Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2024 – 11:18 AM JST

PDB ID	:	4UB8
Title	:	Native structure of photosystem II (dataset-2) by a femtosecond X-ray laser
Authors	:	Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R.
Deposited on	:	2014-08-12
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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 (i)) were used in the production of this report:

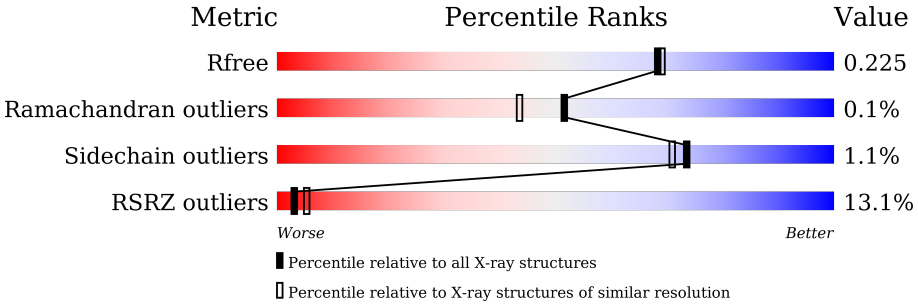
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	13% 97%
1	a	344	17% 97%
2	B	505	8% 99%
2	b	505	10% 99%
3	C	455	6% 98%
3	c	455	8% 99%
4	D	342	18% 100%

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Mol	Chain	Length	Quality of chain
4	d	342	11% 99%
5	E	84	18% 96%
5	e	84	18% 95%
6	F	44	14% 75% 23%
6	f	44	9% 70% 27%
7	H	65	5% 97%
7	h	65	9% 98%
8	I	38	13% 97%
8	i	38	13% 92% 8%
9	J	39	21% 97%
9	j	39	8% 97%
10	K	37	95% 5%
10	k	37	22% 95% 5%
11	L	37	30% 97%
11	l	37	16% 97%
12	M	36	17% 94% 6%
12	m	36	14% 89% 6% 6%
13	O	244	9% 99%
13	o	244	21% 99%
14	T	31	13% 90% 6%
14	t	31	6% 90% 6%
15	U	104	5% 92% 7%
15	u	104	93% 7%
16	V	137	99%
16	v	137	9% 99%

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Mol	Chain	Length	Quality of chain
17	Y	30	30% 97%
17	y	30	30% 93%
18	X	40	20% 98%
18	x	40	28% 98%
19	Z	62	29% 98%
19	z	62	58% 98%
20	R	34	100% 97%

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	CLA	A	405	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	404	X	-	-	-
28	GOL	B	635	-	-	-	X
29	UNL	J	103	-	-	-	X
29	UNL	k	102	-	-	-	X
30	LMT	a	417	-	-	-	X
36	DGD	D	407	-	-	-	X
36	DGD	d	407	-	-	-	X

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 53958 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2631	1725	431	460	15	0	3	0
1	a	334	2634	1727	431	461	15	0	4	0

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	504	4023	2642	667	701	13	0	10	0
2	b	504	4028	2645	668	702	13	0	11	0

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	3506	2296	584	613	13	0	5	0
3	c	455	3544	2323	589	619	13	0	6	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	342	2726	1805	445	464	12	0	0	0
4	d	341	2720	1802	444	462	12	0	1	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	81	668	436	107	125	0	2	0
5	e	81	662	432	107	123	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	34	275	187	45	42	1	0	0	0
6	f	32	257	175	43	38	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	H	65	519	346	85	86	2	0	1	0
7	h	65	511	341	82	86	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	I	38	314	211	48	54	1	0	0	0
8	i	38	314	211	48	54	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	J	38	272	182	42	47	1	0	0	0
9	j	39	282	188	43	49	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	K	37	293	204	43	46	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	k	37	293	204	43	46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	309	207	48	53	1	0	1	0
11	l	37	309	207	48	53	1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	34	274	184	40	49	1	0	1	0
12	m	34	269	179	40	49	1	0	0	0

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	243	1883	1178	315	385	5	0	4	0
13	o	243	1879	1175	315	384	5	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	264	185	36	41	2	0	1	0
14	t	30	264	185	36	41	2	0	1	0

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	U	97	774	491	129	154	0	0	0
15	u	97	774	491	129	154	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	1072	680	180	208	4	0	1	0
16	v	137	1064	675	177	208	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Y	29	215	142	37	33	3	0	0	0
17	y	29	215	142	37	33	3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	X	39	292	196	46	50	0	1	0
18	x	39	287	191	46	50	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	Z	62	479	328	72	77	2	0	0	0
19	z	62	479	328	72	77	2	0	0	0

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	R	34	273	186	47	40	0	0	0

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
21	A	1	1	1	0	0

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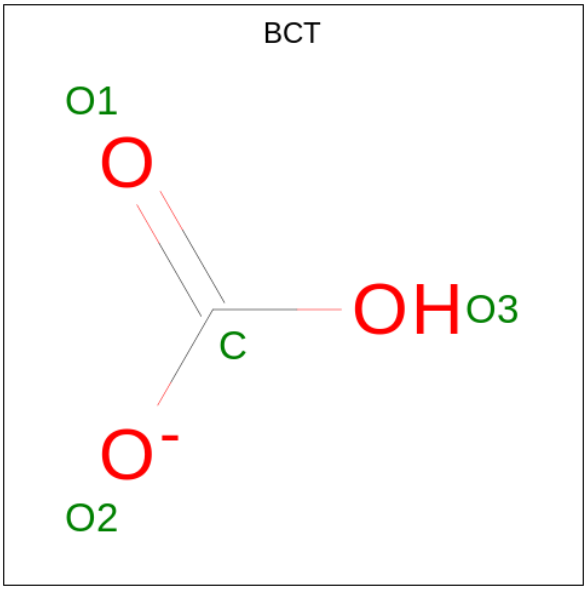
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
21	a	1	1	1	0	0

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
22	A	2	2	2	0	0
			Total	Cl		
22	V	1	1	1	0	0
			Total	Cl		
22	a	2	2	2	0	0
			Total	Cl		
22	u	1	1	1	0	0

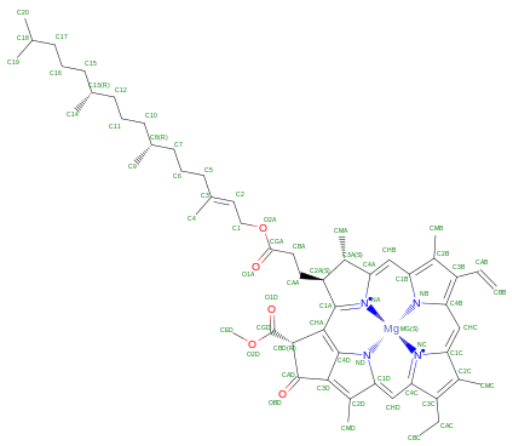
- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).

CLA



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
24	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	D	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	D	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	D	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
24	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0

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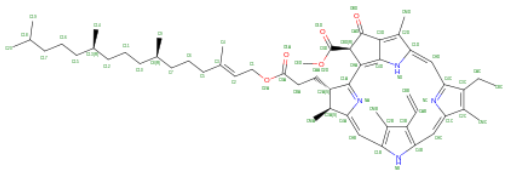
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	d	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	d	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	d	1	65	55	1	4	5	0	0

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).

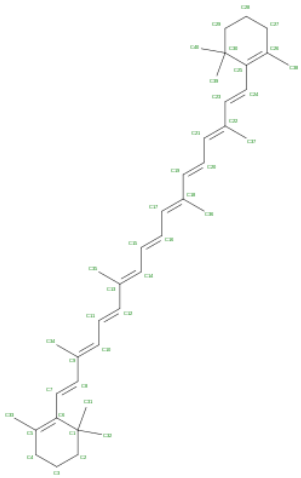
PHO



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
25	A	1	64	55	4	5	0	0
			Total	C	N	O		
25	A	1	64	55	4	5	0	0
			Total	C	N	O		
25	a	1	64	55	4	5	0	0
			Total	C	N	O		
25	d	1	64	55	4	5	0	0

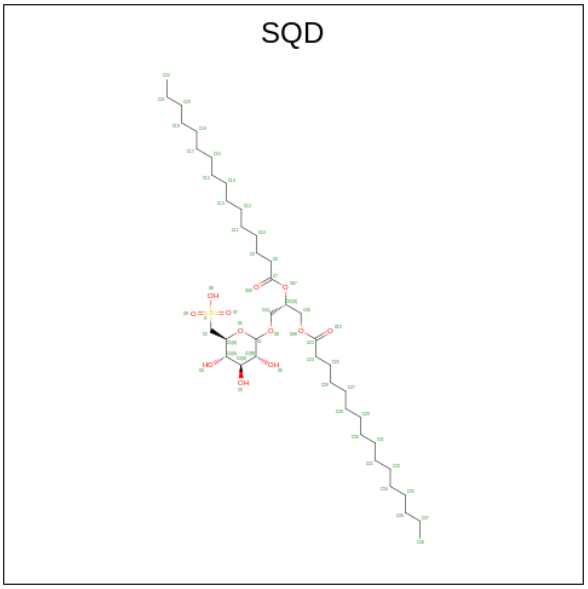
- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

BCR



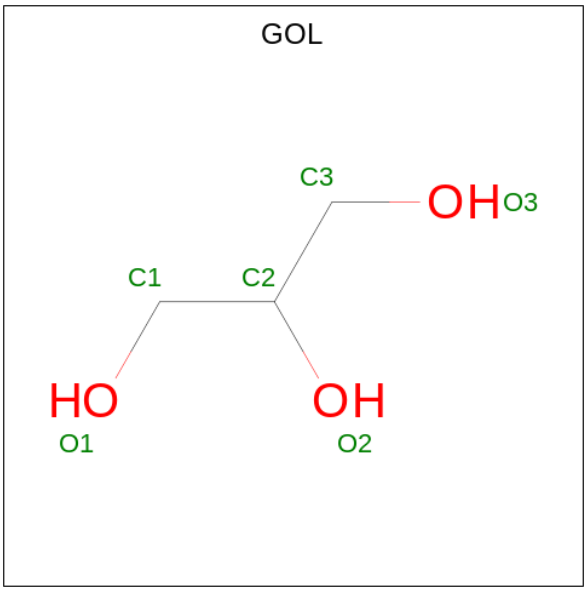
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
26	A	1	40	40	0	0
26	B	1	40	40	0	0
26	B	1	40	40	0	0
26	B	1	40	40	0	0
26	C	1	40	40	0	0
26	C	1	40	40	0	0
26	D	1	40	40	0	0
26	H	1	40	40	0	0
26	K	1	40	40	0	0
26	T	1	40	40	0	0
26	Y	1	40	40	0	0
26	a	1	40	40	0	0
26	b	1	40	40	0	0
26	b	1	40	40	0	0
26	b	1	40	40	0	0
26	c	1	40	40	0	0
26	c	1	40	40	0	0
26	d	1	40	40	0	0
26	h	1	40	40	0	0
26	k	1	40	40	0	0
26	t	1	40	40	0	0
26	y	1	40	40	0	0

- Molecule 27 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				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
			Total	C	O	S		
27	F	1	43	30	12	1	0	0
			Total	C	O	S		
27	a	1	54	41	12	1	0	0
			Total	C	O	S		
27	a	1	54	41	12	1	0	0
			Total	C	O	S		
27	b	1	54	41	12	1	0	0
			Total	C	O	S		
27	f	1	43	30	12	1	0	0
			Total	C	O	S		
27	l	1	54	41	12	1	0	0

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
28	A	1	6	3	3	0	0
			Total	C	O		
28	A	1	6	3	3	0	0
			Total	C	O		
28	A	1	6	3	3	0	0
			Total	C	O		
28	B	1	6	3	3	0	0
			Total	C	O		
28	B	1	6	3	3	0	0
			Total	C	O		
28	B	1	6	3	3	0	0
			Total	C	O		
28	B	1	6	3	3	0	0
			Total	C	O		
28	B	1	6	3	3	0	0
			Total	C	O		
28	B	1	6	3	3	0	0
			Total	C	O		
28	B	1	6	3	3	0	0
			Total	C	O		
28	C	1	6	3	3	0	0
			Total	C	O		
28	C	1	6	3	3	0	0
			Total	C	O		
28	F	1	6	3	3	0	0
			Total	C	O		
28	O	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
28	T	1	6	3	3	0	0
			Total	C	O		
28	T	1	6	3	3	0	0
			Total	C	O		
28	V	1	6	3	3	0	0
			Total	C	O		
28	V	1	6	3	3	0	0
			Total	C	O		
28	V	1	6	3	3	0	0
			Total	C	O		
28	V	1	6	3	3	0	0
			Total	C	O		
28	V	1	6	3	3	0	0
			Total	C	O		
28	a	1	6	3	3	0	0
			Total	C	O		
28	a	1	6	3	3	0	0
			Total	C	O		
28	b	1	6	3	3	0	0
			Total	C	O		
28	b	1	6	3	3	0	0
			Total	C	O		
28	b	1	6	3	3	0	0
			Total	C	O		
28	b	1	6	3	3	0	0
			Total	C	O		
28	b	1	6	3	3	0	0
			Total	C	O		
28	c	1	6	3	3	0	0
			Total	C	O		
28	c	1	6	3	3	0	0
			Total	C	O		
28	c	1	6	3	3	0	0
			Total	C	O		
28	f	1	6	3	3	0	0
			Total	C	O		
28	t	1	6	3	3	0	0
			Total	C	O		
28	v	1	6	3	3	0	0
			Total	C	O		
28	v	1	6	3	3	0	0

