	-	1/37/103/103	0/5/6/6
25	CLA	C	501	-	1/1/15/20	7/37/115/115	-
25	CLA	C	503	-	1/1/15/20	9/37/115/115	-
24	CHL	G	609	21	3/3/19/26	10/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	N	611	26	1/1/14/20	12/31/109/115	-
25	CLA	Y	311	21	1/1/14/20	9/31/109/115	-
25	CLA	G	610	-	1/1/14/20	14/36/114/115	-
25	CLA	B	612	-	1/1/15/20	8/37/115/115	-
25	CLA	B	609	-	1/1/15/20	11/37/115/115	-
25	CLA	G	611	-	1/1/14/20	16/31/109/115	-
28	BCR	D	404	-	-	5/29/63/63	0/2/2/2
25	CLA	g	613	-	1/1/15/20	16/37/115/115	-
24	CHL	Y	306	21	3/3/16/26	9/18/116/137	-
26	LHG	y	301	21	-	16/53/53/53	-
31	PL9	a	410	-	-	2/5/18/73	0/1/1/1
28	BCR	I	101	-	-	5/29/63/63	0/2/2/2
40	NEX	r	617	-	-	6/27/83/83	0/3/3/3
24	CHL	S	302	20	2/2/16/26	4/15/113/137	-
25	CLA	2	604	2,26	1/1/13/20	9/25/103/115	-
40	NEX	n	617	-	-	10/27/83/83	0/3/3/3
28	BCR	i	101	-	-	4/29/63/63	0/2/2/2
28	BCR	K	101	-	-	4/29/63/63	0/2/2/2
30	LMG	a	411	-	-	13/35/55/70	0/1/1/1
25	CLA	r	611	-	1/1/11/20	11/18/96/115	-
25	CLA	S	312	-	1/1/11/20	7/18/96/115	-
26	LHG	c	519	6	-	21/53/53/53	-
24	CHL	n	606	-	2/2/16/26	4/15/113/137	-
25	CLA	R	609	22	1/1/15/20	14/37/115/115	-
24	CHL	R	607	-	3/3/19/26	13/33/131/137	-
25	CLA	g	610	-	1/1/14/20	14/36/114/115	-
24	CHL	G	601	21	2/2/20/26	24/39/137/137	-
24	CHL	N	605	21	3/3/16/26	7/18/116/137	-
24	CHL	N	606	-	2/2/16/26	4/15/113/137	-
39	LUT	R	615	-	-	4/29/67/67	0/2/2/2
39	LUT	n	616	-	-	4/29/67/67	0/2/2/2
25	CLA	c	512	-	1/1/15/20	12/37/115/115	-
26	LHG	S	301	-	-	21/53/53/53	-
25	CLA	G	612	21	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	S	303	20	1/1/14/20	16/33/111/115	-
26	LHG	L	102	-	-	29/53/53/53	-
28	BCR	B	619	-	-	3/29/63/63	0/2/2/2
41	XAT	R	616	-	-	2/31/93/93	0/4/4/4
25	CLA	N	612	-	1/1/14/20	18/31/109/115	-
25	CLA	C	508	-	1/1/15/20	12/37/115/115	-
39	LUT	n	615	-	-	8/29/67/67	0/2/2/2
25	CLA	a	403	-	1/1/15/20	7/37/115/115	-
24	CHL	r	607	-	3/3/19/26	13/33/131/137	-
26	LHG	s	318	25	-	21/53/53/53	-
25	CLA	D	402	-	1/1/15/20	10/37/115/115	-
39	LUT	N	616	-	-	4/29/67/67	0/2/2/2
25	CLA	c	501	-	1/1/15/20	7/37/115/115	-
24	CHL	2	603	2	3/3/16/26	10/15/113/137	-
25	CLA	S	305	-	1/1/12/20	9/19/97/115	-
26	LHG	B	622	-	-	18/53/53/53	-
24	CHL	g	606	-	3/3/16/26	3/20/118/137	-
26	LHG	C	517	-	-	16/53/53/53	-
25	CLA	R	601	-	1/1/11/20	11/18/96/115	-
25	CLA	G	614	-	1/1/11/20	9/17/95/115	-
25	CLA	b	616	-	1/1/15/20	17/37/115/115	-
25	CLA	D	403	-	1/1/15/20	12/37/115/115	-
25	CLA	c	508	-	1/1/15/20	12/37/115/115	-
25	CLA	g	612	21	1/1/14/20	11/31/109/115	-
39	LUT	G	616	-	-	0/29/67/67	0/2/2/2
35	DGD	b	626	-	-	23/51/91/95	0/2/2/2
39	LUT	g	616	-	-	0/29/67/67	0/2/2/2
27	PHO	a	405	-	-	1/37/103/103	0/5/6/6
29	SQD	l	102	-	-	13/37/57/69	0/1/1/1
25	CLA	2	602	2	1/1/14/20	13/31/109/115	-
25	CLA	n	602	21	1/1/15/20	13/37/115/115	-
25	CLA	n	614	-	1/1/11/20	4/17/95/115	-
40	NEX	g	617	25	-	11/27/83/83	0/3/3/3
39	LUT	G	615	-	-	5/29/67/67	0/2/2/2
25	CLA	c	513	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	L	103	-	-	27/49/69/69	0/1/1/1
25	CLA	s	310	20	1/1/13/20	9/25/103/115	-
30	LMG	A	410	-	-	13/35/55/70	0/1/1/1
24	CHL	N	607	-	2/2/20/26	18/39/137/137	-
24	CHL	g	607	-	2/2/16/26	6/15/113/137	-
25	CLA	A	402	-	1/1/15/20	7/37/115/115	-
24	CHL	G	606	-	3/3/16/26	3/20/118/137	-
25	CLA	s	311	26	1/1/13/20	12/27/105/115	-
24	CHL	S	306	-	3/3/16/26	7/15/113/137	-
24	CHL	R	606	-	3/3/16/26	11/15/113/137	-
24	CHL	y	309	-	3/3/20/26	20/39/137/137	-
25	CLA	a	402	-	1/1/15/20	7/37/115/115	-
24	CHL	6	603	2	3/3/16/26	10/15/113/137	-
25	CLA	C	504	-	1/1/14/20	14/31/109/115	-
24	CHL	s	308	-	3/3/16/26	2/15/113/137	-
30	LMG	C	520	-	-	18/46/66/70	0/1/1/1
26	LHG	B	621	-	-	19/51/51/53	-
39	LUT	r	615	-	-	4/29/67/67	0/2/2/2
25	CLA	C	502	-	1/1/15/20	6/37/115/115	-
25	CLA	N	613	-	1/1/14/20	21/31/109/115	-
28	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
40	NEX	Y	318	-	-	7/27/83/83	1/3/3/3
25	CLA	s	312	-	1/1/11/20	7/18/96/115	-
39	LUT	S	315	-	-	4/29/67/67	0/2/2/2
25	CLA	A	401	-	1/1/15/20	7/37/115/115	-
28	BCR	k	101	-	-	4/29/63/63	0/2/2/2
25	CLA	y	304	-	1/1/15/20	22/37/115/115	-
25	CLA	B	606	-	1/1/15/20	11/37/115/115	-
25	CLA	r	604	-	1/1/11/20	4/17/95/115	-
30	LMG	D	407	-	-	16/41/61/70	0/1/1/1
27	PHO	a	404	-	-	12/37/103/103	0/5/6/6
25	CLA	S	311	26	1/1/13/20	12/27/105/115	-
25	CLA	b	611	-	1/1/15/20	10/37/115/115	-
24	CHL	n	609	21	2/2/20/26	15/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	s	301	-	-	21/53/53/53	-
25	CLA	b	607	-	1/1/15/20	16/37/115/115	-
25	CLA	d	403	-	1/1/15/20	12/37/115/115	-
25	CLA	y	303	21	1/1/15/20	12/37/115/115	-
24	CHL	g	605	21	3/3/16/26	9/15/113/137	-
25	CLA	B	605	-	1/1/15/20	7/37/115/115	-
30	LMG	d	407	-	-	16/41/61/70	0/1/1/1
25	CLA	C	506	-	1/1/15/20	11/37/115/115	-
25	CLA	G	603	-	1/1/14/20	12/31/109/115	-
35	DGD	c	516	-	-	28/51/91/95	0/2/2/2
25	CLA	b	606	-	1/1/15/20	11/37/115/115	-
24	CHL	5	301	1	3/3/16/26	4/15/113/137	-
39	LUT	y	317	-	-	3/29/67/67	0/2/2/2
28	BCR	t	101	16	-	17/29/63/63	0/2/2/2
28	BCR	a	407	-	-	5/29/63/63	0/2/2/2

All (2344) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	F	101	HEM	FE-NB	8.66	2.39	1.96
38	f	101	HEM	FE-NB	8.66	2.39	1.96
25	N	610	CLA	C1B-NB	7.29	1.41	1.35
25	n	610	CLA	C1B-NB	7.26	1.41	1.35
25	y	311	CLA	C1B-NB	7.19	1.41	1.35
25	s	312	CLA	C1B-NB	7.17	1.41	1.35
25	S	312	CLA	C1B-NB	7.11	1.41	1.35
25	s	309	CLA	C1B-NB	7.10	1.41	1.35
25	Y	311	CLA	C1B-NB	7.09	1.41	1.35
25	r	614	CLA	C1B-NB	7.06	1.41	1.35
25	r	608	CLA	C1B-NB	7.06	1.41	1.35
25	S	309	CLA	C1B-NB	7.02	1.41	1.35
25	N	602	CLA	C4B-NB	7.00	1.41	1.35
25	n	602	CLA	C4B-NB	7.00	1.41	1.35
25	G	602	CLA	C4B-NB	6.99	1.41	1.35
25	g	602	CLA	C4B-NB	6.99	1.41	1.35
25	R	608	CLA	C1B-NB	6.97	1.41	1.35
25	R	614	CLA	C1B-NB	6.95	1.41	1.35
25	g	612	CLA	C1B-NB	6.88	1.41	1.35
25	C	506	CLA	C1B-NB	6.88	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	C1B-NB	6.88	1.41	1.35
25	y	315	CLA	C4B-NB	6.82	1.41	1.35
25	G	612	CLA	C1B-NB	6.81	1.41	1.35
25	r	614	CLA	C4B-NB	6.81	1.41	1.35
25	s	314	CLA	C1B-NB	6.80	1.41	1.35
25	Y	303	CLA	C4B-NB	6.80	1.41	1.35
25	y	303	CLA	C4B-NB	6.80	1.41	1.35
25	b	602	CLA	C1B-NB	6.80	1.41	1.35
25	B	602	CLA	C1B-NB	6.79	1.41	1.35
25	Y	313	CLA	C1B-NB	6.79	1.41	1.35
25	d	402	CLA	C1B-NB	6.79	1.41	1.35
25	B	615	CLA	C1B-NB	6.77	1.41	1.35
25	b	615	CLA	C1B-NB	6.77	1.41	1.35
25	r	609	CLA	C1B-NB	6.77	1.41	1.35
25	R	614	CLA	C4B-NB	6.77	1.41	1.35
25	R	609	CLA	C1B-NB	6.76	1.41	1.35
25	R	611	CLA	MG-ND	-6.76	1.92	2.05
25	D	402	CLA	C1B-NB	6.75	1.41	1.35
25	y	313	CLA	C1B-NB	6.74	1.41	1.35
25	r	611	CLA	MG-ND	-6.71	1.92	2.05
25	Y	315	CLA	C4B-NB	6.71	1.41	1.35
25	S	314	CLA	C1B-NB	6.70	1.41	1.35
25	B	610	CLA	C1B-NB	6.67	1.41	1.35
25	b	610	CLA	C1B-NB	6.67	1.41	1.35
25	N	612	CLA	C1B-NB	6.64	1.41	1.35
25	n	612	CLA	C1B-NB	6.64	1.41	1.35
25	Y	303	CLA	C1B-NB	6.62	1.41	1.35
25	y	303	CLA	C1B-NB	6.62	1.41	1.35
25	G	612	CLA	C4B-NB	6.61	1.41	1.35
25	y	305	CLA	C4B-NB	6.55	1.41	1.35
25	Y	305	CLA	C4B-NB	6.54	1.41	1.35
25	b	602	CLA	C4B-NB	6.53	1.41	1.35
25	n	602	CLA	C1B-NB	6.52	1.41	1.35
25	Y	313	CLA	C4B-NB	6.52	1.41	1.35
25	B	602	CLA	C4B-NB	6.52	1.41	1.35
25	c	505	CLA	C4B-NB	6.51	1.41	1.35
25	g	612	CLA	C4B-NB	6.50	1.41	1.35
25	y	313	CLA	C4B-NB	6.49	1.41	1.35
25	S	303	CLA	C1B-NB	6.49	1.41	1.35
25	s	303	CLA	C1B-NB	6.49	1.41	1.35
25	B	616	CLA	C4B-NB	6.47	1.41	1.35
25	b	616	CLA	C4B-NB	6.47	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	305	CLA	C1B-NB	6.47	1.41	1.35
25	S	310	CLA	C1B-NB	6.45	1.41	1.35
25	g	602	CLA	C1B-NB	6.44	1.41	1.35
25	S	310	CLA	C4B-NB	6.43	1.40	1.35
25	s	310	CLA	C4B-NB	6.43	1.40	1.35
25	G	614	CLA	C4B-NB	6.42	1.40	1.35
25	g	614	CLA	C4B-NB	6.42	1.40	1.35
25	N	610	CLA	C4B-NB	6.42	1.40	1.35
25	n	610	CLA	C4B-NB	6.42	1.40	1.35
25	N	602	CLA	C1B-NB	6.42	1.40	1.35
25	B	610	CLA	C4B-NB	6.41	1.40	1.35
25	C	505	CLA	C4B-NB	6.41	1.40	1.35
25	C	506	CLA	C4B-NB	6.41	1.40	1.35
25	Y	305	CLA	C1B-NB	6.40	1.40	1.35
25	c	513	CLA	C4B-NB	6.40	1.40	1.35
25	g	604	CLA	C4B-NB	6.40	1.40	1.35
25	S	303	CLA	C4B-NB	6.39	1.40	1.35
25	s	303	CLA	C4B-NB	6.39	1.40	1.35
25	S	314	CLA	C4B-NB	6.39	1.40	1.35
25	b	608	CLA	C4B-NB	6.39	1.40	1.35
25	s	314	CLA	C4B-NB	6.39	1.40	1.35
25	n	611	CLA	C4B-NB	6.38	1.40	1.35
25	C	513	CLA	C4B-NB	6.37	1.40	1.35
25	c	506	CLA	C4B-NB	6.37	1.40	1.35
25	G	602	CLA	C1B-NB	6.36	1.40	1.35
25	s	312	CLA	C4B-NB	6.36	1.40	1.35
25	s	310	CLA	C1B-NB	6.35	1.40	1.35
25	R	602	CLA	C4B-NB	6.35	1.40	1.35
25	r	602	CLA	C4B-NB	6.35	1.40	1.35
25	Y	312	CLA	C4B-NB	6.35	1.40	1.35
25	y	312	CLA	C4B-NB	6.35	1.40	1.35
25	B	613	CLA	C4B-NB	6.35	1.40	1.35
25	b	613	CLA	C4B-NB	6.35	1.40	1.35
25	G	604	CLA	C1B-NB	6.34	1.40	1.35
25	b	610	CLA	C4B-NB	6.34	1.40	1.35
25	g	604	CLA	C1B-NB	6.34	1.40	1.35
25	N	612	CLA	C4B-NB	6.33	1.40	1.35
25	n	612	CLA	C4B-NB	6.33	1.40	1.35
25	C	507	CLA	C4B-NB	6.33	1.40	1.35
25	c	507	CLA	C4B-NB	6.33	1.40	1.35
25	c	502	CLA	C4B-NB	6.33	1.40	1.35
25	Y	311	CLA	C4B-NB	6.33	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	311	CLA	C4B-NB	6.33	1.40	1.35
25	S	312	CLA	C4B-NB	6.32	1.40	1.35
25	Y	312	CLA	C1B-NB	6.32	1.40	1.35
25	y	312	CLA	C1B-NB	6.32	1.40	1.35
25	N	611	CLA	C4B-NB	6.32	1.40	1.35
25	R	602	CLA	C1B-NB	6.31	1.40	1.35
25	B	612	CLA	C4B-NB	6.30	1.40	1.35
25	r	608	CLA	C4B-NB	6.30	1.40	1.35
25	b	607	CLA	C4B-NB	6.30	1.40	1.35
25	R	609	CLA	C4B-NB	6.30	1.40	1.35
25	r	609	CLA	C4B-NB	6.30	1.40	1.35
25	G	604	CLA	C4B-NB	6.30	1.40	1.35
25	R	610	CLA	MG-ND	-6.29	1.93	2.05
25	r	602	CLA	C1B-NB	6.29	1.40	1.35
25	B	608	CLA	C4B-NB	6.29	1.40	1.35
25	B	607	CLA	C4B-NB	6.28	1.40	1.35
25	Y	315	CLA	C1B-NB	6.28	1.40	1.35
25	y	315	CLA	C1B-NB	6.28	1.40	1.35
25	B	609	CLA	C4B-NB	6.28	1.40	1.35
25	b	609	CLA	C4B-NB	6.28	1.40	1.35
25	C	502	CLA	C4B-NB	6.27	1.40	1.35
25	C	505	CLA	C1B-NB	6.27	1.40	1.35
25	R	608	CLA	C4B-NB	6.27	1.40	1.35
25	B	603	CLA	C4B-NB	6.26	1.40	1.35
25	R	601	CLA	MG-ND	-6.26	1.93	2.05
25	r	610	CLA	MG-ND	-6.26	1.93	2.05
25	S	309	CLA	C4B-NB	6.25	1.40	1.35
25	d	402	CLA	C4B-NB	6.25	1.40	1.35
25	B	614	CLA	C4B-NB	6.24	1.40	1.35
25	b	614	CLA	C4B-NB	6.24	1.40	1.35
25	b	603	CLA	C4B-NB	6.24	1.40	1.35
25	b	612	CLA	C4B-NB	6.23	1.40	1.35
25	r	601	CLA	MG-ND	-6.23	1.93	2.05
25	N	611	CLA	C1B-NB	6.22	1.40	1.35
25	n	611	CLA	C1B-NB	6.22	1.40	1.35
25	B	615	CLA	C4B-NB	6.22	1.40	1.35
25	b	615	CLA	C4B-NB	6.22	1.40	1.35
25	s	309	CLA	C4B-NB	6.21	1.40	1.35
25	C	509	CLA	C4B-NB	6.20	1.40	1.35
25	c	509	CLA	C4B-NB	6.20	1.40	1.35
25	D	402	CLA	C4B-NB	6.19	1.40	1.35
25	y	304	CLA	C4B-NB	6.18	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	604	CLA	C4B-NB	6.17	1.40	1.35
25	b	604	CLA	C4B-NB	6.17	1.40	1.35
25	2	605	CLA	C4B-NB	6.17	1.40	1.35
25	6	605	CLA	C4B-NB	6.17	1.40	1.35
25	B	608	CLA	C1B-NB	6.14	1.40	1.35
25	N	603	CLA	C4B-NB	6.14	1.40	1.35
25	n	603	CLA	C4B-NB	6.14	1.40	1.35
25	Y	304	CLA	C4B-NB	6.13	1.40	1.35
25	c	505	CLA	C1B-NB	6.12	1.40	1.35
25	R	603	CLA	MG-ND	-6.12	1.93	2.05
25	r	603	CLA	MG-ND	-6.12	1.93	2.05
25	B	603	CLA	C1B-NB	6.11	1.40	1.35
25	A	401	CLA	C4B-NB	6.11	1.40	1.35
25	a	402	CLA	C4B-NB	6.11	1.40	1.35
25	G	614	CLA	C1B-NB	6.10	1.40	1.35
25	N	604	CLA	C4B-NB	6.09	1.40	1.35
25	c	503	CLA	C4B-NB	6.07	1.40	1.35
25	B	611	CLA	C4B-NB	6.07	1.40	1.35
25	b	611	CLA	C4B-NB	6.07	1.40	1.35
25	A	405	CLA	C4B-NB	6.07	1.40	1.35
25	a	406	CLA	C4B-NB	6.07	1.40	1.35
25	S	305	CLA	MG-ND	-6.06	1.93	2.05
25	s	305	CLA	MG-ND	-6.06	1.93	2.05
25	d	403	CLA	MG-ND	-6.06	1.93	2.05
25	b	603	CLA	C1B-NB	6.06	1.40	1.35
25	n	604	CLA	C4B-NB	6.06	1.40	1.35
25	g	614	CLA	C1B-NB	6.06	1.40	1.35
25	S	304	CLA	C4B-NB	6.06	1.40	1.35
25	s	304	CLA	C4B-NB	6.06	1.40	1.35
25	B	613	CLA	C1B-NB	6.05	1.40	1.35
25	b	613	CLA	C1B-NB	6.05	1.40	1.35
25	S	311	CLA	C4B-NB	6.05	1.40	1.35
25	D	403	CLA	MG-ND	-6.05	1.93	2.05
25	B	604	CLA	C1B-NB	6.04	1.40	1.35
25	B	616	CLA	C1B-NB	6.04	1.40	1.35
25	b	604	CLA	C1B-NB	6.04	1.40	1.35
25	b	616	CLA	C1B-NB	6.04	1.40	1.35
25	Y	304	CLA	C1B-NB	6.04	1.40	1.35
25	C	507	CLA	C1B-NB	6.03	1.40	1.35
25	b	608	CLA	C1B-NB	6.03	1.40	1.35
25	C	513	CLA	C1B-NB	6.02	1.40	1.35
25	c	513	CLA	C1B-NB	6.02	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	607	CLA	C1B-NB	6.01	1.40	1.35
25	C	504	CLA	MG-ND	-6.01	1.93	2.05
25	c	509	CLA	C1B-NB	6.01	1.40	1.35
25	y	304	CLA	C1B-NB	6.01	1.40	1.35
25	c	510	CLA	C4B-NB	6.00	1.40	1.35
25	B	614	CLA	C1B-NB	6.00	1.40	1.35
25	b	614	CLA	C1B-NB	6.00	1.40	1.35
25	s	311	CLA	C4B-NB	5.99	1.40	1.35
25	C	503	CLA	C4B-NB	5.99	1.40	1.35
25	c	503	CLA	C1B-NB	5.99	1.40	1.35
25	c	504	CLA	MG-ND	-5.99	1.93	2.05
25	A	405	CLA	C1B-NB	5.99	1.40	1.35
25	a	406	CLA	C1B-NB	5.99	1.40	1.35
25	c	507	CLA	C1B-NB	5.99	1.40	1.35
25	C	512	CLA	C4B-NB	5.98	1.40	1.35
25	c	512	CLA	C4B-NB	5.98	1.40	1.35
25	2	602	CLA	MG-ND	-5.98	1.93	2.05
25	6	602	CLA	MG-ND	-5.98	1.93	2.05
25	B	607	CLA	C1B-NB	5.97	1.40	1.35
25	C	503	CLA	C1B-NB	5.97	1.40	1.35
25	B	605	CLA	C4B-NB	5.94	1.40	1.35
25	G	603	CLA	C4B-NB	5.94	1.40	1.35
25	g	603	CLA	C4B-NB	5.94	1.40	1.35
25	C	510	CLA	C4B-NB	5.93	1.40	1.35
25	C	509	CLA	C1B-NB	5.93	1.40	1.35
25	2	605	CLA	C1B-NB	5.92	1.40	1.35
25	6	605	CLA	C1B-NB	5.92	1.40	1.35
25	C	512	CLA	C1B-NB	5.92	1.40	1.35
25	c	512	CLA	C1B-NB	5.92	1.40	1.35
25	C	502	CLA	C1B-NB	5.91	1.40	1.35
25	c	502	CLA	C1B-NB	5.91	1.40	1.35
25	d	401	CLA	C4B-NB	5.91	1.40	1.35
25	D	401	CLA	C4B-NB	5.90	1.40	1.35
25	b	605	CLA	C4B-NB	5.90	1.40	1.35
25	N	603	CLA	C1B-NB	5.90	1.40	1.35
25	B	611	CLA	C1B-NB	5.89	1.40	1.35
25	b	611	CLA	C1B-NB	5.89	1.40	1.35
25	G	603	CLA	C1B-NB	5.89	1.40	1.35
25	Y	314	CLA	C4B-NB	5.89	1.40	1.35
25	y	314	CLA	C4B-NB	5.89	1.40	1.35
25	B	612	CLA	C1B-NB	5.86	1.40	1.35
25	N	614	CLA	C4B-NB	5.86	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	612	CLA	C1B-NB	5.86	1.40	1.35
25	C	508	CLA	C4B-NB	5.86	1.40	1.35
25	c	508	CLA	C4B-NB	5.86	1.40	1.35
25	n	603	CLA	C1B-NB	5.86	1.40	1.35
25	n	614	CLA	C4B-NB	5.86	1.40	1.35
25	S	304	CLA	C1B-NB	5.84	1.40	1.35
25	s	304	CLA	C1B-NB	5.84	1.40	1.35
25	B	605	CLA	C1B-NB	5.83	1.40	1.35
25	A	402	CLA	C4B-NB	5.83	1.40	1.35
25	a	403	CLA	C4B-NB	5.83	1.40	1.35
25	c	511	CLA	C4B-NB	5.81	1.40	1.35
25	C	501	CLA	MG-ND	-5.81	1.94	2.05
25	c	501	CLA	MG-ND	-5.81	1.94	2.05
25	B	606	CLA	C4B-NB	5.80	1.40	1.35
25	b	606	CLA	C4B-NB	5.80	1.40	1.35
25	g	603	CLA	C1B-NB	5.79	1.40	1.35
25	G	610	CLA	C4B-NB	5.79	1.40	1.35
25	g	610	CLA	C4B-NB	5.79	1.40	1.35
25	C	511	CLA	C4B-NB	5.78	1.40	1.35
25	b	605	CLA	C1B-NB	5.76	1.40	1.35
25	n	604	CLA	C1B-NB	5.75	1.40	1.35
25	C	511	CLA	C1B-NB	5.74	1.40	1.35
25	A	401	CLA	C1B-NB	5.74	1.40	1.35
25	a	402	CLA	C1B-NB	5.74	1.40	1.35
25	S	311	CLA	C1B-NB	5.74	1.40	1.35
25	B	606	CLA	C1B-NB	5.73	1.40	1.35
25	b	606	CLA	C1B-NB	5.73	1.40	1.35
25	G	611	CLA	C4B-NB	5.73	1.40	1.35
25	C	510	CLA	C1B-NB	5.72	1.40	1.35
25	g	611	CLA	C4B-NB	5.71	1.40	1.35
25	2	604	CLA	MG-ND	-5.71	1.94	2.05
25	D	401	CLA	C1B-NB	5.71	1.40	1.35
25	d	401	CLA	C1B-NB	5.71	1.40	1.35
25	B	601	CLA	C4B-NB	5.70	1.40	1.35
25	B	609	CLA	C1B-NB	5.70	1.40	1.35
25	b	609	CLA	C1B-NB	5.70	1.40	1.35
25	S	313	CLA	C4B-NB	5.69	1.40	1.35
25	s	313	CLA	C4B-NB	5.69	1.40	1.35
25	A	402	CLA	C1B-NB	5.68	1.40	1.35
25	a	403	CLA	C1B-NB	5.68	1.40	1.35
25	y	314	CLA	C1B-NB	5.67	1.40	1.35
25	r	612	CLA	C4B-NB	5.67	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	C1B-NB	5.67	1.40	1.35
25	6	604	CLA	MG-ND	-5.67	1.94	2.05
25	s	311	CLA	C1B-NB	5.66	1.40	1.35
25	R	612	CLA	C4B-NB	5.65	1.40	1.35
25	S	313	CLA	C1B-NB	5.65	1.40	1.35
25	N	604	CLA	C1B-NB	5.64	1.40	1.35
25	b	601	CLA	C4B-NB	5.62	1.40	1.35
25	B	601	CLA	C1B-NB	5.60	1.40	1.35
25	b	601	CLA	C1B-NB	5.60	1.40	1.35
25	c	511	CLA	C1B-NB	5.60	1.40	1.35
25	c	501	CLA	C4B-NB	5.57	1.40	1.35
25	s	313	CLA	C1B-NB	5.57	1.40	1.35
25	G	613	CLA	C1B-NB	5.56	1.40	1.35
25	g	613	CLA	C1B-NB	5.56	1.40	1.35
25	N	613	CLA	C1B-NB	5.56	1.40	1.35
25	n	613	CLA	C1B-NB	5.56	1.40	1.35
25	C	501	CLA	C4B-NB	5.55	1.40	1.35
25	R	604	CLA	C4B-NB	5.53	1.40	1.35
25	r	604	CLA	C4B-NB	5.52	1.40	1.35
25	Y	314	CLA	C1B-NB	5.52	1.40	1.35
24	Y	308	CHL	CMC-C2C	5.48	1.56	1.45
24	y	308	CHL	CMC-C2C	5.48	1.56	1.45
25	N	613	CLA	C4B-NB	5.48	1.40	1.35
24	5	302	CHL	CMC-C2C	5.47	1.56	1.45
25	C	508	CLA	C1B-NB	5.45	1.40	1.35
25	c	508	CLA	C1B-NB	5.45	1.40	1.35
25	n	613	CLA	C4B-NB	5.45	1.40	1.35
24	G	607	CHL	CMC-C2C	5.45	1.56	1.45
24	g	607	CHL	CMC-C2C	5.45	1.56	1.45
24	6	601	CHL	CMC-C2C	5.44	1.56	1.45
24	R	613	CHL	CMC-C2C	5.44	1.56	1.45
25	R	603	CLA	C4B-NB	5.44	1.40	1.35
24	n	601	CHL	CMC-C2C	5.43	1.56	1.45
24	N	601	CHL	CMC-C2C	5.43	1.56	1.45
25	g	613	CLA	C4B-NB	5.43	1.40	1.35
25	G	613	CLA	C4B-NB	5.42	1.40	1.35
24	r	607	CHL	CMC-C2C	5.42	1.56	1.45
24	1	302	CHL	CMC-C2C	5.41	1.56	1.45
24	1	301	CHL	CMC-C2C	5.41	1.56	1.45
24	R	607	CHL	CMC-C2C	5.40	1.56	1.45
24	5	301	CHL	CMC-C2C	5.40	1.56	1.45
24	g	609	CHL	CMC-C2C	5.40	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	601	CHL	CMC-C2C	5.40	1.56	1.45
24	S	308	CHL	CMC-C2C	5.40	1.56	1.45
24	s	308	CHL	CMC-C2C	5.40	1.56	1.45
25	r	612	CLA	C1B-NB	5.39	1.40	1.35
24	r	606	CHL	CMC-C2C	5.39	1.56	1.45
25	C	504	CLA	C4B-NB	5.39	1.40	1.35
40	n	617	NEX	C10-C9	5.39	1.42	1.35
25	D	403	CLA	C4B-NB	5.39	1.40	1.35
24	r	613	CHL	CMC-C2C	5.39	1.56	1.45
24	S	306	CHL	CMC-C2C	5.38	1.56	1.45
24	S	307	CHL	CMC-C2C	5.38	1.56	1.45
24	s	307	CHL	CMC-C2C	5.38	1.56	1.45
24	G	606	CHL	CMC-C2C	5.38	1.56	1.45
24	g	606	CHL	CMC-C2C	5.38	1.56	1.45
40	N	617	NEX	C10-C9	5.38	1.42	1.35
24	R	606	CHL	CMC-C2C	5.38	1.56	1.45
24	s	302	CHL	CMC-C2C	5.37	1.56	1.45
24	Y	309	CHL	CMC-C2C	5.37	1.56	1.45
24	N	605	CHL	CMC-C2C	5.37	1.56	1.45
24	n	605	CHL	CMC-C2C	5.37	1.56	1.45
25	c	504	CLA	C4B-NB	5.37	1.40	1.35
24	G	609	CHL	CMC-C2C	5.37	1.56	1.45
25	R	612	CLA	C1B-NB	5.36	1.40	1.35
25	r	603	CLA	C4B-NB	5.36	1.40	1.35
24	n	608	CHL	CMC-C2C	5.36	1.56	1.45
24	N	609	CHL	CMC-C2C	5.36	1.56	1.45
24	n	609	CHL	CMC-C2C	5.36	1.56	1.45
24	Y	306	CHL	CMC-C2C	5.36	1.56	1.45
24	N	606	CHL	CMC-C2C	5.36	1.56	1.45
24	n	606	CHL	CMC-C2C	5.36	1.56	1.45
24	y	309	CHL	CMC-C2C	5.36	1.56	1.45
24	G	608	CHL	CMC-C2C	5.35	1.56	1.45
24	g	608	CHL	CMC-C2C	5.35	1.56	1.45
24	y	306	CHL	CMC-C2C	5.35	1.56	1.45
25	2	602	CLA	MG-NA	-5.35	1.93	2.06
25	6	602	CLA	MG-NA	-5.35	1.93	2.06
25	d	403	CLA	C4B-NB	5.35	1.40	1.35
24	s	306	CHL	CMC-C2C	5.35	1.56	1.45
25	r	601	CLA	C4B-NB	5.35	1.40	1.35
24	N	608	CHL	CMC-C2C	5.34	1.56	1.45
24	Y	302	CHL	CMC-C2C	5.34	1.56	1.45
24	y	302	CHL	CMC-C2C	5.34	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	605	CHL	CMC-C2C	5.34	1.56	1.45
24	N	607	CHL	CMC-C2C	5.34	1.56	1.45
24	n	607	CHL	CMC-C2C	5.34	1.56	1.45
24	G	605	CHL	CMC-C2C	5.33	1.56	1.45
24	S	302	CHL	CMC-C2C	5.33	1.56	1.45
24	Y	307	CHL	CMC-C2C	5.33	1.56	1.45
24	Y	310	CHL	CMC-C2C	5.33	1.56	1.45
24	y	310	CHL	CMC-C2C	5.33	1.56	1.45
25	R	611	CLA	MG-NA	-5.32	1.93	2.06
25	r	611	CLA	MG-NA	-5.32	1.93	2.06
24	R	605	CHL	CMC-C2C	5.32	1.56	1.45
24	G	601	CHL	CMC-C2C	5.32	1.56	1.45
24	g	601	CHL	CMC-C2C	5.32	1.56	1.45
24	y	307	CHL	CMC-C2C	5.32	1.56	1.45
25	2	602	CLA	MG-NC	-5.31	1.93	2.06
25	6	602	CLA	MG-NC	-5.31	1.93	2.06
25	r	610	CLA	C4B-NB	5.30	1.39	1.35
25	R	601	CLA	C4B-NB	5.29	1.39	1.35
25	S	305	CLA	C4B-NB	5.29	1.39	1.35
25	s	305	CLA	C4B-NB	5.29	1.39	1.35
24	g	605	CHL	CMC-C2C	5.28	1.56	1.45
25	R	611	CLA	MG-NC	-5.28	1.93	2.06
25	r	611	CLA	MG-NC	-5.28	1.93	2.06
40	y	318	NEX	C10-C9	5.26	1.42	1.35
25	R	610	CLA	C4B-NB	5.23	1.39	1.35
25	2	604	CLA	C4B-NB	5.22	1.39	1.35
25	6	604	CLA	C4B-NB	5.22	1.39	1.35
40	Y	318	NEX	C10-C9	5.21	1.42	1.35
25	G	611	CLA	MG-ND	-5.18	1.95	2.05
25	g	611	CLA	MG-ND	-5.18	1.95	2.05
25	r	604	CLA	C1B-NB	5.18	1.39	1.35
25	R	604	CLA	C1B-NB	5.18	1.39	1.35
25	r	610	CLA	MG-NA	-5.17	1.94	2.06
25	g	610	CLA	MG-ND	-5.14	1.95	2.05
25	R	610	CLA	MG-NA	-5.13	1.94	2.06
24	2	603	CHL	CMC-C2C	5.13	1.56	1.45
25	g	610	CLA	C1B-NB	5.13	1.39	1.35
25	G	610	CLA	MG-ND	-5.10	1.95	2.05
25	2	604	CLA	C1B-NB	5.10	1.39	1.35
25	6	604	CLA	C1B-NB	5.10	1.39	1.35
24	6	603	CHL	CMC-C2C	5.09	1.55	1.45
25	g	611	CLA	C1B-NB	5.08	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	305	CLA	MG-NA	-5.06	1.94	2.06
25	s	305	CLA	MG-NA	-5.06	1.94	2.06
25	G	610	CLA	C1B-NB	5.04	1.39	1.35
40	R	617	NEX	C10-C9	5.04	1.42	1.35
40	r	617	NEX	C10-C9	5.04	1.42	1.35
25	G	611	CLA	C1B-NB	5.00	1.39	1.35
25	R	611	CLA	C4B-NB	4.99	1.39	1.35
25	R	604	CLA	MG-ND	-4.99	1.95	2.05
25	R	610	CLA	MG-NC	-4.94	1.94	2.06
25	r	604	CLA	MG-ND	-4.93	1.96	2.05
25	R	612	CLA	MG-ND	-4.93	1.96	2.05
25	r	610	CLA	MG-NC	-4.92	1.94	2.06
25	D	403	CLA	MG-NA	-4.91	1.94	2.06
25	c	504	CLA	MG-NA	-4.91	1.94	2.06
25	r	612	CLA	MG-ND	-4.90	1.96	2.05
25	d	403	CLA	MG-NA	-4.90	1.94	2.06
25	C	504	CLA	MG-NA	-4.89	1.94	2.06
25	s	305	CLA	MG-NC	-4.89	1.94	2.06
25	r	603	CLA	MG-NA	-4.88	1.94	2.06
40	s	317	NEX	C10-C9	4.88	1.42	1.35
25	R	603	CLA	MG-NA	-4.87	1.94	2.06
25	r	611	CLA	C4B-NB	4.87	1.39	1.35
25	S	305	CLA	MG-NC	-4.86	1.94	2.06
40	S	317	NEX	C10-C9	4.85	1.42	1.35
25	R	601	CLA	MG-NA	-4.85	1.94	2.06
25	r	601	CLA	MG-NA	-4.85	1.94	2.06
25	d	403	CLA	MG-NC	-4.82	1.94	2.06
25	r	601	CLA	MG-NC	-4.81	1.94	2.06
25	n	614	CLA	MG-ND	-4.81	1.96	2.05
25	D	403	CLA	MG-NC	-4.79	1.94	2.06
25	N	614	CLA	MG-ND	-4.79	1.96	2.05
25	s	313	CLA	MG-ND	-4.79	1.96	2.05
25	R	601	CLA	MG-NC	-4.78	1.94	2.06
40	g	617	NEX	C10-C9	4.76	1.42	1.35
25	C	504	CLA	MG-NC	-4.76	1.95	2.06
25	g	613	CLA	MG-NA	-4.75	1.95	2.06
25	c	504	CLA	MG-NC	-4.75	1.95	2.06
25	S	313	CLA	MG-ND	-4.75	1.96	2.05
25	R	603	CLA	MG-NC	-4.75	1.95	2.06
25	r	603	CLA	MG-NC	-4.75	1.95	2.06
25	6	602	CLA	C4B-NB	4.72	1.39	1.35
25	B	601	CLA	MG-ND	-4.72	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	601	CLA	MG-ND	-4.72	1.96	2.05
25	N	614	CLA	C1B-NB	4.71	1.39	1.35
25	G	613	CLA	MG-NA	-4.71	1.95	2.06
25	2	602	CLA	C1B-NB	4.69	1.39	1.35
25	6	602	CLA	C1B-NB	4.69	1.39	1.35
25	2	602	CLA	C4B-NB	4.69	1.39	1.35
25	g	613	CLA	MG-ND	-4.68	1.96	2.05
25	C	501	CLA	MG-NA	-4.67	1.95	2.06
25	c	501	CLA	MG-NA	-4.67	1.95	2.06
25	G	613	CLA	MG-ND	-4.64	1.96	2.05
25	2	604	CLA	MG-NC	-4.62	1.95	2.06
25	6	604	CLA	MG-NC	-4.62	1.95	2.06
25	n	614	CLA	C1B-NB	4.60	1.39	1.35
25	C	501	CLA	MG-NC	-4.59	1.95	2.06
25	c	501	CLA	MG-NC	-4.59	1.95	2.06
25	c	507	CLA	MG-ND	-4.58	1.96	2.05
25	C	507	CLA	MG-ND	-4.57	1.96	2.05
25	R	611	CLA	C1B-NB	4.56	1.39	1.35
25	C	508	CLA	MG-ND	-4.55	1.96	2.05
25	c	508	CLA	MG-ND	-4.55	1.96	2.05
25	A	402	CLA	MG-ND	-4.55	1.96	2.05
25	N	612	CLA	MG-NA	-4.54	1.95	2.06
29	A	411	SQD	O8-S	4.54	1.63	1.47
29	a	412	SQD	O8-S	4.54	1.63	1.47
29	A	407	SQD	O8-S	4.54	1.63	1.47
29	a	408	SQD	O8-S	4.54	1.63	1.47
29	L	103	SQD	O8-S	4.54	1.63	1.47
29	l	101	SQD	O8-S	4.54	1.63	1.47
25	B	606	CLA	MG-ND	-4.53	1.96	2.05
25	b	606	CLA	MG-ND	-4.53	1.96	2.05
29	l	102	SQD	O8-S	4.53	1.63	1.47
25	a	403	CLA	MG-ND	-4.52	1.96	2.05
29	L	101	SQD	O8-S	4.51	1.63	1.47
25	S	311	CLA	MG-ND	-4.51	1.96	2.05
25	n	612	CLA	MG-NA	-4.51	1.95	2.06
25	r	611	CLA	C1B-NB	4.49	1.39	1.35
25	C	512	CLA	MG-ND	-4.49	1.96	2.05
25	c	512	CLA	MG-ND	-4.49	1.96	2.05
25	r	609	CLA	MG-ND	-4.49	1.96	2.05
25	C	511	CLA	MG-ND	-4.49	1.96	2.05
25	c	511	CLA	MG-ND	-4.49	1.96	2.05
25	6	604	CLA	MG-NA	-4.49	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	MG-ND	-4.49	1.96	2.05
25	2	604	CLA	MG-NA	-4.48	1.95	2.06
25	C	510	CLA	MG-ND	-4.48	1.96	2.05
25	s	311	CLA	MG-ND	-4.47	1.96	2.05
25	D	401	CLA	MG-ND	-4.46	1.96	2.05
25	d	401	CLA	MG-ND	-4.46	1.96	2.05
25	6	605	CLA	MG-ND	-4.46	1.97	2.05
40	Y	318	NEX	C14-C13	4.45	1.41	1.35
25	A	401	CLA	MG-ND	-4.45	1.97	2.05
25	a	402	CLA	MG-ND	-4.45	1.97	2.05
25	B	605	CLA	MG-ND	-4.44	1.97	2.05
25	b	605	CLA	MG-ND	-4.44	1.97	2.05
25	2	605	CLA	MG-ND	-4.43	1.97	2.05
40	y	318	NEX	C14-C13	4.43	1.41	1.35
25	R	609	CLA	MG-ND	-4.43	1.97	2.05
25	C	509	CLA	MG-ND	-4.42	1.97	2.05
25	s	304	CLA	MG-ND	-4.42	1.97	2.05
25	c	509	CLA	MG-ND	-4.41	1.97	2.05
25	S	312	CLA	MG-NA	-4.41	1.95	2.06
25	s	312	CLA	MG-NA	-4.41	1.95	2.06
25	B	612	CLA	MG-ND	-4.41	1.97	2.05
25	b	612	CLA	MG-ND	-4.41	1.97	2.05
25	S	304	CLA	MG-ND	-4.40	1.97	2.05
25	B	604	CLA	MG-ND	-4.39	1.97	2.05
25	b	604	CLA	MG-ND	-4.39	1.97	2.05
25	y	304	CLA	MG-ND	-4.36	1.97	2.05
25	N	613	CLA	MG-NA	-4.34	1.96	2.06
25	n	613	CLA	MG-NA	-4.34	1.96	2.06
25	n	613	CLA	MG-ND	-4.34	1.97	2.05
25	B	615	CLA	MG-NA	-4.32	1.96	2.06
25	b	615	CLA	MG-NA	-4.32	1.96	2.06
25	D	402	CLA	MG-ND	-4.31	1.97	2.05
25	d	402	CLA	MG-ND	-4.31	1.97	2.05
25	N	613	CLA	MG-ND	-4.31	1.97	2.05
25	Y	304	CLA	MG-ND	-4.30	1.97	2.05
25	A	405	CLA	MG-ND	-4.28	1.97	2.05
25	a	406	CLA	MG-ND	-4.28	1.97	2.05
25	N	604	CLA	MG-ND	-4.27	1.97	2.05
25	n	604	CLA	MG-ND	-4.27	1.97	2.05
25	G	611	CLA	C1D-C2D	-4.27	1.36	1.45
25	C	513	CLA	MG-ND	-4.27	1.97	2.05
25	R	612	CLA	MG-NA	-4.26	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	611	CLA	C1D-C2D	-4.26	1.36	1.45
25	b	602	CLA	MG-ND	-4.25	1.97	2.05
25	C	503	CLA	MG-ND	-4.25	1.97	2.05
25	c	503	CLA	MG-ND	-4.25	1.97	2.05
25	N	603	CLA	MG-ND	-4.25	1.97	2.05
25	n	603	CLA	MG-ND	-4.25	1.97	2.05
25	S	310	CLA	MG-ND	-4.25	1.97	2.05
25	s	310	CLA	MG-ND	-4.25	1.97	2.05
25	R	608	CLA	MG-ND	-4.25	1.97	2.05
25	r	612	CLA	MG-NA	-4.24	1.96	2.06
25	r	608	CLA	MG-ND	-4.24	1.97	2.05
25	c	513	CLA	MG-ND	-4.23	1.97	2.05
25	B	611	CLA	MG-ND	-4.23	1.97	2.05
25	b	611	CLA	MG-ND	-4.23	1.97	2.05
25	b	615	CLA	MG-ND	-4.22	1.97	2.05
25	G	603	CLA	MG-ND	-4.22	1.97	2.05
25	B	602	CLA	MG-ND	-4.22	1.97	2.05
25	b	609	CLA	MG-ND	-4.21	1.97	2.05
25	N	611	CLA	MG-ND	-4.20	1.97	2.05
25	D	402	CLA	MG-NA	-4.20	1.96	2.06
25	S	309	CLA	MG-ND	-4.19	1.97	2.05
25	d	402	CLA	MG-NA	-4.19	1.96	2.06
25	B	615	CLA	MG-ND	-4.18	1.97	2.05
25	S	303	CLA	MG-ND	-4.17	1.97	2.05
25	s	303	CLA	MG-ND	-4.17	1.97	2.05
25	g	603	CLA	MG-ND	-4.17	1.97	2.05
25	S	313	CLA	MG-NA	-4.17	1.96	2.06
25	n	611	CLA	MG-ND	-4.17	1.97	2.05
40	n	617	NEX	C14-C13	4.17	1.41	1.35
25	R	602	CLA	MG-ND	-4.16	1.97	2.05
25	b	607	CLA	MG-ND	-4.16	1.97	2.05
40	N	617	NEX	C14-C13	4.16	1.41	1.35
25	S	312	CLA	MG-ND	-4.16	1.97	2.05
25	b	603	CLA	MG-ND	-4.16	1.97	2.05
25	s	313	CLA	MG-NA	-4.15	1.96	2.06
25	s	309	CLA	MG-ND	-4.14	1.97	2.05
25	Y	315	CLA	MG-ND	-4.14	1.97	2.05
25	B	607	CLA	MG-ND	-4.14	1.97	2.05
25	B	609	CLA	MG-ND	-4.14	1.97	2.05
25	n	612	CLA	MG-ND	-4.14	1.97	2.05
25	Y	312	CLA	MG-ND	-4.14	1.97	2.05
25	y	315	CLA	MG-ND	-4.14	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	609	CLA	MG-NA	-4.13	1.96	2.06
25	G	604	CLA	MG-ND	-4.12	1.97	2.05
25	g	604	CLA	MG-ND	-4.12	1.97	2.05
25	B	603	CLA	MG-ND	-4.12	1.97	2.05
25	y	312	CLA	MG-ND	-4.12	1.97	2.05
25	B	613	CLA	MG-ND	-4.11	1.97	2.05
25	s	312	CLA	MG-ND	-4.11	1.97	2.05
25	y	314	CLA	MG-ND	-4.11	1.97	2.05
25	S	309	CLA	MG-NA	-4.11	1.96	2.06
25	s	309	CLA	MG-NA	-4.11	1.96	2.06
25	B	608	CLA	MG-ND	-4.10	1.97	2.05
25	r	602	CLA	MG-ND	-4.10	1.97	2.05
25	C	502	CLA	MG-ND	-4.10	1.97	2.05
25	c	502	CLA	MG-ND	-4.10	1.97	2.05
25	R	609	CLA	MG-NA	-4.10	1.96	2.06
25	g	612	CLA	MG-NA	-4.09	1.96	2.06
25	b	608	CLA	MG-ND	-4.09	1.97	2.05
25	R	604	CLA	MG-NA	-4.09	1.96	2.06
25	r	604	CLA	MG-NA	-4.09	1.96	2.06
40	r	617	NEX	C14-C13	4.09	1.41	1.35
25	c	506	CLA	MG-ND	-4.08	1.97	2.05
25	G	610	CLA	MG-NA	-4.08	1.96	2.06
25	N	612	CLA	MG-ND	-4.07	1.97	2.05
25	g	610	CLA	MG-NA	-4.07	1.96	2.06
25	C	511	CLA	MG-NA	-4.07	1.96	2.06
25	c	511	CLA	MG-NA	-4.07	1.96	2.06
25	Y	314	CLA	MG-ND	-4.07	1.97	2.05
25	b	613	CLA	MG-ND	-4.06	1.97	2.05
40	R	617	NEX	C14-C13	4.06	1.41	1.35
25	B	614	CLA	MG-ND	-4.06	1.97	2.05
25	b	614	CLA	MG-ND	-4.06	1.97	2.05
25	B	601	CLA	MG-NA	-4.05	1.96	2.06
25	S	314	CLA	MG-ND	-4.05	1.97	2.05
25	s	314	CLA	MG-ND	-4.05	1.97	2.05
25	G	612	CLA	MG-NA	-4.05	1.96	2.06
25	B	610	CLA	MG-ND	-4.04	1.97	2.05
25	g	614	CLA	MG-ND	-4.04	1.97	2.05
25	G	611	CLA	MG-NA	-4.03	1.96	2.06
25	g	611	CLA	MG-NA	-4.03	1.96	2.06
25	C	506	CLA	MG-ND	-4.03	1.97	2.05
25	b	616	CLA	MG-ND	-4.03	1.97	2.05
25	r	614	CLA	MG-NA	-4.02	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	601	CLA	MG-NA	-4.02	1.96	2.06
25	G	614	CLA	MG-ND	-4.02	1.97	2.05
25	R	614	CLA	MG-NA	-4.01	1.96	2.06
25	s	310	CLA	MG-NA	-4.01	1.96	2.06
25	N	602	CLA	MG-ND	-4.01	1.97	2.05
25	B	616	CLA	MG-ND	-4.01	1.97	2.05
25	b	610	CLA	MG-ND	-4.00	1.97	2.05
25	S	310	CLA	MG-NA	-4.00	1.96	2.06
24	R	613	CHL	C4B-NB	3.99	1.38	1.35
24	r	613	CHL	C4B-NB	3.99	1.38	1.35
25	Y	305	CLA	MG-ND	-3.98	1.97	2.05
25	y	305	CLA	MG-ND	-3.98	1.97	2.05
25	n	602	CLA	MG-ND	-3.98	1.97	2.05
24	R	605	CHL	C4B-NB	3.98	1.38	1.35
25	Y	311	CLA	MG-ND	-3.97	1.97	2.05
25	y	311	CLA	MG-ND	-3.97	1.97	2.05
25	y	312	CLA	C1D-C2D	-3.97	1.37	1.45
25	B	610	CLA	MG-NA	-3.96	1.96	2.06
25	b	610	CLA	MG-NA	-3.96	1.96	2.06
25	Y	312	CLA	C1D-C2D	-3.96	1.37	1.45
25	y	303	CLA	MG-NA	-3.95	1.96	2.06
25	N	610	CLA	MG-ND	-3.94	1.98	2.05
25	n	610	CLA	MG-ND	-3.94	1.98	2.05
25	Y	313	CLA	MG-ND	-3.93	1.98	2.05
24	s	306	CHL	C4B-NB	3.93	1.38	1.35
25	Y	303	CLA	MG-NA	-3.93	1.96	2.06
25	c	507	CLA	MG-NA	-3.93	1.96	2.06
25	y	313	CLA	MG-ND	-3.92	1.98	2.05
24	G	606	CHL	C4B-NB	3.92	1.38	1.35
24	g	606	CHL	C4B-NB	3.92	1.38	1.35
25	G	602	CLA	MG-ND	-3.91	1.98	2.05
24	r	605	CHL	C4B-NB	3.91	1.38	1.35
24	1	302	CHL	C4B-NB	3.91	1.38	1.35
24	5	302	CHL	C4B-NB	3.91	1.38	1.35
25	C	507	CLA	MG-NA	-3.90	1.97	2.06
25	N	611	CLA	C1D-C2D	-3.90	1.37	1.45
25	n	611	CLA	C1D-C2D	-3.90	1.37	1.45
25	g	602	CLA	MG-ND	-3.90	1.98	2.05
24	S	306	CHL	C4B-NB	3.89	1.38	1.35
24	G	605	CHL	C4B-NB	3.89	1.38	1.35
24	G	608	CHL	C4B-NB	3.89	1.38	1.35
24	g	608	CHL	C4B-NB	3.89	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	306	CHL	C4B-NB	3.89	1.38	1.35
24	G	609	CHL	C4B-NB	3.89	1.38	1.35
24	g	609	CHL	C4B-NB	3.89	1.38	1.35
24	Y	310	CHL	C4B-NB	3.89	1.38	1.35
24	y	310	CHL	C4B-NB	3.89	1.38	1.35
24	y	307	CHL	C3B-C2B	-3.89	1.35	1.40
25	C	505	CLA	MG-ND	-3.89	1.98	2.05
25	c	505	CLA	MG-ND	-3.89	1.98	2.05
25	N	602	CLA	MG-NA	-3.88	1.97	2.06
24	s	307	CHL	C4B-NB	3.88	1.38	1.35
25	n	602	CLA	MG-NA	-3.87	1.97	2.06
24	R	606	CHL	C4B-NB	3.87	1.38	1.35
24	r	606	CHL	C4B-NB	3.87	1.38	1.35
24	N	606	CHL	C4B-NB	3.87	1.38	1.35
24	n	606	CHL	C4B-NB	3.87	1.38	1.35
25	Y	303	CLA	MG-ND	-3.87	1.98	2.05
25	y	303	CLA	MG-ND	-3.87	1.98	2.05
25	S	312	CLA	MG-NC	-3.87	1.97	2.06
25	s	312	CLA	MG-NC	-3.87	1.97	2.06
25	n	612	CLA	MG-NC	-3.86	1.97	2.06
25	s	311	CLA	MG-NA	-3.86	1.97	2.06
25	N	612	CLA	MG-NC	-3.86	1.97	2.06
25	S	311	CLA	MG-NA	-3.85	1.97	2.06
25	R	612	CLA	MG-NC	-3.85	1.97	2.06
25	g	602	CLA	MG-NA	-3.85	1.97	2.06
24	S	308	CHL	C4B-NB	3.85	1.38	1.35
24	s	308	CHL	C4B-NB	3.85	1.38	1.35
24	S	307	CHL	C4B-NB	3.85	1.38	1.35
25	s	313	CLA	MG-NC	-3.85	1.97	2.06
28	B	617	BCR	C1-C6	-3.84	1.48	1.53
28	b	617	BCR	C1-C6	-3.84	1.48	1.53
24	Y	307	CHL	C3B-C2B	-3.84	1.35	1.40
25	c	508	CLA	MG-NA	-3.84	1.97	2.06
24	N	605	CHL	C4B-NB	3.84	1.38	1.35
24	n	605	CHL	C4B-NB	3.84	1.38	1.35
25	B	615	CLA	MG-NC	-3.84	1.97	2.06
25	b	615	CLA	MG-NC	-3.84	1.97	2.06
24	y	306	CHL	C4B-NB	3.84	1.38	1.35
25	G	612	CLA	MG-ND	-3.83	1.98	2.05
38	F	101	HEM	C1B-NB	-3.83	1.33	1.40
25	A	402	CLA	MG-NA	-3.83	1.97	2.06
25	a	403	CLA	MG-NA	-3.83	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	610	CLA	MG-NC	-3.83	1.97	2.06
24	r	607	CHL	C4B-NB	3.83	1.38	1.35
25	6	605	CLA	MG-NA	-3.83	1.97	2.06
25	r	612	CLA	MG-NC	-3.82	1.97	2.06
25	G	602	CLA	MG-NA	-3.82	1.97	2.06
24	1	301	CHL	C4B-NB	3.82	1.38	1.35
25	C	508	CLA	MG-NA	-3.82	1.97	2.06
25	S	313	CLA	MG-NC	-3.82	1.97	2.06
25	d	402	CLA	MG-NC	-3.82	1.97	2.06
24	g	605	CHL	C4B-NB	3.82	1.38	1.35
25	G	610	CLA	MG-NC	-3.82	1.97	2.06
38	f	101	HEM	C4D-ND	-3.82	1.33	1.40
25	C	507	CLA	MG-NC	-3.82	1.97	2.06
25	R	604	CLA	MG-NC	-3.82	1.97	2.06
25	B	604	CLA	MG-NA	-3.81	1.97	2.06
25	D	402	CLA	MG-NC	-3.81	1.97	2.06
25	b	604	CLA	MG-NA	-3.81	1.97	2.06
25	N	614	CLA	MG-NA	-3.81	1.97	2.06
25	n	614	CLA	MG-NA	-3.81	1.97	2.06
25	Y	313	CLA	C1D-C2D	-3.80	1.37	1.45
25	y	313	CLA	C1D-C2D	-3.80	1.37	1.45
40	Y	318	NEX	C34-C33	3.80	1.40	1.35
28	D	404	BCR	C1-C6	-3.80	1.48	1.53
28	d	404	BCR	C1-C6	-3.80	1.48	1.53
25	g	612	CLA	MG-ND	-3.79	1.98	2.05
25	c	507	CLA	MG-NC	-3.79	1.97	2.06
25	r	604	CLA	MG-NC	-3.79	1.97	2.06
25	y	313	CLA	MG-NA	-3.79	1.97	2.06
24	n	607	CHL	C4B-NB	3.78	1.38	1.35
24	g	607	CHL	C4B-NB	3.78	1.38	1.35
25	B	605	CLA	MG-NA	-3.78	1.97	2.06
24	y	309	CHL	C4B-NB	3.77	1.38	1.35
25	n	614	CLA	MG-NC	-3.77	1.97	2.06
25	N	614	CLA	MG-NC	-3.77	1.97	2.06
38	f	101	HEM	C1B-NB	-3.77	1.33	1.40
24	N	607	CHL	C4B-NB	3.77	1.38	1.35
25	2	605	CLA	MG-NA	-3.77	1.97	2.06
25	R	614	CLA	MG-ND	-3.77	1.98	2.05
25	D	401	CLA	MG-NA	-3.77	1.97	2.06
25	d	401	CLA	MG-NA	-3.77	1.97	2.06
24	N	608	CHL	C4B-NB	3.76	1.38	1.35
24	5	301	CHL	C4B-NB	3.76	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	608	CHL	C4B-NB	3.76	1.38	1.35
25	c	506	CLA	MG-NA	-3.76	1.97	2.06
25	R	602	CLA	MG-NA	-3.76	1.97	2.06
25	Y	313	CLA	MG-NA	-3.76	1.97	2.06
38	F	101	HEM	C4D-ND	-3.75	1.33	1.40
25	s	304	CLA	MG-NA	-3.75	1.97	2.06
25	r	614	CLA	MG-ND	-3.75	1.98	2.05
25	R	609	CLA	MG-NC	-3.75	1.97	2.06
25	A	401	CLA	MG-NA	-3.74	1.97	2.06
25	a	402	CLA	MG-NA	-3.74	1.97	2.06
25	r	602	CLA	MG-NA	-3.74	1.97	2.06
25	S	304	CLA	MG-NA	-3.74	1.97	2.06
25	b	605	CLA	MG-NA	-3.74	1.97	2.06
24	R	607	CHL	C4B-NB	3.73	1.38	1.35
40	y	318	NEX	C34-C33	3.73	1.40	1.35
25	Y	314	CLA	MG-NA	-3.73	1.97	2.06
25	y	314	CLA	MG-NA	-3.73	1.97	2.06
25	C	506	CLA	MG-NA	-3.73	1.97	2.06
25	B	606	CLA	MG-NA	-3.72	1.97	2.06
25	b	606	CLA	MG-NA	-3.72	1.97	2.06
24	Y	309	CHL	C4B-NB	3.72	1.38	1.35
25	C	510	CLA	MG-NA	-3.71	1.97	2.06
25	c	510	CLA	MG-NA	-3.71	1.97	2.06
25	S	305	CLA	C1B-NB	3.71	1.38	1.35
25	s	305	CLA	C1B-NB	3.71	1.38	1.35
24	G	607	CHL	C4B-NB	3.71	1.38	1.35
25	r	609	CLA	MG-NC	-3.71	1.97	2.06
25	r	614	CLA	MG-NC	-3.70	1.97	2.06
25	C	512	CLA	MG-NA	-3.70	1.97	2.06
25	c	512	CLA	MG-NA	-3.70	1.97	2.06
24	2	601	CHL	C4B-NB	3.69	1.38	1.35
24	6	601	CHL	C4B-NB	3.69	1.38	1.35
25	S	309	CLA	MG-NC	-3.69	1.97	2.06
25	s	309	CLA	MG-NC	-3.69	1.97	2.06
24	2	603	CHL	C4B-NB	3.68	1.38	1.35
28	i	101	BCR	C1-C6	-3.68	1.48	1.53
25	R	614	CLA	MG-NC	-3.68	1.97	2.06
25	b	601	CLA	MG-NC	-3.68	1.97	2.06
25	C	513	CLA	MG-NA	-3.67	1.97	2.06
25	c	513	CLA	MG-NA	-3.67	1.97	2.06
25	A	405	CLA	MG-NA	-3.67	1.97	2.06
25	a	406	CLA	MG-NA	-3.67	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	501	CLA	C1B-NB	3.66	1.38	1.35
24	N	609	CHL	C4B-NB	3.66	1.38	1.35
24	n	609	CHL	C4B-NB	3.66	1.38	1.35
25	B	602	CLA	MG-NA	-3.65	1.97	2.06
25	b	602	CLA	MG-NA	-3.65	1.97	2.06
25	S	314	CLA	MG-NA	-3.65	1.97	2.06
25	s	314	CLA	MG-NA	-3.65	1.97	2.06
24	2	603	CHL	OBD-CAD	3.64	1.28	1.22
24	6	603	CHL	OBD-CAD	3.64	1.28	1.22
25	B	601	CLA	MG-NC	-3.64	1.97	2.06
25	B	610	CLA	MG-NC	-3.64	1.97	2.06
25	b	610	CLA	MG-NC	-3.64	1.97	2.06
25	d	403	CLA	C1B-NB	3.64	1.38	1.35
25	B	603	CLA	MG-NA	-3.64	1.97	2.06
25	b	603	CLA	MG-NA	-3.64	1.97	2.06
25	g	603	CLA	MG-NA	-3.63	1.97	2.06
25	B	612	CLA	MG-NA	-3.63	1.97	2.06
28	I	101	BCR	C1-C6	-3.63	1.48	1.53
28	T	101	BCR	C1-C6	-3.63	1.48	1.53
28	t	101	BCR	C1-C6	-3.63	1.48	1.53
25	b	612	CLA	MG-NA	-3.63	1.97	2.06
25	C	503	CLA	MG-NA	-3.62	1.97	2.06
25	c	503	CLA	MG-NA	-3.62	1.97	2.06
25	C	502	CLA	C1D-C2D	-3.62	1.38	1.45
25	c	502	CLA	C1D-C2D	-3.62	1.38	1.45
25	B	610	CLA	C1D-C2D	-3.62	1.38	1.45
25	b	610	CLA	C1D-C2D	-3.62	1.38	1.45
25	G	603	CLA	MG-NA	-3.62	1.97	2.06
25	n	610	CLA	C1D-C2D	-3.61	1.38	1.45
25	C	501	CLA	C1B-NB	3.61	1.38	1.35
25	C	511	CLA	MG-NC	-3.61	1.97	2.06
25	c	511	CLA	MG-NC	-3.61	1.97	2.06
25	n	604	CLA	MG-NA	-3.61	1.97	2.06
25	g	612	CLA	C1D-C2D	-3.61	1.38	1.45
25	N	614	CLA	C1D-C2D	-3.60	1.38	1.45
25	n	614	CLA	C1D-C2D	-3.60	1.38	1.45
25	n	603	CLA	MG-NA	-3.60	1.97	2.06
24	N	607	CHL	O2D-CGD	3.60	1.42	1.33
24	n	607	CHL	O2D-CGD	3.60	1.42	1.33
25	n	610	CLA	MG-NA	-3.60	1.97	2.06
24	6	603	CHL	C4B-NB	3.60	1.38	1.35
25	y	304	CLA	MG-NA	-3.60	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	514	BCR	C1-C6	-3.60	1.48	1.53
28	c	514	BCR	C1-C6	-3.60	1.48	1.53
25	N	610	CLA	C1D-C2D	-3.59	1.38	1.45
25	R	603	CLA	C1B-NB	3.59	1.38	1.35
25	N	604	CLA	MG-NA	-3.59	1.97	2.06
24	Y	302	CHL	C4B-NB	3.59	1.38	1.35
24	y	302	CHL	C4B-NB	3.59	1.38	1.35
25	Y	311	CLA	C1D-C2D	-3.59	1.38	1.45
24	g	601	CHL	C4B-NB	3.59	1.38	1.35
25	g	604	CLA	MG-NA	-3.58	1.97	2.06
25	N	610	CLA	MG-NA	-3.58	1.97	2.06
25	R	601	CLA	C1B-NB	3.58	1.38	1.35
25	r	601	CLA	C1B-NB	3.58	1.38	1.35
25	y	311	CLA	C1D-C2D	-3.58	1.38	1.45
25	Y	304	CLA	C1D-C2D	-3.58	1.38	1.45
25	S	303	CLA	MG-NA	-3.58	1.97	2.06
25	s	303	CLA	MG-NA	-3.58	1.97	2.06
25	Y	303	CLA	C1D-C2D	-3.57	1.38	1.45
25	y	303	CLA	C1D-C2D	-3.57	1.38	1.45
25	Y	311	CLA	MG-NA	-3.57	1.97	2.06
25	y	311	CLA	MG-NA	-3.57	1.97	2.06
25	Y	304	CLA	MG-NA	-3.57	1.97	2.06
25	c	509	CLA	MG-NA	-3.57	1.97	2.06
25	C	509	CLA	MG-NA	-3.57	1.97	2.06
25	S	310	CLA	C1D-C2D	-3.57	1.38	1.45
25	N	603	CLA	MG-NA	-3.57	1.97	2.06
24	Y	308	CHL	O2D-CGD	3.57	1.41	1.33
24	y	308	CHL	O2D-CGD	3.57	1.41	1.33
25	G	612	CLA	MG-NC	-3.56	1.97	2.06
25	G	604	CLA	MG-NA	-3.56	1.97	2.06
25	B	615	CLA	C1D-C2D	-3.56	1.38	1.45
25	s	310	CLA	C1D-C2D	-3.55	1.38	1.45
25	N	611	CLA	MG-NA	-3.55	1.97	2.06
25	n	611	CLA	MG-NA	-3.55	1.97	2.06
25	N	612	CLA	C1D-C2D	-3.55	1.38	1.45
25	2	605	CLA	MG-NC	-3.55	1.97	2.06
25	b	607	CLA	MG-NA	-3.55	1.97	2.06
25	B	612	CLA	MG-NC	-3.55	1.97	2.06
25	b	612	CLA	MG-NC	-3.55	1.97	2.06
25	G	603	CLA	C1D-C2D	-3.55	1.38	1.45
25	g	603	CLA	C1D-C2D	-3.55	1.38	1.45
25	N	602	CLA	C1D-C2D	-3.55	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	g	617	NEX	C14-C13	3.55	1.40	1.35
25	B	606	CLA	MG-NC	-3.55	1.97	2.06
25	b	606	CLA	MG-NC	-3.55	1.97	2.06
24	N	601	CHL	C4B-NB	3.54	1.38	1.35
25	B	611	CLA	MG-NA	-3.54	1.97	2.06
25	b	611	CLA	MG-NA	-3.54	1.97	2.06
25	B	613	CLA	C1D-C2D	-3.54	1.38	1.45
25	b	613	CLA	C1D-C2D	-3.54	1.38	1.45
25	C	508	CLA	MG-NC	-3.54	1.97	2.06
25	A	402	CLA	MG-NC	-3.54	1.97	2.06
25	a	403	CLA	MG-NC	-3.54	1.97	2.06
25	g	614	CLA	MG-NA	-3.54	1.97	2.06
25	y	304	CLA	C1D-C2D	-3.54	1.38	1.45
25	G	614	CLA	MG-NA	-3.54	1.97	2.06
24	1	301	CHL	O2D-CGD	3.53	1.41	1.33
24	5	301	CHL	O2D-CGD	3.53	1.41	1.33
25	D	403	CLA	C1B-NB	3.53	1.38	1.35
25	G	602	CLA	C1D-C2D	-3.53	1.38	1.45
25	g	602	CLA	C1D-C2D	-3.53	1.38	1.45
25	g	612	CLA	MG-NC	-3.53	1.97	2.06
24	g	606	CHL	O2D-CGD	3.53	1.41	1.33
28	I	101	BCR	C30-C25	-3.53	1.48	1.53
25	S	311	CLA	MG-NC	-3.53	1.97	2.06
25	c	508	CLA	MG-NC	-3.53	1.97	2.06
25	b	616	CLA	C1D-C2D	-3.52	1.38	1.45
25	B	616	CLA	C1D-C2D	-3.52	1.38	1.45
25	n	602	CLA	C1D-C2D	-3.52	1.38	1.45
24	S	302	CHL	C4B-NB	3.52	1.38	1.35
24	s	302	CHL	C4B-NB	3.52	1.38	1.35
25	Y	315	CLA	C1D-C2D	-3.52	1.38	1.45
25	y	315	CLA	C1D-C2D	-3.52	1.38	1.45
25	s	311	CLA	MG-NC	-3.52	1.97	2.06
24	y	310	CHL	O2D-CGD	3.52	1.41	1.33
25	G	612	CLA	C1D-C2D	-3.52	1.38	1.45
25	b	604	CLA	MG-NC	-3.52	1.97	2.06
25	Y	305	CLA	C1D-C2D	-3.52	1.38	1.45
25	y	305	CLA	C1D-C2D	-3.52	1.38	1.45
24	N	601	CHL	O2D-CGD	3.52	1.41	1.33
28	k	101	BCR	C30-C25	-3.52	1.48	1.53
25	B	607	CLA	MG-NA	-3.52	1.97	2.06
25	b	615	CLA	C1D-C2D	-3.52	1.38	1.45
25	n	612	CLA	C1D-C2D	-3.52	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	609	CLA	MG-NA	-3.52	1.97	2.06
25	C	509	CLA	MG-NC	-3.51	1.97	2.06
24	Y	310	CHL	O2D-CGD	3.51	1.41	1.33
25	c	510	CLA	MG-NC	-3.51	1.97	2.06
24	Y	309	CHL	O2D-CGD	3.51	1.41	1.33
28	B	619	BCR	C1-C6	-3.51	1.48	1.53
28	b	619	BCR	C1-C6	-3.51	1.48	1.53
25	C	504	CLA	C1B-NB	3.51	1.38	1.35
25	c	504	CLA	C1B-NB	3.51	1.38	1.35
28	i	101	BCR	C30-C25	-3.51	1.48	1.53
25	6	605	CLA	MG-NC	-3.51	1.97	2.06
24	6	601	CHL	O2D-CGD	3.51	1.41	1.33
24	n	601	CHL	C4B-NB	3.51	1.38	1.35
24	G	606	CHL	O2D-CGD	3.51	1.41	1.33
24	y	309	CHL	O2D-CGD	3.50	1.41	1.33
25	Y	311	CLA	MG-NC	-3.50	1.97	2.06
25	C	505	CLA	C1D-C2D	-3.50	1.38	1.45
25	c	505	CLA	C1D-C2D	-3.50	1.38	1.45
25	C	502	CLA	MG-NA	-3.50	1.98	2.06
25	c	502	CLA	MG-NA	-3.50	1.98	2.06
24	R	613	CHL	O2D-CGD	3.50	1.41	1.33
24	G	608	CHL	O2D-CGD	3.50	1.41	1.33
25	s	314	CLA	C1D-C2D	-3.50	1.38	1.45
25	B	604	CLA	MG-NC	-3.50	1.98	2.06
25	C	506	CLA	C1D-C2D	-3.50	1.38	1.45
25	c	506	CLA	C1D-C2D	-3.50	1.38	1.45
25	R	608	CLA	C1D-C2D	-3.50	1.38	1.45
25	b	609	CLA	MG-NA	-3.50	1.98	2.06
25	B	608	CLA	C1D-C2D	-3.50	1.38	1.45
25	A	405	CLA	C1D-C2D	-3.49	1.38	1.45
25	y	305	CLA	MG-NA	-3.49	1.98	2.06
24	Y	308	CHL	C4B-NB	3.49	1.38	1.35
24	y	308	CHL	C4B-NB	3.49	1.38	1.35
24	s	308	CHL	O2D-CGD	3.49	1.41	1.33
25	c	509	CLA	MG-NC	-3.49	1.98	2.06
25	g	614	CLA	C1D-C2D	-3.49	1.38	1.45
25	S	314	CLA	C1D-C2D	-3.49	1.38	1.45
25	r	603	CLA	C1B-NB	3.49	1.38	1.35
24	S	302	CHL	O2D-CGD	3.49	1.41	1.33
24	s	302	CHL	O2D-CGD	3.49	1.41	1.33
24	R	606	CHL	O2D-CGD	3.49	1.41	1.33
24	r	606	CHL	O2D-CGD	3.49	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	614	CLA	C1D-C2D	-3.49	1.38	1.45
25	Y	305	CLA	MG-NA	-3.49	1.98	2.06
25	y	311	CLA	MG-NC	-3.49	1.98	2.06
24	g	601	CHL	O2D-CGD	3.49	1.41	1.33
25	C	509	CLA	C1D-C2D	-3.49	1.38	1.45
25	c	509	CLA	C1D-C2D	-3.49	1.38	1.45
24	1	302	CHL	O2D-CGD	3.49	1.41	1.33
24	5	302	CHL	O2D-CGD	3.49	1.41	1.33
24	r	607	CHL	O2D-CGD	3.49	1.41	1.33
25	A	401	CLA	MG-NC	-3.48	1.98	2.06
25	a	402	CLA	MG-NC	-3.48	1.98	2.06
24	G	605	CHL	O2D-CGD	3.48	1.41	1.33
24	g	605	CHL	O2D-CGD	3.48	1.41	1.33
24	N	606	CHL	O2D-CGD	3.48	1.41	1.33
24	n	601	CHL	O2D-CGD	3.48	1.41	1.33
25	a	406	CLA	C1D-C2D	-3.48	1.38	1.45
24	y	307	CHL	MG-NA	3.48	2.14	2.06
25	n	603	CLA	C1D-C2D	-3.48	1.38	1.45
25	b	608	CLA	C1D-C2D	-3.48	1.38	1.45
25	B	608	CLA	MG-NA	-3.48	1.98	2.06
25	C	510	CLA	MG-NC	-3.48	1.98	2.06
28	A	406	BCR	C30-C25	-3.48	1.49	1.53
25	G	604	CLA	C1D-C2D	-3.48	1.38	1.45
25	R	608	CLA	MG-NA	-3.48	1.98	2.06
24	Y	307	CHL	MG-NA	3.48	2.14	2.06
25	S	309	CLA	C1D-C2D	-3.48	1.38	1.45
25	b	612	CLA	C1D-C2D	-3.48	1.38	1.45
25	s	309	CLA	C1D-C2D	-3.48	1.38	1.45
24	2	601	CHL	O2D-CGD	3.48	1.41	1.33
24	r	613	CHL	O2D-CGD	3.48	1.41	1.33
24	R	605	CHL	O2D-CGD	3.47	1.41	1.33
24	r	605	CHL	O2D-CGD	3.47	1.41	1.33
25	Y	312	CLA	MG-NA	-3.47	1.98	2.06
25	y	312	CLA	MG-NA	-3.47	1.98	2.06
24	S	307	CHL	O2D-CGD	3.47	1.41	1.33
24	s	307	CHL	O2D-CGD	3.47	1.41	1.33
24	G	601	CHL	O2D-CGD	3.47	1.41	1.33
28	H	101	BCR	C1-C6	-3.47	1.49	1.53
28	h	101	BCR	C1-C6	-3.47	1.49	1.53
24	g	608	CHL	O2D-CGD	3.47	1.41	1.33
24	Y	302	CHL	O2D-CGD	3.47	1.41	1.33
24	y	302	CHL	O2D-CGD	3.47	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	608	CLA	C1D-C2D	-3.47	1.38	1.45
25	B	614	CLA	MG-NA	-3.47	1.98	2.06
25	b	614	CLA	MG-NA	-3.47	1.98	2.06
25	N	613	CLA	C1D-C2D	-3.46	1.38	1.45
28	K	101	BCR	C1-C6	-3.46	1.49	1.53
28	k	101	BCR	C1-C6	-3.46	1.49	1.53
24	S	308	CHL	O2D-CGD	3.46	1.41	1.33
24	2	603	CHL	C3B-C2B	-3.46	1.35	1.40
24	6	603	CHL	C3B-C2B	-3.46	1.35	1.40
25	C	513	CLA	C1D-C2D	-3.46	1.38	1.45
24	Y	306	CHL	O2D-CGD	3.46	1.41	1.33
24	y	306	CHL	O2D-CGD	3.46	1.41	1.33
24	g	607	CHL	O2D-CGD	3.46	1.41	1.33
25	N	610	CLA	MG-NC	-3.46	1.98	2.06
25	n	610	CLA	MG-NC	-3.46	1.98	2.06
24	Y	307	CHL	C4B-NB	3.46	1.38	1.35
24	N	608	CHL	O2D-CGD	3.46	1.41	1.33
24	n	608	CHL	O2D-CGD	3.46	1.41	1.33
25	n	613	CLA	C1D-C2D	-3.46	1.38	1.45
25	C	511	CLA	C1D-C2D	-3.46	1.38	1.45
25	c	511	CLA	C1D-C2D	-3.46	1.38	1.45
25	B	609	CLA	C1D-C2D	-3.45	1.38	1.45
28	K	101	BCR	C30-C25	-3.45	1.49	1.53
28	B	618	BCR	C1-C6	-3.45	1.49	1.53
28	b	618	BCR	C1-C6	-3.45	1.49	1.53
25	C	507	CLA	C1D-C2D	-3.45	1.38	1.45
25	N	603	CLA	C1D-C2D	-3.45	1.38	1.45
24	R	607	CHL	O2D-CGD	3.45	1.41	1.33
25	D	402	CLA	C1D-C2D	-3.45	1.38	1.45
25	d	402	CLA	C1D-C2D	-3.45	1.38	1.45
25	g	604	CLA	C1D-C2D	-3.45	1.38	1.45
24	G	601	CHL	C4B-NB	3.45	1.38	1.35
25	r	608	CLA	MG-NA	-3.45	1.98	2.06
24	N	605	CHL	O2D-CGD	3.45	1.41	1.33
24	n	605	CHL	O2D-CGD	3.45	1.41	1.33
25	R	602	CLA	MG-NC	-3.45	1.98	2.06
25	B	614	CLA	C1D-C2D	-3.45	1.38	1.45
25	S	312	CLA	C1D-C2D	-3.45	1.38	1.45
25	b	614	CLA	C1D-C2D	-3.45	1.38	1.45
25	s	312	CLA	C1D-C2D	-3.45	1.38	1.45
25	C	506	CLA	MG-NC	-3.44	1.98	2.06
25	c	506	CLA	MG-NC	-3.44	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	407	BCR	C30-C25	-3.44	1.49	1.53
25	B	613	CLA	MG-NA	-3.44	1.98	2.06
25	b	613	CLA	MG-NA	-3.44	1.98	2.06
40	s	317	NEX	C14-C13	3.44	1.40	1.35
24	S	306	CHL	O2D-CGD	3.44	1.41	1.33
25	b	604	CLA	C1D-C2D	-3.44	1.38	1.45
25	c	513	CLA	C1D-C2D	-3.44	1.38	1.45
25	B	607	CLA	C1D-C2D	-3.44	1.38	1.45
25	b	607	CLA	C1D-C2D	-3.44	1.38	1.45
24	Y	307	CHL	O2D-CGD	3.44	1.41	1.33
24	n	606	CHL	O2D-CGD	3.44	1.41	1.33
24	y	307	CHL	O2D-CGD	3.44	1.41	1.33
24	n	609	CHL	O2D-CGD	3.43	1.41	1.33
28	A	406	BCR	C1-C6	-3.43	1.49	1.53
28	a	407	BCR	C1-C6	-3.43	1.49	1.53
25	b	608	CLA	MG-NA	-3.43	1.98	2.06
24	G	607	CHL	O2D-CGD	3.43	1.41	1.33
24	N	609	CHL	O2D-CGD	3.43	1.41	1.33
25	S	304	CLA	MG-NC	-3.43	1.98	2.06
25	s	304	CLA	MG-NC	-3.43	1.98	2.06
25	b	609	CLA	C1D-C2D	-3.43	1.38	1.45
25	b	611	CLA	C1D-C2D	-3.43	1.38	1.45
25	c	507	CLA	C1D-C2D	-3.43	1.38	1.45
25	B	605	CLA	MG-NC	-3.43	1.98	2.06
25	b	605	CLA	MG-NC	-3.43	1.98	2.06
25	r	602	CLA	MG-NC	-3.43	1.98	2.06
25	r	608	CLA	MG-NC	-3.43	1.98	2.06
25	B	612	CLA	C1D-C2D	-3.43	1.38	1.45
24	s	306	CHL	O2D-CGD	3.42	1.41	1.33
40	R	617	NEX	C34-C33	3.42	1.40	1.35
24	y	307	CHL	C4B-NB	3.42	1.38	1.35
25	s	314	CLA	MG-NC	-3.42	1.98	2.06
25	D	401	CLA	MG-NC	-3.42	1.98	2.06
25	d	401	CLA	MG-NC	-3.42	1.98	2.06
24	G	609	CHL	O2D-CGD	3.42	1.41	1.33
25	2	605	CLA	C1D-C2D	-3.42	1.38	1.45
25	G	610	CLA	C1D-C2D	-3.42	1.38	1.45
25	6	605	CLA	C1D-C2D	-3.42	1.38	1.45
24	2	603	CHL	O2D-CGD	3.42	1.41	1.33
24	6	603	CHL	O2D-CGD	3.42	1.41	1.33
24	g	609	CHL	O2D-CGD	3.42	1.41	1.33
25	S	303	CLA	C1D-C2D	-3.41	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	613	CHL	C3B-C2B	-3.41	1.35	1.40
24	Y	306	CHL	C3B-C2B	-3.41	1.35	1.40
25	C	505	CLA	MG-NA	-3.41	1.98	2.06
25	c	505	CLA	MG-NA	-3.41	1.98	2.06
24	S	306	CHL	C3B-C2B	-3.41	1.35	1.40
24	s	306	CHL	C3B-C2B	-3.41	1.35	1.40
25	g	610	CLA	C1D-C2D	-3.41	1.38	1.45
24	S	308	CHL	C3B-C2B	-3.41	1.35	1.40
25	S	311	CLA	C1D-C2D	-3.40	1.38	1.45
25	R	614	CLA	C1D-C2D	-3.40	1.38	1.45
25	r	614	CLA	C1D-C2D	-3.40	1.38	1.45
25	B	611	CLA	C1D-C2D	-3.40	1.38	1.45
25	R	608	CLA	MG-NC	-3.40	1.98	2.06
25	b	603	CLA	C1D-C2D	-3.40	1.38	1.45
25	Y	314	CLA	C1D-C2D	-3.39	1.38	1.45
25	y	314	CLA	C1D-C2D	-3.39	1.38	1.45
25	B	604	CLA	C1D-C2D	-3.39	1.38	1.45
25	S	314	CLA	MG-NC	-3.39	1.98	2.06
25	C	513	CLA	MG-NC	-3.39	1.98	2.06
25	c	513	CLA	MG-NC	-3.39	1.98	2.06
25	B	603	CLA	C1D-C2D	-3.39	1.38	1.45
25	c	503	CLA	C1D-C2D	-3.39	1.38	1.45
24	r	606	CHL	O2A-CGA	3.39	1.42	1.30
40	s	317	NEX	C12-C13	-3.39	1.38	1.45
25	g	613	CLA	C1D-C2D	-3.39	1.38	1.45
40	S	317	NEX	C14-C13	3.39	1.40	1.35
24	s	308	CHL	C3B-C2B	-3.39	1.35	1.40
25	b	616	CLA	MG-NA	-3.38	1.98	2.06
24	R	605	CHL	O2A-CGA	3.38	1.42	1.30
24	r	605	CHL	O2A-CGA	3.38	1.42	1.30
25	n	604	CLA	C1D-C2D	-3.38	1.38	1.45
25	d	401	CLA	C1D-C2D	-3.38	1.38	1.45
25	r	609	CLA	C1D-C2D	-3.38	1.38	1.45
25	G	613	CLA	C1D-C2D	-3.38	1.38	1.45
25	C	512	CLA	C1D-C2D	-3.37	1.38	1.45
25	c	512	CLA	C1D-C2D	-3.37	1.38	1.45
25	s	303	CLA	C1D-C2D	-3.37	1.38	1.45
24	5	301	CHL	O2A-CGA	3.37	1.42	1.30
24	r	605	CHL	C3B-C2B	-3.37	1.35	1.40
28	Z	101	BCR	C1-C6	-3.37	1.49	1.53
25	D	401	CLA	C1D-C2D	-3.37	1.38	1.45
24	1	301	CHL	O2A-CGA	3.37	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	605	CHL	O2A-CGA	3.37	1.42	1.30
24	g	605	CHL	O2A-CGA	3.37	1.42	1.30
40	r	617	NEX	C34-C33	3.37	1.40	1.35
24	S	307	CHL	O2A-CGA	3.37	1.42	1.30
24	Y	310	CHL	C3B-C2B	-3.37	1.35	1.40
24	y	310	CHL	C3B-C2B	-3.37	1.35	1.40
25	R	610	CLA	C1B-NB	3.37	1.38	1.35
25	r	610	CLA	C1B-NB	3.37	1.38	1.35
24	S	302	CHL	O2A-CGA	3.37	1.42	1.30
24	s	302	CHL	O2A-CGA	3.37	1.42	1.30
40	S	317	NEX	C12-C13	-3.37	1.38	1.45
24	2	603	CHL	O2A-CGA	3.36	1.42	1.30
24	6	603	CHL	O2A-CGA	3.36	1.42	1.30
24	1	302	CHL	O2A-CGA	3.36	1.42	1.30
24	5	302	CHL	O2A-CGA	3.36	1.42	1.30
24	Y	308	CHL	C3B-C2B	-3.36	1.35	1.40
24	s	307	CHL	O2A-CGA	3.36	1.42	1.30
24	y	302	CHL	C3B-C2B	-3.36	1.35	1.40
25	s	311	CLA	C1D-C2D	-3.36	1.38	1.45
25	N	604	CLA	MG-NC	-3.36	1.98	2.06
25	A	402	CLA	C1D-C2D	-3.36	1.38	1.45
25	a	403	CLA	C1D-C2D	-3.36	1.38	1.45
24	S	308	CHL	O2A-CGA	3.36	1.42	1.30
24	s	308	CHL	O2A-CGA	3.36	1.42	1.30
24	N	605	CHL	C3B-C2B	-3.36	1.35	1.40
24	n	605	CHL	C3B-C2B	-3.36	1.35	1.40
24	R	606	CHL	O2A-CGA	3.36	1.42	1.30
25	R	609	CLA	C1D-C2D	-3.36	1.38	1.45
24	N	606	CHL	O2A-CGA	3.35	1.42	1.30
24	S	306	CHL	O2A-CGA	3.35	1.42	1.30
24	s	306	CHL	O2A-CGA	3.35	1.42	1.30
25	r	602	CLA	C1D-C2D	-3.35	1.38	1.45
25	B	616	CLA	MG-NA	-3.35	1.98	2.06
25	B	607	CLA	MG-NC	-3.35	1.98	2.06
25	C	503	CLA	C1D-C2D	-3.35	1.38	1.45
25	A	401	CLA	C1D-C2D	-3.35	1.38	1.45
25	a	402	CLA	C1D-C2D	-3.35	1.38	1.45
25	S	303	CLA	MG-NC	-3.34	1.98	2.06
25	s	303	CLA	MG-NC	-3.34	1.98	2.06
24	y	306	CHL	C3B-C2B	-3.34	1.35	1.40
25	N	604	CLA	C1D-C2D	-3.34	1.38	1.45
24	n	606	CHL	O2A-CGA	3.34	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	602	CLA	C1D-C2D	-3.34	1.38	1.45
25	B	605	CLA	C1D-C2D	-3.34	1.38	1.45
25	b	605	CLA	C1D-C2D	-3.34	1.38	1.45
25	C	512	CLA	MG-NC	-3.34	1.98	2.06
25	c	512	CLA	MG-NC	-3.34	1.98	2.06
25	a	406	CLA	MG-NC	-3.33	1.98	2.06
28	z	101	BCR	C1-C6	-3.33	1.49	1.53
25	n	604	CLA	MG-NC	-3.33	1.98	2.06
25	B	616	CLA	MG-NC	-3.33	1.98	2.06
24	R	605	CHL	C3B-C2B	-3.33	1.35	1.40
25	R	610	CLA	C1D-C2D	-3.33	1.38	1.45
25	r	610	CLA	C1D-C2D	-3.33	1.38	1.45
25	C	501	CLA	C1D-C2D	-3.32	1.38	1.45
25	c	501	CLA	C1D-C2D	-3.32	1.38	1.45
25	N	611	CLA	MG-NC	-3.32	1.98	2.06
24	y	308	CHL	C3B-C2B	-3.32	1.35	1.40
25	c	508	CLA	C1D-C2D	-3.32	1.38	1.45
25	C	503	CLA	MG-NC	-3.32	1.98	2.06
25	c	503	CLA	MG-NC	-3.32	1.98	2.06
40	g	617	NEX	C12-C13	-3.32	1.38	1.45
25	B	611	CLA	MG-NC	-3.31	1.98	2.06
24	g	609	CHL	C3B-C2B	-3.31	1.35	1.40
24	r	613	CHL	C3B-C2B	-3.31	1.35	1.40
25	B	602	CLA	MG-NC	-3.31	1.98	2.06
25	b	602	CLA	MG-NC	-3.31	1.98	2.06
25	b	611	CLA	MG-NC	-3.31	1.98	2.06
24	N	607	CHL	C3B-C2B	-3.31	1.35	1.40
25	b	607	CLA	MG-NC	-3.31	1.98	2.06
25	b	616	CLA	MG-NC	-3.31	1.98	2.06
24	G	609	CHL	C3B-C2B	-3.31	1.35	1.40
25	n	611	CLA	MG-NC	-3.31	1.98	2.06
25	c	510	CLA	C1D-C2D	-3.31	1.38	1.45
25	B	606	CLA	C1D-C2D	-3.30	1.38	1.45
25	b	606	CLA	C1D-C2D	-3.30	1.38	1.45
25	A	405	CLA	MG-NC	-3.30	1.98	2.06
25	C	510	CLA	C1D-C2D	-3.30	1.38	1.45
24	G	607	CHL	O2A-CGA	3.30	1.41	1.30
25	B	603	CLA	MG-NC	-3.30	1.98	2.06
25	b	603	CLA	MG-NC	-3.30	1.98	2.06
25	S	304	CLA	C1D-C2D	-3.30	1.38	1.45
25	s	304	CLA	C1D-C2D	-3.30	1.38	1.45
25	C	508	CLA	C1D-C2D	-3.30	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	G	617	NEX	C14-C13	3.30	1.40	1.35
24	g	607	CHL	O2A-CGA	3.29	1.41	1.30
24	y	309	CHL	C3B-C2B	-3.29	1.35	1.40
28	C	514	BCR	C30-C25	-3.29	1.49	1.53
28	c	514	BCR	C30-C25	-3.29	1.49	1.53
24	R	607	CHL	C3B-C2B	-3.29	1.35	1.40
24	r	607	CHL	C3B-C2B	-3.29	1.35	1.40
24	n	607	CHL	C3B-C2B	-3.29	1.35	1.40
24	g	601	CHL	C3B-C2B	-3.29	1.35	1.40
25	G	604	CLA	MG-NC	-3.29	1.98	2.06
25	Y	305	CLA	MG-NC	-3.28	1.98	2.06
25	B	602	CLA	C1D-C2D	-3.28	1.38	1.45
25	b	602	CLA	C1D-C2D	-3.28	1.38	1.45
24	N	609	CHL	C3B-C2B	-3.28	1.35	1.40
24	Y	302	CHL	C3B-C2B	-3.28	1.35	1.40
24	n	609	CHL	C3B-C2B	-3.28	1.35	1.40
25	B	601	CLA	C1D-C2D	-3.28	1.38	1.45
25	b	601	CLA	C1D-C2D	-3.28	1.38	1.45
25	S	310	CLA	MG-NC	-3.28	1.98	2.06
25	Y	314	CLA	MG-NC	-3.28	1.98	2.06
25	Y	315	CLA	MG-NA	-3.27	1.98	2.06
25	B	613	CLA	MG-NC	-3.27	1.98	2.06
24	S	302	CHL	C3B-C2B	-3.27	1.35	1.40
24	1	301	CHL	C3B-C2B	-3.27	1.35	1.40
24	5	301	CHL	C3B-C2B	-3.27	1.35	1.40
25	c	505	CLA	MG-NC	-3.27	1.98	2.06
25	b	613	CLA	MG-NC	-3.27	1.98	2.06
24	G	601	CHL	C3B-C2B	-3.27	1.35	1.40
24	S	307	CHL	C3B-C2B	-3.27	1.35	1.40
24	s	307	CHL	C3B-C2B	-3.27	1.35	1.40
25	y	305	CLA	MG-NC	-3.26	1.98	2.06
25	g	604	CLA	MG-NC	-3.26	1.98	2.06
25	Y	303	CLA	MG-NC	-3.26	1.98	2.06
25	y	303	CLA	MG-NC	-3.26	1.98	2.06
25	C	504	CLA	C1D-C2D	-3.26	1.38	1.45
25	s	310	CLA	MG-NC	-3.26	1.98	2.06
24	g	608	CHL	C3B-C2B	-3.26	1.35	1.40
25	B	614	CLA	MG-NC	-3.26	1.98	2.06
25	b	614	CLA	MG-NC	-3.26	1.98	2.06
24	G	605	CHL	C3B-C2B	-3.26	1.35	1.40
24	Y	309	CHL	C3B-C2B	-3.25	1.35	1.40
25	Y	313	CLA	MG-NC	-3.25	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	602	CLA	MG-NC	-3.25	1.98	2.06
25	C	505	CLA	MG-NC	-3.25	1.98	2.06
25	y	314	CLA	MG-NC	-3.25	1.98	2.06
28	B	618	BCR	C30-C25	-3.25	1.49	1.53
28	b	618	BCR	C30-C25	-3.25	1.49	1.53
24	G	606	CHL	C3B-C2B	-3.25	1.35	1.40
24	g	606	CHL	C3B-C2B	-3.25	1.35	1.40
24	R	606	CHL	C3B-C2B	-3.25	1.35	1.40
25	D	403	CLA	C1D-C2D	-3.25	1.38	1.45
25	d	403	CLA	C1D-C2D	-3.25	1.38	1.45
25	n	602	CLA	MG-NC	-3.24	1.98	2.06
25	y	315	CLA	MG-NA	-3.24	1.98	2.06
25	R	603	CLA	C1D-C2D	-3.24	1.38	1.45
25	b	608	CLA	MG-NC	-3.24	1.98	2.06
25	b	609	CLA	MG-NC	-3.24	1.98	2.06
25	y	313	CLA	MG-NC	-3.23	1.98	2.06
25	C	502	CLA	MG-NC	-3.23	1.98	2.06
25	c	502	CLA	MG-NC	-3.23	1.98	2.06
24	G	608	CHL	C3B-C2B	-3.23	1.35	1.40
24	g	605	CHL	C3B-C2B	-3.23	1.35	1.40
25	S	313	CLA	C1D-C2D	-3.22	1.39	1.45
25	R	604	CLA	C1D-C2D	-3.22	1.39	1.45
25	r	604	CLA	C1D-C2D	-3.22	1.39	1.45
25	c	504	CLA	C1D-C2D	-3.22	1.39	1.45
28	B	619	BCR	C30-C25	-3.22	1.49	1.53
28	b	619	BCR	C30-C25	-3.22	1.49	1.53
25	s	313	CLA	C1D-C2D	-3.21	1.39	1.45
24	N	606	CHL	C3B-C2B	-3.21	1.35	1.40
24	n	606	CHL	C3B-C2B	-3.21	1.35	1.40
25	B	609	CLA	MG-NC	-3.21	1.98	2.06
25	Y	304	CLA	MG-NC	-3.20	1.98	2.06
25	y	304	CLA	MG-NC	-3.20	1.98	2.06
24	N	601	CHL	C3B-C2B	-3.20	1.35	1.40
24	r	606	CHL	C3B-C2B	-3.20	1.35	1.40
25	B	608	CLA	MG-NC	-3.20	1.98	2.06
25	G	603	CLA	MG-NC	-3.20	1.98	2.06
25	g	603	CLA	MG-NC	-3.20	1.98	2.06
25	r	603	CLA	C1D-C2D	-3.20	1.39	1.45
25	G	611	CLA	MG-NC	-3.19	1.98	2.06
25	g	611	CLA	MG-NC	-3.19	1.98	2.06
25	N	603	CLA	MG-NC	-3.18	1.98	2.06
25	n	603	CLA	MG-NC	-3.18	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	302	CHL	C3B-C2B	-3.18	1.36	1.40
25	R	612	CLA	C1D-C2D	-3.17	1.39	1.45
25	r	612	CLA	C1D-C2D	-3.17	1.39	1.45
24	R	613	CHL	MG-NA	3.17	2.13	2.06
24	N	608	CHL	C3B-C2B	-3.16	1.36	1.40
24	n	601	CHL	C3B-C2B	-3.16	1.36	1.40
25	G	614	CLA	MG-NC	-3.16	1.98	2.06
25	g	614	CLA	MG-NC	-3.16	1.98	2.06
25	r	601	CLA	C1D-C2D	-3.16	1.39	1.45
25	G	602	CLA	MG-NC	-3.15	1.98	2.06
24	2	601	CHL	C3B-C2B	-3.15	1.36	1.40
24	6	601	CHL	C3B-C2B	-3.15	1.36	1.40
24	r	613	CHL	MG-NA	3.15	2.13	2.06
25	S	305	CLA	C1D-C2D	-3.14	1.39	1.45
25	s	305	CLA	C1D-C2D	-3.14	1.39	1.45
25	y	315	CLA	MG-NC	-3.14	1.98	2.06
25	g	602	CLA	MG-NC	-3.14	1.98	2.06
24	n	608	CHL	C3B-C2B	-3.13	1.36	1.40
25	Y	312	CLA	MG-NC	-3.12	1.98	2.06
25	y	312	CLA	MG-NC	-3.12	1.98	2.06
40	G	617	NEX	C10-C9	3.11	1.39	1.35
24	Y	310	CHL	MG-NA	3.11	2.13	2.06
24	y	310	CHL	MG-NA	3.11	2.13	2.06
25	R	601	CLA	C1D-C2D	-3.11	1.39	1.45
40	N	617	NEX	C34-C33	3.11	1.39	1.35
40	G	617	NEX	C11-C12	3.10	1.42	1.34
40	n	617	NEX	C34-C33	3.10	1.39	1.35
24	1	302	CHL	C3B-C2B	-3.10	1.36	1.40
24	5	302	CHL	C3B-C2B	-3.10	1.36	1.40
25	6	604	CLA	C1D-C2D	-3.10	1.39	1.45
25	Y	315	CLA	MG-NC	-3.09	1.98	2.06
24	g	609	CHL	MG-NA	3.09	2.13	2.06
24	R	606	CHL	MG-NA	3.08	2.13	2.06
24	r	606	CHL	MG-NA	3.08	2.13	2.06
40	G	617	NEX	C12-C13	-3.08	1.39	1.45
28	T	101	BCR	C30-C25	-3.08	1.49	1.53
28	t	101	BCR	C30-C25	-3.07	1.49	1.53
24	r	605	CHL	MG-NA	3.06	2.13	2.06
24	S	306	CHL	MG-NA	3.06	2.13	2.06
24	s	306	CHL	MG-NA	3.06	2.13	2.06
25	2	604	CLA	C1D-C2D	-3.05	1.39	1.45
24	S	307	CHL	MG-NA	3.05	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	307	CHL	MG-NA	3.05	2.13	2.06
24	R	605	CHL	MG-NA	3.05	2.13	2.06
24	G	609	CHL	MG-NA	3.04	2.13	2.06
24	N	609	CHL	MG-NA	3.04	2.13	2.06
28	B	617	BCR	C30-C25	-3.04	1.49	1.53
28	b	617	BCR	C30-C25	-3.04	1.49	1.53
24	s	308	CHL	MG-NA	3.04	2.13	2.06
24	n	609	CHL	MG-NA	3.03	2.13	2.06
24	S	308	CHL	MG-NA	3.03	2.13	2.06
24	Y	307	CHL	O2A-CGA	3.02	1.42	1.33
25	n	613	CLA	MG-NC	-3.00	1.99	2.06
40	r	617	NEX	C12-C13	-3.00	1.39	1.45
24	Y	306	CHL	MG-NA	3.00	2.13	2.06
24	y	306	CHL	MG-NA	3.00	2.13	2.06
40	R	617	NEX	C12-C13	-2.99	1.39	1.45
28	z	101	BCR	C30-C25	-2.99	1.49	1.53
24	N	605	CHL	MG-NA	2.99	2.13	2.06
24	n	605	CHL	MG-NA	2.99	2.13	2.06
24	y	307	CHL	O2A-CGA	2.99	1.42	1.33
24	N	605	CHL	O2A-CGA	2.98	1.42	1.33
25	2	602	CLA	C1D-C2D	-2.98	1.39	1.45
25	6	602	CLA	C1D-C2D	-2.98	1.39	1.45
24	R	607	CHL	MG-NA	2.98	2.13	2.06
24	r	607	CHL	MG-NA	2.98	2.13	2.06
24	G	608	CHL	O2A-CGA	2.98	1.42	1.33
24	Y	308	CHL	O2A-CGA	2.98	1.42	1.33
24	g	608	CHL	O2A-CGA	2.98	1.42	1.33
25	N	613	CLA	MG-NC	-2.97	1.99	2.06
24	y	308	CHL	O2A-CGA	2.97	1.42	1.33
24	n	605	CHL	O2A-CGA	2.97	1.42	1.33
24	r	607	CHL	O2A-CGA	2.97	1.42	1.33
24	2	601	CHL	O2A-CGA	2.97	1.42	1.33
24	6	601	CHL	O2A-CGA	2.97	1.42	1.33
25	g	613	CLA	MG-NC	-2.96	1.99	2.06
24	Y	306	CHL	O2A-CGA	2.96	1.42	1.33
24	Y	310	CHL	O2A-CGA	2.96	1.42	1.33
24	y	310	CHL	O2A-CGA	2.96	1.42	1.33
24	G	606	CHL	O2A-CGA	2.96	1.42	1.33
24	g	606	CHL	O2A-CGA	2.96	1.42	1.33
24	G	605	CHL	MG-NA	2.95	2.13	2.06
24	g	605	CHL	MG-NA	2.95	2.13	2.06
28	Z	101	BCR	C30-C25	-2.95	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	601	CHL	O2A-CGA	2.95	1.42	1.33
24	y	306	CHL	O2A-CGA	2.95	1.42	1.33
24	5	301	CHL	MG-NA	2.95	2.13	2.06
24	N	608	CHL	O2A-CGA	2.95	1.41	1.33
24	Y	309	CHL	O2A-CGA	2.95	1.41	1.33
24	y	309	CHL	O2A-CGA	2.95	1.41	1.33
24	n	608	CHL	O2A-CGA	2.95	1.41	1.33
24	R	607	CHL	O2A-CGA	2.94	1.41	1.33
24	G	609	CHL	O2A-CGA	2.94	1.41	1.33
24	g	609	CHL	O2A-CGA	2.94	1.41	1.33
25	G	613	CLA	MG-NC	-2.93	1.99	2.06
24	n	601	CHL	O2A-CGA	2.93	1.41	1.33
24	G	607	CHL	MG-NA	2.93	2.13	2.06
24	Y	308	CHL	MG-NA	2.93	2.13	2.06
24	y	308	CHL	MG-NA	2.93	2.13	2.06
24	G	608	CHL	MG-NA	2.93	2.13	2.06
24	n	609	CHL	O2A-CGA	2.93	1.41	1.33
24	g	607	CHL	MG-NA	2.92	2.13	2.06
24	N	609	CHL	O2A-CGA	2.92	1.41	1.33
40	Y	318	NEX	C11-C12	2.92	1.42	1.34
24	g	608	CHL	MG-NA	2.91	2.13	2.06
40	y	318	NEX	C11-C12	2.91	1.42	1.34
24	N	607	CHL	MG-NA	2.91	2.13	2.06
24	g	606	CHL	MG-NA	2.91	2.13	2.06
40	N	617	NEX	C11-C12	2.91	1.42	1.34
24	1	301	CHL	MG-NA	2.91	2.13	2.06
24	n	607	CHL	MG-NA	2.91	2.13	2.06
24	Y	302	CHL	O2A-CGA	2.91	1.41	1.33
24	y	302	CHL	O2A-CGA	2.91	1.41	1.33
28	D	404	BCR	C30-C25	-2.90	1.49	1.53
28	d	404	BCR	C30-C25	-2.90	1.49	1.53
24	n	606	CHL	MG-NA	2.89	2.13	2.06
24	g	601	CHL	O2A-CGA	2.89	1.41	1.33
40	n	617	NEX	C11-C12	2.89	1.42	1.34
24	G	606	CHL	MG-NA	2.89	2.13	2.06
24	n	608	CHL	MG-NA	2.88	2.13	2.06
24	G	601	CHL	O2A-CGA	2.88	1.41	1.33
24	N	608	CHL	MG-NA	2.87	2.13	2.06
24	Y	309	CHL	MG-NA	2.87	2.13	2.06
25	Y	313	CLA	C4B-CHC	-2.87	1.33	1.41
24	6	601	CHL	MG-NA	2.87	2.13	2.06
28	H	101	BCR	C30-C25	-2.86	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	h	101	BCR	C30-C25	-2.86	1.49	1.53
24	N	606	CHL	MG-NA	2.86	2.13	2.06
24	n	607	CHL	O2A-CGA	2.86	1.41	1.33
24	5	302	CHL	MG-NC	2.85	2.13	2.06
24	2	601	CHL	MG-NA	2.85	2.13	2.06
24	N	607	CHL	O2A-CGA	2.85	1.41	1.33
24	y	309	CHL	MG-NA	2.84	2.13	2.06
24	s	302	CHL	MG-NA	2.83	2.13	2.06
25	y	313	CLA	C4B-CHC	-2.83	1.33	1.41
24	1	302	CHL	MG-NC	2.83	2.13	2.06
40	g	617	NEX	C34-C33	2.82	1.39	1.35
24	y	302	CHL	MG-NA	2.82	2.13	2.06
24	S	302	CHL	MG-NA	2.81	2.12	2.06
40	G	617	NEX	C34-C33	2.79	1.39	1.35
24	G	601	CHL	MG-NA	2.79	2.12	2.06
24	g	601	CHL	MG-NA	2.79	2.12	2.06
24	Y	302	CHL	MG-NA	2.79	2.12	2.06
25	y	315	CLA	C4B-CHC	-2.78	1.33	1.41
25	R	611	CLA	C1D-C2D	-2.77	1.39	1.45
25	r	611	CLA	C1D-C2D	-2.75	1.39	1.45
25	Y	315	CLA	C4B-CHC	-2.73	1.33	1.41
24	N	601	CHL	MG-NA	2.73	2.12	2.06
24	n	601	CHL	MG-NA	2.73	2.12	2.06
24	1	302	CHL	MG-NA	2.72	2.12	2.06
24	5	302	CHL	MG-NA	2.72	2.12	2.06
25	B	609	CLA	C4B-CHC	-2.72	1.33	1.41
25	b	609	CLA	C4B-CHC	-2.72	1.33	1.41
40	R	617	NEX	C11-C12	2.71	1.41	1.34
40	r	617	NEX	C11-C12	2.71	1.41	1.34
39	R	615	LUT	C23-C24	2.71	1.54	1.50
39	r	615	LUT	C23-C24	2.71	1.54	1.50
24	G	607	CHL	C3B-C2B	-2.70	1.36	1.40
24	g	607	CHL	C3B-C2B	-2.70	1.36	1.40
40	N	617	NEX	O24-C25	-2.69	1.42	1.46
24	2	603	CHL	CHD-C1D	2.69	1.43	1.38
24	6	603	CHL	CHD-C1D	2.69	1.43	1.38
25	G	603	CLA	C4B-CHC	-2.68	1.33	1.41
25	g	603	CLA	C4B-CHC	-2.68	1.33	1.41
40	S	317	NEX	C32-C33	-2.68	1.40	1.45
40	n	617	NEX	C12-C13	-2.67	1.40	1.45
40	N	617	NEX	C12-C13	-2.66	1.40	1.45
40	n	617	NEX	O24-C25	-2.66	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	s	317	NEX	C32-C33	-2.65	1.40	1.45
25	c	505	CLA	C4B-CHC	-2.65	1.33	1.41
24	Y	307	CHL	C1B-NB	2.65	1.37	1.35
25	G	604	CLA	C4B-CHC	-2.65	1.33	1.41
25	N	613	CLA	C4B-CHC	-2.65	1.33	1.41
25	n	613	CLA	C4B-CHC	-2.65	1.33	1.41
25	G	614	CLA	C4B-CHC	-2.65	1.33	1.41
25	g	604	CLA	C4B-CHC	-2.65	1.33	1.41
25	g	614	CLA	C4B-CHC	-2.65	1.33	1.41
40	y	318	NEX	C12-C13	-2.65	1.40	1.45
25	y	304	CLA	C4B-CHC	-2.64	1.33	1.41
40	Y	318	NEX	C12-C13	-2.64	1.40	1.45
40	S	317	NEX	C34-C33	2.64	1.39	1.35
40	s	317	NEX	C34-C33	2.64	1.39	1.35
40	g	617	NEX	O24-C25	-2.64	1.42	1.46
25	b	608	CLA	C4B-CHC	-2.63	1.33	1.41
25	B	614	CLA	C4B-CHC	-2.63	1.33	1.41
25	b	614	CLA	C4B-CHC	-2.63	1.33	1.41
25	Y	304	CLA	C4B-CHC	-2.63	1.33	1.41
25	C	505	CLA	C4B-CHC	-2.62	1.33	1.41
25	B	608	CLA	C4B-CHC	-2.62	1.33	1.41
25	Y	312	CLA	C4B-CHC	-2.62	1.33	1.41
25	C	502	CLA	C4B-CHC	-2.62	1.33	1.41
25	c	502	CLA	C4B-CHC	-2.62	1.33	1.41
25	N	603	CLA	C4B-CHC	-2.61	1.33	1.41
25	n	603	CLA	C4B-CHC	-2.61	1.33	1.41
39	n	616	LUT	C23-C24	2.61	1.53	1.50
25	g	613	CLA	C4C-C3C	-2.61	1.40	1.45
40	G	617	NEX	O24-C25	-2.61	1.42	1.46
25	B	613	CLA	C4B-CHC	-2.61	1.33	1.41
41	R	616	XAT	O24-C25	-2.60	1.42	1.46
25	g	613	CLA	C4B-CHC	-2.60	1.33	1.41
25	y	312	CLA	C4B-CHC	-2.60	1.33	1.41
40	y	318	NEX	O24-C25	-2.60	1.42	1.46
25	N	613	CLA	C4C-C3C	-2.60	1.40	1.45
25	G	613	CLA	C4B-CHC	-2.60	1.33	1.41
25	C	513	CLA	C4C-C3C	-2.59	1.40	1.45
25	B	611	CLA	C4B-CHC	-2.59	1.33	1.41
25	b	611	CLA	C4B-CHC	-2.59	1.33	1.41
25	N	610	CLA	C4C-C3C	-2.59	1.40	1.45
25	n	610	CLA	C4C-C3C	-2.59	1.40	1.45
40	s	317	NEX	O24-C25	-2.59	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	513	CLA	C4C-C3C	-2.58	1.40	1.45
25	Y	305	CLA	C4B-CHC	-2.58	1.33	1.41
25	y	305	CLA	C4B-CHC	-2.58	1.33	1.41
25	g	602	CLA	C4C-C3C	-2.58	1.40	1.45
25	G	602	CLA	C4C-C3C	-2.58	1.40	1.45
25	b	613	CLA	C4B-CHC	-2.58	1.33	1.41
24	G	607	CHL	CHC-C1C	2.58	1.41	1.35
25	b	610	CLA	C4C-C3C	-2.58	1.40	1.45
25	b	616	CLA	C4B-CHC	-2.58	1.33	1.41
24	6	603	CHL	MG-NA	2.58	2.12	2.06
25	Y	314	CLA	C4B-CHC	-2.57	1.33	1.41
24	g	607	CHL	CHC-C1C	2.57	1.41	1.35
25	G	613	CLA	C4C-C3C	-2.57	1.40	1.45
25	A	405	CLA	C4B-CHC	-2.57	1.33	1.41
25	a	406	CLA	C4B-CHC	-2.57	1.33	1.41
41	r	616	XAT	O24-C25	-2.57	1.42	1.46
24	2	603	CHL	MG-NA	2.57	2.12	2.06
25	y	314	CLA	C4C-C3C	-2.57	1.40	1.45
40	Y	318	NEX	O24-C25	-2.57	1.42	1.46
25	D	401	CLA	C4B-CHC	-2.56	1.33	1.41
25	C	503	CLA	C4B-CHC	-2.56	1.33	1.41
25	c	503	CLA	C4B-CHC	-2.56	1.33	1.41
39	N	616	LUT	C23-C24	2.56	1.53	1.50
24	y	307	CHL	C1B-NB	2.56	1.37	1.35
24	N	607	CHL	CHC-C1C	2.56	1.41	1.35
24	n	607	CHL	CHC-C1C	2.56	1.41	1.35
25	y	314	CLA	C4B-CHC	-2.56	1.33	1.41
25	B	616	CLA	C4B-CHC	-2.56	1.33	1.41
40	S	317	NEX	O24-C25	-2.56	1.42	1.46
25	A	405	CLA	C4C-C3C	-2.56	1.40	1.45
25	a	406	CLA	C4C-C3C	-2.56	1.40	1.45
39	Y	317	LUT	C23-C24	2.56	1.53	1.50
25	C	502	CLA	C4C-C3C	-2.56	1.40	1.45
25	c	502	CLA	C4C-C3C	-2.56	1.40	1.45
25	y	305	CLA	C4C-C3C	-2.56	1.40	1.45
25	B	607	CLA	C4B-CHC	-2.56	1.33	1.41
25	b	607	CLA	C4B-CHC	-2.56	1.33	1.41
41	R	616	XAT	O4-C5	-2.55	1.42	1.46
41	r	616	XAT	O4-C5	-2.55	1.42	1.46
25	Y	311	CLA	C4C-C3C	-2.55	1.40	1.45
24	2	601	CHL	CHC-C1C	2.55	1.41	1.35
25	n	613	CLA	C4C-C3C	-2.55	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	303	CLA	C4B-CHC	-2.55	1.33	1.41
25	S	303	CLA	C4B-CHC	-2.55	1.33	1.41
25	R	614	CLA	C4B-CHC	-2.55	1.33	1.41
25	Y	314	CLA	C4C-C3C	-2.55	1.40	1.45
25	b	603	CLA	C4C-C3C	-2.55	1.40	1.45
25	C	512	CLA	C4B-CHC	-2.55	1.33	1.41
25	c	512	CLA	C4B-CHC	-2.55	1.33	1.41
25	y	311	CLA	C4C-C3C	-2.54	1.40	1.45
25	B	604	CLA	C4C-C3C	-2.54	1.40	1.45
25	R	608	CLA	C4B-CHC	-2.54	1.33	1.41
25	d	401	CLA	C4B-CHC	-2.54	1.33	1.41
25	g	602	CLA	C4B-CHC	-2.54	1.33	1.41
25	y	303	CLA	C4B-CHC	-2.54	1.33	1.41
25	B	603	CLA	C4B-CHC	-2.54	1.33	1.41
25	b	603	CLA	C4B-CHC	-2.54	1.33	1.41
25	R	614	CLA	C4C-C3C	-2.53	1.40	1.45
25	B	610	CLA	C4C-C3C	-2.53	1.40	1.45
40	R	617	NEX	O24-C25	-2.53	1.42	1.46
40	r	617	NEX	O24-C25	-2.53	1.42	1.46
24	R	607	CHL	C2-C3	2.53	1.39	1.33
25	y	311	CLA	C4B-CHC	-2.53	1.34	1.41
25	Y	303	CLA	C4C-C3C	-2.53	1.40	1.45
25	r	614	CLA	C4C-C3C	-2.53	1.40	1.45
24	y	308	CHL	C2-C3	2.53	1.39	1.33
25	s	303	CLA	C4B-CHC	-2.53	1.34	1.41
24	6	601	CHL	CHC-C1C	2.53	1.41	1.35
24	n	601	CHL	C2-C3	2.52	1.39	1.33
25	N	610	CLA	C4B-CHC	-2.52	1.34	1.41
24	Y	308	CHL	C2-C3	2.52	1.39	1.33
25	Y	311	CLA	C4B-CHC	-2.52	1.34	1.41
25	N	604	CLA	C4B-CHC	-2.52	1.34	1.41
25	C	506	CLA	C4B-CHC	-2.52	1.34	1.41
25	r	608	CLA	C4B-CHC	-2.52	1.34	1.41
25	y	303	CLA	C4C-C3C	-2.52	1.40	1.45
25	G	602	CLA	C4B-CHC	-2.52	1.34	1.41
25	C	509	CLA	C4C-C3C	-2.52	1.40	1.45
25	c	509	CLA	C4C-C3C	-2.52	1.40	1.45
24	g	608	CHL	C2-C3	2.52	1.39	1.33
25	r	614	CLA	C4B-CHC	-2.52	1.34	1.41
25	a	402	CLA	C4B-CHC	-2.51	1.34	1.41
24	N	601	CHL	C2-C3	2.51	1.39	1.33
25	s	314	CLA	C4B-CHC	-2.51	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	616	CLA	C4C-C3C	-2.51	1.40	1.45
38	F	101	HEM	C1D-ND	-2.51	1.33	1.38
38	f	101	HEM	C1D-ND	-2.51	1.33	1.38
25	n	604	CLA	C4C-C3C	-2.51	1.40	1.45
25	b	605	CLA	C4B-CHC	-2.51	1.34	1.41
39	y	317	LUT	C23-C24	2.51	1.53	1.50
25	A	402	CLA	C4C-C3C	-2.51	1.40	1.45
39	G	616	LUT	C23-C24	2.51	1.53	1.50
39	g	616	LUT	C23-C24	2.51	1.53	1.50
25	B	601	CLA	C4C-C3C	-2.50	1.40	1.45
24	G	608	CHL	C1B-NB	2.50	1.37	1.35
25	B	605	CLA	C4B-CHC	-2.50	1.34	1.41
25	b	604	CLA	C4C-C3C	-2.50	1.40	1.45
24	N	608	CHL	C2-C3	2.50	1.39	1.33
24	n	608	CHL	C2-C3	2.50	1.39	1.33
25	G	612	CLA	C4B-CHC	-2.50	1.34	1.41
25	g	612	CLA	C4B-CHC	-2.50	1.34	1.41
25	n	611	CLA	C4B-CHC	-2.50	1.34	1.41
25	S	314	CLA	C4C-C3C	-2.50	1.40	1.45
25	S	304	CLA	C4B-CHC	-2.50	1.34	1.41
25	s	304	CLA	C4B-CHC	-2.50	1.34	1.41
25	n	610	CLA	C4B-CHC	-2.50	1.34	1.41
25	N	611	CLA	C4C-C3C	-2.50	1.40	1.45
25	n	611	CLA	C4C-C3C	-2.50	1.40	1.45
25	S	314	CLA	C4B-CHC	-2.50	1.34	1.41
25	C	505	CLA	C4C-C3C	-2.50	1.40	1.45
25	c	505	CLA	C4C-C3C	-2.50	1.40	1.45
24	G	608	CHL	C2-C3	2.50	1.39	1.33
25	c	511	CLA	C4C-C3C	-2.50	1.40	1.45
25	S	310	CLA	C4B-CHC	-2.50	1.34	1.41
25	B	604	CLA	C4B-CHC	-2.49	1.34	1.41
25	b	604	CLA	C4B-CHC	-2.49	1.34	1.41
40	g	617	NEX	C11-C12	2.49	1.41	1.34
25	N	602	CLA	C4C-C3C	-2.49	1.40	1.45
25	n	602	CLA	C4C-C3C	-2.49	1.40	1.45
25	B	609	CLA	C4C-C3C	-2.49	1.40	1.45
25	Y	305	CLA	C4C-C3C	-2.49	1.40	1.45
25	b	609	CLA	C4C-C3C	-2.49	1.40	1.45
24	r	607	CHL	C2-C3	2.49	1.39	1.33
25	c	506	CLA	C4B-CHC	-2.49	1.34	1.41
24	Y	309	CHL	C2-C3	2.49	1.39	1.33
25	N	614	CLA	C4C-C3C	-2.49	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	309	CHL	C2-C3	2.49	1.39	1.33
25	R	602	CLA	C4B-CHC	-2.49	1.34	1.41
25	r	602	CLA	C4B-CHC	-2.49	1.34	1.41
24	N	609	CHL	CHC-C1C	2.49	1.41	1.35
24	n	609	CHL	CHC-C1C	2.49	1.41	1.35
25	B	603	CLA	C4C-C3C	-2.49	1.40	1.45
25	B	614	CLA	C4C-C3C	-2.49	1.40	1.45
25	A	402	CLA	C4B-CHC	-2.49	1.34	1.41
25	a	403	CLA	C4B-CHC	-2.49	1.34	1.41
25	B	607	CLA	C4C-C3C	-2.49	1.40	1.45
25	n	604	CLA	C4B-CHC	-2.49	1.34	1.41
24	1	301	CHL	CHC-C1C	2.49	1.41	1.35
25	G	603	CLA	C4C-C3C	-2.49	1.40	1.45
25	n	614	CLA	C4C-C3C	-2.49	1.40	1.45
24	y	309	CHL	CHC-C1C	2.48	1.41	1.35
24	g	601	CHL	CHC-C1C	2.48	1.41	1.35
25	N	611	CLA	C4B-CHC	-2.48	1.34	1.41
24	Y	310	CHL	C2-C3	2.48	1.38	1.33
24	y	310	CHL	C2-C3	2.48	1.38	1.33
25	g	603	CLA	C4C-C3C	-2.48	1.40	1.45
24	g	608	CHL	CHC-C1C	2.48	1.41	1.35
25	N	604	CLA	C4C-C3C	-2.48	1.40	1.45
24	2	601	CHL	C2-C3	2.48	1.38	1.33
24	6	601	CHL	C2-C3	2.48	1.38	1.33
25	R	602	CLA	C4C-C3C	-2.48	1.40	1.45
25	r	602	CLA	C4C-C3C	-2.48	1.40	1.45
25	A	401	CLA	C4B-CHC	-2.48	1.34	1.41
25	C	513	CLA	C4B-CHC	-2.48	1.34	1.41
24	y	302	CHL	C2-C3	2.48	1.38	1.33
24	5	301	CHL	CHC-C1C	2.48	1.41	1.35
24	g	609	CHL	C2-C3	2.47	1.38	1.33
24	N	609	CHL	C2-C3	2.47	1.38	1.33
24	n	609	CHL	C2-C3	2.47	1.38	1.33
25	G	604	CLA	C4C-C3C	-2.47	1.40	1.45
25	s	310	CLA	C4B-CHC	-2.47	1.34	1.41
25	c	508	CLA	C4C-C3C	-2.47	1.40	1.45
24	R	605	CHL	CHC-C1C	2.47	1.41	1.35
24	r	605	CHL	CHC-C1C	2.47	1.41	1.35
25	G	610	CLA	C4C-C3C	-2.47	1.40	1.45
40	g	617	NEX	C32-C33	-2.47	1.40	1.45
40	S	317	NEX	C11-C12	2.47	1.40	1.34
40	s	317	NEX	C11-C12	2.47	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	610	CLA	C4C-C3C	-2.47	1.40	1.45
25	b	616	CLA	C4C-C3C	-2.47	1.40	1.45
25	C	508	CLA	C4C-C3C	-2.47	1.40	1.45
25	N	603	CLA	C4C-C3C	-2.46	1.40	1.45
25	n	603	CLA	C4C-C3C	-2.46	1.40	1.45
24	G	601	CHL	CHC-C1C	2.46	1.41	1.35
40	G	617	NEX	C32-C33	-2.46	1.40	1.45
24	S	306	CHL	CHC-C1C	2.46	1.41	1.35
24	s	306	CHL	CHC-C1C	2.46	1.41	1.35
25	y	312	CLA	C4C-C3C	-2.46	1.40	1.45
25	R	609	CLA	C4C-C3C	-2.46	1.40	1.45
25	r	609	CLA	C4C-C3C	-2.46	1.40	1.45
25	D	401	CLA	C4C-C3C	-2.46	1.40	1.45
25	d	401	CLA	C4C-C3C	-2.46	1.40	1.45
24	S	308	CHL	CHC-C1C	2.46	1.41	1.35
24	s	308	CHL	CHC-C1C	2.46	1.41	1.35
25	B	615	CLA	C4C-C3C	-2.46	1.40	1.45
25	b	615	CLA	C4C-C3C	-2.46	1.40	1.45
24	G	609	CHL	C2-C3	2.45	1.38	1.33
25	Y	312	CLA	C4C-C3C	-2.45	1.40	1.45
25	a	403	CLA	C4C-C3C	-2.45	1.40	1.45
24	G	608	CHL	CHC-C1C	2.45	1.41	1.35
24	R	605	CHL	CBA-CGA	2.45	1.56	1.50
24	r	605	CHL	CBA-CGA	2.45	1.56	1.50
25	b	601	CLA	C4C-C3C	-2.45	1.40	1.45
25	s	314	CLA	C4C-C3C	-2.45	1.40	1.45
24	g	608	CHL	C1B-NB	2.45	1.37	1.35
25	C	508	CLA	C4B-CHC	-2.45	1.34	1.41
25	c	508	CLA	C4B-CHC	-2.45	1.34	1.41
25	B	613	CLA	C4C-C3C	-2.45	1.40	1.45
25	b	613	CLA	C4C-C3C	-2.45	1.40	1.45
25	c	506	CLA	C4C-C3C	-2.45	1.40	1.45
24	n	608	CHL	CHC-C1C	2.45	1.41	1.35
25	c	513	CLA	C4B-CHC	-2.45	1.34	1.41
25	b	614	CLA	C4C-C3C	-2.45	1.40	1.45
25	g	604	CLA	C4C-C3C	-2.45	1.40	1.45
24	N	601	CHL	CHC-C1C	2.45	1.41	1.35
24	n	601	CHL	CHC-C1C	2.45	1.41	1.35
25	C	511	CLA	C4C-C3C	-2.44	1.40	1.45
25	n	612	CLA	C4B-CHC	-2.44	1.34	1.41
24	1	301	CHL	CBA-CGA	2.44	1.56	1.50
25	N	612	CLA	C4B-CHC	-2.44	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	310	CLA	C4C-C3C	-2.44	1.40	1.45
25	s	311	CLA	C4B-CHC	-2.44	1.34	1.41
25	b	605	CLA	C4C-C3C	-2.44	1.40	1.45
24	N	608	CHL	CHC-C1C	2.44	1.41	1.35
25	B	612	CLA	C4C-C3C	-2.44	1.40	1.45
25	b	612	CLA	C4C-C3C	-2.44	1.40	1.45
24	5	301	CHL	CBA-CGA	2.44	1.56	1.50
24	Y	309	CHL	CHC-C1C	2.44	1.41	1.35
24	G	605	CHL	CHC-C1C	2.44	1.41	1.35
24	g	605	CHL	CHC-C1C	2.44	1.41	1.35
24	6	603	CHL	CHD-C4C	2.44	1.44	1.39
25	S	304	CLA	C4C-C3C	-2.44	1.40	1.45
24	r	607	CHL	CHC-C1C	2.44	1.41	1.35
25	B	605	CLA	C4C-C3C	-2.44	1.40	1.45
25	b	612	CLA	C4B-CHC	-2.44	1.34	1.41
25	S	311	CLA	C4C-C3C	-2.44	1.40	1.45
25	s	311	CLA	C4C-C3C	-2.44	1.40	1.45
25	G	611	CLA	C4C-C3C	-2.43	1.40	1.45
25	g	611	CLA	C4C-C3C	-2.43	1.40	1.45
24	S	302	CHL	CBA-CGA	2.43	1.56	1.50
24	s	302	CHL	CBA-CGA	2.43	1.56	1.50
24	G	606	CHL	CHC-C1C	2.43	1.41	1.35
24	g	606	CHL	CHC-C1C	2.43	1.41	1.35
25	C	510	CLA	C4B-CHC	-2.43	1.34	1.41
25	c	510	CLA	C4B-CHC	-2.43	1.34	1.41
24	R	606	CHL	CBA-CGA	2.43	1.56	1.50
25	b	607	CLA	C4C-C3C	-2.43	1.40	1.45
39	s	315	LUT	C23-C24	2.43	1.53	1.50
24	Y	310	CHL	CHC-C1C	2.43	1.41	1.35
24	1	302	CHL	CBA-CGA	2.43	1.56	1.50
25	B	612	CLA	C4B-CHC	-2.43	1.34	1.41
25	s	304	CLA	C4C-C3C	-2.43	1.40	1.45
25	S	311	CLA	C4B-CHC	-2.43	1.34	1.41
25	R	611	CLA	C3D-C4D	-2.42	1.38	1.44
24	S	308	CHL	CBA-CGA	2.42	1.56	1.50
25	B	611	CLA	C4C-C3C	-2.42	1.40	1.45
25	S	310	CLA	C4C-C3C	-2.42	1.40	1.45
25	C	503	CLA	C4C-C3C	-2.42	1.40	1.45
25	C	506	CLA	C4C-C3C	-2.42	1.40	1.45
25	c	503	CLA	C4C-C3C	-2.42	1.40	1.45
24	N	606	CHL	CHC-C1C	2.42	1.41	1.35
24	n	606	CHL	CHC-C1C	2.42	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	609	CHL	CHC-C1C	2.42	1.41	1.35
24	g	609	CHL	CHC-C1C	2.42	1.41	1.35
24	S	302	CHL	CHC-C1C	2.42	1.41	1.35
24	R	607	CHL	CHC-C1C	2.42	1.41	1.35
39	S	316	LUT	C23-C24	2.42	1.53	1.50
39	s	316	LUT	C23-C24	2.42	1.53	1.50
24	s	302	CHL	CHC-C1C	2.42	1.41	1.35
24	S	307	CHL	CBA-CGA	2.42	1.56	1.50
40	R	617	NEX	C32-C33	-2.41	1.40	1.45
40	r	617	NEX	C32-C33	-2.41	1.40	1.45
38	F	101	HEM	FE-ND	-2.41	1.84	1.96
38	f	101	HEM	FE-ND	-2.41	1.84	1.96
24	R	606	CHL	CHC-C1C	2.41	1.41	1.35
25	S	303	CLA	C4C-C3C	-2.41	1.40	1.45
25	s	303	CLA	C4C-C3C	-2.41	1.40	1.45
24	S	307	CHL	CHC-C1C	2.41	1.41	1.35
24	s	307	CHL	CHC-C1C	2.41	1.41	1.35
24	s	307	CHL	CBA-CGA	2.41	1.56	1.50
24	n	606	CHL	CBA-CGA	2.41	1.56	1.50
24	Y	302	CHL	C2-C3	2.41	1.38	1.33
25	b	611	CLA	C4C-C3C	-2.41	1.40	1.45
24	S	306	CHL	CBA-CGA	2.41	1.56	1.50
24	s	306	CHL	CBA-CGA	2.41	1.56	1.50
24	Y	308	CHL	CHC-C1C	2.41	1.41	1.35
24	y	308	CHL	CHC-C1C	2.41	1.41	1.35
25	Y	313	CLA	C4C-C3C	-2.41	1.40	1.45
25	d	402	CLA	C4C-C3C	-2.41	1.40	1.45
25	y	313	CLA	C4C-C3C	-2.41	1.40	1.45
24	N	606	CHL	CBA-CGA	2.41	1.56	1.50
24	n	607	CHL	C2-C3	2.41	1.38	1.33
24	G	605	CHL	CBA-CGA	2.41	1.56	1.50
24	g	605	CHL	CBA-CGA	2.41	1.56	1.50
25	c	501	CLA	C4C-C3C	-2.41	1.40	1.45
24	G	601	CHL	C2-C3	2.41	1.38	1.33
24	r	606	CHL	CBA-CGA	2.41	1.56	1.50
39	S	315	LUT	C23-C24	2.40	1.53	1.50
24	5	302	CHL	CBA-CGA	2.40	1.56	1.50
25	C	509	CLA	C4B-CHC	-2.40	1.34	1.41
25	c	509	CLA	C4B-CHC	-2.40	1.34	1.41
24	2	603	CHL	CHD-C4C	2.40	1.44	1.39
25	G	611	CLA	C4B-CHC	-2.40	1.34	1.41
24	N	607	CHL	C2-C3	2.40	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	605	CHL	CHC-C1C	2.40	1.41	1.35
24	n	605	CHL	CHC-C1C	2.40	1.41	1.35
25	R	608	CLA	C4C-C3C	-2.39	1.40	1.45
25	r	608	CLA	C4C-C3C	-2.39	1.40	1.45
24	r	606	CHL	CHC-C1C	2.39	1.41	1.35
25	r	612	CLA	C4C-C3C	-2.39	1.40	1.45
25	2	605	CLA	C4C-C3C	-2.39	1.40	1.45
25	6	605	CLA	C4C-C3C	-2.39	1.40	1.45
24	g	601	CHL	C2-C3	2.39	1.38	1.33
24	R	613	CHL	CHC-C1C	2.39	1.41	1.35
24	r	613	CHL	CHC-C1C	2.39	1.41	1.35
25	C	507	CLA	C4C-C3C	-2.39	1.40	1.45
25	c	507	CLA	C4C-C3C	-2.39	1.40	1.45
24	y	310	CHL	CHC-C1C	2.39	1.41	1.35
24	Y	302	CHL	CHC-C1C	2.39	1.41	1.35
24	y	302	CHL	CHC-C1C	2.39	1.41	1.35
24	s	308	CHL	CBA-CGA	2.39	1.56	1.50
25	B	608	CLA	C4C-C3C	-2.39	1.40	1.45
25	b	608	CLA	C4C-C3C	-2.39	1.40	1.45
25	g	614	CLA	C4C-C3C	-2.39	1.40	1.45
25	B	610	CLA	C4B-CHC	-2.39	1.34	1.41
25	r	611	CLA	C3D-C4D	-2.39	1.38	1.44
24	Y	306	CHL	CHC-C1C	2.38	1.41	1.35
25	Y	304	CLA	C4C-C3C	-2.38	1.40	1.45
25	c	511	CLA	C4B-CHC	-2.38	1.34	1.41
25	b	610	CLA	C4B-CHC	-2.38	1.34	1.41
25	D	402	CLA	C4C-C3C	-2.38	1.40	1.45
25	B	606	CLA	C4B-CHC	-2.38	1.34	1.41
25	b	606	CLA	C4B-CHC	-2.38	1.34	1.41
24	y	306	CHL	CHC-C1C	2.38	1.41	1.35
25	B	601	CLA	C4B-CHC	-2.38	1.34	1.41
25	b	602	CLA	C4C-C3C	-2.37	1.40	1.45
25	2	605	CLA	C4B-CHC	-2.37	1.34	1.41
25	R	612	CLA	C4C-C3C	-2.37	1.41	1.45
25	C	507	CLA	C4B-CHC	-2.37	1.34	1.41
25	c	507	CLA	C4B-CHC	-2.37	1.34	1.41
39	N	615	LUT	C5-C6	2.37	1.38	1.34
24	2	603	CHL	CBA-CGA	2.37	1.56	1.50
24	2	603	CHL	CHC-C1C	2.37	1.41	1.35
24	G	607	CHL	CBA-CGA	2.37	1.56	1.50
25	C	501	CLA	C4C-C3C	-2.36	1.41	1.45
24	6	603	CHL	CBA-CGA	2.36	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	602	CLA	C4B-CHC	-2.36	1.34	1.41
25	N	602	CLA	C4B-CHC	-2.36	1.34	1.41
25	n	602	CLA	C4B-CHC	-2.36	1.34	1.41
25	S	312	CLA	C4C-C3C	-2.36	1.41	1.45
25	R	604	CLA	C4C-C3C	-2.36	1.41	1.45
25	g	611	CLA	C4B-CHC	-2.36	1.34	1.41
25	S	309	CLA	C4B-CHC	-2.35	1.34	1.41
25	s	312	CLA	C4C-C3C	-2.35	1.41	1.45
25	C	511	CLA	C4B-CHC	-2.35	1.34	1.41
25	s	309	CLA	C4B-CHC	-2.35	1.34	1.41
25	D	403	CLA	C4C-C3C	-2.35	1.41	1.45
25	R	610	CLA	C4C-C3C	-2.35	1.41	1.45
25	d	403	CLA	C4C-C3C	-2.35	1.41	1.45
25	r	610	CLA	C4C-C3C	-2.35	1.41	1.45
39	N	615	LUT	C23-C24	2.35	1.53	1.50
39	n	615	LUT	C23-C24	2.35	1.53	1.50
25	A	401	CLA	C4C-C3C	-2.35	1.41	1.45
25	a	402	CLA	C4C-C3C	-2.35	1.41	1.45
38	F	101	HEM	C4B-NB	-2.35	1.34	1.38
25	S	309	CLA	C4C-C3C	-2.35	1.41	1.45
25	c	504	CLA	C4C-C3C	-2.35	1.41	1.45
25	s	309	CLA	C4C-C3C	-2.35	1.41	1.45
25	r	609	CLA	C4B-CHC	-2.35	1.34	1.41
25	y	304	CLA	C4C-C3C	-2.35	1.41	1.45
25	6	605	CLA	C4B-CHC	-2.34	1.34	1.41
39	G	616	LUT	C5-C6	2.34	1.38	1.34
39	g	616	LUT	C5-C6	2.34	1.38	1.34
25	C	504	CLA	C4C-C3C	-2.34	1.41	1.45
38	f	101	HEM	C4B-NB	-2.34	1.34	1.38
24	S	302	CHL	MG-NC	2.34	2.11	2.06
25	Y	315	CLA	C4C-C3C	-2.34	1.41	1.45
24	y	308	CHL	MG-NC	2.34	2.11	2.06
24	6	603	CHL	CHC-C1C	2.34	1.41	1.35
24	Y	307	CHL	MG-NC	2.34	2.11	2.06
39	G	615	LUT	C23-C24	2.34	1.53	1.50
39	g	615	LUT	C23-C24	2.34	1.53	1.50
25	b	601	CLA	C4B-CHC	-2.33	1.34	1.41
25	b	602	CLA	C4B-CHC	-2.33	1.34	1.41
24	1	302	CHL	CHC-C1C	2.33	1.40	1.35
24	5	302	CHL	CHC-C1C	2.33	1.40	1.35
25	C	512	CLA	C4C-C3C	-2.33	1.41	1.45
25	G	614	CLA	C4C-C3C	-2.33	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	512	CLA	C4C-C3C	-2.33	1.41	1.45
25	C	510	CLA	C4C-C3C	-2.32	1.41	1.45
39	n	615	LUT	C5-C6	2.32	1.38	1.34
25	c	510	CLA	C4C-C3C	-2.32	1.41	1.45
24	s	302	CHL	MG-NC	2.32	2.11	2.06
24	y	307	CHL	MG-NC	2.32	2.11	2.06
24	n	608	CHL	C1B-NB	2.32	1.37	1.35
25	R	609	CLA	C4B-CHC	-2.32	1.34	1.41
24	Y	308	CHL	MG-NC	2.32	2.11	2.06
25	B	602	CLA	C4C-C3C	-2.32	1.41	1.45
25	S	313	CLA	C4C-C3C	-2.31	1.41	1.45
25	s	313	CLA	C4C-C3C	-2.31	1.41	1.45
24	g	607	CHL	CBA-CGA	2.31	1.56	1.50
25	B	606	CLA	C4C-C3C	-2.31	1.41	1.45
25	b	606	CLA	C4C-C3C	-2.31	1.41	1.45
39	y	317	LUT	C5-C6	2.31	1.38	1.34
40	N	617	NEX	C32-C33	-2.31	1.41	1.45
25	y	315	CLA	C4C-C3C	-2.31	1.41	1.45
40	n	617	NEX	C32-C33	-2.30	1.41	1.45
25	B	608	CLA	C1C-C2C	-2.30	1.40	1.44
41	r	616	XAT	C14-C13	2.29	1.38	1.35
25	G	612	CLA	C4C-C3C	-2.29	1.41	1.45
25	B	609	CLA	C1C-C2C	-2.29	1.40	1.44
25	s	305	CLA	C4C-C3C	-2.29	1.41	1.45
24	S	307	CHL	MG-NC	2.29	2.11	2.06
25	C	502	CLA	C1C-C2C	-2.28	1.40	1.44
25	b	609	CLA	C1C-C2C	-2.28	1.40	1.44
39	S	315	LUT	C5-C6	2.28	1.38	1.34
39	N	616	LUT	C5-C6	2.27	1.38	1.34
39	n	616	LUT	C5-C6	2.27	1.38	1.34
25	N	614	CLA	C4B-CHC	-2.27	1.34	1.41
25	g	612	CLA	C4C-C3C	-2.27	1.41	1.45
25	2	604	CLA	C3D-C4D	-2.27	1.39	1.44
25	6	604	CLA	C3D-C4D	-2.27	1.39	1.44
41	R	616	XAT	C32-C33	-2.27	1.41	1.45
41	r	616	XAT	C32-C33	-2.27	1.41	1.45
25	B	614	CLA	C1C-C2C	-2.27	1.40	1.44
25	r	604	CLA	C4C-C3C	-2.27	1.41	1.45
24	s	307	CHL	MG-NC	2.27	2.11	2.06
25	B	611	CLA	C1C-C2C	-2.27	1.40	1.44
25	b	611	CLA	C1C-C2C	-2.27	1.40	1.44
24	R	613	CHL	MG-NC	2.27	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	614	CLA	C4B-CHC	-2.26	1.34	1.41
25	R	604	CLA	C4B-CHC	-2.26	1.34	1.41
41	R	616	XAT	C12-C13	-2.26	1.41	1.45
41	r	616	XAT	C12-C13	-2.26	1.41	1.45
25	r	603	CLA	C4C-C3C	-2.26	1.41	1.45
39	Y	317	LUT	C5-C6	2.26	1.38	1.34
25	S	305	CLA	C4C-C3C	-2.26	1.41	1.45
24	y	307	CHL	CHC-C1C	2.26	1.40	1.35
24	G	607	CHL	MG-NC	2.26	2.11	2.06
24	g	607	CHL	MG-NC	2.26	2.11	2.06
24	r	613	CHL	MG-NC	2.26	2.11	2.06
25	b	608	CLA	C1C-C2C	-2.26	1.40	1.44
25	c	502	CLA	C1C-C2C	-2.25	1.40	1.44
25	g	603	CLA	C1C-C2C	-2.25	1.40	1.44
25	S	303	CLA	C1C-C2C	-2.25	1.40	1.44
25	s	303	CLA	C1C-C2C	-2.25	1.40	1.44
25	C	505	CLA	C1C-C2C	-2.25	1.40	1.44
25	c	505	CLA	C1C-C2C	-2.25	1.40	1.44
24	1	301	CHL	MG-NC	2.25	2.11	2.06
25	D	402	CLA	C4B-CHC	-2.25	1.34	1.41
24	R	606	CHL	MG-NC	2.25	2.11	2.06
24	r	606	CHL	MG-NC	2.25	2.11	2.06
24	N	607	CHL	MG-NC	2.25	2.11	2.06
24	n	607	CHL	MG-NC	2.25	2.11	2.06
25	N	603	CLA	C1C-C2C	-2.25	1.40	1.44
25	n	603	CLA	C1C-C2C	-2.25	1.40	1.44
25	d	402	CLA	C4B-CHC	-2.25	1.34	1.41
25	b	614	CLA	C1C-C2C	-2.25	1.40	1.44
40	G	617	NEX	C11-C10	-2.25	1.36	1.43
25	R	603	CLA	C4C-C3C	-2.25	1.41	1.45
24	Y	307	CHL	CHC-C1C	2.24	1.40	1.35
24	N	608	CHL	C1B-NB	2.24	1.37	1.35
24	Y	309	CHL	C1B-NB	2.24	1.37	1.35
24	y	309	CHL	C1B-NB	2.24	1.37	1.35
41	R	616	XAT	C14-C13	2.24	1.38	1.35
24	G	609	CHL	MG-NC	2.24	2.11	2.06
24	g	609	CHL	MG-NC	2.24	2.11	2.06
25	c	503	CLA	C1C-C2C	-2.24	1.40	1.44
25	G	603	CLA	C1C-C2C	-2.24	1.40	1.44
25	c	512	CLA	C1C-C2C	-2.24	1.40	1.44
25	r	604	CLA	C4B-CHC	-2.24	1.34	1.41
25	Y	304	CLA	C1C-C2C	-2.24	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	304	CLA	C1C-C2C	-2.24	1.40	1.44
39	R	615	LUT	C26-C27	2.24	1.53	1.50
25	B	613	CLA	C1C-C2C	-2.24	1.40	1.44
25	Y	313	CLA	C1C-C2C	-2.24	1.40	1.44
25	b	613	CLA	C1C-C2C	-2.24	1.40	1.44
25	y	313	CLA	C1C-C2C	-2.24	1.40	1.44
25	N	613	CLA	CHD-C1D	-2.24	1.34	1.38
39	r	615	LUT	C26-C27	2.24	1.53	1.50
39	y	316	LUT	C23-C24	2.24	1.53	1.50
25	r	612	CLA	C4B-CHC	-2.23	1.34	1.41
24	1	302	CHL	C1B-NB	2.23	1.37	1.35
25	S	312	CLA	C4B-CHC	-2.23	1.34	1.41
25	S	313	CLA	C4B-CHC	-2.23	1.34	1.41
25	s	313	CLA	C4B-CHC	-2.23	1.34	1.41
25	G	604	CLA	C1C-C2C	-2.23	1.40	1.44
25	N	604	CLA	C1C-C2C	-2.23	1.40	1.44
25	g	604	CLA	C1C-C2C	-2.23	1.40	1.44
24	N	609	CHL	MG-NC	2.23	2.11	2.06
24	n	609	CHL	MG-NC	2.23	2.11	2.06
39	R	615	LUT	C5-C6	2.22	1.38	1.34
39	g	615	LUT	C5-C6	2.22	1.38	1.34
39	S	316	LUT	C5-C6	2.22	1.38	1.34
39	s	316	LUT	C5-C6	2.22	1.38	1.34
41	R	616	XAT	C34-C33	2.22	1.38	1.35
41	r	616	XAT	C34-C33	2.22	1.38	1.35
25	G	602	CLA	CHD-C1D	-2.22	1.34	1.38
25	g	602	CLA	CHD-C1D	-2.22	1.34	1.38
39	G	615	LUT	C5-C6	2.22	1.38	1.34
25	Y	315	CLA	C1C-C2C	-2.22	1.40	1.44
25	a	403	CLA	C1C-C2C	-2.22	1.40	1.44
25	y	315	CLA	C1C-C2C	-2.22	1.40	1.44
25	C	503	CLA	C1C-C2C	-2.22	1.40	1.44
25	s	312	CLA	C4B-CHC	-2.22	1.34	1.41
25	G	610	CLA	C4B-CHC	-2.21	1.34	1.41
25	g	610	CLA	C4B-CHC	-2.21	1.34	1.41
25	A	401	CLA	C1C-C2C	-2.21	1.40	1.44
25	a	402	CLA	C1C-C2C	-2.21	1.40	1.44
25	G	602	CLA	C1C-C2C	-2.21	1.40	1.44
25	g	602	CLA	C1C-C2C	-2.21	1.40	1.44
25	d	401	CLA	C1C-C2C	-2.21	1.40	1.44
25	C	508	CLA	C1C-C2C	-2.21	1.40	1.44
25	c	508	CLA	C1C-C2C	-2.21	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	306	CHL	MG-NC	2.21	2.11	2.06
24	Y	310	CHL	MG-NC	2.21	2.11	2.06
39	s	315	LUT	C5-C6	2.21	1.38	1.34
25	R	612	CLA	C4B-CHC	-2.21	1.34	1.41
24	R	605	CHL	MG-NC	2.21	2.11	2.06
25	n	613	CLA	CHD-C1D	-2.21	1.34	1.38
24	S	306	CHL	MG-NC	2.21	2.11	2.06
24	s	306	CHL	MG-NC	2.21	2.11	2.06
25	G	614	CLA	C1C-C2C	-2.21	1.40	1.44
25	g	614	CLA	C1C-C2C	-2.21	1.40	1.44
25	A	402	CLA	C1C-C2C	-2.20	1.40	1.44
39	r	615	LUT	C5-C6	2.20	1.38	1.34
25	r	611	CLA	C4D-ND	-2.20	1.34	1.37
25	C	512	CLA	C1C-C2C	-2.20	1.40	1.44
25	b	603	CLA	C1C-C2C	-2.20	1.40	1.44
24	5	302	CHL	C1B-NB	2.19	1.37	1.35
24	y	310	CHL	MG-NC	2.19	2.11	2.06
24	5	301	CHL	MG-NC	2.19	2.11	2.06
25	c	507	CLA	C1C-C2C	-2.19	1.40	1.44
24	r	605	CHL	MG-NC	2.19	2.11	2.06
25	B	612	CLA	C1C-C2C	-2.19	1.40	1.44
25	b	612	CLA	C1C-C2C	-2.19	1.40	1.44
25	C	510	CLA	C1C-C2C	-2.19	1.40	1.44
40	Y	318	NEX	C31-C32	2.19	1.40	1.34
25	B	616	CLA	C1C-C2C	-2.19	1.40	1.44
25	b	616	CLA	C1C-C2C	-2.19	1.40	1.44
24	N	605	CHL	MG-NC	2.19	2.11	2.06
24	n	605	CHL	MG-NC	2.19	2.11	2.06
24	s	308	CHL	MG-NC	2.19	2.11	2.06
24	N	606	CHL	MG-NC	2.18	2.11	2.06
24	n	606	CHL	MG-NC	2.18	2.11	2.06
39	S	315	LUT	C26-C27	2.18	1.53	1.50
24	S	308	CHL	MG-NC	2.18	2.11	2.06
25	R	601	CLA	C4C-C3C	-2.18	1.41	1.45
25	r	601	CLA	C4C-C3C	-2.18	1.41	1.45
25	B	607	CLA	C1C-C2C	-2.18	1.40	1.44
25	C	507	CLA	C1C-C2C	-2.18	1.40	1.44
25	b	607	CLA	C1C-C2C	-2.18	1.40	1.44
24	G	606	CHL	C1B-NB	2.18	1.37	1.35
25	R	611	CLA	C4C-C3C	-2.18	1.41	1.45
25	r	611	CLA	C4C-C3C	-2.18	1.41	1.45
25	S	314	CLA	C1C-C2C	-2.18	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	603	CHL	C1B-NB	2.18	1.37	1.35
24	6	603	CHL	C1B-NB	2.18	1.37	1.35
24	g	606	CHL	C1B-NB	2.18	1.37	1.35
25	R	611	CLA	C4D-ND	-2.18	1.34	1.37
24	R	607	CHL	MG-NC	2.18	2.11	2.06
24	r	607	CHL	MG-NC	2.18	2.11	2.06
25	y	312	CLA	CHD-C1D	-2.17	1.34	1.38
25	D	401	CLA	C1C-C2C	-2.17	1.40	1.44
40	Y	318	NEX	C32-C33	-2.17	1.41	1.45
39	Y	316	LUT	C23-C24	2.17	1.53	1.50
39	s	315	LUT	C26-C27	2.17	1.53	1.50
25	2	602	CLA	C4C-C3C	-2.17	1.41	1.45
25	6	602	CLA	C4C-C3C	-2.17	1.41	1.45
25	n	612	CLA	C1C-C2C	-2.17	1.40	1.44
25	c	506	CLA	C1C-C2C	-2.17	1.40	1.44
24	y	306	CHL	MG-NC	2.17	2.11	2.06
25	2	602	CLA	C3D-C4D	-2.17	1.39	1.44
25	S	304	CLA	C1C-C2C	-2.17	1.40	1.44
25	A	405	CLA	C1C-C2C	-2.17	1.40	1.44
25	a	406	CLA	C1C-C2C	-2.17	1.40	1.44
24	G	606	CHL	MG-NC	2.17	2.11	2.06
24	g	606	CHL	MG-NC	2.17	2.11	2.06
25	B	615	CLA	C4B-CHC	-2.17	1.35	1.41
25	b	615	CLA	C4B-CHC	-2.17	1.35	1.41
25	Y	314	CLA	C1C-C2C	-2.16	1.40	1.44
25	y	314	CLA	C1C-C2C	-2.16	1.40	1.44
39	G	616	LUT	C1-C6	2.16	1.56	1.53
39	g	616	LUT	C1-C6	2.16	1.56	1.53
25	B	603	CLA	C1C-C2C	-2.16	1.40	1.44
25	N	612	CLA	C1C-C2C	-2.16	1.40	1.44
25	b	605	CLA	C1C-C2C	-2.16	1.40	1.44
25	R	608	CLA	C1C-C2C	-2.16	1.40	1.44
25	s	311	CLA	C1C-C2C	-2.16	1.40	1.44
25	n	604	CLA	C1C-C2C	-2.16	1.40	1.44
25	r	608	CLA	C1C-C2C	-2.16	1.40	1.44
25	Y	315	CLA	C1B-CHB	-2.16	1.35	1.41
25	y	315	CLA	C1B-CHB	-2.16	1.35	1.41
25	c	510	CLA	C1C-C2C	-2.16	1.40	1.44
24	N	601	CHL	MG-NC	2.15	2.11	2.06
24	n	601	CHL	MG-NC	2.15	2.11	2.06
40	y	318	NEX	C31-C32	2.15	1.40	1.34
25	s	304	CLA	C1C-C2C	-2.15	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	308	CHL	C3B-CAB	-2.15	1.43	1.47
24	y	308	CHL	C3B-CAB	-2.15	1.43	1.47
25	B	605	CLA	C1C-C2C	-2.15	1.40	1.44
25	b	604	CLA	C1C-C2C	-2.15	1.40	1.44
25	r	602	CLA	C1C-C2C	-2.15	1.40	1.44
25	c	509	CLA	C1C-C2C	-2.15	1.40	1.44
25	C	506	CLA	C1C-C2C	-2.14	1.40	1.44
25	6	602	CLA	C3D-C4D	-2.14	1.39	1.44
25	s	314	CLA	C1C-C2C	-2.14	1.40	1.44
24	G	605	CHL	MG-NC	2.14	2.11	2.06
24	g	605	CHL	MG-NC	2.14	2.11	2.06
25	Y	312	CLA	C1C-C2C	-2.14	1.40	1.44
25	y	312	CLA	C1C-C2C	-2.14	1.40	1.44
24	N	608	CHL	MG-NC	2.14	2.11	2.06
24	n	608	CHL	MG-NC	2.14	2.11	2.06
25	R	611	CLA	CHC-C1C	2.14	1.40	1.35
25	r	611	CLA	CHC-C1C	2.14	1.40	1.35
25	n	612	CLA	C4C-C3C	-2.14	1.41	1.45
25	Y	312	CLA	CHD-C1D	-2.14	1.34	1.38
24	Y	302	CHL	MG-NC	2.14	2.11	2.06
24	N	607	CHL	C3B-CAB	-2.14	1.43	1.47
25	B	602	CLA	C1C-C2C	-2.14	1.40	1.44
25	S	311	CLA	C1C-C2C	-2.14	1.40	1.44
25	g	613	CLA	C1C-C2C	-2.14	1.40	1.44
24	n	607	CHL	C3B-CAB	-2.13	1.43	1.47
39	Y	316	LUT	C5-C6	2.13	1.38	1.34
40	y	318	NEX	C32-C33	-2.13	1.41	1.45
25	B	604	CLA	C1C-C2C	-2.13	1.40	1.44
25	C	513	CLA	C1C-C2C	-2.13	1.40	1.44
25	c	513	CLA	C1C-C2C	-2.13	1.40	1.44
25	C	511	CLA	C1C-C2C	-2.13	1.40	1.44
25	c	511	CLA	C1C-C2C	-2.13	1.40	1.44
25	Y	305	CLA	C1C-C2C	-2.13	1.40	1.44
25	y	305	CLA	C1C-C2C	-2.13	1.40	1.44
25	2	605	CLA	C1C-C2C	-2.13	1.40	1.44
25	S	305	CLA	C3D-C4D	-2.13	1.39	1.44
38	F	101	HEM	CHB-C1B	2.13	1.40	1.35
25	C	509	CLA	C1C-C2C	-2.12	1.40	1.44
40	S	317	NEX	C11-C10	-2.12	1.36	1.43
40	s	317	NEX	C11-C10	-2.12	1.36	1.43
25	s	305	CLA	C3D-C4D	-2.12	1.39	1.44
40	g	617	NEX	C11-C10	-2.12	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	614	CLA	C1C-C2C	-2.12	1.40	1.44
25	D	403	CLA	C3D-C4D	-2.12	1.39	1.44
24	N	606	CHL	C1B-NB	2.12	1.37	1.35
24	n	606	CHL	C1B-NB	2.12	1.37	1.35
25	N	602	CLA	CHD-C1D	-2.12	1.34	1.38
25	n	602	CLA	CHD-C1D	-2.12	1.34	1.38
24	G	608	CHL	MG-NC	2.12	2.11	2.06
24	Y	309	CHL	MG-NC	2.11	2.11	2.06
38	f	101	HEM	CHB-C1B	2.11	1.40	1.35
24	y	302	CHL	MG-NC	2.11	2.11	2.06
25	R	602	CLA	C1C-C2C	-2.11	1.40	1.44
39	y	316	LUT	C5-C6	2.10	1.38	1.34
25	S	309	CLA	C1C-C2C	-2.10	1.40	1.44
39	S	316	LUT	C26-C27	2.10	1.53	1.50
39	s	316	LUT	C26-C27	2.10	1.53	1.50
24	g	608	CHL	MG-NC	2.10	2.11	2.06
25	d	403	CLA	C3D-C4D	-2.10	1.39	1.44
25	6	605	CLA	C1C-C2C	-2.10	1.40	1.44
25	R	601	CLA	C3D-C4D	-2.10	1.39	1.44
25	r	601	CLA	C3D-C4D	-2.10	1.39	1.44
24	y	309	CHL	MG-NC	2.10	2.11	2.06
25	S	313	CLA	C1C-C2C	-2.10	1.40	1.44
25	Y	303	CLA	CHD-C1D	-2.09	1.34	1.38
25	Y	313	CLA	CHD-C1D	-2.09	1.34	1.38
25	y	303	CLA	CHD-C1D	-2.09	1.34	1.38
25	y	313	CLA	CHD-C1D	-2.09	1.34	1.38
25	N	614	CLA	C1C-C2C	-2.09	1.40	1.44
25	N	612	CLA	C4C-C3C	-2.09	1.41	1.45
25	B	610	CLA	C1C-C2C	-2.09	1.40	1.44
25	b	610	CLA	C1C-C2C	-2.09	1.40	1.44
25	C	504	CLA	C3D-C4D	-2.09	1.39	1.44
25	c	504	CLA	C3D-C4D	-2.09	1.39	1.44
24	G	601	CHL	MG-NC	2.09	2.11	2.06
24	g	601	CHL	MG-NC	2.09	2.11	2.06
25	N	611	CLA	CHD-C1D	-2.09	1.34	1.38
25	n	611	CLA	CHD-C1D	-2.09	1.34	1.38
25	G	613	CLA	C1C-C2C	-2.09	1.40	1.44
25	C	501	CLA	C3D-C4D	-2.09	1.39	1.44
25	b	602	CLA	C1C-C2C	-2.09	1.40	1.44
25	S	313	CLA	C3D-C4D	-2.08	1.39	1.44
25	N	613	CLA	C1C-C2C	-2.08	1.40	1.44
25	n	613	CLA	C1C-C2C	-2.08	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	612	CLA	C3D-C4D	-2.08	1.39	1.44
24	2	603	CHL	O1D-CGD	2.08	1.26	1.21
24	6	603	CHL	O1D-CGD	2.08	1.26	1.21
25	D	402	CLA	C1C-C2C	-2.08	1.40	1.44
25	d	402	CLA	C1C-C2C	-2.08	1.40	1.44
24	Y	310	CHL	C3B-CAB	-2.08	1.43	1.47
25	s	309	CLA	C1C-C2C	-2.08	1.40	1.44
25	r	609	CLA	C1C-C2C	-2.08	1.40	1.44
25	Y	303	CLA	C1C-C2C	-2.08	1.40	1.44
25	y	303	CLA	C1C-C2C	-2.08	1.40	1.44
25	b	601	CLA	C1C-C2C	-2.07	1.40	1.44
25	S	312	CLA	C1C-C2C	-2.07	1.40	1.44
38	F	101	HEM	C3B-C4B	2.07	1.49	1.44
38	f	101	HEM	C3B-C4B	2.07	1.49	1.44
25	R	609	CLA	C1C-C2C	-2.07	1.40	1.44
25	c	512	CLA	C3D-C4D	-2.07	1.39	1.44
25	A	402	CLA	C3D-C4D	-2.07	1.39	1.44
25	a	403	CLA	C3D-C4D	-2.07	1.39	1.44
25	N	602	CLA	C1C-C2C	-2.07	1.40	1.44
25	n	602	CLA	C1C-C2C	-2.07	1.40	1.44
24	2	601	CHL	O1D-CGD	2.06	1.26	1.21
24	6	601	CHL	O1D-CGD	2.06	1.26	1.21
25	g	613	CLA	CHD-C1D	-2.06	1.34	1.38
25	r	612	CLA	C3D-C4D	-2.06	1.39	1.44
25	G	613	CLA	CHD-C1D	-2.06	1.34	1.38
24	N	607	CHL	C1B-NB	2.06	1.37	1.35
25	y	311	CLA	C1C-C2C	-2.06	1.40	1.44
25	Y	311	CLA	C1C-C2C	-2.06	1.40	1.44
25	R	604	CLA	C1C-C2C	-2.06	1.40	1.44
24	G	609	CHL	O1D-CGD	2.06	1.26	1.21
25	S	310	CLA	C1C-C2C	-2.05	1.40	1.44
25	s	310	CLA	C1C-C2C	-2.05	1.40	1.44
25	B	606	CLA	C1C-C2C	-2.05	1.40	1.44
25	b	606	CLA	C1C-C2C	-2.05	1.40	1.44
25	C	509	CLA	C3D-C4D	-2.05	1.39	1.44
25	c	509	CLA	C3D-C4D	-2.05	1.39	1.44
25	s	313	CLA	C1C-C2C	-2.05	1.40	1.44
25	Y	304	CLA	C3D-C4D	-2.05	1.39	1.44
25	c	501	CLA	C3D-C4D	-2.05	1.39	1.44
25	y	304	CLA	C3D-C4D	-2.05	1.39	1.44
24	G	608	CHL	C3B-CAB	-2.05	1.43	1.47
24	g	608	CHL	O1D-CGD	2.05	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	301	CHL	O1D-CGD	2.05	1.26	1.21
24	S	308	CHL	O1D-CGD	2.05	1.26	1.21
25	r	612	CLA	C1C-C2C	-2.05	1.40	1.44
24	G	605	CHL	O1D-CGD	2.05	1.26	1.21
24	Y	309	CHL	C3B-CAB	-2.05	1.43	1.47
25	R	603	CLA	C3D-C4D	-2.05	1.39	1.44
25	r	603	CLA	C3D-C4D	-2.05	1.39	1.44
25	R	610	CLA	C3D-C4D	-2.05	1.39	1.44
24	Y	302	CHL	C3B-CAB	-2.05	1.43	1.47
24	g	605	CHL	O1D-CGD	2.05	1.26	1.21
24	R	613	CHL	O1D-CGD	2.04	1.26	1.21
24	R	607	CHL	O1D-CGD	2.04	1.26	1.21
24	r	607	CHL	O1D-CGD	2.04	1.26	1.21
24	Y	306	CHL	C3B-CAB	-2.04	1.43	1.47
24	y	306	CHL	C3B-CAB	-2.04	1.43	1.47
24	Y	307	CHL	C3B-CAB	-2.04	1.43	1.47
39	Y	317	LUT	C1-C6	2.04	1.56	1.53
25	s	312	CLA	C1C-C2C	-2.04	1.40	1.44
25	n	604	CLA	C3D-C4D	-2.04	1.39	1.44
39	S	316	LUT	C1-C6	2.04	1.56	1.53
24	g	601	CHL	O1D-CGD	2.04	1.26	1.21
25	b	612	CLA	C3D-C4D	-2.04	1.39	1.44
24	y	310	CHL	C3B-CAB	-2.04	1.43	1.47
24	G	607	CHL	C3B-CAB	-2.04	1.43	1.47
25	s	313	CLA	C3D-C4D	-2.04	1.39	1.44
24	g	605	CHL	C1B-NB	2.04	1.37	1.35
24	R	607	CHL	C3B-CAB	-2.04	1.43	1.47
24	r	607	CHL	C3B-CAB	-2.04	1.43	1.47
24	r	613	CHL	O1D-CGD	2.04	1.26	1.21
24	n	606	CHL	C3B-CAB	-2.04	1.43	1.47
25	D	402	CLA	C3D-C4D	-2.04	1.39	1.44
25	d	402	CLA	C3D-C4D	-2.04	1.39	1.44
25	D	401	CLA	C3D-C4D	-2.03	1.39	1.44
25	d	401	CLA	C3D-C4D	-2.03	1.39	1.44
24	1	302	CHL	O1D-CGD	2.03	1.26	1.21
24	5	302	CHL	O1D-CGD	2.03	1.26	1.21
24	R	605	CHL	C3B-CAB	-2.03	1.43	1.47
24	n	606	CHL	O1D-CGD	2.03	1.26	1.21
25	C	512	CLA	C3D-C4D	-2.03	1.39	1.44
25	B	604	CLA	C3D-C4D	-2.03	1.39	1.44
25	C	510	CLA	C3D-C4D	-2.03	1.39	1.44
25	S	314	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	612	CLA	C3D-C4D	-2.03	1.39	1.44
24	s	308	CHL	O1D-CGD	2.03	1.26	1.21
25	G	612	CLA	C1C-C2C	-2.03	1.40	1.44
25	A	405	CLA	C3D-C4D	-2.03	1.39	1.44
25	a	406	CLA	C3D-C4D	-2.03	1.39	1.44
24	y	310	CHL	O1D-CGD	2.03	1.26	1.21
24	6	601	CHL	C3B-CAB	-2.03	1.43	1.47
24	S	306	CHL	C1B-NB	2.03	1.37	1.35
24	G	601	CHL	O1D-CGD	2.03	1.26	1.21
24	n	607	CHL	C1B-NB	2.02	1.37	1.35
24	G	608	CHL	O1D-CGD	2.02	1.26	1.21
24	S	308	CHL	C3B-CAB	-2.02	1.43	1.47
24	s	308	CHL	C3B-CAB	-2.02	1.43	1.47
25	B	601	CLA	C1C-C2C	-2.02	1.40	1.44
24	R	605	CHL	O1D-CGD	2.02	1.26	1.21
24	5	301	CHL	O1D-CGD	2.02	1.26	1.21
24	r	605	CHL	O1D-CGD	2.02	1.26	1.21
24	y	307	CHL	C4C-C3C	-2.02	1.41	1.45
25	g	611	CLA	CHD-C1D	-2.02	1.34	1.38
25	2	602	CLA	CHC-C1C	2.02	1.40	1.35
25	6	602	CLA	CHC-C1C	2.02	1.40	1.35
25	c	510	CLA	C3D-C4D	-2.02	1.39	1.44
24	s	306	CHL	O1D-CGD	2.02	1.26	1.21
39	N	616	LUT	C26-C27	2.02	1.53	1.50
39	n	616	LUT	C26-C27	2.02	1.53	1.50
24	n	601	CHL	C3B-CAB	-2.02	1.43	1.47
39	Y	317	LUT	C26-C27	2.02	1.53	1.50
25	r	604	CLA	C1C-C2C	-2.02	1.40	1.44
25	2	604	CLA	C4C-C3C	-2.02	1.41	1.45
25	6	604	CLA	C4C-C3C	-2.02	1.41	1.45
24	s	302	CHL	C3B-CAB	-2.02	1.43	1.47
24	N	605	CHL	O1D-CGD	2.02	1.26	1.21
38	f	101	HEM	CHA-C4D	2.02	1.40	1.35
24	S	307	CHL	C3B-CAB	-2.02	1.43	1.47
24	s	307	CHL	C3B-CAB	-2.02	1.43	1.47
25	r	610	CLA	C3D-C4D	-2.02	1.39	1.44
25	N	604	CLA	C3D-C4D	-2.02	1.39	1.44
25	n	610	CLA	C1C-C2C	-2.02	1.40	1.44
24	s	306	CHL	C1B-NB	2.02	1.37	1.35
24	N	605	CHL	C3B-CAB	-2.02	1.43	1.47
24	n	605	CHL	C3B-CAB	-2.02	1.43	1.47
40	y	318	NEX	C35-C15	2.02	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	r	617	NEX	C31-C32	2.02	1.39	1.34
24	n	609	CHL	O1D-CGD	2.02	1.26	1.21
24	y	309	CHL	C3B-CAB	-2.02	1.43	1.47
24	G	609	CHL	C3B-CAB	-2.02	1.43	1.47
24	N	606	CHL	O1D-CGD	2.01	1.26	1.21
25	R	612	CLA	C1C-C2C	-2.01	1.40	1.44
39	y	317	LUT	C1-C6	2.01	1.56	1.53
25	N	610	CLA	CHD-C1D	-2.01	1.34	1.38
24	2	601	CHL	MG-NC	2.01	2.11	2.06
24	6	601	CHL	MG-NC	2.01	2.11	2.06
28	T	101	BCR	C33-C5	-2.01	1.47	1.50
25	A	401	CLA	C3D-C4D	-2.01	1.39	1.44
25	a	402	CLA	C3D-C4D	-2.01	1.39	1.44
24	S	306	CHL	C3B-CAB	-2.01	1.43	1.47
24	N	601	CHL	C3B-CAB	-2.01	1.43	1.47
24	s	306	CHL	C3B-CAB	-2.01	1.43	1.47
24	S	306	CHL	O1D-CGD	2.01	1.26	1.21
24	Y	306	CHL	O1D-CGD	2.01	1.26	1.21
24	y	306	CHL	O1D-CGD	2.01	1.26	1.21
25	B	608	CLA	C3D-C4D	-2.01	1.39	1.44
25	S	303	CLA	C3D-C4D	-2.01	1.39	1.44
25	b	608	CLA	C3D-C4D	-2.01	1.39	1.44
28	t	101	BCR	C33-C5	-2.01	1.47	1.50
24	N	601	CHL	O1D-CGD	2.01	1.26	1.21
24	s	307	CHL	O1D-CGD	2.01	1.26	1.21
25	c	513	CLA	C3D-C4D	-2.01	1.39	1.44
39	G	615	LUT	C26-C27	2.01	1.53	1.50
25	R	601	CLA	C1C-C2C	-2.01	1.40	1.44
25	r	601	CLA	C1C-C2C	-2.01	1.40	1.44
24	S	308	CHL	C1B-NB	2.01	1.37	1.35
24	s	308	CHL	C1B-NB	2.01	1.37	1.35
39	s	316	LUT	C1-C6	2.01	1.56	1.53
24	r	613	CHL	C1B-NB	2.01	1.37	1.35
25	N	611	CLA	C1C-C2C	-2.01	1.40	1.44
25	n	611	CLA	C1C-C2C	-2.01	1.40	1.44
25	s	314	CLA	C3D-C4D	-2.01	1.39	1.44
24	1	301	CHL	C3B-CAB	-2.00	1.43	1.47
24	Y	302	CHL	O1D-CGD	2.00	1.26	1.21
24	g	609	CHL	O1D-CGD	2.00	1.26	1.21
24	n	601	CHL	O1D-CGD	2.00	1.26	1.21
25	g	611	CLA	C1C-C2C	-2.00	1.40	1.44
24	G	601	CHL	C3B-CAB	-2.00	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	608	CHL	C3B-CAB	-2.00	1.43	1.47
24	S	302	CHL	O1D-CGD	2.00	1.26	1.21
24	s	302	CHL	O1D-CGD	2.00	1.26	1.21
25	C	513	CLA	C3D-C4D	-2.00	1.39	1.44
24	y	308	CHL	C1B-NB	2.00	1.37	1.35
24	y	302	CHL	O1D-CGD	2.00	1.26	1.21
25	R	604	CLA	C3D-C4D	-2.00	1.39	1.44
24	N	606	CHL	C3B-CAB	-2.00	1.43	1.47
25	S	304	CLA	C3D-C4D	-2.00	1.39	1.44
25	c	502	CLA	C1B-CHB	-2.00	1.35	1.41
24	R	606	CHL	O1D-CGD	2.00	1.26	1.21
24	y	302	CHL	C3B-CAB	-2.00	1.43	1.47
25	N	603	CLA	C3D-C4D	-2.00	1.39	1.44
25	n	603	CLA	C3D-C4D	-2.00	1.39	1.44