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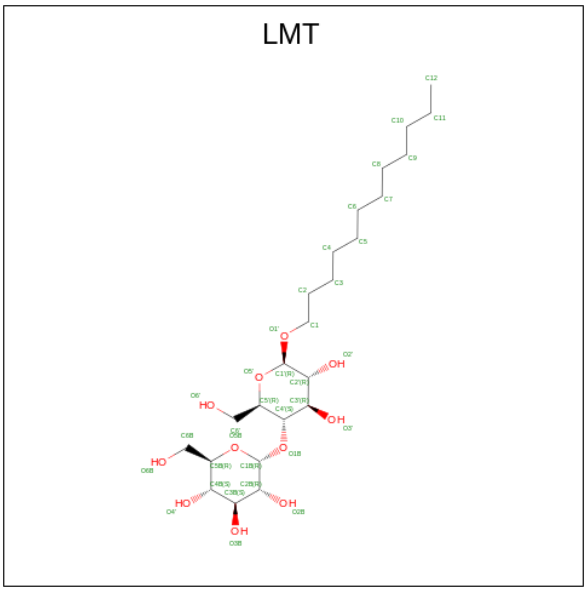
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	v	1	Total C O 6 3 3	0	0
28	v	1	Total C O 6 3 3	0	0

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

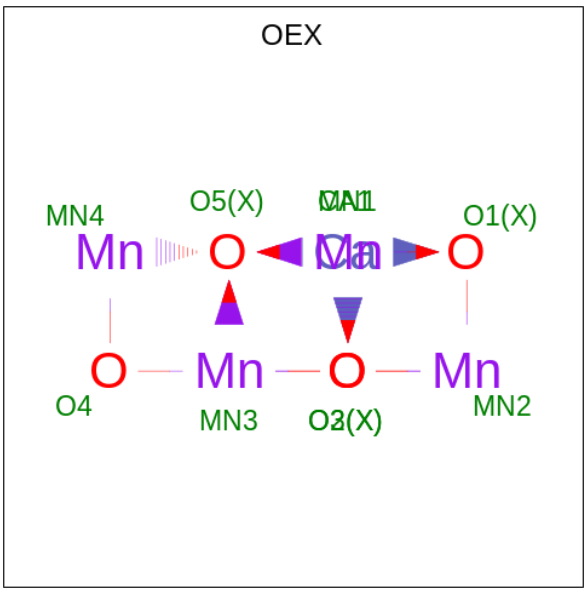
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 28 23 5	0	0
29	B	1	Total C O 33 28 5	0	0
29	C	1	Total C O 34 29 5	0	0
29	D	2	Total C O 57 51 6	0	0
29	I	1	Total C O 40 35 5	0	0
29	J	1	Total C 10 10	0	0
29	M	1	Total C 10 10	0	0
29	X	1	Total C 10 10	0	0
29	a	1	Total C O 30 25 5	0	0
29	b	1	Total C O 33 28 5	0	0
29	d	2	Total C O 53 47 6	0	0
29	i	1	Total C O 40 35 5	0	0
29	j	1	Total C 10 10	0	0
29	k	2	Total C O 42 37 5	0	0
29	m	1	Total C 10 10	0	0
29	x	1	Total C 10 10	0	0

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



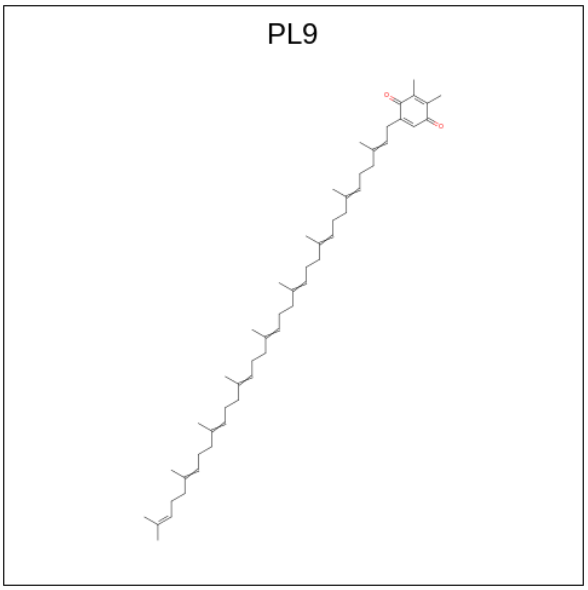
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
30	A	1	33	22	11	0	0
30	B	1	25	19	6	0	0
30	D	1	35	24	11	0	0
30	E	1	35	24	11	0	0
30	I	1	35	24	11	0	0
30	M	1	35	24	11	0	0
30	M	1	35	24	11	0	0
30	a	1	35	24	11	0	0
30	a	1	35	24	11	0	0
30	b	1	25	19	6	0	0
30	b	1	25	19	6	0	0
30	f	1	35	24	11	0	0
30	m	1	35	24	11	0	0
30	m	1	35	24	11	0	0

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 32 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: $C_{53}H_{80}O_2$).

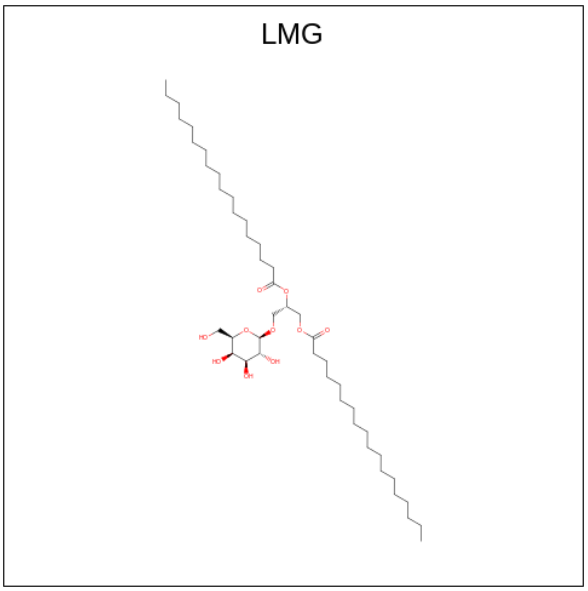


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
32	A	1	55	53	2	0	0
32	D	1	55	53	2	0	0
32	a	1	55	53	2	0	0
32	d	1	55	53	2	0	0

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
33	B	1	1	1	0	0
33	F	1	1	1	0	0
33	O	1	1	1	0	0
33	b	1	1	1	0	0
33	c	1	1	1	0	0
33	f	1	1	1	0	0
33	o	1	1	1	0	0

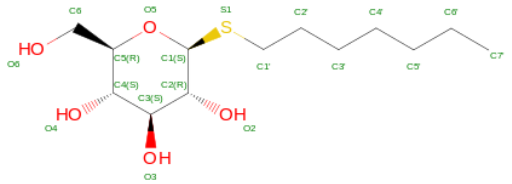
- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	B	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	J	1	51	41	10	0	0
34	Z	1	37	27	10	0	0
34	b	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	j	1	51	41	10	0	0
34	z	1	39	29	10	0	0

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).

HTG



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	B	1	19	13	5	1	0	0
			Total	C	O	S		
35	B	1	19	13	5	1	0	0
			Total	C	O	S		
35	B	1	19	13	5	1	0	0
			Total	C	O	S		
35	B	1	19	13	5	1	0	0
			Total	C	O	S		
35	B	1	19	13	5	1	0	0
			Total	C	O	S		
35	C	1	19	13	5	1	0	0
			Total	C	O	S		
35	C	1	19	13	5	1	0	0
			Total	C	O	S		
35	D	1	16	10	5	1	0	0
			Total	C	O	S		
35	O	1	19	13	5	1	0	0
			Total	C	O	S		
35	V	1	19	13	5	1	0	0
			Total	C	O	S		
35	b	1	19	13	5	1	0	0
			Total	C	O	S		
35	b	1	19	13	5	1	0	0
			Total	C	O	S		
35	b	1	19	13	5	1	0	0
			Total	C	O	S		
35	b	1	19	13	5	1	0	0

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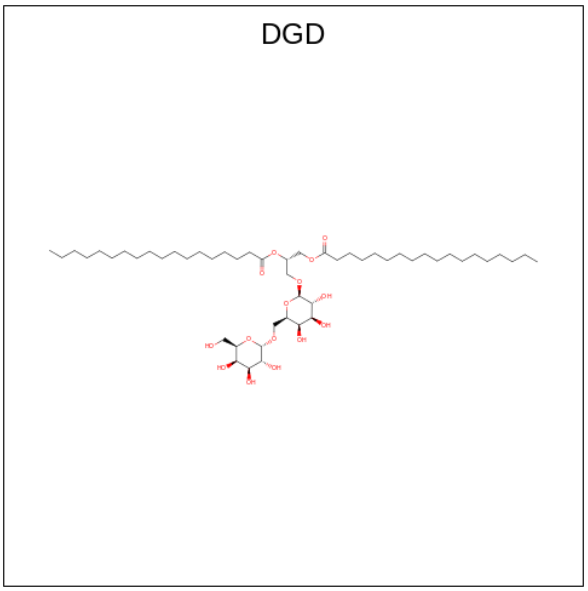
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
35	c	1	19	13	5	1	0	0
			Total	C	O	S		
35	c	1	19	13	5	1	0	0
			Total	C	O	S		
35	d	1	16	10	5	1	0	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
36	C	1	62	47	15	0	0
			Total	C	O		
36	C	1	62	47	15	0	0
			Total	C	O		
36	C	1	62	47	15	0	0
			Total	C	O		
36	D	1	62	47	15	0	0
			Total	C	O		
36	H	1	62	47	15	0	0
			Total	C	O		
36	c	1	62	47	15	0	0
			Total	C	O		
36	c	1	62	47	15	0	0
			Total	C	O		
36	c	1	62	47	15	0	0

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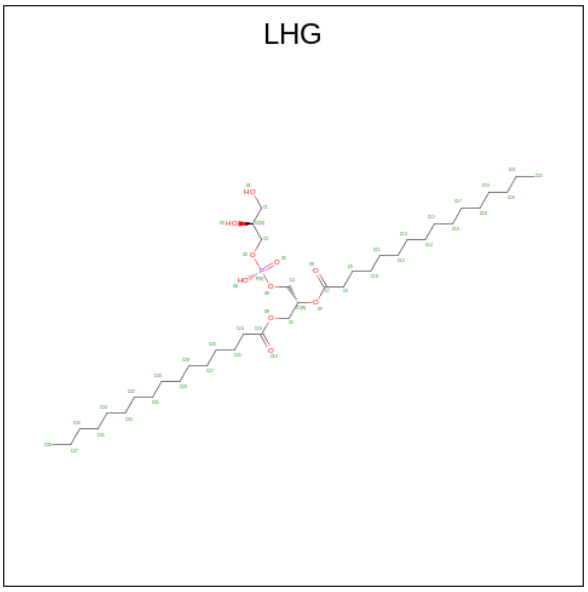
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
36	d	1	62	47	15	0	0
			Total	C	O		
36	h	1	62	47	15	0	0

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
37	D	1	49	38	10	1	0	0
			Total	C	O	P		
37	D	1	49	38	10	1	0	0
			Total	C	O	P		
37	D	1	49	38	10	1	0	0
			Total	C	O	P		
37	E	1	42	31	10	1	0	0
			Total	C	O	P		
37	L	1	49	38	10	1	0	0
			Total	C	O	P		
37	d	1	49	38	10	1	0	0
			Total	C	O	P		
37	d	1	49	38	10	1	0	0
			Total	C	O	P		
37	d	1	49	38	10	1	0	0
			Total	C	O	P		
37	e	1	42	31	10	1	0	0

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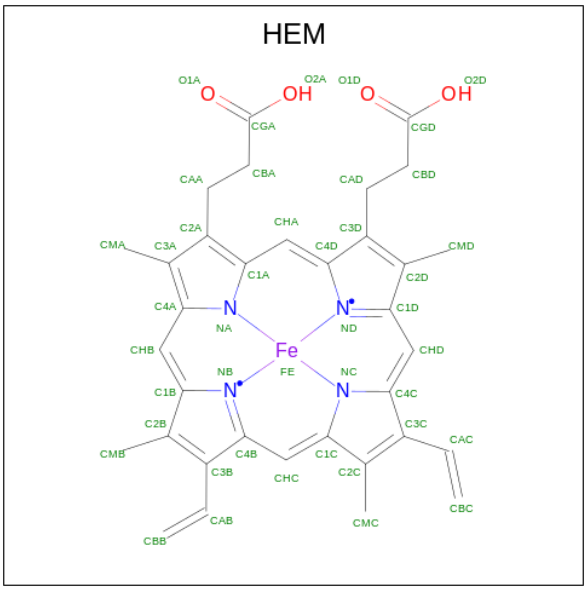
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
37	l	1	49	38	10	1	0	0

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

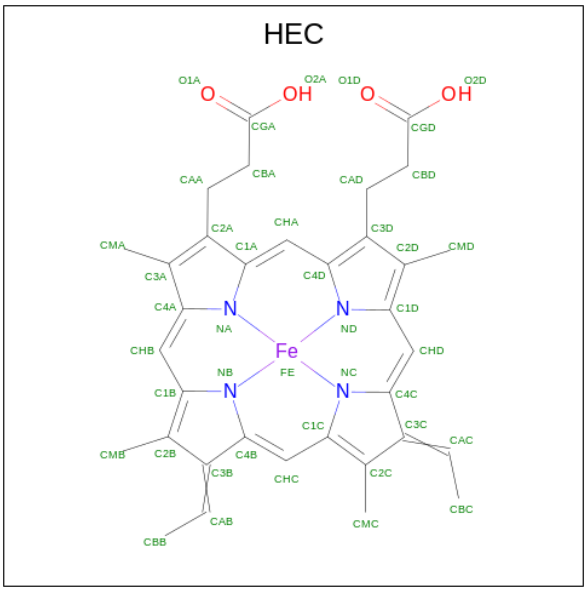


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
38	E	1	43	34	1	4	4	0	0
38	e	1	43	34	1	4	4	0	0

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
39	J	1	1	1	0	0
39	j	1	1	1	0	0

- Molecule 40 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
40	V	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
40	v	1	43	34	1	4	4	0	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	A	146	149	149	0	3
			Total	O		
41	B	277	280	280	0	3
			Total	O		
41	C	206	209	209	0	3
			Total	O		
41	D	157	161	161	0	4
			Total	O		
41	E	28	28	28	0	0
			Total	O		
41	F	7	7	7	0	0
			Total	O		
41	H	39	40	40	0	1
			Total	O		
41	I	8	8	8	0	0
			Total	O		
41	J	12	12	12	0	0
			Total	O		
41	K	6	6	6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	12	Total O 12 12	0	0
41	M	15	Total O 15 15	0	0
41	O	164	Total O 165 165	0	1
41	T	12	Total O 13 13	0	1
41	U	75	Total O 76 76	0	1
41	V	111	Total O 111 111	0	0
41	Y	1	Total O 1 1	0	0
41	X	8	Total O 8 8	0	0
41	a	151	Total O 151 151	0	0
41	b	247	Total O 249 249	0	2
41	c	187	Total O 189 189	0	2
41	d	136	Total O 139 139	0	3
41	e	15	Total O 15 15	0	0
41	f	7	Total O 7 7	0	0
41	h	36	Total O 36 36	0	0
41	i	5	Total O 5 5	0	0
41	j	7	Total O 7 7	0	0
41	k	3	Total O 3 3	0	0
41	l	10	Total O 10 10	0	0
41	m	12	Total O 12 12	0	0
41	o	137	Total O 137 137	0	0

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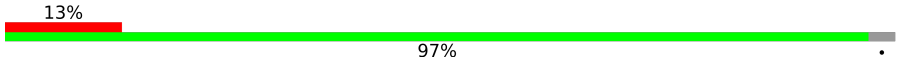
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	t	10	Total O 10 10	0	0
41	u	89	Total O 89 89	0	0
41	v	80	Total O 80 80	0	0
41	y	4	Total O 4 4	0	0
41	x	5	Total O 5 5	0	0

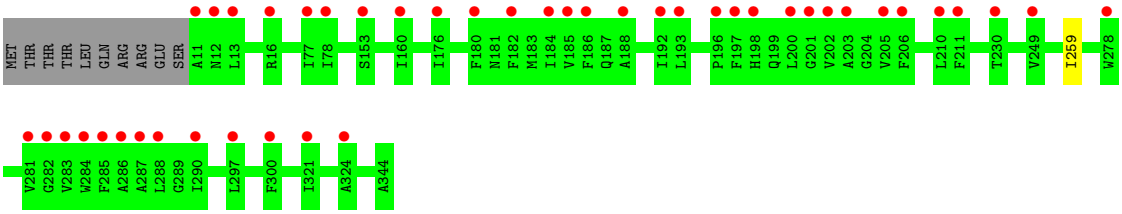
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem Q(B) protein

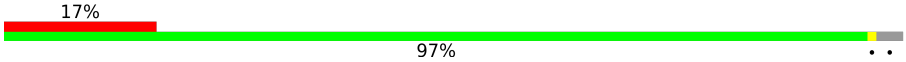
Chain A:

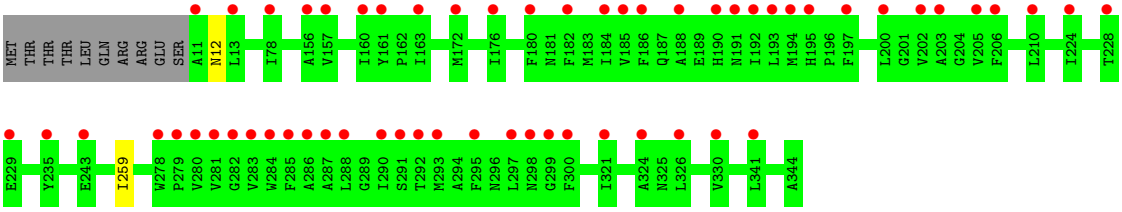




• Molecule 1: Photosystem Q(B) protein

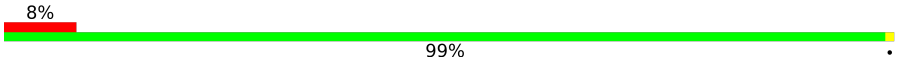
Chain a:

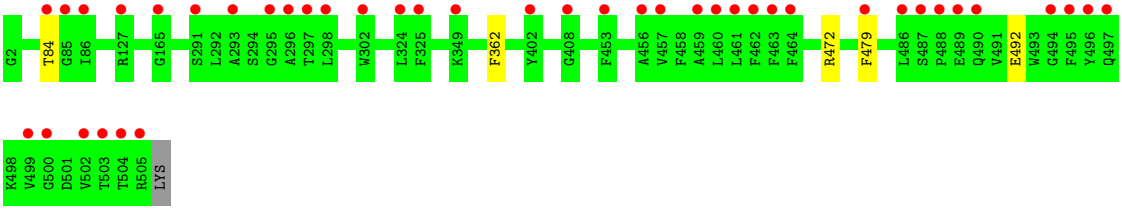




• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

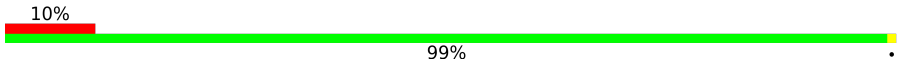
Chain B:

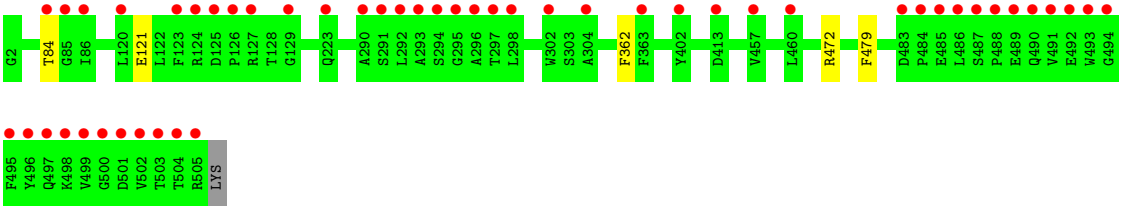




• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

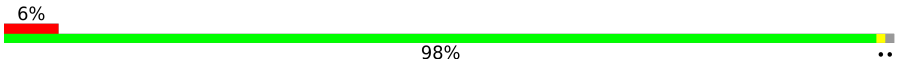
Chain b:

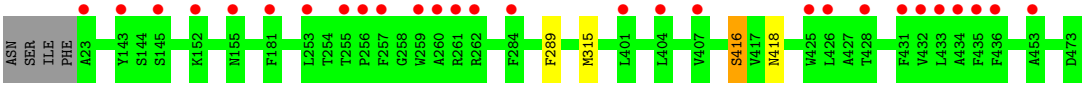




• Molecule 3: Photosystem II 44 kDa reaction center protein

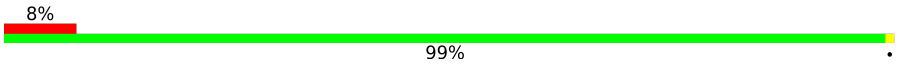
Chain C:

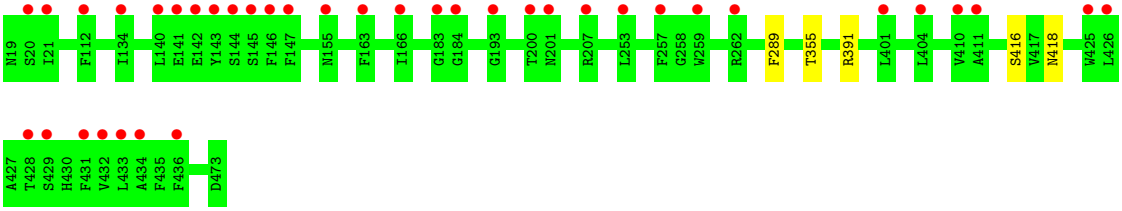




• Molecule 3: Photosystem II 44 kDa reaction center protein

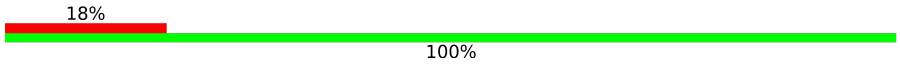
Chain c:

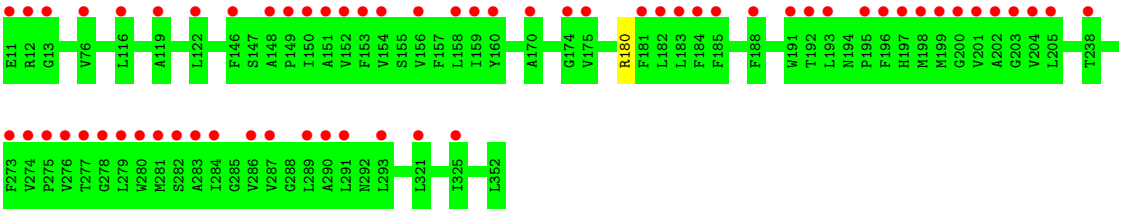




• Molecule 4: Photosystem II D2 protein

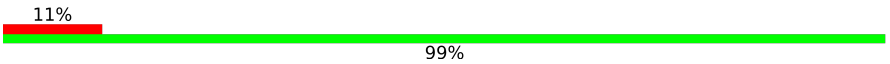
Chain D:

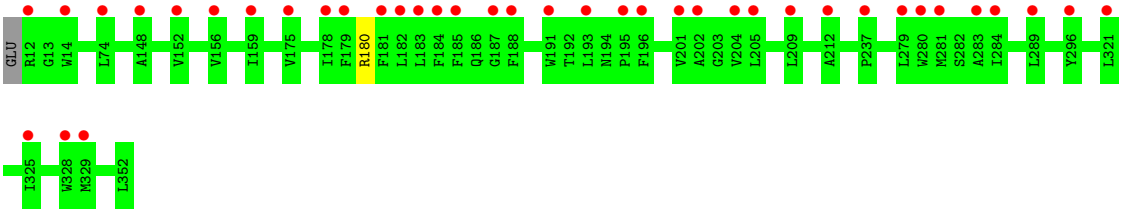




• Molecule 4: Photosystem II D2 protein

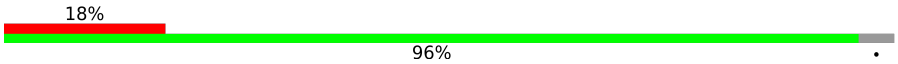
Chain d:

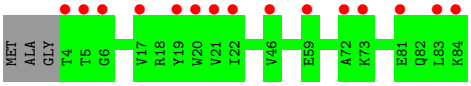




• Molecule 5: Cytochrome b559 subunit alpha

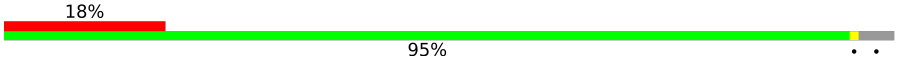
Chain E:

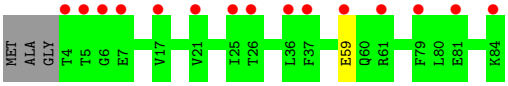




• Molecule 5: Cytochrome b559 subunit alpha

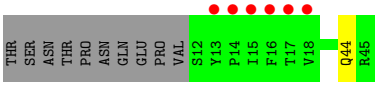
Chain e:





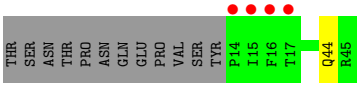
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



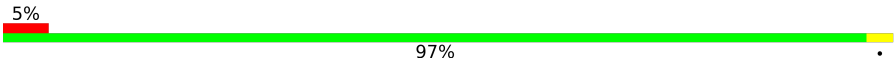
• Molecule 6: Cytochrome b559 subunit beta

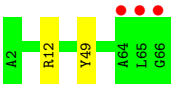
Chain f:



• Molecule 7: Photosystem II reaction center protein H

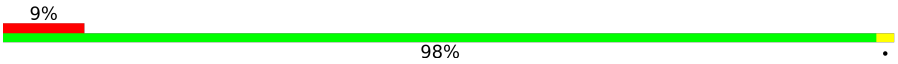
Chain H:

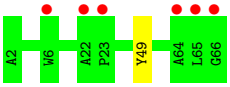




• Molecule 7: Photosystem II reaction center protein H

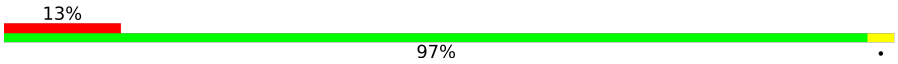
Chain h:

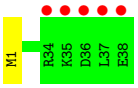




• Molecule 8: Photosystem II reaction center protein I

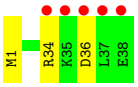
Chain I:





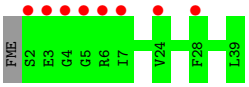
• Molecule 8: Photosystem II reaction center protein I

Chain i: 13% 92% 8%



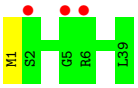
• Molecule 9: Photosystem II reaction center protein J

Chain J: 21% 97%



• Molecule 9: Photosystem II reaction center protein J

Chain j: 8% 97%

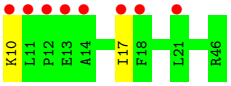


• Molecule 10: Photosystem II reaction center protein K

Chain K: 95% 5%

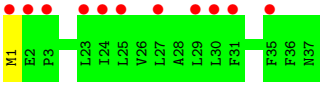
• Molecule 10: Photosystem II reaction center protein K

Chain k: 22% 95% 5%



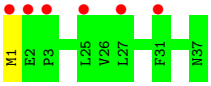
• Molecule 11: Photosystem II reaction center protein L

Chain L: 30% 97%



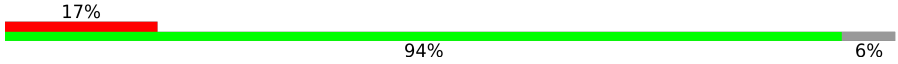
• Molecule 11: Photosystem II reaction center protein L

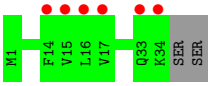
Chain l: 16% 97%



• Molecule 12: Photosystem II reaction center protein M

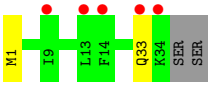
Chain M:





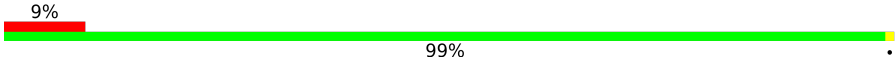
• Molecule 12: Photosystem II reaction center protein M

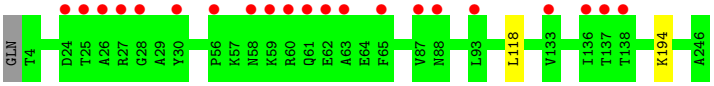
Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

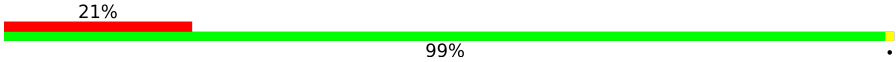
Chain O:

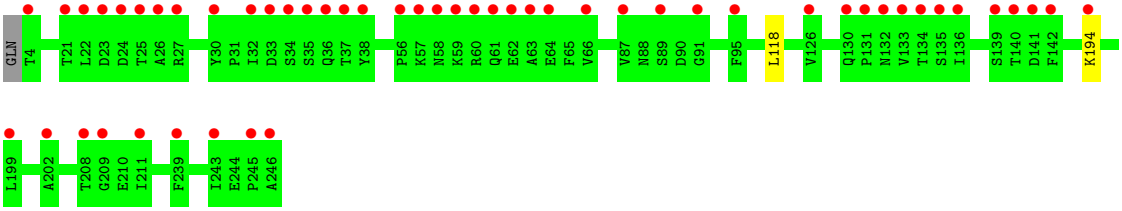




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

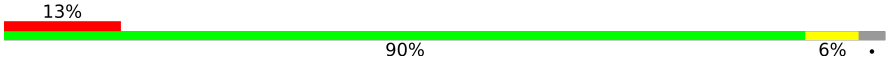
Chain o:

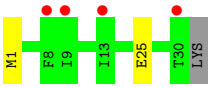




• Molecule 14: Photosystem II reaction center protein T

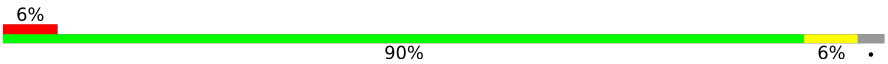
Chain T:

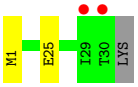




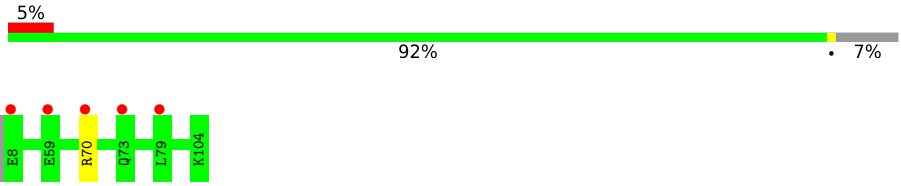
• Molecule 14: Photosystem II reaction center protein T

Chain t:

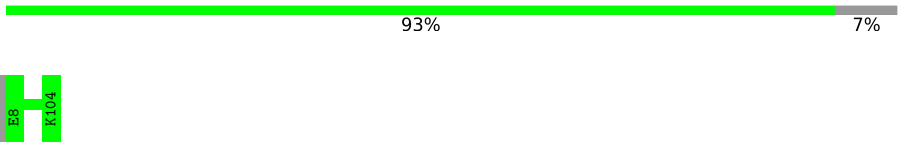




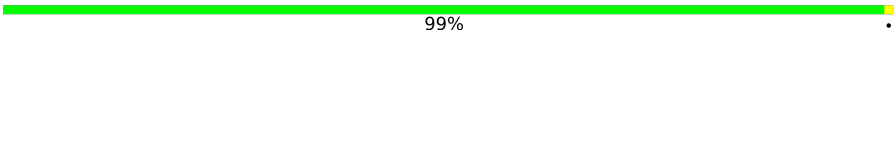
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 

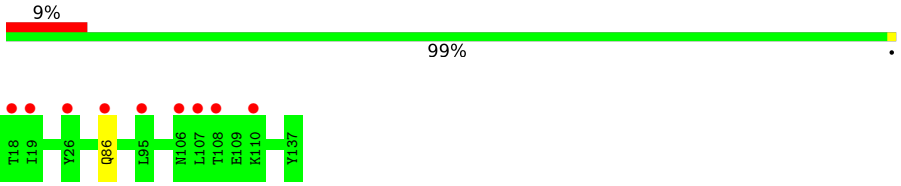
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 

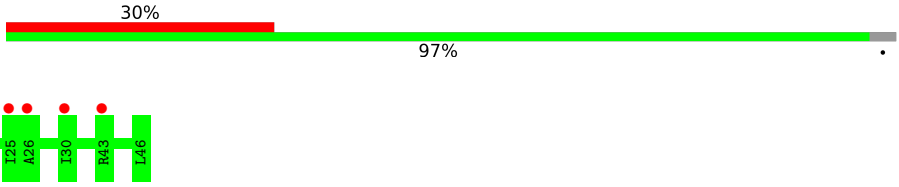
• Molecule 16: Cytochrome c-550

Chain V: 

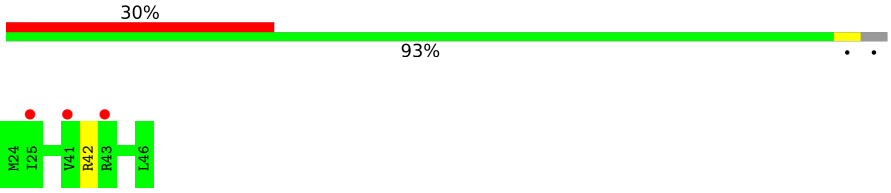
• Molecule 16: Cytochrome c-550

Chain v: 

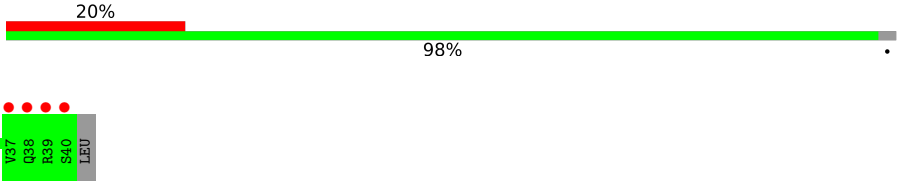
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 

• Molecule 17: Photosystem II reaction center protein Ycf12

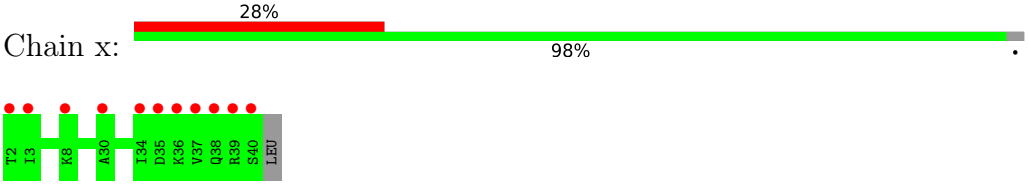
Chain y: 

• Molecule 18: Photosystem II reaction center protein X

Chain X: 

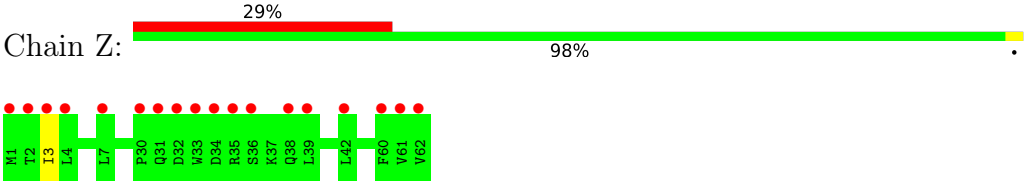
• Molecule 18: Photosystem II reaction center protein X

Chain x:



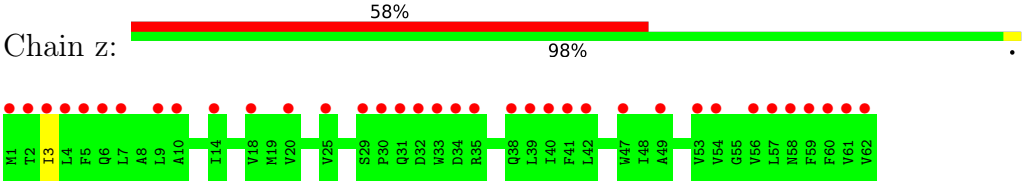
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