All (4029) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	305	CLA	C4A-NA-C1A	-18.81	98.25	106.71
25	S	305	CLA	C4A-NA-C1A	-18.75	98.28	106.71
25	r	601	CLA	C4A-NA-C1A	-17.30	98.93	106.71
25	R	601	CLA	C4A-NA-C1A	-17.14	99.00	106.71
25	R	610	CLA	C4A-NA-C1A	-16.34	99.36	106.71
25	r	610	CLA	C4A-NA-C1A	-16.34	99.36	106.71
25	D	403	CLA	C4A-NA-C1A	-16.26	99.40	106.71
25	d	403	CLA	C4A-NA-C1A	-16.26	99.40	106.71
25	R	611	CLA	C4A-NA-C1A	-16.04	99.50	106.71
25	r	611	CLA	C4A-NA-C1A	-16.04	99.50	106.71
25	r	603	CLA	C4A-NA-C1A	-15.47	99.75	106.71
25	R	603	CLA	C4A-NA-C1A	-15.35	99.80	106.71
25	c	504	CLA	C4A-NA-C1A	-15.03	99.95	106.71
25	C	504	CLA	C4A-NA-C1A	-14.98	99.97	106.71
25	C	501	CLA	C4A-NA-C1A	-14.34	100.26	106.71
25	c	501	CLA	C4A-NA-C1A	-14.34	100.26	106.71
24	6	601	CHL	C4A-NA-C1A	11.88	112.05	106.71
24	2	601	CHL	C4A-NA-C1A	11.81	112.02	106.71
25	C	511	CLA	C4A-NA-C1A	-11.60	101.49	106.71
25	c	511	CLA	C4A-NA-C1A	-11.48	101.54	106.71
24	r	605	CHL	C4A-NA-C1A	10.70	111.52	106.71
24	s	308	CHL	C4A-NA-C1A	10.67	111.50	106.71
24	R	605	CHL	C4A-NA-C1A	10.66	111.50	106.71
25	S	313	CLA	C4A-NA-C1A	-10.66	101.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	313	CLA	C4A-NA-C1A	-10.66	101.92	106.71
24	S	308	CHL	C4A-NA-C1A	10.63	111.48	106.71
24	S	307	CHL	C4A-NA-C1A	10.35	111.36	106.71
24	g	609	CHL	C4A-NA-C1A	10.31	111.34	106.71
24	g	606	CHL	C4A-NA-C1A	10.27	111.32	106.71
24	s	307	CHL	C4A-NA-C1A	10.26	111.32	106.71
25	2	602	CLA	C4A-NA-C1A	10.25	111.31	106.71
25	6	602	CLA	C4A-NA-C1A	10.25	111.31	106.71
24	G	606	CHL	C4A-NA-C1A	10.19	111.29	106.71
24	G	609	CHL	C4A-NA-C1A	10.18	111.28	106.71
24	R	607	CHL	C4A-NA-C1A	10.16	111.28	106.71
24	S	306	CHL	C4A-NA-C1A	10.11	111.25	106.71
24	s	306	CHL	C4A-NA-C1A	10.11	111.25	106.71
24	1	302	CHL	C4A-NA-C1A	10.09	111.24	106.71
24	5	302	CHL	C4A-NA-C1A	10.09	111.24	106.71
24	r	607	CHL	C4A-NA-C1A	10.08	111.24	106.71
25	S	311	CLA	C4A-NA-C1A	-10.06	102.18	106.71
25	s	311	CLA	C4A-NA-C1A	-10.06	102.18	106.71
24	6	603	CHL	C4A-NA-C1A	10.04	111.22	106.71
24	2	603	CHL	C4A-NA-C1A	9.97	111.19	106.71
24	n	606	CHL	C4A-NA-C1A	9.88	111.15	106.71
24	R	613	CHL	C4A-NA-C1A	9.86	111.14	106.71
24	r	613	CHL	C4A-NA-C1A	9.86	111.14	106.71
24	N	606	CHL	C4A-NA-C1A	9.78	111.10	106.71
24	Y	302	CHL	C4A-NA-C1A	9.67	111.05	106.71
24	y	302	CHL	C4A-NA-C1A	9.67	111.05	106.71
24	N	605	CHL	C4A-NA-C1A	9.64	111.04	106.71
24	G	608	CHL	C4A-NA-C1A	9.60	111.02	106.71
24	Y	306	CHL	C4A-NA-C1A	9.60	111.02	106.71
40	r	617	NEX	C15-C14-C13	-9.59	113.62	127.31
40	R	617	NEX	C15-C14-C13	-9.59	113.63	127.31
24	n	605	CHL	C4A-NA-C1A	9.58	111.01	106.71
24	y	306	CHL	C4A-NA-C1A	9.58	111.01	106.71
24	n	608	CHL	C4A-NA-C1A	9.57	111.01	106.71
24	S	302	CHL	C4A-NA-C1A	9.56	111.00	106.71
24	s	302	CHL	C4A-NA-C1A	9.56	111.00	106.71
24	N	608	CHL	C4A-NA-C1A	9.55	111.00	106.71
25	R	611	CLA	C4D-CHA-C1A	-9.54	109.64	121.25
25	r	611	CLA	C4D-CHA-C1A	-9.54	109.64	121.25
24	g	608	CHL	C4A-NA-C1A	9.50	110.97	106.71
24	5	301	CHL	C4A-NA-C1A	9.47	110.96	106.71
24	g	605	CHL	C4A-NA-C1A	9.46	110.96	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	301	CHL	C4A-NA-C1A	9.38	110.92	106.71
24	G	605	CHL	C4A-NA-C1A	9.37	110.92	106.71
40	S	317	NEX	O24-C25-C24	9.29	120.36	113.38
40	s	317	NEX	O24-C25-C24	9.27	120.34	113.38
24	R	606	CHL	C4A-NA-C1A	9.21	110.85	106.71
24	y	308	CHL	C4A-NA-C1A	9.18	110.83	106.71
25	N	614	CLA	C4A-NA-C1A	-9.15	102.59	106.71
24	r	606	CHL	C4A-NA-C1A	9.13	110.81	106.71
24	Y	308	CHL	C4A-NA-C1A	9.12	110.81	106.71
25	g	610	CLA	C4A-NA-C1A	-9.09	102.62	106.71
24	Y	309	CHL	C4A-NA-C1A	9.02	110.76	106.71
24	G	601	CHL	C4A-NA-C1A	9.00	110.75	106.71
24	g	601	CHL	C4A-NA-C1A	9.00	110.75	106.71
25	G	610	CLA	C4A-NA-C1A	-9.00	102.66	106.71
25	n	614	CLA	C4A-NA-C1A	-9.00	102.66	106.71
40	g	617	NEX	C11-C10-C9	-8.90	114.61	127.31
40	n	617	NEX	O24-C25-C24	8.89	120.06	113.38
24	N	607	CHL	C4A-NA-C1A	8.88	110.70	106.71
24	y	309	CHL	C4A-NA-C1A	8.85	110.68	106.71
40	N	617	NEX	O24-C25-C24	8.84	120.02	113.38
24	n	607	CHL	C4A-NA-C1A	8.84	110.68	106.71
40	G	617	NEX	O24-C25-C24	8.81	120.00	113.38
40	g	617	NEX	O24-C25-C24	8.77	119.97	113.38
40	G	617	NEX	C11-C10-C9	-8.74	114.84	127.31
24	y	310	CHL	C4A-NA-C1A	8.64	110.59	106.71
24	Y	310	CHL	C4A-NA-C1A	8.62	110.58	106.71
25	R	601	CLA	C1B-CHB-C4A	-8.42	113.44	130.12
25	r	601	CLA	C1B-CHB-C4A	-8.38	113.52	130.12
24	N	609	CHL	C4A-NA-C1A	8.16	110.37	106.71
24	n	609	CHL	C4A-NA-C1A	8.14	110.37	106.71
25	Y	314	CLA	C4A-NA-C1A	-8.03	103.09	106.71
25	y	314	CLA	C4A-NA-C1A	-8.03	103.09	106.71
25	N	604	CLA	C4A-NA-C1A	-7.88	103.16	106.71
24	N	601	CHL	C4A-NA-C1A	7.87	110.24	106.71
40	R	617	NEX	C35-C34-C33	-7.86	116.10	127.31
40	r	617	NEX	C35-C34-C33	-7.86	116.10	127.31
25	n	604	CLA	C4A-NA-C1A	-7.80	103.20	106.71
24	n	601	CHL	C4A-NA-C1A	7.78	110.20	106.71
41	R	616	XAT	O24-C25-C24	7.71	119.17	113.38
41	r	616	XAT	O24-C25-C24	7.71	119.17	113.38
24	G	607	CHL	C4A-NA-C1A	7.70	110.17	106.71
24	g	607	CHL	C4A-NA-C1A	7.68	110.16	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	613	CLA	C4A-NA-C1A	-7.61	103.28	106.71
25	S	305	CLA	C1B-CHB-C4A	-7.51	115.24	130.12
25	B	606	CLA	CHD-C1D-ND	-7.51	117.55	124.45
25	b	606	CLA	CHD-C1D-ND	-7.51	117.55	124.45
25	s	305	CLA	C1B-CHB-C4A	-7.50	115.26	130.12
25	G	613	CLA	C4A-NA-C1A	-7.50	103.34	106.71
40	R	617	NEX	O24-C25-C24	7.44	118.97	113.38
40	r	617	NEX	O24-C25-C24	7.43	118.97	113.38
25	r	612	CLA	CHD-C1D-ND	-7.42	117.64	124.45
40	y	318	NEX	C31-C30-C29	-7.40	116.75	127.31
40	Y	318	NEX	C31-C30-C29	-7.40	116.75	127.31
25	R	612	CLA	CHD-C1D-ND	-7.36	117.69	124.45
25	r	604	CLA	CHD-C1D-ND	-7.36	117.69	124.45
25	R	604	CLA	CHD-C1D-ND	-7.35	117.70	124.45
25	R	612	CLA	C4A-NA-C1A	-7.29	103.43	106.71
25	B	601	CLA	CHD-C1D-ND	-7.20	117.83	124.45
25	S	304	CLA	C4A-NA-C1A	-7.20	103.47	106.71
25	s	304	CLA	C4A-NA-C1A	-7.20	103.47	106.71
25	D	403	CLA	C1B-CHB-C4A	-7.19	115.87	130.12
25	d	403	CLA	C1B-CHB-C4A	-7.19	115.87	130.12
25	R	611	CLA	CHD-C1D-ND	-7.19	117.85	124.45
25	b	601	CLA	CHD-C1D-ND	-7.18	117.86	124.45
25	r	612	CLA	C4A-NA-C1A	-7.18	103.48	106.71
25	r	611	CLA	CHD-C1D-ND	-7.17	117.86	124.45
40	g	617	NEX	C27-C28-C29	-7.13	114.47	125.53
25	d	401	CLA	C4A-NA-C1A	-7.11	103.51	106.71
25	D	401	CLA	C4A-NA-C1A	-7.10	103.51	106.71
27	A	403	PHO	O2D-CGD-CBD	7.10	119.99	111.00
27	a	404	PHO	O2D-CGD-CBD	7.10	119.99	111.00
27	A	404	PHO	O2D-CGD-CBD	7.10	119.99	111.00
40	G	617	NEX	C27-C28-C29	-7.06	114.57	125.53
27	a	405	PHO	O2D-CGD-CBD	7.06	119.94	111.00
40	G	617	NEX	C31-C30-C29	-7.05	117.25	127.31
25	r	610	CLA	C1B-CHB-C4A	-7.01	116.24	130.12
25	r	603	CLA	C1B-CHB-C4A	-6.99	116.27	130.12
25	C	510	CLA	CHD-C1D-ND	-6.99	118.03	124.45
25	c	510	CLA	CHD-C1D-ND	-6.99	118.03	124.45
40	g	617	NEX	C31-C30-C29	-6.98	117.34	127.31
25	R	603	CLA	C1B-CHB-C4A	-6.98	116.30	130.12
25	R	610	CLA	C1B-CHB-C4A	-6.98	116.31	130.12
25	B	605	CLA	C4A-NA-C1A	-6.83	103.63	106.71
25	S	313	CLA	CHD-C1D-ND	-6.83	118.18	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	313	CLA	CHD-C1D-ND	-6.83	118.18	124.45
25	c	508	CLA	CHD-C1D-ND	-6.82	118.19	124.45
25	C	508	CLA	CHD-C1D-ND	-6.72	118.28	124.45
25	c	507	CLA	CHD-C1D-ND	-6.72	118.28	124.45
25	b	605	CLA	C4A-NA-C1A	-6.69	103.70	106.71
25	C	507	CLA	CHD-C1D-ND	-6.69	118.31	124.45
25	A	401	CLA	CHD-C1D-ND	-6.68	118.32	124.45
25	a	402	CLA	CHD-C1D-ND	-6.68	118.32	124.45
25	B	605	CLA	CHD-C1D-ND	-6.67	118.32	124.45
25	b	605	CLA	CHD-C1D-ND	-6.67	118.32	124.45
25	S	310	CLA	CHD-C1D-ND	-6.67	118.33	124.45
25	s	310	CLA	CHD-C1D-ND	-6.66	118.33	124.45
41	r	616	XAT	O4-C5-C4	6.65	118.38	113.38
41	R	616	XAT	O4-C5-C4	6.63	118.36	113.38
25	c	509	CLA	C4A-NA-C1A	-6.63	103.72	106.71
25	N	612	CLA	CHD-C1D-ND	-6.62	118.37	124.45
25	s	304	CLA	CHD-C1D-ND	-6.60	118.39	124.45
25	n	612	CLA	CHD-C1D-ND	-6.59	118.40	124.45
25	b	604	CLA	CHD-C1D-ND	-6.58	118.41	124.45
25	C	509	CLA	C4A-NA-C1A	-6.58	103.75	106.71
25	g	604	CLA	C4A-NA-C1A	-6.55	103.76	106.71
25	R	609	CLA	CHD-C1D-ND	-6.55	118.44	124.45
25	G	604	CLA	C4A-NA-C1A	-6.53	103.77	106.71
25	c	504	CLA	C1B-CHB-C4A	-6.53	117.19	130.12
25	r	609	CLA	CHD-C1D-ND	-6.53	118.45	124.45
25	S	304	CLA	CHD-C1D-ND	-6.52	118.46	124.45
25	B	604	CLA	CHD-C1D-ND	-6.51	118.47	124.45
25	C	504	CLA	C1B-CHB-C4A	-6.50	117.24	130.12
25	B	601	CLA	C4A-NA-C1A	-6.48	103.79	106.71
25	A	402	CLA	CHD-C1D-ND	-6.45	118.52	124.45
25	C	502	CLA	C4A-NA-C1A	-6.44	103.81	106.71
25	c	502	CLA	C4A-NA-C1A	-6.44	103.81	106.71
25	R	602	CLA	C4A-NA-C1A	-6.44	103.81	106.71
25	r	602	CLA	C4A-NA-C1A	-6.44	103.81	106.71
25	a	403	CLA	CHD-C1D-ND	-6.43	118.55	124.45
40	N	617	NEX	C15-C14-C13	-6.42	118.14	127.31
25	C	512	CLA	CHD-C1D-ND	-6.41	118.56	124.45
40	n	617	NEX	C15-C14-C13	-6.40	118.17	127.31
25	c	512	CLA	CHD-C1D-ND	-6.40	118.57	124.45
25	b	601	CLA	C4A-NA-C1A	-6.39	103.83	106.71
25	c	503	CLA	CHD-C1D-ND	-6.39	118.58	124.45
41	R	616	XAT	C35-C34-C33	-6.39	118.20	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	r	616	XAT	C35-C34-C33	-6.39	118.20	127.31
25	B	614	CLA	C4A-NA-C1A	-6.37	103.84	106.71
25	6	605	CLA	C4A-NA-C1A	-6.37	103.84	106.71
25	2	605	CLA	C4A-NA-C1A	-6.35	103.85	106.71
25	b	614	CLA	C4A-NA-C1A	-6.35	103.85	106.71
25	C	503	CLA	CHD-C1D-ND	-6.35	118.62	124.45
25	R	611	CLA	C2D-C1D-ND	-6.35	105.43	110.10
25	S	311	CLA	CHD-C1D-ND	-6.35	118.62	124.45
25	c	508	CLA	C4A-NA-C1A	-6.33	103.86	106.71
25	C	508	CLA	C4A-NA-C1A	-6.28	103.88	106.71
25	s	311	CLA	CHD-C1D-ND	-6.27	118.69	124.45
25	r	611	CLA	C2D-C1D-ND	-6.27	105.48	110.10
25	n	613	CLA	C4A-NA-C1A	-6.27	103.89	106.71
25	A	405	CLA	CHD-C1D-ND	-6.26	118.70	124.45
25	N	613	CLA	C4A-NA-C1A	-6.25	103.90	106.71
25	a	406	CLA	CHD-C1D-ND	-6.24	118.72	124.45
25	B	609	CLA	C4A-NA-C1A	-6.23	103.90	106.71
25	b	609	CLA	C4A-NA-C1A	-6.23	103.90	106.71
25	G	613	CLA	CHD-C1D-ND	-6.19	118.77	124.45
25	g	613	CLA	CHD-C1D-ND	-6.15	118.81	124.45
25	s	313	CLA	C1B-CHB-C4A	-6.14	117.96	130.12
25	S	309	CLA	C4A-NA-C1A	-6.14	103.95	106.71
25	s	309	CLA	C4A-NA-C1A	-6.12	103.95	106.71
25	b	607	CLA	CHD-C1D-ND	-6.11	118.83	124.45
25	c	503	CLA	C4A-NA-C1A	-6.11	103.96	106.71
25	S	313	CLA	C1B-CHB-C4A	-6.11	118.02	130.12
25	2	602	CLA	CHD-C1D-ND	-6.07	118.88	124.45
25	6	602	CLA	CHD-C1D-ND	-6.07	118.88	124.45
25	B	607	CLA	CHD-C1D-ND	-6.07	118.88	124.45
25	C	503	CLA	C4A-NA-C1A	-6.04	103.99	106.71
25	C	511	CLA	CHD-C1D-ND	-6.02	118.92	124.45
25	c	511	CLA	CHD-C1D-ND	-6.02	118.92	124.45
25	N	613	CLA	CHD-C1D-ND	-6.00	118.94	124.45
25	n	613	CLA	CHD-C1D-ND	-6.00	118.94	124.45
25	C	501	CLA	C1B-CHB-C4A	-5.97	118.30	130.12
25	c	501	CLA	C1B-CHB-C4A	-5.97	118.30	130.12
25	D	401	CLA	CHD-C1D-ND	-5.92	119.01	124.45
25	R	608	CLA	CHD-C1D-ND	-5.92	119.01	124.45
25	d	401	CLA	CHD-C1D-ND	-5.92	119.01	124.45
25	C	504	CLA	CHD-C1D-ND	-5.91	119.02	124.45
25	c	505	CLA	CHD-C1D-ND	-5.90	119.03	124.45
25	2	604	CLA	CHD-C1D-ND	-5.90	119.03	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	604	CLA	CHD-C1D-ND	-5.90	119.03	124.45
25	c	504	CLA	CHD-C1D-ND	-5.90	119.04	124.45
25	r	608	CLA	CHD-C1D-ND	-5.90	119.04	124.45
25	c	513	CLA	CHD-C1D-ND	-5.88	119.05	124.45
25	B	611	CLA	CHD-C1D-ND	-5.88	119.05	124.45
25	b	611	CLA	CHD-C1D-ND	-5.88	119.05	124.45
25	D	403	CLA	CHD-C1D-ND	-5.87	119.06	124.45
25	R	602	CLA	CHD-C1D-ND	-5.87	119.06	124.45
25	d	403	CLA	CHD-C1D-ND	-5.87	119.06	124.45
25	C	513	CLA	CHD-C1D-ND	-5.86	119.07	124.45
25	r	602	CLA	CHD-C1D-ND	-5.85	119.07	124.45
25	C	505	CLA	CHD-C1D-ND	-5.84	119.08	124.45
25	b	603	CLA	CHD-C1D-ND	-5.83	119.10	124.45
25	S	303	CLA	CHD-C1D-ND	-5.81	119.12	124.45
25	B	611	CLA	C4A-NA-C1A	-5.79	104.10	106.71
25	b	611	CLA	C4A-NA-C1A	-5.79	104.10	106.71
25	N	604	CLA	CHD-C1D-ND	-5.79	119.13	124.45
25	n	604	CLA	CHD-C1D-ND	-5.78	119.14	124.45
25	B	603	CLA	CHD-C1D-ND	-5.78	119.14	124.45
25	R	603	CLA	CHD-C1D-ND	-5.77	119.15	124.45
25	s	303	CLA	CHD-C1D-ND	-5.76	119.16	124.45
25	6	602	CLA	C4D-CHA-C1A	-5.76	114.24	121.25
25	2	602	CLA	C4D-CHA-C1A	-5.74	114.27	121.25
25	C	501	CLA	CHD-C1D-ND	-5.73	119.19	124.45
25	c	501	CLA	CHD-C1D-ND	-5.73	119.19	124.45
25	b	612	CLA	CHD-C1D-ND	-5.73	119.19	124.45
25	R	610	CLA	CHD-C1D-ND	-5.72	119.20	124.45
25	B	614	CLA	CHD-C1D-ND	-5.72	119.20	124.45
25	b	614	CLA	CHD-C1D-ND	-5.72	119.20	124.45
25	s	305	CLA	CHD-C1D-ND	-5.72	119.20	124.45
25	S	305	CLA	CHD-C1D-ND	-5.70	119.21	124.45
25	r	603	CLA	CHD-C1D-ND	-5.70	119.22	124.45
25	r	610	CLA	CHD-C1D-ND	-5.69	119.22	124.45
25	G	603	CLA	C4A-NA-C1A	-5.66	104.16	106.71
33	A	413	BCT	O2-C-O1	5.66	134.22	119.55
33	a	414	BCT	O2-C-O1	5.66	134.22	119.55
25	B	612	CLA	C4A-NA-C1A	-5.65	104.17	106.71
25	b	612	CLA	C4A-NA-C1A	-5.65	104.17	106.71
25	B	612	CLA	CHD-C1D-ND	-5.65	119.26	124.45
25	g	603	CLA	C4A-NA-C1A	-5.64	104.17	106.71
25	n	603	CLA	CHD-C1D-ND	-5.61	119.30	124.45
25	N	603	CLA	CHD-C1D-ND	-5.58	119.33	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	314	CLA	CHD-C1D-ND	-5.57	119.33	124.45
25	B	608	CLA	CHD-C1D-ND	-5.57	119.33	124.45
25	b	608	CLA	CHD-C1D-ND	-5.57	119.33	124.45
25	r	601	CLA	C2A-C3A-C4A	-5.57	92.87	101.87
25	Y	314	CLA	CHD-C1D-ND	-5.57	119.34	124.45
25	R	601	CLA	C2A-C3A-C4A	-5.56	92.88	101.87
25	r	601	CLA	CHD-C1D-ND	-5.56	119.35	124.45
25	y	311	CLA	CHD-C1D-ND	-5.53	119.37	124.45
25	R	601	CLA	CHD-C1D-ND	-5.52	119.38	124.45
25	Y	311	CLA	CHD-C1D-ND	-5.51	119.39	124.45
25	c	509	CLA	CHD-C1D-ND	-5.50	119.40	124.45
25	C	509	CLA	CHD-C1D-ND	-5.50	119.40	124.45
25	b	609	CLA	CHD-C1D-ND	-5.47	119.42	124.45
25	R	608	CLA	C4A-NA-C1A	-5.47	104.25	106.71
25	r	608	CLA	C4A-NA-C1A	-5.47	104.25	106.71
25	c	511	CLA	C1B-CHB-C4A	-5.46	119.31	130.12
25	G	612	CLA	C1D-ND-C4D	-5.44	102.47	106.33
25	g	612	CLA	C1D-ND-C4D	-5.44	102.47	106.33
25	B	609	CLA	CHD-C1D-ND	-5.44	119.46	124.45
25	n	610	CLA	CHD-C1D-ND	-5.43	119.47	124.45
25	C	511	CLA	C1B-CHB-C4A	-5.43	119.37	130.12
25	b	602	CLA	CHD-C1D-ND	-5.41	119.48	124.45
29	l	101	SQD	O8-S-C6	-5.40	97.13	105.74
25	N	610	CLA	CHD-C1D-ND	-5.40	119.50	124.45
29	L	103	SQD	O8-S-C6	-5.39	97.16	105.74
25	R	612	CLA	C1B-CHB-C4A	-5.38	119.46	130.12
25	B	602	CLA	CHD-C1D-ND	-5.38	119.51	124.45
25	r	612	CLA	C1B-CHB-C4A	-5.37	119.48	130.12
25	G	610	CLA	CHD-C1D-ND	-5.36	119.53	124.45
25	y	313	CLA	C1D-ND-C4D	-5.35	102.53	106.33
25	Y	313	CLA	C1D-ND-C4D	-5.34	102.54	106.33
40	r	617	NEX	C11-C12-C13	-5.32	111.46	126.42
40	R	617	NEX	C27-C28-C29	-5.32	117.27	125.53
25	G	614	CLA	C4A-NA-C1A	-5.32	104.31	106.71
25	g	614	CLA	C4A-NA-C1A	-5.32	104.31	106.71
25	g	610	CLA	CHD-C1D-ND	-5.32	119.57	124.45
40	R	617	NEX	C11-C12-C13	-5.31	111.49	126.42
25	b	608	CLA	C4A-NA-C1A	-5.31	104.32	106.71
25	r	611	CLA	C1B-CHB-C4A	-5.31	119.60	130.12
25	R	611	CLA	C1B-CHB-C4A	-5.31	119.61	130.12
25	R	614	CLA	CHD-C1D-ND	-5.31	119.58	124.45
25	r	614	CLA	CHD-C1D-ND	-5.31	119.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	r	617	NEX	C27-C28-C29	-5.30	117.30	125.53
39	N	615	LUT	C18-C5-C6	5.30	130.48	124.53
39	n	615	LUT	C18-C5-C6	5.30	130.48	124.53
25	G	604	CLA	CHD-C1D-ND	-5.29	119.59	124.45
40	s	317	NEX	C27-C28-C29	-5.28	117.34	125.53
25	2	602	CLA	C2D-C1D-ND	-5.27	106.22	110.10
25	6	602	CLA	C2D-C1D-ND	-5.27	106.22	110.10
40	S	317	NEX	C27-C28-C29	-5.27	117.35	125.53
25	C	505	CLA	O2D-CGD-CBD	5.27	120.64	111.27
25	c	505	CLA	O2D-CGD-CBD	5.27	120.64	111.27
25	B	608	CLA	C4A-NA-C1A	-5.27	104.34	106.71
25	g	604	CLA	CHD-C1D-ND	-5.25	119.63	124.45
25	g	611	CLA	O2D-CGD-CBD	5.24	120.58	111.27
25	g	603	CLA	CHD-C1D-ND	-5.23	119.65	124.45
25	b	605	CLA	O2D-CGD-CBD	5.23	120.56	111.27
25	R	611	CLA	CHD-C1D-C2D	5.22	136.44	125.48
25	Y	304	CLA	CHD-C1D-ND	-5.22	119.65	124.45
25	G	611	CLA	O2D-CGD-CBD	5.21	120.53	111.27
25	B	605	CLA	O2D-CGD-CBD	5.21	120.53	111.27
25	G	603	CLA	CHD-C1D-ND	-5.21	119.67	124.45
25	r	611	CLA	CHD-C1D-C2D	5.19	136.37	125.48
25	S	304	CLA	O2D-CGD-CBD	5.19	120.49	111.27
25	s	304	CLA	O2D-CGD-CBD	5.19	120.49	111.27
38	F	101	HEM	C1B-NB-C4B	5.17	110.41	105.07
25	S	312	CLA	C1B-CHB-C4A	-5.16	119.89	130.12
25	s	312	CLA	C1B-CHB-C4A	-5.16	119.91	130.12
25	B	614	CLA	O2D-CGD-CBD	5.16	120.43	111.27
25	b	614	CLA	O2D-CGD-CBD	5.16	120.43	111.27
25	G	612	CLA	CHD-C1D-ND	-5.15	119.72	124.45
25	g	612	CLA	CHD-C1D-ND	-5.15	119.72	124.45
24	R	613	CHL	CAA-C2A-C3A	-5.15	104.08	116.10
24	r	613	CHL	CAA-C2A-C3A	-5.15	104.08	116.10
25	y	304	CLA	CHD-C1D-ND	-5.14	119.73	124.45
25	N	612	CLA	C4D-CHA-C1A	-5.13	115.00	121.25
24	y	307	CHL	C4A-NA-C1A	5.13	109.01	106.71
38	f	101	HEM	C1B-NB-C4B	5.11	110.35	105.07
25	n	612	CLA	C4D-CHA-C1A	-5.11	115.03	121.25
39	G	616	LUT	C18-C5-C6	5.11	130.26	124.53
39	g	616	LUT	C18-C5-C6	5.11	130.26	124.53
25	c	506	CLA	CHD-C1D-ND	-5.10	119.77	124.45
25	B	616	CLA	CHD-C1D-ND	-5.09	119.77	124.45
25	b	616	CLA	CHD-C1D-ND	-5.09	119.77	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	614	CLA	CHD-C1D-ND	-5.09	119.78	124.45
25	g	614	CLA	CHD-C1D-ND	-5.09	119.78	124.45
25	B	616	CLA	C4A-NA-C1A	-5.09	104.42	106.71
25	b	616	CLA	C4A-NA-C1A	-5.09	104.42	106.71
25	Y	305	CLA	CHD-C1D-ND	-5.08	119.79	124.45
25	y	305	CLA	CHD-C1D-ND	-5.08	119.79	124.45
25	C	506	CLA	CHD-C1D-ND	-5.07	119.79	124.45
25	2	604	CLA	C4D-CHA-C1A	-5.07	115.08	121.25
25	6	604	CLA	C4D-CHA-C1A	-5.07	115.08	121.25
25	A	405	CLA	C4A-NA-C1A	-5.07	104.43	106.71
25	a	406	CLA	C4A-NA-C1A	-5.07	104.43	106.71
25	S	305	CLA	C4D-CHA-C1A	-5.06	115.09	121.25
29	A	411	SQD	O8-S-C6	-5.05	97.69	105.74
29	a	412	SQD	O8-S-C6	-5.05	97.69	105.74
24	Y	307	CHL	C4A-NA-C1A	5.04	108.97	106.71
25	s	305	CLA	C4D-CHA-C1A	-5.04	115.11	121.25
25	G	604	CLA	O2D-CGD-CBD	5.03	120.21	111.27
25	B	601	CLA	O2D-CGD-CBD	5.03	120.20	111.27
25	b	601	CLA	O2D-CGD-CBD	5.03	120.20	111.27
25	b	604	CLA	O2D-CGD-CBD	5.02	120.19	111.27
25	S	311	CLA	O2D-CGD-CBD	5.02	120.19	111.27
25	B	604	CLA	O2D-CGD-CBD	5.02	120.18	111.27
25	C	510	CLA	O2D-CGD-CBD	5.01	120.17	111.27
25	c	510	CLA	O2D-CGD-CBD	5.01	120.17	111.27
25	s	311	CLA	O2D-CGD-CBD	5.01	120.17	111.27
25	g	604	CLA	O2D-CGD-CBD	5.01	120.17	111.27
25	S	314	CLA	CHD-C1D-ND	-5.00	119.86	124.45
25	s	314	CLA	CHD-C1D-ND	-5.00	119.86	124.45
25	Y	311	CLA	O2D-CGD-CBD	5.00	120.14	111.27
25	b	602	CLA	C4A-NA-C1A	-4.99	104.46	106.71
25	y	311	CLA	O2D-CGD-CBD	4.98	120.11	111.27
29	l	102	SQD	O8-S-C6	-4.97	97.81	105.74
25	B	602	CLA	C4A-NA-C1A	-4.97	104.47	106.71
25	b	616	CLA	C1D-ND-C4D	-4.96	102.81	106.33
29	L	101	SQD	O8-S-C6	-4.96	97.84	105.74
25	Y	304	CLA	O2D-CGD-CBD	4.96	120.08	111.27
25	r	601	CLA	C2D-C1D-ND	-4.95	106.45	110.10
25	b	607	CLA	C4A-NA-C1A	-4.95	104.48	106.71
25	B	607	CLA	O2D-CGD-CBD	4.95	120.06	111.27
25	b	607	CLA	O2D-CGD-CBD	4.95	120.06	111.27
39	N	616	LUT	C18-C5-C6	4.94	130.08	124.53
39	n	616	LUT	C18-C5-C6	4.94	130.08	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	f	101	HEM	C4D-ND-C1D	4.94	110.18	105.07
25	y	304	CLA	O2D-CGD-CBD	4.94	120.05	111.27
25	R	601	CLA	C2D-C1D-ND	-4.94	106.46	110.10
25	6	605	CLA	C4D-CHA-C1A	-4.93	115.25	121.25
25	G	602	CLA	C1D-ND-C4D	-4.93	102.83	106.33
25	g	602	CLA	C1D-ND-C4D	-4.93	102.83	106.33
25	B	602	CLA	O2D-CGD-CBD	4.93	120.03	111.27
25	b	602	CLA	O2D-CGD-CBD	4.93	120.03	111.27
25	B	616	CLA	C1D-ND-C4D	-4.93	102.83	106.33
25	c	505	CLA	C4A-NA-C1A	-4.92	104.49	106.71
24	N	607	CHL	O2D-CGD-CBD	4.92	120.01	111.27
24	n	607	CHL	O2D-CGD-CBD	4.92	120.01	111.27
25	2	605	CLA	C4D-CHA-C1A	-4.91	115.27	121.25
39	s	315	LUT	C18-C5-C6	4.91	130.04	124.53
39	S	315	LUT	C18-C5-C6	4.91	130.04	124.53
38	F	101	HEM	C4D-ND-C1D	4.90	110.14	105.07
25	D	402	CLA	O2D-CGD-CBD	4.90	119.98	111.27
25	d	402	CLA	O2D-CGD-CBD	4.90	119.98	111.27
39	g	616	LUT	C38-C25-C24	-4.90	113.08	123.56
39	G	616	LUT	C38-C25-C24	-4.90	113.08	123.56
25	B	610	CLA	C1D-ND-C4D	-4.89	102.86	106.33
24	Y	308	CHL	O2D-CGD-CBD	4.89	119.96	111.27
24	y	308	CHL	O2D-CGD-CBD	4.89	119.96	111.27
25	a	406	CLA	O2D-CGD-CBD	4.89	119.96	111.27
25	C	505	CLA	C1D-ND-C4D	-4.89	102.86	106.33
25	c	505	CLA	C1D-ND-C4D	-4.89	102.86	106.33
25	A	405	CLA	O2D-CGD-CBD	4.89	119.95	111.27
25	Y	312	CLA	C1D-ND-C4D	-4.88	102.87	106.33
40	R	617	NEX	C35-C15-C14	4.88	133.47	123.47
40	r	617	NEX	C35-C15-C14	4.88	133.47	123.47
25	A	401	CLA	O2D-CGD-CBD	4.86	119.91	111.27
25	a	402	CLA	O2D-CGD-CBD	4.86	119.91	111.27
25	B	607	CLA	C4A-NA-C1A	-4.86	104.52	106.71
39	r	615	LUT	C18-C5-C6	4.86	129.98	124.53
39	S	315	LUT	C38-C25-C24	-4.86	113.17	123.56
39	s	315	LUT	C38-C25-C24	-4.85	113.18	123.56
25	Y	312	CLA	O2D-CGD-CBD	4.85	119.88	111.27
25	2	605	CLA	CHD-C1D-ND	-4.85	120.00	124.45
25	G	610	CLA	O2D-CGD-CBD	4.84	119.87	111.27
25	6	605	CLA	CHD-C1D-ND	-4.83	120.01	124.45
25	R	611	CLA	C2A-C3A-C4A	-4.83	94.06	101.87
25	y	312	CLA	O2D-CGD-CBD	4.83	119.85	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	314	CLA	O2D-CGD-CBD	4.83	119.84	111.27
25	b	610	CLA	C1D-ND-C4D	-4.82	102.91	106.33
29	A	407	SQD	O8-S-C6	-4.82	98.06	105.74
29	a	408	SQD	O8-S-C6	-4.82	98.06	105.74
39	Y	316	LUT	C18-C5-C6	4.82	129.94	124.53
25	B	613	CLA	C1D-ND-C4D	-4.81	102.92	106.33
25	b	613	CLA	C1D-ND-C4D	-4.81	102.92	106.33
25	S	314	CLA	O2D-CGD-CBD	4.81	119.82	111.27
25	g	610	CLA	O2D-CGD-CBD	4.81	119.82	111.27
25	S	309	CLA	O2D-CGD-CBD	4.81	119.81	111.27
25	C	505	CLA	C4A-NA-C1A	-4.81	104.54	106.71
25	y	315	CLA	CHD-C1D-ND	-4.81	120.04	124.45
39	R	615	LUT	C18-C5-C6	4.80	129.91	124.53
25	s	309	CLA	O2D-CGD-CBD	4.80	119.79	111.27
25	Y	315	CLA	CHD-C1D-ND	-4.79	120.05	124.45
25	r	611	CLA	C2A-C3A-C4A	-4.79	94.13	101.87
39	y	316	LUT	C18-C5-C6	4.79	129.91	124.53
25	y	312	CLA	C1D-ND-C4D	-4.79	102.93	106.33
39	s	316	LUT	C38-C25-C24	-4.79	113.31	123.56
25	B	603	CLA	O2D-CGD-CBD	4.79	119.78	111.27
25	b	603	CLA	O2D-CGD-CBD	4.79	119.78	111.27
25	y	313	CLA	O2D-CGD-CBD	4.79	119.78	111.27
25	Y	313	CLA	O2D-CGD-CBD	4.78	119.77	111.27
25	a	403	CLA	C4A-NA-C1A	-4.78	104.56	106.71
39	S	316	LUT	C38-C25-C24	-4.77	113.35	123.56
25	n	602	CLA	C4A-NA-C1A	-4.77	104.56	106.71
25	c	512	CLA	O2D-CGD-CBD	4.77	119.74	111.27
25	C	512	CLA	O2D-CGD-CBD	4.77	119.74	111.27
25	B	606	CLA	O2D-CGD-CBD	4.77	119.74	111.27
25	b	606	CLA	O2D-CGD-CBD	4.77	119.74	111.27
39	n	616	LUT	C38-C25-C24	-4.77	113.36	123.56
25	C	511	CLA	O2D-CGD-CBD	4.76	119.73	111.27
25	N	613	CLA	O2D-CGD-CBD	4.76	119.73	111.27
25	n	613	CLA	O2D-CGD-CBD	4.76	119.73	111.27
25	D	402	CLA	C1B-CHB-C4A	-4.76	120.69	130.12
25	A	402	CLA	C4A-NA-C1A	-4.76	104.57	106.71
25	c	511	CLA	O2D-CGD-CBD	4.76	119.72	111.27
25	y	305	CLA	C4A-NA-C1A	-4.76	104.57	106.71
24	G	609	CHL	O2D-CGD-CBD	4.75	119.70	111.27
39	N	616	LUT	C38-C25-C24	-4.75	113.40	123.56
25	S	312	CLA	O2D-CGD-CBD	4.75	119.70	111.27
25	s	312	CLA	O2D-CGD-CBD	4.74	119.70	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	402	CLA	C1B-CHB-C4A	-4.74	120.72	130.12
25	2	604	CLA	C4A-NA-C1A	4.74	108.84	106.71
25	B	615	CLA	C1B-CHB-C4A	-4.74	120.73	130.12
24	g	609	CHL	O2D-CGD-CBD	4.74	119.69	111.27
25	Y	305	CLA	C1D-ND-C4D	-4.73	102.97	106.33
25	y	305	CLA	C1D-ND-C4D	-4.73	102.97	106.33
25	C	502	CLA	CHD-C1D-ND	-4.73	120.11	124.45
25	c	502	CLA	CHD-C1D-ND	-4.73	120.11	124.45
39	G	615	LUT	C18-C5-C6	4.73	129.84	124.53
25	N	610	CLA	O2D-CGD-CBD	4.73	119.67	111.27
25	n	610	CLA	O2D-CGD-CBD	4.73	119.67	111.27
25	Y	303	CLA	CHD-C1D-ND	-4.72	120.11	124.45
25	y	303	CLA	CHD-C1D-ND	-4.72	120.11	124.45
40	R	617	NEX	C12-C13-C14	4.72	126.19	118.94
39	g	615	LUT	C18-C5-C6	4.72	129.83	124.53
25	b	615	CLA	C1B-CHB-C4A	-4.72	120.78	130.12
25	6	604	CLA	C4A-NA-C1A	4.72	108.83	106.71
39	R	615	LUT	C38-C25-C24	-4.71	113.47	123.56
40	r	617	NEX	C12-C13-C14	4.71	126.17	118.94
25	G	602	CLA	CHD-C1D-ND	-4.71	120.12	124.45
25	g	602	CLA	CHD-C1D-ND	-4.71	120.12	124.45
39	g	615	LUT	C38-C25-C24	-4.70	113.50	123.56
39	r	615	LUT	C38-C25-C24	-4.70	113.50	123.56
25	N	611	CLA	C1D-ND-C4D	-4.70	103.00	106.33
25	Y	303	CLA	C1D-ND-C4D	-4.70	103.00	106.33
25	N	602	CLA	C4A-NA-C1A	-4.69	104.60	106.71
39	G	615	LUT	C38-C25-C24	-4.69	113.52	123.56
25	C	506	CLA	O2D-CGD-CBD	4.68	119.59	111.27
25	c	506	CLA	O2D-CGD-CBD	4.68	119.59	111.27
25	y	303	CLA	C1D-ND-C4D	-4.68	103.01	106.33
25	Y	303	CLA	O2D-CGD-CBD	4.68	119.59	111.27
25	y	303	CLA	O2D-CGD-CBD	4.68	119.59	111.27
25	y	311	CLA	C1D-ND-C4D	-4.67	103.01	106.33
25	r	604	CLA	O2D-CGD-CBD	4.67	119.57	111.27
25	n	610	CLA	C1D-ND-C4D	-4.67	103.02	106.33
39	N	615	LUT	C38-C25-C24	-4.67	113.57	123.56
25	y	304	CLA	C4A-NA-C1A	-4.67	104.61	106.71
25	R	604	CLA	O2D-CGD-CBD	4.67	119.56	111.27
39	n	615	LUT	C38-C25-C24	-4.67	113.58	123.56
25	N	610	CLA	C1D-ND-C4D	-4.67	103.02	106.33
25	S	313	CLA	C2A-C3A-C4A	-4.66	94.34	101.87
25	s	313	CLA	C2A-C3A-C4A	-4.66	94.34	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	310	CLA	O2D-CGD-CBD	4.66	119.55	111.27
25	s	310	CLA	O2D-CGD-CBD	4.66	119.55	111.27
39	y	317	LUT	C38-C25-C24	-4.66	113.59	123.56
39	S	316	LUT	C18-C5-C6	4.66	129.76	124.53
39	Y	317	LUT	C38-C25-C24	-4.65	113.61	123.56
25	r	608	CLA	O2D-CGD-CBD	4.65	119.53	111.27
25	n	611	CLA	C1D-ND-C4D	-4.65	103.03	106.33
25	g	611	CLA	CHD-C1D-ND	-4.64	120.19	124.45
25	G	611	CLA	CHD-C1D-ND	-4.64	120.19	124.45
39	s	316	LUT	C18-C5-C6	4.64	129.74	124.53
25	n	611	CLA	O2D-CGD-CBD	4.64	119.51	111.27
25	S	309	CLA	CHD-C1D-ND	-4.63	120.20	124.45
25	B	615	CLA	O2D-CGD-CBD	4.63	119.49	111.27
25	D	402	CLA	CHD-C1D-ND	-4.63	120.20	124.45
25	d	402	CLA	CHD-C1D-ND	-4.63	120.20	124.45
25	b	610	CLA	O2D-CGD-CBD	4.63	119.49	111.27
39	Y	317	LUT	C18-C5-C6	4.62	129.71	124.53
24	G	607	CHL	O2D-CGD-CBD	4.62	119.47	111.27
25	b	615	CLA	O2D-CGD-CBD	4.61	119.46	111.27
39	y	317	LUT	C18-C5-C6	4.61	129.71	124.53
25	R	608	CLA	O2D-CGD-CBD	4.61	119.46	111.27
24	g	607	CHL	O2D-CGD-CBD	4.61	119.46	111.27
25	B	610	CLA	O2D-CGD-CBD	4.61	119.45	111.27
25	N	611	CLA	O2D-CGD-CBD	4.61	119.45	111.27
25	s	309	CLA	CHD-C1D-ND	-4.61	120.22	124.45
25	C	508	CLA	O2D-CGD-CBD	4.60	119.45	111.27
25	c	508	CLA	O2D-CGD-CBD	4.60	119.45	111.27
25	S	314	CLA	C1D-ND-C4D	-4.60	103.07	106.33
25	Y	311	CLA	C1D-ND-C4D	-4.60	103.07	106.33
25	Y	305	CLA	C4A-NA-C1A	-4.59	104.64	106.71
25	B	611	CLA	O2D-CGD-CBD	4.59	119.43	111.27
25	b	611	CLA	O2D-CGD-CBD	4.59	119.43	111.27
25	c	513	CLA	C4A-NA-C1A	-4.59	104.64	106.71
25	B	606	CLA	C1B-CHB-C4A	-4.59	121.03	130.12
25	b	606	CLA	C1B-CHB-C4A	-4.59	121.03	130.12
25	A	402	CLA	O2D-CGD-CBD	4.59	119.42	111.27
25	a	403	CLA	O2D-CGD-CBD	4.59	119.42	111.27
25	R	612	CLA	O2D-CGD-CBD	4.59	119.42	111.27
25	r	612	CLA	O2D-CGD-CBD	4.59	119.42	111.27
25	C	513	CLA	C4A-NA-C1A	-4.58	104.64	106.71
25	N	602	CLA	C1D-ND-C4D	-4.58	103.08	106.33
39	y	316	LUT	C38-C25-C24	-4.58	113.77	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	614	CLA	C1D-ND-C4D	-4.57	103.09	106.33
25	S	305	CLA	C2D-C1D-ND	-4.57	106.73	110.10
25	r	614	CLA	C1D-ND-C4D	-4.57	103.09	106.33
25	2	602	CLA	O2D-CGD-CBD	4.57	119.39	111.27
39	Y	316	LUT	C38-C25-C24	-4.57	113.79	123.56
24	y	307	CHL	C1D-ND-C4D	-4.56	103.09	106.33
25	s	305	CLA	C2D-C1D-ND	-4.56	106.74	110.10
25	C	502	CLA	O2D-CGD-CBD	4.56	119.37	111.27
25	c	502	CLA	O2D-CGD-CBD	4.56	119.37	111.27
25	s	314	CLA	C1D-ND-C4D	-4.56	103.10	106.33
25	n	602	CLA	C1D-ND-C4D	-4.56	103.10	106.33
25	6	602	CLA	O2D-CGD-CBD	4.54	119.34	111.27
25	Y	304	CLA	C4A-NA-C1A	-4.54	104.67	106.71
25	c	513	CLA	O2D-CGD-CBD	4.53	119.31	111.27
25	N	603	CLA	O2D-CGD-CBD	4.52	119.31	111.27
40	y	318	NEX	C5-C6-C1	-4.52	115.21	119.70
25	B	613	CLA	CHD-C1D-ND	-4.52	120.30	124.45
25	b	613	CLA	CHD-C1D-ND	-4.52	120.30	124.45
25	B	616	CLA	O2D-CGD-CBD	4.51	119.29	111.27
25	S	313	CLA	O2D-CGD-CBD	4.51	119.29	111.27
25	C	513	CLA	O2D-CGD-CBD	4.51	119.28	111.27
40	Y	318	NEX	C5-C6-C1	-4.51	115.22	119.70
25	b	616	CLA	O2D-CGD-CBD	4.51	119.27	111.27
25	B	608	CLA	O2D-CGD-CBD	4.50	119.27	111.27
25	n	610	CLA	C4A-NA-C1A	-4.50	104.68	106.71
25	S	303	CLA	O2D-CGD-CBD	4.50	119.26	111.27
25	b	608	CLA	O2D-CGD-CBD	4.50	119.26	111.27
25	s	303	CLA	O2D-CGD-CBD	4.50	119.26	111.27
25	s	313	CLA	O2D-CGD-CBD	4.50	119.26	111.27
24	Y	307	CHL	C1D-ND-C4D	-4.50	103.14	106.33
25	c	506	CLA	C1D-ND-C4D	-4.49	103.14	106.33
25	r	610	CLA	C2D-C1D-ND	-4.49	106.79	110.10
25	n	603	CLA	O2D-CGD-CBD	4.49	119.25	111.27
35	B	626	DGD	C3G-O3G-C1D	-4.49	104.97	113.74
35	b	626	DGD	C3G-O3G-C1D	-4.49	104.97	113.74
41	r	616	XAT	C31-C30-C29	-4.48	120.91	127.31
25	S	312	CLA	CHD-C1D-ND	-4.48	120.34	124.45
25	Y	313	CLA	CHD-C1D-ND	-4.48	120.34	124.45
25	y	313	CLA	CHD-C1D-ND	-4.48	120.34	124.45
25	d	401	CLA	O2D-CGD-CBD	4.48	119.23	111.27
25	G	612	CLA	O2D-CGD-CBD	4.48	119.22	111.27
25	b	609	CLA	O2D-CGD-CBD	4.48	119.22	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	609	CLA	O2D-CGD-CBD	4.47	119.21	111.27
25	S	305	CLA	O2D-CGD-CBD	4.46	119.20	111.27
25	c	503	CLA	O2D-CGD-CBD	4.46	119.20	111.27
25	s	312	CLA	CHD-C1D-ND	-4.46	120.36	124.45
41	R	616	XAT	C31-C30-C29	-4.46	120.95	127.31
25	R	610	CLA	C2D-C1D-ND	-4.45	106.82	110.10
25	g	602	CLA	O1D-CGD-CBD	-4.45	115.38	124.48
25	s	305	CLA	O2D-CGD-CBD	4.45	119.17	111.27
25	C	503	CLA	O2D-CGD-CBD	4.45	119.17	111.27
25	g	612	CLA	O2D-CGD-CBD	4.44	119.17	111.27
25	D	401	CLA	O2D-CGD-CBD	4.44	119.16	111.27
25	S	305	CLA	C1-C2-C3	-4.44	119.57	126.75
25	N	610	CLA	C4A-NA-C1A	-4.43	104.71	106.71
24	G	606	CHL	O2D-CGD-CBD	4.43	119.14	111.27
25	B	601	CLA	C1B-CHB-C4A	-4.43	121.34	130.12
39	Y	316	LUT	C3-C4-C5	4.43	120.68	111.85
39	G	615	LUT	C3-C4-C5	4.43	120.67	111.85
39	g	615	LUT	C3-C4-C5	4.43	120.67	111.85
24	g	606	CHL	O2D-CGD-CBD	4.42	119.13	111.27
25	n	614	CLA	CHD-C1D-ND	-4.42	120.39	124.45
39	y	316	LUT	C3-C4-C5	4.42	120.66	111.85
25	g	602	CLA	O2D-CGD-CBD	4.42	119.12	111.27
25	G	602	CLA	O1D-CGD-CBD	-4.42	115.44	124.48
25	s	305	CLA	C1-C2-C3	-4.42	119.60	126.75
25	B	610	CLA	CHD-C1D-ND	-4.42	120.39	124.45
25	g	614	CLA	O2D-CGD-CBD	4.42	119.12	111.27
25	r	603	CLA	C2D-C1D-ND	-4.41	106.85	110.10
25	b	601	CLA	C1B-CHB-C4A	-4.41	121.38	130.12
24	2	603	CHL	CHD-C1D-ND	-4.41	120.40	124.45
24	6	603	CHL	CHD-C1D-ND	-4.41	120.40	124.45
25	C	506	CLA	C1D-ND-C4D	-4.40	103.21	106.33
25	R	610	CLA	O2D-CGD-CBD	4.40	119.09	111.27
25	r	610	CLA	O2D-CGD-CBD	4.40	119.09	111.27
25	G	614	CLA	C1D-ND-C4D	-4.40	103.21	106.33
25	g	614	CLA	C1D-ND-C4D	-4.40	103.21	106.33
25	N	614	CLA	CHD-C1D-ND	-4.40	120.41	124.45
25	b	610	CLA	CHD-C1D-ND	-4.40	120.41	124.45
25	R	603	CLA	C2D-C1D-ND	-4.40	106.86	110.10
25	r	611	CLA	C4D-C3D-CAD	-4.39	102.92	108.10
25	G	614	CLA	O2D-CGD-CBD	4.39	119.07	111.27
25	S	309	CLA	C4D-CHA-C1A	-4.39	115.91	121.25
40	S	317	NEX	C35-C34-C33	-4.38	121.05	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	s	317	NEX	C35-C34-C33	-4.38	121.05	127.31
25	G	602	CLA	O2D-CGD-CBD	4.38	119.06	111.27
25	s	309	CLA	C4D-CHA-C1A	-4.38	115.91	121.25
25	2	602	CLA	CHD-C1D-C2D	4.37	134.65	125.48
25	6	602	CLA	CHD-C1D-C2D	4.37	134.65	125.48
25	B	612	CLA	O2D-CGD-CBD	4.37	119.04	111.27
25	b	612	CLA	O2D-CGD-CBD	4.37	119.04	111.27
25	c	507	CLA	O2D-CGD-CBD	4.37	119.03	111.27
25	N	602	CLA	CHD-C1D-ND	-4.37	120.44	124.45
25	R	611	CLA	C4D-C3D-CAD	-4.37	102.95	108.10
25	B	615	CLA	CHD-C1D-ND	-4.36	120.44	124.45
25	c	509	CLA	O2D-CGD-CBD	4.36	119.02	111.27
40	Y	318	NEX	C15-C14-C13	-4.36	121.09	127.31
25	C	509	CLA	O2D-CGD-CBD	4.36	119.01	111.27
25	6	605	CLA	O2D-CGD-CBD	4.36	119.01	111.27
25	C	507	CLA	O2D-CGD-CBD	4.35	119.00	111.27
39	N	615	LUT	C3-C4-C5	4.35	120.52	111.85
39	n	615	LUT	C3-C4-C5	4.35	120.52	111.85
25	6	604	CLA	O2D-CGD-CBD	4.35	119.00	111.27
40	r	617	NEX	C28-C29-C30	4.35	125.62	118.94
25	2	604	CLA	O2D-CGD-CBD	4.35	118.99	111.27
25	n	602	CLA	CHD-C1D-ND	-4.35	120.46	124.45
40	R	617	NEX	C28-C29-C30	4.35	125.61	118.94
25	2	605	CLA	O2D-CGD-CBD	4.35	118.99	111.27
25	y	315	CLA	C1D-ND-C4D	-4.34	103.25	106.33
41	r	616	XAT	C15-C14-C13	-4.34	121.12	127.31
25	C	513	CLA	C4D-CHA-C1A	-4.34	115.97	121.25
25	c	513	CLA	C4D-CHA-C1A	-4.33	115.97	121.25
25	N	604	CLA	C1-C2-C3	-4.33	119.74	126.75
41	R	616	XAT	C15-C14-C13	-4.33	121.13	127.31
25	n	604	CLA	C1-C2-C3	-4.33	119.75	126.75
24	y	307	CHL	C2D-C1D-ND	4.32	113.29	110.10
25	Y	305	CLA	O2D-CGD-CBD	4.32	118.94	111.27
25	y	305	CLA	O2D-CGD-CBD	4.32	118.94	111.27
40	y	318	NEX	C15-C14-C13	-4.32	121.15	127.31
25	N	602	CLA	O2D-CGD-CBD	4.32	118.94	111.27
25	Y	315	CLA	C1D-ND-C4D	-4.32	103.27	106.33
25	n	602	CLA	O2D-CGD-CBD	4.32	118.94	111.27
25	R	611	CLA	O2D-CGD-CBD	4.30	118.91	111.27
25	c	501	CLA	C1-C2-C3	-4.30	118.60	126.04
25	6	604	CLA	C2D-C1D-ND	-4.30	106.94	110.10
24	G	607	CHL	CMB-C2B-C1B	-4.29	121.86	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	403	CLA	O2D-CGD-CBD	4.29	118.90	111.27
25	r	611	CLA	O2D-CGD-CBD	4.29	118.89	111.27
25	d	403	CLA	O2D-CGD-CBD	4.29	118.89	111.27
25	C	501	CLA	C1-C2-C3	-4.29	118.63	126.04
25	b	615	CLA	CHD-C1D-ND	-4.28	120.52	124.45
25	2	604	CLA	C2D-C1D-ND	-4.28	106.95	110.10
25	b	609	CLA	C1D-ND-C4D	-4.28	103.29	106.33
40	r	617	NEX	C15-C35-C34	4.28	132.24	123.47
40	R	617	NEX	C15-C35-C34	4.28	132.23	123.47
24	g	607	CHL	CMB-C2B-C1B	-4.28	121.89	128.46
39	r	615	LUT	C3-C4-C5	4.27	120.36	111.85
39	R	615	LUT	C3-C4-C5	4.27	120.36	111.85
25	Y	303	CLA	O1D-CGD-CBD	-4.27	115.75	124.48
25	y	303	CLA	O1D-CGD-CBD	-4.27	115.75	124.48
24	Y	307	CHL	C2D-C1D-ND	4.25	113.24	110.10
25	D	402	CLA	C4A-NA-C1A	-4.25	104.79	106.71
40	r	617	NEX	C20-C13-C14	-4.24	116.99	122.92
25	g	604	CLA	C1D-ND-C4D	-4.23	103.33	106.33
40	R	617	NEX	C20-C13-C14	-4.23	117.00	122.92
25	Y	311	CLA	C4A-NA-C1A	-4.23	104.80	106.71
25	B	609	CLA	C1D-ND-C4D	-4.23	103.33	106.33
25	g	613	CLA	C4D-CHA-C1A	-4.23	116.11	121.25
39	y	316	LUT	C2-C3-C4	4.23	116.09	110.30
25	B	614	CLA	C1D-ND-C4D	-4.22	103.33	106.33
25	b	614	CLA	C1D-ND-C4D	-4.22	103.33	106.33
26	R	618	LHG	O7-C7-C8	4.22	120.59	111.50
25	D	401	CLA	C1-C2-C3	-4.22	119.93	126.75
39	Y	316	LUT	C2-C3-C4	4.21	116.07	110.30
25	d	401	CLA	C1-C2-C3	-4.21	119.94	126.75
25	G	613	CLA	C4D-CHA-C1A	-4.20	116.13	121.25
26	r	618	LHG	O7-C7-C8	4.20	120.56	111.50
25	d	402	CLA	C4A-NA-C1A	-4.19	104.82	106.71
25	C	501	CLA	O2D-CGD-CBD	4.19	118.72	111.27
25	c	501	CLA	O2D-CGD-CBD	4.19	118.72	111.27
25	R	609	CLA	O2D-CGD-CBD	4.18	118.70	111.27
25	r	609	CLA	O2D-CGD-CBD	4.18	118.69	111.27
25	b	603	CLA	C1D-ND-C4D	-4.18	103.37	106.33
25	G	604	CLA	C1D-ND-C4D	-4.18	103.37	106.33
25	y	311	CLA	C4A-NA-C1A	-4.17	104.83	106.71
25	D	403	CLA	C2D-C1D-ND	-4.17	107.03	110.10
25	d	403	CLA	C2D-C1D-ND	-4.17	107.03	110.10
25	B	608	CLA	C1D-ND-C4D	-4.17	103.38	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	608	CLA	C1D-ND-C4D	-4.17	103.38	106.33
25	G	602	CLA	C4A-NA-C1A	-4.16	104.83	106.71
25	g	602	CLA	C4A-NA-C1A	-4.16	104.83	106.71
25	n	603	CLA	C4A-NA-C1A	-4.16	104.84	106.71
25	g	613	CLA	O2D-CGD-CBD	4.16	118.66	111.27
25	D	401	CLA	C4D-CHA-C1A	-4.16	116.19	121.25
25	d	401	CLA	C4D-CHA-C1A	-4.16	116.19	121.25
25	y	314	CLA	O2D-CGD-CBD	4.15	118.65	111.27
25	S	303	CLA	C1D-ND-C4D	-4.15	103.38	106.33
25	s	303	CLA	C1D-ND-C4D	-4.15	103.38	106.33
25	G	613	CLA	O2D-CGD-CBD	4.15	118.65	111.27
25	Y	314	CLA	O2D-CGD-CBD	4.14	118.62	111.27
25	c	504	CLA	C2D-C1D-ND	-4.14	107.06	110.10
26	C	517	LHG	O7-C7-C8	4.13	120.40	111.50
26	c	517	LHG	O7-C7-C8	4.13	120.40	111.50
25	D	403	CLA	C2A-C3A-C4A	-4.13	95.20	101.87
25	d	403	CLA	C2A-C3A-C4A	-4.13	95.20	101.87
25	G	603	CLA	O2D-CGD-CBD	4.12	118.59	111.27
25	g	603	CLA	O2D-CGD-CBD	4.12	118.59	111.27
24	2	603	CHL	C3C-C4C-NC	-4.12	105.95	110.57
25	r	601	CLA	O2D-CGD-CBD	4.11	118.57	111.27
25	B	603	CLA	C1D-ND-C4D	-4.11	103.42	106.33
40	n	617	NEX	C20-C13-C14	-4.11	117.17	122.92
25	s	314	CLA	C4A-NA-C1A	-4.11	104.86	106.71
25	B	604	CLA	C1-C2-C3	-4.11	118.94	126.04
25	b	604	CLA	C1-C2-C3	-4.11	118.94	126.04
40	n	617	NEX	C12-C13-C14	4.11	125.24	118.94
25	C	504	CLA	C2D-C1D-ND	-4.10	107.08	110.10
25	S	311	CLA	C1B-CHB-C4A	-4.10	122.00	130.12
25	s	311	CLA	C1B-CHB-C4A	-4.10	122.00	130.12
24	6	603	CHL	C3C-C4C-NC	-4.10	105.98	110.57
30	C	520	LMG	O7-C10-C11	4.09	120.33	111.50
30	c	520	LMG	O7-C10-C11	4.09	120.33	111.50
25	c	509	CLA	C1B-CHB-C4A	-4.09	122.01	130.12
25	C	509	CLA	C1B-CHB-C4A	-4.09	122.01	130.12
40	N	617	NEX	C20-C13-C14	-4.09	117.19	122.92
25	R	602	CLA	C1D-ND-C4D	-4.09	103.43	106.33
25	S	314	CLA	C4A-NA-C1A	-4.09	104.87	106.71
24	2	603	CHL	OBD-CAD-C3D	4.09	138.36	128.52
24	6	603	CHL	OBD-CAD-C3D	4.09	138.36	128.52
25	R	601	CLA	O2D-CGD-CBD	4.09	118.53	111.27
35	C	516	DGD	C1D-O6D-C5D	-4.08	105.68	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	516	DGD	C1D-O6D-C5D	-4.08	105.68	113.69
25	C	502	CLA	C1D-ND-C4D	-4.08	103.44	106.33
25	c	502	CLA	C1D-ND-C4D	-4.08	103.44	106.33
25	r	603	CLA	O2D-CGD-CBD	4.07	118.50	111.27
40	G	617	NEX	C38-C25-C26	-4.07	115.44	122.26
25	r	602	CLA	C1D-ND-C4D	-4.07	103.44	106.33
26	B	622	LHG	O7-C7-C8	4.07	120.27	111.50
26	b	622	LHG	O7-C7-C8	4.07	120.27	111.50
39	G	615	LUT	C2-C3-C4	4.07	115.87	110.30
39	g	615	LUT	C2-C3-C4	4.07	115.87	110.30
25	N	603	CLA	C4A-NA-C1A	-4.07	104.88	106.71
40	N	617	NEX	C12-C13-C14	4.07	125.18	118.94
25	R	603	CLA	O2D-CGD-CBD	4.06	118.49	111.27
24	N	601	CHL	O2D-CGD-CBD	4.06	118.48	111.27
40	g	617	NEX	C38-C25-C26	-4.05	115.47	122.26
25	Y	312	CLA	CHD-C1D-ND	-4.05	120.73	124.45
25	r	602	CLA	C1-C2-C3	-4.05	119.04	126.04
40	r	617	NEX	C39-C29-C30	-4.04	117.26	122.92
25	C	511	CLA	C2A-C3A-C4A	-4.04	95.34	101.87
26	Y	301	LHG	O7-C7-C8	4.04	120.21	111.50
40	R	617	NEX	C39-C29-C30	-4.04	117.26	122.92
40	y	318	NEX	O24-C25-C24	4.04	116.42	113.38
25	r	601	CLA	CHD-C1D-C2D	4.04	133.95	125.48
25	r	612	CLA	CHD-C1D-C2D	4.04	133.95	125.48
26	B	621	LHG	O7-C7-C8	4.04	120.20	111.50
26	b	621	LHG	O7-C7-C8	4.04	120.20	111.50
26	Y	319	LHG	O7-C7-C8	4.03	120.19	111.50
26	y	301	LHG	O7-C7-C8	4.03	120.18	111.50
26	y	319	LHG	O7-C7-C8	4.02	120.17	111.50
25	r	601	CLA	C4D-CHA-C1A	-4.02	116.35	121.25
24	1	302	CHL	O2D-CGD-CBD	4.02	118.41	111.27
25	R	601	CLA	CHD-C1D-C2D	4.02	133.91	125.48
27	A	403	PHO	C1-C2-C3	-4.02	119.10	126.04
27	a	404	PHO	C1-C2-C3	-4.02	119.10	126.04
25	R	602	CLA	C1-C2-C3	-4.02	119.10	126.04
25	R	601	CLA	C4D-CHA-C1A	-4.01	116.36	121.25
25	R	612	CLA	CHD-C1D-C2D	4.01	133.89	125.48
24	n	601	CHL	O2D-CGD-CBD	4.01	118.40	111.27
24	5	302	CHL	O2D-CGD-CBD	4.01	118.39	111.27
25	R	604	CLA	C1B-CHB-C4A	-4.01	122.18	130.12
25	r	604	CLA	C1B-CHB-C4A	-4.01	122.18	130.12
25	y	312	CLA	CHD-C1D-ND	-4.01	120.77	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	511	CLA	C2A-C3A-C4A	-4.01	95.40	101.87
25	G	603	CLA	C1D-ND-C4D	-4.00	103.49	106.33
25	g	603	CLA	C1D-ND-C4D	-4.00	103.49	106.33
25	n	612	CLA	O2D-CGD-CBD	4.00	118.38	111.27
25	b	605	CLA	C1B-CHB-C4A	-4.00	122.20	130.12
25	B	603	CLA	C4A-NA-C1A	-3.99	104.91	106.71
25	b	603	CLA	C4A-NA-C1A	-3.99	104.91	106.71
24	y	310	CHL	O2D-CGD-CBD	3.98	118.35	111.27
25	y	305	CLA	C1-C2-C3	-3.98	120.31	126.75
30	b	623	LMG	O7-C10-C11	3.98	120.08	111.50
25	r	604	CLA	CHD-C1D-C2D	3.98	133.83	125.48
25	S	305	CLA	CHD-C1D-C2D	3.98	133.83	125.48
25	s	305	CLA	CHD-C1D-C2D	3.98	133.83	125.48
25	N	604	CLA	C4D-CHA-C1A	-3.98	116.41	121.25
25	N	612	CLA	O2D-CGD-CBD	3.98	118.34	111.27
39	n	615	LUT	C18-C5-C4	-3.98	106.99	114.36
25	B	605	CLA	C1B-CHB-C4A	-3.98	122.24	130.12
25	b	613	CLA	C4A-NA-C1A	-3.97	104.92	106.71
26	B	625	LHG	O7-C7-C8	3.97	120.06	111.50
26	b	625	LHG	O7-C7-C8	3.97	120.06	111.50
24	r	606	CHL	O2D-CGD-CBD	3.97	118.33	111.27
25	n	604	CLA	C4D-CHA-C1A	-3.97	116.42	121.25
24	R	606	CHL	O2D-CGD-CBD	3.97	118.33	111.27
25	C	504	CLA	O2D-CGD-CBD	3.97	118.32	111.27
39	N	615	LUT	C18-C5-C4	-3.97	107.00	114.36
25	c	504	CLA	O2D-CGD-CBD	3.97	118.32	111.27
25	R	604	CLA	CHD-C1D-C2D	3.97	133.80	125.48
30	A	410	LMG	O7-C10-C11	3.96	120.04	111.50
30	a	411	LMG	O7-C10-C11	3.96	120.04	111.50
30	B	623	LMG	O7-C10-C11	3.96	120.04	111.50
24	Y	310	CHL	O2D-CGD-CBD	3.96	118.31	111.27
25	Y	305	CLA	C1-C2-C3	-3.96	120.35	126.75
25	S	312	CLA	C1D-ND-C4D	-3.96	103.53	106.33
25	R	610	CLA	CHD-C1D-C2D	3.95	133.77	125.48
25	r	610	CLA	CHD-C1D-C2D	3.95	133.77	125.48
24	Y	306	CHL	O2D-CGD-CBD	3.95	118.29	111.27
24	y	306	CHL	O2D-CGD-CBD	3.95	118.29	111.27
39	Y	317	LUT	C18-C5-C4	-3.95	107.04	114.36
26	l	103	LHG	O7-C7-C8	3.95	120.00	111.50
25	C	504	CLA	C1-C2-C3	-3.94	119.22	126.04
25	y	312	CLA	C4A-NA-C1A	-3.94	104.93	106.71
25	6	604	CLA	CHD-C1D-C2D	3.94	133.75	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	603	CLA	CHD-C1D-C2D	3.94	133.74	125.48
39	y	317	LUT	C18-C5-C4	-3.94	107.06	114.36
25	2	604	CLA	CHD-C1D-C2D	3.93	133.73	125.48
25	B	604	CLA	C4A-NA-C1A	-3.93	104.94	106.71
25	b	604	CLA	C4A-NA-C1A	-3.93	104.94	106.71
25	c	504	CLA	C1-C2-C3	-3.93	119.24	126.04
25	B	615	CLA	C1D-ND-C4D	-3.93	103.54	106.33
25	n	603	CLA	C1D-ND-C4D	-3.93	103.54	106.33
26	L	102	LHG	O7-C7-C8	3.93	119.97	111.50
40	Y	318	NEX	O24-C25-C24	3.93	116.33	113.38
25	Y	313	CLA	C1-C2-C3	-3.92	119.26	126.04
30	A	408	LMG	O7-C10-C11	3.92	119.96	111.50
25	B	612	CLA	C1B-CHB-C4A	-3.92	122.35	130.12
26	d	406	LHG	O7-C7-C8	3.92	119.95	111.50
30	B	620	LMG	O7-C10-C11	3.92	119.95	111.50
30	b	620	LMG	O7-C10-C11	3.92	119.95	111.50
39	n	616	LUT	C18-C5-C4	-3.92	107.09	114.36
26	D	406	LHG	O7-C7-C8	3.92	119.94	111.50
25	r	603	CLA	CHD-C1D-C2D	3.91	133.69	125.48
39	N	616	LUT	C18-C5-C4	-3.91	107.11	114.36
25	B	613	CLA	C4A-NA-C1A	-3.91	104.95	106.71
25	D	403	CLA	CHD-C1D-C2D	3.91	133.68	125.48
25	d	403	CLA	CHD-C1D-C2D	3.91	133.68	125.48
25	b	612	CLA	C1B-CHB-C4A	-3.91	122.38	130.12
25	C	504	CLA	CHD-C1D-C2D	3.90	133.67	125.48
25	c	504	CLA	CHD-C1D-C2D	3.90	133.67	125.48
25	S	310	CLA	C1D-ND-C4D	-3.90	103.56	106.33
25	N	603	CLA	C1D-ND-C4D	-3.90	103.56	106.33
25	b	612	CLA	C1D-ND-C4D	-3.90	103.56	106.33
25	n	614	CLA	O2D-CGD-CBD	3.90	118.19	111.27
30	a	409	LMG	O7-C10-C11	3.90	119.90	111.50
39	g	615	LUT	C18-C5-C4	-3.90	107.14	114.36
25	N	611	CLA	CHD-C1D-ND	-3.90	120.87	124.45
39	G	615	LUT	C18-C5-C4	-3.90	107.14	114.36
25	y	313	CLA	C1-C2-C3	-3.90	119.31	126.04
25	c	509	CLA	C1D-ND-C4D	-3.90	103.57	106.33
25	C	509	CLA	C1D-ND-C4D	-3.89	103.57	106.33
25	s	310	CLA	C1D-ND-C4D	-3.89	103.57	106.33
25	n	611	CLA	CHD-C1D-ND	-3.89	120.88	124.45
25	b	615	CLA	C1D-ND-C4D	-3.89	103.58	106.33
25	N	614	CLA	O2D-CGD-CBD	3.88	118.17	111.27
25	s	312	CLA	C1D-ND-C4D	-3.88	103.58	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	603	CLA	C1-C2-C3	-3.88	119.34	126.04
25	R	614	CLA	O2D-CGD-CBD	3.87	118.15	111.27
25	r	614	CLA	O2D-CGD-CBD	3.87	118.15	111.27
25	Y	304	CLA	C1D-ND-C4D	-3.87	103.58	106.33
26	s	301	LHG	O7-C7-C8	3.87	119.84	111.50
26	c	518	LHG	O7-C7-C8	3.87	119.83	111.50
25	G	602	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
26	S	301	LHG	O7-C7-C8	3.86	119.83	111.50
26	C	518	LHG	O7-C7-C8	3.86	119.82	111.50
24	2	601	CHL	CAA-C2A-C3A	-3.86	102.20	112.78
25	g	602	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
25	s	309	CLA	C1B-CHB-C4A	-3.86	122.48	130.12
35	A	415	DGD	C6D-O5D-C1E	-3.86	106.21	113.74
35	a	401	DGD	C6D-O5D-C1E	-3.86	106.21	113.74
25	B	612	CLA	C1D-ND-C4D	-3.85	103.60	106.33
40	y	318	NEX	C25-C24-C23	-3.85	105.13	112.75
25	S	309	CLA	C1B-CHB-C4A	-3.85	122.49	130.12
39	r	615	LUT	C18-C5-C4	-3.85	107.22	114.36
24	r	613	CHL	O2D-CGD-CBD	3.85	118.11	111.27
24	g	605	CHL	O2D-CGD-CBD	3.85	118.11	111.27
40	N	617	NEX	C38-C25-C26	-3.85	115.81	122.26
39	R	615	LUT	C2-C3-C4	3.85	115.57	110.30
25	R	603	CLA	C1-C2-C3	-3.84	119.39	126.04
39	R	615	LUT	C18-C5-C4	-3.84	107.23	114.36
24	6	601	CHL	CAA-C2A-C3A	-3.84	102.26	112.78
30	D	407	LMG	O7-C10-C11	3.84	119.78	111.50
30	d	407	LMG	O7-C10-C11	3.84	119.78	111.50
39	r	615	LUT	C2-C3-C4	3.84	115.56	110.30
24	R	613	CHL	O2D-CGD-CBD	3.84	118.09	111.27
40	Y	318	NEX	C25-C24-C23	-3.83	105.16	112.75
25	B	607	CLA	C1D-ND-C4D	-3.83	103.61	106.33
25	b	607	CLA	C1D-ND-C4D	-3.83	103.61	106.33
24	G	605	CHL	O2D-CGD-CBD	3.83	118.08	111.27
40	n	617	NEX	C38-C25-C26	-3.83	115.84	122.26
40	n	617	NEX	C27-C28-C29	-3.83	119.58	125.53
39	y	316	LUT	C18-C5-C4	-3.83	107.26	114.36
40	Y	318	NEX	C38-C25-C26	-3.83	115.84	122.26
40	y	318	NEX	C38-C25-C26	-3.83	115.84	122.26
25	B	615	CLA	C1-C2-C3	-3.83	119.42	126.04
25	b	615	CLA	C1-C2-C3	-3.83	119.42	126.04
25	r	610	CLA	C4D-CHA-C1A	-3.83	116.59	121.25
24	n	608	CHL	O2D-CGD-CBD	3.82	118.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	312	CLA	C4A-NA-C1A	-3.82	104.99	106.71
39	Y	316	LUT	C18-C5-C4	-3.82	107.27	114.36
25	y	304	CLA	C1D-ND-C4D	-3.82	103.62	106.33
25	n	611	CLA	C1-C2-C3	-3.82	119.44	126.04
25	n	604	CLA	C1D-ND-C4D	-3.82	103.62	106.33
25	2	604	CLA	C1-C2-C3	-3.81	119.44	126.04
25	6	604	CLA	C1-C2-C3	-3.81	119.44	126.04
25	B	613	CLA	O2D-CGD-CBD	3.81	118.05	111.27
25	b	613	CLA	O2D-CGD-CBD	3.81	118.05	111.27
24	N	608	CHL	O2D-CGD-CBD	3.81	118.04	111.27
25	N	611	CLA	C1-C2-C3	-3.81	119.45	126.04
40	N	617	NEX	C27-C28-C29	-3.81	119.62	125.53
26	2	606	LHG	O7-C7-C8	3.81	119.70	111.50
25	G	604	CLA	C4D-CHA-C1A	-3.81	116.62	121.25
24	N	609	CHL	O2D-CGD-CBD	3.81	118.03	111.27
26	6	606	LHG	O7-C7-C8	3.81	119.70	111.50
25	D	403	CLA	C1-C2-C3	-3.81	119.46	126.04
25	d	403	CLA	C1-C2-C3	-3.81	119.46	126.04
25	S	312	CLA	C2A-C3A-C4A	-3.80	95.72	101.87
24	R	605	CHL	O2D-CGD-CBD	3.80	118.02	111.27
24	r	605	CHL	O2D-CGD-CBD	3.80	118.02	111.27
24	n	609	CHL	O2D-CGD-CBD	3.80	118.02	111.27
35	c	515	DGD	O2G-C1B-C2B	3.80	119.69	111.50
25	s	312	CLA	C2A-C3A-C4A	-3.79	95.74	101.87
25	R	610	CLA	C4D-CHA-C1A	-3.79	116.63	121.25
24	6	603	CHL	CAC-C3C-C4C	3.79	129.73	124.81
24	2	601	CHL	CHD-C1D-ND	-3.79	120.97	124.45
24	6	601	CHL	CHD-C1D-ND	-3.79	120.97	124.45
25	C	502	CLA	C1-C2-C3	-3.79	119.49	126.04
35	C	515	DGD	O2G-C1B-C2B	3.79	119.66	111.50
25	C	501	CLA	C2D-C1D-ND	-3.78	107.31	110.10
25	c	501	CLA	C2D-C1D-ND	-3.78	107.31	110.10
26	s	318	LHG	O7-C7-C8	3.78	119.65	111.50
26	S	318	LHG	O7-C7-C8	3.78	119.64	111.50
40	S	317	NEX	C38-C25-C26	-3.77	115.94	122.26
40	s	317	NEX	C38-C25-C26	-3.77	115.94	122.26
24	2	603	CHL	CAC-C3C-C4C	3.77	129.71	124.81
25	g	604	CLA	C4D-CHA-C1A	-3.77	116.66	121.25
25	C	503	CLA	C1D-ND-C4D	-3.77	103.66	106.33
25	c	502	CLA	C1-C2-C3	-3.77	119.53	126.04
25	C	513	CLA	C1-C2-C3	-3.77	119.53	126.04
25	c	513	CLA	C1-C2-C3	-3.77	119.53	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	S	315	LUT	C3-C4-C5	3.76	119.35	111.85
39	s	315	LUT	C3-C4-C5	3.76	119.35	111.85
25	G	611	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
24	N	605	CHL	O2D-CGD-CBD	3.76	117.95	111.27
25	C	508	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
25	c	508	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
25	S	309	CLA	C1D-ND-C4D	-3.76	103.67	106.33
25	y	304	CLA	C1-C2-C3	-3.76	119.55	126.04
30	B	623	LMG	C7-O1-C1	-3.75	106.41	113.74
30	b	623	LMG	C7-O1-C1	-3.75	106.41	113.74
39	s	315	LUT	C18-C5-C4	-3.75	107.40	114.36
25	C	503	CLA	C1B-CHB-C4A	-3.75	122.69	130.12
25	c	503	CLA	C1B-CHB-C4A	-3.75	122.69	130.12
25	N	604	CLA	C1D-ND-C4D	-3.75	103.67	106.33
24	S	307	CHL	O2D-CGD-CBD	3.74	117.92	111.27
25	S	303	CLA	C1-C2-C3	-3.74	119.57	126.04
24	s	307	CHL	O2D-CGD-CBD	3.74	117.92	111.27
25	g	611	CLA	C1B-CHB-C4A	-3.74	122.70	130.12
25	r	608	CLA	C1-C2-C3	-3.74	119.57	126.04
39	S	315	LUT	C18-C5-C4	-3.74	107.42	114.36
40	S	317	NEX	C19-C9-C10	-3.74	117.68	122.92
25	S	304	CLA	C1B-CHB-C4A	-3.74	122.71	130.12
25	s	304	CLA	C1B-CHB-C4A	-3.74	122.71	130.12
25	B	606	CLA	CHD-C1D-C2D	3.74	133.33	125.48
25	b	606	CLA	CHD-C1D-C2D	3.74	133.33	125.48
24	n	605	CHL	O2D-CGD-CBD	3.74	117.91	111.27
24	S	308	CHL	O2D-CGD-CBD	3.74	117.91	111.27
25	R	608	CLA	C1-C2-C3	-3.73	119.59	126.04
40	s	317	NEX	C19-C9-C10	-3.73	117.69	122.92
25	C	506	CLA	C1-C2-C3	-3.73	119.59	126.04
25	c	506	CLA	C1-C2-C3	-3.73	119.59	126.04
25	s	313	CLA	CHD-C1D-C2D	3.73	133.31	125.48
35	c	516	DGD	O2G-C1B-C2B	3.73	119.54	111.50
25	A	405	CLA	C1D-ND-C4D	-3.73	103.69	106.33
25	B	611	CLA	C1D-ND-C4D	-3.73	103.69	106.33
35	C	516	DGD	O2G-C1B-C2B	3.72	119.53	111.50
25	B	601	CLA	CHD-C1D-C2D	3.72	133.29	125.48
25	s	309	CLA	CHB-C4A-NA	-3.72	119.37	124.51
25	S	313	CLA	CHD-C1D-C2D	3.72	133.28	125.48
25	c	503	CLA	C1D-ND-C4D	-3.72	103.69	106.33
25	s	303	CLA	C1-C2-C3	-3.72	119.61	126.04
25	S	309	CLA	CHB-C4A-NA	-3.72	119.37	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	610	CLA	C4D-CHA-C1A	-3.72	116.72	121.25
25	b	611	CLA	C1D-ND-C4D	-3.71	103.70	106.33
25	b	601	CLA	CHD-C1D-C2D	3.71	133.27	125.48
25	a	406	CLA	C1D-ND-C4D	-3.71	103.70	106.33
25	C	501	CLA	CHD-C1D-C2D	3.71	133.25	125.48
25	c	501	CLA	CHD-C1D-C2D	3.71	133.25	125.48
25	y	314	CLA	C1D-ND-C4D	-3.71	103.70	106.33
24	s	308	CHL	O2D-CGD-CBD	3.70	117.85	111.27
25	R	603	CLA	C2A-C3A-C4A	-3.70	95.89	101.87
25	r	603	CLA	C2A-C3A-C4A	-3.70	95.89	101.87
25	Y	304	CLA	C1-C2-C3	-3.70	119.65	126.04
25	N	604	CLA	O2D-CGD-CBD	3.69	117.83	111.27
25	G	603	CLA	C1-C2-C3	-3.69	119.66	126.04
41	r	616	XAT	C18-C5-C6	-3.69	116.07	122.26
25	D	402	CLA	C1-C2-C3	-3.69	119.66	126.04
24	2	603	CHL	O2D-CGD-O1D	-3.69	116.62	123.84
24	6	603	CHL	O2D-CGD-O1D	-3.69	116.62	123.84
25	B	602	CLA	CHB-C4A-NA	-3.69	119.41	124.51
25	n	604	CLA	O2D-CGD-CBD	3.69	117.82	111.27
25	g	610	CLA	C4D-CHA-C1A	-3.68	116.77	121.25
25	b	602	CLA	CHB-C4A-NA	-3.68	119.42	124.51
25	6	602	CLA	C1-C2-C3	-3.68	119.68	126.04
25	C	513	CLA	C1D-ND-C4D	-3.68	103.72	106.33
41	R	616	XAT	C18-C5-C6	-3.68	116.10	122.26
25	s	309	CLA	C1D-ND-C4D	-3.68	103.72	106.33
25	2	602	CLA	C1-C2-C3	-3.67	119.69	126.04
25	d	402	CLA	C1-C2-C3	-3.67	119.69	126.04
25	g	603	CLA	C1-C2-C3	-3.67	119.70	126.04
24	Y	302	CHL	O2D-CGD-CBD	3.67	117.78	111.27
25	g	610	CLA	C1-C2-C3	-3.66	119.72	126.04
25	B	605	CLA	C1-C2-C3	-3.66	119.72	126.04
25	c	513	CLA	C1D-ND-C4D	-3.66	103.74	106.33
25	S	309	CLA	C3A-C2A-C1A	-3.66	95.86	101.34
25	s	313	CLA	C1-C2-C3	-3.65	119.72	126.04
39	Y	317	LUT	C11-C10-C9	-3.65	122.10	127.31
24	S	302	CHL	O2D-CGD-CBD	3.65	117.76	111.27
25	G	610	CLA	C1-C2-C3	-3.65	119.73	126.04
39	y	317	LUT	C11-C10-C9	-3.65	122.10	127.31
24	y	302	CHL	O2D-CGD-CBD	3.65	117.75	111.27
25	s	309	CLA	C3A-C2A-C1A	-3.65	95.88	101.34
25	r	609	CLA	C1-C2-C3	-3.65	119.73	126.04
25	n	613	CLA	C1-C2-C3	-3.65	119.74	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	601	CHL	O2D-CGD-CBD	3.65	117.75	111.27
24	s	302	CHL	O2D-CGD-CBD	3.64	117.74	111.27
35	b	626	DGD	O2G-C1B-C2B	3.64	119.35	111.50
25	Y	314	CLA	C1D-ND-C4D	-3.64	103.75	106.33
25	N	613	CLA	C1-C2-C3	-3.64	119.75	126.04
25	S	313	CLA	C1-C2-C3	-3.64	119.75	126.04
25	b	605	CLA	C1-C2-C3	-3.63	119.76	126.04
25	R	609	CLA	C1-C2-C3	-3.63	119.76	126.04
25	A	401	CLA	C1-C2-C3	-3.63	119.77	126.04
24	R	607	CHL	O2D-CGD-CBD	3.63	117.71	111.27
24	6	603	CHL	O1D-CGD-CBD	-3.63	117.06	124.48
35	C	515	DGD	C6D-O5D-C1E	-3.63	106.66	113.74
35	c	515	DGD	C6D-O5D-C1E	-3.63	106.66	113.74
35	B	626	DGD	O2G-C1B-C2B	3.62	119.31	111.50
25	a	402	CLA	C1-C2-C3	-3.62	119.79	126.04
24	g	601	CHL	O2D-CGD-CBD	3.62	117.69	111.27
24	r	607	CHL	O2D-CGD-CBD	3.62	117.69	111.27
24	2	603	CHL	O1D-CGD-CBD	-3.61	117.09	124.48
39	S	316	LUT	C18-C5-C4	-3.61	107.66	114.36
39	s	316	LUT	C18-C5-C4	-3.61	107.66	114.36
40	N	617	NEX	C35-C34-C33	-3.61	122.16	127.31
39	N	615	LUT	C2-C3-C4	3.61	115.24	110.30
25	B	612	CLA	C1-C2-C3	-3.61	119.81	126.04
25	b	612	CLA	C1-C2-C3	-3.61	119.81	126.04
25	Y	311	CLA	C4D-CHA-C1A	-3.60	116.87	121.25
25	y	311	CLA	C4D-CHA-C1A	-3.60	116.87	121.25
41	r	616	XAT	C11-C10-C9	-3.60	122.17	127.31
25	S	305	CLA	C2A-C3A-C4A	-3.59	96.07	101.87
25	B	608	CLA	C1-C2-C3	-3.58	119.84	126.04
25	b	608	CLA	C1-C2-C3	-3.58	119.84	126.04
39	n	615	LUT	C2-C3-C4	3.58	115.21	110.30
39	G	616	LUT	C18-C5-C4	-3.58	107.73	114.36
25	B	606	CLA	C1-C2-C3	-3.58	119.86	126.04
25	b	606	CLA	C1-C2-C3	-3.58	119.86	126.04
25	b	609	CLA	C1-C2-C3	-3.58	119.86	126.04
25	s	305	CLA	C2A-C3A-C4A	-3.58	96.09	101.87
25	B	609	CLA	C1-C2-C3	-3.57	119.86	126.04
35	A	415	DGD	O2G-C1B-C2B	3.57	119.20	111.50
35	a	401	DGD	O2G-C1B-C2B	3.57	119.20	111.50
25	Y	312	CLA	C1-C2-C3	-3.57	119.86	126.04
25	y	312	CLA	C1-C2-C3	-3.57	119.86	126.04
25	n	612	CLA	C1D-ND-C4D	-3.57	103.80	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	410	LMG	C7-O1-C1	-3.57	106.77	113.74
30	a	411	LMG	C7-O1-C1	-3.57	106.77	113.74
25	R	602	CLA	C4D-CHA-C1A	-3.56	116.91	121.25
40	n	617	NEX	C35-C34-C33	-3.56	122.23	127.31
41	R	616	XAT	C11-C10-C9	-3.56	122.23	127.31
39	g	616	LUT	C18-C5-C4	-3.56	107.76	114.36
27	A	404	PHO	C1-C2-C3	-3.56	119.89	126.04
27	a	405	PHO	C1-C2-C3	-3.56	119.89	126.04
30	B	623	LMG	C1-O6-C5	-3.55	106.71	113.69
24	s	306	CHL	O2D-CGD-CBD	3.55	117.58	111.27
25	Y	314	CLA	C4D-CHA-C1A	-3.55	116.93	121.25
25	y	314	CLA	C4D-CHA-C1A	-3.55	116.93	121.25
35	B	626	DGD	C6D-O5D-C1E	-3.55	106.81	113.74
35	b	626	DGD	C6D-O5D-C1E	-3.55	106.81	113.74
26	C	519	LHG	O7-C7-C8	3.55	119.14	111.50
26	c	519	LHG	O7-C7-C8	3.55	119.14	111.50
24	g	608	CHL	O2D-CGD-CBD	3.54	117.56	111.27
30	b	623	LMG	C1-O6-C5	-3.54	106.74	113.69
25	B	611	CLA	C1-C2-C3	-3.54	119.92	126.04
25	b	611	CLA	C1-C2-C3	-3.54	119.92	126.04
25	r	602	CLA	C4D-CHA-C1A	-3.54	116.94	121.25
40	g	617	NEX	C19-C9-C10	-3.54	117.97	122.92
25	N	612	CLA	C1-C2-C3	-3.54	119.93	126.04
25	n	612	CLA	C1-C2-C3	-3.54	119.93	126.04
25	C	510	CLA	CHD-C1D-C2D	3.54	132.90	125.48
25	n	610	CLA	C4D-CHA-C1A	-3.53	116.95	121.25
25	R	611	CLA	CHB-C4A-NA	-3.53	119.63	124.51
25	r	611	CLA	CHB-C4A-NA	-3.53	119.63	124.51
25	n	602	CLA	C1-C2-C3	-3.53	119.93	126.04
25	G	611	CLA	C4A-NA-C1A	-3.53	105.12	106.71
25	g	611	CLA	C4A-NA-C1A	-3.53	105.12	106.71
24	S	306	CHL	O2D-CGD-CBD	3.53	117.54	111.27
25	c	510	CLA	CHD-C1D-C2D	3.53	132.88	125.48
25	Y	304	CLA	C4D-CHA-C1A	-3.53	116.95	121.25
25	y	304	CLA	C4D-CHA-C1A	-3.53	116.95	121.25
25	2	602	CLA	CHC-C1C-NC	-3.53	118.85	124.20
25	6	602	CLA	CHC-C1C-NC	-3.53	118.85	124.20
25	Y	314	CLA	C1-C2-C3	-3.52	119.95	126.04
25	s	311	CLA	C1-C2-C3	-3.52	119.95	126.04
24	G	608	CHL	O2D-CGD-CBD	3.52	117.53	111.27
25	Y	315	CLA	O2D-CGD-CBD	3.52	117.52	111.27
25	y	315	CLA	O2D-CGD-CBD	3.52	117.52	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	610	CLA	C4D-CHA-C1A	-3.52	116.97	121.25
25	y	314	CLA	C1-C2-C3	-3.52	119.96	126.04
25	C	509	CLA	C1-C2-C3	-3.52	119.96	126.04
25	g	611	CLA	C3D-C2D-C1D	3.52	110.63	105.83
25	N	613	CLA	C1D-ND-C4D	-3.51	103.84	106.33
25	n	613	CLA	C1D-ND-C4D	-3.51	103.84	106.33
25	D	402	CLA	C4D-CHA-C1A	-3.51	116.97	121.25
25	d	402	CLA	C4D-CHA-C1A	-3.51	116.97	121.25
25	G	611	CLA	C1-C2-C3	-3.51	119.97	126.04
25	A	405	CLA	C1-C2-C3	-3.51	119.97	126.04
25	a	406	CLA	C1-C2-C3	-3.51	119.97	126.04
25	R	611	CLA	C3D-C4D-CHA	3.51	120.75	112.72
25	r	611	CLA	C3D-C4D-CHA	3.51	120.75	112.72
25	N	602	CLA	C1-C2-C3	-3.51	119.97	126.04
25	r	608	CLA	C1D-ND-C4D	-3.51	103.84	106.33
25	N	612	CLA	C1D-ND-C4D	-3.51	103.84	106.33
40	R	617	NEX	C11-C10-C9	3.50	132.31	127.31
40	r	617	NEX	C11-C10-C9	3.50	132.31	127.31
24	2	603	CHL	CHD-C4C-C3C	3.50	129.99	124.84
24	n	606	CHL	O2D-CGD-CBD	3.50	117.49	111.27
30	D	407	LMG	C7-O1-C1	-3.50	106.90	113.74
30	d	407	LMG	C7-O1-C1	-3.50	106.90	113.74
25	G	611	CLA	C3D-C2D-C1D	3.50	110.60	105.83
24	N	606	CHL	O2D-CGD-CBD	3.49	117.47	111.27
25	g	611	CLA	C1-C2-C3	-3.49	120.00	126.04
25	B	614	CLA	C1-C2-C3	-3.49	120.01	126.04
25	R	612	CLA	C1-C2-C3	-3.49	120.01	126.04
25	c	509	CLA	C1-C2-C3	-3.49	120.01	126.04
24	6	603	CHL	CHD-C4C-C3C	3.48	129.96	124.84
25	S	311	CLA	C1-C2-C3	-3.48	120.02	126.04
25	C	512	CLA	C1-C2-C3	-3.48	120.02	126.04
25	c	512	CLA	C1-C2-C3	-3.48	120.02	126.04
40	Y	318	NEX	C27-C28-C29	-3.48	120.13	125.53
25	r	612	CLA	C1-C2-C3	-3.48	120.03	126.04
25	Y	303	CLA	C4A-NA-C1A	-3.48	105.14	106.71
25	B	603	CLA	C1-C2-C3	-3.48	120.03	126.04
35	C	515	DGD	C3G-O3G-C1D	-3.48	106.95	113.74
35	c	515	DGD	C3G-O3G-C1D	-3.48	106.95	113.74
25	b	614	CLA	C1-C2-C3	-3.48	120.03	126.04
25	y	303	CLA	C1-C2-C3	-3.47	120.03	126.04
25	Y	303	CLA	C1-C2-C3	-3.47	120.03	126.04
25	A	402	CLA	C4D-CHA-C1A	-3.47	117.02	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	403	CLA	C4D-CHA-C1A	-3.47	117.02	121.25
25	R	608	CLA	C1D-ND-C4D	-3.47	103.87	106.33
40	y	318	NEX	C27-C28-C29	-3.47	120.15	125.53
39	S	316	LUT	C22-C23-C24	3.47	115.69	111.74
26	n	618	LHG	O7-C7-C8	3.47	118.97	111.50
24	y	307	CHL	CHD-C1D-ND	-3.46	121.27	124.45
25	b	603	CLA	C1-C2-C3	-3.46	120.06	126.04
25	S	303	CLA	C2A-C1A-CHA	-3.46	117.82	123.86
25	R	602	CLA	O2D-CGD-CBD	3.46	117.41	111.27
25	Y	315	CLA	C4A-NA-C1A	-3.45	105.15	106.71
25	N	602	CLA	O1D-CGD-CBD	-3.45	117.42	124.48
25	c	508	CLA	CHD-C1D-C2D	3.45	132.72	125.48
25	r	602	CLA	O2D-CGD-CBD	3.45	117.40	111.27
39	s	316	LUT	C22-C23-C24	3.45	115.67	111.74
25	s	303	CLA	C2A-C1A-CHA	-3.44	117.84	123.86
25	A	402	CLA	C1-C2-C3	-3.44	120.09	126.04
25	a	403	CLA	C1-C2-C3	-3.44	120.09	126.04
25	b	601	CLA	C1-C2-C3	-3.44	120.09	126.04
26	N	618	LHG	O7-C7-C8	3.44	118.91	111.50
25	D	402	CLA	C1D-ND-C4D	-3.44	103.89	106.33
25	d	402	CLA	C1D-ND-C4D	-3.44	103.89	106.33
25	C	502	CLA	C4D-CHA-C1A	-3.43	117.07	121.25
25	C	508	CLA	CHD-C1D-C2D	3.43	132.68	125.48
25	2	602	CLA	C3D-C2D-C1D	3.43	110.51	105.83
25	6	602	CLA	C3D-C2D-C1D	3.43	110.51	105.83
25	N	614	CLA	C2A-C1A-CHA	-3.43	117.87	123.86
25	B	601	CLA	C1-C2-C3	-3.43	120.12	126.04
25	n	602	CLA	O1D-CGD-CBD	-3.42	117.48	124.48
40	G	617	NEX	C19-C9-C10	-3.42	118.13	122.92
25	c	502	CLA	C4D-CHA-C1A	-3.42	117.09	121.25
41	R	616	XAT	C6-C7-C8	-3.42	118.77	125.99
41	r	616	XAT	C6-C7-C8	-3.41	118.77	125.99
25	s	312	CLA	C4A-NA-C1A	-3.41	105.17	106.71
25	C	503	CLA	C1-C2-C3	-3.41	120.14	126.04
25	c	503	CLA	C1-C2-C3	-3.41	120.14	126.04
25	y	315	CLA	C4D-CHA-C1A	-3.41	117.09	121.25
40	n	617	NEX	C39-C29-C30	-3.41	118.14	122.92
25	y	303	CLA	C4A-NA-C1A	-3.41	105.17	106.71
24	n	605	CHL	CAA-C2A-C3A	-3.41	103.44	112.78
24	N	605	CHL	CAA-C2A-C3A	-3.41	103.44	112.78
25	B	613	CLA	C1-C2-C3	-3.41	120.15	126.04
25	b	613	CLA	C1-C2-C3	-3.41	120.15	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	611	CLA	C4D-CHA-C1A	-3.41	117.10	121.25
25	g	611	CLA	C4D-CHA-C1A	-3.41	117.10	121.25
40	N	617	NEX	C39-C29-C30	-3.40	118.16	122.92
25	S	312	CLA	C4A-NA-C1A	-3.40	105.18	106.71
25	r	611	CLA	C1D-ND-C4D	3.39	108.75	106.33
25	2	604	CLA	C4D-C3D-CAD	-3.39	104.10	108.10
25	6	604	CLA	C4D-C3D-CAD	-3.39	104.10	108.10
25	y	315	CLA	C4A-NA-C1A	-3.39	105.18	106.71
24	5	301	CHL	O2D-CGD-CBD	3.39	117.29	111.27
30	B	620	LMG	C7-O1-C1	-3.39	107.13	113.74
30	b	620	LMG	C7-O1-C1	-3.39	107.13	113.74
24	1	301	CHL	O2D-CGD-CBD	3.38	117.28	111.27
25	n	614	CLA	C2A-C1A-CHA	-3.38	117.94	123.86
24	Y	307	CHL	CHD-C1D-ND	-3.38	121.34	124.45
35	A	415	DGD	C1E-O6E-C5E	-3.37	107.07	113.69
35	a	401	DGD	C1E-O6E-C5E	-3.37	107.07	113.69
40	n	617	NEX	C11-C12-C13	-3.37	116.95	126.42
40	N	617	NEX	C11-C12-C13	-3.37	116.95	126.42
25	Y	315	CLA	C4D-CHA-C1A	-3.36	117.17	121.25
41	R	616	XAT	C38-C25-C26	-3.35	116.64	122.26
25	R	611	CLA	C1D-ND-C4D	3.35	108.72	106.33
39	y	317	LUT	C3-C4-C5	3.35	118.52	111.85
41	r	616	XAT	C38-C25-C26	-3.35	116.65	122.26
39	n	616	LUT	C3-C4-C5	3.35	118.52	111.85
39	N	616	LUT	C3-C4-C5	3.34	118.52	111.85
39	Y	317	LUT	C3-C4-C5	3.34	118.51	111.85
25	G	613	CLA	C1-C2-C3	-3.33	120.29	126.04
25	g	613	CLA	C1-C2-C3	-3.33	120.29	126.04
25	d	401	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
24	R	607	CHL	C1-C2-C3	3.32	131.79	126.04
25	D	401	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
39	S	316	LUT	C3-C4-C5	3.32	118.47	111.85
25	s	304	CLA	C1D-ND-C4D	-3.32	103.98	106.33
25	N	604	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
25	A	401	CLA	CHD-C1D-C2D	3.31	132.43	125.48
25	a	402	CLA	CHD-C1D-C2D	3.31	132.43	125.48
25	c	511	CLA	C1-C2-C3	-3.31	120.32	126.04
25	n	604	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
39	s	316	LUT	C3-C4-C5	3.31	118.44	111.85
25	2	602	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
25	6	602	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
25	B	602	CLA	C1-C2-C3	-3.30	120.34	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	602	CLA	C1-C2-C3	-3.30	120.34	126.04
25	B	605	CLA	CHD-C1D-C2D	3.30	132.40	125.48
25	b	605	CLA	CHD-C1D-C2D	3.30	132.40	125.48
25	C	511	CLA	C1-C2-C3	-3.30	120.34	126.04
25	g	604	CLA	C1-C2-C3	-3.30	121.42	126.75
30	C	520	LMG	C1-O6-C5	-3.29	107.22	113.69
30	c	520	LMG	C1-O6-C5	-3.29	107.22	113.69
25	S	310	CLA	C1-C2-C3	-3.29	120.35	126.04
40	S	317	NEX	C39-C29-C30	-3.29	118.31	122.92
24	r	607	CHL	C1-C2-C3	3.29	131.74	126.04
24	N	609	CHL	CAA-C2A-C3A	-3.29	103.77	112.78
24	n	609	CHL	CAA-C2A-C3A	-3.29	103.77	112.78
40	s	317	NEX	C39-C29-C30	-3.29	118.32	122.92
25	g	610	CLA	C4-C3-C5	3.28	120.80	115.27
30	A	410	LMG	C1-O6-C5	-3.28	107.24	113.69
30	a	411	LMG	C1-O6-C5	-3.28	107.24	113.69
24	Y	310	CHL	CAA-C2A-C3A	-3.28	103.79	112.78
25	Y	311	CLA	C1-C2-C3	-3.28	120.37	126.04
25	y	311	CLA	C1-C2-C3	-3.28	120.37	126.04
25	R	609	CLA	CHD-C1D-C2D	3.28	132.35	125.48
25	s	310	CLA	C1-C2-C3	-3.28	120.38	126.04
25	b	604	CLA	CHD-C1D-C2D	3.27	132.35	125.48
24	y	310	CHL	CAA-C2A-C3A	-3.27	103.81	112.78
25	G	604	CLA	C1-C2-C3	-3.27	121.47	126.75
25	s	314	CLA	C4D-CHA-C1A	-3.27	117.27	121.25
25	g	612	CLA	C1-C2-C3	-3.26	120.40	126.04
25	G	610	CLA	C4-C3-C5	3.26	120.75	115.27
24	G	608	CHL	CAA-C2A-C3A	-3.26	103.86	112.78
25	S	304	CLA	C1D-ND-C4D	-3.26	104.02	106.33
25	b	602	CLA	C1D-ND-C4D	-3.25	104.02	106.33
25	r	609	CLA	CHD-C1D-C2D	3.25	132.30	125.48
25	S	314	CLA	C4D-CHA-C1A	-3.25	117.29	121.25
25	B	604	CLA	CHD-C1D-C2D	3.25	132.29	125.48
24	g	608	CHL	CAA-C2A-C3A	-3.25	103.89	112.78
24	g	606	CHL	CAA-C2A-C3A	-3.24	103.89	112.78
25	G	612	CLA	C1-C2-C3	-3.24	120.43	126.04
25	B	607	CLA	C1-C2-C3	-3.24	120.43	126.04
25	R	611	CLA	C3D-C2D-C1D	3.24	110.25	105.83
24	G	606	CHL	CAA-C2A-C3A	-3.24	103.91	112.78
30	C	520	LMG	C7-O1-C1	-3.24	107.42	113.74
25	N	611	CLA	C4A-NA-C1A	-3.24	105.25	106.71
24	S	302	CHL	CAA-C2A-C3A	-3.24	103.92	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	403	CLA	CHD-C1D-C2D	3.23	132.26	125.48
25	n	611	CLA	C4A-NA-C1A	-3.23	105.25	106.71
24	G	607	CHL	O1D-CGD-CBD	-3.23	117.87	124.48
25	c	508	CLA	C1-C2-C3	-3.23	120.46	126.04
25	A	402	CLA	CHD-C1D-C2D	3.23	132.25	125.48
25	G	612	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
35	b	626	DGD	C1D-O6D-C5D	-3.22	107.36	113.69
24	R	606	CHL	CAA-C2A-C3A	-3.22	103.95	112.78
25	r	601	CLA	C3D-C2D-C1D	3.22	110.23	105.83
25	N	612	CLA	C1B-CHB-C4A	-3.22	123.73	130.12
24	Y	307	CHL	O2D-CGD-CBD	3.22	117.00	111.27
24	y	307	CHL	O2D-CGD-CBD	3.22	117.00	111.27
35	C	516	DGD	C3G-O3G-C1D	-3.22	107.44	113.74
24	S	307	CHL	CAA-C2A-C3A	-3.22	103.96	112.78
24	s	307	CHL	CAA-C2A-C3A	-3.22	103.96	112.78
25	a	403	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
25	C	508	CLA	C1-C2-C3	-3.22	120.48	126.04
25	b	607	CLA	C1-C2-C3	-3.22	120.48	126.04
35	B	626	DGD	C1D-O6D-C5D	-3.21	107.38	113.69
25	c	507	CLA	CHD-C1D-C2D	3.21	132.22	125.48
24	y	306	CHL	CAA-C2A-C3A	-3.21	103.98	112.78
39	y	316	LUT	C35-C15-C14	-3.21	116.90	123.47
25	s	304	CLA	CHD-C1D-C2D	3.21	132.21	125.48
24	s	302	CHL	CAA-C2A-C3A	-3.21	103.99	112.78
25	g	612	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
24	r	606	CHL	CAA-C2A-C3A	-3.21	104.00	112.78
30	c	520	LMG	C7-O1-C1	-3.21	107.48	113.74
35	c	516	DGD	C3G-O3G-C1D	-3.20	107.48	113.74
40	r	617	NEX	C38-C25-C26	-3.20	116.89	122.26
25	A	402	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
25	C	507	CLA	C1-C2-C3	-3.20	120.51	126.04
25	c	507	CLA	C1-C2-C3	-3.20	120.51	126.04
40	g	617	NEX	C40-C33-C32	3.20	123.12	118.08
25	r	610	CLA	C3D-C2D-C1D	3.20	110.20	105.83
25	r	611	CLA	C3D-C2D-C1D	3.20	110.20	105.83
24	Y	306	CHL	CAA-C2A-C3A	-3.20	104.02	112.78
25	n	612	CLA	C1B-CHB-C4A	-3.20	123.79	130.12
25	y	304	CLA	C3D-C2D-C1D	3.20	110.19	105.83
25	C	507	CLA	CHD-C1D-C2D	3.20	132.18	125.48
25	C	512	CLA	CHD-C1D-C2D	3.19	132.18	125.48
25	S	305	CLA	C3D-C2D-C1D	3.19	110.19	105.83
25	s	305	CLA	C3D-C2D-C1D	3.19	110.19	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	607	CHL	O1D-CGD-CBD	-3.19	117.95	124.48
25	R	601	CLA	C3D-C2D-C1D	3.19	110.18	105.83
39	Y	316	LUT	C35-C15-C14	-3.19	116.94	123.47
40	G	617	NEX	C40-C33-C32	3.19	123.10	118.08
25	c	512	CLA	CHD-C1D-C2D	3.19	132.17	125.48
40	R	617	NEX	C38-C25-C26	-3.19	116.92	122.26
24	r	605	CHL	CAA-C2A-C3A	-3.19	104.05	112.78
24	R	605	CHL	CAA-C2A-C3A	-3.18	104.06	112.78
25	Y	303	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
25	y	303	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
25	Y	304	CLA	C3D-C2D-C1D	3.18	110.17	105.83
25	S	304	CLA	CHD-C1D-C2D	3.18	132.15	125.48
25	S	311	CLA	CHD-C1D-C2D	3.18	132.15	125.48
24	G	601	CHL	CHD-C1D-ND	-3.18	121.53	124.45
25	B	602	CLA	C1D-ND-C4D	-3.18	104.08	106.33
25	B	610	CLA	C4A-NA-C1A	-3.18	105.28	106.71
25	b	610	CLA	C4A-NA-C1A	-3.18	105.28	106.71
25	2	602	CLA	C3C-C4C-NC	-3.18	107.01	110.57
25	6	602	CLA	C3C-C4C-NC	-3.18	107.01	110.57
25	R	610	CLA	C3D-C2D-C1D	3.17	110.16	105.83
25	2	605	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
25	R	603	CLA	C3D-C2D-C1D	3.17	110.16	105.83
24	S	306	CHL	CAA-C2A-C3A	-3.17	104.11	112.78
28	A	406	BCR	C15-C14-C13	-3.17	122.79	127.31
28	a	407	BCR	C15-C14-C13	-3.17	122.79	127.31
25	Y	304	CLA	C2A-C1A-CHA	-3.16	118.33	123.86
25	y	304	CLA	C2A-C1A-CHA	-3.16	118.33	123.86
25	G	613	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
24	R	607	CHL	CAA-C2A-C3A	-3.16	104.12	112.78
25	r	603	CLA	C3D-C2D-C1D	3.16	110.14	105.83
24	s	306	CHL	CAA-C2A-C3A	-3.16	104.13	112.78
25	s	312	CLA	C3D-C2D-C1D	3.16	110.14	105.83
24	Y	309	CHL	O2D-CGD-CBD	3.16	116.88	111.27
25	n	612	CLA	CHD-C1D-C2D	3.16	132.10	125.48
25	N	613	CLA	C4D-CHA-C1A	-3.15	117.41	121.25
25	6	605	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
25	d	403	CLA	C3D-C2D-C1D	3.15	110.13	105.83
25	s	311	CLA	CHD-C1D-C2D	3.15	132.09	125.48
30	A	408	LMG	C7-O1-C1	-3.15	107.58	113.74
30	a	409	LMG	C7-O1-C1	-3.15	107.58	113.74
25	D	403	CLA	C3D-C2D-C1D	3.15	110.12	105.83
25	n	603	CLA	C1-C2-C3	-3.14	120.61	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	613	CLA	C4D-CHA-C1A	-3.14	117.42	121.25
25	N	612	CLA	CHD-C1D-C2D	3.14	132.07	125.48
24	y	307	CHL	O2A-CGA-CBA	3.14	121.77	111.91
24	S	308	CHL	CAA-C2A-C3A	-3.14	104.17	112.78
24	s	308	CHL	CAA-C2A-C3A	-3.14	104.17	112.78
24	r	607	CHL	CAA-C2A-C3A	-3.14	104.18	112.78
24	Y	307	CHL	O2A-CGA-CBA	3.14	121.76	111.91
24	y	302	CHL	CHD-C1D-ND	-3.14	121.57	124.45
24	y	309	CHL	O2D-CGD-CBD	3.14	116.85	111.27
24	Y	302	CHL	CHD-C1D-ND	-3.13	121.57	124.45
25	n	612	CLA	C3D-C2D-C1D	3.13	110.10	105.83
25	g	613	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
25	S	312	CLA	C3D-C2D-C1D	3.13	110.10	105.83
24	Y	309	CHL	CAA-C2A-C3A	-3.13	104.22	112.78
24	N	608	CHL	CAA-C2A-C3A	-3.12	104.22	112.78
25	b	615	CLA	C2A-C3A-C4A	-3.12	96.83	101.87
24	n	606	CHL	CAA-C2A-C3A	-3.12	104.23	112.78
24	g	608	CHL	C1-C2-C3	3.12	131.44	126.04
25	6	602	CLA	C4D-C3D-CAD	-3.12	104.42	108.10
24	y	309	CHL	CAA-C2A-C3A	-3.12	104.24	112.78
25	b	610	CLA	C1-C2-C3	-3.12	120.65	126.04
38	F	101	HEM	CHC-C4B-NB	3.12	127.82	124.43
25	B	615	CLA	C2A-C3A-C4A	-3.12	96.84	101.87
25	6	604	CLA	C3D-C2D-C1D	3.11	110.08	105.83
24	2	601	CHL	O2D-CGD-CBD	3.11	116.80	111.27
24	n	601	CHL	CHD-C1D-ND	-3.11	121.60	124.45
25	N	603	CLA	C1-C2-C3	-3.11	120.67	126.04
25	C	512	CLA	C2A-C1A-CHA	-3.11	118.42	123.86
24	N	606	CHL	CAA-C2A-C3A	-3.11	104.27	112.78
25	B	608	CLA	C2A-C1A-CHA	-3.11	118.42	123.86
25	b	608	CLA	C2A-C1A-CHA	-3.11	118.42	123.86
25	s	313	CLA	C3D-C2D-C1D	3.11	110.07	105.83
24	G	608	CHL	C1-C2-C3	3.11	131.41	126.04
24	y	309	CHL	C1-C2-C3	3.10	131.41	126.04
25	B	610	CLA	C1-C2-C3	-3.10	120.67	126.04
24	g	601	CHL	CHD-C1D-ND	-3.10	121.60	124.45
35	C	516	DGD	C6D-O5D-C1E	-3.10	107.68	113.74
24	n	608	CHL	CAA-C2A-C3A	-3.10	104.28	112.78
25	2	604	CLA	C3D-C2D-C1D	3.10	110.06	105.83
25	c	504	CLA	C3D-C2D-C1D	3.10	110.06	105.83
24	6	601	CHL	O2D-CGD-CBD	3.10	116.78	111.27
24	R	605	CHL	CHD-C1D-ND	-3.10	121.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	309	CHL	C1-C2-C3	3.10	131.41	126.04
25	C	504	CLA	C3D-C2D-C1D	3.10	110.06	105.83
25	C	506	CLA	C1B-CHB-C4A	-3.10	123.99	130.12
25	c	506	CLA	C1B-CHB-C4A	-3.10	123.99	130.12
35	c	516	DGD	C6D-O5D-C1E	-3.09	107.69	113.74
40	G	617	NEX	C5-C4-C3	-3.09	108.08	111.75
25	Y	313	CLA	C3D-C2D-C1D	3.09	110.05	105.83
25	y	313	CLA	C3D-C2D-C1D	3.09	110.05	105.83
25	C	510	CLA	C1-C2-C3	-3.09	120.70	126.04
24	Y	308	CHL	C1-C2-C3	3.09	131.39	126.04
25	C	501	CLA	C3D-C2D-C1D	3.09	110.05	105.83
25	N	612	CLA	C3D-C2D-C1D	3.09	110.05	105.83
25	c	501	CLA	C3D-C2D-C1D	3.09	110.05	105.83
40	R	617	NEX	C10-C11-C12	3.09	132.85	123.22
40	r	617	NEX	C10-C11-C12	3.09	132.85	123.22
39	S	315	LUT	C2-C3-C4	3.08	114.53	110.30
24	s	308	CHL	CHD-C1D-ND	-3.08	121.62	124.45
25	B	607	CLA	C4-C3-C5	3.08	120.46	115.27
25	c	512	CLA	C2A-C1A-CHA	-3.08	118.47	123.86
25	N	614	CLA	C4D-CHA-C1A	-3.08	117.50	121.25
25	c	501	CLA	C4D-CHA-C1A	-3.08	117.50	121.25
25	r	614	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
30	B	620	LMG	C1-O6-C5	-3.08	107.64	113.69
30	b	620	LMG	C1-O6-C5	-3.08	107.64	113.69
25	2	602	CLA	C4D-C3D-CAD	-3.08	104.47	108.10
25	R	614	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
25	R	610	CLA	C4D-C3D-CAD	-3.08	104.47	108.10
24	y	308	CHL	C1-C2-C3	3.08	131.37	126.04
24	g	607	CHL	CHD-C1D-ND	-3.08	121.63	124.45
25	c	510	CLA	C1-C2-C3	-3.08	120.72	126.04
39	s	315	LUT	C2-C3-C4	3.08	114.51	110.30
25	b	607	CLA	C4-C3-C5	3.08	120.44	115.27
25	B	608	CLA	C4D-CHA-C1A	-3.07	117.51	121.25
25	b	608	CLA	C4D-CHA-C1A	-3.07	117.51	121.25
25	D	402	CLA	C3D-C2D-C1D	3.07	110.03	105.83
25	b	615	CLA	C3D-C2D-C1D	3.07	110.03	105.83
25	d	402	CLA	C3D-C2D-C1D	3.07	110.03	105.83
25	R	603	CLA	O1D-CGD-CBD	-3.07	118.19	124.48
24	N	601	CHL	CHD-C1D-ND	-3.07	121.63	124.45
25	r	603	CLA	O1D-CGD-CBD	-3.07	118.19	124.48
40	y	318	NEX	C20-C13-C14	-3.07	118.62	122.92
24	r	605	CHL	CHD-C1D-ND	-3.07	121.63	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	Y	318	NEX	C20-C13-C14	-3.07	118.63	122.92
24	g	606	CHL	CHD-C1D-ND	-3.07	121.64	124.45
25	S	313	CLA	C3D-C2D-C1D	3.07	110.02	105.83
25	B	603	CLA	C2A-C1A-CHA	-3.06	118.50	123.86
25	b	603	CLA	C2A-C1A-CHA	-3.06	118.50	123.86
35	C	516	DGD	C1E-O6E-C5E	-3.06	107.68	113.69
35	c	516	DGD	C1E-O6E-C5E	-3.06	107.68	113.69
25	c	505	CLA	C2A-C1A-CHA	-3.06	118.51	123.86
25	C	501	CLA	C4D-CHA-C1A	-3.06	117.53	121.25
25	y	315	CLA	O1D-CGD-CBD	-3.06	118.23	124.48
24	R	613	CHL	C2A-C3A-C4A	3.05	105.68	101.78
25	B	615	CLA	C3D-C2D-C1D	3.05	110.00	105.83
24	S	308	CHL	CHD-C1D-ND	-3.05	121.65	124.45
38	f	101	HEM	CHC-C4B-NB	3.05	127.75	124.43
41	R	616	XAT	C26-C27-C28	-3.05	119.54	125.99
24	g	609	CHL	CAA-C2A-C3A	-3.05	104.43	112.78
25	y	312	CLA	C3D-C2D-C1D	3.05	109.99	105.83
25	N	602	CLA	C4D-CHA-C1A	-3.05	117.54	121.25
25	n	614	CLA	C4D-CHA-C1A	-3.05	117.54	121.25
24	N	601	CHL	C1-C2-C3	3.05	131.31	126.04
24	G	609	CHL	CAA-C2A-C3A	-3.05	104.44	112.78
25	D	401	CLA	C1D-ND-C4D	-3.05	104.17	106.33
25	d	401	CLA	C1D-ND-C4D	-3.05	104.17	106.33
25	C	505	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
24	G	607	CHL	CHD-C1D-ND	-3.04	121.66	124.45
25	n	610	CLA	C1-C2-C3	-3.04	120.78	126.04
24	N	607	CHL	CHD-C1D-ND	-3.04	121.66	124.45
24	n	607	CHL	CHD-C1D-ND	-3.04	121.66	124.45
25	N	603	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
25	n	603	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
41	r	616	XAT	C26-C27-C28	-3.04	119.57	125.99
25	r	610	CLA	C4D-C3D-CAD	-3.04	104.52	108.10
25	Y	315	CLA	O1D-CGD-CBD	-3.04	118.27	124.48
25	s	309	CLA	C2A-C3A-C4A	-3.04	96.97	101.87
25	c	504	CLA	O1D-CGD-CBD	-3.03	118.28	124.48
40	R	617	NEX	C40-C33-C34	-3.03	118.67	122.92
24	r	613	CHL	C2A-C3A-C4A	3.03	105.65	101.78
25	N	610	CLA	C1-C2-C3	-3.03	120.80	126.04
35	B	626	DGD	C1E-O6E-C5E	-3.03	107.74	113.69
35	b	626	DGD	C1E-O6E-C5E	-3.03	107.74	113.69
25	G	613	CLA	CHD-C1D-C2D	3.03	131.83	125.48
25	c	503	CLA	CHD-C1D-C2D	3.02	131.82	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	602	CLA	C4D-CHA-C1A	-3.02	117.57	121.25
25	n	614	CLA	C1D-ND-C4D	-3.02	104.19	106.33
25	R	601	CLA	C4D-C3D-CAD	-3.02	104.53	108.10
25	C	511	CLA	CHD-C1D-C2D	3.02	131.82	125.48
25	c	511	CLA	CHD-C1D-C2D	3.02	131.82	125.48
25	S	309	CLA	C2A-C3A-C4A	-3.02	96.99	101.87
24	n	601	CHL	C1-C2-C3	3.02	131.27	126.04
25	r	601	CLA	C4D-C3D-CAD	-3.02	104.54	108.10
25	C	504	CLA	O1D-CGD-CBD	-3.02	118.31	124.48
25	y	315	CLA	C2A-C1A-CHA	-3.01	118.59	123.86
28	z	101	BCR	C2-C1-C6	3.01	115.12	110.48
25	n	611	CLA	C3D-C2D-C1D	3.01	109.94	105.83
24	Y	308	CHL	CAA-C2A-C3A	-3.01	104.54	112.78
40	y	318	NEX	C39-C29-C30	-3.01	118.71	122.92
25	r	609	CLA	C4-C3-C5	3.01	120.33	115.27
25	Y	312	CLA	C3D-C2D-C1D	3.01	109.93	105.83
25	R	612	CLA	C3D-C2D-C1D	3.01	109.93	105.83
25	r	612	CLA	C3D-C2D-C1D	3.01	109.93	105.83
28	Z	101	BCR	C2-C1-C6	3.00	115.11	110.48
24	G	606	CHL	CHD-C1D-ND	-3.00	121.69	124.45
24	2	603	CHL	C4D-CHA-C1A	3.00	124.90	121.25
25	Y	311	CLA	C4-C3-C5	3.00	120.32	115.27
25	C	506	CLA	CHB-C4A-NA	-3.00	120.36	124.51
25	c	506	CLA	CHB-C4A-NA	-3.00	120.36	124.51
24	n	609	CHL	CHD-C1D-ND	-3.00	121.69	124.45
25	S	303	CLA	C4A-NA-C1A	-3.00	105.36	106.71
40	r	617	NEX	C40-C33-C34	-3.00	118.72	122.92
25	y	311	CLA	C4-C3-C5	3.00	120.32	115.27
25	g	613	CLA	CHD-C1D-C2D	3.00	131.77	125.48
25	A	401	CLA	C1D-ND-C4D	-3.00	104.20	106.33
25	a	402	CLA	C1D-ND-C4D	-3.00	104.20	106.33
24	y	308	CHL	CAA-C2A-C3A	-3.00	104.57	112.78
24	s	306	CHL	CHD-C1D-ND	-3.00	121.70	124.45
25	C	503	CLA	CHD-C1D-C2D	3.00	131.76	125.48
24	G	607	CHL	CMB-C2B-C3B	3.00	130.28	124.68
27	A	404	PHO	C4-C3-C5	2.99	120.31	115.27
27	a	405	PHO	C4-C3-C5	2.99	120.31	115.27
38	F	101	HEM	CHD-C1D-ND	2.99	127.68	124.43
38	f	101	HEM	CHD-C1D-ND	2.99	127.68	124.43
25	B	605	CLA	C1D-ND-C4D	-2.99	104.21	106.33
25	N	603	CLA	C3D-C2D-C1D	2.99	109.91	105.83
25	N	611	CLA	C3D-C2D-C1D	2.99	109.91	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	604	CLA	CHC-C1C-NC	-2.99	119.66	124.20
25	N	614	CLA	C1D-ND-C4D	-2.99	104.21	106.33
28	b	617	BCR	C15-C14-C13	-2.99	123.04	127.31
24	S	302	CHL	CHD-C1D-ND	-2.99	121.71	124.45
25	n	603	CLA	C3D-C2D-C1D	2.99	109.91	105.83
24	1	302	CHL	C1D-ND-C4D	-2.99	104.21	106.33
25	C	504	CLA	C4D-CHA-C1A	-2.99	117.61	121.25
25	b	604	CLA	C1D-ND-C4D	-2.99	104.21	106.33
25	s	310	CLA	CHD-C1D-C2D	2.99	131.74	125.48
24	S	306	CHL	CHD-C1D-ND	-2.99	121.71	124.45
28	B	617	BCR	C15-C14-C13	-2.98	123.05	127.31
24	n	608	CHL	C1-C2-C3	2.98	131.20	126.04
25	2	604	CLA	CHC-C1C-NC	-2.98	119.68	124.20
25	S	311	CLA	C3D-C2D-C1D	2.98	109.90	105.83
25	b	604	CLA	C3D-C2D-C1D	2.98	109.90	105.83
24	G	605	CHL	CAA-C2A-C3A	-2.98	104.62	112.78
40	Y	318	NEX	C39-C29-C30	-2.98	118.75	122.92
24	g	607	CHL	CMB-C2B-C3B	2.98	130.25	124.68
24	g	605	CHL	CAA-C2A-C3A	-2.98	104.62	112.78
24	N	606	CHL	CHD-C1D-ND	-2.97	121.72	124.45
24	n	606	CHL	CHD-C1D-ND	-2.97	121.72	124.45
24	6	603	CHL	C4D-CHA-C1A	2.97	124.87	121.25
25	Y	315	CLA	C2A-C1A-CHA	-2.97	118.66	123.86
25	b	605	CLA	C1D-ND-C4D	-2.97	104.22	106.33
24	N	608	CHL	C1-C2-C3	2.97	131.18	126.04
25	s	311	CLA	C3D-C2D-C1D	2.97	109.88	105.83
24	G	608	CHL	O2A-CGA-CBA	2.97	121.22	111.91
24	g	608	CHL	O2A-CGA-CBA	2.97	121.22	111.91
24	N	609	CHL	CHD-C1D-ND	-2.97	121.73	124.45
25	R	609	CLA	C4-C3-C5	2.97	120.26	115.27
25	Y	311	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
25	y	311	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
25	G	610	CLA	C3D-C2D-C1D	2.96	109.87	105.83
24	5	301	CHL	CAA-C2A-C3A	-2.96	104.67	112.78
24	1	301	CHL	CHD-C1D-ND	-2.96	121.73	124.45
25	C	511	CLA	C3D-C2D-C1D	2.96	109.87	105.83
25	c	511	CLA	C3D-C2D-C1D	2.96	109.87	105.83
25	2	602	CLA	CHA-C1A-NA	-2.96	119.62	126.40
25	C	508	CLA	C3D-C2D-C1D	2.96	109.87	105.83
24	S	307	CHL	CHD-C1D-ND	-2.96	121.74	124.45
24	s	307	CHL	CHD-C1D-ND	-2.96	121.74	124.45
28	T	101	BCR	C15-C16-C17	-2.96	117.42	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	510	CLA	C2A-C1A-CHA	-2.96	118.69	123.86
24	2	603	CHL	CBC-CAC-C3C	-2.96	104.28	112.43
24	6	603	CHL	CBC-CAC-C3C	-2.96	104.28	112.43
25	G	603	CLA	C3D-C2D-C1D	2.96	109.86	105.83
25	g	603	CLA	C3D-C2D-C1D	2.96	109.86	105.83
25	C	510	CLA	C3D-C2D-C1D	2.95	109.86	105.83
25	S	314	CLA	C2A-C1A-CHA	-2.95	118.69	123.86
25	s	314	CLA	C2A-C1A-CHA	-2.95	118.69	123.86
24	5	301	CHL	CHD-C1D-ND	-2.95	121.74	124.45
24	G	609	CHL	O2A-CGA-CBA	2.95	121.18	111.91
25	c	504	CLA	C4D-CHA-C1A	-2.95	117.65	121.25
25	2	605	CLA	C1D-ND-C4D	-2.95	104.24	106.33
25	G	602	CLA	C4-C3-C5	2.95	120.24	115.27
24	1	301	CHL	CAA-C2A-C3A	-2.95	104.69	112.78
25	S	310	CLA	CHD-C1D-C2D	2.95	131.67	125.48
25	d	401	CLA	CHD-C1D-C2D	2.95	131.67	125.48
28	t	101	BCR	C15-C16-C17	-2.95	117.43	123.47
25	6	602	CLA	CHA-C1A-NA	-2.95	119.64	126.40
25	g	602	CLA	C4-C3-C5	2.95	120.23	115.27
25	B	604	CLA	C1D-ND-C4D	-2.95	104.24	106.33
25	s	303	CLA	C4A-NA-C1A	-2.94	105.38	106.71
25	G	610	CLA	CHD-C1D-C2D	2.94	131.65	125.48
25	N	604	CLA	O1D-CGD-CBD	-2.94	118.46	124.48
25	c	510	CLA	C3D-C2D-C1D	2.94	109.85	105.83
25	n	611	CLA	O1D-CGD-CBD	-2.94	118.47	124.48
25	D	401	CLA	CHD-C1D-C2D	2.94	131.65	125.48
24	g	609	CHL	O2A-CGA-CBA	2.94	121.14	111.91
25	g	614	CLA	C3D-C2D-C1D	2.94	109.84	105.83
25	r	609	CLA	C3D-C2D-C1D	2.94	109.84	105.83
25	B	604	CLA	C3D-C2D-C1D	2.94	109.84	105.83
24	1	302	CHL	CAA-C2A-C3A	-2.94	104.73	112.78
24	5	302	CHL	CAA-C2A-C3A	-2.94	104.73	112.78
25	g	610	CLA	C3D-C2D-C1D	2.94	109.84	105.83
25	A	401	CLA	C3D-C2D-C1D	2.94	109.84	105.83
25	a	402	CLA	C3D-C2D-C1D	2.94	109.84	105.83
24	n	608	CHL	O2A-CGA-CBA	2.93	121.12	111.91
25	s	309	CLA	C3D-C2D-C1D	2.93	109.83	105.83
24	N	608	CHL	O2A-CGA-CBA	2.93	121.11	111.91
25	n	604	CLA	O1D-CGD-CBD	-2.93	118.48	124.48
25	s	305	CLA	C4D-C3D-CAD	-2.93	104.64	108.10
25	6	605	CLA	C1D-ND-C4D	-2.93	104.25	106.33
24	2	601	CHL	C1-C2-C3	2.93	131.11	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	601	CHL	C1-C2-C3	2.93	131.11	126.04
25	B	601	CLA	C4-C3-C5	2.93	120.20	115.27
25	b	601	CLA	C4-C3-C5	2.93	120.20	115.27
25	C	513	CLA	C3D-C2D-C1D	2.93	109.83	105.83
24	6	601	CHL	O2A-CGA-CBA	2.93	121.10	111.91
25	2	605	CLA	C3D-C2D-C1D	2.93	109.83	105.83
25	6	605	CLA	C3D-C2D-C1D	2.93	109.83	105.83
25	A	402	CLA	C1D-ND-C4D	-2.93	104.25	106.33
25	c	508	CLA	C3D-C2D-C1D	2.93	109.83	105.83
25	d	401	CLA	C3D-C2D-C1D	2.93	109.82	105.83
25	C	506	CLA	C4A-NA-C1A	-2.92	105.39	106.71
25	c	506	CLA	C4A-NA-C1A	-2.92	105.39	106.71
25	S	309	CLA	C3D-C2D-C1D	2.92	109.82	105.83
25	S	305	CLA	C4D-C3D-CAD	-2.92	104.65	108.10
40	s	317	NEX	C15-C14-C13	-2.92	123.14	127.31
24	2	601	CHL	O2A-CGA-CBA	2.92	121.08	111.91
25	N	611	CLA	O1D-CGD-CBD	-2.92	118.50	124.48
25	s	314	CLA	C3D-C2D-C1D	2.92	109.82	105.83
25	a	406	CLA	CHD-C1D-C2D	2.92	131.61	125.48
25	B	606	CLA	C1D-CHD-C4C	-2.92	119.76	126.06
25	b	606	CLA	C1D-CHD-C4C	-2.92	119.76	126.06
25	B	616	CLA	C1-C2-C3	-2.92	120.99	126.04
25	b	616	CLA	C1-C2-C3	-2.92	120.99	126.04
25	C	507	CLA	C1D-ND-C4D	-2.92	104.26	106.33
25	R	609	CLA	C3D-C2D-C1D	2.92	109.82	105.83
25	c	510	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
24	s	302	CHL	CHD-C1D-ND	-2.92	121.77	124.45
28	B	617	BCR	C33-C5-C6	-2.92	121.25	124.53
28	b	617	BCR	C33-C5-C6	-2.92	121.25	124.53
25	A	405	CLA	CHD-C1D-C2D	2.92	131.60	125.48
25	g	610	CLA	CHD-C1D-C2D	2.92	131.60	125.48
25	c	512	CLA	C1D-ND-C4D	-2.92	104.26	106.33
25	B	609	CLA	C3D-C2D-C1D	2.91	109.81	105.83
25	r	609	CLA	C1D-ND-C4D	-2.91	104.27	106.33
28	I	101	BCR	C15-C16-C17	-2.91	117.50	123.47
25	A	402	CLA	C3D-C2D-C1D	2.91	109.81	105.83
25	a	403	CLA	C3D-C2D-C1D	2.91	109.81	105.83
25	g	613	CLA	C3D-C2D-C1D	2.91	109.81	105.83
40	S	317	NEX	C15-C14-C13	-2.91	123.15	127.31
24	5	302	CHL	C1D-ND-C4D	-2.91	104.27	106.33
25	n	604	CLA	C3D-C2D-C1D	2.91	109.80	105.83
25	r	602	CLA	C3D-C2D-C1D	2.91	109.80	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	508	CLA	C4-C3-C5	2.91	120.16	115.27
24	r	606	CHL	CHD-C1D-ND	-2.91	121.78	124.45
25	R	602	CLA	C3D-C2D-C1D	2.91	109.80	105.83
28	D	404	BCR	C33-C5-C6	-2.91	121.26	124.53
28	d	404	BCR	C33-C5-C6	-2.91	121.26	124.53
28	b	617	BCR	C15-C16-C17	-2.91	117.52	123.47
24	y	309	CHL	O2A-CGA-CBA	2.90	121.02	111.91
28	B	617	BCR	C15-C16-C17	-2.90	117.53	123.47
25	S	304	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	s	304	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	D	401	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	B	601	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	N	604	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	b	601	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	B	610	CLA	C3D-C2D-C1D	2.90	109.79	105.83
25	b	610	CLA	C3D-C2D-C1D	2.90	109.79	105.83
24	Y	309	CHL	O2A-CGA-CBA	2.90	121.00	111.91
25	A	405	CLA	C4-C3-C5	2.90	120.15	115.27
25	a	406	CLA	C4-C3-C5	2.90	120.15	115.27
28	i	101	BCR	C15-C16-C17	-2.90	117.54	123.47
25	G	613	CLA	C3D-C2D-C1D	2.89	109.78	105.83
25	n	613	CLA	C4-C3-C5	2.89	120.14	115.27
24	1	302	CHL	C2D-C1D-ND	2.89	112.24	110.10
25	y	312	CLA	C2A-C1A-CHA	-2.89	118.80	123.86
25	B	614	CLA	C2A-C1A-CHA	-2.89	118.80	123.86
25	b	614	CLA	C2A-C1A-CHA	-2.89	118.80	123.86
25	S	311	CLA	C1D-ND-C4D	-2.89	104.28	106.33
25	c	507	CLA	C1D-ND-C4D	-2.89	104.28	106.33
24	n	601	CHL	CAA-C2A-C3A	-2.89	104.86	112.78
25	B	605	CLA	C3D-C2D-C1D	2.89	109.78	105.83
25	B	608	CLA	C3D-C2D-C1D	2.89	109.78	105.83
25	b	605	CLA	C3D-C2D-C1D	2.89	109.78	105.83
25	b	614	CLA	C4-C3-C5	2.89	120.13	115.27
25	R	604	CLA	C3D-C2D-C1D	2.89	109.78	105.83
25	r	604	CLA	C3D-C2D-C1D	2.89	109.78	105.83
25	Y	305	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
25	D	402	CLA	CHB-C4A-NA	-2.89	120.52	124.51
25	B	614	CLA	C4-C3-C5	2.89	120.13	115.27
25	R	611	CLA	C3C-C4C-NC	-2.89	107.33	110.57
25	r	611	CLA	C3C-C4C-NC	-2.89	107.33	110.57
24	R	606	CHL	CHD-C1D-ND	-2.89	121.80	124.45
25	S	314	CLA	C3D-C2D-C1D	2.89	109.77	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	610	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
25	b	610	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
25	B	607	CLA	C3D-C2D-C1D	2.89	109.77	105.83
25	C	512	CLA	C3D-C2D-C1D	2.89	109.77	105.83
25	b	607	CLA	C3D-C2D-C1D	2.89	109.77	105.83
25	c	512	CLA	C3D-C2D-C1D	2.89	109.77	105.83
24	N	601	CHL	CAA-C2A-C3A	-2.89	104.88	112.78
25	B	615	CLA	C4A-NA-C1A	-2.88	105.41	106.71
25	b	615	CLA	C4A-NA-C1A	-2.88	105.41	106.71
24	N	608	CHL	CMB-C2B-C1B	-2.88	124.03	128.46
25	a	403	CLA	C1D-ND-C4D	-2.88	104.29	106.33
25	Y	312	CLA	C2A-C1A-CHA	-2.88	118.82	123.86
25	R	608	CLA	C4D-CHA-C1A	-2.88	117.75	121.25
25	G	604	CLA	C3D-C2D-C1D	2.88	109.76	105.83
25	G	614	CLA	C3D-C2D-C1D	2.88	109.76	105.83
25	C	508	CLA	C4-C3-C5	2.88	120.11	115.27
25	C	502	CLA	C3D-C2D-C1D	2.88	109.76	105.83
25	N	613	CLA	C4-C3-C5	2.87	120.11	115.27
25	C	505	CLA	C3D-C2D-C1D	2.87	109.75	105.83
24	n	608	CHL	CMB-C2B-C1B	-2.87	124.05	128.46
24	N	605	CHL	CHD-C1D-ND	-2.87	121.81	124.45
24	n	605	CHL	CHD-C1D-ND	-2.87	121.81	124.45
25	b	608	CLA	C3D-C2D-C1D	2.87	109.75	105.83
25	b	608	CLA	C4-C3-C5	2.87	120.10	115.27
27	A	403	PHO	O1D-CGD-CBD	-2.87	119.96	124.74
27	a	404	PHO	O1D-CGD-CBD	-2.87	119.96	124.74
25	S	303	CLA	C3D-C2D-C1D	2.87	109.75	105.83
24	R	613	CHL	CHD-C1D-ND	-2.87	121.81	124.45
24	n	605	CHL	O2A-CGA-CBA	2.87	120.92	111.91
25	b	611	CLA	C3D-C2D-C1D	2.87	109.75	105.83
25	c	502	CLA	C3D-C2D-C1D	2.87	109.75	105.83
25	B	603	CLA	C4-C3-C5	2.87	120.10	115.27
25	G	610	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
24	n	609	CHL	O2A-CGA-CBA	2.87	120.91	111.91
25	c	503	CLA	C3D-C2D-C1D	2.87	109.75	105.83
25	C	512	CLA	C1D-ND-C4D	-2.87	104.30	106.33
24	y	308	CHL	CHD-C1D-ND	-2.87	121.82	124.45
25	N	612	CLA	C4A-NA-C1A	-2.87	105.42	106.71
25	n	612	CLA	C4A-NA-C1A	-2.87	105.42	106.71
25	6	604	CLA	CHA-C1A-NA	-2.87	119.83	126.40
25	B	608	CLA	C4-C3-C5	2.87	120.09	115.27
25	R	612	CLA	C4-C3-C5	2.87	120.09	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	602	CLA	C3D-C2D-C1D	2.87	109.74	105.83
25	b	609	CLA	C3D-C2D-C1D	2.87	109.74	105.83
24	N	605	CHL	O2A-CGA-CBA	2.86	120.90	111.91
24	y	307	CHL	CAA-C2A-C3A	-2.86	104.94	112.78
25	B	611	CLA	C3D-C2D-C1D	2.86	109.74	105.83
25	B	614	CLA	C3D-C2D-C1D	2.86	109.74	105.83
25	b	614	CLA	C3D-C2D-C1D	2.86	109.74	105.83
25	b	612	CLA	C3D-C2D-C1D	2.86	109.74	105.83
24	R	606	CHL	CMB-C2B-C1B	-2.86	124.07	128.46
30	D	407	LMG	C1-O6-C5	-2.86	108.07	113.69
30	d	407	LMG	C1-O6-C5	-2.86	108.07	113.69
25	B	612	CLA	C3D-C2D-C1D	2.86	109.73	105.83
25	c	513	CLA	C3D-C2D-C1D	2.86	109.73	105.83
25	b	607	CLA	CHD-C1D-C2D	2.86	131.47	125.48
24	N	609	CHL	O2A-CGA-CBA	2.86	120.88	111.91
25	y	305	CLA	C2A-C1A-CHA	-2.86	118.86	123.86
25	Y	314	CLA	C4-C3-C5	2.86	120.08	115.27
25	s	311	CLA	C1D-ND-C4D	-2.86	104.31	106.33
24	Y	307	CHL	CAA-C2A-C3A	-2.86	104.96	112.78
25	N	610	CLA	C2A-C1A-CHA	-2.86	118.87	123.86
25	c	506	CLA	C3D-C2D-C1D	2.85	109.73	105.83
25	g	610	CLA	C1B-CHB-C4A	-2.85	124.46	130.12
25	C	503	CLA	C3D-C2D-C1D	2.85	109.72	105.83
25	C	506	CLA	C3D-C2D-C1D	2.85	109.72	105.83
25	2	604	CLA	CHA-C1A-NA	-2.85	119.86	126.40
25	b	602	CLA	C3D-C2D-C1D	2.85	109.72	105.83
25	d	402	CLA	CHB-C4A-NA	-2.85	120.57	124.51
25	c	505	CLA	C3D-C2D-C1D	2.85	109.72	105.83
25	s	303	CLA	C3D-C2D-C1D	2.85	109.72	105.83
25	b	610	CLA	C4-C3-C5	2.85	120.06	115.27
25	y	314	CLA	C4-C3-C5	2.85	120.06	115.27
25	n	610	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
25	R	603	CLA	C4D-C3D-CAD	-2.85	104.74	108.10
25	r	603	CLA	C4D-C3D-CAD	-2.85	104.74	108.10
25	C	508	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	c	508	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	r	613	CHL	CHD-C1D-ND	-2.85	121.84	124.45
25	B	610	CLA	C4-C3-C5	2.84	120.06	115.27
25	C	508	CLA	O1D-CGD-CBD	-2.84	118.67	124.48
25	c	508	CLA	O1D-CGD-CBD	-2.84	118.67	124.48
41	R	616	XAT	C27-C28-C29	-2.84	121.12	125.53
24	r	606	CHL	CMB-C2B-C1B	-2.84	124.09	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	514	BCR	C33-C5-C6	-2.84	121.34	124.53
25	N	611	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
25	n	611	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
25	R	609	CLA	C1D-ND-C4D	-2.84	104.32	106.33
25	y	305	CLA	C4D-CHA-C1A	-2.84	117.79	121.25
25	R	608	CLA	C3D-C2D-C1D	2.84	109.71	105.83
25	b	603	CLA	C3D-C2D-C1D	2.84	109.71	105.83
25	b	603	CLA	C4-C3-C5	2.84	120.05	115.27
25	a	406	CLA	C3D-C2D-C1D	2.84	109.71	105.83
24	Y	308	CHL	CHD-C1D-ND	-2.84	121.84	124.45
25	N	613	CLA	C3D-C2D-C1D	2.84	109.71	105.83
25	c	504	CLA	C4-C3-C5	2.84	120.05	115.27
25	B	607	CLA	CHD-C1D-C2D	2.84	131.43	125.48
25	R	603	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	r	603	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	n	602	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	C	505	CLA	C1-C2-C3	-2.84	121.14	126.04
25	c	505	CLA	C1-C2-C3	-2.84	121.14	126.04
25	A	405	CLA	C3D-C2D-C1D	2.83	109.70	105.83
25	R	610	CLA	C3B-C4B-NB	-2.83	105.55	109.21
28	T	101	BCR	C11-C10-C9	-2.83	123.27	127.31
25	r	612	CLA	C4-C3-C5	2.83	120.03	115.27
25	r	601	CLA	O1D-CGD-CBD	-2.83	118.69	124.48
27	A	404	PHO	O1D-CGD-CBD	-2.83	120.03	124.74
25	r	610	CLA	C3B-C4B-NB	-2.83	105.55	109.21
25	g	604	CLA	C3D-C2D-C1D	2.83	109.69	105.83
24	g	606	CHL	O1D-CGD-CBD	-2.83	118.70	124.48
25	y	305	CLA	C3D-C2D-C1D	2.83	109.69	105.83
25	b	609	CLA	C4-C3-C5	2.83	120.03	115.27
25	Y	305	CLA	C4D-CHA-C1A	-2.83	117.81	121.25
24	N	601	CHL	O2A-CGA-CBA	2.83	120.78	111.91
25	g	612	CLA	C3D-C2D-C1D	2.83	109.69	105.83
27	a	405	PHO	O1D-CGD-CBD	-2.82	120.03	124.74
25	g	613	CLA	O1D-CGD-CBD	-2.82	118.70	124.48
25	Y	305	CLA	C3D-C2D-C1D	2.82	109.69	105.83
24	n	601	CHL	O2A-CGA-CBA	2.82	120.77	111.91
25	C	509	CLA	C3D-C2D-C1D	2.82	109.68	105.83
25	Y	314	CLA	C3D-C2D-C1D	2.82	109.68	105.83
25	c	509	CLA	C3D-C2D-C1D	2.82	109.68	105.83
25	y	314	CLA	C3D-C2D-C1D	2.82	109.68	105.83
25	r	608	CLA	C3D-C2D-C1D	2.82	109.68	105.83
24	G	606	CHL	O1D-CGD-CBD	-2.82	118.71	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	602	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
24	R	607	CHL	CHD-C1D-ND	-2.82	121.86	124.45
25	Y	315	CLA	C3D-C2D-C1D	2.82	109.68	105.83
24	g	601	CHL	CAA-C2A-C3A	-2.82	105.06	112.78
24	5	302	CHL	C2D-C1D-ND	2.82	112.18	110.10
25	C	504	CLA	C4-C3-C5	2.82	120.01	115.27
25	G	613	CLA	O1D-CGD-CBD	-2.82	118.72	124.48
28	c	514	BCR	C33-C5-C6	-2.82	121.36	124.53
25	g	603	CLA	O1D-CGD-CBD	-2.82	118.72	124.48
25	c	502	CLA	C4-C3-C5	2.82	120.01	115.27
25	y	303	CLA	C4-C3-C5	2.82	120.01	115.27
25	B	603	CLA	C3D-C2D-C1D	2.82	109.68	105.83
25	Y	303	CLA	C4-C3-C5	2.82	120.01	115.27
25	B	609	CLA	C4-C3-C5	2.81	120.01	115.27
25	R	601	CLA	O1D-CGD-CBD	-2.81	118.73	124.48
24	N	609	CHL	C1-C2-C3	2.81	130.91	126.04
24	n	609	CHL	C1-C2-C3	2.81	130.91	126.04
25	g	612	CLA	C4-C3-C5	2.81	120.00	115.27
25	y	311	CLA	C3D-C2D-C1D	2.81	109.66	105.83
24	G	601	CHL	CAA-C2A-C3A	-2.81	105.09	112.78
24	r	607	CHL	CHD-C1D-ND	-2.81	121.87	124.45
25	B	606	CLA	C3D-C2D-C1D	2.81	109.66	105.83
25	b	606	CLA	C3D-C2D-C1D	2.81	109.66	105.83
25	C	502	CLA	C4-C3-C5	2.80	119.99	115.27
25	S	310	CLA	C4-C3-C5	2.80	119.99	115.27
25	G	603	CLA	C4D-CHA-C1A	-2.80	117.84	121.25
25	g	603	CLA	C4D-CHA-C1A	-2.80	117.84	121.25
25	B	604	CLA	C4-C3-C5	2.80	119.99	115.27
25	b	604	CLA	C4-C3-C5	2.80	119.99	115.27
25	r	608	CLA	C4D-CHA-C1A	-2.80	117.84	121.25
25	B	616	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
25	b	616	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
25	B	611	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
25	b	611	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
28	B	617	BCR	C11-C10-C9	-2.80	123.31	127.31
28	b	617	BCR	C11-C10-C9	-2.80	123.31	127.31
25	G	612	CLA	C3D-C2D-C1D	2.80	109.65	105.83
25	y	315	CLA	C3D-C2D-C1D	2.80	109.65	105.83
41	r	616	XAT	C27-C28-C29	-2.80	121.19	125.53
25	G	603	CLA	O1D-CGD-CBD	-2.80	118.76	124.48
25	B	607	CLA	C2A-C1A-CHA	-2.80	118.97	123.86
25	b	607	CLA	C2A-C1A-CHA	-2.80	118.97	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	613	CLA	C3D-C2D-C1D	2.80	109.65	105.83
25	d	403	CLA	C4-C3-C5	2.79	119.97	115.27
25	r	608	CLA	CHD-C1D-C2D	2.79	131.34	125.48
25	Y	311	CLA	C3D-C2D-C1D	2.79	109.64	105.83
25	r	603	CLA	C4D-CHA-C1A	-2.79	117.85	121.25
25	R	608	CLA	CHD-C1D-C2D	2.79	131.34	125.48
28	t	101	BCR	C11-C10-C9	-2.79	123.32	127.31
25	r	611	CLA	CHD-C4C-C3C	2.79	128.94	124.84
25	G	612	CLA	C4-C3-C5	2.79	119.97	115.27
25	s	310	CLA	C4-C3-C5	2.79	119.97	115.27
35	c	515	DGD	C1E-O6E-C5E	-2.79	108.21	113.69
25	r	602	CLA	C4-C3-C5	2.79	119.97	115.27
35	C	515	DGD	C1E-O6E-C5E	-2.79	108.21	113.69
24	Y	306	CHL	O2A-CGA-CBA	2.79	120.66	111.91
25	R	603	CLA	C4D-CHA-C1A	-2.79	117.86	121.25
25	R	602	CLA	C4-C3-C5	2.79	119.96	115.27
35	A	415	DGD	C3G-O3G-C1D	-2.79	108.29	113.74
35	a	401	DGD	C3G-O3G-C1D	-2.79	108.29	113.74
24	n	608	CHL	CHD-C1D-ND	-2.79	121.89	124.45
25	C	513	CLA	CHD-C1D-C2D	2.79	131.32	125.48
25	B	613	CLA	C4-C3-C5	2.79	119.96	115.27
25	b	613	CLA	C4-C3-C5	2.79	119.96	115.27
24	Y	302	CHL	O2A-CGA-CBA	2.78	120.65	111.91
24	y	302	CHL	O2A-CGA-CBA	2.78	120.65	111.91
25	A	402	CLA	C4-C3-C5	2.78	119.95	115.27
25	a	403	CLA	C4-C3-C5	2.78	119.95	115.27
41	R	616	XAT	C40-C33-C34	-2.78	119.03	122.92
25	D	403	CLA	C4-C3-C5	2.78	119.95	115.27
25	n	610	CLA	C4-C3-C5	2.78	119.95	115.27
40	y	318	NEX	C12-C13-C14	2.78	123.21	118.94
25	N	610	CLA	C4-C3-C5	2.78	119.95	115.27
25	S	305	CLA	O1D-CGD-CBD	-2.78	118.80	124.48
25	S	313	CLA	O1D-CGD-CBD	-2.78	118.80	124.48
25	s	305	CLA	O1D-CGD-CBD	-2.78	118.80	124.48
25	n	610	CLA	C3D-C2D-C1D	2.78	109.62	105.83
25	G	610	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
25	G	611	CLA	C4-C3-C5	2.78	119.94	115.27
25	n	613	CLA	C3D-C2D-C1D	2.78	109.62	105.83
41	r	616	XAT	C40-C33-C34	-2.78	119.03	122.92
25	Y	313	CLA	C4-C3-C5	2.78	119.94	115.27
28	K	101	BCR	C15-C16-C17	-2.78	117.79	123.47
24	R	613	CHL	CMA-C3A-C2A	-2.78	109.62	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	613	CHL	CMA-C3A-C2A	-2.78	109.62	116.10
25	C	506	CLA	C4-C3-C5	2.78	119.94	115.27
25	b	605	CLA	C4-C3-C5	2.78	119.94	115.27
25	c	506	CLA	C4-C3-C5	2.78	119.94	115.27
40	Y	318	NEX	C12-C13-C14	2.77	123.20	118.94
25	g	603	CLA	C4-C3-C5	2.77	119.94	115.27
40	s	317	NEX	C28-C29-C30	2.77	123.20	118.94
25	R	610	CLA	C2A-C3A-C4A	-2.77	97.39	101.87
25	r	610	CLA	C2A-C3A-C4A	-2.77	97.39	101.87
25	N	612	CLA	C4-C3-C5	2.77	119.93	115.27
25	c	513	CLA	CHD-C1D-C2D	2.77	131.29	125.48
25	B	616	CLA	O2A-CGA-CBA	2.77	120.60	111.91
25	b	616	CLA	O2A-CGA-CBA	2.77	120.60	111.91
25	R	604	CLA	O2A-CGA-CBA	2.77	120.60	111.91
25	r	604	CLA	O2A-CGA-CBA	2.77	120.60	111.91
25	Y	314	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
25	D	403	CLA	C4D-CHA-C1A	-2.77	117.88	121.25
25	c	507	CLA	C4D-CHA-C1A	-2.77	117.88	121.25
25	d	403	CLA	C4D-CHA-C1A	-2.77	117.88	121.25
24	y	306	CHL	O2A-CGA-CBA	2.77	120.59	111.91
25	b	613	CLA	C3D-C2D-C1D	2.77	109.61	105.83
24	Y	309	CHL	CHD-C1D-ND	-2.77	121.91	124.45
40	S	317	NEX	C28-C29-C30	2.77	123.19	118.94
25	B	616	CLA	C3D-C2D-C1D	2.77	109.61	105.83
25	B	604	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
25	b	604	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
25	c	505	CLA	C4-C3-C5	2.77	119.92	115.27
25	s	313	CLA	O1D-CGD-CBD	-2.76	118.83	124.48
25	6	605	CLA	O1D-CGD-CBD	-2.76	118.83	124.48
25	B	611	CLA	CHD-C1D-C2D	2.76	131.28	125.48
28	k	101	BCR	C15-C16-C17	-2.76	117.81	123.47
25	n	612	CLA	C4-C3-C5	2.76	119.92	115.27
25	R	614	CLA	C3D-C2D-C1D	2.76	109.60	105.83
25	r	614	CLA	C3D-C2D-C1D	2.76	109.60	105.83
25	g	610	CLA	C2A-C1A-CHA	-2.76	119.03	123.86
25	D	402	CLA	C2A-C3A-C4A	-2.76	97.41	101.87
25	d	402	CLA	C2A-C3A-C4A	-2.76	97.41	101.87
25	Y	312	CLA	C4-C3-C5	2.76	119.92	115.27
25	g	611	CLA	C4-C3-C5	2.76	119.92	115.27
25	2	605	CLA	O1D-CGD-CBD	-2.76	118.83	124.48
24	y	306	CHL	CHD-C1D-ND	-2.76	121.92	124.45
25	R	611	CLA	CHD-C4C-C3C	2.76	128.90	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	609	CHL	C1-C2-C3	2.76	130.82	126.04
25	G	603	CLA	C4-C3-C5	2.76	119.92	115.27
35	c	515	DGD	C1D-O6D-C5D	-2.76	108.27	113.69
25	N	614	CLA	C3D-C2D-C1D	2.76	109.60	105.83
25	n	614	CLA	C3D-C2D-C1D	2.76	109.60	105.83
25	b	611	CLA	CHD-C1D-C2D	2.76	131.27	125.48
25	2	602	CLA	CHD-C4C-C3C	2.76	128.90	124.84
25	6	602	CLA	CHD-C4C-C3C	2.76	128.90	124.84
25	N	610	CLA	C3D-C2D-C1D	2.76	109.59	105.83
28	T	101	BCR	C33-C5-C6	-2.76	121.43	124.53
25	y	313	CLA	C4-C3-C5	2.76	119.91	115.27
25	y	303	CLA	C3D-C2D-C1D	2.76	109.59	105.83
39	s	315	LUT	C22-C23-C24	2.76	114.88	111.74
24	6	603	CHL	CHC-C1C-NC	2.75	128.38	124.20
25	b	616	CLA	C3D-C2D-C1D	2.75	109.59	105.83
25	y	314	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
24	Y	302	CHL	CAA-C2A-C3A	-2.75	105.25	112.78
24	y	302	CHL	CAA-C2A-C3A	-2.75	105.25	112.78
25	y	312	CLA	C4-C3-C5	2.75	119.90	115.27
39	S	315	LUT	C22-C23-C24	2.75	114.87	111.74
28	A	406	BCR	C33-C5-C6	-2.75	121.44	124.53
28	a	407	BCR	C33-C5-C6	-2.75	121.44	124.53
24	N	608	CHL	CHD-C1D-ND	-2.75	121.93	124.45
25	N	611	CLA	C4-C3-C5	2.75	119.89	115.27
25	N	603	CLA	C4-C3-C5	2.75	119.89	115.27
25	6	604	CLA	C4-C3-C5	2.75	119.89	115.27
24	G	605	CHL	CHD-C1D-ND	-2.75	121.93	124.45
24	g	605	CHL	CHD-C1D-ND	-2.75	121.93	124.45
25	Y	303	CLA	C3D-C2D-C1D	2.74	109.58	105.83
25	n	603	CLA	C4-C3-C5	2.74	119.89	115.27
25	A	401	CLA	C4A-NA-C1A	-2.74	105.47	106.71
35	C	515	DGD	C1D-O6D-C5D	-2.74	108.31	113.69
24	Y	302	CHL	C1-C2-C3	2.74	130.79	126.04
24	y	302	CHL	C1-C2-C3	2.74	130.79	126.04
25	c	509	CLA	C4-C3-C5	2.74	119.88	115.27
24	G	601	CHL	O2A-CGA-CBA	2.74	120.51	111.91
24	g	601	CHL	O2A-CGA-CBA	2.74	120.51	111.91
24	G	609	CHL	C1-C2-C3	2.74	130.78	126.04
24	Y	306	CHL	CHD-C1D-ND	-2.74	121.94	124.45
28	t	101	BCR	C33-C5-C6	-2.74	121.45	124.53
25	y	313	CLA	O1D-CGD-CBD	-2.74	118.88	124.48
25	n	611	CLA	C4-C3-C5	2.74	119.88	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	402	CLA	C4A-NA-C1A	-2.74	105.47	106.71
25	G	604	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
24	S	307	CHL	CMB-C2B-C1B	-2.74	124.25	128.46
24	s	307	CHL	CMB-C2B-C1B	-2.74	124.25	128.46
25	C	505	CLA	C4-C3-C5	2.74	119.88	115.27
25	R	608	CLA	O2A-CGA-CBA	2.74	120.50	111.91
25	B	605	CLA	C4-C3-C5	2.74	119.88	115.27
24	2	603	CHL	CHC-C1C-NC	2.74	128.36	124.20
25	N	604	CLA	CHD-C1D-C2D	2.74	131.22	125.48
25	b	609	CLA	C2A-C1A-CHA	-2.74	119.08	123.86
25	r	608	CLA	O2A-CGA-CBA	2.73	120.49	111.91
25	C	513	CLA	C4-C3-C5	2.73	119.87	115.27
24	N	607	CHL	CMB-C2B-C1B	-2.73	124.27	128.46
25	b	612	CLA	CHD-C1D-C2D	2.73	131.21	125.48
25	c	510	CLA	C4-C3-C5	2.73	119.86	115.27
28	Z	101	BCR	C24-C23-C22	-2.73	122.11	126.23
28	z	101	BCR	C24-C23-C22	-2.73	122.11	126.23
28	B	619	BCR	C33-C5-C6	-2.73	121.46	124.53
28	b	619	BCR	C33-C5-C6	-2.73	121.46	124.53
25	n	604	CLA	CHD-C1D-C2D	2.73	131.20	125.48
25	B	611	CLA	C4D-CHA-C1A	-2.73	117.93	121.25
28	A	406	BCR	C27-C26-C25	2.73	126.69	122.73
28	a	407	BCR	C27-C26-C25	2.73	126.69	122.73
25	B	602	CLA	C4-C3-C5	2.73	119.86	115.27
25	c	513	CLA	C4-C3-C5	2.73	119.86	115.27
25	C	510	CLA	C1D-ND-C4D	-2.73	104.40	106.33
25	c	510	CLA	C1D-ND-C4D	-2.73	104.40	106.33
25	C	510	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
25	c	510	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
25	N	613	CLA	CHD-C1D-C2D	2.72	131.19	125.48
28	K	101	BCR	C33-C5-C6	-2.72	121.47	124.53
28	k	101	BCR	C33-C5-C6	-2.72	121.47	124.53
25	C	509	CLA	C4-C3-C5	2.72	119.85	115.27
25	C	507	CLA	C3D-C2D-C1D	2.72	109.55	105.83
25	A	405	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
25	a	406	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
24	n	607	CHL	CMB-C2B-C1B	-2.72	124.28	128.46
24	6	601	CHL	C2A-C1A-CHA	2.72	128.62	123.86
25	B	609	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
25	R	614	CLA	O1D-CGD-CBD	-2.72	118.91	124.48
25	b	611	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
25	C	511	CLA	C1D-ND-C4D	-2.72	104.40	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	511	CLA	C1D-ND-C4D	-2.72	104.40	106.33
25	C	507	CLA	C4D-CHA-C1A	-2.72	117.94	121.25
24	y	309	CHL	CHD-C1D-ND	-2.72	121.95	124.45
25	r	614	CLA	O1D-CGD-CBD	-2.72	118.92	124.48
28	A	406	BCR	C11-C10-C9	-2.72	123.43	127.31
28	a	407	BCR	C11-C10-C9	-2.72	123.43	127.31
28	B	619	BCR	C24-C23-C22	-2.72	122.13	126.23
28	b	619	BCR	C24-C23-C22	-2.72	122.13	126.23
25	N	614	CLA	CBA-CAA-C2A	-2.72	105.84	113.86
25	B	611	CLA	C2A-C1A-CHA	-2.72	119.11	123.86
25	g	613	CLA	C1D-ND-C4D	-2.72	104.41	106.33
24	R	607	CHL	O2A-CGA-CBA	2.72	120.43	111.91
25	b	611	CLA	C4D-CHA-C1A	-2.72	117.94	121.25
25	R	602	CLA	CHD-C1D-C2D	2.72	131.18	125.48
25	s	311	CLA	C4-C3-C5	2.72	119.84	115.27
25	A	401	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
25	a	402	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
24	n	607	CHL	O2A-CGA-O1A	-2.72	116.74	123.59
26	s	318	LHG	O8-C23-C24	2.72	120.43	111.91
24	N	607	CHL	O2A-CGA-O1A	-2.71	116.74	123.59
25	B	613	CLA	O1D-CGD-CBD	-2.71	118.93	124.48
25	b	613	CLA	O1D-CGD-CBD	-2.71	118.93	124.48
25	2	604	CLA	C4-C3-C5	2.71	119.84	115.27
25	c	507	CLA	C3D-C2D-C1D	2.71	109.53	105.83
25	B	604	CLA	C4D-CHA-C1A	-2.71	117.95	121.25
25	b	604	CLA	C4D-CHA-C1A	-2.71	117.95	121.25
24	Y	310	CHL	CHD-C1D-ND	-2.71	121.96	124.45
26	S	318	LHG	O8-C23-C24	2.71	120.42	111.91
25	C	504	CLA	C4D-C3D-CAD	-2.71	104.90	108.10
25	c	504	CLA	C4D-C3D-CAD	-2.71	104.90	108.10
25	S	313	CLA	C4-C3-C5	2.71	119.83	115.27
25	s	313	CLA	C4-C3-C5	2.71	119.83	115.27
24	y	307	CHL	OMC-CMC-C2C	-2.71	119.56	125.69
24	Y	308	CHL	CMB-C2B-C1B	-2.71	124.30	128.46
25	r	602	CLA	CHD-C1D-C2D	2.71	131.16	125.48
40	g	617	NEX	C5-C4-C3	-2.71	108.54	111.75
25	Y	313	CLA	O1D-CGD-CBD	-2.71	118.94	124.48
28	I	101	BCR	C27-C26-C25	2.71	126.66	122.73
25	B	612	CLA	CHD-C1D-C2D	2.71	131.16	125.48
25	n	612	CLA	C1D-CHD-C4C	-2.71	120.22	126.06
24	Y	309	CHL	C2A-C1A-CHA	2.71	128.59	123.86
30	C	520	LMG	O8-C28-C29	2.71	120.40	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	315	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
25	b	602	CLA	C4-C3-C5	2.71	119.82	115.27
24	Y	310	CHL	C1-C2-C3	2.70	130.72	126.04
24	y	310	CHL	C1-C2-C3	2.70	130.72	126.04
25	S	311	CLA	C4-C3-C5	2.70	119.82	115.27
24	G	608	CHL	CHD-C1D-ND	-2.70	121.97	124.45
24	g	608	CHL	CHD-C1D-ND	-2.70	121.97	124.45
25	S	312	CLA	O2A-CGA-CBA	2.70	120.39	111.91
25	n	613	CLA	CHD-C1D-C2D	2.70	131.15	125.48
28	i	101	BCR	C27-C26-C25	2.70	126.66	122.73
25	n	614	CLA	CBA-CAA-C2A	-2.70	105.89	113.86
24	g	606	CHL	O2A-CGA-CBA	2.70	120.39	111.91
24	y	309	CHL	C2A-C1A-CHA	2.70	128.58	123.86
30	c	520	LMG	O8-C28-C29	2.70	120.38	111.91
25	g	604	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
26	2	606	LHG	P-O6-C4	-2.70	105.85	121.68
25	G	613	CLA	C1D-ND-C4D	-2.70	104.42	106.33
25	R	601	CLA	C3D-C4D-CHA	2.70	118.90	112.72
25	r	601	CLA	C3D-C4D-CHA	2.70	118.90	112.72
26	Y	301	LHG	O8-C23-C24	2.70	120.38	111.91
26	D	406	LHG	P-O6-C4	-2.70	105.86	121.68
26	d	406	LHG	P-O6-C4	-2.70	105.86	121.68
26	6	606	LHG	P-O6-C4	-2.70	105.86	121.68
24	r	607	CHL	O2A-CGA-CBA	2.70	120.38	111.91
25	C	510	CLA	C4-C3-C5	2.70	119.81	115.27
25	r	611	CLA	C3B-C4B-NB	-2.70	105.72	109.21
24	2	601	CHL	C2A-C1A-CHA	2.70	128.57	123.86
25	N	602	CLA	C3D-C2D-C1D	2.70	109.51	105.83
24	G	606	CHL	O2A-CGA-CBA	2.69	120.36	111.91
25	R	611	CLA	C3B-C4B-NB	-2.69	105.73	109.21
25	y	315	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
25	y	305	CLA	O1D-CGD-CBD	-2.69	118.97	124.48
26	y	301	LHG	O8-C23-C24	2.69	120.36	111.91
30	a	409	LMG	C1-O6-C5	-2.69	108.41	113.69
25	Y	305	CLA	O1D-CGD-CBD	-2.69	118.98	124.48
25	N	612	CLA	C1D-CHD-C4C	-2.69	120.25	126.06
28	Z	101	BCR	C28-C27-C26	-2.69	109.28	114.08
30	A	408	LMG	C1-O6-C5	-2.69	108.41	113.69
28	I	101	BCR	C33-C5-C6	-2.69	121.51	124.53
28	K	101	BCR	C27-C26-C25	2.69	126.63	122.73
25	C	512	CLA	O1D-CGD-CBD	-2.69	118.99	124.48
25	c	512	CLA	O1D-CGD-CBD	-2.69	118.99	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	303	CLA	CHD-C1D-C2D	2.68	131.11	125.48
24	y	310	CHL	CHD-C1D-ND	-2.68	121.99	124.45
25	s	312	CLA	O2A-CGA-CBA	2.68	120.32	111.91
25	C	504	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
40	g	617	NEX	C39-C29-C30	-2.68	119.17	122.92
25	B	602	CLA	CHD-C1D-C2D	2.68	131.10	125.48
25	b	602	CLA	CHD-C1D-C2D	2.68	131.10	125.48
25	S	313	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
25	s	313	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	y	308	CHL	CMB-C2B-C1B	-2.68	124.35	128.46
25	G	602	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
25	g	602	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
25	d	403	CLA	C4D-C3D-CAD	-2.68	104.94	108.10
28	H	101	BCR	C2-C1-C6	2.68	114.60	110.48
25	c	507	CLA	O2A-CGA-CBA	2.68	120.31	111.91
25	a	402	CLA	C4-C3-C5	2.68	119.77	115.27
25	c	511	CLA	C4-C3-C5	2.68	119.77	115.27
24	g	601	CHL	C1-C2-C3	2.67	130.67	126.04
28	H	101	BCR	C24-C23-C22	-2.67	122.20	126.23
25	A	401	CLA	C4-C3-C5	2.67	119.77	115.27
25	c	503	CLA	O1D-CGD-CBD	-2.67	119.02	124.48
24	y	309	CHL	CMB-C2B-C1B	-2.67	124.36	128.46
28	K	101	BCR	C2-C1-C6	2.67	114.59	110.48
28	k	101	BCR	C2-C1-C6	2.67	114.59	110.48
40	N	617	NEX	C28-C29-C30	2.67	123.04	118.94
25	b	615	CLA	C4D-CHA-C1A	-2.67	118.00	121.25
25	b	603	CLA	CHD-C1D-C2D	2.67	131.08	125.48
25	n	602	CLA	C3D-C2D-C1D	2.67	109.47	105.83
40	n	617	NEX	C28-C29-C30	2.67	123.03	118.94
41	r	616	XAT	C20-C13-C14	-2.66	119.19	122.92
28	k	101	BCR	C27-C26-C25	2.66	126.60	122.73
25	C	507	CLA	O2A-CGA-CBA	2.66	120.27	111.91
28	z	101	BCR	C28-C27-C26	-2.66	109.32	114.08
24	Y	307	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
25	C	511	CLA	C4-C3-C5	2.66	119.75	115.27
28	h	101	BCR	C24-C23-C22	-2.66	122.22	126.23
25	C	501	CLA	C4-C3-C5	2.66	119.75	115.27
28	h	101	BCR	C2-C1-C6	2.66	114.58	110.48
25	6	602	CLA	C3D-C4D-CHA	2.66	118.81	112.72
25	Y	304	CLA	C4-C3-C5	2.66	119.74	115.27
27	A	403	PHO	C4-C3-C5	2.66	119.74	115.27
27	a	404	PHO	C4-C3-C5	2.66	119.74	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	607	CHL	CMB-C2B-C1B	-2.66	124.38	128.46
24	r	607	CHL	CMB-C2B-C1B	-2.66	124.38	128.46
25	y	304	CLA	C4-C3-C5	2.66	119.74	115.27
25	g	602	CLA	C1-C2-C3	-2.66	121.45	126.04
25	S	303	CLA	C4-C3-C5	2.66	119.74	115.27
28	B	618	BCR	C33-C5-C6	-2.66	121.55	124.53
28	b	618	BCR	C33-C5-C6	-2.66	121.55	124.53
25	6	602	CLA	O1D-CGD-CBD	-2.66	119.05	124.48
24	1	302	CHL	CMB-C2B-C1B	-2.66	124.38	128.46
25	y	312	CLA	O2A-CGA-CBA	2.66	120.24	111.91
25	G	602	CLA	C3D-C2D-C1D	2.65	109.45	105.83
25	g	602	CLA	C3D-C2D-C1D	2.65	109.45	105.83
25	C	506	CLA	O2A-CGA-CBA	2.65	120.23	111.91
25	c	506	CLA	O2A-CGA-CBA	2.65	120.23	111.91
25	S	303	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
25	c	504	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
25	2	604	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
25	6	604	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
25	s	303	CLA	CHD-C1D-C2D	2.65	131.04	125.48
28	D	404	BCR	C28-C27-C26	-2.65	109.34	114.08
25	2	602	CLA	C3D-C4D-CHA	2.65	118.79	112.72
25	s	303	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
25	n	603	CLA	CHD-C1D-C2D	2.65	131.04	125.48
24	G	601	CHL	C1-C2-C3	2.65	130.62	126.04
41	R	616	XAT	C20-C13-C14	-2.65	119.21	122.92
25	S	311	CLA	C4D-CHA-C1A	-2.65	118.03	121.25
25	s	311	CLA	C4D-CHA-C1A	-2.65	118.03	121.25
27	A	403	PHO	O2A-CGA-CBA	2.65	120.22	111.91
25	Y	313	CLA	O2A-CGA-CBA	2.65	120.21	111.91
25	C	510	CLA	O2A-CGA-CBA	2.65	120.21	111.91
24	5	302	CHL	CMB-C2B-C1B	-2.64	124.40	128.46
25	c	510	CLA	O2A-CGA-CBA	2.64	120.21	111.91
25	2	602	CLA	O1D-CGD-CBD	-2.64	119.07	124.48
24	Y	309	CHL	CMB-C2B-C1B	-2.64	124.40	128.46
25	B	615	CLA	C4D-CHA-C1A	-2.64	118.03	121.25
27	a	404	PHO	O2A-CGA-CBA	2.64	120.20	111.91
25	N	603	CLA	CHD-C1D-C2D	2.64	131.02	125.48
25	D	403	CLA	C4D-C3D-CAD	-2.64	104.98	108.10
25	B	606	CLA	C4-C3-C5	2.64	119.72	115.27
25	b	606	CLA	C4-C3-C5	2.64	119.72	115.27
25	c	501	CLA	C4-C3-C5	2.64	119.72	115.27
26	S	318	LHG	P-O6-C4	-2.64	106.19	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	613	CLA	C4-C3-C5	2.64	119.71	115.27
26	Y	301	LHG	P-O3-C3	-2.64	106.20	121.68
26	y	301	LHG	P-O3-C3	-2.64	106.20	121.68
25	B	603	CLA	CHD-C1D-C2D	2.64	131.02	125.48
40	N	617	NEX	C2-C1-C6	2.64	111.78	109.21
25	N	604	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
25	Y	312	CLA	O2A-CGA-CBA	2.64	120.18	111.91
25	s	303	CLA	C4-C3-C5	2.64	119.70	115.27
25	n	613	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
25	c	508	CLA	C1D-ND-C4D	-2.63	104.46	106.33
24	n	607	CHL	CAA-C2A-C3A	-2.63	105.57	112.78
26	s	318	LHG	P-O6-C4	-2.63	106.24	121.68
26	B	625	LHG	P-O6-C4	-2.63	106.24	121.68
39	G	615	LUT	C35-C15-C14	-2.63	118.08	123.47
39	g	615	LUT	C35-C15-C14	-2.63	118.08	123.47
25	b	606	CLA	O2A-CGA-CBA	2.63	120.16	111.91
25	B	613	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
25	b	613	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
25	G	602	CLA	C1-C2-C3	-2.63	121.49	126.04
25	n	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	C	518	LHG	O8-C23-C24	2.63	120.16	111.91
25	G	613	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
25	N	613	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
28	B	618	BCR	C15-C16-C17	-2.63	118.09	123.47
28	b	618	BCR	C15-C16-C17	-2.63	118.09	123.47
39	r	615	LUT	C1-C2-C3	2.63	119.58	113.64
24	N	607	CHL	CAA-C2A-C3A	-2.63	105.59	112.78
25	c	512	CLA	C4-C3-C5	2.62	119.69	115.27
26	b	625	LHG	P-O6-C4	-2.62	106.30	121.68
28	A	406	BCR	C24-C23-C22	-2.62	122.27	126.23
28	a	407	BCR	C24-C23-C22	-2.62	122.27	126.23
28	d	404	BCR	C28-C27-C26	-2.62	109.39	114.08
25	C	503	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
24	y	310	CHL	C2A-C1A-CHA	2.62	128.44	123.86
29	l	101	SQD	O7-S-C6	2.62	110.06	106.94
25	R	610	CLA	C3D-C4D-CHA	2.62	118.72	112.72
25	C	501	CLA	O2A-CGA-CBA	2.62	120.13	111.91
25	b	611	CLA	C4-C3-C5	2.62	119.68	115.27
25	C	509	CLA	CHD-C1D-C2D	2.62	130.98	125.48
25	A	405	CLA	C4D-CHA-C1A	-2.62	118.06	121.25
25	a	406	CLA	C4D-CHA-C1A	-2.62	118.06	121.25
25	B	606	CLA	O2A-CGA-CBA	2.62	120.13	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	g	612	CLA	O2A-CGA-CBA	2.62	120.13	111.91
25	r	609	CLA	O2A-CGA-CBA	2.62	120.13	111.91
28	k	101	BCR	C24-C23-C22	-2.62	122.28	126.23
39	R	615	LUT	C1-C2-C3	2.62	119.55	113.64
25	c	509	CLA	CHD-C1D-C2D	2.62	130.97	125.48
25	r	614	CLA	C4A-NA-C1A	-2.62	105.53	106.71
25	y	313	CLA	O2A-CGA-CBA	2.62	120.12	111.91
25	A	402	CLA	O2A-CGA-CBA	2.62	120.11	111.91
24	g	607	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
25	a	403	CLA	O2A-CGA-CBA	2.61	120.11	111.91
26	c	518	LHG	O8-C23-C24	2.61	120.11	111.91
25	S	310	CLA	C1D-CHD-C4C	-2.61	120.42	126.06
25	R	609	CLA	O2A-CGA-CBA	2.61	120.11	111.91
28	i	101	BCR	C33-C5-C6	-2.61	121.59	124.53
40	n	617	NEX	C2-C1-C6	2.61	111.75	109.21
24	Y	310	CHL	CMB-C2B-C1B	-2.61	124.45	128.46
40	G	617	NEX	C39-C29-C30	-2.61	119.27	122.92
25	g	613	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	c	504	CLA	C2A-C3A-C4A	-2.61	97.65	101.87
25	c	501	CLA	C4D-C3D-CAD	-2.61	105.02	108.10
25	B	616	CLA	C4-C3-C5	2.61	119.66	115.27
25	b	616	CLA	C4-C3-C5	2.61	119.66	115.27
25	Y	314	CLA	CHD-C1D-C2D	2.61	130.95	125.48
25	y	314	CLA	CHD-C1D-C2D	2.61	130.95	125.48
25	G	613	CLA	C4-C3-C5	2.61	119.66	115.27
29	L	103	SQD	O7-S-C6	2.61	110.04	106.94
28	k	101	BCR	C15-C14-C13	-2.61	123.59	127.31
24	n	609	CHL	C4D-CHA-C1A	2.61	124.42	121.25
26	L	102	LHG	O8-C23-C24	2.61	120.09	111.91
26	l	103	LHG	O8-C23-C24	2.61	120.09	111.91
25	G	612	CLA	O2A-CGA-CBA	2.61	120.08	111.91
40	g	617	NEX	C20-C13-C12	2.60	122.18	118.08
25	r	608	CLA	C4-C3-C5	2.60	119.65	115.27
24	g	609	CHL	CHD-C1D-ND	-2.60	122.06	124.45
25	B	611	CLA	C4-C3-C5	2.60	119.65	115.27
25	C	512	CLA	C4-C3-C5	2.60	119.65	115.27
40	G	617	NEX	C10-C11-C12	2.60	131.34	123.22
25	R	608	CLA	C4-C3-C5	2.60	119.65	115.27
25	c	501	CLA	O2A-CGA-CBA	2.60	120.07	111.91
28	K	101	BCR	C24-C23-C22	-2.60	122.31	126.23
24	N	605	CHL	CMB-C2B-C1B	-2.60	124.47	128.46
24	n	605	CHL	CMB-C2B-C1B	-2.60	124.47	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	603	CHL	CAA-C2A-C3A	-2.60	105.66	112.78
24	6	603	CHL	CAA-C2A-C3A	-2.60	105.66	112.78
28	K	101	BCR	C15-C14-C13	-2.60	123.60	127.31
25	R	611	CLA	C2C-C1C-NC	-2.60	107.54	109.97
26	n	618	LHG	P-O6-C4	-2.60	106.45	121.68
25	r	611	CLA	CAD-C3D-C2D	2.60	153.33	140.80
26	Y	319	LHG	P-O3-C3	-2.60	106.46	121.68
26	y	319	LHG	P-O3-C3	-2.60	106.46	121.68
25	a	406	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
24	2	603	CHL	CMB-C2B-C1B	-2.60	124.47	128.46
24	6	603	CHL	CMB-C2B-C1B	-2.60	124.47	128.46
25	s	310	CLA	C3D-C2D-C1D	2.59	109.37	105.83
25	C	504	CLA	C2A-C3A-C4A	-2.59	97.68	101.87
25	B	614	CLA	CHD-C1D-C2D	2.59	130.92	125.48
25	b	614	CLA	CHD-C1D-C2D	2.59	130.92	125.48
24	y	310	CHL	CMB-C2B-C1B	-2.59	124.48	128.46
24	G	608	CHL	CMB-C2B-C1B	-2.59	124.48	128.46
25	G	614	CLA	O2A-CGA-CBA	2.59	120.04	111.91
25	g	614	CLA	O2A-CGA-CBA	2.59	120.04	111.91
24	Y	310	CHL	C2A-C1A-CHA	2.59	128.39	123.86
25	r	610	CLA	C3D-C4D-CHA	2.59	118.65	112.72
25	B	612	CLA	C4-C3-C5	2.59	119.63	115.27
25	b	612	CLA	C4-C3-C5	2.59	119.63	115.27
25	s	310	CLA	C1D-CHD-C4C	-2.59	120.47	126.06
24	G	605	CHL	OMC-CMC-C2C	-2.59	119.83	125.69
25	R	611	CLA	CAD-C3D-C2D	2.59	153.30	140.80
24	N	609	CHL	CMB-C2B-C1B	-2.59	124.48	128.46
26	N	618	LHG	P-O6-C4	-2.59	106.50	121.68
26	b	621	LHG	P-O3-C3	-2.59	106.50	121.68
26	B	621	LHG	P-O3-C3	-2.59	106.50	121.68
26	n	618	LHG	O8-C23-C24	2.59	120.03	111.91
25	C	512	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
35	B	626	DGD	O1G-C1A-C2A	2.59	120.03	111.91
26	C	518	LHG	P-O3-C3	-2.59	106.51	121.68
24	N	609	CHL	C4D-CHA-C1A	2.59	124.40	121.25
26	c	518	LHG	P-O3-C3	-2.59	106.52	121.68
25	c	512	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
24	1	301	CHL	CMB-C2B-C1B	-2.58	124.49	128.46
25	R	602	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
25	r	602	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
28	I	101	BCR	C15-C14-C13	-2.58	123.62	127.31
25	C	511	CLA	C4D-CHA-C1A	-2.58	118.11	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	605	CHL	C2A-C1A-CHA	2.58	128.38	123.86
28	B	618	BCR	C15-C14-C13	-2.58	123.62	127.31
28	b	618	BCR	C15-C14-C13	-2.58	123.62	127.31
24	g	608	CHL	CMB-C2B-C1B	-2.58	124.50	128.46
28	Z	101	BCR	C33-C5-C6	-2.58	121.63	124.53
40	N	617	NEX	C40-C33-C34	-2.58	119.31	122.92
25	C	508	CLA	C1D-ND-C4D	-2.58	104.50	106.33
24	R	605	CHL	CMB-C2B-C1B	-2.58	124.50	128.46
25	N	614	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
35	c	516	DGD	O1G-C1A-C2A	2.58	120.00	111.91
35	b	626	DGD	O1G-C1A-C2A	2.58	120.00	111.91
24	G	605	CHL	CMB-C2B-C1B	-2.58	124.50	128.46
25	C	502	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
25	B	610	CLA	C4D-CHA-C1A	-2.58	118.11	121.25
25	b	610	CLA	C4D-CHA-C1A	-2.58	118.11	121.25
24	Y	310	CHL	O2A-CGA-CBA	2.57	119.98	111.91
24	y	310	CHL	O2A-CGA-CBA	2.57	119.98	111.91
26	s	301	LHG	P-O6-C4	-2.57	106.59	121.68
24	n	609	CHL	CMB-C2B-C1B	-2.57	124.51	128.46
25	c	511	CLA	C4D-CHA-C1A	-2.57	118.12	121.25
26	2	606	LHG	O8-C23-C24	2.57	119.98	111.91
25	B	610	CLA	O1D-CGD-CBD	-2.57	119.22	124.48
25	b	610	CLA	O1D-CGD-CBD	-2.57	119.22	124.48
24	G	607	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
28	z	101	BCR	C33-C5-C6	-2.57	121.64	124.53
25	C	501	CLA	C4D-C3D-CAD	-2.57	105.07	108.10
24	g	605	CHL	OMC-CMC-C2C	-2.57	119.88	125.69
25	2	605	CLA	O2A-CGA-CBA	2.57	119.97	111.91
25	6	605	CLA	O2A-CGA-CBA	2.57	119.97	111.91
25	r	611	CLA	C2C-C1C-NC	-2.57	107.56	109.97
24	r	605	CHL	CMB-C2B-C1B	-2.57	124.52	128.46
25	n	603	CLA	O2A-CGA-CBA	2.57	119.97	111.91
26	N	618	LHG	O8-C23-C24	2.57	119.97	111.91
35	C	516	DGD	O1G-C1A-C2A	2.57	119.96	111.91
26	B	622	LHG	P-O6-C4	-2.57	106.63	121.68
26	b	622	LHG	P-O6-C4	-2.57	106.63	121.68
28	i	101	BCR	C15-C14-C13	-2.57	123.65	127.31
26	l	103	LHG	P-O6-C4	-2.57	106.64	121.68
24	5	301	CHL	CMB-C2B-C1B	-2.57	124.52	128.46
25	y	312	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
24	S	306	CHL	CMB-C2B-C1B	-2.56	124.52	128.46
24	s	306	CHL	CMB-C2B-C1B	-2.56	124.52	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	301	LHG	P-O3-C3	-2.56	106.64	121.68
26	s	301	LHG	P-O3-C3	-2.56	106.64	121.68
39	N	616	LUT	C2-C3-C4	2.56	113.81	110.30
24	n	608	CHL	C2A-C1A-CHA	2.56	128.34	123.86
26	S	301	LHG	P-O6-C4	-2.56	106.65	121.68
24	6	601	CHL	CMB-C2B-C1B	-2.56	124.52	128.46
24	n	601	CHL	C4D-CHA-C1A	2.56	124.37	121.25
26	L	102	LHG	P-O6-C4	-2.56	106.66	121.68
25	b	609	CLA	O1D-CGD-CBD	-2.56	119.24	124.48
25	n	614	CLA	O1D-CGD-CBD	-2.56	119.24	124.48
25	A	405	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
24	S	308	CHL	CMB-C2B-C1B	-2.56	124.53	128.46
24	g	601	CHL	CMB-C2B-C1B	-2.56	124.53	128.46
24	s	308	CHL	CMB-C2B-C1B	-2.56	124.53	128.46
25	c	502	CLA	O1D-CGD-CBD	-2.56	119.25	124.48
25	Y	304	CLA	CHD-C1D-C2D	2.56	130.85	125.48
24	2	601	CHL	CMB-C2B-C1B	-2.56	124.53	128.46
24	G	605	CHL	C2A-C1A-CHA	2.56	128.33	123.86
25	6	602	CLA	C4-C3-C5	2.56	119.57	115.27
26	d	406	LHG	O8-C23-C24	2.56	119.93	111.91
25	b	612	CLA	O2A-CGA-CBA	2.56	119.93	111.91
24	G	608	CHL	C2A-C1A-CHA	2.56	128.33	123.86
25	N	603	CLA	O2A-CGA-CBA	2.56	119.93	111.91
24	g	608	CHL	C2A-C1A-CHA	2.56	128.33	123.86
26	D	406	LHG	O8-C23-C24	2.56	119.93	111.91
25	2	602	CLA	C4-C3-C5	2.55	119.57	115.27
24	N	608	CHL	C2A-C1A-CHA	2.55	128.32	123.86
25	s	303	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
26	6	606	LHG	O8-C23-C24	2.55	119.92	111.91
25	S	310	CLA	C3D-C2D-C1D	2.55	109.31	105.83
26	b	621	LHG	P-O6-C4	-2.55	106.71	121.68
24	N	607	CHL	OMC-CMC-C2C	-2.55	119.92	125.69
25	B	608	CLA	CHD-C1D-C2D	2.55	130.83	125.48
39	n	616	LUT	C2-C3-C4	2.55	113.80	110.30
25	B	609	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
25	B	602	CLA	O2A-CGA-CBA	2.55	119.92	111.91
24	G	601	CHL	CMB-C2B-C1B	-2.55	124.54	128.46
24	g	605	CHL	CMB-C2B-C1B	-2.55	124.54	128.46
25	B	612	CLA	O2A-CGA-CBA	2.55	119.91	111.91
25	c	512	CLA	C4A-NA-C1A	-2.55	105.56	106.71
25	b	608	CLA	CHD-C1D-C2D	2.55	130.83	125.48
24	n	607	CHL	OMC-CMC-C2C	-2.55	119.92	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	602	CLA	O2A-CGA-CBA	2.55	119.91	111.91
25	y	304	CLA	CHD-C1D-C2D	2.55	130.82	125.48
25	C	503	CLA	C4-C3-C5	2.55	119.56	115.27
25	c	503	CLA	C4-C3-C5	2.55	119.56	115.27
25	r	601	CLA	O2A-CGA-CBA	2.54	119.89	111.91
25	Y	312	CLA	O1D-CGD-CBD	-2.54	119.28	124.48
24	S	302	CHL	CMB-C2B-C1B	-2.54	124.56	128.46
24	R	613	CHL	CMB-C2B-C1B	-2.54	124.56	128.46
26	B	621	LHG	P-O6-C4	-2.54	106.77	121.68
25	N	603	CLA	C4D-CHA-C1A	-2.54	118.15	121.25
25	n	603	CLA	C4D-CHA-C1A	-2.54	118.15	121.25
24	N	601	CHL	C2C-C3C-C4C	2.54	108.30	106.49
25	C	502	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
25	g	604	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
28	I	101	BCR	C11-C10-C9	-2.54	123.69	127.31
28	i	101	BCR	C11-C10-C9	-2.54	123.69	127.31
25	R	612	CLA	C2D-C1D-ND	-2.54	108.23	110.10
25	r	612	CLA	C2D-C1D-ND	-2.54	108.23	110.10
40	N	617	NEX	C10-C11-C12	2.54	131.14	123.22
25	a	402	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
25	s	310	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
30	A	408	LMG	O8-C28-C29	2.54	119.87	111.91
40	n	617	NEX	C10-C11-C12	2.54	131.14	123.22
40	n	617	NEX	C40-C33-C34	-2.54	119.37	122.92
25	S	303	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
25	Y	313	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
24	g	609	CHL	CMB-C2B-C1B	-2.54	124.57	128.46
25	C	512	CLA	C4A-NA-C1A	-2.54	105.57	106.71
30	A	410	LMG	O8-C28-C29	2.53	119.86	111.91
30	a	411	LMG	O8-C28-C29	2.53	119.86	111.91
24	n	601	CHL	C2C-C3C-C4C	2.53	108.30	106.49
25	G	613	CLA	O2A-CGA-CBA	2.53	119.86	111.91
25	R	601	CLA	O2A-CGA-CBA	2.53	119.86	111.91
25	c	505	CLA	CHD-C1D-C2D	2.53	130.79	125.48
30	a	409	LMG	O8-C28-C29	2.53	119.85	111.91
24	G	609	CHL	CHD-C1D-ND	-2.53	122.13	124.45
38	f	101	HEM	CHA-C4D-ND	2.53	127.51	124.38
25	S	305	CLA	C3D-C4D-CHA	2.53	118.51	112.72
26	B	625	LHG	O8-C23-C24	2.53	119.84	111.91
26	b	625	LHG	O8-C23-C24	2.53	119.84	111.91
24	R	607	CHL	C2A-C3A-C4A	2.53	105.95	101.87
25	y	313	CLA	O2D-CGD-O1D	-2.53	118.90	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	613	CHL	CMB-C2B-C1B	-2.53	124.58	128.46
25	n	602	CLA	C4-C3-C5	2.52	119.52	115.27
25	R	614	CLA	C4A-NA-C1A	-2.52	105.57	106.71
25	G	604	CLA	O1D-CGD-CBD	-2.52	119.32	124.48
25	D	402	CLA	C4-C3-C5	2.52	119.52	115.27
25	S	310	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
25	G	603	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
26	c	519	LHG	P-O3-C3	-2.52	106.89	121.68
28	H	101	BCR	C33-C5-C6	-2.52	121.69	124.53
28	h	101	BCR	C33-C5-C6	-2.52	121.69	124.53
30	d	407	LMG	O8-C28-C29	2.52	119.82	111.91
24	Y	306	CHL	CMB-C2B-C1B	-2.52	124.59	128.46
26	2	606	LHG	P-O3-C3	-2.52	106.89	121.68
26	S	318	LHG	P-O3-C3	-2.52	106.90	121.68
26	s	318	LHG	P-O3-C3	-2.52	106.90	121.68
25	c	502	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
26	6	606	LHG	P-O3-C3	-2.52	106.90	121.68
26	C	517	LHG	P-O6-C4	-2.52	106.91	121.68
24	G	609	CHL	CMB-C2B-C1B	-2.52	124.59	128.46
24	N	601	CHL	C4D-CHA-C1A	2.52	124.31	121.25
25	R	609	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
25	r	609	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
26	C	519	LHG	P-O3-C3	-2.52	106.92	121.68
26	c	517	LHG	P-O6-C4	-2.52	106.92	121.68
25	d	402	CLA	C4-C3-C5	2.52	119.50	115.27
26	c	517	LHG	P-O3-C3	-2.52	106.93	121.68
24	s	302	CHL	CMB-C2B-C1B	-2.52	124.60	128.46
25	N	602	CLA	C4-C3-C5	2.52	119.50	115.27
25	s	305	CLA	C3D-C4D-CHA	2.52	118.48	112.72
30	D	407	LMG	O8-C28-C29	2.51	119.80	111.91
25	A	401	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
40	y	318	NEX	C30-C31-C32	2.51	131.06	123.22
24	r	607	CHL	C2A-C3A-C4A	2.51	105.93	101.87
26	C	517	LHG	P-O3-C3	-2.51	106.94	121.68
25	B	606	CLA	C1D-ND-C4D	-2.51	104.55	106.33
25	b	606	CLA	C1D-ND-C4D	-2.51	104.55	106.33
26	B	625	LHG	P-O3-C3	-2.51	106.95	121.68
26	b	625	LHG	P-O3-C3	-2.51	106.95	121.68
26	d	406	LHG	P-O3-C3	-2.51	106.95	121.68
40	Y	318	NEX	C30-C31-C32	2.51	131.05	123.22
39	g	616	LUT	C3-C4-C5	2.51	116.85	111.85
25	R	601	CLA	O2D-CGD-O1D	-2.51	118.93	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	406	LHG	P-O3-C3	-2.51	106.97	121.68
24	n	606	CHL	CMB-C2B-C1B	-2.51	124.61	128.46
30	B	620	LMG	O8-C28-C29	2.51	119.78	111.91
25	R	609	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
24	N	606	CHL	CMB-C2B-C1B	-2.51	124.61	128.46
25	C	505	CLA	CHD-C1D-C2D	2.51	130.74	125.48
25	g	613	CLA	O2A-CGA-CBA	2.51	119.77	111.91
25	r	609	CLA	O1D-CGD-CBD	-2.50	119.36	124.48
25	g	603	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
26	B	622	LHG	P-O3-C3	-2.50	107.00	121.68
26	b	622	LHG	P-O3-C3	-2.50	107.00	121.68
30	b	620	LMG	O8-C28-C29	2.50	119.76	111.91
25	D	401	CLA	O2A-CGA-CBA	2.50	119.76	111.91
25	d	401	CLA	O2A-CGA-CBA	2.50	119.76	111.91
25	r	601	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
24	R	605	CHL	C2A-C3A-C4A	2.50	105.91	101.87
26	C	517	LHG	O8-C23-C24	2.50	119.75	111.91
26	c	517	LHG	O8-C23-C24	2.50	119.75	111.91
24	y	306	CHL	CMB-C2B-C1B	-2.50	124.62	128.46
25	n	611	CLA	O2A-CGA-CBA	2.50	119.75	111.91
40	y	318	NEX	C24-C23-C22	-2.50	105.94	110.77
26	C	518	LHG	P-O6-C4	-2.50	107.02	121.68
26	c	518	LHG	P-O6-C4	-2.50	107.02	121.68
28	B	617	BCR	C28-C27-C26	-2.50	109.61	114.08
28	b	617	BCR	C28-C27-C26	-2.50	109.61	114.08
25	R	611	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
25	r	611	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
26	N	618	LHG	P-O3-C3	-2.50	107.04	121.68
26	b	621	LHG	O8-C23-C24	2.50	119.74	111.91
24	r	605	CHL	C2A-C3A-C4A	2.50	105.90	101.87
26	n	618	LHG	P-O3-C3	-2.50	107.05	121.68
24	n	601	CHL	CMB-C2B-C1B	-2.50	124.63	128.46
39	G	616	LUT	C3-C4-C5	2.49	116.82	111.85
25	n	611	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
40	n	617	NEX	C26-C27-C28	-2.49	120.72	125.99
26	C	519	LHG	O8-C23-C24	2.49	119.73	111.91
26	c	519	LHG	O8-C23-C24	2.49	119.73	111.91
25	N	611	CLA	O2A-CGA-CBA	2.49	119.73	111.91
25	C	510	CLA	O1D-CGD-CBD	-2.49	119.38	124.48
25	c	510	CLA	O1D-CGD-CBD	-2.49	119.38	124.48
25	N	612	CLA	O2A-CGA-CBA	2.49	119.73	111.91
25	2	602	CLA	O2A-CGA-CBA	2.49	119.73	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	602	CLA	O2A-CGA-CBA	2.49	119.73	111.91
25	R	608	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
25	r	608	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
28	C	514	BCR	C15-C16-C17	-2.49	118.37	123.47
28	c	514	BCR	C15-C16-C17	-2.49	118.37	123.47
39	S	315	LUT	C1-C2-C3	2.49	119.27	113.64
25	S	312	CLA	C4D-CHA-C1A	-2.49	118.22	121.25
25	s	312	CLA	C4D-CHA-C1A	-2.49	118.22	121.25
28	T	101	BCR	C27-C26-C25	2.49	126.35	122.73
28	t	101	BCR	C27-C26-C25	2.49	126.35	122.73
40	Y	318	NEX	C24-C23-C22	-2.49	105.97	110.77
25	s	314	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
25	R	611	CLA	O2A-CGA-CBA	2.49	119.72	111.91
25	B	609	CLA	CHD-C1D-C2D	2.49	130.70	125.48
25	S	311	CLA	O2A-CGA-CBA	2.49	119.72	111.91
26	B	621	LHG	O8-C23-C24	2.49	119.72	111.91
28	B	619	BCR	C2-C1-C6	2.49	114.31	110.48
28	b	619	BCR	C2-C1-C6	2.49	114.31	110.48
25	N	611	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
25	r	611	CLA	O2A-CGA-CBA	2.49	119.71	111.91
39	s	315	LUT	C1-C2-C3	2.49	119.26	113.64
26	L	102	LHG	P-O3-C3	-2.49	107.10	121.68
39	G	615	LUT	C1-C2-C3	2.49	119.26	113.64
26	l	103	LHG	P-O3-C3	-2.49	107.11	121.68
25	r	604	CLA	O1D-CGD-CBD	-2.48	119.40	124.48
25	S	312	CLA	CHB-C4A-NA	-2.48	121.08	124.51
24	2	603	CHL	CHD-C1D-C2D	2.48	130.69	125.48
24	6	603	CHL	CHD-C1D-C2D	2.48	130.69	125.48
25	C	509	CLA	O2A-CGA-CBA	2.48	119.69	111.91
25	s	311	CLA	O2A-CGA-CBA	2.48	119.69	111.91
25	C	512	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
25	c	512	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
25	N	603	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
25	C	503	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
25	g	604	CLA	C5-C3-C4	2.48	120.08	114.60
24	N	601	CHL	CMB-C2B-C1B	-2.48	124.65	128.46
25	R	604	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
24	S	308	CHL	C2A-C3A-C4A	2.48	105.87	101.87
24	s	308	CHL	C2A-C3A-C4A	2.48	105.87	101.87
25	r	614	CLA	C4D-CHA-C1A	-2.48	118.23	121.25
25	C	510	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
25	c	510	CLA	O2D-CGD-O1D	-2.48	119.00	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	614	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
25	B	602	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
25	b	602	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
25	R	609	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
25	s	312	CLA	CHB-C4A-NA	-2.48	121.09	124.51
39	g	615	LUT	C1-C2-C3	2.48	119.23	113.64
25	n	612	CLA	O2A-CGA-CBA	2.47	119.67	111.91
25	c	509	CLA	O2A-CGA-CBA	2.47	119.67	111.91
40	N	617	NEX	C26-C27-C28	-2.47	120.76	125.99
38	F	101	HEM	CHA-C4D-ND	2.47	127.44	124.38
25	G	604	CLA	C5-C3-C4	2.47	120.07	114.60
25	R	604	CLA	CAA-CBA-CGA	-2.47	106.03	113.25
25	r	604	CLA	CAA-CBA-CGA	-2.47	106.03	113.25
24	G	606	CHL	C2C-C3C-C4C	2.47	108.25	106.49
25	b	609	CLA	CHD-C1D-C2D	2.47	130.66	125.48
30	B	623	LMG	O8-C28-C29	2.47	119.66	111.91
30	b	623	LMG	O8-C28-C29	2.47	119.66	111.91
25	G	612	CLA	C4D-CHA-C1A	-2.47	118.24	121.25
39	n	616	LUT	C11-C10-C9	-2.47	123.79	127.31
26	y	319	LHG	O8-C23-C24	2.46	119.64	111.91
25	n	603	CLA	O1D-CGD-CBD	-2.46	119.44	124.48
25	2	605	CLA	CHD-C1D-C2D	2.46	130.65	125.48
40	Y	318	NEX	C19-C9-C10	-2.46	119.47	122.92
26	r	618	LHG	P-O3-C3	-2.46	107.24	121.68
24	G	609	CHL	OMC-CMC-C2C	-2.46	120.12	125.69
25	B	615	CLA	C4-C3-C5	2.46	119.41	115.27
25	b	615	CLA	C4-C3-C5	2.46	119.41	115.27
25	r	608	CLA	C2A-C3A-C4A	-2.46	97.89	101.87
25	y	304	CLA	O2A-CGA-CBA	2.46	119.63	111.91
24	y	302	CHL	CMB-C2B-C1B	-2.46	124.68	128.46
25	g	611	CLA	CHD-C1D-C2D	2.46	130.64	125.48
27	A	404	PHO	O2A-CGA-CBA	2.46	119.62	111.91
27	a	405	PHO	O2A-CGA-CBA	2.46	119.62	111.91
25	r	601	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
25	r	609	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
26	R	618	LHG	O8-C23-C24	2.46	119.62	111.91
39	y	316	LUT	C1-C2-C3	2.46	119.19	113.64
26	Y	319	LHG	O8-C23-C24	2.46	119.62	111.91
25	Y	304	CLA	O2A-CGA-CBA	2.46	119.62	111.91
24	y	306	CHL	OMC-CMC-C2C	-2.46	120.13	125.69
39	Y	316	LUT	C1-C2-C3	2.46	119.19	113.64
25	D	403	CLA	O1D-CGD-CBD	-2.45	119.46	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	S	317	NEX	C1-C2-C3	-2.45	108.10	113.64
25	6	605	CLA	CHD-C1D-C2D	2.45	130.63	125.48
25	S	314	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
28	A	406	BCR	C15-C16-C17	-2.45	118.45	123.47
28	a	407	BCR	C15-C16-C17	-2.45	118.45	123.47
24	N	606	CHL	OMC-CMC-C2C	-2.45	120.14	125.69
25	c	503	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
40	y	318	NEX	C19-C9-C10	-2.45	119.49	122.92
26	R	618	LHG	P-O3-C3	-2.45	107.31	121.68
25	A	402	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
25	a	403	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
25	B	601	CLA	O2A-CGA-CBA	2.45	119.60	111.91
25	b	601	CLA	O2A-CGA-CBA	2.45	119.60	111.91
28	A	406	BCR	C2-C1-C6	2.45	114.25	110.48
28	a	407	BCR	C2-C1-C6	2.45	114.25	110.48
25	g	611	CLA	CMD-C2D-C1D	-2.45	120.40	124.71
40	R	617	NEX	C1-C2-C3	-2.45	108.11	113.64
24	g	606	CHL	C2C-C3C-C4C	2.45	108.23	106.49
24	g	609	CHL	OMC-CMC-C2C	-2.45	120.15	125.69
25	R	608	CLA	C2A-C3A-C4A	-2.45	97.92	101.87
24	n	606	CHL	OMC-CMC-C2C	-2.45	120.15	125.69
24	s	307	CHL	C2A-C3A-C4A	2.45	105.82	101.87
25	n	613	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
40	s	317	NEX	C1-C2-C3	-2.45	108.12	113.64
25	s	309	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
24	y	310	CHL	O2A-CGA-O1A	-2.45	117.42	123.59
26	s	301	LHG	O8-C23-C24	2.45	119.58	111.91
25	d	403	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
25	B	615	CLA	O2A-CGA-CBA	2.44	119.58	111.91
25	b	615	CLA	O2A-CGA-CBA	2.44	119.58	111.91
24	Y	310	CHL	O2A-CGA-O1A	-2.44	117.42	123.59
25	S	309	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
25	B	607	CLA	C4D-CHA-C1A	-2.44	118.28	121.25
25	b	607	CLA	C4D-CHA-C1A	-2.44	118.28	121.25
39	N	616	LUT	C11-C10-C9	-2.44	123.83	127.31
25	N	613	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
24	Y	306	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
24	y	302	CHL	C4D-CHA-C1A	2.44	124.22	121.25
25	S	305	CLA	C5-C3-C4	2.44	119.99	114.60
40	R	617	NEX	C32-C33-C34	2.44	122.68	118.94
25	Y	305	CLA	C5-C3-C4	2.44	119.99	114.60
41	r	616	XAT	C31-C32-C33	-2.44	119.57	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	608	CLA	O2A-CGA-CBA	2.44	119.55	111.91
25	b	608	CLA	O2A-CGA-CBA	2.43	119.55	111.91
25	s	305	CLA	C5-C3-C4	2.43	119.98	114.60
25	G	611	CLA	CMD-C2D-C1D	-2.43	120.42	124.71
25	G	611	CLA	CHD-C1D-C2D	2.43	130.59	125.48
25	Y	311	CLA	O2A-CGA-CBA	2.43	119.55	111.91
25	y	311	CLA	O2A-CGA-CBA	2.43	119.55	111.91
25	S	313	CLA	O2A-CGA-CBA	2.43	119.54	111.91
40	r	617	NEX	C1-C2-C3	-2.43	108.15	113.64
25	C	506	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
25	c	506	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
24	S	307	CHL	C2A-C3A-C4A	2.43	105.80	101.87
24	g	609	CHL	C2A-C3A-C4A	2.43	105.80	101.87
25	C	512	CLA	C4D-CHA-C1A	-2.43	118.29	121.25
25	R	602	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
24	Y	302	CHL	C4D-CHA-C1A	2.43	124.20	121.25
25	R	601	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
41	R	616	XAT	C31-C32-C33	-2.43	119.59	126.42
25	s	313	CLA	O2A-CGA-CBA	2.43	119.53	111.91
26	r	618	LHG	O8-C23-C24	2.43	119.53	111.91
25	2	604	CLA	O2A-CGA-CBA	2.43	119.53	111.91
25	6	604	CLA	O2A-CGA-CBA	2.43	119.53	111.91
25	R	603	CLA	C3D-C4D-CHA	2.43	118.28	112.72
25	r	603	CLA	C3D-C4D-CHA	2.43	118.28	112.72
40	r	617	NEX	C32-C33-C34	2.43	122.67	118.94
25	y	303	CLA	O2A-CGA-CBA	2.43	119.52	111.91
25	n	604	CLA	C5-C3-C4	2.43	119.96	114.60
25	A	401	CLA	O2A-CGA-CBA	2.43	119.52	111.91
25	a	402	CLA	O2A-CGA-CBA	2.43	119.52	111.91
25	N	604	CLA	C5-C3-C4	2.42	119.96	114.60
25	Y	314	CLA	O1D-CGD-CBD	-2.42	119.52	124.48
25	y	314	CLA	O1D-CGD-CBD	-2.42	119.52	124.48
25	y	305	CLA	C5-C3-C4	2.42	119.96	114.60
25	N	614	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
24	s	302	CHL	C2A-C3A-C4A	2.42	105.78	101.87
26	S	301	LHG	O8-C23-C24	2.42	119.51	111.91
25	g	612	CLA	C4D-CHA-C1A	-2.42	118.30	121.25
25	G	603	CLA	O2A-CGA-CBA	2.42	119.50	111.91
25	N	602	CLA	O2A-CGA-CBA	2.42	119.50	111.91
24	S	302	CHL	C2A-C3A-C4A	2.42	105.78	101.87
38	F	101	HEM	CHB-C1B-NB	2.42	127.37	124.38
28	K	101	BCR	C38-C26-C25	-2.42	121.81	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	302	CHL	CMB-C2B-C1B	-2.42	124.75	128.46
25	b	610	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
25	Y	303	CLA	O2A-CGA-CBA	2.42	119.49	111.91
25	C	508	CLA	O2A-CGA-CBA	2.42	119.49	111.91
25	c	508	CLA	O2A-CGA-CBA	2.42	119.49	111.91
39	y	317	LUT	C2-C3-C4	2.42	113.61	110.30
25	R	614	CLA	C4D-CHA-C1A	-2.41	118.31	121.25
25	B	607	CLA	O1D-CGD-CBD	-2.41	119.54	124.48
25	b	607	CLA	O1D-CGD-CBD	-2.41	119.54	124.48
24	N	605	CHL	OMC-CMC-C2C	-2.41	120.23	125.69
24	n	605	CHL	OMC-CMC-C2C	-2.41	120.23	125.69
25	n	602	CLA	O2A-CGA-CBA	2.41	119.48	111.91
39	S	316	LUT	C2-C3-C4	2.41	113.61	110.30
39	s	316	LUT	C2-C3-C4	2.41	113.61	110.30
28	B	618	BCR	C24-C23-C22	-2.41	122.59	126.23
28	b	618	BCR	C24-C23-C22	-2.41	122.59	126.23
35	A	415	DGD	O1G-C1A-C2A	2.41	119.48	111.91
35	a	401	DGD	O1G-C1A-C2A	2.41	119.48	111.91
25	S	305	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
24	G	609	CHL	C2A-C3A-C4A	2.41	105.77	101.87
24	G	601	CHL	C4D-CHA-C1A	2.41	124.18	121.25
24	g	601	CHL	C4D-CHA-C1A	2.41	124.18	121.25
25	y	305	CLA	O2A-CGA-CBA	2.41	119.47	111.91
24	n	606	CHL	C2C-C3C-C4C	2.41	108.21	106.49
25	G	603	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
25	g	603	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
24	2	601	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
25	y	313	CLA	C4A-NA-C1A	-2.41	105.62	106.71
25	g	603	CLA	O2A-CGA-CBA	2.41	119.47	111.91
39	S	316	LUT	C37-C21-C22	-2.41	104.88	109.44
39	s	316	LUT	C37-C21-C22	-2.41	104.88	109.44
26	r	618	LHG	P-O6-C4	-2.41	107.56	121.68
26	R	618	LHG	P-O6-C4	-2.41	107.57	121.68
25	Y	305	CLA	O2A-CGA-CBA	2.41	119.46	111.91
25	g	604	CLA	O2A-CGA-CBA	2.41	119.46	111.91
24	G	606	CHL	CMB-C2B-C1B	-2.40	124.77	128.46
28	B	617	BCR	C7-C8-C9	-2.40	122.60	126.23
28	b	617	BCR	C7-C8-C9	-2.40	122.60	126.23
25	r	602	CLA	O1D-CGD-CBD	-2.40	119.56	124.48
25	B	610	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
25	B	609	CLA	O2A-CGA-CBA	2.40	119.44	111.91
25	b	609	CLA	O2A-CGA-CBA	2.40	119.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	604	CLA	O2A-CGA-CBA	2.40	119.44	111.91
25	g	603	CLA	CHD-C1D-C2D	2.40	130.52	125.48
25	n	612	CLA	CHB-C4A-NA	-2.40	121.19	124.51
25	s	305	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
25	G	604	CLA	CHD-C1D-C2D	2.40	130.51	125.48
24	6	601	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
24	Y	308	CHL	O2A-CGA-CBA	2.40	119.43	111.91
25	B	611	CLA	O2A-CGA-CBA	2.40	119.43	111.91
25	b	611	CLA	O2A-CGA-CBA	2.40	119.43	111.91
24	S	302	CHL	C4D-CHA-C1A	2.40	124.17	121.25
25	2	605	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
25	6	605	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
25	G	614	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
25	S	312	CLA	O1D-CGD-CBD	-2.39	119.58	124.48
25	b	605	CLA	O1D-CGD-CBD	-2.39	119.58	124.48
24	r	605	CHL	OMC-CMC-C2C	-2.39	120.27	125.69
25	y	311	CLA	CHD-C1D-C2D	2.39	130.50	125.48
25	D	401	CLA	C5-C3-C4	2.39	119.89	114.60
25	d	401	CLA	C5-C3-C4	2.39	119.89	114.60
25	s	312	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
24	R	605	CHL	OMC-CMC-C2C	-2.39	120.28	125.69
25	G	603	CLA	CHD-C1D-C2D	2.39	130.50	125.48
24	s	302	CHL	C4D-CHA-C1A	2.39	124.16	121.25
28	H	101	BCR	C29-C30-C25	2.39	114.16	110.48
28	h	101	BCR	C29-C30-C25	2.39	114.16	110.48
25	N	612	CLA	CHB-C4A-NA	-2.39	121.20	124.51
25	c	512	CLA	C4D-CHA-C1A	-2.39	118.34	121.25
39	Y	317	LUT	C2-C3-C4	2.39	113.58	110.30
28	B	618	BCR	C27-C26-C25	2.39	126.20	122.73
28	b	618	BCR	C27-C26-C25	2.39	126.20	122.73
25	s	313	CLA	C2D-C1D-ND	-2.39	108.34	110.10
25	Y	314	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
28	k	101	BCR	C38-C26-C25	-2.39	121.85	124.53
25	2	604	CLA	C3D-C4D-CHA	2.39	118.18	112.72
25	6	604	CLA	C3D-C4D-CHA	2.39	118.18	112.72
25	r	604	CLA	C2D-C1D-ND	-2.39	108.34	110.10
24	y	308	CHL	O2A-CGA-CBA	2.39	119.39	111.91
26	B	622	LHG	O8-C23-C24	2.39	119.39	111.91
26	b	622	LHG	O8-C23-C24	2.39	119.39	111.91
25	Y	311	CLA	CHD-C1D-C2D	2.39	130.48	125.48
25	B	608	CLA	O1D-CGD-CBD	-2.38	119.60	124.48
25	C	503	CLA	O2A-CGA-CBA	2.38	119.39	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	503	CLA	O2A-CGA-CBA	2.38	119.39	111.91
25	b	608	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
25	R	610	CLA	O2A-CGA-CBA	2.38	119.38	111.91
35	c	515	DGD	O1G-C1A-C2A	2.38	119.38	111.91
25	D	402	CLA	C3A-C2A-C1A	-2.38	97.77	101.34
25	d	402	CLA	C3A-C2A-C1A	-2.38	97.77	101.34
25	B	605	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
26	y	319	LHG	P-O6-C4	-2.38	107.72	121.68
25	A	401	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
25	a	402	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
25	r	610	CLA	O2A-CGA-CBA	2.38	119.38	111.91
25	y	314	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
24	y	307	CHL	O1D-CGD-CBD	-2.38	119.61	124.48
28	B	618	BCR	C11-C10-C9	-2.38	123.91	127.31
28	b	618	BCR	C11-C10-C9	-2.38	123.91	127.31
24	g	606	CHL	CMB-C2B-C1B	-2.38	124.81	128.46
25	6	602	CLA	C1D-ND-C4D	2.38	108.03	106.33
26	y	301	LHG	P-O6-C4	-2.38	107.73	121.68
24	N	606	CHL	C2C-C3C-C4C	2.38	108.18	106.49
25	g	614	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	g	608	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
35	C	515	DGD	O1G-C1A-C2A	2.38	119.36	111.91
25	S	311	CLA	O1D-CGD-CBD	-2.37	119.62	124.48
26	Y	301	LHG	P-O6-C4	-2.37	107.76	121.68
26	Y	319	LHG	P-O6-C4	-2.37	107.76	121.68
25	2	602	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
40	S	317	NEX	C5-C6-C1	-2.37	117.34	119.70
24	Y	307	CHL	O1D-CGD-CBD	-2.37	119.63	124.48
25	b	609	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	5	302	CHL	OMC-CMC-C2C	-2.37	120.33	125.69
24	N	607	CHL	O2A-CGA-CBA	2.37	119.34	111.91
39	R	615	LUT	C31-C30-C29	-2.37	123.93	127.31
39	r	615	LUT	C31-C30-C29	-2.37	123.93	127.31
24	G	608	CHL	OMC-CMC-C2C	-2.37	120.33	125.69
38	f	101	HEM	CHB-C1B-NB	2.37	127.31	124.38
25	C	504	CLA	C3D-C4D-CHA	2.37	118.14	112.72
25	c	504	CLA	C3D-C4D-CHA	2.37	118.14	112.72
24	g	609	CHL	C2A-C1A-CHA	2.37	128.00	123.86
24	2	601	CHL	O1D-CGD-CBD	-2.37	119.64	124.48
24	6	601	CHL	O1D-CGD-CBD	-2.37	119.64	124.48
25	c	507	CLA	O1D-CGD-CBD	-2.36	119.64	124.48
25	s	311	CLA	O1D-CGD-CBD	-2.36	119.64	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	n	617	NEX	C5-C6-C1	-2.36	117.35	119.70
25	B	609	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
25	R	604	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
25	B	611	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
25	B	615	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
25	b	611	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
25	g	604	CLA	CHD-C1D-C2D	2.36	130.44	125.48
24	n	607	CHL	O2A-CGA-CBA	2.36	119.33	111.91
25	D	402	CLA	CHD-C1D-C2D	2.36	130.44	125.48
25	d	402	CLA	CHD-C1D-C2D	2.36	130.44	125.48
25	g	614	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
25	R	604	CLA	C2D-C1D-ND	-2.36	108.36	110.10
25	r	604	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
25	S	313	CLA	C2D-C1D-ND	-2.36	108.36	110.10
40	Y	318	NEX	O24-C25-C38	2.36	117.88	115.06
25	R	609	CLA	C4D-CHA-C1A	-2.36	118.38	121.25
25	R	612	CLA	O2A-CGA-CBA	2.36	119.31	111.91
25	C	507	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
25	r	612	CLA	O2A-CGA-CBA	2.36	119.31	111.91
24	1	302	CHL	OMC-CMC-C2C	-2.36	120.36	125.69
25	r	614	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
25	N	604	CLA	O2A-CGA-CBA	2.36	119.31	111.91
24	n	607	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
24	N	607	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
25	R	614	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
25	N	610	CLA	O1D-CGD-CBD	-2.36	119.67	124.48
25	n	610	CLA	O1D-CGD-CBD	-2.36	119.67	124.48
25	n	604	CLA	O2A-CGA-CBA	2.35	119.30	111.91
25	Y	305	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
25	b	606	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
40	N	617	NEX	C5-C6-C1	-2.35	117.36	119.70
40	s	317	NEX	C5-C6-C1	-2.35	117.36	119.70
28	H	101	BCR	C11-C10-C9	-2.35	123.95	127.31
28	h	101	BCR	C11-C10-C9	-2.35	123.95	127.31
25	R	614	CLA	C4D-C3D-CAD	-2.35	105.33	108.10
24	Y	302	CHL	C2C-C3C-C4C	2.35	108.16	106.49
24	y	302	CHL	C2C-C3C-C4C	2.35	108.16	106.49
25	b	615	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
25	A	401	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
25	a	402	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
25	N	610	CLA	O2A-CGA-CBA	2.35	119.28	111.91
25	n	610	CLA	O2A-CGA-CBA	2.35	119.28	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	615	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
25	b	615	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
33	A	413	BCT	O3-C-O1	-2.35	113.46	119.55
33	a	414	BCT	O3-C-O1	-2.35	113.46	119.55
24	G	607	CHL	OMC-CMC-C2C	-2.35	120.38	125.69
24	g	607	CHL	OMC-CMC-C2C	-2.35	120.38	125.69
25	N	613	CLA	CHD-C4C-C3C	-2.34	121.39	124.84
25	6	602	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
25	D	402	CLA	O2A-CGA-CBA	2.34	119.26	111.91
25	r	609	CLA	C4D-CHA-C1A	-2.34	118.40	121.25
25	y	305	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
24	s	302	CHL	OMC-CMC-C2C	-2.34	120.40	125.69
25	d	402	CLA	O2A-CGA-CBA	2.34	119.24	111.91
25	Y	313	CLA	C4A-NA-C1A	-2.34	105.66	106.71
24	Y	302	CHL	OMC-CMC-C2C	-2.34	120.40	125.69
24	y	302	CHL	OMC-CMC-C2C	-2.34	120.40	125.69
25	G	611	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
28	A	406	BCR	C38-C26-C25	-2.34	121.91	124.53
28	a	407	BCR	C38-C26-C25	-2.34	121.91	124.53
25	r	614	CLA	C4D-C3D-CAD	-2.34	105.34	108.10
24	y	308	CHL	O1D-CGD-CBD	-2.34	119.70	124.48
25	B	601	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
25	2	602	CLA	C1D-ND-C4D	2.34	107.99	106.33
25	b	601	CLA	O1D-CGD-CBD	-2.34	119.71	124.48
25	c	501	CLA	C2A-C3A-C4A	-2.33	98.10	101.87
28	I	101	BCR	C38-C26-C25	-2.33	121.91	124.53
24	1	302	CHL	CHD-C1D-ND	-2.33	122.31	124.45
25	B	611	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	b	611	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	g	611	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
25	c	507	CLA	C4-C3-C5	2.33	119.19	115.27
25	B	606	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	R	603	CLA	C4-C3-C5	2.33	119.19	115.27
25	r	603	CLA	C4-C3-C5	2.33	119.19	115.27
25	C	513	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
25	c	513	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
25	G	614	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
25	S	305	CLA	O2A-CGA-CBA	2.33	119.22	111.91
25	s	305	CLA	O2A-CGA-CBA	2.33	119.22	111.91
25	Y	303	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
24	S	306	CHL	C2A-C3A-C4A	2.33	105.63	101.87
24	Y	308	CHL	O1D-CGD-CBD	-2.33	119.72	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	610	CLA	O2A-CGA-CBA	2.33	119.21	111.91
28	B	619	BCR	C27-C26-C25	2.33	126.11	122.73
28	H	101	BCR	C27-C26-C25	2.33	126.11	122.73
28	i	101	BCR	C38-C26-C25	-2.33	121.92	124.53
25	B	612	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
25	b	612	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
25	s	304	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
24	s	306	CHL	C2A-C3A-C4A	2.32	105.62	101.87
25	y	312	CLA	C4D-CHA-C1A	-2.32	118.43	121.25
24	S	306	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
25	n	613	CLA	CHD-C4C-C3C	-2.32	121.43	124.84
25	S	304	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
24	s	308	CHL	OMC-CMC-C2C	-2.32	120.45	125.69
24	g	601	CHL	OMC-CMC-C2C	-2.32	120.45	125.69
40	y	318	NEX	O24-C25-C38	2.32	117.83	115.06
24	G	609	CHL	C2A-C1A-CHA	2.32	127.91	123.86
24	G	601	CHL	OMC-CMC-C2C	-2.32	120.45	125.69
24	R	613	CHL	OMC-CMC-C2C	-2.32	120.45	125.69
24	s	306	CHL	OMC-CMC-C2C	-2.32	120.45	125.69
25	B	607	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
25	b	607	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
25	b	613	CLA	O2A-CGA-CBA	2.31	119.17	111.91
25	C	507	CLA	C4-C3-C5	2.31	119.17	115.27
28	b	619	BCR	C27-C26-C25	2.31	126.09	122.73
25	d	403	CLA	C3D-C4D-CHA	2.31	118.02	112.72
25	s	305	CLA	C3C-C4C-NC	-2.31	107.98	110.57
24	S	302	CHL	OMC-CMC-C2C	-2.31	120.46	125.69
24	N	605	CHL	C2A-C3A-C4A	2.31	105.60	101.87
24	s	307	CHL	OMC-CMC-C2C	-2.31	120.46	125.69
24	n	607	CHL	C2C-C3C-C4C	2.31	108.14	106.49
25	n	610	CLA	CHD-C1D-C2D	2.31	130.32	125.48
39	R	615	LUT	C35-C34-C33	-2.31	124.02	127.31
25	B	616	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
25	b	616	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
25	d	401	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
25	C	507	CLA	C1D-CHD-C4C	-2.31	121.08	126.06
25	c	507	CLA	C1D-CHD-C4C	-2.31	121.08	126.06
24	g	607	CHL	CAA-C2A-C3A	-2.31	106.46	112.78
25	B	610	CLA	O2A-CGA-CBA	2.31	119.15	111.91
25	G	614	CLA	C2C-C1C-NC	2.31	112.13	109.97
40	Y	318	NEX	C40-C33-C32	2.31	121.71	118.08
25	n	604	CLA	C2A-C1A-CHA	-2.31	119.83	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	305	CLA	C3C-C4C-NC	-2.31	107.98	110.57
25	B	608	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
25	c	505	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
25	C	513	CLA	O2A-CGA-CBA	2.30	119.14	111.91
25	c	513	CLA	O2A-CGA-CBA	2.30	119.14	111.91
25	y	315	CLA	C2C-C1C-NC	2.30	112.13	109.97
25	D	403	CLA	C3D-C4D-CHA	2.30	118.00	112.72
25	B	613	CLA	O2A-CGA-CBA	2.30	119.14	111.91
25	C	501	CLA	C3D-C4D-CHA	2.30	117.99	112.72
28	h	101	BCR	C27-C26-C25	2.30	126.08	122.73
24	r	613	CHL	OMC-CMC-C2C	-2.30	120.48	125.69
25	C	501	CLA	C2A-C3A-C4A	-2.30	98.15	101.87
28	B	618	BCR	C2-C1-C6	2.30	114.03	110.48
28	b	618	BCR	C2-C1-C6	2.30	114.03	110.48
24	y	309	CHL	OMC-CMC-C2C	-2.30	120.48	125.69
24	S	308	CHL	OMC-CMC-C2C	-2.30	120.48	125.69
24	S	307	CHL	OMC-CMC-C2C	-2.30	120.48	125.69
25	y	303	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
25	c	501	CLA	C3D-C4D-CHA	2.30	117.98	112.72
25	B	603	CLA	O2A-CGA-CBA	2.30	119.12	111.91
25	b	603	CLA	O2A-CGA-CBA	2.30	119.12	111.91
25	G	604	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
25	b	608	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
24	1	302	CHL	O2A-CGA-CBA	2.30	121.41	114.03
24	N	609	CHL	C2A-C3A-C4A	2.30	105.58	101.87
24	n	609	CHL	C2A-C3A-C4A	2.30	105.58	101.87
24	G	607	CHL	CAA-C2A-C3A	-2.30	106.49	112.78
24	N	607	CHL	C2C-C3C-C4C	2.30	108.12	106.49
24	n	605	CHL	C2A-C3A-C4A	2.29	105.58	101.87
25	b	604	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
25	C	505	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
25	r	608	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
24	Y	306	CHL	C2A-C3A-C4A	2.29	105.57	101.87
25	B	604	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
24	Y	309	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
24	N	601	CHL	C2A-C3A-C4A	2.29	105.57	101.87
24	G	606	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
25	A	402	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
25	a	403	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
24	5	302	CHL	O2A-CGA-CBA	2.29	121.38	114.03
25	c	502	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
24	5	302	CHL	CHD-C1D-ND	-2.29	122.35	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	506	CLA	CHD-C1D-C2D	2.29	130.28	125.48
25	c	506	CLA	CHD-C1D-C2D	2.29	130.28	125.48
25	R	604	CLA	C4D-CHA-C1A	-2.29	118.47	121.25
25	r	604	CLA	C4D-CHA-C1A	-2.29	118.47	121.25
39	r	615	LUT	C35-C34-C33	-2.29	124.05	127.31
24	y	306	CHL	C2A-C3A-C4A	2.29	105.56	101.87
25	n	602	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
24	g	606	CHL	OMC-CMC-C2C	-2.29	120.52	125.69
25	Y	303	CLA	C2A-C1A-CHA	-2.28	119.86	123.86
25	y	303	CLA	C2A-C1A-CHA	-2.28	119.86	123.86
25	g	614	CLA	C2C-C1C-NC	2.28	112.11	109.97
25	b	613	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	N	606	CHL	CBC-CAC-C3C	-2.28	106.14	112.43
24	n	606	CHL	CBC-CAC-C3C	-2.28	106.14	112.43
25	N	610	CLA	CHD-C1D-C2D	2.28	130.26	125.48
25	R	612	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
25	S	310	CLA	O2A-CGA-CBA	2.28	119.06	111.91
24	Y	302	CHL	C2A-C3A-C4A	2.28	105.55	101.87
24	y	302	CHL	C2A-C3A-C4A	2.28	105.55	101.87
25	B	606	CLA	O1D-CGD-CBD	-2.28	119.83	124.48
25	g	614	CLA	CHD-C1D-C2D	2.27	130.25	125.48
28	T	101	BCR	C38-C26-C25	-2.27	121.97	124.53
28	t	101	BCR	C38-C26-C25	-2.27	121.97	124.53
25	N	604	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
25	D	401	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
25	Y	315	CLA	C2C-C1C-NC	2.27	112.10	109.97
25	B	601	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
25	b	601	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
25	N	602	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
25	2	602	CLA	CHC-C1C-C2C	2.27	133.01	126.72
25	6	602	CLA	CHC-C1C-C2C	2.27	133.01	126.72
25	2	604	CLA	C3C-C4C-NC	-2.27	108.02	110.57
25	6	604	CLA	C3C-C4C-NC	-2.27	108.02	110.57
25	r	601	CLA	C3C-C4C-NC	-2.27	108.02	110.57
24	y	310	CHL	OMC-CMC-C2C	-2.27	120.55	125.69
24	Y	308	CHL	O2D-CGD-O1D	-2.27	119.40	123.84
25	R	608	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
24	n	605	CHL	C2A-C1A-CHA	2.27	127.83	123.86
25	C	502	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
25	Y	313	CLA	C4D-CHA-C1A	-2.27	118.49	121.25
25	r	612	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
40	y	318	NEX	C40-C33-C32	2.27	121.65	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	304	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
25	S	312	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
24	n	608	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
25	s	310	CLA	O2A-CGA-CBA	2.27	119.02	111.91
28	T	101	BCR	C15-C14-C13	-2.27	124.08	127.31
25	S	314	CLA	C3D-C4D-ND	2.27	113.90	110.24
25	g	610	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
25	r	609	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
25	g	604	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
25	G	611	CLA	CAD-C3D-C2D	2.27	151.73	140.80
25	g	611	CLA	CAD-C3D-C2D	2.27	151.73	140.80
25	B	605	CLA	CBA-CAA-C2A	-2.26	107.18	113.86
25	b	605	CLA	CBA-CAA-C2A	-2.26	107.18	113.86
25	a	402	CLA	C4D-CHA-C1A	-2.26	118.49	121.25
24	Y	310	CHL	OMC-CMC-C2C	-2.26	120.57	125.69
24	n	601	CHL	C2A-C3A-C4A	2.26	105.52	101.87
24	r	607	CHL	OMC-CMC-C2C	-2.26	120.57	125.69
25	R	609	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
25	c	505	CLA	C3D-C4D-ND	2.26	113.89	110.24
25	c	503	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
25	c	513	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
24	y	308	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
25	B	613	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
25	Y	304	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
24	r	606	CHL	OMC-CMC-C2C	-2.26	120.58	125.69
24	5	301	CHL	OMC-CMC-C2C	-2.26	120.58	125.69
25	C	503	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
25	B	614	CLA	O1D-CGD-CBD	-2.26	119.87	124.48
25	b	614	CLA	O1D-CGD-CBD	-2.26	119.87	124.48
25	G	614	CLA	CHD-C1D-C2D	2.26	130.21	125.48
25	R	601	CLA	C3C-C4C-NC	-2.26	108.04	110.57
40	G	617	NEX	C20-C13-C12	2.26	121.63	118.08
25	D	403	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
25	d	403	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
25	C	513	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
24	Y	308	CHL	OMC-CMC-C2C	-2.25	120.59	125.69
24	N	609	CHL	OMC-CMC-C2C	-2.25	120.59	125.69
24	n	609	CHL	OMC-CMC-C2C	-2.25	120.59	125.69
25	2	604	CLA	CAD-C3D-C2D	2.25	151.67	140.80
25	6	604	CLA	CAD-C3D-C2D	2.25	151.67	140.80
24	N	608	CHL	OMC-CMC-C2C	-2.25	120.59	125.69
25	B	605	CLA	O2D-CGD-O1D	-2.25	119.43	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	605	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
25	A	405	CLA	O2A-CGA-CBA	2.25	118.98	111.91
25	a	406	CLA	O2A-CGA-CBA	2.25	118.98	111.91
25	b	606	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
25	n	614	CLA	CHD-C1D-C2D	2.25	130.20	125.48
24	N	606	CHL	C2A-C3A-C4A	2.25	105.51	101.87
24	n	606	CHL	C2A-C3A-C4A	2.25	105.51	101.87
25	s	312	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
25	A	401	CLA	C4D-CHA-C1A	-2.25	118.51	121.25
24	y	308	CHL	OMC-CMC-C2C	-2.25	120.60	125.69
25	D	403	CLA	C3B-C4B-NB	-2.25	106.30	109.21
25	S	311	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
25	s	311	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
25	C	505	CLA	C3D-C4D-ND	2.25	113.88	110.24
25	B	606	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
25	b	606	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	g	601	CHL	O1D-CGD-CBD	-2.25	119.88	124.48
25	c	513	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
25	Y	312	CLA	C4D-CHA-C1A	-2.25	118.51	121.25
24	2	601	CHL	C3C-C4C-NC	-2.25	108.05	110.57
24	6	601	CHL	C3C-C4C-NC	-2.25	108.05	110.57
25	C	513	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
25	C	507	CLA	C4D-C3D-CAD	-2.25	105.45	108.10
25	D	401	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
25	d	401	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
25	s	314	CLA	CHD-C1D-C2D	2.25	130.19	125.48
24	y	307	CHL	CMB-C2B-C1B	-2.25	125.01	128.46
24	N	605	CHL	C2A-C1A-CHA	2.25	127.78	123.86
40	Y	318	NEX	C28-C29-C30	2.25	122.39	118.94
25	S	305	CLA	C3B-C4B-NB	-2.24	106.31	109.21
25	N	614	CLA	CHD-C1D-C2D	2.24	130.19	125.48
25	N	603	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
24	R	607	CHL	OMC-CMC-C2C	-2.24	120.61	125.69
25	G	610	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
25	Y	311	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
24	G	601	CHL	C2C-C3C-C4C	2.24	108.09	106.49
25	D	402	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
25	d	402	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
25	6	604	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
28	h	101	BCR	C38-C26-C25	-2.24	122.01	124.53
25	2	604	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
25	C	506	CLA	O2D-CGD-O1D	-2.24	119.46	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	506	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
24	R	606	CHL	OMC-CMC-C2C	-2.24	120.62	125.69
24	G	601	CHL	O1D-CGD-CBD	-2.24	119.90	124.48
28	H	101	BCR	C38-C26-C25	-2.24	122.01	124.53
25	y	311	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
24	G	606	CHL	O2A-CGA-O1A	-2.24	117.94	123.59
24	Y	307	CHL	CMB-C2B-C1B	-2.24	125.03	128.46
25	n	613	CLA	O2A-CGA-CBA	2.24	118.93	111.91
25	S	309	CLA	CHD-C1D-C2D	2.24	130.17	125.48
25	s	309	CLA	CHD-C1D-C2D	2.24	130.17	125.48
25	S	314	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
25	R	614	CLA	CHD-C1D-C2D	2.24	130.17	125.48
25	r	614	CLA	CHD-C1D-C2D	2.24	130.17	125.48
24	1	301	CHL	O2A-CGA-CBA	2.24	121.21	114.03
24	5	301	CHL	O2A-CGA-CBA	2.24	121.21	114.03
25	r	603	CLA	O2A-CGA-CBA	2.24	118.92	111.91
25	r	603	CLA	C3B-C4B-NB	-2.23	106.32	109.21
25	C	502	CLA	O2A-CGA-CBA	2.23	118.92	111.91
25	c	502	CLA	O2A-CGA-CBA	2.23	118.92	111.91
25	s	314	CLA	C3D-C4D-ND	2.23	113.85	110.24
25	N	614	CLA	O2A-CGA-CBA	2.23	118.92	111.91
25	c	507	CLA	C4D-C3D-CAD	-2.23	105.46	108.10
25	s	305	CLA	C3B-C4B-NB	-2.23	106.32	109.21
25	C	501	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
25	c	501	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
24	Y	309	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
25	S	314	CLA	CHD-C1D-C2D	2.23	130.16	125.48
25	n	614	CLA	O2A-CGA-CBA	2.23	118.91	111.91
25	B	612	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
25	y	313	CLA	C4D-CHA-C1A	-2.23	118.53	121.25
40	y	318	NEX	C28-C29-C30	2.23	122.36	118.94
25	A	401	CLA	C11-C12-C13	-2.23	108.71	115.92
24	Y	307	CHL	CBC-CAC-C3C	-2.23	106.28	112.43
25	g	610	CLA	O2A-CGA-CBA	2.23	118.91	111.91
25	G	610	CLA	O2A-CGA-CBA	2.23	118.91	111.91
28	t	101	BCR	C15-C14-C13	-2.23	124.13	127.31
25	r	614	CLA	C3D-C4D-ND	2.23	113.84	110.24
24	g	606	CHL	O2A-CGA-O1A	-2.23	117.97	123.59
24	R	607	CHL	O1D-CGD-CBD	-2.23	119.93	124.48
24	r	607	CHL	O1D-CGD-CBD	-2.23	119.93	124.48
25	r	608	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
24	S	306	CHL	O2D-CGD-O1D	-2.23	119.48	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	613	CLA	O2A-CGA-CBA	2.23	118.89	111.91
25	n	603	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
25	r	602	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
25	R	614	CLA	CAD-C3D-C2D	2.23	151.54	140.80
25	r	614	CLA	CAD-C3D-C2D	2.23	151.54	140.80
25	b	613	CLA	C4D-CHA-C1A	-2.22	118.54	121.25
25	Y	312	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
25	B	602	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
25	b	602	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
25	a	402	CLA	C11-C12-C13	-2.22	108.73	115.92
25	d	403	CLA	C3B-C4B-NB	-2.22	106.34	109.21
28	D	404	BCR	C7-C8-C9	-2.22	122.88	126.23
28	d	404	BCR	C7-C8-C9	-2.22	122.88	126.23
25	R	614	CLA	C3D-C4D-ND	2.22	113.83	110.24
25	C	509	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
25	c	509	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
24	s	306	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
25	Y	315	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
25	y	315	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
24	y	309	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
25	R	608	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
24	y	307	CHL	CBC-CAC-C3C	-2.22	106.31	112.43
24	1	301	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
25	G	602	CLA	C6-C7-C8	-2.22	108.75	115.92
25	R	603	CLA	C3B-C4B-NB	-2.22	106.34	109.21
25	B	614	CLA	O2A-CGA-CBA	2.22	118.87	111.91
25	b	614	CLA	O2A-CGA-CBA	2.22	118.87	111.91
24	R	607	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
25	g	602	CLA	C6-C7-C8	-2.22	108.75	115.92
25	B	613	CLA	C4D-CHA-C1A	-2.22	118.55	121.25
25	n	613	CLA	C6-C7-C8	-2.22	108.75	115.92
24	n	601	CHL	C2A-C1A-CHA	2.22	127.73	123.86
25	g	611	CLA	C11-C10-C8	-2.22	108.76	115.92
24	G	601	CHL	O2D-CGD-O1D	-2.22	119.51	123.84
29	l	102	SQD	C1-C2-C3	2.22	114.61	110.00
25	G	602	CLA	C3D-C4D-ND	2.22	113.82	110.24
25	g	602	CLA	C3D-C4D-ND	2.22	113.82	110.24
40	g	617	NEX	C32-C33-C34	-2.22	115.54	118.94
25	s	314	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
28	I	101	BCR	C7-C8-C9	-2.21	122.89	126.23
24	s	306	CHL	O1D-CGD-CBD	-2.21	119.95	124.48
28	A	406	BCR	C7-C8-C9	-2.21	122.89	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	407	BCR	C7-C8-C9	-2.21	122.89	126.23
24	S	306	CHL	O1D-CGD-CBD	-2.21	119.96	124.48
28	B	619	BCR	C15-C16-C17	-2.21	118.94	123.47
28	b	619	BCR	C15-C16-C17	-2.21	118.94	123.47
24	G	608	CHL	C2C-C3C-C4C	2.21	108.07	106.49
40	G	617	NEX	C32-C33-C34	-2.21	115.55	118.94
25	G	611	CLA	C11-C10-C8	-2.21	108.77	115.92
25	C	505	CLA	O2A-CGA-CBA	2.21	118.85	111.91
28	c	514	BCR	C15-C14-C13	-2.21	124.15	127.31
29	L	101	SQD	C1-C2-C3	2.21	114.60	110.00
40	N	617	NEX	C5-C4-C3	-2.21	109.13	111.75
39	n	615	LUT	C1-C2-C3	2.21	118.63	113.64
25	c	505	CLA	O2A-CGA-CBA	2.21	118.84	111.91
40	n	617	NEX	C17-C1-C6	-2.21	108.50	110.47
25	d	401	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
25	S	312	CLA	CHD-C1D-C2D	2.21	130.11	125.48
25	s	312	CLA	CHD-C1D-C2D	2.21	130.11	125.48
25	D	401	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
25	Y	312	CLA	C3D-C4D-ND	2.21	113.81	110.24
28	D	404	BCR	C11-C10-C9	-2.21	124.16	127.31
28	d	404	BCR	C11-C10-C9	-2.21	124.16	127.31
24	g	607	CHL	C2A-C3A-C4A	2.21	105.44	101.87
24	s	307	CHL	C4D-CHA-C1A	2.21	123.94	121.25
24	r	607	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
24	y	308	CHL	C2A-C3A-C4A	2.21	105.43	101.87
28	C	514	BCR	C8-C7-C6	-2.21	121.01	127.20
25	R	603	CLA	O2A-CGA-CBA	2.21	118.83	111.91
40	n	617	NEX	C5-C4-C3	-2.21	109.13	111.75
24	n	607	CHL	C2A-C1A-CHA	2.20	127.71	123.86
25	s	312	CLA	C3A-C2A-C1A	-2.20	98.04	101.34
25	N	613	CLA	C6-C7-C8	-2.20	108.80	115.92
24	N	607	CHL	C2A-C1A-CHA	2.20	127.71	123.86
24	n	609	CHL	O1D-CGD-CBD	-2.20	119.98	124.48
24	6	601	CHL	OMC-CMC-C2C	-2.20	120.71	125.69
25	6	602	CLA	CAD-C3D-C2D	2.20	151.42	140.80
25	B	605	CLA	O2A-CGA-CBA	2.20	118.81	111.91
25	b	605	CLA	O2A-CGA-CBA	2.20	118.81	111.91
25	b	612	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
28	i	101	BCR	C7-C8-C9	-2.20	122.91	126.23
39	N	615	LUT	C1-C2-C3	2.20	118.61	113.64
25	R	602	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
24	N	601	CHL	OMC-CMC-C2C	-2.20	120.72	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	612	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
24	S	307	CHL	C4D-CHA-C1A	2.20	123.92	121.25
24	N	609	CHL	O1D-CGD-CBD	-2.20	119.99	124.48
25	r	604	CLA	C4D-C3D-CAD	-2.19	105.51	108.10
25	2	602	CLA	CAD-C3D-C2D	2.19	151.39	140.80
25	S	312	CLA	C3A-C2A-C1A	-2.19	98.05	101.34
25	r	610	CLA	CAD-C3D-C2D	2.19	151.39	140.80
24	g	601	CHL	C2C-C3C-C4C	2.19	108.05	106.49
28	C	514	BCR	C2-C1-C6	2.19	113.86	110.48
24	n	606	CHL	C4D-CHA-C1A	2.19	123.92	121.25
25	C	504	CLA	C6-C7-C8	-2.19	108.83	115.92
24	2	601	CHL	C2C-C3C-C4C	2.19	108.05	106.49
25	G	602	CLA	C2C-C1C-NC	2.19	112.03	109.97
25	g	602	CLA	C2C-C1C-NC	2.19	112.03	109.97
24	2	601	CHL	OMC-CMC-C2C	-2.19	120.73	125.69
24	R	607	CHL	C2C-C3C-C4C	2.19	108.05	106.49
25	R	610	CLA	CAD-C3D-C2D	2.19	151.37	140.80
24	n	606	CHL	C2A-C1A-CHA	2.19	127.69	123.86
28	c	514	BCR	C8-C7-C6	-2.19	121.05	127.20
25	r	612	CLA	C4D-CHA-C1A	-2.19	118.58	121.25
25	Y	305	CLA	CHD-C1D-C2D	2.19	130.07	125.48
25	y	305	CLA	CHD-C1D-C2D	2.19	130.07	125.48
28	C	514	BCR	C15-C14-C13	-2.19	124.19	127.31
24	N	606	CHL	C2A-C1A-CHA	2.19	127.69	123.86
25	y	312	CLA	C3D-C4D-ND	2.19	113.78	110.24
28	c	514	BCR	C2-C1-C6	2.19	113.85	110.48
28	B	618	BCR	C38-C26-C25	-2.19	122.07	124.53
28	b	618	BCR	C38-C26-C25	-2.19	122.07	124.53
25	R	612	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
25	y	312	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
25	y	314	CLA	O2A-CGA-CBA	2.19	118.77	111.91
25	G	612	CLA	O1D-CGD-CBD	-2.18	120.01	124.48
25	g	612	CLA	O1D-CGD-CBD	-2.18	120.01	124.48
25	c	504	CLA	C6-C7-C8	-2.18	108.86	115.92
24	g	601	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
25	B	616	CLA	CHD-C1D-C2D	2.18	130.06	125.48
25	C	505	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
25	Y	305	CLA	C3D-C4D-ND	2.18	113.77	110.24
24	n	601	CHL	OMC-CMC-C2C	-2.18	120.76	125.69
25	S	303	CLA	C3D-C4D-ND	2.18	113.77	110.24
25	g	612	CLA	C3D-C4D-ND	2.18	113.77	110.24
24	Y	307	CHL	C1B-CHB-C4A	-2.18	125.80	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	610	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
25	G	610	CLA	C1D-ND-C4D	-2.18	104.79	106.33
25	g	610	CLA	C1D-ND-C4D	-2.18	104.79	106.33
24	y	309	CHL	C2C-C3C-C4C	2.18	108.04	106.49
25	Y	314	CLA	O2A-CGA-CBA	2.18	118.75	111.91
24	N	606	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
28	K	101	BCR	C8-C7-C6	-2.18	121.08	127.20
25	G	603	CLA	C11-C10-C8	-2.18	108.88	115.92
28	B	619	BCR	C38-C26-C25	-2.18	122.08	124.53
28	b	619	BCR	C38-C26-C25	-2.18	122.08	124.53
24	Y	308	CHL	C2A-C3A-C4A	2.18	105.39	101.87
28	Z	101	BCR	C37-C22-C21	-2.18	119.87	122.92
25	C	511	CLA	O2A-CGA-CBA	2.18	118.74	111.91
25	c	511	CLA	O2A-CGA-CBA	2.18	118.74	111.91
25	R	611	CLA	CHA-C4D-ND	-2.18	127.94	132.50
25	s	303	CLA	C3D-C4D-ND	2.18	113.76	110.24
28	k	101	BCR	C8-C7-C6	-2.18	121.09	127.20
25	r	604	CLA	C2A-C1A-CHA	-2.18	120.06	123.86
24	y	307	CHL	C1B-CHB-C4A	-2.17	125.81	130.12
24	y	310	CHL	C2A-C3A-C4A	2.17	105.38	101.87
24	N	601	CHL	C2A-C1A-CHA	2.17	127.66	123.86
25	G	602	CLA	O2A-CGA-CBA	2.17	118.73	111.91
25	r	614	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
24	g	608	CHL	O1D-CGD-CBD	-2.17	120.04	124.48
39	R	615	LUT	C22-C23-C24	2.17	114.21	111.74
39	r	615	LUT	C22-C23-C24	2.17	114.21	111.74
25	n	610	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
25	Y	312	CLA	C11-C10-C8	-2.17	108.90	115.92
25	y	312	CLA	C11-C10-C8	-2.17	108.90	115.92
28	z	101	BCR	C37-C22-C21	-2.17	119.88	122.92
25	G	612	CLA	C3D-C4D-ND	2.17	113.75	110.24
25	c	505	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
25	R	604	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
25	B	604	CLA	O2A-CGA-CBA	2.17	118.72	111.91
40	s	317	NEX	C35-C15-C14	-2.17	119.03	123.47
25	g	602	CLA	O2A-CGA-CBA	2.17	118.71	111.91
25	A	401	CLA	C11-C10-C8	-2.17	108.91	115.92
25	a	402	CLA	C11-C10-C8	-2.17	108.91	115.92
25	b	616	CLA	CHD-C1D-C2D	2.17	130.03	125.48
25	6	602	CLA	C6-C7-C8	-2.17	108.91	115.92
25	y	314	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
25	y	315	CLA	CHD-C1D-C2D	2.17	130.02	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	609	CLA	C3D-C4D-ND	2.17	113.74	110.24
24	6	601	CHL	C2C-C3C-C4C	2.17	108.03	106.49
24	G	608	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
40	N	617	NEX	C17-C1-C6	-2.17	108.53	110.47
25	b	604	CLA	O2A-CGA-CBA	2.17	118.70	111.91
25	s	305	CLA	CAD-C3D-C2D	2.17	151.25	140.80
28	Z	101	BCR	C8-C7-C6	-2.17	121.12	127.20
24	G	605	CHL	O2A-CGA-CBA	2.16	120.98	114.03
24	g	605	CHL	O2A-CGA-CBA	2.16	120.98	114.03
25	2	604	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
25	6	604	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
24	N	606	CHL	C4D-CHA-C1A	2.16	123.88	121.25
25	2	602	CLA	C6-C7-C8	-2.16	108.93	115.92
25	B	609	CLA	C3D-C4D-ND	2.16	113.74	110.24
25	y	305	CLA	C3D-C4D-ND	2.16	113.74	110.24
24	r	607	CHL	C2C-C3C-C4C	2.16	108.03	106.49
25	g	603	CLA	C11-C10-C8	-2.16	108.93	115.92
24	g	608	CHL	O2D-CGD-O1D	-2.16	119.61	123.84
25	2	602	CLA	C2C-C1C-NC	-2.16	107.95	109.97
25	6	602	CLA	C2C-C1C-NC	-2.16	107.95	109.97
25	R	610	CLA	C3C-C4C-NC	-2.16	108.15	110.57
25	r	610	CLA	C3C-C4C-NC	-2.16	108.15	110.57
25	A	402	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
25	a	403	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
24	Y	308	CHL	O2A-CGA-O1A	-2.16	118.14	123.59
24	y	308	CHL	O2A-CGA-O1A	-2.16	118.14	123.59
25	r	611	CLA	CHA-C4D-ND	-2.16	127.98	132.50
25	S	305	CLA	CAD-C3D-C2D	2.16	151.22	140.80
40	S	317	NEX	C35-C15-C14	-2.16	119.05	123.47
24	N	609	CHL	C2C-C3C-C4C	2.16	108.03	106.49
24	n	609	CHL	C2C-C3C-C4C	2.16	108.03	106.49
25	c	506	CLA	C3D-C4D-ND	2.16	113.73	110.24
25	N	613	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
25	r	601	CLA	CAD-C3D-C2D	2.16	151.21	140.80
25	Y	315	CLA	CHD-C1D-C2D	2.16	130.01	125.48
24	6	603	CHL	C2C-C3C-C4C	2.16	108.03	106.49
24	G	607	CHL	C2A-C3A-C4A	2.16	105.35	101.87
24	Y	310	CHL	C2A-C3A-C4A	2.16	105.35	101.87
25	B	613	CLA	C6-C7-C8	-2.16	108.95	115.92
25	b	613	CLA	C6-C7-C8	-2.16	108.95	115.92
25	Y	314	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
25	r	601	CLA	C3B-C4B-NB	-2.16	106.42	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	512	CLA	O2A-CGA-CBA	2.16	118.67	111.91
25	R	604	CLA	C4A-NA-C1A	-2.16	105.74	106.71
25	r	604	CLA	C4A-NA-C1A	-2.16	105.74	106.71
25	c	504	CLA	C3B-C4B-NB	-2.15	106.42	109.21
25	B	602	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
25	b	602	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
25	C	504	CLA	C3B-C4B-NB	-2.15	106.42	109.21
25	n	613	CLA	C2C-C1C-NC	2.15	111.99	109.97
25	y	303	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
24	Y	307	CHL	C2A-C3A-C4A	2.15	105.35	101.87
24	y	307	CHL	C2A-C3A-C4A	2.15	105.35	101.87
24	2	603	CHL	C2C-C3C-C4C	2.15	108.02	106.49
25	c	512	CLA	O2A-CGA-CBA	2.15	118.66	111.91
25	R	601	CLA	CAD-C3D-C2D	2.15	151.18	140.80
28	z	101	BCR	C8-C7-C6	-2.15	121.16	127.20
25	b	602	CLA	C11-C10-C8	-2.15	108.97	115.92
25	R	608	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
25	C	502	CLA	CHD-C1D-C2D	2.15	129.99	125.48
25	c	502	CLA	CHD-C1D-C2D	2.15	129.99	125.48
24	s	308	CHL	C4D-CHA-C1A	2.15	123.86	121.25
25	C	509	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
39	n	615	LUT	C15-C35-C34	-2.15	119.07	123.47
41	r	616	XAT	C11-C12-C13	-2.15	120.38	126.42
25	B	612	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
25	b	612	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
39	N	615	LUT	C15-C35-C34	-2.15	119.08	123.47
25	G	611	CLA	C6-C7-C8	-2.15	108.98	115.92
25	R	604	CLA	C4D-C3D-CAD	-2.15	105.57	108.10
25	N	602	CLA	C16-C15-C13	-2.15	108.98	115.92
25	R	614	CLA	C2A-C1A-CHA	-2.15	120.11	123.86
25	c	513	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
25	B	604	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
25	b	604	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
25	n	602	CLA	C16-C15-C13	-2.14	108.99	115.92
24	y	306	CHL	C4D-CHA-C1A	2.14	123.86	121.25
24	G	608	CHL	O1D-CGD-CBD	-2.14	120.10	124.48
24	N	607	CHL	C1-C2-C3	2.14	129.75	126.04
24	Y	308	CHL	C3C-C4C-NC	-2.14	108.17	110.57
24	S	306	CHL	C4D-CHA-C1A	2.14	123.86	121.25
24	s	306	CHL	C4D-CHA-C1A	2.14	123.86	121.25
25	Y	313	CLA	C2C-C1C-NC	2.14	111.98	109.97
25	R	603	CLA	C3C-C4C-NC	-2.14	108.17	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	606	CHL	O2A-CGA-CBA	2.14	120.91	114.03
25	n	613	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
25	G	610	CLA	C2D-C1D-ND	-2.14	108.53	110.10
25	b	616	CLA	C3D-C4D-ND	2.14	113.70	110.24
25	C	513	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
41	R	616	XAT	C11-C12-C13	-2.14	120.41	126.42
25	g	611	CLA	C6-C7-C8	-2.14	109.01	115.92
25	Y	303	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
24	R	606	CHL	C2C-C3C-C4C	2.14	108.01	106.49
24	N	606	CHL	O2A-CGA-CBA	2.14	120.89	114.03
25	S	314	CLA	O2A-CGA-CBA	2.14	118.61	111.91
25	s	314	CLA	O2A-CGA-CBA	2.14	118.61	111.91
40	g	617	NEX	C10-C11-C12	2.14	129.88	123.22
25	c	504	CLA	C3C-C4C-NC	-2.13	108.18	110.57
25	B	602	CLA	C11-C10-C8	-2.13	109.02	115.92
25	B	615	CLA	CHD-C1D-C2D	2.13	129.96	125.48
25	B	604	CLA	CBA-CAA-C2A	-2.13	107.57	113.86
25	b	604	CLA	CBA-CAA-C2A	-2.13	107.57	113.86
24	n	606	CHL	O2A-CGA-CBA	2.13	120.88	114.03
25	c	512	CLA	CBA-CAA-C2A	-2.13	107.57	113.86
24	y	308	CHL	C3C-C4C-NC	-2.13	108.18	110.57
25	r	608	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
24	r	606	CHL	O2A-CGA-CBA	2.13	120.88	114.03
25	r	602	CLA	C3D-C4D-ND	2.13	113.69	110.24
25	s	310	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
25	R	612	CLA	C4D-CHA-C1A	-2.13	118.65	121.25
25	G	611	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
25	g	611	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
25	S	310	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
25	N	612	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
24	g	601	CHL	O2A-CGA-O1A	-2.13	118.22	123.59
25	R	603	CLA	CAD-C3D-C2D	2.13	151.07	140.80
25	r	603	CLA	CAD-C3D-C2D	2.13	151.07	140.80
29	l	101	SQD	O9-S-O7	2.13	121.32	113.95
24	Y	302	CHL	O1D-CGD-CBD	-2.13	120.13	124.48
28	B	619	BCR	C8-C7-C6	-2.13	121.22	127.20
28	b	619	BCR	C8-C7-C6	-2.13	121.22	127.20
25	B	603	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
25	b	603	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
28	z	101	BCR	C29-C30-C25	2.13	113.75	110.48
24	S	302	CHL	C2C-C3C-C4C	2.13	108.00	106.49
24	s	302	CHL	C2C-C3C-C4C	2.13	108.00	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	614	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
25	b	614	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
25	C	511	CLA	C11-C12-C13	-2.13	109.05	115.92
25	R	602	CLA	C3D-C4D-ND	2.13	113.68	110.24
24	N	605	CHL	O1D-CGD-CBD	-2.13	120.13	124.48
25	R	611	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
25	N	611	CLA	C3D-C4D-ND	2.12	113.67	110.24
25	c	509	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
25	n	612	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
25	D	403	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
25	d	403	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
24	g	607	CHL	O2A-CGA-O1A	-2.12	118.00	123.30
24	G	601	CHL	O2A-CGA-O1A	-2.12	118.23	123.59
24	y	302	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
25	C	508	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
24	s	307	CHL	O2A-CGA-CBA	2.12	120.85	114.03
25	G	602	CLA	C16-C15-C13	-2.12	109.06	115.92
25	y	311	CLA	C3D-C4D-ND	2.12	113.67	110.24
24	n	606	CHL	O2D-CGD-O1D	-2.12	119.69	123.84
25	c	511	CLA	C11-C12-C13	-2.12	109.06	115.92
25	n	613	CLA	C11-C10-C8	-2.12	109.07	115.92
25	c	508	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
25	r	602	CLA	O2A-CGA-CBA	2.12	118.56	111.91
24	6	601	CHL	C2A-C3A-C4A	2.12	105.29	101.87
24	g	609	CHL	C2C-C3C-C4C	2.12	108.00	106.49
25	B	616	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
25	g	602	CLA	C16-C15-C13	-2.12	109.07	115.92
25	C	506	CLA	C3D-C4D-ND	2.12	113.67	110.24
25	N	611	CLA	C6-C7-C8	-2.12	109.07	115.92
25	n	611	CLA	C6-C7-C8	-2.12	109.07	115.92
24	Y	306	CHL	C4D-CHA-C1A	2.12	123.83	121.25
29	L	103	SQD	O9-S-O7	2.12	121.28	113.95
28	c	514	BCR	C24-C23-C22	-2.12	123.03	126.23
24	S	308	CHL	C4D-CHA-C1A	2.12	123.83	121.25
25	g	610	CLA	C2D-C1D-ND	-2.12	108.54	110.10
25	R	601	CLA	C3B-C4B-NB	-2.12	106.47	109.21
24	S	307	CHL	O2A-CGA-CBA	2.12	120.83	114.03
40	G	617	NEX	C15-C35-C34	-2.12	119.14	123.47
29	l	102	SQD	O9-S-O7	2.12	121.28	113.95
25	C	512	CLA	CBA-CAA-C2A	-2.12	107.61	113.86
25	G	611	CLA	C1D-ND-C4D	-2.12	104.83	106.33
28	D	404	BCR	C29-C30-C25	2.12	113.74	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d	404	BCR	C29-C30-C25	2.12	113.74	110.48
25	C	504	CLA	C3C-C4C-NC	-2.12	108.20	110.57
29	A	411	SQD	O9-S-O7	2.12	121.27	113.95
29	a	412	SQD	O9-S-O7	2.12	121.27	113.95
24	Y	306	CHL	O2A-CGA-O1A	-2.12	118.25	123.59
25	r	602	CLA	CAA-CBA-CGA	-2.12	107.07	113.25
25	G	602	CLA	CHD-C4C-C3C	-2.12	121.73	124.84
25	R	609	CLA	CAA-CBA-CGA	-2.11	107.07	113.25
25	b	616	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
25	r	611	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
25	Y	311	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
40	g	617	NEX	C15-C35-C34	-2.11	119.14	123.47
40	y	318	NEX	C11-C12-C13	-2.11	120.48	126.42
25	N	613	CLA	C2C-C1C-NC	2.11	111.95	109.97
25	y	313	CLA	C2C-C1C-NC	2.11	111.95	109.97
25	g	611	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
25	G	611	CLA	C4D-C3D-CAD	-2.11	105.61	108.10
25	g	611	CLA	C4D-C3D-CAD	-2.11	105.61	108.10
25	N	611	CLA	C4D-CHA-C1A	-2.11	118.68	121.25
25	n	611	CLA	C4D-CHA-C1A	-2.11	118.68	121.25
25	Y	312	CLA	C2C-C1C-NC	2.11	111.95	109.97
25	y	312	CLA	C2C-C1C-NC	2.11	111.95	109.97
25	C	506	CLA	C11-C12-C13	-2.11	109.09	115.92
25	c	506	CLA	C11-C12-C13	-2.11	109.09	115.92
25	r	612	CLA	C2A-C3A-C4A	-2.11	98.46	101.87
25	R	612	CLA	C11-C10-C8	-2.11	109.09	115.92
25	b	615	CLA	CHD-C1D-C2D	2.11	129.91	125.48
28	h	101	BCR	C16-C15-C14	-2.11	119.15	123.47
24	5	301	CHL	O2D-CGD-O1D	-2.11	119.71	123.84
25	D	403	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
25	d	403	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
28	C	514	BCR	C24-C23-C22	-2.11	123.05	126.23
29	L	101	SQD	O9-S-O7	2.11	121.25	113.95
24	2	601	CHL	C2A-C3A-C4A	2.11	105.28	101.87
25	R	610	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
25	r	610	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
25	B	604	CLA	C16-C15-C13	-2.11	109.11	115.92
25	b	604	CLA	C16-C15-C13	-2.11	109.11	115.92
40	Y	318	NEX	C11-C12-C13	-2.11	120.49	126.42
25	R	602	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
25	N	610	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
25	n	610	CLA	O2D-CGD-O1D	-2.11	119.72	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	612	CLA	C2A-C3A-C4A	-2.11	98.47	101.87
24	g	605	CHL	C2C-C3C-C4C	2.11	107.99	106.49
25	Y	303	CLA	C3D-C4D-ND	2.11	113.65	110.24
25	d	403	CLA	CAD-C3D-C2D	2.11	150.97	140.80
25	N	613	CLA	CBA-CAA-C2A	-2.11	107.64	113.86
25	c	507	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
24	1	301	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
39	s	316	LUT	C12-C13-C14	-2.11	115.71	118.94
24	G	607	CHL	O2A-CGA-O1A	-2.11	118.05	123.30
24	g	608	CHL	C2C-C3C-C4C	2.11	107.99	106.49
24	n	605	CHL	O1D-CGD-CBD	-2.11	120.18	124.48
25	c	504	CLA	O2A-CGA-CBA	2.10	118.51	111.91
24	n	607	CHL	C1-C2-C3	2.10	129.68	126.04
25	R	602	CLA	O2A-CGA-CBA	2.10	118.51	111.91
25	a	406	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
25	c	510	CLA	C11-C10-C8	-2.10	109.12	115.92
24	S	308	CHL	O2A-CGA-CBA	2.10	120.79	114.03
24	Y	309	CHL	O1D-CGD-CBD	-2.10	120.18	124.48
28	Z	101	BCR	C29-C30-C25	2.10	113.72	110.48
24	s	308	CHL	O2A-CGA-CBA	2.10	120.78	114.03
25	C	510	CLA	C11-C10-C8	-2.10	109.12	115.92
25	N	602	CLA	C2C-C1C-NC	2.10	111.94	109.97
25	n	602	CLA	C2C-C1C-NC	2.10	111.94	109.97
24	N	605	CHL	C2C-C3C-C4C	2.10	107.99	106.49
24	n	605	CHL	C2C-C3C-C4C	2.10	107.99	106.49
39	N	615	LUT	C7-C8-C9	2.10	129.41	126.23
25	G	614	CLA	C4D-CHA-C1A	-2.10	118.69	121.25
25	g	614	CLA	C4D-CHA-C1A	-2.10	118.69	121.25
25	N	613	CLA	C11-C10-C8	-2.10	109.13	115.92
25	n	602	CLA	C11-C12-C13	-2.10	109.13	115.92
25	y	303	CLA	C3D-C4D-ND	2.10	113.64	110.24
25	G	614	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
25	G	611	CLA	O2A-CGA-CBA	2.10	118.50	111.91
24	2	603	CHL	C3D-C4D-ND	2.10	113.64	110.24
25	D	403	CLA	CAD-C3D-C2D	2.10	150.93	140.80
25	A	405	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
25	c	513	CLA	C6-C7-C8	-2.10	109.13	115.92
25	g	611	CLA	O2A-CGA-CBA	2.10	118.50	111.91
25	b	603	CLA	C3D-C4D-ND	2.10	113.63	110.24
24	y	309	CHL	O1D-CGD-CBD	-2.10	120.19	124.48
25	Y	304	CLA	C16-C15-C13	-2.10	109.13	115.92
24	2	603	CHL	O2A-CGA-CBA	2.10	120.77	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	101	BCR	C16-C15-C14	-2.10	119.17	123.47
25	C	504	CLA	O2A-CGA-CBA	2.10	118.50	111.91
25	c	511	CLA	C6-C7-C8	-2.10	109.14	115.92
24	Y	309	CHL	C2C-C3C-C4C	2.10	107.98	106.49
25	r	612	CLA	C11-C10-C8	-2.10	109.14	115.92
25	N	602	CLA	C11-C12-C13	-2.10	109.14	115.92
25	n	611	CLA	C3D-C4D-ND	2.10	113.63	110.24
28	K	101	BCR	C11-C10-C9	-2.10	124.32	127.31
24	6	603	CHL	O2A-CGA-CBA	2.10	120.77	114.03
25	r	609	CLA	CAA-CBA-CGA	-2.10	107.13	113.25
25	C	511	CLA	C6-C7-C8	-2.10	109.14	115.92
24	G	607	CHL	C2C-C3C-C4C	2.10	107.98	106.49
25	C	513	CLA	C6-C7-C8	-2.10	109.14	115.92
25	g	614	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
25	y	311	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
39	S	316	LUT	C12-C13-C14	-2.09	115.73	118.94
24	y	306	CHL	O2A-CGA-O1A	-2.09	118.31	123.59
24	1	301	CHL	O2D-CGD-O1D	-2.09	119.74	123.84
24	5	301	CHL	O1D-CGD-CBD	-2.09	120.20	124.48
24	1	301	CHL	C2A-C1A-CHA	2.09	127.52	123.86
39	n	615	LUT	C7-C8-C9	2.09	129.40	126.23
25	g	611	CLA	C1D-ND-C4D	-2.09	104.85	106.33
25	n	613	CLA	CBA-CAA-C2A	-2.09	107.69	113.86
25	C	501	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
25	c	501	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
39	S	315	LUT	C37-C21-C22	-2.09	105.47	109.44
39	s	315	LUT	C37-C21-C22	-2.09	105.47	109.44
24	6	603	CHL	C3D-C4D-ND	2.09	113.62	110.24
28	B	619	BCR	C15-C14-C13	-2.09	124.33	127.31
28	b	619	BCR	C15-C14-C13	-2.09	124.33	127.31
25	c	512	CLA	C11-C12-C13	-2.09	109.16	115.92
28	H	101	BCR	C8-C7-C6	-2.09	121.33	127.20
28	h	101	BCR	C8-C7-C6	-2.09	121.33	127.20
25	C	507	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
24	R	613	CHL	C2C-C3C-C4C	2.09	107.98	106.49
26	c	519	LHG	P-O6-C4	-2.09	109.42	121.68
25	S	304	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
25	y	304	CLA	C16-C15-C13	-2.09	109.17	115.92
26	C	519	LHG	P-O6-C4	-2.09	109.43	121.68
24	y	306	CHL	C2C-C3C-C4C	2.09	107.98	106.49
25	Y	304	CLA	C3D-C4D-ND	2.09	113.61	110.24
25	y	304	CLA	C3D-C4D-ND	2.09	113.61	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	603	CLA	C3C-C4C-NC	-2.09	108.23	110.57
25	B	607	CLA	O2A-CGA-CBA	2.09	118.46	111.91
25	b	607	CLA	O2A-CGA-CBA	2.09	118.46	111.91
25	C	504	CLA	CAD-C3D-C2D	2.09	150.87	140.80
25	B	616	CLA	C3D-C4D-ND	2.09	113.61	110.24
25	N	603	CLA	C3D-C4D-ND	2.09	113.61	110.24
25	n	603	CLA	C3D-C4D-ND	2.09	113.61	110.24
25	D	402	CLA	C16-C15-C13	-2.09	109.17	115.92
25	d	402	CLA	C16-C15-C13	-2.09	109.17	115.92
24	S	306	CHL	O2A-CGA-O1A	-2.09	118.10	123.30
25	Y	313	CLA	C3D-C4D-ND	2.09	113.61	110.24
24	G	609	CHL	C2C-C3C-C4C	2.09	107.98	106.49
25	C	512	CLA	C11-C12-C13	-2.09	109.18	115.92
25	G	611	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
24	R	607	CHL	O2A-CGA-O1A	-2.09	118.33	123.59
25	Y	311	CLA	C3D-C4D-ND	2.09	113.61	110.24
25	c	504	CLA	CAD-C3D-C2D	2.09	150.86	140.80
25	s	304	CLA	O2D-CGD-O1D	-2.08	119.76	123.84
24	S	308	CHL	C2C-C3C-C4C	2.08	107.97	106.49
25	b	601	CLA	C1D-CHD-C4C	-2.08	121.56	126.06
25	B	603	CLA	C3D-C4D-ND	2.08	113.61	110.24
25	R	609	CLA	C11-C12-C13	-2.08	109.19	115.92
25	c	508	CLA	C16-C15-C13	-2.08	109.19	115.92
25	C	503	CLA	C11-C10-C8	-2.08	109.19	115.92
25	c	503	CLA	C11-C10-C8	-2.08	109.19	115.92
25	B	607	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
25	B	606	CLA	C11-C10-C8	-2.08	109.19	115.92
25	b	606	CLA	C11-C10-C8	-2.08	109.19	115.92
25	S	303	CLA	O2A-CGA-CBA	2.08	118.44	111.91
25	s	303	CLA	O2A-CGA-CBA	2.08	118.44	111.91
25	n	611	CLA	C11-C10-C8	-2.08	109.19	115.92
25	d	403	CLA	C6-C7-C8	-2.08	109.19	115.92
25	y	313	CLA	C3D-C4D-ND	2.08	113.60	110.24
24	r	606	CHL	C2C-C3C-C4C	2.08	107.97	106.49
25	R	602	CLA	C11-C10-C8	-2.08	109.19	115.92
24	r	605	CHL	C4D-CHA-C1A	2.08	123.78	121.25
24	s	306	CHL	O2A-CGA-O1A	-2.08	118.12	123.30
25	r	609	CLA	C11-C12-C13	-2.08	109.20	115.92
25	Y	313	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
25	B	608	CLA	C3D-C4D-ND	2.08	113.60	110.24
25	b	608	CLA	C3D-C4D-ND	2.08	113.60	110.24
25	B	601	CLA	C1D-CHD-C4C	-2.08	121.57	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	604	CLA	C3D-C4D-ND	2.08	113.60	110.24
25	A	405	CLA	C6-C7-C8	-2.08	109.20	115.92
25	g	602	CLA	CHD-C4C-C3C	-2.08	121.79	124.84
24	r	607	CHL	O2A-CGA-O1A	-2.08	118.35	123.59
28	B	618	BCR	C29-C30-C25	2.08	113.68	110.48
28	b	618	BCR	C29-C30-C25	2.08	113.68	110.48
25	D	403	CLA	C3C-C4C-NC	-2.08	108.24	110.57
25	d	403	CLA	C3C-C4C-NC	-2.08	108.24	110.57
25	C	508	CLA	C16-C15-C13	-2.08	109.21	115.92
24	r	613	CHL	C2C-C3C-C4C	2.08	107.97	106.49
25	N	611	CLA	C11-C10-C8	-2.08	109.21	115.92
25	N	610	CLA	C3D-C4D-ND	2.08	113.60	110.24
25	n	610	CLA	C3D-C4D-ND	2.08	113.60	110.24
25	B	609	CLA	C11-C12-C13	-2.08	109.21	115.92
25	b	609	CLA	C11-C12-C13	-2.08	109.21	115.92
24	g	607	CHL	C2C-C3C-C4C	2.07	107.97	106.49
24	R	605	CHL	O1D-CGD-CBD	-2.07	120.24	124.48
24	r	605	CHL	O1D-CGD-CBD	-2.07	120.24	124.48
28	k	101	BCR	C11-C10-C9	-2.07	124.35	127.31
25	B	609	CLA	C16-C15-C13	-2.07	109.22	115.92
25	b	609	CLA	C16-C15-C13	-2.07	109.22	115.92
28	C	514	BCR	C27-C26-C25	2.07	125.74	122.73
28	c	514	BCR	C27-C26-C25	2.07	125.74	122.73
25	6	602	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
25	a	406	CLA	C6-C7-C8	-2.07	109.22	115.92
24	S	302	CHL	O2A-CGA-CBA	2.07	120.69	114.03
24	s	302	CHL	O2A-CGA-CBA	2.07	120.69	114.03
29	A	407	SQD	O9-S-C6	2.07	109.40	106.94
29	a	408	SQD	O9-S-C6	2.07	109.40	106.94
25	y	312	CLA	CAD-C3D-C2D	2.07	150.79	140.80
25	a	403	CLA	C6-C7-C8	-2.07	109.23	115.92
25	S	314	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
25	B	603	CLA	C6-C7-C8	-2.07	109.23	115.92
25	b	603	CLA	C6-C7-C8	-2.07	109.23	115.92
25	c	501	CLA	C6-C7-C8	-2.07	109.23	115.92
25	D	403	CLA	C6-C7-C8	-2.07	109.23	115.92
25	6	602	CLA	C3B-C4B-NB	-2.07	106.54	109.21
28	T	101	BCR	C24-C23-C22	-2.07	123.11	126.23
28	t	101	BCR	C24-C23-C22	-2.07	123.11	126.23
25	r	602	CLA	C11-C10-C8	-2.07	109.24	115.92
24	R	605	CHL	O2A-CGA-O1A	-2.07	118.15	123.30
24	r	605	CHL	O2A-CGA-O1A	-2.07	118.15	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	313	CLA	CAD-C3D-C2D	2.07	150.77	140.80
40	n	617	NEX	C11-C10-C9	2.07	130.26	127.31
25	y	313	CLA	C1B-CHB-C4A	-2.07	126.03	130.12
24	y	302	CHL	O2D-CGD-O1D	-2.07	119.80	123.84
24	R	605	CHL	O2A-CGA-CBA	2.06	120.66	114.03
24	r	605	CHL	O2A-CGA-CBA	2.06	120.66	114.03
25	b	607	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
24	1	301	CHL	C4D-CHA-C1A	2.06	123.76	121.25
25	A	402	CLA	C6-C7-C8	-2.06	109.25	115.92
25	Y	312	CLA	CAD-C3D-C2D	2.06	150.75	140.80
25	R	608	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
25	s	313	CLA	C4D-CHA-C1A	-2.06	118.74	121.25
25	B	609	CLA	C11-C10-C8	-2.06	109.25	115.92
25	C	501	CLA	C6-C7-C8	-2.06	109.25	115.92
25	b	612	CLA	C11-C10-C8	-2.06	109.25	115.92
24	Y	302	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
25	2	602	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
25	c	501	CLA	CAD-C3D-C2D	2.06	150.74	140.80
25	B	612	CLA	C11-C10-C8	-2.06	109.26	115.92
25	C	505	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
25	g	612	CLA	CHD-C1D-C2D	2.06	129.80	125.48
24	5	301	CHL	C2A-C1A-CHA	2.06	127.46	123.86
25	G	612	CLA	CHD-C1D-C2D	2.06	129.80	125.48
25	c	513	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
24	R	605	CHL	C2C-C3C-C4C	2.06	107.96	106.49
24	s	308	CHL	C2C-C3C-C4C	2.06	107.96	106.49
25	B	615	CLA	C11-C12-C13	-2.06	109.27	115.92
25	b	615	CLA	C11-C12-C13	-2.06	109.27	115.92
25	B	614	CLA	C3D-C4D-ND	2.06	113.57	110.24
25	b	614	CLA	C3D-C4D-ND	2.06	113.57	110.24
25	y	315	CLA	C3D-C4D-ND	2.06	113.57	110.24
25	C	511	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
25	c	511	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
25	B	603	CLA	C4D-CHA-C1A	-2.06	118.75	121.25
25	b	603	CLA	C4D-CHA-C1A	-2.06	118.75	121.25
25	C	513	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
25	B	602	CLA	C11-C12-C13	-2.06	109.27	115.92
25	B	612	CLA	C16-C15-C13	-2.06	109.27	115.92
25	b	612	CLA	C16-C15-C13	-2.06	109.27	115.92
25	g	613	CLA	C11-C10-C8	-2.06	109.27	115.92
25	S	313	CLA	C4D-CHA-C1A	-2.06	118.75	121.25
25	B	601	CLA	C1D-ND-C4D	-2.06	104.87	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	601	CLA	C1D-ND-C4D	-2.06	104.87	106.33
25	g	604	CLA	C3D-C4D-ND	2.06	113.56	110.24
40	G	617	NEX	C35-C15-C14	-2.06	119.26	123.47
25	G	613	CLA	C11-C10-C8	-2.06	109.28	115.92
25	C	501	CLA	CAD-C3D-C2D	2.05	150.71	140.80
40	g	617	NEX	C12-C13-C14	-2.05	115.79	118.94
25	C	508	CLA	C6-C7-C8	-2.05	109.28	115.92
25	A	405	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
25	a	406	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
24	G	605	CHL	C2C-C3C-C4C	2.05	107.95	106.49
25	S	313	CLA	CAD-C3D-C2D	2.05	150.70	140.80
24	n	606	CHL	O1D-CGD-CBD	-2.05	120.29	124.48
24	R	605	CHL	C4D-CHA-C1A	2.05	123.75	121.25
24	5	301	CHL	C4D-CHA-C1A	2.05	123.75	121.25
25	c	502	CLA	C2C-C1C-NC	2.05	111.89	109.97
25	2	602	CLA	C3B-C4B-NB	-2.05	106.56	109.21
25	b	602	CLA	C11-C12-C13	-2.05	109.30	115.92
25	N	604	CLA	C3D-C4D-ND	2.05	113.55	110.24
24	g	609	CHL	O1D-CGD-CBD	-2.05	120.29	124.48
25	b	609	CLA	C11-C10-C8	-2.05	109.30	115.92
40	N	617	NEX	C11-C10-C9	2.05	130.23	127.31
40	y	318	NEX	C31-C32-C33	2.05	132.17	126.42
25	c	508	CLA	C6-C7-C8	-2.05	109.30	115.92
25	Y	311	CLA	C6-C7-C8	-2.05	109.31	115.92
25	y	311	CLA	C6-C7-C8	-2.05	109.31	115.92
24	G	606	CHL	CBC-CAC-C3C	-2.05	106.79	112.43
28	I	101	BCR	C2-C1-C6	2.05	113.63	110.48
25	g	614	CLA	C3D-C4D-ND	2.05	113.55	110.24
25	G	610	CLA	C4D-C3D-CAD	-2.04	105.69	108.10
25	g	610	CLA	C4D-C3D-CAD	-2.04	105.69	108.10
24	s	308	CHL	O1D-CGD-CBD	-2.04	120.30	124.48
39	Y	316	LUT	C22-C23-C24	2.04	114.07	111.74
25	C	510	CLA	CAC-C3C-C4C	2.04	127.46	124.81
25	G	611	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
25	c	505	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
24	g	606	CHL	CBC-CAC-C3C	-2.04	106.80	112.43
25	n	611	CLA	CAD-C3D-C2D	2.04	150.66	140.80
25	C	502	CLA	C16-C15-C13	-2.04	109.32	115.92
25	Y	315	CLA	C3D-C4D-ND	2.04	113.54	110.24
24	S	307	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
24	Y	307	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
25	r	608	CLA	C2A-C1A-CHA	-2.04	120.29	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	502	CLA	C16-C15-C13	-2.04	109.32	115.92
24	G	609	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
25	Y	313	CLA	C11-C10-C8	-2.04	109.33	115.92
24	y	307	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
24	S	308	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
25	c	508	CLA	C4D-CHA-C1A	-2.04	118.77	121.25
40	g	617	NEX	C35-C15-C14	-2.04	119.30	123.47
25	S	303	CLA	C6-C7-C8	-2.04	109.33	115.92
25	B	601	CLA	CAD-C3D-C2D	2.04	150.64	140.80
25	b	601	CLA	CAD-C3D-C2D	2.04	150.64	140.80
24	s	306	CHL	C2C-C3C-C4C	2.04	107.94	106.49
25	B	607	CLA	C6-C7-C8	-2.04	109.33	115.92
25	C	503	CLA	C11-C12-C13	-2.04	109.33	115.92
25	c	503	CLA	C11-C12-C13	-2.04	109.33	115.92
25	N	611	CLA	CAD-C3D-C2D	2.04	150.63	140.80
24	Y	306	CHL	C2C-C3C-C4C	2.04	107.94	106.49
25	g	611	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
25	b	608	CLA	C16-C15-C13	-2.04	109.34	115.92
25	R	609	CLA	C11-C10-C8	-2.04	109.34	115.92
25	b	607	CLA	C6-C7-C8	-2.04	109.34	115.92
30	a	409	LMG	C6-C5-C4	-2.04	108.23	113.00
28	b	618	BCR	C8-C7-C6	-2.04	121.48	127.20
24	r	605	CHL	C2C-C3C-C4C	2.04	107.94	106.49
39	N	615	LUT	C35-C34-C33	2.04	130.22	127.31
25	N	603	CLA	C11-C12-C13	-2.04	109.34	115.92
25	n	603	CLA	C11-C12-C13	-2.04	109.34	115.92
25	y	313	CLA	C11-C10-C8	-2.04	109.34	115.92
25	B	608	CLA	C16-C15-C13	-2.04	109.34	115.92
25	C	505	CLA	C11-C10-C8	-2.03	109.34	115.92
24	n	605	CHL	C4D-CHA-C1A	2.03	123.72	121.25
25	s	314	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
24	1	302	CHL	C2A-C1A-CHA	2.03	127.41	123.86
25	c	512	CLA	C11-C10-C8	-2.03	109.35	115.92
25	s	303	CLA	C6-C7-C8	-2.03	109.35	115.92
25	C	512	CLA	C11-C10-C8	-2.03	109.35	115.92
25	B	602	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
25	B	611	CLA	C11-C12-C13	-2.03	109.36	115.92
25	C	501	CLA	C16-C15-C13	-2.03	109.36	115.92
25	b	611	CLA	C11-C12-C13	-2.03	109.36	115.92
25	c	501	CLA	C16-C15-C13	-2.03	109.36	115.92
24	s	307	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
24	N	609	CHL	O2D-CGD-O1D	-2.03	119.87	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	302	CHL	O2A-CGA-O1A	-2.03	118.24	123.30
24	s	302	CHL	O2A-CGA-O1A	-2.03	118.24	123.30
25	n	612	CLA	CAD-C3D-C2D	2.03	150.59	140.80
28	i	101	BCR	C2-C1-C6	2.03	113.61	110.48
25	S	304	CLA	CAD-C3D-C2D	2.03	150.59	140.80
25	s	304	CLA	CAD-C3D-C2D	2.03	150.59	140.80
27	A	404	PHO	C16-C15-C13	-2.03	109.36	115.92
27	a	405	PHO	C16-C15-C13	-2.03	109.36	115.92
28	B	618	BCR	C8-C7-C6	-2.03	121.50	127.20
25	G	610	CLA	C11-C10-C8	-2.03	109.36	115.92
28	A	406	BCR	C20-C21-C22	-2.03	124.42	127.31
28	a	407	BCR	C20-C21-C22	-2.03	124.42	127.31
40	Y	318	NEX	C31-C32-C33	2.03	132.11	126.42
25	G	614	CLA	C3D-C4D-ND	2.03	113.52	110.24
25	r	604	CLA	CAD-C3D-C2D	2.03	150.58	140.80
28	T	101	BCR	C8-C7-C6	-2.03	121.51	127.20
29	A	407	SQD	O9-S-O7	2.03	120.96	113.95
29	a	408	SQD	O9-S-O7	2.03	120.96	113.95
24	Y	309	CHL	O2A-CGA-O1A	-2.03	118.48	123.59
24	y	309	CHL	O2A-CGA-O1A	-2.03	118.48	123.59
25	N	612	CLA	CAD-C3D-C2D	2.03	150.57	140.80
24	S	306	CHL	C2C-C3C-C4C	2.03	107.93	106.49
25	C	507	CLA	CAD-C3D-C2D	2.03	150.57	140.80
25	B	609	CLA	C6-C7-C8	-2.02	109.37	115.92
25	b	609	CLA	C6-C7-C8	-2.02	109.37	115.92
24	n	609	CHL	O2D-CGD-O1D	-2.02	119.88	123.84
25	c	505	CLA	C11-C10-C8	-2.02	109.38	115.92
25	C	511	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
25	r	609	CLA	C11-C10-C8	-2.02	109.38	115.92
25	C	503	CLA	C3D-C4D-ND	2.02	113.51	110.24
24	S	308	CHL	C2A-C1A-CHA	2.02	127.40	123.86
24	s	308	CHL	C2A-C1A-CHA	2.02	127.40	123.86
25	B	615	CLA	C16-C15-C13	-2.02	109.38	115.92
25	b	615	CLA	C16-C15-C13	-2.02	109.38	115.92
28	t	101	BCR	C8-C7-C6	-2.02	121.52	127.20
25	S	309	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
25	R	604	CLA	CAD-C3D-C2D	2.02	150.56	140.80
25	c	507	CLA	CAD-C3D-C2D	2.02	150.56	140.80
25	C	513	CLA	C11-C12-C13	-2.02	109.38	115.92
25	c	513	CLA	C11-C12-C13	-2.02	109.38	115.92
25	n	603	CLA	C6-C7-C8	-2.02	109.39	115.92
28	I	101	BCR	C8-C7-C6	-2.02	121.53	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	604	CLA	C3D-C4D-ND	2.02	113.51	110.24
25	R	602	CLA	C6-C7-C8	-2.02	109.39	115.92
27	a	405	PHO	C11-C12-C13	-2.02	109.39	115.92
25	C	501	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
25	c	501	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
25	B	603	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
25	b	603	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
25	C	508	CLA	C4D-CHA-C1A	-2.02	118.79	121.25
25	c	511	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
24	r	606	CHL	C2A-C3A-C4A	2.02	105.13	101.87
27	A	404	PHO	C11-C12-C13	-2.02	109.40	115.92
24	S	306	CHL	O2A-CGA-CBA	2.02	120.51	114.03
24	s	306	CHL	O2A-CGA-CBA	2.02	120.51	114.03
25	R	604	CLA	C1D-CHD-C4C	-2.02	121.71	126.06
28	z	101	BCR	C16-C15-C14	-2.02	119.34	123.47
25	N	602	CLA	C11-C10-C8	-2.02	109.40	115.92
25	n	602	CLA	C11-C10-C8	-2.02	109.40	115.92
25	r	602	CLA	C6-C7-C8	-2.02	109.40	115.92
25	G	613	CLA	CHD-C4C-C3C	-2.02	121.88	124.84
25	C	510	CLA	CAD-C3D-C2D	2.02	150.53	140.80
25	c	510	CLA	CAD-C3D-C2D	2.02	150.53	140.80
24	G	609	CHL	O2D-CGD-O1D	-2.02	119.90	123.84
24	r	613	CHL	C2A-C1A-CHA	2.02	127.37	123.85
25	n	610	CLA	C11-C10-C8	-2.01	109.41	115.92
25	s	309	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
25	c	504	CLA	C11-C10-C8	-2.01	109.41	115.92
25	C	504	CLA	C11-C10-C8	-2.01	109.41	115.92
25	R	609	CLA	C6-C7-C8	-2.01	109.41	115.92
25	B	611	CLA	C16-C15-C13	-2.01	109.41	115.92
25	b	611	CLA	C16-C15-C13	-2.01	109.41	115.92
25	S	310	CLA	CHB-C4A-NA	-2.01	121.73	124.51
25	B	601	CLA	C4D-C3D-CAD	-2.01	105.72	108.10
25	b	601	CLA	C4D-C3D-CAD	-2.01	105.72	108.10
24	N	605	CHL	C4D-CHA-C1A	2.01	123.70	121.25
25	B	613	CLA	C3D-C4D-ND	2.01	113.49	110.24
25	r	609	CLA	C6-C7-C8	-2.01	109.41	115.92
25	r	612	CLA	CAD-C3D-C2D	2.01	150.51	140.80
25	Y	311	CLA	C11-C10-C8	-2.01	109.41	115.92
25	c	510	CLA	CAC-C3C-C4C	2.01	127.42	124.81
25	c	512	CLA	C16-C15-C13	-2.01	109.42	115.92
25	G	610	CLA	CAD-C3D-C2D	2.01	150.50	140.80
25	N	603	CLA	C6-C7-C8	-2.01	109.42	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	311	CLA	C11-C10-C8	-2.01	109.42	115.92
25	b	613	CLA	C3D-C4D-ND	2.01	113.49	110.24
28	i	101	BCR	C8-C7-C6	-2.01	121.56	127.20
25	N	610	CLA	C11-C10-C8	-2.01	109.42	115.92
39	n	615	LUT	C35-C34-C33	2.01	130.18	127.31
25	N	602	CLA	C3D-C4D-ND	2.01	113.49	110.24
24	G	606	CHL	C2A-C1A-CHA	2.01	127.37	123.86
39	y	316	LUT	C22-C23-C24	2.01	114.03	111.74
25	2	605	CLA	C2A-C3A-C4A	-2.01	98.62	101.87
25	B	610	CLA	C16-C15-C13	-2.01	109.43	115.92
25	b	605	CLA	C16-C15-C13	-2.01	109.43	115.92
25	b	610	CLA	C16-C15-C13	-2.01	109.43	115.92
25	s	303	CLA	C11-C10-C8	-2.01	109.43	115.92
25	g	610	CLA	CAD-C3D-C2D	2.01	150.49	140.80
30	A	408	LMG	C6-C5-C4	-2.01	108.30	113.00
24	Y	302	CHL	C3C-C4C-NC	-2.01	108.32	110.57
24	y	302	CHL	C3C-C4C-NC	-2.01	108.32	110.57
24	s	307	CHL	O2D-CGD-O1D	-2.01	119.91	123.84
25	n	602	CLA	C3D-C4D-ND	2.01	113.48	110.24
25	R	612	CLA	CAD-C3D-C2D	2.01	150.48	140.80
25	B	602	CLA	C4D-CHA-C1A	-2.01	118.81	121.25
24	Y	302	CHL	O2A-CGA-O1A	-2.01	118.53	123.59
24	y	302	CHL	O2A-CGA-O1A	-2.01	118.53	123.59
25	Y	304	CLA	CAD-C3D-C2D	2.01	150.48	140.80
25	y	304	CLA	CAD-C3D-C2D	2.01	150.48	140.80
25	C	509	CLA	C11-C12-C13	-2.01	109.44	115.92
25	b	604	CLA	C11-C10-C8	-2.01	109.44	115.92
25	C	512	CLA	C16-C15-C13	-2.00	109.44	115.92
25	C	502	CLA	C2C-C1C-NC	2.00	111.85	109.97
41	R	616	XAT	C32-C33-C34	2.00	122.02	118.94
41	r	616	XAT	C32-C33-C34	2.00	122.02	118.94
24	G	601	CHL	C3C-C4C-NC	-2.00	108.32	110.57
25	r	602	CLA	CAD-C3D-C2D	2.00	150.47	140.80
25	C	511	CLA	C11-C10-C8	-2.00	109.44	115.92
24	R	605	CHL	O2D-CGD-O1D	-2.00	119.92	123.84
24	r	605	CHL	O2D-CGD-O1D	-2.00	119.92	123.84
25	D	402	CLA	C6-C7-C8	-2.00	109.44	115.92
25	d	402	CLA	C6-C7-C8	-2.00	109.44	115.92
25	B	605	CLA	C16-C15-C13	-2.00	109.44	115.92
24	R	613	CHL	C2A-C1A-CHA	2.00	127.35	123.85
28	Z	101	BCR	C16-C15-C14	-2.00	119.37	123.47
25	Y	303	CLA	CHD-C1D-C2D	2.00	129.68	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	303	CLA	CHD-C1D-C2D	2.00	129.68	125.48
39	G	615	LUT	C37-C21-C22	-2.00	105.64	109.44
39	g	615	LUT	C37-C21-C22	-2.00	105.64	109.44
25	b	602	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
25	R	602	CLA	CAD-C3D-C2D	2.00	150.46	140.80
24	R	606	CHL	C2A-C3A-C4A	2.00	105.10	101.87
25	r	604	CLA	C1D-CHD-C4C	-2.00	121.74	126.06
25	C	506	CLA	C11-C10-C8	-2.00	109.45	115.92
25	C	508	CLA	C11-C10-C8	-2.00	109.45	115.92
25	c	506	CLA	C11-C10-C8	-2.00	109.45	115.92
39	Y	316	LUT	C37-C21-C22	-2.00	105.65	109.44
25	c	503	CLA	C3D-C4D-ND	2.00	113.47	110.24
25	A	402	CLA	CAD-C3D-C2D	2.00	150.45	140.80
25	a	403	CLA	CAD-C3D-C2D	2.00	150.45	140.80
25	C	512	CLA	C6-C7-C8	-2.00	109.45	115.92

All (324) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	301	CHL	ND
24	1	301	CHL	NA
24	1	301	CHL	NC
24	1	302	CHL	ND
24	1	302	CHL	NA
24	1	302	CHL	NC
24	2	601	CHL	ND
24	2	601	CHL	NA
24	2	601	CHL	NC
24	2	603	CHL	ND
24	2	603	CHL	NA
24	2	603	CHL	NC
24	S	302	CHL	ND
24	S	302	CHL	NC
24	S	306	CHL	ND
24	S	306	CHL	NA
24	S	306	CHL	NC
24	S	307	CHL	ND
24	S	307	CHL	NA
24	S	307	CHL	NC
24	S	308	CHL	ND
24	S	308	CHL	NA
24	S	308	CHL	NC

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Mol	Chain	Res	Type	Atom
24	G	601	CHL	ND
24	G	601	CHL	NC
24	G	605	CHL	ND
24	G	605	CHL	NA
24	G	605	CHL	NC
24	G	606	CHL	ND
24	G	606	CHL	NA
24	G	606	CHL	NC
24	G	607	CHL	ND
24	G	607	CHL	NC
24	G	608	CHL	ND
24	G	608	CHL	NA
24	G	608	CHL	NC
24	G	609	CHL	ND
24	G	609	CHL	NA
24	G	609	CHL	NC
24	N	601	CHL	ND
24	N	601	CHL	NC
24	N	605	CHL	ND
24	N	605	CHL	NA
24	N	605	CHL	NC
24	N	606	CHL	ND
24	N	606	CHL	NC
24	N	607	CHL	ND
24	N	607	CHL	NC
24	N	608	CHL	ND
24	N	608	CHL	NA
24	N	608	CHL	NC
24	N	609	CHL	ND
24	N	609	CHL	NC
24	Y	302	CHL	ND
24	Y	302	CHL	NC
24	Y	306	CHL	ND
24	Y	306	CHL	NA
24	Y	306	CHL	NC
24	Y	307	CHL	NC
24	Y	307	CHL	ND
24	Y	307	CHL	NA
24	Y	308	CHL	ND
24	Y	308	CHL	NC
24	Y	309	CHL	ND
24	Y	309	CHL	NA

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Mol	Chain	Res	Type	Atom
24	Y	309	CHL	NC
24	Y	310	CHL	ND
24	Y	310	CHL	NA
24	Y	310	CHL	NC
24	R	605	CHL	ND
24	R	605	CHL	NA
24	R	605	CHL	NC
24	R	606	CHL	ND
24	R	606	CHL	NA
24	R	606	CHL	NC
24	R	607	CHL	ND
24	R	607	CHL	NA
24	R	607	CHL	NC
24	R	613	CHL	ND
24	R	613	CHL	NA
24	R	613	CHL	NC
24	5	301	CHL	ND
24	5	301	CHL	NA
24	5	301	CHL	NC
24	5	302	CHL	ND
24	5	302	CHL	NA
24	5	302	CHL	NC
24	6	601	CHL	ND
24	6	601	CHL	NA
24	6	601	CHL	NC
24	6	603	CHL	ND
24	6	603	CHL	NA
24	6	603	CHL	NC
24	s	302	CHL	ND
24	s	302	CHL	NC
24	s	306	CHL	ND
24	s	306	CHL	NA
24	s	306	CHL	NC
24	s	307	CHL	ND
24	s	307	CHL	NA
24	s	307	CHL	NC
24	s	308	CHL	ND
24	s	308	CHL	NA
24	s	308	CHL	NC
24	g	601	CHL	ND
24	g	601	CHL	NC
24	g	605	CHL	ND

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Mol	Chain	Res	Type	Atom
24	g	605	CHL	NA
24	g	605	CHL	NC
24	g	606	CHL	ND
24	g	606	CHL	NA
24	g	606	CHL	NC
24	g	607	CHL	ND
24	g	607	CHL	NC
24	g	608	CHL	ND
24	g	608	CHL	NA
24	g	608	CHL	NC
24	g	609	CHL	ND
24	g	609	CHL	NA
24	g	609	CHL	NC
24	n	601	CHL	ND
24	n	601	CHL	NC
24	n	605	CHL	ND
24	n	605	CHL	NA
24	n	605	CHL	NC
24	n	606	CHL	ND
24	n	606	CHL	NC
24	n	607	CHL	ND
24	n	607	CHL	NC
24	n	608	CHL	ND
24	n	608	CHL	NA
24	n	608	CHL	NC
24	n	609	CHL	ND
24	n	609	CHL	NC
24	y	302	CHL	ND
24	y	302	CHL	NC
24	y	306	CHL	ND
24	y	306	CHL	NA
24	y	306	CHL	NC
24	y	307	CHL	NC
24	y	307	CHL	ND
24	y	307	CHL	NA
24	y	308	CHL	ND
24	y	308	CHL	NC
24	y	309	CHL	ND
24	y	309	CHL	NA
24	y	309	CHL	NC
24	y	310	CHL	ND
24	y	310	CHL	NA

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Mol	Chain	Res	Type	Atom
24	y	310	CHL	NC
24	r	605	CHL	ND
24	r	605	CHL	NA
24	r	605	CHL	NC
24	r	606	CHL	ND
24	r	606	CHL	NA
24	r	606	CHL	NC
24	r	607	CHL	ND
24	r	607	CHL	NA
24	r	607	CHL	NC
24	r	613	CHL	ND
24	r	613	CHL	NA
24	r	613	CHL	NC
25	2	602	CLA	ND
25	2	604	CLA	ND
25	2	605	CLA	ND
25	A	401	CLA	ND
25	A	402	CLA	ND
25	A	405	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND

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Mol	Chain	Res	Type	Atom
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	401	CLA	ND
25	D	402	CLA	ND
25	D	403	CLA	ND
25	S	303	CLA	ND
25	S	304	CLA	ND
25	S	305	CLA	ND
25	S	309	CLA	ND
25	S	310	CLA	ND
25	S	311	CLA	ND
25	S	312	CLA	ND
25	S	313	CLA	ND
25	S	314	CLA	ND
25	G	602	CLA	ND
25	G	603	CLA	ND
25	G	604	CLA	ND
25	G	610	CLA	ND
25	G	611	CLA	ND
25	G	612	CLA	ND
25	G	613	CLA	ND
25	G	614	CLA	ND
25	N	602	CLA	ND
25	N	603	CLA	ND
25	N	604	CLA	ND
25	N	610	CLA	ND
25	N	611	CLA	ND
25	N	612	CLA	ND
25	N	613	CLA	ND
25	N	614	CLA	ND
25	Y	303	CLA	ND
25	Y	304	CLA	ND
25	Y	305	CLA	ND
25	Y	311	CLA	ND
25	Y	312	CLA	ND
25	Y	313	CLA	ND
25	Y	314	CLA	ND
25	Y	315	CLA	ND

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Mol	Chain	Res	Type	Atom
25	R	601	CLA	ND
25	R	602	CLA	ND
25	R	603	CLA	ND
25	R	604	CLA	ND
25	R	608	CLA	ND
25	R	609	CLA	ND
25	R	610	CLA	ND
25	R	611	CLA	ND
25	R	612	CLA	ND
25	R	614	CLA	ND
25	6	602	CLA	ND
25	6	604	CLA	ND
25	6	605	CLA	ND
25	a	402	CLA	ND
25	a	403	CLA	ND
25	a	406	CLA	ND
25	b	601	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND

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Mol	Chain	Res	Type	Atom
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	401	CLA	ND
25	d	402	CLA	ND
25	d	403	CLA	ND
25	s	303	CLA	ND
25	s	304	CLA	ND
25	s	305	CLA	ND
25	s	309	CLA	ND
25	s	310	CLA	ND
25	s	311	CLA	ND
25	s	312	CLA	ND
25	s	313	CLA	ND
25	s	314	CLA	ND
25	g	602	CLA	ND
25	g	603	CLA	ND
25	g	604	CLA	ND
25	g	610	CLA	ND
25	g	611	CLA	ND
25	g	612	CLA	ND
25	g	613	CLA	ND
25	g	614	CLA	ND
25	n	602	CLA	ND
25	n	603	CLA	ND
25	n	604	CLA	ND
25	n	610	CLA	ND
25	n	611	CLA	ND
25	n	612	CLA	ND
25	n	613	CLA	ND
25	n	614	CLA	ND
25	y	303	CLA	ND
25	y	304	CLA	ND
25	y	305	CLA	ND
25	y	311	CLA	ND
25	y	312	CLA	ND
25	y	313	CLA	ND
25	y	314	CLA	ND
25	y	315	CLA	ND
25	r	601	CLA	ND
25	r	602	CLA	ND
25	r	603	CLA	ND

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Mol	Chain	Res	Type	Atom
25	r	604	CLA	ND
25	r	608	CLA	ND
25	r	609	CLA	ND
25	r	610	CLA	ND
25	r	611	CLA	ND
25	r	612	CLA	ND
25	r	614	CLA	ND

All (3889) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	302	CHL	C1A-C2A-CAA-CBA
24	1	302	CHL	C3A-C2A-CAA-CBA
24	2	601	CHL	C1C-C2C-CMC-OMC
24	2	601	CHL	C3C-C2C-CMC-OMC
24	2	601	CHL	CHA-CBD-CGD-O2D
24	2	601	CHL	CBD-CGD-O2D-CED
24	2	601	CHL	C6-C7-C8-C10
24	2	603	CHL	C1C-C2C-CMC-OMC
24	2	603	CHL	C3C-C2C-CMC-OMC
24	2	603	CHL	CAD-CBD-CGD-O1D
24	2	603	CHL	CBD-CGD-O2D-CED
24	S	302	CHL	CHA-CBD-CGD-O2D
24	S	306	CHL	CHA-CBD-CGD-O1D
24	S	306	CHL	CAD-CBD-CGD-O1D
24	S	307	CHL	C1A-C2A-CAA-CBA
24	S	307	CHL	C3A-C2A-CAA-CBA
24	G	601	CHL	C3C-C2C-CMC-OMC
24	G	601	CHL	C2-C3-C5-C6
24	G	601	CHL	C11-C10-C8-C7
24	G	605	CHL	C1A-C2A-CAA-CBA
24	G	605	CHL	C3A-C2A-CAA-CBA
24	G	605	CHL	C1C-C2C-CMC-OMC
24	G	605	CHL	CHA-CBD-CGD-O2D
24	G	607	CHL	CHA-CBD-CGD-O1D
24	G	608	CHL	C1A-C2A-CAA-CBA
24	G	608	CHL	C3A-C2A-CAA-CBA
24	G	608	CHL	C1C-C2C-CMC-OMC
24	G	608	CHL	C3C-C2C-CMC-OMC
24	G	608	CHL	CBD-CGD-O2D-CED
24	G	609	CHL	C1C-C2C-CMC-OMC
24	G	609	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	N	601	CHL	C1A-C2A-CAA-CBA
24	N	601	CHL	C1C-C2C-CMC-OMC
24	N	601	CHL	C3C-C2C-CMC-OMC
24	N	601	CHL	CHA-CBD-CGD-O1D
24	N	601	CHL	CHA-CBD-CGD-O2D
24	N	601	CHL	C2-C3-C5-C6
24	N	601	CHL	C4-C3-C5-C6
24	N	606	CHL	CHA-CBD-CGD-O2D
24	N	607	CHL	C1A-C2A-CAA-CBA
24	N	607	CHL	C3A-C2A-CAA-CBA
24	N	607	CHL	CAD-CBD-CGD-O2D
24	N	607	CHL	C4-C3-C5-C6
24	N	608	CHL	C1A-C2A-CAA-CBA
24	N	608	CHL	C1C-C2C-CMC-OMC
24	N	608	CHL	CHA-CBD-CGD-O2D
24	N	609	CHL	C1A-C2A-CAA-CBA
24	N	609	CHL	C3A-C2A-CAA-CBA
24	N	609	CHL	C11-C10-C8-C9
24	Y	302	CHL	C1C-C2C-CMC-OMC
24	Y	302	CHL	C3C-C2C-CMC-OMC
24	Y	302	CHL	CHA-CBD-CGD-O2D
24	Y	309	CHL	C1A-C2A-CAA-CBA
24	Y	309	CHL	C1C-C2C-CMC-OMC
24	Y	309	CHL	CHA-CBD-CGD-O2D
24	Y	309	CHL	C14-C13-C15-C16
24	Y	310	CHL	C1A-C2A-CAA-CBA
24	R	606	CHL	C1A-C2A-CAA-CBA
24	R	606	CHL	CHA-CBD-CGD-O1D
24	R	606	CHL	CHA-CBD-CGD-O2D
24	R	607	CHL	CBA-CGA-O2A-C1
24	R	607	CHL	O1A-CGA-O2A-C1
24	R	613	CHL	CHA-CBD-CGD-O1D
24	R	613	CHL	CHA-CBD-CGD-O2D
24	R	613	CHL	CAD-CBD-CGD-O1D
24	5	302	CHL	C1A-C2A-CAA-CBA
24	5	302	CHL	C3A-C2A-CAA-CBA
24	6	601	CHL	C1C-C2C-CMC-OMC
24	6	601	CHL	C3C-C2C-CMC-OMC
24	6	601	CHL	CHA-CBD-CGD-O2D
24	6	601	CHL	CBD-CGD-O2D-CED
24	6	601	CHL	C6-C7-C8-C10
24	6	603	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	6	603	CHL	C3C-C2C-CMC-OMC
24	6	603	CHL	CAD-CBD-CGD-O1D
24	6	603	CHL	CBD-CGD-O2D-CED
24	s	302	CHL	CHA-CBD-CGD-O2D
24	s	306	CHL	CHA-CBD-CGD-O1D
24	s	306	CHL	CAD-CBD-CGD-O1D
24	s	307	CHL	C1A-C2A-CAA-CBA
24	s	307	CHL	C3A-C2A-CAA-CBA
24	g	601	CHL	C3C-C2C-CMC-OMC
24	g	601	CHL	C2-C3-C5-C6
24	g	601	CHL	C11-C10-C8-C7
24	g	605	CHL	C1A-C2A-CAA-CBA
24	g	605	CHL	C3A-C2A-CAA-CBA
24	g	605	CHL	C1C-C2C-CMC-OMC
24	g	605	CHL	CHA-CBD-CGD-O2D
24	g	607	CHL	CHA-CBD-CGD-O1D
24	g	608	CHL	C1A-C2A-CAA-CBA
24	g	608	CHL	C3A-C2A-CAA-CBA
24	g	608	CHL	C1C-C2C-CMC-OMC
24	g	608	CHL	C3C-C2C-CMC-OMC
24	g	608	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	C1C-C2C-CMC-OMC
24	g	609	CHL	C3C-C2C-CMC-OMC
24	n	601	CHL	C1C-C2C-CMC-OMC
24	n	601	CHL	C3C-C2C-CMC-OMC
24	n	601	CHL	CHA-CBD-CGD-O1D
24	n	601	CHL	CHA-CBD-CGD-O2D
24	n	601	CHL	C2-C3-C5-C6
24	n	601	CHL	C4-C3-C5-C6
24	n	606	CHL	CHA-CBD-CGD-O2D
24	n	607	CHL	C1A-C2A-CAA-CBA
24	n	607	CHL	C3A-C2A-CAA-CBA
24	n	607	CHL	CAD-CBD-CGD-O2D
24	n	607	CHL	C4-C3-C5-C6
24	n	608	CHL	C1A-C2A-CAA-CBA
24	n	608	CHL	C1C-C2C-CMC-OMC
24	n	608	CHL	CHA-CBD-CGD-O2D
24	n	609	CHL	C1A-C2A-CAA-CBA
24	n	609	CHL	C3A-C2A-CAA-CBA
24	n	609	CHL	C11-C10-C8-C9
24	y	302	CHL	C1C-C2C-CMC-OMC
24	y	302	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	y	302	CHL	CHA-CBD-CGD-O2D
24	y	309	CHL	C1A-C2A-CAA-CBA
24	y	309	CHL	C1C-C2C-CMC-OMC
24	y	309	CHL	CHA-CBD-CGD-O2D
24	y	309	CHL	C14-C13-C15-C16
24	y	310	CHL	C1A-C2A-CAA-CBA
24	r	606	CHL	C1A-C2A-CAA-CBA
24	r	606	CHL	CHA-CBD-CGD-O1D
24	r	606	CHL	CHA-CBD-CGD-O2D
24	r	607	CHL	CBA-CGA-O2A-C1
24	r	607	CHL	O1A-CGA-O2A-C1
24	r	613	CHL	CHA-CBD-CGD-O1D
24	r	613	CHL	CHA-CBD-CGD-O2D
24	r	613	CHL	CAD-CBD-CGD-O1D
25	2	602	CLA	C1A-C2A-CAA-CBA
25	2	602	CLA	C3A-C2A-CAA-CBA
25	2	602	CLA	CAD-CBD-CGD-O1D
25	2	602	CLA	CAD-CBD-CGD-O2D
25	2	604	CLA	CBD-CGD-O2D-CED
25	2	604	CLA	C2-C3-C5-C6
25	2	605	CLA	C1A-C2A-CAA-CBA
25	2	605	CLA	C3A-C2A-CAA-CBA
25	A	402	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	CHA-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	602	CLA	C2-C3-C5-C6
25	B	602	CLA	C6-C7-C8-C9
25	B	604	CLA	C1A-C2A-CAA-CBA
25	B	604	CLA	C6-C7-C8-C9
25	B	604	CLA	C11-C12-C13-C15
25	B	609	CLA	C1A-C2A-CAA-CBA
25	B	609	CLA	C3A-C2A-CAA-CBA
25	B	612	CLA	C1A-C2A-CAA-CBA
25	B	612	CLA	C3A-C2A-CAA-CBA
25	B	614	CLA	CHA-CBD-CGD-O1D
25	B	614	CLA	CHA-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	C4-C3-C5-C6
25	C	506	CLA	C14-C13-C15-C16
25	C	507	CLA	C2-C3-C5-C6
25	C	507	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	D	401	CLA	CHA-CBD-CGD-O2D
25	D	402	CLA	C1A-C2A-CAA-CBA
25	D	402	CLA	C3A-C2A-CAA-CBA
25	D	403	CLA	C1A-C2A-CAA-CBA
25	D	403	CLA	C3A-C2A-CAA-CBA
25	S	303	CLA	C1A-C2A-CAA-CBA
25	S	305	CLA	C3A-C2A-CAA-CBA
25	S	305	CLA	CHA-CBD-CGD-O2D
25	S	305	CLA	CBD-CGD-O2D-CED
25	S	310	CLA	C1-C2-C3-C4
25	S	310	CLA	C2-C3-C5-C6
25	S	311	CLA	C1A-C2A-CAA-CBA
25	S	311	CLA	CHA-CBD-CGD-O1D
25	S	311	CLA	CAD-CBD-CGD-O1D
25	S	311	CLA	CAD-CBD-CGD-O2D
25	S	313	CLA	C1A-C2A-CAA-CBA
25	S	313	CLA	C3A-C2A-CAA-CBA
25	G	604	CLA	CBD-CGD-O2D-CED
25	G	610	CLA	CBD-CGD-O2D-CED
25	G	611	CLA	C3A-C2A-CAA-CBA
25	G	611	CLA	CAD-CBD-CGD-O1D
25	G	611	CLA	CAD-CBD-CGD-O2D
25	G	611	CLA	C2-C3-C5-C6
25	G	613	CLA	C1A-C2A-CAA-CBA
25	G	614	CLA	C1A-C2A-CAA-CBA
25	G	614	CLA	C3A-C2A-CAA-CBA
25	G	614	CLA	CAD-CBD-CGD-O1D
25	N	604	CLA	C1A-C2A-CAA-CBA
25	N	604	CLA	C3A-C2A-CAA-CBA
25	N	610	CLA	C1A-C2A-CAA-CBA
25	N	610	CLA	C1-C2-C3-C4
25	N	610	CLA	C4-C3-C5-C6
25	N	611	CLA	C1A-C2A-CAA-CBA
25	N	611	CLA	C3A-C2A-CAA-CBA
25	N	613	CLA	CHA-CBD-CGD-O1D
25	N	613	CLA	CBD-CGD-O2D-CED
25	N	614	CLA	CBD-CGD-O2D-CED
25	Y	304	CLA	CHA-CBD-CGD-O2D
25	Y	305	CLA	CBD-CGD-O2D-CED
25	Y	311	CLA	CBD-CGD-O2D-CED
25	Y	312	CLA	CBA-CGA-O2A-C1
25	Y	312	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	Y	314	CLA	CHA-CBD-CGD-O1D
25	Y	314	CLA	C14-C13-C15-C16
25	Y	315	CLA	C1A-C2A-CAA-CBA
25	Y	315	CLA	CHA-CBD-CGD-O2D
25	Y	315	CLA	CBD-CGD-O2D-CED
25	Y	315	CLA	O1D-CGD-O2D-CED
25	R	601	CLA	C1A-C2A-CAA-CBA
25	R	601	CLA	C3A-C2A-CAA-CBA
25	R	602	CLA	CHA-CBD-CGD-O1D
25	R	603	CLA	CBD-CGD-O2D-CED
25	R	603	CLA	C6-C7-C8-C9
25	R	608	CLA	CHA-CBD-CGD-O2D
25	R	608	CLA	CBD-CGD-O2D-CED
25	R	609	CLA	C1A-C2A-CAA-CBA
25	R	610	CLA	C3A-C2A-CAA-CBA
25	R	611	CLA	C3A-C2A-CAA-CBA
25	R	611	CLA	CHA-CBD-CGD-O1D
25	R	611	CLA	CBD-CGD-O2D-CED
25	R	612	CLA	CHA-CBD-CGD-O1D
25	R	614	CLA	C1A-C2A-CAA-CBA
25	6	602	CLA	C1A-C2A-CAA-CBA
25	6	602	CLA	C3A-C2A-CAA-CBA
25	6	602	CLA	CAD-CBD-CGD-O1D
25	6	602	CLA	CAD-CBD-CGD-O2D
25	6	604	CLA	CBD-CGD-O2D-CED
25	6	604	CLA	C2-C3-C5-C6
25	6	605	CLA	C1A-C2A-CAA-CBA
25	6	605	CLA	C3A-C2A-CAA-CBA
25	a	403	CLA	CHA-CBD-CGD-O2D
25	b	601	CLA	CHA-CBD-CGD-O1D
25	b	601	CLA	CAD-CBD-CGD-O1D
25	b	601	CLA	CAD-CBD-CGD-O2D
25	b	602	CLA	C2-C3-C5-C6
25	b	602	CLA	C6-C7-C8-C9
25	b	604	CLA	C1A-C2A-CAA-CBA
25	b	604	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C12-C13-C15
25	b	609	CLA	C1A-C2A-CAA-CBA
25	b	609	CLA	C3A-C2A-CAA-CBA
25	b	612	CLA	C1A-C2A-CAA-CBA
25	b	612	CLA	C3A-C2A-CAA-CBA
25	b	614	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	CHA-CBD-CGD-O2D
25	b	614	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	C4-C3-C5-C6
25	c	506	CLA	C14-C13-C15-C16
25	c	507	CLA	C2-C3-C5-C6
25	c	507	CLA	C11-C10-C8-C9
25	d	401	CLA	CHA-CBD-CGD-O2D
25	d	402	CLA	C1A-C2A-CAA-CBA
25	d	402	CLA	C3A-C2A-CAA-CBA
25	d	403	CLA	C1A-C2A-CAA-CBA
25	d	403	CLA	C3A-C2A-CAA-CBA
25	s	303	CLA	C1A-C2A-CAA-CBA
25	s	305	CLA	C3A-C2A-CAA-CBA
25	s	305	CLA	CHA-CBD-CGD-O2D
25	s	305	CLA	CBD-CGD-O2D-CED
25	s	310	CLA	C1-C2-C3-C4
25	s	310	CLA	C2-C3-C5-C6
25	s	311	CLA	C1A-C2A-CAA-CBA
25	s	311	CLA	CHA-CBD-CGD-O1D
25	s	311	CLA	CAD-CBD-CGD-O1D
25	s	311	CLA	CAD-CBD-CGD-O2D
25	s	313	CLA	C1A-C2A-CAA-CBA
25	s	313	CLA	C3A-C2A-CAA-CBA
25	g	604	CLA	CBD-CGD-O2D-CED
25	g	610	CLA	CBD-CGD-O2D-CED
25	g	611	CLA	C3A-C2A-CAA-CBA
25	g	611	CLA	CAD-CBD-CGD-O1D
25	g	611	CLA	CAD-CBD-CGD-O2D
25	g	611	CLA	C2-C3-C5-C6
25	g	613	CLA	C1A-C2A-CAA-CBA
25	g	614	CLA	C1A-C2A-CAA-CBA
25	g	614	CLA	C3A-C2A-CAA-CBA
25	g	614	CLA	CAD-CBD-CGD-O1D
25	n	604	CLA	C1A-C2A-CAA-CBA
25	n	604	CLA	C3A-C2A-CAA-CBA
25	n	610	CLA	C1A-C2A-CAA-CBA
25	n	610	CLA	C1-C2-C3-C4
25	n	610	CLA	C4-C3-C5-C6
25	n	611	CLA	C1A-C2A-CAA-CBA
25	n	611	CLA	C3A-C2A-CAA-CBA
25	n	613	CLA	CHA-CBD-CGD-O1D
25	n	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	n	614	CLA	CBD-CGD-O2D-CED
25	y	304	CLA	CHA-CBD-CGD-O2D
25	y	305	CLA	CBD-CGD-O2D-CED
25	y	311	CLA	CBD-CGD-O2D-CED
25	y	312	CLA	CBA-CGA-O2A-C1
25	y	312	CLA	O1A-CGA-O2A-C1
25	y	314	CLA	CHA-CBD-CGD-O1D
25	y	314	CLA	C14-C13-C15-C16
25	y	315	CLA	C1A-C2A-CAA-CBA
25	y	315	CLA	CHA-CBD-CGD-O2D
25	y	315	CLA	CBD-CGD-O2D-CED
25	y	315	CLA	O1D-CGD-O2D-CED
25	r	601	CLA	C1A-C2A-CAA-CBA
25	r	601	CLA	C3A-C2A-CAA-CBA
25	r	602	CLA	CHA-CBD-CGD-O1D
25	r	603	CLA	CBD-CGD-O2D-CED
25	r	603	CLA	C6-C7-C8-C9
25	r	608	CLA	CHA-CBD-CGD-O2D
25	r	608	CLA	CBD-CGD-O2D-CED
25	r	609	CLA	C1A-C2A-CAA-CBA
25	r	610	CLA	C3A-C2A-CAA-CBA
25	r	611	CLA	C3A-C2A-CAA-CBA
25	r	611	CLA	CHA-CBD-CGD-O1D
25	r	611	CLA	CBD-CGD-O2D-CED
25	r	612	CLA	CHA-CBD-CGD-O1D
25	r	614	CLA	C1A-C2A-CAA-CBA
26	2	606	LHG	C3-O3-P-O4
26	2	606	LHG	C3-O3-P-O6
26	2	606	LHG	O7-C5-C6-O8
26	C	517	LHG	C1-C2-C3-O3
26	C	518	LHG	C3-O3-P-O6
26	C	518	LHG	C8-C7-O7-C5
26	C	519	LHG	C4-O6-P-O4
26	C	519	LHG	C4-O6-P-O5
26	C	519	LHG	C8-C7-O7-C5
26	D	406	LHG	O1-C1-C2-O2
26	D	406	LHG	O1-C1-C2-C3
26	D	406	LHG	C1-C2-C3-O3
26	L	102	LHG	C4-O6-P-O4
26	L	102	LHG	C4-O6-P-O5
26	S	301	LHG	O1-C1-C2-C3
26	S	318	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	N	618	LHG	O1-C1-C2-C3
26	Y	301	LHG	C1-C2-C3-O3
26	Y	319	LHG	O1-C1-C2-C3
26	Y	319	LHG	C3-O3-P-O4
26	Y	319	LHG	C3-O3-P-O5
26	Y	319	LHG	C3-O3-P-O6
26	6	606	LHG	C3-O3-P-O4
26	6	606	LHG	C3-O3-P-O6
26	6	606	LHG	O7-C5-C6-O8
26	c	517	LHG	C1-C2-C3-O3
26	c	518	LHG	C3-O3-P-O6
26	c	518	LHG	C8-C7-O7-C5
26	c	519	LHG	C4-O6-P-O5
26	c	519	LHG	C8-C7-O7-C5
26	d	406	LHG	O1-C1-C2-O2
26	d	406	LHG	O1-C1-C2-C3
26	d	406	LHG	C1-C2-C3-O3
26	l	103	LHG	C4-O6-P-O4
26	l	103	LHG	C4-O6-P-O5
26	s	301	LHG	O1-C1-C2-C3
26	s	318	LHG	O1-C1-C2-C3
26	n	618	LHG	O1-C1-C2-C3
26	y	301	LHG	C1-C2-C3-O3
26	y	319	LHG	O1-C1-C2-C3
26	y	319	LHG	C3-O3-P-O4
26	y	319	LHG	C3-O3-P-O5
26	y	319	LHG	C3-O3-P-O6
27	A	403	PHO	O1A-CGA-O2A-C1
27	a	404	PHO	O1A-CGA-O2A-C1
28	A	406	BCR	C14-C15-C16-C17
28	A	406	BCR	C16-C17-C18-C19
28	A	406	BCR	C16-C17-C18-C36
28	B	618	BCR	C23-C24-C25-C30
28	D	404	BCR	C1-C6-C7-C8
28	D	404	BCR	C7-C8-C9-C10
28	H	101	BCR	C7-C8-C9-C10
28	H	101	BCR	C7-C8-C9-C34
28	H	101	BCR	C22-C23-C24-C25
28	I	101	BCR	C20-C21-C22-C37
28	K	101	BCR	C7-C8-C9-C10
28	T	101	BCR	C11-C10-C9-C8
28	T	101	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
28	T	101	BCR	C11-C12-C13-C35
28	T	101	BCR	C13-C14-C15-C16
28	T	101	BCR	C21-C22-C23-C24
28	T	101	BCR	C37-C22-C23-C24
28	T	101	BCR	C22-C23-C24-C25
28	Z	101	BCR	C1-C6-C7-C8
28	Z	101	BCR	C7-C8-C9-C34
28	Z	101	BCR	C11-C12-C13-C35
28	Z	101	BCR	C20-C21-C22-C37
28	Z	101	BCR	C21-C22-C23-C24
28	Z	101	BCR	C37-C22-C23-C24
28	a	407	BCR	C14-C15-C16-C17
28	a	407	BCR	C16-C17-C18-C19
28	a	407	BCR	C16-C17-C18-C36
28	b	618	BCR	C23-C24-C25-C30
28	d	404	BCR	C1-C6-C7-C8
28	d	404	BCR	C7-C8-C9-C10
28	h	101	BCR	C7-C8-C9-C10
28	h	101	BCR	C7-C8-C9-C34
28	h	101	BCR	C22-C23-C24-C25
28	i	101	BCR	C20-C21-C22-C37
28	k	101	BCR	C7-C8-C9-C10
28	t	101	BCR	C11-C10-C9-C8
28	t	101	BCR	C11-C10-C9-C34
28	t	101	BCR	C11-C12-C13-C35
28	t	101	BCR	C13-C14-C15-C16
28	t	101	BCR	C21-C22-C23-C24
28	t	101	BCR	C37-C22-C23-C24
28	t	101	BCR	C22-C23-C24-C25
28	z	101	BCR	C1-C6-C7-C8
28	z	101	BCR	C7-C8-C9-C34
28	z	101	BCR	C11-C12-C13-C35
28	z	101	BCR	C20-C21-C22-C37
28	z	101	BCR	C21-C22-C23-C24
28	z	101	BCR	C37-C22-C23-C24
29	A	407	SQD	C2-C1-O6-C44
29	A	407	SQD	O5-C1-O6-C44
29	A	407	SQD	O49-C7-O47-C45
29	A	407	SQD	O5-C5-C6-S
29	A	411	SQD	O5-C1-O6-C44
29	A	411	SQD	O5-C5-C6-S
29	L	101	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
29	L	103	SQD	C2-C1-O6-C44
29	L	103	SQD	O5-C1-O6-C44
29	L	103	SQD	O49-C7-O47-C45
29	L	103	SQD	C8-C7-O47-C45
29	L	103	SQD	O5-C5-C6-S
29	a	408	SQD	C2-C1-O6-C44
29	a	408	SQD	O5-C1-O6-C44
29	a	408	SQD	O49-C7-O47-C45
29	a	408	SQD	O5-C5-C6-S
29	a	412	SQD	O5-C1-O6-C44
29	a	412	SQD	O5-C5-C6-S
29	l	101	SQD	C2-C1-O6-C44
29	l	101	SQD	O5-C1-O6-C44
29	l	101	SQD	O49-C7-O47-C45
29	l	101	SQD	C8-C7-O47-C45
29	l	101	SQD	O5-C5-C6-S
29	l	102	SQD	O47-C45-C46-O48
30	A	410	LMG	O7-C8-C9-O8
30	B	623	LMG	C2-C1-O1-C7
30	B	623	LMG	O6-C1-O1-C7
30	B	623	LMG	O9-C10-O7-C8
30	C	520	LMG	C2-C1-O1-C7
30	C	520	LMG	O9-C10-O7-C8
30	a	411	LMG	O7-C8-C9-O8
30	b	623	LMG	C2-C1-O1-C7
30	b	623	LMG	O6-C1-O1-C7
30	b	623	LMG	O9-C10-O7-C8
30	c	520	LMG	C2-C1-O1-C7
30	c	520	LMG	O9-C10-O7-C8
35	A	415	DGD	C2A-C1A-O1G-C1G
35	A	415	DGD	O1A-C1A-O1G-C1G
35	A	415	DGD	C2B-C1B-O2G-C2G
35	A	415	DGD	C2D-C1D-O3G-C3G
35	A	415	DGD	O6D-C1D-O3G-C3G
35	C	516	DGD	C2D-C1D-O3G-C3G
35	C	516	DGD	C2E-C1E-O5D-C6D
35	C	516	DGD	O6E-C1E-O5D-C6D
35	a	401	DGD	C2A-C1A-O1G-C1G
35	a	401	DGD	O1A-C1A-O1G-C1G
35	a	401	DGD	C2B-C1B-O2G-C2G
35	a	401	DGD	C2D-C1D-O3G-C3G
35	a	401	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
35	c	516	DGD	C2D-C1D-O3G-C3G
35	c	516	DGD	C2E-C1E-O5D-C6D
35	c	516	DGD	O6E-C1E-O5D-C6D
39	N	616	LUT	C7-C8-C9-C10
39	N	616	LUT	C7-C8-C9-C19
39	n	616	LUT	C7-C8-C9-C10
39	n	616	LUT	C7-C8-C9-C19
40	S	317	NEX	C11-C12-C13-C14
40	S	317	NEX	C11-C12-C13-C20
40	G	617	NEX	C9-C10-C11-C12
40	G	617	NEX	C11-C12-C13-C20
40	G	617	NEX	C21-C26-C27-C28
40	G	617	NEX	C25-C26-C27-C28
40	G	617	NEX	C27-C28-C29-C30
40	G	617	NEX	C27-C28-C29-C39
40	N	617	NEX	C7-C8-C9-C10
40	N	617	NEX	C27-C28-C29-C30
40	N	617	NEX	C27-C28-C29-C39
40	N	617	NEX	C31-C32-C33-C34
40	N	617	NEX	C31-C32-C33-C40
40	Y	318	NEX	C9-C10-C11-C12
40	Y	318	NEX	C21-C26-C27-C28
40	Y	318	NEX	C27-C28-C29-C30
40	Y	318	NEX	C27-C28-C29-C39
40	R	617	NEX	C9-C10-C11-C12
40	R	617	NEX	C11-C12-C13-C14
40	R	617	NEX	C11-C12-C13-C20
40	s	317	NEX	C11-C12-C13-C14
40	s	317	NEX	C11-C12-C13-C20
40	g	617	NEX	C9-C10-C11-C12
40	g	617	NEX	C11-C12-C13-C20
40	g	617	NEX	C21-C26-C27-C28
40	g	617	NEX	C25-C26-C27-C28
40	g	617	NEX	C27-C28-C29-C30
40	g	617	NEX	C27-C28-C29-C39
40	n	617	NEX	C7-C8-C9-C10
40	n	617	NEX	C27-C28-C29-C30
40	n	617	NEX	C27-C28-C29-C39
40	n	617	NEX	C31-C32-C33-C34
40	n	617	NEX	C31-C32-C33-C40
40	y	318	NEX	C9-C10-C11-C12
40	y	318	NEX	C21-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
40	y	318	NEX	C27-C28-C29-C30
40	y	318	NEX	C27-C28-C29-C39
40	r	617	NEX	C9-C10-C11-C12
40	r	617	NEX	C11-C12-C13-C14
40	r	617	NEX	C11-C12-C13-C20
24	Y	308	CHL	C2C-C3C-CAC-CBC
24	Y	308	CHL	C4C-C3C-CAC-CBC
24	y	308	CHL	C2C-C3C-CAC-CBC
24	y	308	CHL	C4C-C3C-CAC-CBC
25	N	602	CLA	C4C-C3C-CAC-CBC
25	n	602	CLA	C4C-C3C-CAC-CBC
25	2	604	CLA	O1D-CGD-O2D-CED
25	2	605	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	O1D-CGD-O2D-CED
25	S	305	CLA	O1D-CGD-O2D-CED
25	G	604	CLA	O1D-CGD-O2D-CED
25	G	610	CLA	O1D-CGD-O2D-CED
25	Y	311	CLA	O1D-CGD-O2D-CED
25	6	604	CLA	O1D-CGD-O2D-CED
25	6	605	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
25	s	305	CLA	O1D-CGD-O2D-CED
25	g	604	CLA	O1D-CGD-O2D-CED
25	g	610	CLA	O1D-CGD-O2D-CED
25	y	311	CLA	O1D-CGD-O2D-CED
25	G	614	CLA	C2C-C3C-CAC-CBC
25	G	614	CLA	C4C-C3C-CAC-CBC
25	N	602	CLA	C2C-C3C-CAC-CBC
25	g	614	CLA	C2C-C3C-CAC-CBC
25	g	614	CLA	C4C-C3C-CAC-CBC
25	n	602	CLA	C2C-C3C-CAC-CBC
24	2	601	CHL	O1D-CGD-O2D-CED
24	N	608	CHL	O1D-CGD-O2D-CED
24	6	601	CHL	O1D-CGD-O2D-CED
24	n	608	CHL	O1D-CGD-O2D-CED
25	A	401	CLA	O1D-CGD-O2D-CED
25	S	313	CLA	O1D-CGD-O2D-CED
25	N	613	CLA	O1D-CGD-O2D-CED
25	R	603	CLA	O1D-CGD-O2D-CED
25	R	611	CLA	O1D-CGD-O2D-CED
25	a	402	CLA	O1D-CGD-O2D-CED
25	s	313	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	n	613	CLA	O1D-CGD-O2D-CED
25	r	603	CLA	O1D-CGD-O2D-CED
25	r	611	CLA	O1D-CGD-O2D-CED
24	N	607	CHL	CBD-CGD-O2D-CED
24	N	608	CHL	CBD-CGD-O2D-CED
24	Y	309	CHL	CBD-CGD-O2D-CED
24	Y	310	CHL	CBD-CGD-O2D-CED
24	R	606	CHL	CBD-CGD-O2D-CED
24	n	607	CHL	CBD-CGD-O2D-CED
24	n	608	CHL	CBD-CGD-O2D-CED
24	y	309	CHL	CBD-CGD-O2D-CED
24	y	310	CHL	CBD-CGD-O2D-CED
24	r	606	CHL	CBD-CGD-O2D-CED
25	2	605	CLA	CBD-CGD-O2D-CED
25	A	401	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	CBD-CGD-O2D-CED
25	C	502	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	S	304	CLA	CBD-CGD-O2D-CED
25	S	309	CLA	CBD-CGD-O2D-CED
25	S	313	CLA	CBD-CGD-O2D-CED
25	G	613	CLA	CBD-CGD-O2D-CED
25	N	604	CLA	CBD-CGD-O2D-CED
25	N	610	CLA	CBD-CGD-O2D-CED
25	N	611	CLA	CBD-CGD-O2D-CED
25	R	609	CLA	CBD-CGD-O2D-CED
25	6	605	CLA	CBD-CGD-O2D-CED
25	a	402	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	c	502	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	s	304	CLA	CBD-CGD-O2D-CED
25	s	309	CLA	CBD-CGD-O2D-CED
25	s	313	CLA	CBD-CGD-O2D-CED
25	g	613	CLA	CBD-CGD-O2D-CED
25	n	604	CLA	CBD-CGD-O2D-CED
25	n	610	CLA	CBD-CGD-O2D-CED
25	n	611	CLA	CBD-CGD-O2D-CED
25	r	609	CLA	CBD-CGD-O2D-CED
25	2	602	CLA	O1A-CGA-O2A-C1
25	2	604	CLA	O1A-CGA-O2A-C1
25	2	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	G	614	CLA	O1A-CGA-O2A-C1
25	6	602	CLA	O1A-CGA-O2A-C1
25	6	604	CLA	O1A-CGA-O2A-C1
25	6	605	CLA	O1A-CGA-O2A-C1
25	g	614	CLA	O1A-CGA-O2A-C1
24	G	608	CHL	O1D-CGD-O2D-CED
24	Y	309	CHL	O1D-CGD-O2D-CED
24	g	608	CHL	O1D-CGD-O2D-CED
24	y	309	CHL	O1D-CGD-O2D-CED
25	S	304	CLA	O1D-CGD-O2D-CED
25	G	613	CLA	O1D-CGD-O2D-CED
25	N	614	CLA	O1D-CGD-O2D-CED
25	R	608	CLA	O1D-CGD-O2D-CED
25	s	304	CLA	O1D-CGD-O2D-CED
25	g	613	CLA	O1D-CGD-O2D-CED
25	n	614	CLA	O1D-CGD-O2D-CED
25	r	608	CLA	O1D-CGD-O2D-CED
24	S	307	CHL	C4C-C3C-CAC-CBC
24	s	307	CHL	C4C-C3C-CAC-CBC
25	R	608	CLA	C4C-C3C-CAC-CBC
25	r	608	CLA	C4C-C3C-CAC-CBC
25	C	502	CLA	O1D-CGD-O2D-CED
25	N	610	CLA	O1D-CGD-O2D-CED
25	N	611	CLA	O1D-CGD-O2D-CED
25	Y	314	CLA	O1D-CGD-O2D-CED
25	c	502	CLA	O1D-CGD-O2D-CED
25	n	610	CLA	O1D-CGD-O2D-CED
25	n	611	CLA	O1D-CGD-O2D-CED
25	y	314	CLA	O1D-CGD-O2D-CED
25	2	604	CLA	CBA-CGA-O2A-C1
25	2	605	CLA	CBA-CGA-O2A-C1
25	G	614	CLA	CBA-CGA-O2A-C1
25	6	604	CLA	CBA-CGA-O2A-C1
25	6	605	CLA	CBA-CGA-O2A-C1
25	g	614	CLA	CBA-CGA-O2A-C1
24	R	607	CHL	CBD-CGD-O2D-CED
24	r	607	CHL	CBD-CGD-O2D-CED
25	B	613	CLA	CBD-CGD-O2D-CED
25	N	602	CLA	CBD-CGD-O2D-CED
25	Y	314	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
25	n	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	y	314	CLA	CBD-CGD-O2D-CED
24	S	307	CHL	C2C-C3C-CAC-CBC
24	s	307	CHL	C2C-C3C-CAC-CBC
25	N	613	CLA	C2C-C3C-CAC-CBC
25	N	613	CLA	C4C-C3C-CAC-CBC
25	n	613	CLA	C2C-C3C-CAC-CBC
25	n	613	CLA	C4C-C3C-CAC-CBC
25	B	616	CLA	O1A-CGA-O2A-C1
25	R	608	CLA	O1A-CGA-O2A-C1
25	R	610	CLA	O1A-CGA-O2A-C1
25	R	611	CLA	O1A-CGA-O2A-C1
25	b	616	CLA	O1A-CGA-O2A-C1
25	r	608	CLA	O1A-CGA-O2A-C1
25	r	610	CLA	O1A-CGA-O2A-C1
25	r	611	CLA	O1A-CGA-O2A-C1
26	L	102	LHG	O10-C23-O8-C6
26	l	103	LHG	O10-C23-O8-C6
24	2	603	CHL	O1D-CGD-O2D-CED
24	R	606	CHL	O1D-CGD-O2D-CED
24	6	603	CHL	O1D-CGD-O2D-CED
24	r	606	CHL	O1D-CGD-O2D-CED
25	B	613	CLA	O1D-CGD-O2D-CED
25	S	309	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
25	s	309	CLA	O1D-CGD-O2D-CED
25	R	608	CLA	C2C-C3C-CAC-CBC
25	r	608	CLA	C2C-C3C-CAC-CBC
26	C	518	LHG	O9-C7-O7-C5
26	C	519	LHG	O9-C7-O7-C5
26	c	518	LHG	O9-C7-O7-C5
26	c	519	LHG	O9-C7-O7-C5
35	A	415	DGD	O1B-C1B-O2G-C2G
35	a	401	DGD	O1B-C1B-O2G-C2G
24	G	609	CHL	C3-C5-C6-C7
24	N	608	CHL	C3-C5-C6-C7
24	Y	308	CHL	C3-C5-C6-C7
24	g	609	CHL	C3-C5-C6-C7
24	n	608	CHL	C3-C5-C6-C7
24	y	308	CHL	C3-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
25	C	512	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	C3-C5-C6-C7
25	b	616	CLA	C3-C5-C6-C7
25	c	512	CLA	C3-C5-C6-C7
25	B	616	CLA	CBA-CGA-O2A-C1
25	G	612	CLA	CBA-CGA-O2A-C1
25	R	610	CLA	CBA-CGA-O2A-C1
25	R	611	CLA	CBA-CGA-O2A-C1
25	b	616	CLA	CBA-CGA-O2A-C1
25	g	612	CLA	CBA-CGA-O2A-C1
25	r	610	CLA	CBA-CGA-O2A-C1
25	r	611	CLA	CBA-CGA-O2A-C1
26	L	102	LHG	C24-C23-O8-C6
26	l	103	LHG	C24-C23-O8-C6
27	A	403	PHO	CBA-CGA-O2A-C1
27	a	404	PHO	CBA-CGA-O2A-C1
29	L	103	SQD	C24-C23-O48-C46
29	l	101	SQD	C24-C23-O48-C46
24	N	601	CHL	C2C-C3C-CAC-CBC
24	n	601	CHL	C2C-C3C-CAC-CBC
29	A	407	SQD	C8-C7-O47-C45
29	a	408	SQD	C8-C7-O47-C45
30	B	623	LMG	C11-C10-O7-C8
30	C	520	LMG	C11-C10-O7-C8
30	b	623	LMG	C11-C10-O7-C8
30	c	520	LMG	C11-C10-O7-C8
25	G	603	CLA	CBD-CGD-O2D-CED
25	g	603	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	C2C-C3C-CAC-CBC
25	b	616	CLA	C2C-C3C-CAC-CBC
25	D	403	CLA	O1A-CGA-O2A-C1
25	d	403	CLA	O1A-CGA-O2A-C1
26	C	519	LHG	O10-C23-O8-C6
26	c	519	LHG	O10-C23-O8-C6
25	y	304	CLA	C2C-C3C-CAC-CBC
25	Y	304	CLA	C2C-C3C-CAC-CBC
25	2	604	CLA	C4-C3-C5-C6
25	B	602	CLA	C4-C3-C5-C6
25	S	303	CLA	C4-C3-C5-C6
25	G	611	CLA	C4-C3-C5-C6
25	R	609	CLA	C4-C3-C5-C6
25	6	604	CLA	C4-C3-C5-C6
25	b	602	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	s	303	CLA	C4-C3-C5-C6
25	g	611	CLA	C4-C3-C5-C6
25	r	609	CLA	C4-C3-C5-C6
30	A	408	LMG	C4-C5-C6-O5
30	a	409	LMG	C4-C5-C6-O5
24	N	607	CHL	C2-C3-C5-C6
24	n	607	CHL	C2-C3-C5-C6
25	C	504	CLA	C2-C3-C5-C6
25	c	504	CLA	C2-C3-C5-C6
24	G	608	CHL	C2A-CAA-CBA-CGA
24	Y	306	CHL	C2A-CAA-CBA-CGA
24	R	606	CHL	C2A-CAA-CBA-CGA
24	g	608	CHL	C2A-CAA-CBA-CGA
24	y	306	CHL	C2A-CAA-CBA-CGA
24	r	606	CHL	C2A-CAA-CBA-CGA
25	2	602	CLA	C2A-CAA-CBA-CGA
25	B	601	CLA	C2A-CAA-CBA-CGA
25	C	512	CLA	C2A-CAA-CBA-CGA
25	G	614	CLA	C2A-CAA-CBA-CGA
25	R	609	CLA	C2A-CAA-CBA-CGA
25	R	611	CLA	C2A-CAA-CBA-CGA
25	6	602	CLA	C2A-CAA-CBA-CGA
25	b	601	CLA	C2A-CAA-CBA-CGA
25	c	512	CLA	C2A-CAA-CBA-CGA
25	g	614	CLA	C2A-CAA-CBA-CGA
25	r	609	CLA	C2A-CAA-CBA-CGA
25	r	611	CLA	C2A-CAA-CBA-CGA
24	G	608	CHL	C3-C5-C6-C7
24	N	601	CHL	C3-C5-C6-C7
24	R	607	CHL	C3-C5-C6-C7
24	g	608	CHL	C3-C5-C6-C7
24	n	601	CHL	C3-C5-C6-C7
24	r	607	CHL	C3-C5-C6-C7
25	C	504	CLA	C3-C5-C6-C7
25	c	504	CLA	C3-C5-C6-C7
25	S	312	CLA	CBA-CGA-O2A-C1
25	s	312	CLA	CBA-CGA-O2A-C1
35	C	515	DGD	C4E-C5E-C6E-O5E
35	c	515	DGD	C4E-C5E-C6E-O5E
24	N	601	CHL	C4C-C3C-CAC-CBC
24	n	601	CHL	C4C-C3C-CAC-CBC
24	Y	310	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	y	310	CHL	O1D-CGD-O2D-CED
25	B	601	CLA	O1A-CGA-O2A-C1
25	C	504	CLA	O1A-CGA-O2A-C1
25	S	312	CLA	O1A-CGA-O2A-C1
25	b	601	CLA	O1A-CGA-O2A-C1
25	c	504	CLA	O1A-CGA-O2A-C1
25	s	312	CLA	O1A-CGA-O2A-C1
29	L	103	SQD	O10-C23-O48-C46
29	l	101	SQD	O10-C23-O48-C46
25	Y	305	CLA	C2C-C3C-CAC-CBC
25	y	305	CLA	C2C-C3C-CAC-CBC
39	S	316	LUT	C33-C34-C35-C15
39	s	316	LUT	C33-C34-C35-C15
40	N	617	NEX	C9-C10-C11-C12
40	n	617	NEX	C9-C10-C11-C12
29	L	101	SQD	C10-C11-C12-C13
29	l	102	SQD	C10-C11-C12-C13
35	C	516	DGD	CCA-CDA-CEA-CFA
35	c	516	DGD	CCA-CDA-CEA-CFA
25	C	504	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	CBD-CGD-O2D-CED
25	c	504	CLA	CBD-CGD-O2D-CED
25	c	508	CLA	CBD-CGD-O2D-CED
26	B	622	LHG	O2-C2-C3-O3
26	C	517	LHG	O2-C2-C3-O3
26	D	406	LHG	O2-C2-C3-O3
26	S	301	LHG	O2-C2-C3-O3
26	b	622	LHG	O2-C2-C3-O3
26	c	517	LHG	O2-C2-C3-O3
26	d	406	LHG	O2-C2-C3-O3
26	s	301	LHG	O2-C2-C3-O3
25	N	613	CLA	C3-C5-C6-C7
25	R	603	CLA	C3-C5-C6-C7
25	R	608	CLA	C3-C5-C6-C7
25	n	613	CLA	C3-C5-C6-C7
25	r	603	CLA	C3-C5-C6-C7
25	r	608	CLA	C3-C5-C6-C7
24	Y	310	CHL	CBA-CGA-O2A-C1
24	y	310	CHL	CBA-CGA-O2A-C1
25	2	602	CLA	CBA-CGA-O2A-C1
25	B	601	CLA	CBA-CGA-O2A-C1
25	6	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	b	601	CLA	CBA-CGA-O2A-C1
26	C	519	LHG	C24-C23-O8-C6
26	c	519	LHG	C24-C23-O8-C6
25	C	510	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
26	2	606	LHG	C8-C7-O7-C5
26	C	517	LHG	C8-C7-O7-C5
26	6	606	LHG	C8-C7-O7-C5
26	c	517	LHG	C8-C7-O7-C5
29	L	101	SQD	C8-C7-O47-C45
29	l	102	SQD	C8-C7-O47-C45
29	L	103	SQD	C10-C11-C12-C13
29	l	101	SQD	C10-C11-C12-C13
30	B	620	LMG	C39-C40-C41-C42
35	B	626	DGD	O6E-C5E-C6E-O5E
35	b	626	DGD	O6E-C5E-C6E-O5E
30	b	620	LMG	C39-C40-C41-C42
25	B	601	CLA	C3-C5-C6-C7
25	b	601	CLA	C3-C5-C6-C7
24	N	607	CHL	CBA-CGA-O2A-C1
24	n	607	CHL	CBA-CGA-O2A-C1
25	C	510	CLA	CBA-CGA-O2A-C1
25	R	608	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
25	r	608	CLA	CBA-CGA-O2A-C1
30	A	408	LMG	O6-C5-C6-O5
30	a	409	LMG	O6-C5-C6-O5
35	C	515	DGD	O6E-C5E-C6E-O5E
35	c	515	DGD	O6E-C5E-C6E-O5E
24	G	608	CHL	C2C-C3C-CAC-CBC
24	g	608	CHL	C2C-C3C-CAC-CBC
25	G	612	CLA	O1A-CGA-O2A-C1
25	g	612	CLA	O1A-CGA-O2A-C1
24	2	601	CHL	C4-C3-C5-C6
24	G	601	CHL	C4-C3-C5-C6
24	6	601	CHL	C4-C3-C5-C6
24	g	601	CHL	C4-C3-C5-C6
25	C	507	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
24	2	601	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	6	601	CHL	C2-C3-C5-C6
25	N	610	CLA	C2-C3-C5-C6
25	n	610	CLA	C2-C3-C5-C6
24	1	301	CHL	C2A-CAA-CBA-CGA
24	5	301	CHL	C2A-CAA-CBA-CGA
25	S	303	CLA	C2A-CAA-CBA-CGA
25	N	613	CLA	C2A-CAA-CBA-CGA
25	Y	311	CLA	C2A-CAA-CBA-CGA
25	R	601	CLA	C2A-CAA-CBA-CGA
25	R	602	CLA	C2A-CAA-CBA-CGA
25	R	610	CLA	C2A-CAA-CBA-CGA
25	R	614	CLA	C2A-CAA-CBA-CGA
25	s	303	CLA	C2A-CAA-CBA-CGA
25	n	613	CLA	C2A-CAA-CBA-CGA
25	y	311	CLA	C2A-CAA-CBA-CGA
25	r	602	CLA	C2A-CAA-CBA-CGA
25	r	610	CLA	C2A-CAA-CBA-CGA
25	r	614	CLA	C2A-CAA-CBA-CGA
30	A	408	LMG	O6-C1-O1-C7
30	a	409	LMG	O6-C1-O1-C7
27	A	403	PHO	C3-C5-C6-C7
27	a	404	PHO	C3-C5-C6-C7
26	Y	319	LHG	C29-C30-C31-C32
26	y	319	LHG	C29-C30-C31-C32
25	B	616	CLA	C4C-C3C-CAC-CBC
25	Y	304	CLA	C4C-C3C-CAC-CBC
25	b	616	CLA	C4C-C3C-CAC-CBC
25	y	304	CLA	C4C-C3C-CAC-CBC
24	Y	302	CHL	C2C-C3C-CAC-CBC
24	y	302	CHL	C2C-C3C-CAC-CBC
25	G	611	CLA	C2C-C3C-CAC-CBC
25	g	611	CLA	C2C-C3C-CAC-CBC
26	B	622	LHG	C1-C2-C3-O3
26	L	102	LHG	C1-C2-C3-O3
26	S	301	LHG	C1-C2-C3-O3
26	b	622	LHG	C1-C2-C3-O3
26	l	103	LHG	C1-C2-C3-O3
26	s	301	LHG	C1-C2-C3-O3
26	C	517	LHG	O9-C7-O7-C5
26	c	517	LHG	O9-C7-O7-C5
29	L	101	SQD	O49-C7-O47-C45
29	l	102	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
25	N	603	CLA	C3-C5-C6-C7
25	n	603	CLA	C3-C5-C6-C7
24	N	607	CHL	O1D-CGD-O2D-CED
24	n	607	CHL	O1D-CGD-O2D-CED
25	C	504	CLA	CBA-CGA-O2A-C1
25	C	511	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	CBA-CGA-O2A-C1
25	D	403	CLA	CBA-CGA-O2A-C1
25	N	611	CLA	CBA-CGA-O2A-C1
25	c	504	CLA	CBA-CGA-O2A-C1
25	c	511	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	d	403	CLA	CBA-CGA-O2A-C1
25	n	611	CLA	CBA-CGA-O2A-C1
26	B	622	LHG	C24-C23-O8-C6
26	Y	319	LHG	C24-C23-O8-C6
26	b	622	LHG	C24-C23-O8-C6
26	y	319	LHG	C24-C23-O8-C6
25	R	602	CLA	CBD-CGD-O2D-CED
25	R	614	CLA	CBD-CGD-O2D-CED
25	r	602	CLA	CBD-CGD-O2D-CED
25	r	614	CLA	CBD-CGD-O2D-CED
39	N	615	LUT	C9-C10-C11-C12
25	N	604	CLA	C2C-C3C-CAC-CBC
25	n	604	CLA	C2C-C3C-CAC-CBC
24	G	609	CHL	C10-C11-C12-C13
24	g	609	CHL	C10-C11-C12-C13
35	C	515	DGD	C2A-C3A-C4A-C5A
35	c	515	DGD	C2A-C3A-C4A-C5A
24	R	607	CHL	C5-C6-C7-C8
24	r	607	CHL	C5-C6-C7-C8
25	S	303	CLA	C10-C11-C12-C13
25	Y	304	CLA	C13-C15-C16-C17
25	s	303	CLA	C10-C11-C12-C13
25	y	304	CLA	C13-C15-C16-C17
26	L	102	LHG	O2-C2-C3-O3
26	l	103	LHG	O2-C2-C3-O3
25	G	612	CLA	C3-C5-C6-C7
26	Y	301	LHG	C23-C24-C25-C26
26	R	618	LHG	C23-C24-C25-C26
26	y	301	LHG	C23-C24-C25-C26
26	r	618	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	A	408	LMG	C2-C1-O1-C7
30	a	409	LMG	C2-C1-O1-C7
26	S	301	LHG	C14-C15-C16-C17
26	s	301	LHG	C14-C15-C16-C17
24	n	607	CHL	O1A-CGA-O2A-C1
25	N	611	CLA	O1A-CGA-O2A-C1
25	n	611	CLA	O1A-CGA-O2A-C1
25	R	609	CLA	C2-C3-C5-C6
25	r	609	CLA	C2-C3-C5-C6
24	G	601	CHL	C11-C12-C13-C14
24	G	608	CHL	C11-C10-C8-C9
24	G	608	CHL	C14-C13-C15-C16
24	G	609	CHL	C6-C7-C8-C9
24	N	608	CHL	C11-C10-C8-C9
24	N	609	CHL	C11-C12-C13-C14
24	Y	302	CHL	C11-C12-C13-C14
24	Y	309	CHL	C11-C10-C8-C9
24	g	601	CHL	C11-C12-C13-C14
24	g	608	CHL	C11-C10-C8-C9
24	g	608	CHL	C14-C13-C15-C16
24	g	609	CHL	C6-C7-C8-C9
24	n	608	CHL	C11-C10-C8-C9
24	n	609	CHL	C11-C12-C13-C14
24	y	302	CHL	C11-C12-C13-C14
24	y	309	CHL	C11-C10-C8-C9
25	A	402	CLA	C14-C13-C15-C16
25	B	602	CLA	C11-C12-C13-C14
25	B	602	CLA	C14-C13-C15-C16
25	B	607	CLA	C14-C13-C15-C16
25	B	608	CLA	C14-C13-C15-C16
25	B	609	CLA	C6-C7-C8-C9
25	B	613	CLA	C11-C12-C13-C14
25	B	613	CLA	C14-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C9
25	B	614	CLA	C14-C13-C15-C16
25	B	615	CLA	C11-C10-C8-C9
25	C	501	CLA	C14-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C9
25	C	506	CLA	C6-C7-C8-C9
25	C	507	CLA	C11-C12-C13-C14
25	C	509	CLA	C6-C7-C8-C9
25	C	511	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C14-C13-C15-C16
25	S	303	CLA	C11-C10-C8-C9
25	N	602	CLA	C6-C7-C8-C9
25	N	612	CLA	C6-C7-C8-C9
25	N	612	CLA	C11-C10-C8-C9
25	Y	303	CLA	C11-C10-C8-C9
25	Y	304	CLA	C11-C10-C8-C9
25	Y	312	CLA	C6-C7-C8-C9
25	Y	314	CLA	C6-C7-C8-C9
25	R	603	CLA	C11-C10-C8-C9
25	R	608	CLA	C6-C7-C8-C9
25	R	612	CLA	C6-C7-C8-C9
25	a	403	CLA	C14-C13-C15-C16
25	b	602	CLA	C11-C12-C13-C14
25	b	602	CLA	C14-C13-C15-C16
25	b	607	CLA	C14-C13-C15-C16
25	b	608	CLA	C14-C13-C15-C16
25	b	609	CLA	C6-C7-C8-C9
25	b	613	CLA	C11-C12-C13-C14
25	b	613	CLA	C14-C13-C15-C16
25	b	614	CLA	C6-C7-C8-C9
25	b	614	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C10-C8-C9
25	c	501	CLA	C14-C13-C15-C16
25	c	503	CLA	C11-C10-C8-C9
25	c	506	CLA	C6-C7-C8-C9
25	c	507	CLA	C11-C12-C13-C14
25	c	509	CLA	C6-C7-C8-C9
25	c	511	CLA	C11-C10-C8-C9
25	c	513	CLA	C14-C13-C15-C16
25	s	303	CLA	C11-C10-C8-C9
25	n	602	CLA	C6-C7-C8-C9
25	n	612	CLA	C6-C7-C8-C9
25	n	612	CLA	C11-C10-C8-C9
25	y	303	CLA	C11-C10-C8-C9
25	y	304	CLA	C11-C10-C8-C9
25	y	312	CLA	C6-C7-C8-C9
25	y	314	CLA	C6-C7-C8-C9
25	r	603	CLA	C11-C10-C8-C9
25	r	608	CLA	C6-C7-C8-C9
25	r	612	CLA	C6-C7-C8-C9
27	A	403	PHO	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	a	404	PHO	C14-C13-C15-C16
25	C	505	CLA	C15-C16-C17-C18
25	c	505	CLA	C15-C16-C17-C18
25	r	601	CLA	C2A-CAA-CBA-CGA
28	H	101	BCR	C37-C22-C23-C24
28	K	101	BCR	C7-C8-C9-C34
28	h	101	BCR	C37-C22-C23-C24
28	k	101	BCR	C7-C8-C9-C34
39	N	615	LUT	C11-C12-C13-C20
39	Y	317	LUT	C7-C8-C9-C19
39	n	615	LUT	C11-C12-C13-C20
39	y	317	LUT	C7-C8-C9-C19
28	H	101	BCR	C21-C22-C23-C24
28	h	101	BCR	C21-C22-C23-C24
39	N	615	LUT	C11-C12-C13-C14
39	Y	317	LUT	C7-C8-C9-C10
39	n	615	LUT	C11-C12-C13-C14
39	y	317	LUT	C7-C8-C9-C10
26	2	606	LHG	O9-C7-O7-C5
26	6	606	LHG	O9-C7-O7-C5
25	R	614	CLA	C2C-C3C-CAC-CBC
25	r	614	CLA	C2C-C3C-CAC-CBC
29	L	103	SQD	C23-C24-C25-C26
29	l	101	SQD	C23-C24-C25-C26
24	N	607	CHL	O1A-CGA-O2A-C1
24	N	607	CHL	C8-C10-C11-C12
24	Y	302	CHL	C8-C10-C11-C12
24	n	607	CHL	C8-C10-C11-C12
24	y	302	CHL	C8-C10-C11-C12
25	B	616	CLA	C5-C6-C7-C8
25	b	616	CLA	C5-C6-C7-C8
24	G	601	CHL	C2C-C3C-CAC-CBC
24	g	601	CHL	C2C-C3C-CAC-CBC
25	g	612	CLA	C3-C5-C6-C7
24	Y	302	CHL	CBA-CGA-O2A-C1
24	y	302	CHL	CBA-CGA-O2A-C1
24	2	601	CHL	C10-C11-C12-C13
24	G	601	CHL	C8-C10-C11-C12
24	G	608	CHL	C10-C11-C12-C13
24	G	608	CHL	C13-C15-C16-C17
24	6	601	CHL	C10-C11-C12-C13
24	g	601	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	g	608	CHL	C10-C11-C12-C13
24	g	608	CHL	C13-C15-C16-C17
25	B	611	CLA	C13-C15-C16-C17
25	B	611	CLA	C15-C16-C17-C18
25	B	613	CLA	C13-C15-C16-C17
25	N	603	CLA	C10-C11-C12-C13
25	N	613	CLA	C5-C6-C7-C8
25	Y	314	CLA	C13-C15-C16-C17
25	b	611	CLA	C13-C15-C16-C17
25	b	611	CLA	C15-C16-C17-C18
25	b	613	CLA	C13-C15-C16-C17
25	n	603	CLA	C10-C11-C12-C13
25	n	613	CLA	C5-C6-C7-C8
25	y	314	CLA	C13-C15-C16-C17
26	B	625	LHG	C7-C8-C9-C10
26	b	625	LHG	C7-C8-C9-C10
30	B	620	LMG	C28-C29-C30-C31
30	b	620	LMG	C28-C29-C30-C31
24	R	606	CHL	C2C-C3C-CAC-CBC
24	r	606	CHL	C2C-C3C-CAC-CBC
26	Y	319	LHG	C33-C34-C35-C36
26	y	319	LHG	C33-C34-C35-C36
30	D	407	LMG	O6-C5-C6-O5
30	d	407	LMG	O6-C5-C6-O5
24	N	601	CHL	C5-C6-C7-C8
24	N	607	CHL	C10-C11-C12-C13
24	N	609	CHL	C13-C15-C16-C17
24	n	601	CHL	C5-C6-C7-C8
24	n	607	CHL	C10-C11-C12-C13
24	n	609	CHL	C13-C15-C16-C17
25	B	601	CLA	C10-C11-C12-C13
25	B	607	CLA	C8-C10-C11-C12
25	B	614	CLA	C5-C6-C7-C8
25	C	503	CLA	C5-C6-C7-C8
25	D	403	CLA	C10-C11-C12-C13
25	S	310	CLA	C5-C6-C7-C8
25	G	612	CLA	C10-C11-C12-C13
25	N	602	CLA	C5-C6-C7-C8
25	N	602	CLA	C8-C10-C11-C12
25	N	603	CLA	C5-C6-C7-C8
25	Y	311	CLA	C8-C10-C11-C12
25	b	601	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	b	607	CLA	C8-C10-C11-C12
25	b	614	CLA	C5-C6-C7-C8
25	c	503	CLA	C5-C6-C7-C8
25	d	403	CLA	C10-C11-C12-C13
25	s	310	CLA	C5-C6-C7-C8
25	g	612	CLA	C10-C11-C12-C13
25	n	602	CLA	C5-C6-C7-C8
25	n	602	CLA	C8-C10-C11-C12
25	n	603	CLA	C5-C6-C7-C8
25	y	311	CLA	C8-C10-C11-C12
26	N	618	LHG	O1-C1-C2-O2
26	n	618	LHG	O1-C1-C2-O2
26	B	621	LHG	C7-C8-C9-C10
26	C	518	LHG	C7-C8-C9-C10
26	C	519	LHG	C23-C24-C25-C26
26	b	621	LHG	C7-C8-C9-C10
26	c	518	LHG	C7-C8-C9-C10
26	c	519	LHG	C23-C24-C25-C26
30	B	623	LMG	C28-C29-C30-C31
30	b	623	LMG	C28-C29-C30-C31
24	G	608	CHL	C5-C6-C7-C8
24	g	608	CHL	C5-C6-C7-C8
25	A	405	CLA	C10-C11-C12-C13
25	a	406	CLA	C10-C11-C12-C13
25	B	604	CLA	C3-C5-C6-C7
25	b	604	CLA	C3-C5-C6-C7
25	y	305	CLA	C4C-C3C-CAC-CBC
25	Y	305	CLA	C4C-C3C-CAC-CBC
25	Y	313	CLA	C10-C11-C12-C13
25	y	313	CLA	C10-C11-C12-C13
26	2	606	LHG	C23-C24-C25-C26
26	B	622	LHG	C7-C8-C9-C10
26	6	606	LHG	C23-C24-C25-C26
26	b	622	LHG	C7-C8-C9-C10
29	L	101	SQD	C23-C24-C25-C26
29	l	102	SQD	C23-C24-C25-C26
25	N	612	CLA	CBD-CGD-O2D-CED
25	n	612	CLA	CBD-CGD-O2D-CED
26	S	301	LHG	C31-C32-C33-C34
26	s	301	LHG	C31-C32-C33-C34
25	B	607	CLA	C5-C6-C7-C8
25	S	303	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	b	607	CLA	C5-C6-C7-C8
25	s	303	CLA	C8-C10-C11-C12
24	G	601	CHL	C12-C13-C15-C16
24	N	607	CHL	C6-C7-C8-C10
24	N	609	CHL	C11-C12-C13-C15
24	g	601	CHL	C12-C13-C15-C16
24	n	607	CHL	C6-C7-C8-C10
24	n	609	CHL	C11-C12-C13-C15
25	B	607	CLA	C11-C12-C13-C15
25	B	611	CLA	C12-C13-C15-C16
25	B	613	CLA	C11-C10-C8-C7
25	C	503	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C12-C13-C15
25	D	403	CLA	C12-C13-C15-C16
25	S	303	CLA	C11-C12-C13-C15
25	G	603	CLA	C6-C7-C8-C10
25	N	602	CLA	C6-C7-C8-C10
25	Y	313	CLA	C6-C7-C8-C10
25	b	607	CLA	C11-C12-C13-C15
25	b	611	CLA	C12-C13-C15-C16
25	b	613	CLA	C11-C10-C8-C7
25	c	503	CLA	C11-C10-C8-C7
25	c	510	CLA	C11-C12-C13-C15
25	d	403	CLA	C12-C13-C15-C16
25	s	303	CLA	C11-C12-C13-C15
25	g	603	CLA	C6-C7-C8-C10
25	n	602	CLA	C6-C7-C8-C10
25	y	313	CLA	C6-C7-C8-C10
26	Y	319	LHG	O10-C23-O8-C6
26	y	319	LHG	O10-C23-O8-C6
39	S	316	LUT	C13-C14-C15-C35
39	s	316	LUT	C13-C14-C15-C35
39	n	615	LUT	C9-C10-C11-C12
40	N	617	NEX	C33-C34-C35-C15
40	n	617	NEX	C33-C34-C35-C15
25	S	312	CLA	C2A-CAA-CBA-CGA
25	Y	304	CLA	C2A-CAA-CBA-CGA
25	Y	314	CLA	C2A-CAA-CBA-CGA
25	s	312	CLA	C2A-CAA-CBA-CGA
25	y	304	CLA	C2A-CAA-CBA-CGA
25	y	314	CLA	C2A-CAA-CBA-CGA
25	Y	305	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	y	305	CLA	O1D-CGD-O2D-CED
25	B	610	CLA	C15-C16-C17-C18
25	C	507	CLA	C13-C15-C16-C17
25	C	510	CLA	C13-C15-C16-C17
25	b	610	CLA	C15-C16-C17-C18
25	c	507	CLA	C13-C15-C16-C17
25	c	510	CLA	C13-C15-C16-C17
35	C	516	DGD	C8B-C9B-CAB-CBB
35	c	516	DGD	C8B-C9B-CAB-CBB
26	B	622	LHG	O10-C23-O8-C6
26	b	622	LHG	O10-C23-O8-C6
25	R	601	CLA	CBD-CGD-O2D-CED
25	r	601	CLA	CBD-CGD-O2D-CED
25	G	602	CLA	C10-C11-C12-C13
25	g	602	CLA	C10-C11-C12-C13
30	D	407	LMG	C31-C32-C33-C34
30	d	407	LMG	C31-C32-C33-C34
26	N	618	LHG	O2-C2-C3-O3
26	n	618	LHG	O2-C2-C3-O3
25	2	604	CLA	C3-C5-C6-C7
25	B	607	CLA	C3-C5-C6-C7
25	6	604	CLA	C3-C5-C6-C7
25	b	607	CLA	C3-C5-C6-C7
24	Y	310	CHL	C5-C6-C7-C8
24	y	310	CHL	C5-C6-C7-C8
25	B	607	CLA	C10-C11-C12-C13
25	D	402	CLA	C15-C16-C17-C18
25	Y	303	CLA	C10-C11-C12-C13
25	Y	304	CLA	C10-C11-C12-C13
25	Y	311	CLA	C5-C6-C7-C8
25	b	607	CLA	C10-C11-C12-C13
25	d	402	CLA	C15-C16-C17-C18
25	y	303	CLA	C10-C11-C12-C13
25	y	304	CLA	C10-C11-C12-C13
25	y	311	CLA	C5-C6-C7-C8
30	B	623	LMG	C29-C28-O8-C9
30	b	623	LMG	C29-C28-O8-C9
24	G	601	CHL	C10-C11-C12-C13
24	N	609	CHL	C8-C10-C11-C12
24	Y	309	CHL	C8-C10-C11-C12
24	g	601	CHL	C10-C11-C12-C13
24	n	609	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	y	309	CHL	C8-C10-C11-C12
25	B	607	CLA	C13-C15-C16-C17
25	B	611	CLA	C8-C10-C11-C12
25	C	503	CLA	C15-C16-C17-C18
25	N	613	CLA	C10-C11-C12-C13
25	Y	313	CLA	C8-C10-C11-C12
25	R	603	CLA	C8-C10-C11-C12
25	b	607	CLA	C13-C15-C16-C17
25	b	611	CLA	C8-C10-C11-C12
25	c	503	CLA	C15-C16-C17-C18
25	n	613	CLA	C10-C11-C12-C13
25	y	313	CLA	C8-C10-C11-C12
25	r	603	CLA	C8-C10-C11-C12
26	C	517	LHG	C10-C11-C12-C13
26	c	517	LHG	C10-C11-C12-C13
35	C	516	DGD	O6D-C5D-C6D-O5D
35	c	516	DGD	O6D-C5D-C6D-O5D
29	A	411	SQD	C8-C7-O47-C45
29	a	412	SQD	C8-C7-O47-C45
24	Y	309	CHL	C13-C15-C16-C17
24	y	309	CHL	C13-C15-C16-C17
25	B	604	CLA	C5-C6-C7-C8
25	B	609	CLA	C15-C16-C17-C18
25	B	616	CLA	C13-C15-C16-C17
25	C	513	CLA	C8-C10-C11-C12
25	G	610	CLA	C8-C10-C11-C12
25	N	612	CLA	C5-C6-C7-C8
25	R	608	CLA	C8-C10-C11-C12
25	R	612	CLA	C10-C11-C12-C13
25	b	604	CLA	C5-C6-C7-C8
25	b	609	CLA	C15-C16-C17-C18
25	b	616	CLA	C13-C15-C16-C17
25	c	513	CLA	C8-C10-C11-C12
25	g	610	CLA	C8-C10-C11-C12
25	n	612	CLA	C5-C6-C7-C8
25	r	608	CLA	C8-C10-C11-C12
25	r	612	CLA	C10-C11-C12-C13
24	N	607	CHL	C1-C2-C3-C5
24	n	607	CHL	C1-C2-C3-C5
26	C	519	LHG	C4-O6-P-O3
26	L	102	LHG	C4-O6-P-O3
26	N	618	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
26	c	519	LHG	C4-O6-P-O3
26	l	103	LHG	C4-O6-P-O3
26	n	618	LHG	C3-O3-P-O6
26	Y	319	LHG	C23-C24-C25-C26
26	y	319	LHG	C23-C24-C25-C26
25	C	510	CLA	C15-C16-C17-C18
25	G	613	CLA	C15-C16-C17-C18
25	c	510	CLA	C15-C16-C17-C18
26	N	618	LHG	C1-C2-C3-O3
26	n	618	LHG	C1-C2-C3-O3
29	A	411	SQD	O49-C7-O47-C45
29	a	412	SQD	O49-C7-O47-C45
25	S	310	CLA	C4-C3-C5-C6
25	s	310	CLA	C4-C3-C5-C6
25	C	504	CLA	C5-C6-C7-C8
25	c	504	CLA	C5-C6-C7-C8
25	g	613	CLA	C15-C16-C17-C18
31	A	409	PL9	C2-C3-C7-C8
31	a	410	PL9	C2-C3-C7-C8
25	A	401	CLA	C2C-C3C-CAC-CBC
25	N	603	CLA	C2C-C3C-CAC-CBC
25	a	402	CLA	C2C-C3C-CAC-CBC
25	n	603	CLA	C2C-C3C-CAC-CBC
30	A	410	LMG	C35-C36-C37-C38
30	a	411	LMG	C35-C36-C37-C38
25	C	513	CLA	C2A-CAA-CBA-CGA
25	S	310	CLA	C2A-CAA-CBA-CGA
25	N	610	CLA	C2A-CAA-CBA-CGA
25	c	513	CLA	C2A-CAA-CBA-CGA
25	s	310	CLA	C2A-CAA-CBA-CGA
25	n	610	CLA	C2A-CAA-CBA-CGA
25	C	504	CLA	C11-C12-C13-C14
25	G	613	CLA	C16-C17-C18-C19
25	R	609	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C14
25	g	613	CLA	C16-C17-C18-C19
25	r	609	CLA	C16-C17-C18-C20
30	A	410	LMG	O6-C5-C6-O5
30	a	411	LMG	O6-C5-C6-O5
24	G	601	CHL	CBA-CGA-O2A-C1
24	g	601	CHL	CBA-CGA-O2A-C1
35	C	516	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
35	c	516	DGD	C4D-C5D-C6D-O5D
26	Y	319	LHG	C11-C12-C13-C14
26	y	319	LHG	C11-C12-C13-C14
29	A	407	SQD	C11-C12-C13-C14
29	a	408	SQD	C11-C12-C13-C14
24	G	608	CHL	C8-C10-C11-C12
28	H	101	BCR	C20-C21-C22-C37
28	T	101	BCR	C35-C13-C14-C15
28	h	101	BCR	C20-C21-C22-C37
28	t	101	BCR	C35-C13-C14-C15
26	2	606	LHG	C15-C16-C17-C18
26	B	625	LHG	C25-C26-C27-C28
26	C	517	LHG	C34-C35-C36-C37
26	L	102	LHG	C27-C28-C29-C30
26	6	606	LHG	C15-C16-C17-C18
26	b	625	LHG	C25-C26-C27-C28
26	c	517	LHG	C34-C35-C36-C37
26	l	103	LHG	C27-C28-C29-C30
29	L	103	SQD	C11-C10-C9-C8
29	L	103	SQD	C9-C10-C11-C12
29	l	101	SQD	C11-C10-C9-C8
29	l	101	SQD	C9-C10-C11-C12
30	A	410	LMG	C37-C38-C39-C40
30	D	407	LMG	C13-C14-C15-C16
30	a	411	LMG	C37-C38-C39-C40
30	d	407	LMG	C13-C14-C15-C16
24	n	609	CHL	O1D-CGD-O2D-CED
24	Y	302	CHL	C16-C17-C18-C19
24	y	302	CHL	C16-C17-C18-C19
25	B	608	CLA	C16-C17-C18-C19
25	N	612	CLA	C11-C12-C13-C14
25	b	608	CLA	C16-C17-C18-C19
25	n	612	CLA	C11-C12-C13-C14
25	y	313	CLA	C11-C12-C13-C15
26	S	301	LHG	C26-C27-C28-C29
26	s	301	LHG	C26-C27-C28-C29
26	y	301	LHG	C26-C27-C28-C29
30	A	408	LMG	C30-C31-C32-C33
30	D	407	LMG	C12-C13-C14-C15
30	a	409	LMG	C30-C31-C32-C33
35	C	515	DGD	C5A-C6A-C7A-C8A
35	C	515	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
35	c	515	DGD	C5A-C6A-C7A-C8A
35	c	515	DGD	C7B-C8B-C9B-CAB
26	C	519	LHG	C4-C5-O7-C7
26	c	519	LHG	C4-C5-O7-C7
24	N	609	CHL	O1D-CGD-O2D-CED
24	g	608	CHL	C8-C10-C11-C12
25	G	614	CLA	CBD-CGD-O2D-CED
25	g	614	CLA	CBD-CGD-O2D-CED
26	Y	301	LHG	C26-C27-C28-C29
30	B	623	LMG	C31-C32-C33-C34
30	b	623	LMG	C31-C32-C33-C34
30	d	407	LMG	C12-C13-C14-C15
35	C	515	DGD	C4A-C5A-C6A-C7A
35	c	515	DGD	C4A-C5A-C6A-C7A
24	G	608	CHL	C4C-C3C-CAC-CBC
24	g	608	CHL	C4C-C3C-CAC-CBC
26	2	606	LHG	C14-C15-C16-C17
26	B	621	LHG	C26-C27-C28-C29
26	D	406	LHG	C33-C34-C35-C36
26	N	618	LHG	C26-C27-C28-C29
26	N	618	LHG	C27-C28-C29-C30
26	Y	319	LHG	C13-C14-C15-C16
26	6	606	LHG	C14-C15-C16-C17
26	b	621	LHG	C26-C27-C28-C29
26	d	406	LHG	C33-C34-C35-C36
26	n	618	LHG	C26-C27-C28-C29
26	n	618	LHG	C27-C28-C29-C30
26	y	319	LHG	C13-C14-C15-C16
25	C	503	CLA	O1D-CGD-O2D-CED
26	Y	301	LHG	O2-C2-C3-O3
26	Y	319	LHG	O2-C2-C3-O3
26	y	301	LHG	O2-C2-C3-O3
26	y	319	LHG	O2-C2-C3-O3
26	R	618	LHG	C9-C10-C11-C12
26	r	618	LHG	C9-C10-C11-C12
35	C	516	DGD	CBB-CCB-CDB-CEB
35	c	516	DGD	CBB-CCB-CDB-CEB
35	C	516	DGD	C1A-C2A-C3A-C4A
35	c	516	DGD	C1A-C2A-C3A-C4A
25	c	503	CLA	O1D-CGD-O2D-CED
28	T	101	BCR	C20-C21-C22-C23
28	t	101	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
26	B	622	LHG	C13-C14-C15-C16
26	B	622	LHG	C18-C19-C20-C21
26	C	519	LHG	C28-C29-C30-C31
26	b	622	LHG	C13-C14-C15-C16
26	b	622	LHG	C18-C19-C20-C21
26	c	519	LHG	C28-C29-C30-C31
29	L	101	SQD	C27-C28-C29-C30
35	B	626	DGD	CBB-CCB-CDB-CEB
35	b	626	DGD	CBB-CCB-CDB-CEB
24	Y	310	CHL	O1A-CGA-O2A-C1
24	y	310	CHL	O1A-CGA-O2A-C1
25	A	405	CLA	C11-C12-C13-C14
25	B	612	CLA	C16-C17-C18-C20
25	Y	313	CLA	C11-C12-C13-C15
25	a	406	CLA	C11-C12-C13-C14
25	b	612	CLA	C16-C17-C18-C20
25	Y	304	CLA	C4-C3-C5-C6
25	Y	312	CLA	C4-C3-C5-C6
25	y	304	CLA	C4-C3-C5-C6
25	y	312	CLA	C4-C3-C5-C6
26	B	621	LHG	C27-C28-C29-C30
26	B	622	LHG	C12-C13-C14-C15
26	S	318	LHG	C33-C34-C35-C36
26	b	621	LHG	C27-C28-C29-C30
26	b	622	LHG	C12-C13-C14-C15
26	s	318	LHG	C33-C34-C35-C36
26	n	618	LHG	C32-C33-C34-C35
29	A	411	SQD	C11-C12-C13-C14
29	A	411	SQD	C12-C13-C14-C15
29	a	412	SQD	C11-C12-C13-C14
29	a	412	SQD	C12-C13-C14-C15
29	l	102	SQD	C27-C28-C29-C30
30	B	623	LMG	C32-C33-C34-C35
30	b	623	LMG	C32-C33-C34-C35
24	G	601	CHL	C11-C10-C8-C9
24	g	601	CHL	C11-C10-C8-C9
25	B	604	CLA	C11-C10-C8-C9
25	S	303	CLA	C11-C12-C13-C14
25	G	603	CLA	C6-C7-C8-C9
25	N	603	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C10-C8-C9
25	s	303	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	g	603	CLA	C6-C7-C8-C9
25	n	603	CLA	C6-C7-C8-C9
24	S	307	CHL	O1D-CGD-O2D-CED
24	s	307	CHL	O1D-CGD-O2D-CED
26	D	406	LHG	C7-C8-C9-C10
26	d	406	LHG	C7-C8-C9-C10
26	2	606	LHG	C30-C31-C32-C33
26	B	625	LHG	C10-C11-C12-C13
26	S	318	LHG	C10-C11-C12-C13
26	N	618	LHG	C32-C33-C34-C35
26	6	606	LHG	C30-C31-C32-C33
26	b	625	LHG	C10-C11-C12-C13
26	s	318	LHG	C10-C11-C12-C13
29	L	103	SQD	C13-C14-C15-C16
29	l	101	SQD	C13-C14-C15-C16
30	B	620	LMG	C18-C19-C20-C21
30	b	620	LMG	C18-C19-C20-C21
35	B	626	DGD	C7B-C8B-C9B-CAB
35	C	516	DGD	CAB-CBB-CCB-CDB
35	b	626	DGD	C7B-C8B-C9B-CAB
35	c	516	DGD	CAB-CBB-CCB-CDB
25	2	602	CLA	C8-C10-C11-C12
25	6	602	CLA	C8-C10-C11-C12
30	C	520	LMG	O6-C5-C6-O5
25	B	606	CLA	C2A-CAA-CBA-CGA
25	G	611	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	g	611	CLA	C2A-CAA-CBA-CGA
25	B	607	CLA	O1A-CGA-O2A-C1
25	b	607	CLA	O1A-CGA-O2A-C1
26	L	102	LHG	C30-C31-C32-C33
26	l	103	LHG	C30-C31-C32-C33
26	B	621	LHG	O1-C1-C2-C3
26	B	625	LHG	O1-C1-C2-C3
26	C	519	LHG	O1-C1-C2-C3
26	b	621	LHG	O1-C1-C2-C3
26	b	625	LHG	O1-C1-C2-C3
26	c	519	LHG	O1-C1-C2-C3
28	T	101	BCR	C11-C12-C13-C14
28	t	101	BCR	C11-C12-C13-C14
40	G	617	NEX	C11-C12-C13-C14
40	g	617	NEX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	B	623	LMG	C33-C34-C35-C36
30	C	520	LMG	C16-C17-C18-C19
30	b	623	LMG	C33-C34-C35-C36
30	c	520	LMG	C16-C17-C18-C19
35	c	516	DGD	C8A-C9A-CAA-CBA
26	S	301	LHG	C7-C8-C9-C10
26	s	301	LHG	C7-C8-C9-C10
26	S	318	LHG	C12-C13-C14-C15
26	s	318	LHG	C12-C13-C14-C15
26	n	618	LHG	C15-C16-C17-C18
30	A	408	LMG	C36-C37-C38-C39
30	a	409	LMG	C36-C37-C38-C39
35	C	516	DGD	C8A-C9A-CAA-CBA
30	c	520	LMG	O6-C5-C6-O5
25	C	504	CLA	C11-C12-C13-C15
25	G	613	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C15
25	g	613	CLA	C16-C17-C18-C20
30	B	623	LMG	C8-C9-O8-C28
30	b	623	LMG	C8-C9-O8-C28
25	D	402	CLA	C13-C15-C16-C17
25	d	402	CLA	C13-C15-C16-C17
26	2	606	LHG	C12-C13-C14-C15
26	B	621	LHG	C25-C26-C27-C28
26	B	621	LHG	C32-C33-C34-C35
26	C	518	LHG	C32-C33-C34-C35
26	D	406	LHG	C32-C33-C34-C35
26	N	618	LHG	C15-C16-C17-C18
26	6	606	LHG	C12-C13-C14-C15
26	b	621	LHG	C25-C26-C27-C28
26	b	621	LHG	C32-C33-C34-C35
26	c	518	LHG	C32-C33-C34-C35
26	d	406	LHG	C32-C33-C34-C35
29	L	103	SQD	C32-C33-C34-C35
29	l	101	SQD	C32-C33-C34-C35
35	A	415	DGD	C8B-C9B-CAB-CBB
35	a	401	DGD	C8B-C9B-CAB-CBB
24	R	605	CHL	CBD-CGD-O2D-CED
24	r	605	CHL	CBD-CGD-O2D-CED
29	A	411	SQD	C23-C24-C25-C26
29	a	412	SQD	C23-C24-C25-C26
25	C	506	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	C13-C15-C16-C17
26	S	318	LHG	C11-C12-C13-C14
26	s	318	LHG	C11-C12-C13-C14
26	n	618	LHG	C34-C35-C36-C37
26	y	319	LHG	C24-C25-C26-C27
29	A	411	SQD	C16-C17-C18-C19
29	a	412	SQD	C16-C17-C18-C19
25	g	611	CLA	C3-C5-C6-C7
26	C	517	LHG	C24-C23-O8-C6
26	c	517	LHG	C24-C23-O8-C6
26	N	618	LHG	C34-C35-C36-C37
26	Y	319	LHG	C24-C25-C26-C27
35	A	415	DGD	C8A-C9A-CAA-CBA
35	a	401	DGD	C8A-C9A-CAA-CBA
24	2	603	CHL	C3A-C2A-CAA-CBA
24	G	607	CHL	C3A-C2A-CAA-CBA
24	N	608	CHL	C3A-C2A-CAA-CBA
24	Y	309	CHL	C3A-C2A-CAA-CBA
24	R	605	CHL	C3A-C2A-CAA-CBA
24	R	606	CHL	C3A-C2A-CAA-CBA
24	6	603	CHL	C3A-C2A-CAA-CBA
24	g	607	CHL	C3A-C2A-CAA-CBA
24	n	608	CHL	C3A-C2A-CAA-CBA
24	y	309	CHL	C3A-C2A-CAA-CBA
24	r	605	CHL	C3A-C2A-CAA-CBA
24	r	606	CHL	C3A-C2A-CAA-CBA
25	S	303	CLA	C3A-C2A-CAA-CBA
25	Y	304	CLA	C3A-C2A-CAA-CBA
25	Y	315	CLA	C3A-C2A-CAA-CBA
25	R	609	CLA	C3A-C2A-CAA-CBA
25	R	614	CLA	C3A-C2A-CAA-CBA
25	s	303	CLA	C3A-C2A-CAA-CBA
25	y	304	CLA	C3A-C2A-CAA-CBA
25	y	315	CLA	C3A-C2A-CAA-CBA
25	r	609	CLA	C3A-C2A-CAA-CBA
25	r	614	CLA	C3A-C2A-CAA-CBA
25	C	508	CLA	C13-C15-C16-C17
25	c	508	CLA	C13-C15-C16-C17
26	B	621	LHG	C24-C25-C26-C27
26	C	519	LHG	C25-C26-C27-C28
26	b	621	LHG	C24-C25-C26-C27
26	c	519	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
30	B	623	LMG	C11-C12-C13-C14
30	b	623	LMG	C11-C12-C13-C14
30	B	623	LMG	O10-C28-O8-C9
30	b	623	LMG	O10-C28-O8-C9
25	B	608	CLA	C16-C17-C18-C20
25	N	613	CLA	C11-C12-C13-C14
25	b	608	CLA	C16-C17-C18-C20
25	n	613	CLA	C11-C12-C13-C14
24	2	603	CHL	C2C-C3C-CAC-CBC
24	R	613	CHL	C2C-C3C-CAC-CBC
24	6	603	CHL	C2C-C3C-CAC-CBC
30	A	408	LMG	C16-C17-C18-C19
30	A	408	LMG	C34-C35-C36-C37
30	a	409	LMG	C16-C17-C18-C19
30	a	409	LMG	C34-C35-C36-C37
35	B	626	DGD	CBA-CCA-CDA-CEA
35	b	626	DGD	CBA-CCA-CDA-CEA
26	S	301	LHG	C4-C5-C6-O8
26	s	301	LHG	C4-C5-C6-O8
26	C	517	LHG	C27-C28-C29-C30
26	C	519	LHG	C9-C10-C11-C12
26	S	318	LHG	C17-C18-C19-C20
26	c	517	LHG	C27-C28-C29-C30
26	c	519	LHG	C9-C10-C11-C12
26	s	318	LHG	C17-C18-C19-C20
30	B	623	LMG	C30-C31-C32-C33
25	A	405	CLA	C3-C5-C6-C7
25	G	611	CLA	C3-C5-C6-C7
25	a	406	CLA	C3-C5-C6-C7
30	D	407	LMG	C28-C29-C30-C31
30	d	407	LMG	C28-C29-C30-C31
24	r	613	CHL	C2C-C3C-CAC-CBC
30	b	623	LMG	C30-C31-C32-C33
25	B	606	CLA	C2-C3-C5-C6
25	B	609	CLA	C2-C3-C5-C6
25	C	510	CLA	C2-C3-C5-C6
25	S	311	CLA	C2-C3-C5-C6
25	N	612	CLA	C2-C3-C5-C6
25	b	606	CLA	C2-C3-C5-C6
25	b	609	CLA	C2-C3-C5-C6
25	c	510	CLA	C2-C3-C5-C6
25	s	311	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	n	612	CLA	C2-C3-C5-C6
26	Y	301	LHG	C8-C7-O7-C5
26	y	301	LHG	C8-C7-O7-C5
24	Y	306	CHL	C2C-C3C-CAC-CBC
24	y	306	CHL	C2C-C3C-CAC-CBC
26	S	301	LHG	O1-C1-C2-O2
26	S	318	LHG	O1-C1-C2-O2
26	Y	319	LHG	O1-C1-C2-O2
26	s	301	LHG	O1-C1-C2-O2
26	s	318	LHG	O1-C1-C2-O2
26	y	319	LHG	O1-C1-C2-O2
26	L	102	LHG	C29-C30-C31-C32
26	l	103	LHG	C29-C30-C31-C32
29	L	103	SQD	C26-C27-C28-C29
29	l	101	SQD	C26-C27-C28-C29
35	C	515	DGD	C6B-C7B-C8B-C9B
35	c	515	DGD	C6B-C7B-C8B-C9B
25	B	610	CLA	O1A-CGA-O2A-C1
25	b	610	CLA	O1A-CGA-O2A-C1
35	C	516	DGD	O6E-C5E-C6E-O5E
35	c	516	DGD	O6E-C5E-C6E-O5E
26	S	318	LHG	O2-C2-C3-O3
26	s	318	LHG	O2-C2-C3-O3
24	Y	302	CHL	C4C-C3C-CAC-CBC
24	y	302	CHL	C4C-C3C-CAC-CBC
26	S	301	LHG	C24-C25-C26-C27
26	s	301	LHG	C24-C25-C26-C27
26	L	102	LHG	C31-C32-C33-C34
26	c	518	LHG	C31-C32-C33-C34
26	l	103	LHG	C31-C32-C33-C34
30	a	409	LMG	C13-C14-C15-C16
25	B	610	CLA	C13-C15-C16-C17
25	b	610	CLA	C13-C15-C16-C17
26	C	518	LHG	C31-C32-C33-C34
30	A	408	LMG	C13-C14-C15-C16
30	B	623	LMG	C16-C17-C18-C19
30	b	623	LMG	C16-C17-C18-C19
24	N	608	CHL	C2-C1-O2A-CGA
24	n	608	CHL	C2-C1-O2A-CGA
35	B	626	DGD	C4E-C5E-C6E-O5E
35	b	626	DGD	C4E-C5E-C6E-O5E
25	G	611	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	g	611	CLA	C4C-C3C-CAC-CBC
25	r	614	CLA	C4C-C3C-CAC-CBC
26	L	102	LHG	C28-C29-C30-C31
26	L	102	LHG	C34-C35-C36-C37
26	l	103	LHG	C28-C29-C30-C31
26	l	103	LHG	C34-C35-C36-C37
35	B	626	DGD	CCB-CDB-CEB-CFB
35	C	516	DGD	C3B-C4B-C5B-C6B
35	b	626	DGD	CCB-CDB-CEB-CFB
25	B	602	CLA	C8-C10-C11-C12
25	C	505	CLA	C5-C6-C7-C8
25	b	602	CLA	C8-C10-C11-C12
25	c	505	CLA	C5-C6-C7-C8
25	R	614	CLA	C4C-C3C-CAC-CBC
35	c	516	DGD	C3B-C4B-C5B-C6B
28	B	617	BCR	C1-C6-C7-C8
28	B	617	BCR	C5-C6-C7-C8
28	B	618	BCR	C23-C24-C25-C26
28	B	619	BCR	C23-C24-C25-C30
28	D	404	BCR	C5-C6-C7-C8
28	T	101	BCR	C23-C24-C25-C26
28	T	101	BCR	C23-C24-C25-C30
28	Z	101	BCR	C5-C6-C7-C8
28	b	617	BCR	C1-C6-C7-C8
28	b	617	BCR	C5-C6-C7-C8
28	b	618	BCR	C23-C24-C25-C26
28	b	619	BCR	C23-C24-C25-C30
28	d	404	BCR	C5-C6-C7-C8
28	t	101	BCR	C23-C24-C25-C26
28	t	101	BCR	C23-C24-C25-C30
28	z	101	BCR	C5-C6-C7-C8
39	G	615	LUT	C5-C6-C7-C8
39	N	615	LUT	C1-C6-C7-C8
39	N	615	LUT	C5-C6-C7-C8
39	N	616	LUT	C1-C6-C7-C8
39	N	616	LUT	C5-C6-C7-C8
39	Y	316	LUT	C1-C6-C7-C8
39	Y	316	LUT	C5-C6-C7-C8
39	R	615	LUT	C5-C6-C7-C8
39	g	615	LUT	C5-C6-C7-C8
39	n	615	LUT	C1-C6-C7-C8
39	n	615	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
39	n	616	LUT	C1-C6-C7-C8
39	n	616	LUT	C5-C6-C7-C8
39	y	316	LUT	C1-C6-C7-C8
39	y	316	LUT	C5-C6-C7-C8
39	r	615	LUT	C5-C6-C7-C8
25	N	604	CLA	C4C-C3C-CAC-CBC
25	G	603	CLA	C5-C6-C7-C8
25	G	603	CLA	C10-C11-C12-C13
25	g	603	CLA	C5-C6-C7-C8
25	g	603	CLA	C10-C11-C12-C13
30	D	407	LMG	C11-C10-O7-C8
30	d	407	LMG	C11-C10-O7-C8
29	A	411	SQD	C29-C30-C31-C32
29	L	103	SQD	C27-C28-C29-C30
29	a	412	SQD	C29-C30-C31-C32
29	l	101	SQD	C27-C28-C29-C30
26	s	318	LHG	C23-C24-C25-C26
35	A	415	DGD	C1B-C2B-C3B-C4B
35	a	401	DGD	C1B-C2B-C3B-C4B
25	n	604	CLA	C4C-C3C-CAC-CBC
26	D	406	LHG	C26-C27-C28-C29
26	d	406	LHG	C26-C27-C28-C29
24	Y	309	CHL	C10-C11-C12-C13
24	y	309	CHL	C10-C11-C12-C13
25	A	401	CLA	C15-C16-C17-C18
25	B	605	CLA	C5-C6-C7-C8
25	C	511	CLA	C10-C11-C12-C13
25	a	402	CLA	C15-C16-C17-C18
25	b	605	CLA	C5-C6-C7-C8
25	c	511	CLA	C10-C11-C12-C13
25	N	612	CLA	C4-C3-C5-C6
25	R	608	CLA	C4-C3-C5-C6
25	n	612	CLA	C4-C3-C5-C6
25	r	608	CLA	C4-C3-C5-C6
24	N	609	CHL	C2-C3-C5-C6
24	n	609	CHL	C2-C3-C5-C6
25	A	405	CLA	C6-C7-C8-C10
25	B	602	CLA	C11-C12-C13-C15
25	B	602	CLA	C12-C13-C15-C16
25	B	604	CLA	C11-C10-C8-C7
25	B	610	CLA	C11-C10-C8-C7
25	B	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	B	615	CLA	C2-C3-C5-C6
25	C	501	CLA	C12-C13-C15-C16
25	C	507	CLA	C12-C13-C15-C16
25	S	303	CLA	C11-C10-C8-C7
25	S	313	CLA	C2-C3-C5-C6
25	G	602	CLA	C11-C10-C8-C7
25	G	602	CLA	C12-C13-C15-C16
25	Y	303	CLA	C11-C10-C8-C7
25	Y	304	CLA	C6-C7-C8-C10
25	Y	312	CLA	C2-C3-C5-C6
25	R	608	CLA	C6-C7-C8-C10
25	a	406	CLA	C6-C7-C8-C10
25	b	602	CLA	C12-C13-C15-C16
25	b	604	CLA	C11-C10-C8-C7
25	b	610	CLA	C11-C10-C8-C7
25	b	611	CLA	C2-C3-C5-C6
25	b	615	CLA	C2-C3-C5-C6
25	c	501	CLA	C12-C13-C15-C16
25	c	507	CLA	C12-C13-C15-C16
25	s	303	CLA	C11-C10-C8-C7
25	s	313	CLA	C2-C3-C5-C6
25	g	602	CLA	C11-C10-C8-C7
25	g	602	CLA	C12-C13-C15-C16
25	y	303	CLA	C11-C10-C8-C7
25	y	304	CLA	C6-C7-C8-C10
25	y	312	CLA	C2-C3-C5-C6
25	r	608	CLA	C6-C7-C8-C10
26	C	517	LHG	O10-C23-O8-C6
26	c	517	LHG	O10-C23-O8-C6
30	B	623	LMG	C17-C18-C19-C20
30	b	623	LMG	C17-C18-C19-C20
24	N	608	CHL	C15-C16-C17-C18
24	n	608	CHL	C15-C16-C17-C18
25	G	611	CLA	C8-C10-C11-C12
25	R	609	CLA	C13-C15-C16-C17
25	g	611	CLA	C8-C10-C11-C12
25	r	609	CLA	C13-C15-C16-C17
24	R	607	CHL	C11-C12-C13-C14
24	r	607	CHL	C11-C12-C13-C14
25	R	602	CLA	C11-C12-C13-C15
25	R	609	CLA	C16-C17-C18-C19
25	r	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	r	609	CLA	C16-C17-C18-C19
26	S	318	LHG	C23-C24-C25-C26
30	D	407	LMG	C20-C21-C22-C23
30	d	407	LMG	C20-C21-C22-C23
25	2	605	CLA	C2A-CAA-CBA-CGA
25	6	605	CLA	C2A-CAA-CBA-CGA
25	C	513	CLA	C5-C6-C7-C8
25	c	513	CLA	C5-C6-C7-C8
27	A	403	PHO	C13-C15-C16-C17
27	a	404	PHO	C13-C15-C16-C17
26	D	406	LHG	C25-C26-C27-C28
26	d	406	LHG	C25-C26-C27-C28
30	A	408	LMG	C35-C36-C37-C38
30	a	409	LMG	C35-C36-C37-C38
24	y	309	CHL	O1A-CGA-O2A-C1
30	D	407	LMG	C29-C30-C31-C32
30	d	407	LMG	C29-C30-C31-C32
25	S	311	CLA	C11-C10-C8-C7
25	s	311	CLA	C11-C10-C8-C7
29	L	103	SQD	C12-C13-C14-C15
29	l	101	SQD	C12-C13-C14-C15
30	C	520	LMG	C11-C12-C13-C14
30	c	520	LMG	C11-C12-C13-C14
24	Y	309	CHL	O1A-CGA-O2A-C1
26	B	625	LHG	C32-C33-C34-C35
26	b	625	LHG	C32-C33-C34-C35
30	A	408	LMG	C29-C30-C31-C32
30	a	409	LMG	C29-C30-C31-C32
26	L	102	LHG	O6-C4-C5-O7
26	l	103	LHG	O6-C4-C5-O7
26	S	318	LHG	C31-C32-C33-C34
26	s	318	LHG	C31-C32-C33-C34
29	A	407	SQD	C17-C18-C19-C20
29	a	408	SQD	C17-C18-C19-C20
35	C	516	DGD	CCB-CDB-CEB-CFB
35	c	516	DGD	CCB-CDB-CEB-CFB
25	C	508	CLA	C15-C16-C17-C18
25	N	602	CLA	C10-C11-C12-C13
25	n	602	CLA	C10-C11-C12-C13
25	C	512	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
26	B	625	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	C	519	LHG	C12-C13-C14-C15
26	c	519	LHG	C12-C13-C14-C15
25	G	613	CLA	C3-C5-C6-C7
25	g	613	CLA	C3-C5-C6-C7
26	b	625	LHG	C15-C16-C17-C18
29	L	103	SQD	C15-C16-C17-C18
29	l	101	SQD	C15-C16-C17-C18
25	c	508	CLA	C15-C16-C17-C18
26	S	301	LHG	O7-C5-C6-O8
26	s	301	LHG	O7-C5-C6-O8
29	A	411	SQD	O6-C44-C45-O47
29	a	412	SQD	O6-C44-C45-O47
30	B	623	LMG	C19-C20-C21-C22
30	b	623	LMG	C19-C20-C21-C22
35	A	415	DGD	CBB-CCB-CDB-CEB
35	B	626	DGD	C3B-C4B-C5B-C6B
35	a	401	DGD	CBB-CCB-CDB-CEB
35	b	626	DGD	C3B-C4B-C5B-C6B
25	G	610	CLA	C2-C3-C5-C6
25	Y	311	CLA	C2-C3-C5-C6
25	g	610	CLA	C2-C3-C5-C6
25	y	311	CLA	C2-C3-C5-C6
31	D	405	PL9	C4-C3-C7-C8
31	d	405	PL9	C4-C3-C7-C8
24	N	607	CHL	C6-C7-C8-C9
24	n	607	CHL	C6-C7-C8-C9
25	A	405	CLA	C6-C7-C8-C9
25	B	603	CLA	C6-C7-C8-C9
25	B	604	CLA	C11-C12-C13-C14
25	B	607	CLA	C11-C12-C13-C14
25	B	611	CLA	C14-C13-C15-C16
25	B	615	CLA	C14-C13-C15-C16
25	C	507	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C12-C13-C14
25	G	602	CLA	C14-C13-C15-C16
25	G	603	CLA	C11-C10-C8-C9
25	G	610	CLA	C14-C13-C15-C16
25	N	603	CLA	C14-C13-C15-C16
25	N	610	CLA	C11-C12-C13-C14
25	a	406	CLA	C6-C7-C8-C9
25	b	603	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	b	607	CLA	C11-C12-C13-C14
25	b	611	CLA	C14-C13-C15-C16
25	b	615	CLA	C14-C13-C15-C16
25	c	507	CLA	C14-C13-C15-C16
25	c	510	CLA	C11-C12-C13-C14
25	g	602	CLA	C14-C13-C15-C16
25	g	603	CLA	C11-C10-C8-C9
25	g	610	CLA	C14-C13-C15-C16
25	n	603	CLA	C14-C13-C15-C16
25	n	610	CLA	C11-C12-C13-C14
27	A	403	PHO	C11-C10-C8-C9
27	a	404	PHO	C11-C10-C8-C9
24	G	601	CHL	C4C-C3C-CAC-CBC
26	S	318	LHG	C29-C30-C31-C32
26	s	318	LHG	C29-C30-C31-C32
24	N	605	CHL	C2A-CAA-CBA-CGA
24	n	605	CHL	C2A-CAA-CBA-CGA
25	B	603	CLA	C2A-CAA-CBA-CGA
25	B	614	CLA	C2A-CAA-CBA-CGA
25	S	305	CLA	C2A-CAA-CBA-CGA
25	S	314	CLA	C2A-CAA-CBA-CGA
25	b	603	CLA	C2A-CAA-CBA-CGA
25	b	614	CLA	C2A-CAA-CBA-CGA
25	s	305	CLA	C2A-CAA-CBA-CGA
25	s	314	CLA	C2A-CAA-CBA-CGA
24	S	306	CHL	O1D-CGD-O2D-CED
24	s	306	CHL	O1D-CGD-O2D-CED
24	G	601	CHL	C13-C15-C16-C17
24	g	601	CHL	C13-C15-C16-C17
25	C	506	CLA	C10-C11-C12-C13
25	N	613	CLA	C8-C10-C11-C12
25	c	506	CLA	C10-C11-C12-C13
25	n	613	CLA	C8-C10-C11-C12
24	g	601	CHL	C4C-C3C-CAC-CBC
26	C	519	LHG	C30-C31-C32-C33
26	c	519	LHG	C30-C31-C32-C33
35	A	415	DGD	C7A-C8A-C9A-CAA
35	a	401	DGD	C7A-C8A-C9A-CAA
24	2	603	CHL	C1A-C2A-CAA-CBA
24	R	605	CHL	C1A-C2A-CAA-CBA
24	6	603	CHL	C1A-C2A-CAA-CBA
24	n	601	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	r	605	CHL	C1A-C2A-CAA-CBA
25	A	402	CLA	C1A-C2A-CAA-CBA
25	B	611	CLA	C1A-C2A-CAA-CBA
25	C	506	CLA	C1A-C2A-CAA-CBA
25	S	305	CLA	C1A-C2A-CAA-CBA
25	S	310	CLA	C1A-C2A-CAA-CBA
25	G	604	CLA	C1A-C2A-CAA-CBA
25	G	610	CLA	C1A-C2A-CAA-CBA
25	G	611	CLA	C1A-C2A-CAA-CBA
25	Y	304	CLA	C1A-C2A-CAA-CBA
25	Y	311	CLA	C1A-C2A-CAA-CBA
25	Y	314	CLA	C1A-C2A-CAA-CBA
25	R	604	CLA	C1A-C2A-CAA-CBA
25	R	610	CLA	C1A-C2A-CAA-CBA
25	R	611	CLA	C1A-C2A-CAA-CBA
25	a	403	CLA	C1A-C2A-CAA-CBA
25	b	611	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C1A-C2A-CAA-CBA
25	s	305	CLA	C1A-C2A-CAA-CBA
25	s	310	CLA	C1A-C2A-CAA-CBA
25	g	604	CLA	C1A-C2A-CAA-CBA
25	g	610	CLA	C1A-C2A-CAA-CBA
25	g	611	CLA	C1A-C2A-CAA-CBA
25	y	304	CLA	C1A-C2A-CAA-CBA
25	y	311	CLA	C1A-C2A-CAA-CBA
25	y	314	CLA	C1A-C2A-CAA-CBA
25	r	604	CLA	C1A-C2A-CAA-CBA
25	r	610	CLA	C1A-C2A-CAA-CBA
25	r	611	CLA	C1A-C2A-CAA-CBA
25	N	613	CLA	C11-C12-C13-C15
25	R	602	CLA	C11-C12-C13-C14
25	R	603	CLA	C11-C12-C13-C14
25	n	613	CLA	C11-C12-C13-C15
25	r	602	CLA	C11-C12-C13-C14
25	r	603	CLA	C11-C12-C13-C14
26	Y	301	LHG	O9-C7-O7-C5
26	y	301	LHG	O9-C7-O7-C5
30	D	407	LMG	O9-C10-O7-C8
30	d	407	LMG	O9-C10-O7-C8
26	L	102	LHG	C8-C7-O7-C5
26	l	103	LHG	C8-C7-O7-C5
24	N	607	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	n	607	CHL	C13-C15-C16-C17
24	2	601	CHL	C3-C5-C6-C7
24	G	601	CHL	C3-C5-C6-C7
24	6	601	CHL	C3-C5-C6-C7
24	g	601	CHL	C3-C5-C6-C7
24	r	606	CHL	C4C-C3C-CAC-CBC
25	C	512	CLA	O1A-CGA-O2A-C1
25	B	602	CLA	C5-C6-C7-C8
25	b	602	CLA	C5-C6-C7-C8
25	d	403	CLA	C8-C10-C11-C12
26	S	301	LHG	O6-C4-C5-C6
26	N	618	LHG	O6-C4-C5-C6
26	s	301	LHG	O6-C4-C5-C6
26	n	618	LHG	O6-C4-C5-C6
24	R	606	CHL	C4C-C3C-CAC-CBC
30	B	620	LMG	C17-C18-C19-C20
30	b	620	LMG	C17-C18-C19-C20
25	D	403	CLA	C8-C10-C11-C12
26	C	517	LHG	C14-C15-C16-C17
26	c	517	LHG	C14-C15-C16-C17
29	L	103	SQD	C31-C32-C33-C34
29	l	101	SQD	C31-C32-C33-C34
35	A	415	DGD	C9B-CAB-CBB-CCB
35	a	401	DGD	C9B-CAB-CBB-CCB
24	G	609	CHL	O1D-CGD-O2D-CED
25	Y	312	CLA	C10-C11-C12-C13
25	y	312	CLA	C10-C11-C12-C13
26	Y	319	LHG	C25-C26-C27-C28
35	A	415	DGD	C6B-C7B-C8B-C9B
35	a	401	DGD	C6B-C7B-C8B-C9B
26	S	318	LHG	C1-C2-C3-O3
26	Y	319	LHG	C1-C2-C3-O3
26	s	318	LHG	C1-C2-C3-O3
26	y	319	LHG	C1-C2-C3-O3
24	N	609	CHL	C4-C3-C5-C6
24	n	609	CHL	C4-C3-C5-C6
26	c	518	LHG	C24-C25-C26-C27
26	y	319	LHG	C25-C26-C27-C28
30	B	620	LMG	C37-C38-C39-C40
25	c	512	CLA	O1A-CGA-O2A-C1
26	C	518	LHG	C24-C25-C26-C27
30	b	620	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
24	1	302	CHL	C2A-CAA-CBA-CGA
24	R	607	CHL	C2A-CAA-CBA-CGA
24	r	607	CHL	C2A-CAA-CBA-CGA
25	B	608	CLA	C2A-CAA-CBA-CGA
25	N	611	CLA	C2A-CAA-CBA-CGA
25	b	608	CLA	C2A-CAA-CBA-CGA
25	n	611	CLA	C2A-CAA-CBA-CGA
25	B	603	CLA	C16-C17-C18-C20
25	C	513	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C20
25	c	513	CLA	C16-C17-C18-C19
24	g	609	CHL	O1D-CGD-O2D-CED
26	B	621	LHG	C4-C5-C6-O8
26	b	621	LHG	C4-C5-C6-O8
30	A	408	LMG	C7-C8-C9-O8
30	a	409	LMG	C7-C8-C9-O8
35	B	626	DGD	C1G-C2G-C3G-O3G
35	b	626	DGD	C1G-C2G-C3G-O3G
26	2	606	LHG	C29-C30-C31-C32
26	6	606	LHG	C29-C30-C31-C32
24	g	601	CHL	C5-C6-C7-C8
25	B	603	CLA	C15-C16-C17-C18
25	B	606	CLA	C13-C15-C16-C17
25	C	504	CLA	C10-C11-C12-C13
25	R	609	CLA	C5-C6-C7-C8
25	b	603	CLA	C15-C16-C17-C18
25	b	606	CLA	C13-C15-C16-C17
25	c	504	CLA	C10-C11-C12-C13
25	r	609	CLA	C5-C6-C7-C8
25	S	303	CLA	C14-C13-C15-C16
25	s	303	CLA	C14-C13-C15-C16
26	Y	319	LHG	C34-C35-C36-C37
26	y	319	LHG	C34-C35-C36-C37
35	B	626	DGD	C1A-C2A-C3A-C4A
35	b	626	DGD	C1A-C2A-C3A-C4A
24	G	601	CHL	C5-C6-C7-C8
26	S	318	LHG	C25-C26-C27-C28
26	s	318	LHG	C25-C26-C27-C28
25	C	504	CLA	C8-C10-C11-C12
25	c	504	CLA	C8-C10-C11-C12
30	B	623	LMG	O6-C5-C6-O5
30	b	623	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
25	G	613	CLA	C4-C3-C5-C6
25	g	613	CLA	C4-C3-C5-C6
25	n	602	CLA	C4-C3-C5-C6
35	A	415	DGD	C3B-C4B-C5B-C6B
35	a	401	DGD	C3B-C4B-C5B-C6B
25	N	612	CLA	C11-C12-C13-C15
25	n	612	CLA	C11-C12-C13-C15
25	C	513	CLA	CBA-CGA-O2A-C1
25	R	601	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
25	r	601	CLA	CBA-CGA-O2A-C1
29	A	407	SQD	C10-C11-C12-C13
29	a	408	SQD	C10-C11-C12-C13
24	G	609	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	CBD-CGD-O2D-CED
25	B	616	CLA	C8-C10-C11-C12
25	b	616	CLA	C8-C10-C11-C12
26	R	618	LHG	C28-C29-C30-C31
26	r	618	LHG	C28-C29-C30-C31
24	5	302	CHL	C2A-CAA-CBA-CGA
25	N	614	CLA	C2A-CAA-CBA-CGA
25	n	614	CLA	C2A-CAA-CBA-CGA
24	G	601	CHL	C2-C1-O2A-CGA
24	g	601	CHL	C2-C1-O2A-CGA
29	A	411	SQD	C30-C31-C32-C33
35	C	516	DGD	C2A-C1A-O1G-C1G
35	c	516	DGD	C2A-C1A-O1G-C1G
26	C	517	LHG	O6-C4-C5-O7
26	c	517	LHG	O6-C4-C5-O7
25	2	602	CLA	C11-C12-C13-C15
25	6	602	CLA	C11-C12-C13-C15
29	a	412	SQD	C30-C31-C32-C33
24	Y	302	CHL	O1A-CGA-O2A-C1
24	y	302	CHL	O1A-CGA-O2A-C1
26	b	622	LHG	C26-C27-C28-C29
30	A	410	LMG	C36-C37-C38-C39
30	a	411	LMG	C36-C37-C38-C39
35	A	415	DGD	C1A-C2A-C3A-C4A
35	a	401	DGD	C1A-C2A-C3A-C4A
28	I	101	BCR	C20-C21-C22-C23
28	i	101	BCR	C20-C21-C22-C23
25	A	401	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	a	402	CLA	C4C-C3C-CAC-CBC
26	B	622	LHG	C26-C27-C28-C29
26	B	621	LHG	O7-C5-C6-O8
26	N	618	LHG	O7-C5-C6-O8
26	b	621	LHG	O7-C5-C6-O8
26	n	618	LHG	O7-C5-C6-O8
29	A	407	SQD	O6-C44-C45-O47
29	a	408	SQD	O6-C44-C45-O47
30	C	520	LMG	O7-C8-C9-O8
30	c	520	LMG	O7-C8-C9-O8
26	L	102	LHG	C10-C11-C12-C13
26	l	103	LHG	C10-C11-C12-C13
30	A	410	LMG	C40-C41-C42-C43
30	a	411	LMG	C40-C41-C42-C43
35	C	516	DGD	C2B-C3B-C4B-C5B
25	B	606	CLA	C4-C3-C5-C6
25	N	602	CLA	C4-C3-C5-C6
25	Y	313	CLA	C4-C3-C5-C6
25	b	606	CLA	C4-C3-C5-C6
25	y	313	CLA	C4-C3-C5-C6
25	n	603	CLA	C4C-C3C-CAC-CBC
26	N	618	LHG	C31-C32-C33-C34
35	c	516	DGD	C2B-C3B-C4B-C5B
24	G	608	CHL	C11-C10-C8-C7
24	Y	302	CHL	C12-C13-C15-C16
24	Y	309	CHL	C12-C13-C15-C16
24	g	608	CHL	C11-C10-C8-C7
24	y	302	CHL	C12-C13-C15-C16
24	y	309	CHL	C12-C13-C15-C16
25	B	603	CLA	C6-C7-C8-C10
25	B	604	CLA	C6-C7-C8-C10
25	B	613	CLA	C11-C12-C13-C15
25	B	613	CLA	C12-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C10
25	B	615	CLA	C12-C13-C15-C16
25	C	507	CLA	C6-C7-C8-C10
25	C	509	CLA	C6-C7-C8-C10
25	C	509	CLA	C11-C12-C13-C15
25	C	511	CLA	C11-C10-C8-C7
25	C	511	CLA	C11-C12-C13-C15
25	C	512	CLA	C12-C13-C15-C16
25	D	403	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	S	303	CLA	C6-C7-C8-C10
25	G	610	CLA	C12-C13-C15-C16
25	N	603	CLA	C11-C10-C8-C7
25	N	603	CLA	C11-C12-C13-C15
25	Y	304	CLA	C2-C3-C5-C6
25	Y	304	CLA	C11-C10-C8-C7
25	R	603	CLA	C6-C7-C8-C10
25	b	602	CLA	C11-C12-C13-C15
25	b	603	CLA	C6-C7-C8-C10
25	b	604	CLA	C6-C7-C8-C10
25	b	613	CLA	C11-C12-C13-C15
25	b	613	CLA	C12-C13-C15-C16
25	b	614	CLA	C6-C7-C8-C10
25	b	615	CLA	C12-C13-C15-C16
25	c	507	CLA	C6-C7-C8-C10
25	c	509	CLA	C6-C7-C8-C10
25	c	509	CLA	C11-C12-C13-C15
25	c	511	CLA	C11-C10-C8-C7
25	c	511	CLA	C11-C12-C13-C15
25	c	512	CLA	C12-C13-C15-C16
25	d	403	CLA	C2-C3-C5-C6
25	s	303	CLA	C6-C7-C8-C10
25	g	610	CLA	C12-C13-C15-C16
25	n	603	CLA	C11-C10-C8-C7
25	n	603	CLA	C11-C12-C13-C15
25	y	304	CLA	C2-C3-C5-C6
25	y	304	CLA	C11-C10-C8-C7
25	r	603	CLA	C6-C7-C8-C10
25	r	612	CLA	C6-C7-C8-C10
24	Y	310	CHL	C3-C5-C6-C7
24	y	310	CHL	C3-C5-C6-C7
25	N	603	CLA	C4C-C3C-CAC-CBC
26	b	625	LHG	C12-C13-C14-C15
26	n	618	LHG	C31-C32-C33-C34
25	B	601	CLA	C11-C12-C13-C14
25	B	601	CLA	C14-C13-C15-C16
25	B	605	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C9
25	C	508	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C9
25	C	511	CLA	C11-C12-C13-C14
25	C	512	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C11-C10-C8-C9
25	D	403	CLA	C14-C13-C15-C16
25	Y	313	CLA	C6-C7-C8-C9
25	Y	313	CLA	C11-C10-C8-C9
25	b	601	CLA	C11-C12-C13-C14
25	b	601	CLA	C14-C13-C15-C16
25	b	605	CLA	C14-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C9
25	c	508	CLA	C14-C13-C15-C16
25	c	510	CLA	C11-C10-C8-C9
25	c	511	CLA	C11-C12-C13-C14
25	c	512	CLA	C14-C13-C15-C16
25	c	513	CLA	C11-C10-C8-C9
25	d	403	CLA	C14-C13-C15-C16
25	y	313	CLA	C6-C7-C8-C9
25	y	313	CLA	C11-C10-C8-C9
26	B	625	LHG	C12-C13-C14-C15
26	y	301	LHG	C13-C14-C15-C16
25	B	610	CLA	CBA-CGA-O2A-C1
25	N	603	CLA	CBA-CGA-O2A-C1
25	b	610	CLA	CBA-CGA-O2A-C1
25	n	603	CLA	CBA-CGA-O2A-C1
25	R	603	CLA	C10-C11-C12-C13
25	R	612	CLA	C5-C6-C7-C8
25	r	603	CLA	C10-C11-C12-C13
25	r	612	CLA	C5-C6-C7-C8
26	Y	301	LHG	C13-C14-C15-C16
25	R	610	CLA	C2C-C3C-CAC-CBC
25	r	610	CLA	C2C-C3C-CAC-CBC
26	2	606	LHG	C17-C18-C19-C20
26	6	606	LHG	C17-C18-C19-C20
30	B	620	LMG	C22-C23-C24-C25
30	b	620	LMG	C22-C23-C24-C25
26	B	622	LHG	C14-C15-C16-C17
26	b	622	LHG	C14-C15-C16-C17
25	C	513	CLA	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7
25	R	609	CLA	O1D-CGD-O2D-CED
25	r	609	CLA	O1D-CGD-O2D-CED
25	B	611	CLA	C10-C11-C12-C13
25	N	610	CLA	C13-C15-C16-C17
25	b	611	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	B	621	LHG	C11-C10-C9-C8
26	N	618	LHG	C35-C36-C37-C38
26	b	621	LHG	C11-C10-C9-C8
26	n	618	LHG	C35-C36-C37-C38
26	C	519	LHG	C34-C35-C36-C37
26	c	519	LHG	C34-C35-C36-C37
35	C	515	DGD	C4B-C5B-C6B-C7B
25	C	506	CLA	C5-C6-C7-C8
25	c	506	CLA	C5-C6-C7-C8
25	n	610	CLA	C13-C15-C16-C17
35	c	515	DGD	C4B-C5B-C6B-C7B
35	C	516	DGD	O6D-C1D-O3G-C3G
35	c	516	DGD	O6D-C1D-O3G-C3G
26	L	102	LHG	O6-C4-C5-C6
26	l	103	LHG	O6-C4-C5-C6
29	L	103	SQD	C11-C12-C13-C14
29	l	101	SQD	C11-C12-C13-C14
28	T	101	BCR	C10-C11-C12-C13
28	t	101	BCR	C10-C11-C12-C13
24	6	601	CHL	C15-C16-C17-C18
26	N	618	LHG	C16-C17-C18-C19
26	n	618	LHG	C16-C17-C18-C19
35	A	415	DGD	CCB-CDB-CEB-CFB
35	a	401	DGD	CCB-CDB-CEB-CFB
24	R	607	CHL	C4-C3-C5-C6
24	r	607	CHL	C4-C3-C5-C6
25	N	613	CLA	C4-C3-C5-C6
25	Y	311	CLA	C4-C3-C5-C6
25	n	613	CLA	C4-C3-C5-C6
25	y	311	CLA	C4-C3-C5-C6
24	2	601	CHL	C15-C16-C17-C18
26	Y	301	LHG	C32-C33-C34-C35
26	y	301	LHG	C32-C33-C34-C35
25	S	311	CLA	C11-C10-C8-C9
25	s	311	CLA	C11-C10-C8-C9
25	Y	312	CLA	C11-C12-C13-C15
25	y	312	CLA	C11-C12-C13-C15
25	R	604	CLA	C2A-CAA-CBA-CGA
25	r	604	CLA	C2A-CAA-CBA-CGA
25	C	510	CLA	C2C-C3C-CAC-CBC
25	c	510	CLA	C2C-C3C-CAC-CBC
35	A	415	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
35	a	401	DGD	C2A-C3A-C4A-C5A
24	N	601	CHL	C3A-C2A-CAA-CBA
24	Y	306	CHL	C3A-C2A-CAA-CBA
24	R	607	CHL	C3A-C2A-CAA-CBA
24	n	601	CHL	C3A-C2A-CAA-CBA
24	y	306	CHL	C3A-C2A-CAA-CBA
24	r	607	CHL	C3A-C2A-CAA-CBA
25	S	311	CLA	C3A-C2A-CAA-CBA
25	G	604	CLA	C3A-C2A-CAA-CBA
25	G	613	CLA	C3A-C2A-CAA-CBA
25	Y	314	CLA	C3A-C2A-CAA-CBA
25	R	612	CLA	C3A-C2A-CAA-CBA
25	s	311	CLA	C3A-C2A-CAA-CBA
25	g	604	CLA	C3A-C2A-CAA-CBA
25	g	613	CLA	C3A-C2A-CAA-CBA
25	y	314	CLA	C3A-C2A-CAA-CBA
25	r	612	CLA	C3A-C2A-CAA-CBA
24	5	301	CHL	C2C-C3C-CAC-CBC
26	B	625	LHG	C14-C15-C16-C17
26	b	625	LHG	C14-C15-C16-C17
25	2	602	CLA	C11-C12-C13-C14
25	B	603	CLA	C16-C17-C18-C19
25	R	603	CLA	C11-C12-C13-C15
25	b	603	CLA	C16-C17-C18-C19
25	r	603	CLA	C11-C12-C13-C15
24	1	301	CHL	C2C-C3C-CAC-CBC
25	c	512	CLA	C2C-C3C-CAC-CBC
25	2	605	CLA	O2A-C1-C2-C3
25	6	605	CLA	O2A-C1-C2-C3
25	C	510	CLA	C8-C10-C11-C12
25	c	510	CLA	C8-C10-C11-C12
24	n	606	CHL	O1D-CGD-O2D-CED
29	A	411	SQD	O6-C44-C45-C46
29	a	412	SQD	O6-C44-C45-C46
30	B	623	LMG	C7-C8-C9-O8
30	b	623	LMG	C7-C8-C9-O8
26	L	102	LHG	O9-C7-O7-C5
26	l	103	LHG	O9-C7-O7-C5
25	C	512	CLA	C2C-C3C-CAC-CBC
29	A	411	SQD	C25-C26-C27-C28
29	a	412	SQD	C25-C26-C27-C28
26	D	406	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	L	103	SQD	C30-C31-C32-C33
29	l	101	SQD	C30-C31-C32-C33
26	d	406	LHG	C34-C35-C36-C37
35	C	516	DGD	CAA-CBA-CCA-CDA
35	c	516	DGD	CAA-CBA-CCA-CDA
24	N	606	CHL	O1D-CGD-O2D-CED
26	2	606	LHG	C27-C28-C29-C30
26	6	606	LHG	C27-C28-C29-C30
29	L	101	SQD	C29-C30-C31-C32
29	l	102	SQD	C29-C30-C31-C32
25	B	615	CLA	C8-C10-C11-C12
25	b	615	CLA	C8-C10-C11-C12
25	C	513	CLA	C16-C17-C18-C20
25	6	602	CLA	C11-C12-C13-C14
25	c	513	CLA	C16-C17-C18-C20
25	R	608	CLA	C2-C3-C5-C6
25	r	608	CLA	C2-C3-C5-C6
26	2	606	LHG	C35-C36-C37-C38
30	b	623	LMG	C15-C16-C17-C18
26	N	618	LHG	C19-C20-C21-C22
26	6	606	LHG	C35-C36-C37-C38
30	B	623	LMG	C15-C16-C17-C18
24	G	605	CHL	C3C-C2C-CMC-OMC
24	N	608	CHL	C3C-C2C-CMC-OMC
24	Y	306	CHL	C3C-C2C-CMC-OMC
24	Y	309	CHL	C3C-C2C-CMC-OMC
24	g	605	CHL	C3C-C2C-CMC-OMC
24	n	608	CHL	C3C-C2C-CMC-OMC
24	y	306	CHL	C3C-C2C-CMC-OMC
24	y	309	CHL	C3C-C2C-CMC-OMC
26	n	618	LHG	C19-C20-C21-C22
25	Y	303	CLA	C2A-CAA-CBA-CGA
25	y	303	CLA	C2A-CAA-CBA-CGA
26	C	519	LHG	O1-C1-C2-O2
26	c	519	LHG	O1-C1-C2-O2
25	B	612	CLA	C10-C11-C12-C13
25	G	610	CLA	C10-C11-C12-C13
25	N	603	CLA	C8-C10-C11-C12
25	b	612	CLA	C10-C11-C12-C13
25	g	610	CLA	C10-C11-C12-C13
25	n	603	CLA	C8-C10-C11-C12
26	B	621	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
26	S	301	LHG	O6-C4-C5-O7
26	N	618	LHG	O6-C4-C5-O7
26	b	621	LHG	O6-C4-C5-O7
26	s	301	LHG	O6-C4-C5-O7
26	n	618	LHG	O6-C4-C5-O7
24	r	613	CHL	C4C-C3C-CAC-CBC
25	2	605	CLA	C2C-C3C-CAC-CBC
35	C	516	DGD	O1A-C1A-O1G-C1G
35	c	516	DGD	O1A-C1A-O1G-C1G
25	C	503	CLA	C16-C17-C18-C19
25	Y	312	CLA	C11-C12-C13-C14
25	c	503	CLA	C16-C17-C18-C19
25	y	312	CLA	C11-C12-C13-C14
24	R	613	CHL	C4C-C3C-CAC-CBC
25	6	605	CLA	C2C-C3C-CAC-CBC
24	Y	306	CHL	O1A-CGA-O2A-C1
24	y	306	CHL	O1A-CGA-O2A-C1
25	R	612	CLA	C3-C5-C6-C7
26	L	102	LHG	O7-C5-C6-O8
26	l	103	LHG	O7-C5-C6-O8
29	A	407	SQD	O47-C45-C46-O48
29	a	408	SQD	O47-C45-C46-O48
30	B	623	LMG	O7-C8-C9-O8
30	b	623	LMG	O7-C8-C9-O8
24	Y	309	CHL	CBA-CGA-O2A-C1
24	y	309	CHL	CBA-CGA-O2A-C1
25	B	608	CLA	CBA-CGA-O2A-C1
24	Y	306	CHL	CAA-CBA-CGA-O2A
24	y	306	CHL	CAA-CBA-CGA-O2A
35	B	626	DGD	CDB-CEB-CFB-CGB
25	G	602	CLA	C16-C17-C18-C20
25	g	602	CLA	C16-C17-C18-C20
24	Y	306	CHL	C4C-C3C-CAC-CBC
24	y	306	CHL	C4C-C3C-CAC-CBC
26	y	301	LHG	C27-C28-C29-C30
35	b	626	DGD	CDB-CEB-CFB-CGB
35	B	626	DGD	O6D-C1D-O3G-C3G
35	b	626	DGD	O6D-C1D-O3G-C3G
25	B	601	CLA	C5-C6-C7-C8
25	b	601	CLA	C5-C6-C7-C8
26	B	625	LHG	C1-C2-C3-O3
26	b	625	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
29	L	101	SQD	C28-C29-C30-C31
29	l	102	SQD	C28-C29-C30-C31
25	r	612	CLA	C3-C5-C6-C7
24	G	608	CHL	C2-C1-O2A-CGA
24	g	608	CHL	C2-C1-O2A-CGA
25	G	611	CLA	C2-C1-O2A-CGA
25	g	611	CLA	C2-C1-O2A-CGA
25	N	613	CLA	C2-C3-C5-C6
25	n	613	CLA	C2-C3-C5-C6
26	Y	301	LHG	C27-C28-C29-C30
25	B	603	CLA	C5-C6-C7-C8
25	B	607	CLA	C15-C16-C17-C18
25	b	603	CLA	C5-C6-C7-C8
25	b	607	CLA	C15-C16-C17-C18
26	Y	301	LHG	O8-C23-C24-C25
26	y	301	LHG	O8-C23-C24-C25
24	2	601	CHL	C6-C7-C8-C9
24	G	608	CHL	C6-C7-C8-C9
24	6	601	CHL	C6-C7-C8-C9
24	g	608	CHL	C6-C7-C8-C9
25	B	607	CLA	C6-C7-C8-C9
25	B	613	CLA	C11-C10-C8-C9
25	C	502	CLA	C11-C10-C8-C9
25	S	303	CLA	C6-C7-C8-C9
25	G	610	CLA	C11-C12-C13-C14
25	N	602	CLA	C11-C10-C8-C9
25	Y	303	CLA	C11-C12-C13-C14
25	b	607	CLA	C6-C7-C8-C9
25	b	613	CLA	C11-C10-C8-C9
25	c	502	CLA	C11-C10-C8-C9
25	s	303	CLA	C6-C7-C8-C9
25	g	610	CLA	C11-C12-C13-C14
25	n	602	CLA	C11-C10-C8-C9
25	y	303	CLA	C11-C12-C13-C14
27	A	404	PHO	C6-C7-C8-C9
27	a	405	PHO	C6-C7-C8-C9
25	b	608	CLA	CBA-CGA-O2A-C1
26	N	618	LHG	C10-C11-C12-C13
26	R	618	LHG	C16-C17-C18-C19
26	n	618	LHG	C10-C11-C12-C13
26	Y	319	LHG	C17-C18-C19-C20
26	y	319	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
26	r	618	LHG	C16-C17-C18-C19
25	y	312	CLA	C8-C10-C11-C12
26	N	618	LHG	C2-C3-O3-P
26	n	618	LHG	C2-C3-O3-P
26	2	606	LHG	C11-C10-C9-C8
26	S	301	LHG	C17-C18-C19-C20
26	6	606	LHG	C11-C10-C9-C8
26	s	301	LHG	C17-C18-C19-C20
25	S	313	CLA	C6-C7-C8-C10
25	s	313	CLA	C6-C7-C8-C10
28	B	619	BCR	C23-C24-C25-C26
28	K	101	BCR	C1-C6-C7-C8
28	K	101	BCR	C5-C6-C7-C8
28	b	619	BCR	C23-C24-C25-C26
28	k	101	BCR	C1-C6-C7-C8
28	k	101	BCR	C5-C6-C7-C8
39	S	315	LUT	C1-C6-C7-C8
39	R	615	LUT	C1-C6-C7-C8
39	s	315	LUT	C1-C6-C7-C8
39	r	615	LUT	C1-C6-C7-C8
25	Y	312	CLA	C8-C10-C11-C12
28	B	619	BCR	C7-C8-C9-C34
28	b	619	BCR	C7-C8-C9-C34
35	A	415	DGD	O6E-C5E-C6E-O5E
35	a	401	DGD	O6E-C5E-C6E-O5E
26	L	102	LHG	C16-C17-C18-C19
26	S	301	LHG	C30-C31-C32-C33
26	l	103	LHG	C16-C17-C18-C19
26	s	301	LHG	C30-C31-C32-C33
28	A	406	BCR	C17-C18-C19-C20
28	a	407	BCR	C17-C18-C19-C20
24	G	608	CHL	C15-C16-C17-C18
24	g	608	CHL	C15-C16-C17-C18
38	F	101	HEM	C3D-CAD-CBD-CGD
38	f	101	HEM	C3D-CAD-CBD-CGD
26	N	618	LHG	C8-C7-O7-C5
26	n	618	LHG	C8-C7-O7-C5
26	s	301	LHG	C33-C34-C35-C36
25	R	611	CLA	C2C-C3C-CAC-CBC
26	S	301	LHG	C33-C34-C35-C36
24	Y	302	CHL	C16-C17-C18-C20
24	y	302	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	A	405	CLA	C11-C12-C13-C15
25	B	612	CLA	C16-C17-C18-C19
25	N	610	CLA	C16-C17-C18-C19
25	Y	313	CLA	C11-C12-C13-C14
25	a	406	CLA	C11-C12-C13-C15
25	b	612	CLA	C16-C17-C18-C19
25	n	610	CLA	C16-C17-C18-C19
25	y	313	CLA	C11-C12-C13-C14
26	C	517	LHG	C33-C34-C35-C36
26	c	517	LHG	C33-C34-C35-C36
29	A	407	SQD	C13-C14-C15-C16
29	a	408	SQD	C13-C14-C15-C16
25	Y	314	CLA	C8-C10-C11-C12
25	y	314	CLA	C8-C10-C11-C12
26	C	517	LHG	O6-C4-C5-C6
26	c	517	LHG	O6-C4-C5-C6
29	A	407	SQD	C7-C8-C9-C10
29	a	408	SQD	C7-C8-C9-C10
25	r	611	CLA	C2C-C3C-CAC-CBC
24	G	601	CHL	C11-C12-C13-C15
24	G	608	CHL	C12-C13-C15-C16
24	G	609	CHL	C6-C7-C8-C10
24	N	609	CHL	C11-C10-C8-C7
24	Y	302	CHL	C11-C12-C13-C15
24	Y	308	CHL	C6-C7-C8-C10
24	Y	310	CHL	C2-C3-C5-C6
24	g	601	CHL	C11-C12-C13-C15
24	g	608	CHL	C12-C13-C15-C16
24	g	609	CHL	C6-C7-C8-C10
24	n	609	CHL	C11-C10-C8-C7
24	y	302	CHL	C11-C12-C13-C15
24	y	308	CHL	C6-C7-C8-C10
24	y	310	CHL	C2-C3-C5-C6
25	A	402	CLA	C12-C13-C15-C16
25	B	601	CLA	C11-C12-C13-C15
25	B	602	CLA	C6-C7-C8-C10
25	B	606	CLA	C11-C10-C8-C7
25	B	614	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C10-C8-C7
25	B	616	CLA	C12-C13-C15-C16
25	C	505	CLA	C2-C3-C5-C6
25	C	506	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	C11-C10-C8-C7
25	C	507	CLA	C11-C12-C13-C15
25	C	508	CLA	C12-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C7
25	C	513	CLA	C12-C13-C15-C16
25	N	612	CLA	C6-C7-C8-C10
25	N	612	CLA	C11-C10-C8-C7
25	Y	313	CLA	C11-C10-C8-C7
25	Y	314	CLA	C6-C7-C8-C10
25	R	603	CLA	C11-C10-C8-C7
25	R	612	CLA	C6-C7-C8-C10
25	a	403	CLA	C12-C13-C15-C16
25	b	601	CLA	C11-C12-C13-C15
25	b	602	CLA	C6-C7-C8-C10
25	b	606	CLA	C11-C10-C8-C7
25	b	614	CLA	C12-C13-C15-C16
25	b	615	CLA	C11-C10-C8-C7
25	b	616	CLA	C12-C13-C15-C16
25	c	505	CLA	C2-C3-C5-C6
25	c	506	CLA	C12-C13-C15-C16
25	c	507	CLA	C11-C10-C8-C7
25	c	507	CLA	C11-C12-C13-C15
25	c	508	CLA	C12-C13-C15-C16
25	c	509	CLA	C11-C10-C8-C7
25	c	513	CLA	C12-C13-C15-C16
25	n	612	CLA	C6-C7-C8-C10
25	n	612	CLA	C11-C10-C8-C7
25	y	313	CLA	C11-C10-C8-C7
25	y	314	CLA	C6-C7-C8-C10
25	r	603	CLA	C11-C10-C8-C7
27	A	403	PHO	C12-C13-C15-C16
27	a	404	PHO	C12-C13-C15-C16
28	T	101	BCR	C19-C20-C21-C22
28	t	101	BCR	C19-C20-C21-C22
24	r	607	CHL	C11-C12-C13-C15
25	N	603	CLA	C16-C17-C18-C20
25	n	603	CLA	C16-C17-C18-C20
35	B	626	DGD	C8A-C9A-CAA-CBA
35	b	626	DGD	C8A-C9A-CAA-CBA
35	b	626	DGD	CAB-CBB-CCB-CDB
25	A	405	CLA	C5-C6-C7-C8
25	B	613	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	Y	314	CLA	C5-C6-C7-C8
25	a	406	CLA	C5-C6-C7-C8
25	b	613	CLA	C15-C16-C17-C18
25	y	314	CLA	C5-C6-C7-C8
35	B	626	DGD	CAB-CBB-CCB-CDB
24	6	603	CHL	C4C-C3C-CAC-CBC
26	y	301	LHG	C7-C8-C9-C10
24	2	603	CHL	C4C-C3C-CAC-CBC
26	L	102	LHG	C35-C36-C37-C38
26	l	103	LHG	C35-C36-C37-C38
30	c	520	LMG	C35-C36-C37-C38
24	R	607	CHL	C11-C12-C13-C15
25	B	607	CLA	CBA-CGA-O2A-C1
25	R	603	CLA	CBA-CGA-O2A-C1
25	b	607	CLA	CBA-CGA-O2A-C1
25	r	603	CLA	CBA-CGA-O2A-C1
30	C	520	LMG	C35-C36-C37-C38
25	S	303	CLA	C12-C13-C15-C16
25	s	303	CLA	C12-C13-C15-C16
26	n	618	LHG	C33-C34-C35-C36
25	S	303	CLA	CBD-CGD-O2D-CED
25	s	303	CLA	CBD-CGD-O2D-CED
24	Y	308	CHL	CAD-CBD-CGD-O2D
24	R	613	CHL	CAD-CBD-CGD-O2D
24	y	308	CHL	CAD-CBD-CGD-O2D
24	r	613	CHL	CAD-CBD-CGD-O2D
25	B	603	CLA	CAD-CBD-CGD-O2D
25	B	606	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	S	309	CLA	CAD-CBD-CGD-O2D
25	S	312	CLA	CAD-CBD-CGD-O2D
25	G	603	CLA	CAD-CBD-CGD-O2D
25	G	610	CLA	CAD-CBD-CGD-O2D
25	N	602	CLA	CAD-CBD-CGD-O2D
25	N	604	CLA	CAD-CBD-CGD-O2D
25	b	603	CLA	CAD-CBD-CGD-O2D
25	b	606	CLA	CAD-CBD-CGD-O2D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	s	312	CLA	CAD-CBD-CGD-O2D
25	g	603	CLA	CAD-CBD-CGD-O2D
25	g	610	CLA	CAD-CBD-CGD-O2D
25	n	602	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	n	604	CLA	CAD-CBD-CGD-O2D
25	n	614	CLA	CAD-CBD-CGD-O2D
27	A	403	PHO	CAD-CBD-CGD-O2D
27	a	404	PHO	CAD-CBD-CGD-O2D
40	N	617	NEX	C7-C8-C9-C19
40	Y	318	NEX	C7-C8-C9-C19
40	n	617	NEX	C7-C8-C9-C19
40	y	318	NEX	C7-C8-C9-C19
26	Y	301	LHG	C7-C8-C9-C10
29	A	411	SQD	C13-C14-C15-C16
29	a	412	SQD	C13-C14-C15-C16
28	D	404	BCR	C22-C23-C24-C25
28	d	404	BCR	C22-C23-C24-C25
26	D	406	LHG	C24-C23-O8-C6
26	d	406	LHG	C24-C23-O8-C6
25	g	604	CLA	C2C-C3C-CAC-CBC
26	N	618	LHG	C33-C34-C35-C36
29	A	407	SQD	C30-C31-C32-C33
29	a	408	SQD	C30-C31-C32-C33
30	C	520	LMG	C32-C33-C34-C35
30	c	520	LMG	C32-C33-C34-C35
25	B	605	CLA	C15-C16-C17-C18
25	b	605	CLA	C15-C16-C17-C18
26	y	319	LHG	C35-C36-C37-C38
30	B	623	LMG	C29-C30-C31-C32
30	b	623	LMG	C29-C30-C31-C32
26	2	606	LHG	C2-C3-O3-P
26	2	606	LHG	C4-C5-C6-O8
26	L	102	LHG	C4-C5-C6-O8
26	S	318	LHG	C2-C3-O3-P
26	6	606	LHG	C2-C3-O3-P
26	6	606	LHG	C4-C5-C6-O8
26	l	103	LHG	C4-C5-C6-O8
26	s	318	LHG	C2-C3-O3-P
29	L	101	SQD	C44-C45-C46-O48
29	L	103	SQD	O6-C44-C45-C46
29	l	101	SQD	O6-C44-C45-C46
29	l	102	SQD	C44-C45-C46-O48
30	A	410	LMG	C7-C8-C9-O8
30	C	520	LMG	O1-C7-C8-C9
30	a	411	LMG	C7-C8-C9-O8
30	c	520	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	n	601	CHL	O1A-CGA-O2A-C1
26	D	406	LHG	C30-C31-C32-C33
26	Y	319	LHG	C35-C36-C37-C38
26	d	406	LHG	C30-C31-C32-C33
24	Y	302	CHL	C10-C11-C12-C13
24	y	302	CHL	C10-C11-C12-C13
25	A	405	CLA	C8-C10-C11-C12
25	a	406	CLA	C8-C10-C11-C12
25	c	512	CLA	C13-C15-C16-C17
25	S	312	CLA	O2A-C1-C2-C3
25	s	312	CLA	O2A-C1-C2-C3
25	G	604	CLA	C2C-C3C-CAC-CBC
25	C	512	CLA	C13-C15-C16-C17
26	C	518	LHG	C18-C19-C20-C21
26	c	518	LHG	C18-C19-C20-C21
35	C	516	DGD	C7A-C8A-C9A-CAA
35	c	516	DGD	C7A-C8A-C9A-CAA
25	A	402	CLA	C16-C17-C18-C20
25	a	403	CLA	C16-C17-C18-C20
26	C	519	LHG	C33-C34-C35-C36
26	c	519	LHG	C33-C34-C35-C36
26	B	625	LHG	O2-C2-C3-O3
26	b	625	LHG	O2-C2-C3-O3
26	n	618	LHG	O9-C7-O7-C5
24	2	601	CHL	CHA-CBD-CGD-O1D
24	S	306	CHL	CHA-CBD-CGD-O2D
24	G	609	CHL	CHA-CBD-CGD-O1D
24	G	609	CHL	CHA-CBD-CGD-O2D
24	N	608	CHL	CHA-CBD-CGD-O1D
24	6	601	CHL	CHA-CBD-CGD-O1D
24	s	306	CHL	CHA-CBD-CGD-O2D
24	g	609	CHL	CHA-CBD-CGD-O1D
24	g	609	CHL	CHA-CBD-CGD-O2D
24	n	608	CHL	CHA-CBD-CGD-O1D
25	B	604	CLA	CHA-CBD-CGD-O1D
25	B	604	CLA	CHA-CBD-CGD-O2D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	505	CLA	CHA-CBD-CGD-O1D
25	C	505	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	S	305	CLA	CHA-CBD-CGD-O1D
25	G	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	N	603	CLA	CHA-CBD-CGD-O2D
25	N	612	CLA	CHA-CBD-CGD-O2D
25	N	613	CLA	CHA-CBD-CGD-O2D
25	Y	304	CLA	CHA-CBD-CGD-O1D
25	Y	305	CLA	CHA-CBD-CGD-O1D
25	Y	313	CLA	CHA-CBD-CGD-O1D
25	Y	314	CLA	CHA-CBD-CGD-O2D
25	R	601	CLA	CHA-CBD-CGD-O1D
25	R	602	CLA	CHA-CBD-CGD-O2D
25	R	604	CLA	CHA-CBD-CGD-O1D
25	R	611	CLA	CHA-CBD-CGD-O2D
25	R	612	CLA	CHA-CBD-CGD-O2D
25	b	604	CLA	CHA-CBD-CGD-O1D
25	b	604	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	505	CLA	CHA-CBD-CGD-O1D
25	c	505	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	s	305	CLA	CHA-CBD-CGD-O1D
25	g	604	CLA	CHA-CBD-CGD-O1D
25	n	603	CLA	CHA-CBD-CGD-O2D
25	n	612	CLA	CHA-CBD-CGD-O2D
25	n	613	CLA	CHA-CBD-CGD-O2D
25	y	304	CLA	CHA-CBD-CGD-O1D
25	y	305	CLA	CHA-CBD-CGD-O1D
25	y	313	CLA	CHA-CBD-CGD-O1D
25	y	314	CLA	CHA-CBD-CGD-O2D
25	r	601	CLA	CHA-CBD-CGD-O1D
25	r	602	CLA	CHA-CBD-CGD-O2D
25	r	604	CLA	CHA-CBD-CGD-O1D
25	r	611	CLA	CHA-CBD-CGD-O2D
25	r	612	CLA	CHA-CBD-CGD-O2D
25	y	314	CLA	C3-C5-C6-C7
24	G	601	CHL	O1A-CGA-O2A-C1
24	N	601	CHL	O1A-CGA-O2A-C1
30	B	620	LMG	C30-C31-C32-C33
30	b	620	LMG	C30-C31-C32-C33
35	B	626	DGD	C2D-C1D-O3G-C3G
35	b	626	DGD	C2D-C1D-O3G-C3G
35	A	415	DGD	O1G-C1G-C2G-O2G
35	B	626	DGD	O2G-C2G-C3G-O3G
35	a	401	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
35	b	626	DGD	O2G-C2G-C3G-O3G
26	R	618	LHG	C11-C10-C9-C8
26	r	618	LHG	C11-C10-C9-C8
24	g	601	CHL	O1A-CGA-O2A-C1
29	A	407	SQD	C12-C13-C14-C15
29	a	408	SQD	C12-C13-C14-C15
25	G	612	CLA	C11-C12-C13-C14
25	N	610	CLA	C16-C17-C18-C20
25	g	612	CLA	C11-C12-C13-C14
25	n	610	CLA	C16-C17-C18-C20
30	D	407	LMG	C33-C34-C35-C36
30	d	407	LMG	C33-C34-C35-C36
25	Y	314	CLA	C3-C5-C6-C7
24	Y	302	CHL	C4-C3-C5-C6
24	y	302	CHL	C4-C3-C5-C6
25	B	609	CLA	C4-C3-C5-C6
25	S	313	CLA	C4-C3-C5-C6
25	b	609	CLA	C4-C3-C5-C6
25	s	313	CLA	C4-C3-C5-C6
27	A	403	PHO	C4-C3-C5-C6
27	a	404	PHO	C4-C3-C5-C6
30	B	620	LMG	C4-C5-C6-O5
30	b	620	LMG	C4-C5-C6-O5
25	Y	303	CLA	C2-C3-C5-C6
25	y	303	CLA	C2-C3-C5-C6
31	A	409	PL9	C4-C3-C7-C8
31	a	410	PL9	C4-C3-C7-C8
26	N	618	LHG	O9-C7-O7-C5
25	B	606	CLA	C11-C10-C8-C9
25	B	616	CLA	C14-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	b	616	CLA	C14-C13-C15-C16
25	c	509	CLA	C11-C10-C8-C9
26	C	519	LHG	C18-C19-C20-C21
26	c	519	LHG	C18-C19-C20-C21
25	G	612	CLA	C2C-C3C-CAC-CBC
25	g	612	CLA	C2C-C3C-CAC-CBC
26	B	621	LHG	C13-C14-C15-C16
26	b	621	LHG	C13-C14-C15-C16
25	B	606	CLA	C10-C11-C12-C13
25	b	606	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	A	411	SQD	C4-C5-C6-S
29	L	103	SQD	C4-C5-C6-S
29	a	412	SQD	C4-C5-C6-S
29	l	101	SQD	C4-C5-C6-S
28	Z	101	BCR	C7-C8-C9-C10
28	z	101	BCR	C7-C8-C9-C10
26	S	301	LHG	C32-C33-C34-C35
25	R	608	CLA	C1A-C2A-CAA-CBA
25	r	608	CLA	C1A-C2A-CAA-CBA
25	B	616	CLA	C16-C17-C18-C20
25	S	310	CLA	C6-C7-C8-C9
25	Y	304	CLA	C16-C17-C18-C19
25	b	616	CLA	C16-C17-C18-C20
25	s	310	CLA	C6-C7-C8-C9
25	y	304	CLA	C16-C17-C18-C19
25	C	505	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
26	s	301	LHG	C32-C33-C34-C35
26	L	102	LHG	C3-O3-P-O6
26	l	103	LHG	C3-O3-P-O6
27	A	403	PHO	C10-C11-C12-C13
27	a	404	PHO	C10-C11-C12-C13
30	B	620	LMG	C29-C30-C31-C32
30	b	620	LMG	C29-C30-C31-C32
26	2	606	LHG	C3-O3-P-O5
26	N	618	LHG	C3-O3-P-O4
26	6	606	LHG	C3-O3-P-O5
26	c	519	LHG	C4-O6-P-O4
26	n	618	LHG	C3-O3-P-O4
25	C	503	CLA	C16-C17-C18-C20
25	S	313	CLA	C6-C7-C8-C9
25	G	602	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C20
25	s	313	CLA	C6-C7-C8-C9
25	g	602	CLA	C16-C17-C18-C19
26	B	622	LHG	C23-C24-C25-C26
29	a	412	SQD	C31-C32-C33-C34
30	A	410	LMG	O6-C1-O1-C7
30	a	411	LMG	O6-C1-O1-C7
25	B	603	CLA	CBA-CGA-O2A-C1
25	b	603	CLA	CBA-CGA-O2A-C1
26	2	606	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	A	411	SQD	C31-C32-C33-C34
30	B	623	LMG	C21-C22-C23-C24
30	b	623	LMG	C21-C22-C23-C24
25	D	402	CLA	C10-C11-C12-C13
25	d	402	CLA	C10-C11-C12-C13
26	b	622	LHG	C23-C24-C25-C26
25	2	602	CLA	C3-C5-C6-C7
25	Y	304	CLA	C3-C5-C6-C7
25	6	602	CLA	C3-C5-C6-C7
25	y	304	CLA	C3-C5-C6-C7
26	6	606	LHG	C13-C14-C15-C16
25	B	604	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	505	CLA	CAD-CBD-CGD-O1D
25	S	305	CLA	CAD-CBD-CGD-O1D
25	G	604	CLA	CAD-CBD-CGD-O1D
25	Y	305	CLA	CAD-CBD-CGD-O1D
25	R	609	CLA	CAD-CBD-CGD-O1D
25	b	604	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	505	CLA	CAD-CBD-CGD-O1D
25	s	305	CLA	CAD-CBD-CGD-O1D
25	g	604	CLA	CAD-CBD-CGD-O1D
25	y	305	CLA	CAD-CBD-CGD-O1D
25	r	609	CLA	CAD-CBD-CGD-O1D
40	G	617	NEX	C7-C8-C9-C10
40	Y	318	NEX	C7-C8-C9-C10
40	g	617	NEX	C7-C8-C9-C10
40	y	318	NEX	C7-C8-C9-C10
26	C	518	LHG	C11-C12-C13-C14
26	c	518	LHG	C11-C12-C13-C14
30	B	623	LMG	C35-C36-C37-C38
30	b	623	LMG	C35-C36-C37-C38
25	B	608	CLA	C5-C6-C7-C8
26	c	518	LHG	C27-C28-C29-C30
26	C	518	LHG	C27-C28-C29-C30
35	C	515	DGD	C4D-C5D-C6D-O5D
35	c	515	DGD	C4D-C5D-C6D-O5D
26	C	517	LHG	C30-C31-C32-C33
26	S	301	LHG	C11-C12-C13-C14
26	s	301	LHG	C11-C12-C13-C14
30	D	407	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	d	407	LMG	C17-C18-C19-C20
24	Y	309	CHL	C11-C10-C8-C7
24	y	309	CHL	C11-C10-C8-C7
25	B	609	CLA	C6-C7-C8-C10
25	B	614	CLA	C11-C12-C13-C15
25	B	615	CLA	C11-C12-C13-C15
25	C	508	CLA	C11-C12-C13-C15
25	D	402	CLA	C11-C12-C13-C15
25	N	613	CLA	C6-C7-C8-C10
25	N	613	CLA	C11-C10-C8-C7
25	Y	312	CLA	C6-C7-C8-C10
25	R	604	CLA	C3A-C2A-CAA-CBA
25	R	608	CLA	C3A-C2A-CAA-CBA
25	b	609	CLA	C6-C7-C8-C10
25	b	614	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C12-C13-C15
25	c	508	CLA	C11-C12-C13-C15
25	d	402	CLA	C11-C12-C13-C15
25	n	613	CLA	C6-C7-C8-C10
25	n	613	CLA	C11-C10-C8-C7
25	y	312	CLA	C6-C7-C8-C10
25	r	604	CLA	C3A-C2A-CAA-CBA
25	r	608	CLA	C3A-C2A-CAA-CBA
26	c	517	LHG	C30-C31-C32-C33
25	b	608	CLA	C5-C6-C7-C8
28	T	101	BCR	C9-C10-C11-C12
28	t	101	BCR	C9-C10-C11-C12
39	N	615	LUT	C13-C14-C15-C35
39	n	615	LUT	C13-C14-C15-C35
35	C	515	DGD	O6D-C5D-C6D-O5D
35	c	515	DGD	O6D-C5D-C6D-O5D
26	N	618	LHG	C24-C25-C26-C27
26	s	318	LHG	C9-C10-C11-C12
26	n	618	LHG	C24-C25-C26-C27
26	D	406	LHG	O10-C23-O8-C6
26	d	406	LHG	O10-C23-O8-C6
26	S	318	LHG	C9-C10-C11-C12
24	R	607	CHL	C10-C11-C12-C13
24	r	607	CHL	C10-C11-C12-C13
25	y	315	CLA	C2A-CAA-CBA-CGA
29	L	103	SQD	C29-C30-C31-C32
29	l	101	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
24	G	601	CHL	C1C-C2C-CMC-OMC
24	Y	306	CHL	C1C-C2C-CMC-OMC
24	g	601	CHL	C1C-C2C-CMC-OMC
24	y	306	CHL	C1C-C2C-CMC-OMC
29	A	411	SQD	C44-C45-C46-O48
29	a	412	SQD	C44-C45-C46-O48
30	A	408	LMG	O1-C7-C8-C9
30	a	409	LMG	O1-C7-C8-C9
29	A	411	SQD	O47-C45-C46-O48
29	L	103	SQD	O6-C44-C45-O47
29	a	412	SQD	O47-C45-C46-O48
29	l	101	SQD	O6-C44-C45-O47
30	A	408	LMG	O1-C7-C8-O7
30	A	408	LMG	O7-C8-C9-O8
30	C	520	LMG	O1-C7-C8-O7
30	D	407	LMG	O1-C7-C8-O7
30	a	409	LMG	O1-C7-C8-O7
30	a	409	LMG	O7-C8-C9-O8
30	c	520	LMG	O1-C7-C8-O7
30	d	407	LMG	O1-C7-C8-O7
26	S	318	LHG	C11-C10-C9-C8
26	s	318	LHG	C11-C10-C9-C8
25	R	610	CLA	C4C-C3C-CAC-CBC
25	B	608	CLA	C4-C3-C5-C6
25	b	608	CLA	C4-C3-C5-C6
25	r	610	CLA	C4C-C3C-CAC-CBC
25	Y	313	CLA	C2-C3-C5-C6
25	y	313	CLA	C2-C3-C5-C6
24	G	601	CHL	C14-C13-C15-C16
24	g	601	CHL	C14-C13-C15-C16
25	C	507	CLA	C6-C7-C8-C9
25	C	509	CLA	C11-C12-C13-C14
25	D	402	CLA	C11-C10-C8-C9
25	D	402	CLA	C11-C12-C13-C14
25	S	311	CLA	C6-C7-C8-C9
25	N	603	CLA	C11-C12-C13-C14
25	c	507	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	d	402	CLA	C11-C10-C8-C9
25	d	402	CLA	C11-C12-C13-C14
25	s	311	CLA	C6-C7-C8-C9
25	n	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	s	310	CLA	O1A-CGA-O2A-C1
26	N	618	LHG	C18-C19-C20-C21
24	Y	302	CHL	C3-C5-C6-C7
24	y	302	CHL	C3-C5-C6-C7
26	n	618	LHG	C18-C19-C20-C21
29	a	412	SQD	C17-C18-C19-C20
25	S	310	CLA	O1A-CGA-O2A-C1
24	S	307	CHL	C2A-CAA-CBA-CGA
24	s	307	CHL	C2A-CAA-CBA-CGA
25	Y	315	CLA	C2A-CAA-CBA-CGA
26	B	625	LHG	O1-C1-C2-O2
26	b	625	LHG	O1-C1-C2-O2
26	R	618	LHG	C12-C13-C14-C15
26	r	618	LHG	C12-C13-C14-C15
29	A	411	SQD	C17-C18-C19-C20
35	B	626	DGD	C5A-C6A-C7A-C8A
35	b	626	DGD	C5A-C6A-C7A-C8A
40	G	617	NEX	C10-C11-C12-C13
40	G	617	NEX	C30-C31-C32-C33
40	Y	318	NEX	C30-C31-C32-C33
40	g	617	NEX	C10-C11-C12-C13
40	g	617	NEX	C30-C31-C32-C33
40	y	318	NEX	C30-C31-C32-C33
26	s	318	LHG	C15-C16-C17-C18
26	S	318	LHG	C15-C16-C17-C18
26	2	606	LHG	C9-C10-C11-C12
26	6	606	LHG	C9-C10-C11-C12
26	L	102	LHG	C26-C27-C28-C29
26	l	103	LHG	C26-C27-C28-C29
27	A	403	PHO	C2-C3-C5-C6
27	a	404	PHO	C2-C3-C5-C6
25	N	611	CLA	C10-C11-C12-C13
25	n	611	CLA	C10-C11-C12-C13
26	B	621	LHG	C30-C31-C32-C33
26	b	621	LHG	C30-C31-C32-C33
30	A	408	LMG	C32-C33-C34-C35
30	a	409	LMG	C32-C33-C34-C35
24	G	606	CHL	C1-C2-C3-C4
24	Y	307	CHL	C1-C2-C3-C4
24	g	606	CHL	C1-C2-C3-C4
24	y	307	CHL	C1-C2-C3-C4
25	S	312	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
25	R	610	CLA	C1-C2-C3-C4
25	R	611	CLA	C1-C2-C3-C4
25	s	312	CLA	C1-C2-C3-C4
25	r	610	CLA	C1-C2-C3-C4
25	r	611	CLA	C1-C2-C3-C4
29	L	101	SQD	C25-C26-C27-C28
29	l	102	SQD	C25-C26-C27-C28
30	C	520	LMG	C37-C38-C39-C40
30	c	520	LMG	C37-C38-C39-C40
24	y	302	CHL	C15-C16-C17-C18
26	L	102	LHG	C6-C5-O7-C7
26	l	103	LHG	C6-C5-O7-C7
29	L	103	SQD	C44-C45-O47-C7
29	l	101	SQD	C44-C45-O47-C7
25	C	505	CLA	C2A-CAA-CBA-CGA
25	G	602	CLA	C2A-CAA-CBA-CGA
25	c	505	CLA	C2A-CAA-CBA-CGA
25	g	602	CLA	C2A-CAA-CBA-CGA
25	R	601	CLA	C2C-C3C-CAC-CBC
29	A	411	SQD	C32-C33-C34-C35
25	y	304	CLA	CBA-CGA-O2A-C1
24	Y	308	CHL	C2-C1-O2A-CGA
24	y	308	CHL	C2-C1-O2A-CGA
25	A	401	CLA	C2-C1-O2A-CGA
25	B	613	CLA	C2-C1-O2A-CGA
25	a	402	CLA	C2-C1-O2A-CGA
25	b	613	CLA	C2-C1-O2A-CGA
29	a	412	SQD	C32-C33-C34-C35
35	B	626	DGD	C7A-C8A-C9A-CAA
25	r	601	CLA	C2C-C3C-CAC-CBC
26	B	621	LHG	C31-C32-C33-C34
26	b	621	LHG	C31-C32-C33-C34
35	b	626	DGD	C7A-C8A-C9A-CAA
29	l	102	SQD	C11-C12-C13-C14
29	L	101	SQD	C11-C12-C13-C14
24	Y	302	CHL	C15-C16-C17-C18
25	B	604	CLA	C10-C11-C12-C13
25	b	604	CLA	C10-C11-C12-C13
25	y	304	CLA	C15-C16-C17-C18
25	r	612	CLA	C8-C10-C11-C12
25	Y	304	CLA	CBA-CGA-O2A-C1
35	B	626	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
25	G	613	CLA	C10-C11-C12-C13
25	Y	304	CLA	C15-C16-C17-C18
25	R	612	CLA	C8-C10-C11-C12
25	g	613	CLA	C10-C11-C12-C13
31	D	405	PL9	C20-C19-C21-C22
31	d	405	PL9	C20-C19-C21-C22
26	B	622	LHG	C9-C10-C11-C12
26	b	622	LHG	C9-C10-C11-C12
24	N	605	CHL	O1D-CGD-O2D-CED
39	G	615	LUT	C1-C6-C7-C8
39	g	615	LUT	C1-C6-C7-C8
25	G	613	CLA	C2-C3-C5-C6
25	g	613	CLA	C2-C3-C5-C6
25	R	602	CLA	O1A-CGA-O2A-C1
24	n	605	CHL	O1D-CGD-O2D-CED
25	2	605	CLA	C4C-C3C-CAC-CBC
25	6	605	CLA	C4C-C3C-CAC-CBC
35	b	626	DGD	C6B-C7B-C8B-C9B
30	B	620	LMG	C36-C37-C38-C39
30	b	620	LMG	C36-C37-C38-C39
25	N	603	CLA	C16-C17-C18-C19
25	n	603	CLA	C16-C17-C18-C19
29	L	101	SQD	O5-C1-O6-C44
29	l	102	SQD	O5-C1-O6-C44
29	L	101	SQD	C2-C1-O6-C44
29	l	102	SQD	C2-C1-O6-C44
30	A	410	LMG	C2-C1-O1-C7
30	a	411	LMG	C2-C1-O1-C7
24	N	607	CHL	C5-C6-C7-C8
24	n	607	CHL	C5-C6-C7-C8
26	2	606	LHG	C31-C32-C33-C34
26	S	301	LHG	C25-C26-C27-C28
26	B	621	LHG	C4-O6-P-O3
26	B	622	LHG	C3-O3-P-O6
26	C	517	LHG	C3-O3-P-O6
26	D	406	LHG	C3-O3-P-O6
26	S	318	LHG	C3-O3-P-O6
26	N	618	LHG	C4-O6-P-O3
26	Y	301	LHG	C3-O3-P-O6
26	R	618	LHG	C3-O3-P-O6
26	b	621	LHG	C4-O6-P-O3
26	b	622	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
26	c	517	LHG	C3-O3-P-O6
26	d	406	LHG	C3-O3-P-O6
26	s	318	LHG	C3-O3-P-O6
26	n	618	LHG	C4-O6-P-O3
26	y	301	LHG	C3-O3-P-O6
26	r	618	LHG	C3-O3-P-O6
26	6	606	LHG	C31-C32-C33-C34
26	s	301	LHG	C25-C26-C27-C28
30	D	407	LMG	C21-C22-C23-C24
25	r	602	CLA	O1A-CGA-O2A-C1
26	C	518	LHG	C11-C10-C9-C8
26	c	518	LHG	C11-C10-C9-C8
30	d	407	LMG	C21-C22-C23-C24
25	g	602	CLA	CBD-CGD-O2D-CED
26	L	102	LHG	C17-C18-C19-C20
26	l	103	LHG	C17-C18-C19-C20
30	C	520	LMG	C7-C8-C9-O8
30	c	520	LMG	C7-C8-C9-O8
35	A	415	DGD	O1G-C1G-C2G-C3G
35	a	401	DGD	O1G-C1G-C2G-C3G
25	G	603	CLA	C4-C3-C5-C6
25	g	603	CLA	C4-C3-C5-C6
35	A	415	DGD	C5B-C6B-C7B-C8B
35	a	401	DGD	C5B-C6B-C7B-C8B
24	2	601	CHL	C11-C10-C8-C7
24	G	608	CHL	C6-C7-C8-C10
24	6	601	CHL	C11-C10-C8-C7
24	g	608	CHL	C6-C7-C8-C10
25	2	602	CLA	C11-C10-C8-C7
25	B	608	CLA	C12-C13-C15-C16
25	C	505	CLA	C12-C13-C15-C16
25	6	602	CLA	C11-C10-C8-C7
25	b	608	CLA	C12-C13-C15-C16
25	c	505	CLA	C12-C13-C15-C16
24	G	605	CHL	C2C-C3C-CAC-CBC
24	g	605	CHL	C2C-C3C-CAC-CBC
24	Y	302	CHL	C14-C13-C15-C16
24	Y	308	CHL	C6-C7-C8-C9
24	y	302	CHL	C14-C13-C15-C16
24	y	308	CHL	C6-C7-C8-C9
25	B	614	CLA	C11-C12-C13-C14
25	B	615	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	N	613	CLA	C6-C7-C8-C9
25	N	613	CLA	C11-C10-C8-C9
25	b	614	CLA	C11-C12-C13-C14
25	b	615	CLA	C11-C12-C13-C14
25	n	613	CLA	C6-C7-C8-C9
25	n	613	CLA	C11-C10-C8-C9
24	G	601	CHL	C15-C16-C17-C18
24	g	601	CHL	C15-C16-C17-C18
26	c	519	LHG	C14-C15-C16-C17
30	B	620	LMG	C13-C14-C15-C16
30	b	620	LMG	C13-C14-C15-C16
25	G	602	CLA	CBD-CGD-O2D-CED
25	a	403	CLA	C16-C17-C18-C19
26	C	519	LHG	C14-C15-C16-C17
30	C	520	LMG	C31-C32-C33-C34
30	c	520	LMG	C31-C32-C33-C34
26	S	301	LHG	C16-C17-C18-C19
25	G	611	CLA	CAA-CBA-CGA-O2A
25	g	611	CLA	CAA-CBA-CGA-O2A
25	Y	303	CLA	C5-C6-C7-C8
25	y	303	CLA	C5-C6-C7-C8
26	s	301	LHG	C16-C17-C18-C19
24	Y	310	CHL	C4-C3-C5-C6
24	y	310	CHL	C4-C3-C5-C6
25	B	608	CLA	C2-C3-C5-C6
25	b	608	CLA	C2-C3-C5-C6
25	A	402	CLA	C16-C17-C18-C19
25	N	610	CLA	CBA-CGA-O2A-C1
25	n	610	CLA	CBA-CGA-O2A-C1
28	T	101	BCR	C6-C7-C8-C9
28	t	101	BCR	C6-C7-C8-C9
25	R	601	CLA	O1A-CGA-O2A-C1
25	r	601	CLA	O1A-CGA-O2A-C1
25	G	612	CLA	CBD-CGD-O2D-CED
28	A	406	BCR	C13-C14-C15-C16
28	I	101	BCR	C9-C10-C11-C12
28	a	407	BCR	C13-C14-C15-C16
28	i	101	BCR	C9-C10-C11-C12
39	Y	316	LUT	C33-C34-C35-C15
39	y	316	LUT	C33-C34-C35-C15
26	B	625	LHG	C28-C29-C30-C31
26	b	625	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
30	B	623	LMG	C18-C19-C20-C21
30	b	623	LMG	C18-C19-C20-C21
26	L	102	LHG	C32-C33-C34-C35
26	l	103	LHG	C32-C33-C34-C35
25	b	609	CLA	CBD-CGD-O2D-CED
25	g	612	CLA	CBD-CGD-O2D-CED
29	A	407	SQD	C29-C30-C31-C32
29	a	408	SQD	C29-C30-C31-C32
25	R	602	CLA	C4-C3-C5-C6
25	r	602	CLA	C4-C3-C5-C6
25	B	609	CLA	C5-C6-C7-C8
25	G	610	CLA	C13-C15-C16-C17
25	b	609	CLA	C5-C6-C7-C8
25	g	610	CLA	C13-C15-C16-C17
30	B	620	LMG	O9-C10-O7-C8
30	b	620	LMG	O9-C10-O7-C8
24	N	609	CHL	C2-C1-O2A-CGA
24	n	609	CHL	C2-C1-O2A-CGA
25	C	506	CLA	C2-C1-O2A-CGA
25	G	604	CLA	C2-C1-O2A-CGA
25	c	506	CLA	C2-C1-O2A-CGA
25	g	604	CLA	C2-C1-O2A-CGA
24	N	605	CHL	C2C-C3C-CAC-CBC
24	n	605	CHL	C2C-C3C-CAC-CBC
26	C	517	LHG	C35-C36-C37-C38
26	c	517	LHG	C35-C36-C37-C38
24	1	302	CHL	CAA-CBA-CGA-O2A
24	5	302	CHL	CAA-CBA-CGA-O2A
25	B	616	CLA	C2A-CAA-CBA-CGA
25	G	613	CLA	C2A-CAA-CBA-CGA
25	b	616	CLA	C2A-CAA-CBA-CGA
25	g	613	CLA	C2A-CAA-CBA-CGA
25	B	609	CLA	CBD-CGD-O2D-CED
25	B	604	CLA	C3A-C2A-CAA-CBA
25	b	604	CLA	C3A-C2A-CAA-CBA
24	R	606	CHL	CAA-CBA-CGA-O1A
24	r	606	CHL	CAA-CBA-CGA-O1A
25	S	303	CLA	C5-C6-C7-C8
25	s	303	CLA	C5-C6-C7-C8
25	B	615	CLA	C4-C3-C5-C6
25	b	615	CLA	C4-C3-C5-C6
35	B	626	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
35	b	626	DGD	CCA-CDA-CEA-CFA
26	B	622	LHG	C29-C30-C31-C32
26	b	622	LHG	C29-C30-C31-C32
24	Y	302	CHL	C6-C7-C8-C9
24	y	302	CHL	C6-C7-C8-C9
25	A	405	CLA	C11-C10-C8-C9
25	C	504	CLA	C6-C7-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	C	508	CLA	C11-C12-C13-C14
25	G	610	CLA	C6-C7-C8-C9
25	a	406	CLA	C11-C10-C8-C9
25	c	504	CLA	C6-C7-C8-C9
25	c	505	CLA	C14-C13-C15-C16
25	c	508	CLA	C11-C12-C13-C14
25	g	610	CLA	C6-C7-C8-C9
25	Y	311	CLA	C11-C12-C13-C14
25	y	311	CLA	C11-C12-C13-C14
24	Y	309	CHL	C2C-C3C-CAC-CBC
24	y	309	CHL	C2C-C3C-CAC-CBC
35	A	415	DGD	C3A-C4A-C5A-C6A
35	a	401	DGD	C3A-C4A-C5A-C6A
30	D	407	LMG	O1-C7-C8-C9
30	d	407	LMG	O1-C7-C8-C9
35	B	626	DGD	O1G-C1G-C2G-C3G
35	b	626	DGD	O1G-C1G-C2G-C3G
39	S	315	LUT	C40-C33-C34-C35
39	G	615	LUT	C21-C26-C27-C28
39	N	615	LUT	C21-C26-C27-C28
39	R	615	LUT	C20-C13-C14-C15
39	s	315	LUT	C40-C33-C34-C35
39	g	615	LUT	C21-C26-C27-C28
39	n	615	LUT	C21-C26-C27-C28
39	r	615	LUT	C20-C13-C14-C15
40	S	317	NEX	C11-C10-C9-C19
40	S	317	NEX	C39-C29-C30-C31
40	N	617	NEX	C39-C29-C30-C31
40	R	617	NEX	C39-C29-C30-C31
40	s	317	NEX	C11-C10-C9-C19
40	s	317	NEX	C39-C29-C30-C31
40	n	617	NEX	C39-C29-C30-C31
40	r	617	NEX	C39-C29-C30-C31
41	R	616	XAT	C20-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
41	r	616	XAT	C20-C13-C14-C15
24	r	606	CHL	CAA-CBA-CGA-O2A
26	S	301	LHG	C19-C20-C21-C22
26	s	301	LHG	C19-C20-C21-C22
24	R	606	CHL	CAA-CBA-CGA-O2A
25	Y	315	CLA	C2C-C3C-CAC-CBC
35	A	415	DGD	CAB-CBB-CCB-CDB
35	a	401	DGD	CAB-CBB-CCB-CDB
24	S	308	CHL	CAA-CBA-CGA-O1A
24	s	308	CHL	CAA-CBA-CGA-O1A
29	L	103	SQD	C46-C45-O47-C7
29	l	101	SQD	C46-C45-O47-C7
25	S	311	CLA	C4-C3-C5-C6
25	s	311	CLA	C4-C3-C5-C6
24	G	607	CHL	C1A-C2A-CAA-CBA
24	Y	306	CHL	C1A-C2A-CAA-CBA
24	R	607	CHL	C1A-C2A-CAA-CBA
24	g	607	CHL	C1A-C2A-CAA-CBA
24	y	306	CHL	C1A-C2A-CAA-CBA
24	r	607	CHL	C1A-C2A-CAA-CBA
25	G	602	CLA	C1A-C2A-CAA-CBA
25	G	603	CLA	C1A-C2A-CAA-CBA
25	Y	303	CLA	C1A-C2A-CAA-CBA
25	g	602	CLA	C1A-C2A-CAA-CBA
25	g	603	CLA	C1A-C2A-CAA-CBA
25	y	303	CLA	C1A-C2A-CAA-CBA
24	2	601	CHL	C12-C13-C15-C16
24	6	601	CHL	C12-C13-C15-C16
25	A	402	CLA	C11-C12-C13-C15
25	B	607	CLA	C12-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C10
25	D	402	CLA	C12-C13-C15-C16
25	Y	314	CLA	C12-C13-C15-C16
25	a	403	CLA	C11-C12-C13-C15
25	b	607	CLA	C12-C13-C15-C16
25	c	506	CLA	C6-C7-C8-C10
25	d	402	CLA	C12-C13-C15-C16
25	y	314	CLA	C12-C13-C15-C16
35	A	415	DGD	C7B-C8B-C9B-CAB
35	a	401	DGD	C7B-C8B-C9B-CAB
24	S	307	CHL	C3C-C2C-CMC-OMC
24	s	307	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
25	g	604	CLA	C4C-C3C-CAC-CBC
25	y	315	CLA	C2C-C3C-CAC-CBC
25	G	604	CLA	C4C-C3C-CAC-CBC
26	y	319	LHG	C9-C10-C11-C12
24	Y	302	CHL	C2A-CAA-CBA-CGA
24	y	302	CHL	C2A-CAA-CBA-CGA
25	B	610	CLA	C2A-CAA-CBA-CGA
25	N	602	CLA	C2A-CAA-CBA-CGA
25	R	612	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	C2A-CAA-CBA-CGA
25	n	602	CLA	C2A-CAA-CBA-CGA
25	r	612	CLA	C2A-CAA-CBA-CGA
25	C	510	CLA	C10-C11-C12-C13
25	c	510	CLA	C10-C11-C12-C13
25	y	303	CLA	C2C-C3C-CAC-CBC
25	b	602	CLA	C10-C11-C12-C13
26	Y	319	LHG	C9-C10-C11-C12
30	B	620	LMG	C11-C10-O7-C8
30	b	620	LMG	C11-C10-O7-C8
24	G	607	CHL	CAA-CBA-CGA-O2A
24	g	607	CHL	CAA-CBA-CGA-O2A
25	Y	303	CLA	C2C-C3C-CAC-CBC
31	D	405	PL9	C45-C44-C46-C47
31	d	405	PL9	C45-C44-C46-C47
25	B	602	CLA	C10-C11-C12-C13
24	1	302	CHL	CAA-CBA-CGA-O1A
24	5	302	CHL	CAA-CBA-CGA-O1A
24	Y	302	CHL	C5-C6-C7-C8
39	S	315	LUT	C32-C33-C34-C35
39	R	615	LUT	C12-C13-C14-C15
39	s	315	LUT	C32-C33-C34-C35
39	r	615	LUT	C12-C13-C14-C15
40	S	317	NEX	C11-C10-C9-C8
40	S	317	NEX	C28-C29-C30-C31
40	N	617	NEX	C28-C29-C30-C31
40	R	617	NEX	C28-C29-C30-C31
40	s	317	NEX	C11-C10-C9-C8
40	s	317	NEX	C28-C29-C30-C31
40	n	617	NEX	C28-C29-C30-C31
40	r	617	NEX	C28-C29-C30-C31
41	R	616	XAT	C12-C13-C14-C15
41	r	616	XAT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	S	309	CLA	CAA-CBA-CGA-O2A
25	s	309	CLA	CAA-CBA-CGA-O2A
35	C	515	DGD	O2G-C2G-C3G-O3G
35	c	515	DGD	O2G-C2G-C3G-O3G
24	y	302	CHL	C5-C6-C7-C8
39	S	316	LUT	C9-C10-C11-C12
39	s	316	LUT	C9-C10-C11-C12
25	C	505	CLA	C10-C11-C12-C13
25	c	505	CLA	C10-C11-C12-C13
29	a	412	SQD	C14-C15-C16-C17
29	A	411	SQD	C14-C15-C16-C17
24	g	607	CHL	O1D-CGD-O2D-CED
26	b	622	LHG	C25-C26-C27-C28
25	Y	312	CLA	C2-C1-O2A-CGA
25	y	312	CLA	C2-C1-O2A-CGA
24	Y	302	CHL	C2-C3-C5-C6
24	y	302	CHL	C2-C3-C5-C6
25	G	610	CLA	C15-C16-C17-C18
26	B	622	LHG	C25-C26-C27-C28
24	S	302	CHL	CAA-CBA-CGA-O1A
24	s	302	CHL	CAA-CBA-CGA-O1A
24	G	607	CHL	O1D-CGD-O2D-CED
35	B	626	DGD	O2G-C1B-C2B-C3B
25	B	602	CLA	C11-C10-C8-C9
25	B	610	CLA	C11-C10-C8-C9
25	B	613	CLA	C6-C7-C8-C9
25	b	602	CLA	C11-C10-C8-C9
25	b	610	CLA	C11-C10-C8-C9
25	b	613	CLA	C6-C7-C8-C9
25	c	510	CLA	C14-C13-C15-C16
25	g	610	CLA	C15-C16-C17-C18
25	N	612	CLA	C3-C5-C6-C7
25	n	612	CLA	C3-C5-C6-C7
26	B	621	LHG	O8-C23-C24-C25
35	b	626	DGD	O2G-C1B-C2B-C3B
26	B	622	LHG	C32-C33-C34-C35
26	b	622	LHG	C32-C33-C34-C35
30	A	410	LMG	C29-C30-C31-C32
25	S	310	CLA	C6-C7-C8-C10
25	G	612	CLA	C11-C12-C13-C15
25	s	310	CLA	C6-C7-C8-C10
25	g	612	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
28	C	514	BCR	C1-C6-C7-C8
28	c	514	BCR	C1-C6-C7-C8
39	S	315	LUT	C5-C6-C7-C8
39	s	315	LUT	C5-C6-C7-C8
25	R	601	CLA	C4C-C3C-CAC-CBC
30	a	411	LMG	C29-C30-C31-C32
26	b	621	LHG	O8-C23-C24-C25
26	C	519	LHG	C31-C32-C33-C34
26	c	519	LHG	C31-C32-C33-C34
39	Y	317	LUT	C29-C30-C31-C32
39	y	317	LUT	C29-C30-C31-C32
26	R	618	LHG	C27-C28-C29-C30
25	B	613	CLA	C4-C3-C5-C6
25	b	613	CLA	C4-C3-C5-C6
24	R	607	CHL	C2-C3-C5-C6
24	r	607	CHL	C2-C3-C5-C6
25	N	602	CLA	C2-C3-C5-C6
25	n	602	CLA	C2-C3-C5-C6
24	Y	309	CHL	C3-C5-C6-C7
24	y	309	CHL	C3-C5-C6-C7
26	r	618	LHG	C27-C28-C29-C30
30	B	620	LMG	C8-C7-O1-C1
30	b	620	LMG	C8-C7-O1-C1
25	r	601	CLA	C4C-C3C-CAC-CBC
24	S	302	CHL	CAA-CBA-CGA-O2A
24	s	302	CHL	CAA-CBA-CGA-O2A
25	g	610	CLA	C5-C6-C7-C8
30	C	520	LMG	C18-C19-C20-C21
30	c	520	LMG	C18-C19-C20-C21
35	C	515	DGD	C8B-C9B-CAB-CBB
35	c	515	DGD	C8B-C9B-CAB-CBB
25	G	610	CLA	C5-C6-C7-C8
26	B	621	LHG	O6-C4-C5-C6
26	b	621	LHG	O6-C4-C5-C6
24	N	608	CHL	C12-C13-C15-C16
24	n	608	CHL	C12-C13-C15-C16
25	G	602	CLA	C6-C7-C8-C10
25	G	603	CLA	C2-C3-C5-C6
25	R	609	CLA	C11-C12-C13-C15
25	g	602	CLA	C6-C7-C8-C10
25	g	603	CLA	C2-C3-C5-C6
25	r	609	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	B	621	LHG	O1-C1-C2-O2
26	b	621	LHG	O1-C1-C2-O2
25	B	603	CLA	C1-C2-C3-C4
25	B	607	CLA	C1-C2-C3-C4
25	G	612	CLA	C1-C2-C3-C4
25	b	603	CLA	C1-C2-C3-C4
25	b	607	CLA	C1-C2-C3-C4
25	g	612	CLA	C1-C2-C3-C4
24	N	606	CHL	CAA-CBA-CGA-O2A
24	n	606	CHL	CAA-CBA-CGA-O2A
24	n	605	CHL	C2-C1-O2A-CGA
30	B	623	LMG	C41-C42-C43-C44
30	b	623	LMG	C41-C42-C43-C44
30	B	623	LMG	O1-C7-C8-O7
30	b	623	LMG	O1-C7-C8-O7
24	N	605	CHL	C2-C1-O2A-CGA
24	G	605	CHL	C4C-C3C-CAC-CBC
24	S	308	CHL	CAA-CBA-CGA-O2A
24	s	308	CHL	CAA-CBA-CGA-O2A
25	Y	315	CLA	CAA-CBA-CGA-O2A
25	R	601	CLA	O2A-C1-C2-C3
25	r	601	CLA	O2A-C1-C2-C3
25	R	602	CLA	CAA-CBA-CGA-O2A
25	r	602	CLA	CAA-CBA-CGA-O2A
35	C	515	DGD	O2G-C1B-C2B-C3B
24	g	605	CHL	C4C-C3C-CAC-CBC
30	C	520	LMG	C39-C40-C41-C42
30	c	520	LMG	C39-C40-C41-C42
35	C	516	DGD	C5A-C6A-C7A-C8A
35	c	516	DGD	C5A-C6A-C7A-C8A
25	B	606	CLA	C16-C17-C18-C19
25	b	606	CLA	C16-C17-C18-C19
24	G	605	CHL	CAA-CBA-CGA-O2A
24	g	605	CHL	CAA-CBA-CGA-O2A
25	B	612	CLA	O1A-CGA-O2A-C1
25	b	612	CLA	O1A-CGA-O2A-C1
25	s	305	CLA	O1A-CGA-O2A-C1
28	T	101	BCR	C20-C21-C22-C37
28	t	101	BCR	C20-C21-C22-C37
29	L	103	SQD	C16-C17-C18-C19
29	l	101	SQD	C16-C17-C18-C19
25	B	613	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	b	613	CLA	CAA-CBA-CGA-O2A
35	c	515	DGD	O2G-C1B-C2B-C3B
25	Y	303	CLA	C4C-C3C-CAC-CBC
25	b	607	CLA	C4-C3-C5-C6
24	n	609	CHL	C10-C11-C12-C13
25	N	610	CLA	C8-C10-C11-C12
25	n	610	CLA	C8-C10-C11-C12
25	y	315	CLA	CAA-CBA-CGA-O2A
31	D	405	PL9	C43-C44-C46-C47
31	d	405	PL9	C43-C44-C46-C47
24	Y	307	CHL	CAA-CBA-CGA-O2A
24	y	307	CHL	CAA-CBA-CGA-O2A
25	B	616	CLA	CAA-CBA-CGA-O2A
25	b	616	CLA	CAA-CBA-CGA-O2A
25	y	303	CLA	C4C-C3C-CAC-CBC
24	N	607	CHL	C11-C10-C8-C9
24	n	607	CHL	C11-C10-C8-C9
25	B	603	CLA	C14-C13-C15-C16
25	B	611	CLA	C11-C12-C13-C14
25	C	510	CLA	C14-C13-C15-C16
25	G	613	CLA	C14-C13-C15-C16
25	N	611	CLA	C6-C7-C8-C9
25	Y	304	CLA	C6-C7-C8-C9
25	b	603	CLA	C14-C13-C15-C16
25	b	611	CLA	C11-C12-C13-C14
25	g	613	CLA	C14-C13-C15-C16
25	n	611	CLA	C6-C7-C8-C9
25	y	304	CLA	C6-C7-C8-C9
25	S	305	CLA	O1A-CGA-O2A-C1
25	S	309	CLA	CAA-CBA-CGA-O1A
25	s	309	CLA	CAA-CBA-CGA-O1A
29	A	407	SQD	C18-C19-C20-C21
29	a	408	SQD	C18-C19-C20-C21
24	N	605	CHL	C3A-C2A-CAA-CBA
24	n	605	CHL	C3A-C2A-CAA-CBA
25	B	601	CLA	C3A-C2A-CAA-CBA
25	B	608	CLA	C3A-C2A-CAA-CBA
25	C	505	CLA	C3A-C2A-CAA-CBA
25	G	603	CLA	C3A-C2A-CAA-CBA
25	N	613	CLA	C3A-C2A-CAA-CBA
25	b	601	CLA	C3A-C2A-CAA-CBA
25	b	608	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	c	505	CLA	C3A-C2A-CAA-CBA
25	g	603	CLA	C3A-C2A-CAA-CBA
25	n	613	CLA	C3A-C2A-CAA-CBA
26	b	625	LHG	C11-C12-C13-C14
25	B	604	CLA	C13-C15-C16-C17
25	b	604	CLA	C13-C15-C16-C17
25	D	402	CLA	CAA-CBA-CGA-O2A
25	D	403	CLA	CAA-CBA-CGA-O2A
25	d	402	CLA	CAA-CBA-CGA-O2A
25	d	403	CLA	CAA-CBA-CGA-O2A
26	D	406	LHG	C29-C30-C31-C32
26	d	406	LHG	C29-C30-C31-C32
24	2	603	CHL	CAD-CBD-CGD-O2D
24	Y	310	CHL	CAD-CBD-CGD-O2D
24	6	603	CHL	CAD-CBD-CGD-O2D
24	y	310	CHL	CAD-CBD-CGD-O2D
25	2	604	CLA	CAD-CBD-CGD-O2D
25	B	609	CLA	CAD-CBD-CGD-O2D
25	B	610	CLA	CAD-CBD-CGD-O2D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	616	CLA	CAD-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	508	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	D	403	CLA	CAD-CBD-CGD-O2D
25	S	314	CLA	CAD-CBD-CGD-O2D
25	G	604	CLA	CAD-CBD-CGD-O2D
25	N	614	CLA	CAD-CBD-CGD-O2D
25	R	609	CLA	CAD-CBD-CGD-O2D
25	R	610	CLA	CAD-CBD-CGD-O2D
25	6	604	CLA	CAD-CBD-CGD-O2D
25	b	609	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	b	616	CLA	CAD-CBD-CGD-O2D
25	c	501	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	c	508	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CAD-CBD-CGD-O2D
25	d	403	CLA	CAD-CBD-CGD-O2D
25	s	309	CLA	CAD-CBD-CGD-O2D
25	s	314	CLA	CAD-CBD-CGD-O2D
25	g	604	CLA	CAD-CBD-CGD-O2D
25	r	609	CLA	CAD-CBD-CGD-O2D
25	r	610	CLA	CAD-CBD-CGD-O2D
40	R	617	NEX	C7-C8-C9-C19
40	r	617	NEX	C7-C8-C9-C19
25	Y	304	CLA	C16-C17-C18-C20
25	y	304	CLA	C16-C17-C18-C20
26	B	625	LHG	C11-C12-C13-C14
24	N	609	CHL	C10-C11-C12-C13
30	A	408	LMG	O9-C10-O7-C8
30	a	409	LMG	O9-C10-O7-C8
35	C	516	DGD	O1B-C1B-O2G-C2G
35	c	516	DGD	O1B-C1B-O2G-C2G
24	Y	310	CHL	C2-C1-O2A-CGA
24	y	310	CHL	C2-C1-O2A-CGA
25	C	501	CLA	CAA-CBA-CGA-O2A
25	C	512	CLA	CAA-CBA-CGA-O2A
25	Y	304	CLA	CAA-CBA-CGA-O2A
25	c	501	CLA	CAA-CBA-CGA-O2A
25	c	512	CLA	CAA-CBA-CGA-O2A
25	y	304	CLA	CAA-CBA-CGA-O2A
35	A	415	DGD	O2G-C1B-C2B-C3B
35	a	401	DGD	O2G-C1B-C2B-C3B
28	B	617	BCR	C22-C23-C24-C25
28	b	617	BCR	C22-C23-C24-C25
26	n	618	LHG	C29-C30-C31-C32
25	B	607	CLA	C4-C3-C5-C6
25	B	611	CLA	C4-C3-C5-C6
25	b	611	CLA	C4-C3-C5-C6
30	B	620	LMG	O6-C5-C6-O5
30	b	620	LMG	O6-C5-C6-O5
24	y	308	CHL	C5-C6-C7-C8
25	B	608	CLA	C10-C11-C12-C13
25	b	608	CLA	C10-C11-C12-C13
25	S	313	CLA	CAA-CBA-CGA-O2A
25	s	313	CLA	CAA-CBA-CGA-O2A
26	N	618	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
26	n	618	LHG	C4-C5-C6-O8
29	A	407	SQD	O6-C44-C45-C46
29	a	408	SQD	O6-C44-C45-C46
35	C	515	DGD	C1G-C2G-C3G-O3G
35	c	515	DGD	C1G-C2G-C3G-O3G
40	G	617	NEX	O24-C26-C27-C28
40	g	617	NEX	O24-C26-C27-C28
24	y	309	CHL	C4C-C3C-CAC-CBC
26	N	618	LHG	C29-C30-C31-C32
24	N	605	CHL	C4C-C3C-CAC-CBC
24	Y	309	CHL	C4C-C3C-CAC-CBC
24	n	605	CHL	C4C-C3C-CAC-CBC
26	2	606	LHG	O6-C4-C5-O7
26	6	606	LHG	O6-C4-C5-O7
24	Y	308	CHL	C5-C6-C7-C8
26	R	618	LHG	O7-C7-C8-C9
26	r	618	LHG	O7-C7-C8-C9
29	A	407	SQD	O47-C7-C8-C9
29	a	408	SQD	O47-C7-C8-C9
35	C	516	DGD	C6A-C7A-C8A-C9A
25	S	314	CLA	O2A-C1-C2-C3
25	s	314	CLA	O2A-C1-C2-C3
35	c	516	DGD	C6A-C7A-C8A-C9A
24	N	609	CHL	O2A-C1-C2-C3
24	n	609	CHL	O2A-C1-C2-C3
29	A	407	SQD	C14-C15-C16-C17
29	a	408	SQD	C14-C15-C16-C17
24	S	306	CHL	CAA-CBA-CGA-O1A
24	s	306	CHL	CAA-CBA-CGA-O1A
26	6	606	LHG	C24-C25-C26-C27
24	1	301	CHL	CHA-CBD-CGD-O2D
24	G	601	CHL	CHA-CBD-CGD-O2D
24	G	605	CHL	CHA-CBD-CGD-O1D
24	Y	309	CHL	CHA-CBD-CGD-O1D
24	5	301	CHL	CHA-CBD-CGD-O2D
24	g	601	CHL	CHA-CBD-CGD-O2D
24	g	605	CHL	CHA-CBD-CGD-O1D
24	y	309	CHL	CHA-CBD-CGD-O1D
25	2	602	CLA	CHA-CBD-CGD-O1D
25	B	601	CLA	CHA-CBD-CGD-O2D
25	B	607	CLA	CHA-CBD-CGD-O2D
25	B	610	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	616	CLA	CHA-CBD-CGD-O1D
25	C	506	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	D	401	CLA	CHA-CBD-CGD-O1D
25	S	311	CLA	CHA-CBD-CGD-O2D
25	S	312	CLA	CHA-CBD-CGD-O1D
25	S	313	CLA	CHA-CBD-CGD-O2D
25	G	602	CLA	CHA-CBD-CGD-O2D
25	G	611	CLA	CHA-CBD-CGD-O1D
25	G	611	CLA	CHA-CBD-CGD-O2D
25	G	612	CLA	CHA-CBD-CGD-O2D
25	G	613	CLA	CHA-CBD-CGD-O2D
25	N	612	CLA	CHA-CBD-CGD-O1D
25	Y	303	CLA	CHA-CBD-CGD-O2D
25	R	601	CLA	CHA-CBD-CGD-O2D
25	6	602	CLA	CHA-CBD-CGD-O1D
25	b	601	CLA	CHA-CBD-CGD-O2D
25	b	607	CLA	CHA-CBD-CGD-O2D
25	b	610	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	c	506	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	d	401	CLA	CHA-CBD-CGD-O1D
25	s	311	CLA	CHA-CBD-CGD-O2D
25	s	312	CLA	CHA-CBD-CGD-O1D
25	s	313	CLA	CHA-CBD-CGD-O2D
25	g	602	CLA	CHA-CBD-CGD-O2D
25	g	611	CLA	CHA-CBD-CGD-O1D
25	g	611	CLA	CHA-CBD-CGD-O2D
25	g	612	CLA	CHA-CBD-CGD-O2D
25	g	613	CLA	CHA-CBD-CGD-O2D
25	n	612	CLA	CHA-CBD-CGD-O1D
25	y	303	CLA	CHA-CBD-CGD-O2D
25	r	601	CLA	CHA-CBD-CGD-O2D
26	2	606	LHG	C24-C25-C26-C27
26	N	618	LHG	C9-C10-C11-C12
26	n	618	LHG	C9-C10-C11-C12
26	y	319	LHG	C15-C16-C17-C18
35	C	516	DGD	CBA-CCA-CDA-CEA
25	N	612	CLA	CAA-CBA-CGA-O2A
25	n	612	CLA	CAA-CBA-CGA-O2A
26	D	406	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
26	d	406	LHG	O8-C23-C24-C25
30	A	410	LMG	C4-C5-C6-O5
30	a	411	LMG	C4-C5-C6-O5
26	D	406	LHG	C13-C14-C15-C16
35	c	516	DGD	CBA-CCA-CDA-CEA
26	B	622	LHG	O7-C5-C6-O8
26	b	622	LHG	O7-C5-C6-O8
26	L	102	LHG	C23-C24-C25-C26
26	l	103	LHG	C23-C24-C25-C26
24	6	601	CHL	CBA-CGA-O2A-C1
25	N	610	CLA	C5-C6-C7-C8
25	n	610	CLA	C5-C6-C7-C8
24	S	306	CHL	CAA-CBA-CGA-O2A
24	s	306	CHL	CAA-CBA-CGA-O2A
26	Y	319	LHG	C15-C16-C17-C18
26	d	406	LHG	C13-C14-C15-C16
26	2	606	LHG	O10-C23-O8-C6
25	B	612	CLA	CAA-CBA-CGA-O2A
25	G	612	CLA	CAA-CBA-CGA-O2A
25	g	612	CLA	CAA-CBA-CGA-O2A
25	n	603	CLA	CAA-CBA-CGA-O2A
30	C	520	LMG	O8-C28-C29-C30
24	g	601	CHL	C2A-CAA-CBA-CGA
25	D	403	CLA	C2A-CAA-CBA-CGA
25	d	403	CLA	C2A-CAA-CBA-CGA
27	A	403	PHO	CHA-CBD-CGD-O1D
27	a	404	PHO	CHA-CBD-CGD-O1D
30	D	407	LMG	C14-C15-C16-C17
30	d	407	LMG	C14-C15-C16-C17
24	2	601	CHL	CBA-CGA-O2A-C1
25	b	612	CLA	CAA-CBA-CGA-O2A
30	c	520	LMG	O8-C28-C29-C30
30	a	411	LMG	C30-C31-C32-C33
24	G	607	CHL	CAA-CBA-CGA-O1A
24	g	607	CHL	CAA-CBA-CGA-O1A
25	r	614	CLA	CAA-CBA-CGA-O1A
26	6	606	LHG	O10-C23-O8-C6
24	N	608	CHL	C11-C10-C8-C7
24	n	608	CHL	C11-C10-C8-C7
25	C	513	CLA	C11-C12-C13-C15
25	c	513	CLA	C11-C12-C13-C15
31	D	405	PL9	C18-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
31	d	405	PL9	C18-C19-C21-C22
25	B	616	CLA	C16-C17-C18-C19
25	b	616	CLA	C16-C17-C18-C19
25	C	508	CLA	C2C-C3C-CAC-CBC
30	A	410	LMG	C30-C31-C32-C33
24	G	606	CHL	CAA-CBA-CGA-O2A
25	N	603	CLA	CAA-CBA-CGA-O2A
25	R	614	CLA	CAA-CBA-CGA-O1A
25	c	508	CLA	C2C-C3C-CAC-CBC
25	G	602	CLA	C6-C7-C8-C9
25	g	602	CLA	C6-C7-C8-C9
25	Y	305	CLA	CBA-CGA-O2A-C1
25	y	305	CLA	CBA-CGA-O2A-C1
26	2	606	LHG	C24-C23-O8-C6
26	6	606	LHG	C24-C23-O8-C6
24	g	606	CHL	CAA-CBA-CGA-O2A
25	N	611	CLA	CAA-CBA-CGA-O2A
25	n	611	CLA	CAA-CBA-CGA-O2A
26	y	301	LHG	O10-C23-C24-C25
25	B	606	CLA	C16-C17-C18-C20
25	b	606	CLA	C16-C17-C18-C20
24	N	605	CHL	O1A-CGA-O2A-C1
35	C	516	DGD	C2B-C1B-O2G-C2G
35	c	516	DGD	C2B-C1B-O2G-C2G
24	G	601	CHL	C2A-CAA-CBA-CGA
26	C	518	LHG	C23-C24-C25-C26
26	Y	301	LHG	O10-C23-C24-C25
25	C	510	CLA	C4C-C3C-CAC-CBC
28	D	404	BCR	C7-C8-C9-C34
28	I	101	BCR	C7-C8-C9-C34
28	d	404	BCR	C7-C8-C9-C34
25	C	507	CLA	C5-C6-C7-C8
25	g	611	CLA	C11-C12-C13-C14
25	c	510	CLA	C4C-C3C-CAC-CBC
26	c	517	LHG	O1-C1-C2-C3
35	C	515	DGD	CDB-CEB-CFB-CGB
35	C	515	DGD	O1B-C1B-C2B-C3B
35	c	515	DGD	O1B-C1B-C2B-C3B
25	C	507	CLA	CBA-CGA-O2A-C1
25	c	507	CLA	CBA-CGA-O2A-C1
26	Y	319	LHG	C28-C29-C30-C31
35	c	515	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
24	G	601	CHL	C1A-C2A-CAA-CBA
24	g	601	CHL	C1A-C2A-CAA-CBA
25	2	604	CLA	C1A-C2A-CAA-CBA
25	B	602	CLA	C1A-C2A-CAA-CBA
25	B	608	CLA	C1A-C2A-CAA-CBA
25	N	612	CLA	C1A-C2A-CAA-CBA
25	R	612	CLA	C1A-C2A-CAA-CBA
25	6	604	CLA	C1A-C2A-CAA-CBA
25	b	602	CLA	C1A-C2A-CAA-CBA
25	b	608	CLA	C1A-C2A-CAA-CBA
25	n	612	CLA	C1A-C2A-CAA-CBA
25	r	612	CLA	C1A-C2A-CAA-CBA
26	y	319	LHG	C28-C29-C30-C31
24	N	607	CHL	C16-C17-C18-C20
24	n	607	CHL	C16-C17-C18-C20
25	G	611	CLA	C11-C12-C13-C14
35	A	415	DGD	O1B-C1B-C2B-C3B
35	a	401	DGD	O1B-C1B-C2B-C3B
25	c	507	CLA	C5-C6-C7-C8
24	n	605	CHL	O1A-CGA-O2A-C1
25	g	602	CLA	C13-C15-C16-C17
24	y	307	CHL	CAA-CBA-CGA-O1A
25	R	603	CLA	CAA-CBA-CGA-O1A
25	r	603	CLA	CAA-CBA-CGA-O1A
26	Y	319	LHG	C27-C28-C29-C30
26	y	319	LHG	C27-C28-C29-C30
29	A	407	SQD	C44-C45-C46-O48
29	a	408	SQD	C44-C45-C46-O48
30	B	623	LMG	O1-C7-C8-C9
30	b	623	LMG	O1-C7-C8-C9
25	G	602	CLA	C13-C15-C16-C17
25	C	512	CLA	C4C-C3C-CAC-CBC
25	c	512	CLA	C4C-C3C-CAC-CBC
35	C	515	DGD	C5B-C6B-C7B-C8B
24	Y	307	CHL	CAA-CBA-CGA-O1A
25	N	612	CLA	CAA-CBA-CGA-O1A
25	n	612	CLA	CAA-CBA-CGA-O1A
35	c	515	DGD	C5B-C6B-C7B-C8B
25	R	614	CLA	CAA-CBA-CGA-O2A
25	C	509	CLA	C13-C15-C16-C17
25	c	509	CLA	C13-C15-C16-C17
26	c	518	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	A	410	LMG	C34-C35-C36-C37
30	a	411	LMG	C34-C35-C36-C37
25	r	614	CLA	CAA-CBA-CGA-O2A
26	B	625	LHG	C31-C32-C33-C34
26	R	618	LHG	C14-C15-C16-C17
26	r	618	LHG	C14-C15-C16-C17
26	B	621	LHG	C3-O3-P-O5
26	S	318	LHG	C3-O3-P-O5
26	Y	301	LHG	C3-O3-P-O5
26	b	621	LHG	C3-O3-P-O5
26	s	318	LHG	C3-O3-P-O5
26	y	301	LHG	C3-O3-P-O5
30	A	408	LMG	C11-C10-O7-C8
26	b	622	LHG	C16-C17-C18-C19
25	G	613	CLA	CAA-CBA-CGA-O1A
25	N	611	CLA	CAA-CBA-CGA-O1A
25	g	613	CLA	CAA-CBA-CGA-O1A
25	n	611	CLA	CAA-CBA-CGA-O1A
24	n	609	CHL	CAA-CBA-CGA-O2A
25	N	612	CLA	O1A-CGA-O2A-C1
26	B	622	LHG	C16-C17-C18-C19
26	b	625	LHG	C31-C32-C33-C34
28	C	514	BCR	C5-C6-C7-C8
28	c	514	BCR	C5-C6-C7-C8
30	B	623	LMG	C20-C21-C22-C23
30	b	623	LMG	C20-C21-C22-C23
24	G	606	CHL	CAA-CBA-CGA-O1A
24	g	606	CHL	CAA-CBA-CGA-O1A
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	612	CLA	CAA-CBA-CGA-O1A
29	A	407	SQD	O49-C7-C8-C9
29	a	408	SQD	O49-C7-C8-C9
25	C	501	CLA	O1A-CGA-O2A-C1
26	S	318	LHG	C32-C33-C34-C35
30	c	520	LMG	O10-C28-C29-C30
25	c	501	CLA	O1A-CGA-O2A-C1
25	C	508	CLA	C4C-C3C-CAC-CBC
26	s	318	LHG	C32-C33-C34-C35
30	a	409	LMG	C11-C10-O7-C8
35	C	516	DGD	C4E-C5E-C6E-O5E
35	c	516	DGD	C4E-C5E-C6E-O5E
25	n	611	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	c	508	CLA	C4C-C3C-CAC-CBC
24	S	302	CHL	CAD-CBD-CGD-O1D
24	s	302	CHL	CAD-CBD-CGD-O1D
25	B	609	CLA	CAD-CBD-CGD-O1D
25	C	506	CLA	CAD-CBD-CGD-O1D
25	C	508	CLA	CAD-CBD-CGD-O1D
25	N	610	CLA	CAD-CBD-CGD-O1D
25	b	609	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
25	c	508	CLA	CAD-CBD-CGD-O1D
25	n	610	CLA	CAD-CBD-CGD-O1D
26	L	102	LHG	C4-C5-O7-C7
26	l	103	LHG	C4-C5-O7-C7
25	n	612	CLA	O1A-CGA-O2A-C1
25	B	616	CLA	CAA-CBA-CGA-O1A
25	b	616	CLA	CAA-CBA-CGA-O1A
26	R	618	LHG	O9-C7-C8-C9
26	r	618	LHG	O9-C7-C8-C9
30	C	520	LMG	O10-C28-C29-C30
24	N	609	CHL	CAA-CBA-CGA-O2A
25	g	613	CLA	CAA-CBA-CGA-O2A
25	B	601	CLA	C6-C7-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	C	513	CLA	C11-C12-C13-C14
25	G	602	CLA	C11-C10-C8-C9
25	b	601	CLA	C6-C7-C8-C9
25	c	512	CLA	C6-C7-C8-C9
25	c	513	CLA	C11-C12-C13-C14
25	g	602	CLA	C11-C10-C8-C9
25	y	311	CLA	C11-C10-C8-C9
25	c	508	CLA	C5-C6-C7-C8
25	N	611	CLA	C11-C12-C13-C15
25	G	613	CLA	CAA-CBA-CGA-O2A
26	Y	301	LHG	O7-C7-C8-C9
26	y	301	LHG	O7-C7-C8-C9
35	B	626	DGD	C9A-CAA-CBA-CCA
25	C	508	CLA	C5-C6-C7-C8
25	y	303	CLA	C8-C10-C11-C12
35	b	626	DGD	C9A-CAA-CBA-CCA
25	C	501	CLA	CAA-CBA-CGA-O1A
25	c	501	CLA	CAA-CBA-CGA-O1A
24	1	301	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	n	608	CHL	CAA-CBA-CGA-O2A
25	S	311	CLA	CAA-CBA-CGA-O2A
25	Y	314	CLA	CAA-CBA-CGA-O2A
25	s	311	CLA	CAA-CBA-CGA-O2A
25	B	605	CLA	C13-C15-C16-C17
25	b	605	CLA	C13-C15-C16-C17
26	d	406	LHG	O10-C23-C24-C25
25	C	510	CLA	C4-C3-C5-C6
25	c	510	CLA	C4-C3-C5-C6
35	C	516	DGD	C7B-C8B-C9B-CAB
35	c	516	DGD	C7B-C8B-C9B-CAB
24	Y	302	CHL	C6-C7-C8-C10
24	y	302	CHL	C6-C7-C8-C10
25	A	401	CLA	C11-C10-C8-C7
25	B	601	CLA	C6-C7-C8-C10
25	B	602	CLA	C3A-C2A-CAA-CBA
25	B	605	CLA	C11-C12-C13-C15
25	N	603	CLA	C6-C7-C8-C10
25	N	612	CLA	C3A-C2A-CAA-CBA
25	R	602	CLA	C11-C10-C8-C7
25	a	402	CLA	C11-C10-C8-C7
25	b	601	CLA	C6-C7-C8-C10
25	b	602	CLA	C3A-C2A-CAA-CBA
25	b	605	CLA	C11-C12-C13-C15
25	n	603	CLA	C6-C7-C8-C10
25	n	612	CLA	C3A-C2A-CAA-CBA
25	r	602	CLA	C11-C10-C8-C7
39	G	615	LUT	C25-C26-C27-C28
39	N	615	LUT	C25-C26-C27-C28
39	g	615	LUT	C25-C26-C27-C28
39	n	615	LUT	C25-C26-C27-C28
25	n	613	CLA	CAA-CBA-CGA-O1A
26	D	406	LHG	O10-C23-C24-C25
24	5	301	CHL	C4C-C3C-CAC-CBC
24	N	608	CHL	CAA-CBA-CGA-O2A
25	y	314	CLA	CAA-CBA-CGA-O2A
35	c	516	DGD	O2G-C1B-C2B-C3B
25	Y	303	CLA	C8-C10-C11-C12
25	Y	304	CLA	C8-C10-C11-C12
25	y	304	CLA	C8-C10-C11-C12
28	B	618	BCR	C21-C22-C23-C24
28	I	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	b	618	BCR	C21-C22-C23-C24
28	i	101	BCR	C7-C8-C9-C10
25	N	613	CLA	CAA-CBA-CGA-O1A
39	S	316	LUT	C29-C30-C31-C32
39	G	615	LUT	C33-C34-C35-C15
39	s	316	LUT	C29-C30-C31-C32
39	g	615	LUT	C33-C34-C35-C15
29	A	411	SQD	C28-C29-C30-C31
29	a	412	SQD	C28-C29-C30-C31
26	R	618	LHG	O8-C23-C24-C25
35	C	516	DGD	O2G-C1B-C2B-C3B
30	d	407	LMG	C22-C23-C24-C25
35	A	415	DGD	O6E-C1E-O5D-C6D
35	B	626	DGD	O6E-C1E-O5D-C6D
35	a	401	DGD	O6E-C1E-O5D-C6D
35	b	626	DGD	O6E-C1E-O5D-C6D
25	C	501	CLA	C15-C16-C17-C18
25	c	501	CLA	C15-C16-C17-C18
30	D	407	LMG	C22-C23-C24-C25
26	Y	301	LHG	O9-C7-C8-C9
26	y	301	LHG	O9-C7-C8-C9
24	N	606	CHL	CAA-CBA-CGA-O1A
24	n	606	CHL	CAA-CBA-CGA-O1A
25	G	602	CLA	C8-C10-C11-C12
25	g	602	CLA	C8-C10-C11-C12
25	G	604	CLA	CAA-CBA-CGA-O2A
25	B	606	CLA	C15-C16-C17-C18
25	b	606	CLA	C15-C16-C17-C18
24	S	306	CHL	C2A-CAA-CBA-CGA
24	s	306	CHL	C2A-CAA-CBA-CGA
25	B	615	CLA	C13-C15-C16-C17
25	b	615	CLA	C13-C15-C16-C17
26	s	318	LHG	C34-C35-C36-C37
25	G	603	CLA	CAA-CBA-CGA-O2A
25	g	604	CLA	CAA-CBA-CGA-O2A
26	r	618	LHG	O8-C23-C24-C25