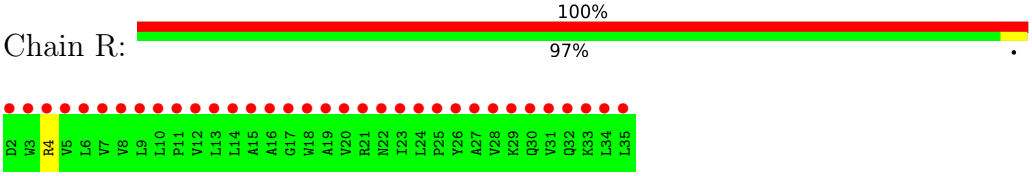
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.81Å 230.00Å 288.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.90 – 1.95 61.90 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.1 (61.90-1.95) 85.6 (61.90-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.08 (at 1.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.188 , 0.225 0.187 , 0.225	Depositor DCC
R_{free} test set	29342 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	53958	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, CA, LHG, LMG, HEM, BCT, CLA, LMT, GOL, MG, DGD, OEX, PHO, UNL, FME, SQD, FE2, HTG, CL, HEC, PL9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.53	0/2725	0.59	0/3716
1	a	0.55	0/2731	0.58	0/3724
2	B	0.49	0/4193	0.56	0/5712
2	b	0.47	0/4201	0.55	0/5723
3	C	0.46	0/3634	0.54	0/4947
3	c	0.46	0/3676	0.54	0/5004
4	D	0.53	0/2821	0.56	0/3844
4	d	0.52	0/2818	0.55	0/3840
5	E	0.36	0/693	0.52	0/944
5	e	0.33	0/681	0.52	0/928
6	F	0.39	0/284	0.48	0/387
6	f	0.37	0/265	0.51	0/360
7	H	0.40	0/535	0.53	0/728
7	h	0.35	0/524	0.50	0/713
8	I	0.38	0/311	0.51	0/419
8	i	0.40	0/311	0.50	0/419
9	J	0.37	0/278	0.46	0/376
9	j	0.38	0/278	0.48	0/376
10	K	0.36	0/303	0.48	0/416
10	k	0.36	0/303	0.51	0/416
11	L	0.48	0/319	0.49	0/433
11	l	0.49	0/319	0.50	0/433
12	M	0.43	0/270	0.58	0/368
12	m	0.47	0/262	0.58	0/357
13	O	0.41	0/1926	0.56	0/2611
13	o	0.40	0/1919	0.57	0/2601
14	T	0.54	0/266	0.56	0/362
14	t	0.54	0/266	0.56	0/362
15	U	0.44	0/785	0.55	0/1064
15	u	0.42	0/785	0.56	0/1064
16	V	0.45	0/1096	0.54	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.41	0/1085	0.53	0/1473
17	Y	0.29	0/216	0.46	0/289
17	y	0.28	0/216	0.46	0/289
18	X	0.34	0/298	0.44	0/403
18	x	0.34	0/290	0.48	0/392
19	Z	0.31	0/490	0.43	0/669
19	z	0.32	0/490	0.43	0/669
20	R	0.24	0/279	0.38	0/383
All	All	0.46	0/43142	0.55	0/58701

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	41	30
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	41	30
2	B	512/505 (101%)	507 (99%)	5 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	454/455 (100%)	445 (98%)	7 (2%)	2 (0%)	34	22
3	c	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	34	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	77 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	1
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	245/244 (100%)	242 (99%)	3 (1%)	0	100	100
13	o	244/244 (100%)	238 (98%)	6 (2%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	29/31 (94%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	130 (96%)	6 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5279/5382 (98%)	5168 (98%)	104 (2%)	7 (0%)	51	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
8	i	36	ASP
1	a	259	ILE
1	A	259	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	272 (100%)	0	100	100
1	a	273/279 (98%)	272 (100%)	1 (0%)	91	90
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	68
2	b	413/403 (102%)	408 (99%)	5 (1%)	71	68
3	C	357/356 (100%)	352 (99%)	5 (1%)	67	62
3	c	362/356 (102%)	358 (99%)	4 (1%)	73	71
4	D	277/277 (100%)	276 (100%)	1 (0%)	91	90
4	d	277/277 (100%)	276 (100%)	1 (0%)	91	90
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	72/73 (99%)	71 (99%)	1 (1%)	67	62
6	F	28/38 (74%)	27 (96%)	1 (4%)	35	23
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	55/54 (102%)	52 (94%)	3 (6%)	21	9
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	50
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	31
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	5
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	5
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	33
11	l	36/35 (103%)	35 (97%)	1 (3%)	43	33
12	M	31/32 (97%)	31 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	26
13	O	210/207 (101%)	208 (99%)	2 (1%)	76	74
13	o	209/207 (101%)	207 (99%)	2 (1%)	76	74
14	T	27/27 (100%)	25 (93%)	2 (7%)	13	4
14	t	27/27 (100%)	25 (93%)	2 (7%)	13	4
15	U	84/89 (94%)	83 (99%)	1 (1%)	71	68
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	80
16	v	117/117 (100%)	116 (99%)	1 (1%)	78	77
17	Y	22/23 (96%)	22 (100%)	0	100	100
17	y	22/23 (96%)	21 (96%)	1 (4%)	27	15
18	X	33/33 (100%)	33 (100%)	0	100	100
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	50
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	50
20	R	29/29 (100%)	28 (97%)	1 (3%)	37	25
All	All	4383/4399 (100%)	4331 (99%)	52 (1%)	73	68

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	84	THR

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Mol	Chain	Res	Type
2	B	362	PHE
2	B	472	ARG
2	B	479	PHE
2	B	492	GLU
3	C	289	PHE
3	C	315	MET
3	C	416[A]	SER
3	C	416[B]	SER
3	C	418	ASN
4	D	180	ARG
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
10	K	10	LYS
10	K	17	ILE
11	L	1	MET
13	O	118	LEU
13	O	194	LYS
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	70	ARG
16	V	86	GLN
19	Z	3	ILE
20	R	4	ARG
1	a	12	ASN
2	b	84	THR
2	b	121	GLU
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
3	c	289	PHE
3	c	355	THR
3	c	391	ARG
3	c	418	ASN
4	d	180	ARG
5	e	59	GLU
6	f	44	GLN
7	h	49	TYR
8	i	34	ARG
10	k	10	LYS
10	k	17	ILE

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Mol	Chain	Res	Type
11	l	1	MET
12	m	33	GLN
13	o	118	LEU
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
16	v	86	GLN
17	y	42	ARG
19	z	3	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	61	HIS
4	D	142	ASN
19	Z	31	GLN
2	b	497	GLN
13	o	109	GLN
15	u	81	HIS
19	z	6	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
14	FME	t	1	14	8,9,10	0.85	0	7,9,11	2.28	4 (57%)
9	FME	j	1	9	8,9,10	0.63	0	7,9,11	1.32	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	M	1	12	8,9,10	0.63	0	7,9,11	1.32	0
12	FME	m	1	12	8,9,10	0.69	0	7,9,11	1.05	1 (14%)
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.32	2 (28%)
8	FME	i	1	8	8,9,10	0.62	0	7,9,11	1.17	1 (14%)
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	1.73	3 (42%)

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
14	FME	t	1	14	-	2/7/9/11	-
9	FME	j	1	9	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	C-CA-N	3.68	116.36	109.73
14	t	1	FME	O-C-CA	-3.00	116.92	124.78
14	T	1	FME	O-C-CA	-2.78	117.48	124.78
14	T	1	FME	C-CA-N	2.35	113.97	109.73
14	T	1	FME	CA-N-CN	-2.29	119.31	122.82
14	t	1	FME	CE-SD-CG	-2.20	92.84	100.40
14	t	1	FME	O1-CN-N	-2.14	119.63	125.27
8	I	1	FME	O-C-CA	-2.12	119.23	124.78
8	I	1	FME	CA-N-CN	-2.11	119.58	122.82
8	i	1	FME	O-C-CA	-2.07	119.36	124.78
9	j	1	FME	C-CA-N	2.04	113.42	109.73
12	m	1	FME	O-C-CA	-2.04	119.43	124.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
14	T	1	FME	O1-CN-N-CA
9	j	1	FME	O1-CN-N-CA
9	j	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
12	m	1	FME	CA-CB-CG-SD
14	t	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 252 ligands modelled in this entry, 17 are monoatomic and 19 are unknown - leaving 216 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	$\#\|Z\| > 2$
24	CLA	c	506	41	65,73,73	2.04	16 (24%)	76,113,113	2.75	27 (35%)
24	CLA	B	610	-	65,73,73	2.00	15 (23%)	76,113,113	2.85	27 (35%)
28	GOL	a	412	-	5,5,5	0.34	0	5,5,5	0.57	0
28	GOL	c	527	-	5,5,5	0.41	0	5,5,5	0.31	0
28	GOL	B	629	-	5,5,5	0.32	0	5,5,5	0.39	0
24	CLA	c	512	-	65,73,73	2.05	15 (23%)	76,113,113	2.71	29 (38%)
28	GOL	A	412	-	5,5,5	0.26	0	5,5,5	0.68	0
24	CLA	c	505	-	65,73,73	2.02	16 (24%)	76,113,113	2.80	26 (34%)
24	CLA	C	510	-	65,73,73	2.14	16 (24%)	76,113,113	2.71	28 (36%)
28	GOL	t	102	-	5,5,5	0.34	0	5,5,5	0.30	0
24	CLA	c	510	-	65,73,73	2.11	16 (24%)	76,113,113	2.76	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	GOL	B	633	-	5,5,5	0.30	0	5,5,5	0.66	0
24	CLA	a	407	41	65,73,73	2.06	16 (24%)	76,113,113	2.77	29 (38%)
26	BCR	A	410	-	41,41,41	1.02	1 (2%)	56,56,56	1.33	7 (12%)
26	BCR	T	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	11 (19%)
28	GOL	b	629	-	5,5,5	0.38	0	5,5,5	0.29	0
30	LMT	M	101	-	36,36,36	0.57	1 (2%)	47,47,47	0.84	0
24	CLA	C	506	-	65,73,73	2.06	16 (24%)	76,113,113	2.57	23 (30%)
24	CLA	C	511	-	65,73,73	2.09	16 (24%)	76,113,113	2.70	28 (36%)
24	CLA	B	614	-	65,73,73	2.06	15 (23%)	76,113,113	2.70	31 (40%)
27	SQD	A	416	-	53,54,54	1.05	3 (5%)	62,65,65	1.15	7 (11%)
24	CLA	b	613	-	65,73,73	2.09	16 (24%)	76,113,113	2.74	30 (39%)
24	CLA	b	618	-	65,73,73	2.05	16 (24%)	76,113,113	2.80	25 (32%)
24	CLA	c	503	-	65,73,73	2.06	16 (24%)	76,113,113	2.77	28 (36%)
26	BCR	b	622	-	41,41,41	1.14	2 (4%)	56,56,56	1.36	4 (7%)
26	BCR	c	526	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	10 (17%)
24	CLA	C	503	-	65,73,73	2.08	16 (24%)	76,113,113	2.66	27 (35%)
30	LMT	m	102	-	36,36,36	0.49	0	47,47,47	0.99	2 (4%)
34	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.14	5 (8%)
30	LMT	B	634	-	25,25,36	0.49	0	30,30,47	0.71	0
24	CLA	C	509	-	65,73,73	2.10	16 (24%)	76,113,113	2.75	26 (34%)
26	BCR	k	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.33	5 (8%)
24	CLA	c	514	-	65,73,73	2.03	16 (24%)	76,113,113	2.81	29 (38%)
26	BCR	c	516	-	41,41,41	1.08	1 (2%)	56,56,56	1.41	9 (16%)
30	LMT	E	102	-	36,36,36	0.46	0	47,47,47	0.75	0
24	CLA	c	504	-	65,73,73	2.00	16 (24%)	76,113,113	2.63	25 (32%)
34	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.44	7 (15%)
35	HTG	O	303	-	19,19,19	1.07	1 (5%)	23,24,24	0.93	1 (4%)
24	CLA	B	606	-	65,73,73	1.99	16 (24%)	76,113,113	2.87	28 (36%)
24	CLA	b	612	41	65,73,73	1.97	15 (23%)	76,113,113	2.72	28 (36%)
28	GOL	B	626	-	5,5,5	0.29	0	5,5,5	0.48	0
24	CLA	b	611	-	65,73,73	2.03	16 (24%)	76,113,113	2.80	29 (38%)
24	CLA	B	607	-	65,73,73	2.06	16 (24%)	76,113,113	2.85	28 (36%)
40	HEC	v	202	16	32,50,50	1.49	4 (12%)	24,82,82	1.34	4 (16%)
32	PL9	A	419	-	55,55,55	0.63	1 (1%)	68,69,69	1.85	19 (27%)
34	LMG	c	520	-	51,51,55	0.95	2 (3%)	59,59,63	0.92	2 (3%)
28	GOL	C	525	-	5,5,5	0.33	0	5,5,5	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	GOL	b	631	-	5,5,5	0.34	0	5,5,5	0.45	0
24	CLA	B	615	-	65,73,73	1.98	17 (26%)	76,113,113	2.96	28 (36%)
25	PHO	A	408	-	51,69,69	1.87	8 (15%)	47,99,99	1.80	10 (21%)
26	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	11 (19%)
28	GOL	c	525	-	5,5,5	0.36	0	5,5,5	0.58	0
28	GOL	v	201	-	5,5,5	0.35	0	5,5,5	0.39	0
24	CLA	B	608	41	65,73,73	2.02	16 (24%)	76,113,113	2.70	30 (39%)
24	CLA	b	606	41	65,73,73	2.10	16 (24%)	76,113,113	2.74	24 (31%)
28	GOL	b	632	-	5,5,5	0.44	0	5,5,5	0.52	0
30	LMT	I	102	-	36,36,36	0.45	0	47,47,47	1.18	4 (8%)
36	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.06	4 (5%)
27	SQD	a	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.60	11 (17%)
28	GOL	F	103	33	5,5,5	0.36	0	5,5,5	0.37	0
32	PL9	a	416	-	55,55,55	0.63	2 (3%)	68,69,69	1.85	18 (26%)
24	CLA	b	607	-	65,73,73	2.08	16 (24%)	76,113,113	2.84	32 (42%)
24	CLA	C	514	-	65,73,73	2.02	16 (24%)	76,113,113	2.73	27 (35%)
34	LMG	b	625	-	51,51,55	0.90	2 (3%)	59,59,63	1.03	4 (6%)
35	HTG	V	204	-	19,19,19	1.00	2 (10%)	23,24,24	1.33	3 (13%)
26	BCR	B	620	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	13 (23%)
25	PHO	A	407	-	51,69,69	1.88	7 (13%)	47,99,99	1.69	9 (19%)
24	CLA	A	406	41	65,73,73	2.10	15 (23%)	76,113,113	2.75	31 (40%)
28	GOL	f	104	33	5,5,5	0.35	0	5,5,5	0.24	0
37	LHG	e	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.04	3 (6%)
26	BCR	B	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.00	3 (5%)
24	CLA	d	401	41	65,73,73	2.04	13 (20%)	76,113,113	2.71	28 (36%)
24	CLA	b	617	-	65,73,73	2.03	17 (26%)	76,113,113	2.64	27 (35%)
24	CLA	B	602	41	65,73,73	2.09	16 (24%)	76,113,113	2.77	28 (36%)
24	CLA	b	621	-	65,73,73	2.10	17 (26%)	76,113,113	2.70	27 (35%)
27	SQD	A	411	-	53,54,54	0.97	3 (5%)	62,65,65	1.58	11 (17%)
24	CLA	B	605	-	65,73,73	1.98	18 (27%)	76,113,113	2.88	26 (34%)
35	HTG	d	411	-	16,16,19	1.21	2 (12%)	20,21,24	1.55	1 (5%)
37	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.16	5 (9%)
26	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.25	5 (8%)
38	HEM	E	103	6,5	41,50,50	1.31	5 (12%)	45,82,82	1.94	14 (31%)
35	HTG	c	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	2 (8%)
28	GOL	v	205	-	5,5,5	0.35	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.86	0
35	HTG	C	522	-	19,19,19	1.01	2 (10%)	23,24,24	1.28	2 (8%)
26	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.39	8 (14%)
24	CLA	b	608	-	65,73,73	2.07	16 (24%)	76,113,113	2.86	30 (39%)
26	BCR	Y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	8 (14%)
35	HTG	c	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.50	2 (8%)
24	CLA	A	405	-	65,73,73	2.08	17 (26%)	76,113,113	2.74	29 (38%)
24	CLA	c	513	3	65,73,73	2.04	15 (23%)	76,113,113	2.68	26 (34%)
26	BCR	d	405	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	13 (23%)
28	GOL	V	208	-	5,5,5	0.37	0	5,5,5	0.27	0
35	HTG	b	603	-	19,19,19	1.07	2 (10%)	23,24,24	1.28	1 (4%)
27	SQD	a	402	-	53,54,54	1.03	3 (5%)	62,65,65	1.19	6 (9%)
30	LMT	b	626	-	25,25,36	0.50	0	30,30,47	0.64	0
37	LHG	D	409	-	48,48,48	0.85	2 (4%)	51,54,54	1.08	5 (9%)
37	LHG	l	102	-	48,48,48	0.95	2 (4%)	51,54,54	1.02	3 (5%)
30	LMT	D	402	-	36,36,36	0.48	0	47,47,47	1.01	3 (6%)
24	CLA	A	409	-	65,73,73	2.03	16 (24%)	76,113,113	2.77	29 (38%)
32	PL9	d	406	-	55,55,55	0.71	1 (1%)	68,69,69	1.55	14 (20%)
28	GOL	c	524	-	5,5,5	0.32	0	5,5,5	0.37	0
24	CLA	B	604	-	65,73,73	2.07	16 (24%)	76,113,113	2.81	31 (40%)
36	DGD	D	407	-	63,63,67	0.96	4 (6%)	77,77,81	1.30	9 (11%)
26	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.33	8 (14%)
24	CLA	C	504	-	65,73,73	2.09	16 (24%)	76,113,113	2.75	26 (34%)
23	BCT	A	404	21	2,3,3	0.65	0	2,3,3	0.87	0
24	CLA	B	612	-	65,73,73	2.07	16 (24%)	76,113,113	2.81	25 (32%)
24	CLA	D	404	-	65,73,73	2.02	15 (23%)	76,113,113	2.76	29 (38%)
24	CLA	C	507	-	65,73,73	2.06	16 (24%)	76,113,113	2.70	29 (38%)
28	GOL	B	627	-	5,5,5	0.34	0	5,5,5	0.71	0
36	DGD	d	407	-	63,63,67	0.94	3 (4%)	77,77,81	1.04	6 (7%)
30	LMT	a	417	-	36,36,36	0.44	0	47,47,47	0.84	2 (4%)
31	OEX	a	415	1,41,3	0,15,15	-	-	-		
28	GOL	V	207	-	5,5,5	0.37	0	5,5,5	0.46	0
24	CLA	C	505	41	65,73,73	2.06	16 (24%)	76,113,113	2.75	26 (34%)
36	DGD	c	519	-	63,63,67	0.89	2 (3%)	77,77,81	0.97	3 (3%)
38	HEM	e	102	6,5	41,50,50	1.32	6 (14%)	45,82,82	1.91	11 (24%)
28	GOL	T	103	-	5,5,5	0.41	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	HTG	b	628	-	19,19,19	1.10	2 (10%)	23,24,24	1.83	3 (13%)
30	LMT	b	602	-	25,25,36	0.46	0	30,30,47	1.26	3 (10%)
37	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.09	3 (6%)
26	BCR	t	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.32	8 (14%)
28	GOL	T	101	-	5,5,5	0.45	0	5,5,5	0.31	0
23	BCT	a	418	21	2,3,3	0.60	0	2,3,3	0.82	0
34	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.11	5 (8%)
36	DGD	c	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	3 (3%)
35	HTG	B	624	-	19,19,19	1.06	2 (10%)	23,24,24	1.89	4 (17%)
40	HEC	V	203	16	32,50,50	1.38	4 (12%)	24,82,82	1.55	4 (16%)
24	CLA	B	611	41	65,73,73	2.05	16 (24%)	76,113,113	2.75	29 (38%)
28	GOL	B	635	-	5,5,5	0.40	0	5,5,5	0.25	0
30	LMT	A	417	-	34,34,36	0.38	0	45,45,47	1.06	3 (6%)
24	CLA	B	603	-	65,73,73	2.05	18 (27%)	76,113,113	2.83	29 (38%)
36	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.02	5 (6%)
24	CLA	B	609	-	65,73,73	2.11	16 (24%)	76,113,113	2.71	28 (36%)
24	CLA	C	502	-	65,73,73	2.00	16 (24%)	76,113,113	2.65	25 (32%)
24	CLA	c	508	-	65,73,73	2.05	17 (26%)	76,113,113	2.67	31 (40%)
36	DGD	c	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.09	6 (7%)
27	SQD	b	601	-	53,54,54	1.02	3 (5%)	62,65,65	1.63	10 (16%)
28	GOL	b	630	-	5,5,5	0.34	0	5,5,5	0.16	0
24	CLA	c	509	41	65,73,73	2.01	15 (23%)	76,113,113	2.74	25 (32%)
26	BCR	b	624	-	41,41,41	0.99	1 (2%)	56,56,56	1.25	8 (14%)
24	CLA	b	609	-	65,73,73	2.09	18 (27%)	76,113,113	2.80	26 (34%)
34	LMG	z	101	-	39,39,55	1.11	2 (5%)	47,47,63	1.17	4 (8%)
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	7 (9%)
27	SQD	F	101	-	42,43,54	1.12	3 (7%)	51,54,65	1.55	9 (17%)
34	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	4 (6%)
24	CLA	B	613	-	65,73,73	2.06	17 (26%)	76,113,113	2.61	24 (31%)
24	CLA	D	403	-	65,73,73	2.05	17 (26%)	76,113,113	2.80	27 (35%)
26	BCR	a	410	-	41,41,41	1.14	1 (2%)	56,56,56	1.35	8 (14%)
37	LHG	d	410	-	48,48,48	0.94	2 (4%)	51,54,54	0.97	3 (5%)
27	SQD	f	101	-	42,43,54	1.18	3 (7%)	51,54,65	1.44	7 (13%)
24	CLA	B	617	-	65,73,73	2.04	16 (24%)	76,113,113	2.72	26 (34%)
24	CLA	c	515	-	65,73,73	2.08	17 (26%)	76,113,113	2.73	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	LMG	c	501	-	51,51,55	0.88	2 (3%)	59,59,63	1.25	6 (10%)
35	HTG	B	631	-	19,19,19	1.03	2 (10%)	23,24,24	1.44	2 (8%)
34	LMG	C	501	-	51,51,55	0.97	2 (3%)	59,59,63	1.10	3 (5%)
24	CLA	b	615	41	65,73,73	2.06	16 (24%)	76,113,113	2.66	27 (35%)
24	CLA	c	507	-	65,73,73	2.00	16 (24%)	76,113,113	2.58	21 (27%)
26	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	5 (8%)
35	HTG	D	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.03	3 (15%)
28	GOL	b	633	-	5,5,5	0.37	0	5,5,5	0.39	0
24	CLA	c	511	-	65,73,73	2.17	16 (24%)	76,113,113	2.72	26 (34%)
30	LMT	m	103	-	36,36,36	0.56	1 (2%)	47,47,47	1.05	4 (8%)
24	CLA	b	616	-	65,73,73	2.04	16 (24%)	76,113,113	2.79	27 (35%)
32	PL9	D	406	-	55,55,55	0.77	2 (3%)	68,69,69	1.50	16 (23%)
35	HTG	B	623	-	19,19,19	0.88	1 (5%)	23,24,24	1.25	3 (13%)
24	CLA	b	620	-	65,73,73	2.07	16 (24%)	76,113,113	2.76	25 (32%)
31	OEX	A	418	1,41,3	0,15,15	-	-	-		
24	CLA	d	402	-	65,73,73	2.07	17 (26%)	76,113,113	2.78	27 (35%)
28	GOL	A	413	-	5,5,5	0.43	0	5,5,5	0.62	0
35	HTG	b	627	-	19,19,19	0.86	1 (5%)	23,24,24	1.35	4 (17%)
37	LHG	D	408	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
34	LMG	J	101	39	51,51,55	0.84	2 (3%)	59,59,63	1.01	4 (6%)
28	GOL	V	201	-	5,5,5	0.38	0	5,5,5	0.43	0
26	BCR	B	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.24	5 (8%)
24	CLA	b	614	-	65,73,73	2.09	15 (23%)	76,113,113	2.77	28 (36%)
36	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	0.89	3 (3%)
24	CLA	C	512	3	65,73,73	2.01	16 (24%)	76,113,113	2.75	24 (31%)
35	HTG	B	630	-	19,19,19	0.97	2 (10%)	23,24,24	1.31	1 (4%)
35	HTG	B	622	-	19,19,19	1.20	1 (5%)	23,24,24	1.43	3 (13%)
37	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.09	5 (9%)
28	GOL	V	206	-	5,5,5	0.37	0	5,5,5	0.46	0
28	GOL	v	203	-	5,5,5	0.27	0	5,5,5	0.49	0
24	CLA	a	409	-	65,73,73	2.03	16 (24%)	76,113,113	2.72	28 (36%)
30	LMT	a	401	-	36,36,36	0.45	0	47,47,47	0.97	3 (6%)
34	LMG	c	521	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	5 (8%)
28	GOL	v	204	-	5,5,5	0.32	0	5,5,5	0.37	0
36	DGD	H	102	-	63,63,67	0.93	3 (4%)	77,77,81	0.90	3 (3%)
24	CLA	C	508	41	65,73,73	2.07	16 (24%)	76,113,113	2.76	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	LMG	j	101	39	51,51,55	0.93	3 (5%)	59,59,63	0.98	3 (5%)
24	CLA	B	616	-	65,73,73	2.03	17 (26%)	76,113,113	2.70	28 (36%)
24	CLA	b	619	-	65,73,73	2.02	16 (24%)	76,113,113	2.82	29 (38%)
28	GOL	C	524	-	5,5,5	0.34	0	5,5,5	0.89	0
24	CLA	D	401	41	65,73,73	2.08	16 (24%)	76,113,113	2.73	31 (40%)
25	PHO	d	403	-	51,69,69	1.87	7 (13%)	47,99,99	1.93	11 (23%)
26	BCR	b	623	-	41,41,41	1.08	1 (2%)	56,56,56	1.13	5 (8%)
24	CLA	d	404	-	65,73,73	2.04	18 (27%)	76,113,113	2.80	27 (35%)
25	PHO	a	408	-	51,69,69	1.83	7 (13%)	47,99,99	1.75	8 (17%)
37	LHG	d	408	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	5 (9%)
28	GOL	B	625	-	5,5,5	0.31	0	5,5,5	0.56	0
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	10 (17%)
24	CLA	b	610	-	65,73,73	1.99	16 (24%)	76,113,113	2.91	28 (36%)
28	GOL	A	414	-	5,5,5	0.41	0	5,5,5	0.20	0
30	LMT	f	102	-	36,36,36	0.47	0	47,47,47	0.77	0
26	BCR	D	405	-	41,41,41	1.05	1 (2%)	56,56,56	1.70	12 (21%)
24	CLA	a	406	-	65,73,73	2.07	16 (24%)	76,113,113	2.73	28 (36%)
27	SQD	l	101	-	53,54,54	1.00	3 (5%)	62,65,65	1.40	9 (14%)
28	GOL	B	628	-	5,5,5	0.40	0	5,5,5	0.29	0
35	HTG	C	523	-	19,19,19	1.02	2 (10%)	23,24,24	1.77	5 (21%)
28	GOL	a	413	-	5,5,5	0.43	0	5,5,5	0.27	0
35	HTG	b	604	-	19,19,19	1.02	2 (10%)	23,24,24	1.10	2 (8%)
37	LHG	D	410	-	48,48,48	0.94	2 (4%)	51,54,54	0.94	3 (5%)
28	GOL	O	302	-	5,5,5	0.36	0	5,5,5	0.35	0
28	GOL	V	205	-	5,5,5	0.37	0	5,5,5	0.30	0
24	CLA	C	513	-	65,73,73	2.04	16 (24%)	76,113,113	2.73	31 (40%)