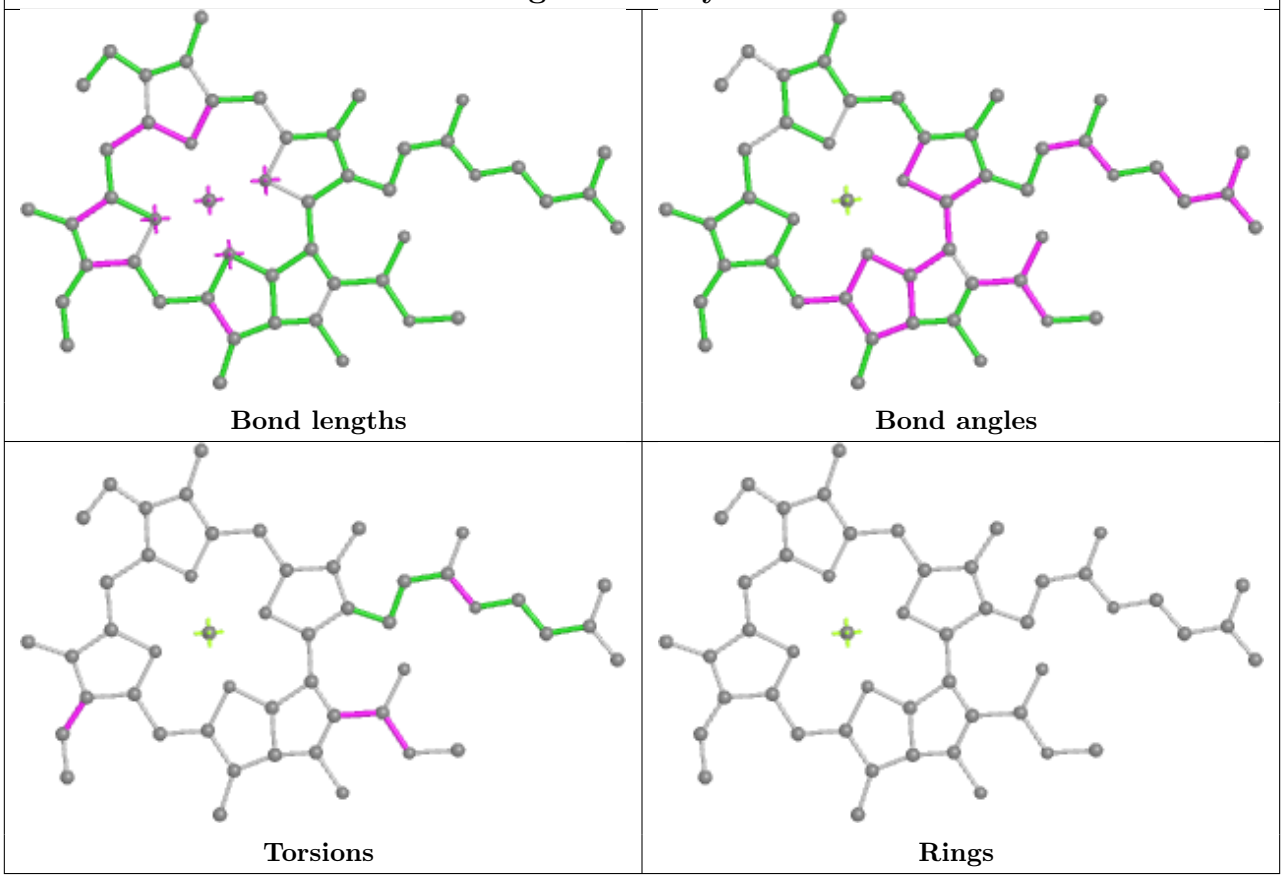
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	Y	318	NEX	C1-C2-C3-C4-C5-C6
40	y	318	NEX	C1-C2-C3-C4-C5-C6

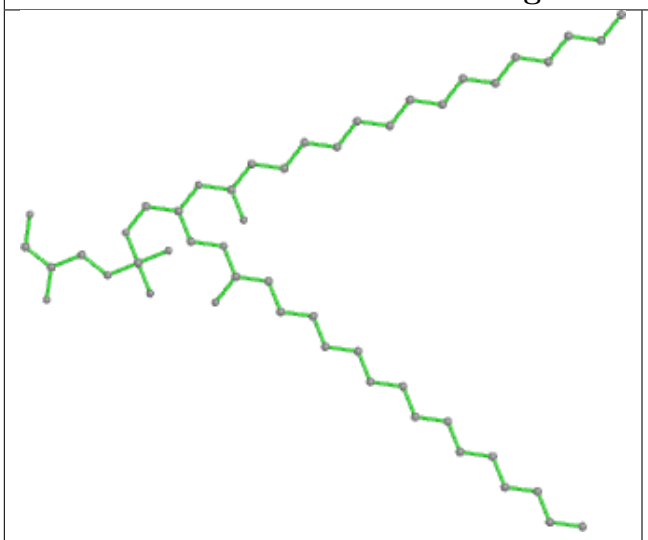
No monomer is involved in short contacts.

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.

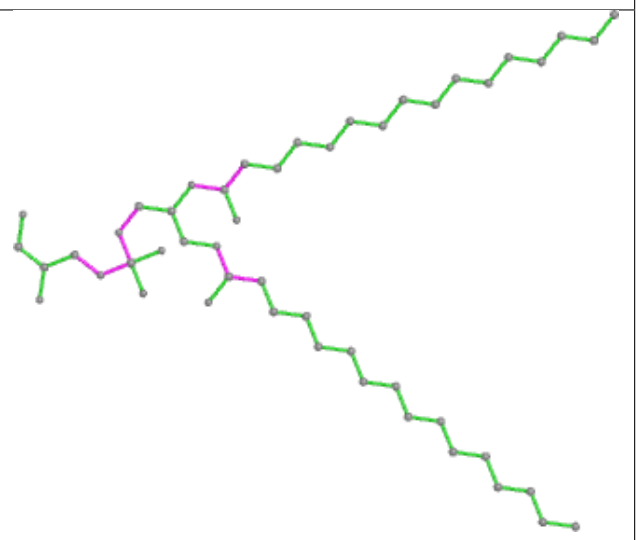
Ligand CLA y 305



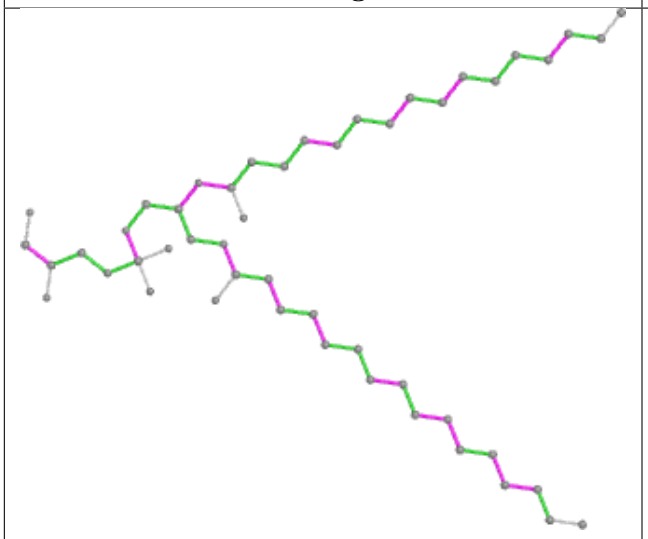
Ligand LHG C 519



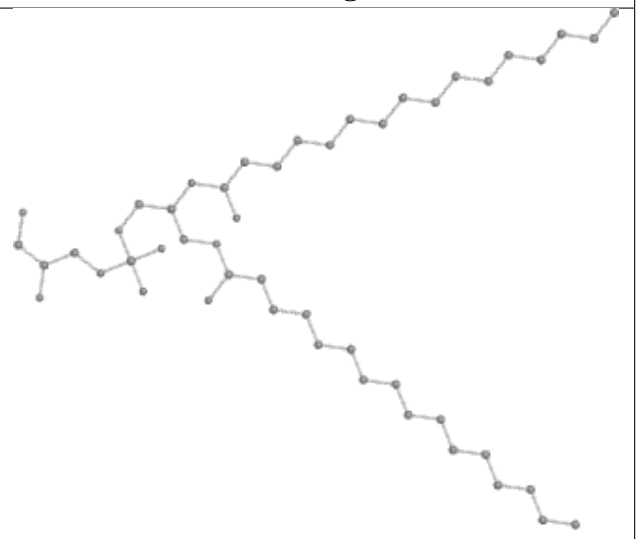
Bond lengths



Bond angles

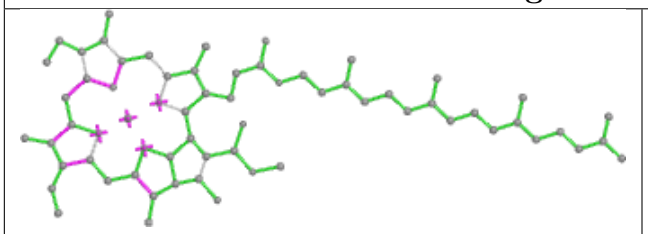


Torsions

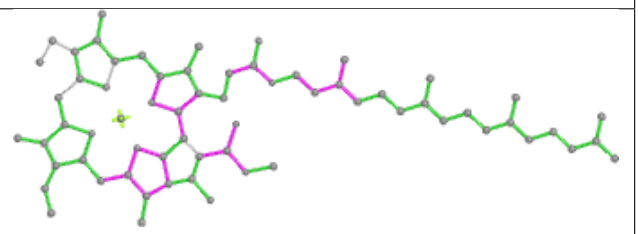


Rings

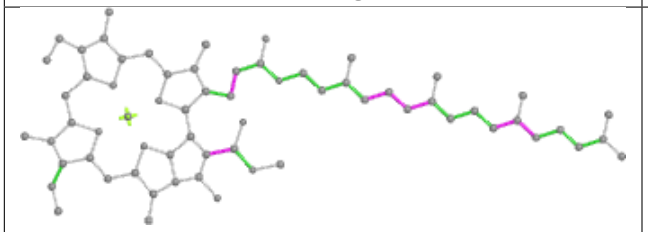
Ligand CLA B 614



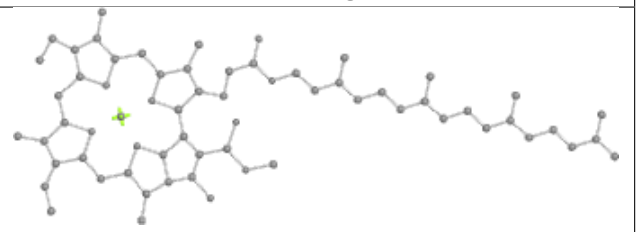
Bond lengths



Bond angles

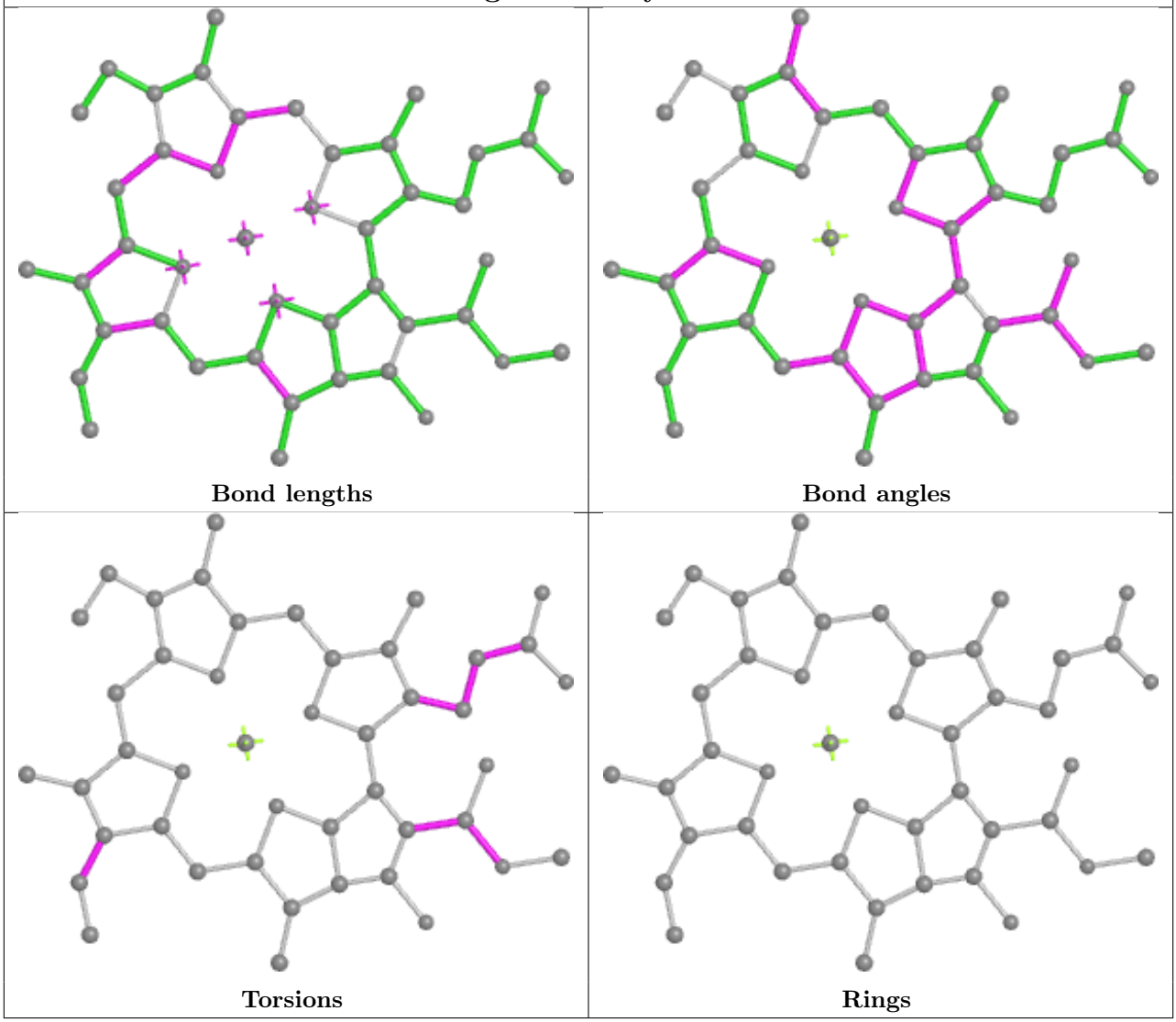


Torsions

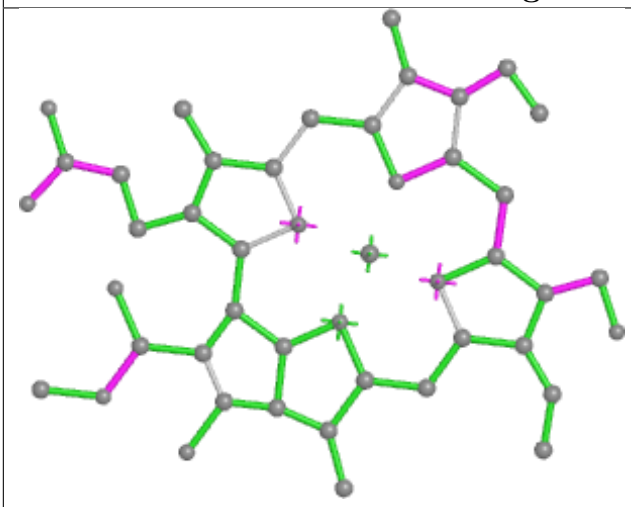


Rings

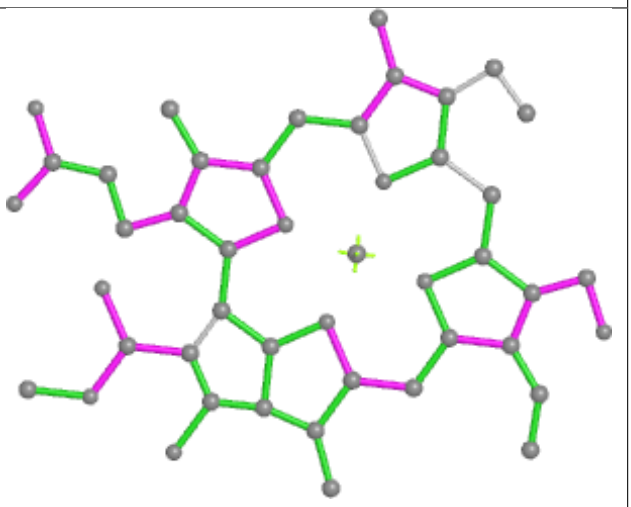
Ligand CLA y 315



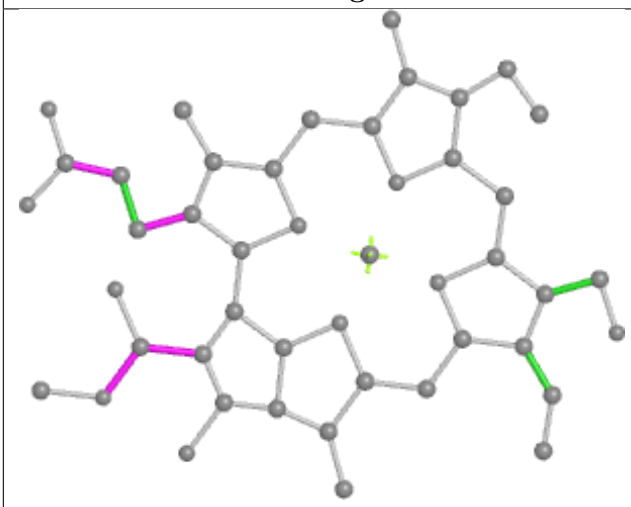
Ligand CHL G 607



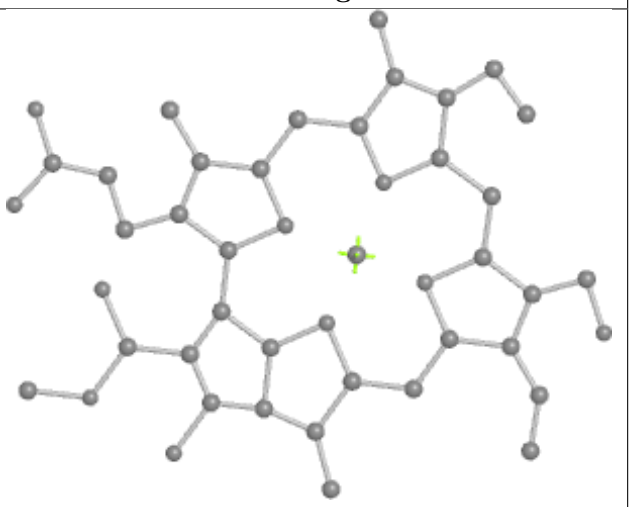
Bond lengths



Bond angles

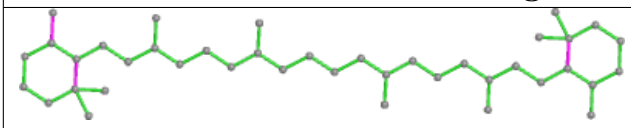


Torsions

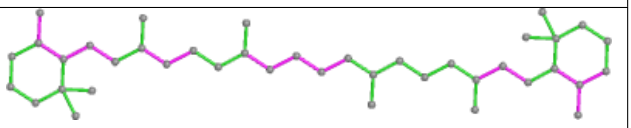


Rings

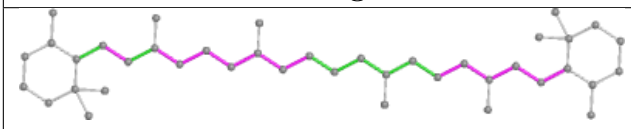
Ligand BCR T 101



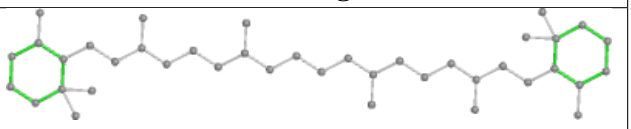
Bond lengths



Bond angles

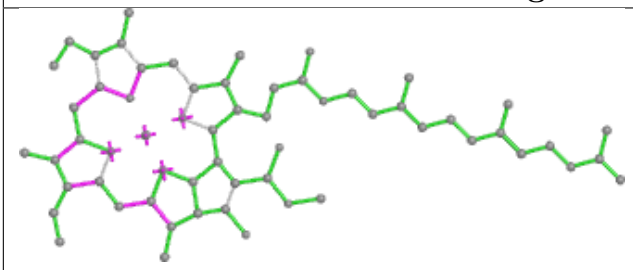


Torsions

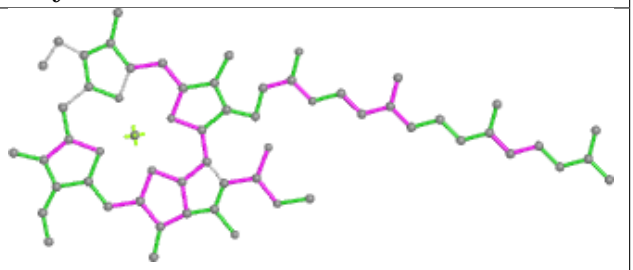


Rings

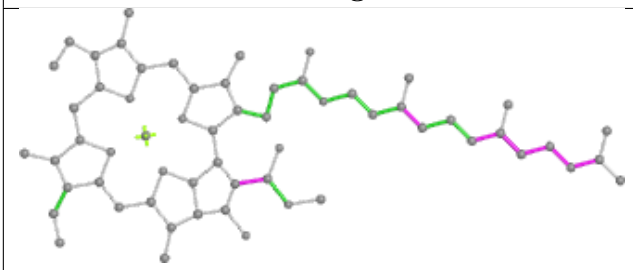
Ligand CLA y 313



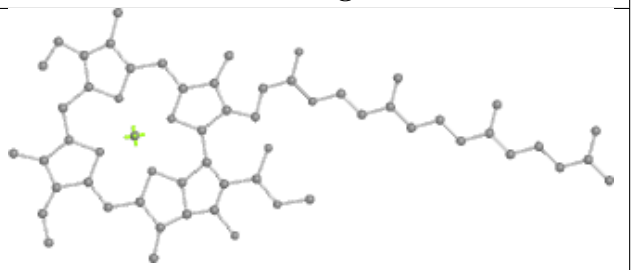
Bond lengths



Bond angles

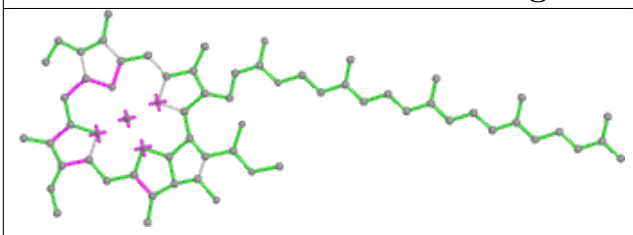


Torsions



Rings

Ligand CLA c 505



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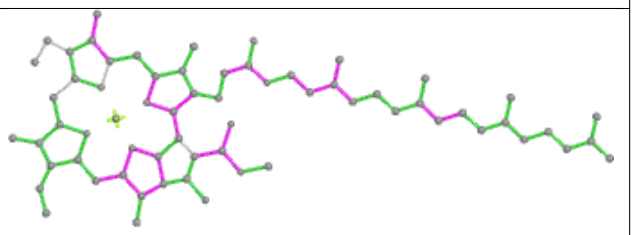
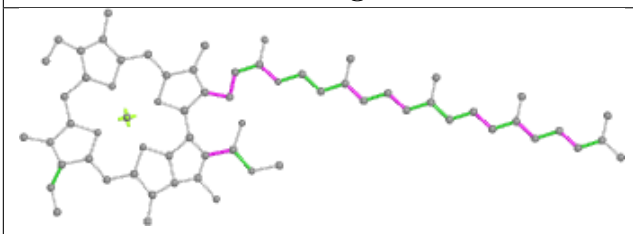
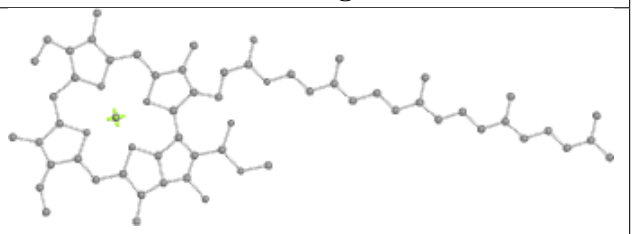


Bond angles

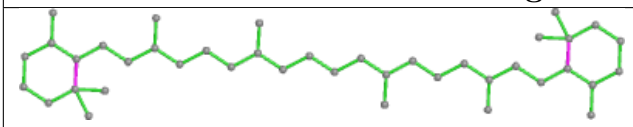


Torsions

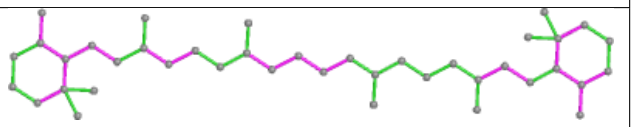


Rings

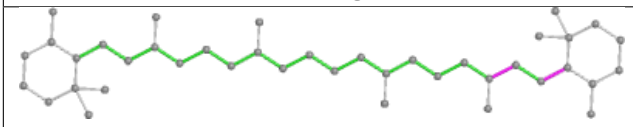
Ligand BCR b 618



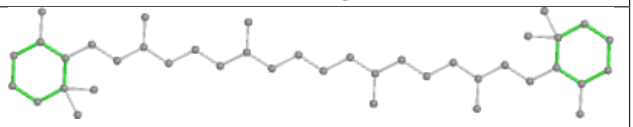
Bond lengths



Bond angles

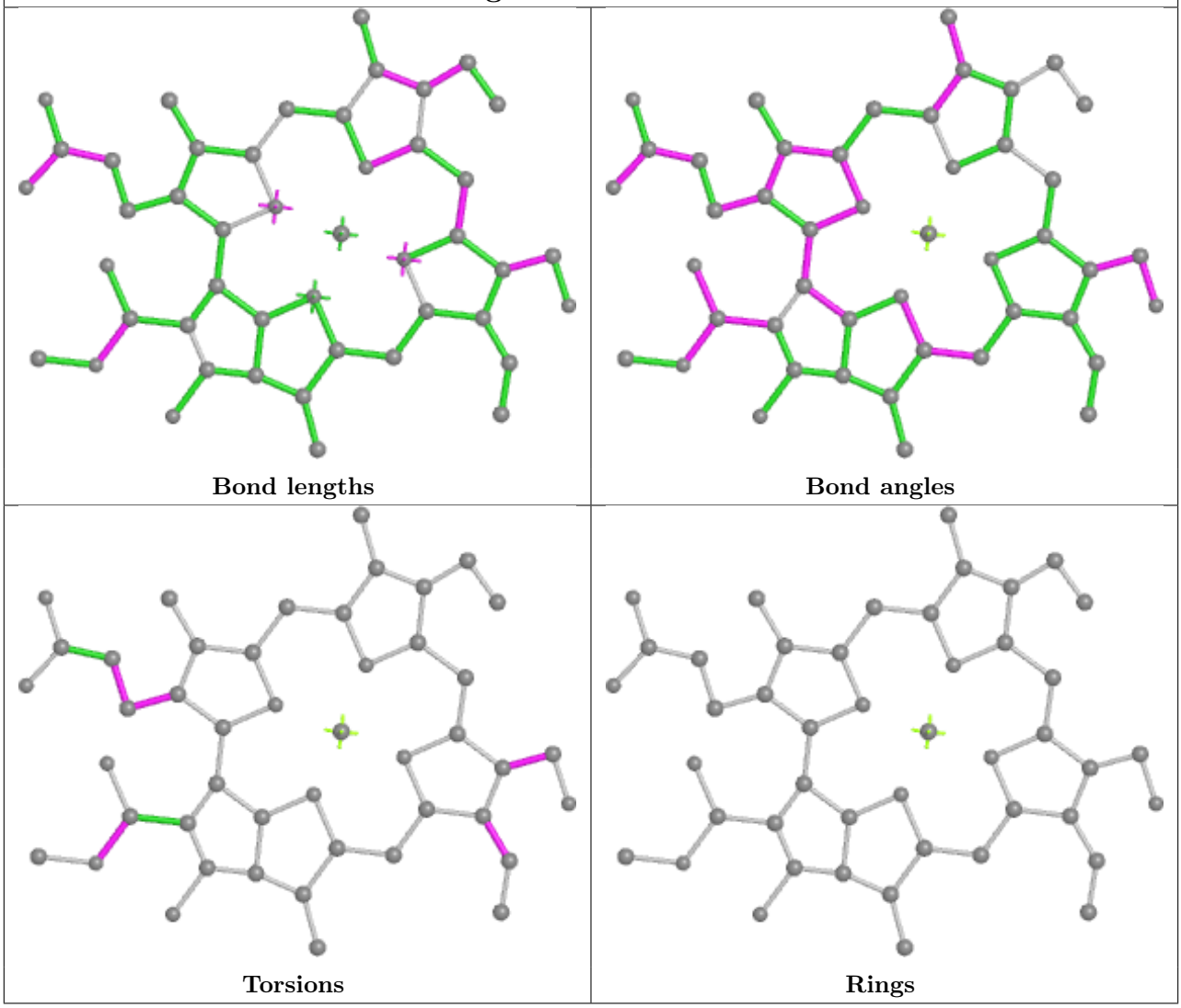


Torsions

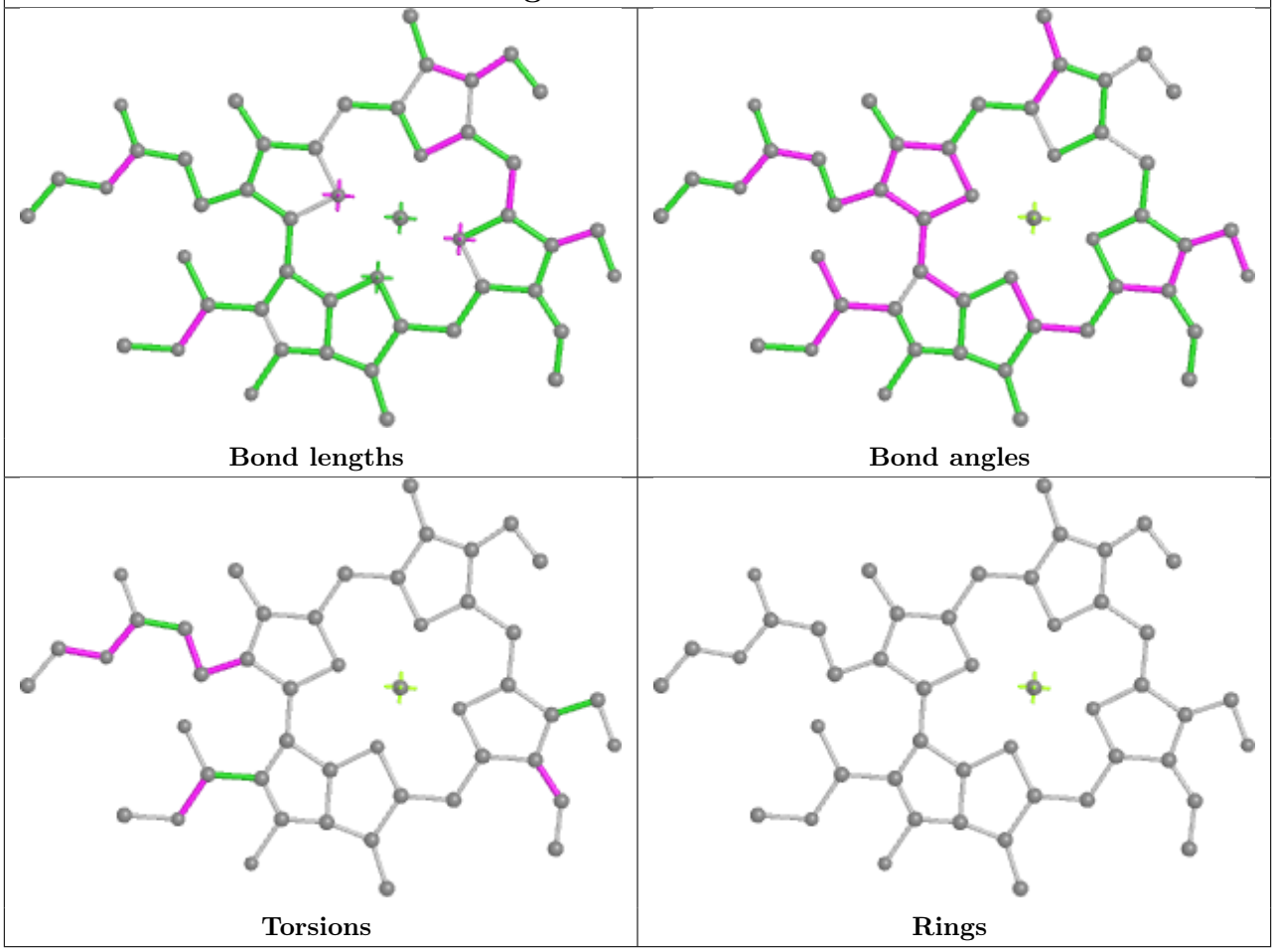


Rings

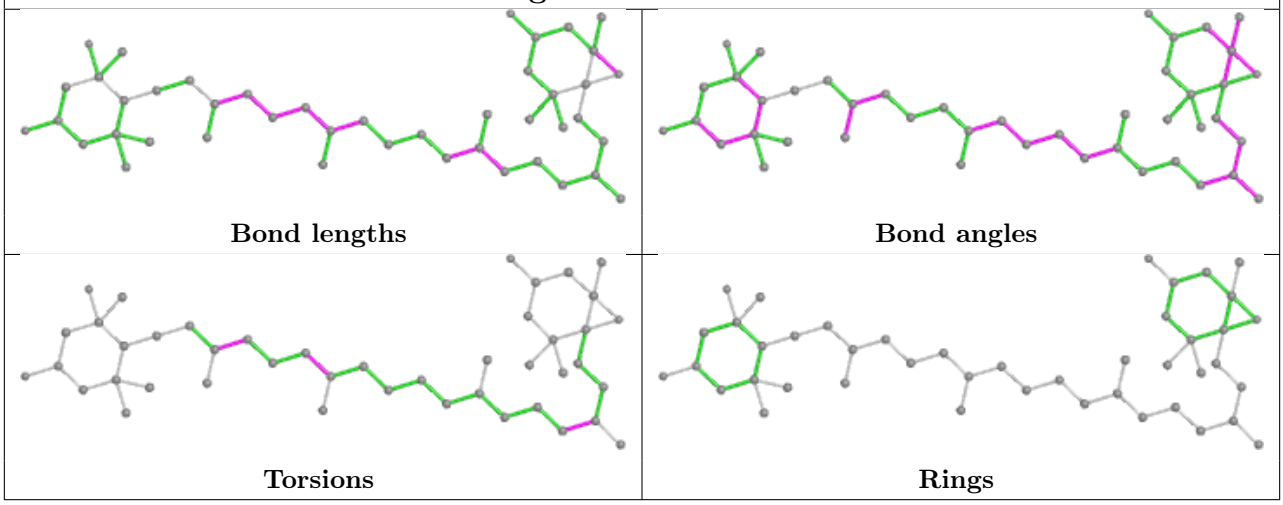
Ligand CHL S 307



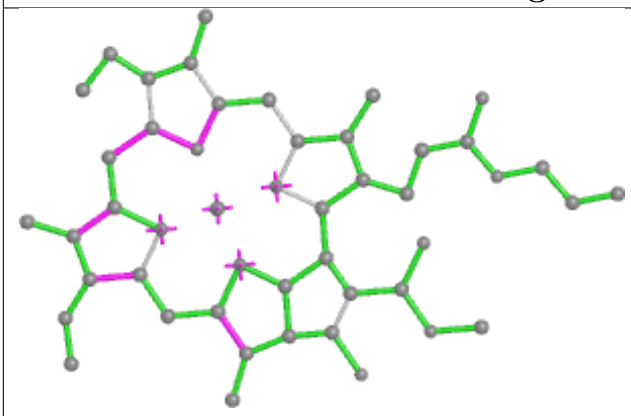
Ligand CHL n 605



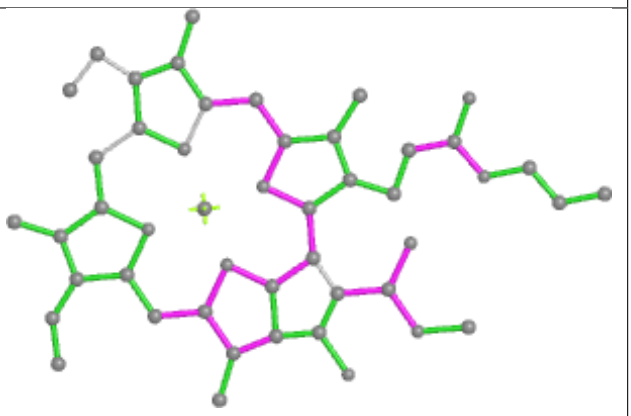
Ligand NEX s 317



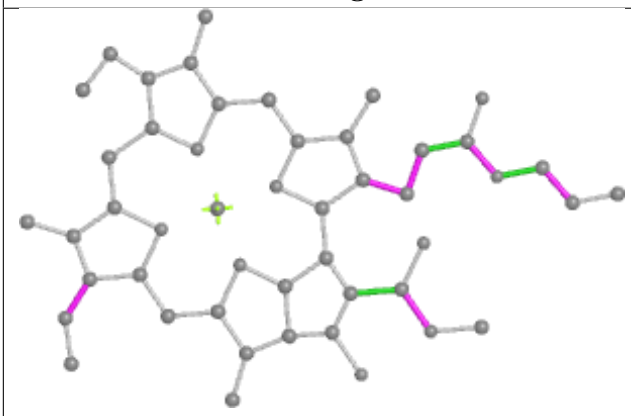
Ligand CLA 6 605



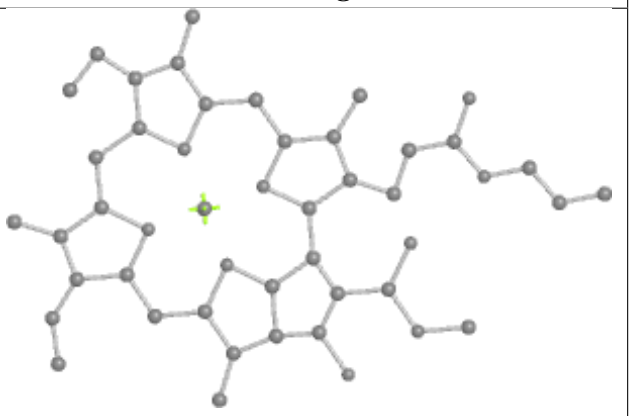
Bond lengths



Bond angles

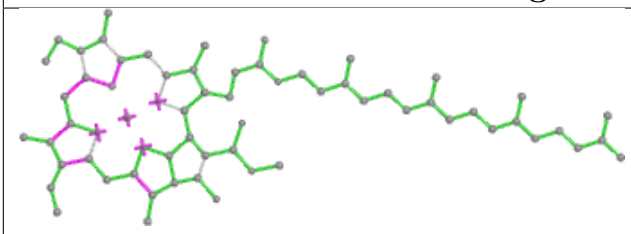


Torsions



Rings

Ligand CLA c 507



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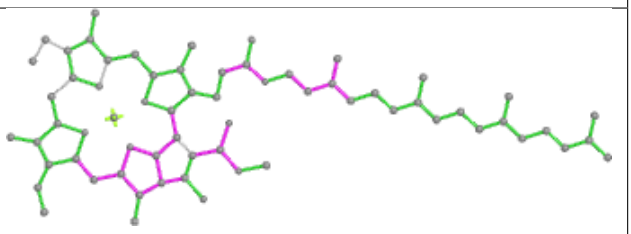
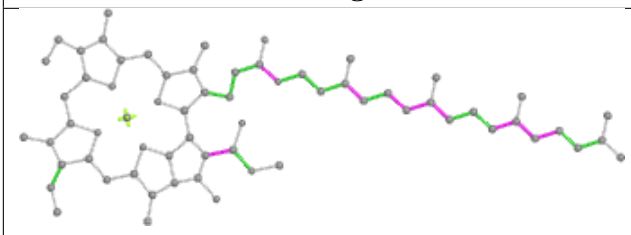
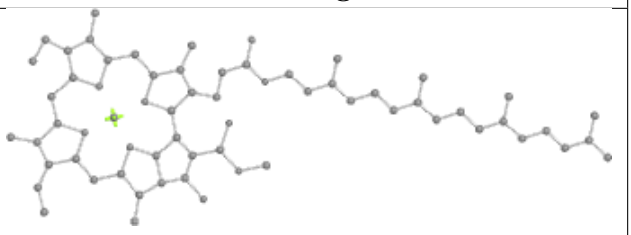


Bond angles

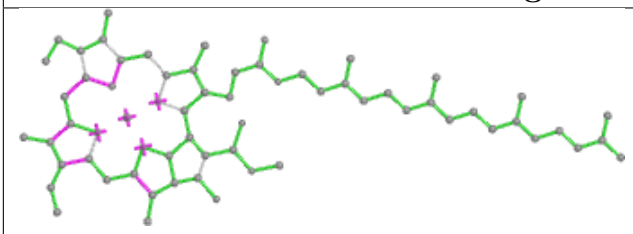


Torsions



Rings

Ligand CLA B 601



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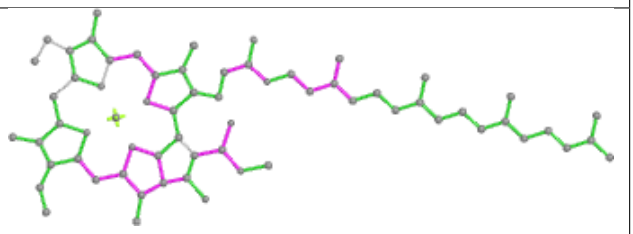
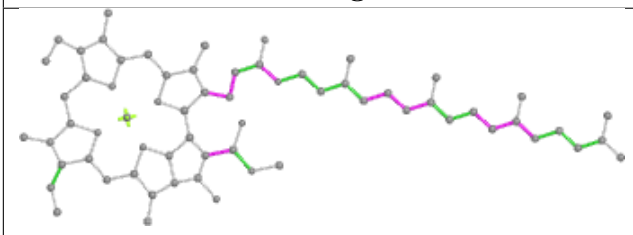


Bond angles



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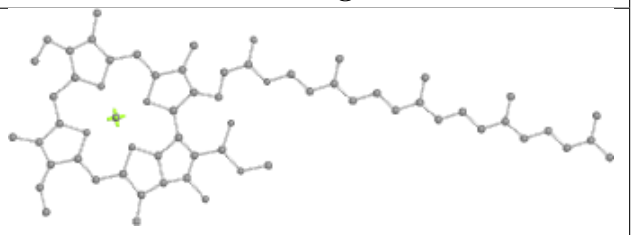
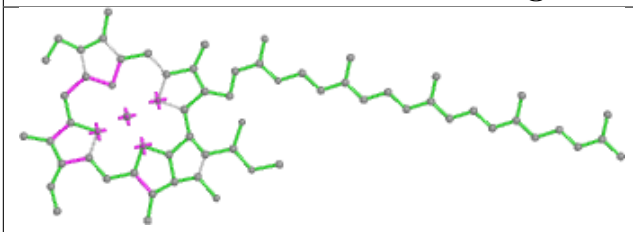
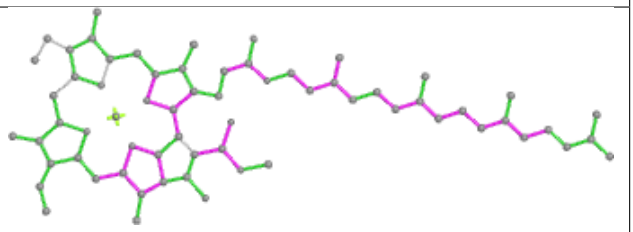


Rings

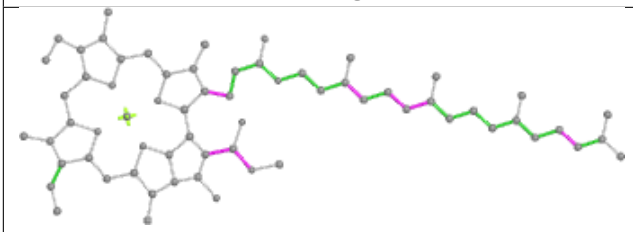
Ligand CLA b 609



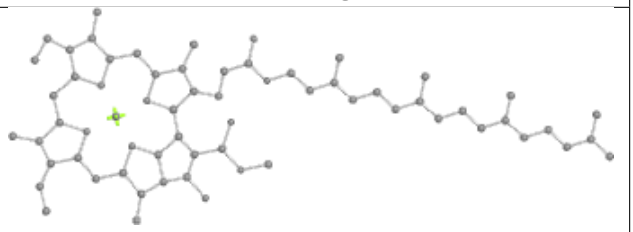
Bond lengths



Bond angles

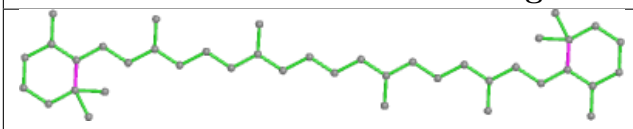


Torsions

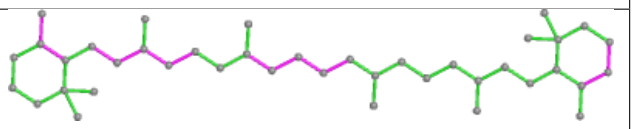


Rings

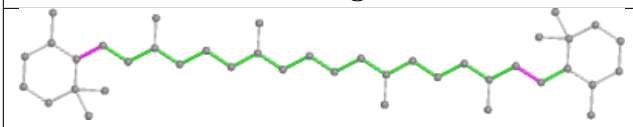
Ligand BCR b 617



Bond lengths



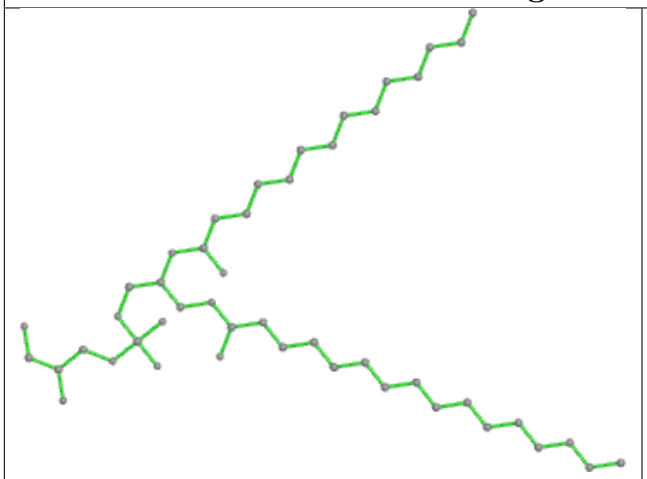
Bond angles



Torsions

Rings

Ligand LHG 2 606



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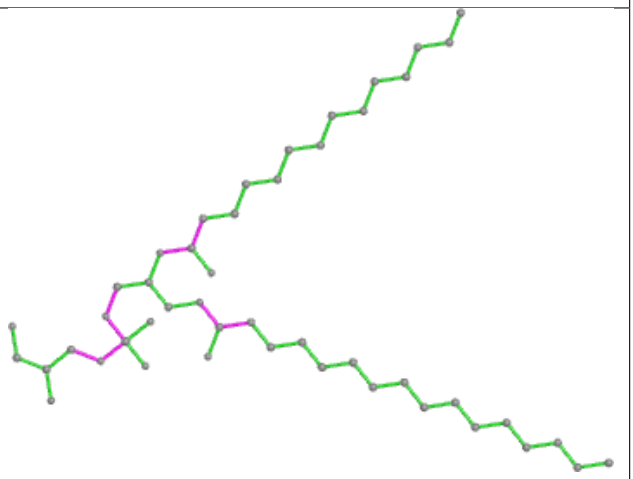
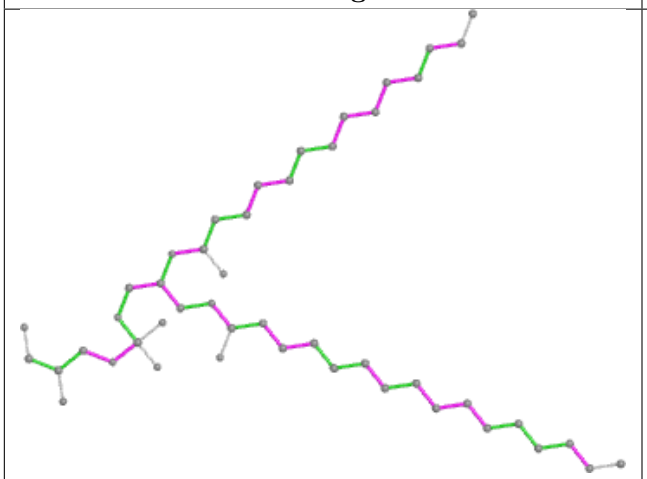
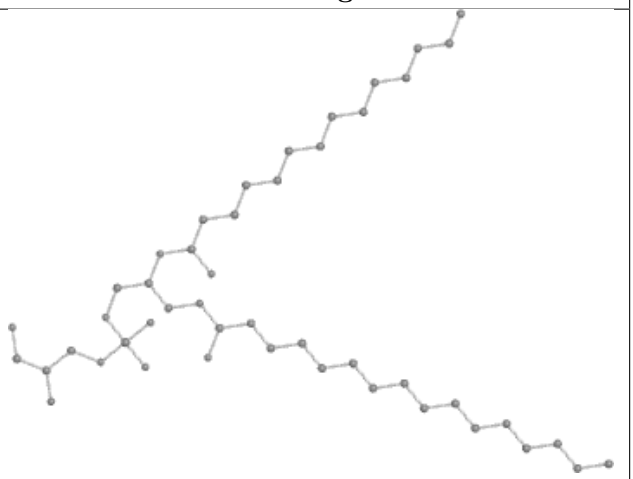


Bond angles

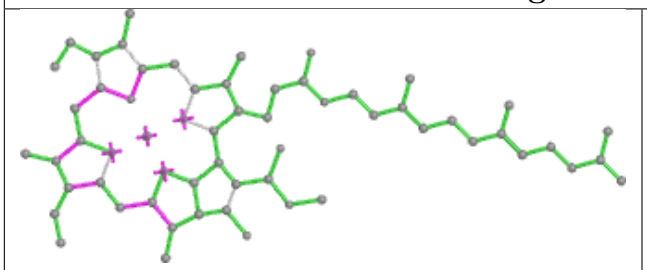


Torsions



Rings

Ligand CLA n 611



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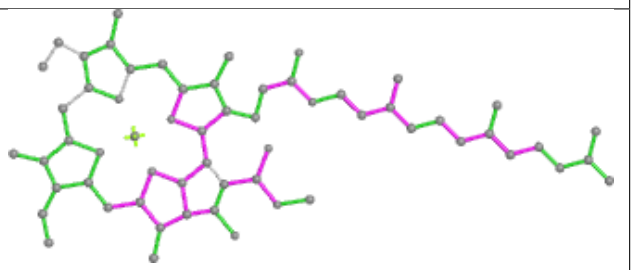
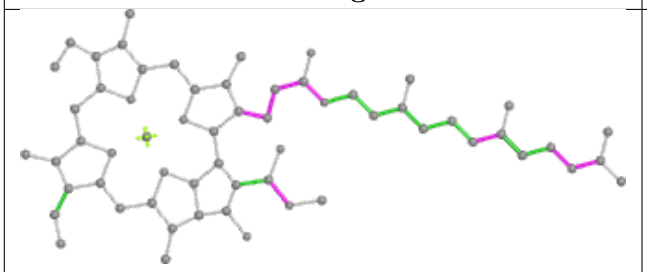
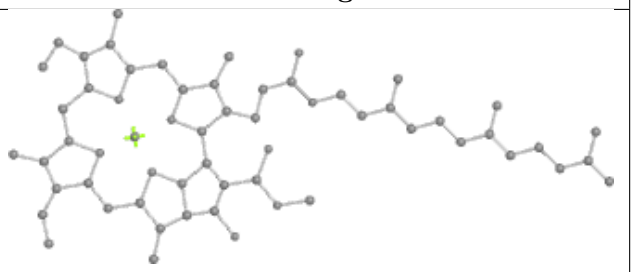


Bond angles

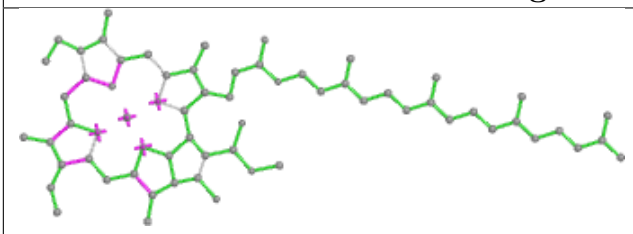


Torsions



Rings

Ligand CLA c 511



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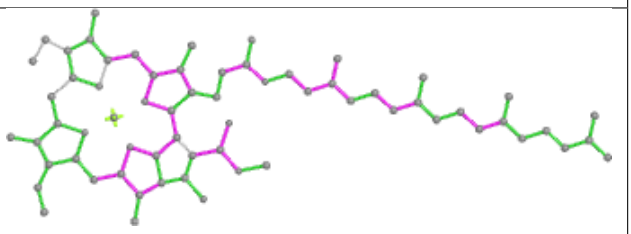
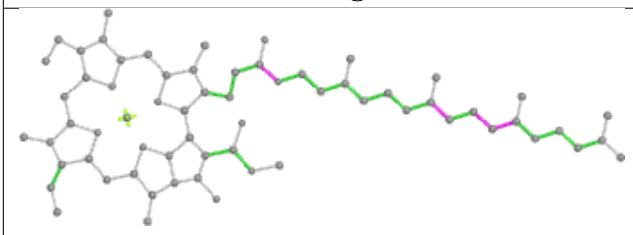
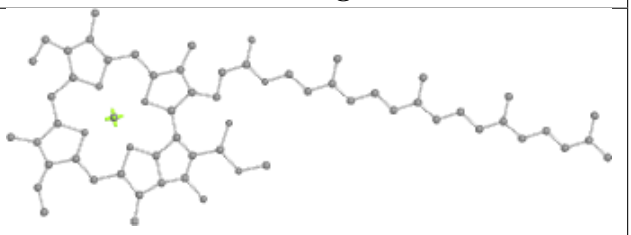


Bond angles

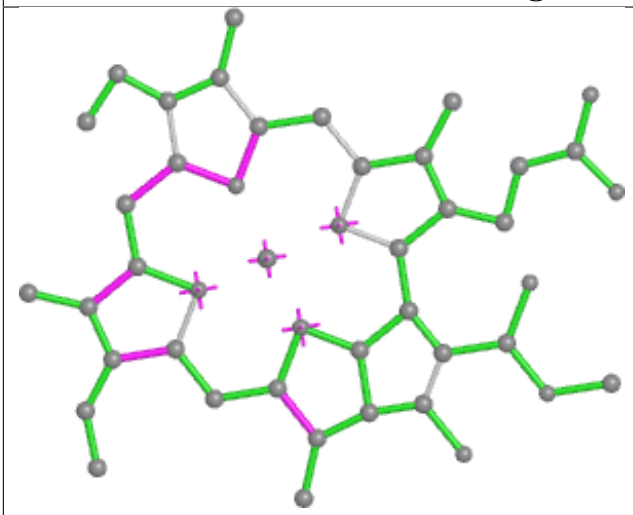


Torsions

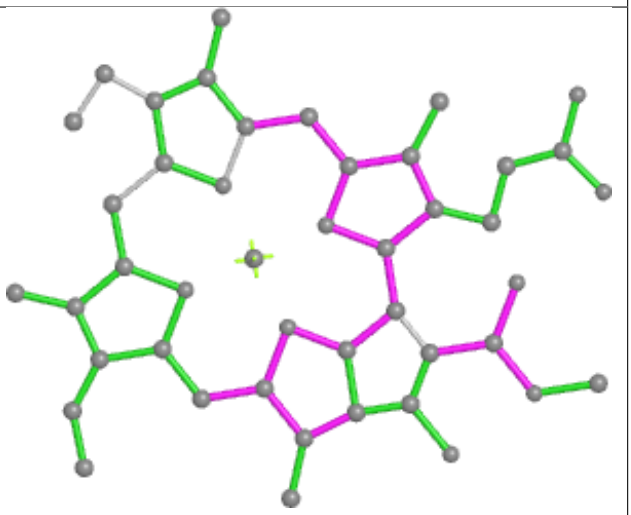


Rings

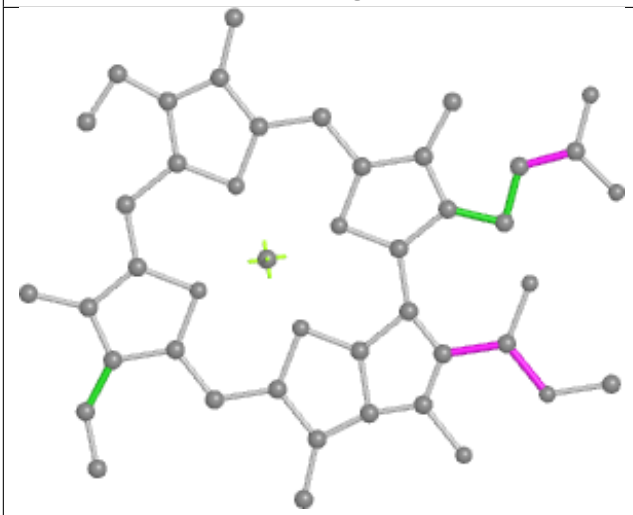
Ligand CLA S 309



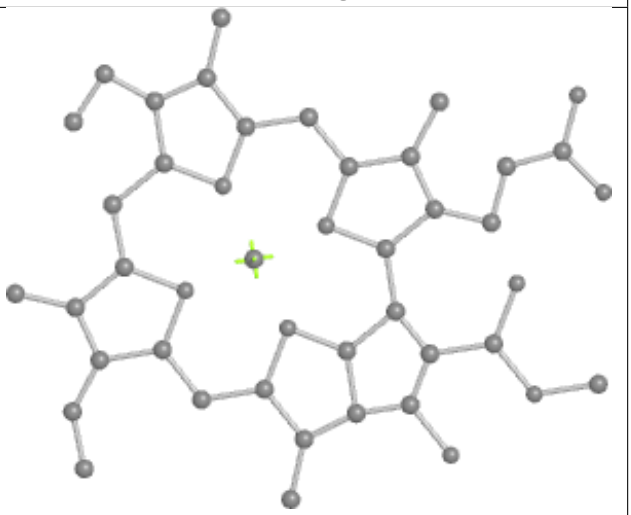
Bond lengths



Bond angles

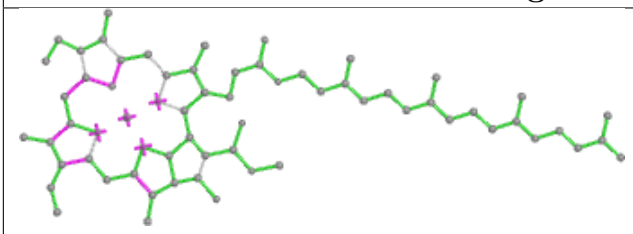


Torsions

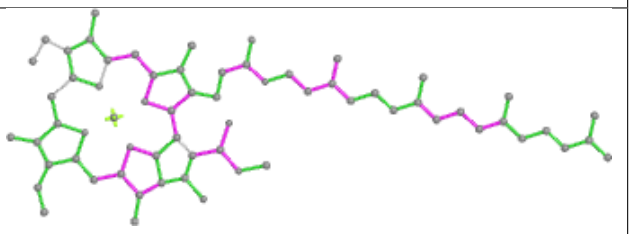


Rings

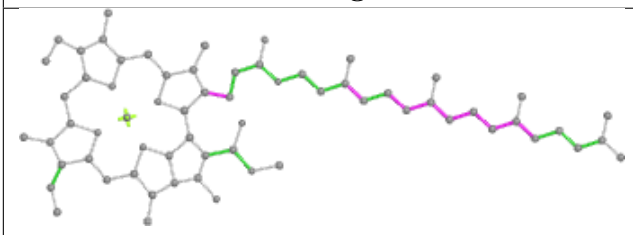
Ligand CLA b 602



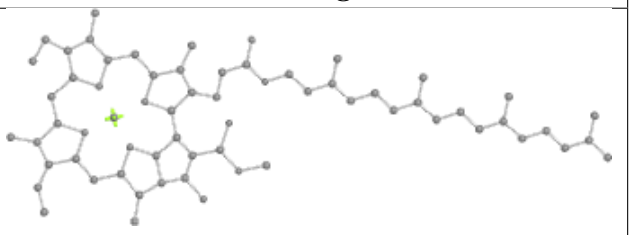
Bond lengths



Bond angles

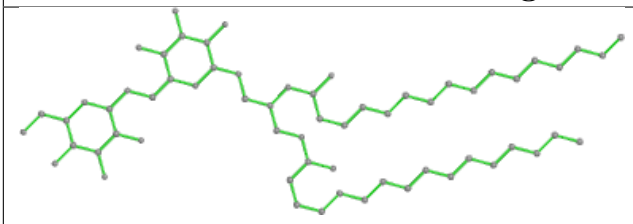


Torsions



Rings

Ligand DGD B 626



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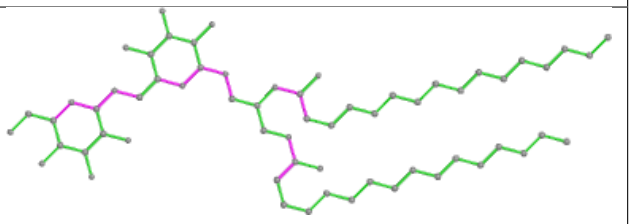

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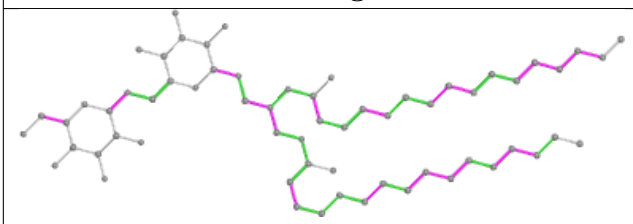

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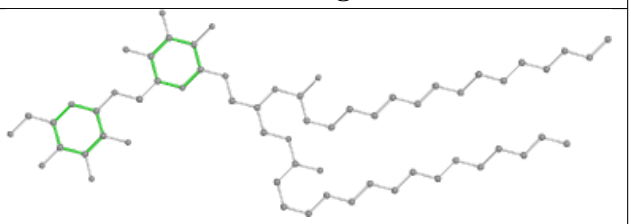
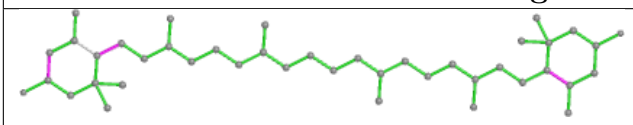


Rings

Ligand LUT s 315



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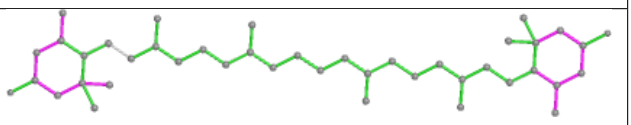
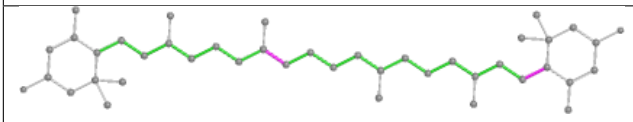


Bond angles



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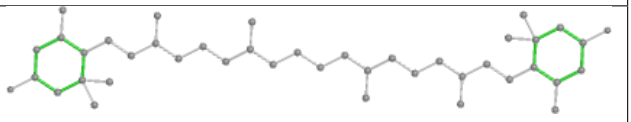
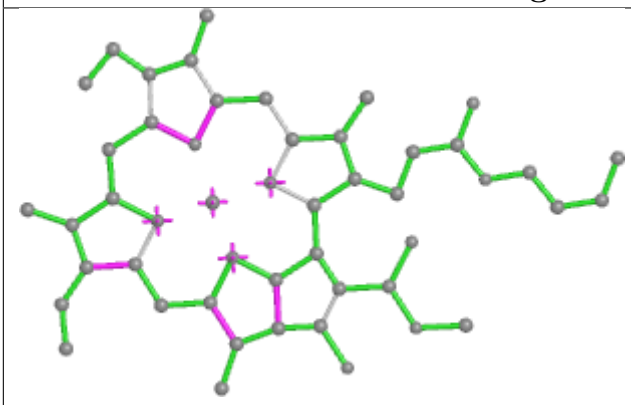


Rings

Ligand CLA r 610



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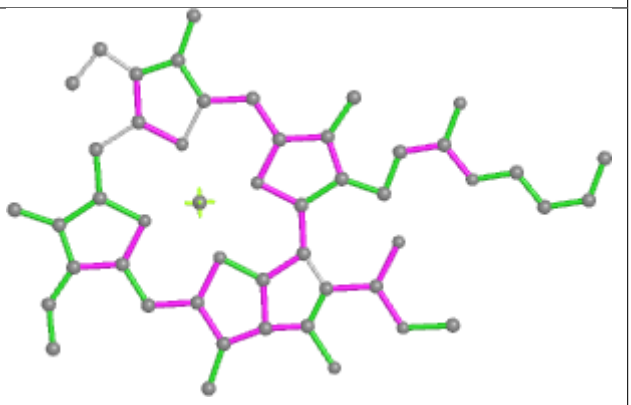

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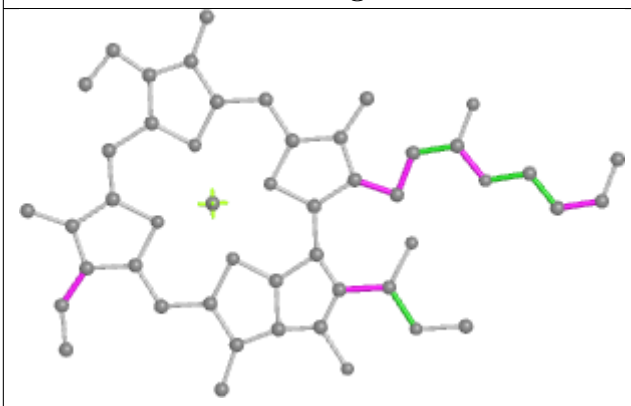

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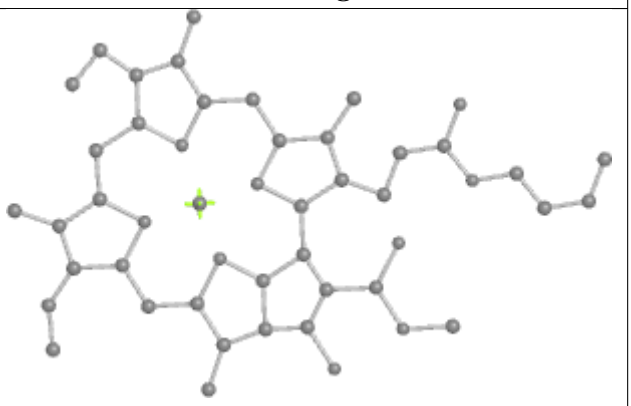
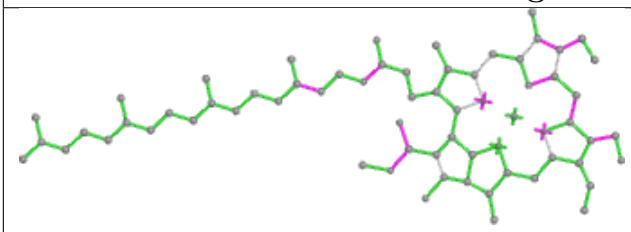


Rings

Ligand CHL y 302



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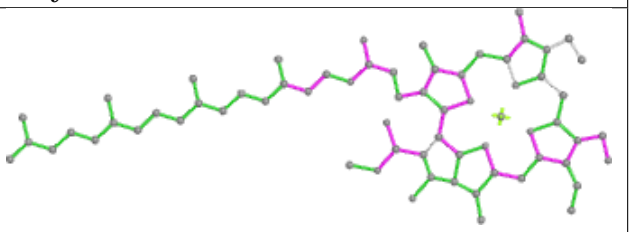

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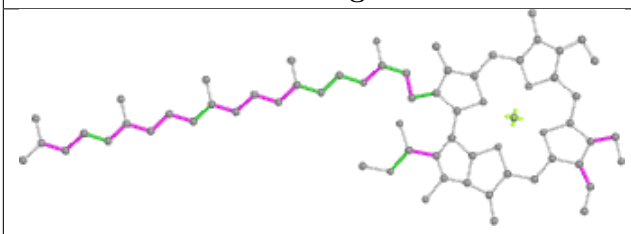

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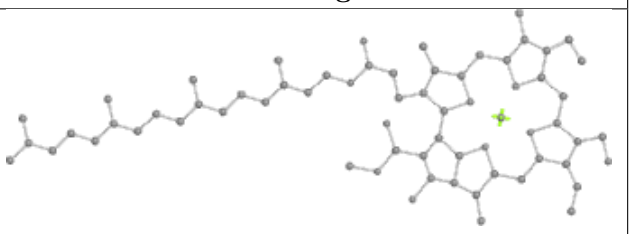
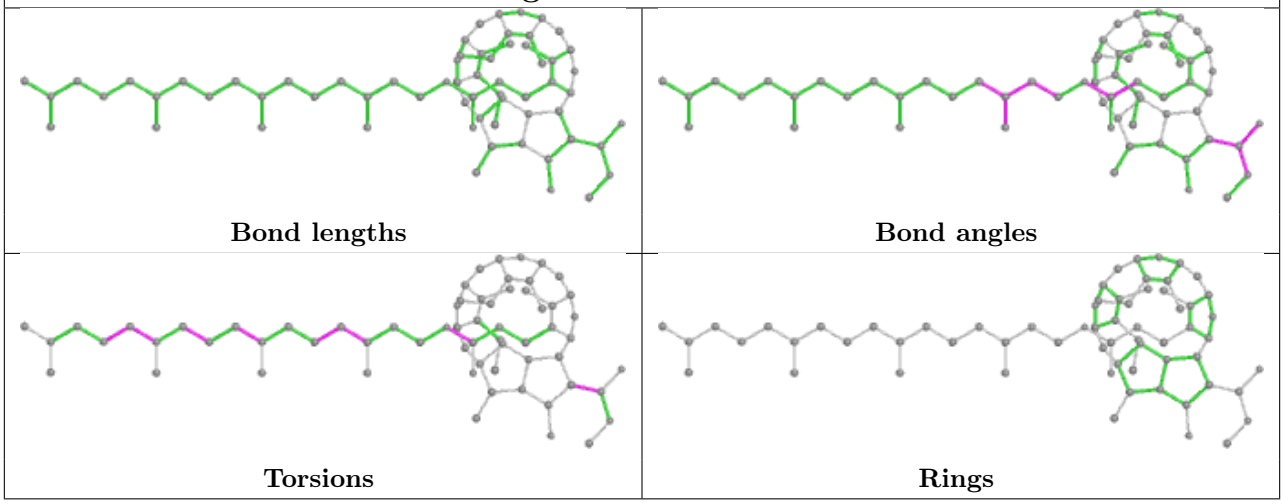
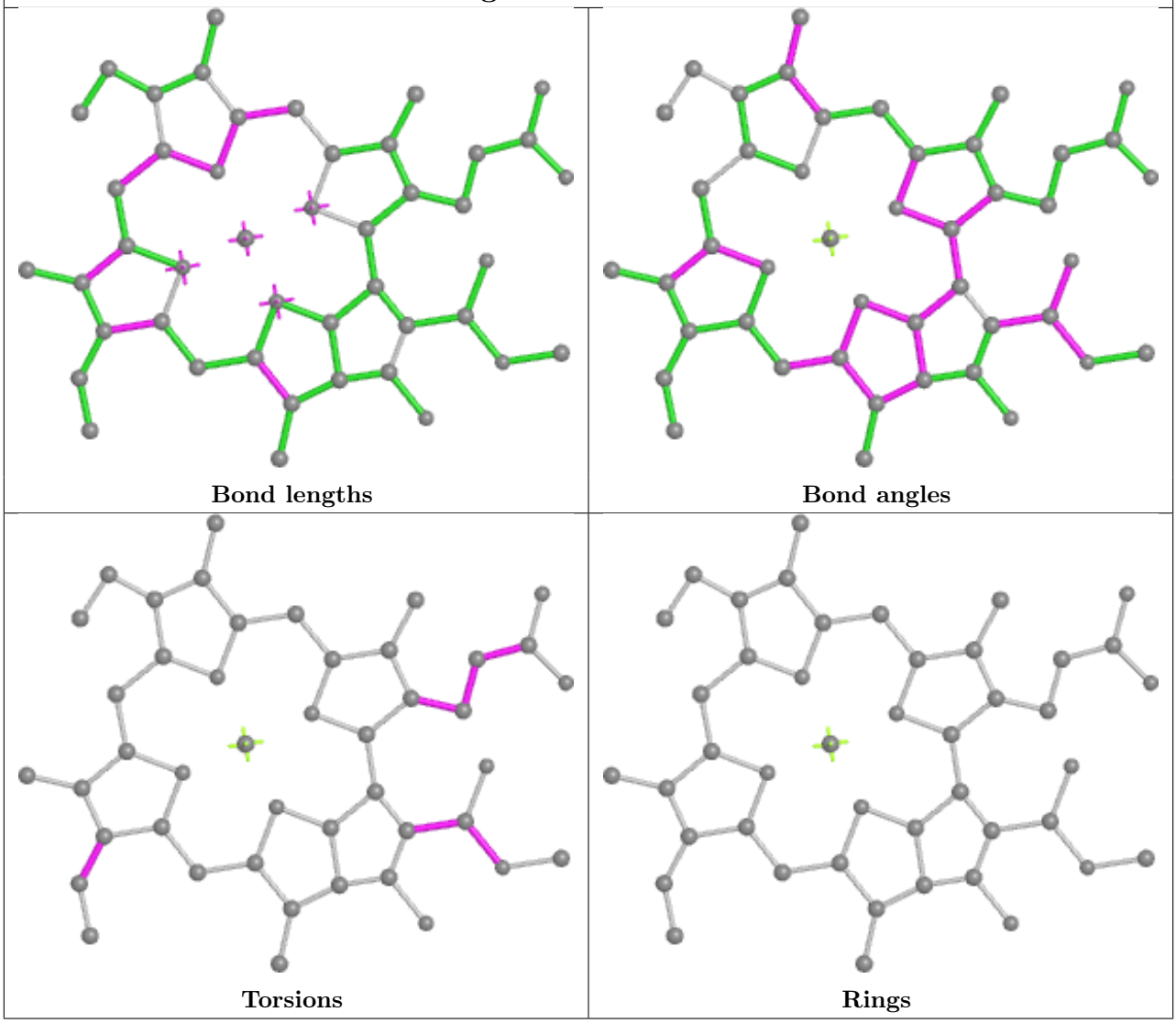


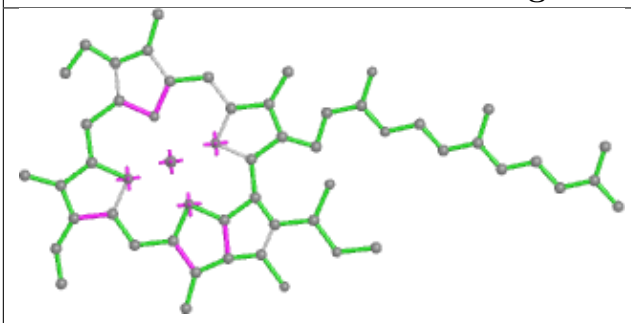
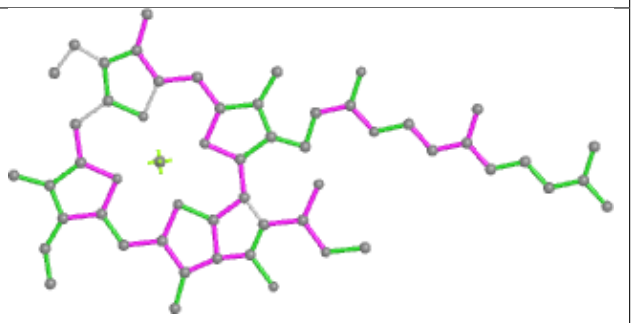
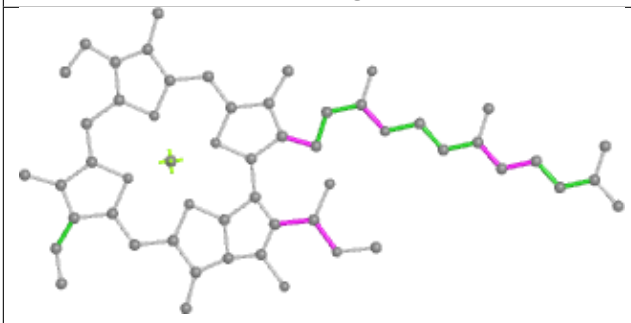
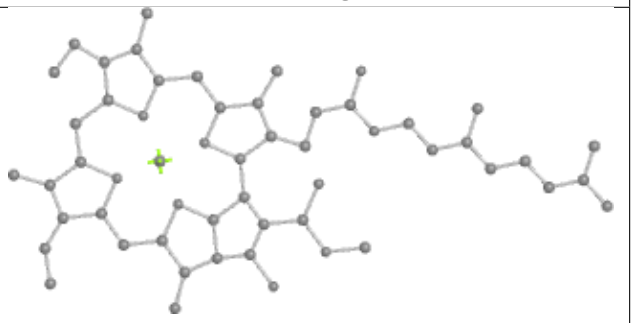
Rings

Ligand PHO A 403



Ligand CLA Y 315



Ligand CLA 6 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

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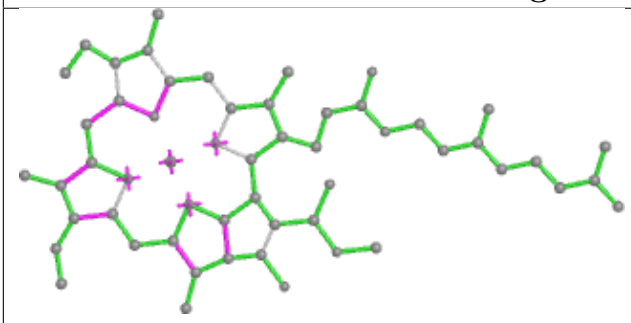
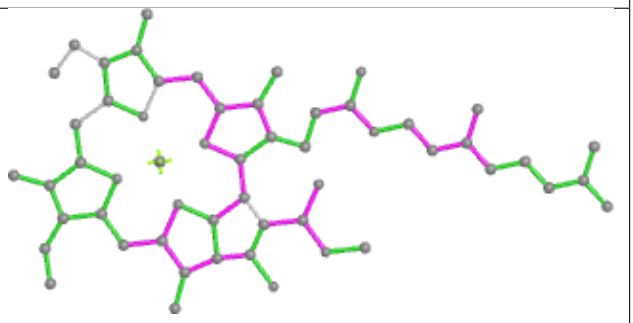
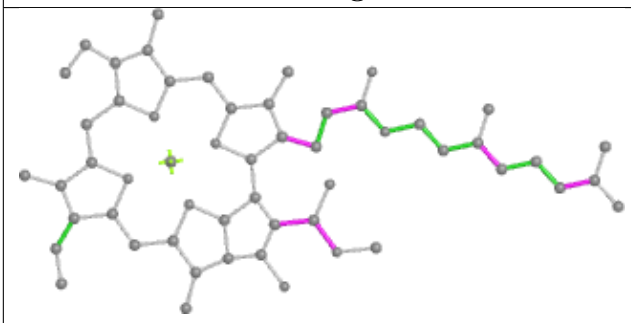
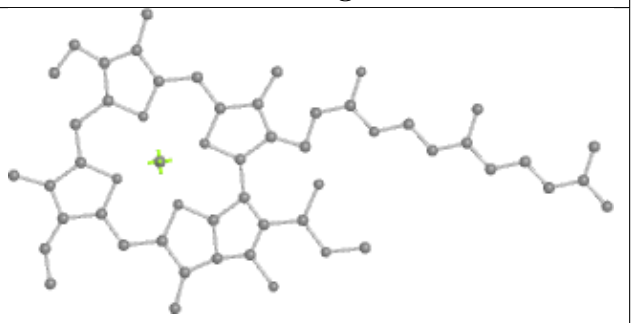
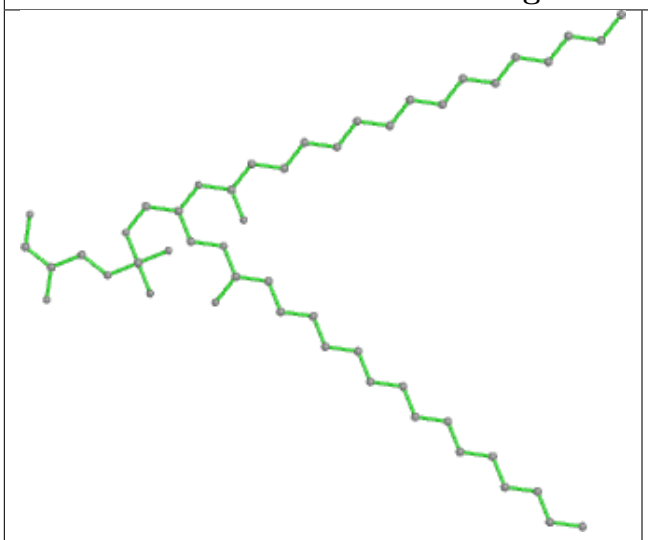
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG D 406



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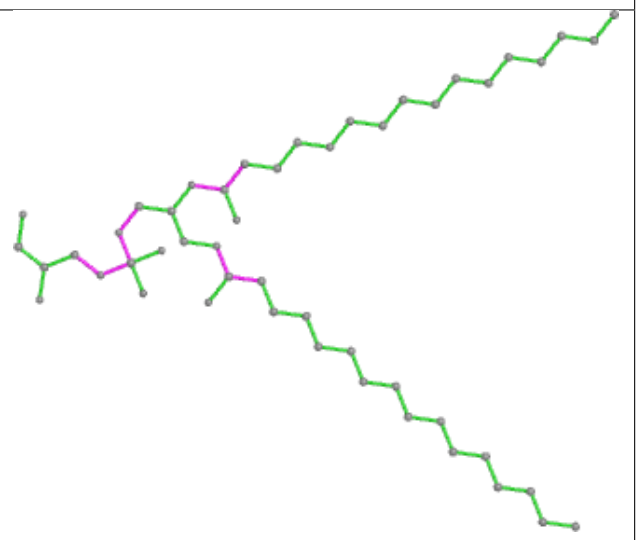
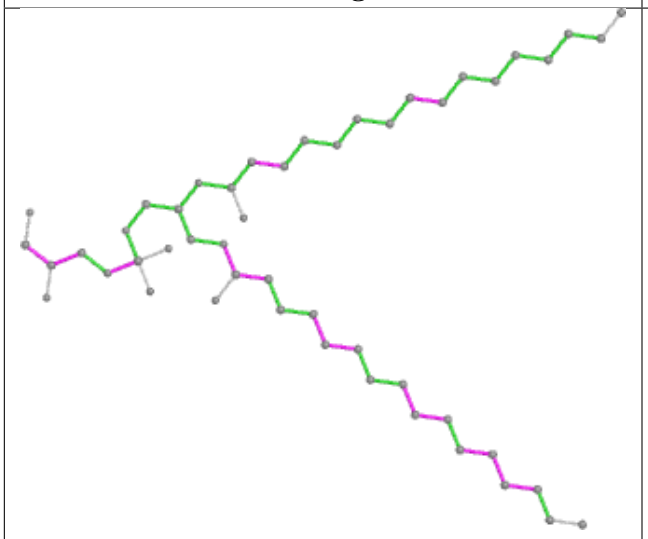


Bond angles



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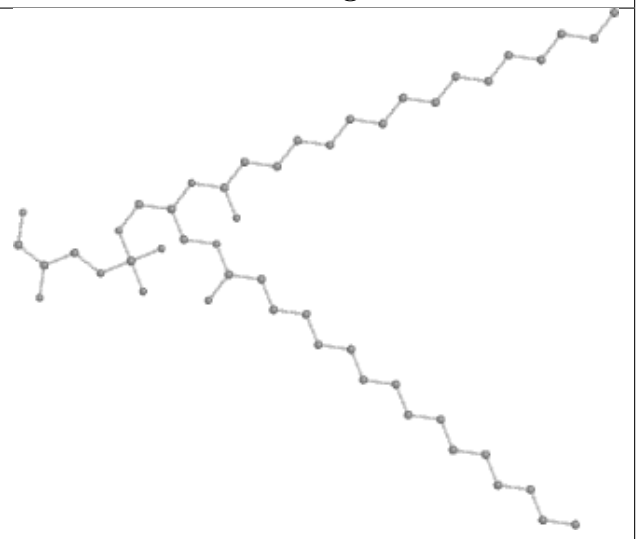
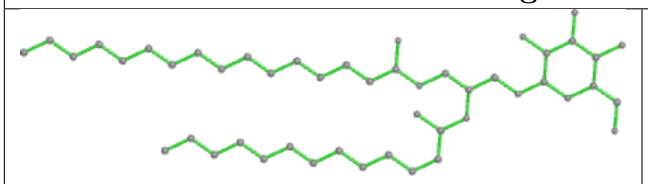


Rings

Ligand LMG A 408



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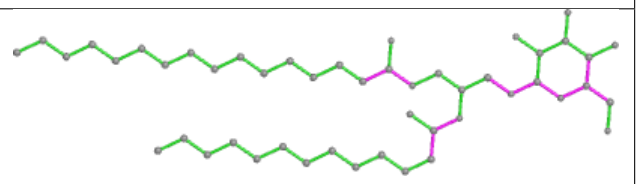

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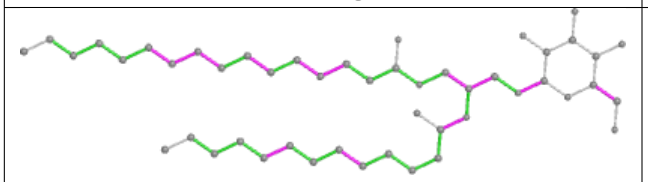

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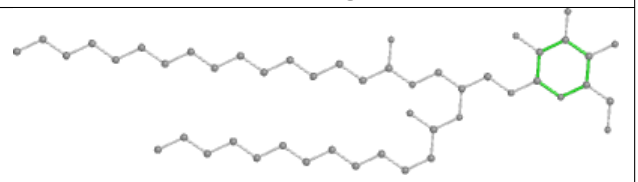
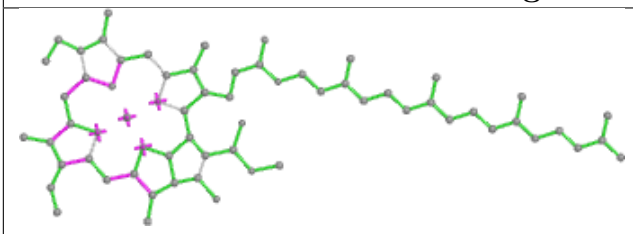


Rings

Ligand CLA G 613



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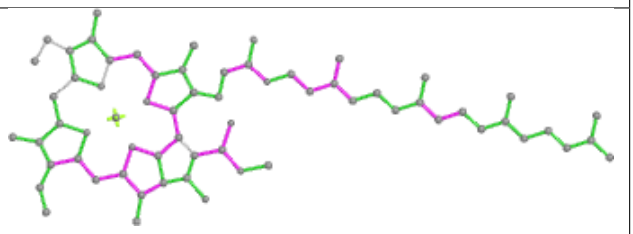
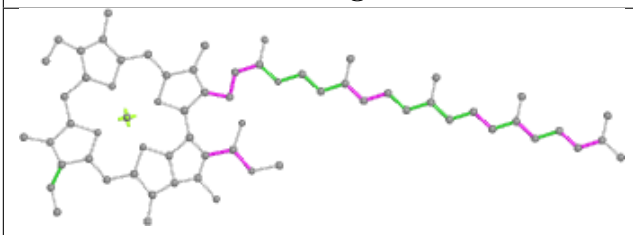


Bond angles



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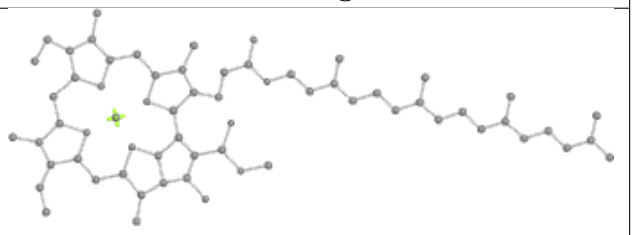
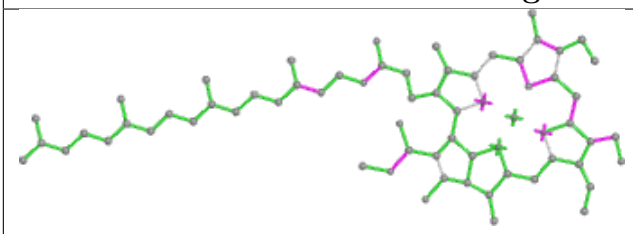


Rings

Ligand CHL N 608



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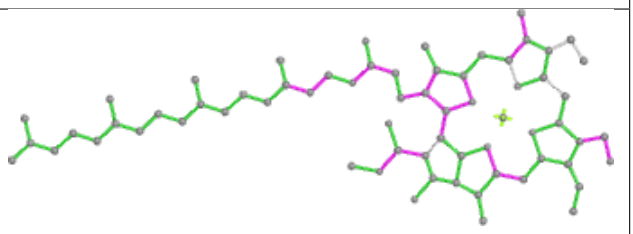
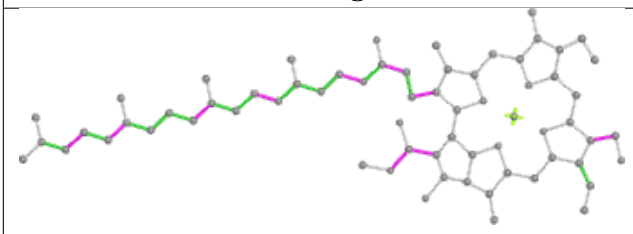


Bond angles



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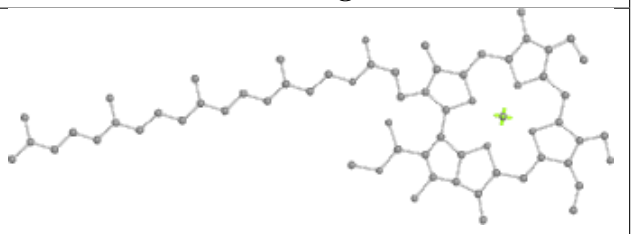
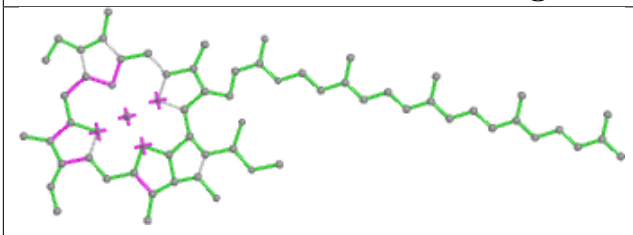


Rings

Ligand CLA c 506



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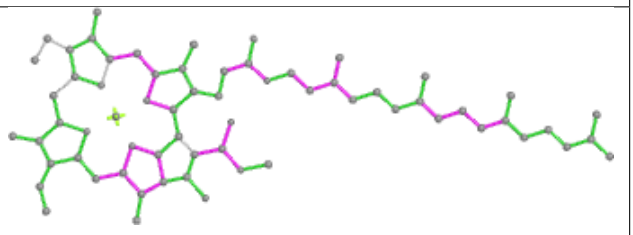
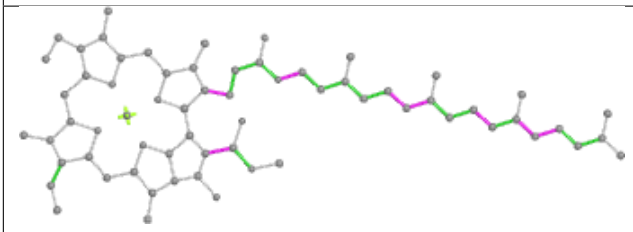


Bond angles



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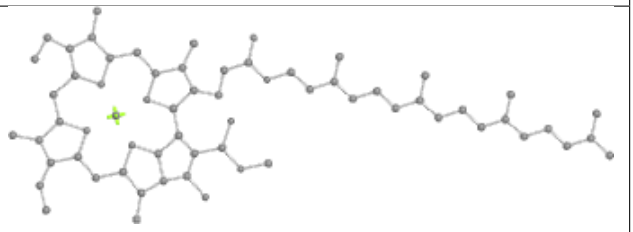
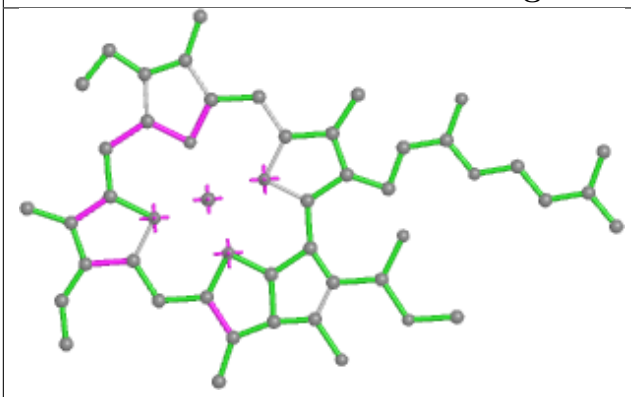


Rings

Ligand CLA Y 305



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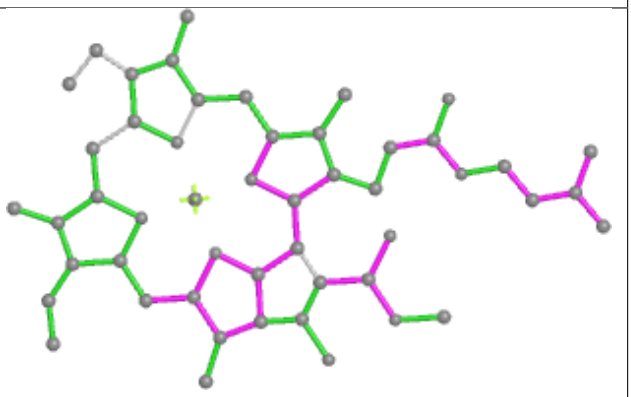
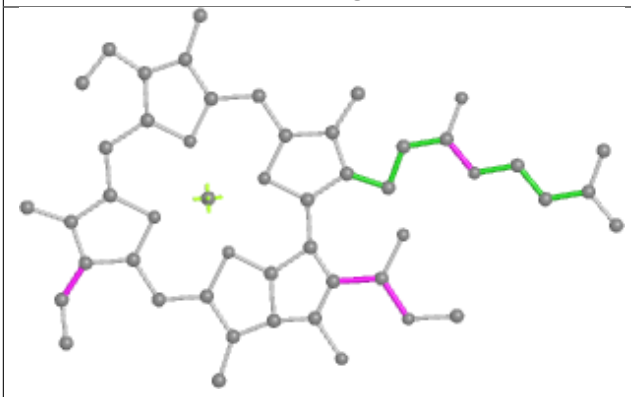
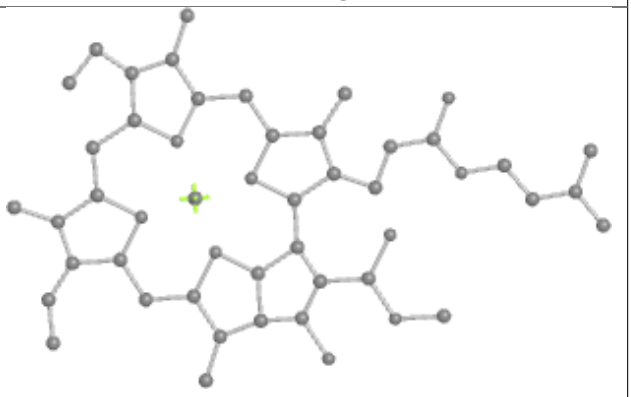


Bond angles

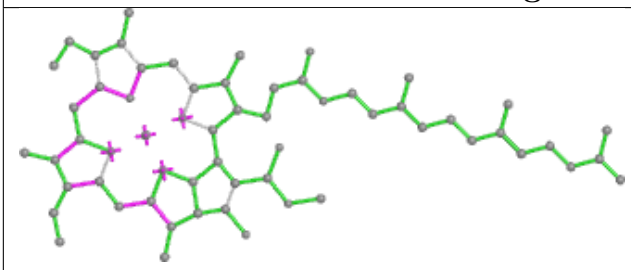


Torsions

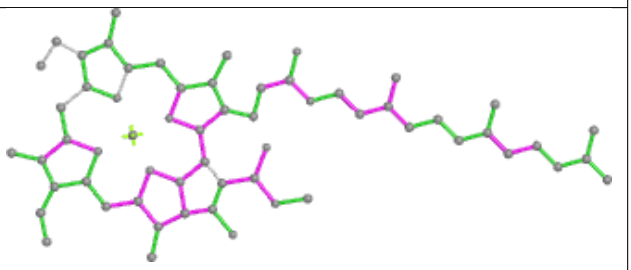


Rings

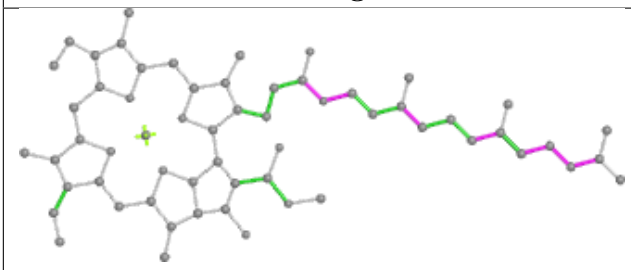
Ligand CLA Y 312



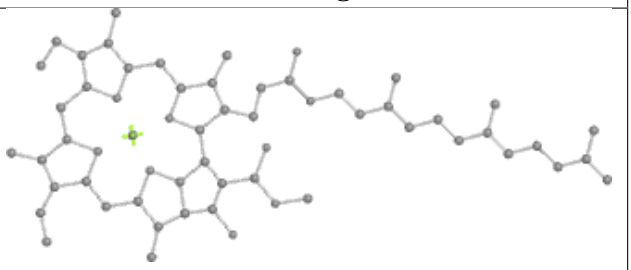
Bond lengths



Bond angles

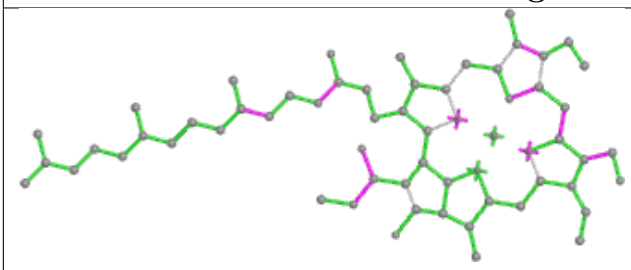


Torsions



Rings

Ligand CHL g 609



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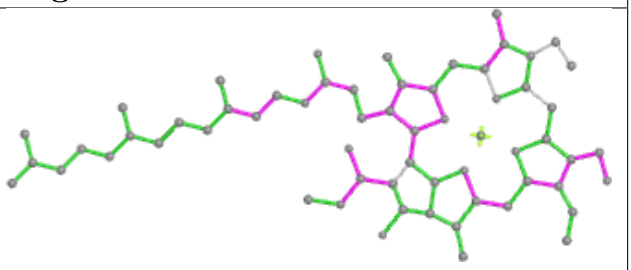
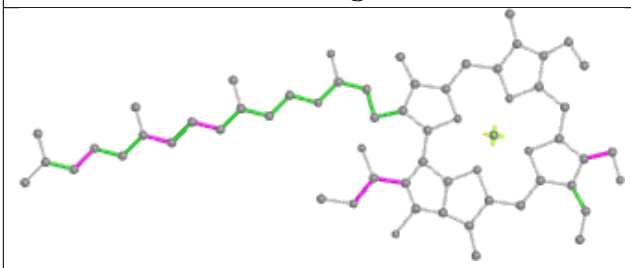


Bond angles



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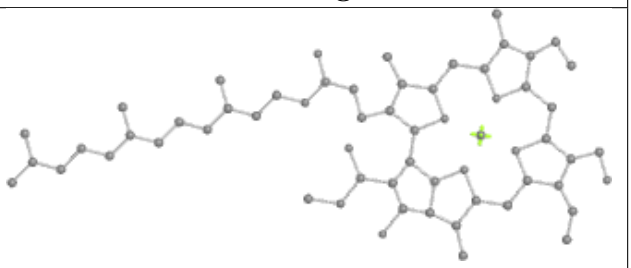
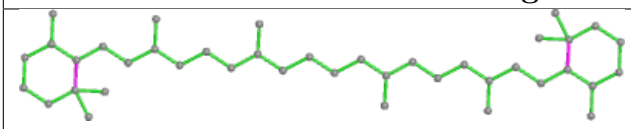


Rings

Ligand BCR H 101



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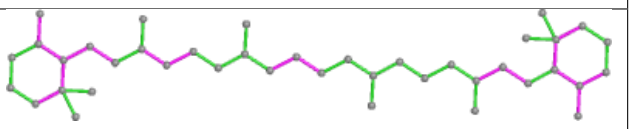
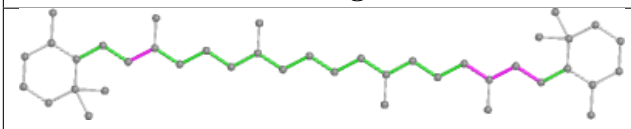


Bond angles



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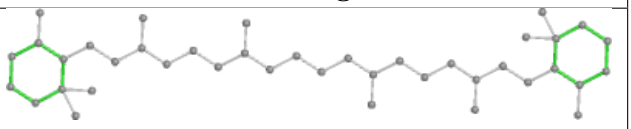
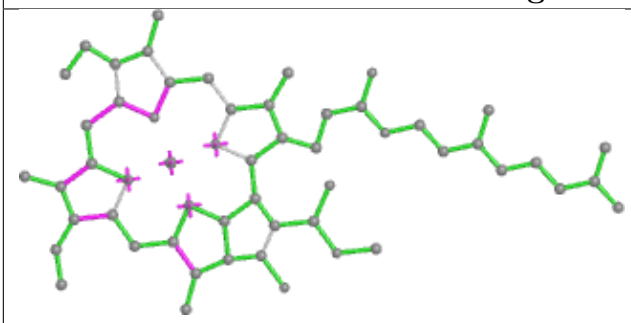


Rings

Ligand CLA S 310



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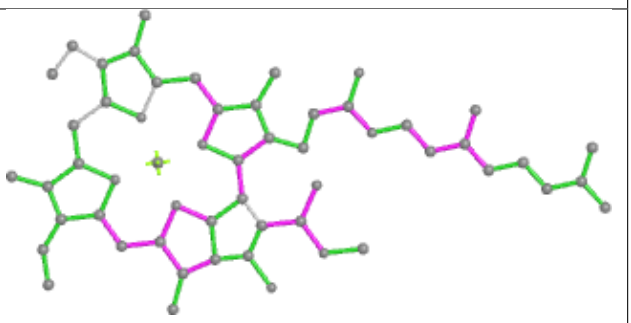

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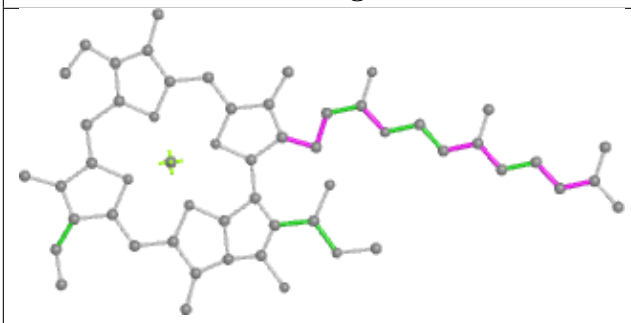

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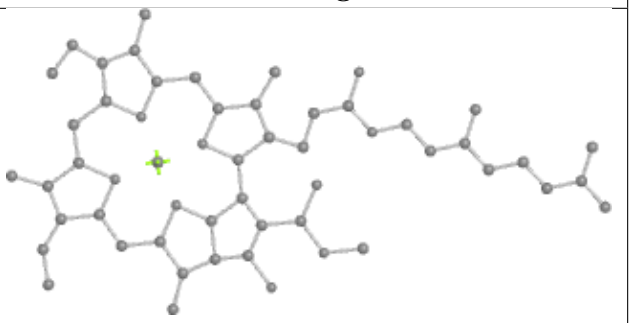
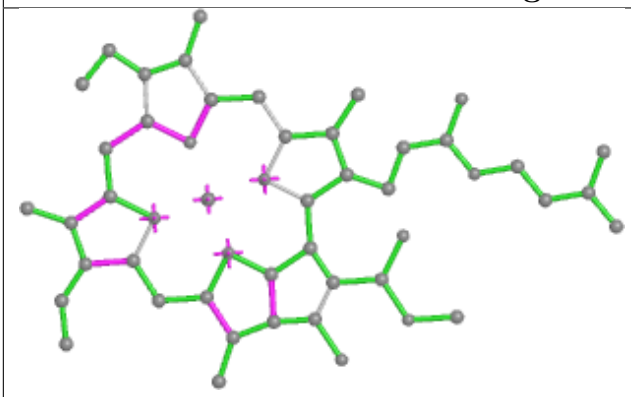
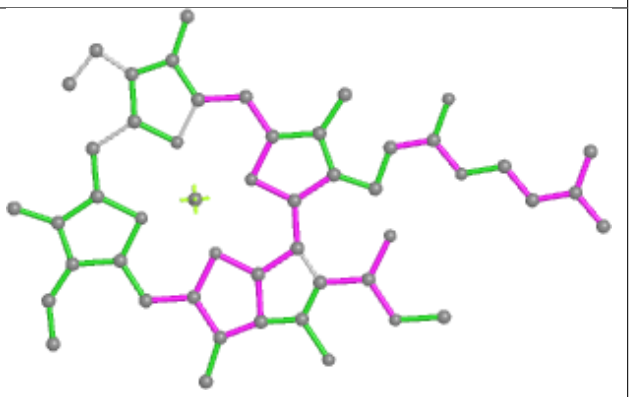
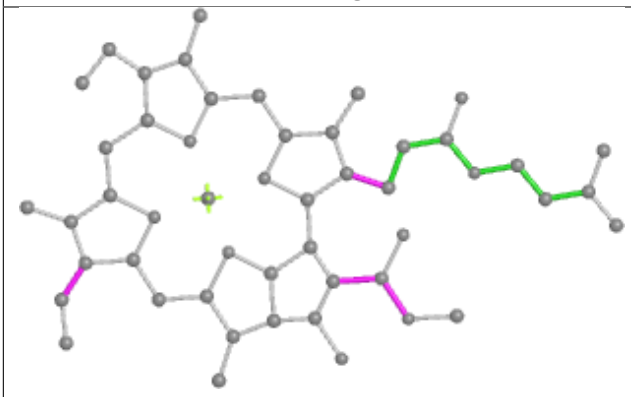
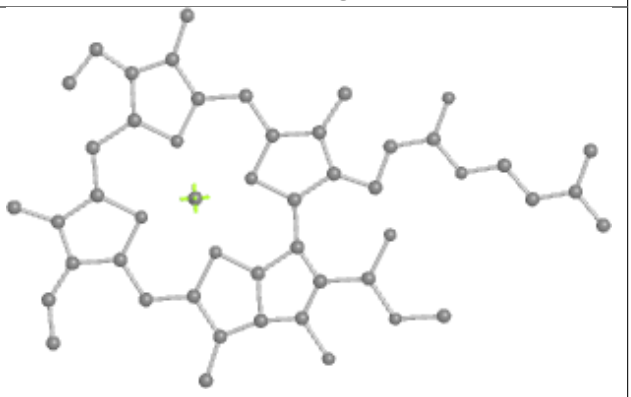


Rings

Ligand CLA N 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

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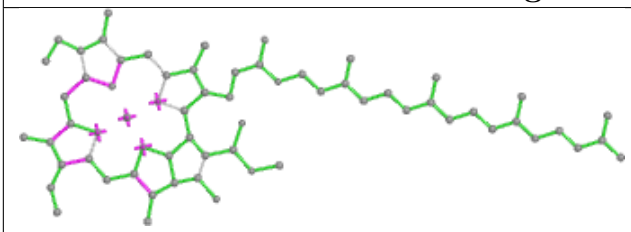
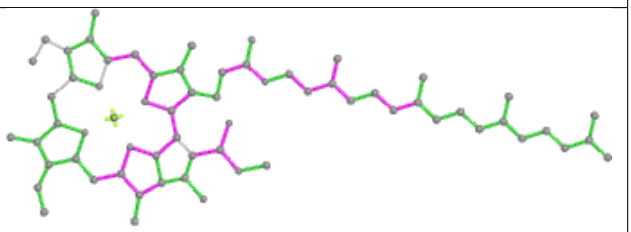
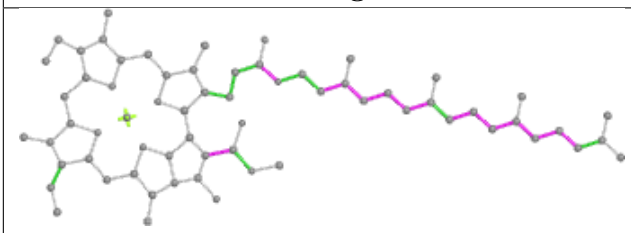
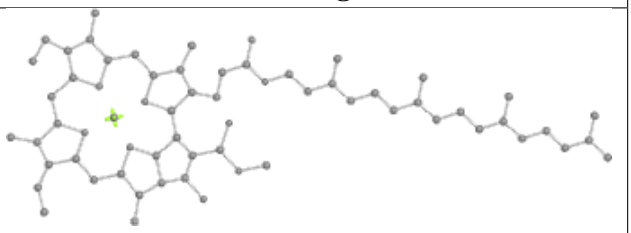
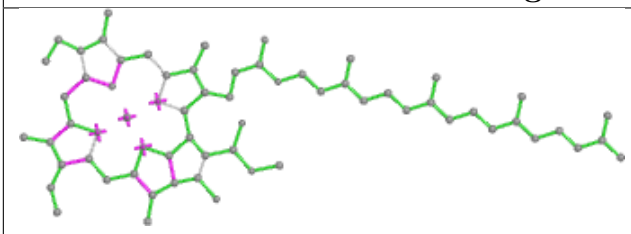
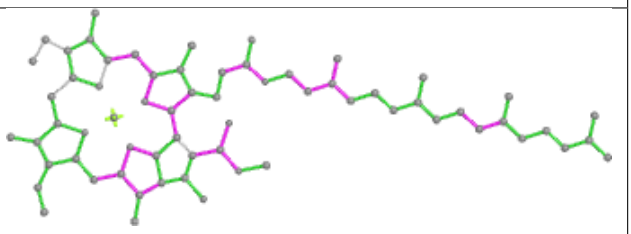
 Bond lengths	 Bond angles
 Torsions	 Rings

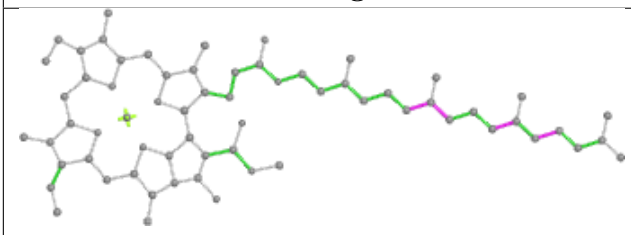
Ligand CLA C 509



Bond lengths



Bond angles



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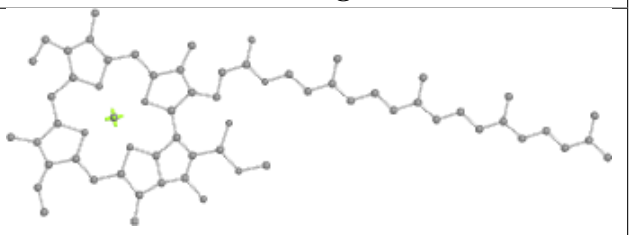
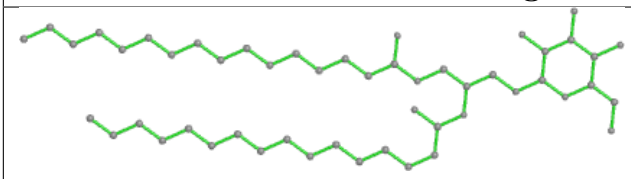


Rings

Ligand LMG b 620



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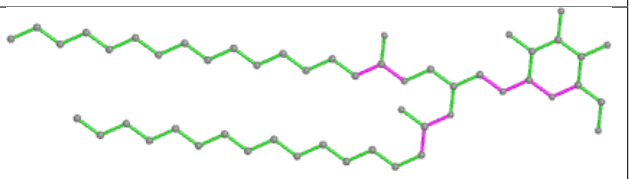
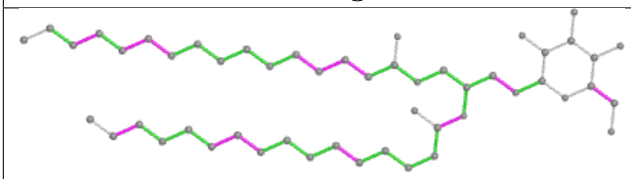


Bond angles



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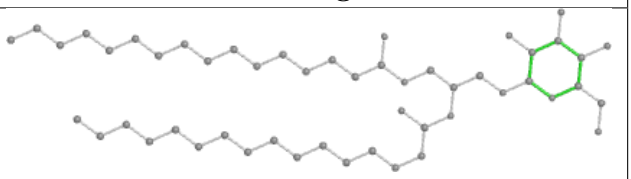
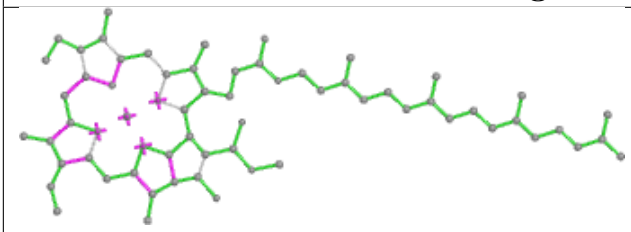
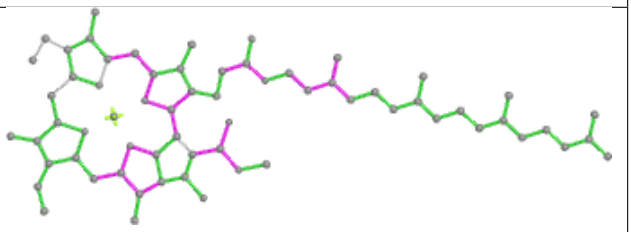


Rings

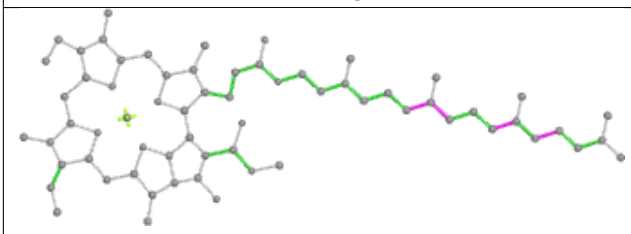
Ligand CLA c 509



Bond lengths



Bond angles



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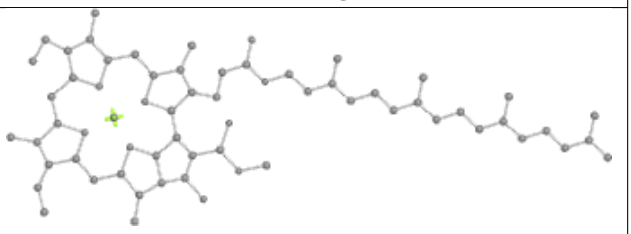
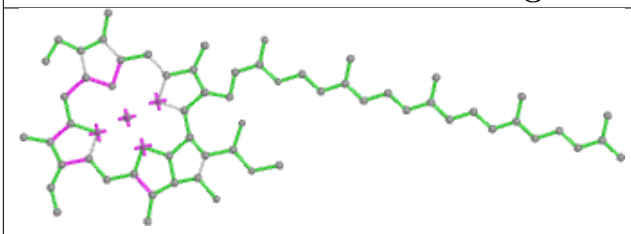
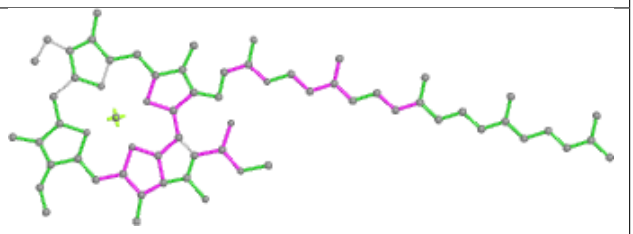
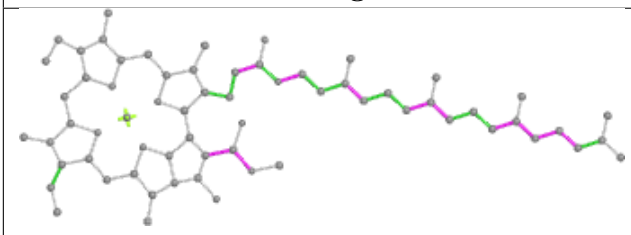
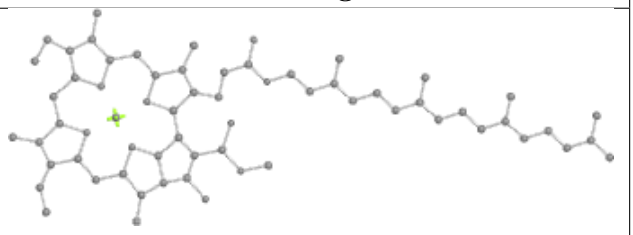
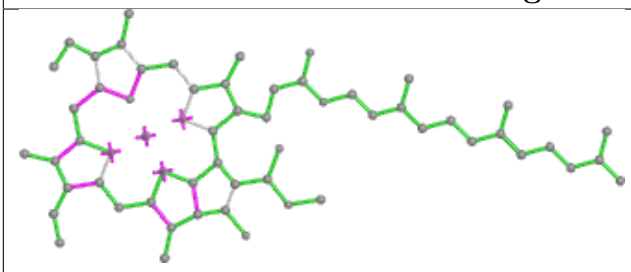
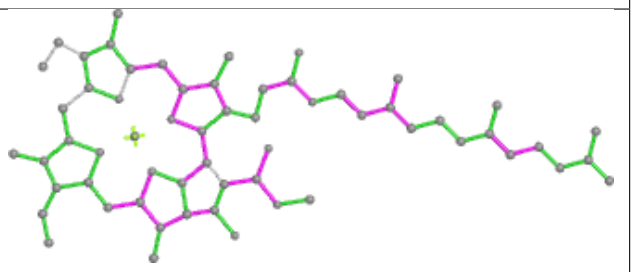
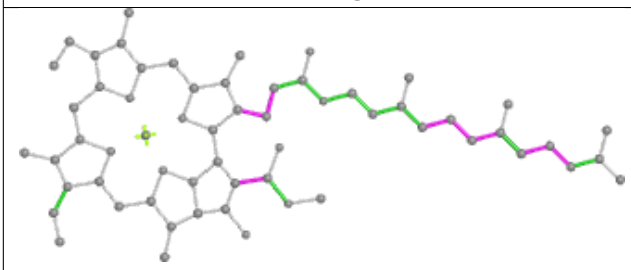
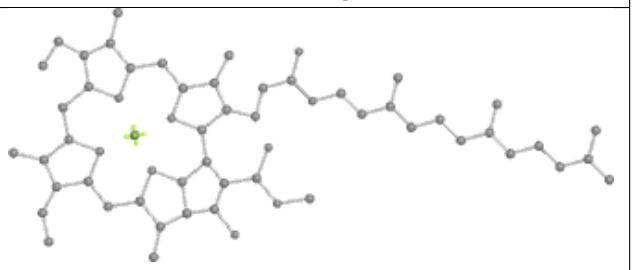
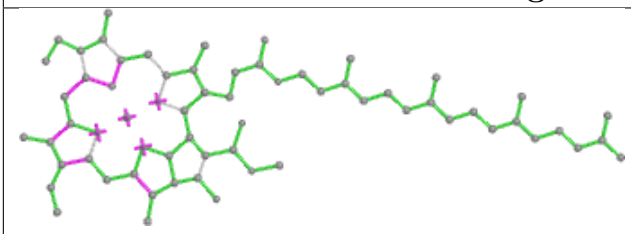
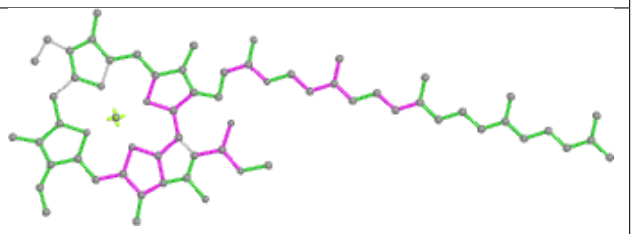
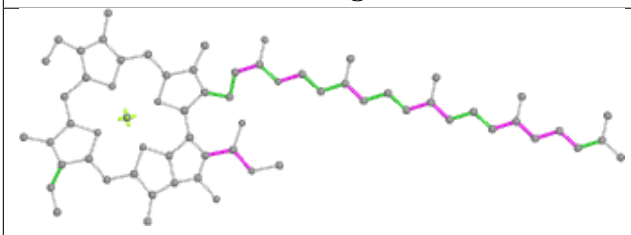
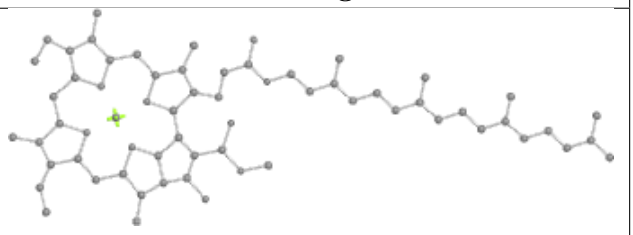
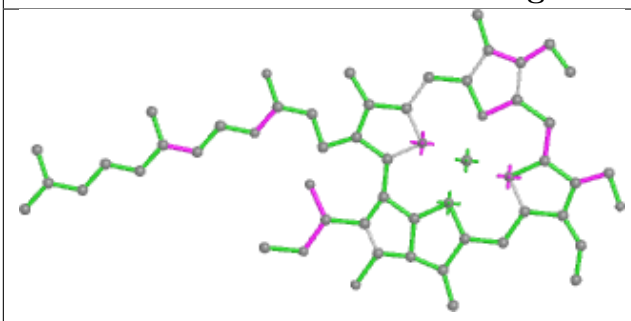
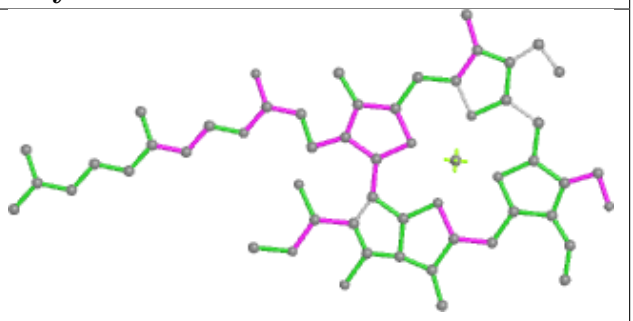
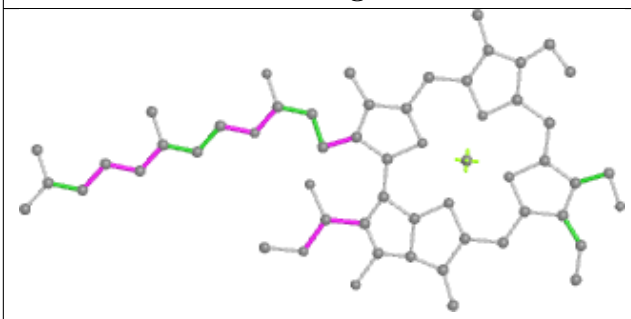
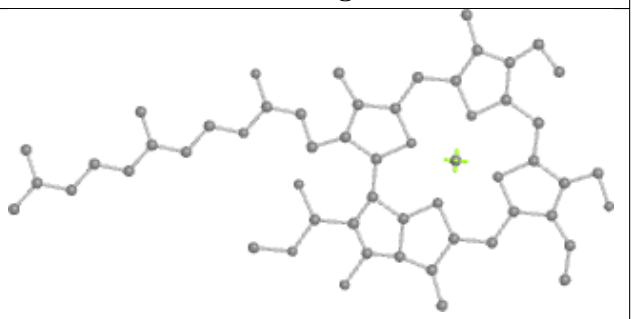


Rings

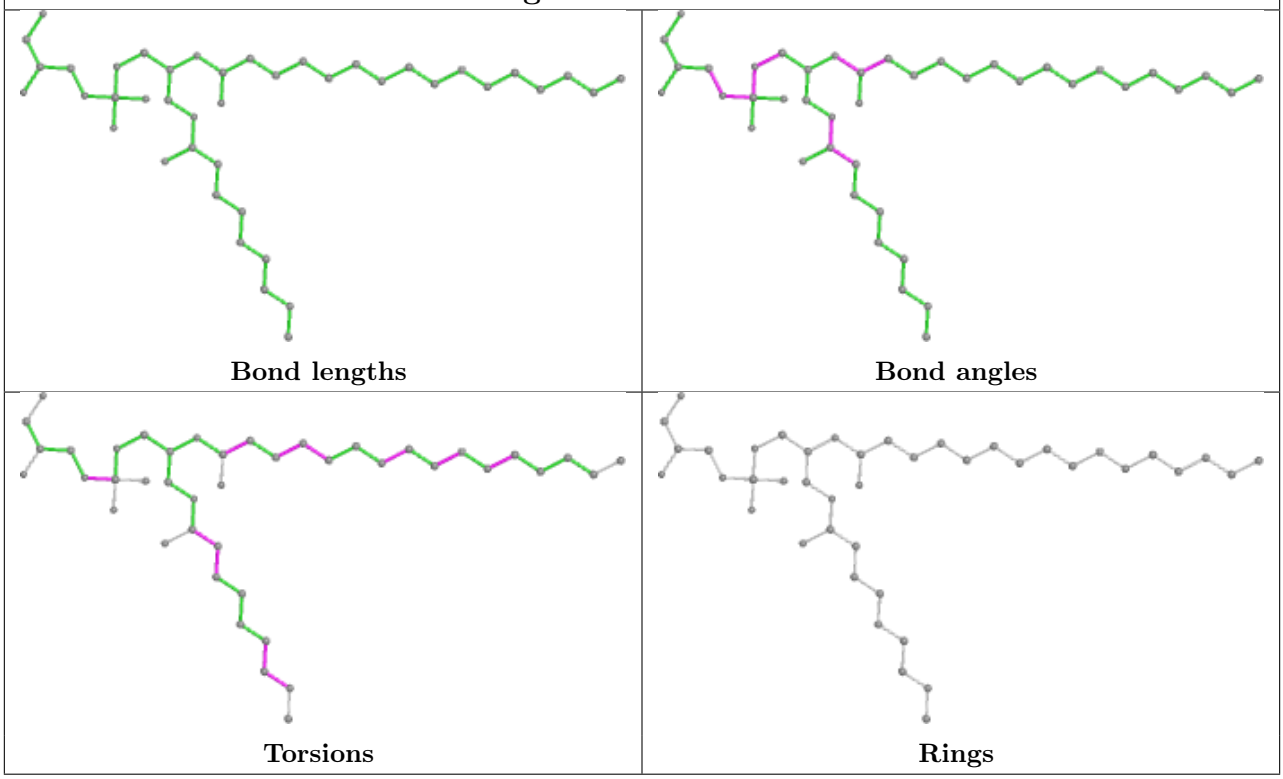
Ligand CLA B 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

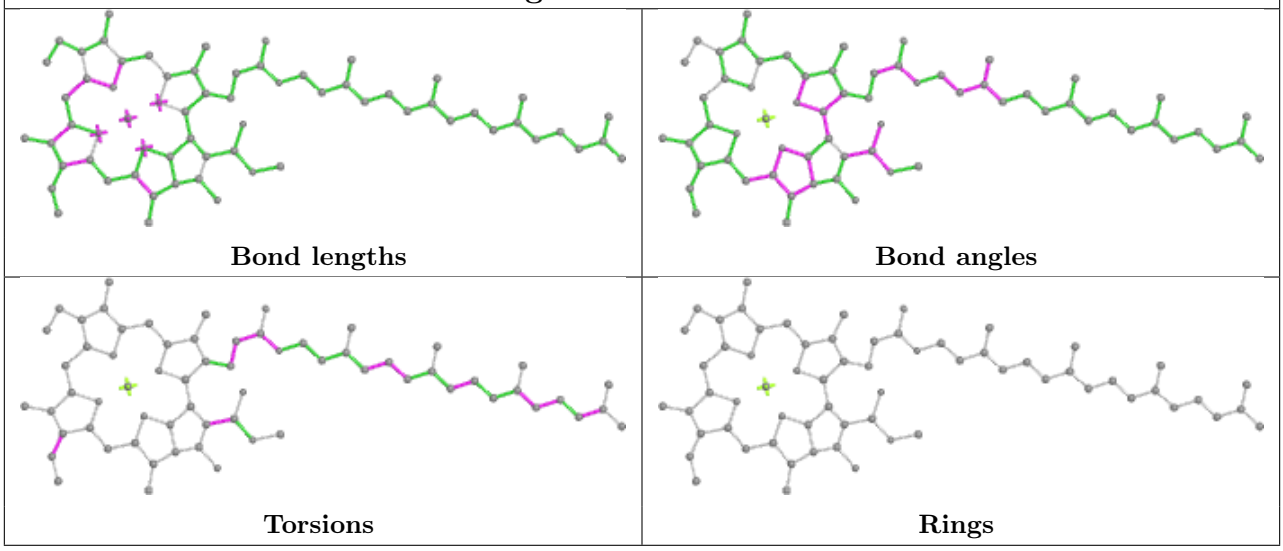
Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

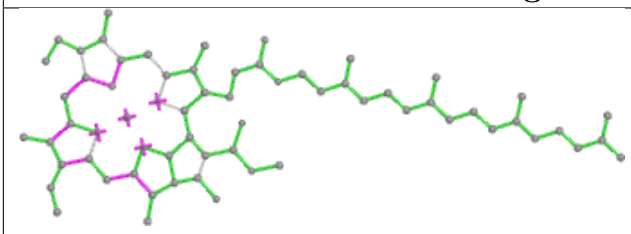
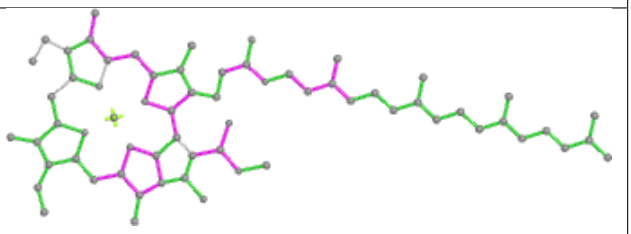
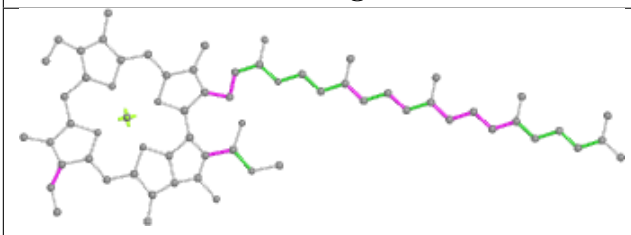
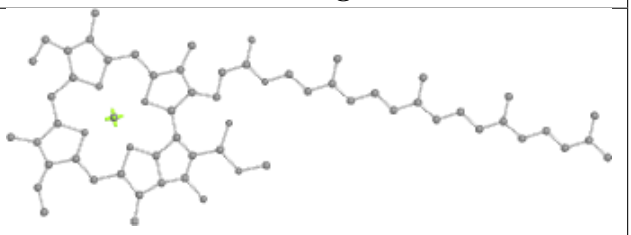
Ligand CHL y 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

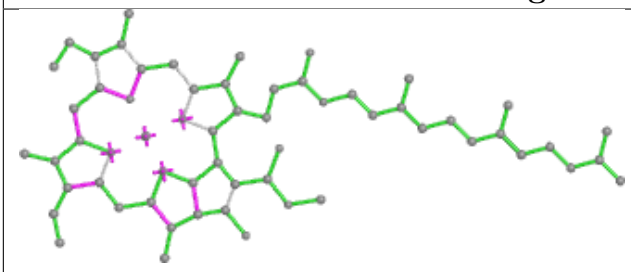
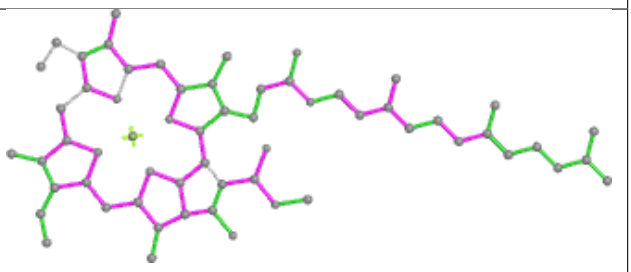
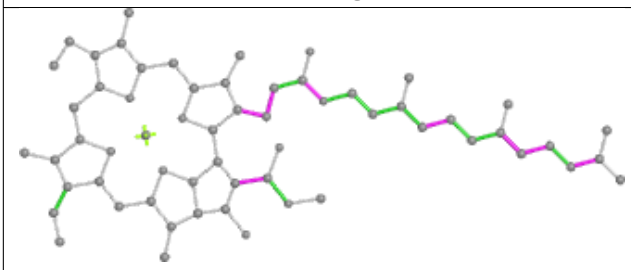
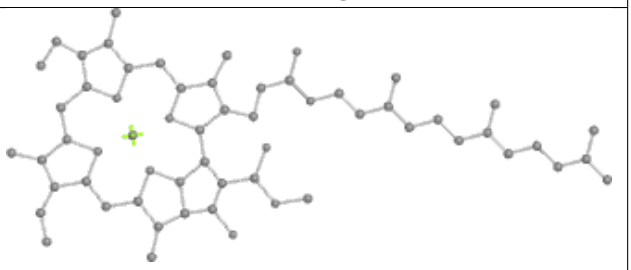
Ligand LHG R 618



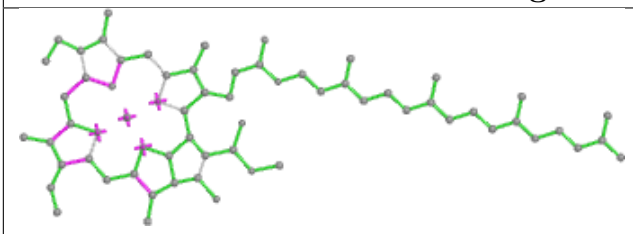
Ligand CLA B 616



Ligand CLA Y 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 503



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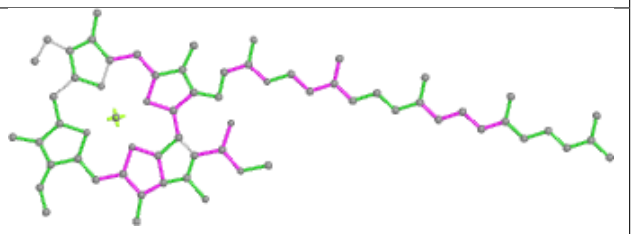

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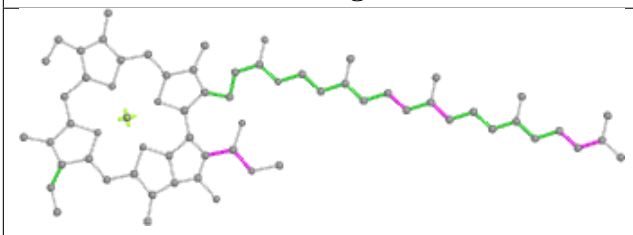

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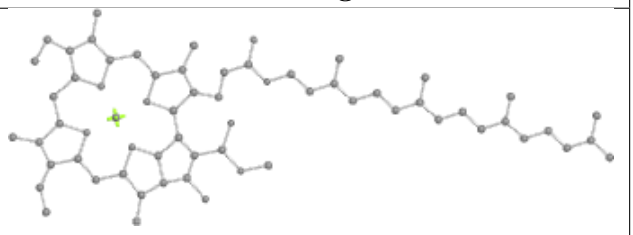
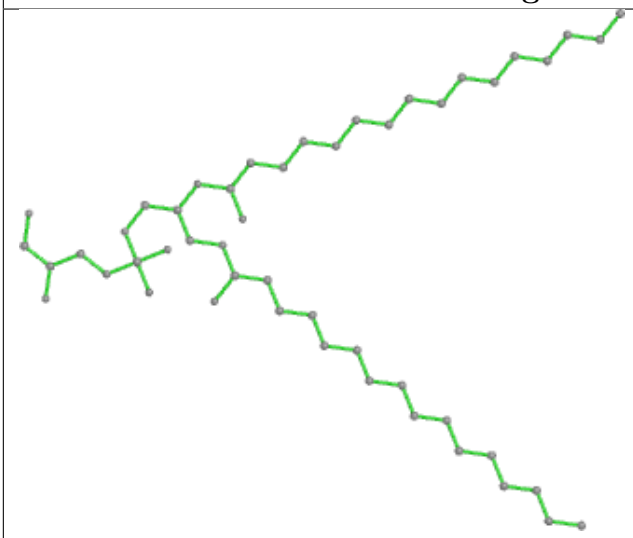


Rings

Ligand LHG Y 319



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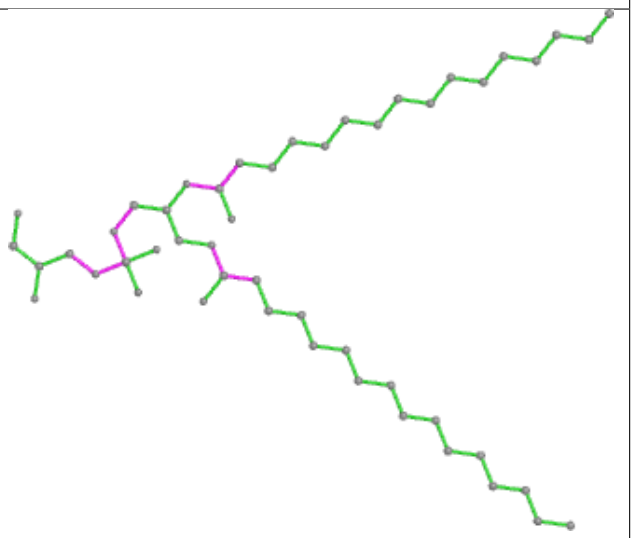
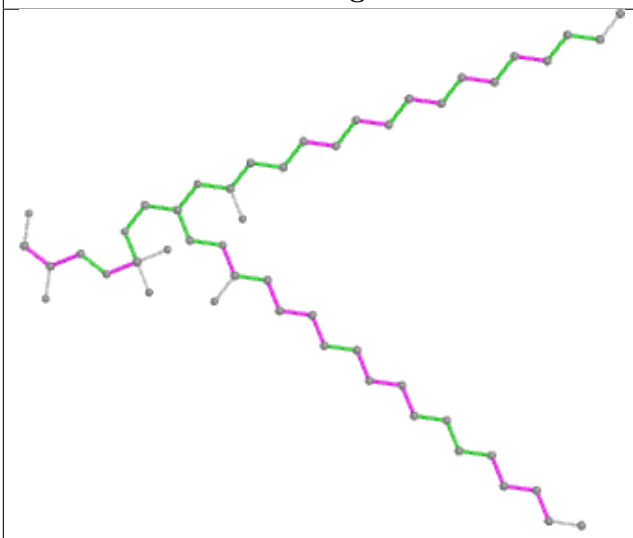


Bond angles



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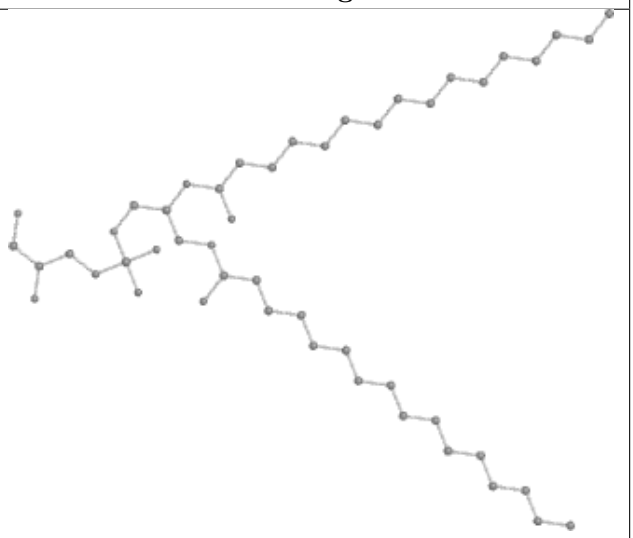
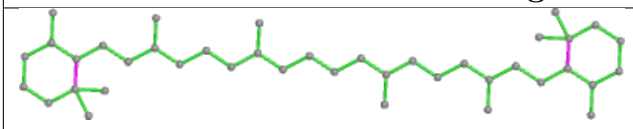


Rings

Ligand BCR c 514



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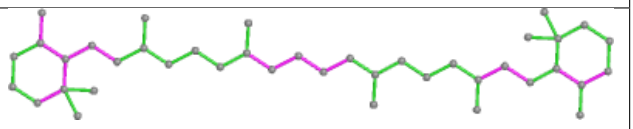
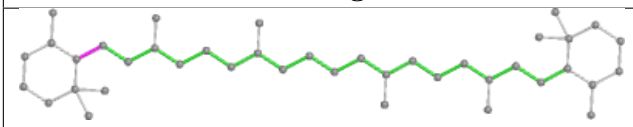


Bond angles



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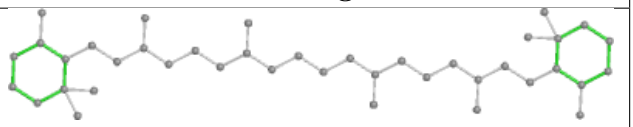
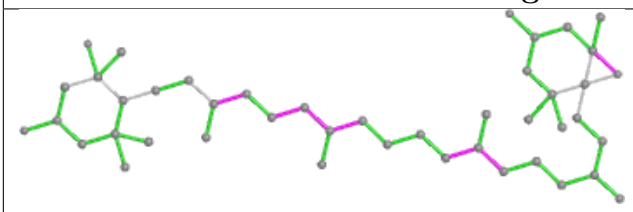


Rings

Ligand NEX R 617



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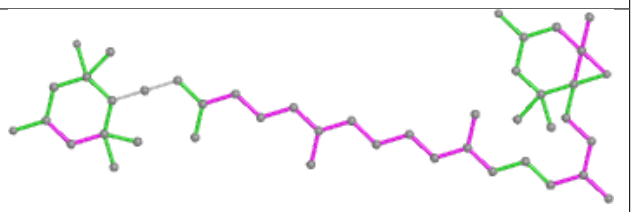
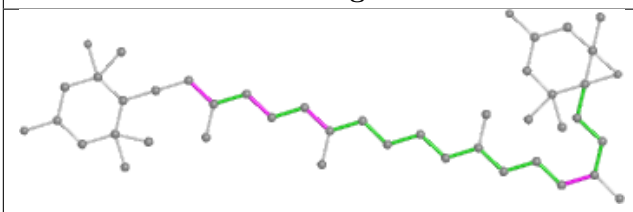


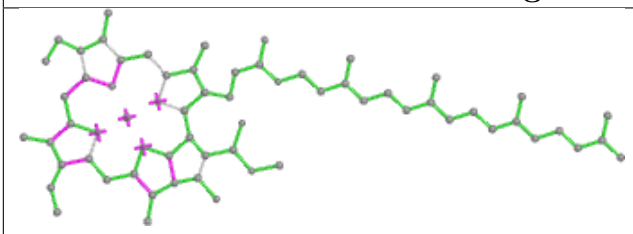
Bond angles



Torsions

Rings

Ligand CLA Y 304



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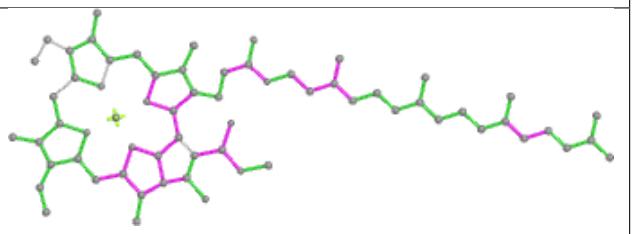
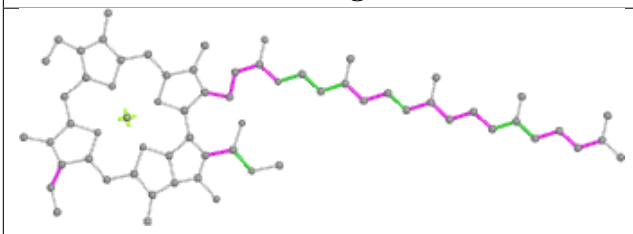


Bond angles



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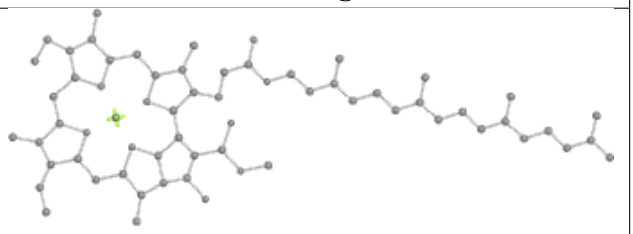
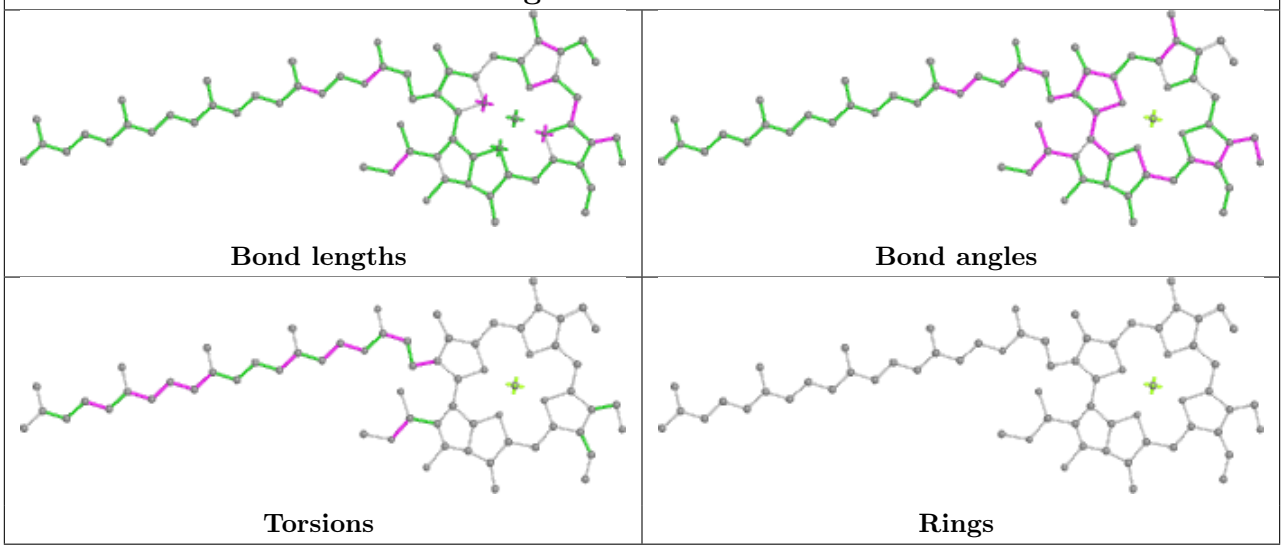
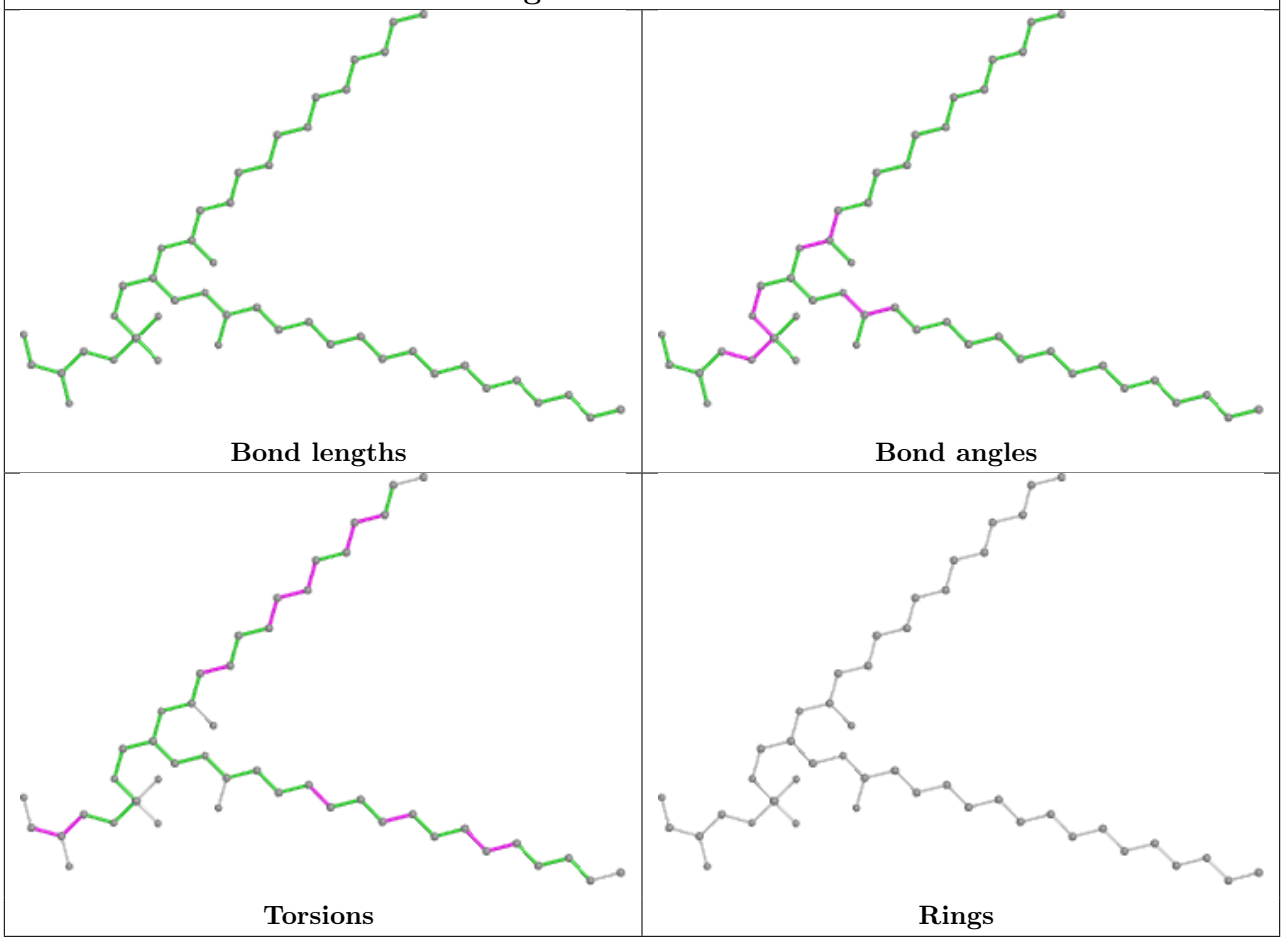


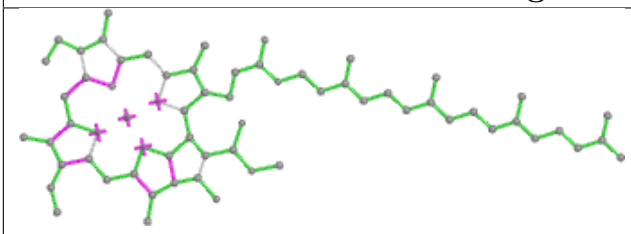
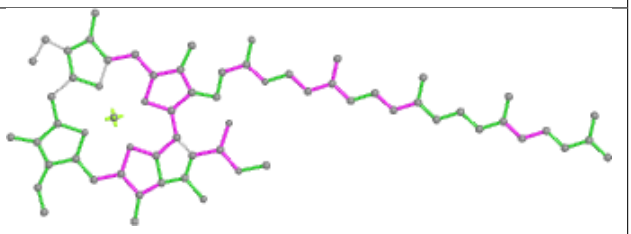
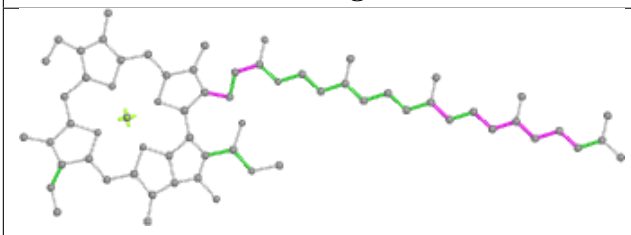
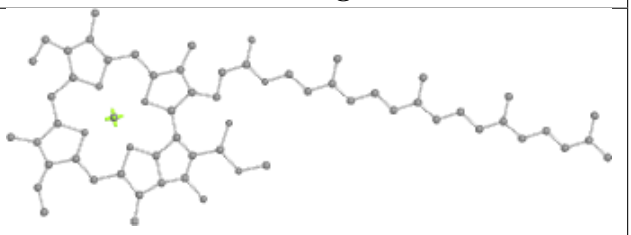
Rings

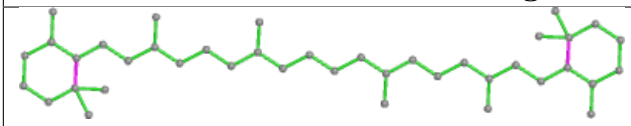
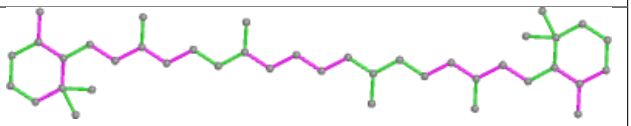
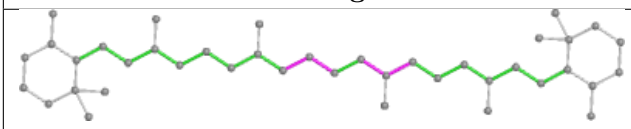
Ligand CHL N 609

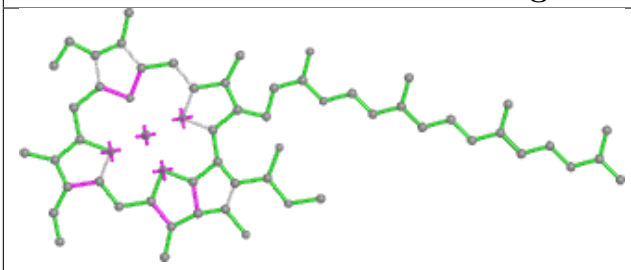
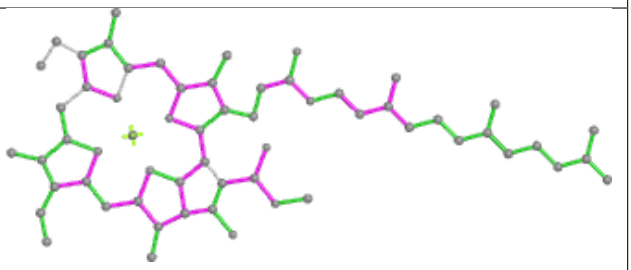
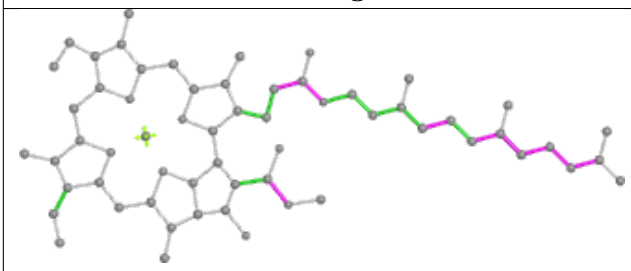
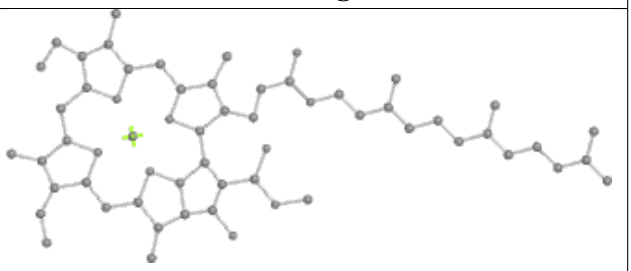


Ligand LHG B 625

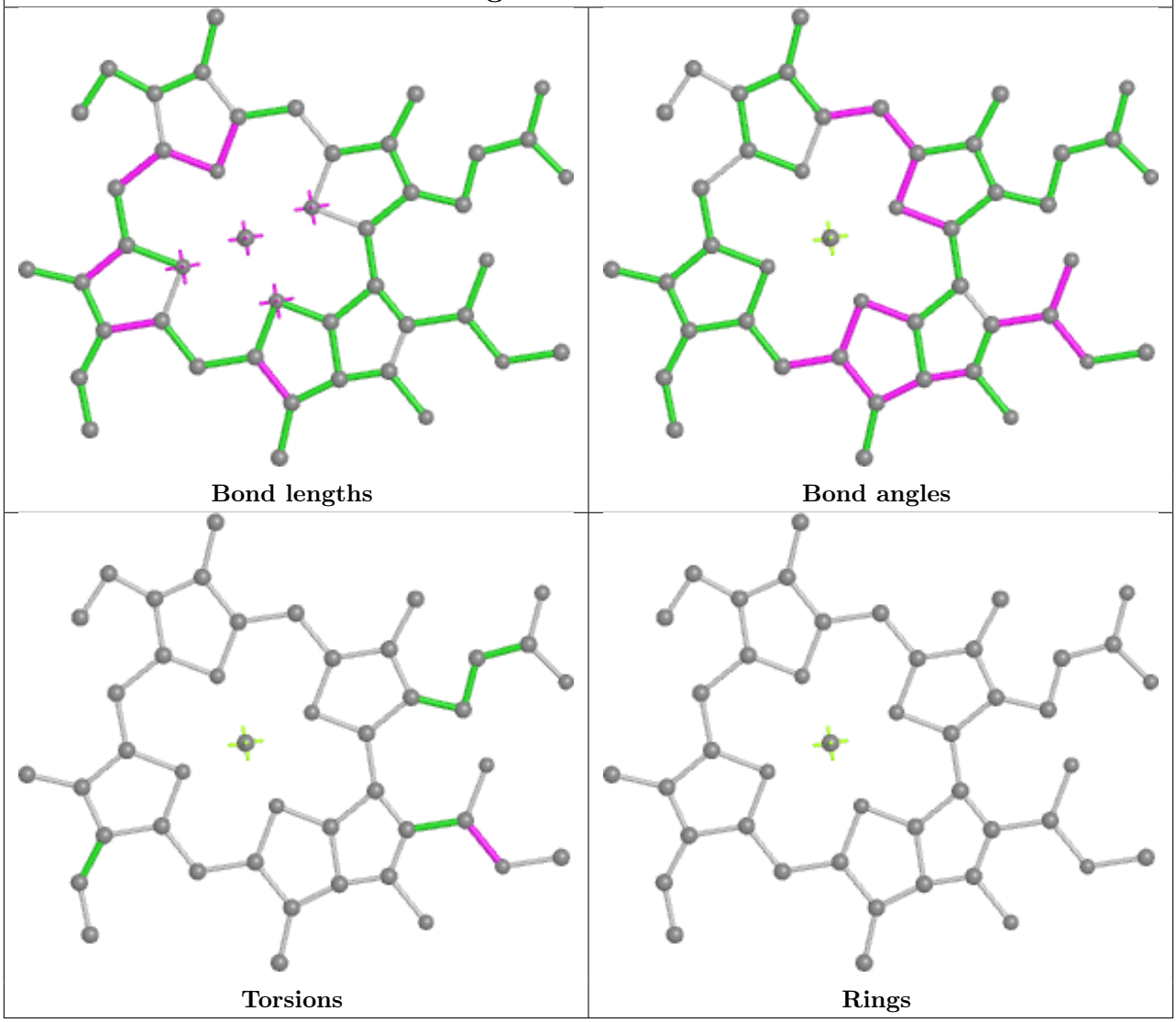


Ligand CLA d 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

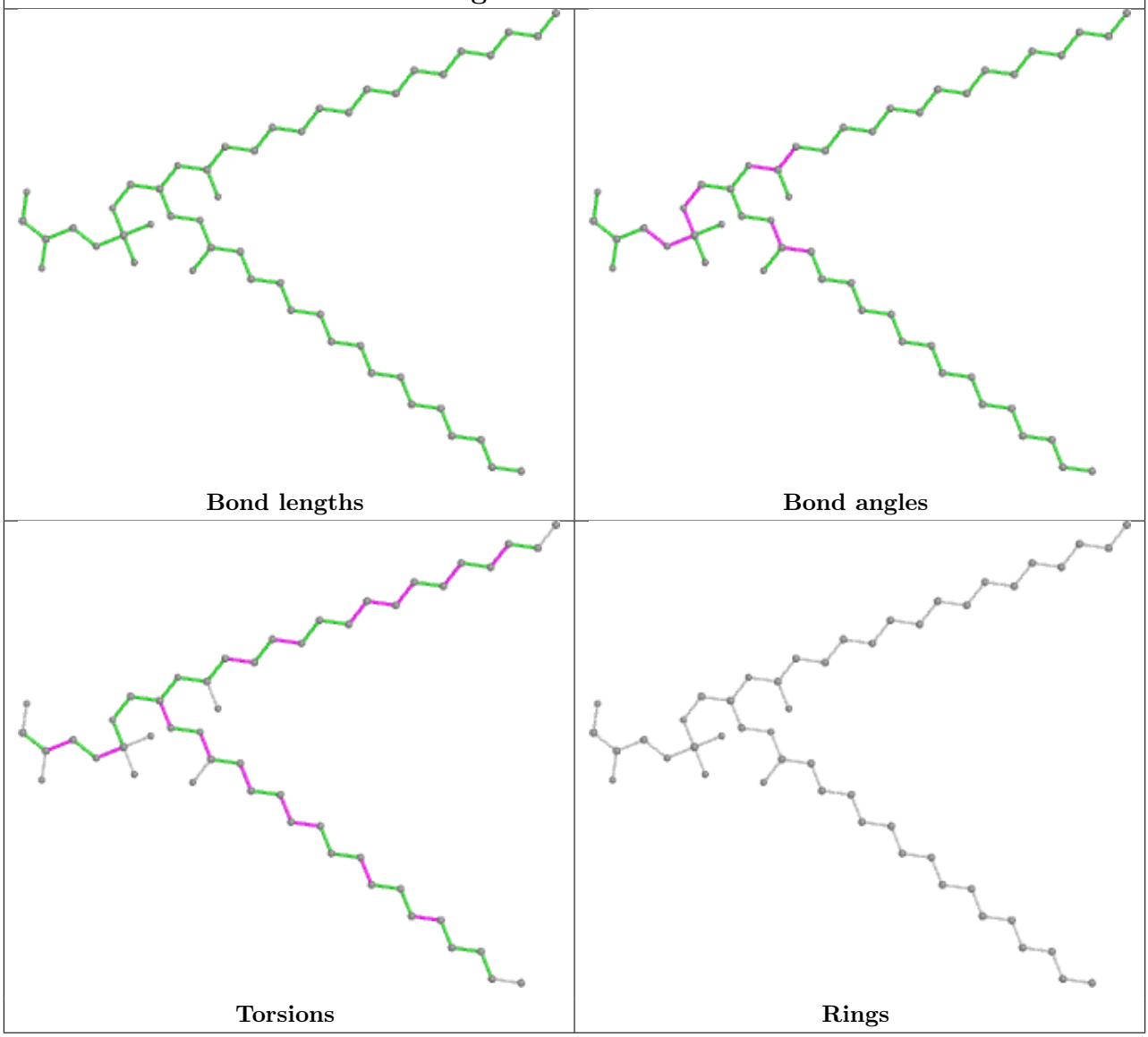
Ligand BCR A 406	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA r 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

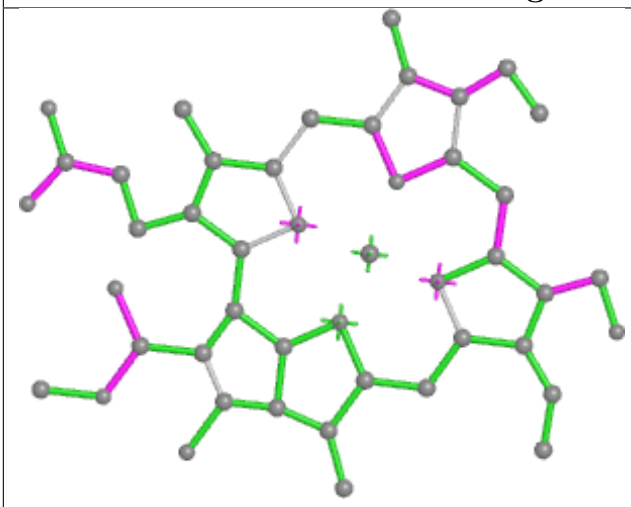
Ligand CLA s 304



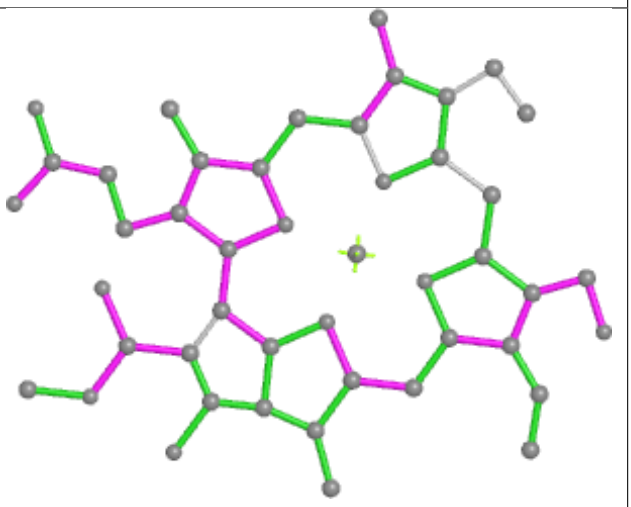
Ligand LHG b 622



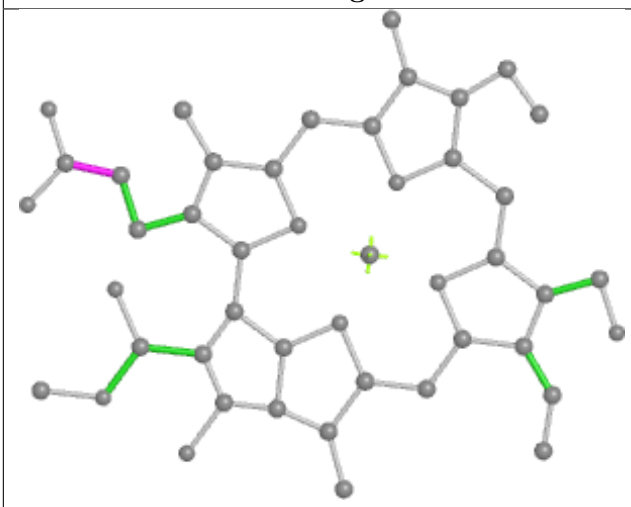
Ligand CHL S 308



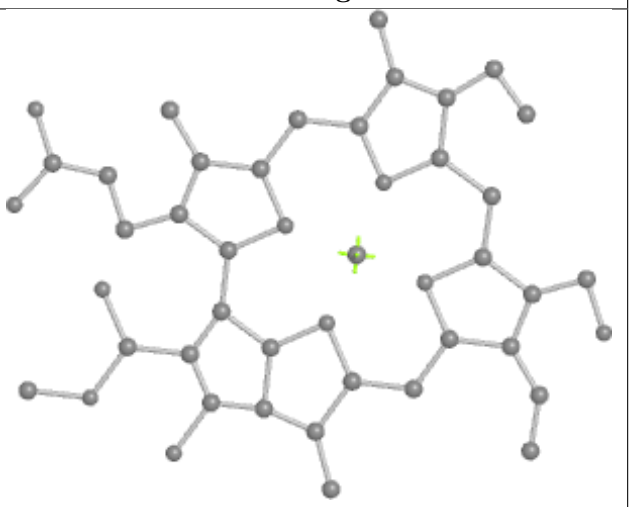
Bond lengths



Bond angles

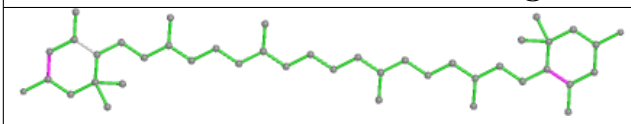


Torsions



Rings

Ligand LUT Y 316



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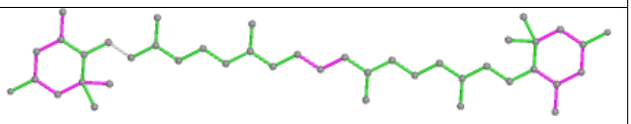
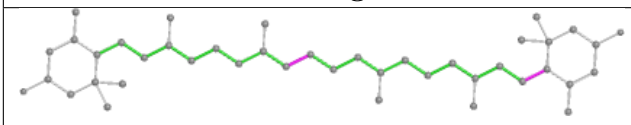
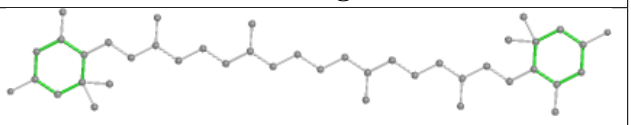


Bond angles

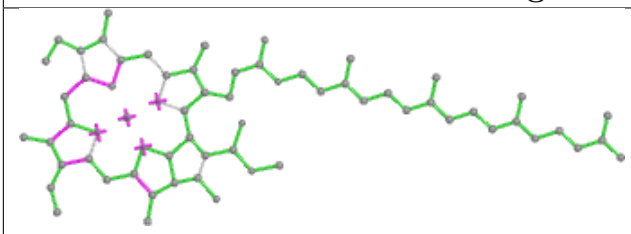


Torsions

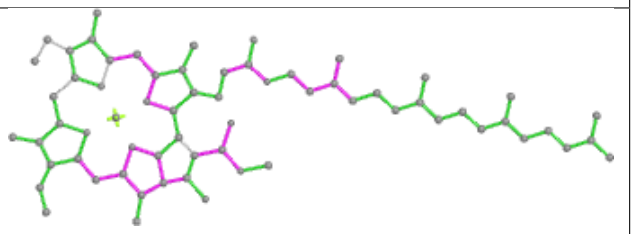


Rings

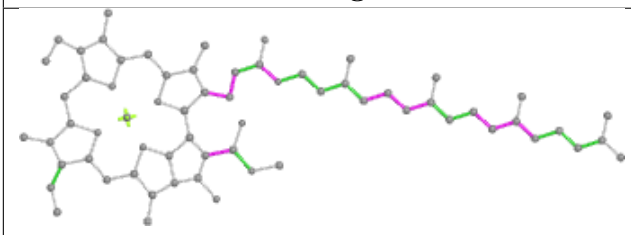
Ligand CLA b 601



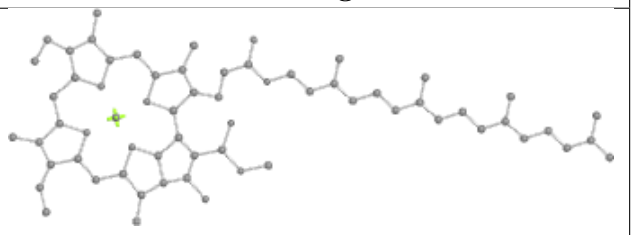
Bond lengths



Bond angles

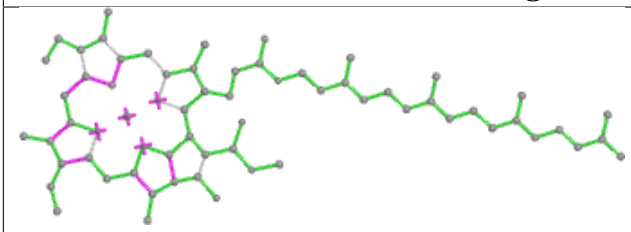


Torsions

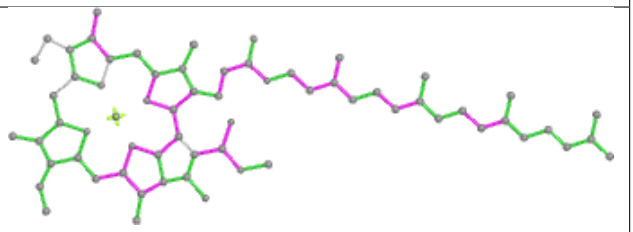


Rings

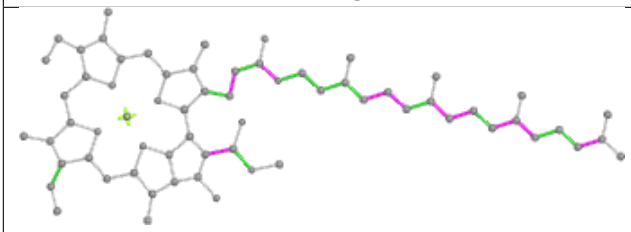
Ligand CLA C 513



Bond lengths



Bond angles



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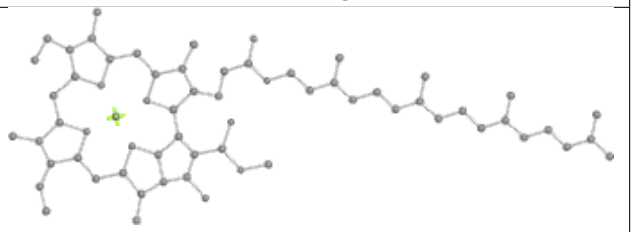
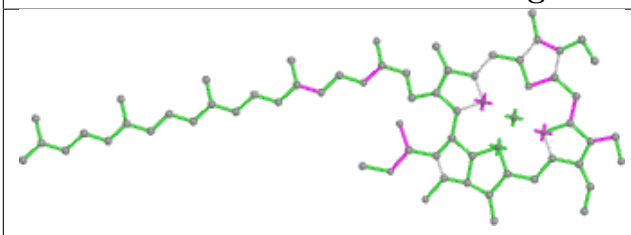


Rings

Ligand CHL g 601



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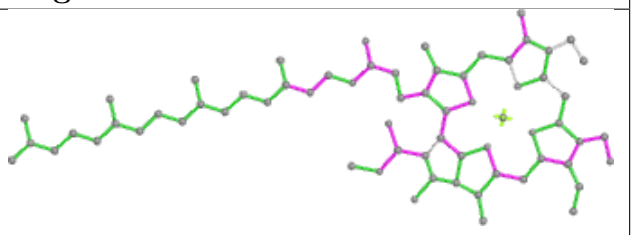
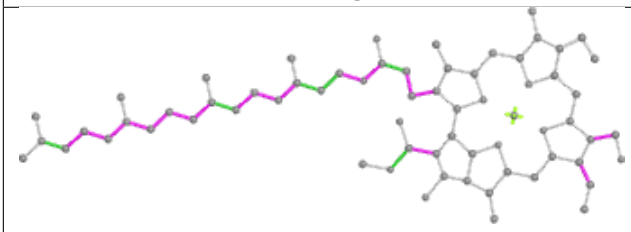


Bond angles



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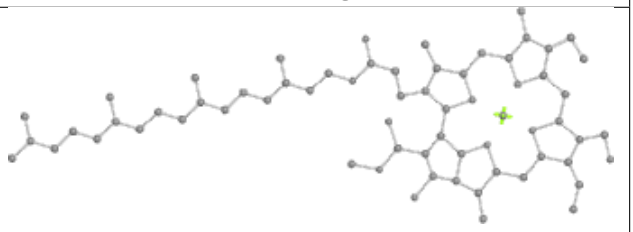
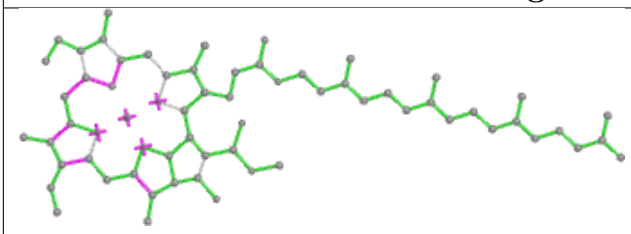
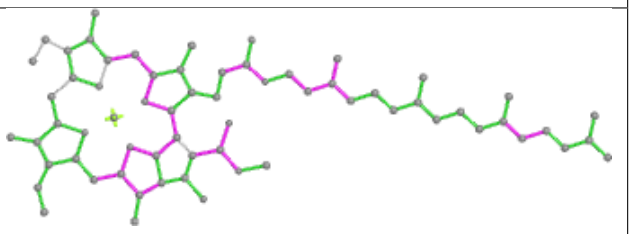
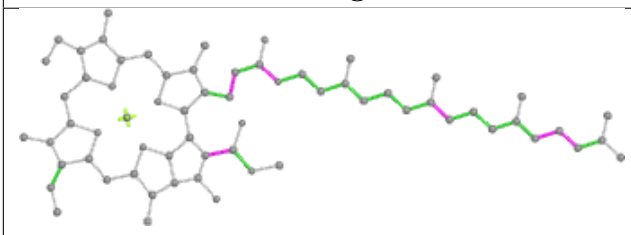
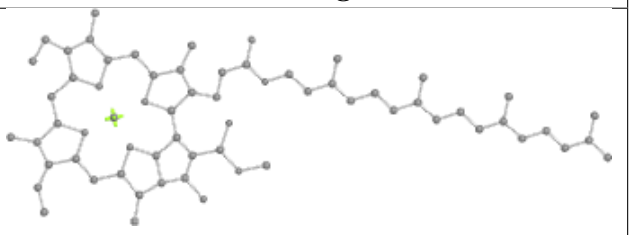
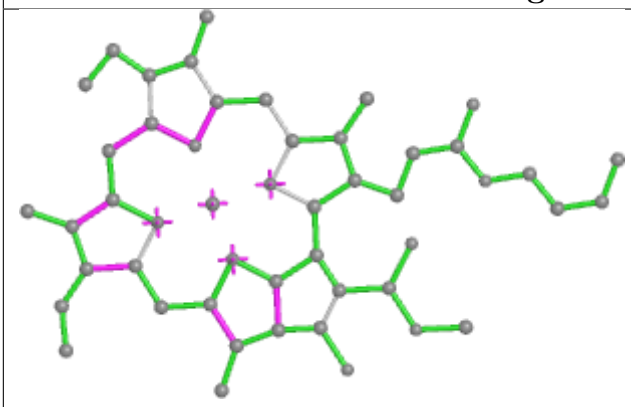
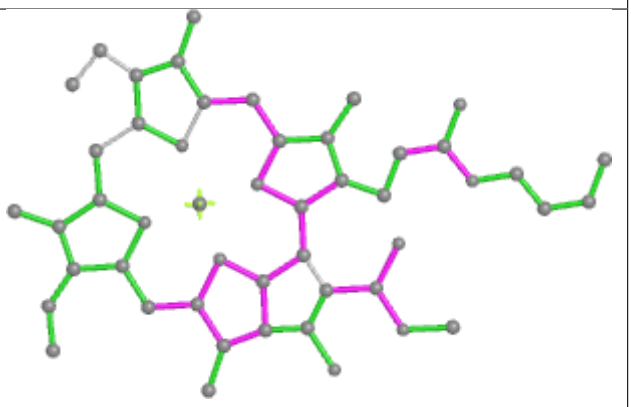
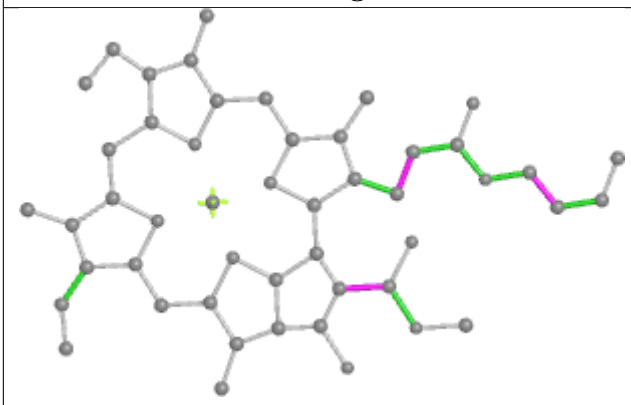
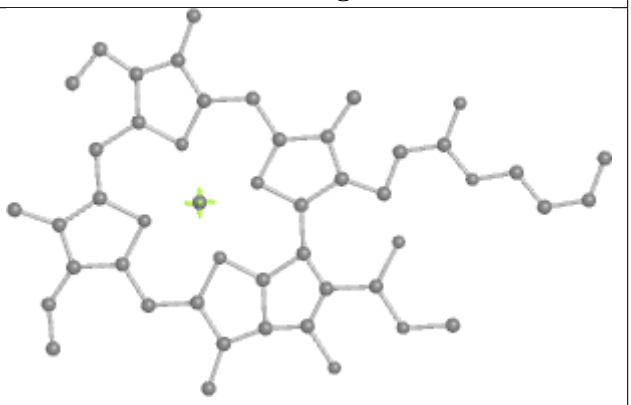
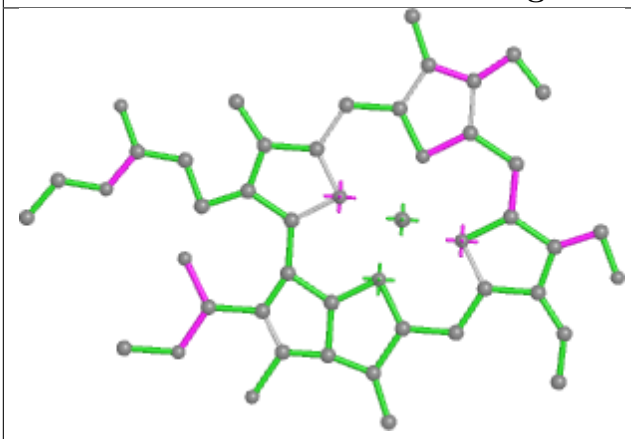
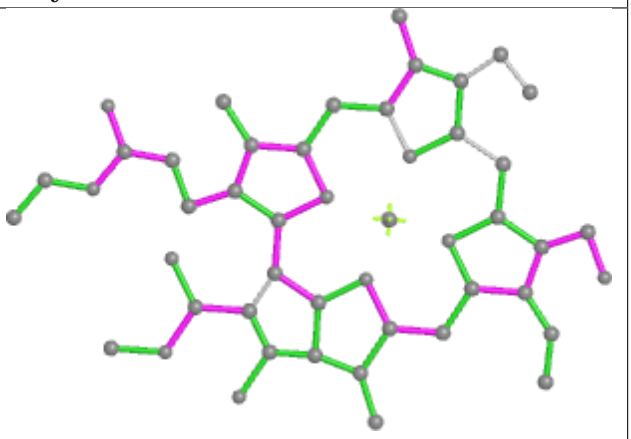
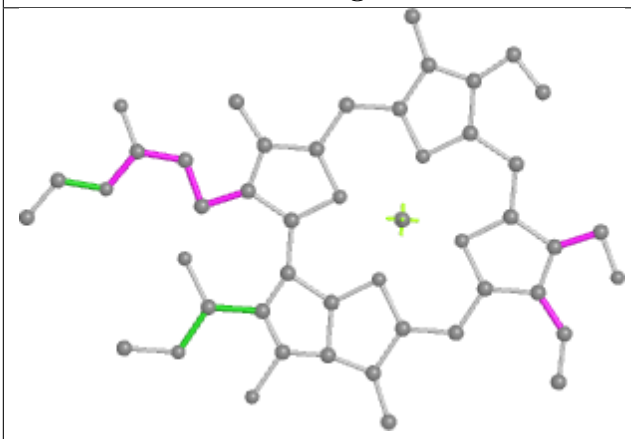
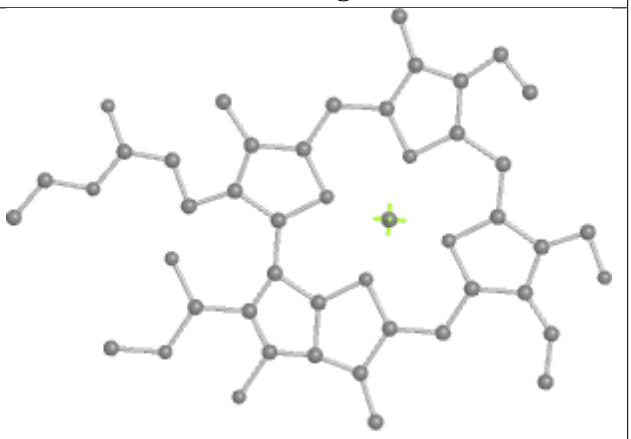


Rings

Ligand CLA b 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL y 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

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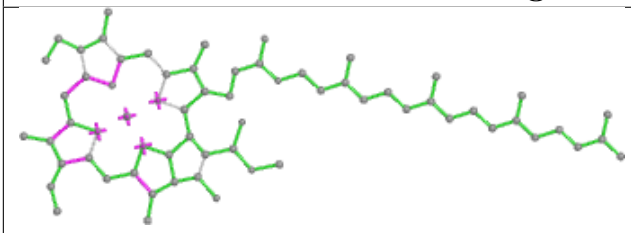
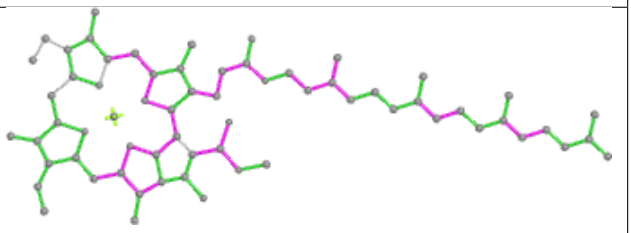
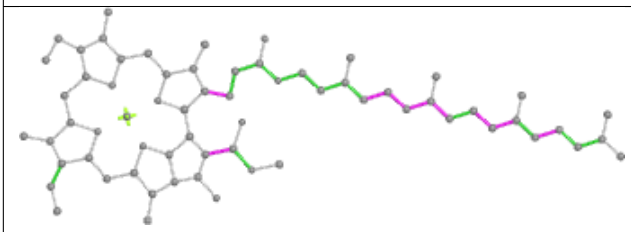
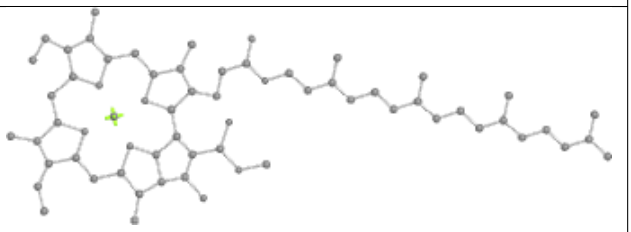
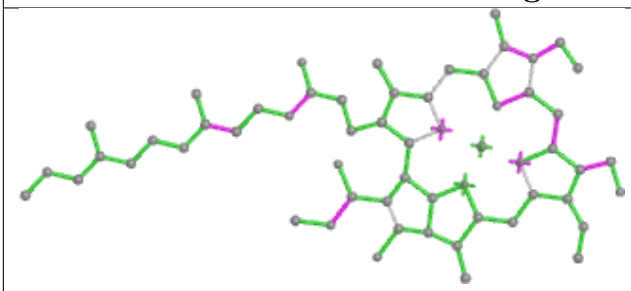
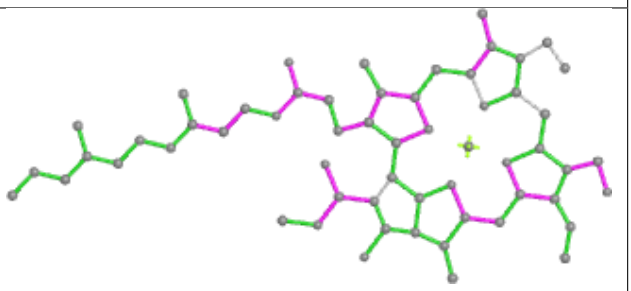
 Bond lengths	 Bond angles
 Torsions	 Rings

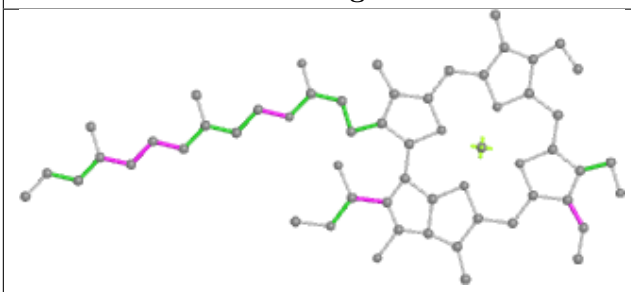
Ligand CHL Y 308



Bond lengths



Bond angles



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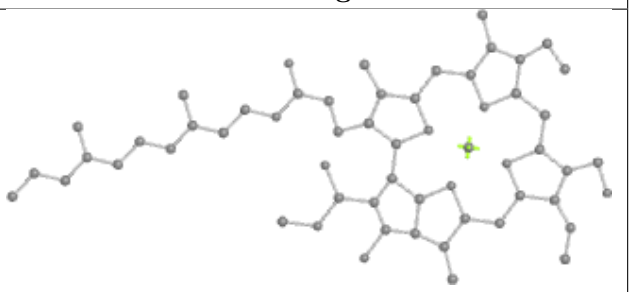
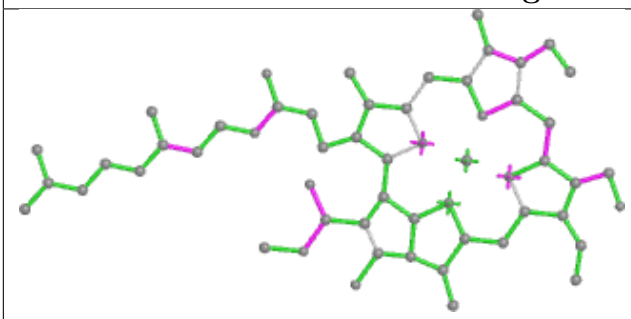


Rings

Ligand CHL N 601



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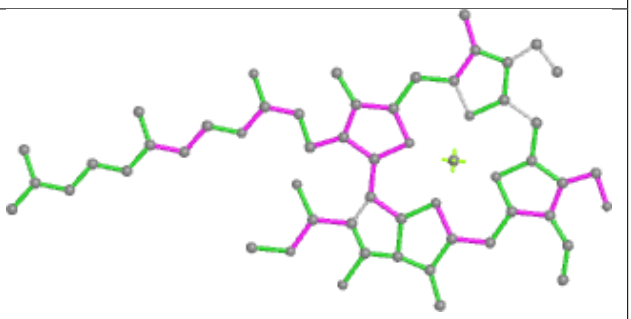
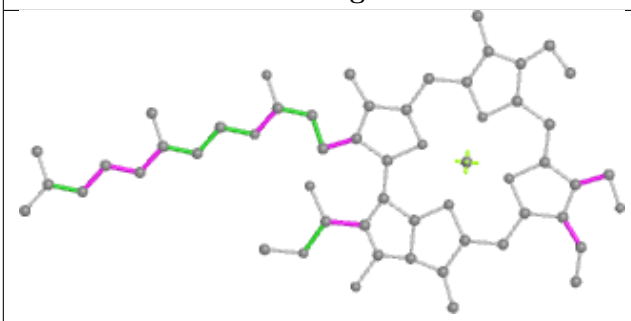


Bond angles



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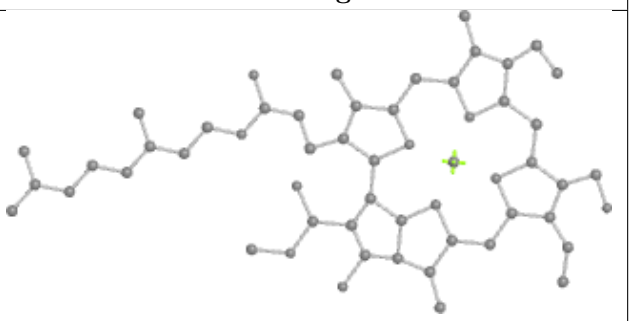
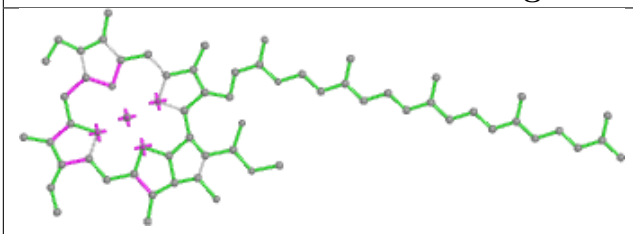


Rings

Ligand CLA Y 314



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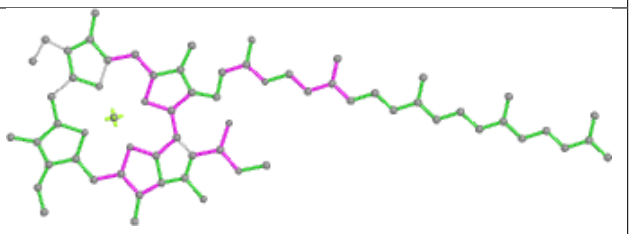
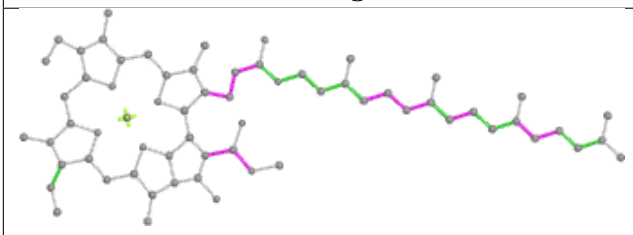


Bond angles



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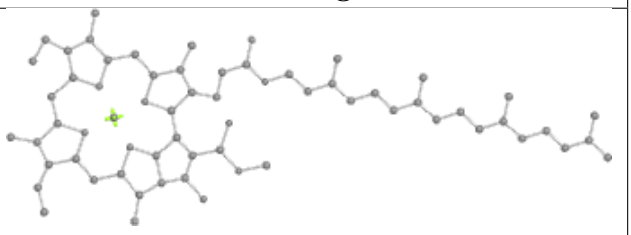
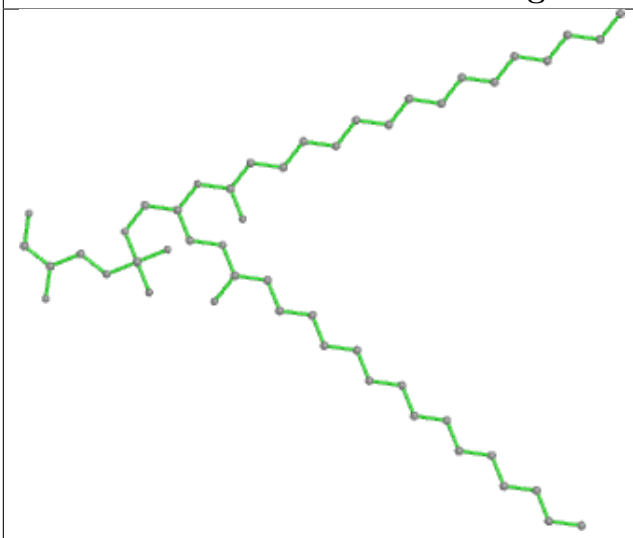


Rings

Ligand LHG c 517



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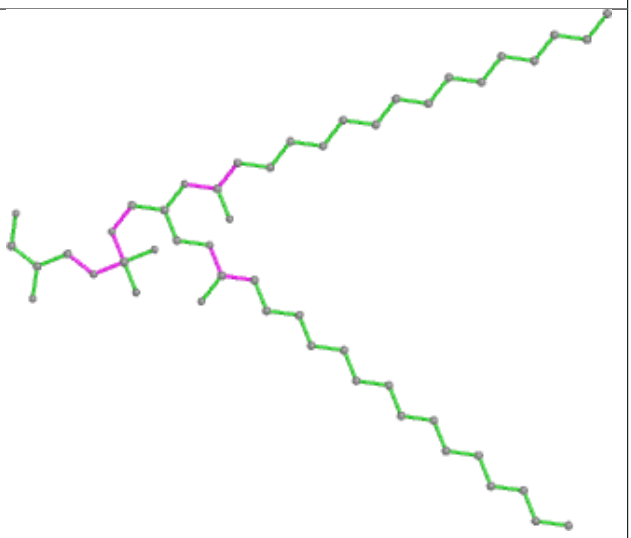
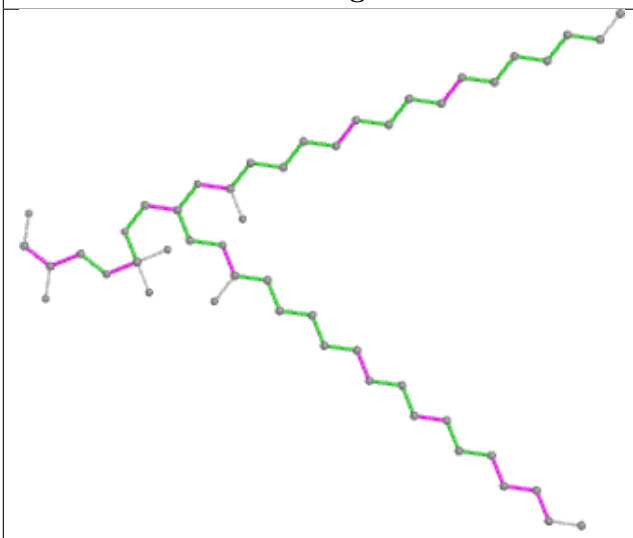


Bond angles



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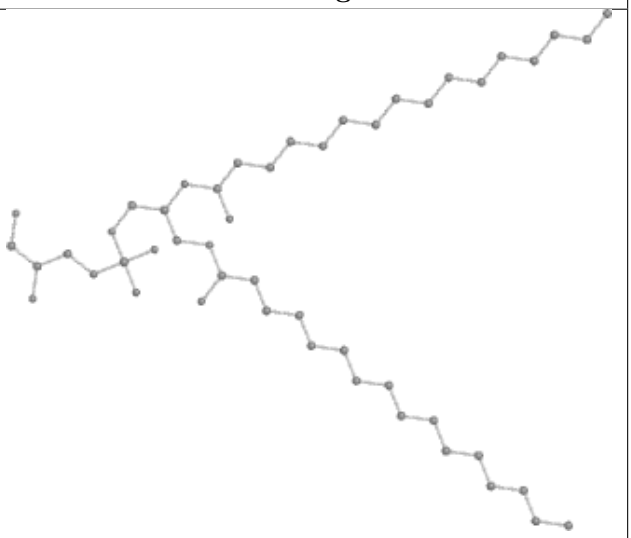
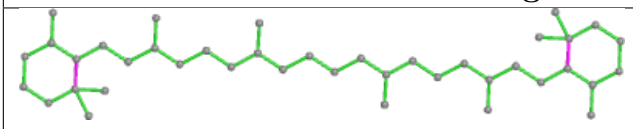


Rings

Ligand BCR B 618



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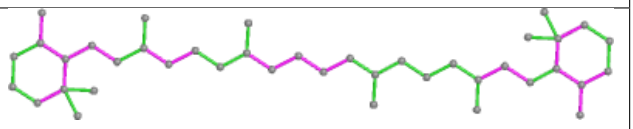
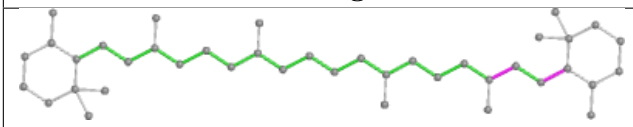


Bond angles



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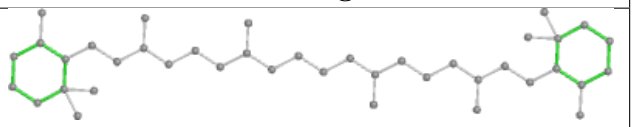
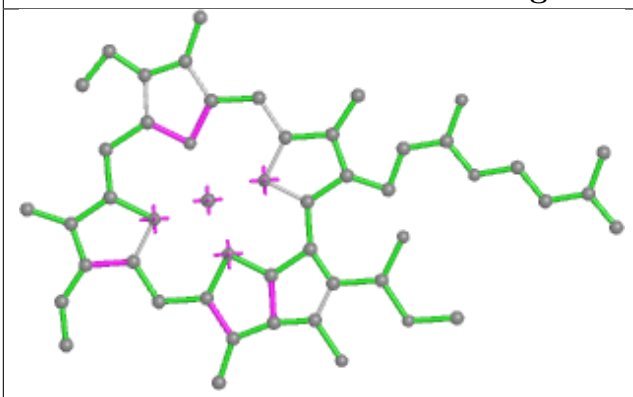


Rings

Ligand CLA s 305



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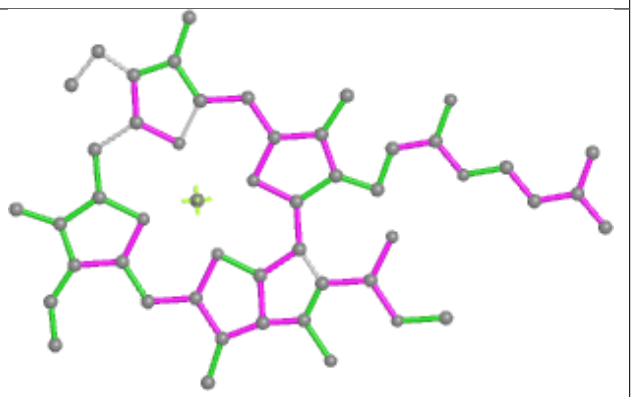
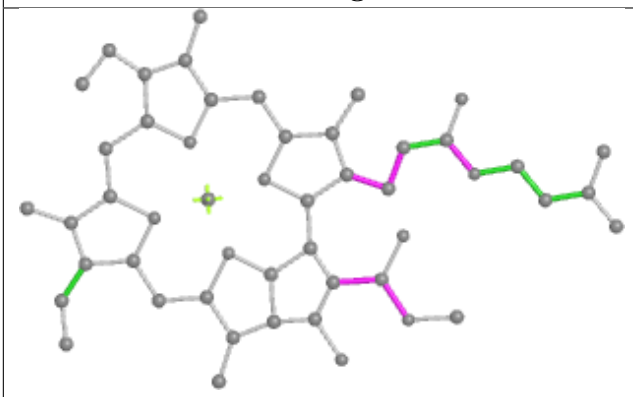


Bond angles



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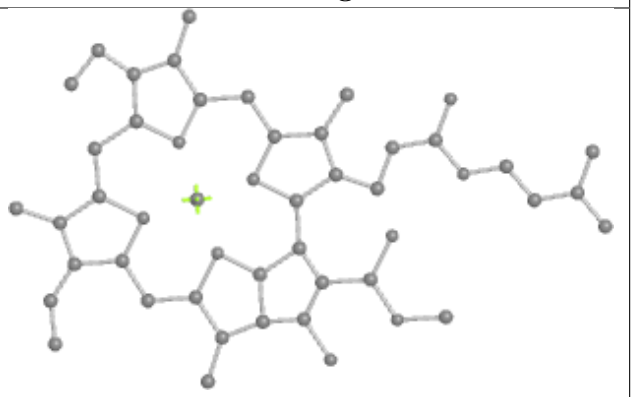
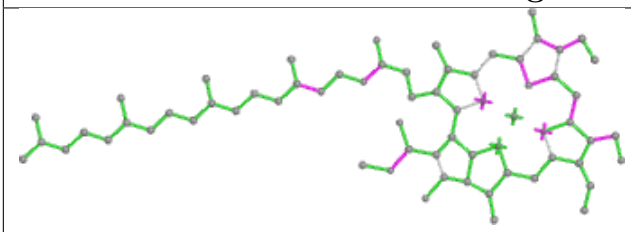
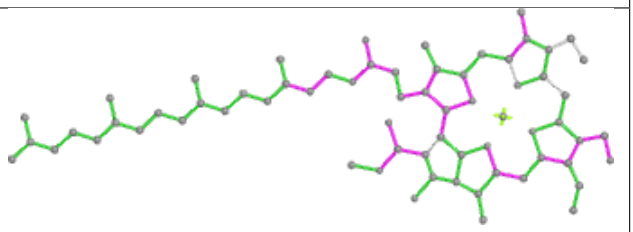
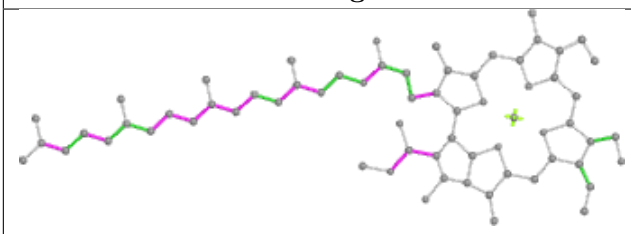
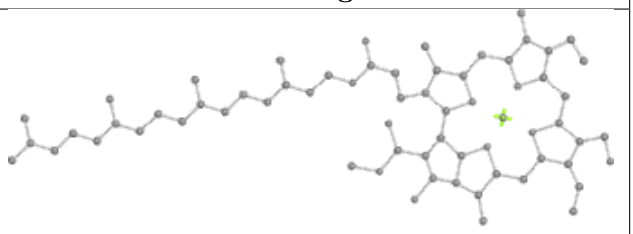
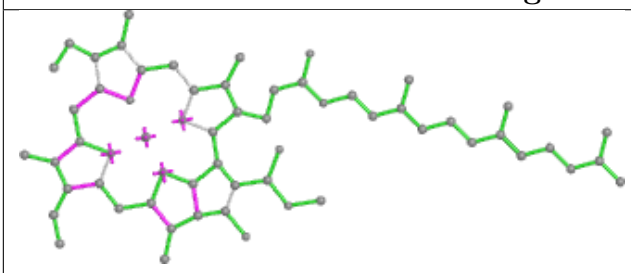
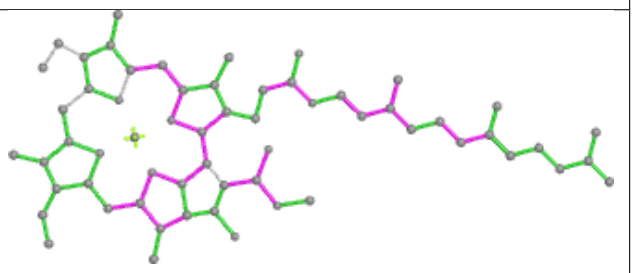
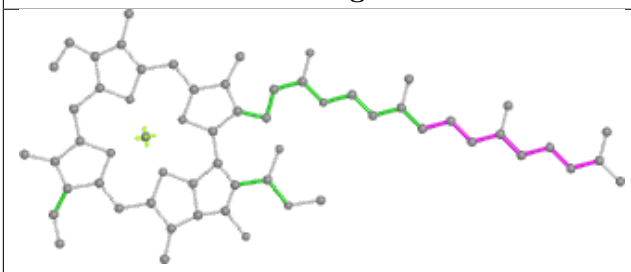
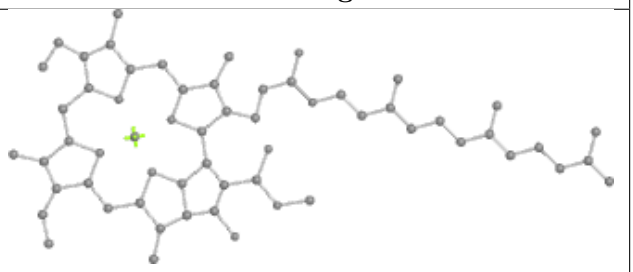
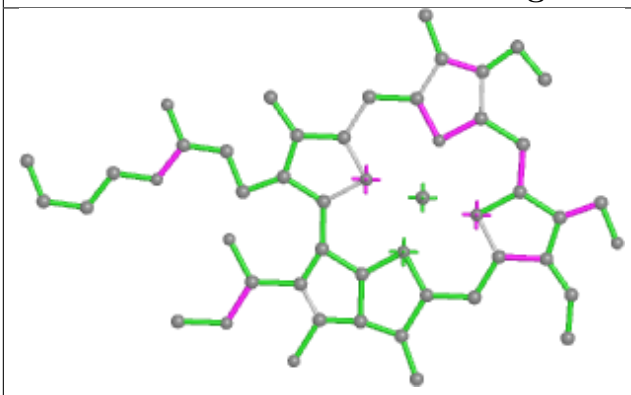


Rings

Ligand CHL n 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL y 307



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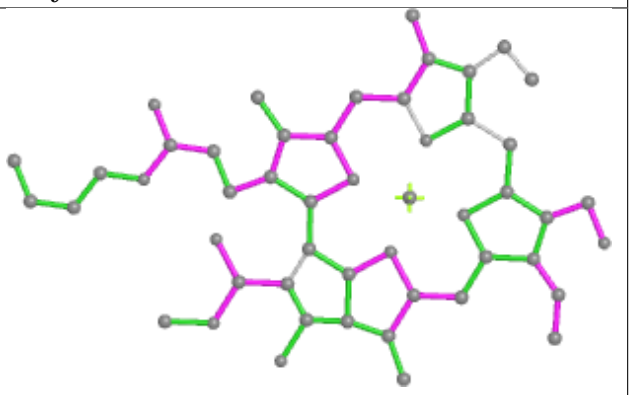

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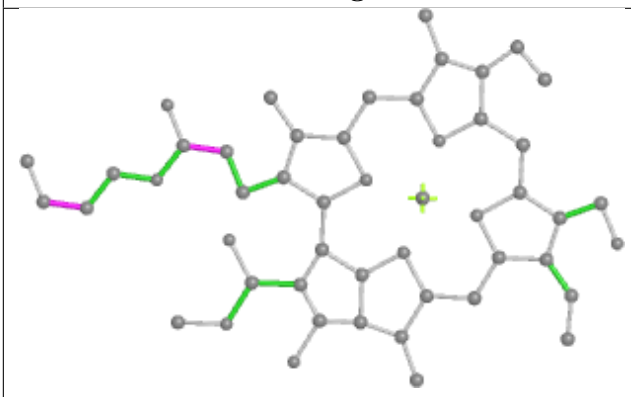

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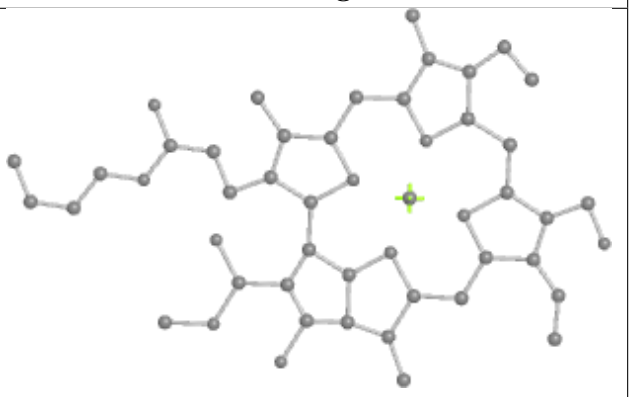
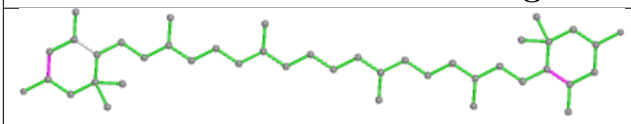


Rings

Ligand LUT N 615



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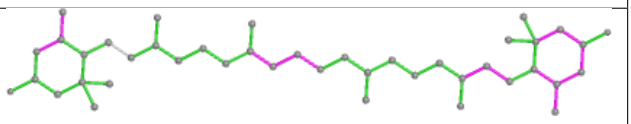

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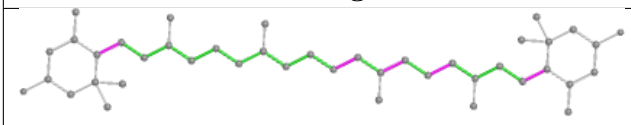
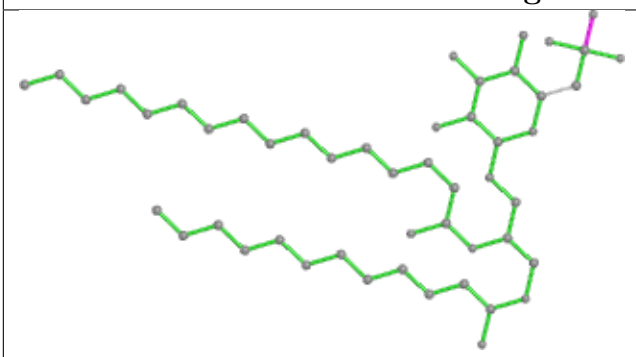
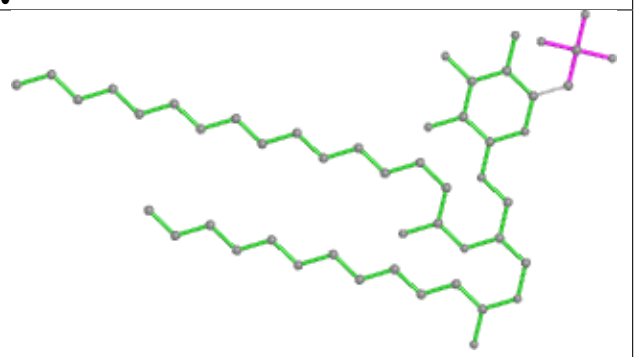
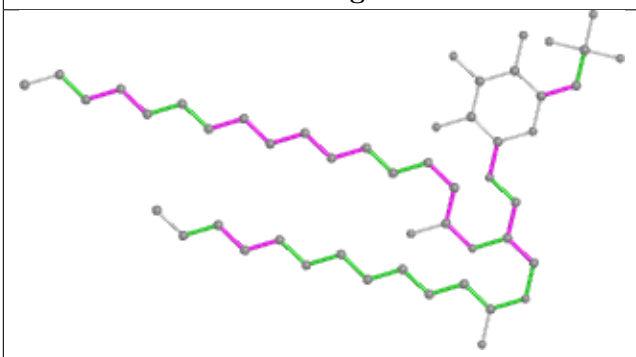
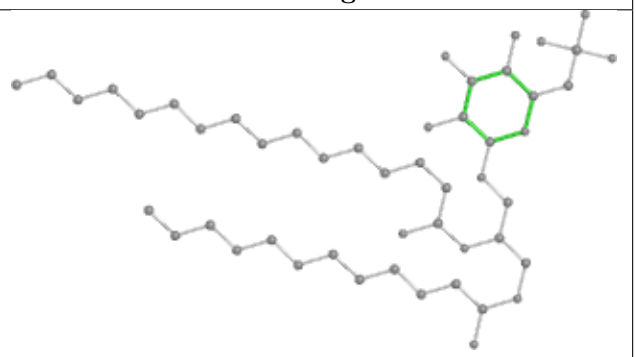
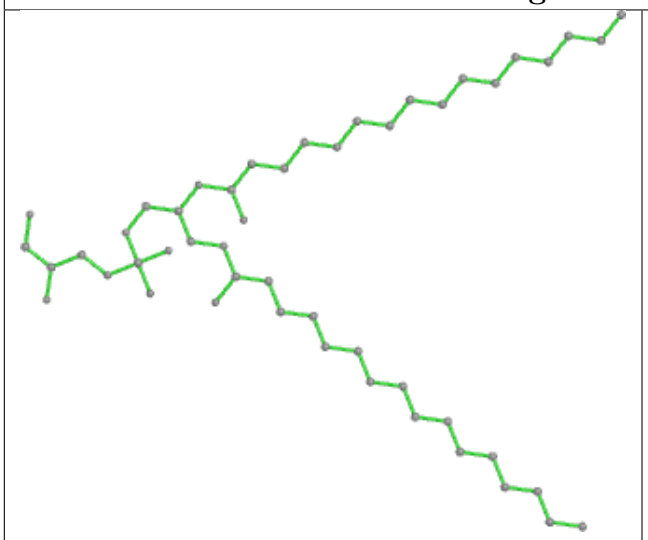


Torsions

Rings

Ligand SQD A 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG c 518



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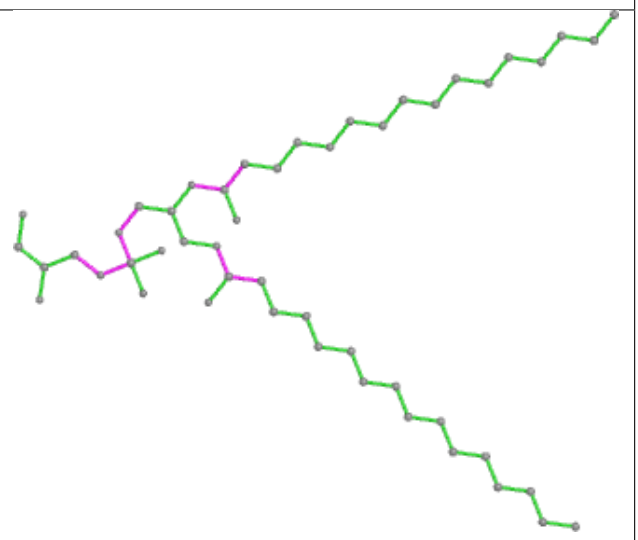

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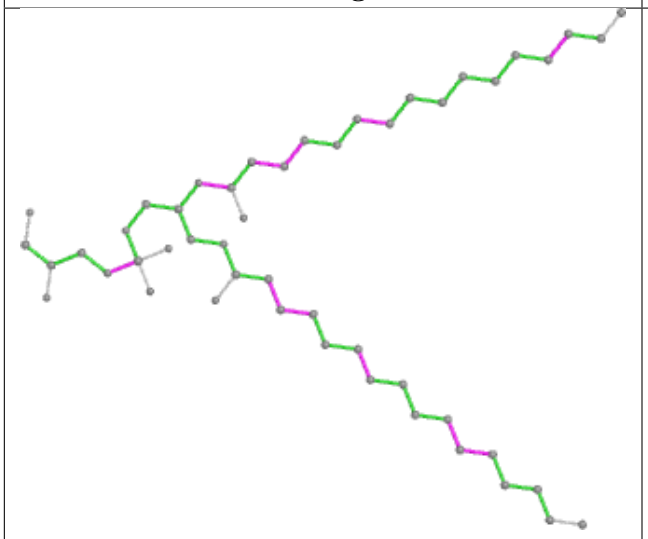

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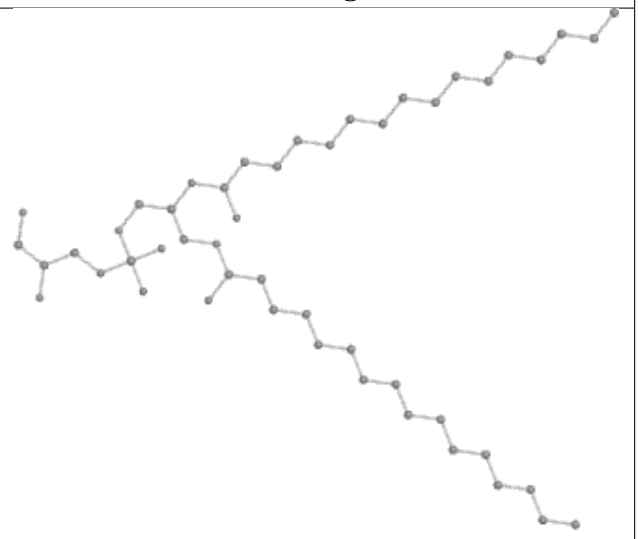
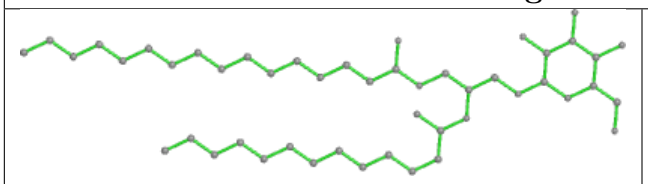


Rings

Ligand LMG a 409



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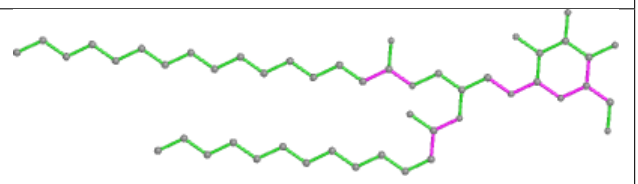

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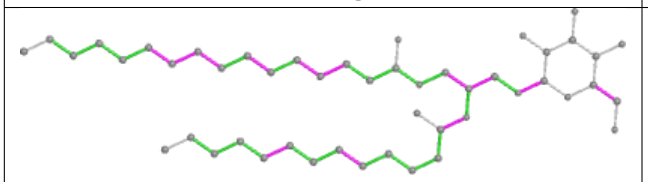

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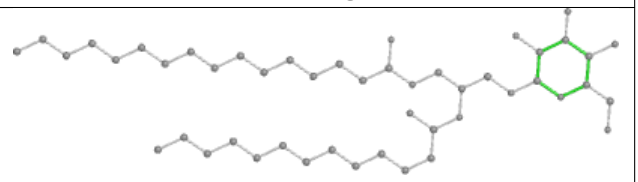

Rings

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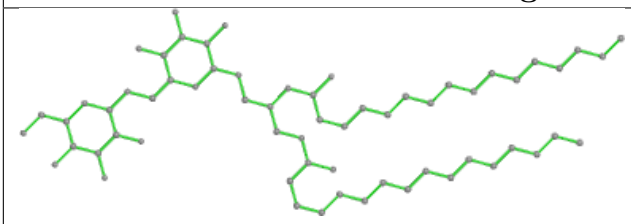

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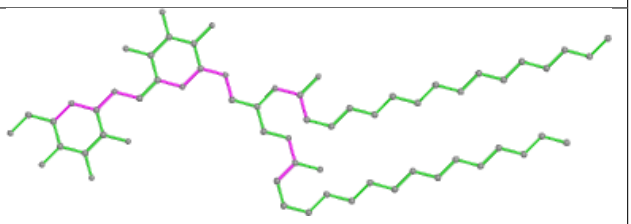

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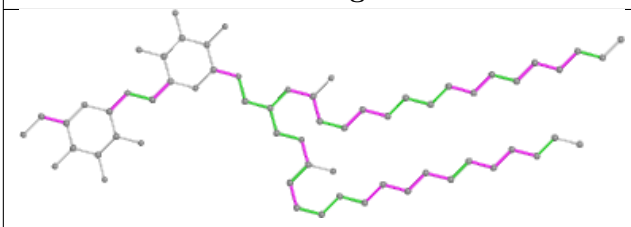

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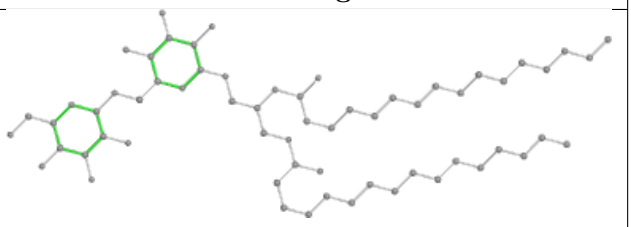
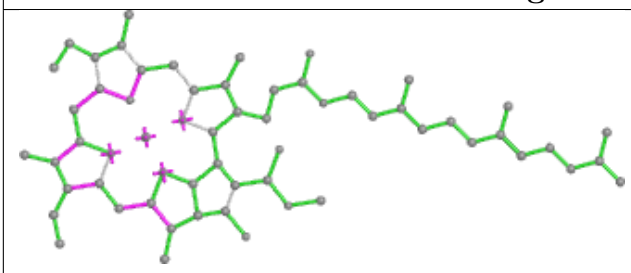


Rings

Ligand CLA n 613



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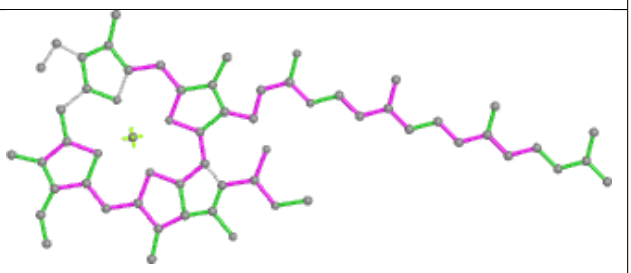

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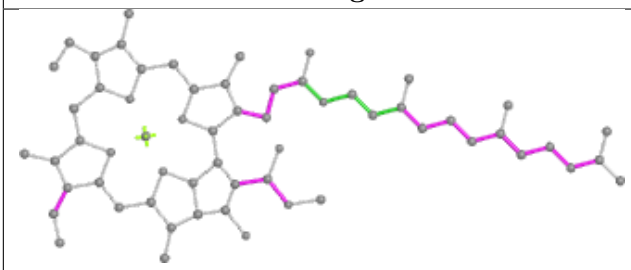

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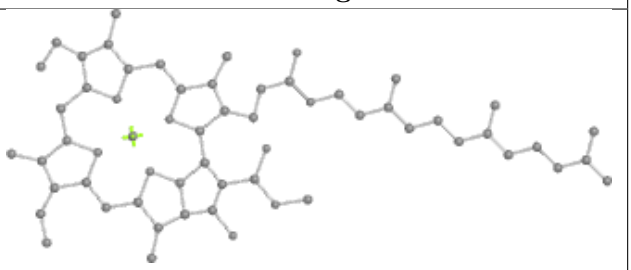

Rings

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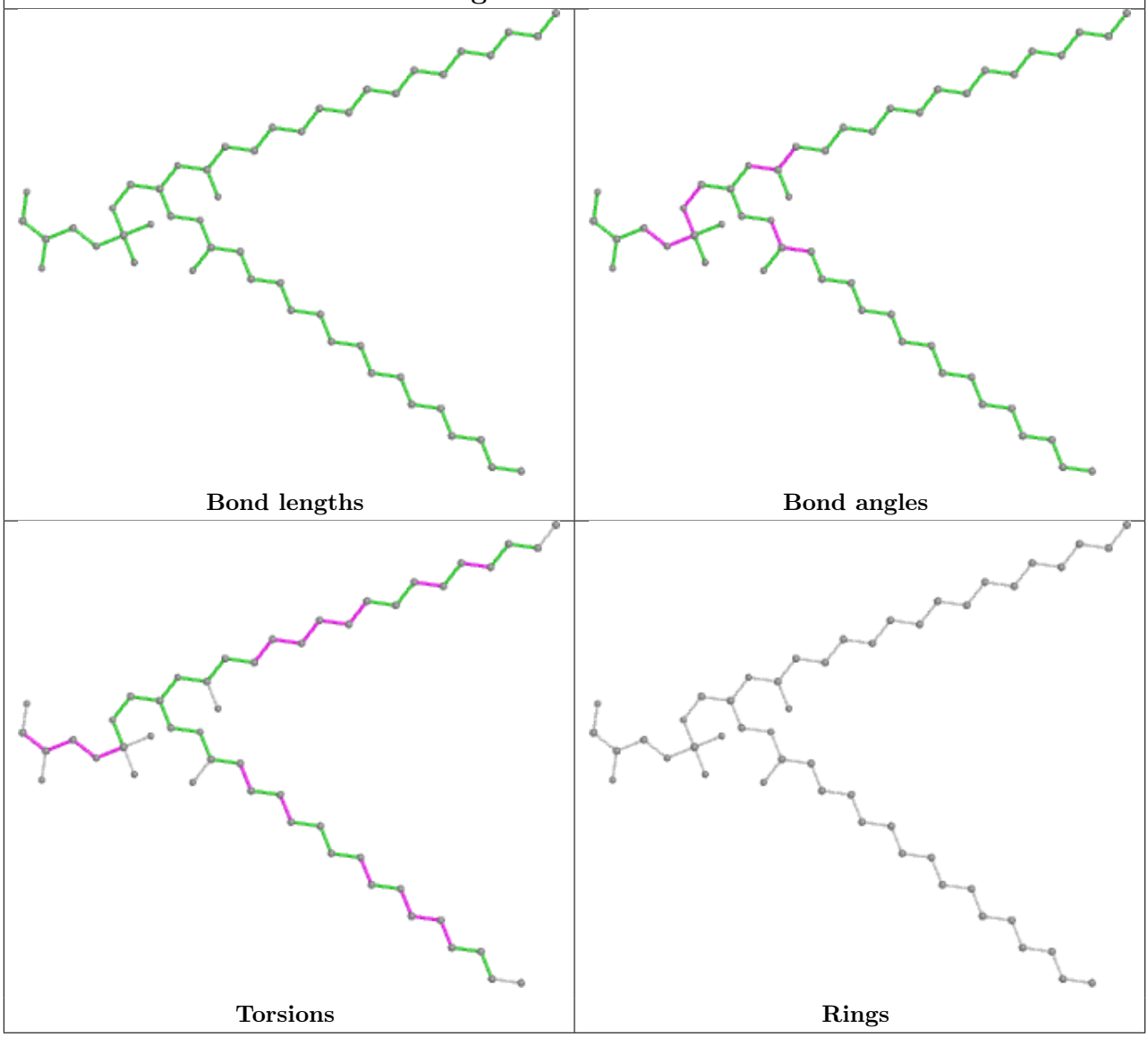

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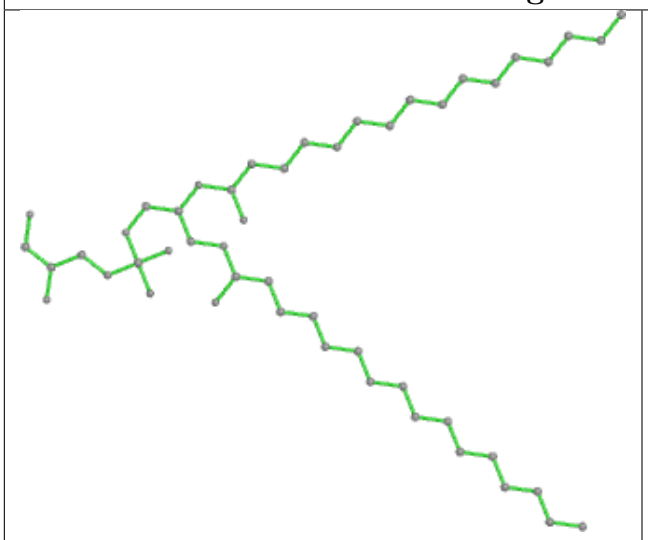

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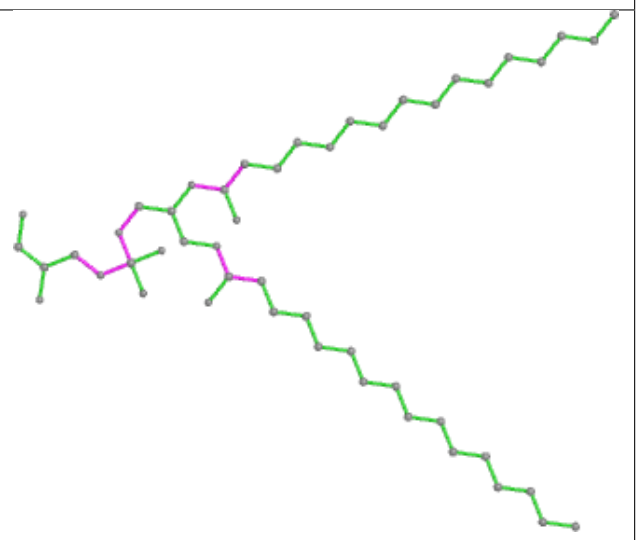

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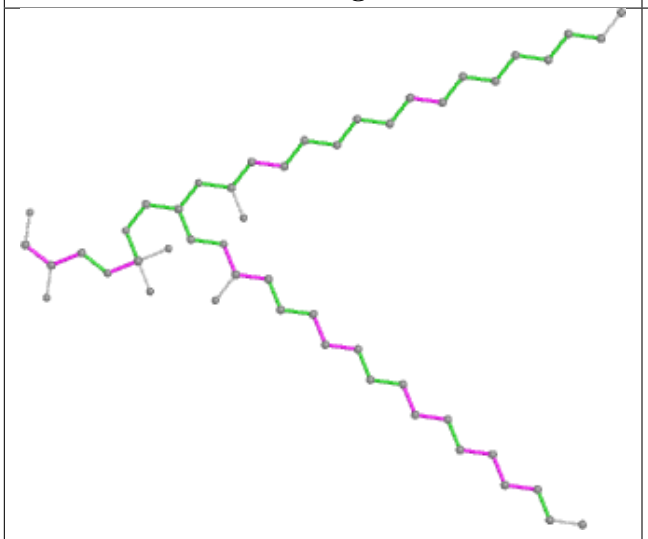

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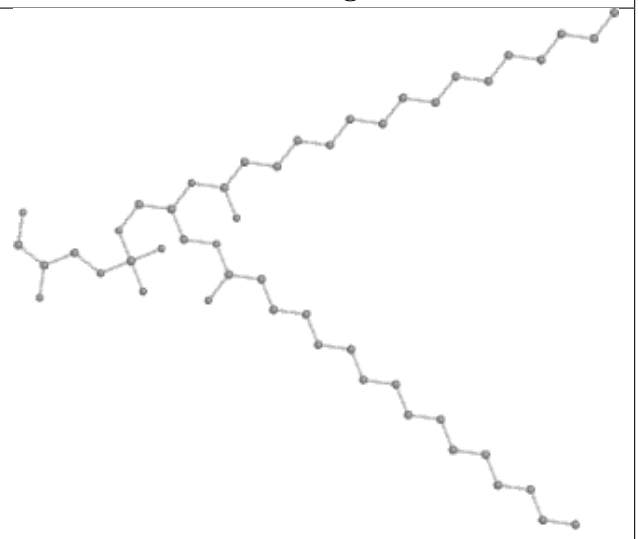
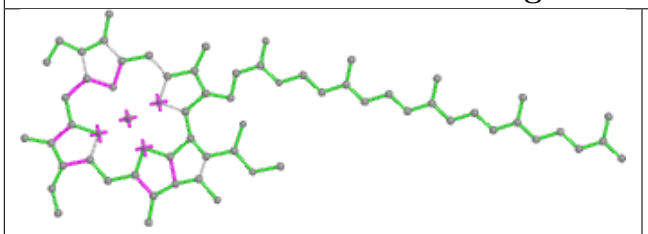


Rings

Ligand CLA N 603



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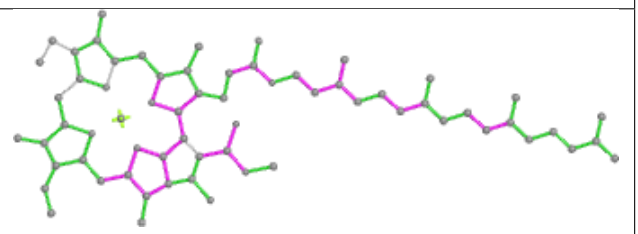

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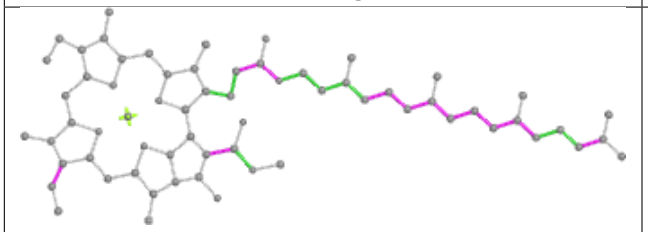

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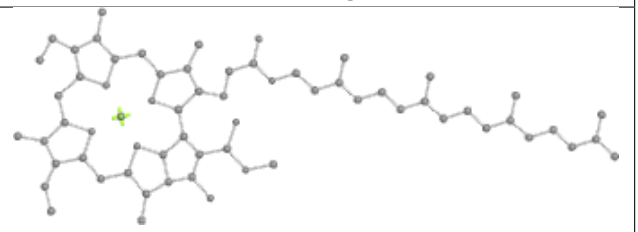
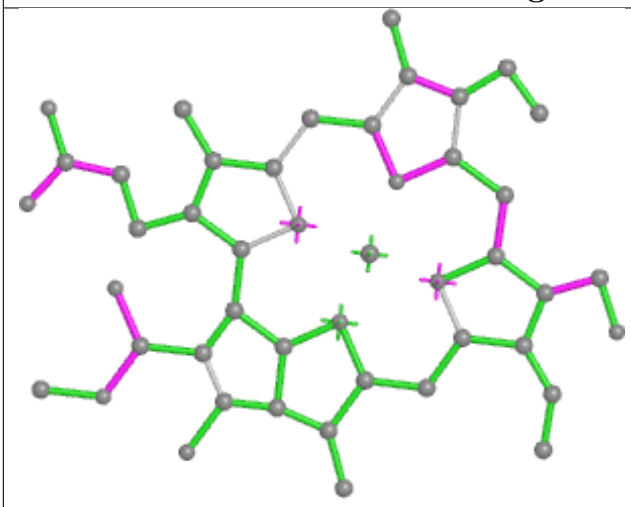


Rings

Ligand CHL 1 302



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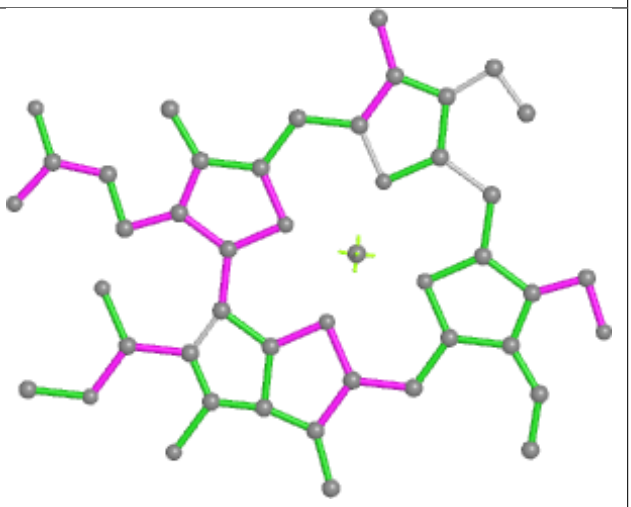

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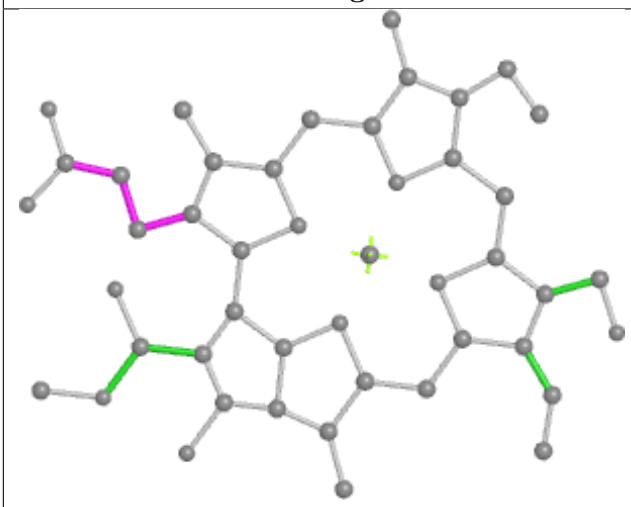

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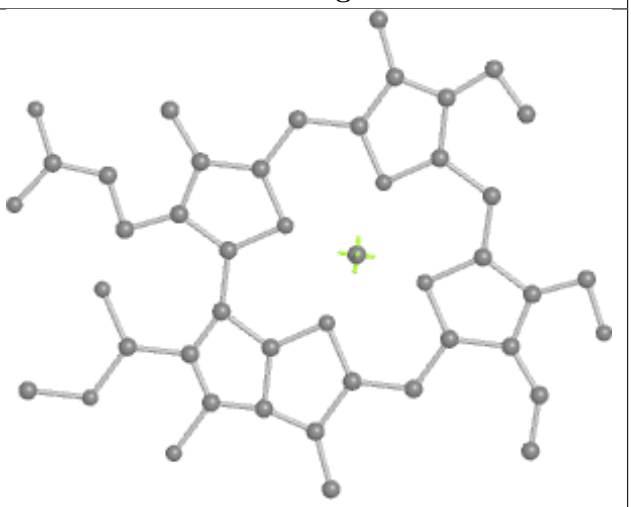
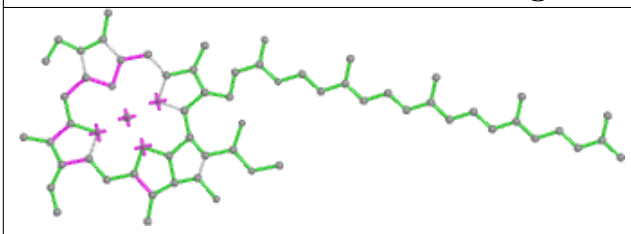


Rings

Ligand CLA c 502



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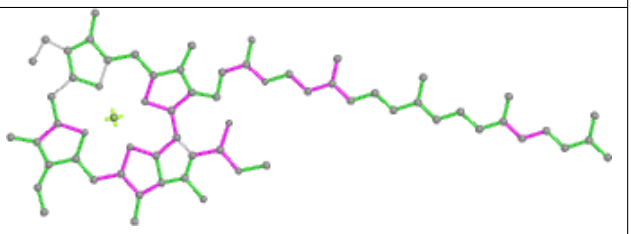

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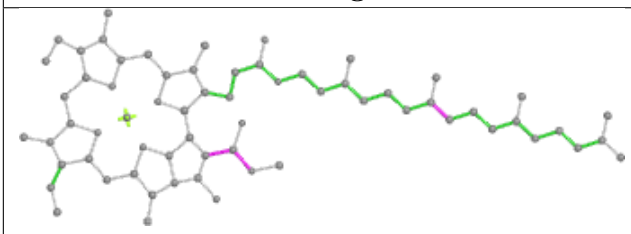

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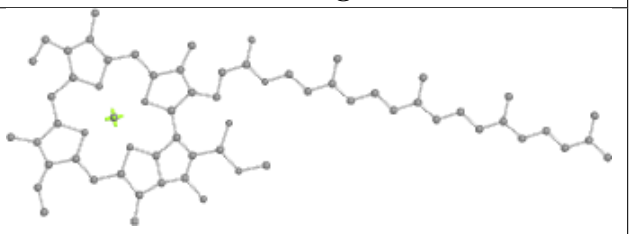
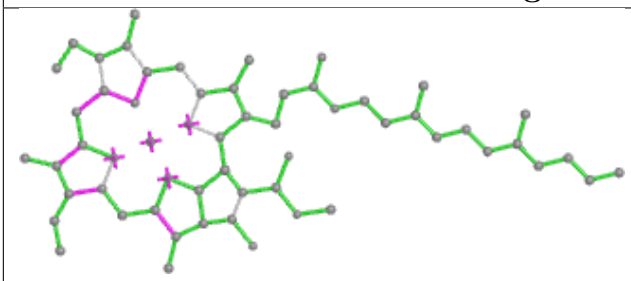
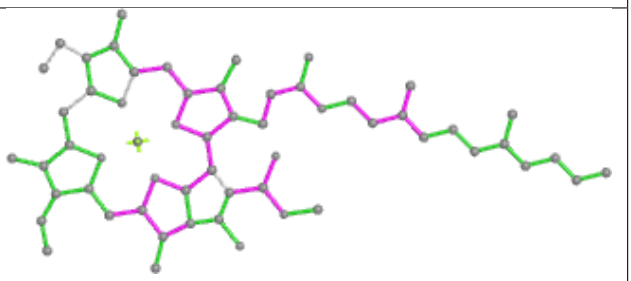
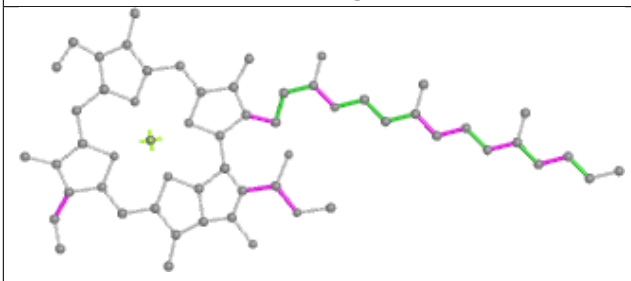
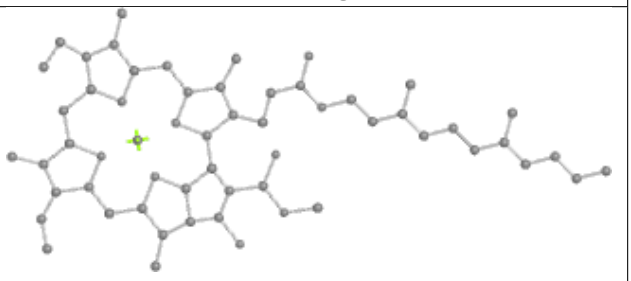
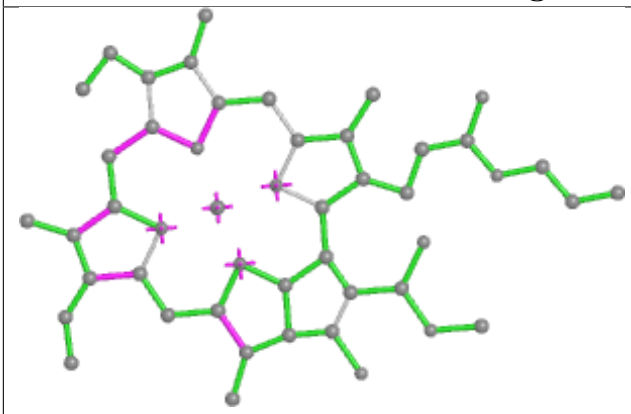
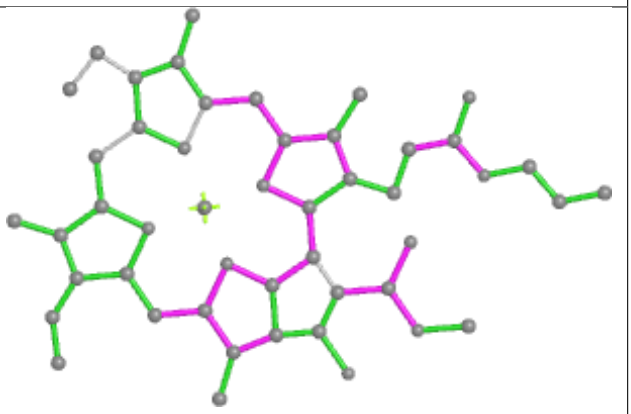
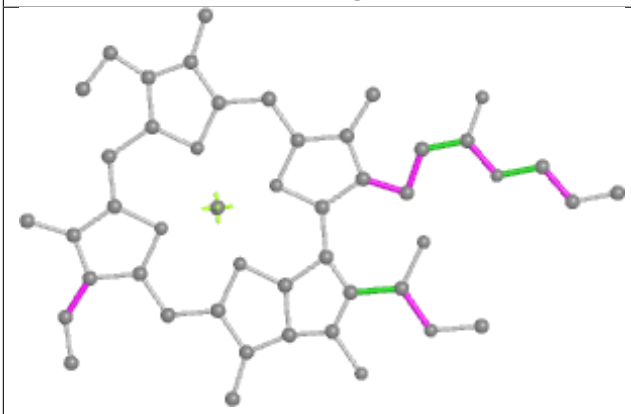
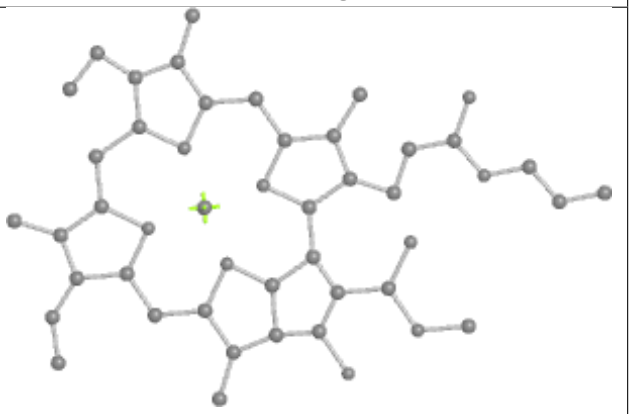
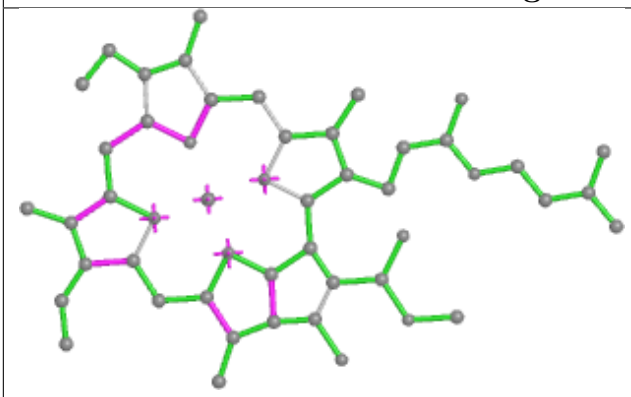


Rings

Ligand CLA R 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA D 401



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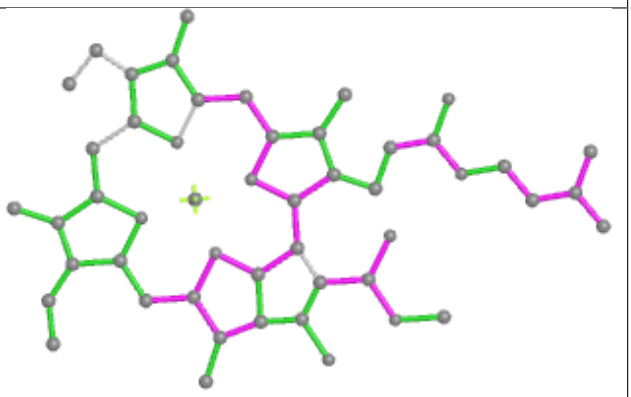

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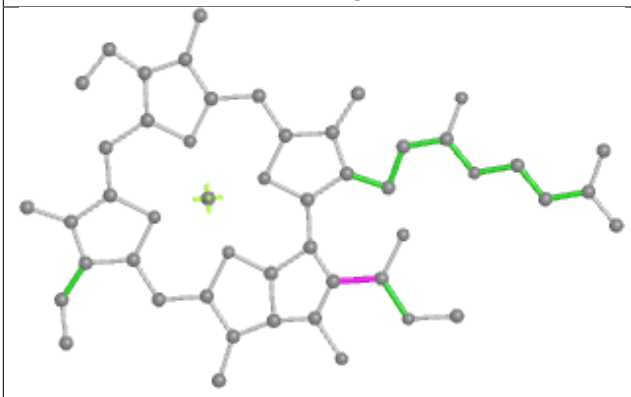

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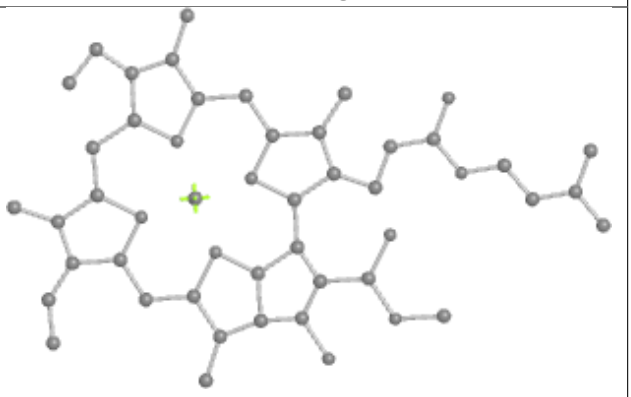
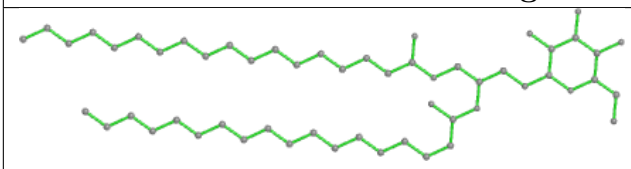


Rings

Ligand LMG B 623



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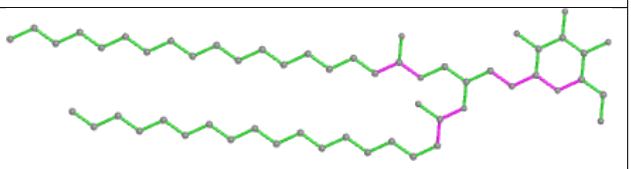

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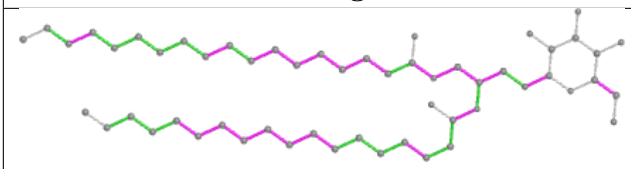
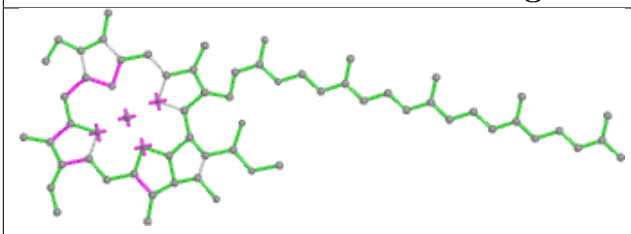
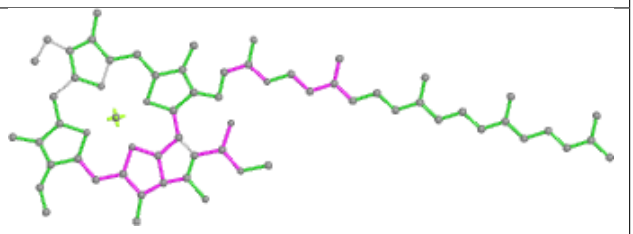
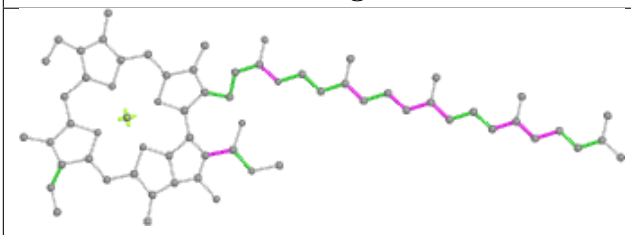
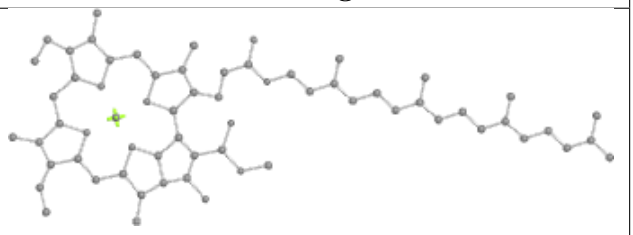


Torsions

Rings

Ligand CLA C 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

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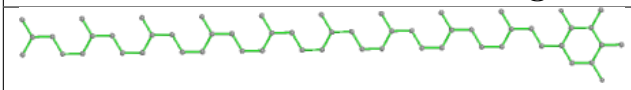
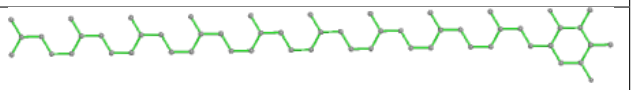
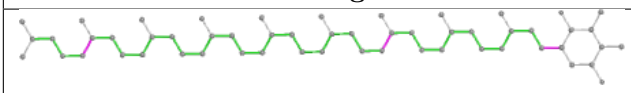
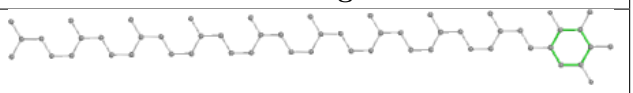
 Bond lengths	 Bond angles
 Torsions	 Rings

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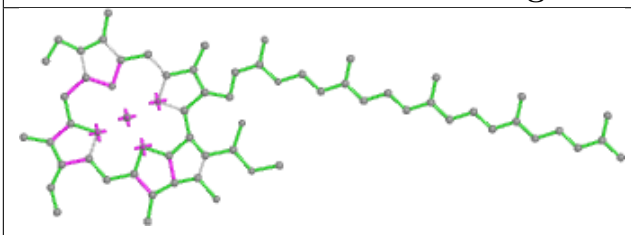
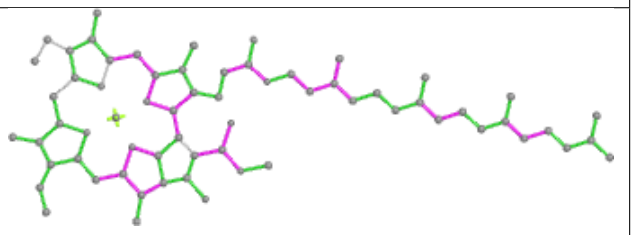
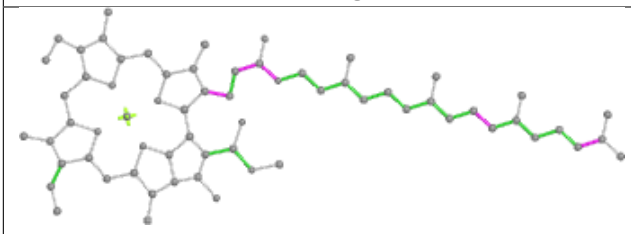
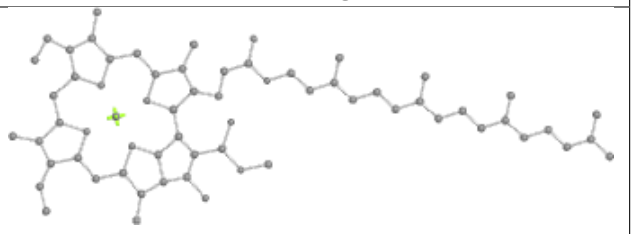
 Bond lengths	 Bond angles
 Torsions	 Rings

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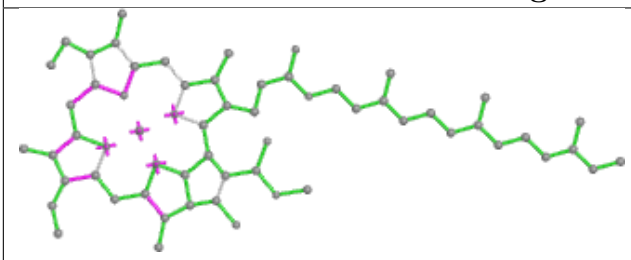
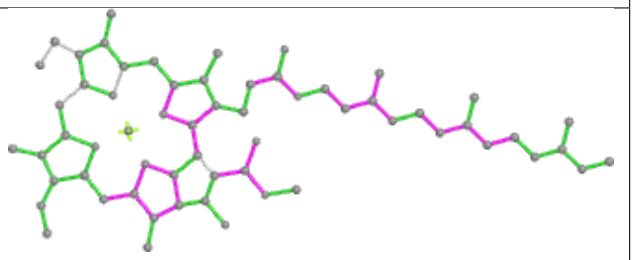
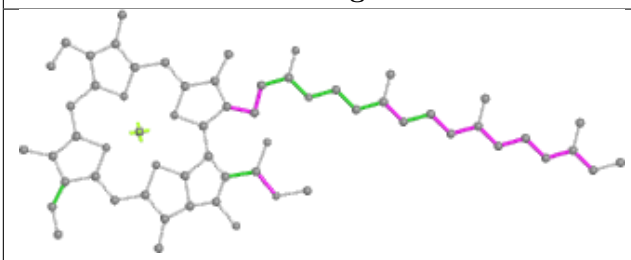
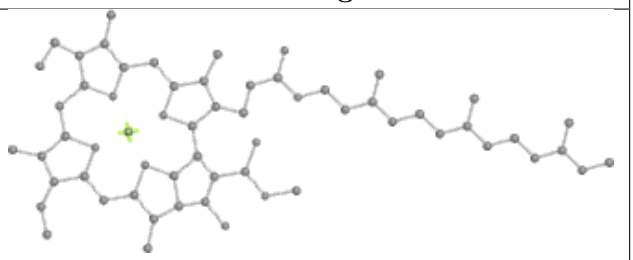
 Bond lengths	 Bond angles
 Torsions	 Rings

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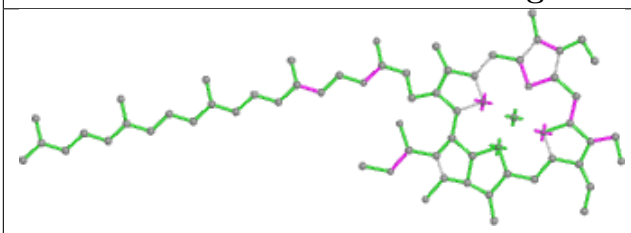
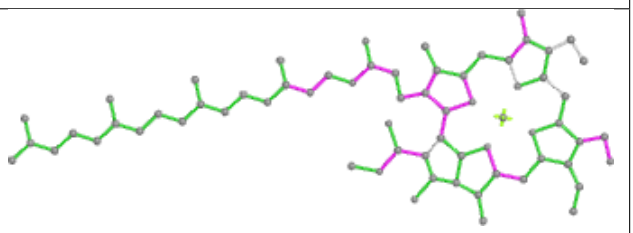
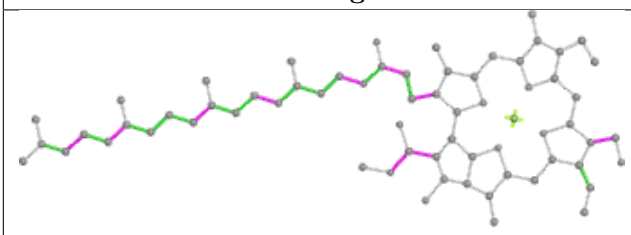
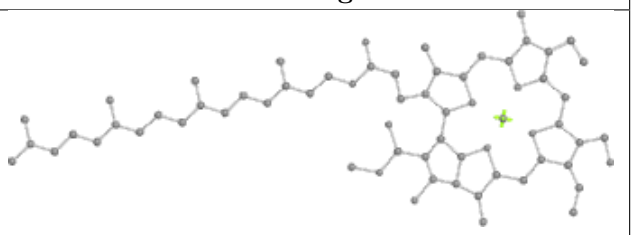
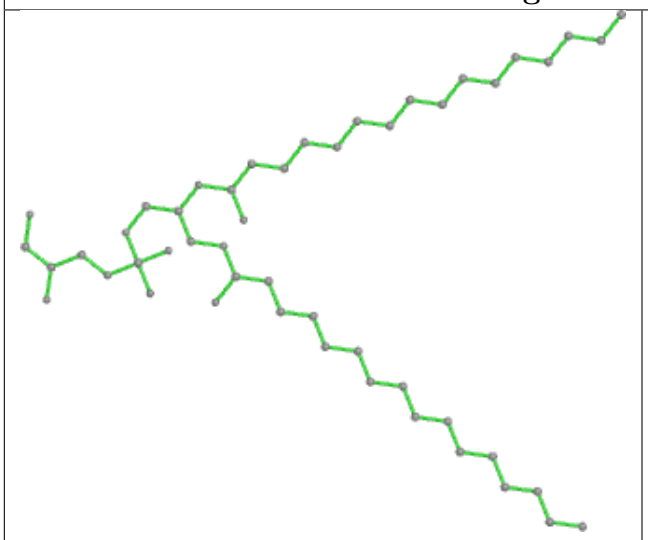
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG Y 301



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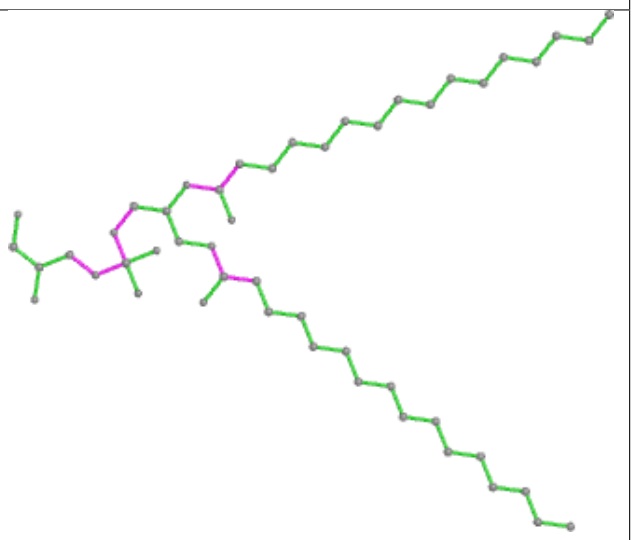

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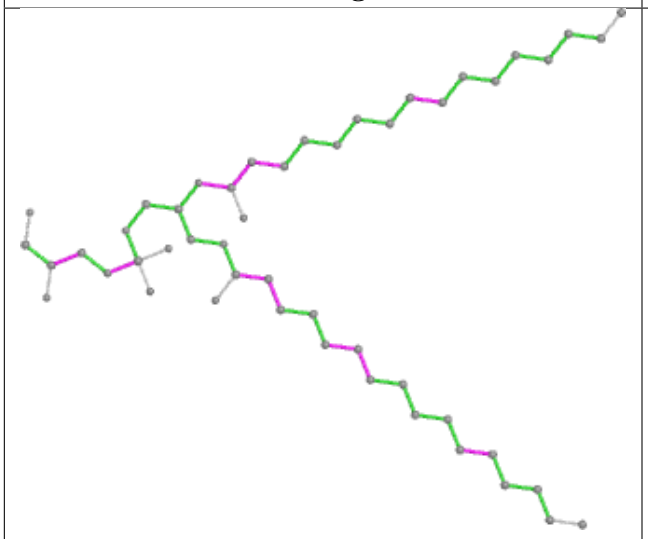

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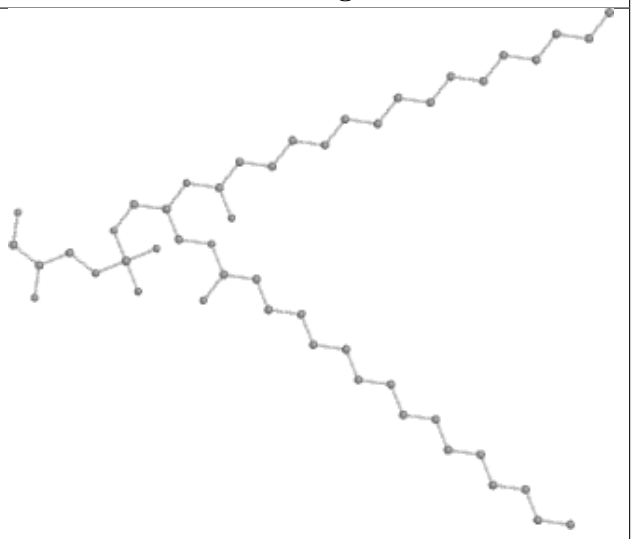
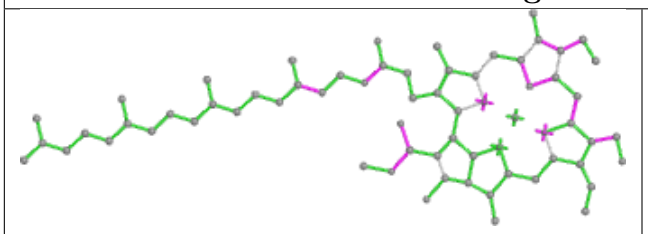


Rings

Ligand CHL G 608



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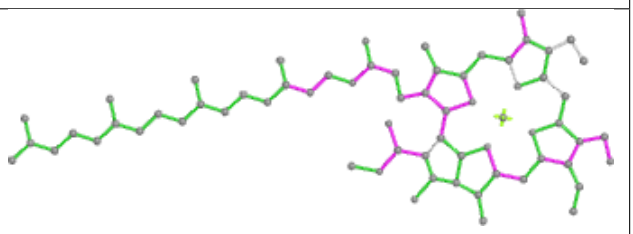

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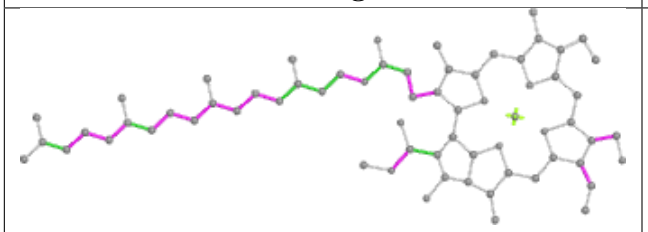

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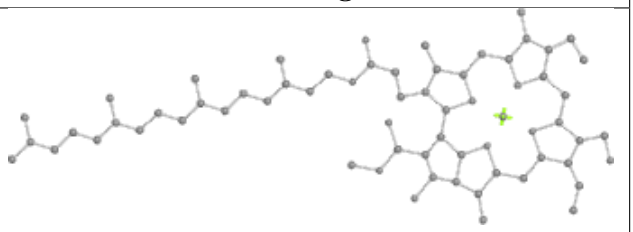
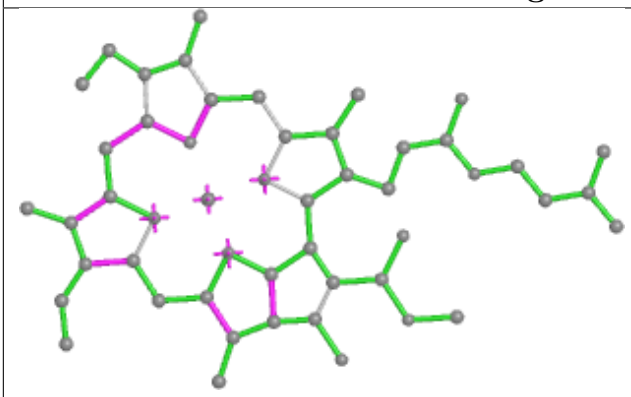
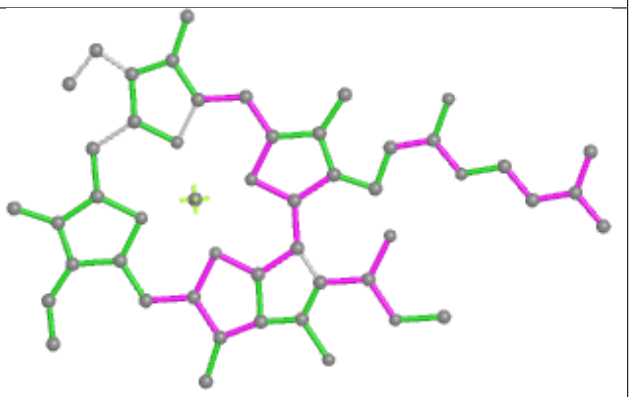
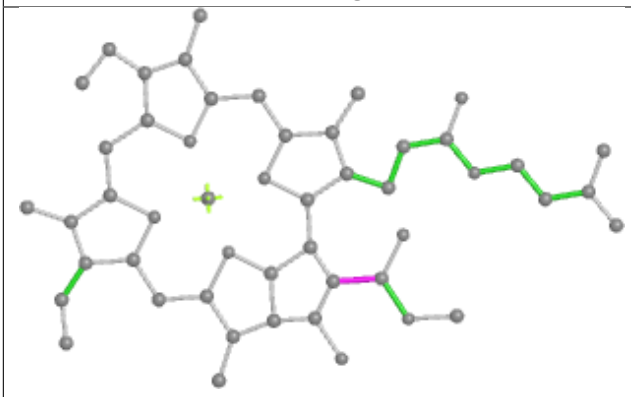
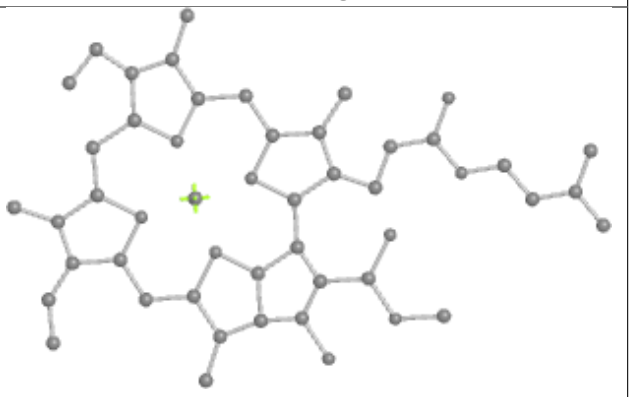


Rings

Ligand CLA d 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

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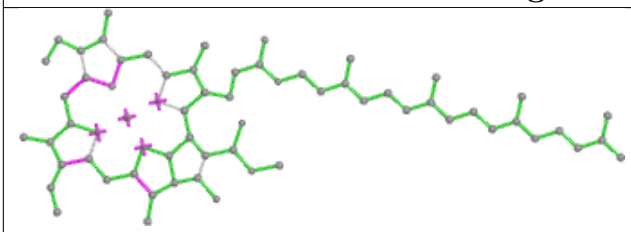
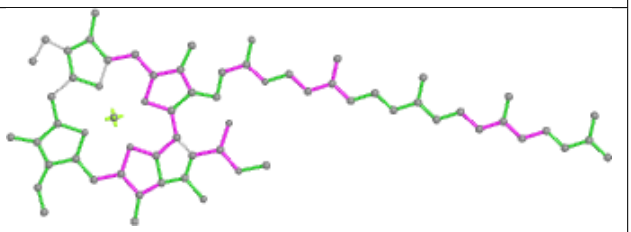
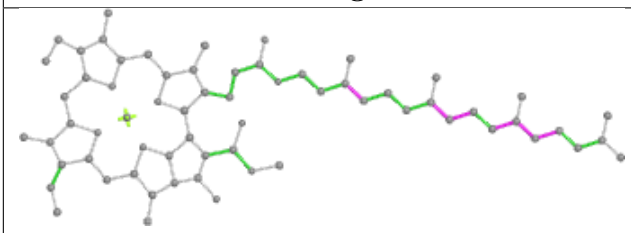
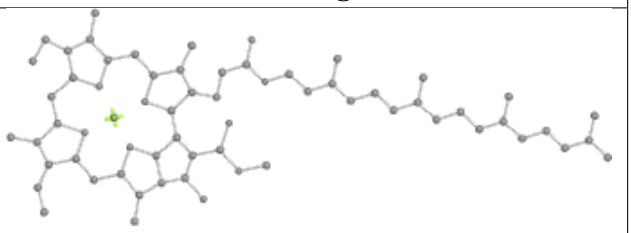
 Bond lengths	 Bond angles
 Torsions	 Rings

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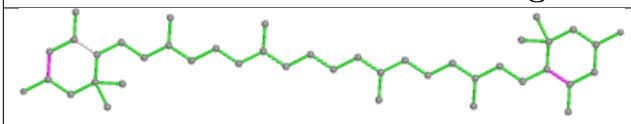
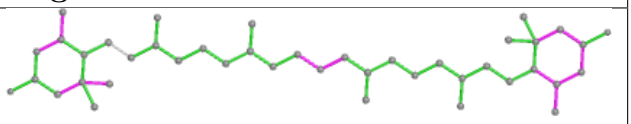
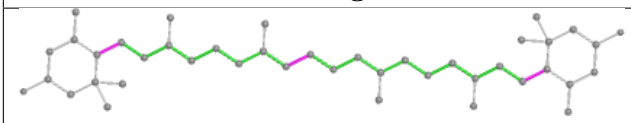
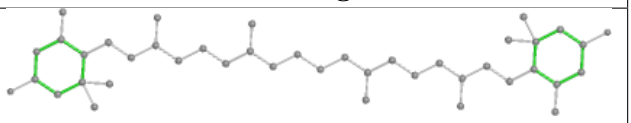
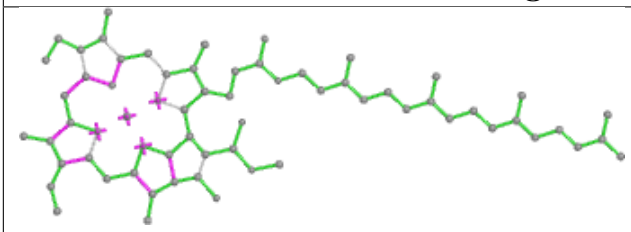
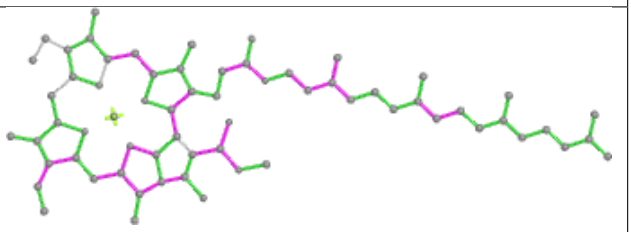
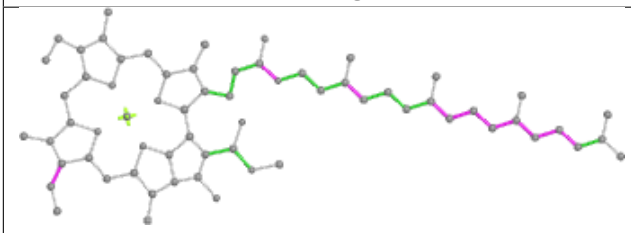
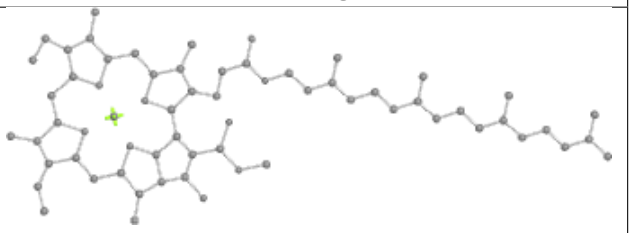
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

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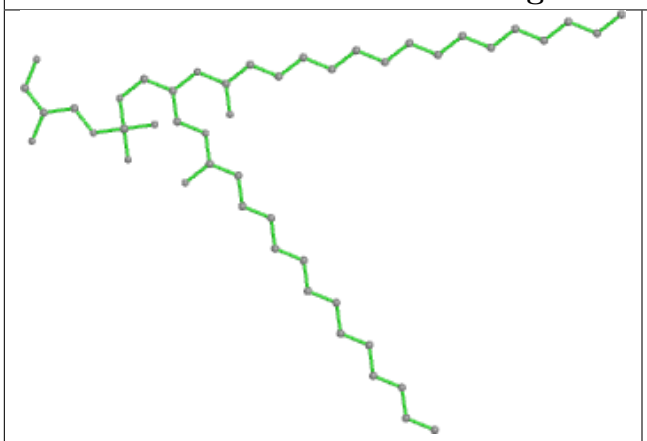
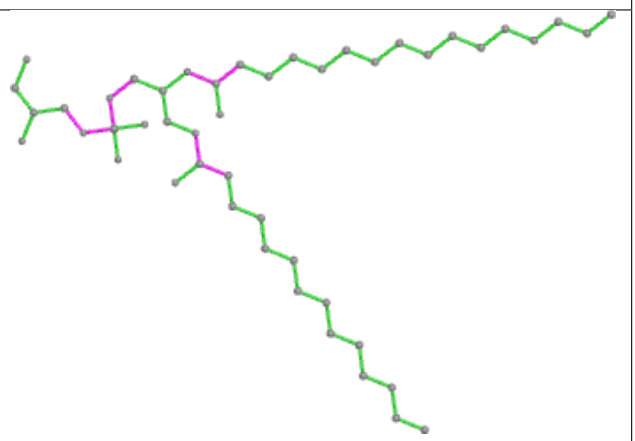
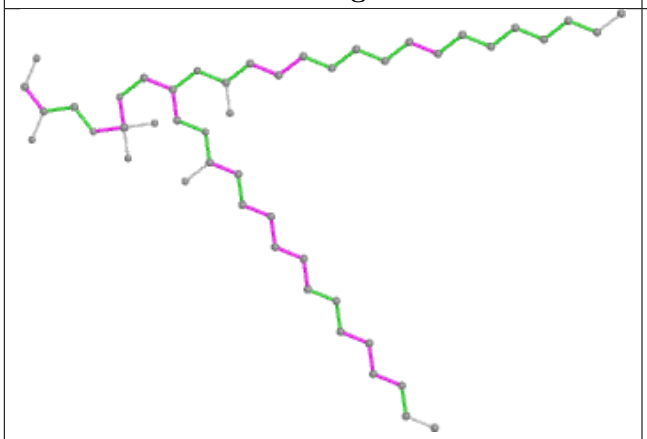
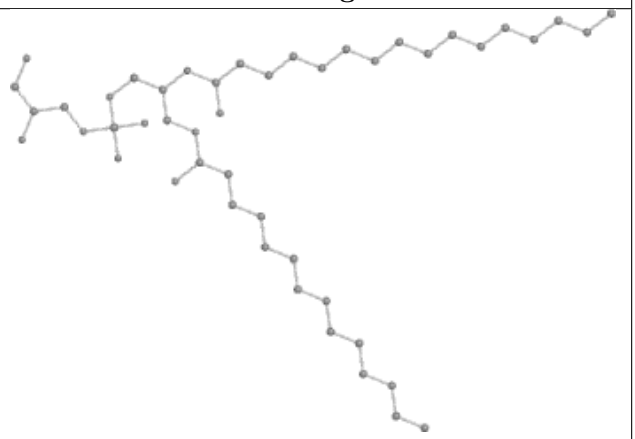
 Bond lengths	 Bond angles
 Torsions	 Rings

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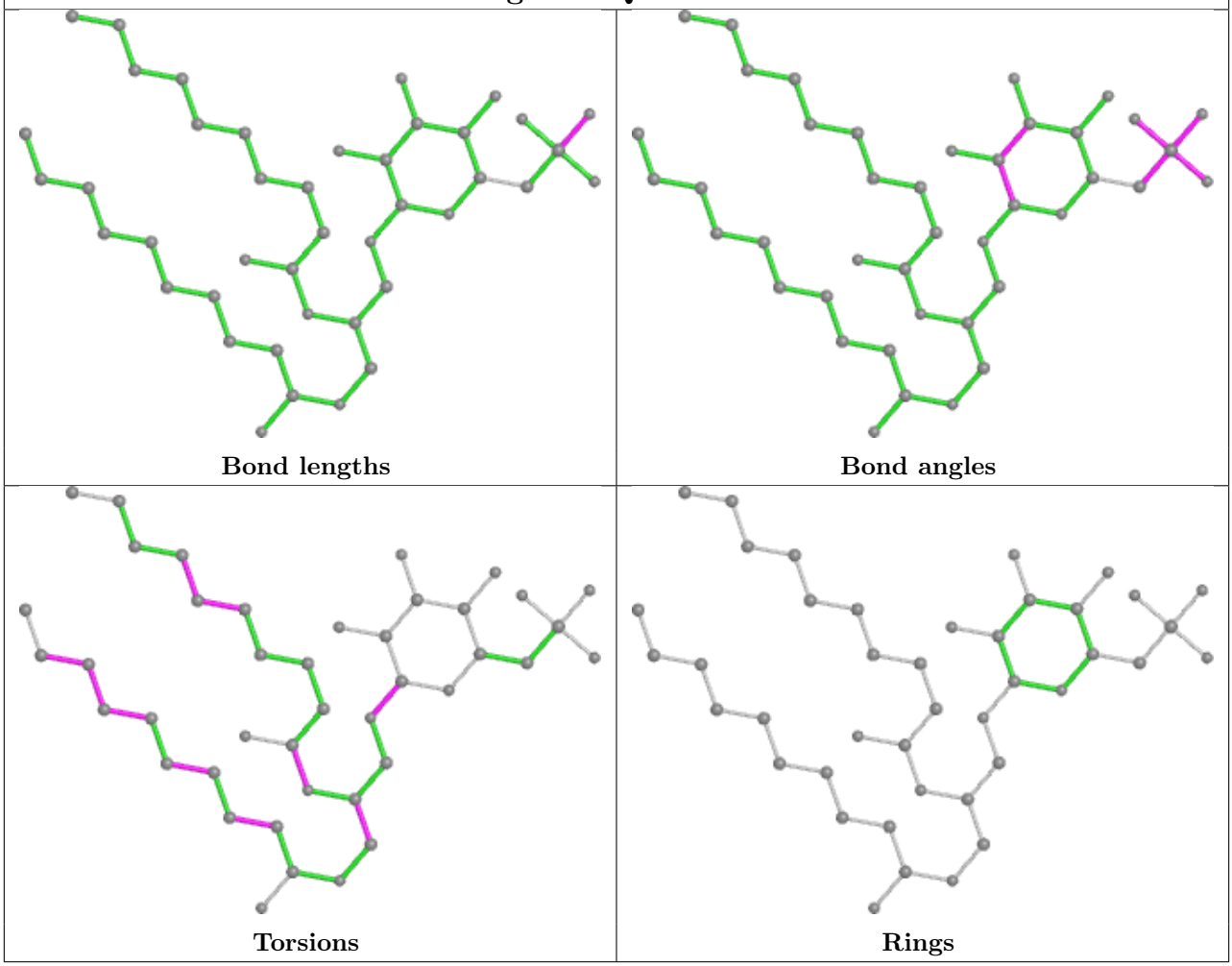
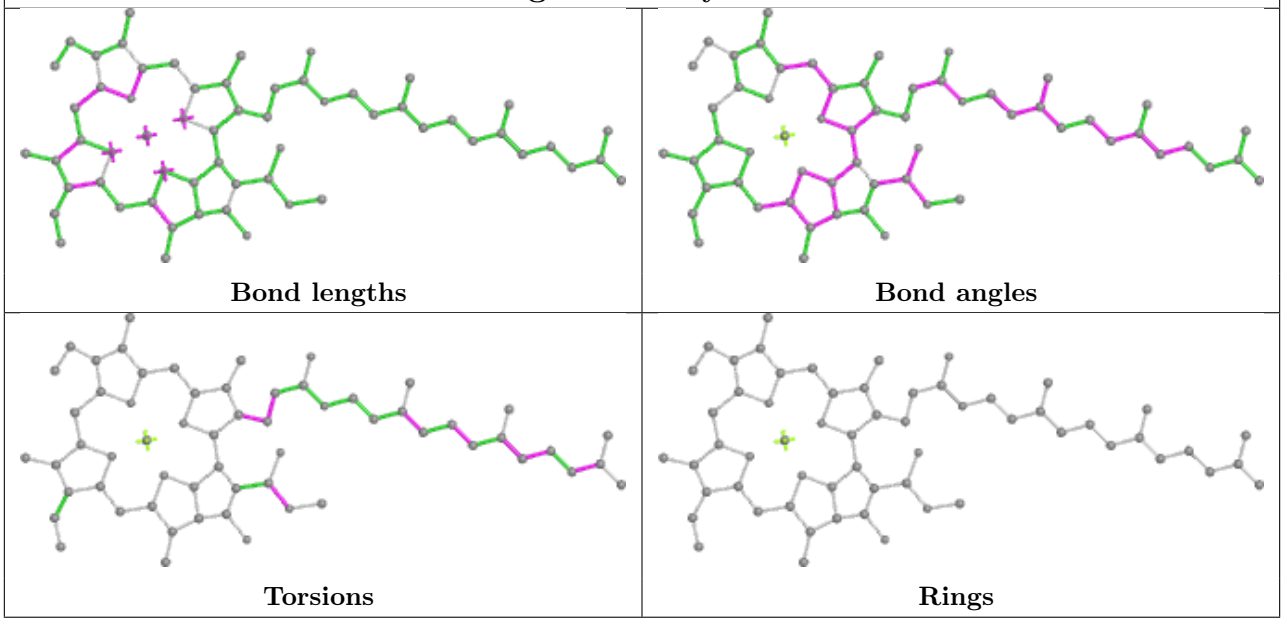


Ligand CLA y 311



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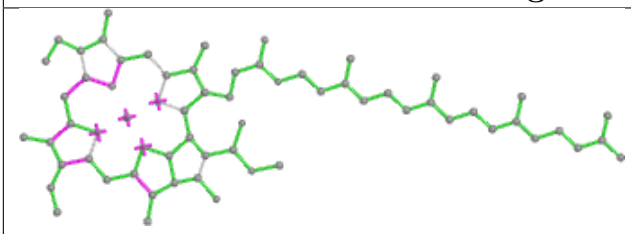
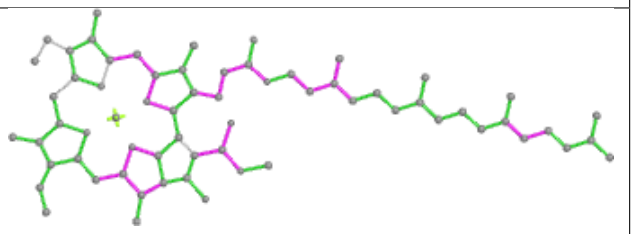
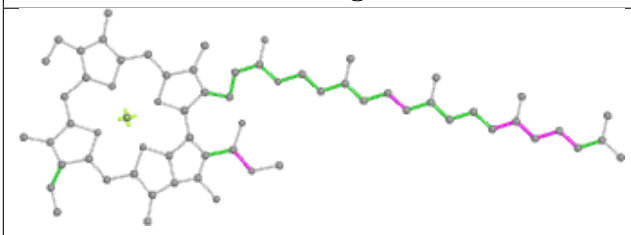
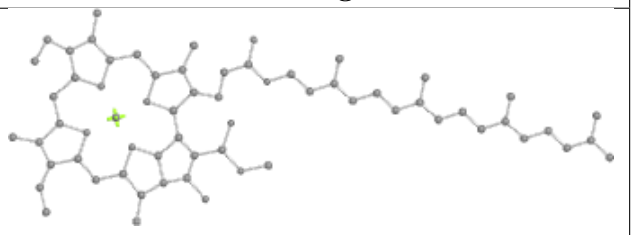
 Bond lengths	 Bond angles
 Torsions	 Rings

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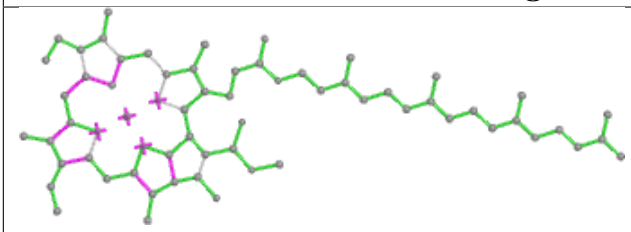
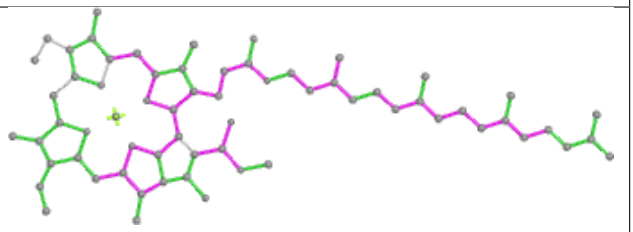
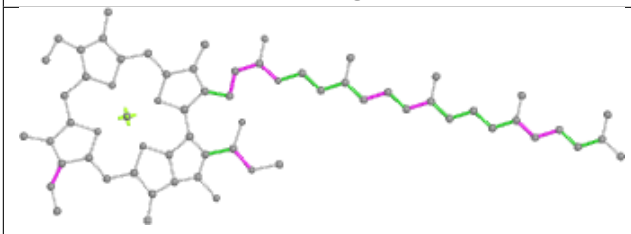
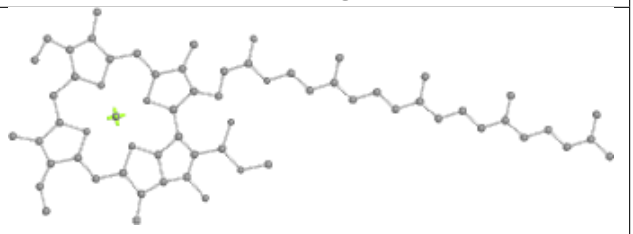
 Bond lengths	 Bond angles
 Torsions	 Rings

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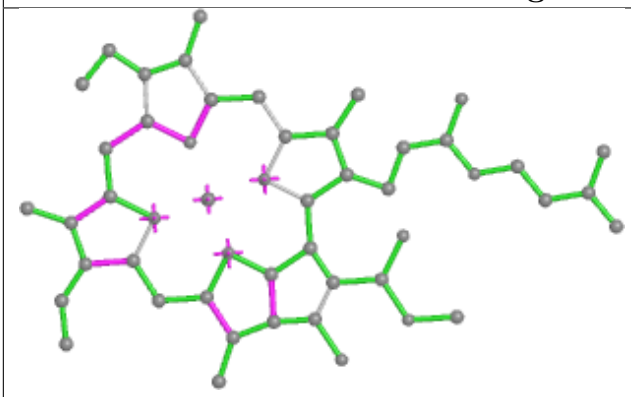
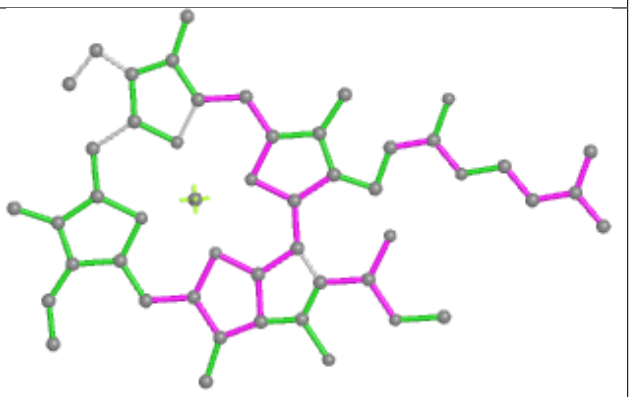
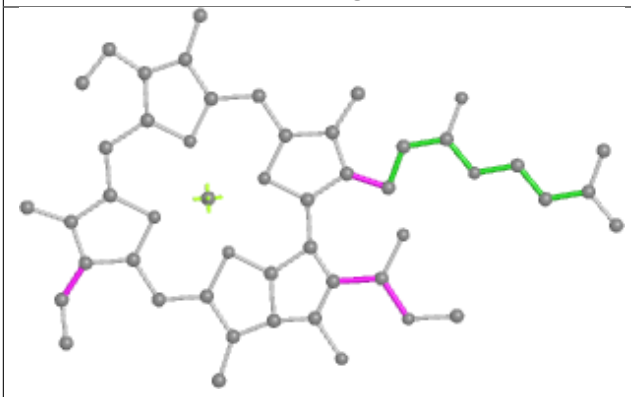
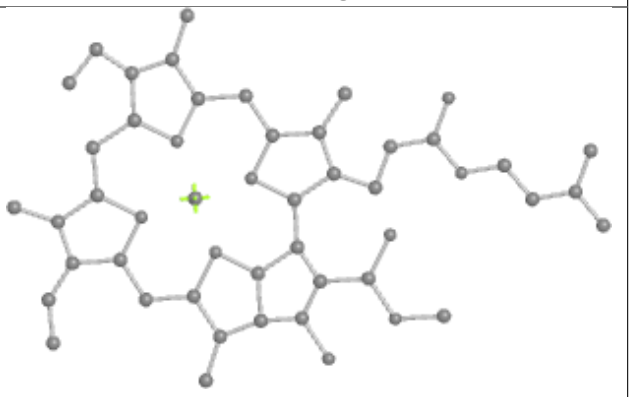
 Bond lengths	 Bond angles
 Torsions	 Rings

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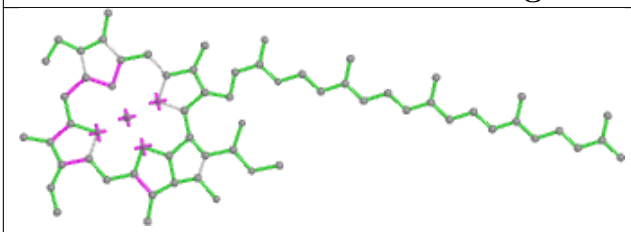
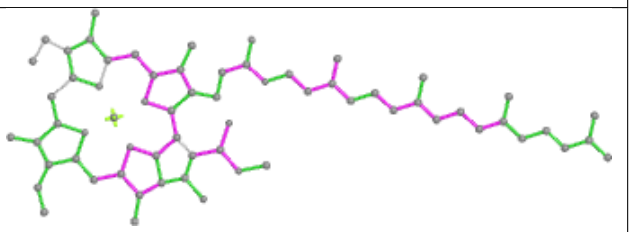
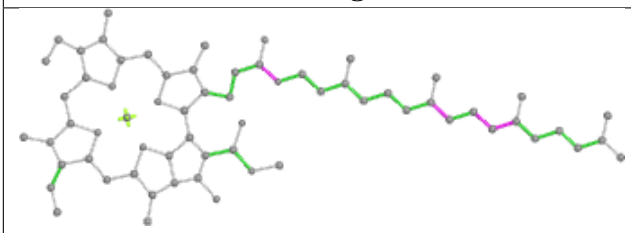
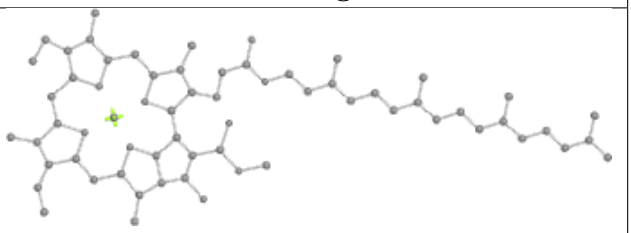
 Bond lengths	 Bond angles
 Torsions	 Rings

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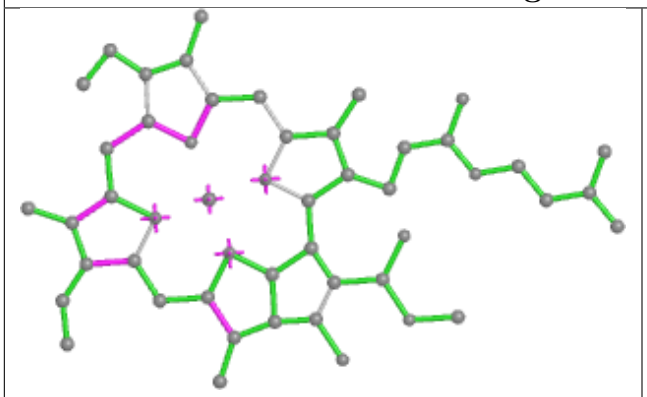

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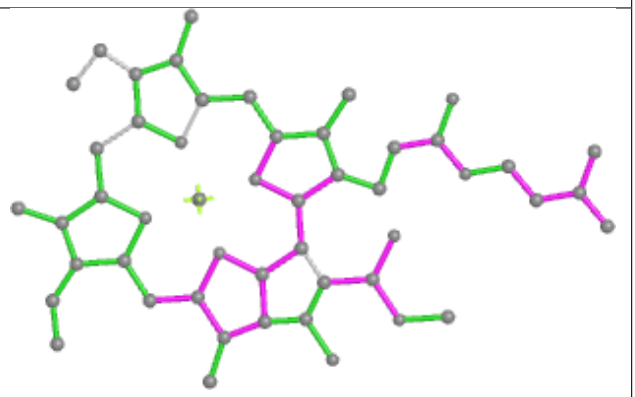

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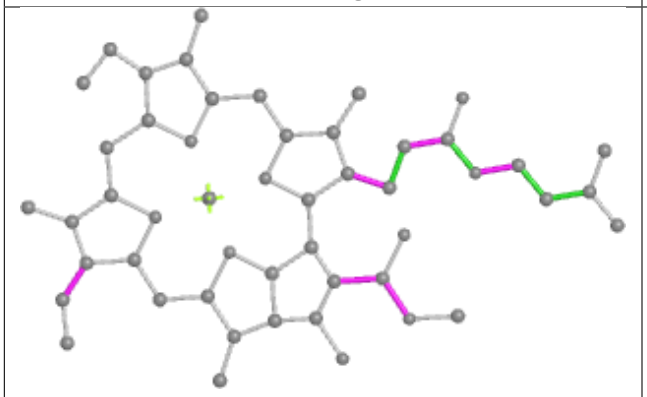

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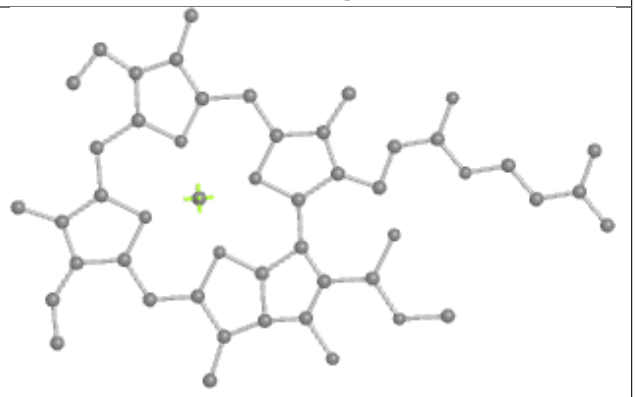
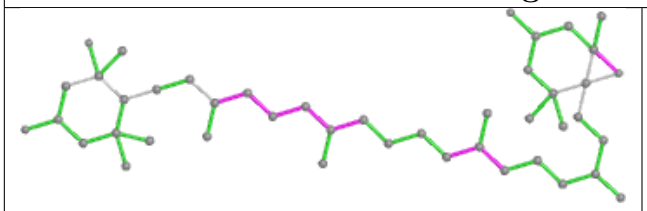


Rings

Ligand NEX G 617



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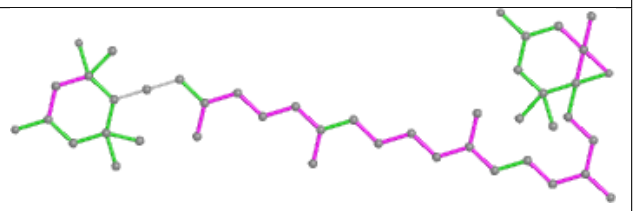

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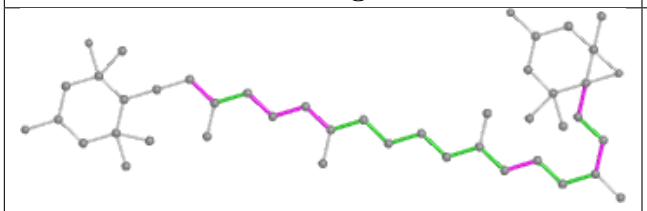