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
24	CLA	c	506	41	1/1/15/20	6/37/115/115	-
24	CLA	B	610	-	1/1/15/20	3/37/115/115	-
28	GOL	a	412	-	-	2/4/4/4	-
28	GOL	c	527	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	629	-	-	0/4/4/4	-
24	CLA	c	512	-	1/1/15/20	7/37/115/115	-
28	GOL	A	412	-	-	2/4/4/4	-
24	CLA	c	505	-	1/1/15/20	4/37/115/115	-
24	CLA	C	510	-	1/1/15/20	4/37/115/115	-
28	GOL	t	102	-	-	0/4/4/4	-
24	CLA	c	510	-	1/1/15/20	2/37/115/115	-
28	GOL	B	633	-	-	0/4/4/4	-
24	CLA	a	407	41	-	3/37/115/115	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
26	BCR	T	102	-	-	0/29/63/63	0/2/2/2
28	GOL	b	629	-	-	2/4/4/4	-
30	LMT	M	101	-	-	8/21/61/61	0/2/2/2
24	CLA	C	506	-	1/1/15/20	5/37/115/115	-
24	CLA	C	511	-	1/1/15/20	8/37/115/115	-
24	CLA	B	614	-	1/1/15/20	9/37/115/115	-
27	SQD	A	416	-	-	17/49/69/69	0/1/1/1
24	CLA	b	613	-	-	2/37/115/115	-
24	CLA	b	618	-	1/1/15/20	6/37/115/115	-
24	CLA	c	503	-	1/1/15/20	3/37/115/115	-
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
26	BCR	c	526	-	-	1/29/63/63	0/2/2/2
24	CLA	C	503	-	-	8/37/115/115	-
30	LMT	m	102	-	-	3/21/61/61	0/2/2/2
34	LMG	C	521	-	-	14/46/66/70	0/1/1/1
30	LMT	B	634	-	-	5/17/37/61	0/1/1/2
24	CLA	C	509	-	-	3/37/115/115	-
26	BCR	k	103	-	-	1/29/63/63	0/2/2/2
24	CLA	c	514	-	1/1/15/20	12/37/115/115	-
26	BCR	c	516	-	-	4/29/63/63	0/2/2/2
30	LMT	E	102	-	-	9/21/61/61	0/2/2/2
24	CLA	c	504	-	1/1/15/20	3/37/115/115	-
34	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
35	HTG	O	303	-	-	2/10/30/30	0/1/1/1
24	CLA	B	606	-	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	612	41	1/1/15/20	3/37/115/115	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	b	611	-	1/1/15/20	8/37/115/115	-
24	CLA	B	607	-	1/1/15/20	4/37/115/115	-
40	HEC	v	202	16	-	2/10/54/54	-
32	PL9	A	419	-	-	8/53/73/73	0/1/1/1
34	LMG	c	520	-	-	5/46/66/70	0/1/1/1
28	GOL	C	525	-	-	0/4/4/4	-
28	GOL	b	631	-	-	2/4/4/4	-
24	CLA	B	615	-	1/1/15/20	14/37/115/115	-
25	PHO	A	408	-	-	1/37/103/103	0/5/6/6
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
28	GOL	c	525	-	-	1/4/4/4	-
28	GOL	v	201	-	-	0/4/4/4	-
24	CLA	B	608	41	1/1/15/20	5/37/115/115	-
24	CLA	b	606	41	1/1/15/20	14/37/115/115	-
28	GOL	b	632	-	-	2/4/4/4	-
30	LMT	I	102	-	-	10/21/61/61	0/2/2/2
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
27	SQD	a	411	-	-	9/49/69/69	0/1/1/1
28	GOL	F	103	33	-	2/4/4/4	-
32	PL9	a	416	-	-	17/53/73/73	0/1/1/1
24	CLA	b	607	-	1/1/15/20	3/37/115/115	-
24	CLA	C	514	-	-	3/37/115/115	-
34	LMG	b	625	-	-	18/46/66/70	0/1/1/1
35	HTG	V	204	-	-	3/10/30/30	0/1/1/1
26	BCR	B	620	-	-	5/29/63/63	0/2/2/2
25	PHO	A	407	-	-	3/37/103/103	0/5/6/6
24	CLA	A	406	41	-	5/37/115/115	-
28	GOL	f	104	33	-	3/4/4/4	-
37	LHG	e	101	-	-	18/46/46/53	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	d	401	41	1/1/15/20	7/37/115/115	-
24	CLA	b	617	-	1/1/15/20	3/37/115/115	-
24	CLA	B	602	41	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	621	-	1/1/15/20	10/37/115/115	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
24	CLA	B	605	-	1/1/15/20	4/37/115/115	-
35	HTG	d	411	-	-	2/7/27/30	0/1/1/1
37	LHG	L	101	-	-	12/53/53/53	-
26	BCR	H	101	-	-	1/29/63/63	0/2/2/2
38	HEM	E	103	6,5	-	2/12/54/54	-
35	HTG	c	523	-	-	1/10/30/30	0/1/1/1
28	GOL	v	205	-	-	2/4/4/4	-
30	LMT	M	102	-	-	5/21/61/61	0/2/2/2
35	HTG	C	522	-	-	2/10/30/30	0/1/1/1
26	BCR	C	516	-	-	3/29/63/63	0/2/2/2
24	CLA	b	608	-	1/1/15/20	7/37/115/115	-
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
35	HTG	c	522	-	-	1/10/30/30	0/1/1/1
24	CLA	A	405	-	1/1/15/20	1/37/115/115	-
24	CLA	c	513	3	1/1/15/20	5/37/115/115	-
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
28	GOL	V	208	-	-	2/4/4/4	-
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
27	SQD	a	402	-	-	17/49/69/69	0/1/1/1
30	LMT	b	626	-	-	6/17/37/61	0/1/1/2
37	LHG	D	409	-	-	9/53/53/53	-
37	LHG	l	102	-	-	18/53/53/53	-
30	LMT	D	402	-	-	9/21/61/61	0/2/2/2
24	CLA	A	409	-	-	11/37/115/115	-
32	PL9	d	406	-	-	3/53/73/73	0/1/1/1
28	GOL	c	524	-	-	0/4/4/4	-
24	CLA	B	604	-	1/1/15/20	3/37/115/115	-
36	DGD	D	407	-	-	17/51/91/95	0/2/2/2
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
24	CLA	C	504	-	-	4/37/115/115	-
24	CLA	B	612	-	-	3/37/115/115	-
24	CLA	D	404	-	1/1/15/20	5/37/115/115	-
24	CLA	C	507	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	627	-	-	2/4/4/4	-
36	DGD	d	407	-	-	20/51/91/95	0/2/2/2
30	LMT	a	417	-	-	2/21/61/61	0/2/2/2
28	GOL	V	207	-	-	0/4/4/4	-
24	CLA	C	505	41	1/1/15/20	4/37/115/115	-
36	DGD	c	519	-	-	12/51/91/95	0/2/2/2
38	HEM	e	102	6,5	-	4/12/54/54	-
28	GOL	T	103	-	-	3/4/4/4	-
35	HTG	b	628	-	-	2/10/30/30	0/1/1/1
30	LMT	b	602	-	-	7/17/37/61	0/1/1/2
37	LHG	E	101	-	-	20/46/46/53	-
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2
28	GOL	T	101	-	-	2/4/4/4	-
34	LMG	C	520	-	-	13/46/66/70	0/1/1/1
36	DGD	c	518	-	-	15/51/91/95	0/2/2/2
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
40	HEC	V	203	16	-	2/10/54/54	-
24	CLA	B	611	41	1/1/15/20	3/37/115/115	-
28	GOL	B	635	-	-	2/4/4/4	-
30	LMT	A	417	-	-	3/19/59/61	0/2/2/2
24	CLA	B	603	-	1/1/15/20	7/37/115/115	-
36	DGD	C	518	-	-	19/51/91/95	0/2/2/2
24	CLA	C	502	-	1/1/15/20	9/37/115/115	-
24	CLA	B	609	-	-	1/37/115/115	-
24	CLA	c	508	-	1/1/15/20	8/37/115/115	-
36	DGD	c	517	-	-	12/51/91/95	0/2/2/2
27	SQD	b	601	-	-	20/49/69/69	0/1/1/1
28	GOL	b	630	-	-	0/4/4/4	-
24	CLA	c	509	41	1/1/15/20	3/37/115/115	-
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
24	CLA	b	609	-	1/1/15/20	3/37/115/115	-
34	LMG	z	101	-	-	13/34/54/70	0/1/1/1
36	DGD	h	102	-	-	9/51/91/95	0/2/2/2
27	SQD	F	101	-	-	12/38/58/69	0/1/1/1
34	LMG	B	621	-	-	7/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	613	-	1/1/15/20	2/37/115/115	-
24	CLA	D	403	-	1/1/15/20	2/37/115/115	-
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
37	LHG	d	410	-	-	13/53/53/53	-
27	SQD	f	101	-	-	16/38/58/69	0/1/1/1
24	CLA	B	617	-	1/1/15/20	9/37/115/115	-
24	CLA	c	515	-	-	4/37/115/115	-
34	LMG	c	501	-	-	14/46/66/70	0/1/1/1
35	HTG	B	631	-	-	1/10/30/30	0/1/1/1
34	LMG	C	501	-	-	16/46/66/70	0/1/1/1
24	CLA	b	615	41	1/1/15/20	6/37/115/115	-
24	CLA	c	507	-	1/1/15/20	3/37/115/115	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
35	HTG	D	411	-	-	1/7/27/30	0/1/1/1
28	GOL	b	633	-	-	2/4/4/4	-
24	CLA	c	511	-	1/1/15/20	9/37/115/115	-
30	LMT	m	103	-	-	6/21/61/61	0/2/2/2
24	CLA	b	616	-	1/1/15/20	2/37/115/115	-
32	PL9	D	406	-	-	1/53/73/73	0/1/1/1
35	HTG	B	623	-	-	5/10/30/30	0/1/1/1
24	CLA	b	620	-	1/1/15/20	4/37/115/115	-
24	CLA	d	402	-	1/1/15/20	1/37/115/115	-
28	GOL	A	413	-	-	2/4/4/4	-
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
37	LHG	D	408	-	-	9/53/53/53	-
34	LMG	J	101	39	-	9/46/66/70	0/1/1/1
28	GOL	V	201	-	-	0/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	b	614	-	1/1/15/20	3/37/115/115	-
36	DGD	C	519	-	-	5/51/91/95	0/2/2/2
24	CLA	C	512	3	1/1/15/20	1/37/115/115	-
35	HTG	B	630	-	-	1/10/30/30	0/1/1/1
35	HTG	B	622	-	-	1/10/30/30	0/1/1/1
37	LHG	d	409	-	-	11/53/53/53	-
28	GOL	V	206	-	-	2/4/4/4	-
28	GOL	v	203	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	409	-	1/1/15/20	11/37/115/115	-
30	LMT	a	401	-	-	9/21/61/61	0/2/2/2
34	LMG	c	521	-	-	6/46/66/70	0/1/1/1
28	GOL	v	204	-	-	2/4/4/4	-
36	DGD	H	102	-	-	11/51/91/95	0/2/2/2
24	CLA	C	508	41	1/1/15/20	11/37/115/115	-
34	LMG	j	101	39	-	12/46/66/70	0/1/1/1
24	CLA	B	616	-	1/1/15/20	8/37/115/115	-
24	CLA	b	619	-	1/1/15/20	14/37/115/115	-
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	D	401	41	1/1/15/20	5/37/115/115	-
25	PHO	d	403	-	-	3/37/103/103	0/5/6/6
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
24	CLA	d	404	-	1/1/15/20	6/37/115/115	-
25	PHO	a	408	-	-	2/37/103/103	0/5/6/6
37	LHG	d	408	-	-	9/53/53/53	-
28	GOL	B	625	-	-	2/4/4/4	-
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
24	CLA	b	610	-	1/1/15/20	5/37/115/115	-
28	GOL	A	414	-	-	2/4/4/4	-
30	LMT	f	102	-	-	7/21/61/61	0/2/2/2
26	BCR	D	405	-	-	6/29/63/63	0/2/2/2
24	CLA	a	406	-	1/1/15/20	3/37/115/115	-
27	SQD	l	101	-	-	20/49/69/69	0/1/1/1
28	GOL	B	628	-	-	2/4/4/4	-
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
28	GOL	a	413	-	-	4/4/4/4	-
35	HTG	b	604	-	-	1/10/30/30	0/1/1/1
37	LHG	D	410	-	-	14/53/53/53	-
28	GOL	O	302	-	-	2/4/4/4	-
28	GOL	V	205	-	-	4/4/4/4	-
24	CLA	C	513	-	1/1/15/20	10/37/115/115	-