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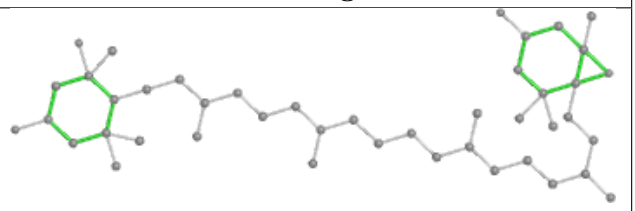
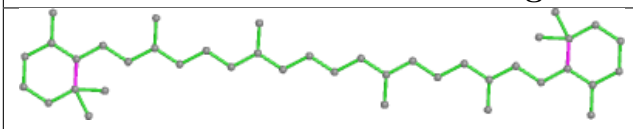


Rings

Ligand BCR d 404



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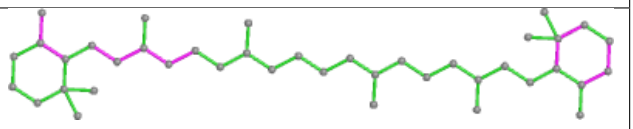

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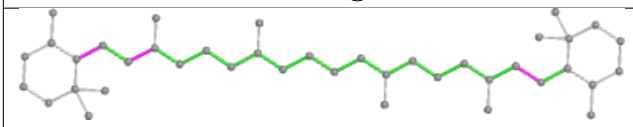

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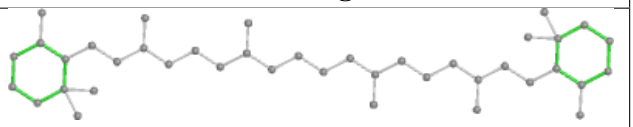
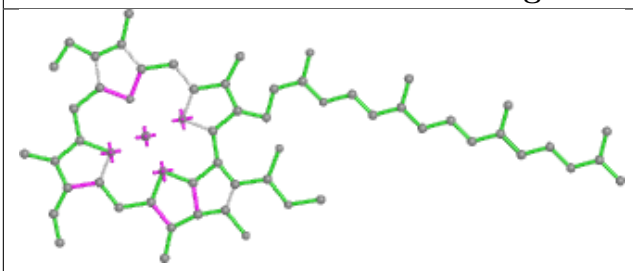


Rings

Ligand CLA R 603



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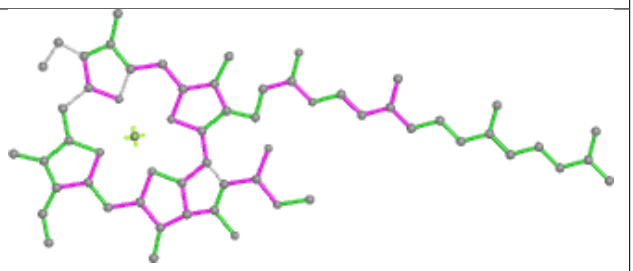

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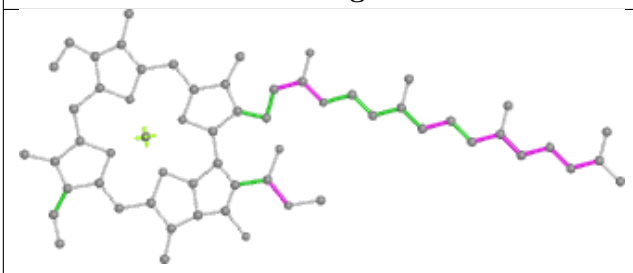

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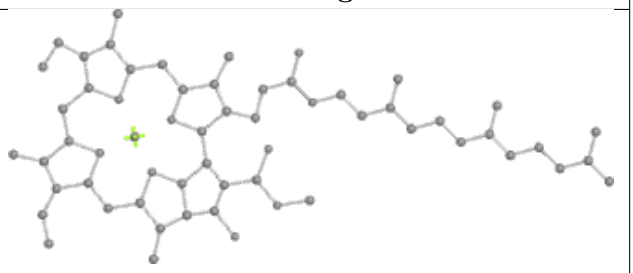
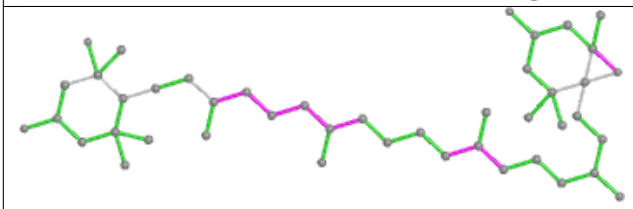


Rings

Ligand NEX S 317



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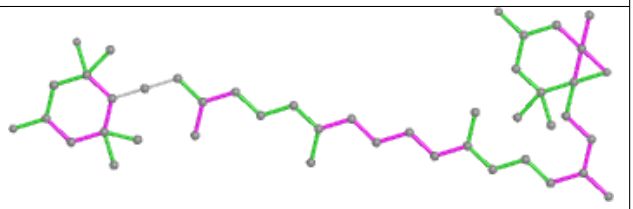

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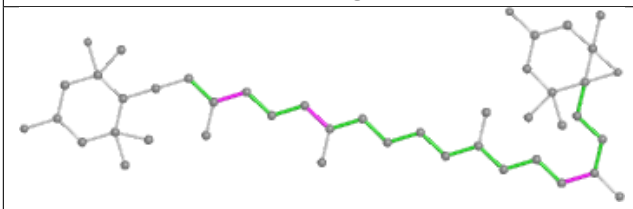

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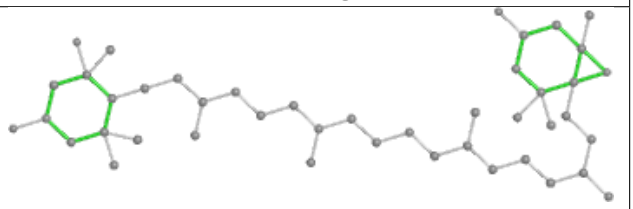
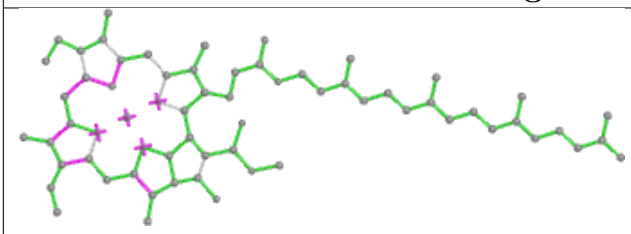
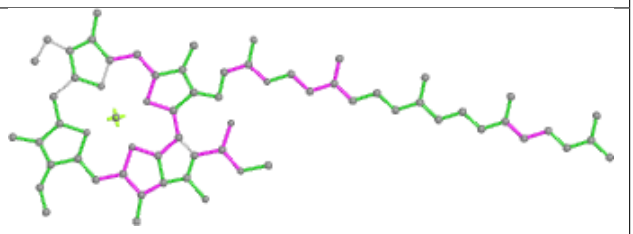
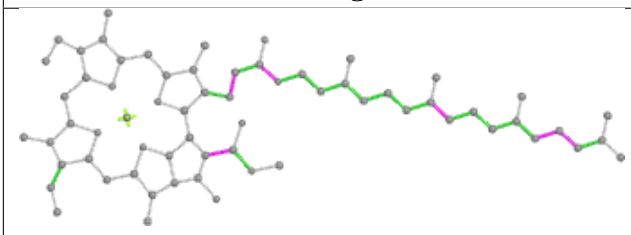
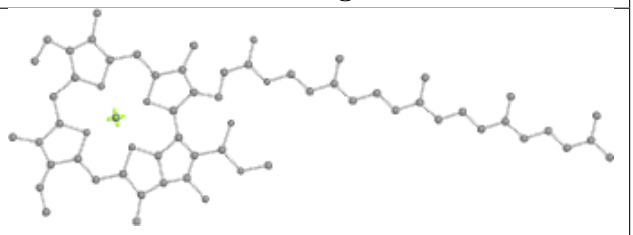


Rings

Ligand CLA B 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

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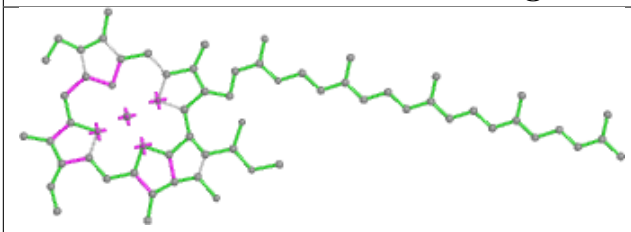
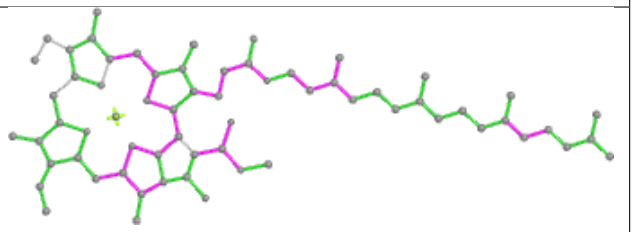
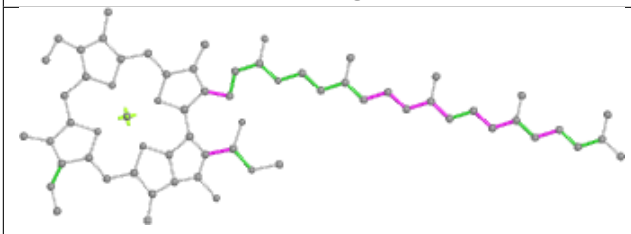
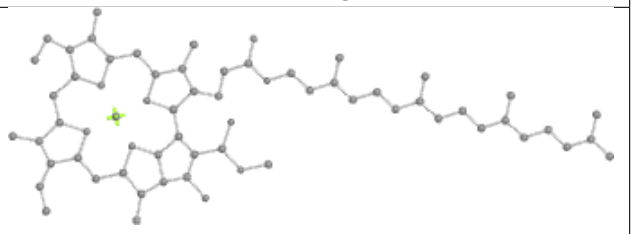
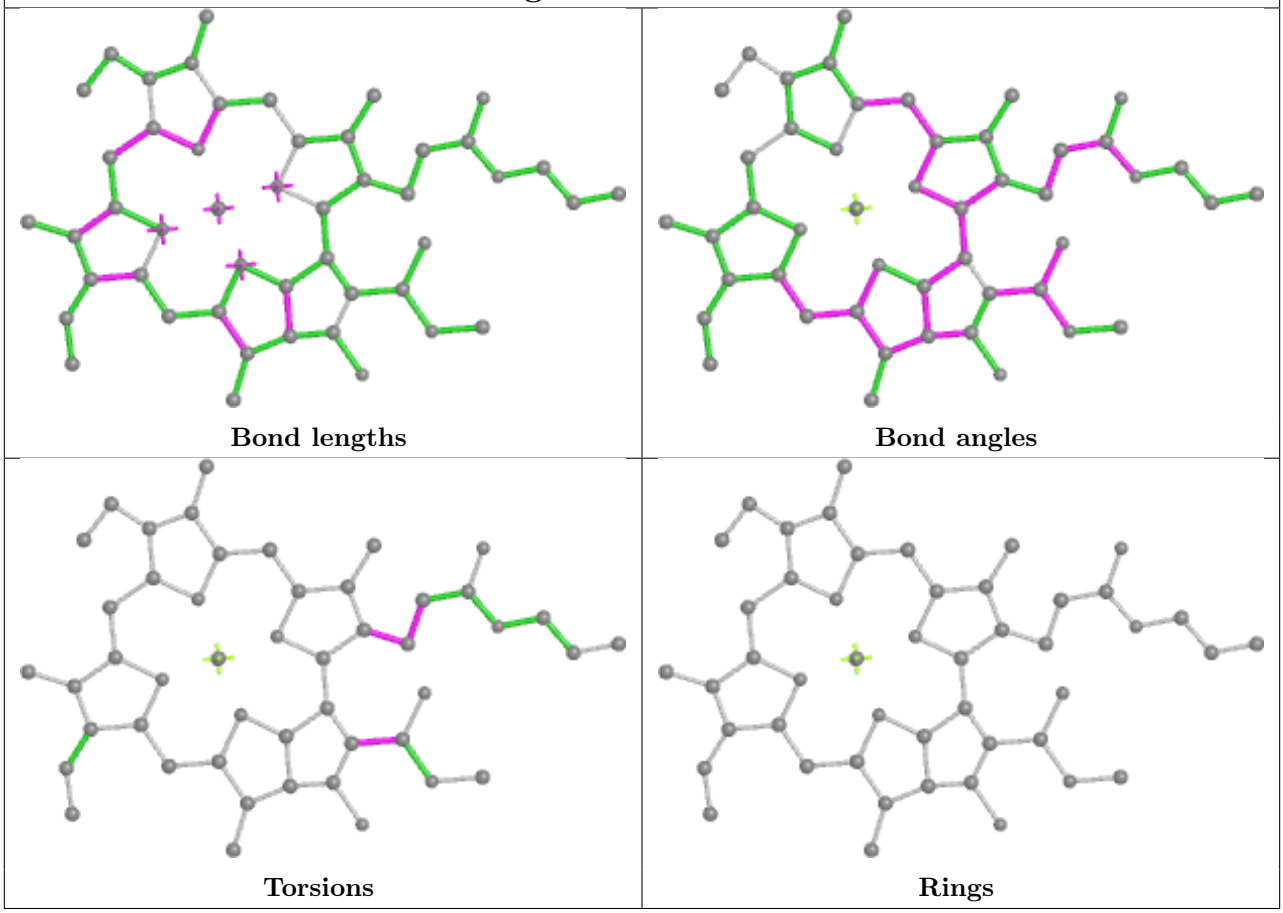
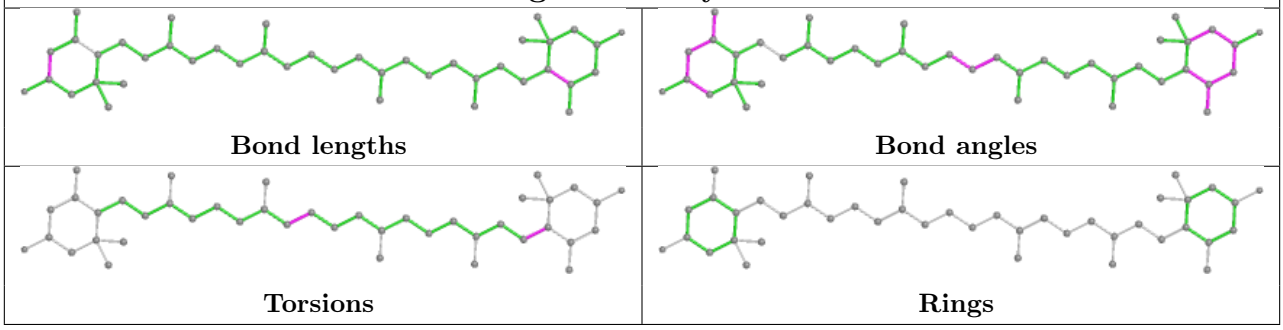
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 604



Ligand LUT y 316



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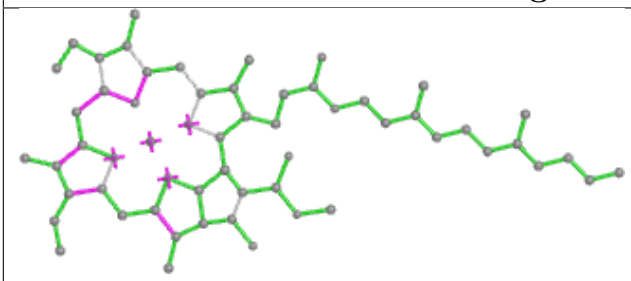
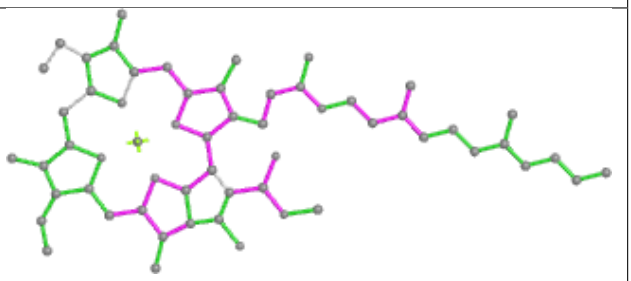
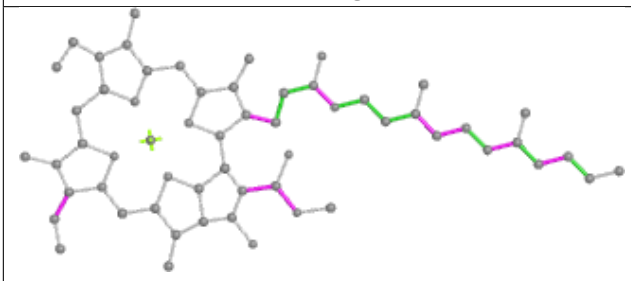
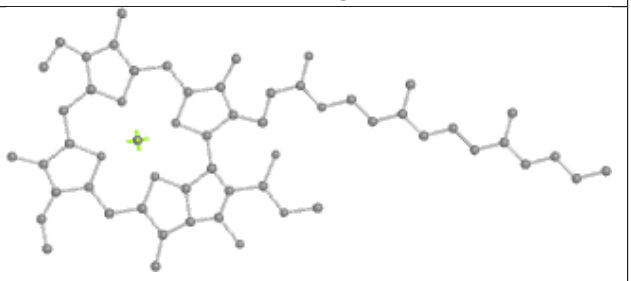
 Bond lengths	 Bond angles
 Torsions	 Rings

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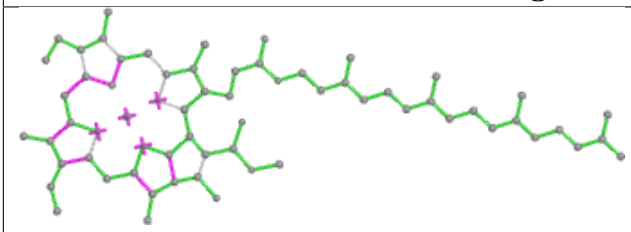
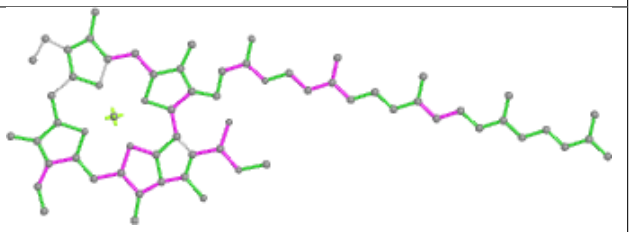
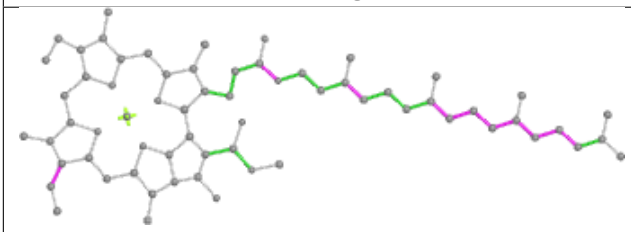
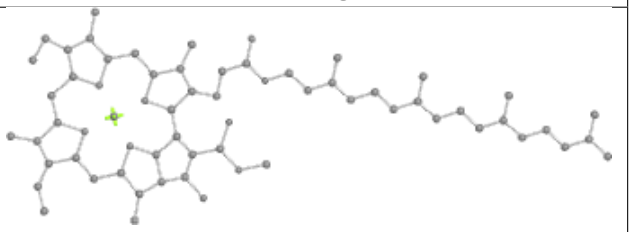
 Bond lengths	 Bond angles
 Torsions	 Rings

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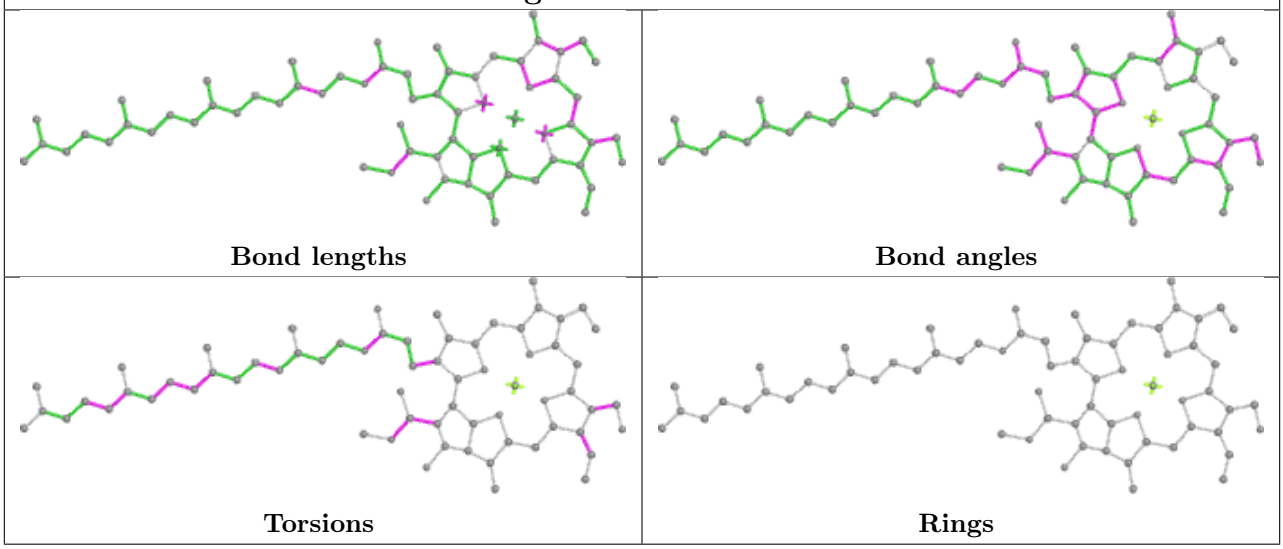

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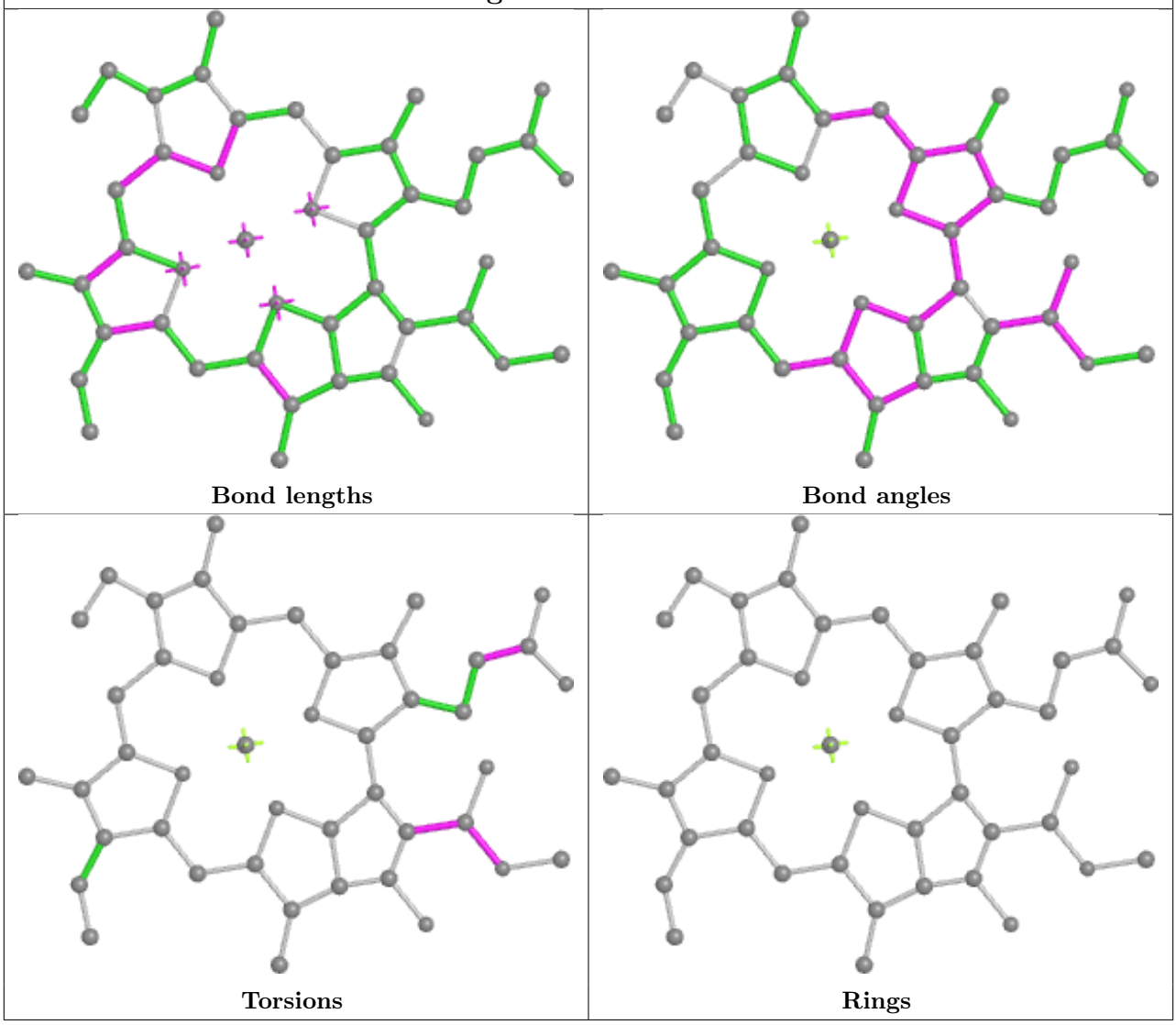
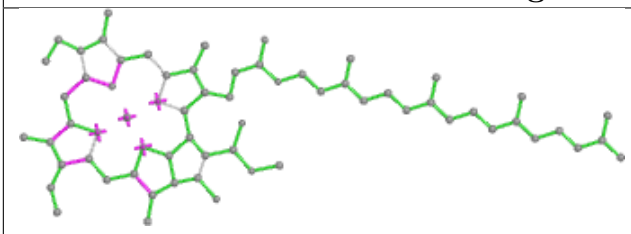
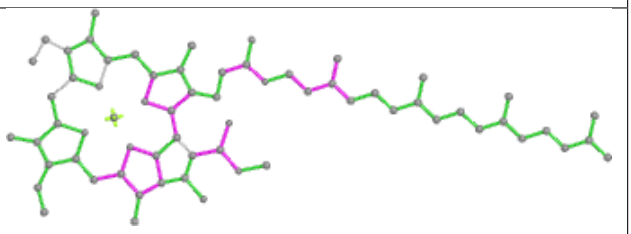


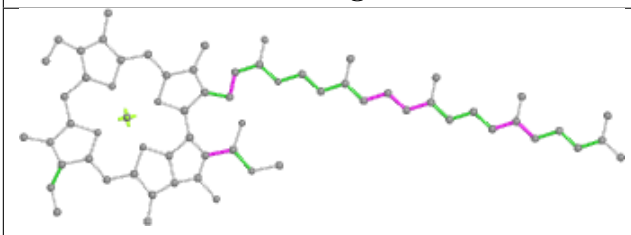
Ligand CLA b 614



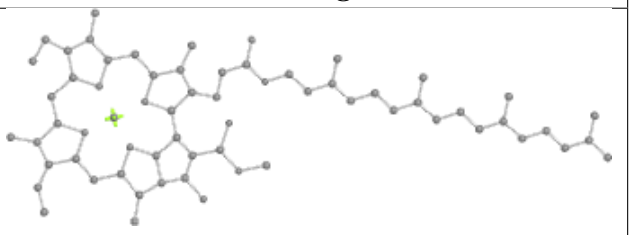
Bond lengths



Bond angles

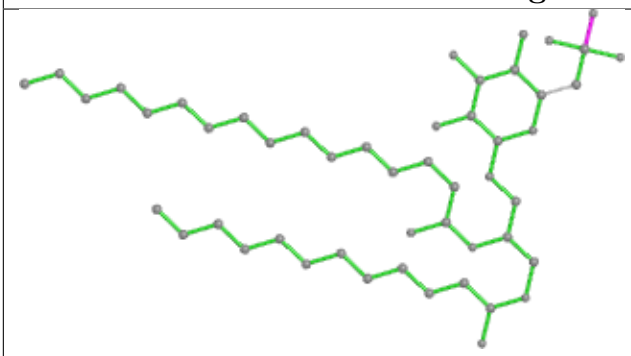


Torsions



Rings

Ligand SQD a 408



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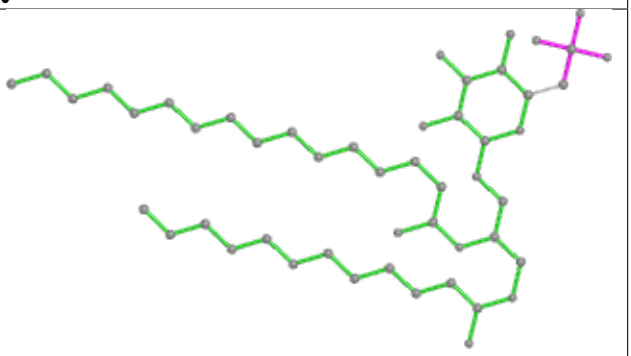
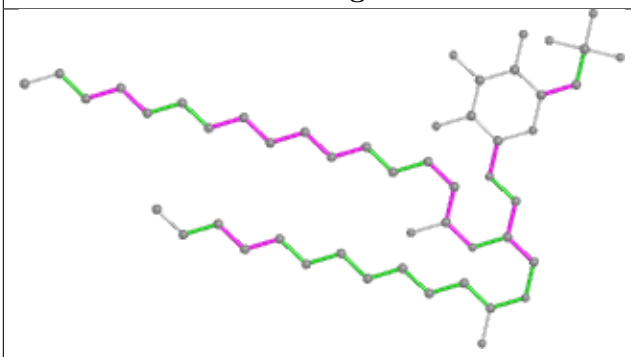


Bond angles



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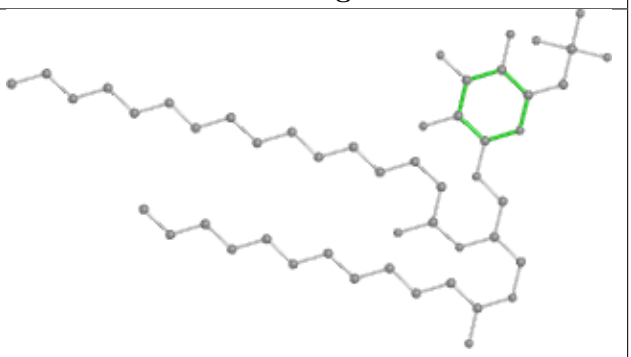
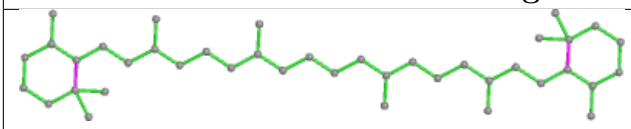


Rings

Ligand BCR C 514



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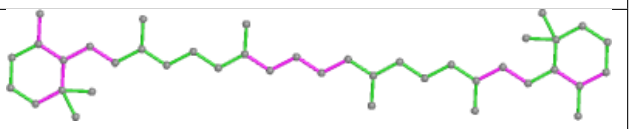
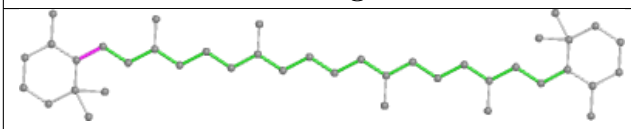


Bond angles



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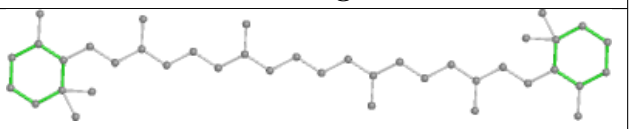
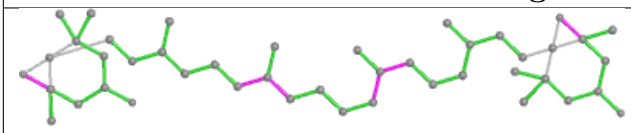


Rings

Ligand XAT r 616



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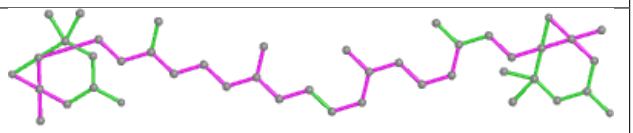
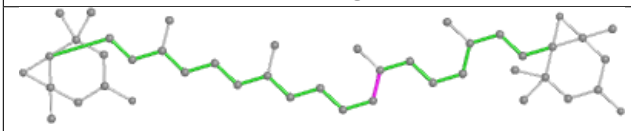


Bond angles



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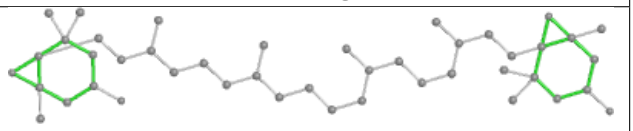
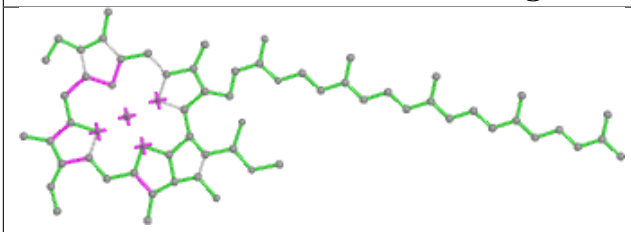


Rings

Ligand CLA B 602



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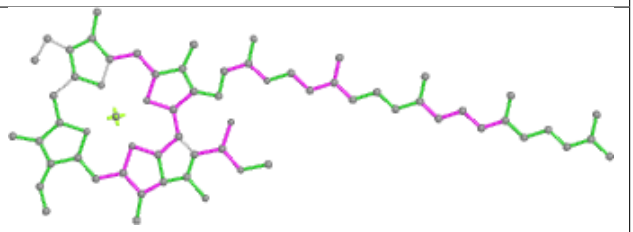

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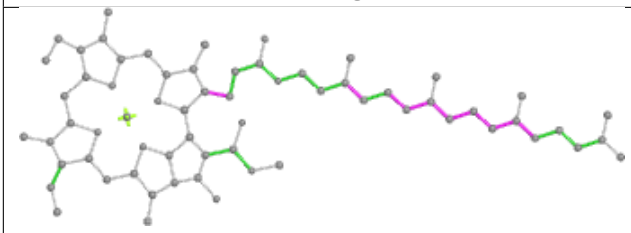

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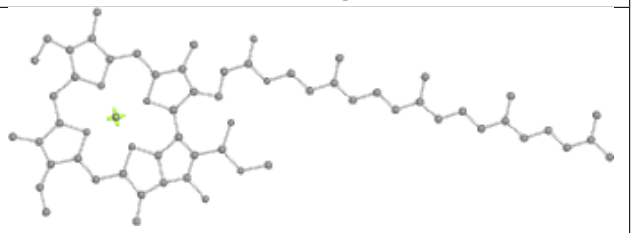
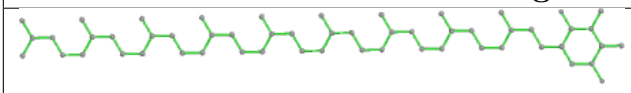


Rings

Ligand PL9 d 405



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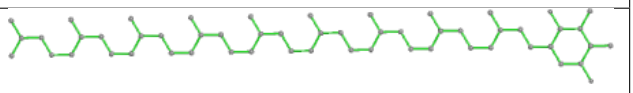

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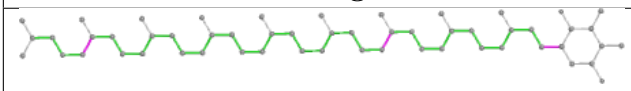

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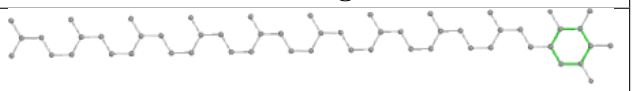
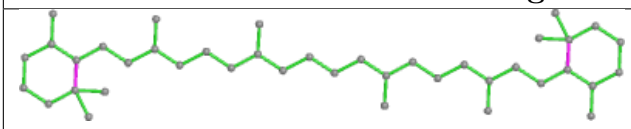


Rings

Ligand BCR z 101



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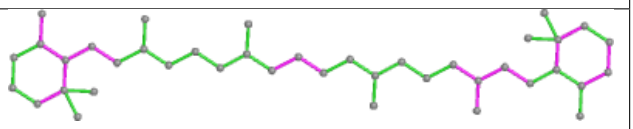

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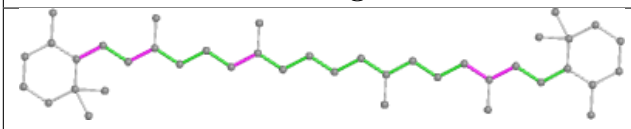

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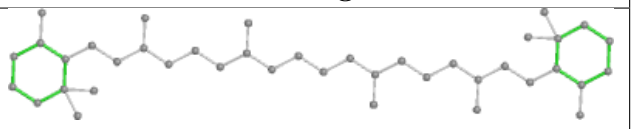
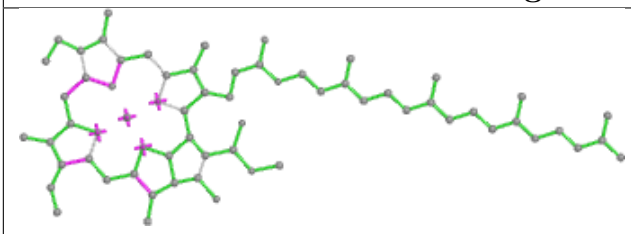
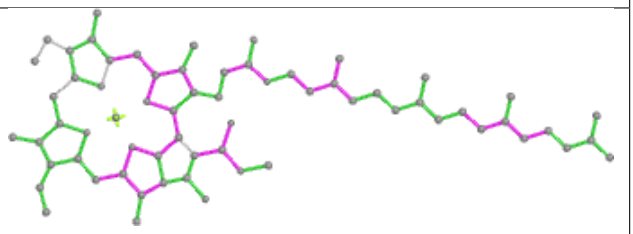
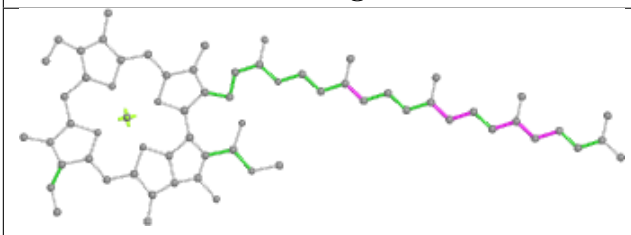
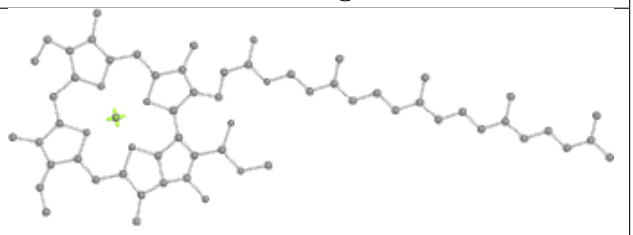


Rings

Ligand CLA B 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

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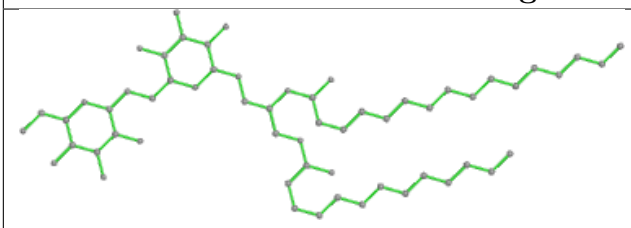
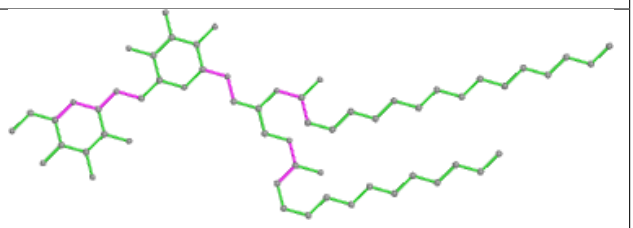
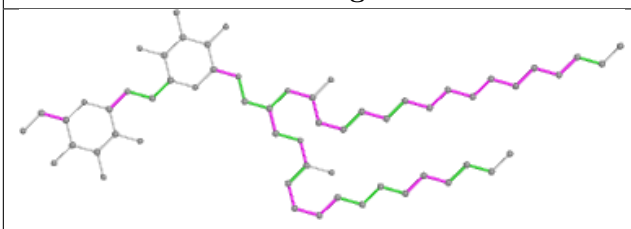
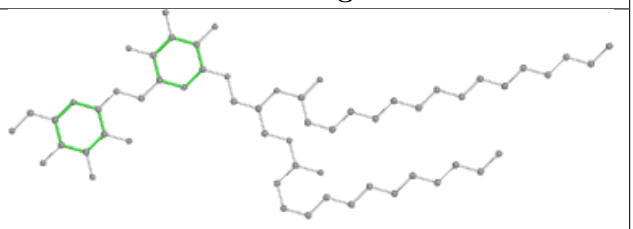
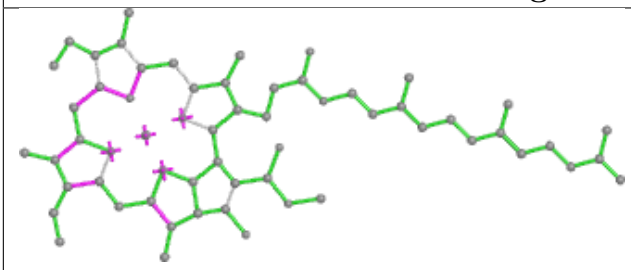
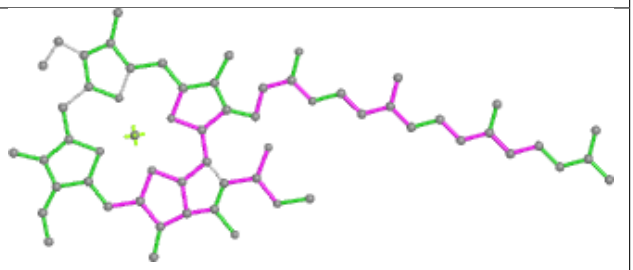
 Bond lengths	 Bond angles
 Torsions	 Rings

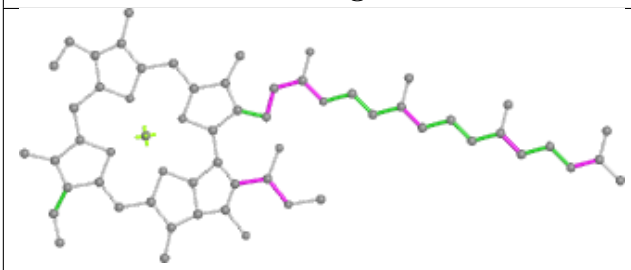
Ligand CLA r 602



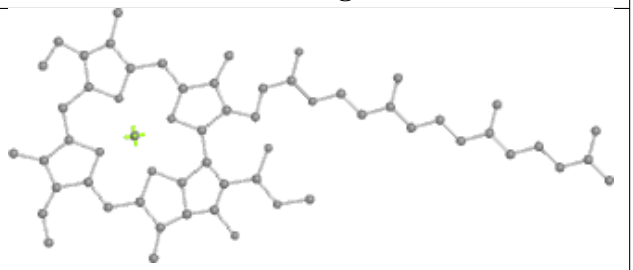
Bond lengths



Bond angles

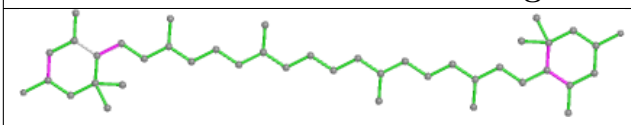


Torsions

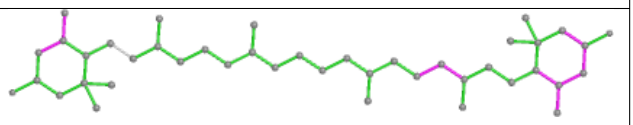


Rings

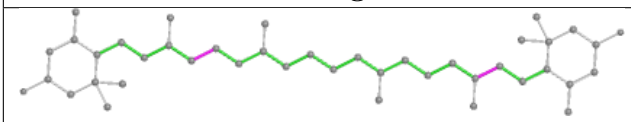
Ligand LUT Y 317



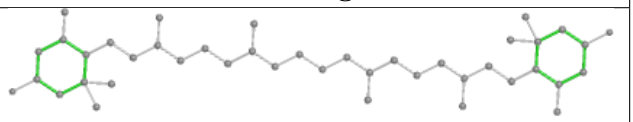
Bond lengths



Bond angles

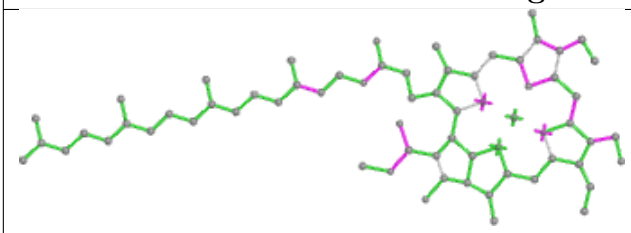


Torsions



Rings

Ligand CHL g 608



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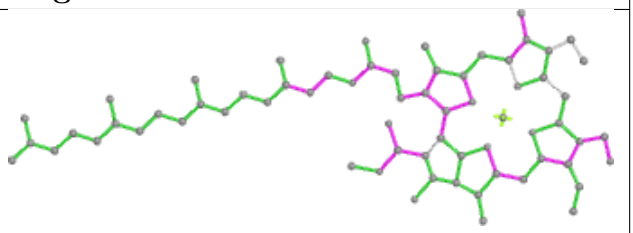
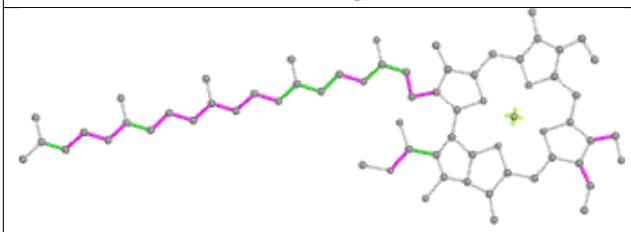
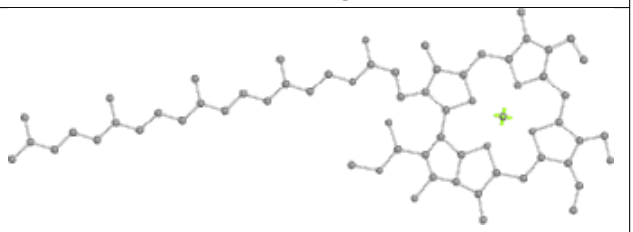


Bond angles

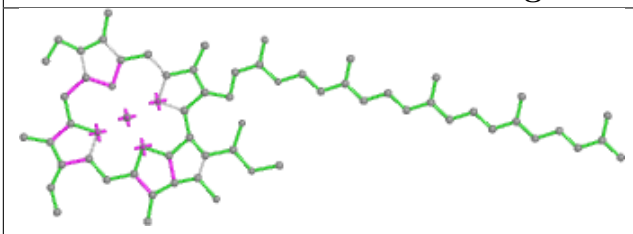


Torsions



Rings

Ligand CLA B 608



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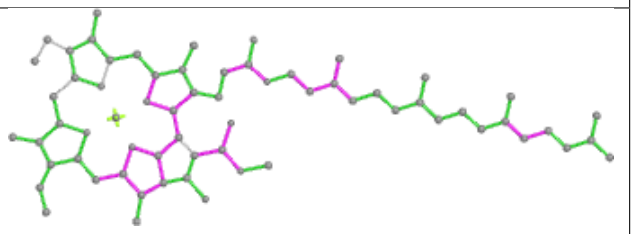
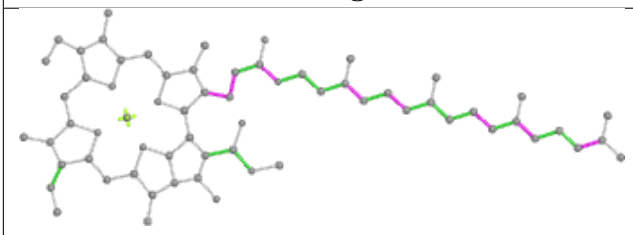


Bond angles



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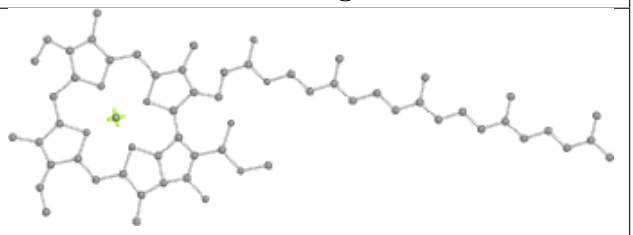
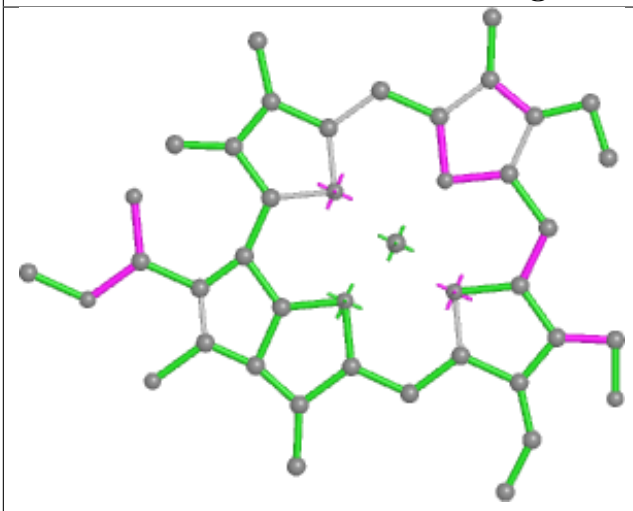


Rings

Ligand CHL r 613



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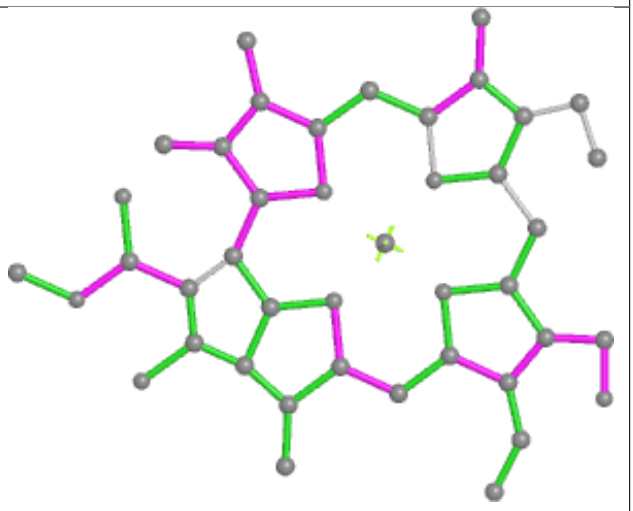
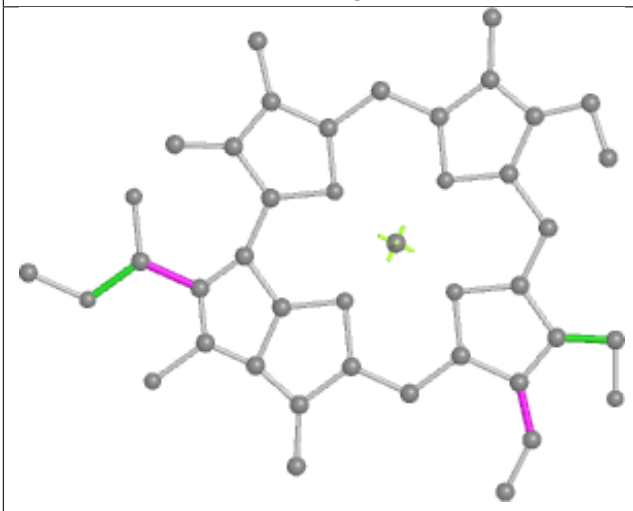


Bond angles



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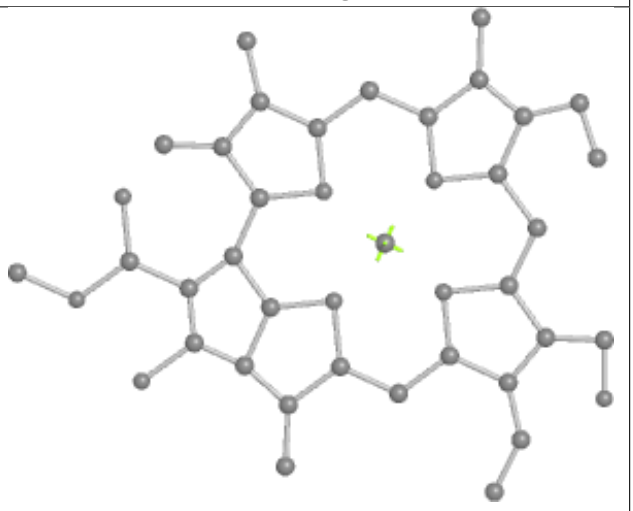
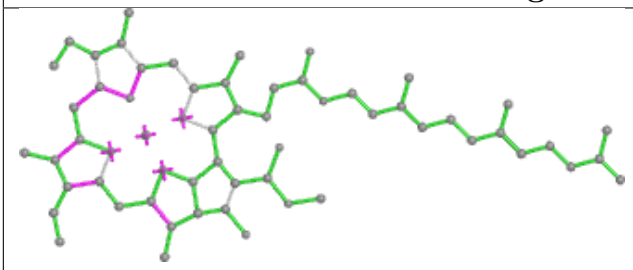


Rings

Ligand CLA n 612



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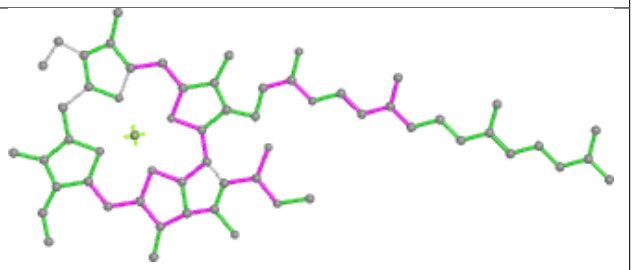
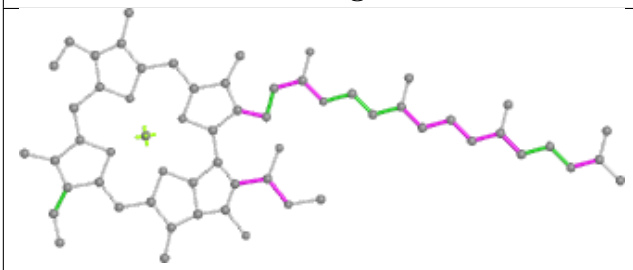


Bond angles



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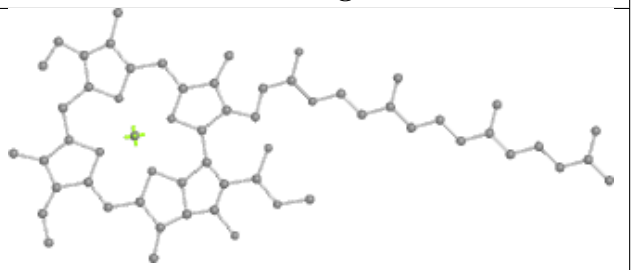
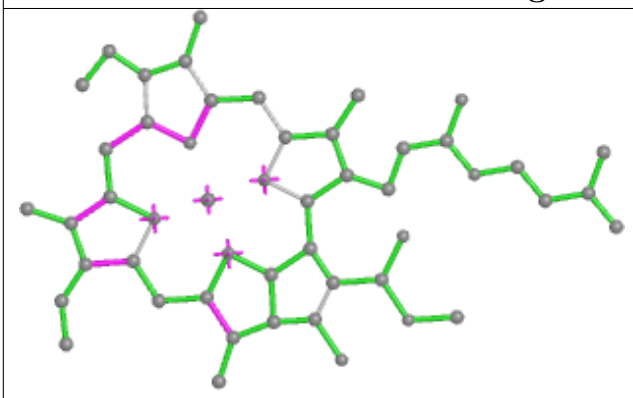


Rings

Ligand CLA g 604



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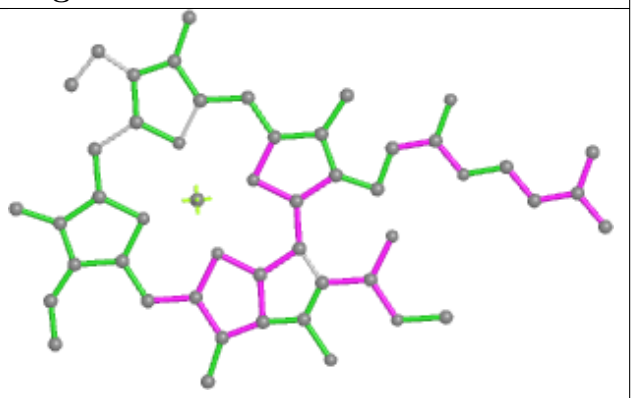
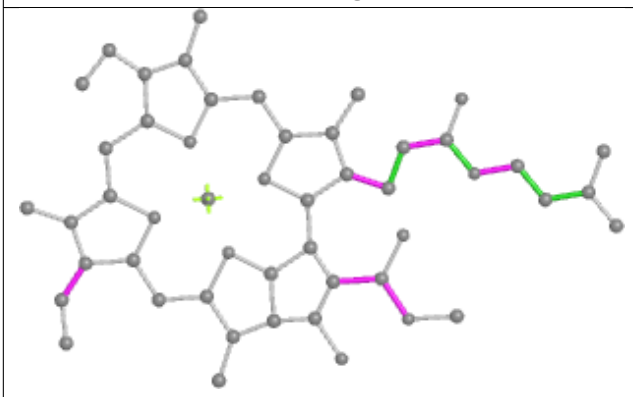


Bond angles



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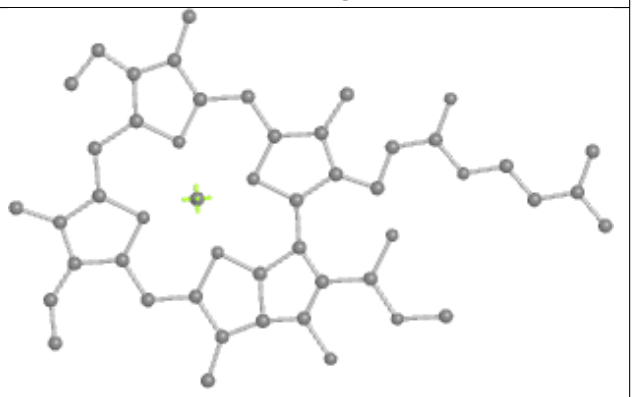
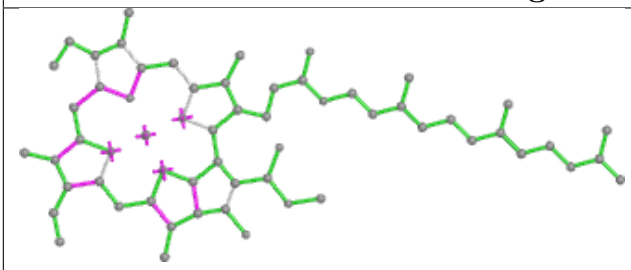


Rings

Ligand CLA a 406



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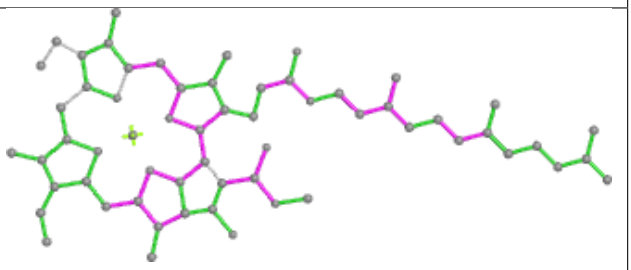
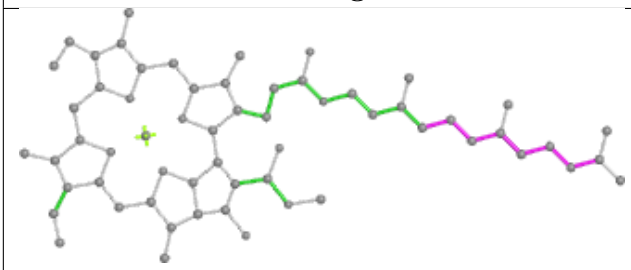


Bond angles



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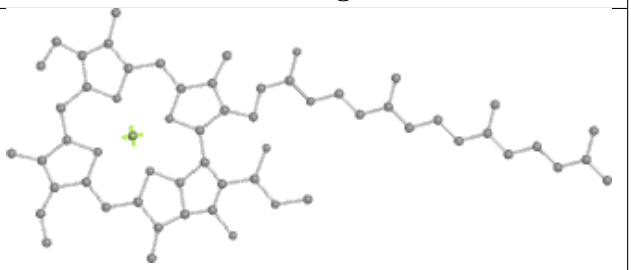
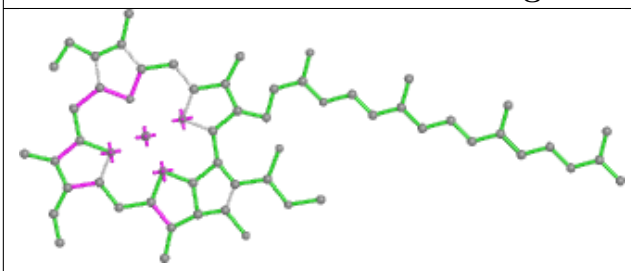


Rings

Ligand CLA R 602



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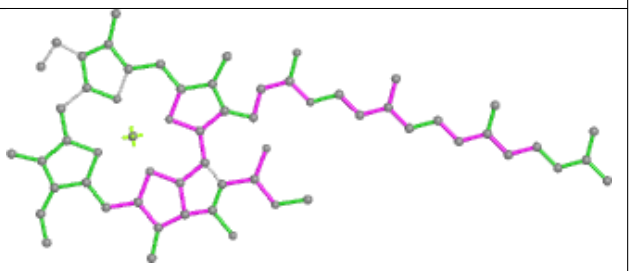
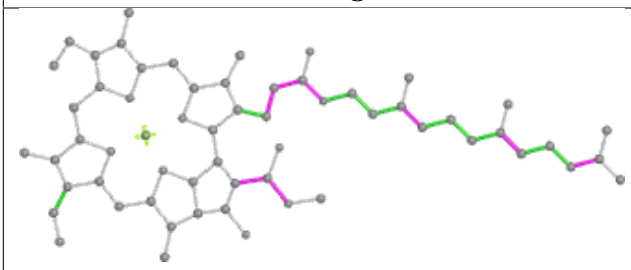
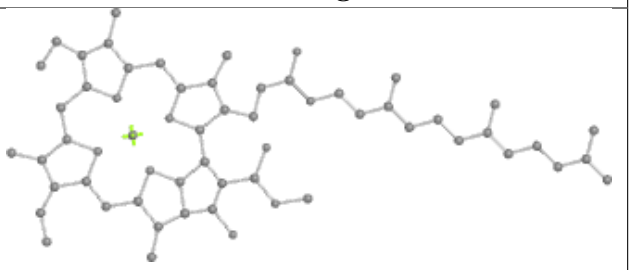


Bond angles

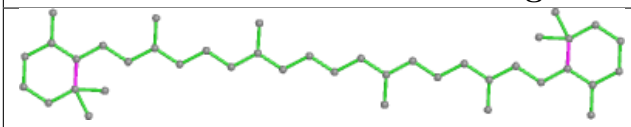


Torsions



Rings

Ligand BCR b 619



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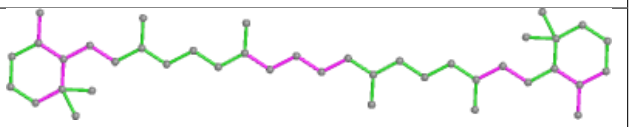
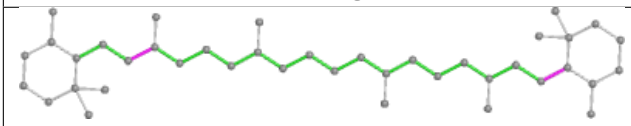


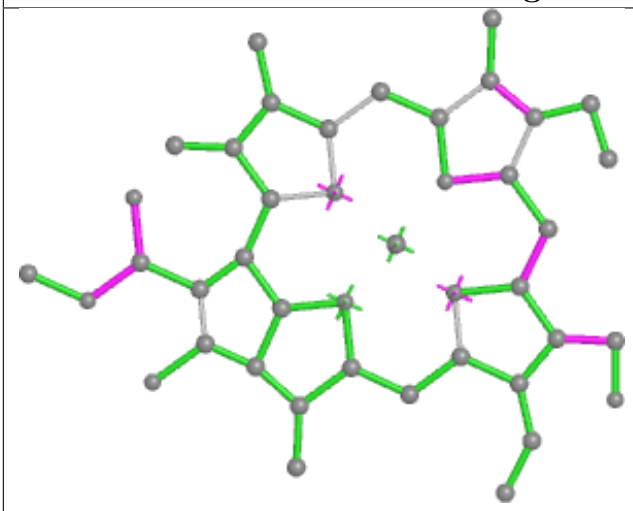
Bond angles



Torsions

Rings

Ligand CHL R 613



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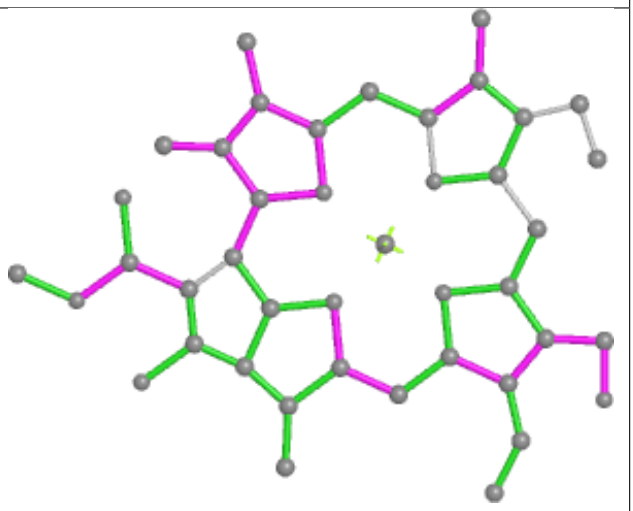
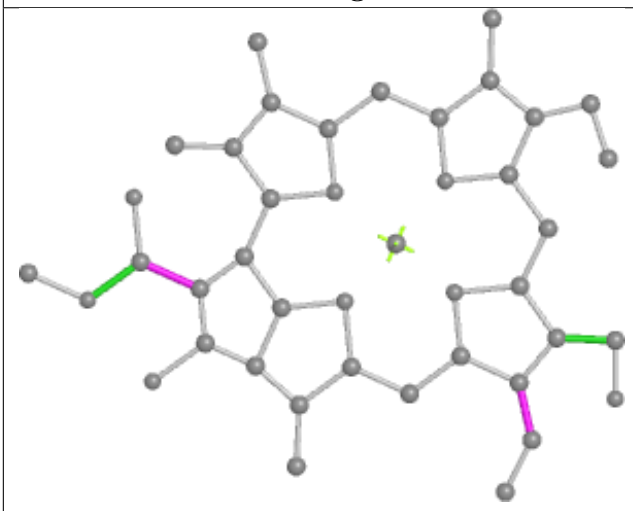
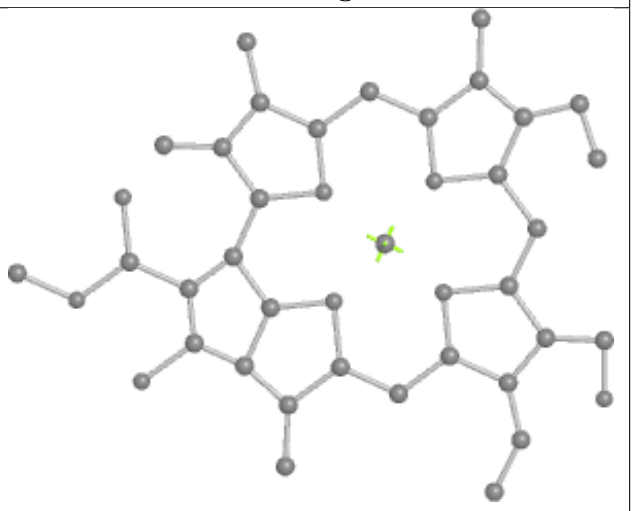


Bond angles

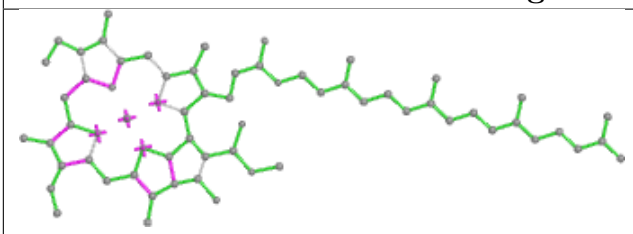


Torsions



Rings

Ligand CLA b 608



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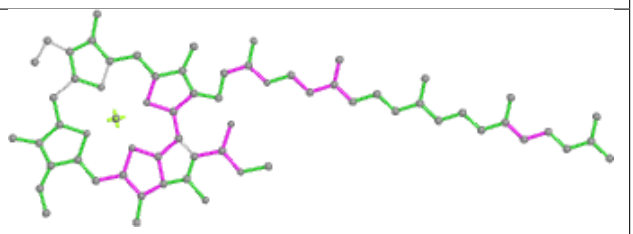
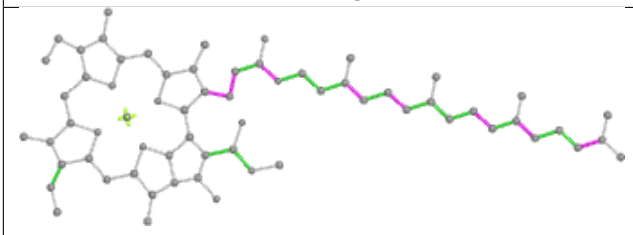


Bond angles



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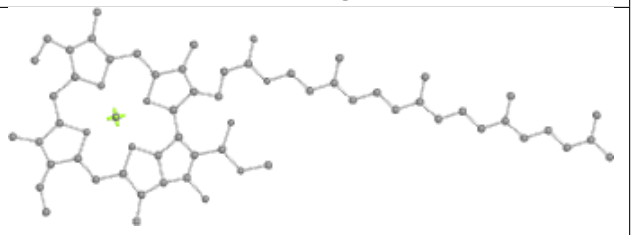
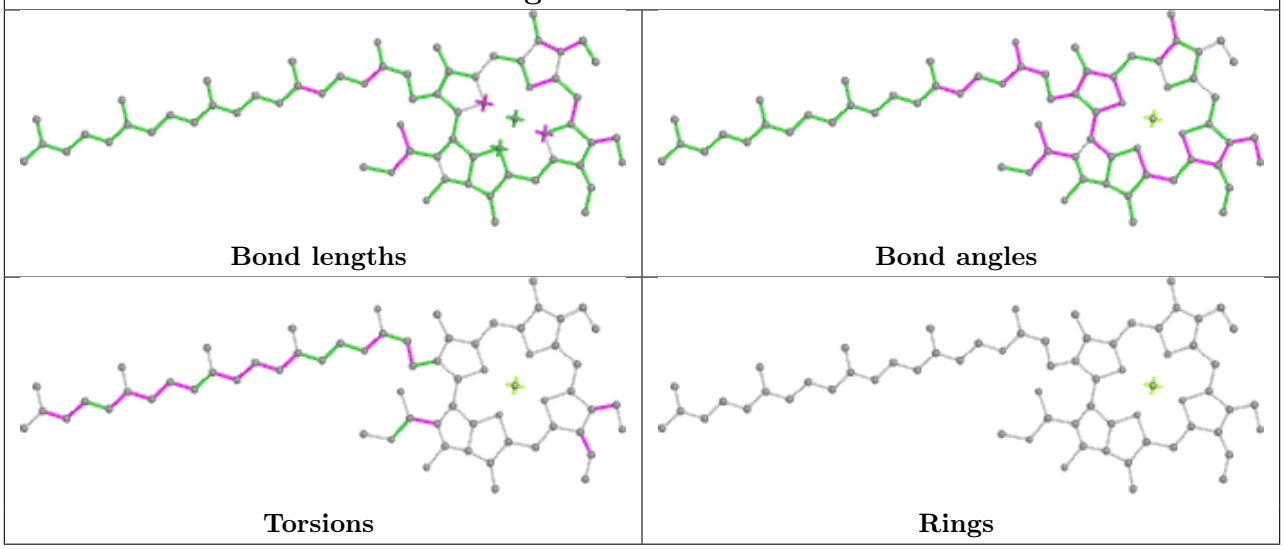
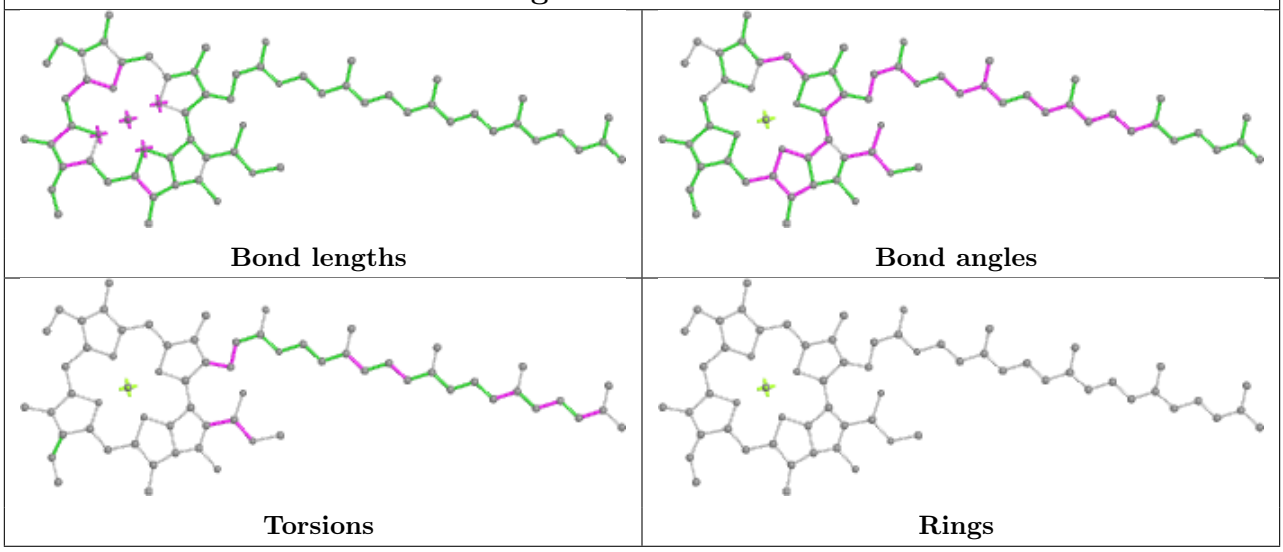


Rings

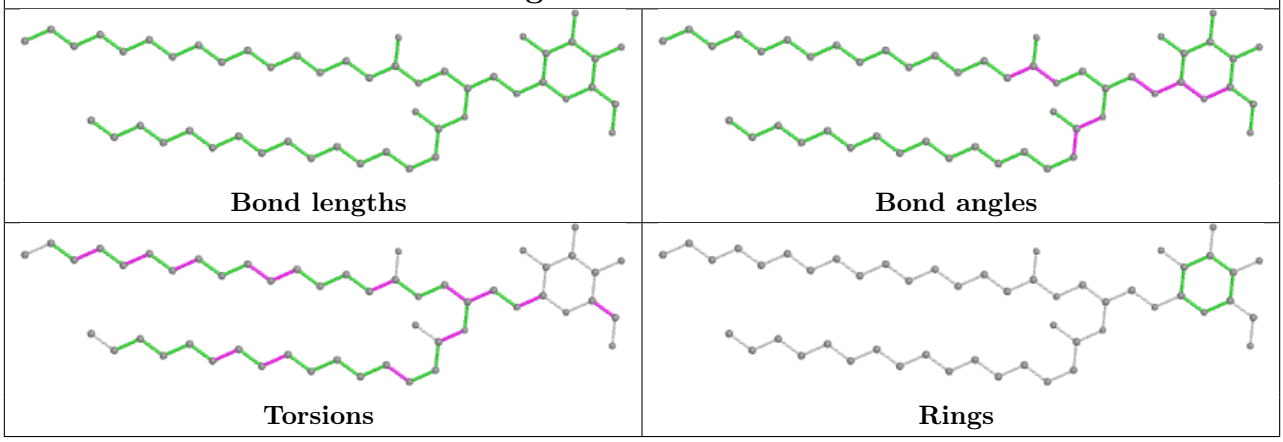
Ligand CHL Y 302



Ligand CLA r 609



Ligand LMG c 520



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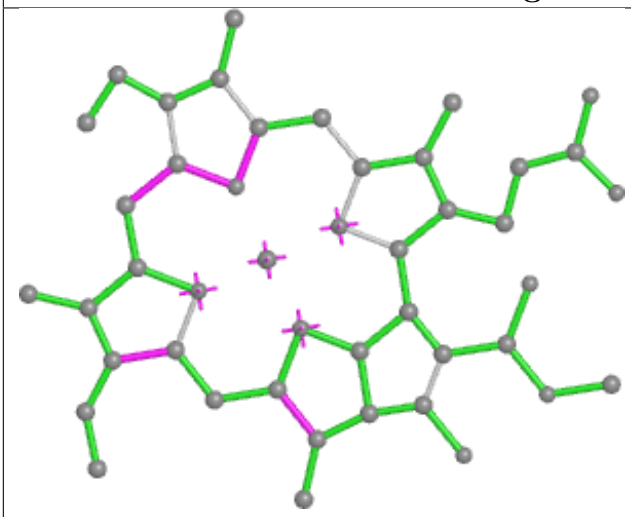
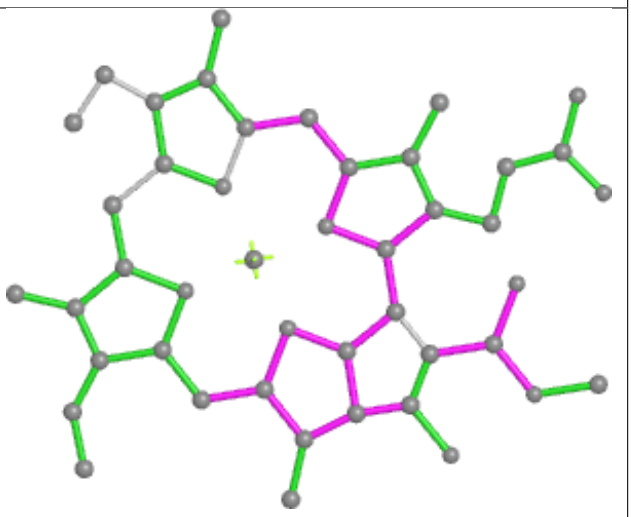
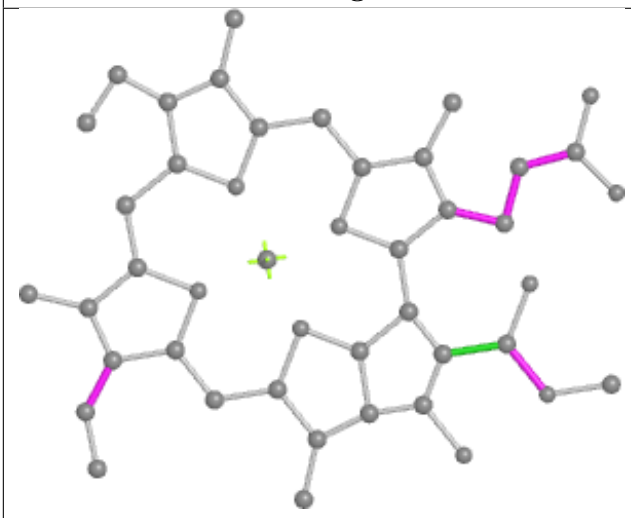


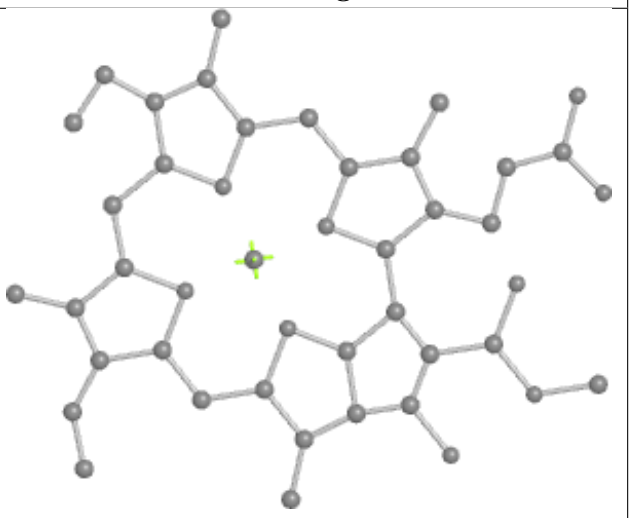
Bond lengths



Bond angles

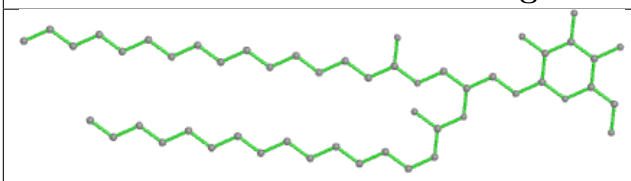


Torsions

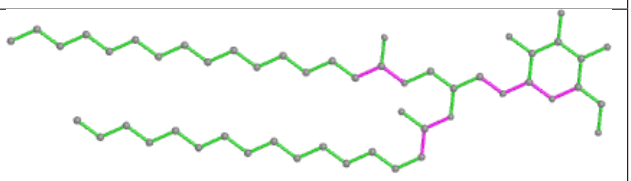


Rings

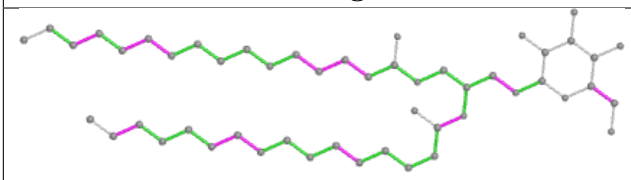
Ligand LMG B 620



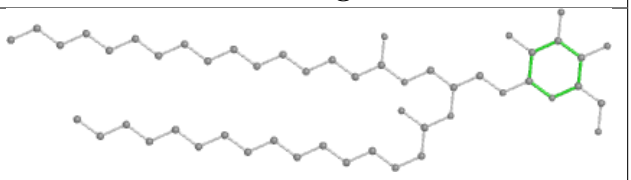
Bond lengths



Bond angles

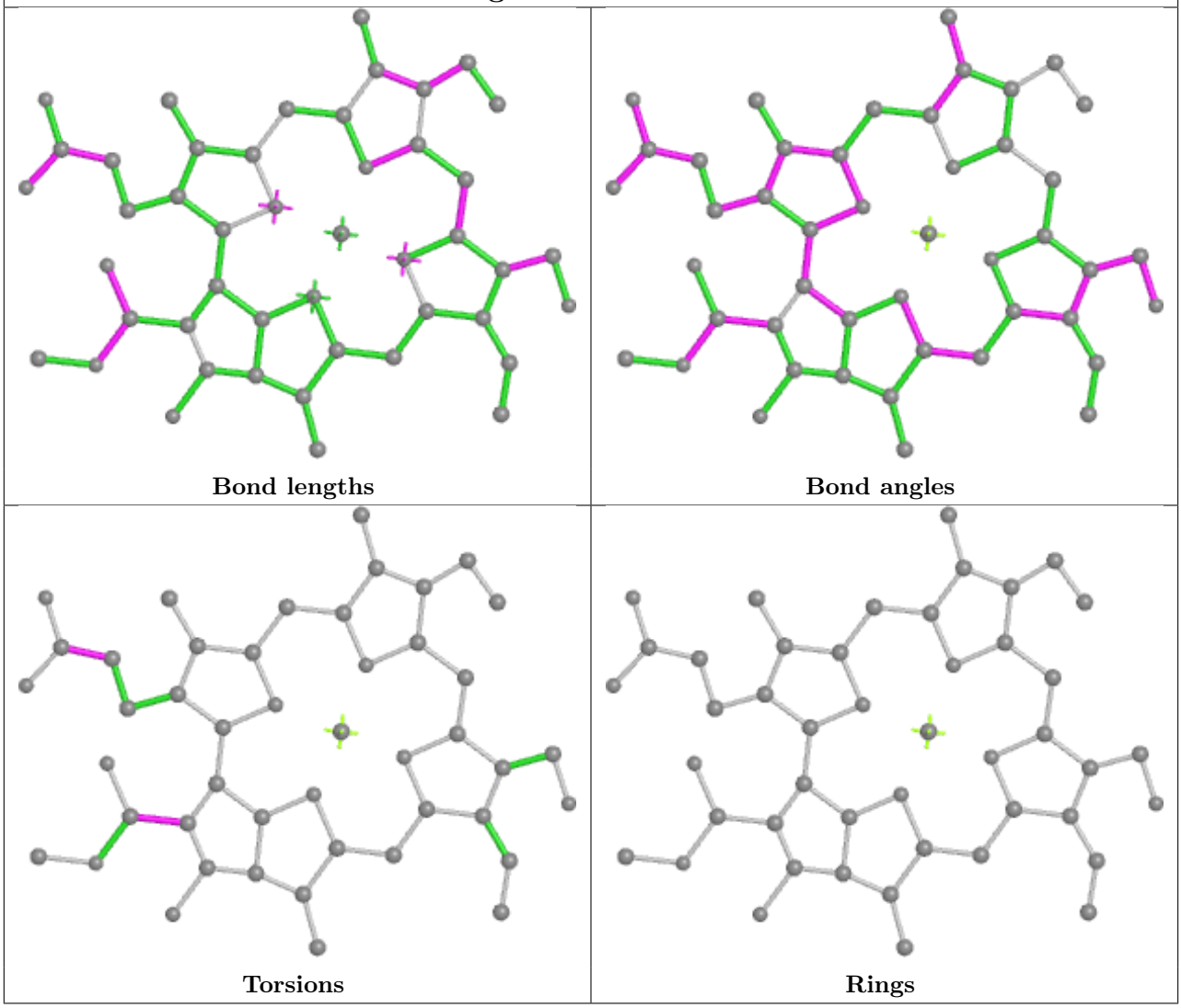


Torsions

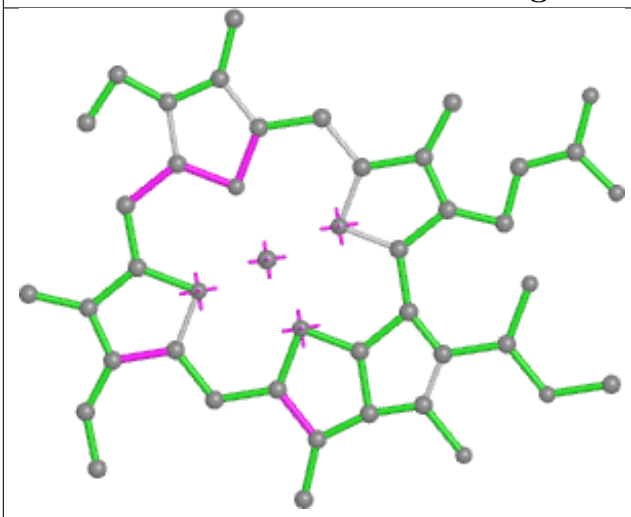


Rings

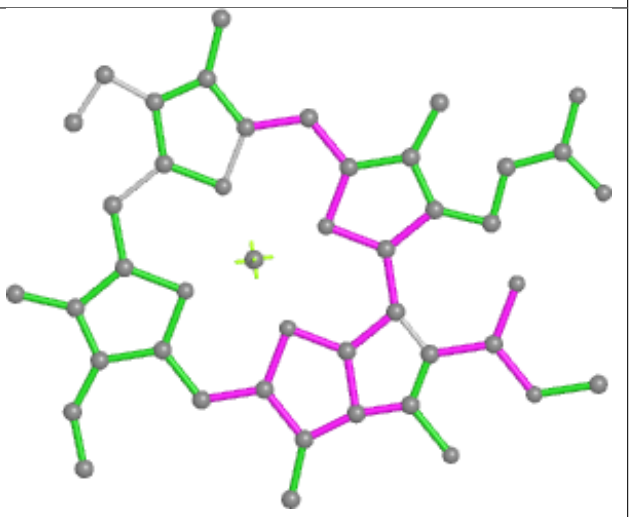
Ligand CHL s 302



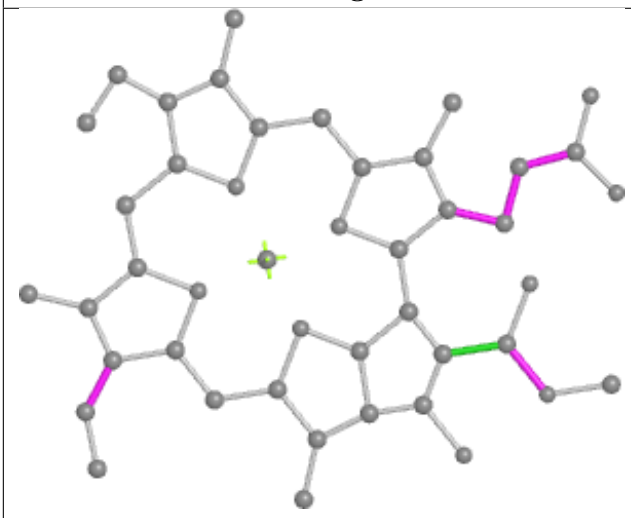
Ligand CLA r 614



Bond lengths



Bond angles



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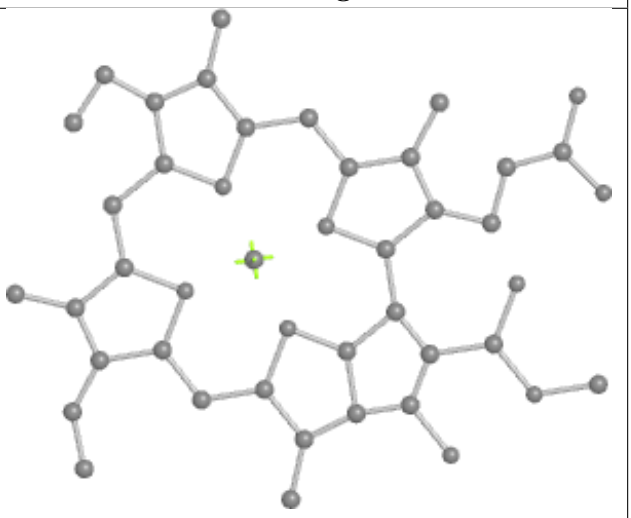
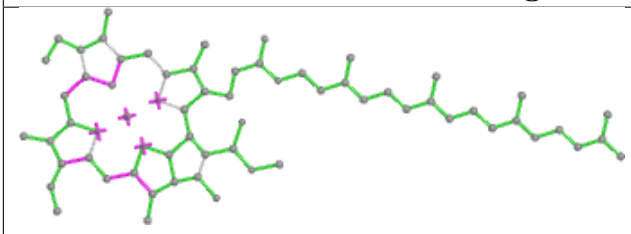
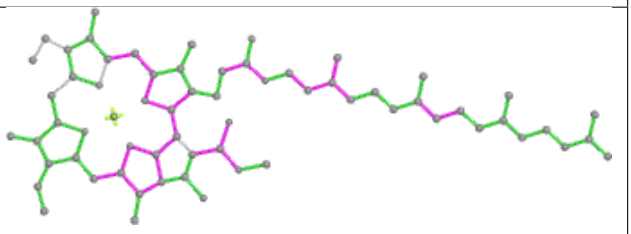


Rings

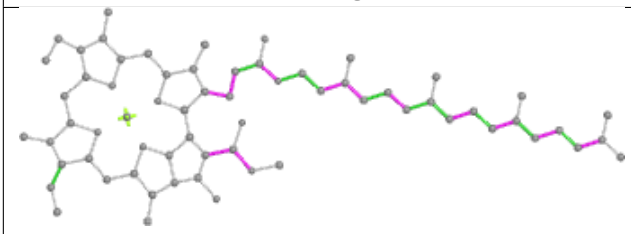
Ligand CLA N 610



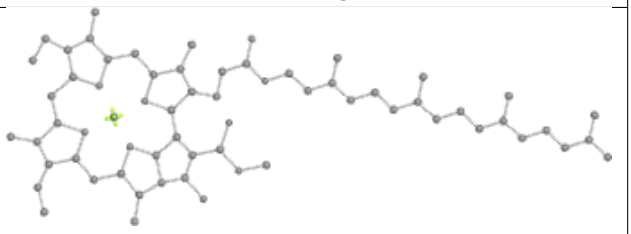
Bond lengths



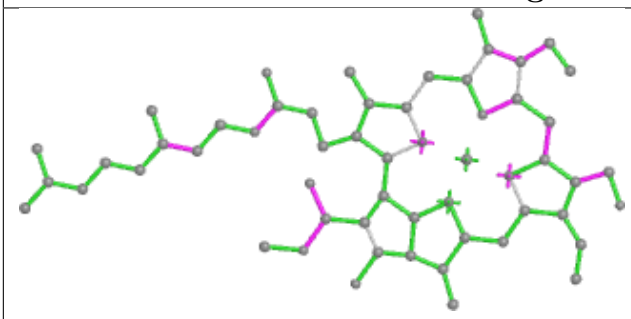
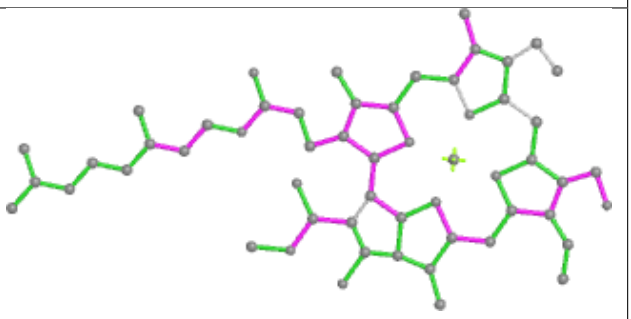
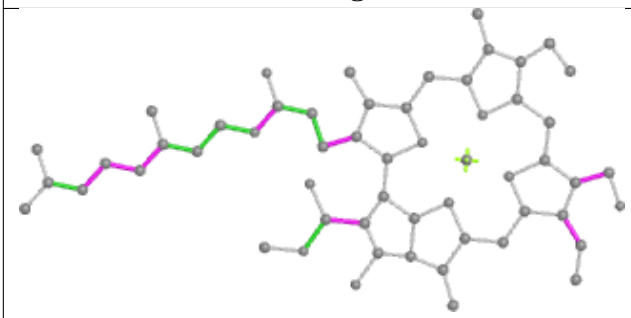
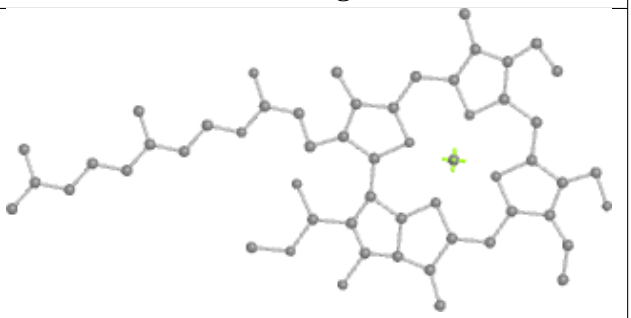
Bond angles

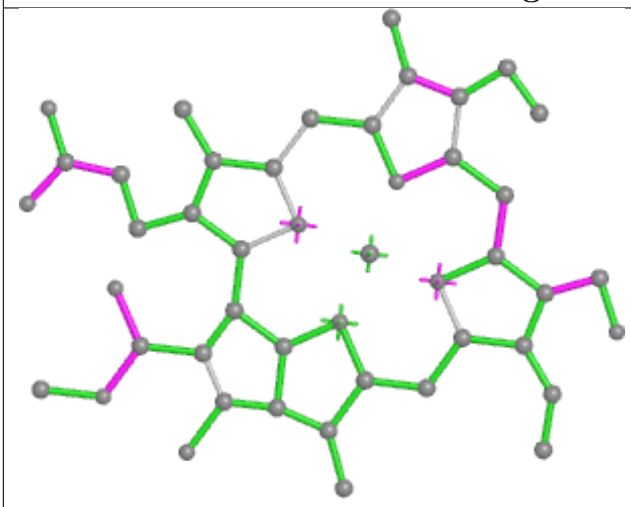
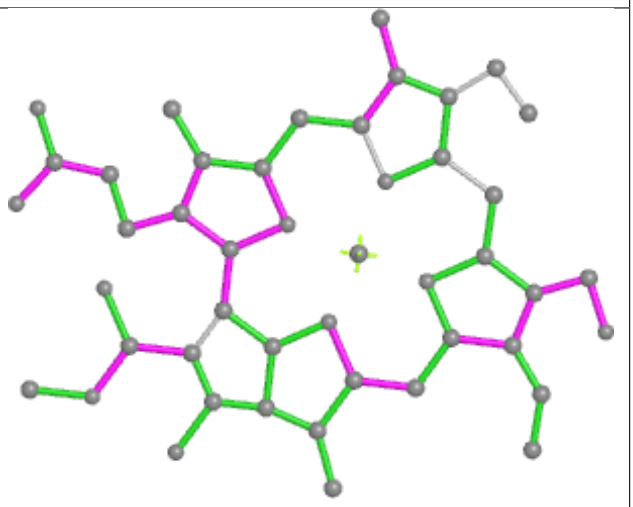
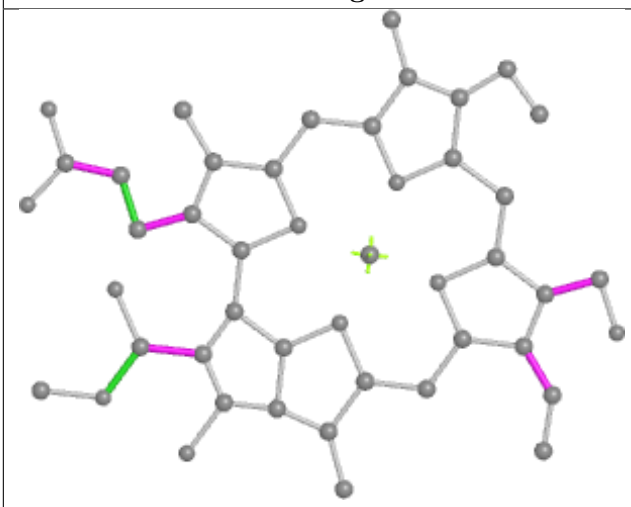
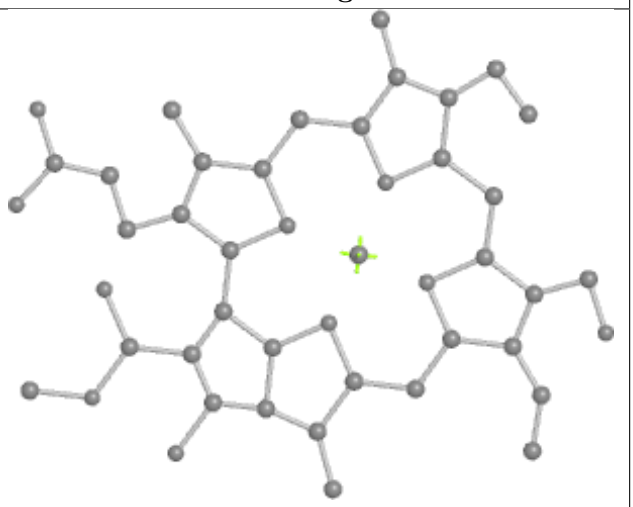


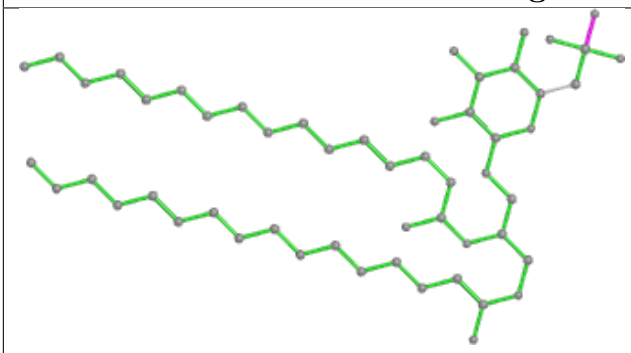
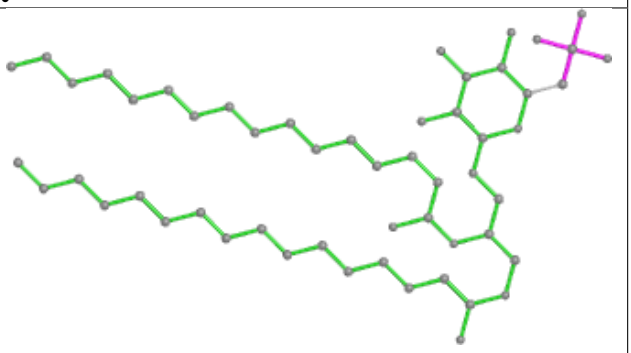
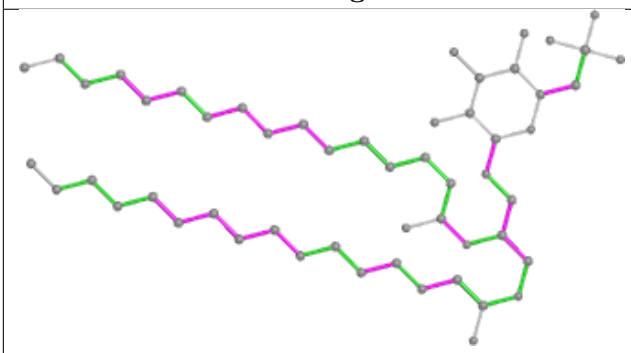
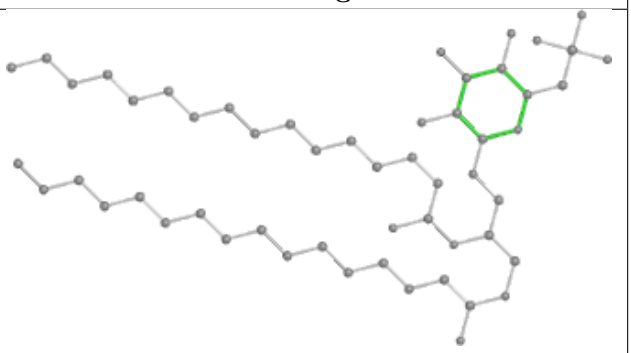
Torsions



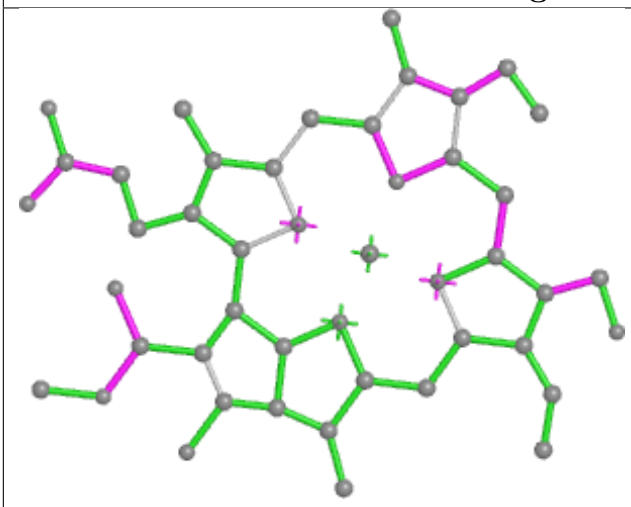
Rings

Ligand CHL n 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

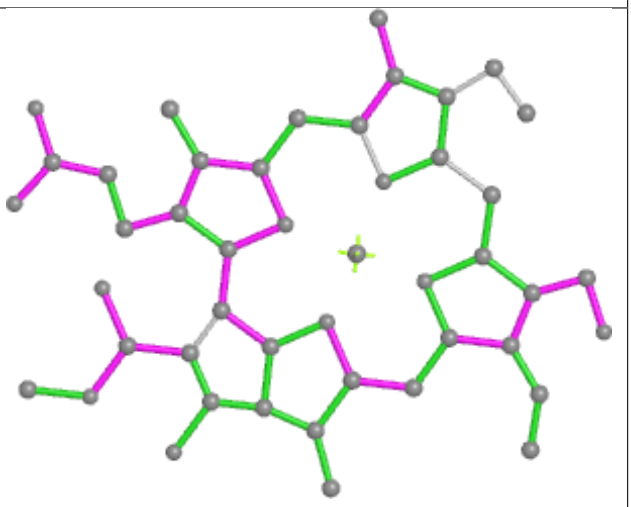
Ligand CHL G 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD a 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

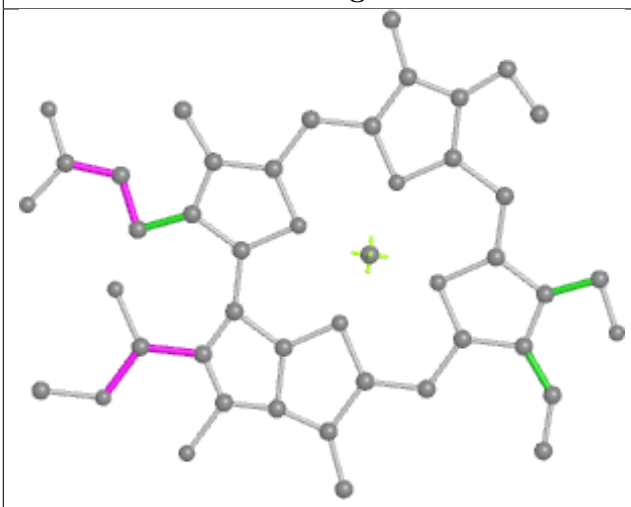
Ligand CHL s 306



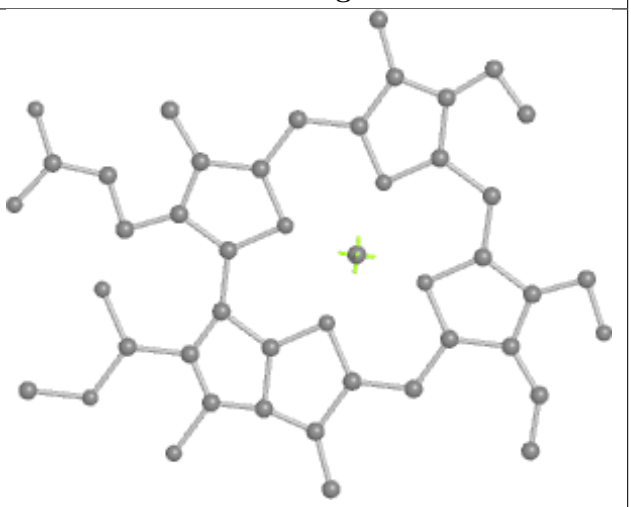
Bond lengths



Bond angles

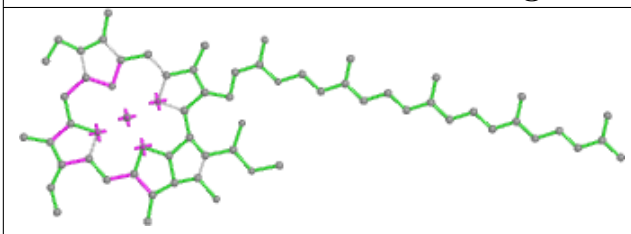


Torsions

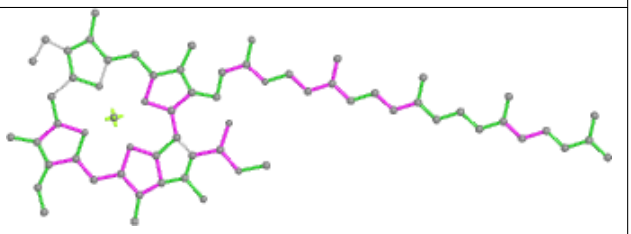


Rings

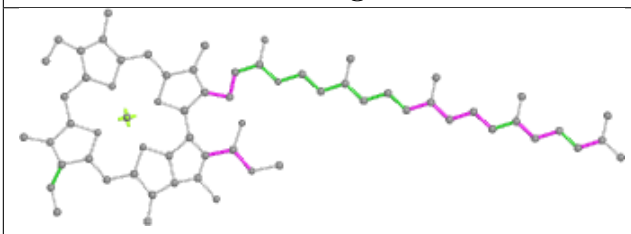
Ligand CLA G 602



Bond lengths



Bond angles



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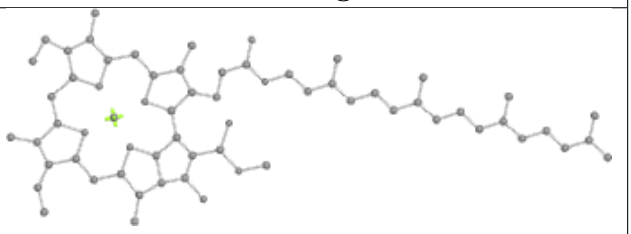
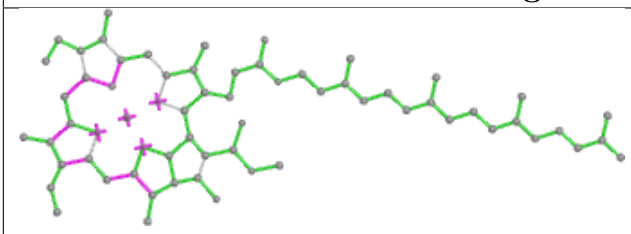
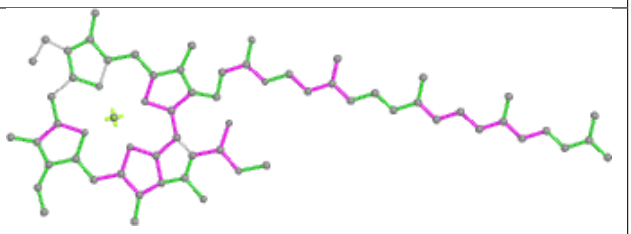
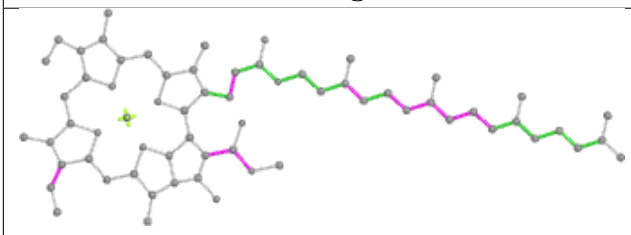
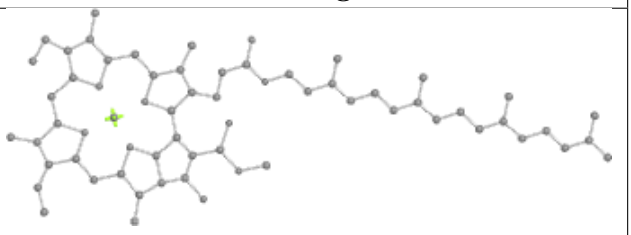


Rings

Ligand CLA N 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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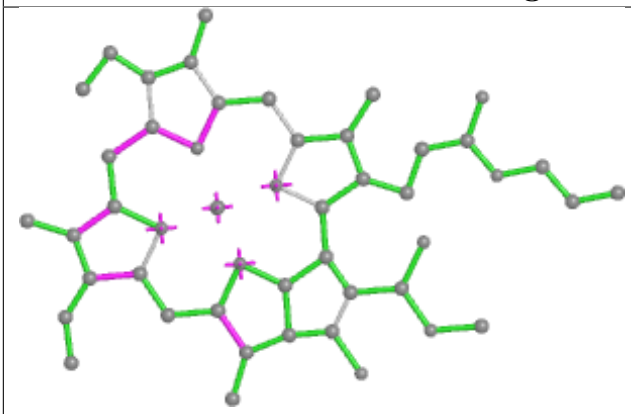
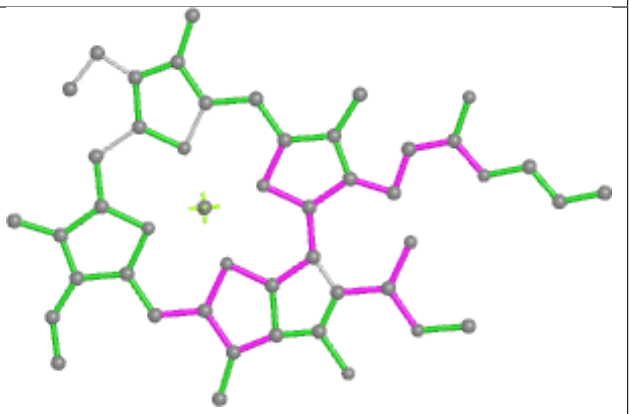
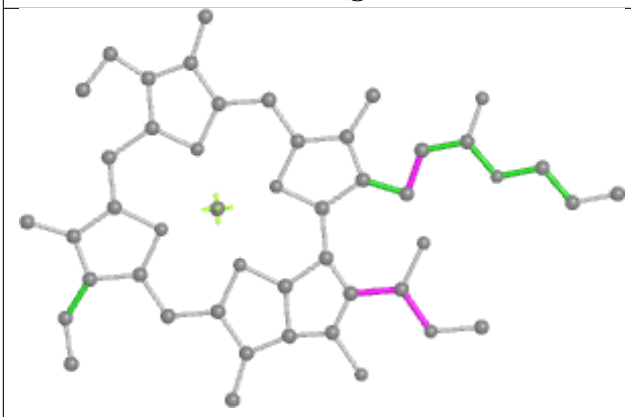
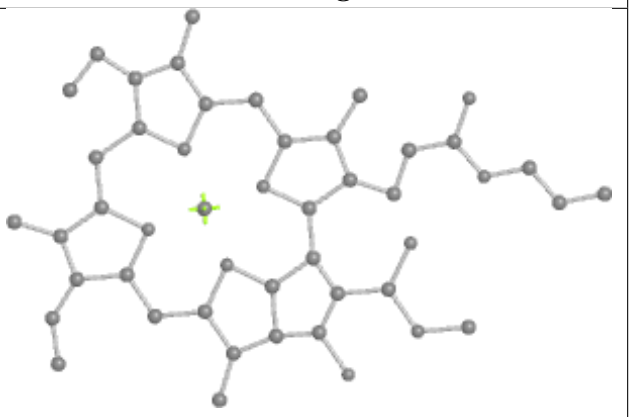
 Bond lengths	 Bond angles
 Torsions	 Rings

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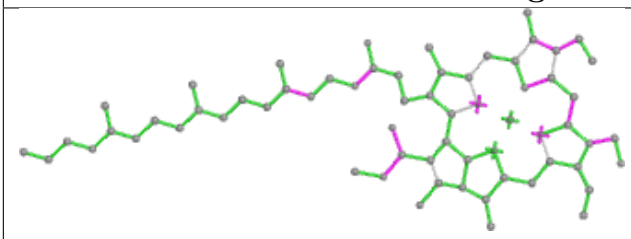
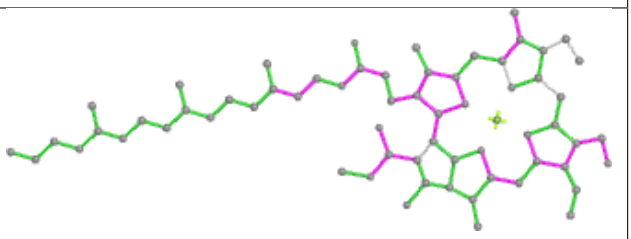
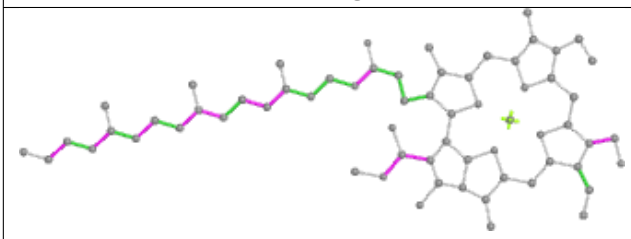
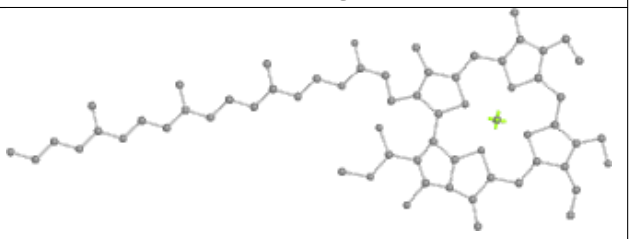
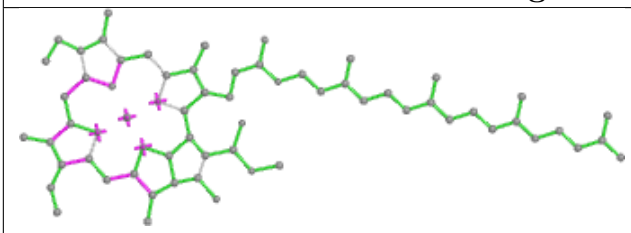
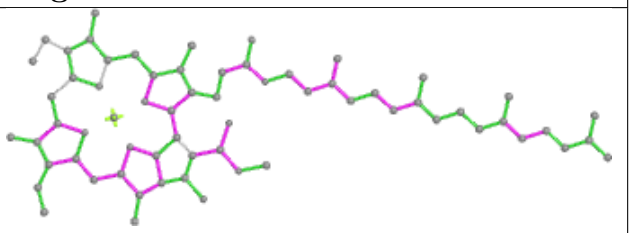
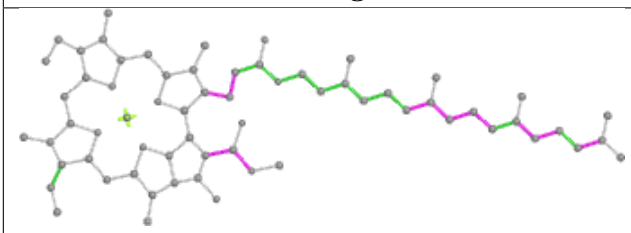
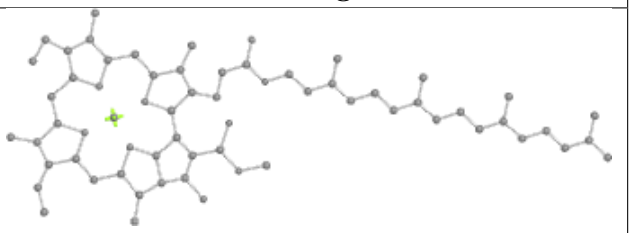
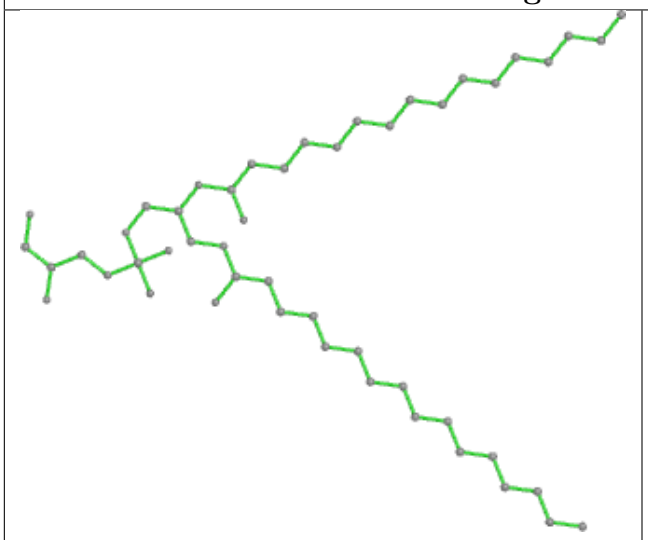
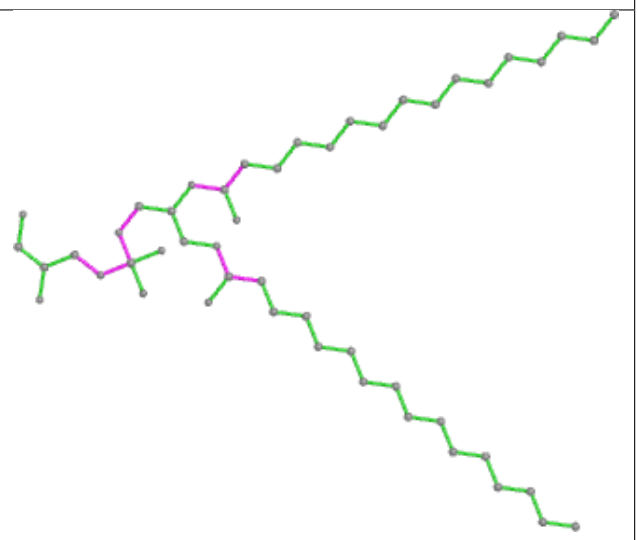
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

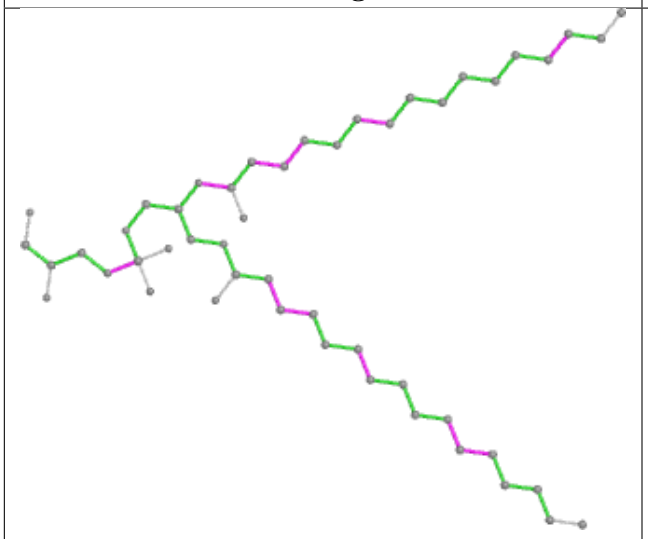
Ligand LHG C 518



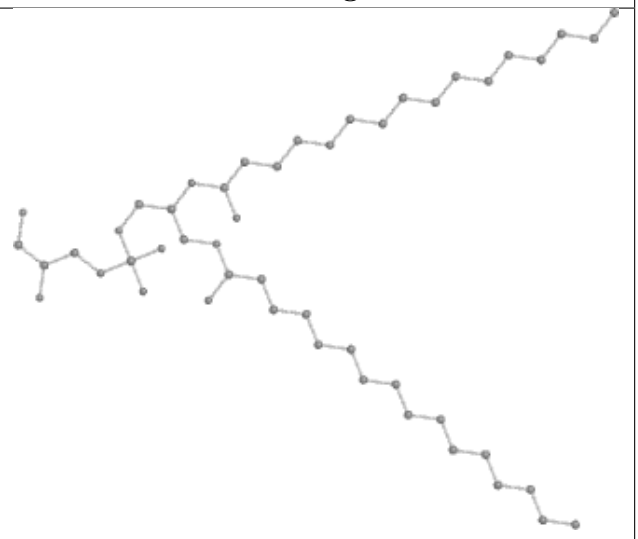
Bond lengths



Bond angles

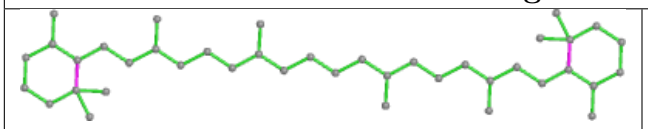


Torsions

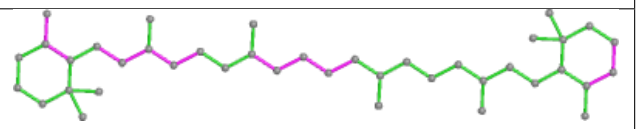


Rings

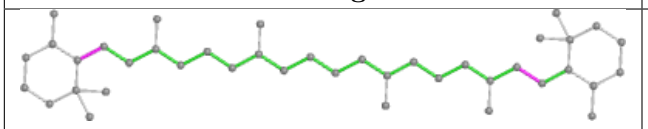
Ligand BCR B 617



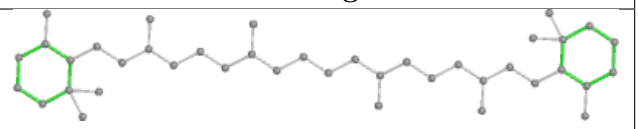
Bond lengths



Bond angles

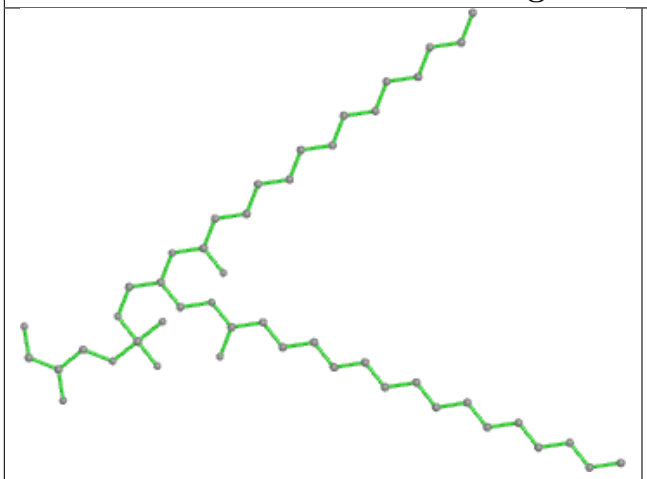


Torsions



Rings

Ligand LHG 6 606



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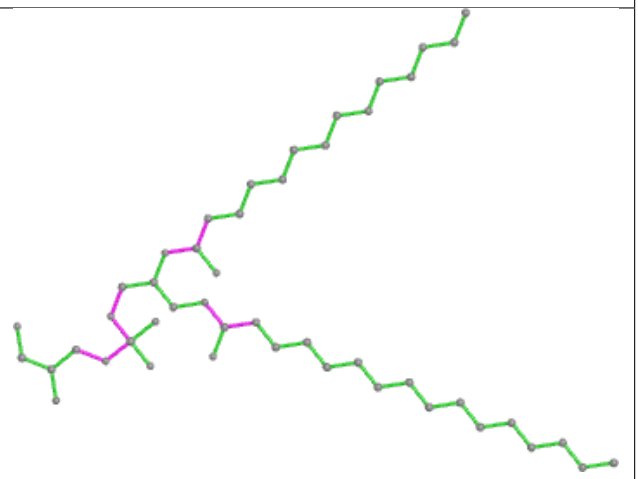
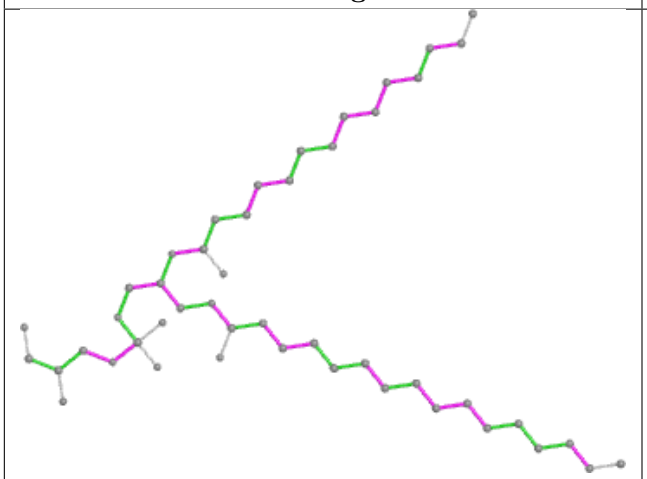
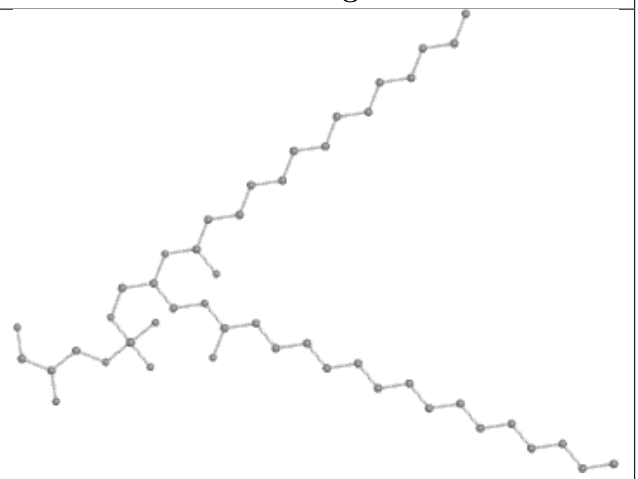


Bond angles

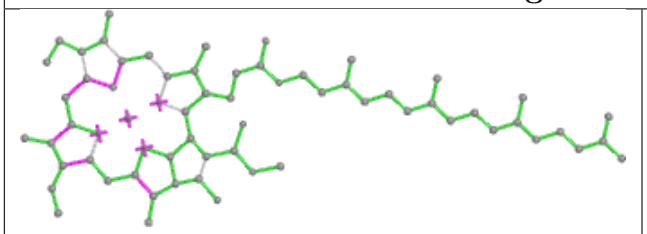


Torsions



Rings

Ligand CLA B 603



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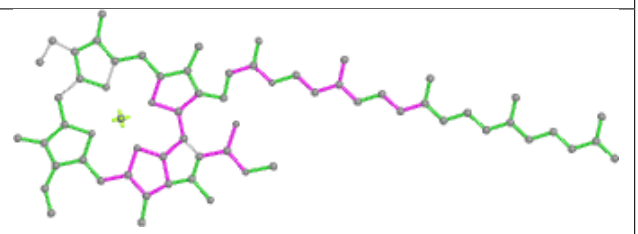

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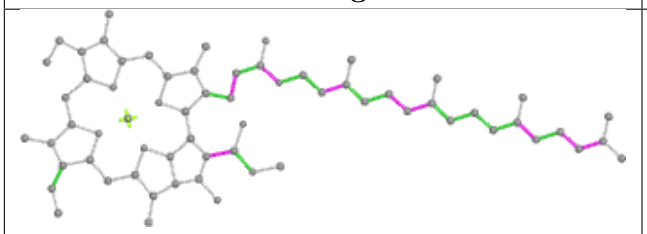

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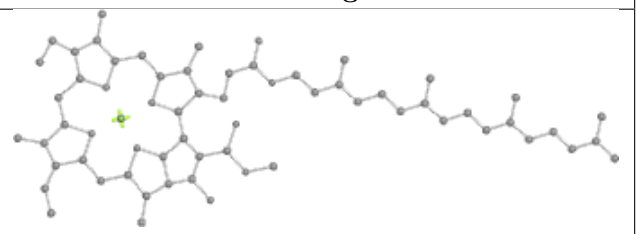
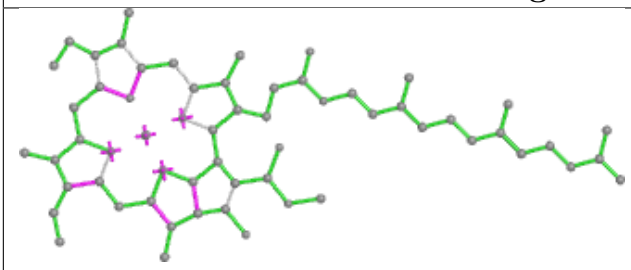


Rings

Ligand CLA c 504



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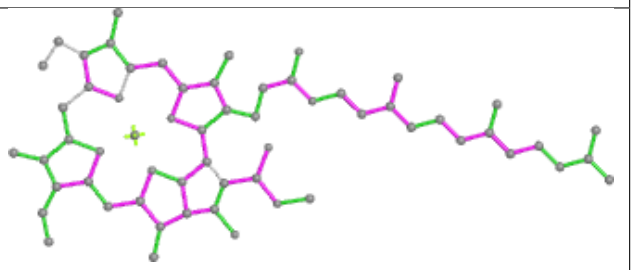
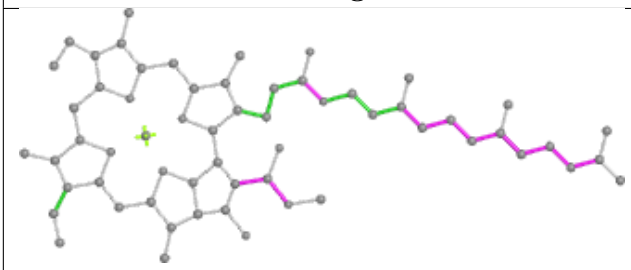


Bond angles



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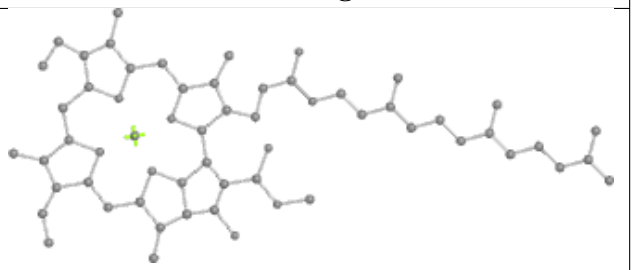
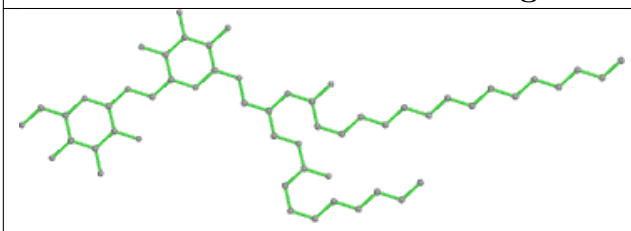


Rings

Ligand DGD C 515



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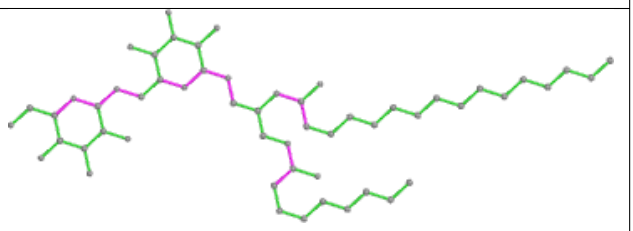

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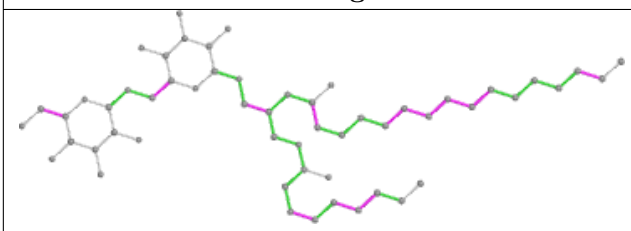

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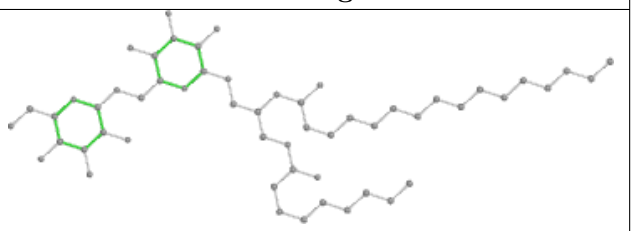
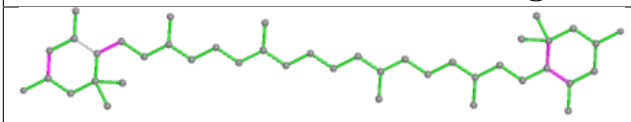


Rings

Ligand LUT S 316



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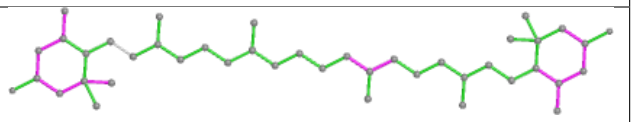
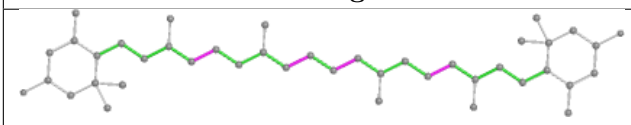


Bond angles



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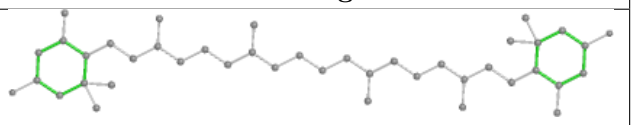
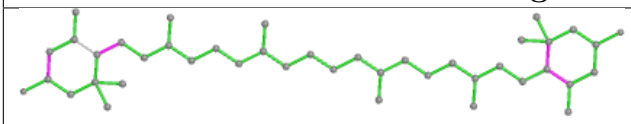
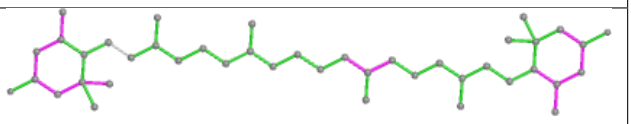
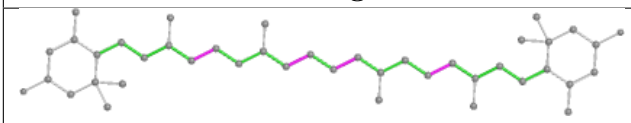
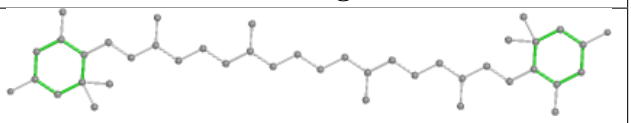
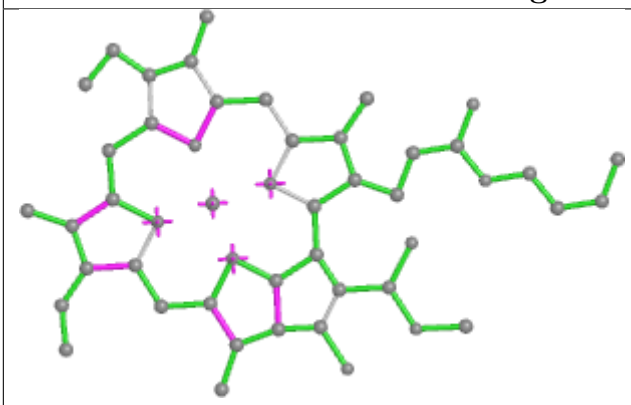
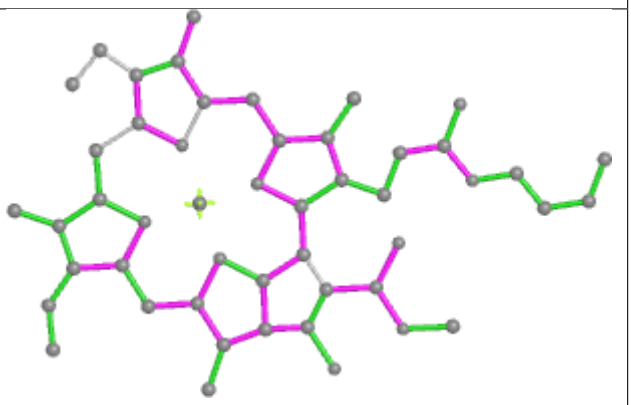
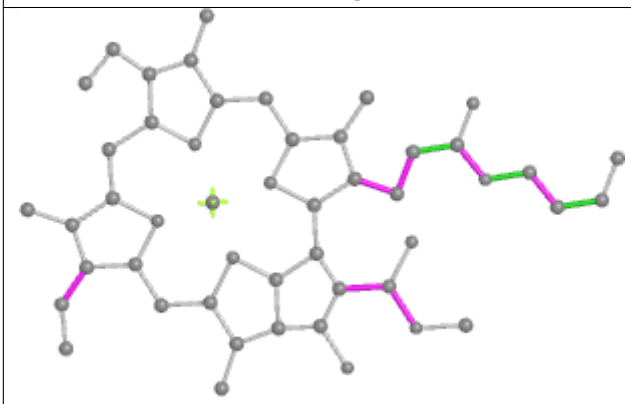
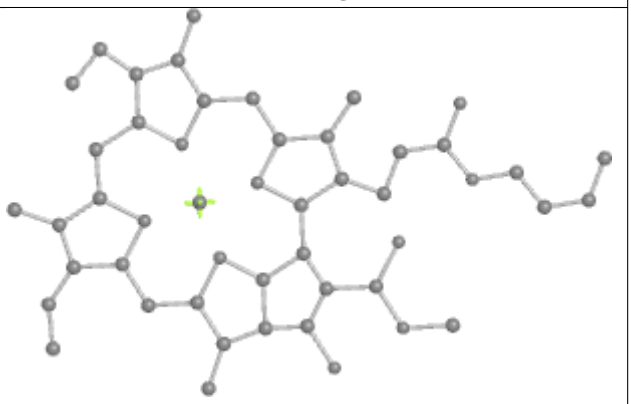
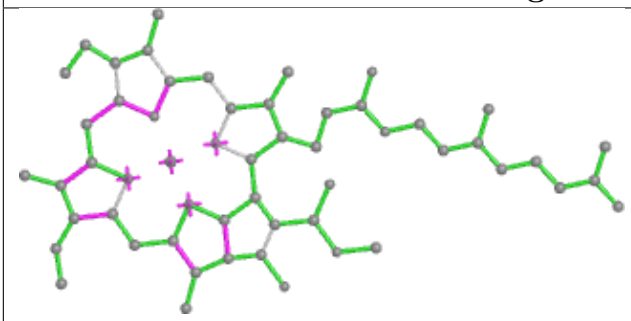


Rings

Ligand LUT s 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 313



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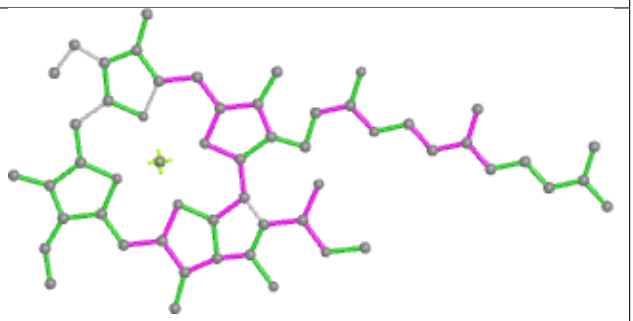
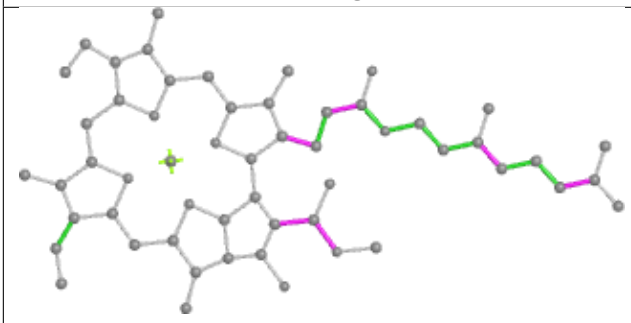


Bond angles



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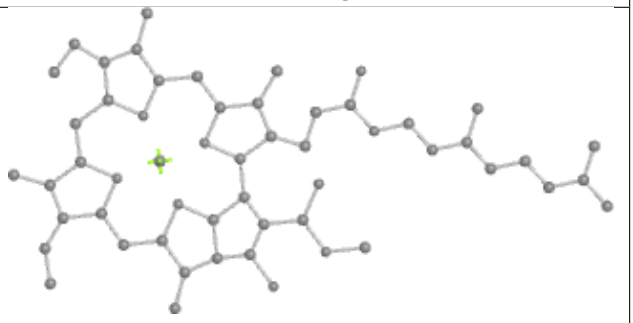
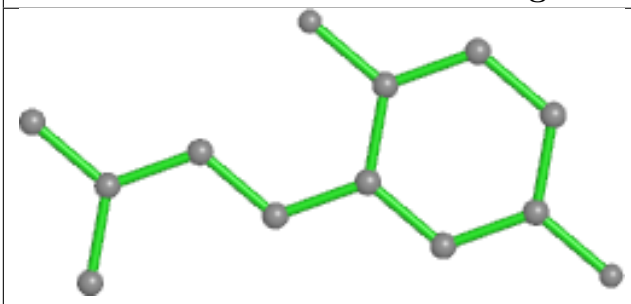


Rings

Ligand PL9 A 409



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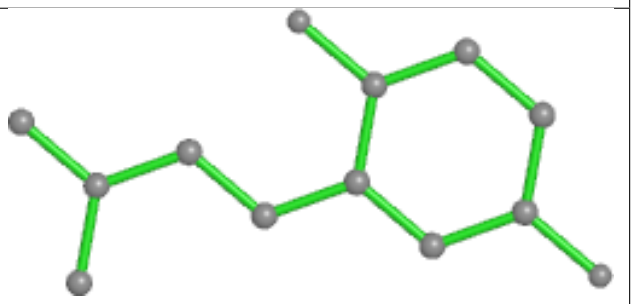
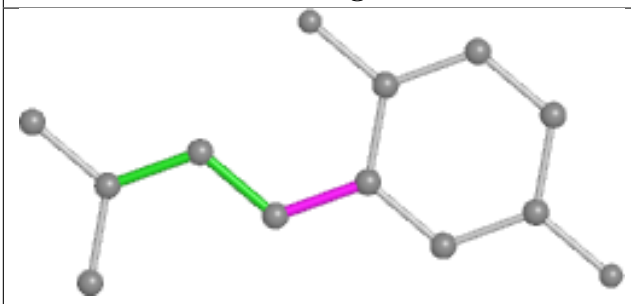


Bond angles



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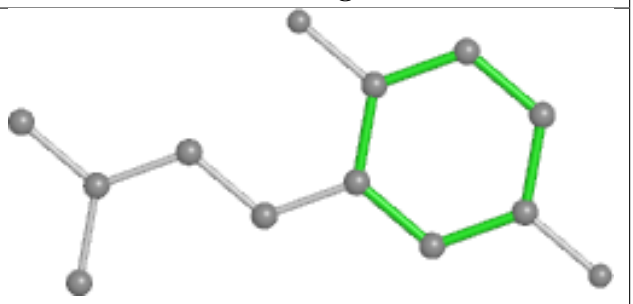
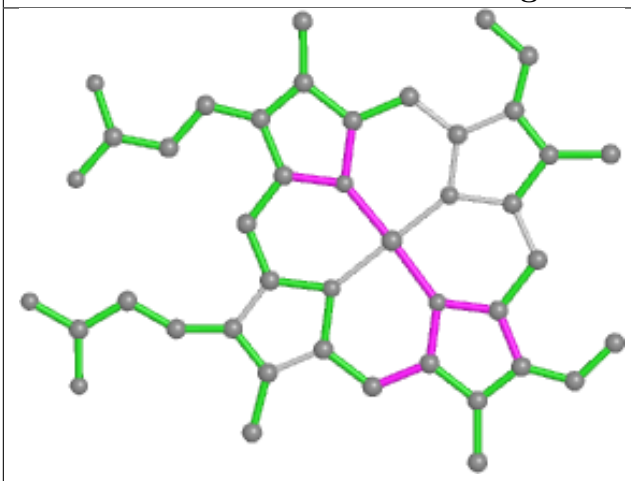


Rings

Ligand HEM F 101



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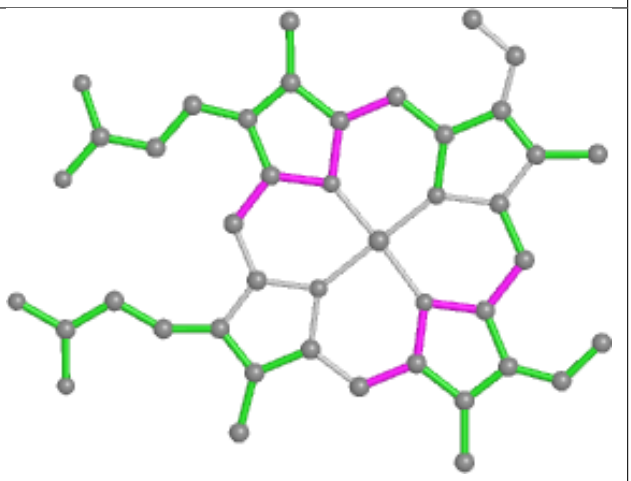
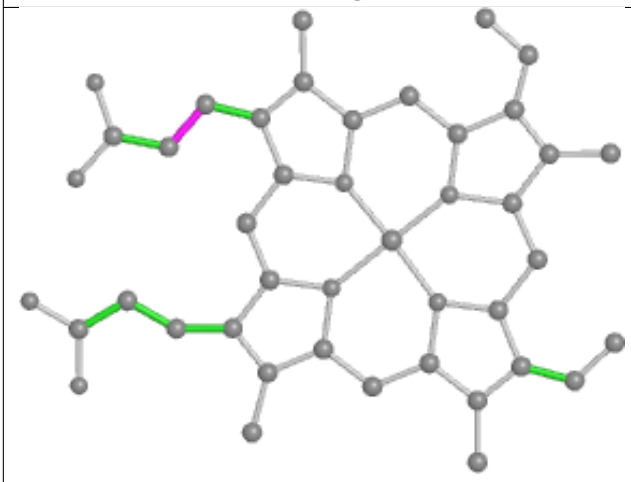


Bond angles



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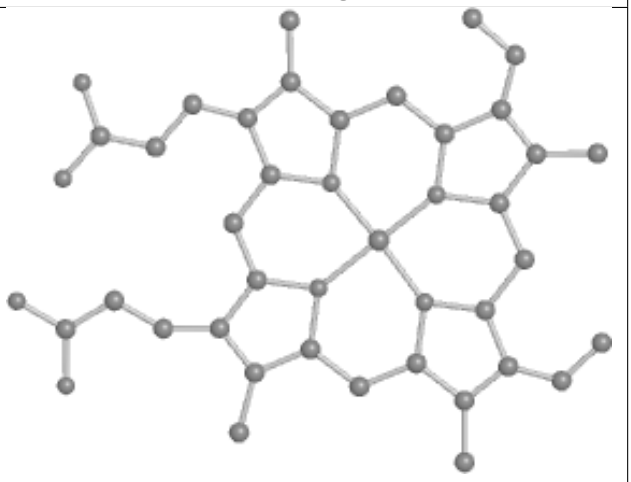
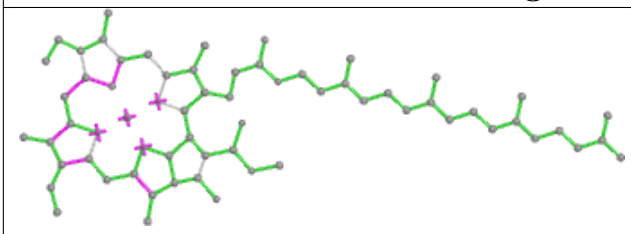
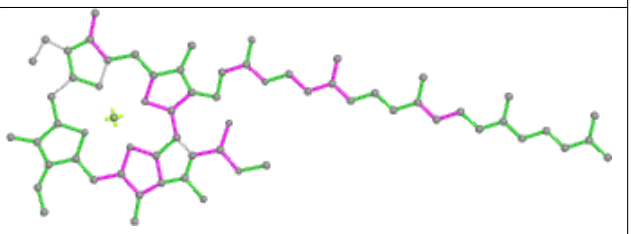


Rings

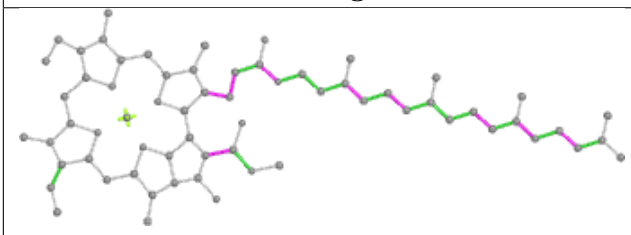
Ligand CLA C 505



Bond lengths



Bond angles



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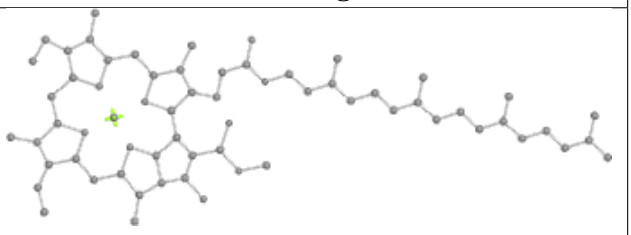
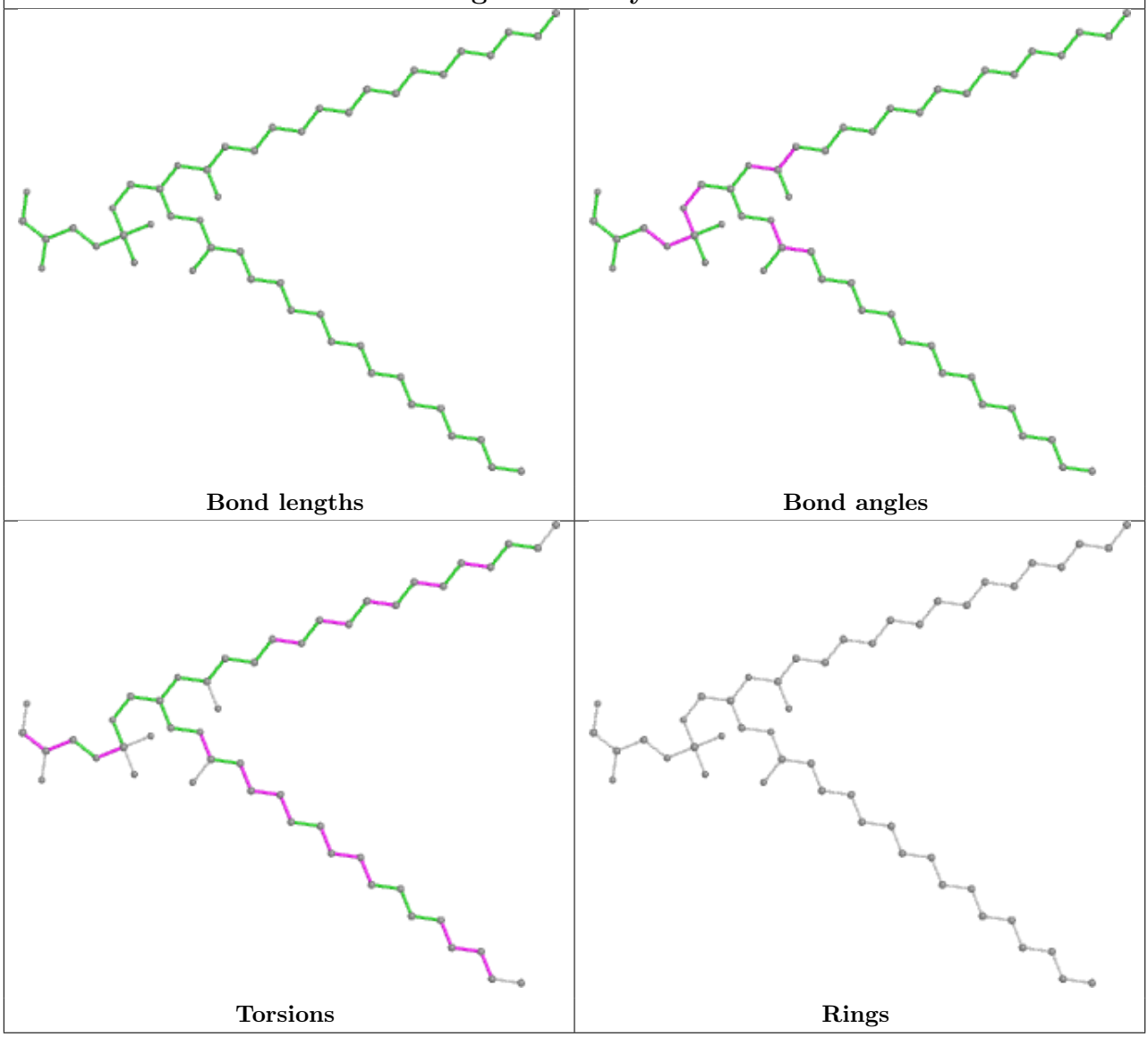
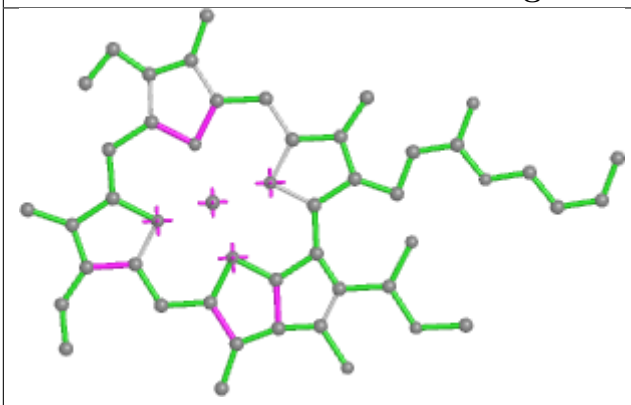
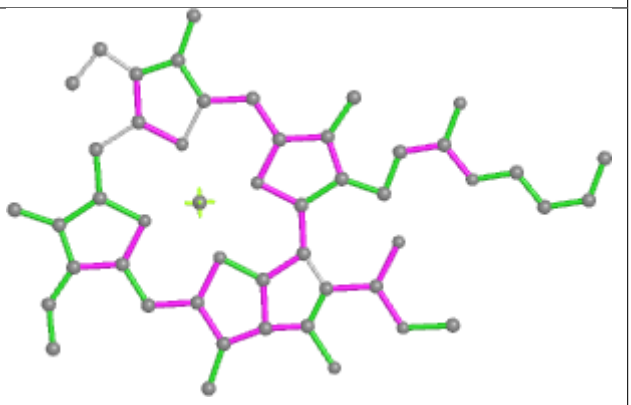
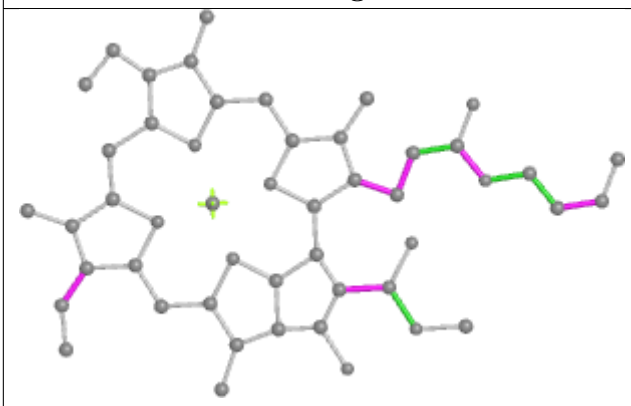
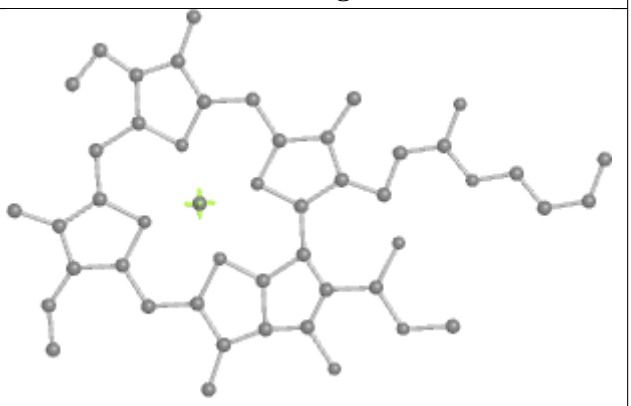
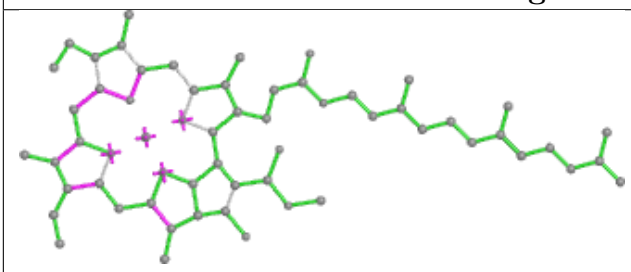
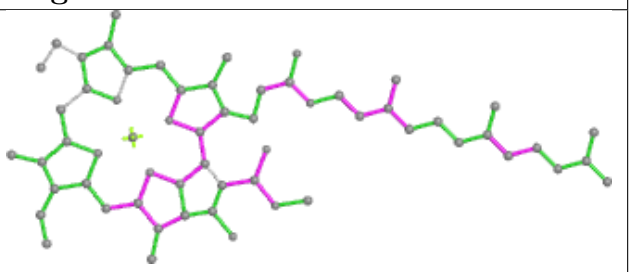
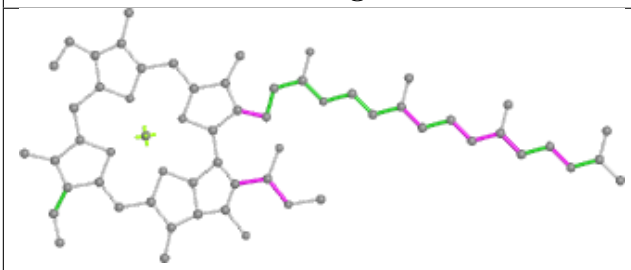
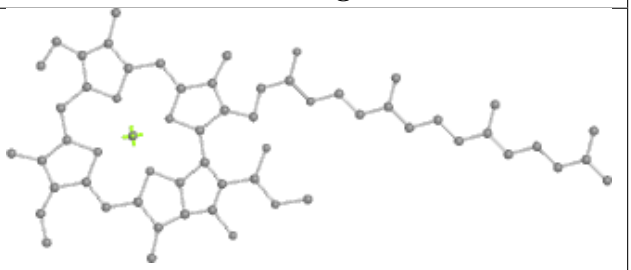


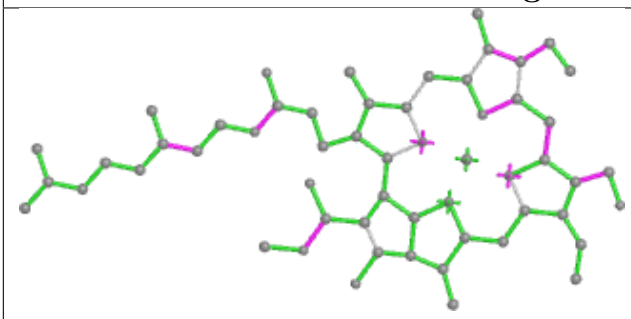
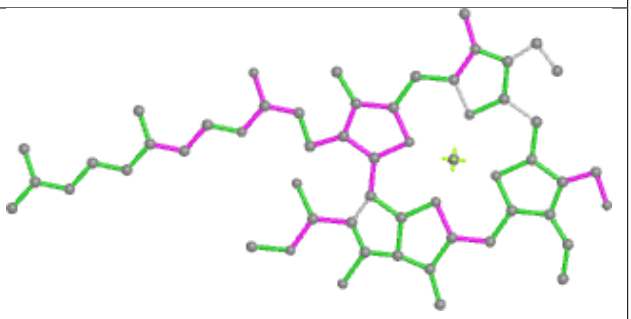
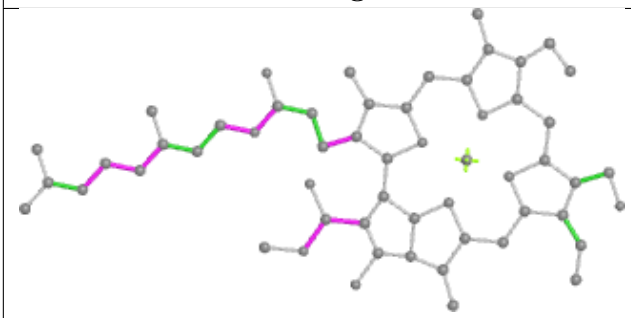
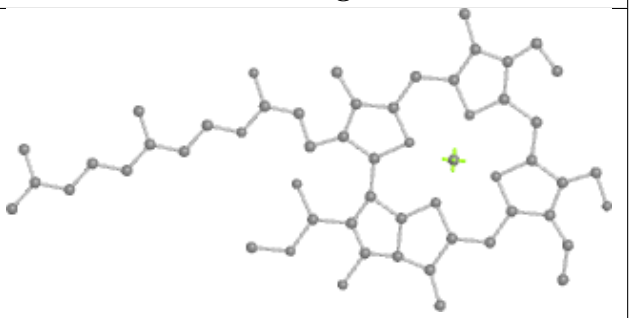
Rings

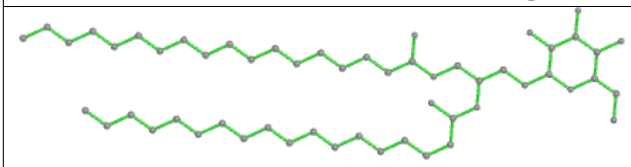
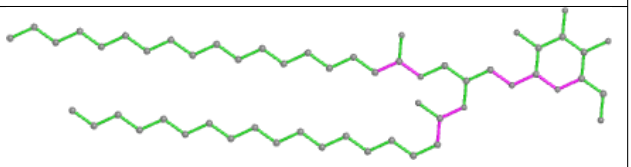
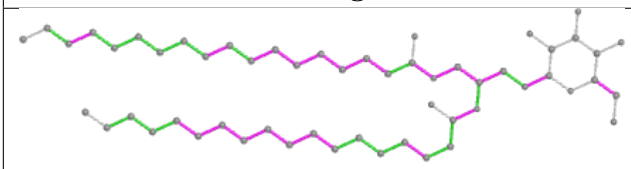
Ligand LHG y 319



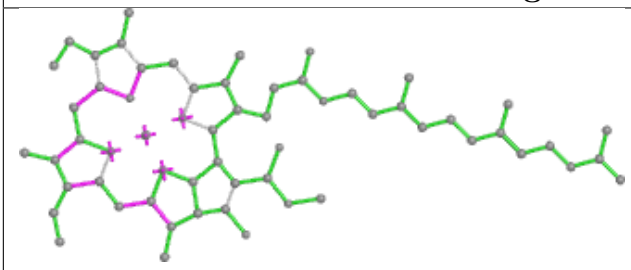
Ligand CLA R 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

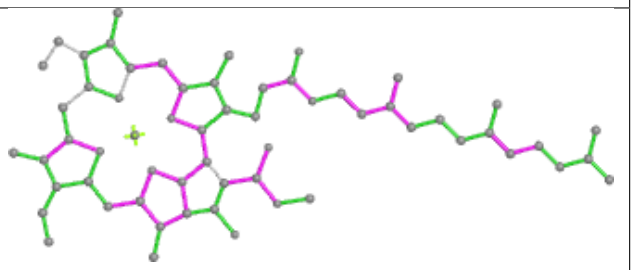
Ligand CHL Y 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG b 623	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA Y 313



Bond lengths



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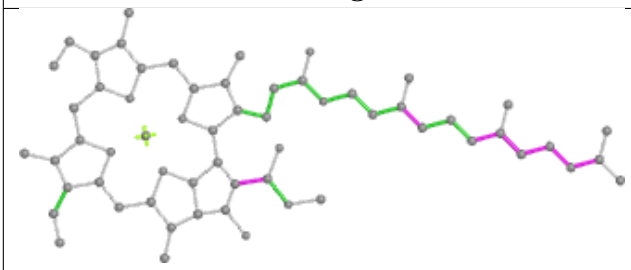
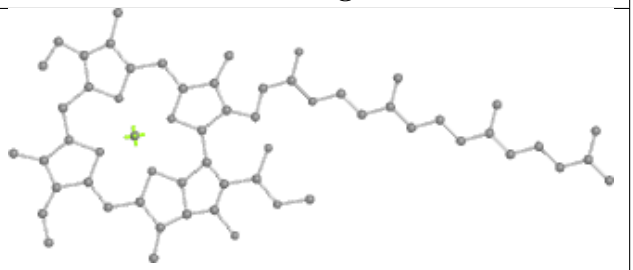
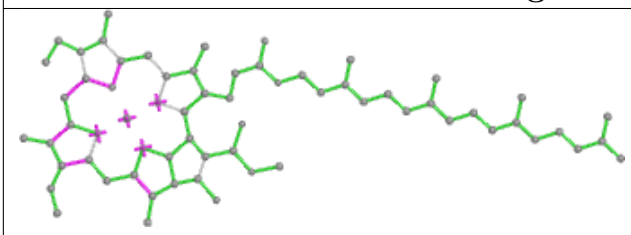


Torsions



Rings

Ligand CLA b 603



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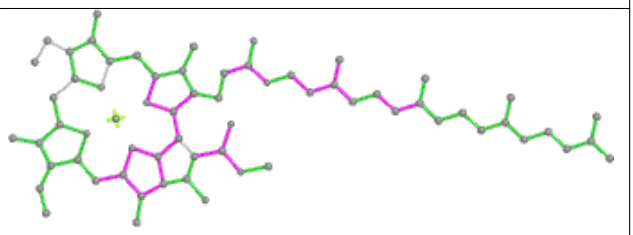
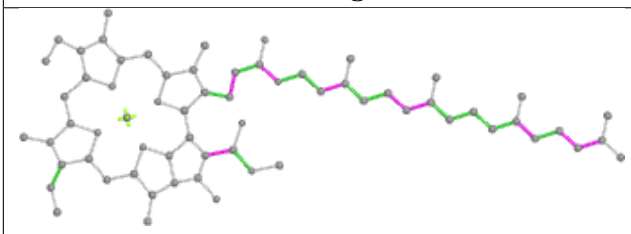


Bond angles



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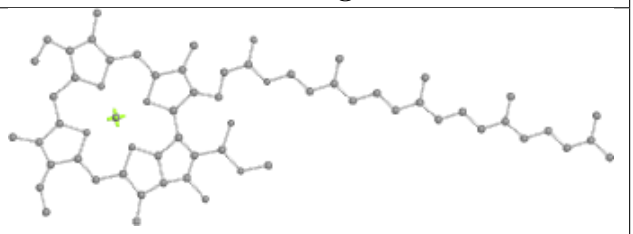
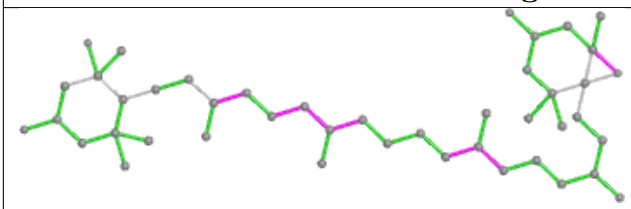


Rings

Ligand NEX N 617



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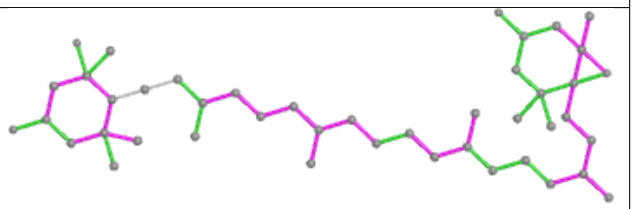
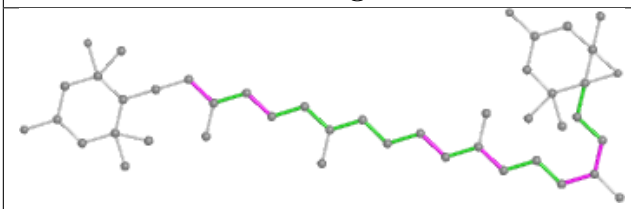


Bond angles



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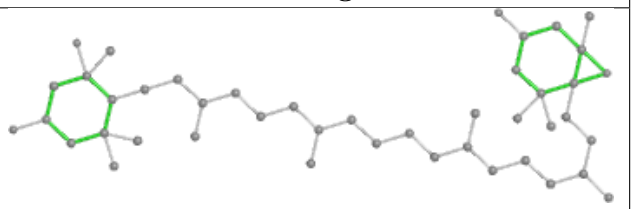
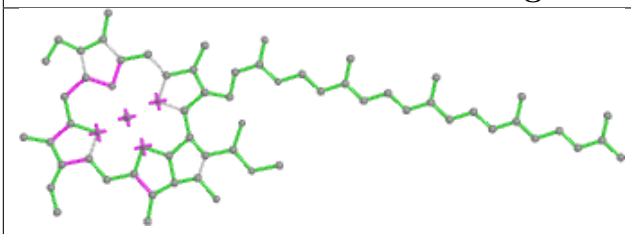
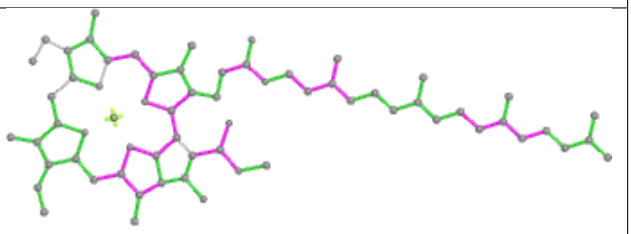
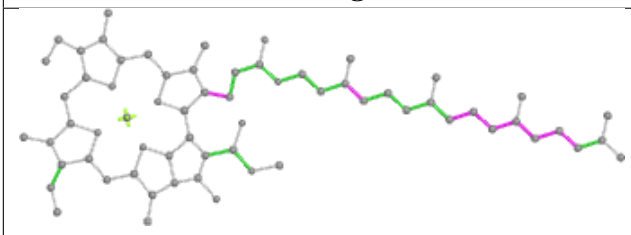
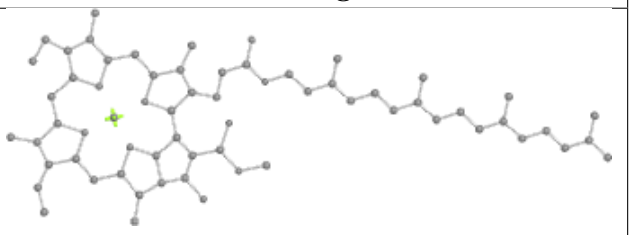
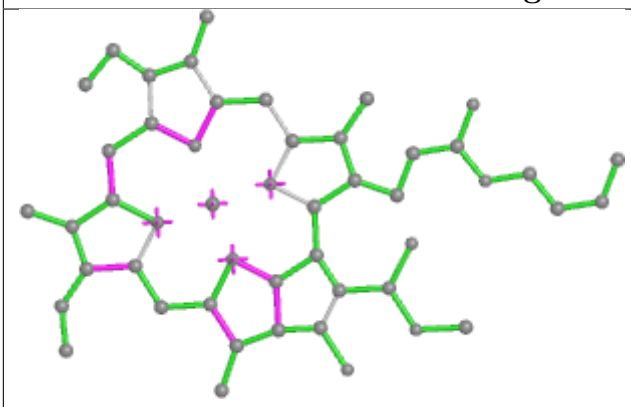
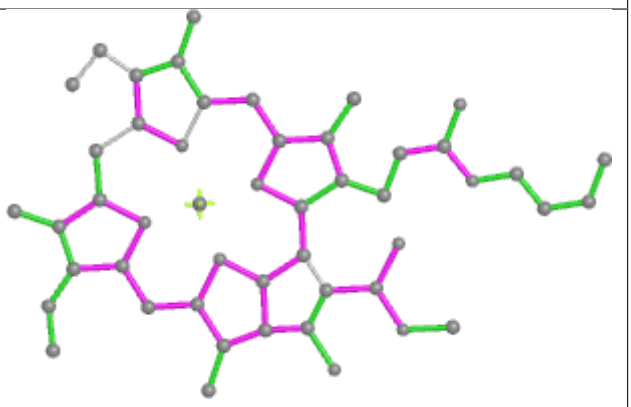
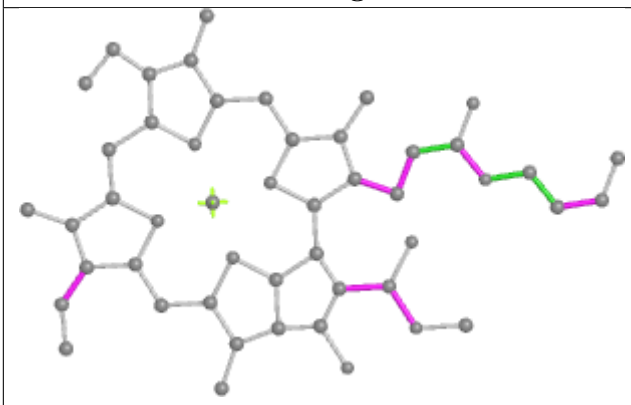
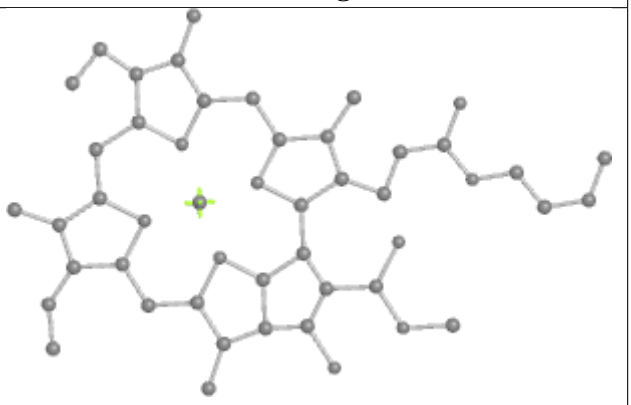
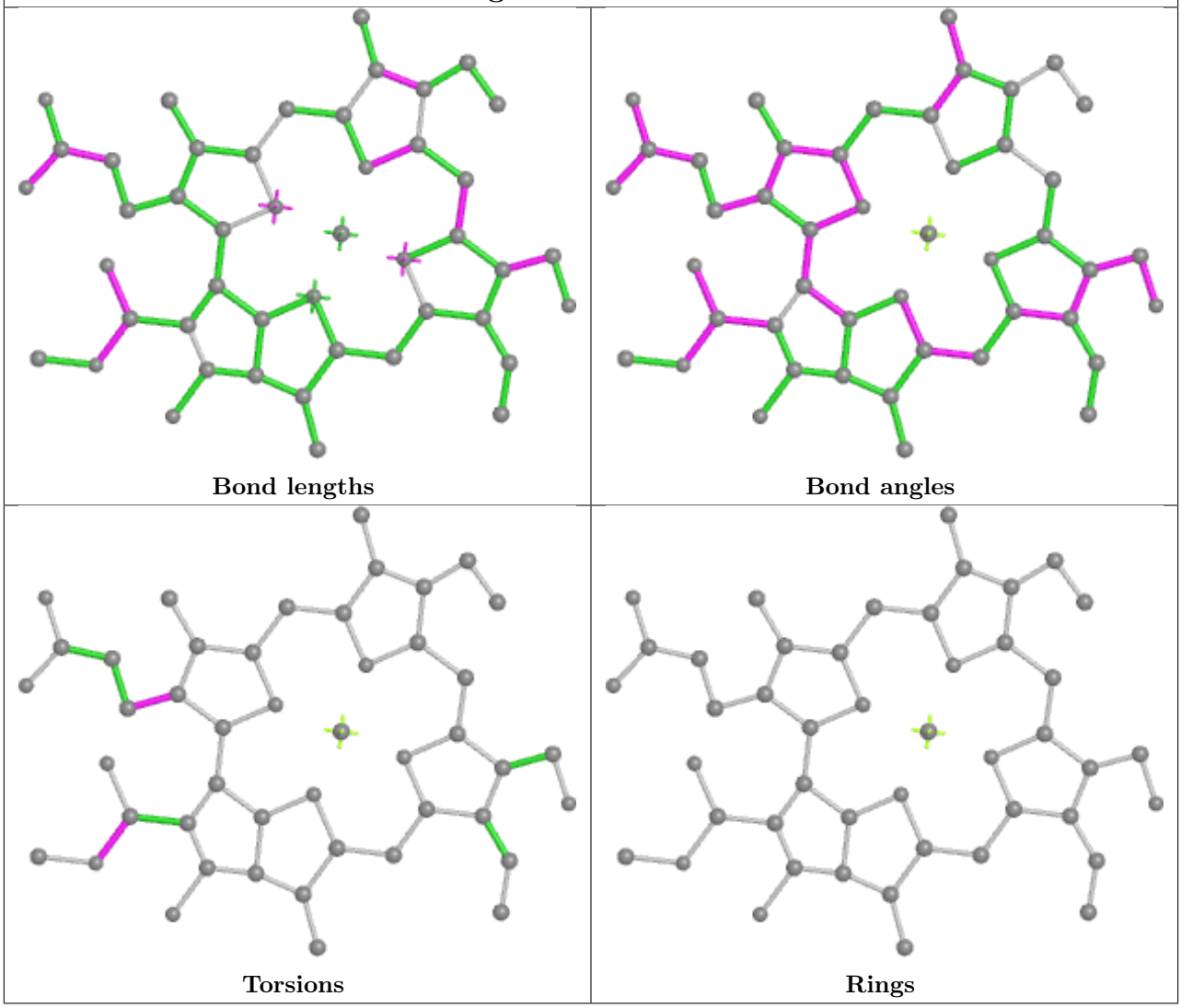


Rings

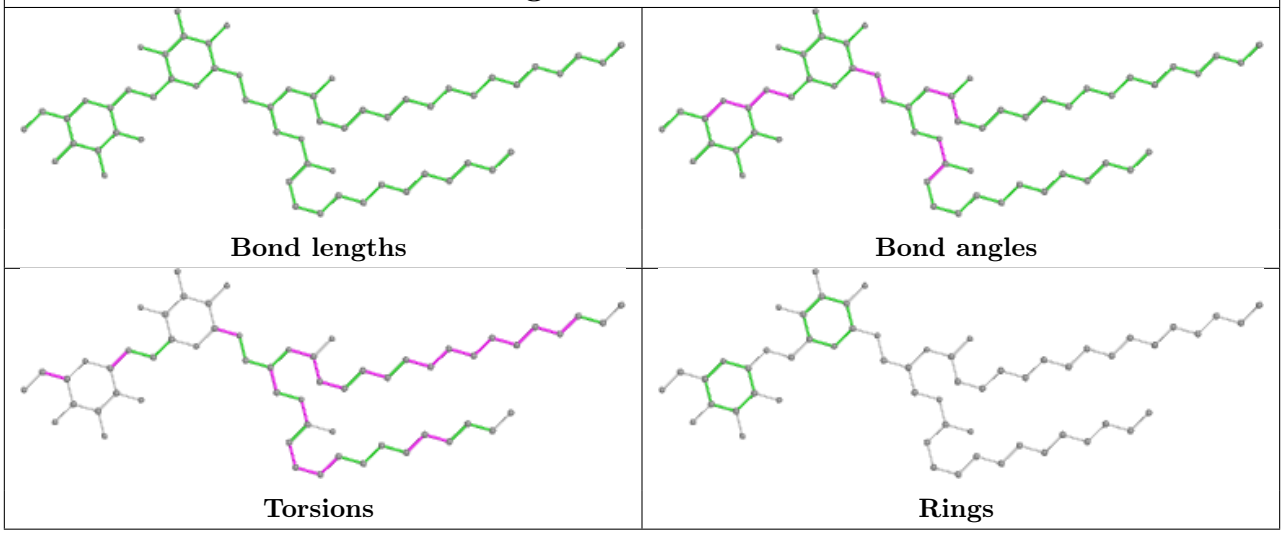
Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

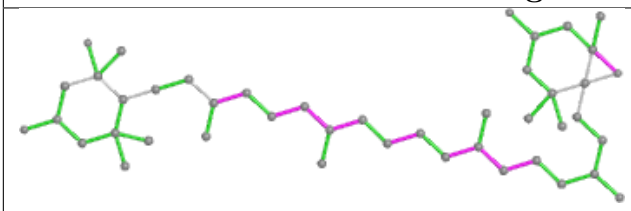
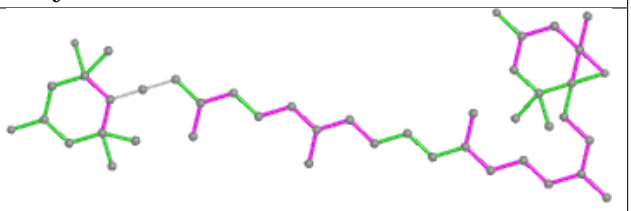
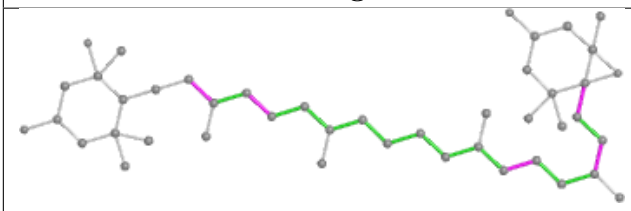
Ligand CLA R 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

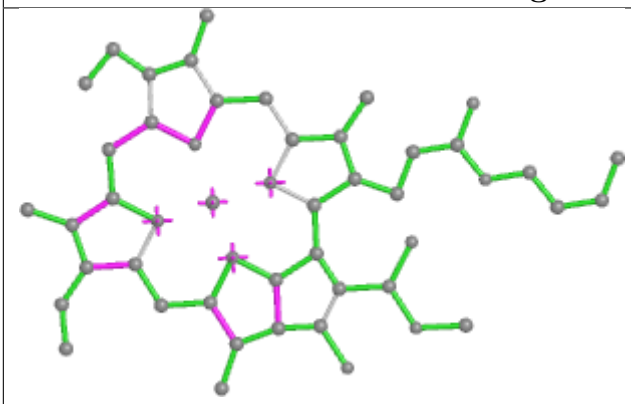
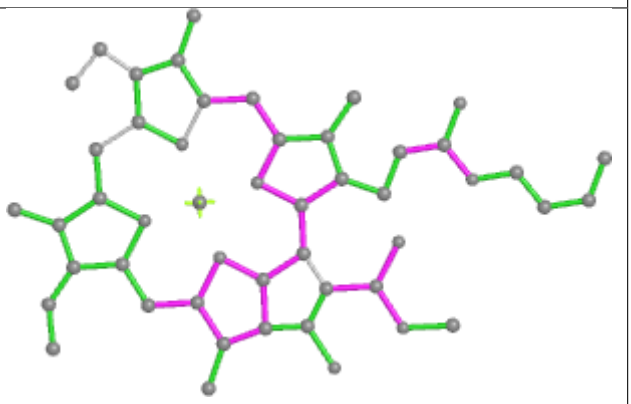
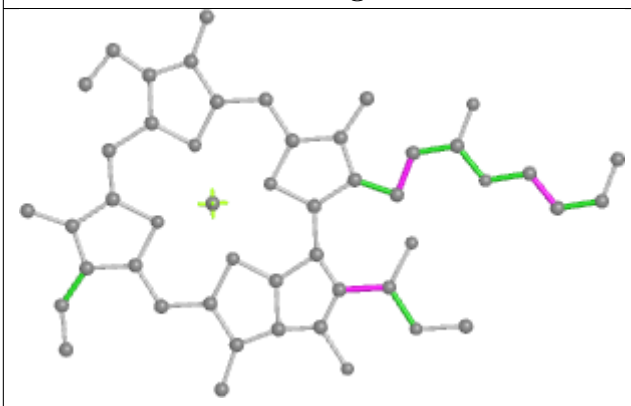
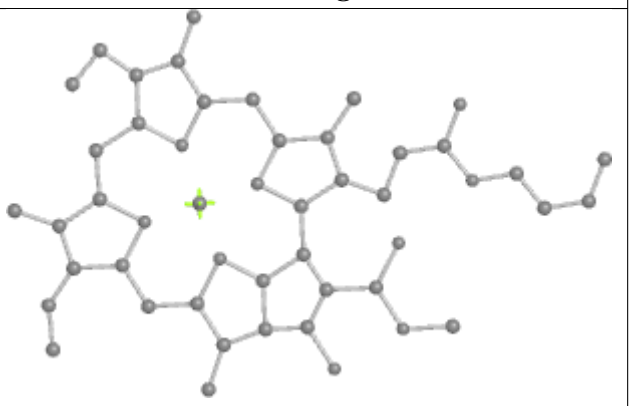
Ligand CHL r 605



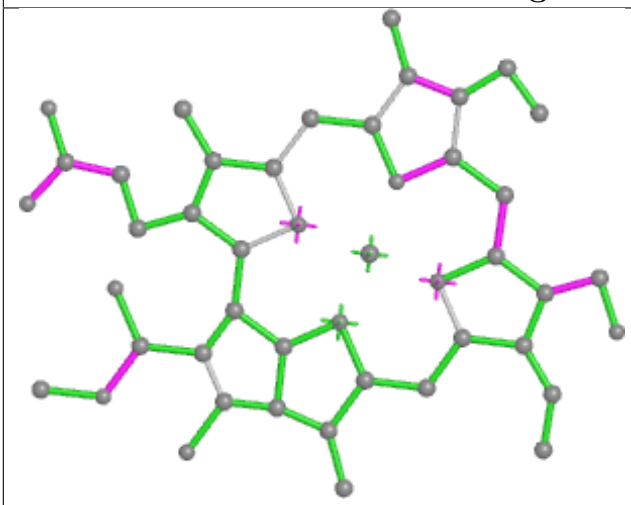
Ligand DGD a 401



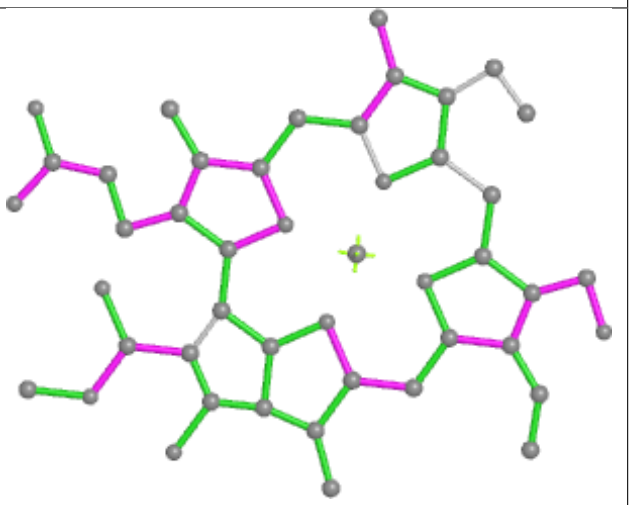
Ligand NEX y 318	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA s 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

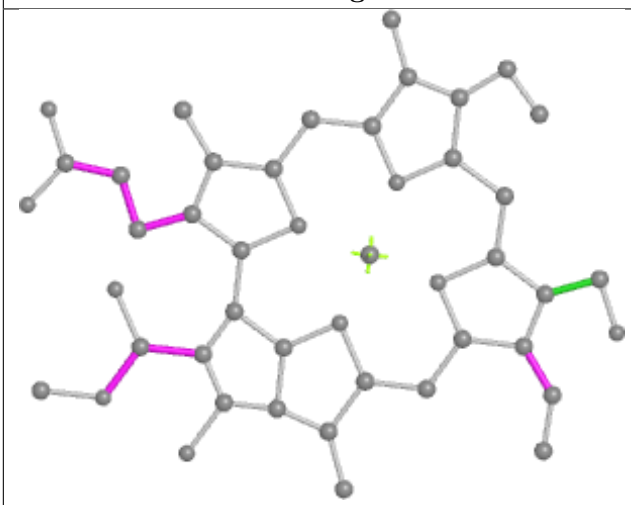
Ligand CHL r 606



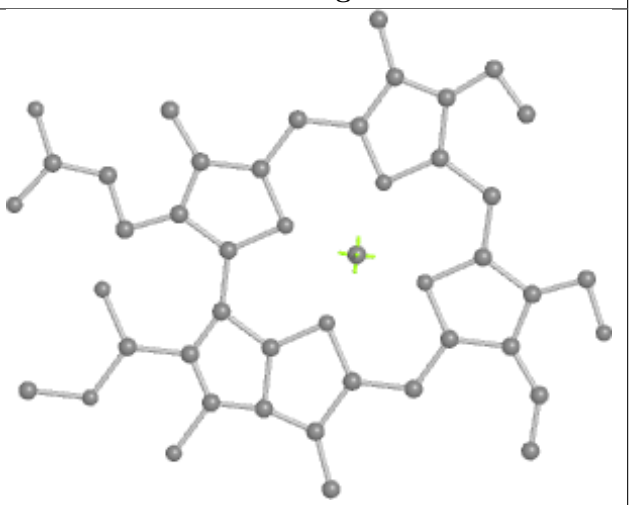
Bond lengths



Bond angles

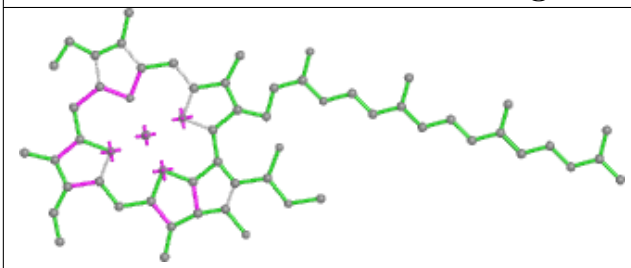


Torsions

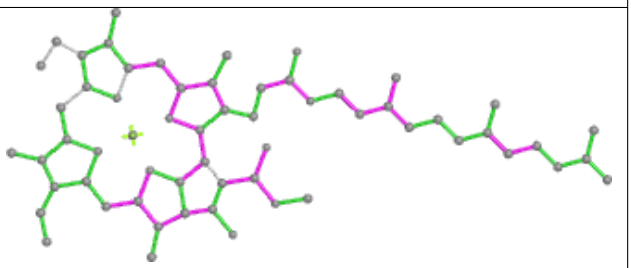


Rings

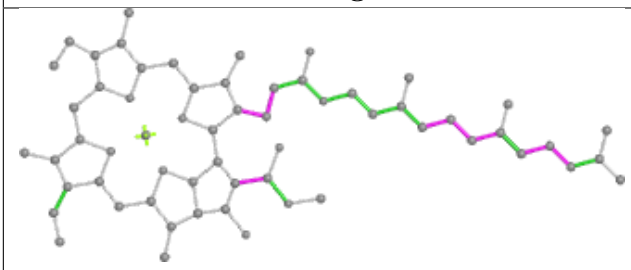
Ligand CLA r 612



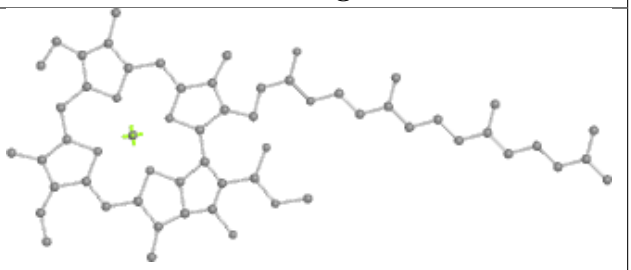
Bond lengths



Bond angles

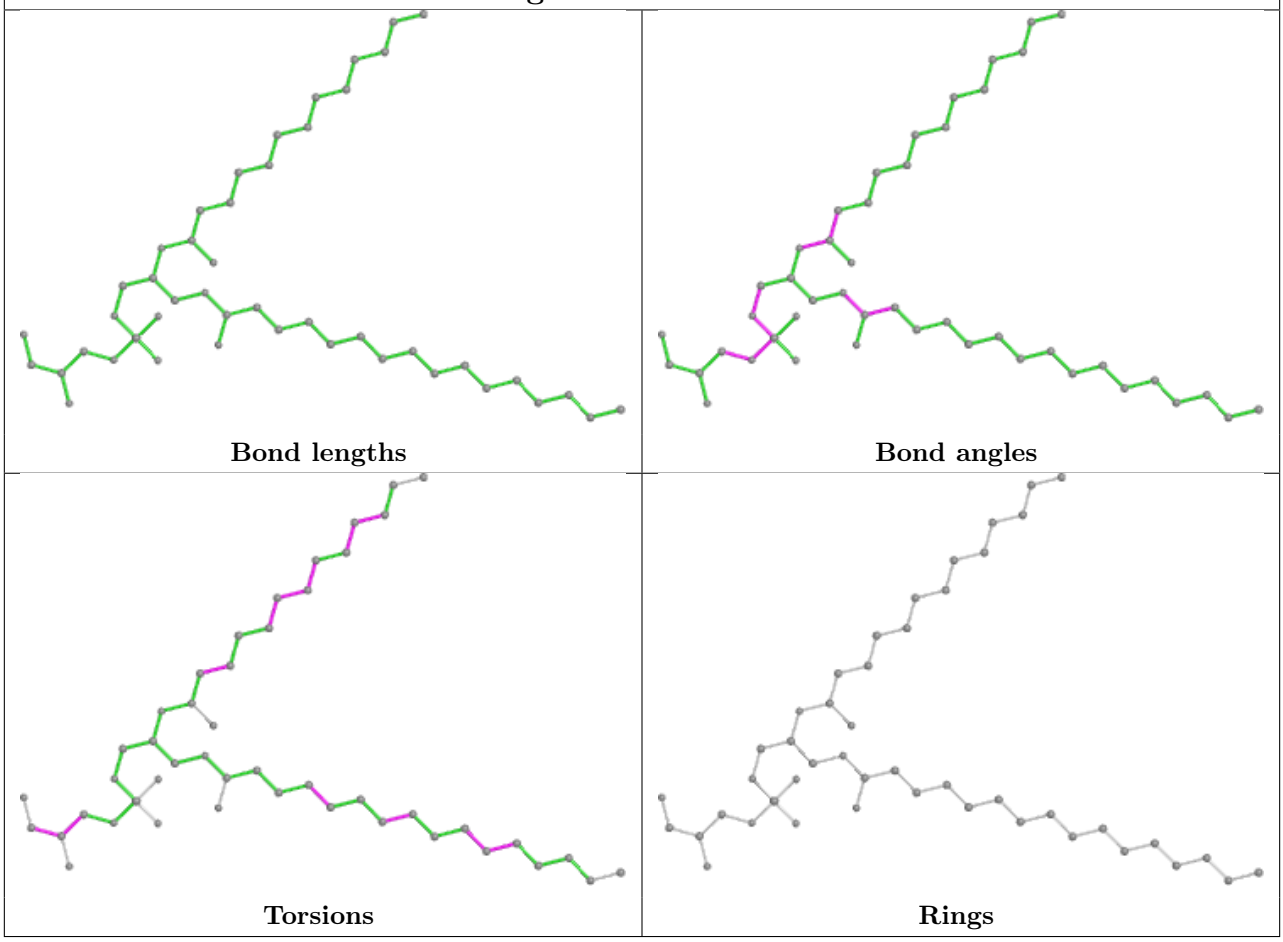


Torsions



Rings

Ligand LHG b 625



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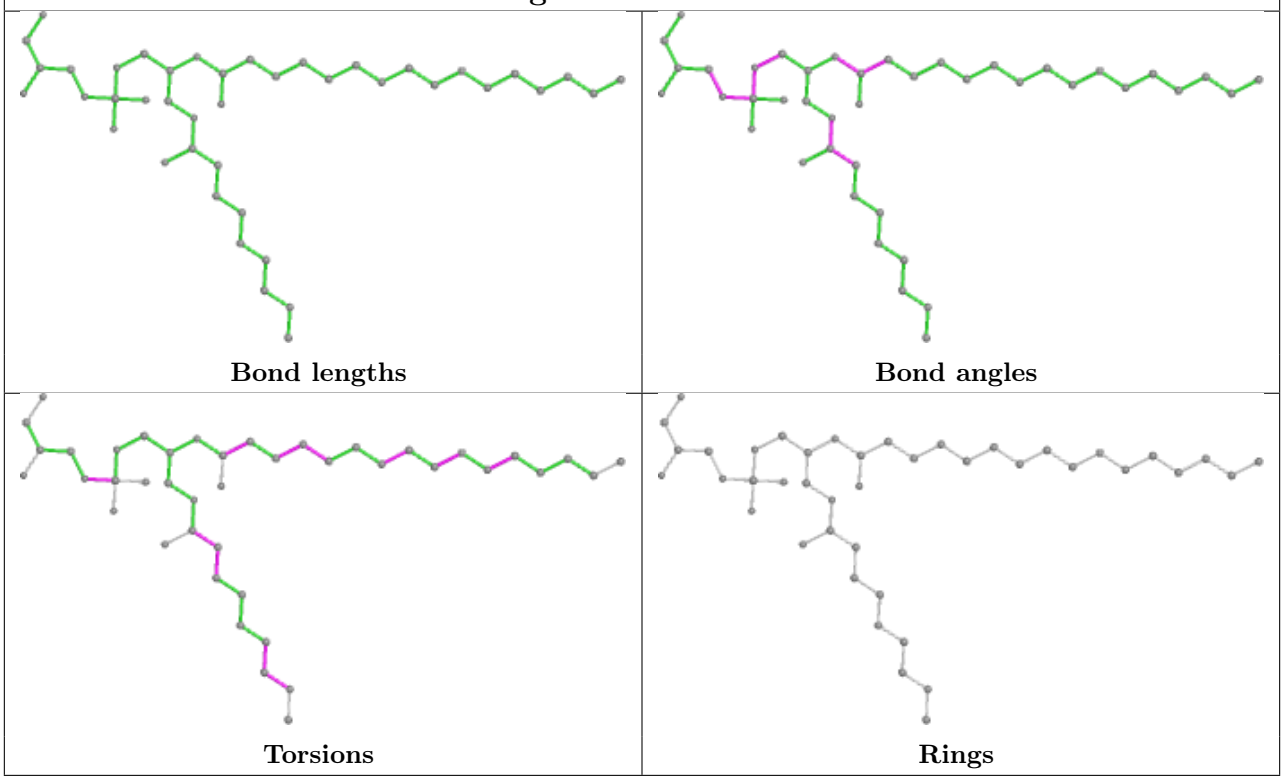
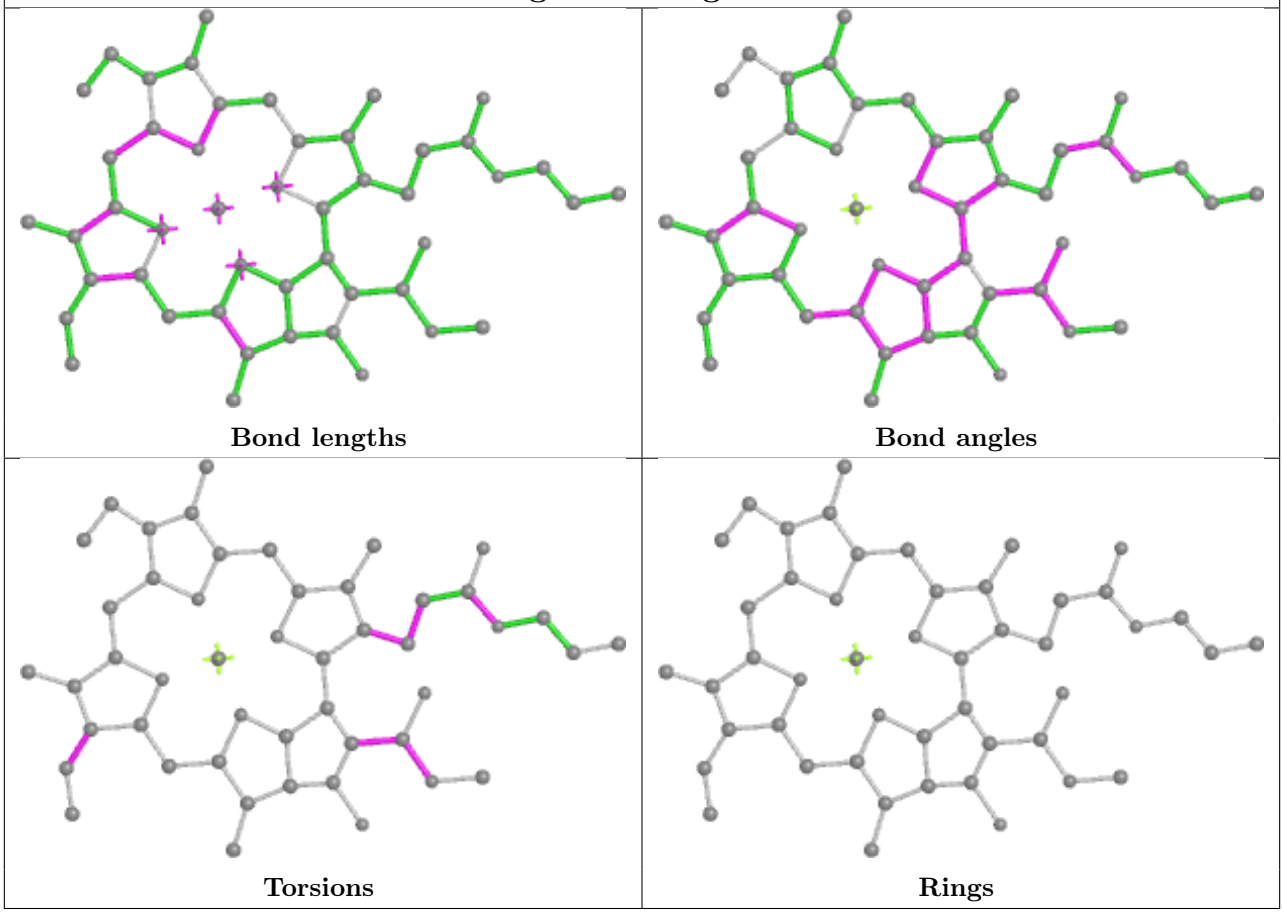
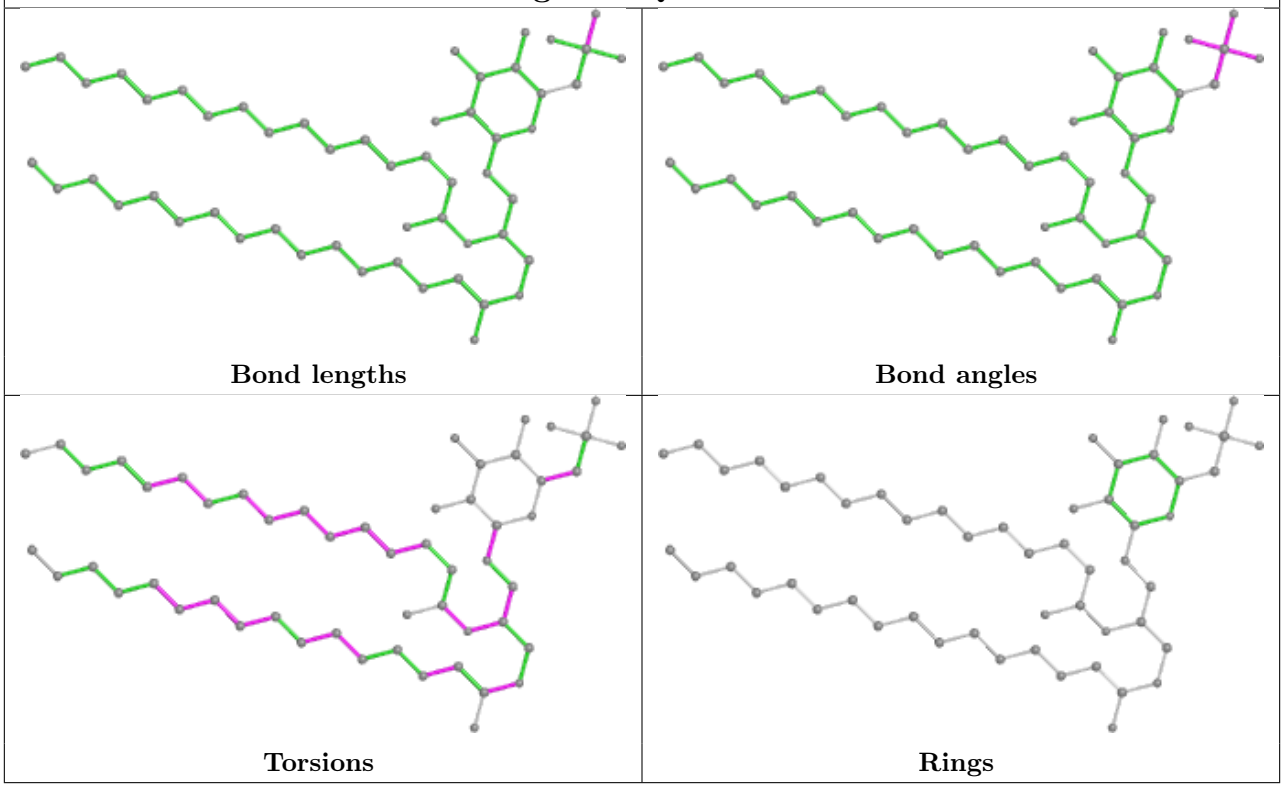


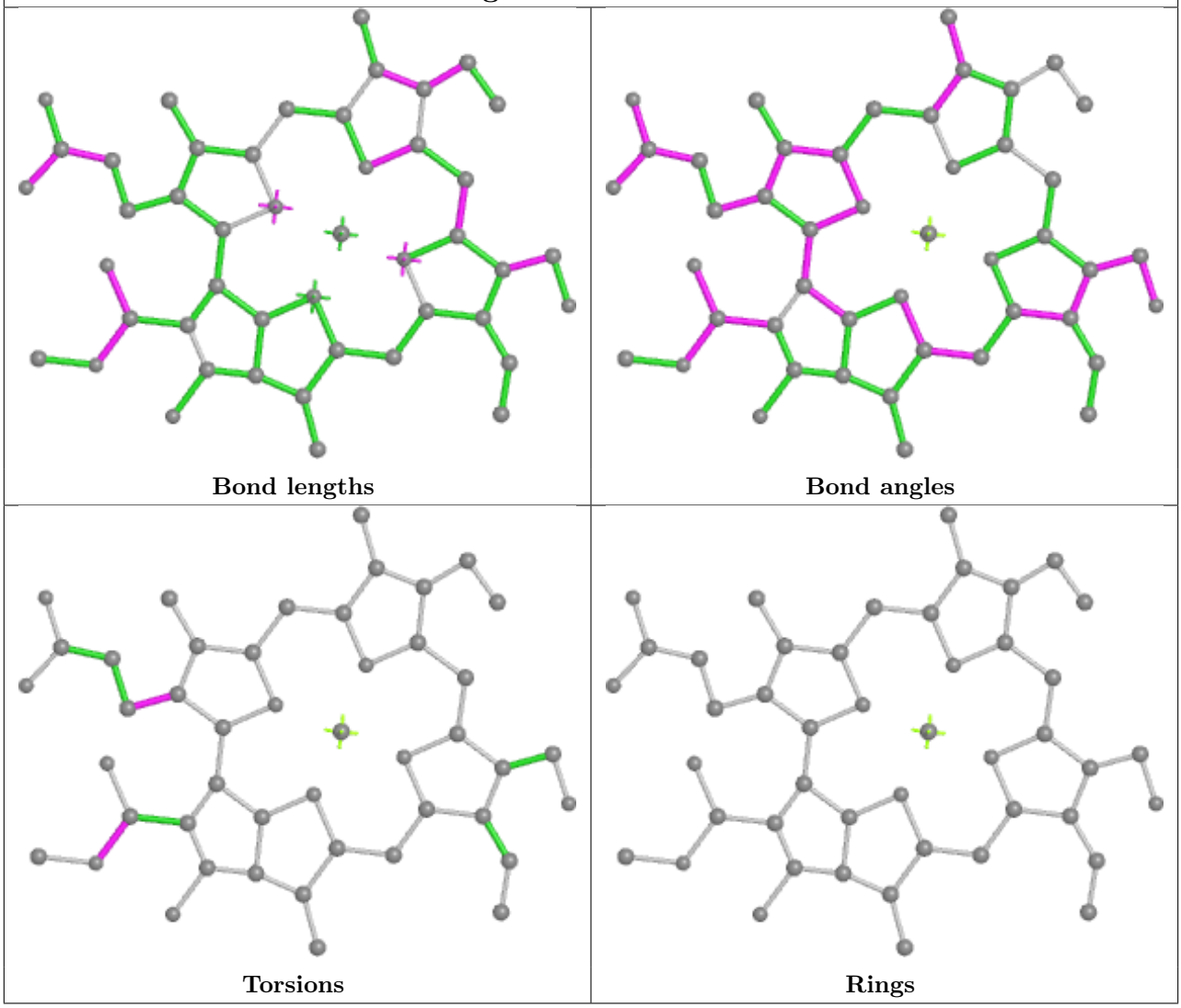
Ligand CLA g 614



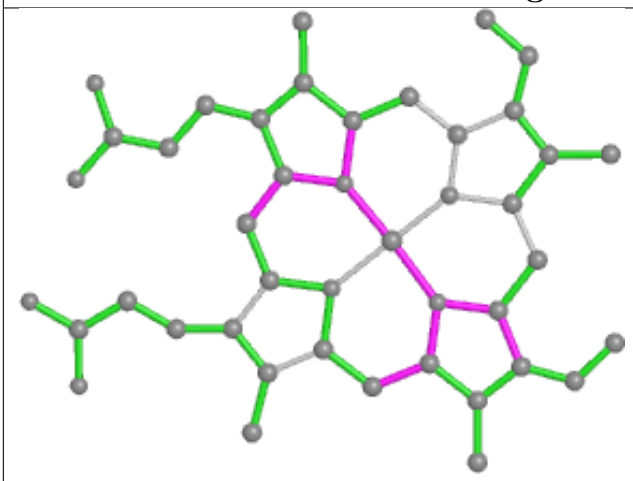
Ligand SQD l 101



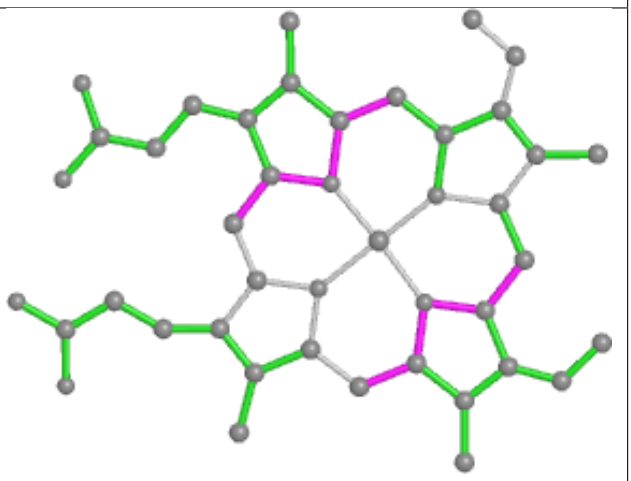
Ligand CHL R 605



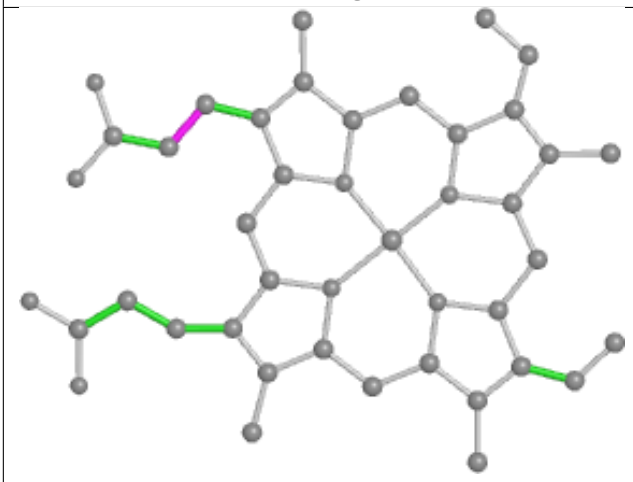
Ligand HEM f 101



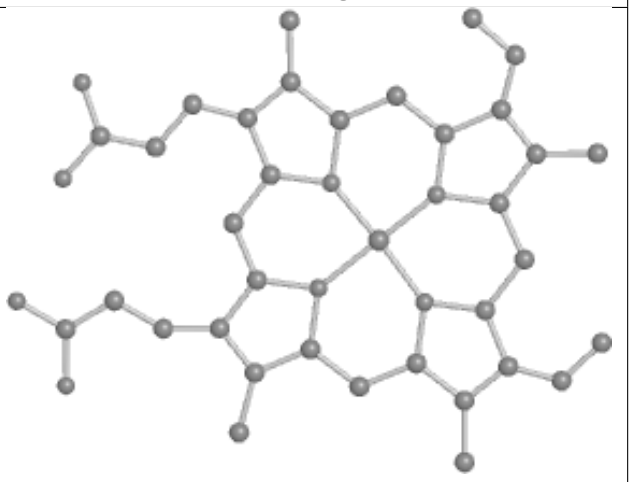
Bond lengths



Bond angles

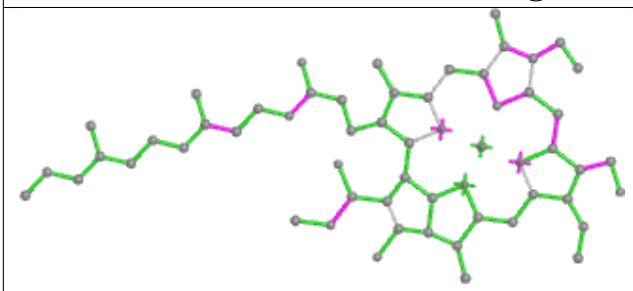


Torsions

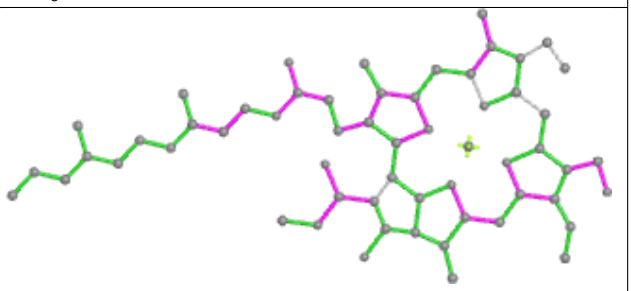


Rings

Ligand CHL y 308



Bond lengths



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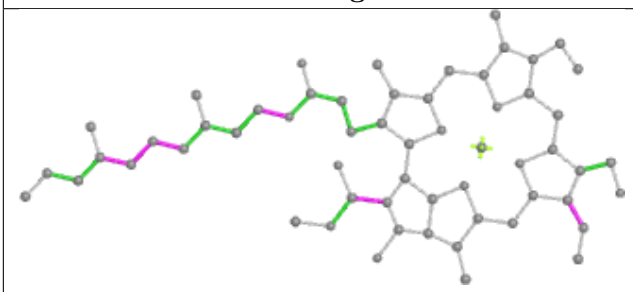
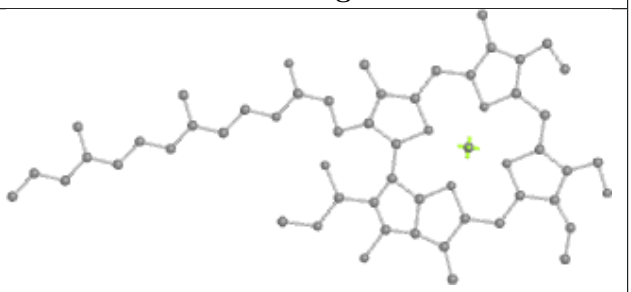
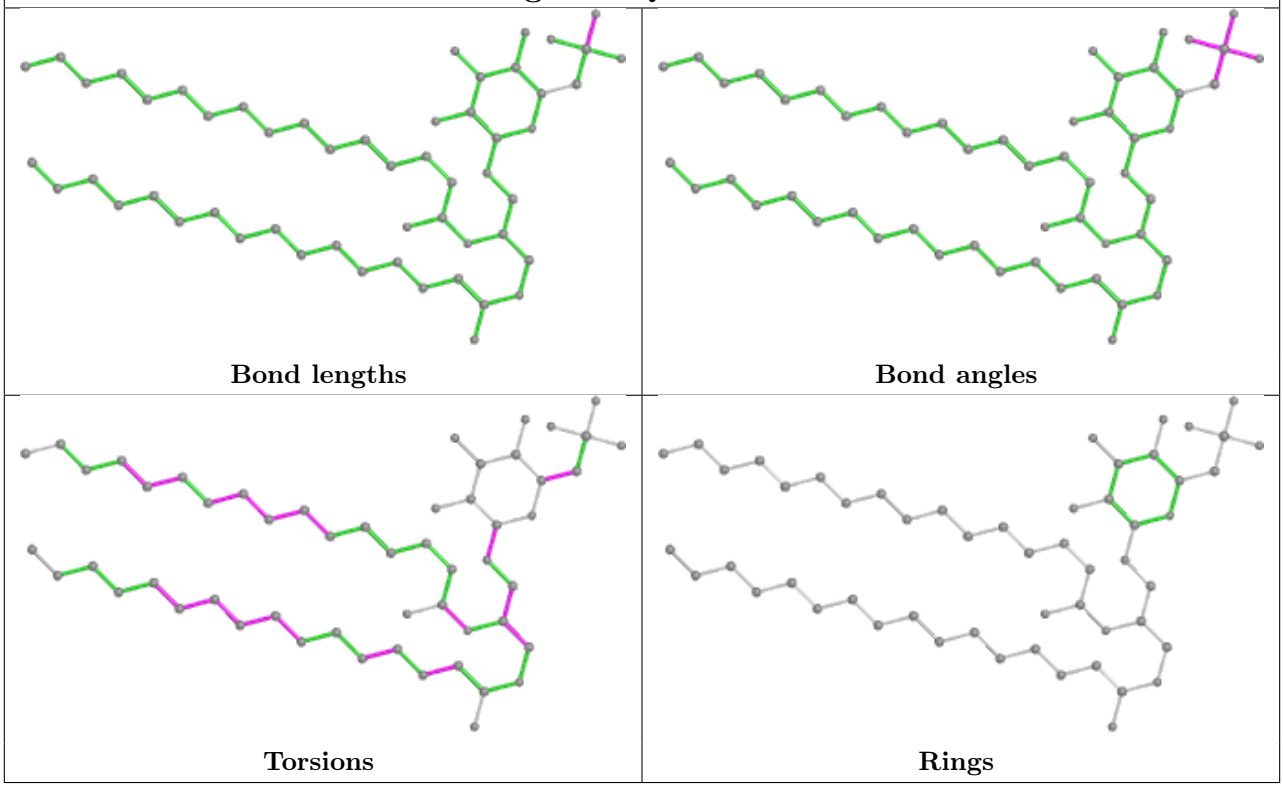


Torsions

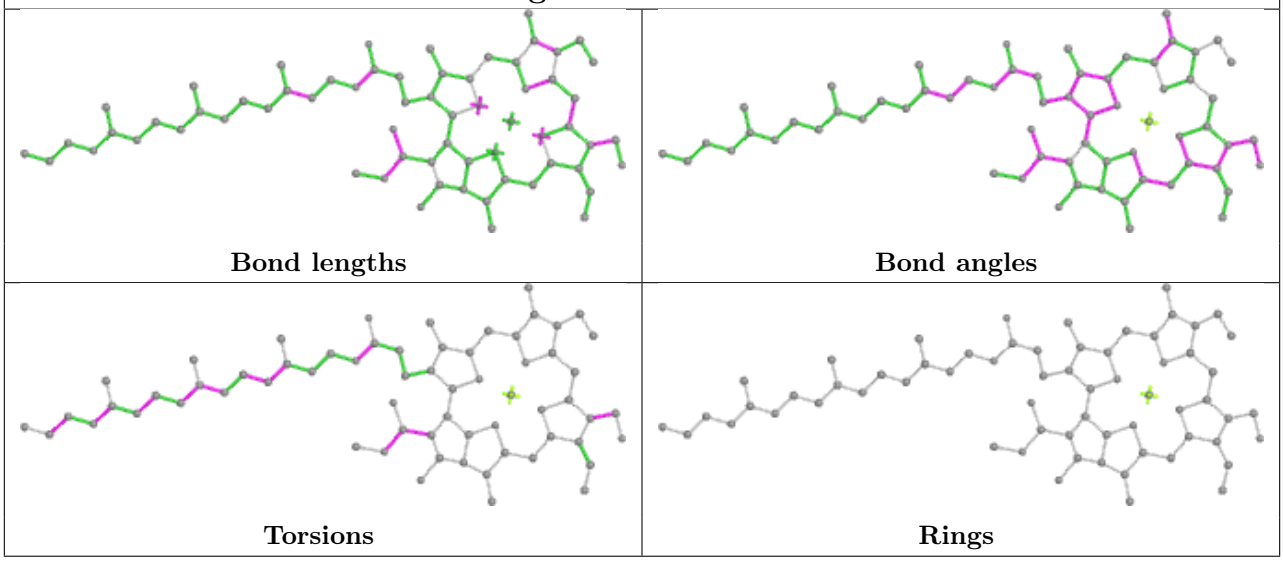


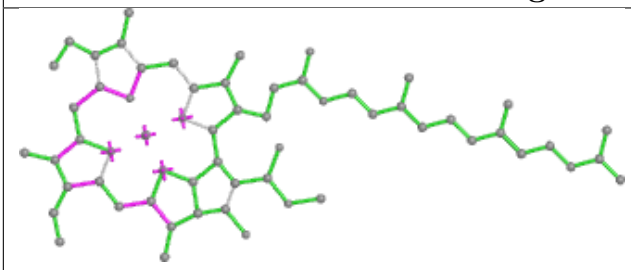
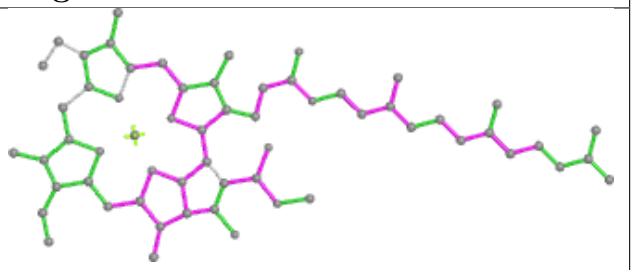
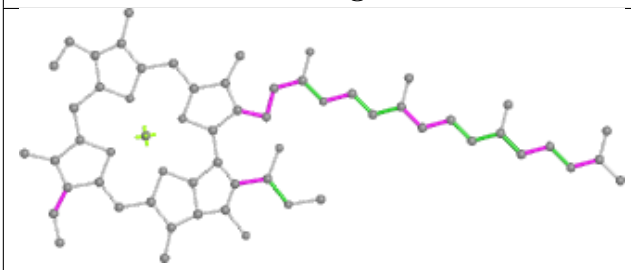
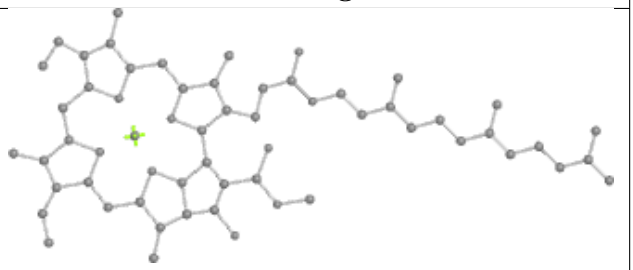
Rings

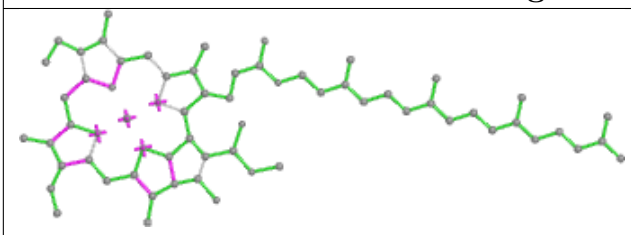
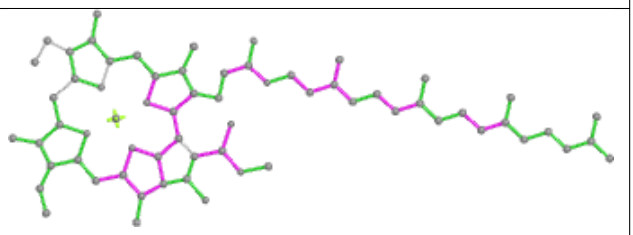
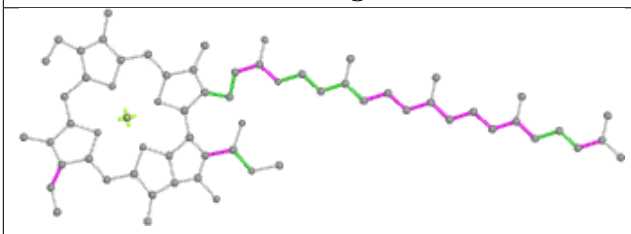
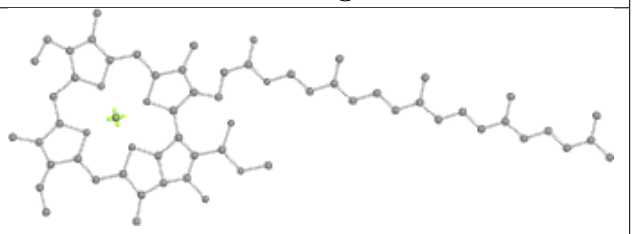
Ligand SQD A 411



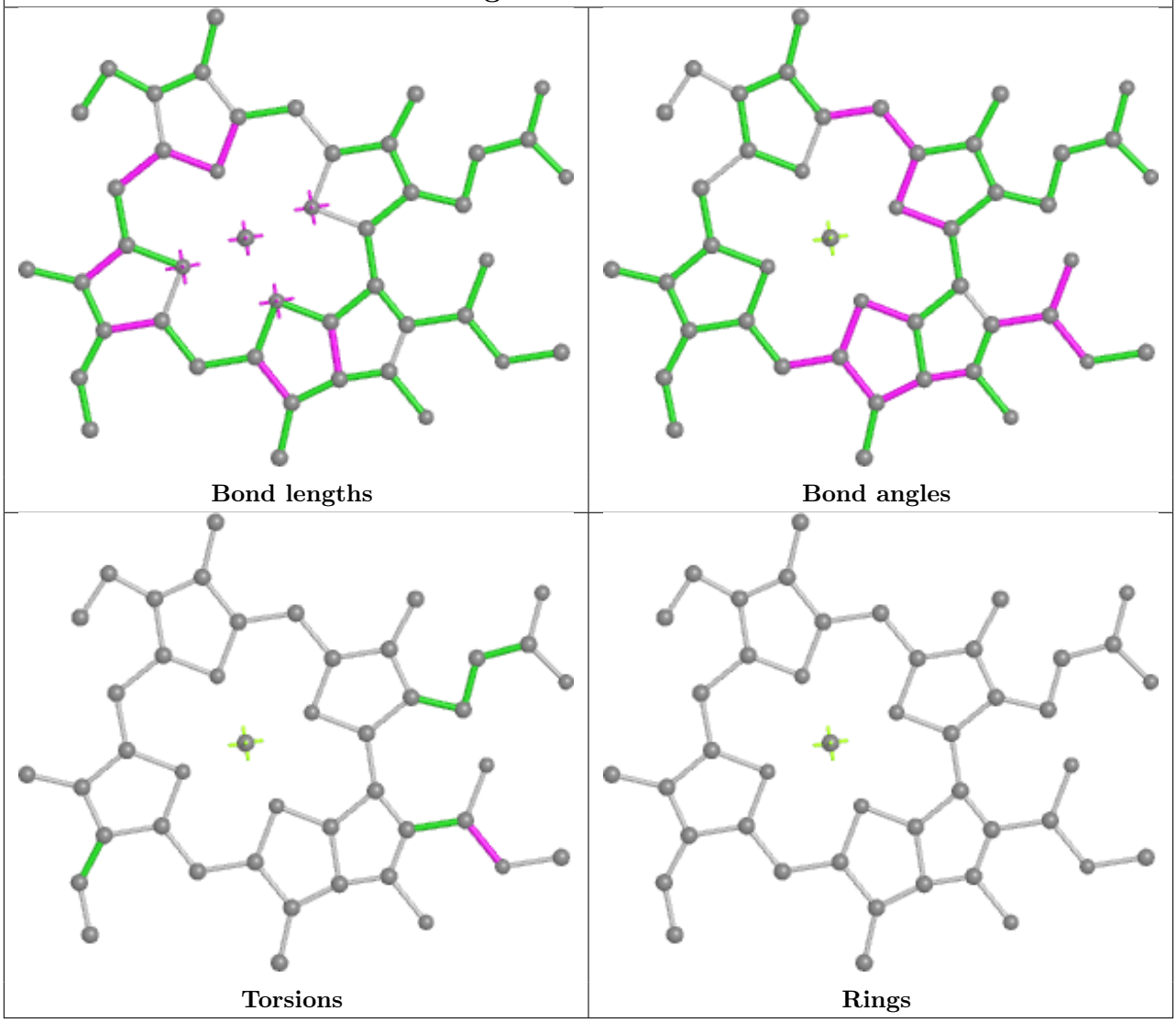
Ligand CHL 2 601



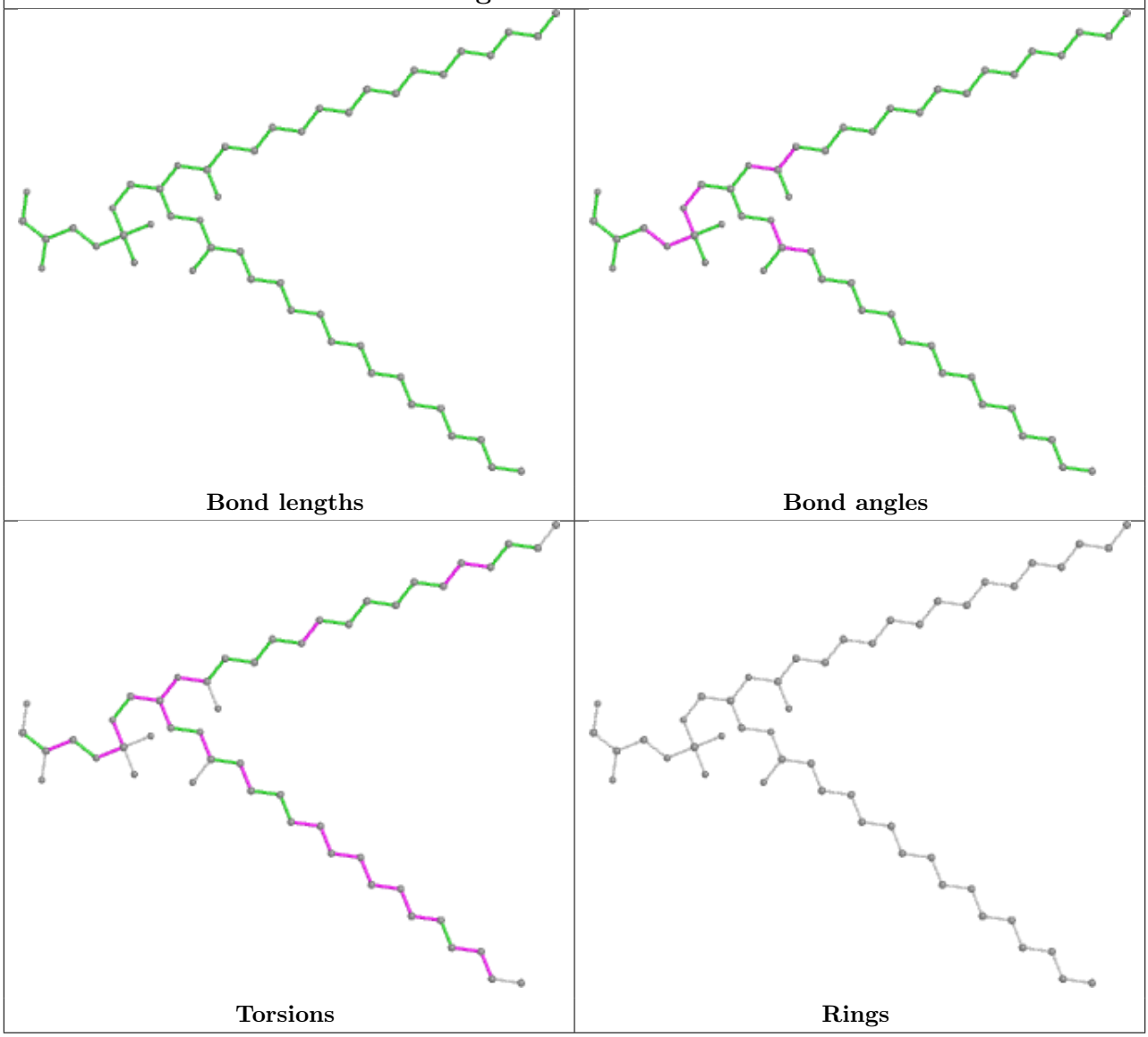
Ligand CLA g 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 304



Ligand LHG l 103



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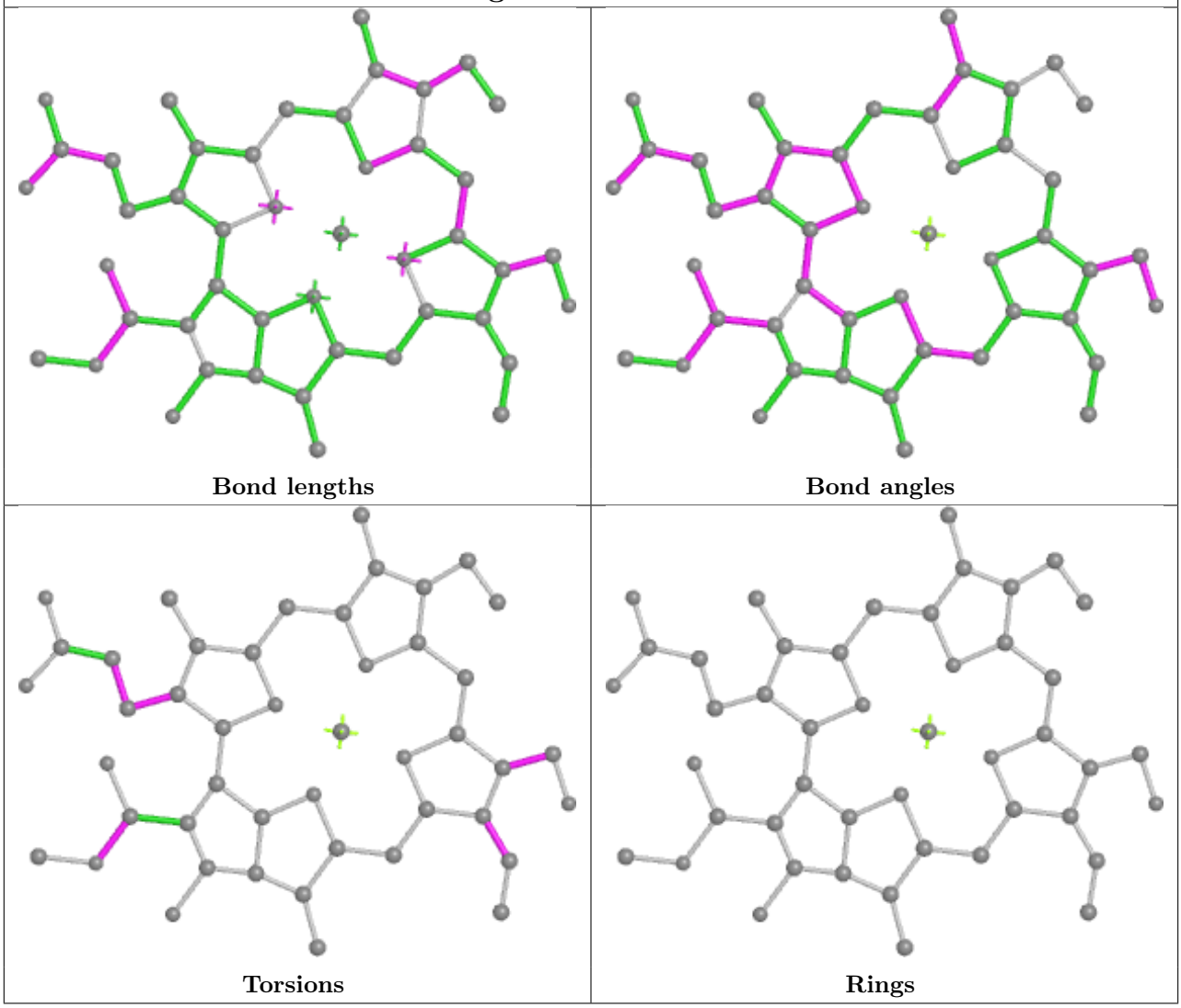

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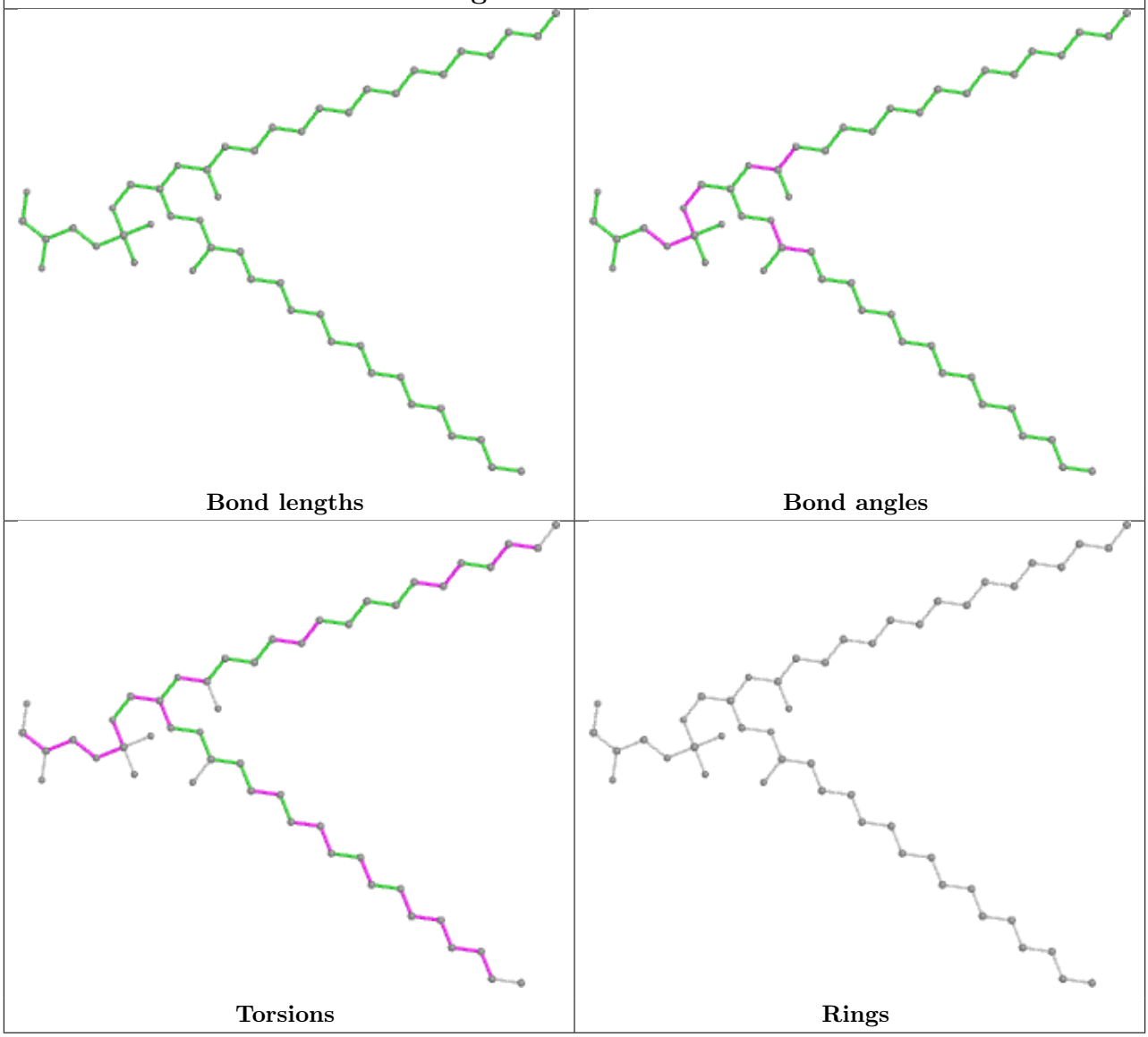

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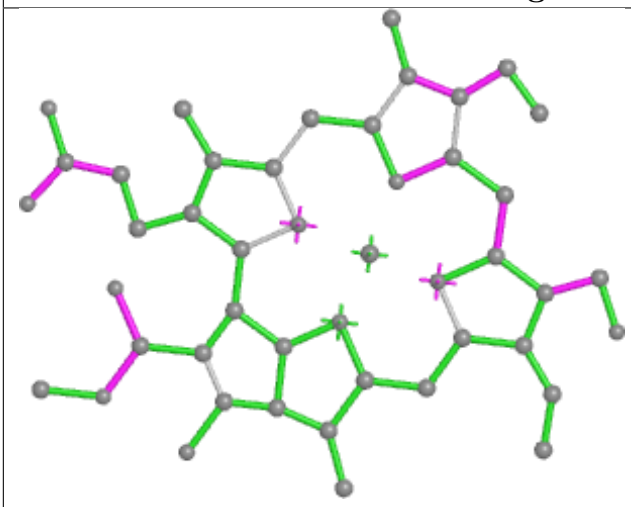
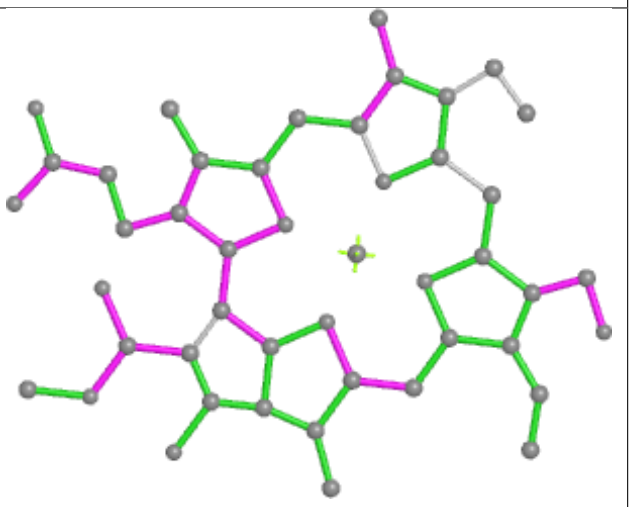
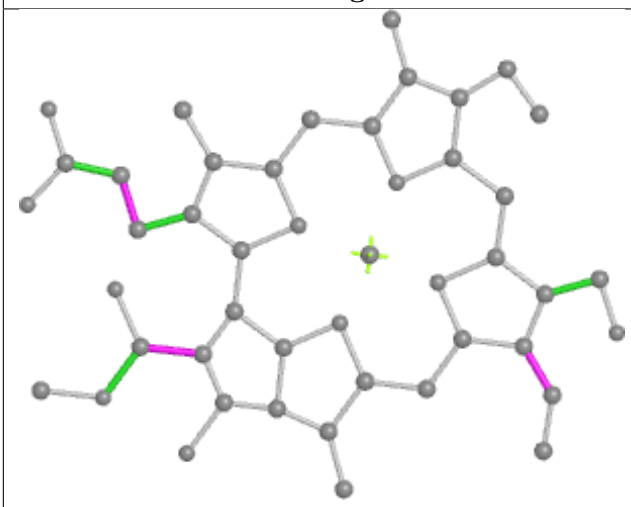


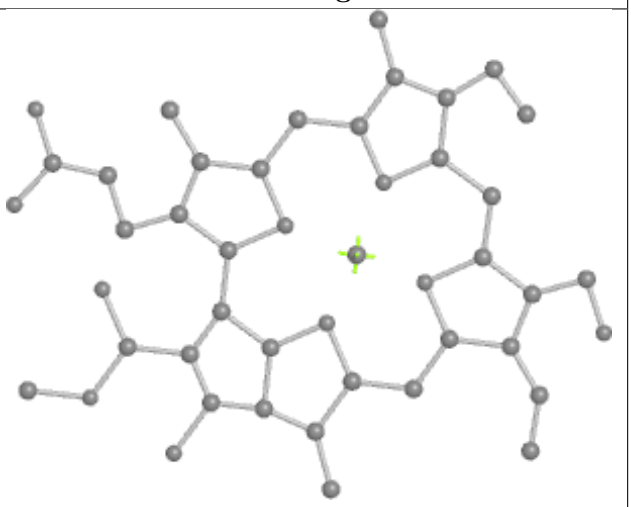
Bond lengths



Bond angles

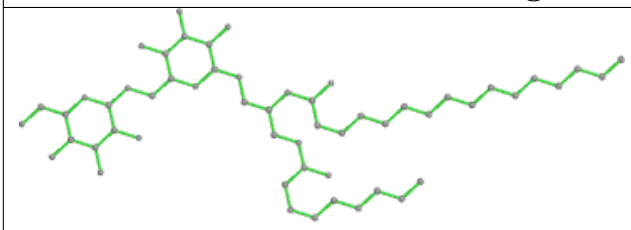


Torsions



Rings

Ligand DGD c 515



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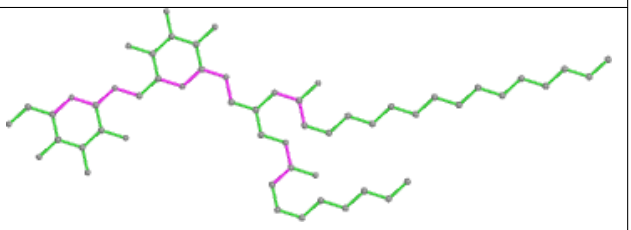
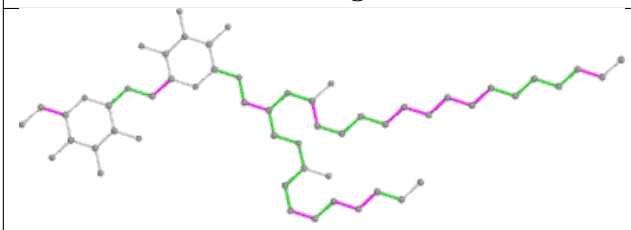


Bond angles



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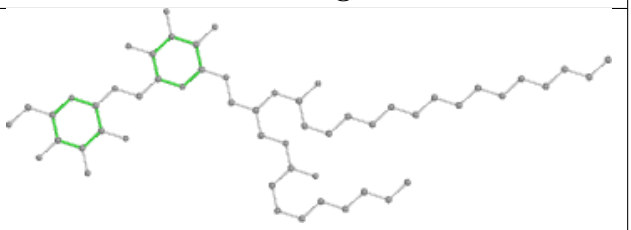

Rings

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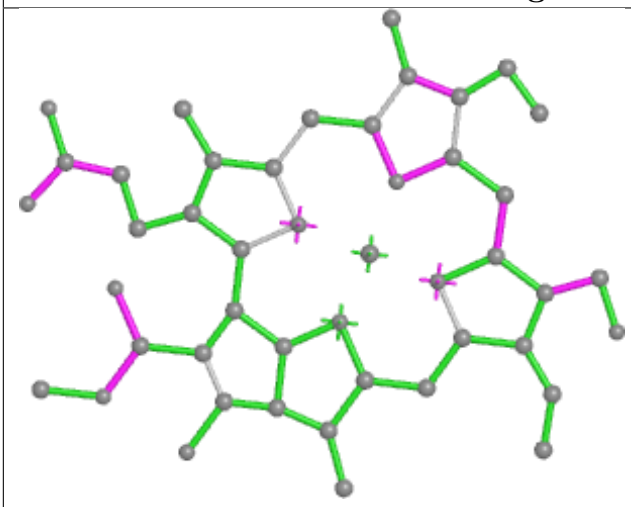

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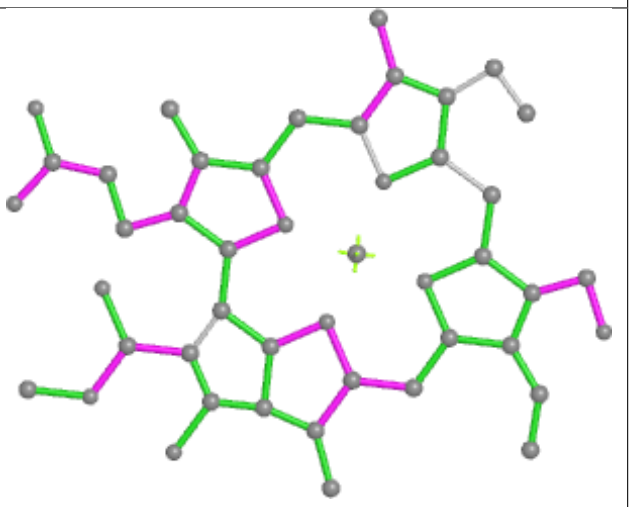
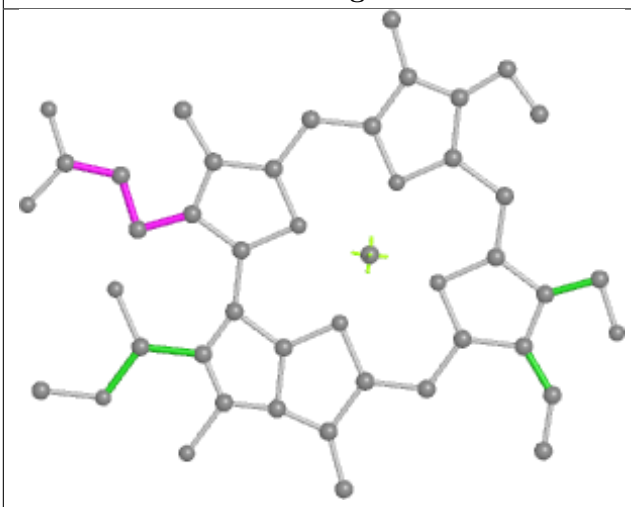


Bond angles



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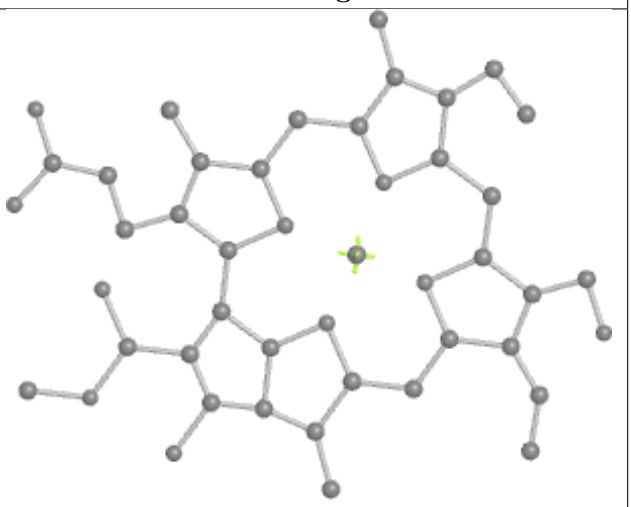
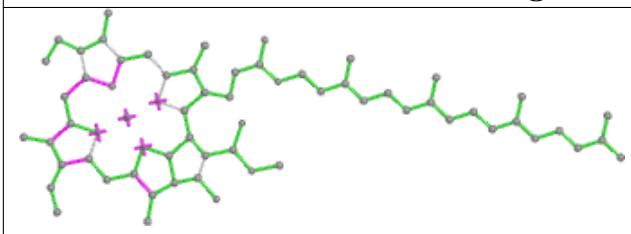
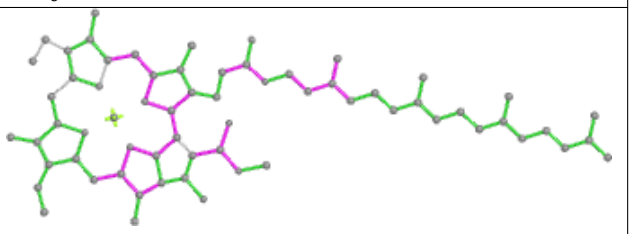


Rings

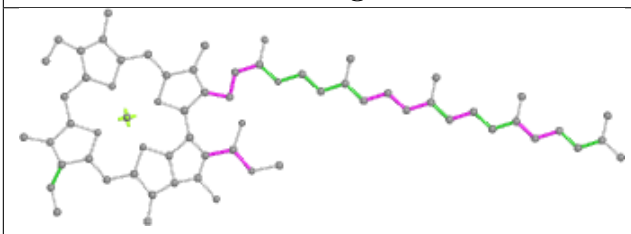
Ligand CLA y 314



Bond lengths



Bond angles



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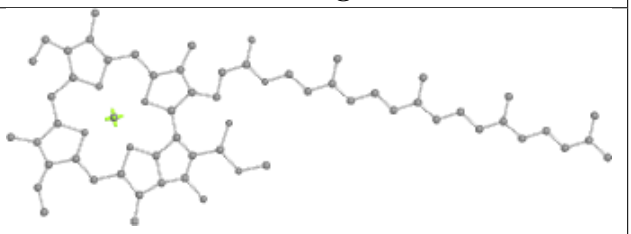
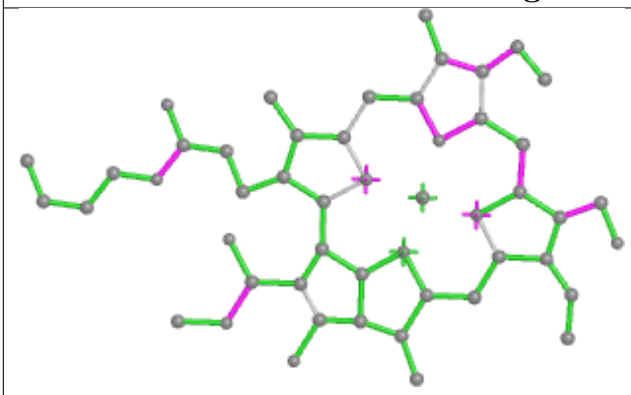
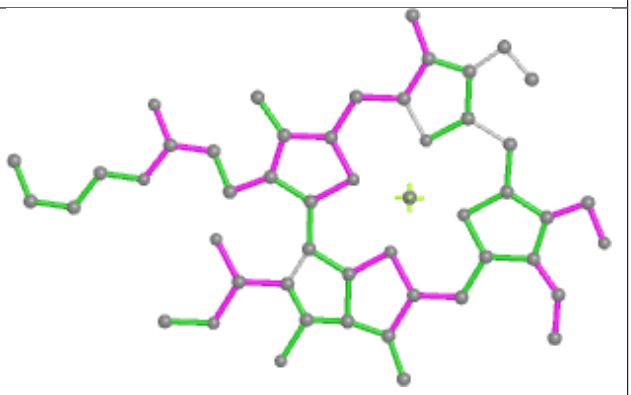
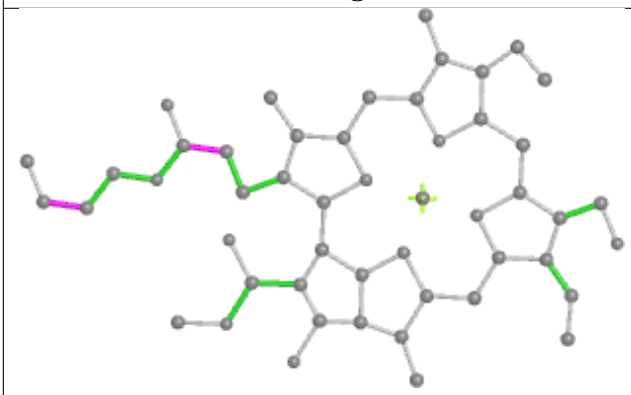
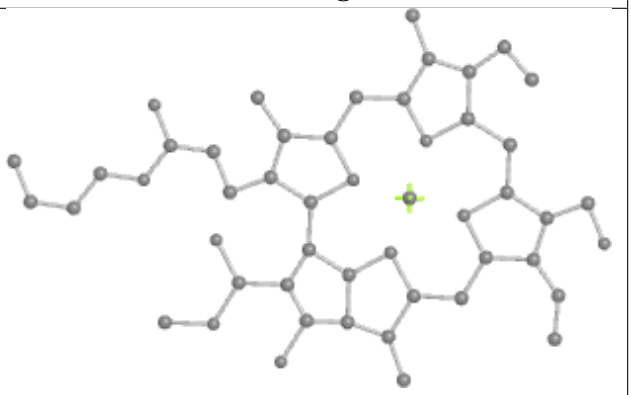
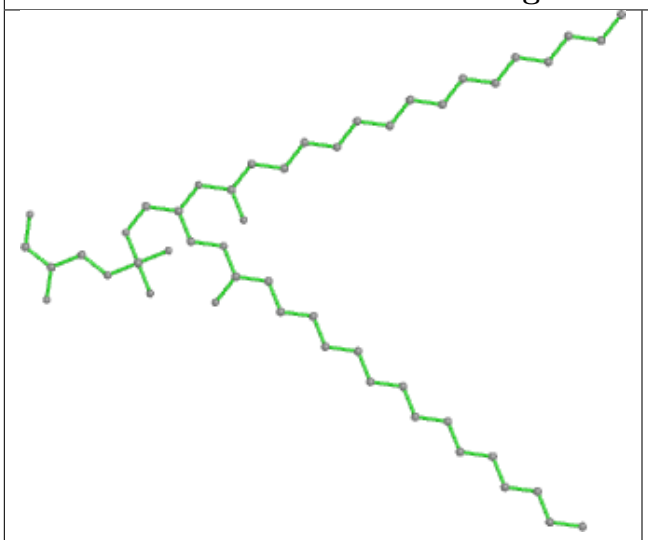


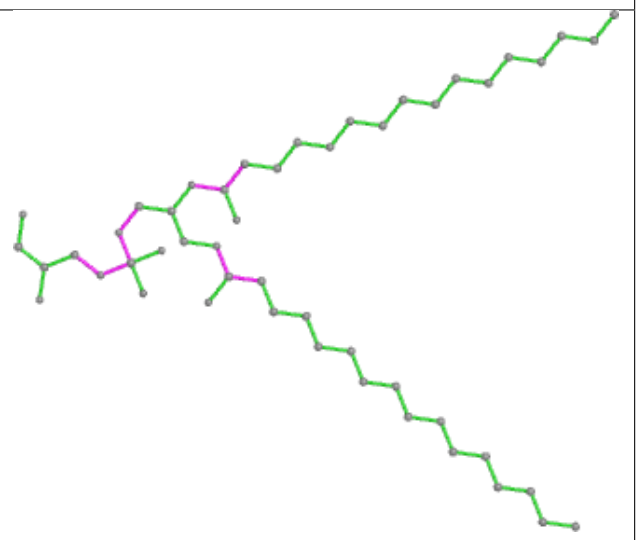
Rings

Ligand CHL Y 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

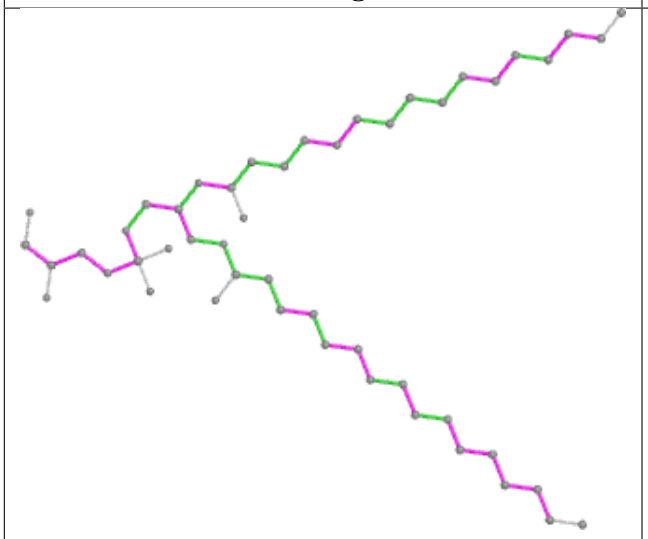
Ligand LHG N 618



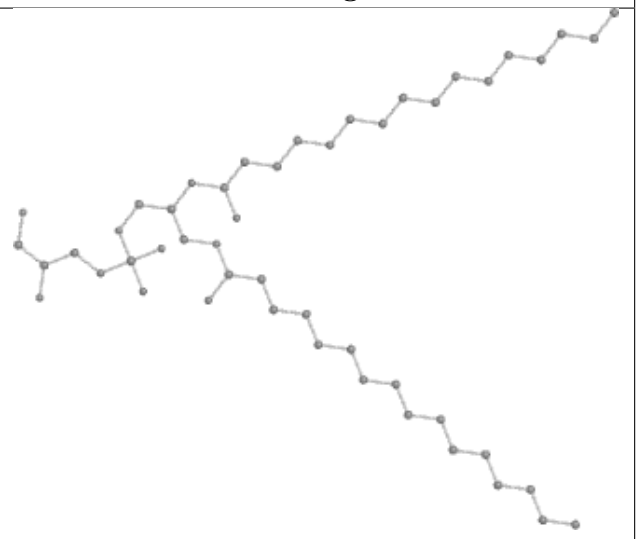
Bond lengths



Bond angles

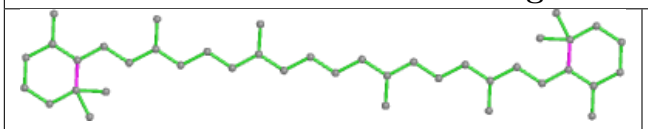


Torsions

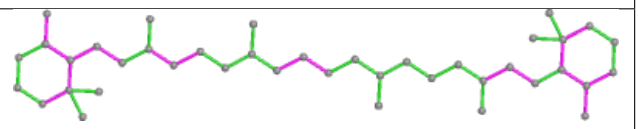


Rings

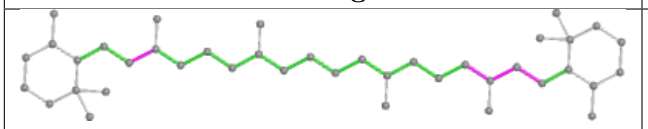
Ligand BCR h 101



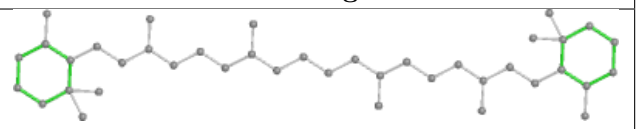
Bond lengths



Bond angles

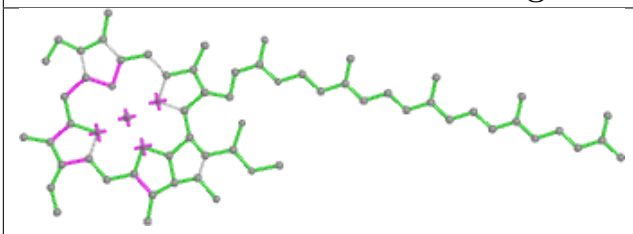


Torsions



Rings

Ligand CLA n 610



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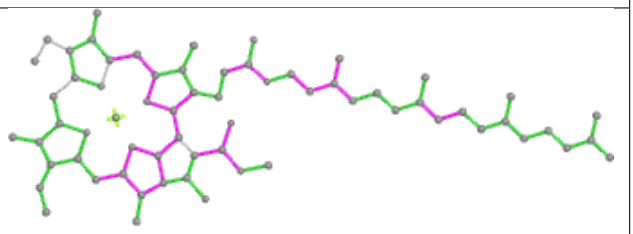
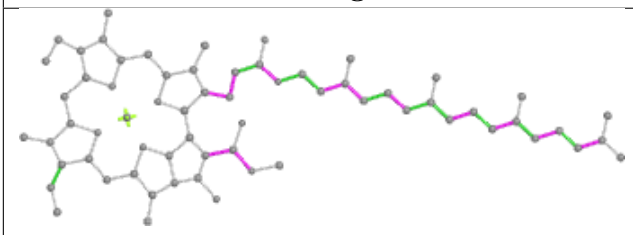
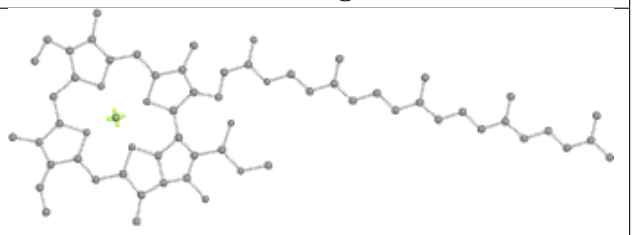


Bond angles

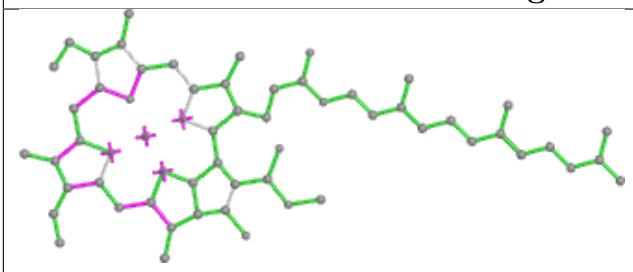


Torsions



Rings

Ligand CLA y 312



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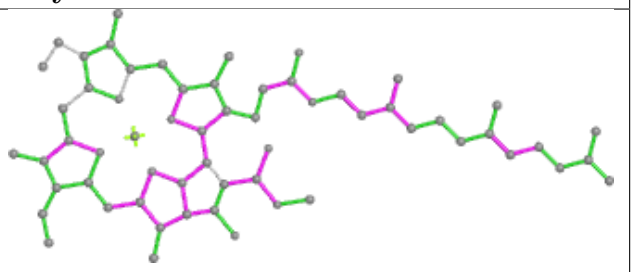

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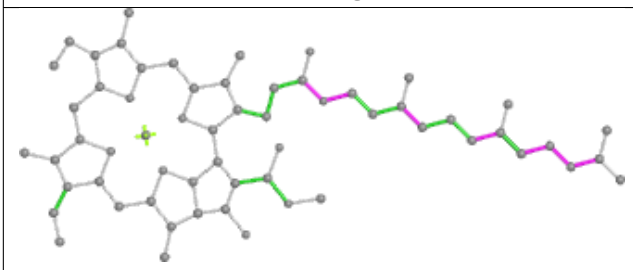

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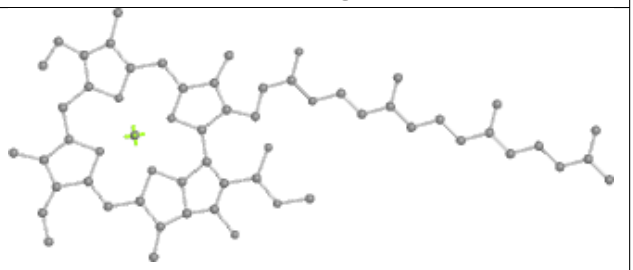
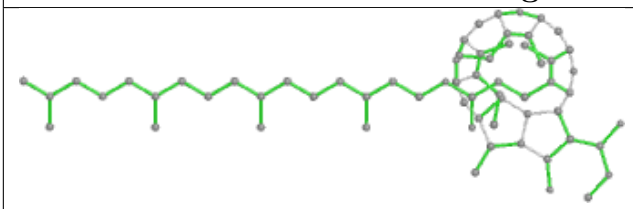


Rings

Ligand PHO A 404



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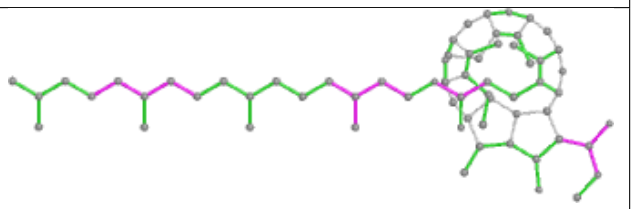
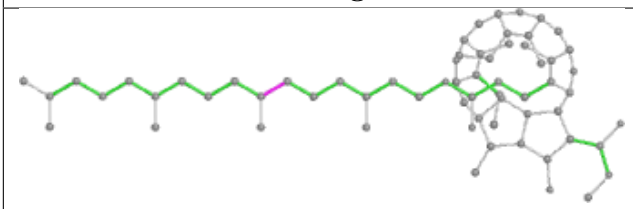


Bond angles



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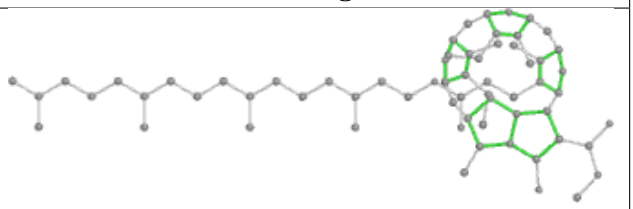

Rings

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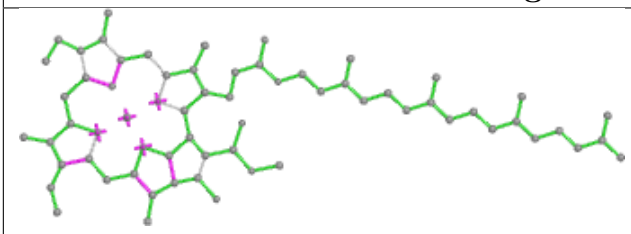
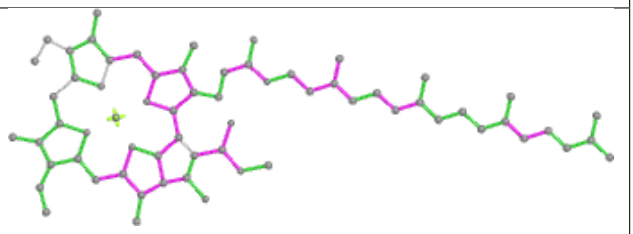
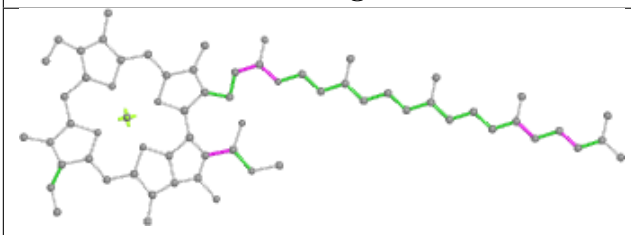
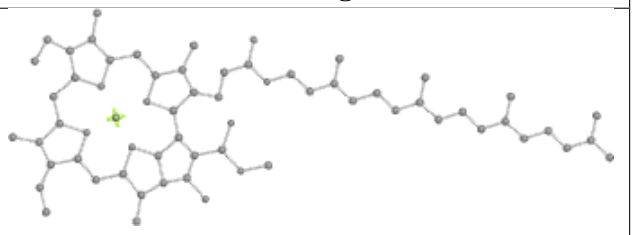
 Bond lengths	 Bond angles
 Torsions	 Rings

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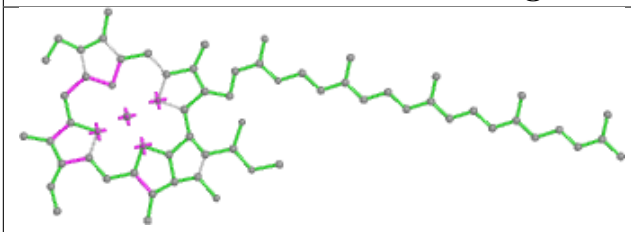
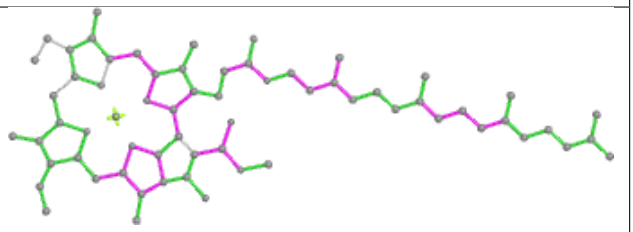
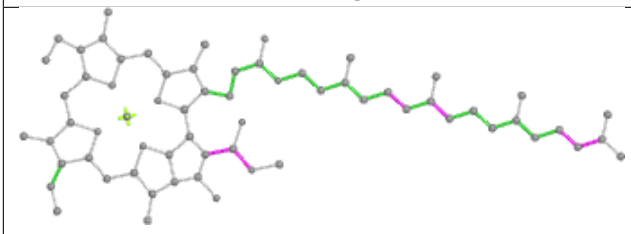
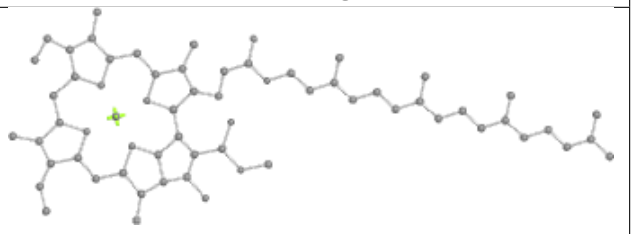
 Bond lengths	 Bond angles
 Torsions	 Rings

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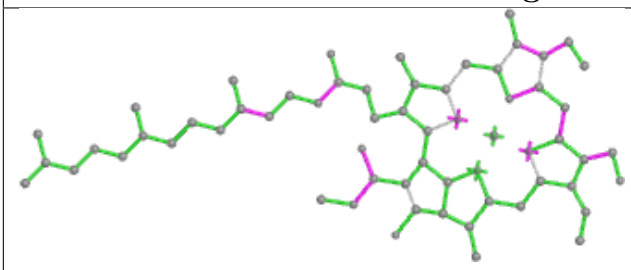
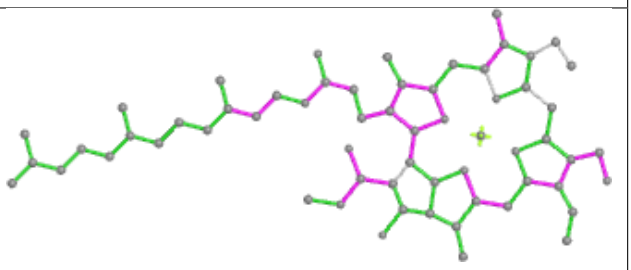
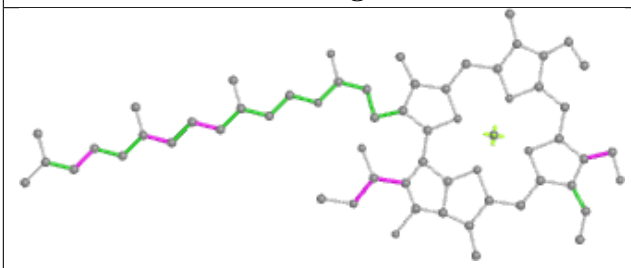
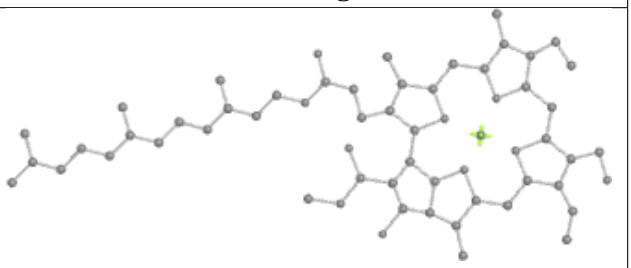
 Bond lengths	 Bond angles
 Torsions	 Rings

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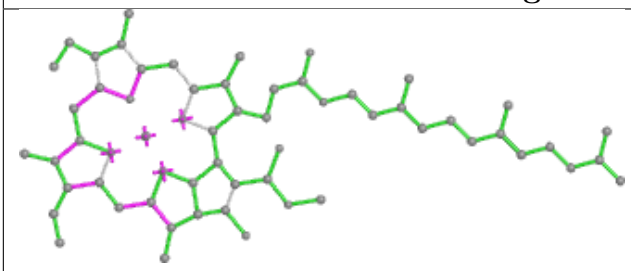
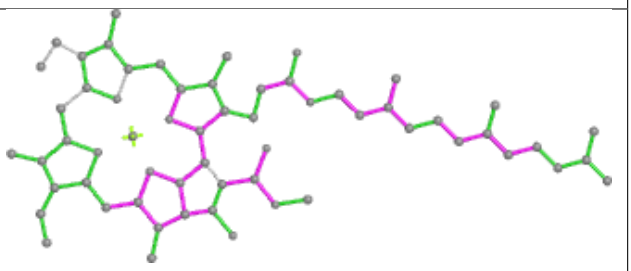
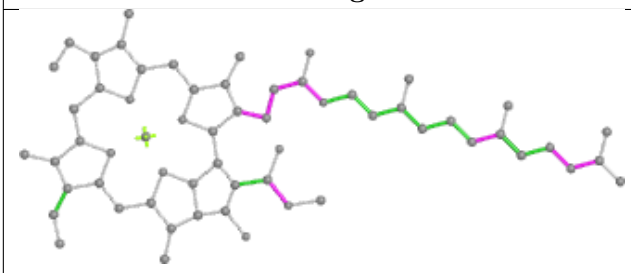
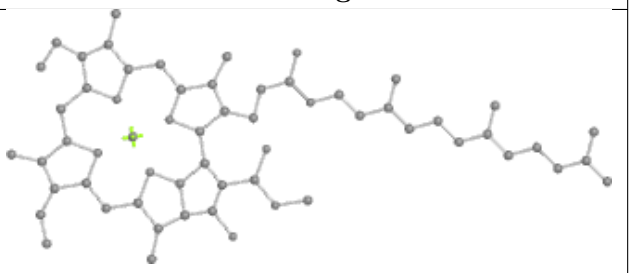
 Bond lengths	 Bond angles
 Torsions	 Rings

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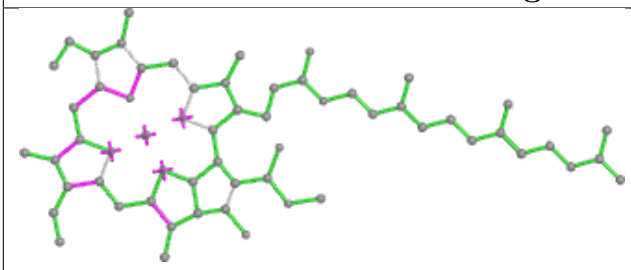
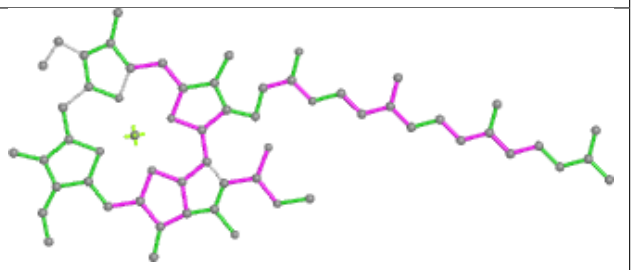
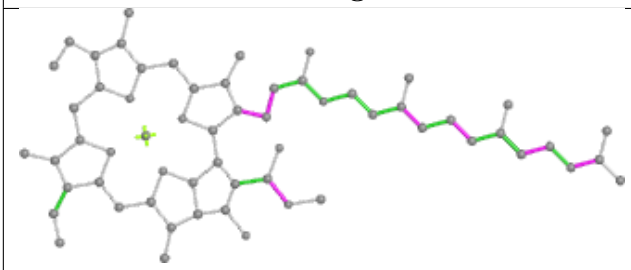
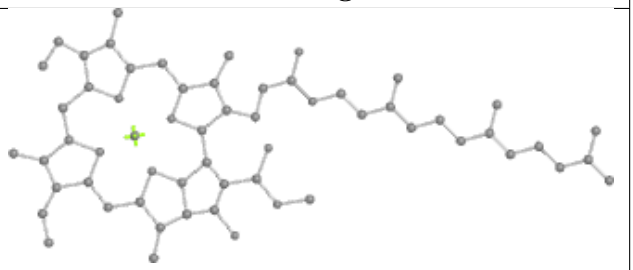
 Bond lengths	 Bond angles
 Torsions	 Rings

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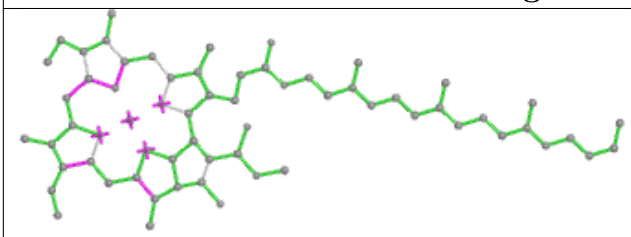
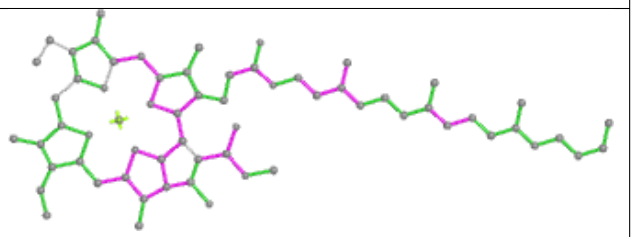
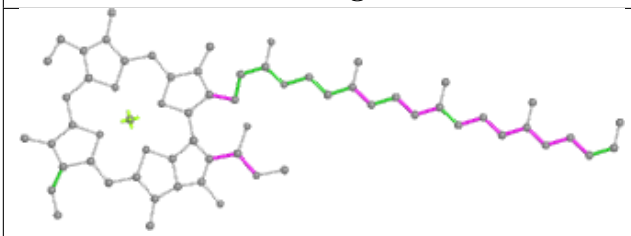
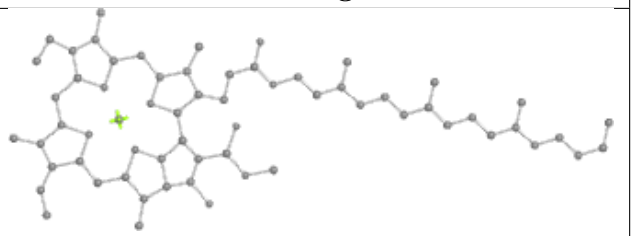
 Bond lengths	 Bond angles
 Torsions	 Rings

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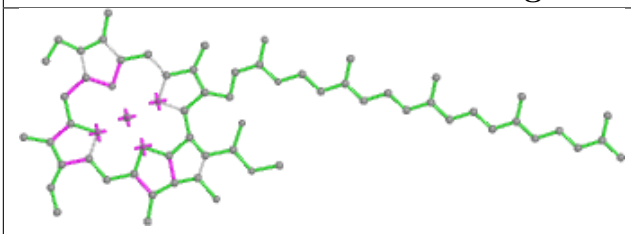
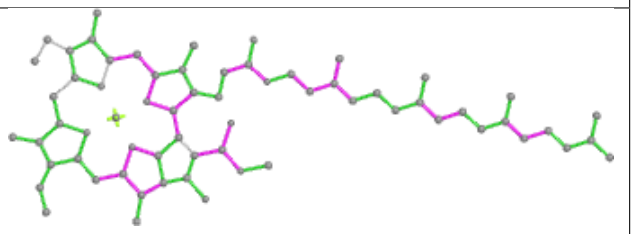
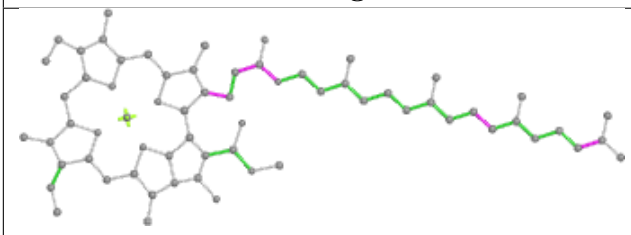
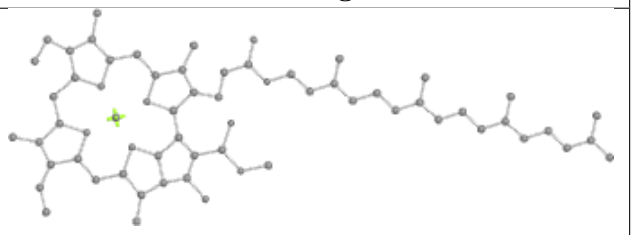
 Bond lengths	 Bond angles
 Torsions	 Rings

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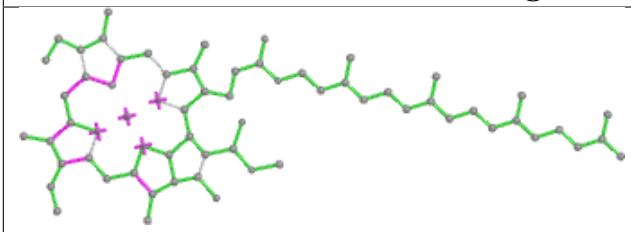
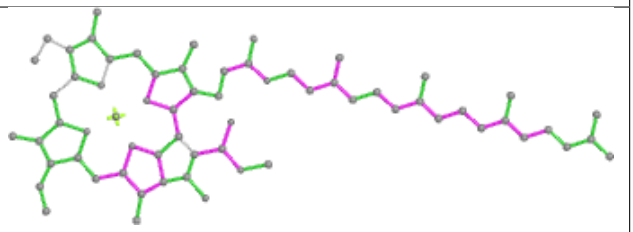
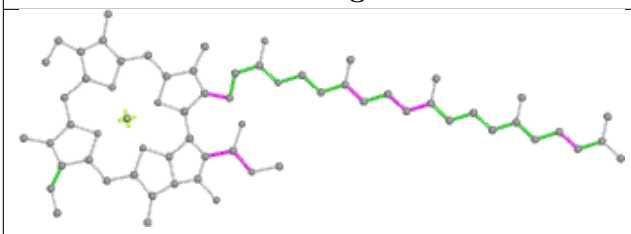
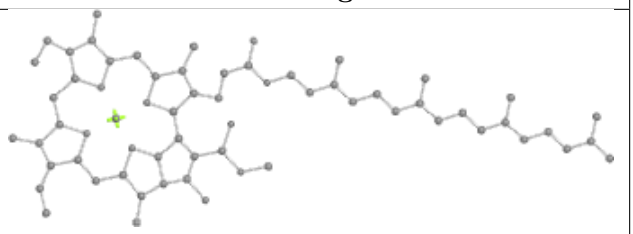
 Bond lengths	 Bond angles
 Torsions	 Rings

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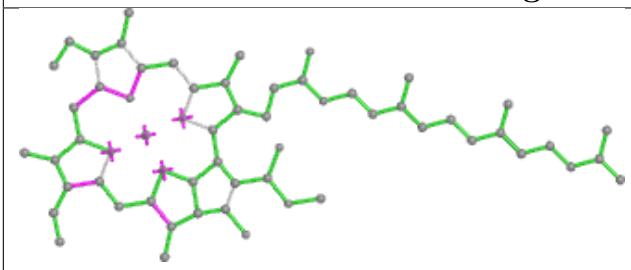

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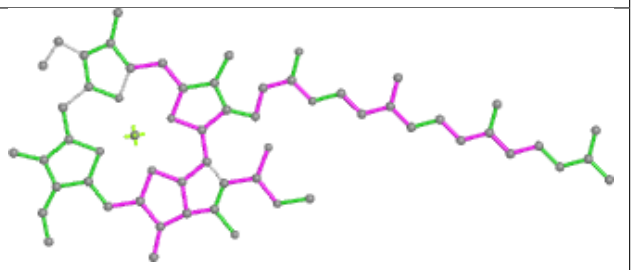
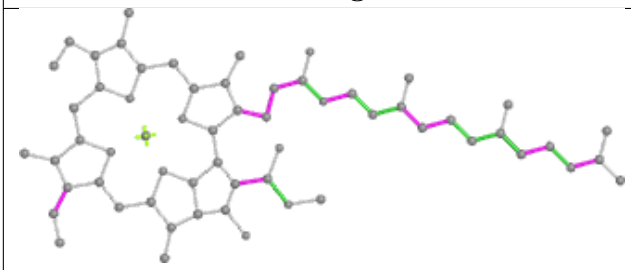


Bond angles



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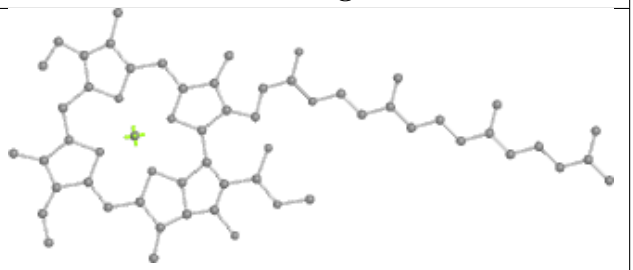
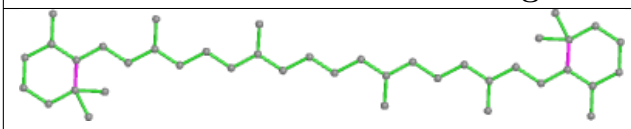


Rings

Ligand BCR D 404



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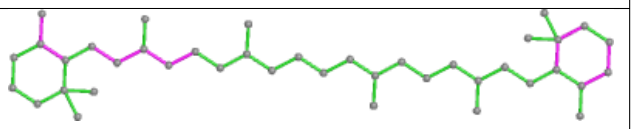
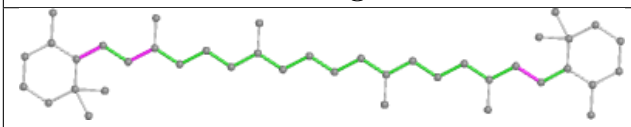


Bond angles



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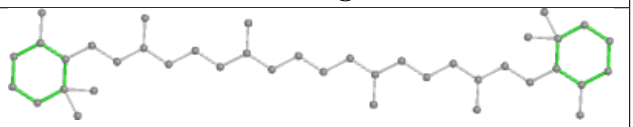
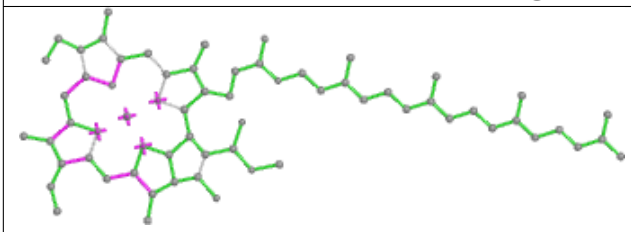


Rings

Ligand CLA g 613



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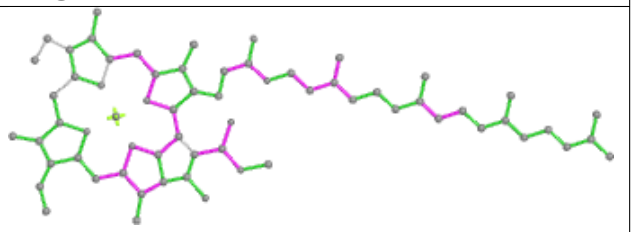
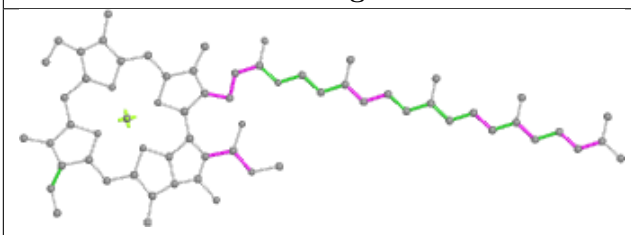
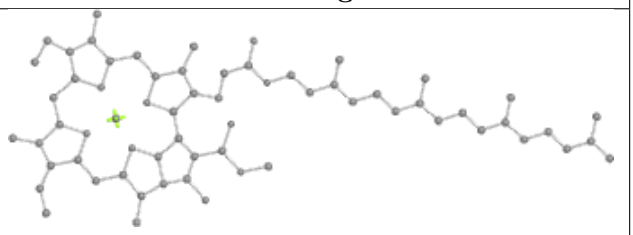


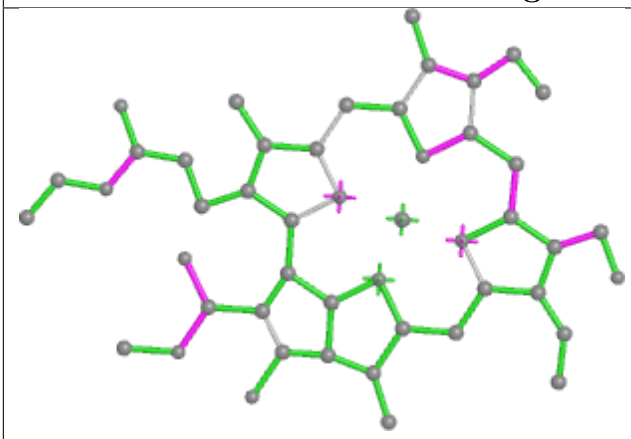
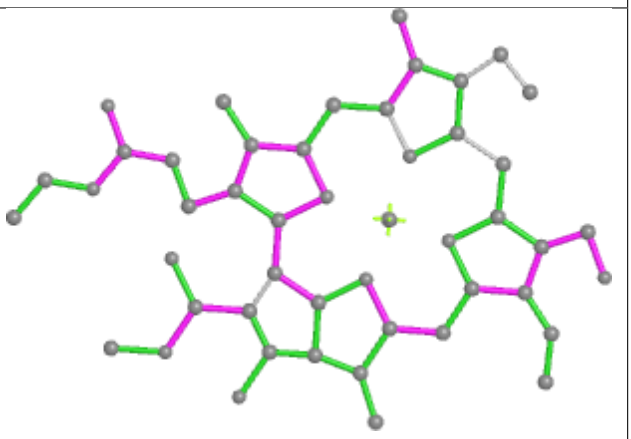
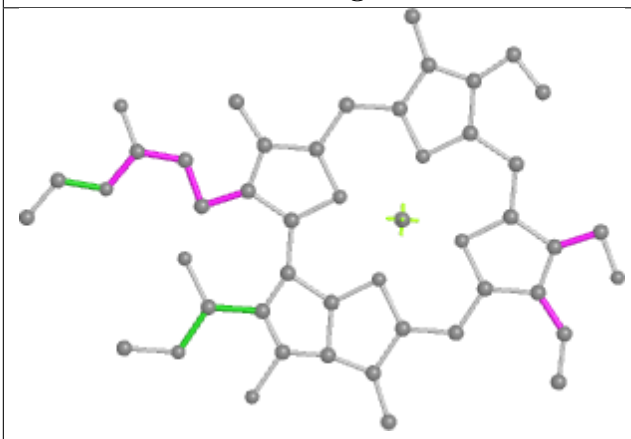
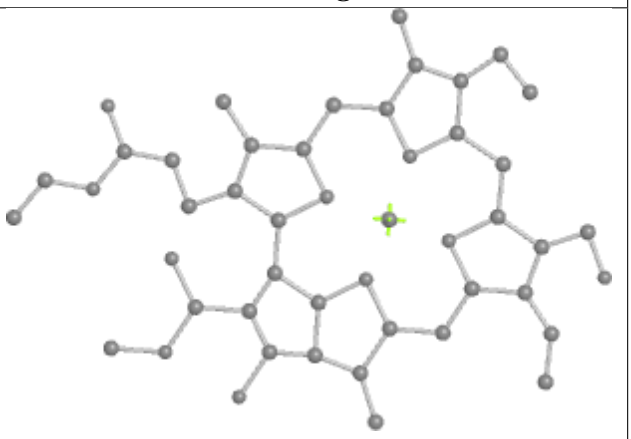
Bond angles



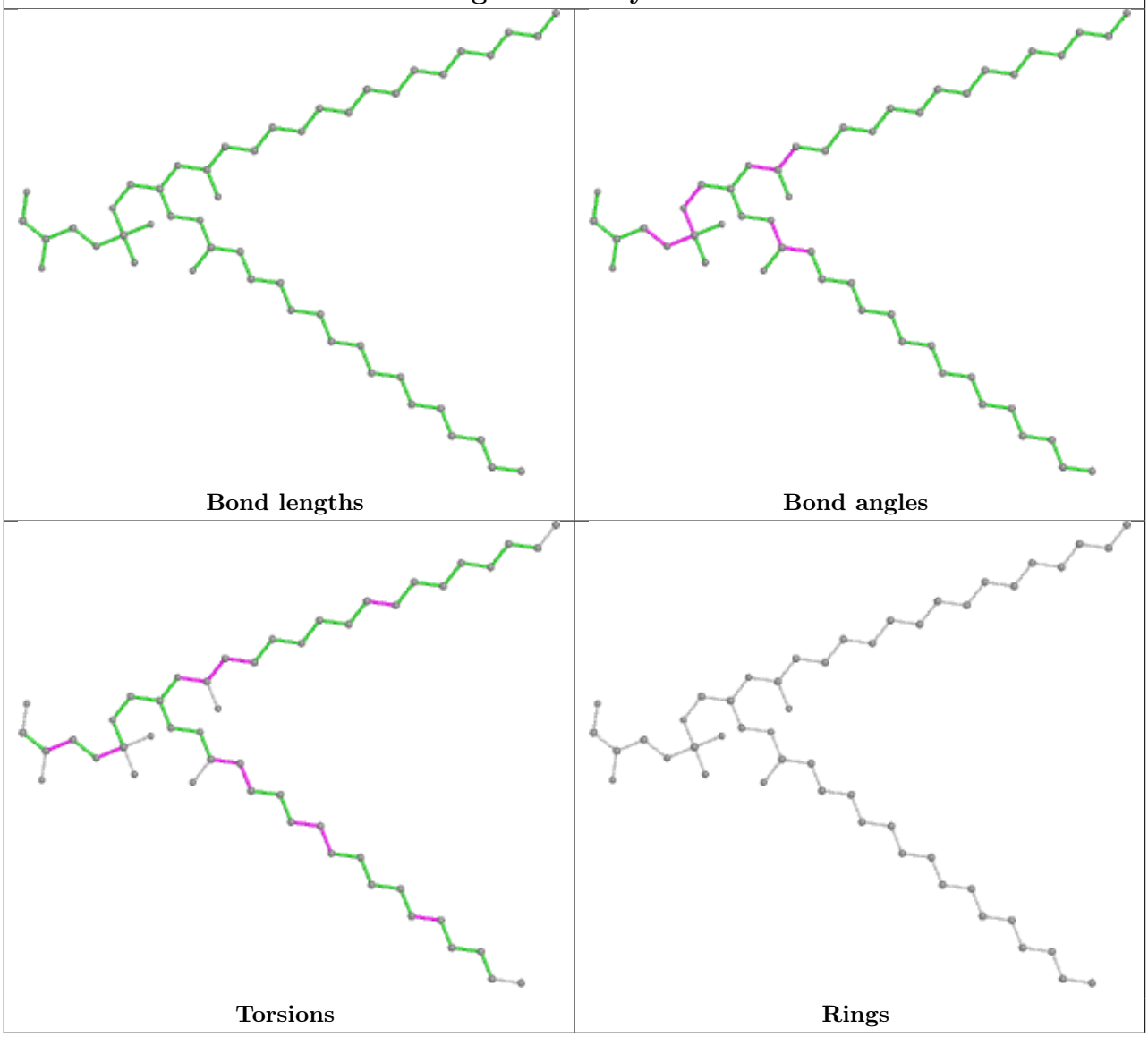
Torsions



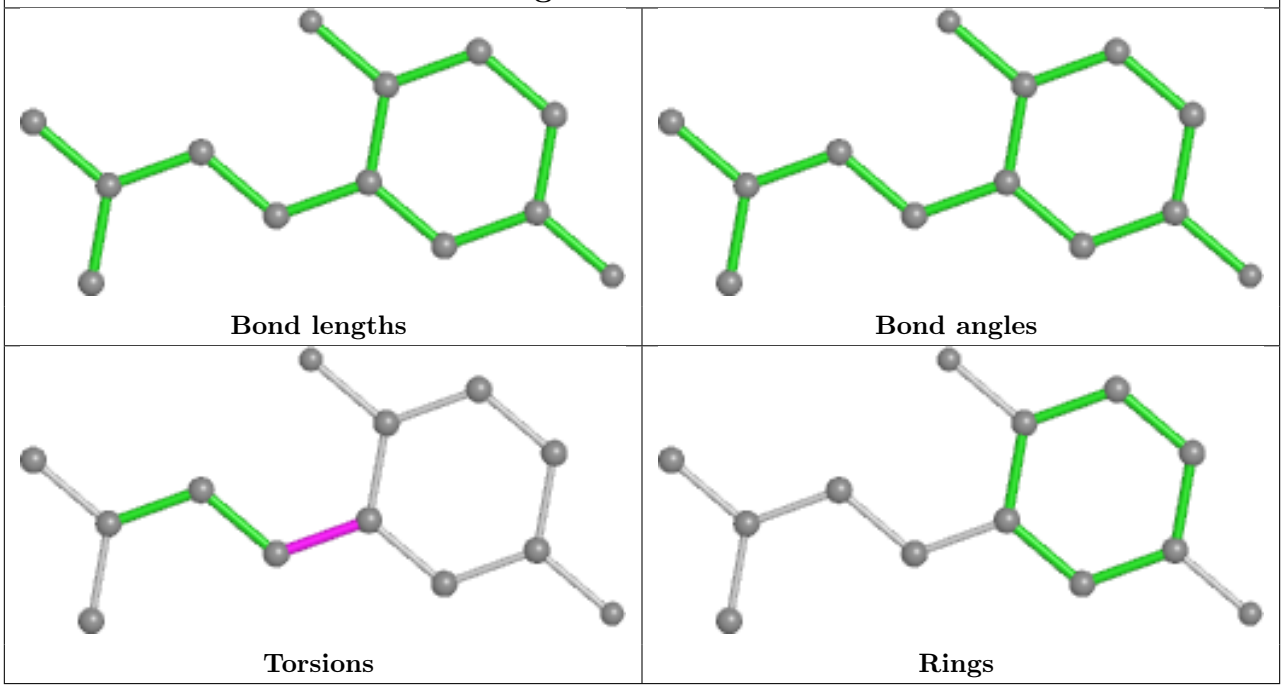
Rings

Ligand CHL Y 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

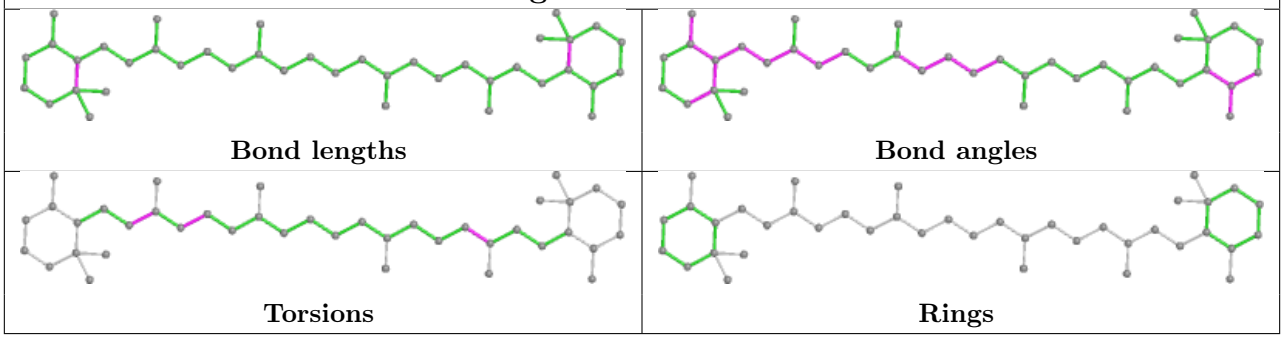
Ligand LHG y 301



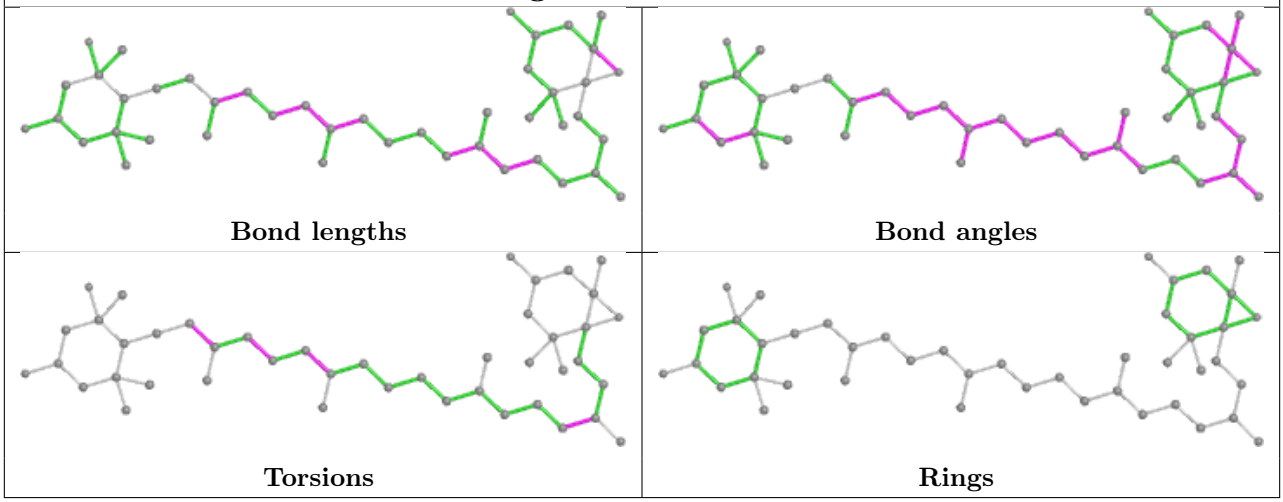
Ligand PL9 a 410



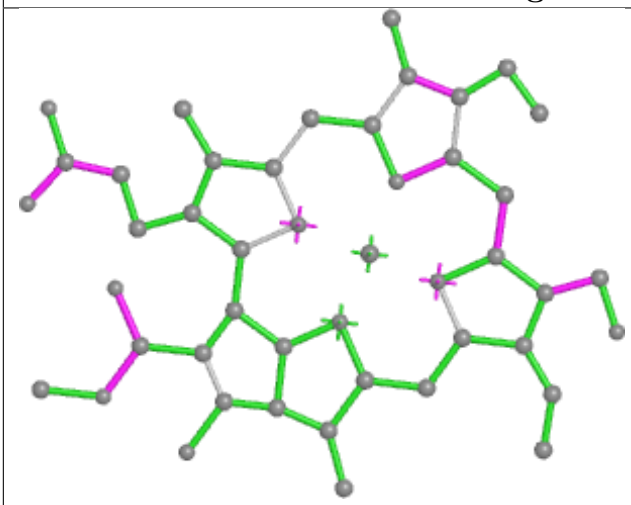
Ligand BCR I 101



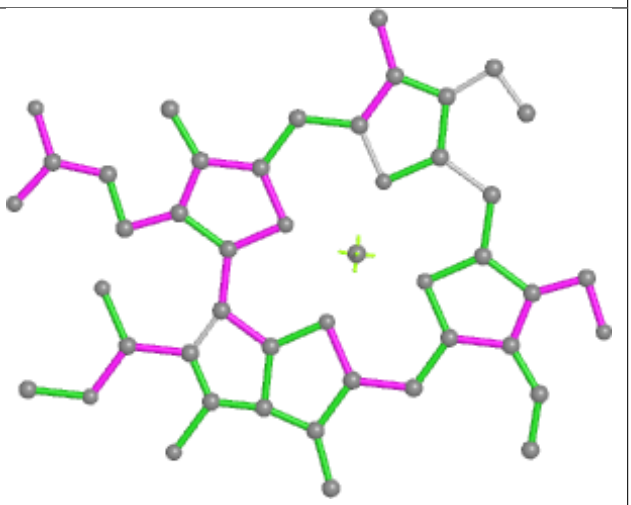
Ligand NEX r 617



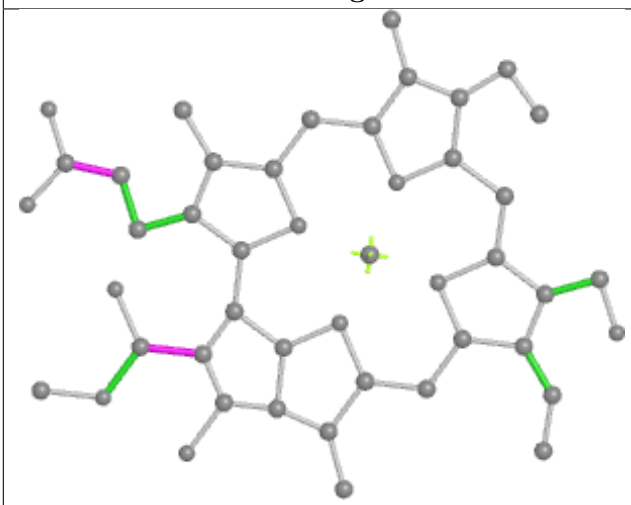
Ligand CHL S 302



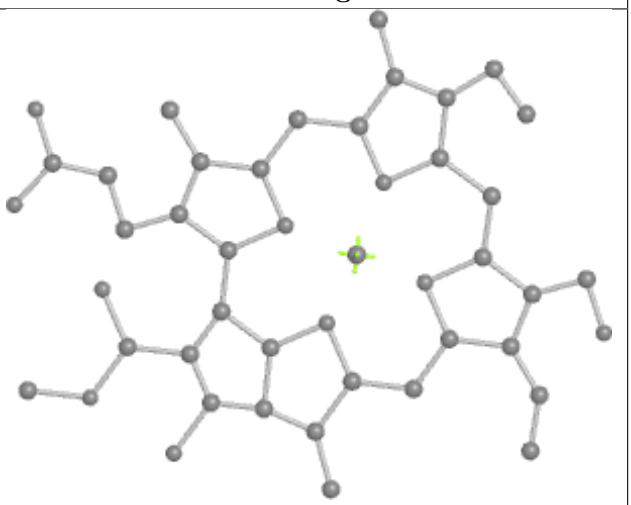
Bond lengths



Bond angles

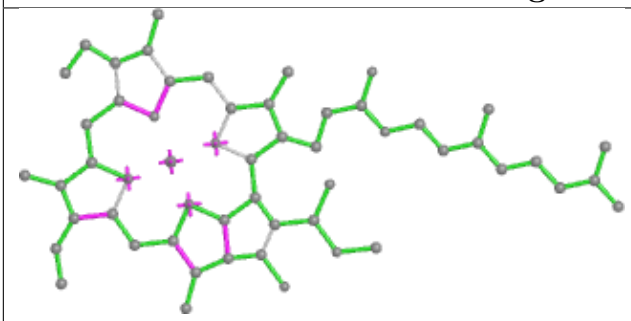


Torsions



Rings

Ligand CLA 2 604



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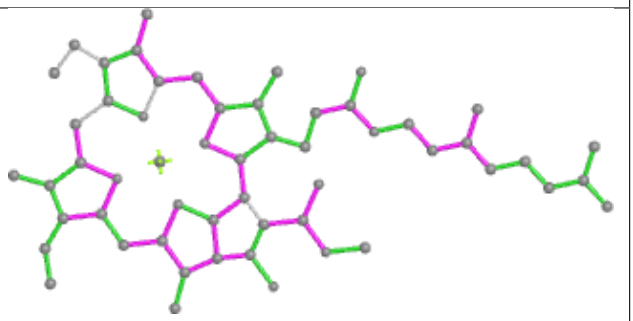
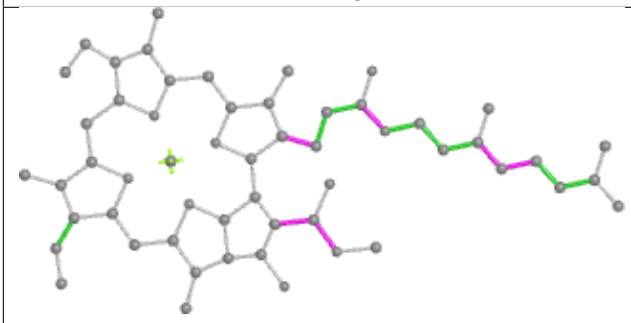


Bond angles



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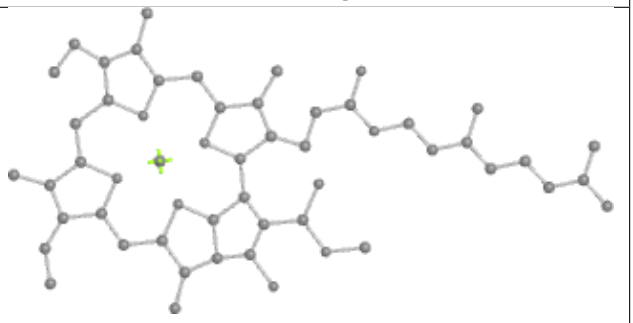
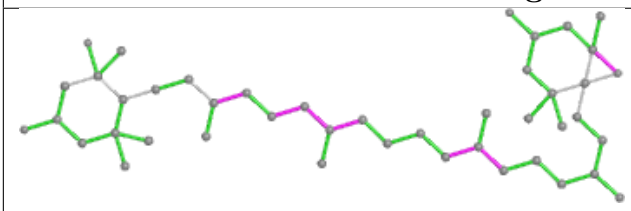


Rings

Ligand NEX n 617



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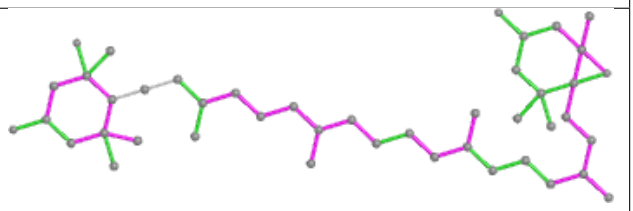
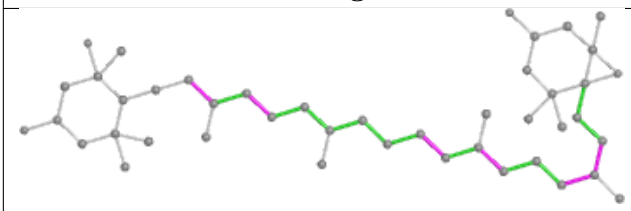


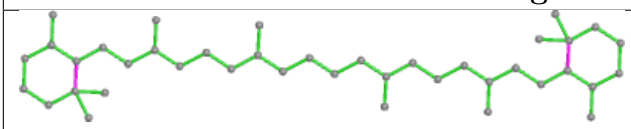
Bond angles



Torsions

Rings

Ligand BCR i 101



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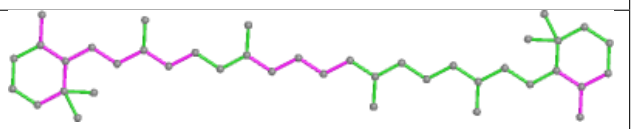
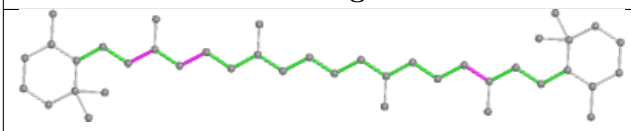
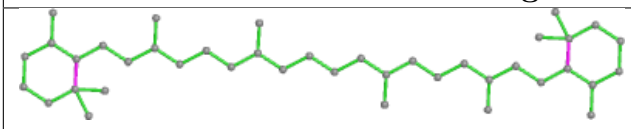
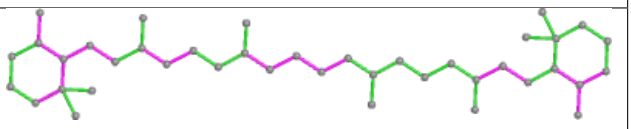
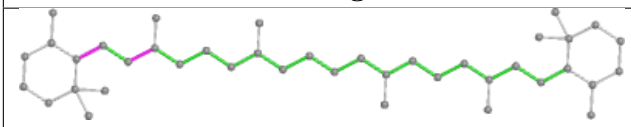


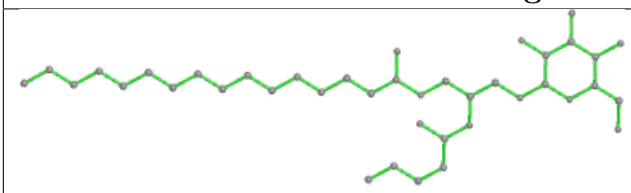
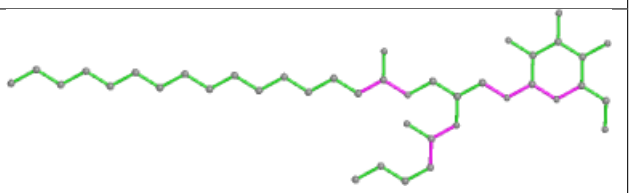
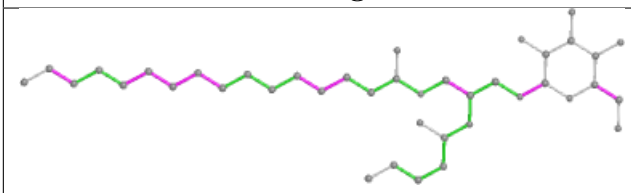
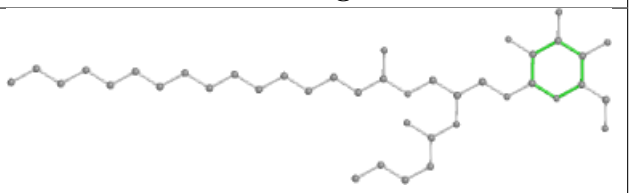
Bond angles

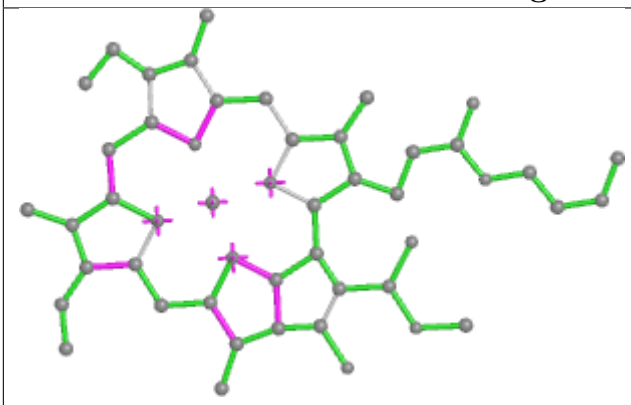
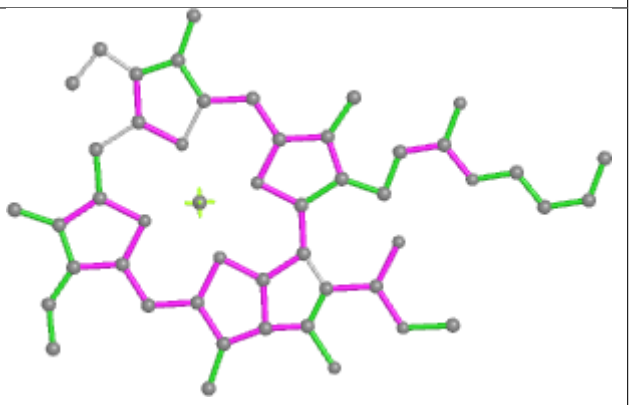
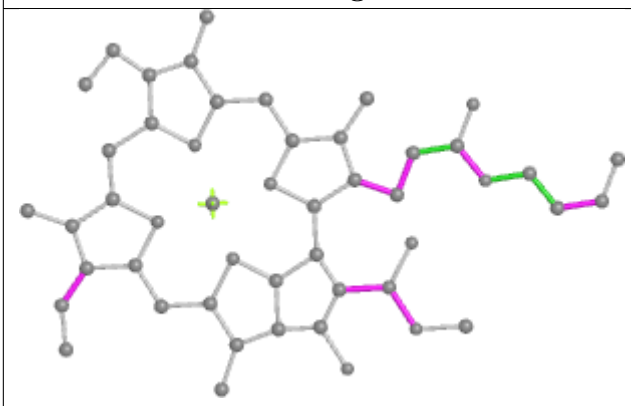
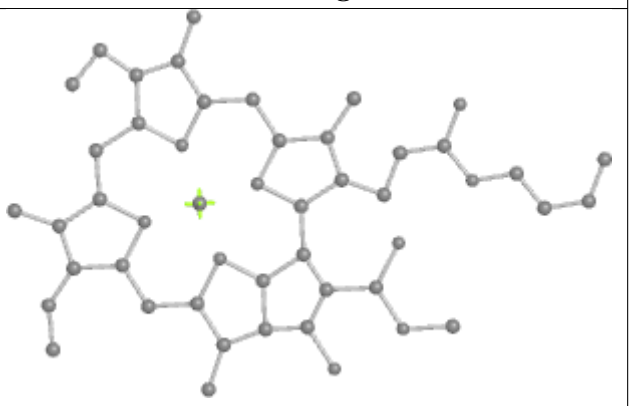


Torsions

Rings

Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LMG a 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

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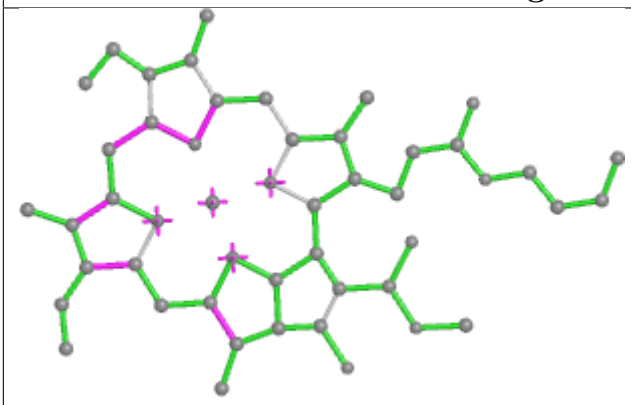
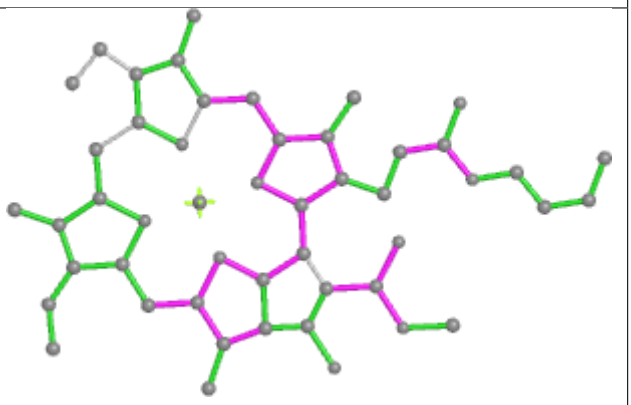
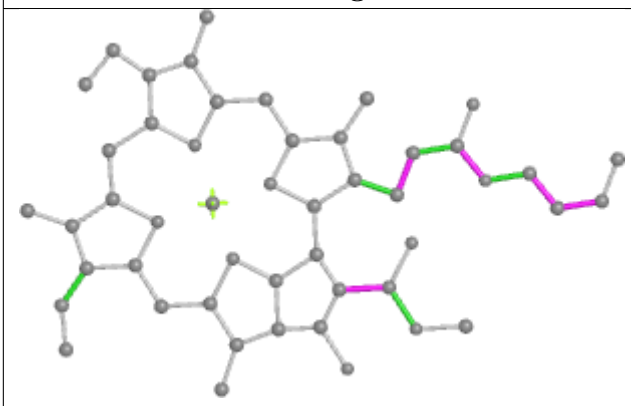
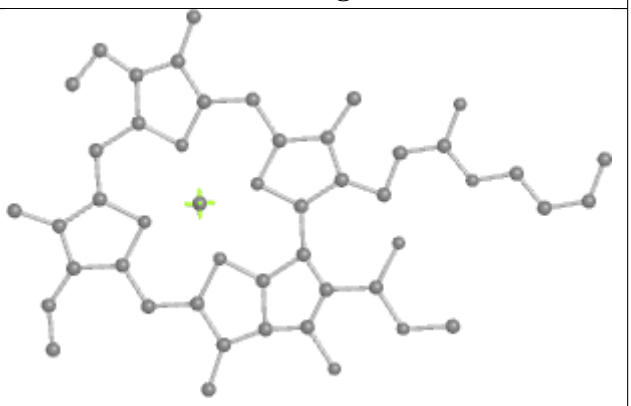
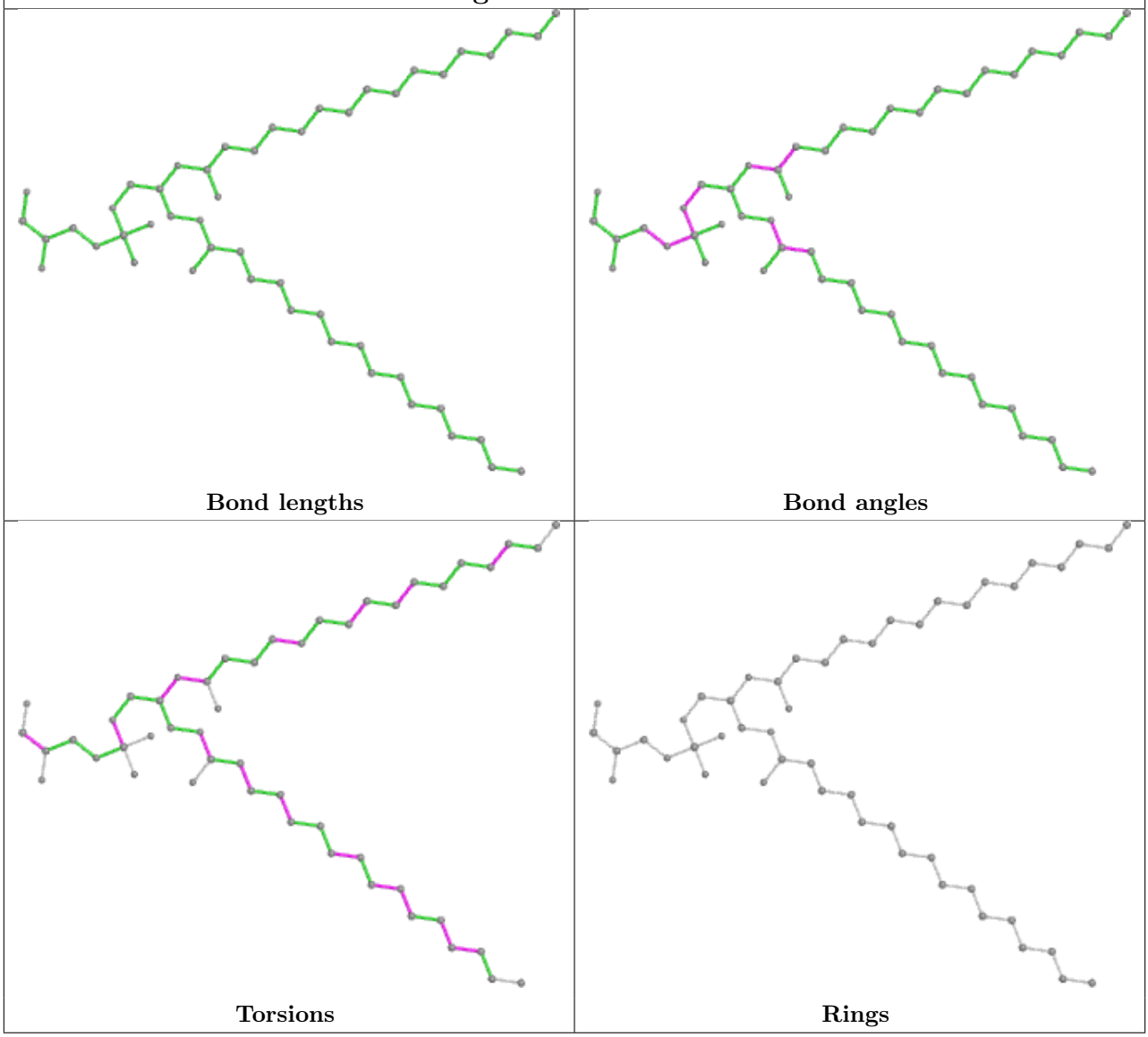
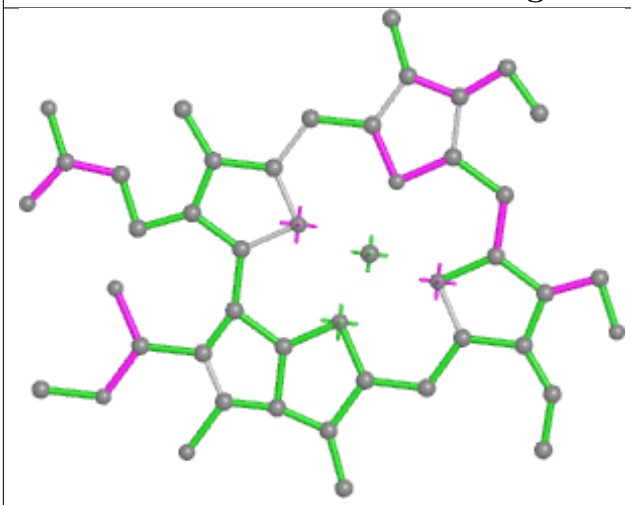
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG c 519



Ligand CHL n 606



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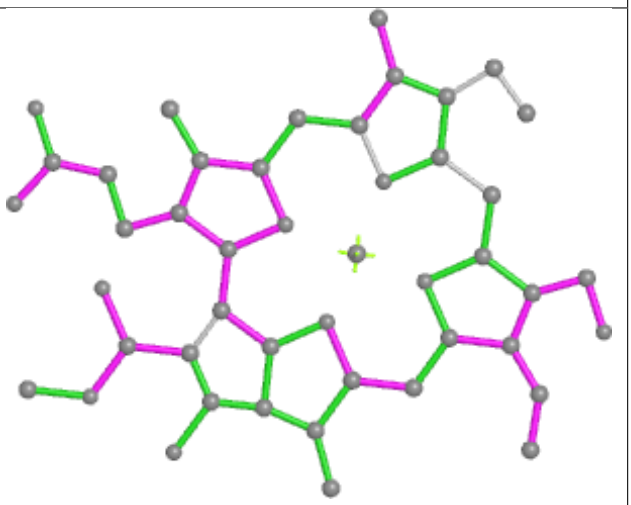
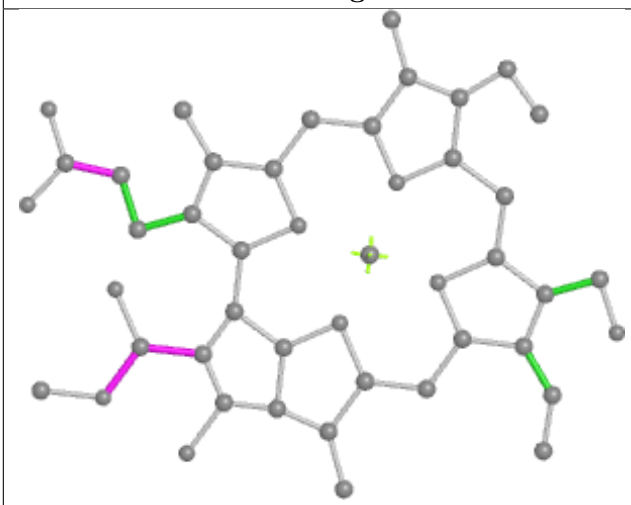
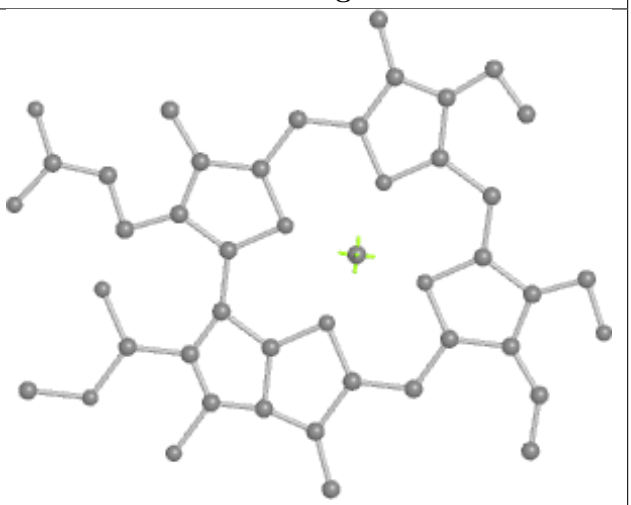


Bond angles

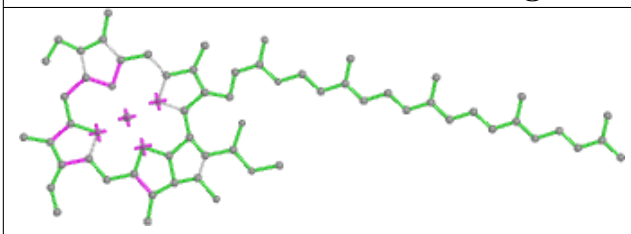


Torsions



Rings

Ligand CLA R 609



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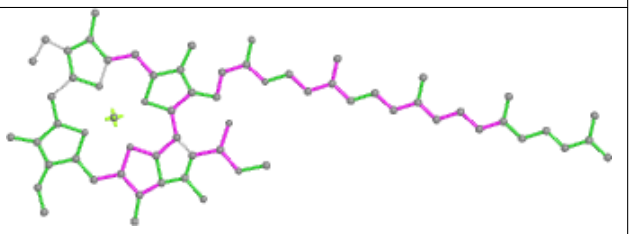
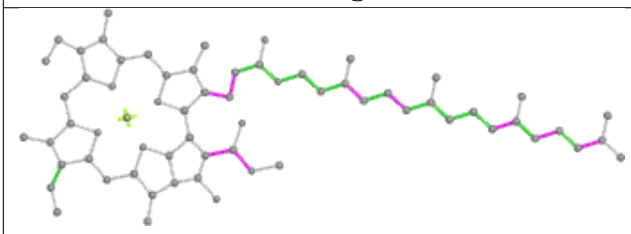


Bond angles



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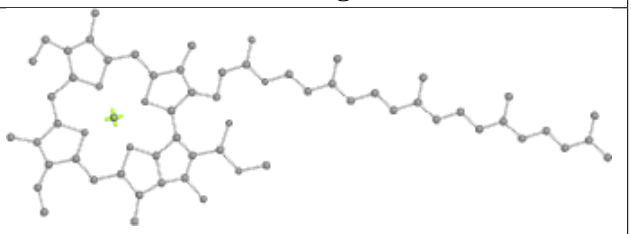
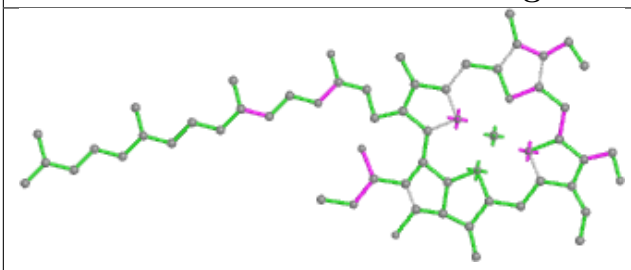
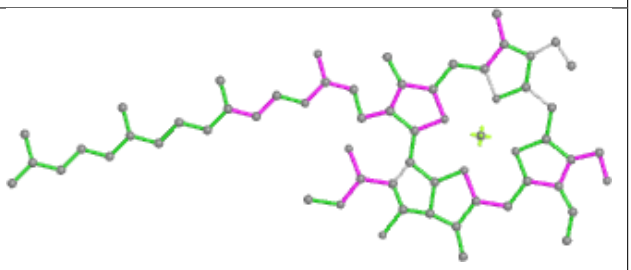
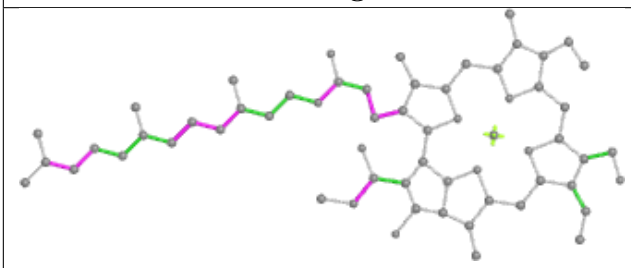
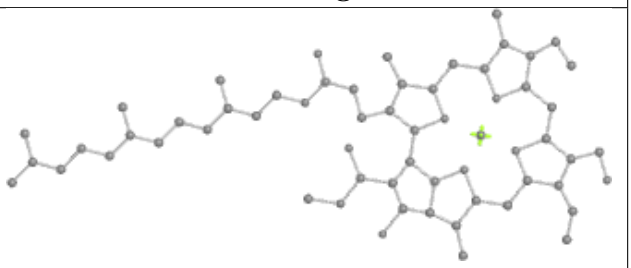


Rings

Ligand CHL R 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

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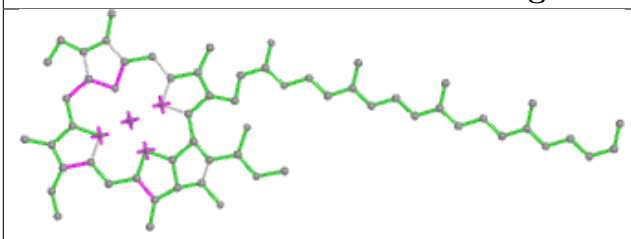
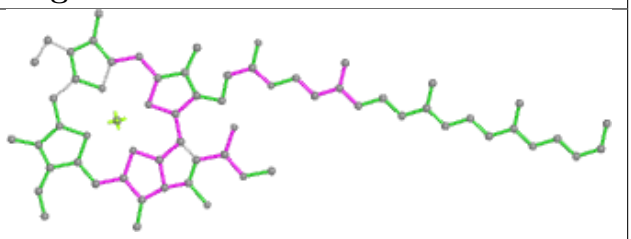
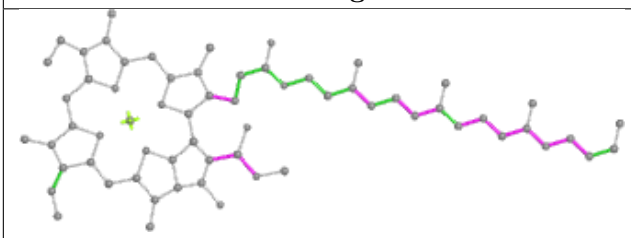
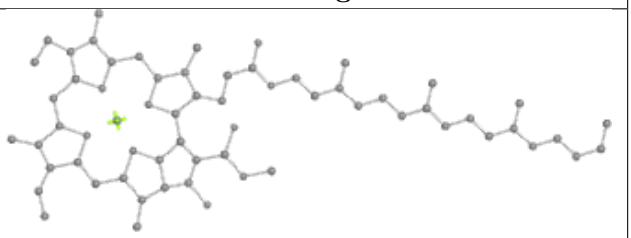
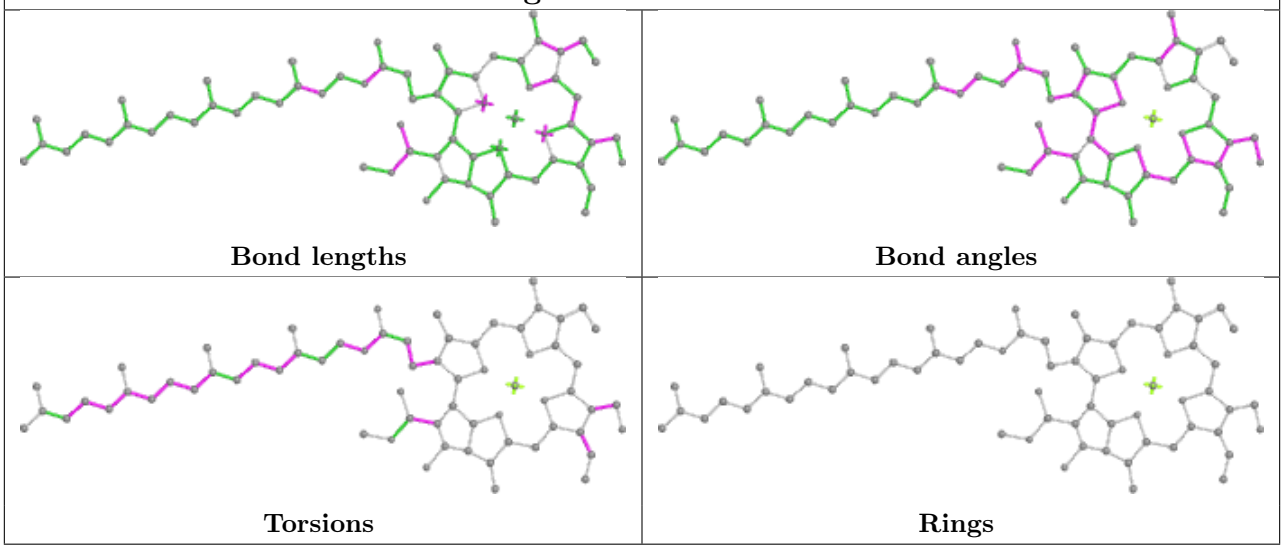
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 601



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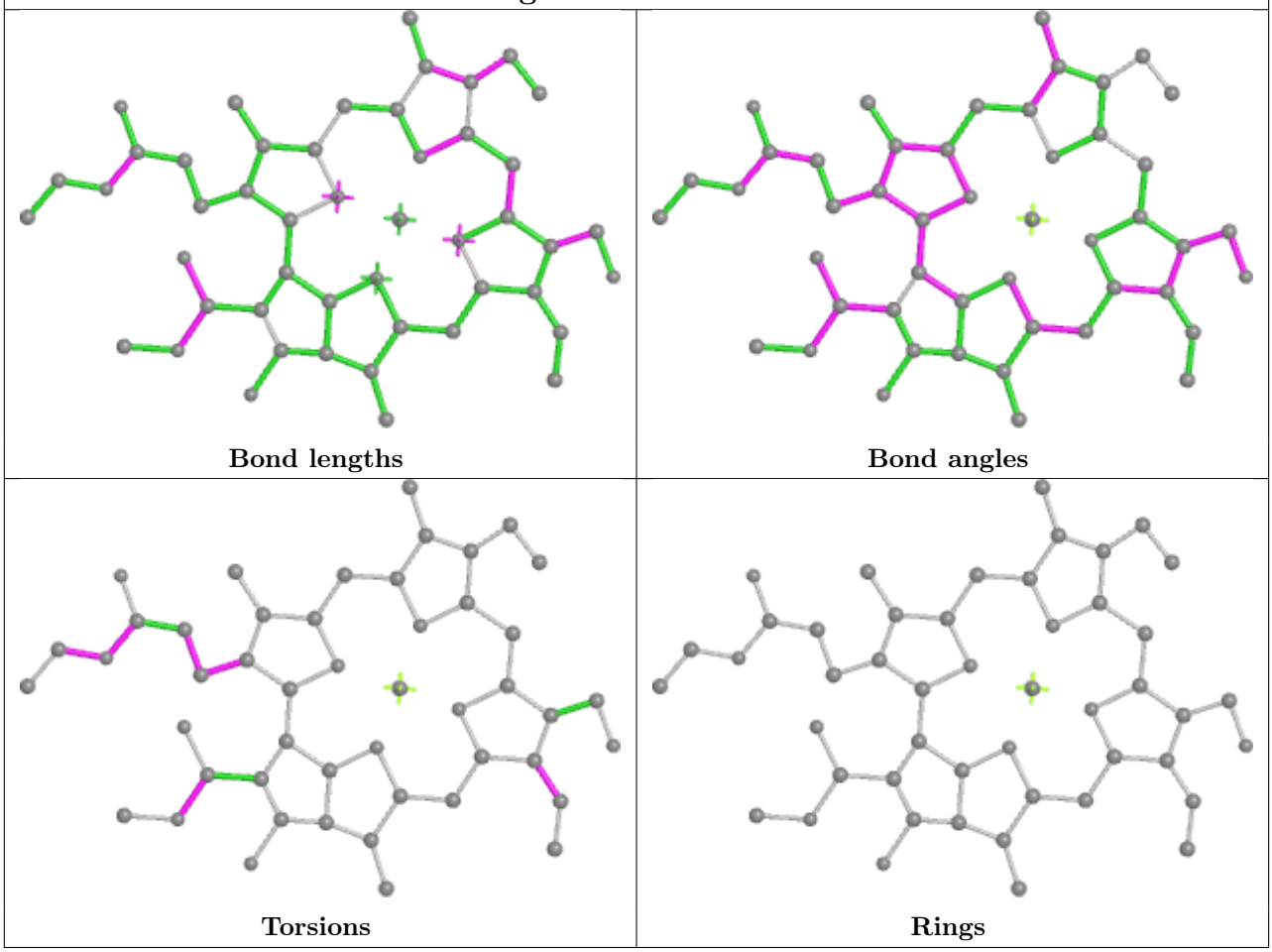

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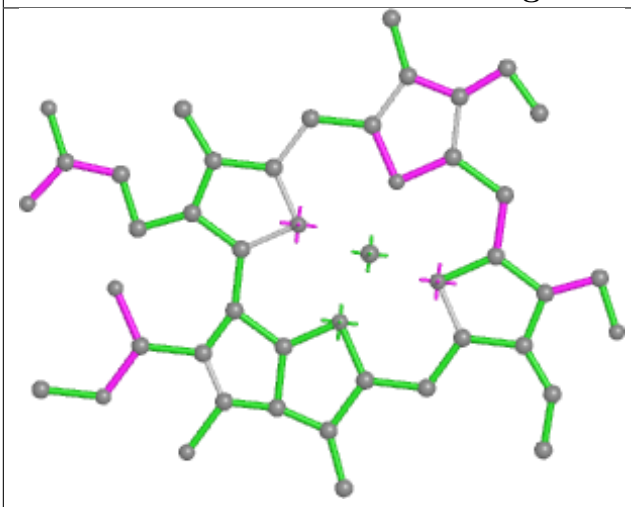
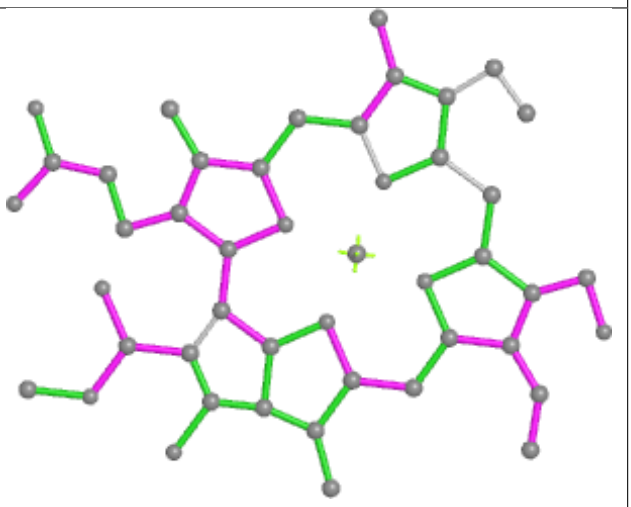
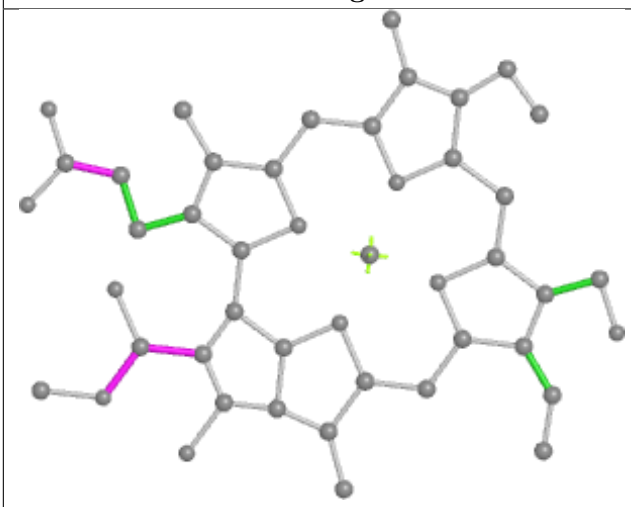


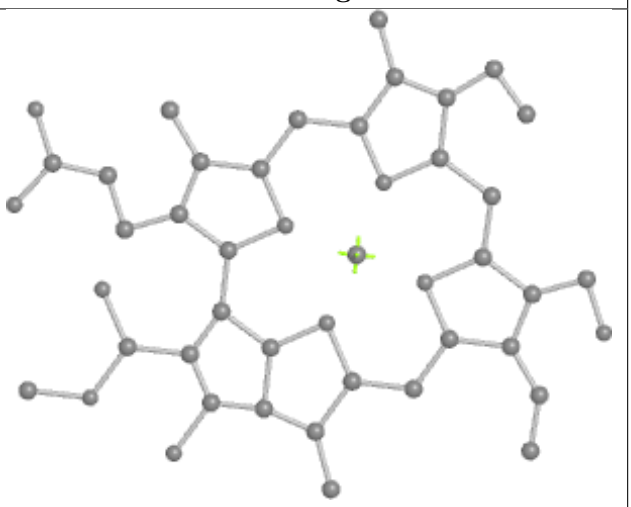
Bond lengths



Bond angles

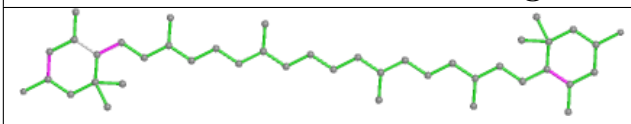


Torsions



Rings

Ligand LUT R 615



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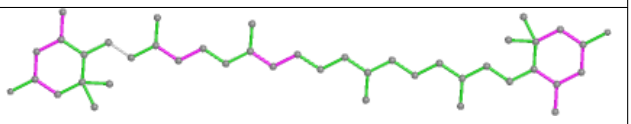
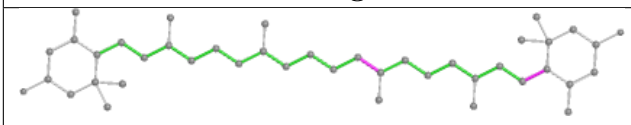


Bond angles



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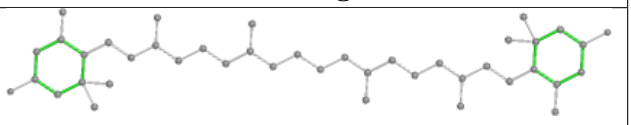
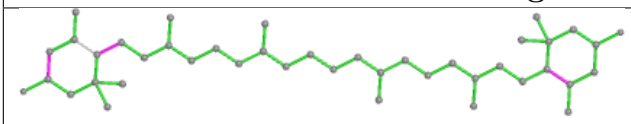
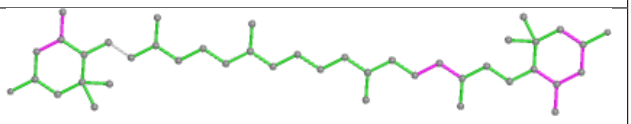
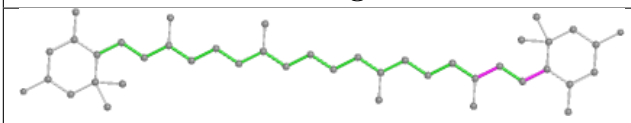
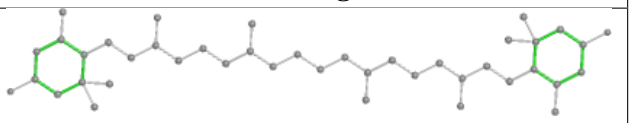


Rings

Ligand LUT n 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

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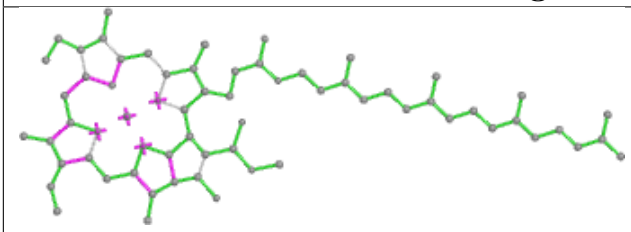
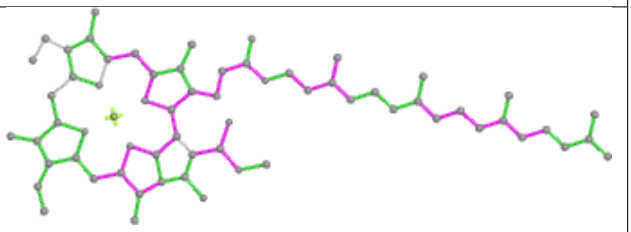
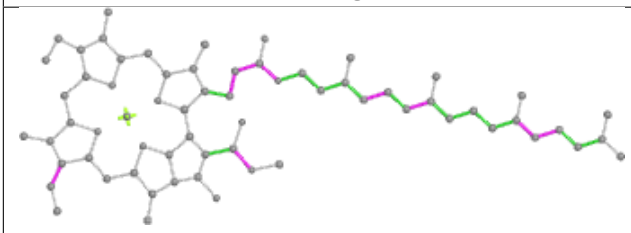
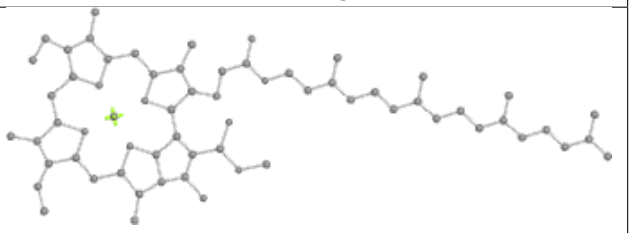
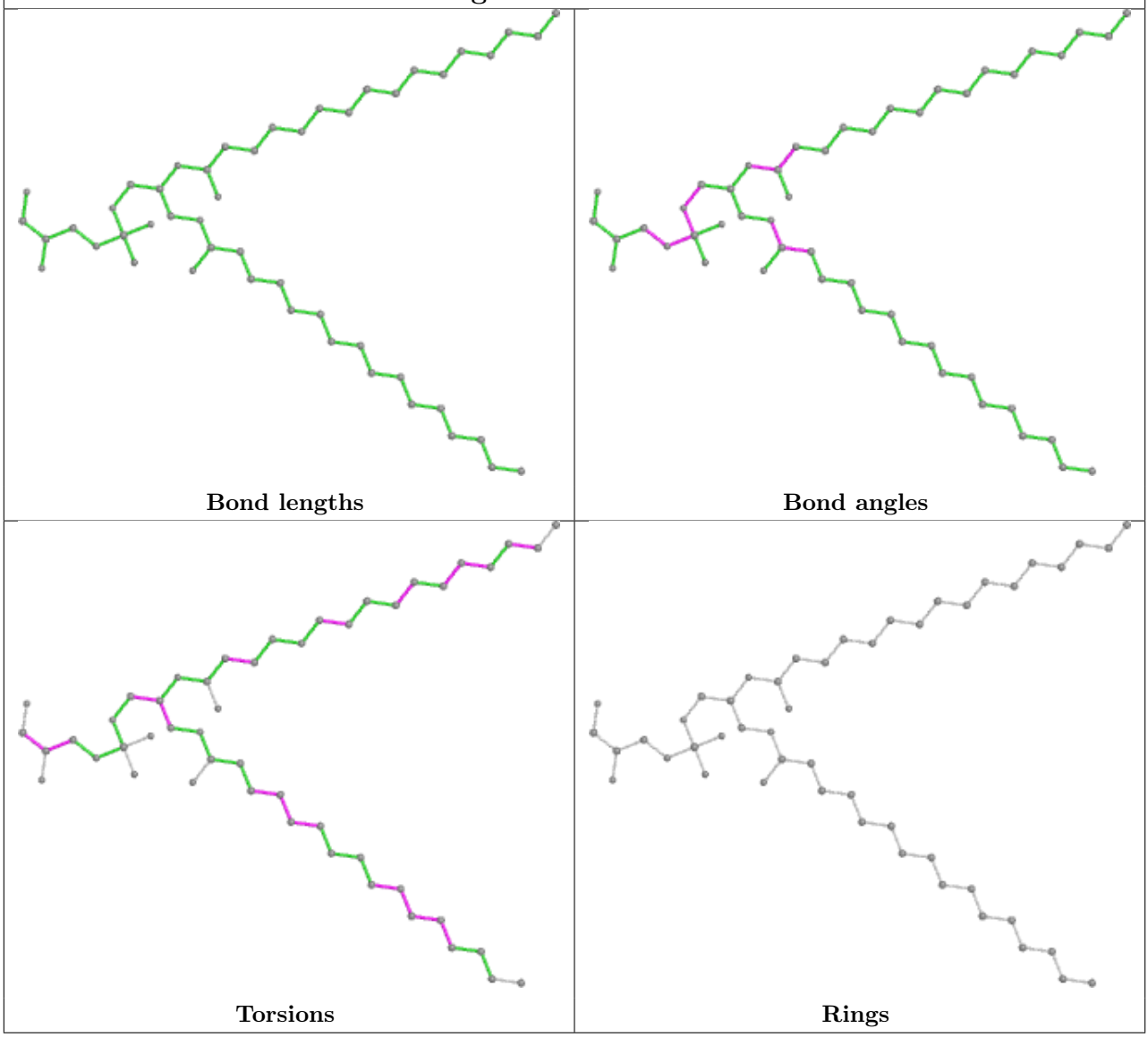
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG S 301



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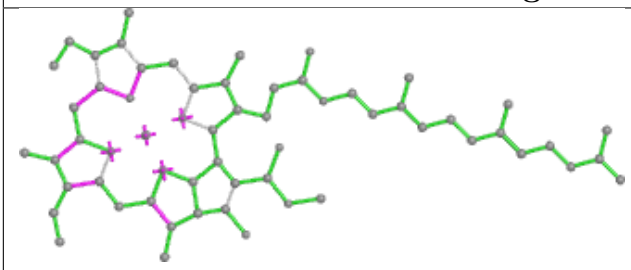
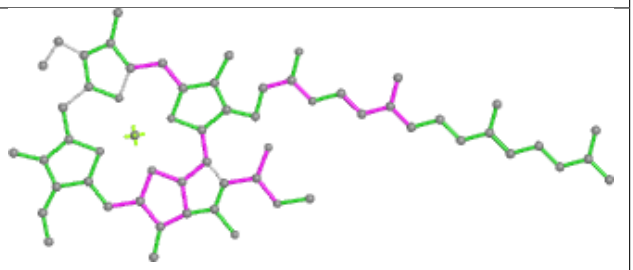
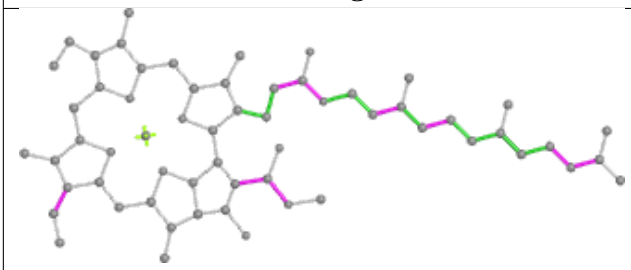
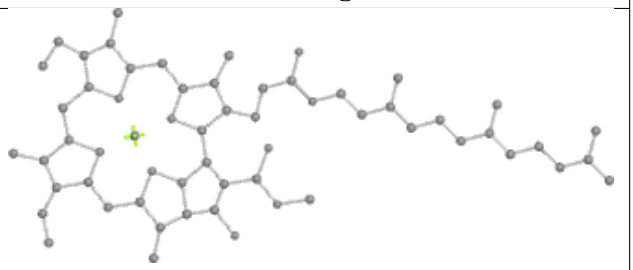
 Bond lengths	 Bond angles
 Torsions	 Rings

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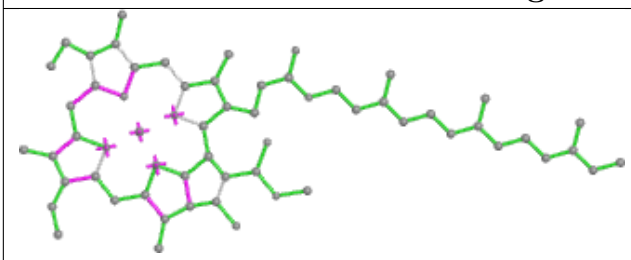
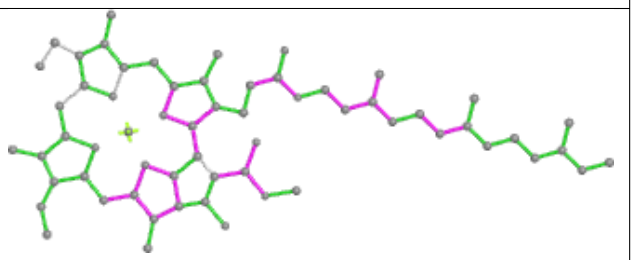
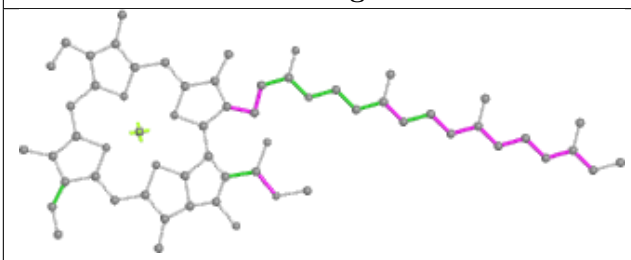
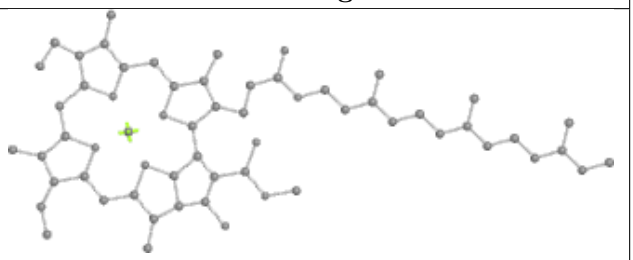
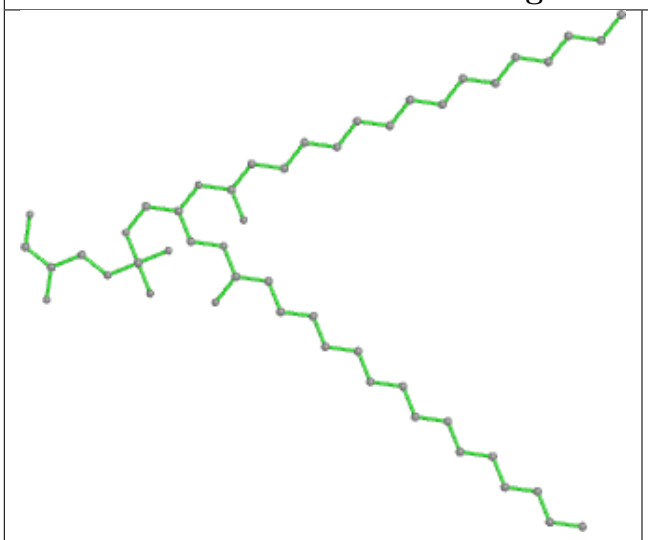
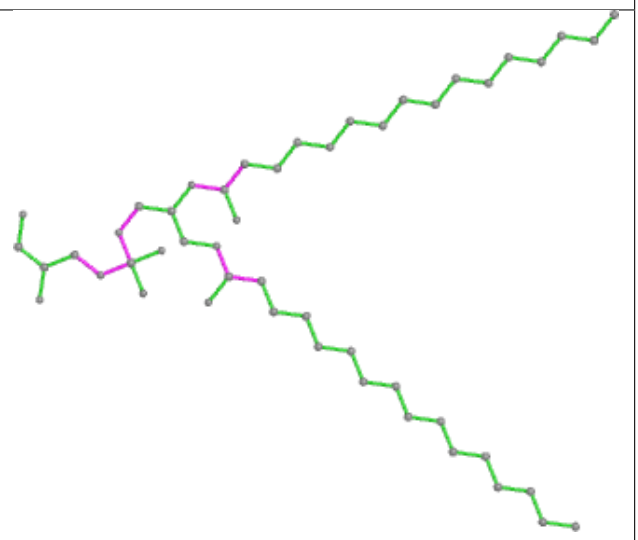
 Bond lengths	 Bond angles
 Torsions	 Rings

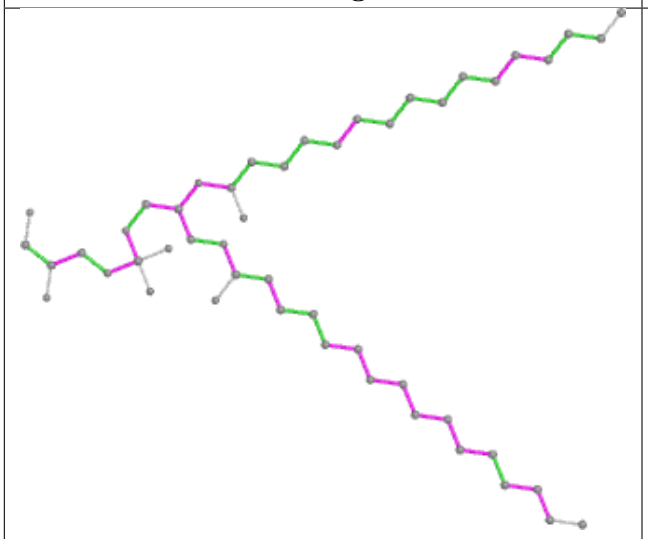
Ligand LHG L 102



Bond lengths



Bond angles



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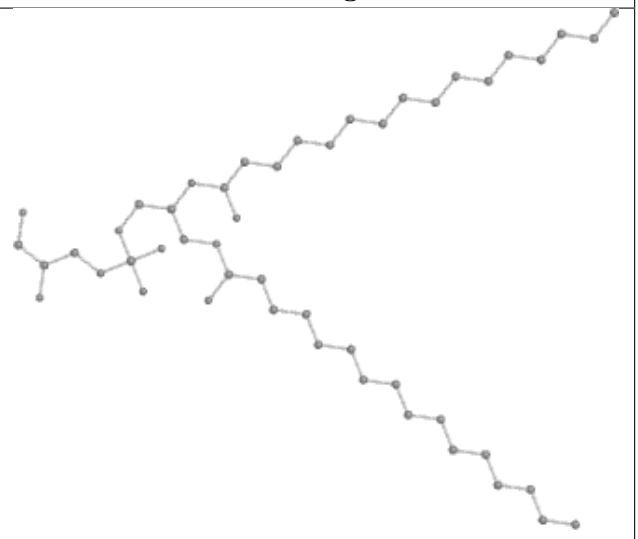

Rings

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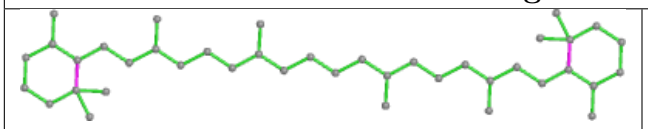

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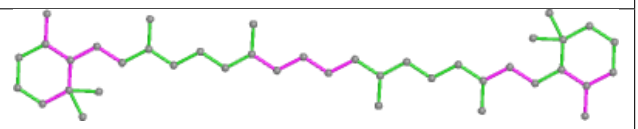
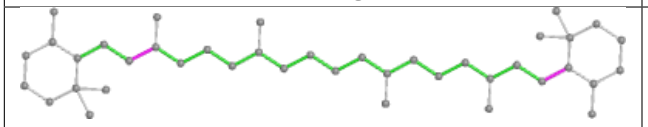


Bond angles



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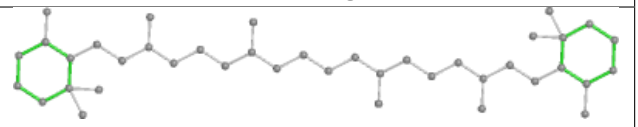
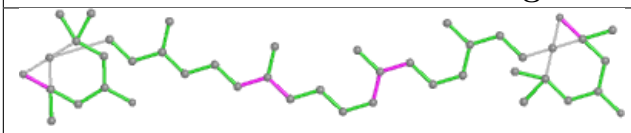


Rings

Ligand XAT R 616



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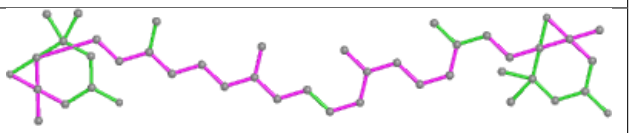

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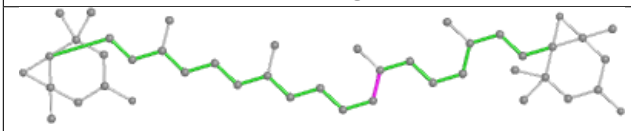

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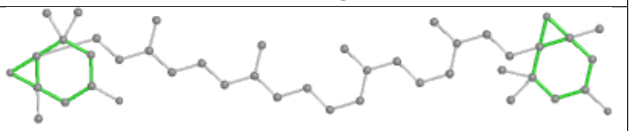

Rings

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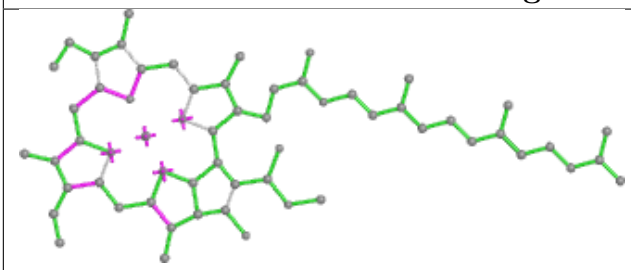

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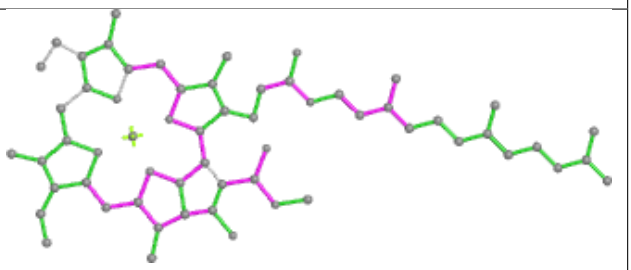
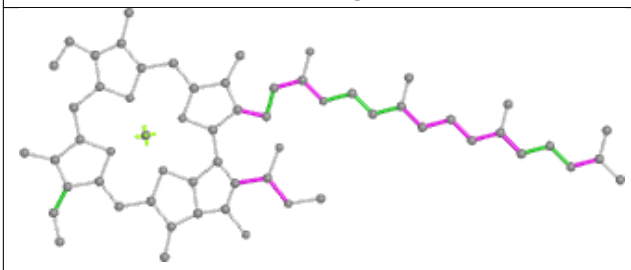


Bond angles



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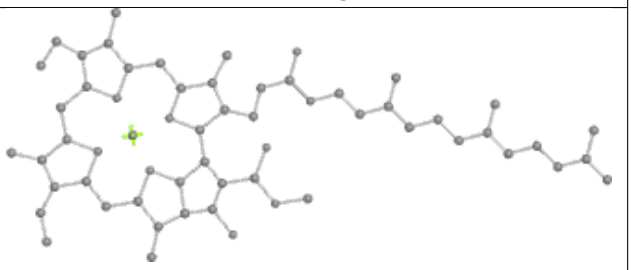

Rings

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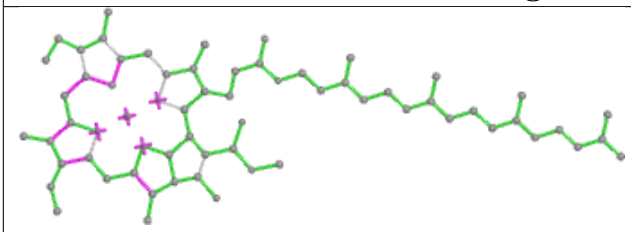

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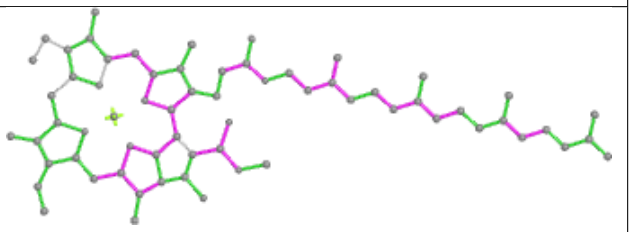
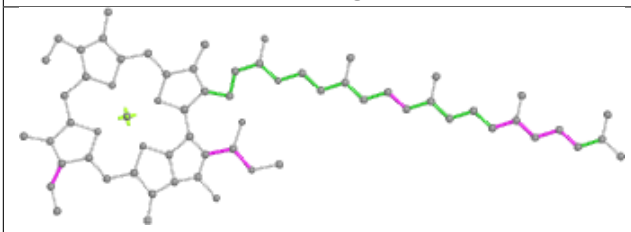


Bond angles



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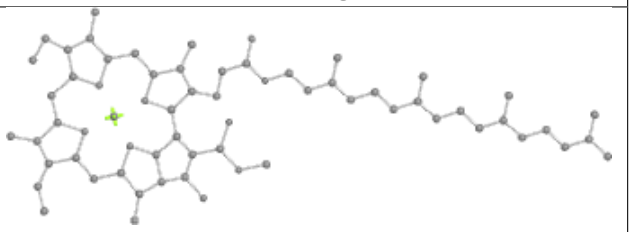
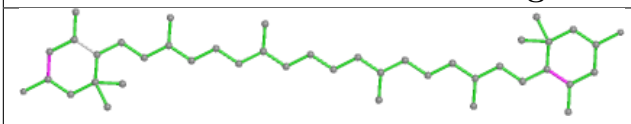


Rings

Ligand LUT n 615



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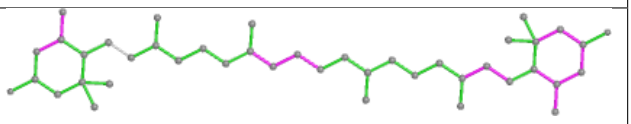
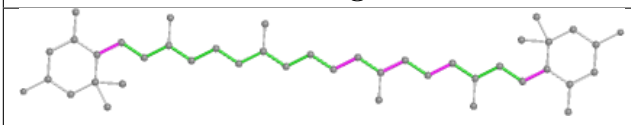
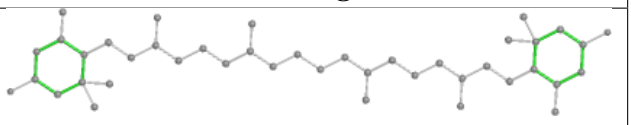


Bond angles

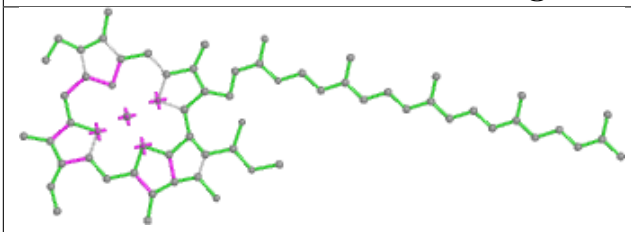


Torsions

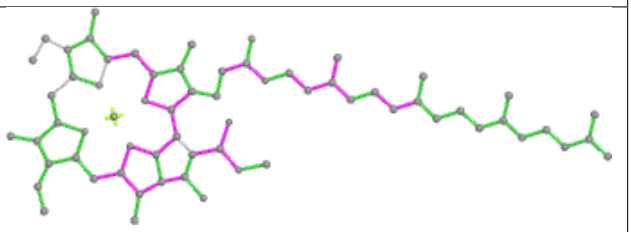


Rings

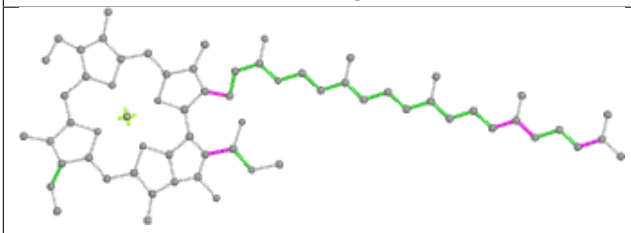
Ligand CLA a 403



Bond lengths



Bond angles



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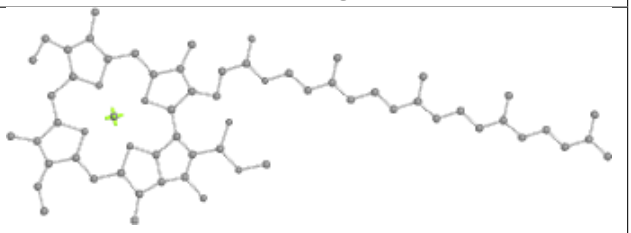
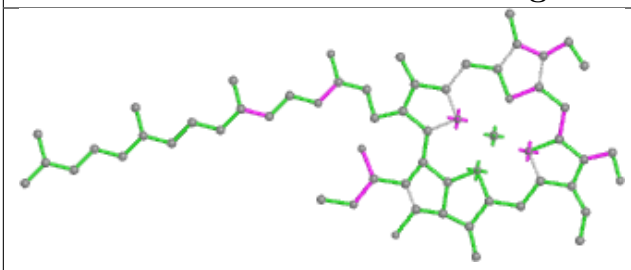


Rings

Ligand CHL r 607



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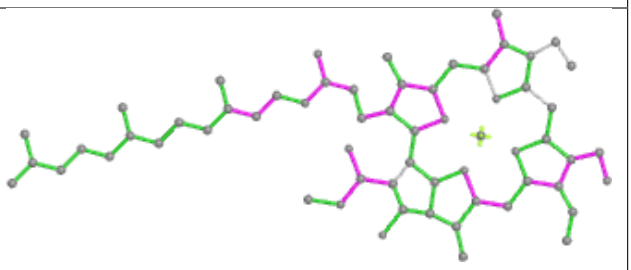
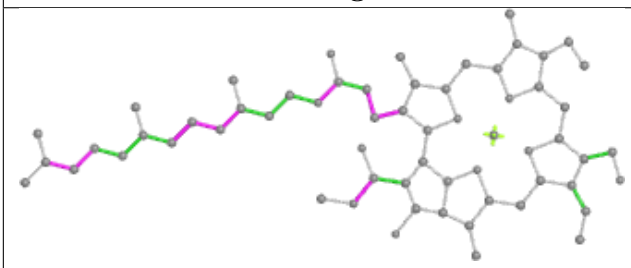


Bond angles



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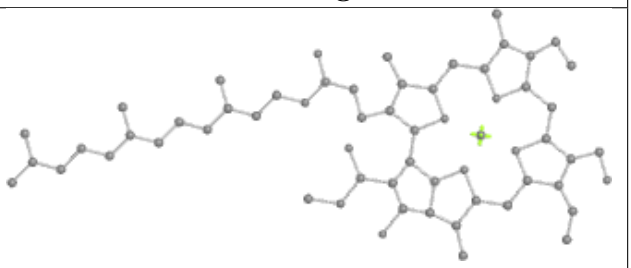
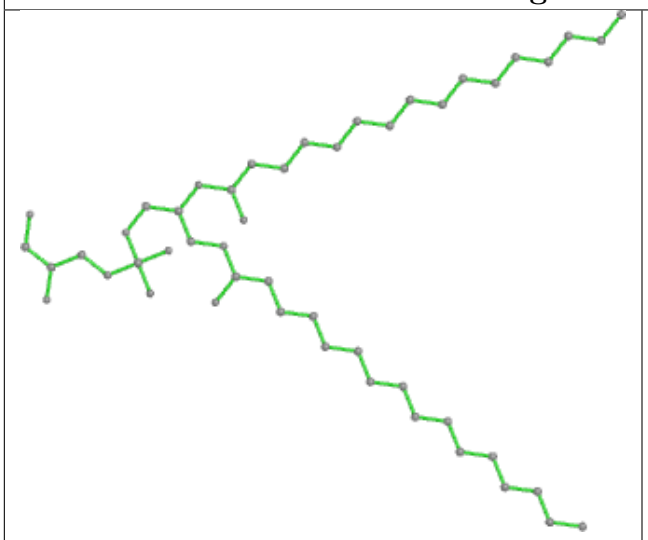
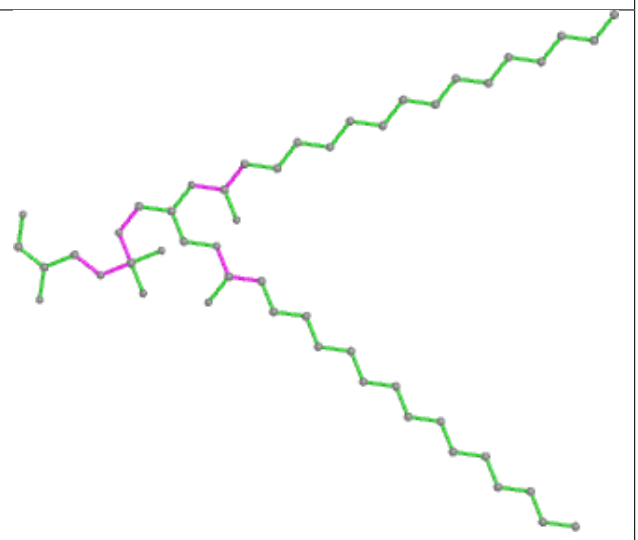


Rings

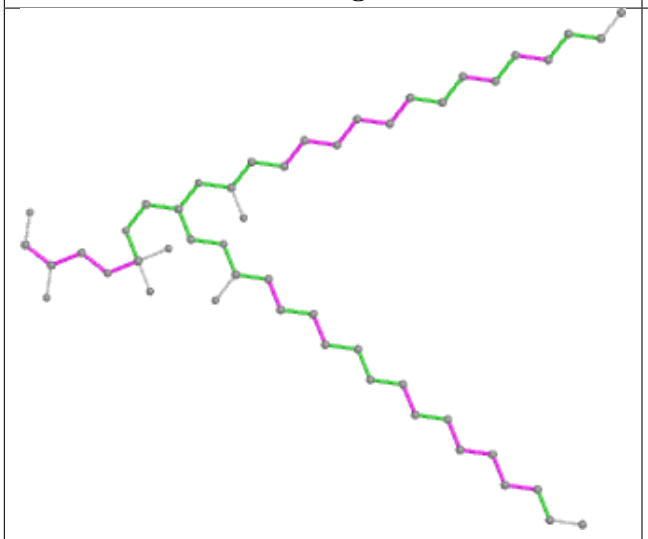
Ligand LHG s 318



Bond lengths



Bond angles



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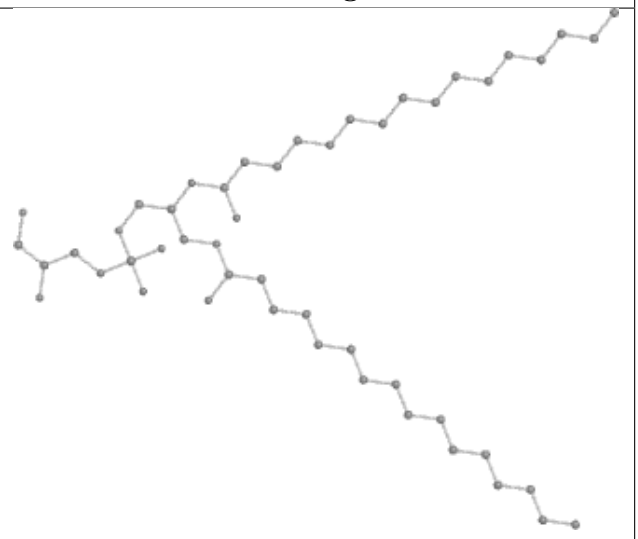
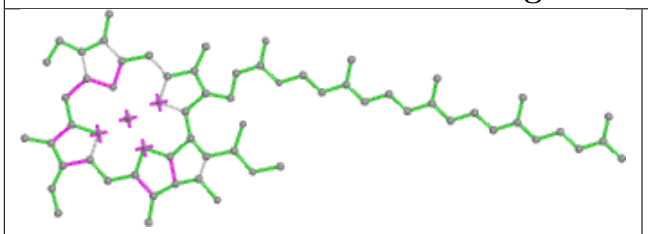


Rings

Ligand CLA D 402



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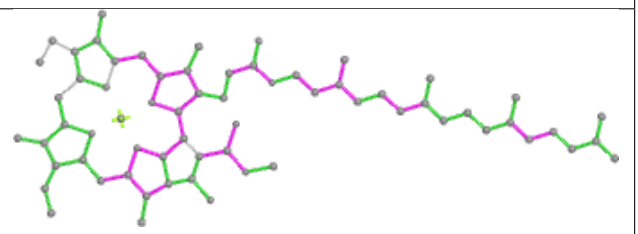
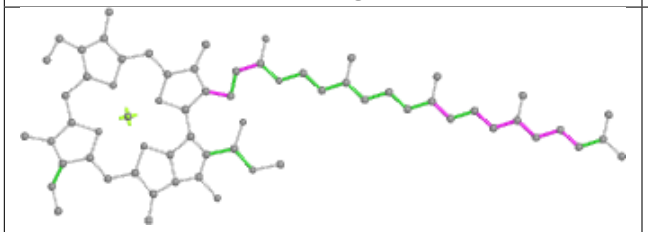


Bond angles



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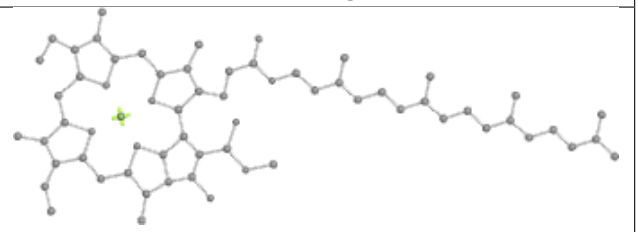
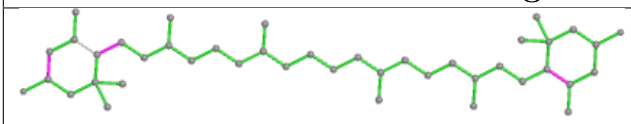
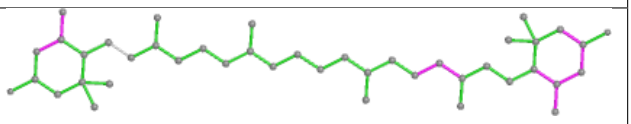
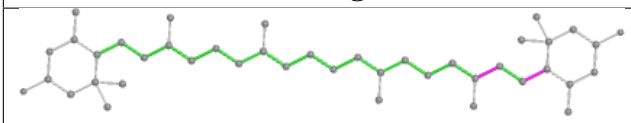
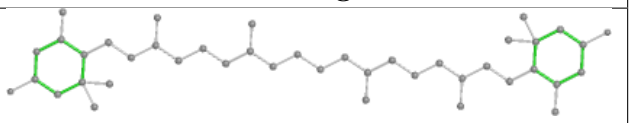


Rings

Ligand LUT N 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

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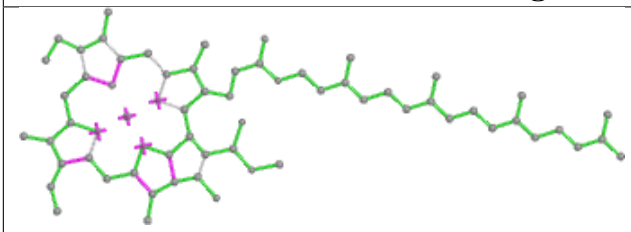
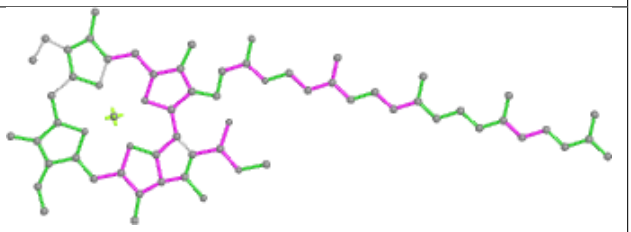
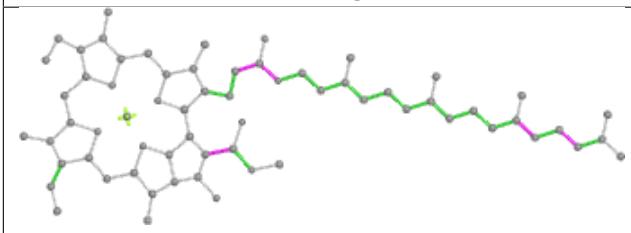
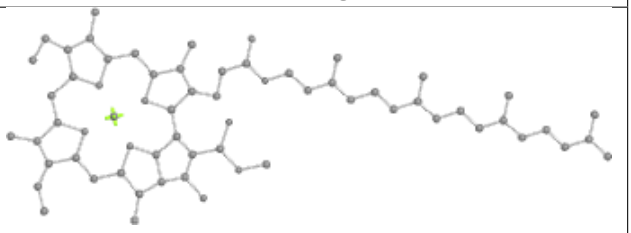
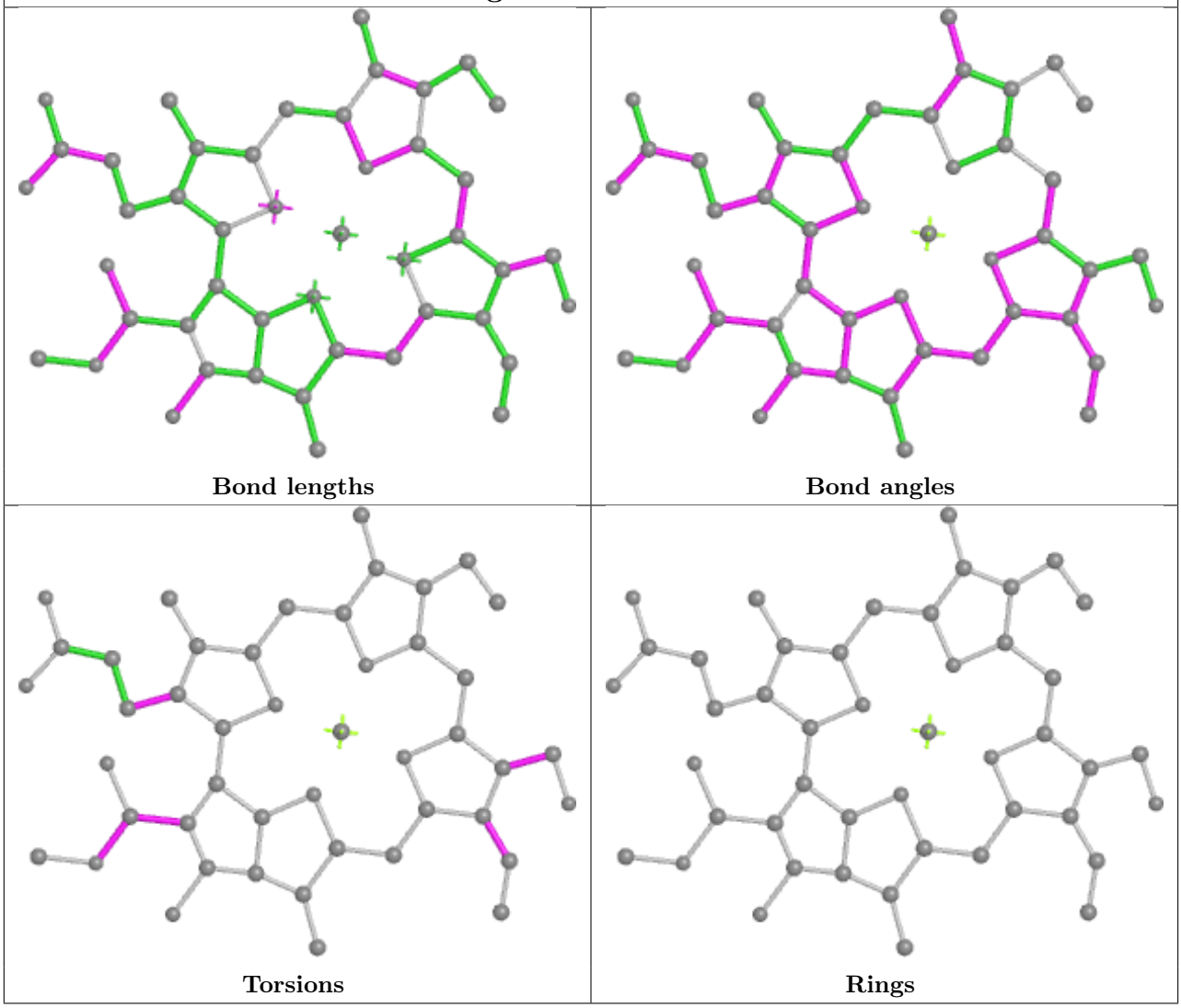
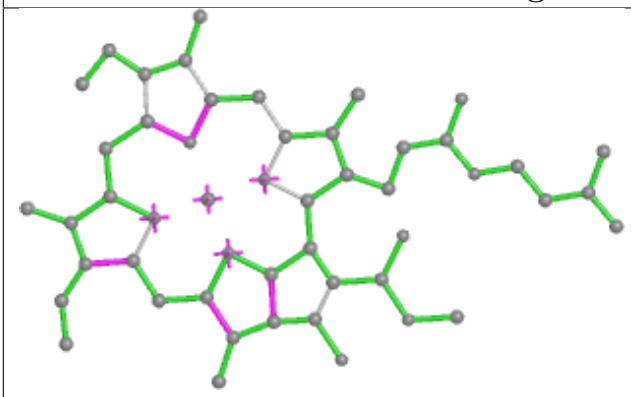
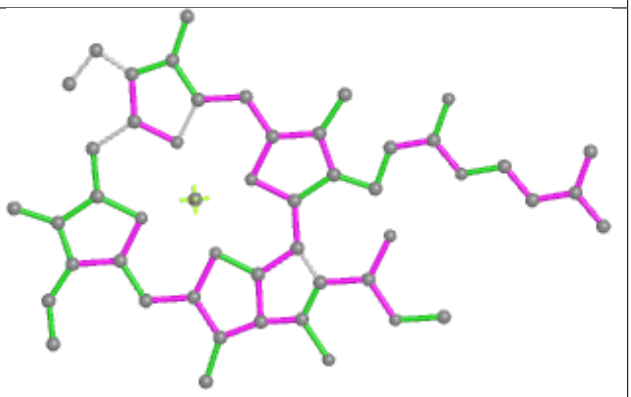
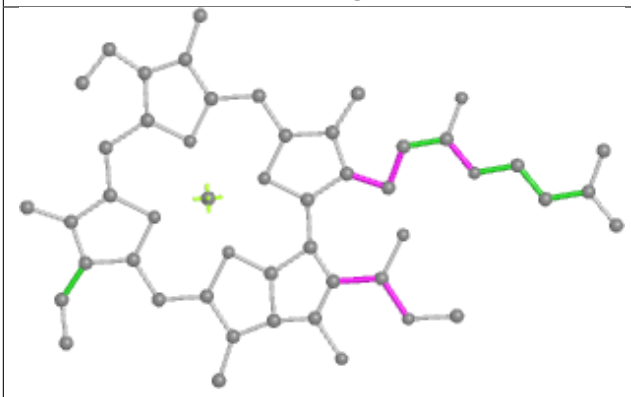
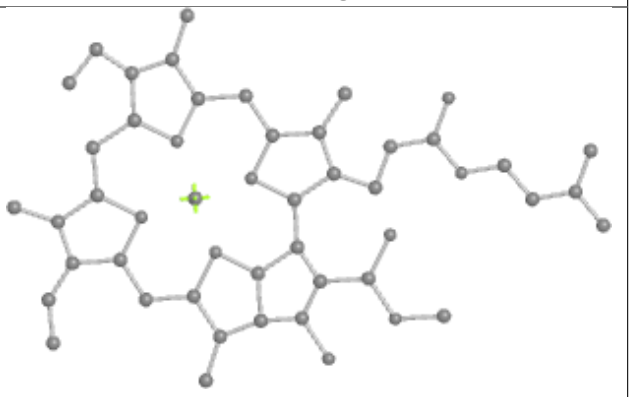
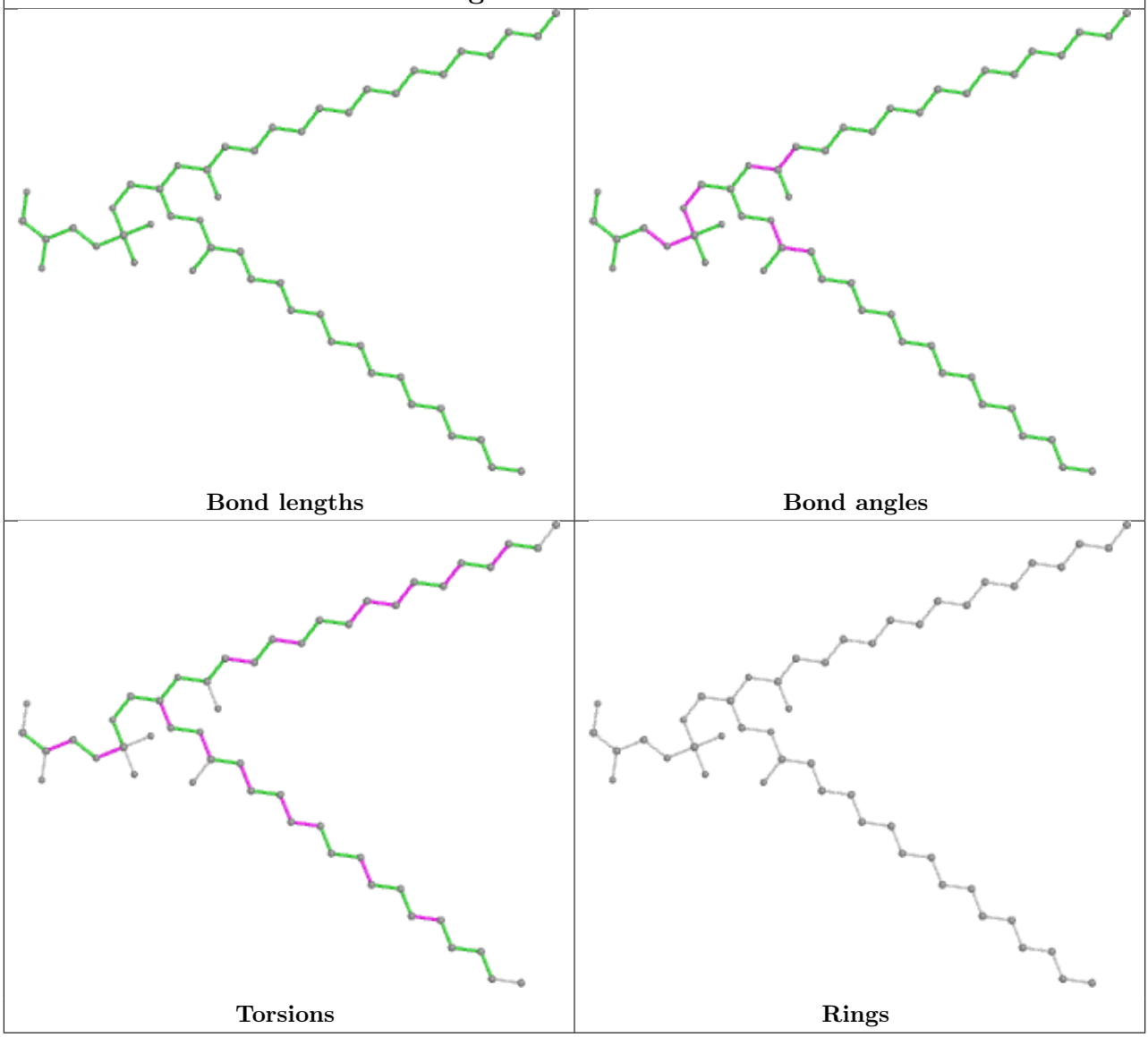
 Bond lengths	 Bond angles
 Torsions	 Rings

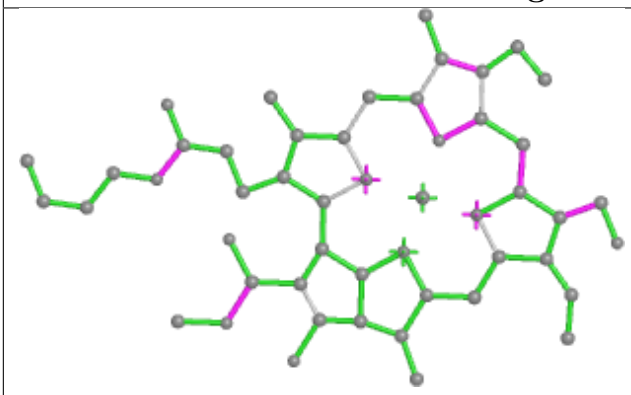
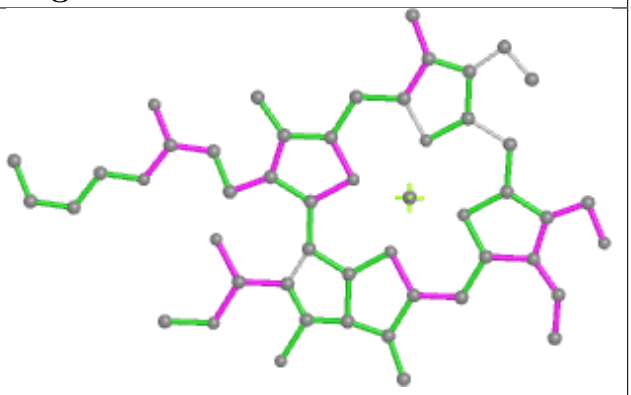
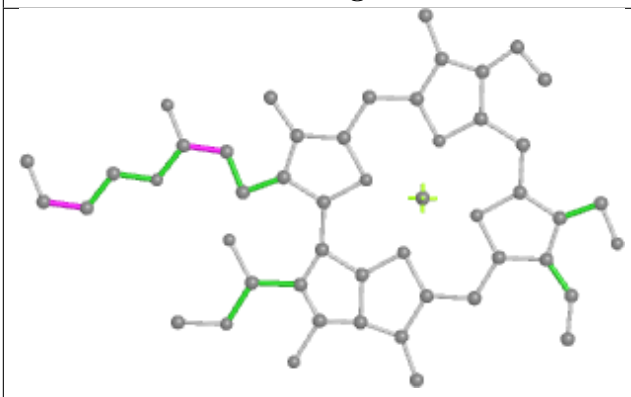
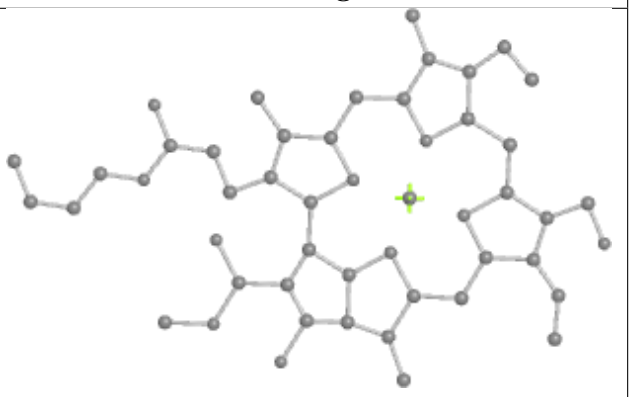
Ligand CHL 2 603



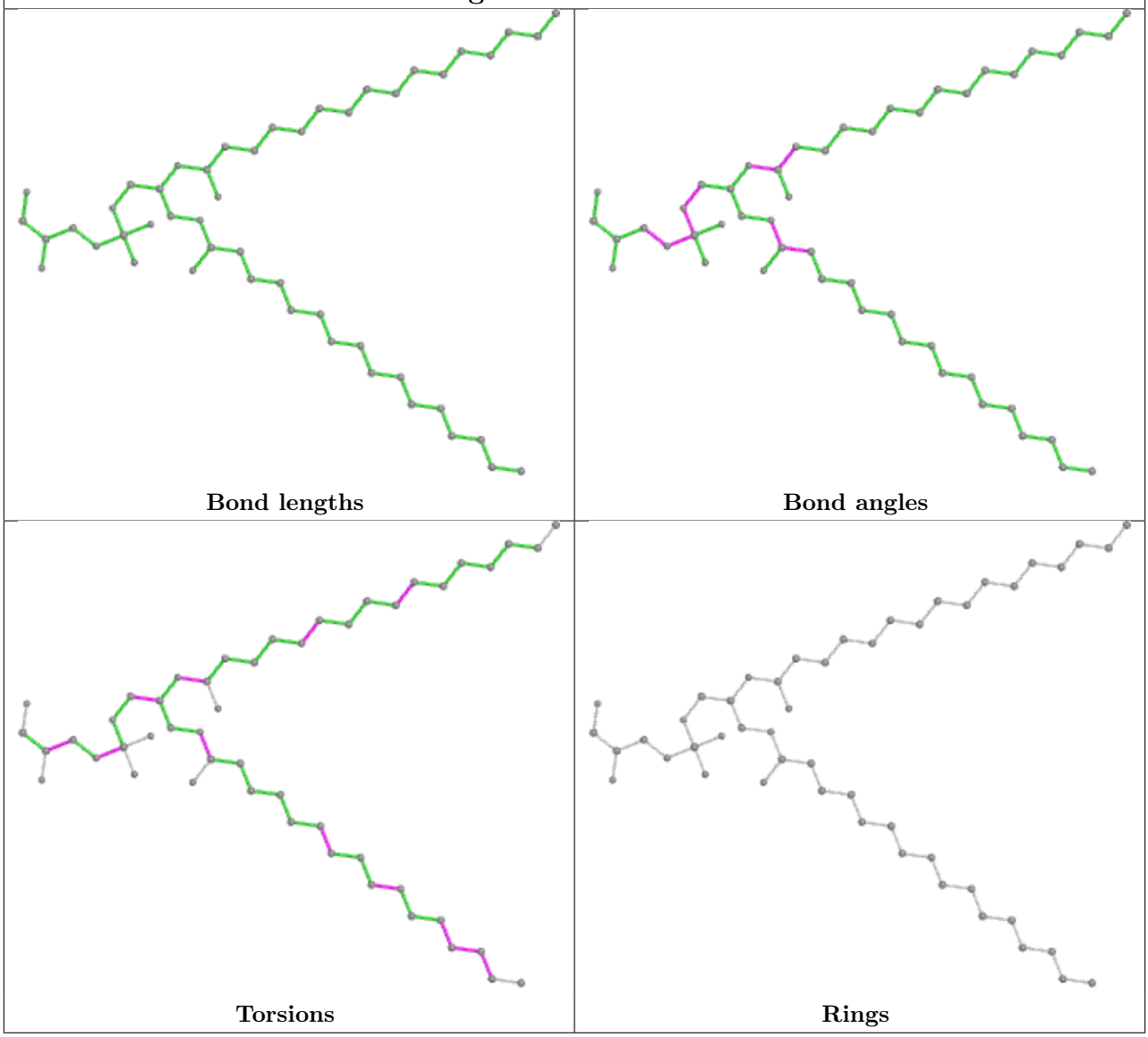
Ligand CLA S 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

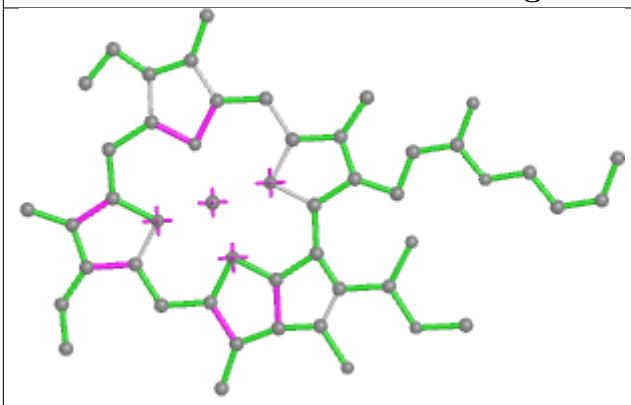
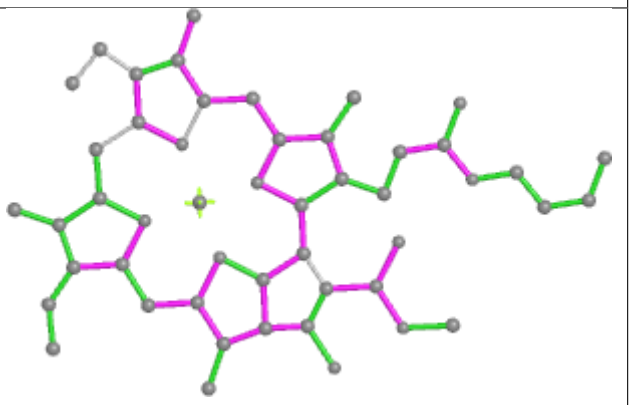
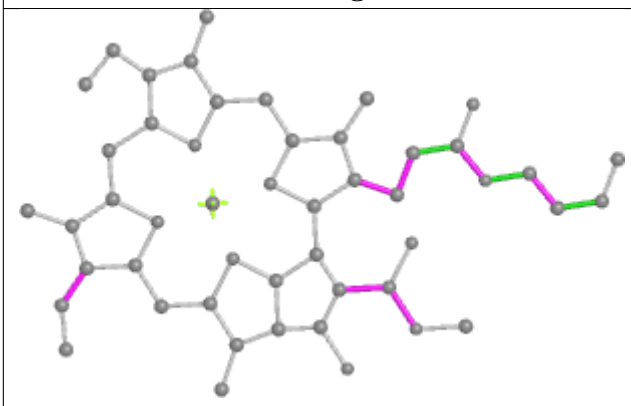
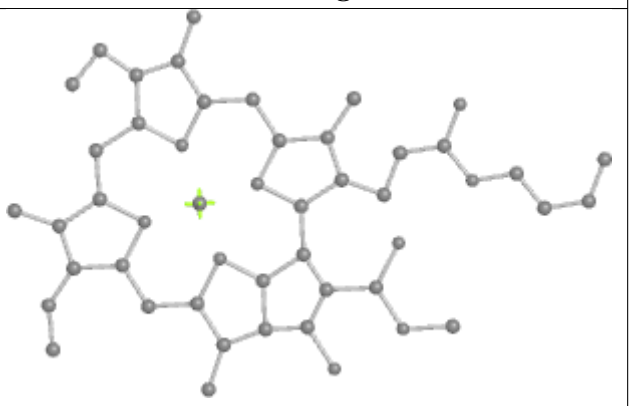
Ligand LHG B 622



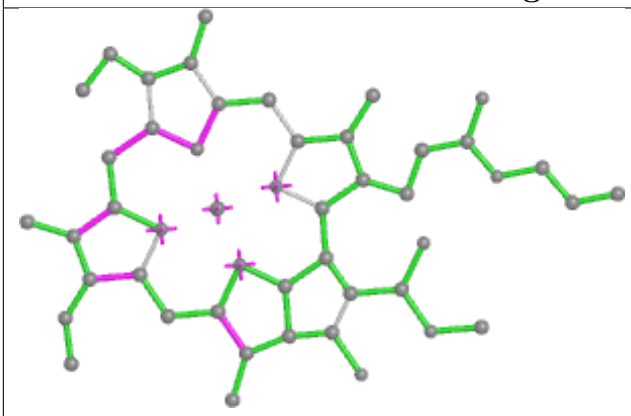
Ligand CHL g 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG C 517

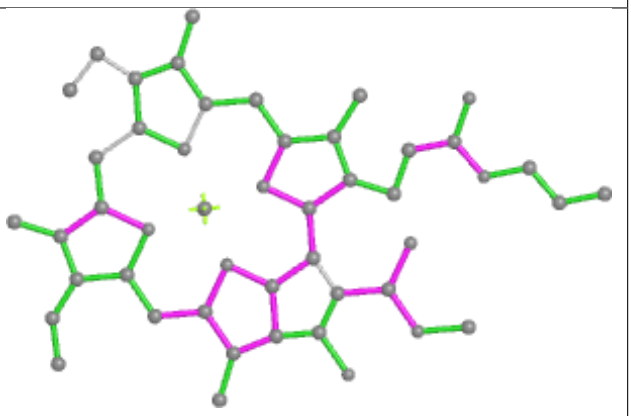


Ligand CLA R 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

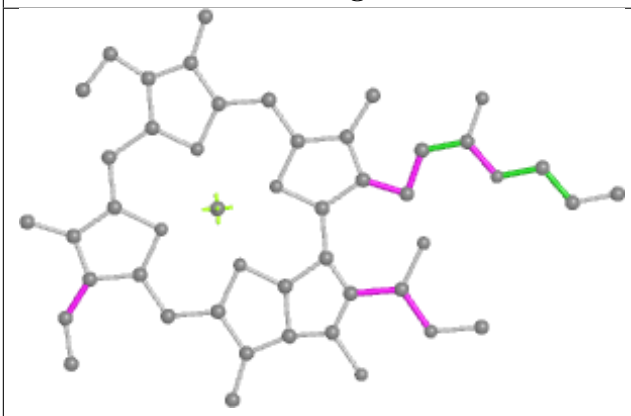
Ligand CLA G 614



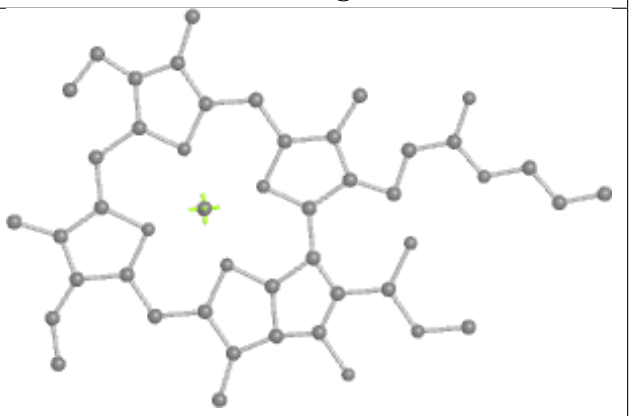
Bond lengths



Bond angles

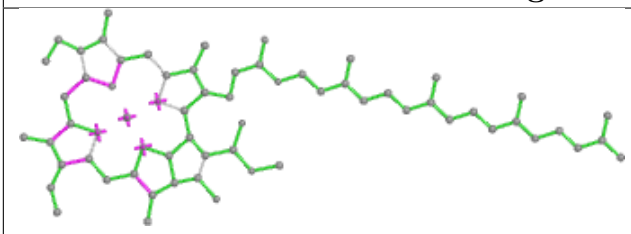


Torsions

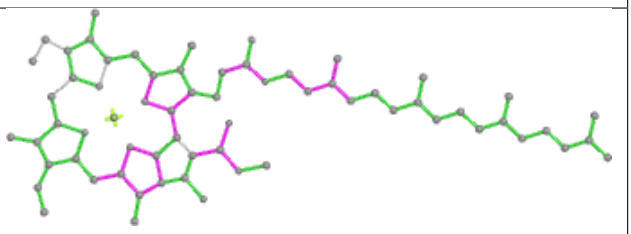


Rings

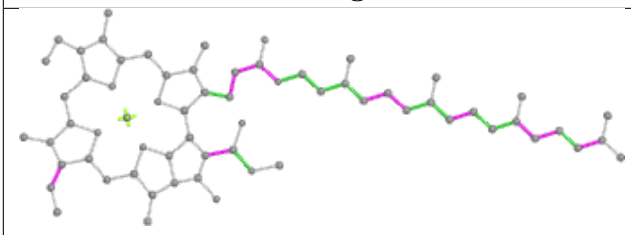
Ligand CLA b 616



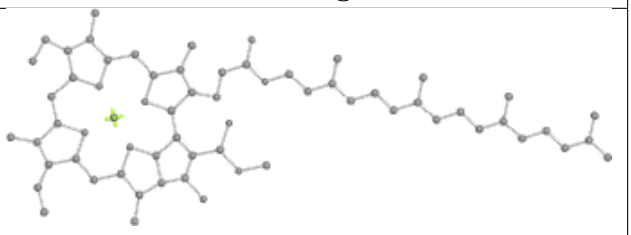
Bond lengths



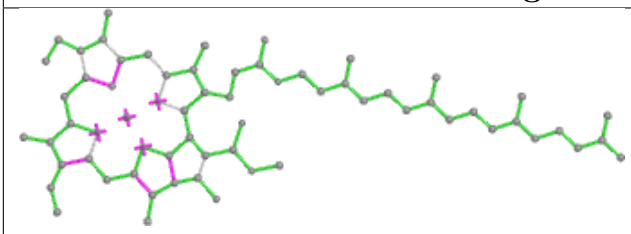
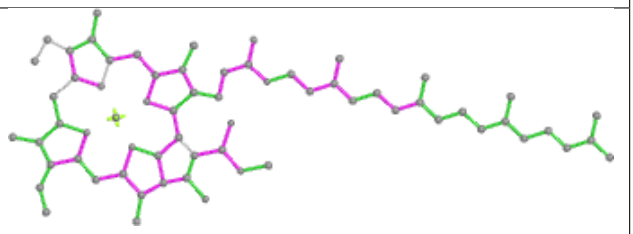
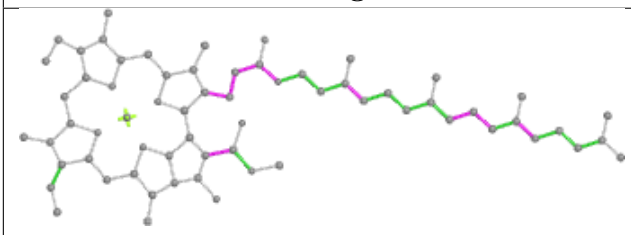
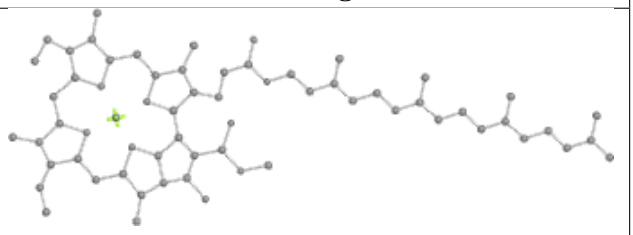
Bond angles

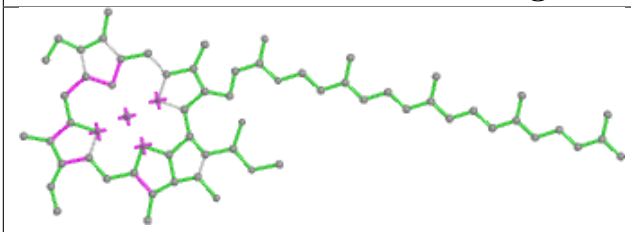
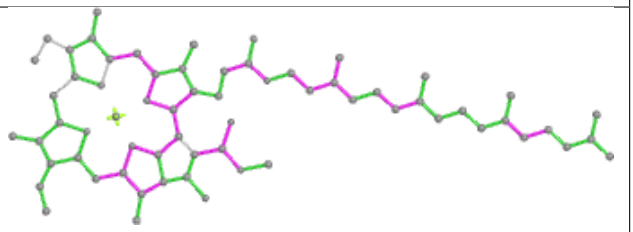
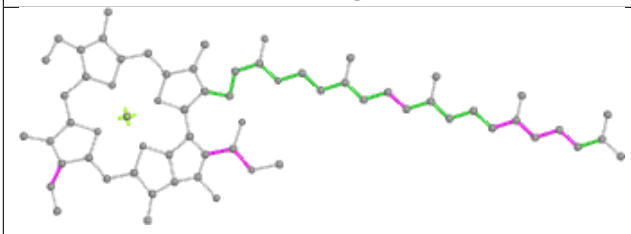
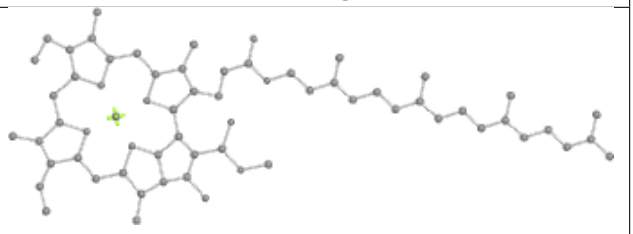


Torsions

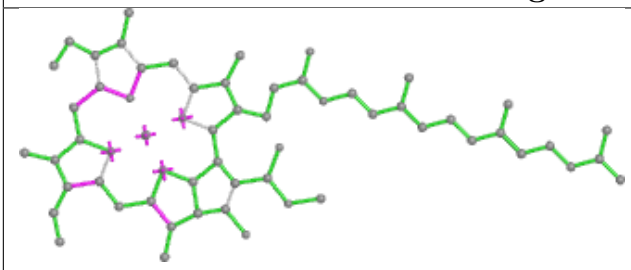


Rings

Ligand CLA D 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 612



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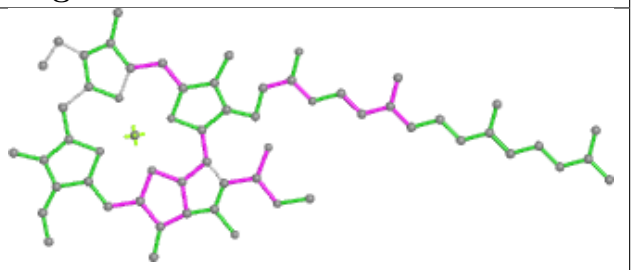
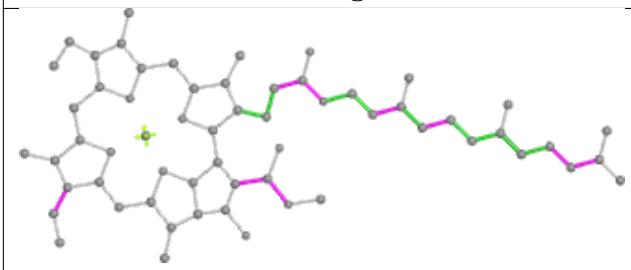


Bond angles



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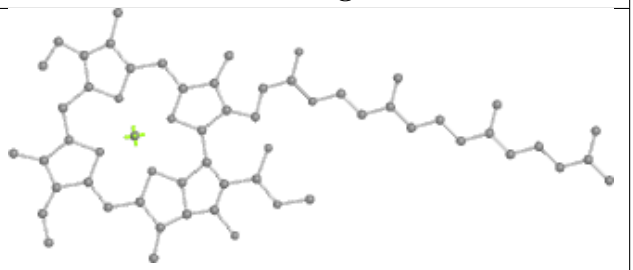
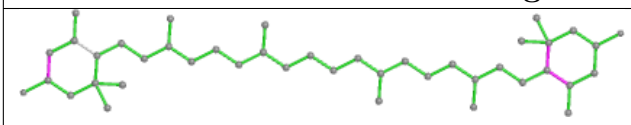


Rings

Ligand LUT G 616



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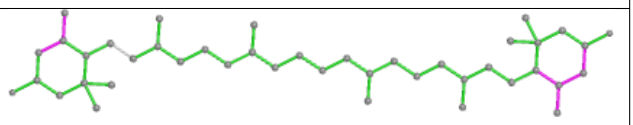

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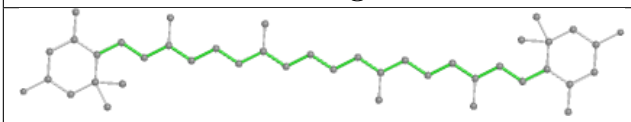

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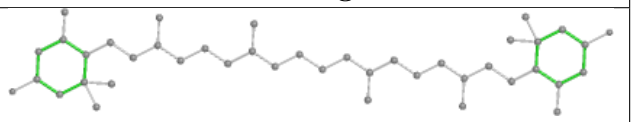
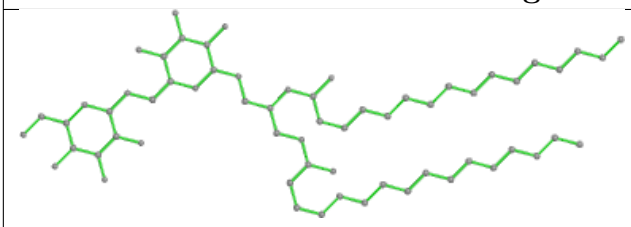


Rings

Ligand DGD b 626



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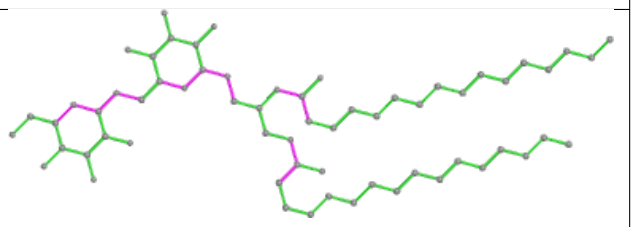
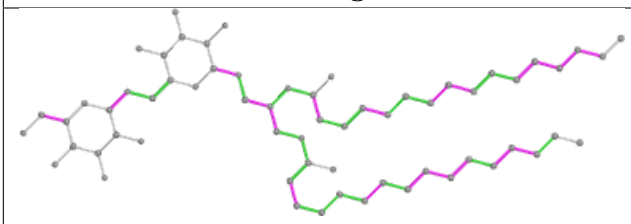


Bond angles



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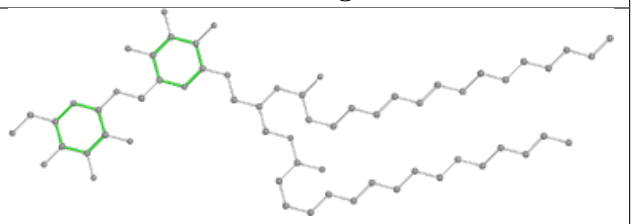

Rings

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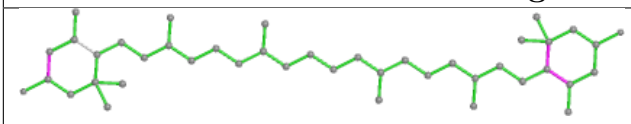
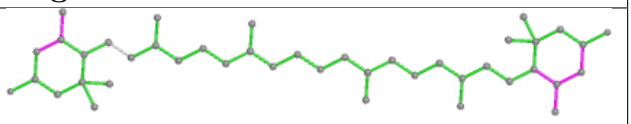
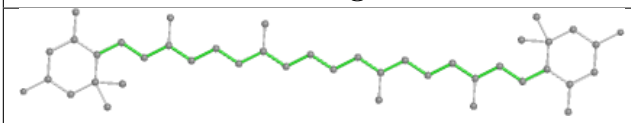
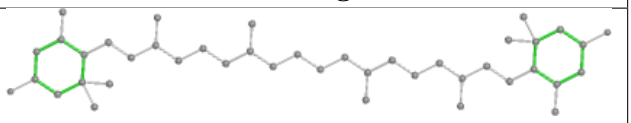
 Bond lengths	 Bond angles
 Torsions	 Rings

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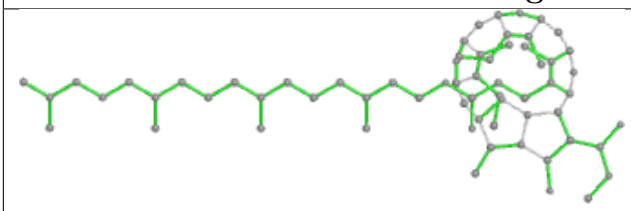
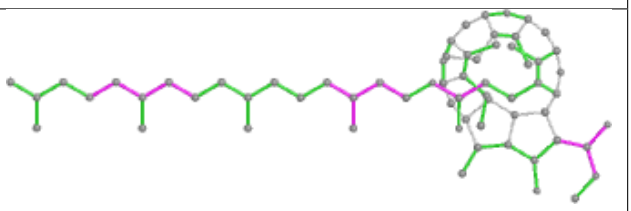
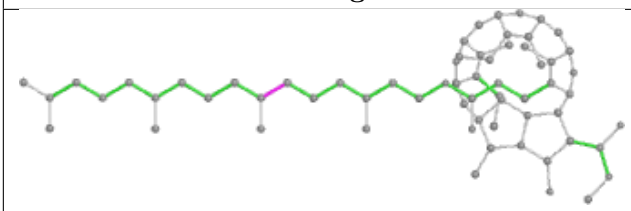
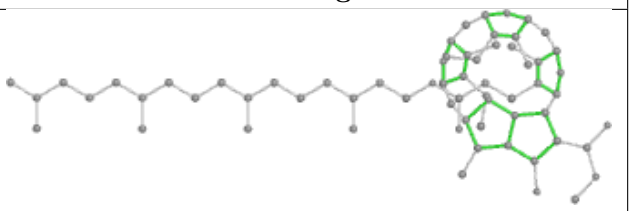
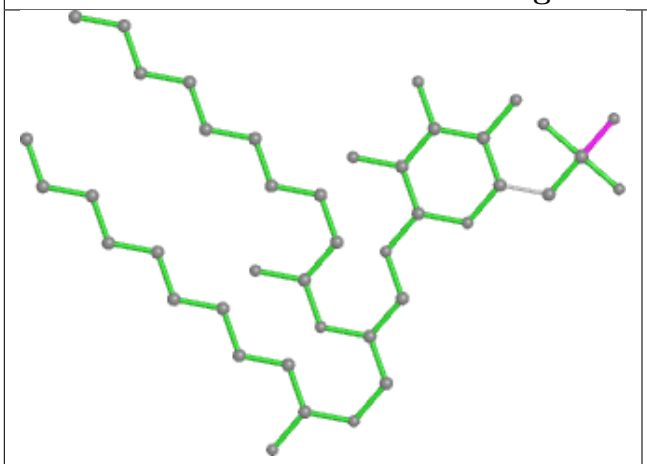
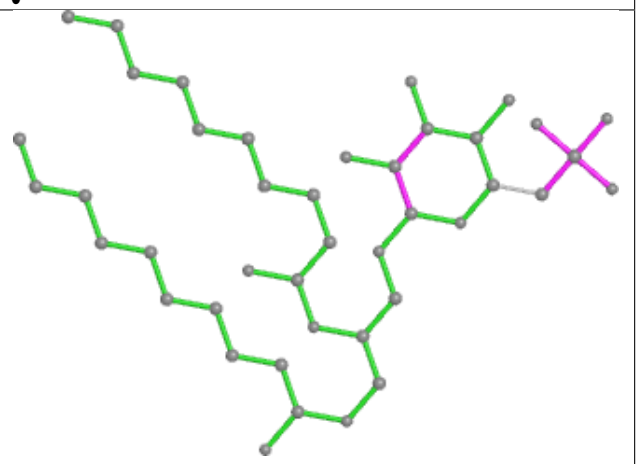
 Bond lengths	 Bond angles
 Torsions	 Rings

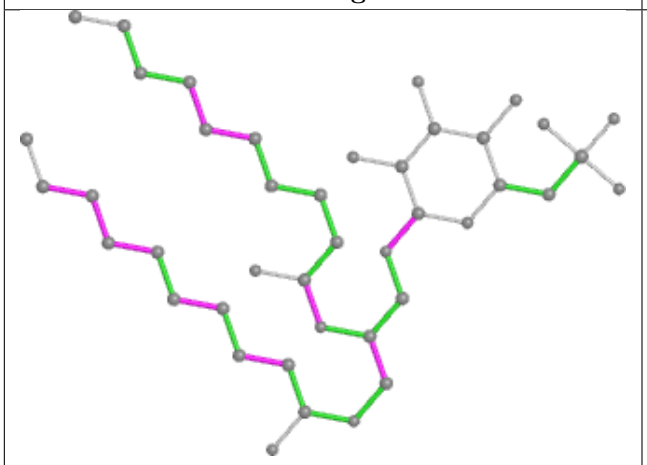
Ligand SQD l 102



Bond lengths



Bond angles



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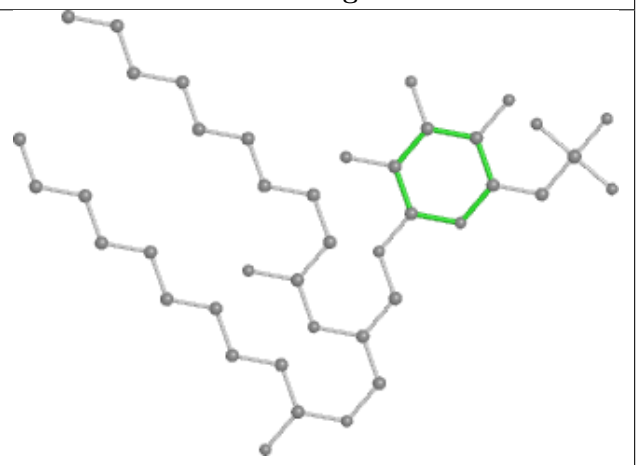
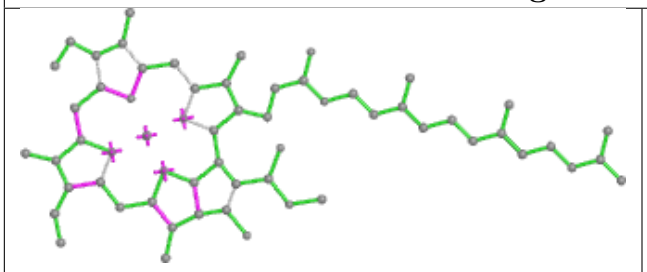


Rings

Ligand CLA 2 602



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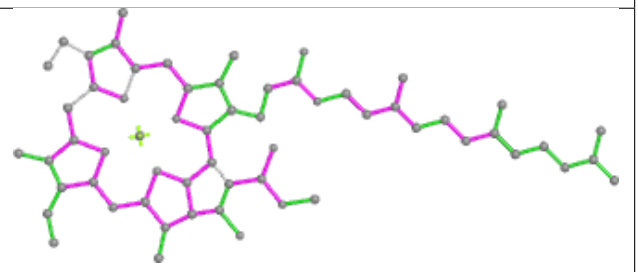
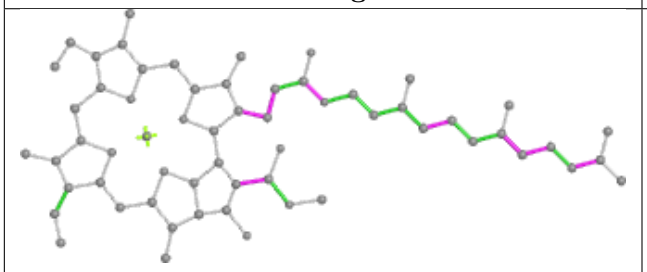


Bond angles



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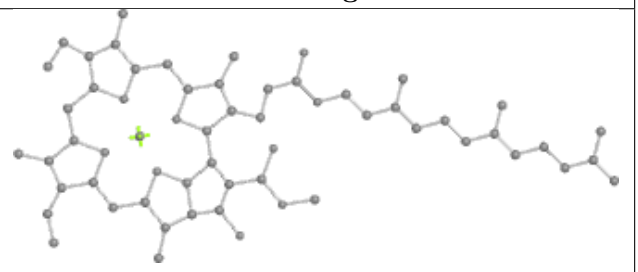
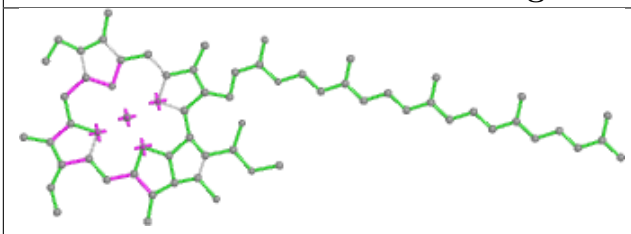
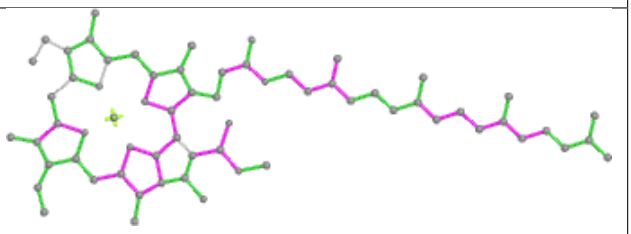
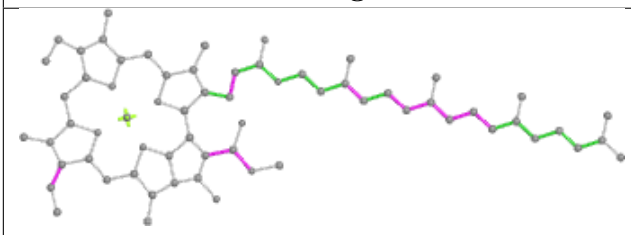
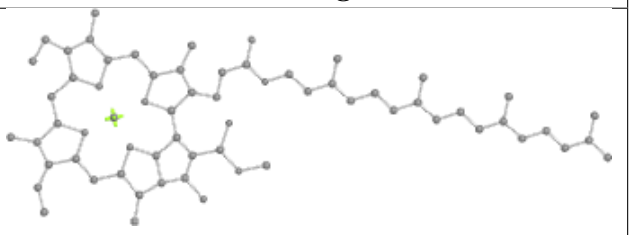
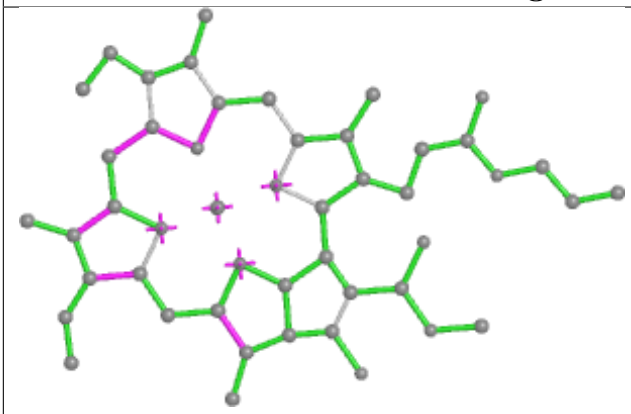
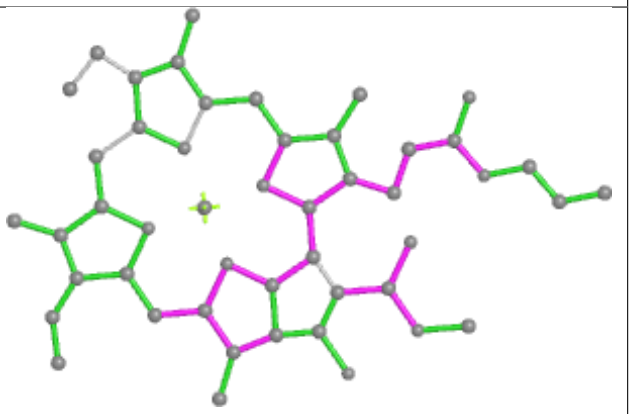
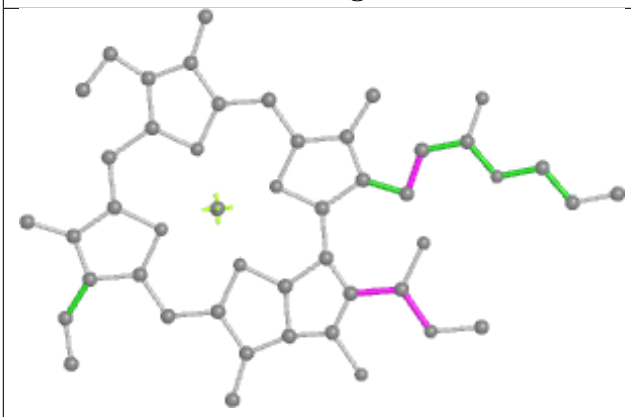
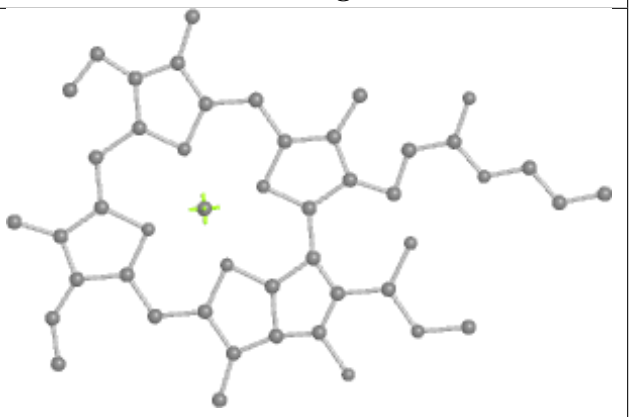
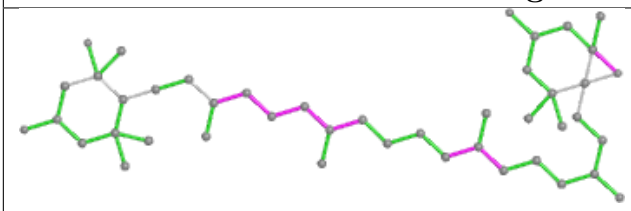
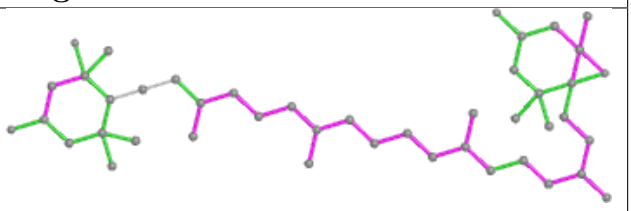
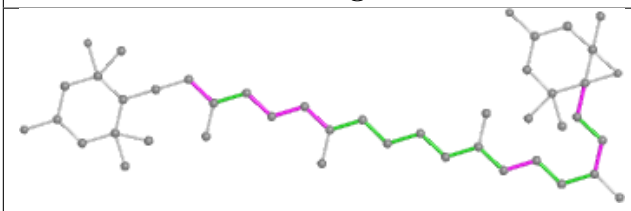
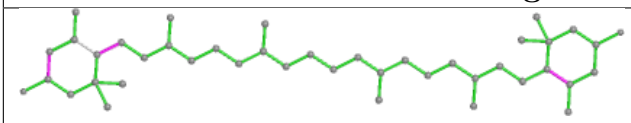
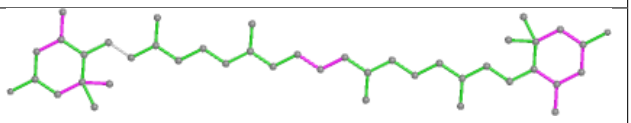
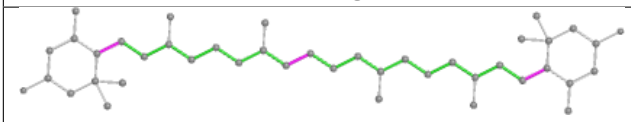
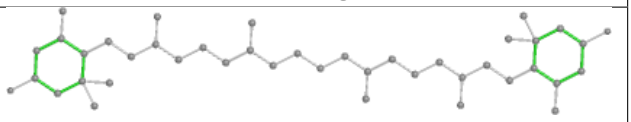


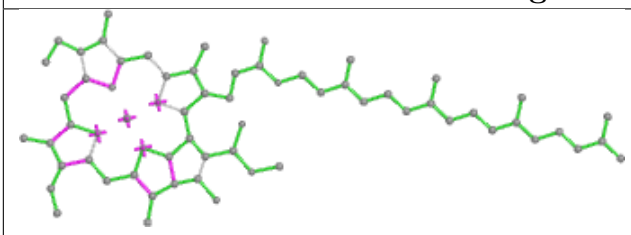
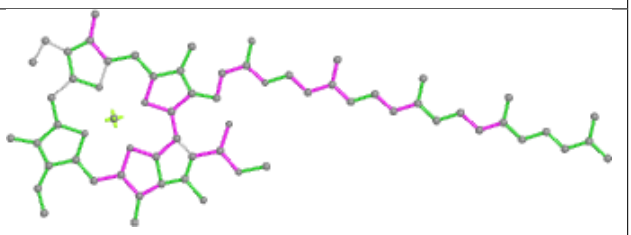
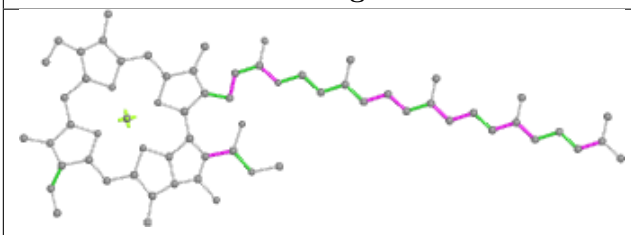
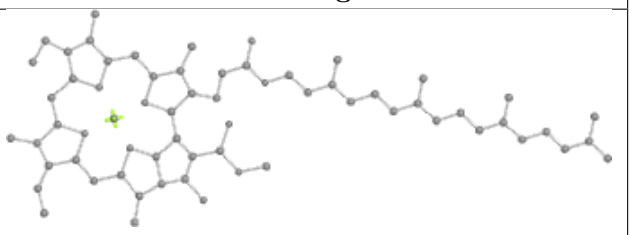
Rings

Ligand CLA n 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

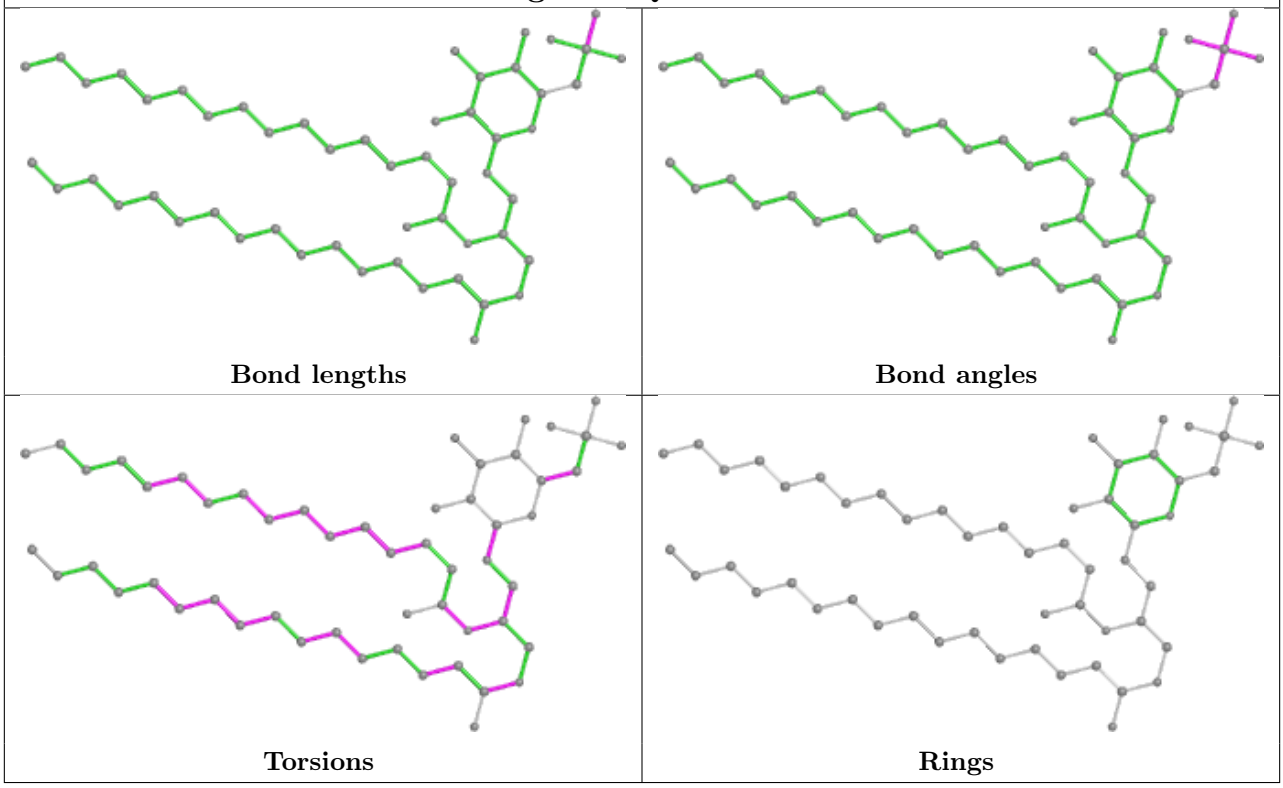
Ligand CLA n 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX g 617	
 Bond lengths	 Bond angles
 Torsions	Rings

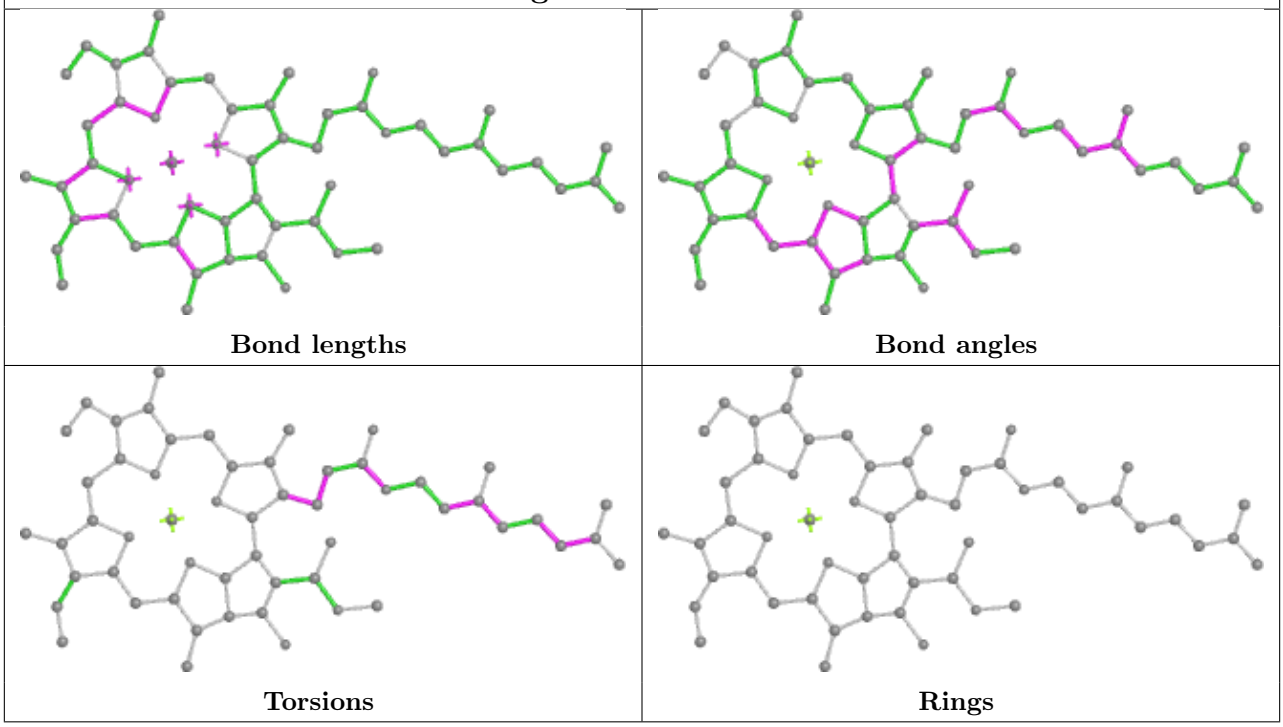
Ligand LUT G 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

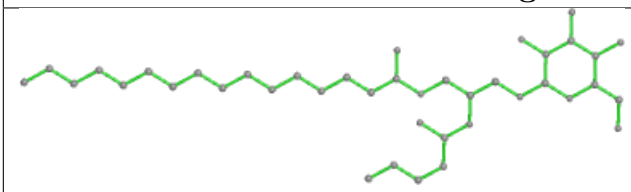
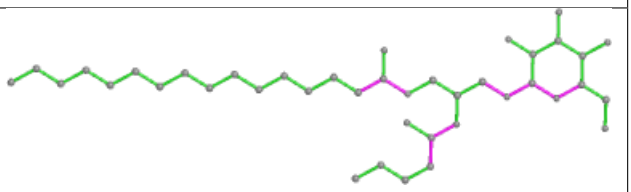
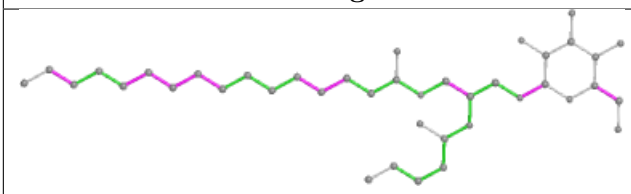
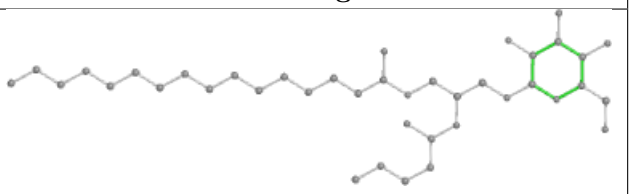
Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

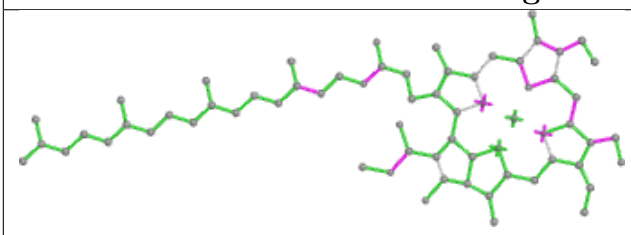
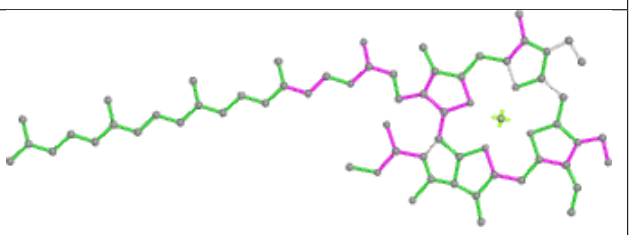
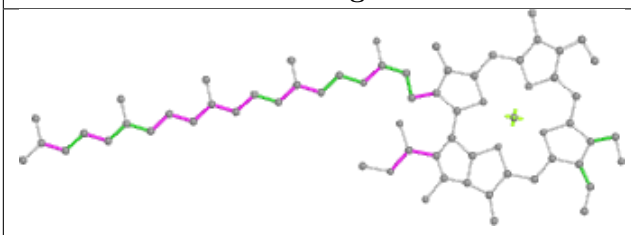
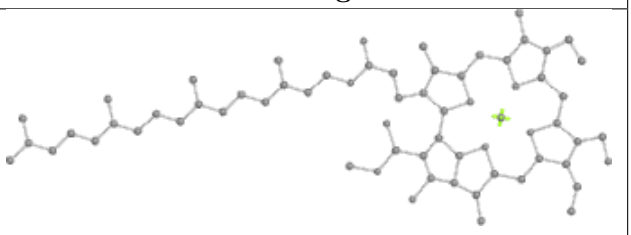
Ligand SQD L 103



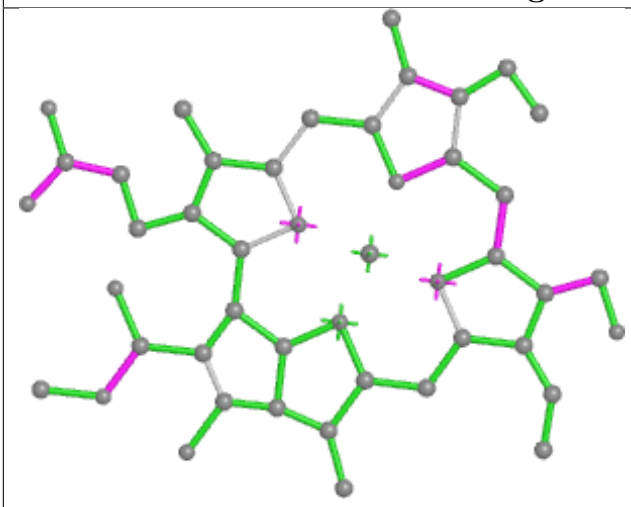
Ligand CLA s 310



Ligand LMG A 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL g 607



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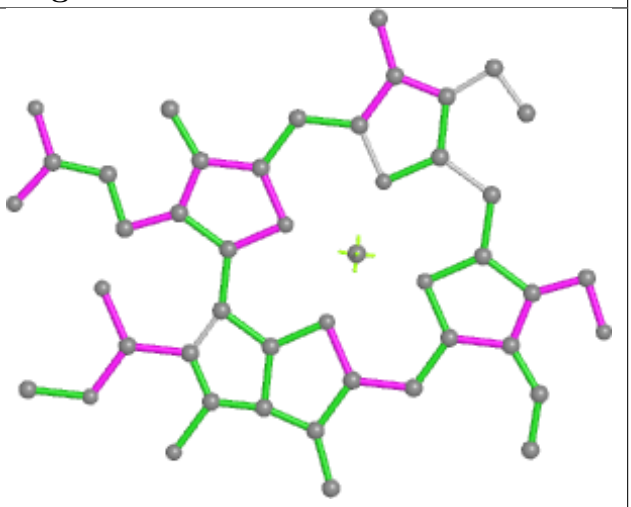

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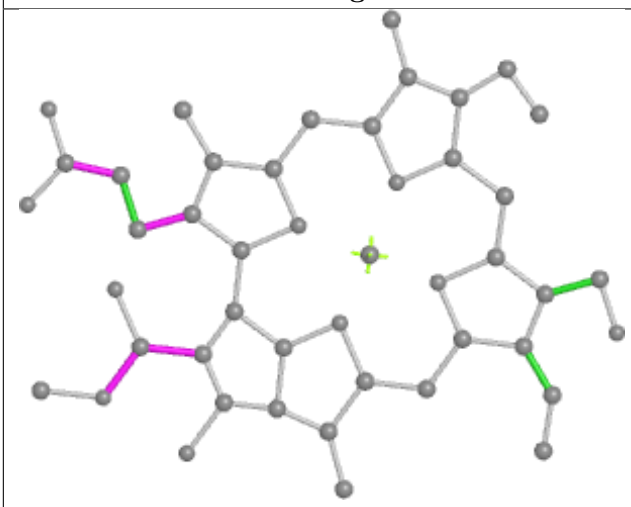

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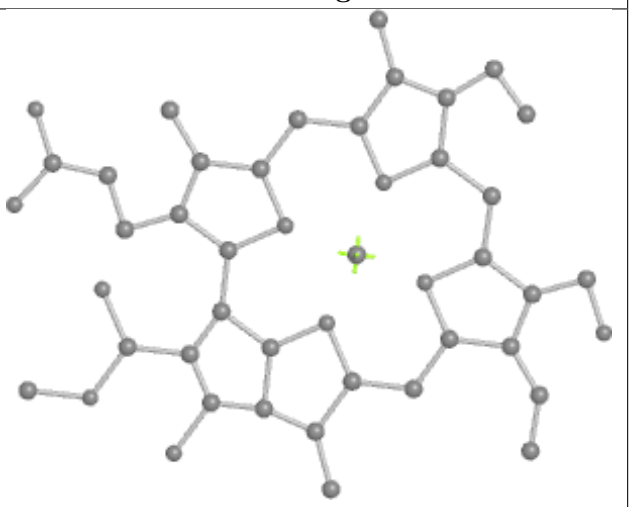
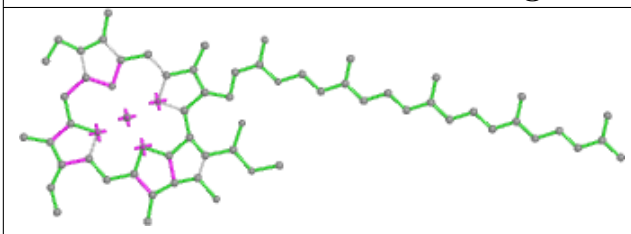


Rings

Ligand CLA A 402



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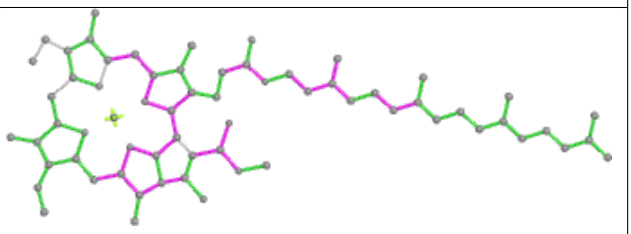

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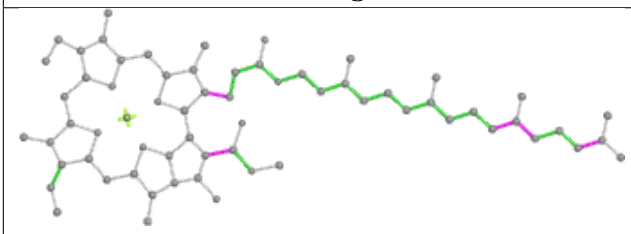

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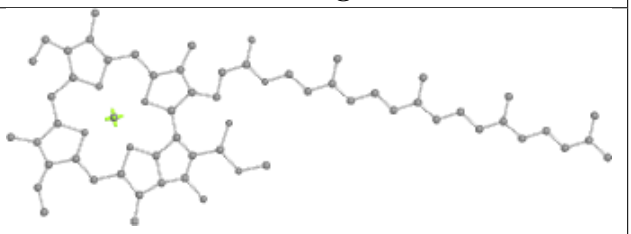
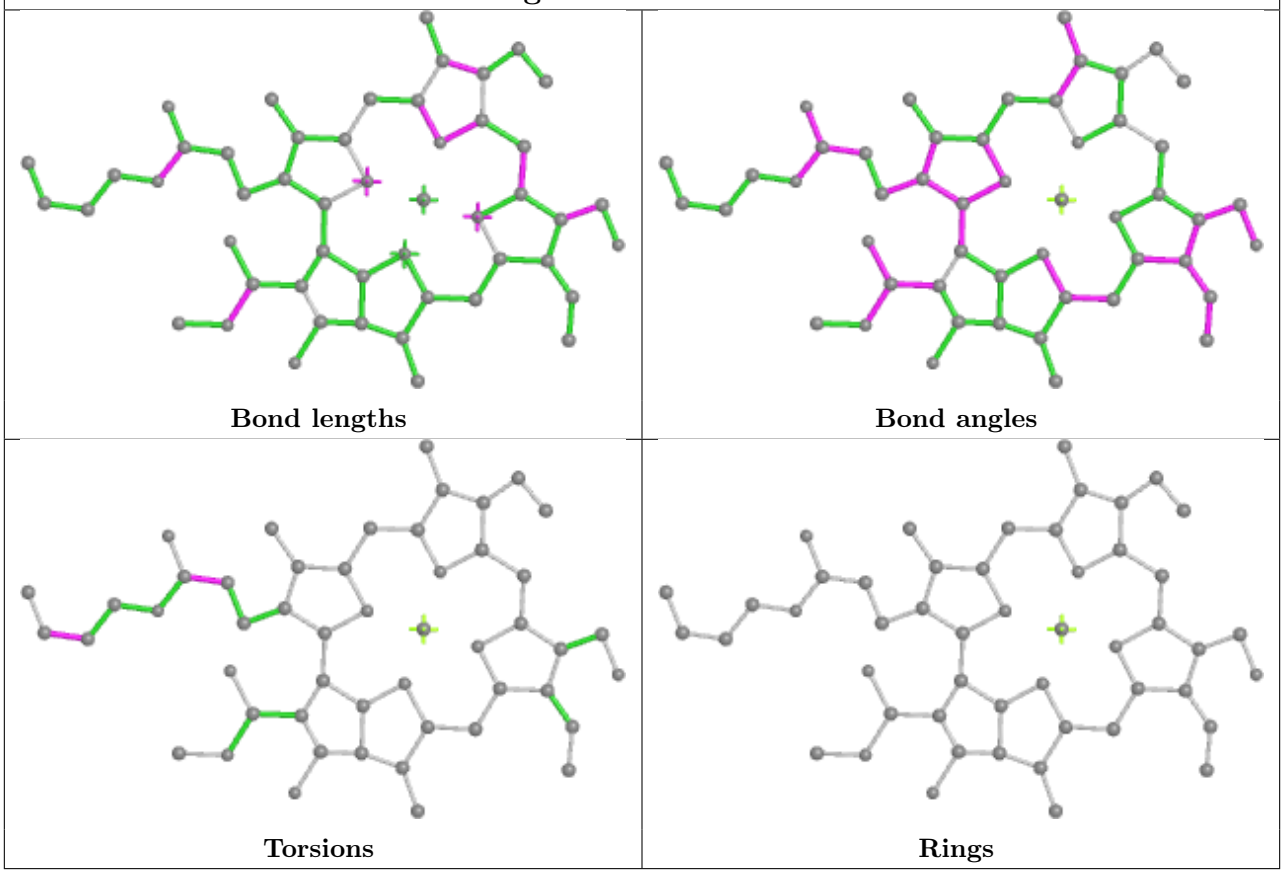
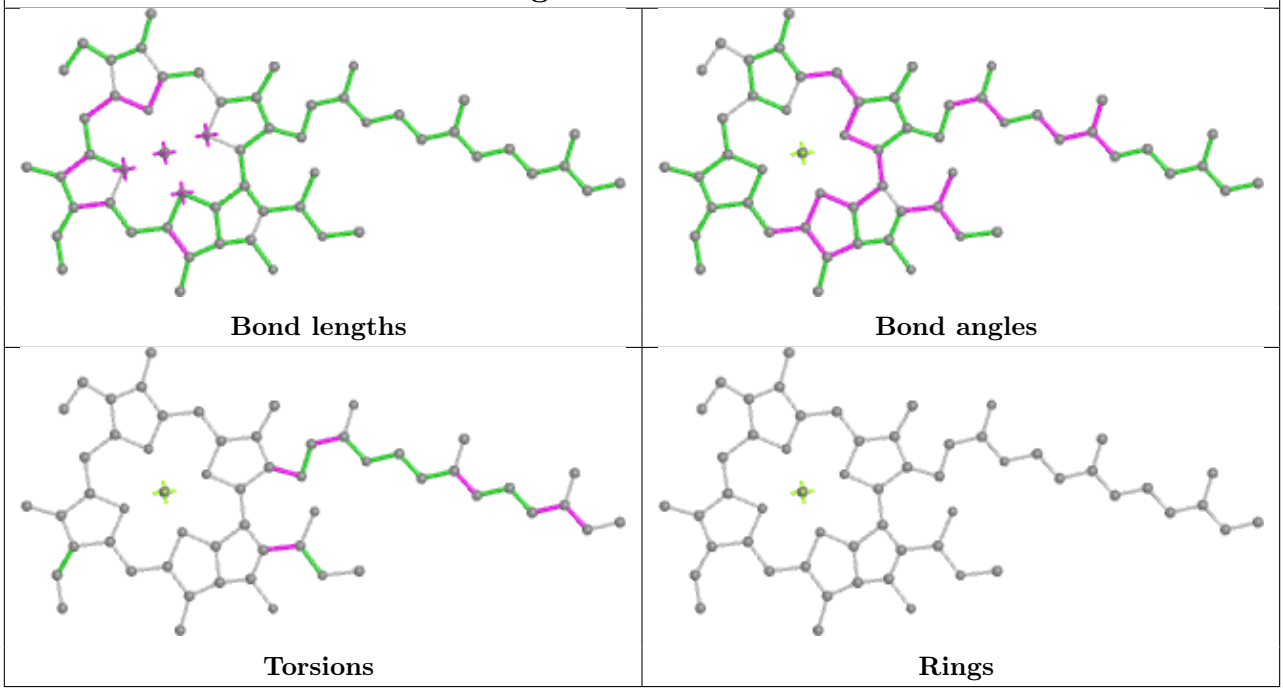


Rings

Ligand CHL G 606



Ligand CLA s 311



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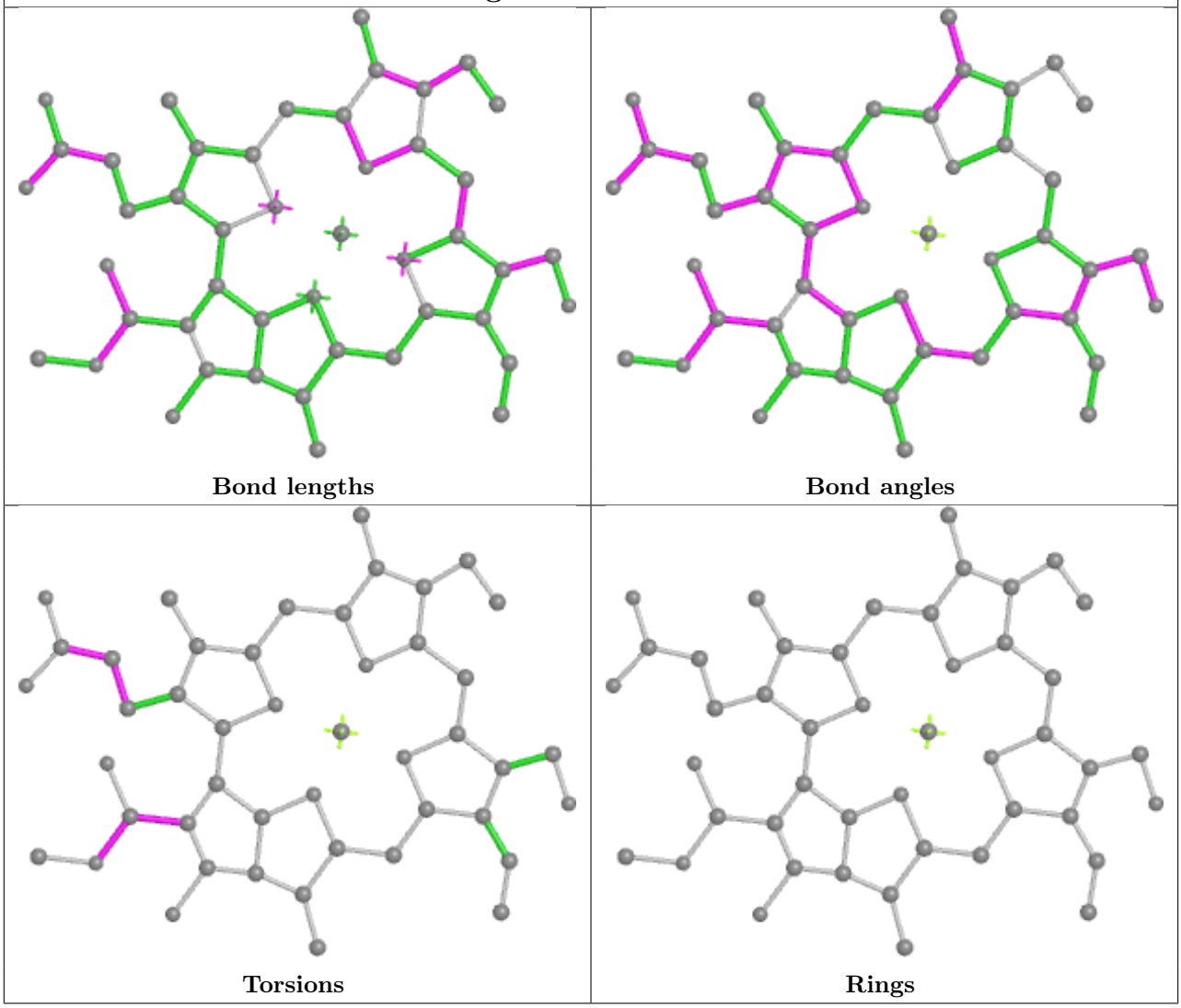

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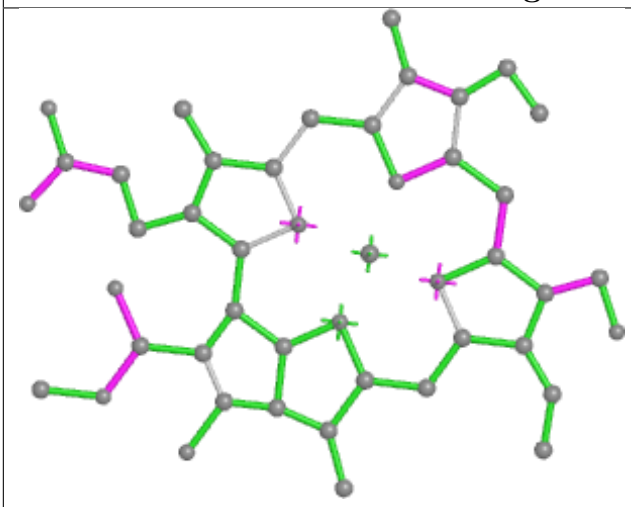
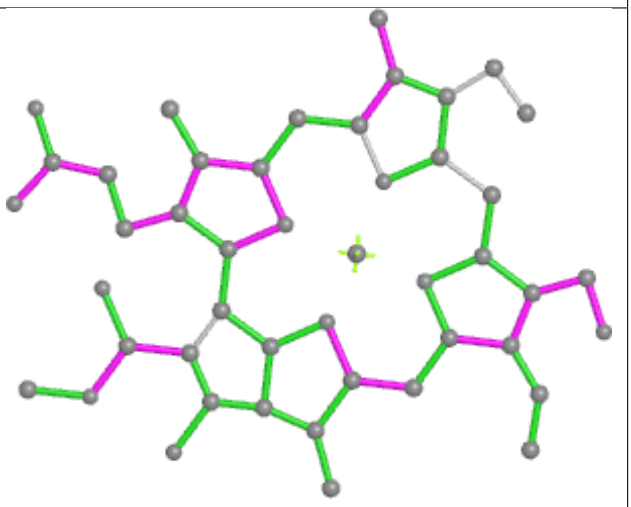
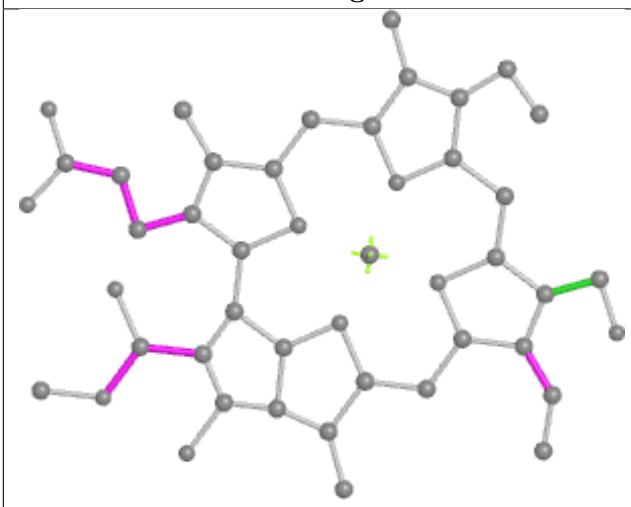


Bond lengths



Bond angles



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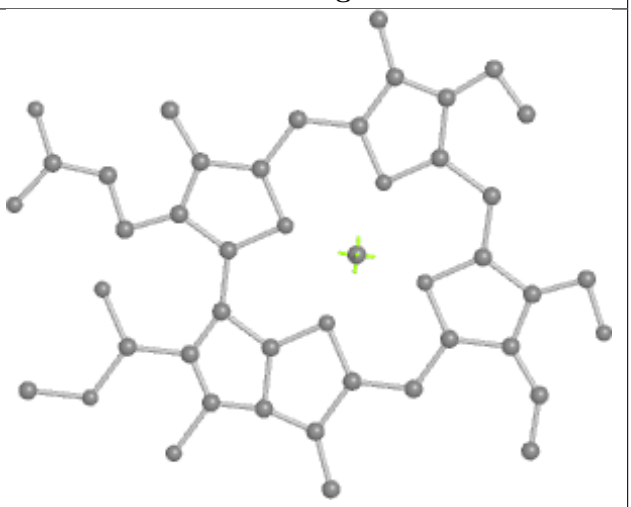
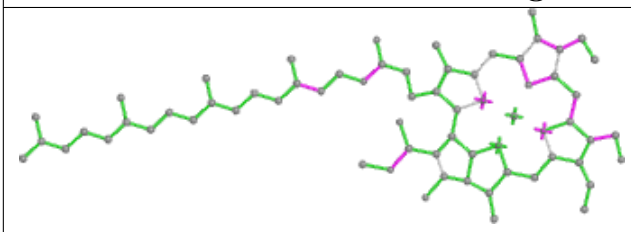


Rings

Ligand CHL y 309



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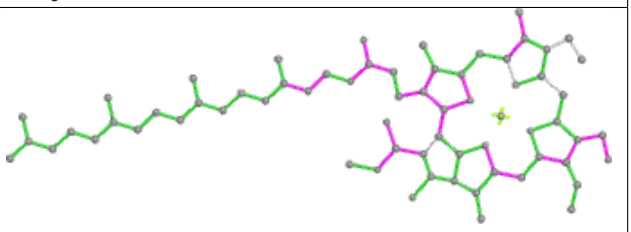
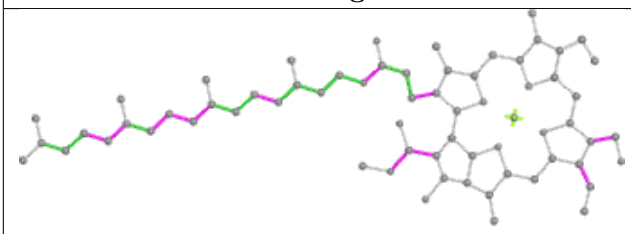


Bond angles



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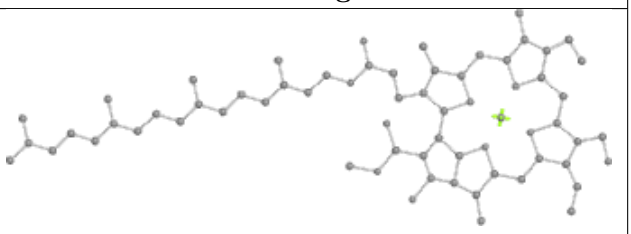
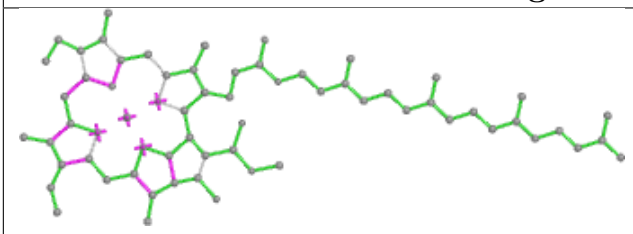


Rings

Ligand CLA a 402



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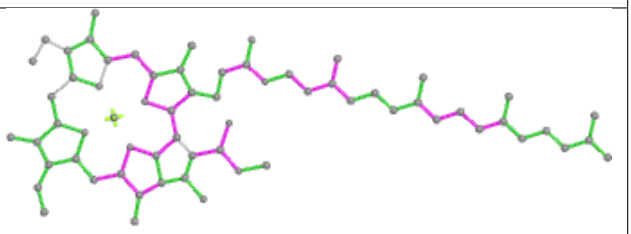

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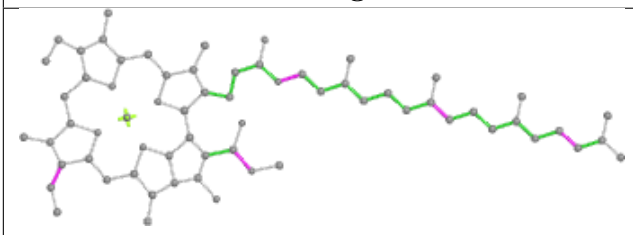

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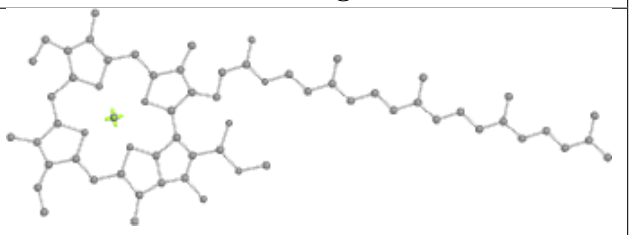
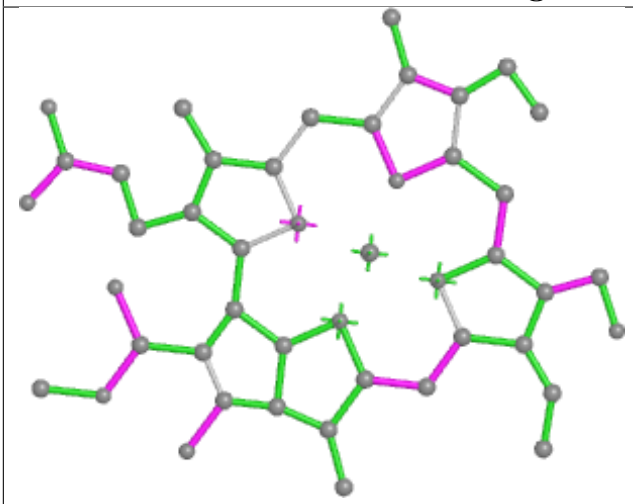


Rings

Ligand CHL 6 603



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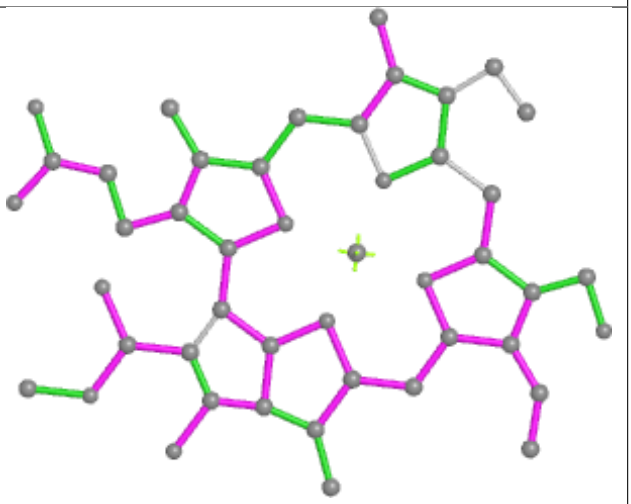

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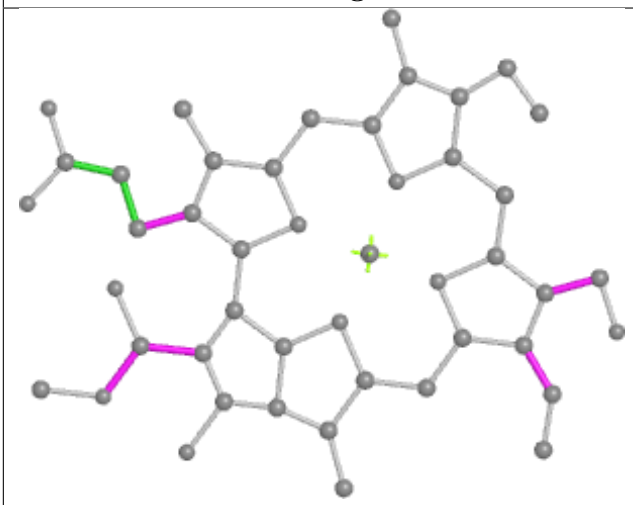

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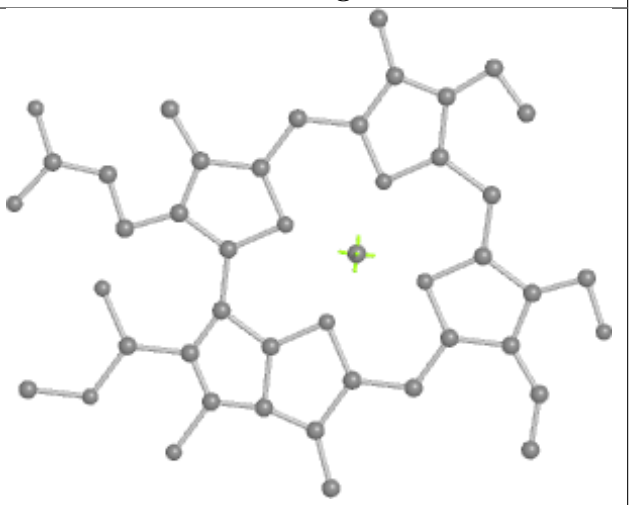
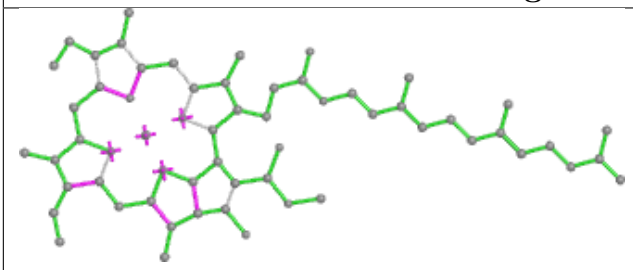


Rings

Ligand CLA C 504



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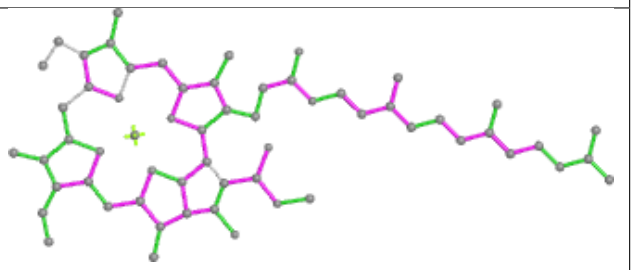

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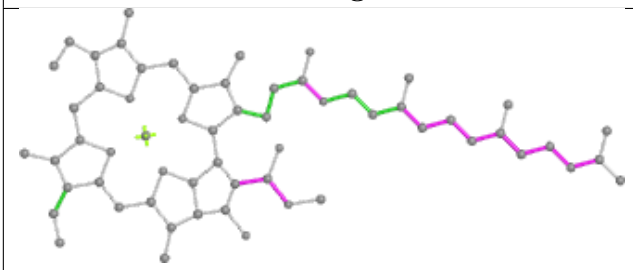

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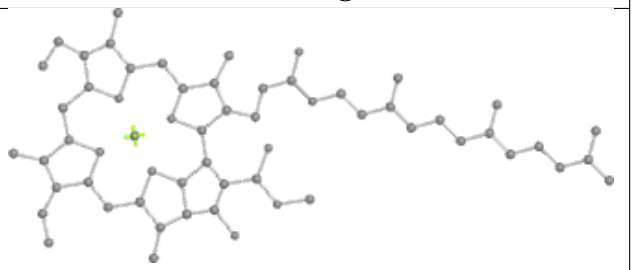
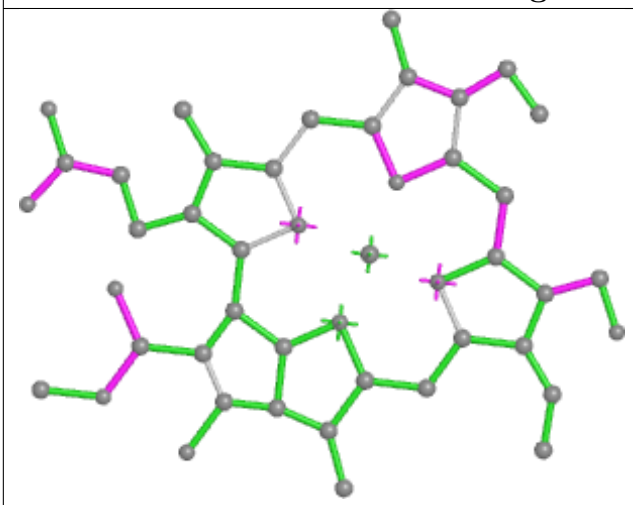


Rings

Ligand CHL s 308



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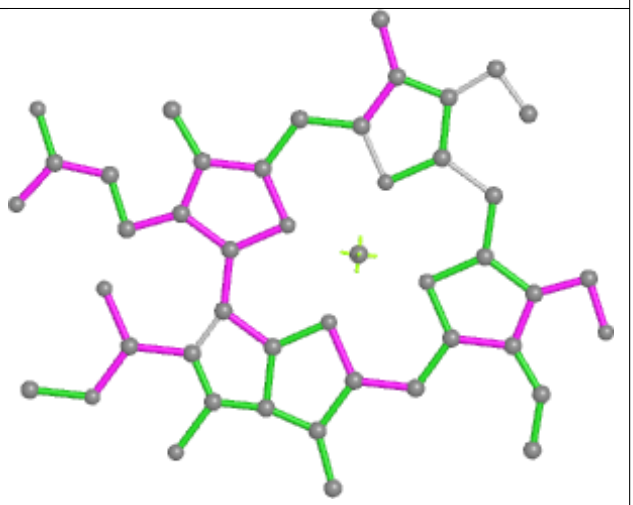
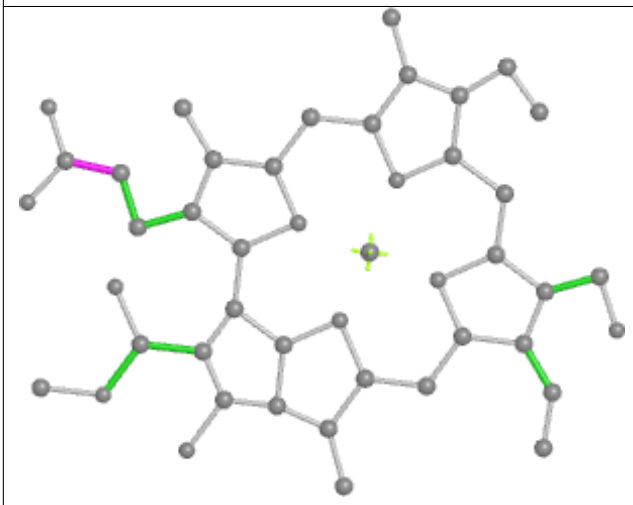


Bond angles



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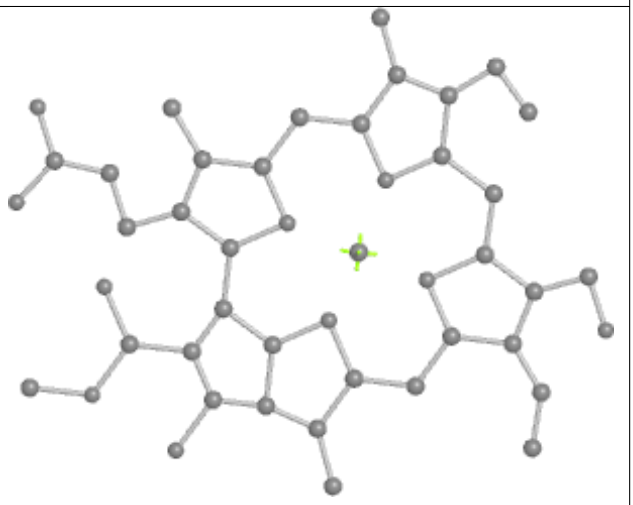
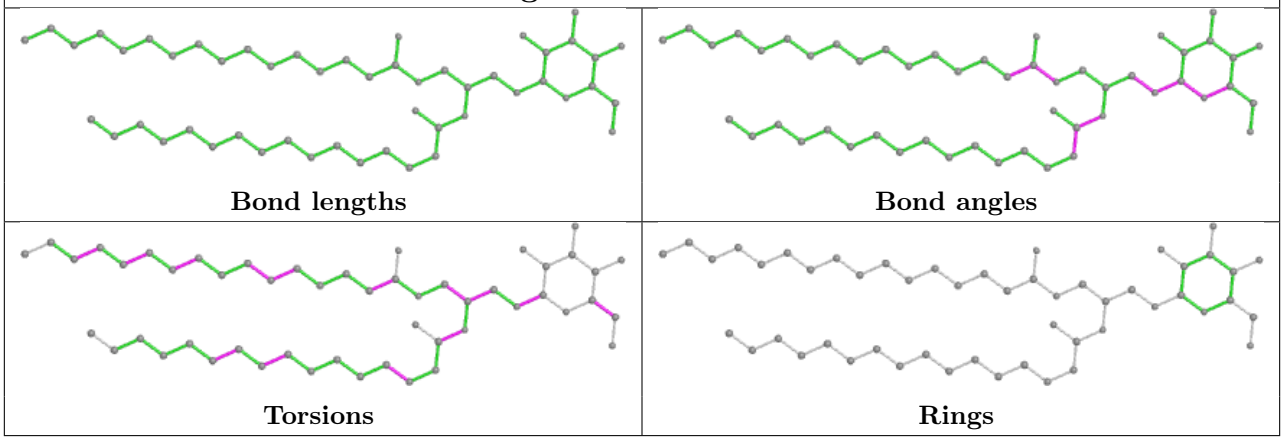
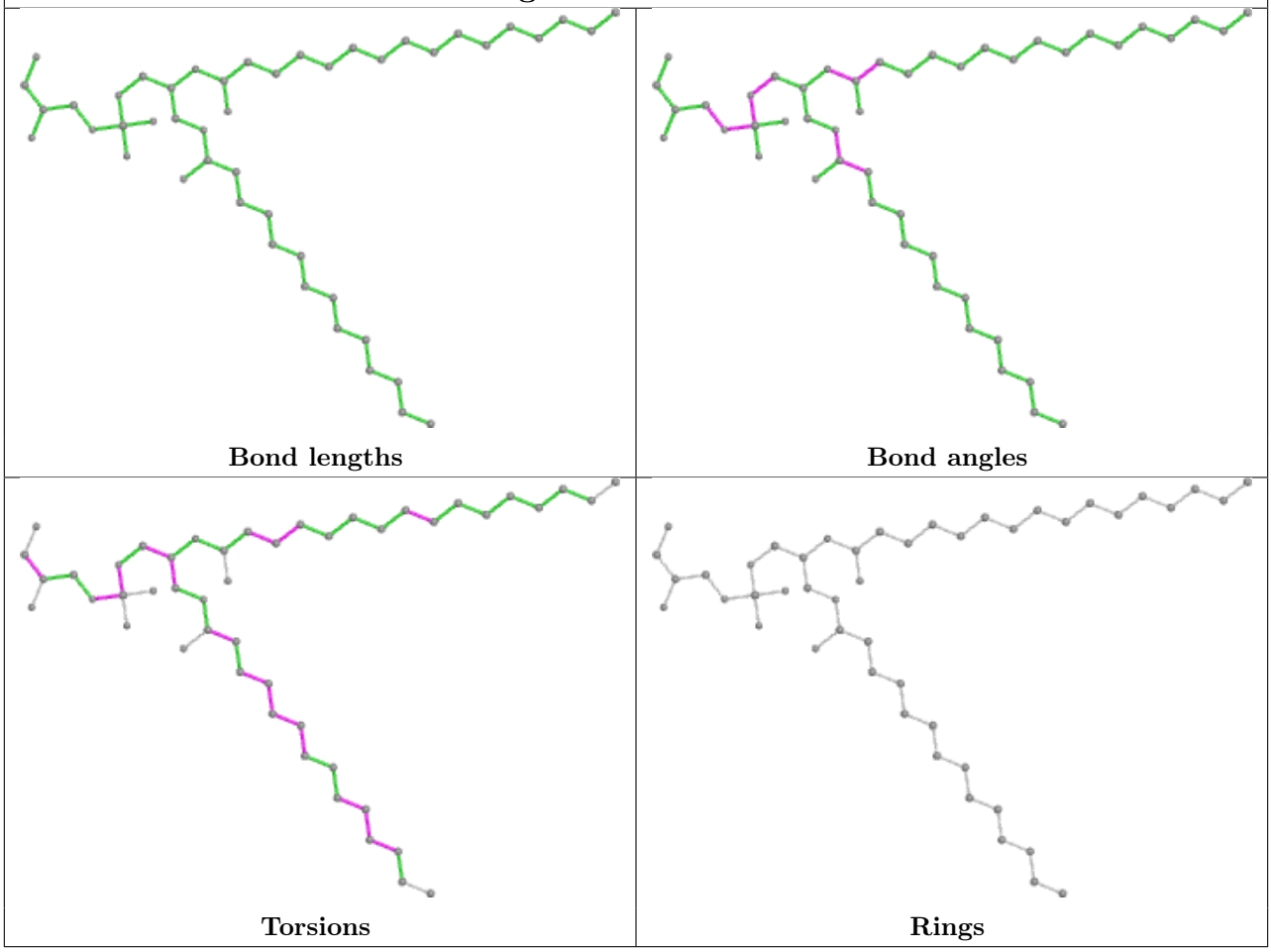


Rings

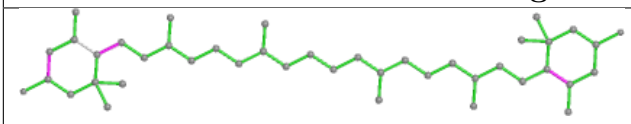
Ligand LMG C 520



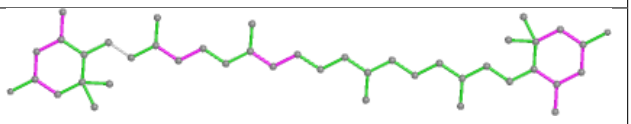
Ligand LHG B 621



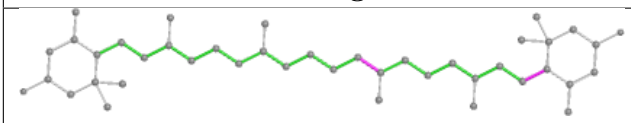
Ligand LUT r 615



Bond lengths



Bond angles



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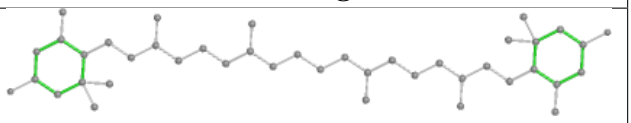
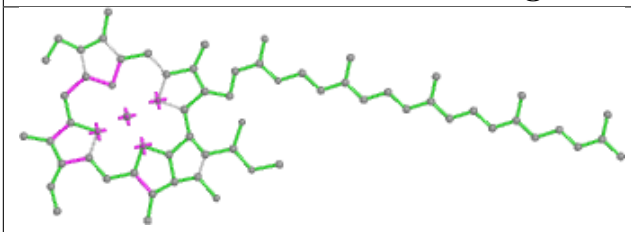
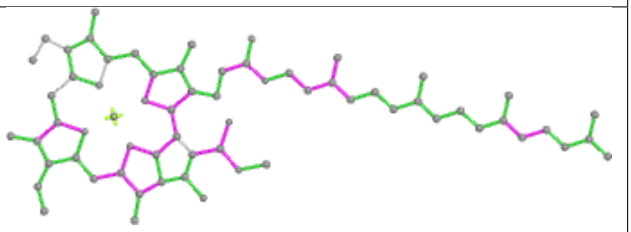


Rings

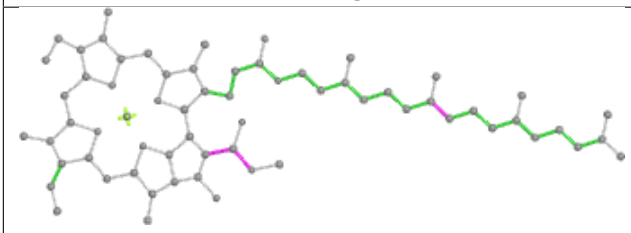
Ligand CLA C 502



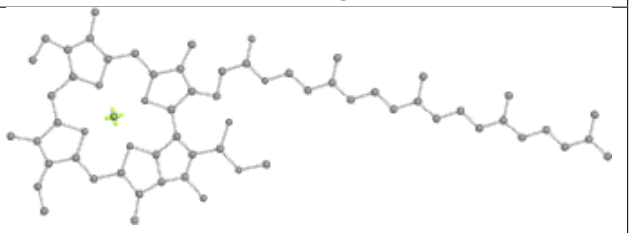
Bond lengths



Bond angles

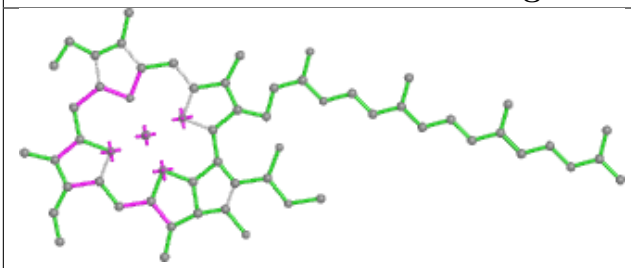


Torsions

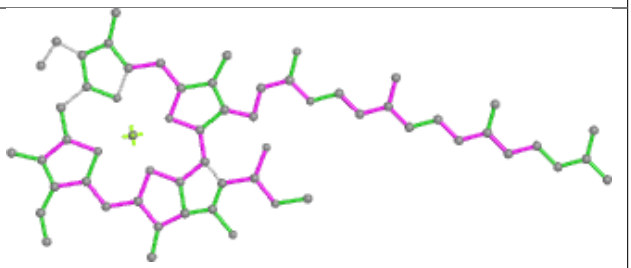


Rings

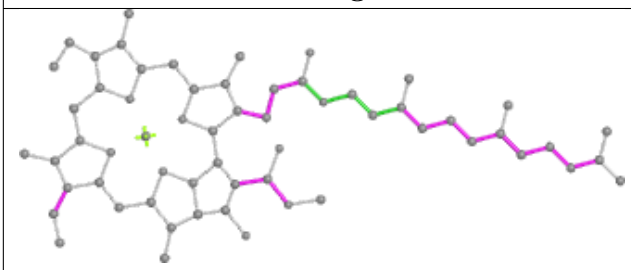
Ligand CLA N 613



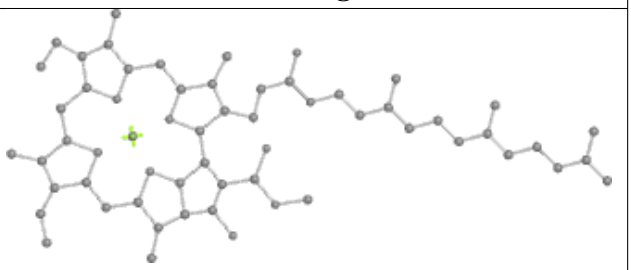
Bond lengths



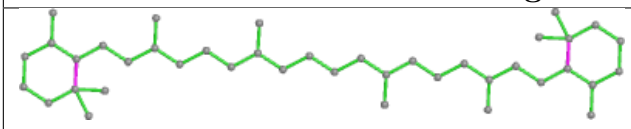
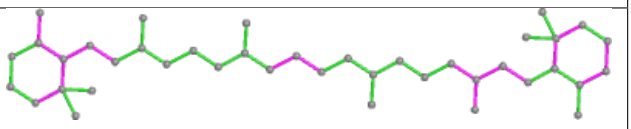
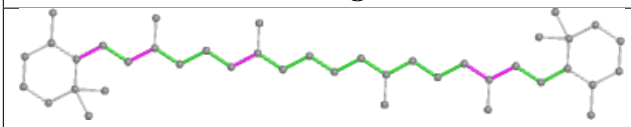
Bond angles

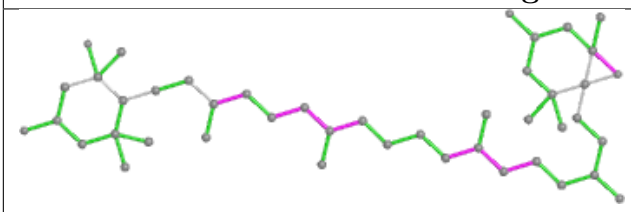
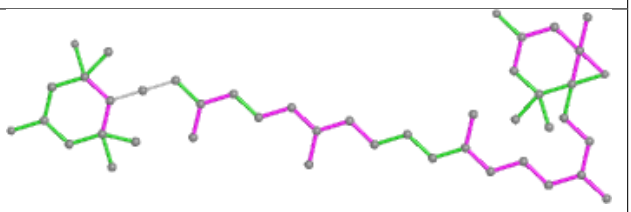
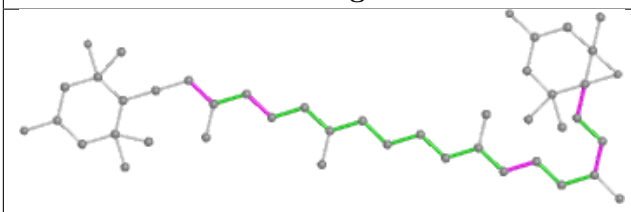


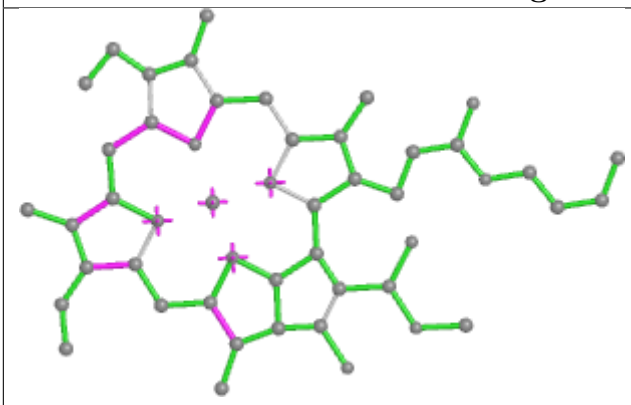
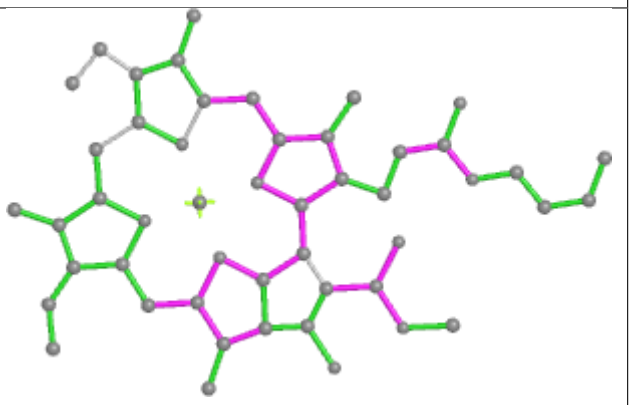
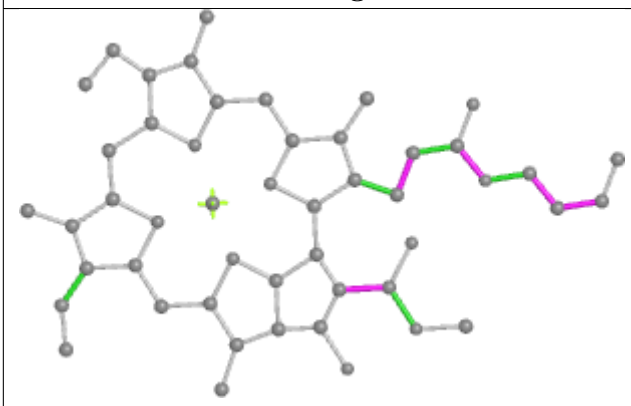
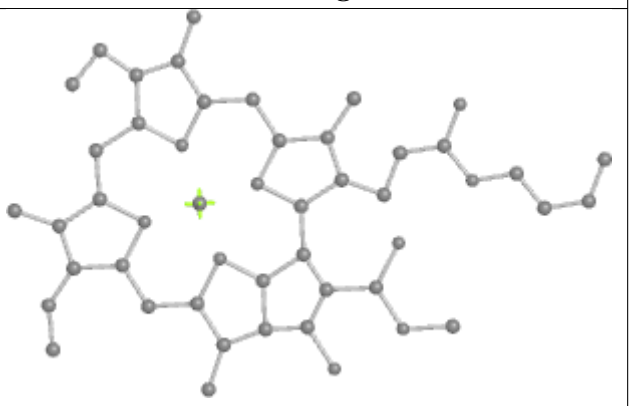
Torsions

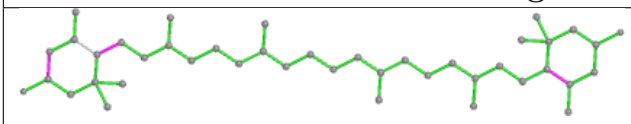
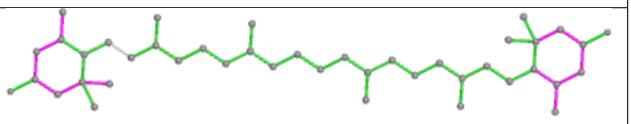
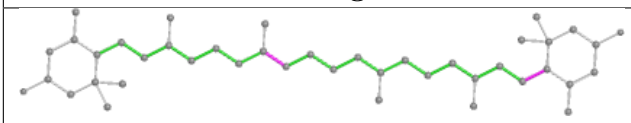
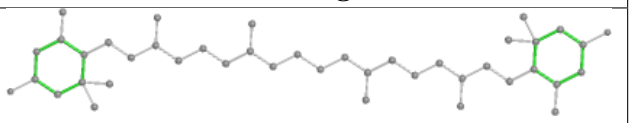


Rings

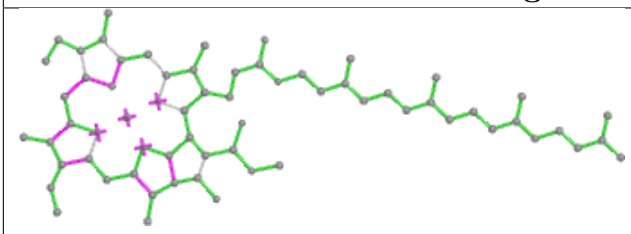
Ligand BCR Z 101	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand NEX Y 318	
 Bond lengths	 Bond angles
 Torsions	Rings

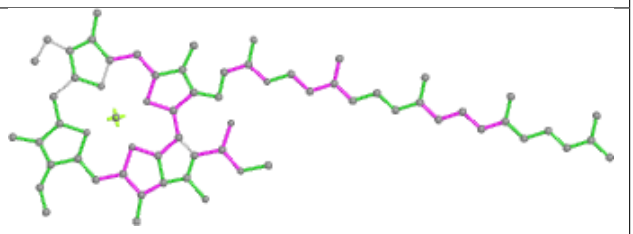
Ligand CLA s 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT S 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

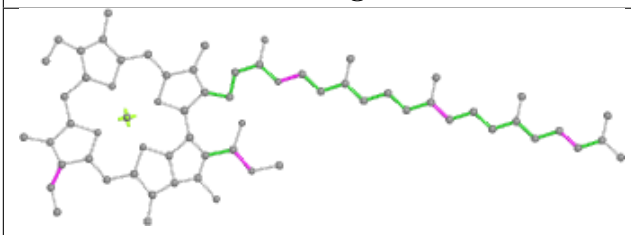
Ligand CLA A 401



Bond lengths



Bond angles



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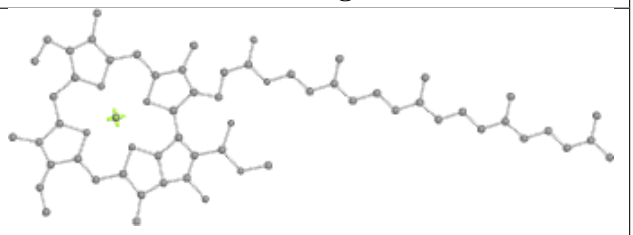
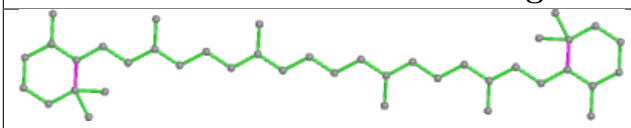


Rings

Ligand BCR k 101



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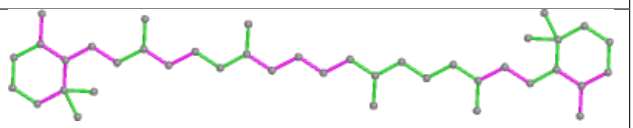
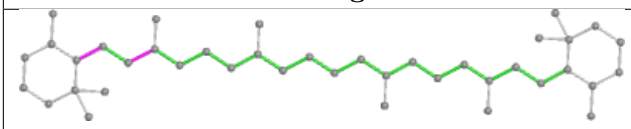


Bond angles



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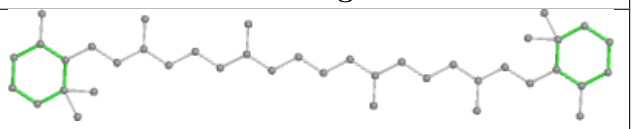
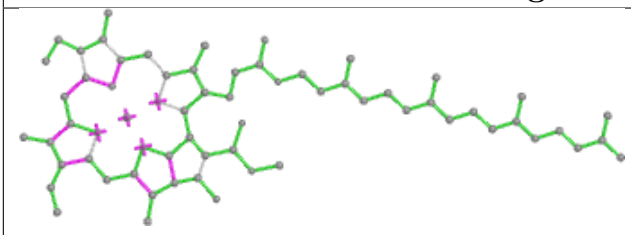


Rings

Ligand CLA y 304



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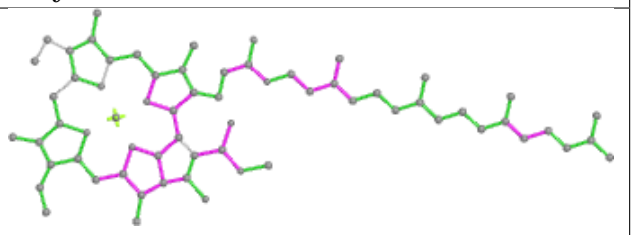
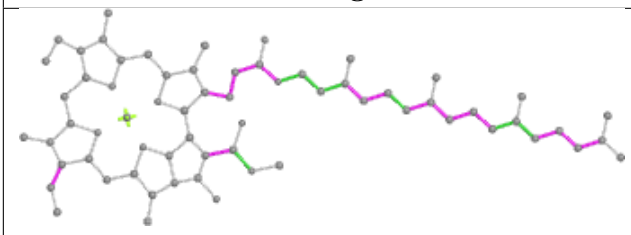


Bond angles



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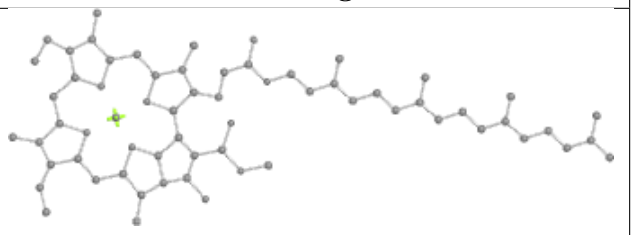
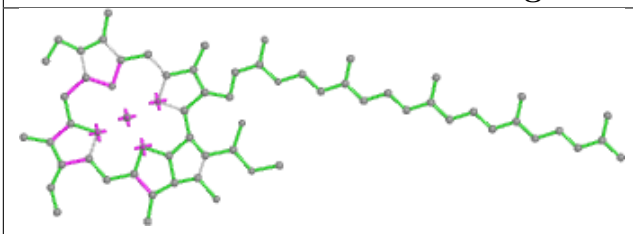
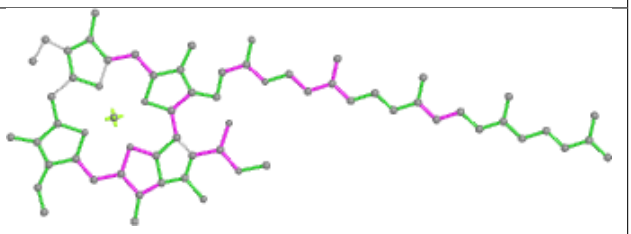


Rings

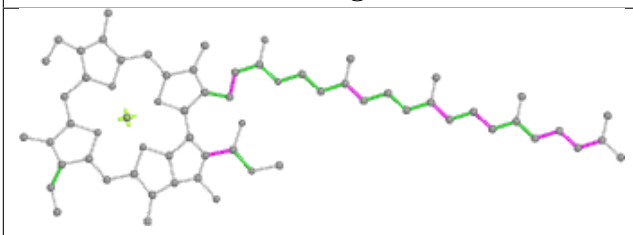
Ligand CLA B 606



Bond lengths



Bond angles



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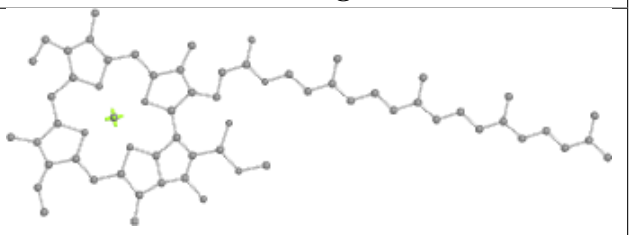
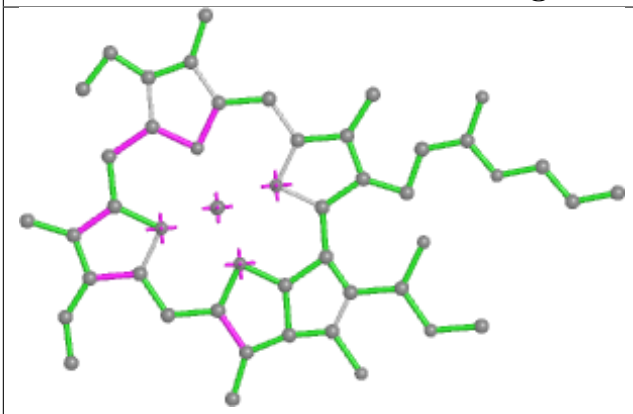
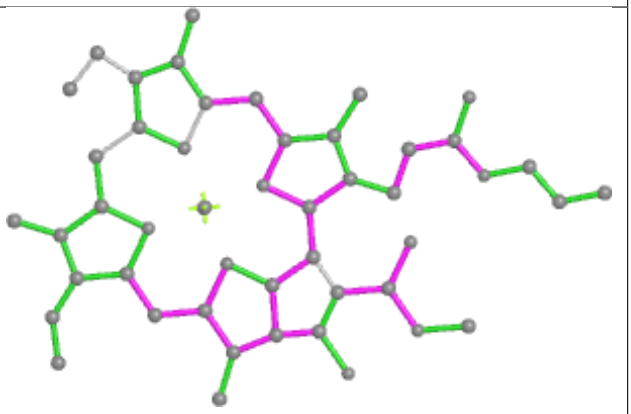


Rings

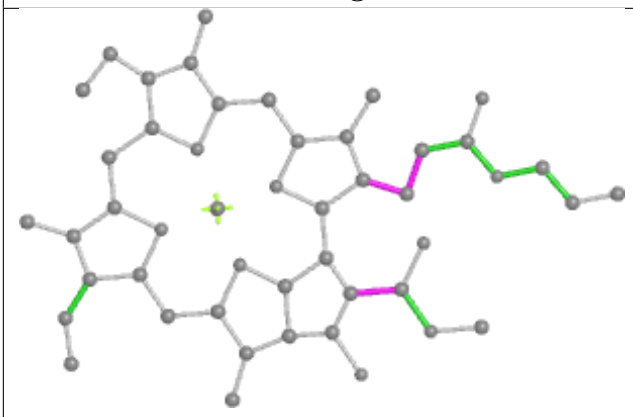
Ligand CLA r 604



Bond lengths



Bond angles



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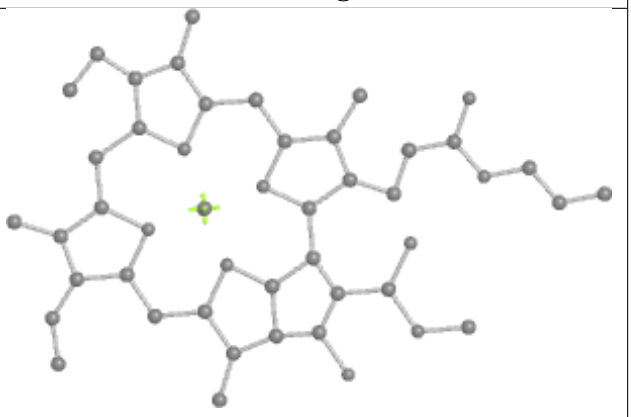
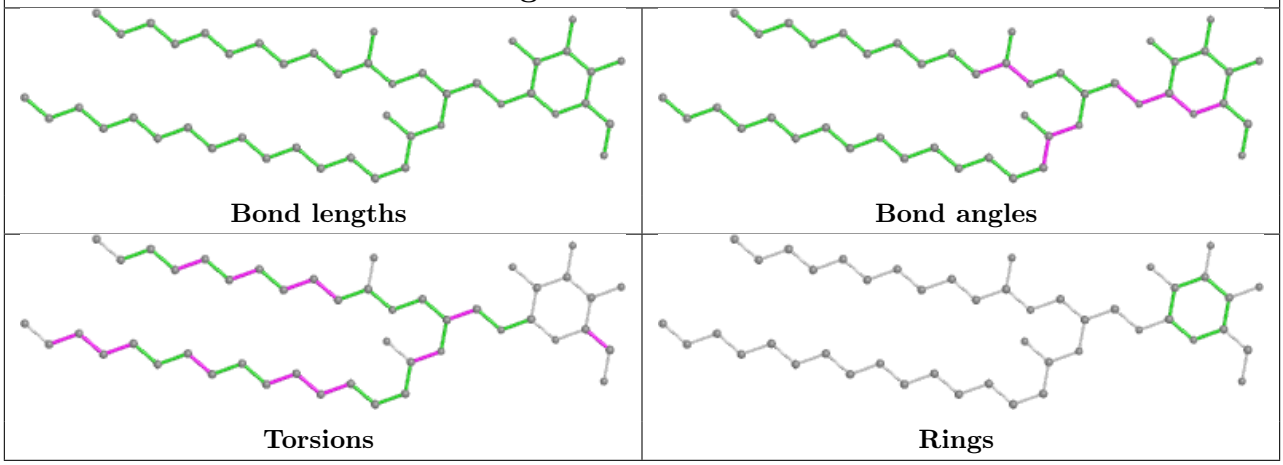
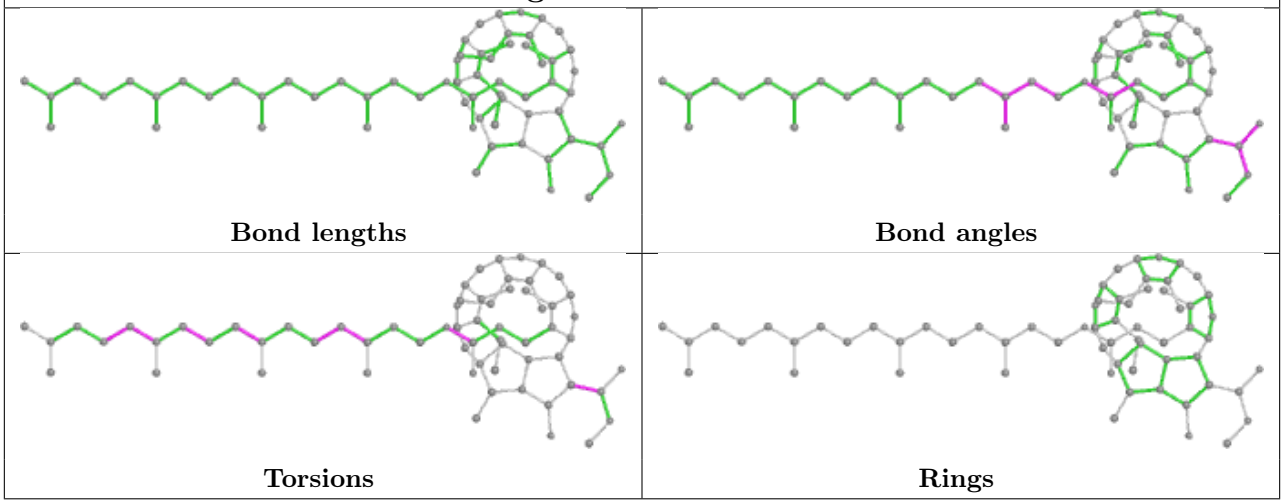


Rings

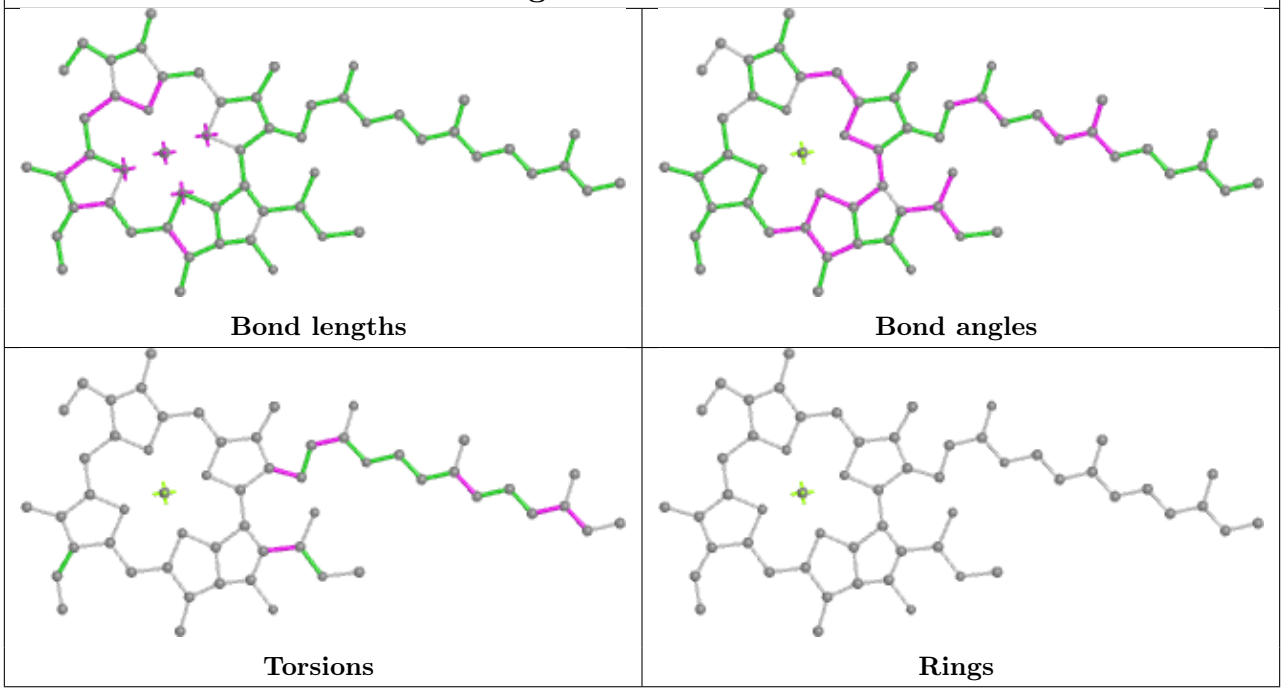
Ligand LMG D 407

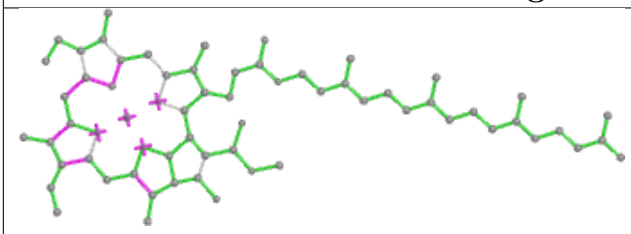
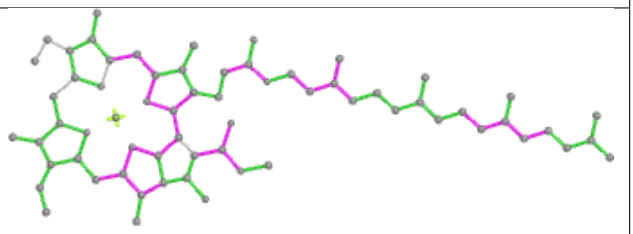
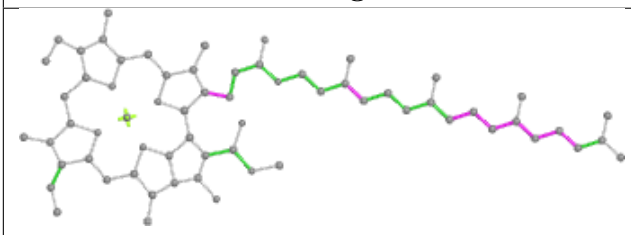
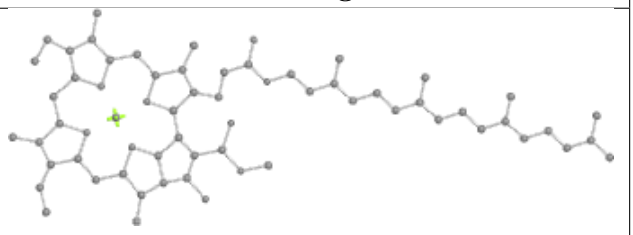


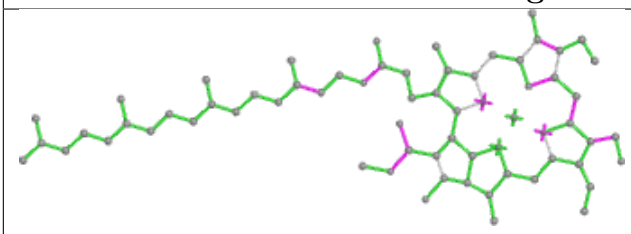
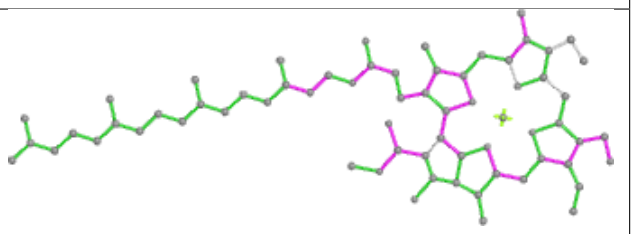
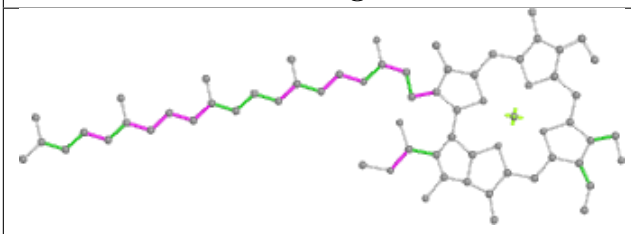
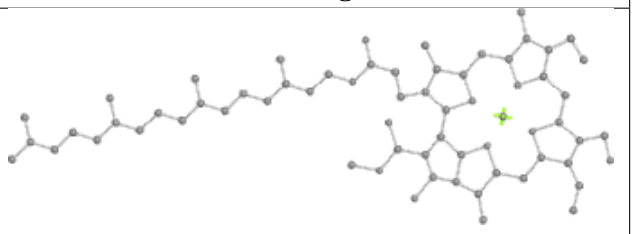
Ligand PHO a 404



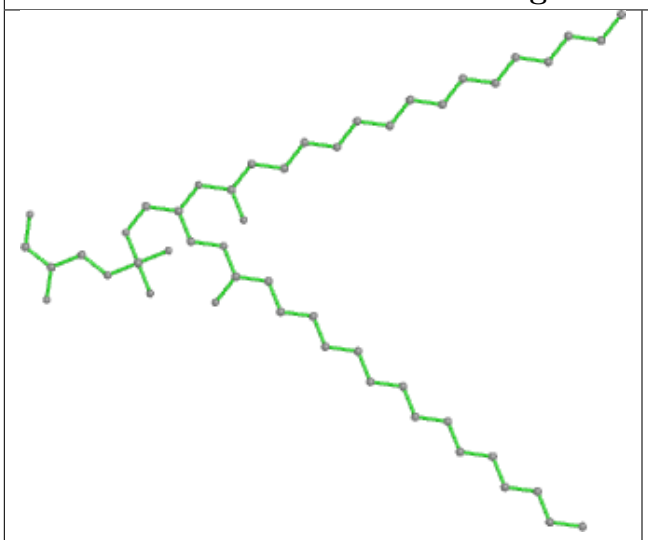
Ligand CLA S 311



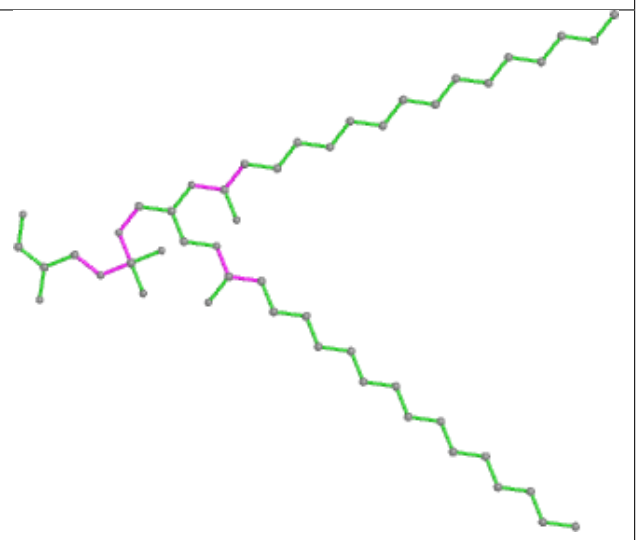
Ligand CLA b 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL n 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

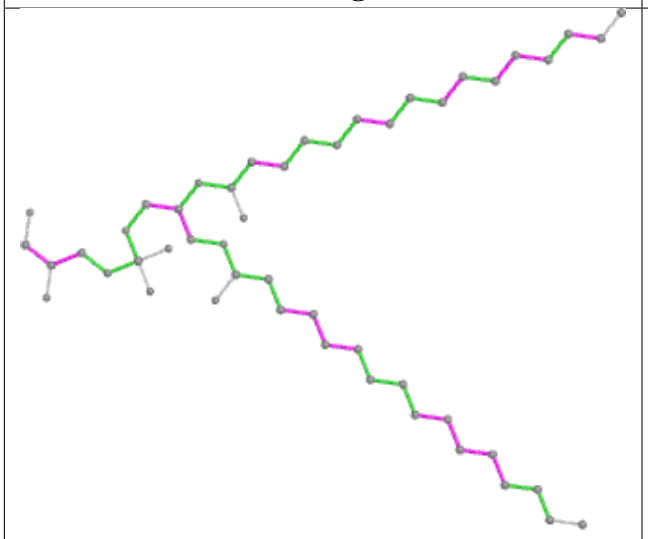
Ligand LHG s 301



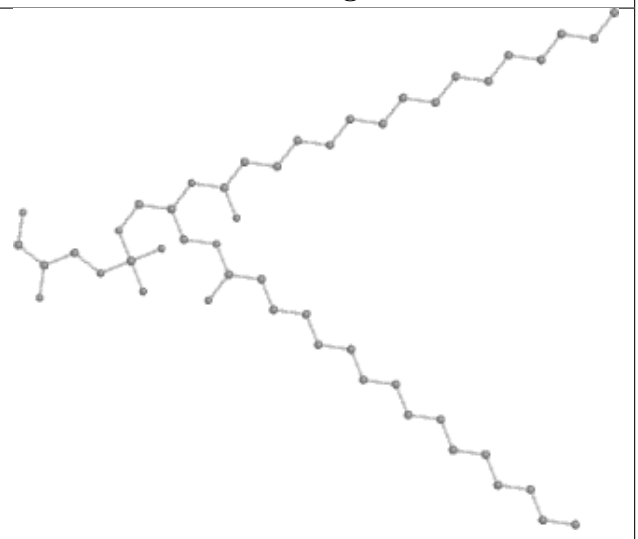
Bond lengths



Bond angles

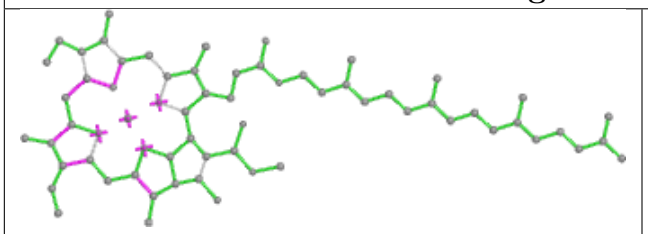


Torsions

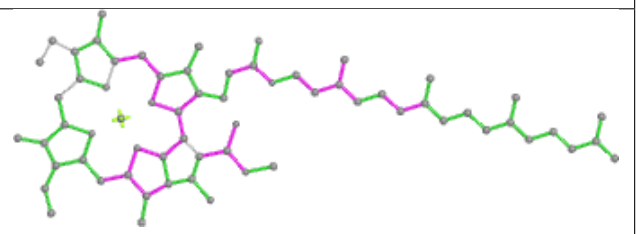


Rings

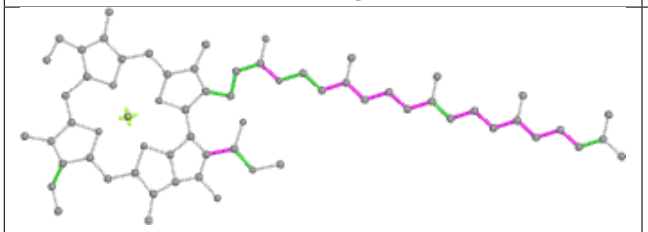
Ligand CLA b 607



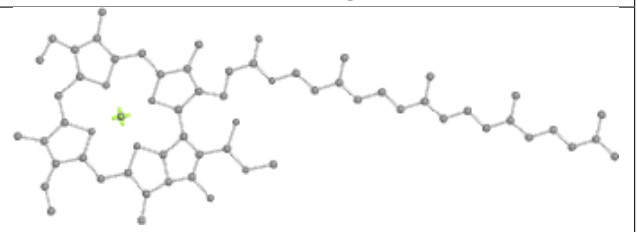
Bond lengths



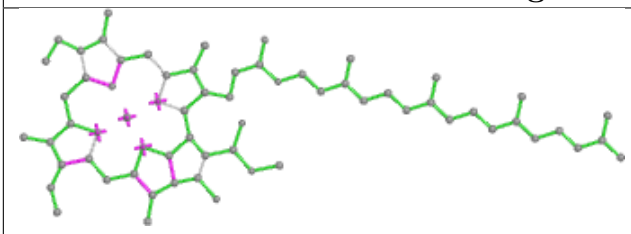
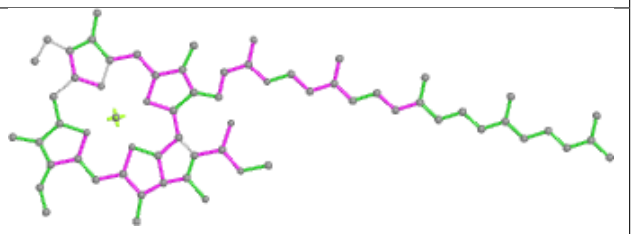
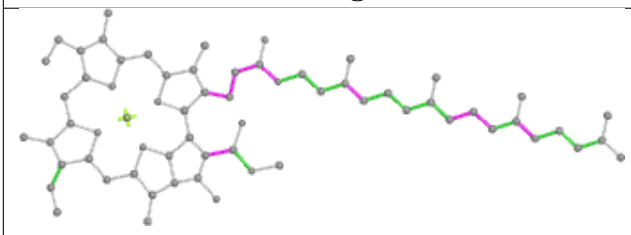
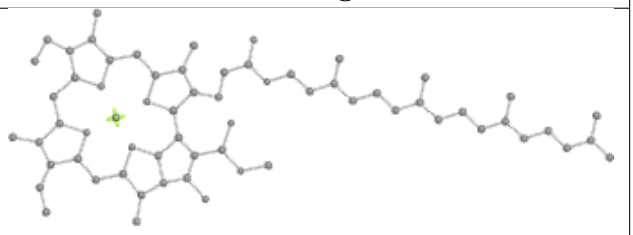
Bond angles

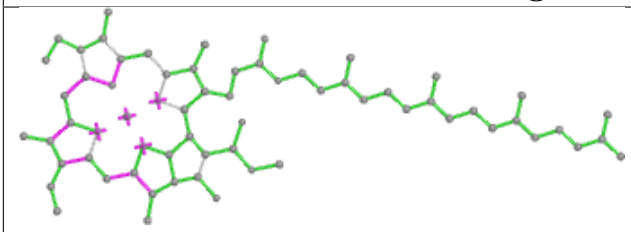
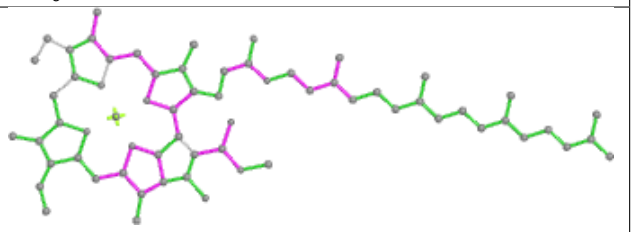
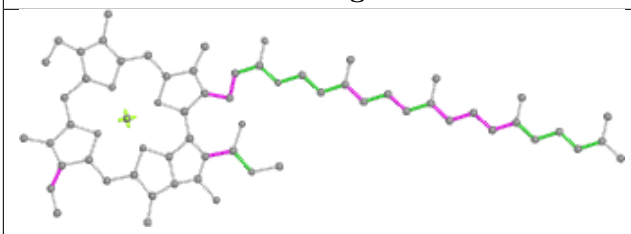
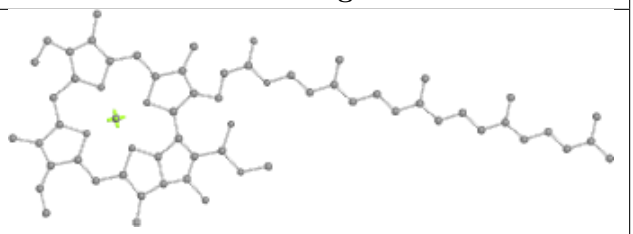


Torsions

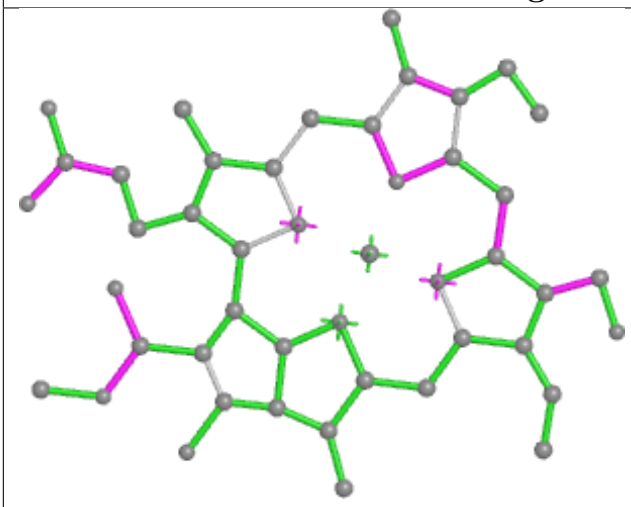


Rings

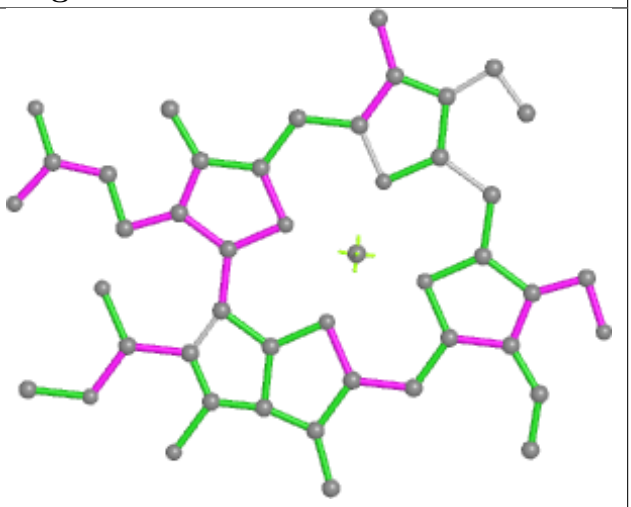
Ligand CLA d 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA y 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

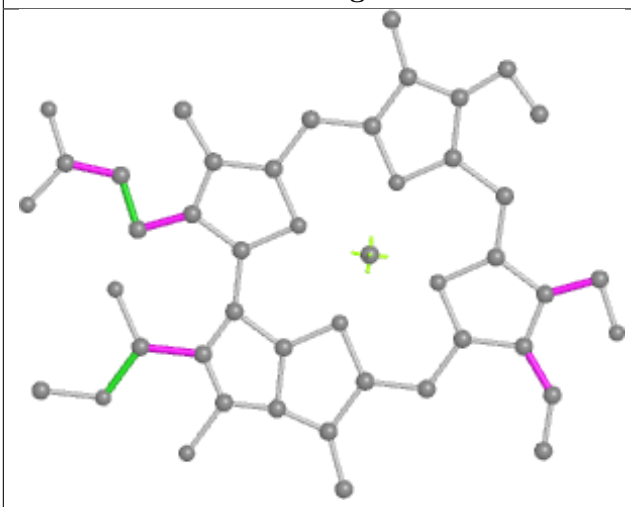
Ligand CHL g 605



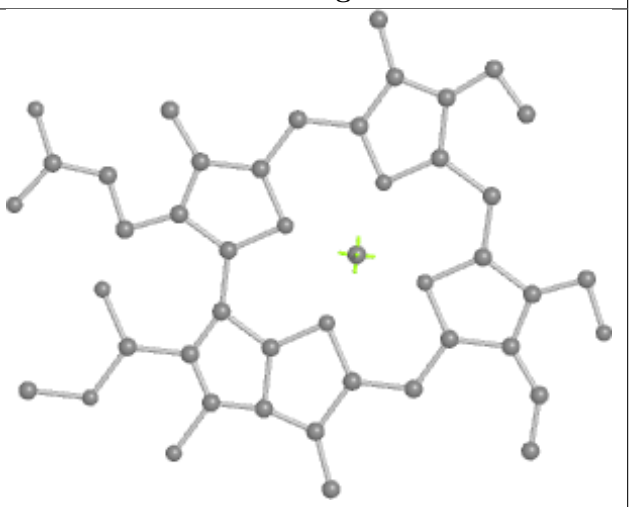
Bond lengths



Bond angles

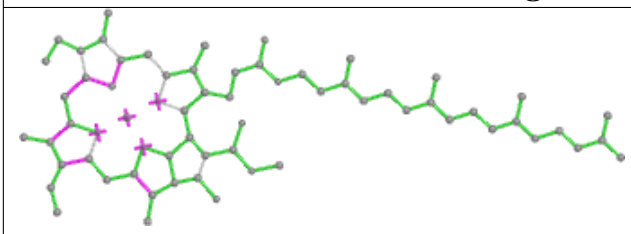


Torsions

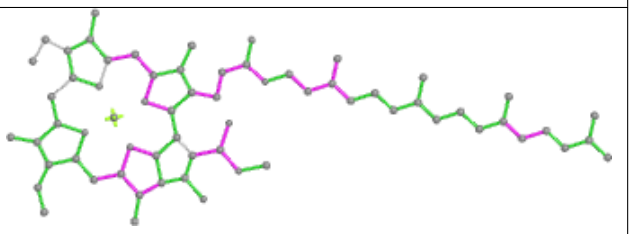


Rings

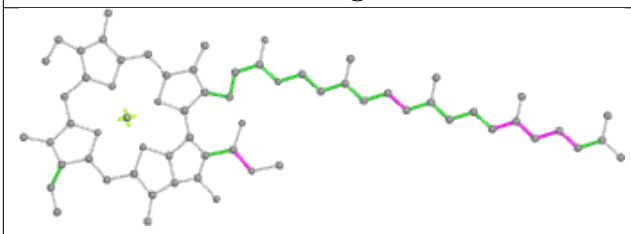
Ligand CLA B 605



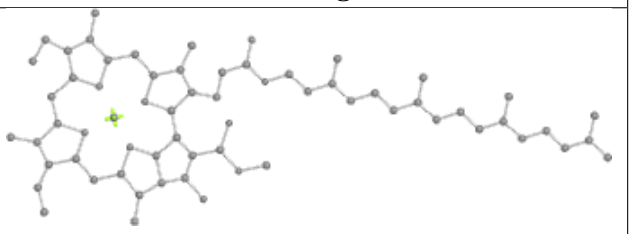
Bond lengths



Bond angles

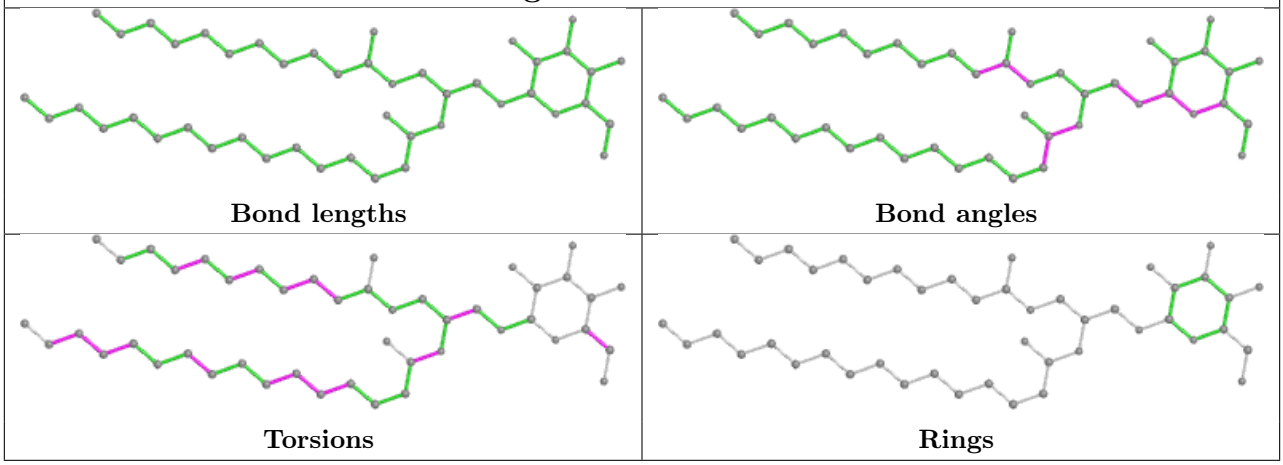


Torsions

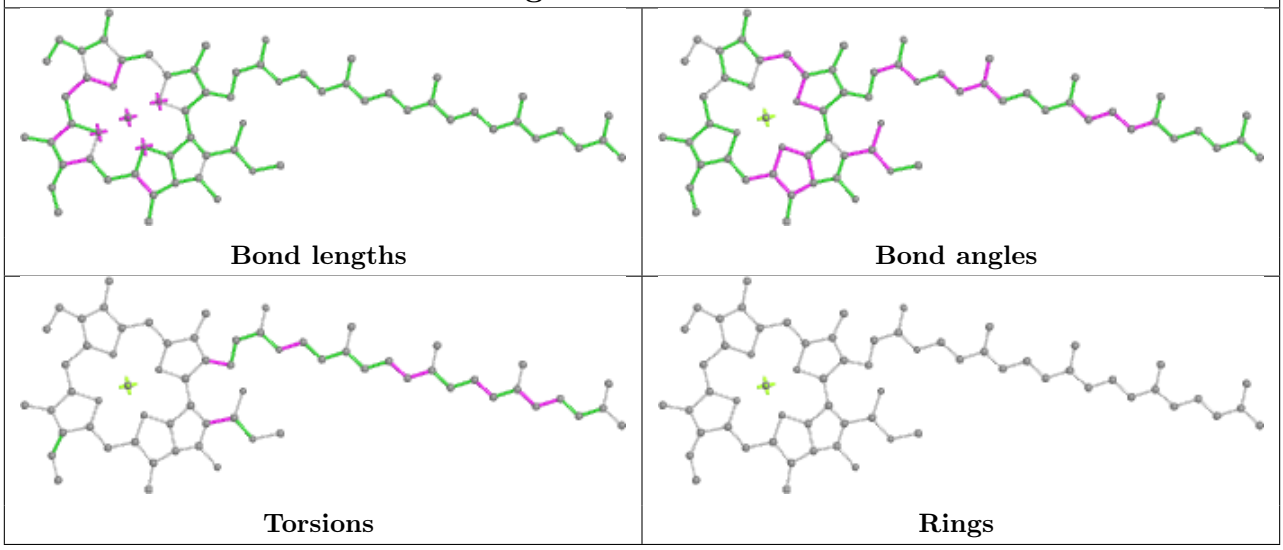


Rings

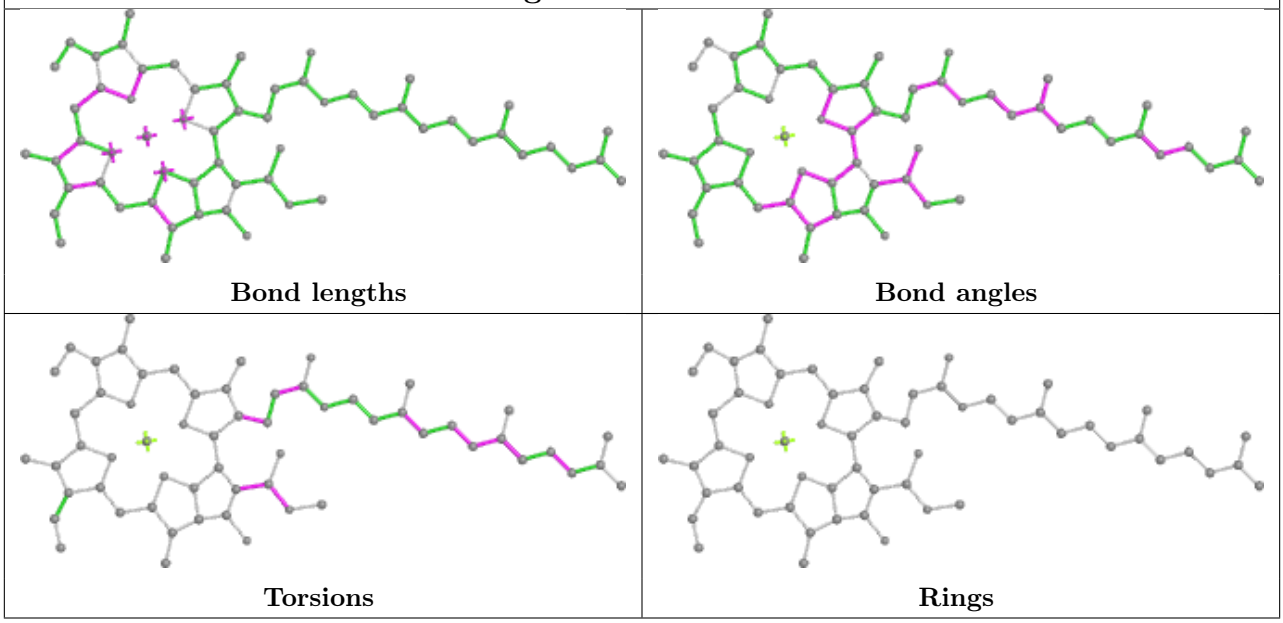
Ligand LMG d 407

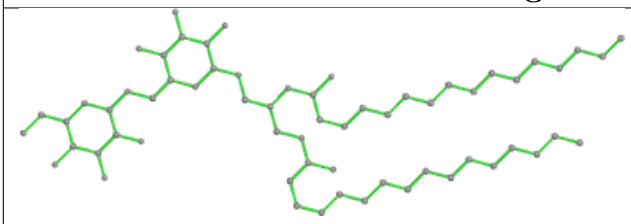
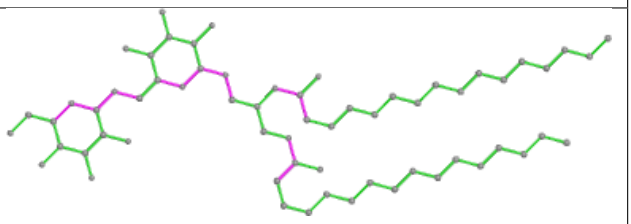
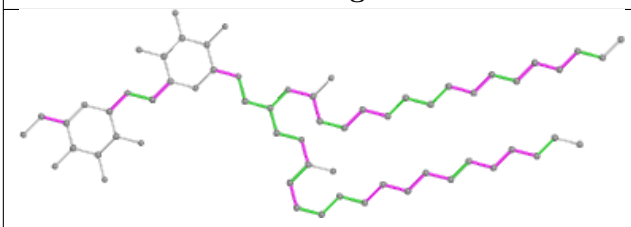
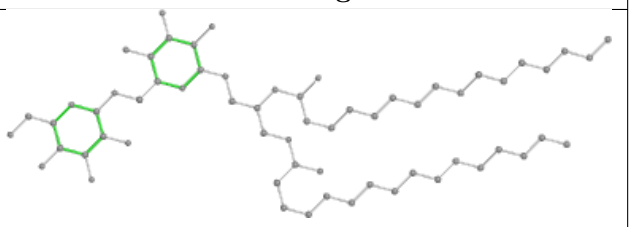


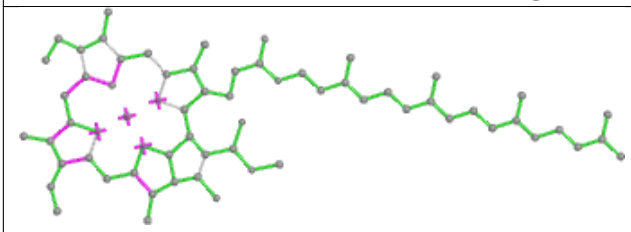
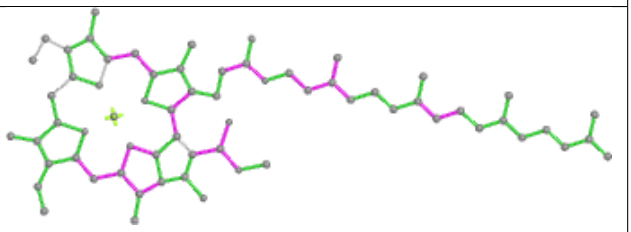
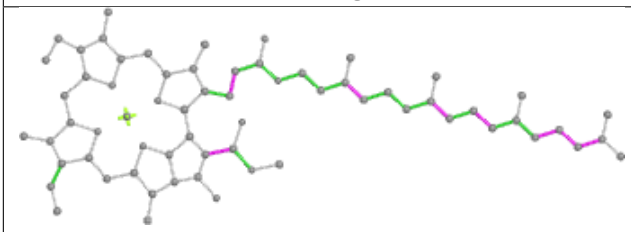
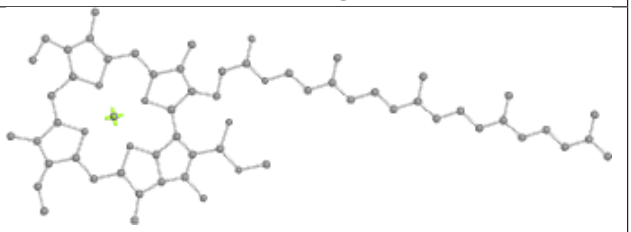
Ligand CLA C 506



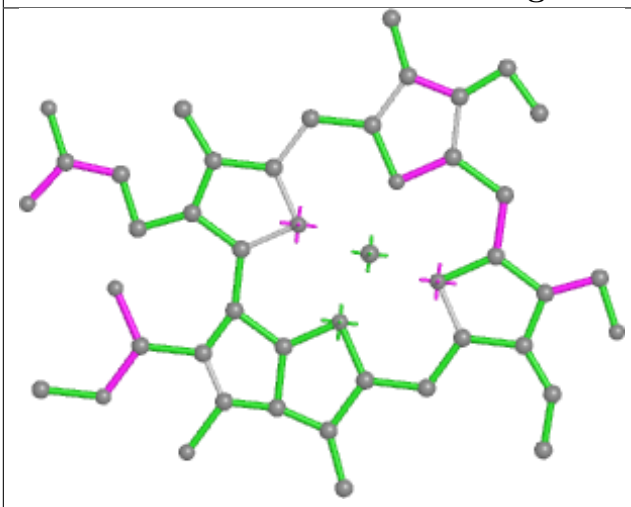
Ligand CLA G 603



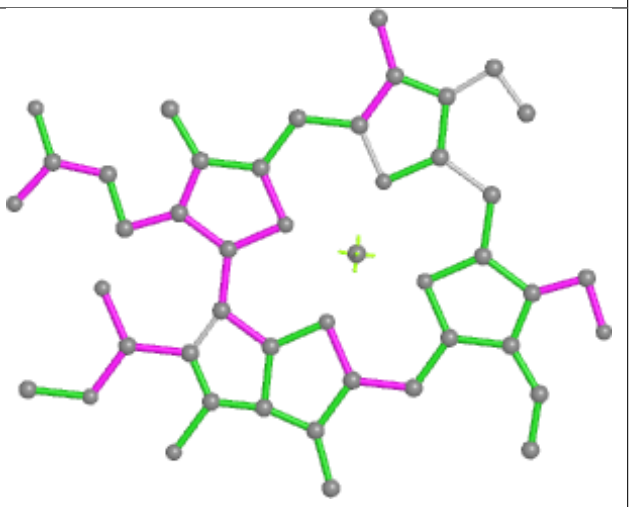
Ligand DGD c 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

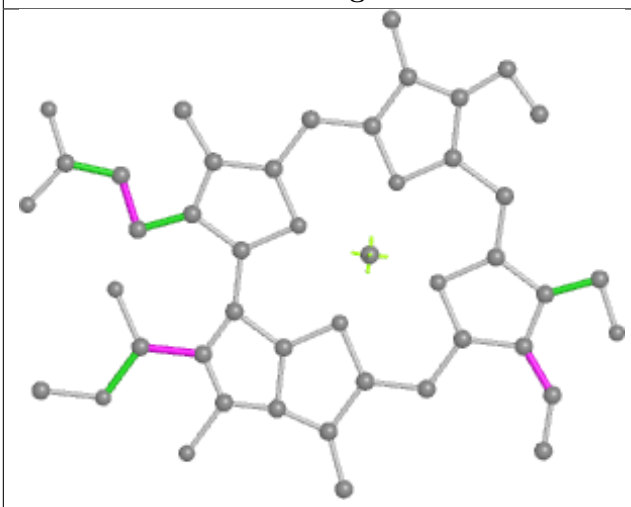
Ligand CHL 5 301



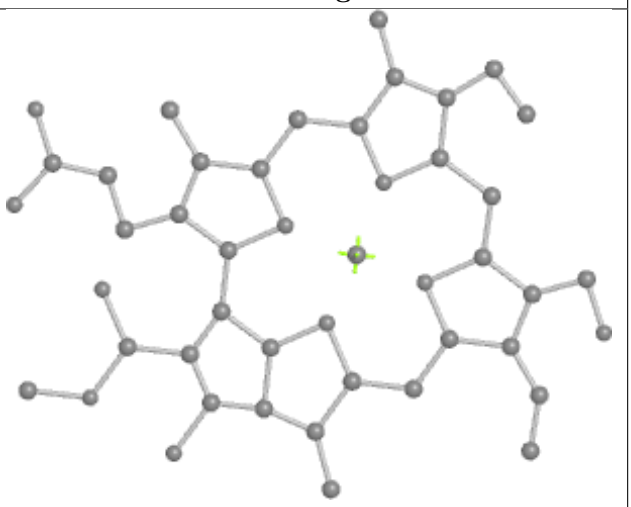
Bond lengths



Bond angles

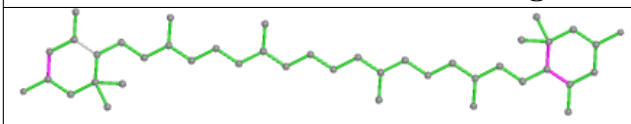


Torsions

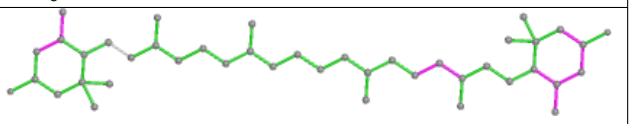


Rings

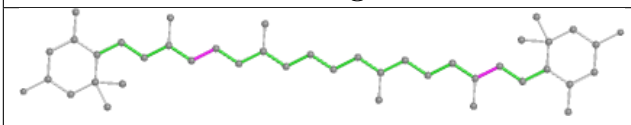
Ligand LUT y 317



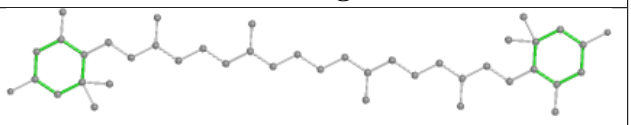
Bond lengths



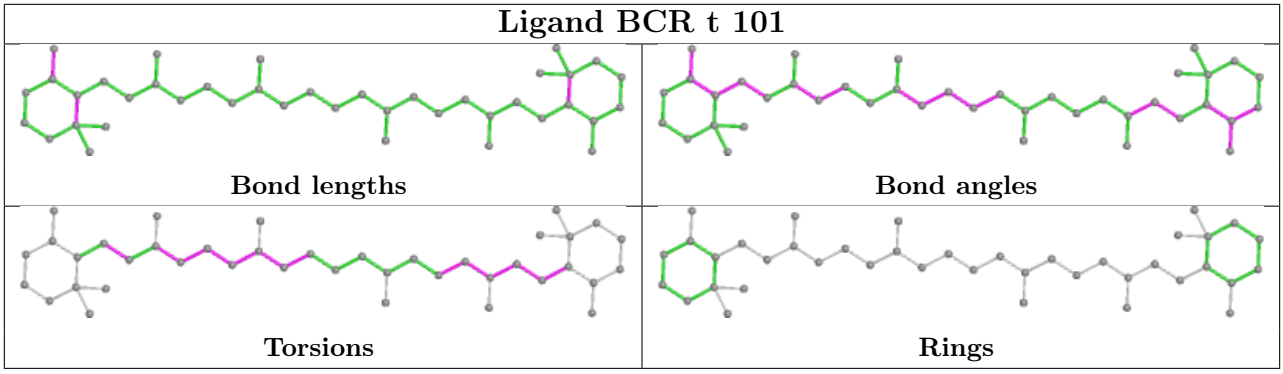
Bond angles

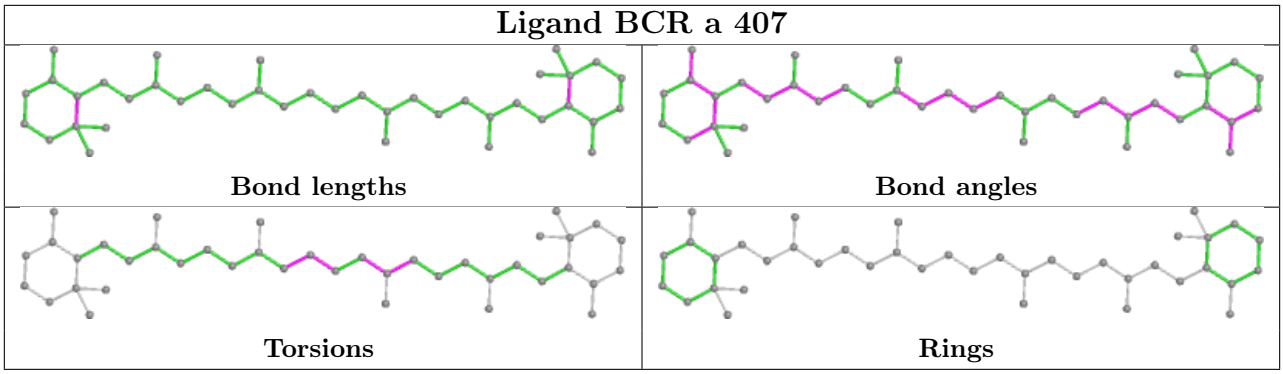


Torsions



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.

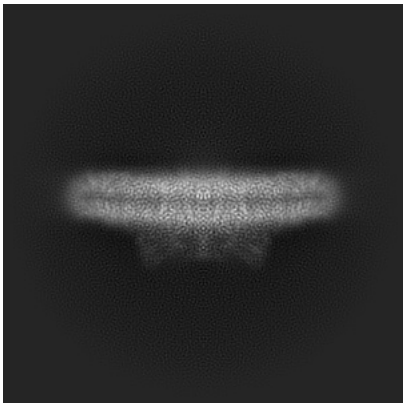
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13078. These allow visual inspection of the internal detail of the map and identification of artifacts.

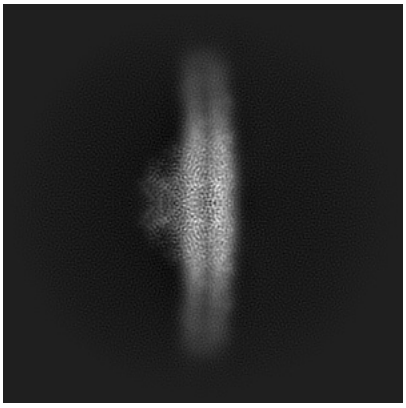
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

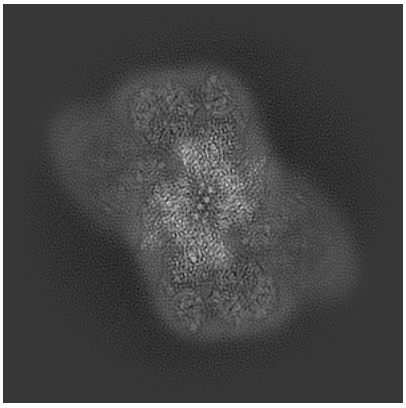
6.1.1 Primary map



X



Y

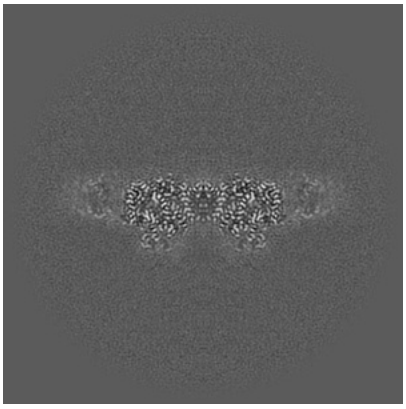


Z

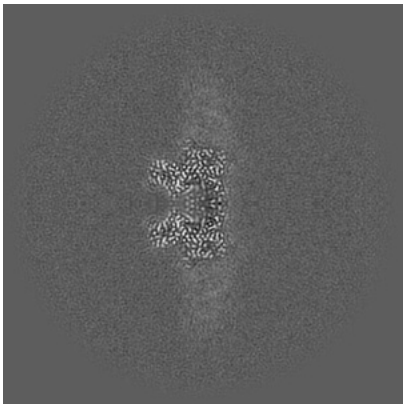
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

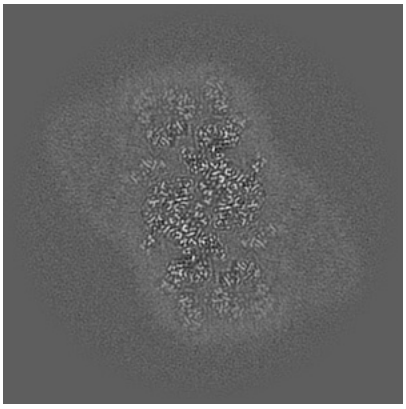
6.2.1 Primary map



X Index: 250



Y Index: 250

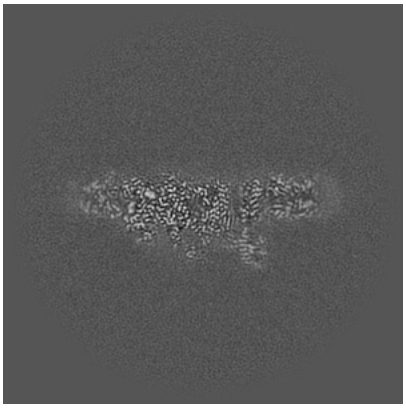


Z Index: 250

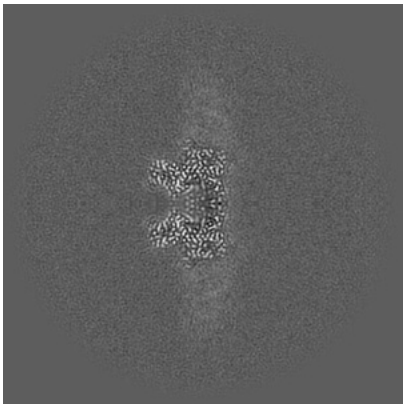
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

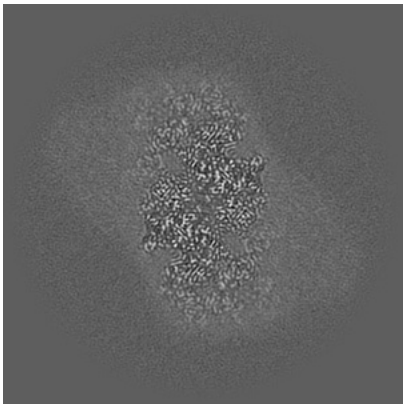
6.3.1 Primary map



X Index: 228



Y Index: 250

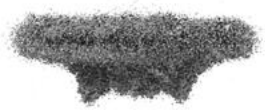


Z Index: 239

The images above show the largest variance slices of the map in three orthogonal directions.

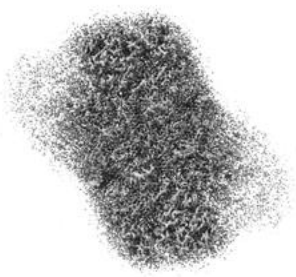
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

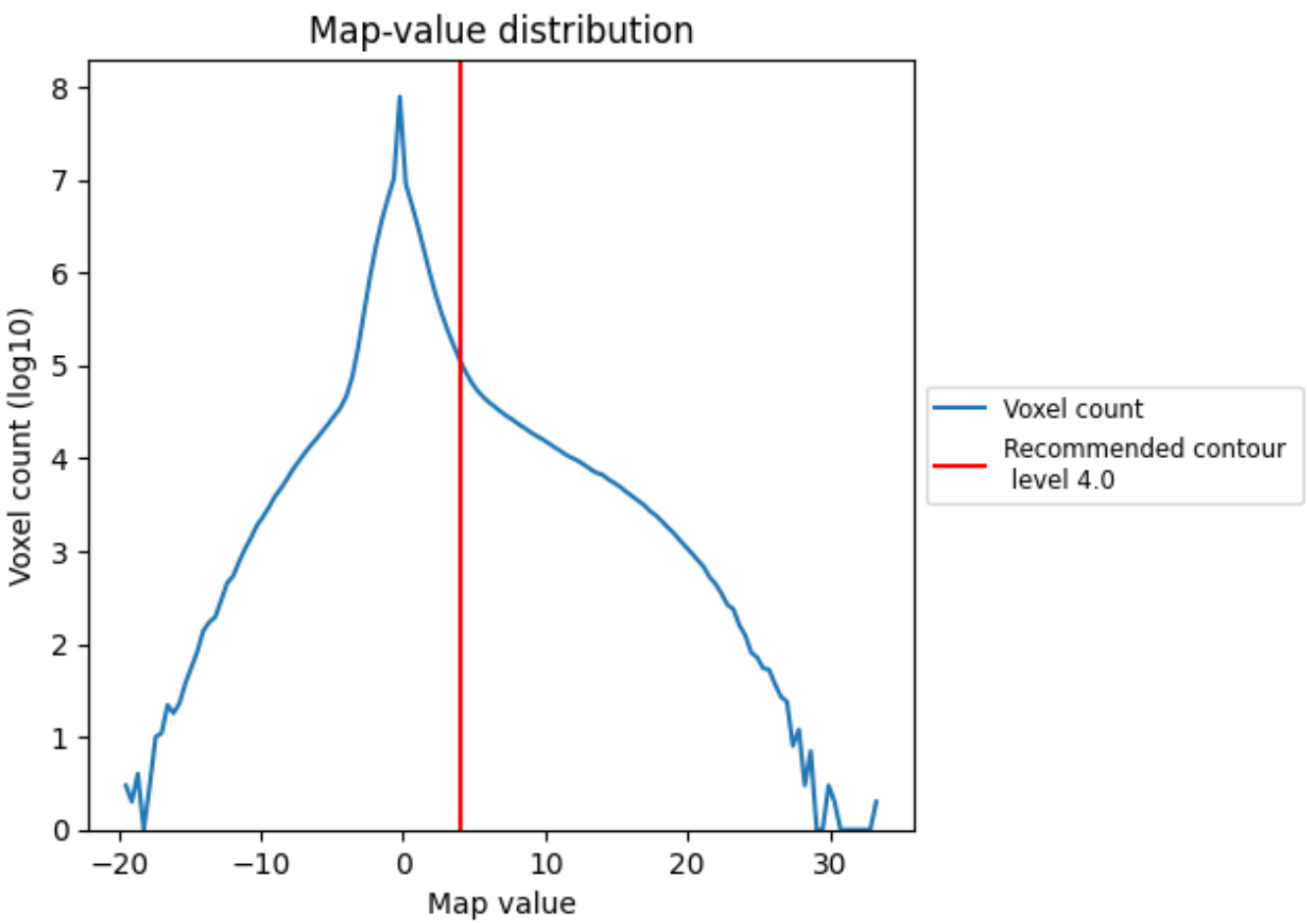
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

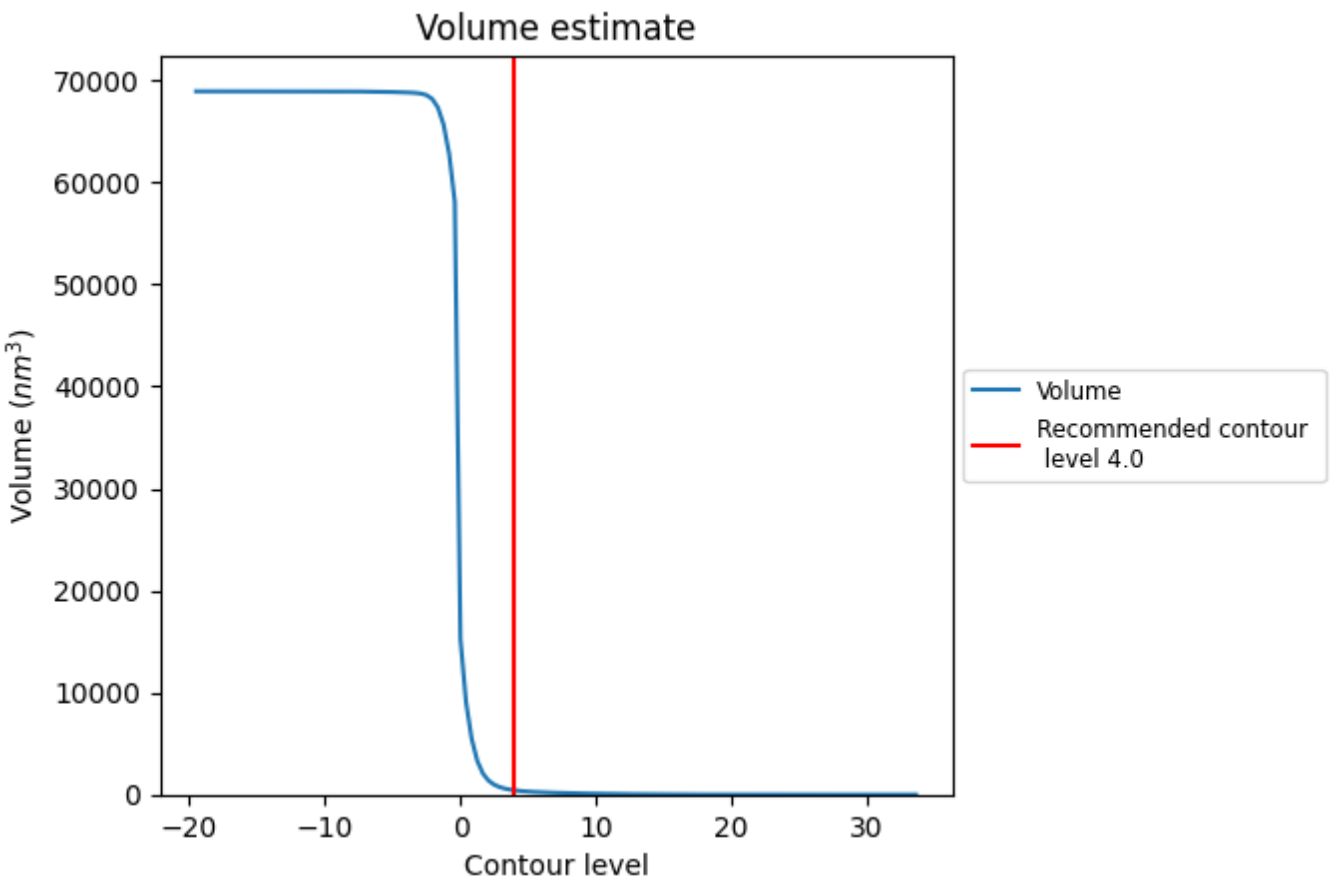
This section contains the results of statistical analysis of the map.

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.

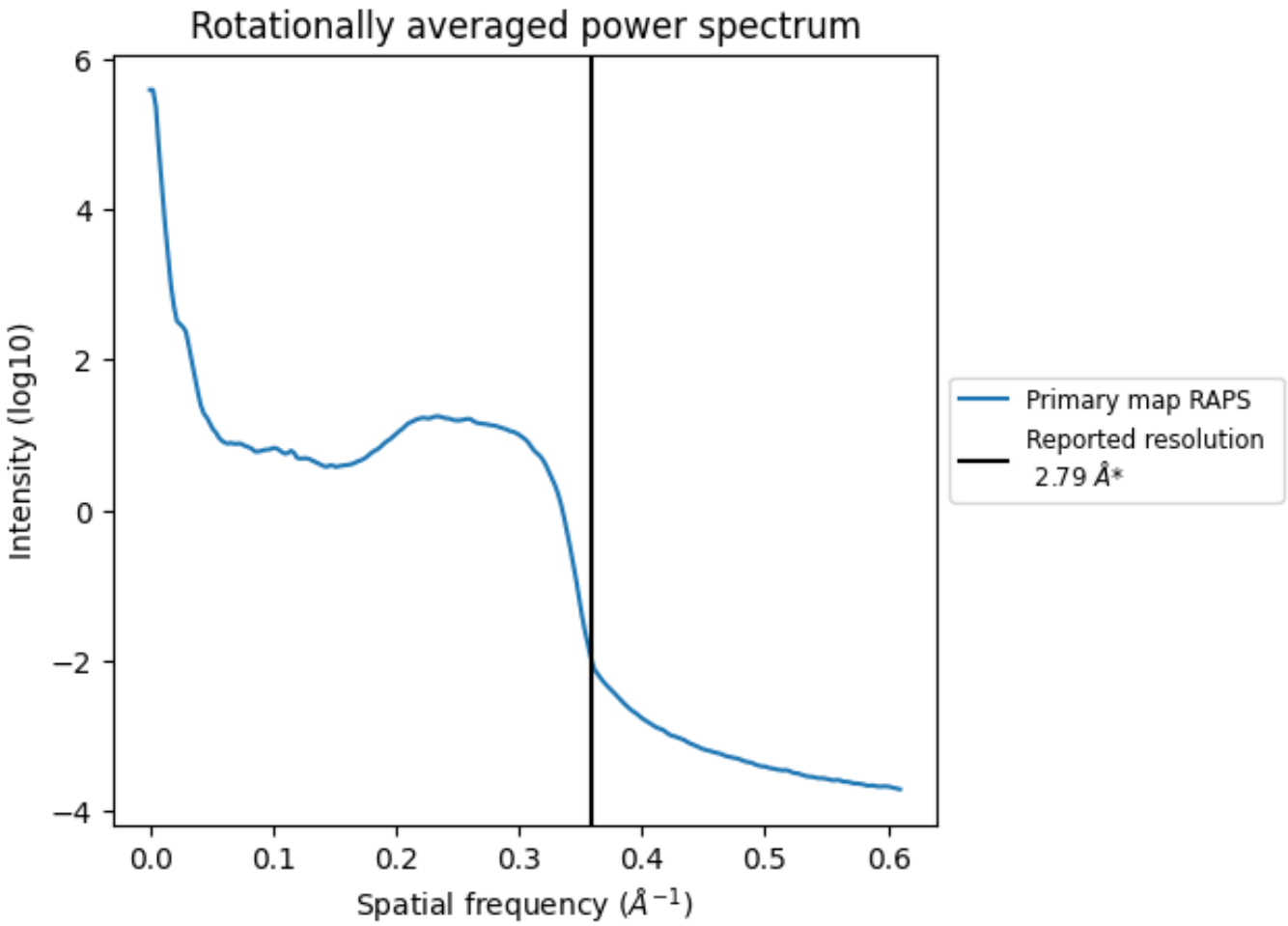
7.2 Volume estimate (i)



The volume at the recommended contour level is 423 nm^3; this corresponds to an approximate mass of 382 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 0.358 Å^{-1}

8 Fourier-Shell correlation (i)

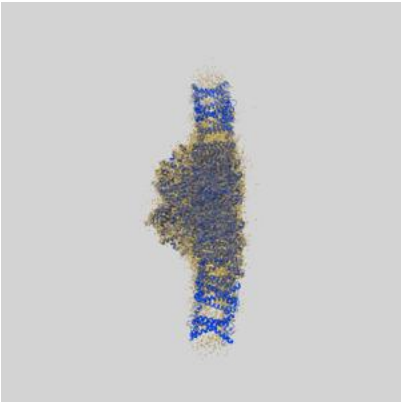
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

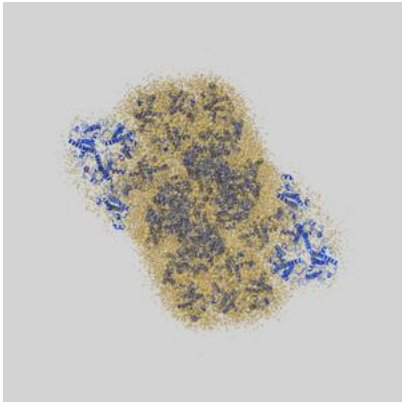
This section contains information regarding the fit between EMDB map EMD-13078 and PDB model 7OUI. Per-residue inclusion information can be found in section 3 on page 42.

9.1 Map-model overlay (i)

X



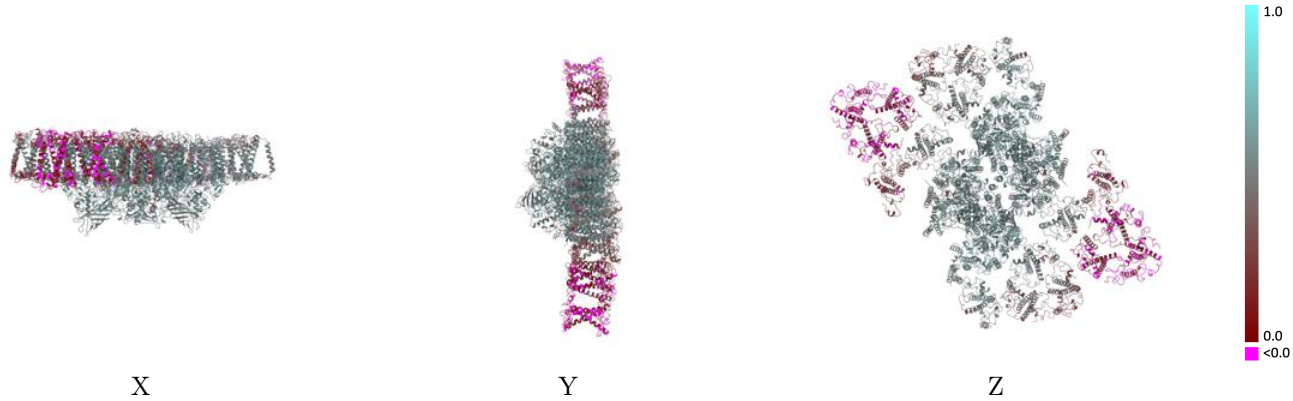
Y



Z

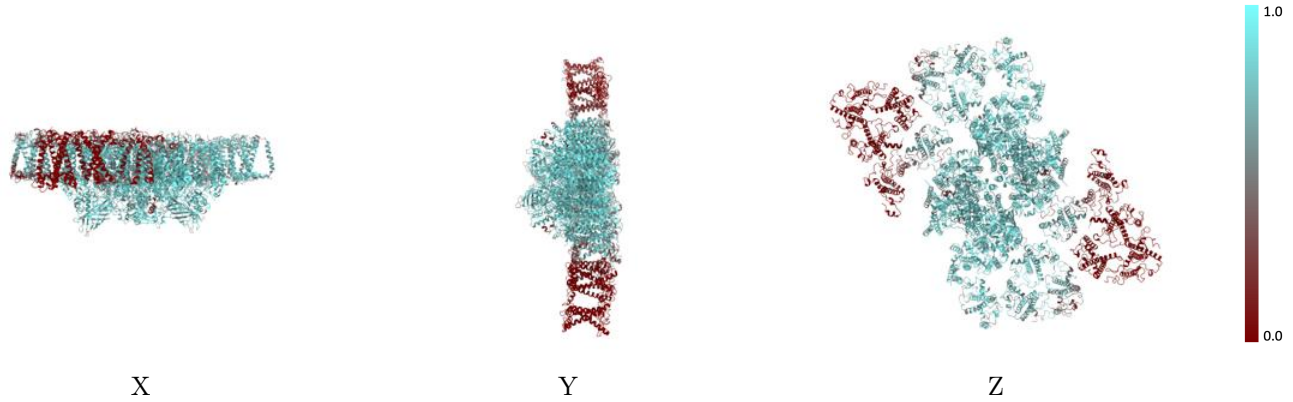
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



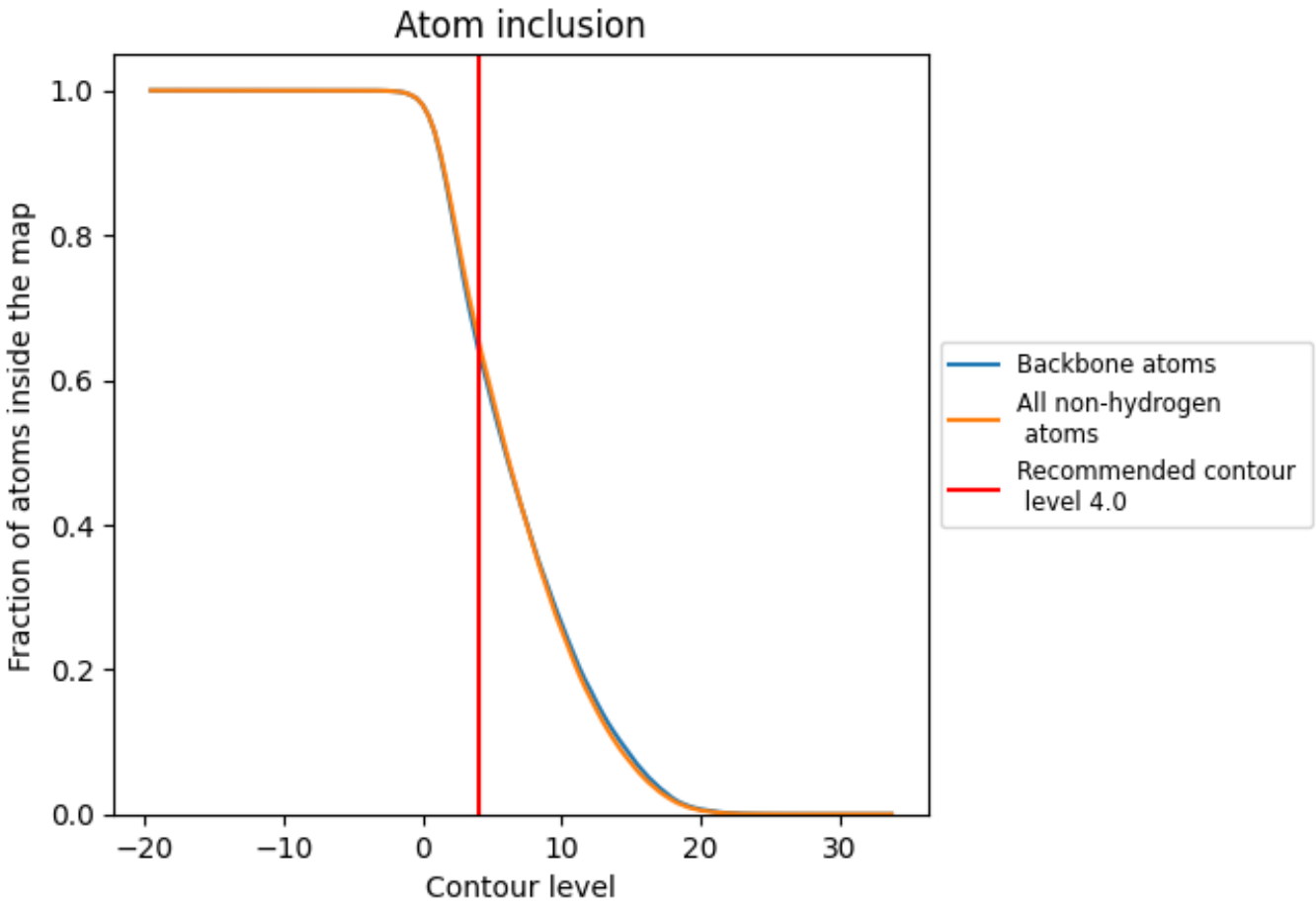
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (4.0).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 66% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6566	0.4650
1	0.0339	0.0670
2	0.0321	0.1050
3	0.0060	0.0400
4	0.0874	0.2440
5	0.0339	0.0680
6	0.0321	0.1040
7	0.0060	0.0410
8	0.0874	0.2450
A	0.8546	0.5740
B	0.8684	0.5810
C	0.8729	0.5820
D	0.8802	0.5890
E	0.7936	0.5260
F	0.7713	0.5100
G	0.5246	0.3940
H	0.7942	0.5510
I	0.8816	0.6010
K	0.8249	0.5570
L	0.8348	0.5430
M	0.8313	0.5620
N	0.6501	0.4540
O	0.7367	0.5090
R	0.6277	0.4770
S	0.7301	0.5110
T	0.8007	0.5660
U	0.2766	0.4110
W	0.8341	0.5810
X	0.6210	0.4490
Y	0.7790	0.5100
Z	0.7271	0.5140
a	0.8555	0.5750
b	0.8677	0.5800
c	0.8696	0.5820
d	0.8762	0.5900

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Chain	Atom inclusion	Q-score
e	0.7917	0.5240
f	0.7752	0.5080
g	0.5271	0.3930
h	0.7921	0.5510
i	0.8941	0.5980
k	0.8398	0.5590
l	0.8348	0.5420
m	0.8233	0.5660
n	0.6505	0.4530
o	0.7360	0.5130
r	0.6250	0.4760
s	0.7257	0.5110
t	0.8080	0.5700
u	0.2819	0.4040
w	0.8341	0.5760
x	0.6250	0.4400
y	0.7772	0.5080
z	0.7151	0.5110