All (1329) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	PHO	C3B-C2B	6.65	1.49	1.40
24	c	511	CLA	C3B-C2B	6.62	1.49	1.40
24	B	617	CLA	C3B-C2B	6.61	1.49	1.40
24	C	511	CLA	C3B-C2B	6.55	1.49	1.40
25	A	408	PHO	C3B-C2B	6.51	1.49	1.40
24	A	405	CLA	C3B-C2B	6.45	1.49	1.40
25	a	408	PHO	C3B-C2B	6.44	1.49	1.40
24	B	609	CLA	C3B-C2B	6.41	1.49	1.40
25	A	407	PHO	C3B-C2B	6.39	1.49	1.40
24	c	510	CLA	C3B-C2B	6.38	1.49	1.40
24	b	618	CLA	C3B-C2B	6.36	1.49	1.40
24	C	504	CLA	C3B-C2B	6.35	1.49	1.40
24	b	621	CLA	C3B-C2B	6.29	1.49	1.40
24	B	613	CLA	C3B-C2B	6.29	1.49	1.40
24	B	614	CLA	C3B-C2B	6.28	1.49	1.40
24	B	603	CLA	C3B-C2B	6.26	1.49	1.40
24	B	612	CLA	C3B-C2B	6.22	1.49	1.40
24	C	508	CLA	C3B-C2B	6.21	1.49	1.40
24	b	608	CLA	C3B-C2B	6.20	1.49	1.40
24	B	604	CLA	C3B-C2B	6.20	1.49	1.40
24	c	503	CLA	C3B-C2B	6.19	1.49	1.40
24	B	602	CLA	C3B-C2B	6.17	1.48	1.40
24	C	506	CLA	C3B-C2B	6.17	1.48	1.40
24	C	513	CLA	C3B-C2B	6.16	1.48	1.40
24	B	605	CLA	C3B-C2B	6.15	1.48	1.40
24	b	615	CLA	C3B-C2B	6.13	1.48	1.40
24	b	619	CLA	C3B-C2B	6.12	1.48	1.40
24	D	401	CLA	C3B-C2B	6.07	1.48	1.40
24	d	401	CLA	C3B-C2B	6.06	1.48	1.40
24	d	402	CLA	C3B-C2B	6.06	1.48	1.40
24	C	509	CLA	C3B-C2B	6.04	1.48	1.40
24	C	514	CLA	C3B-C2B	6.03	1.48	1.40
24	b	607	CLA	C3B-C2B	6.03	1.48	1.40
24	b	606	CLA	C3B-C2B	6.00	1.48	1.40
24	b	609	CLA	C1D-ND	6.00	1.45	1.37
24	B	608	CLA	C3B-C2B	5.98	1.48	1.40
24	b	620	CLA	C3B-C2B	5.98	1.48	1.40
24	C	502	CLA	C3B-C2B	5.96	1.48	1.40
24	b	611	CLA	C3B-C2B	5.96	1.48	1.40
24	b	609	CLA	C3B-C2B	5.95	1.48	1.40
24	B	611	CLA	C3B-C2B	5.93	1.48	1.40
24	c	513	CLA	C3B-C2B	5.91	1.48	1.40
24	B	607	CLA	C3B-C2B	5.90	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	CLA	C3B-C2B	5.89	1.48	1.40
24	C	510	CLA	C3B-C2B	5.89	1.48	1.40
24	C	503	CLA	C3B-C2B	5.88	1.48	1.40
24	b	617	CLA	C3B-C2B	5.87	1.48	1.40
24	D	404	CLA	C3B-C2B	5.86	1.48	1.40
24	c	512	CLA	C3B-C2B	5.86	1.48	1.40
24	c	508	CLA	C3B-C2B	5.84	1.48	1.40
24	c	506	CLA	C3B-C2B	5.83	1.48	1.40
24	b	613	CLA	C3B-C2B	5.81	1.48	1.40
24	c	514	CLA	C3B-C2B	5.80	1.48	1.40
24	D	403	CLA	C3B-C2B	5.78	1.48	1.40
24	A	406	CLA	C1D-ND	5.75	1.44	1.37
24	c	515	CLA	C3B-C2B	5.75	1.48	1.40
24	a	407	CLA	C3B-C2B	5.74	1.48	1.40
24	C	507	CLA	C3B-C2B	5.74	1.48	1.40
24	A	406	CLA	C3B-C2B	5.74	1.48	1.40
24	c	509	CLA	C3B-C2B	5.74	1.48	1.40
24	c	511	CLA	C1D-ND	5.72	1.44	1.37
24	A	409	CLA	C3B-C2B	5.71	1.48	1.40
24	b	612	CLA	C3B-C2B	5.69	1.48	1.40
24	b	614	CLA	C1D-ND	5.68	1.44	1.37
24	b	606	CLA	C3C-C2C	5.67	1.48	1.36
24	C	505	CLA	C3B-C2B	5.63	1.48	1.40
25	A	408	PHO	C3D-C2D	5.63	1.49	1.39
24	b	616	CLA	C3B-C2B	5.62	1.48	1.40
24	B	609	CLA	C3C-C2C	5.61	1.48	1.36
24	A	409	CLA	C3C-C2C	5.60	1.48	1.36
24	a	406	CLA	C1D-ND	5.58	1.44	1.37
25	d	403	PHO	C3D-C2D	5.58	1.49	1.39
24	B	605	CLA	C1D-ND	5.54	1.44	1.37
24	B	612	CLA	C3C-C2C	5.51	1.48	1.36
24	b	614	CLA	C3B-C2B	5.50	1.48	1.40
24	B	602	CLA	C3C-C2C	5.50	1.48	1.36
24	B	615	CLA	C3B-C2B	5.48	1.48	1.40
24	C	504	CLA	C1D-ND	5.47	1.44	1.37
24	C	512	CLA	C3B-C2B	5.46	1.47	1.40
24	B	611	CLA	C3C-C2C	5.45	1.48	1.36
24	C	509	CLA	C3C-C2C	5.45	1.48	1.36
24	B	609	CLA	C1D-ND	5.43	1.44	1.37
24	C	506	CLA	C3C-C2C	5.42	1.48	1.36
24	c	506	CLA	C3C-C2C	5.42	1.48	1.36
24	d	404	CLA	C3B-C2B	5.41	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	409	CLA	C3B-C2B	5.40	1.47	1.40
24	C	503	CLA	C3C-C2C	5.40	1.48	1.36
24	c	511	CLA	C3C-C2C	5.39	1.48	1.36
24	C	504	CLA	C3C-C2C	5.38	1.48	1.36
24	b	620	CLA	C3C-C2C	5.38	1.48	1.36
24	c	503	CLA	C3C-C2C	5.37	1.48	1.36
24	B	610	CLA	CHC-C1C	5.37	1.48	1.35
24	a	406	CLA	C3C-C2C	5.35	1.48	1.36
24	b	617	CLA	C3C-C2C	5.35	1.48	1.36
25	A	407	PHO	C3D-C2D	5.35	1.49	1.39
24	D	404	CLA	C3C-C2C	5.35	1.48	1.36
24	B	606	CLA	C3B-C2B	5.35	1.47	1.40
24	b	618	CLA	C3C-C2C	5.35	1.48	1.36
24	c	514	CLA	C3C-C2C	5.35	1.48	1.36
24	B	616	CLA	C1D-ND	5.34	1.44	1.37
24	a	407	CLA	C1D-ND	5.34	1.44	1.37
24	b	610	CLA	C1D-ND	5.34	1.44	1.37
24	c	505	CLA	C3B-C2B	5.34	1.47	1.40
24	c	512	CLA	C3C-C2C	5.34	1.48	1.36
24	b	614	CLA	O2D-CGD	5.34	1.46	1.33
24	b	606	CLA	C1D-ND	5.33	1.44	1.37
24	c	508	CLA	C1D-ND	5.33	1.44	1.37
24	b	613	CLA	C3C-C2C	5.33	1.48	1.36
24	d	402	CLA	C3C-C2C	5.32	1.48	1.36
24	c	504	CLA	C3C-C2C	5.32	1.48	1.36
24	b	621	CLA	C1D-ND	5.32	1.44	1.37
24	a	409	CLA	C3C-C2C	5.32	1.48	1.36
24	B	613	CLA	CHC-C1C	5.31	1.48	1.35
24	b	620	CLA	C1D-ND	5.31	1.44	1.37
24	C	510	CLA	C3C-C2C	5.30	1.48	1.36
24	c	509	CLA	C3C-C2C	5.30	1.48	1.36
24	c	504	CLA	C3B-C2B	5.28	1.47	1.40
24	b	617	CLA	CHC-C1C	5.28	1.48	1.35
24	C	513	CLA	C3C-C2C	5.28	1.48	1.36
24	b	607	CLA	C3C-C2C	5.27	1.47	1.36
24	B	607	CLA	C1D-ND	5.27	1.44	1.37
24	c	510	CLA	C3C-C2C	5.26	1.47	1.36
24	C	510	CLA	O2D-CGD	5.26	1.46	1.33
24	B	610	CLA	C3B-C2B	5.26	1.47	1.40
24	B	604	CLA	C3C-C2C	5.26	1.47	1.36
24	C	511	CLA	C3C-C2C	5.25	1.47	1.36
24	B	606	CLA	O2D-CGD	5.25	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	C3C-C2C	5.25	1.47	1.36
24	b	606	CLA	O2D-CGD	5.25	1.46	1.33
24	b	611	CLA	CHC-C1C	5.23	1.48	1.35
24	C	505	CLA	C3C-C2C	5.23	1.47	1.36
24	c	515	CLA	CHC-C1C	5.22	1.48	1.35
24	c	505	CLA	CHC-C1C	5.22	1.48	1.35
24	C	507	CLA	C3C-C2C	5.22	1.47	1.36
24	c	505	CLA	C1D-ND	5.22	1.44	1.37
24	b	616	CLA	CHC-C1C	5.21	1.48	1.35
25	A	407	PHO	OBD-CAD	5.21	1.29	1.22
24	b	607	CLA	CHC-C1C	5.21	1.48	1.35
24	b	608	CLA	C1D-ND	5.21	1.44	1.37
24	b	615	CLA	C3C-C2C	5.21	1.47	1.36
24	b	608	CLA	CHC-C1C	5.20	1.48	1.35
24	B	602	CLA	O2D-CGD	5.20	1.45	1.33
24	a	407	CLA	CHC-C1C	5.19	1.48	1.35
24	B	610	CLA	C3C-C2C	5.19	1.47	1.36
24	B	602	CLA	CHC-C1C	5.19	1.48	1.35
24	B	616	CLA	CHC-C1C	5.19	1.48	1.35
24	b	608	CLA	C3C-C2C	5.19	1.47	1.36
24	c	505	CLA	C3C-C2C	5.19	1.47	1.36
24	D	401	CLA	C3C-C2C	5.18	1.47	1.36
24	c	515	CLA	C3C-C2C	5.18	1.47	1.36
24	c	514	CLA	CHC-C1C	5.18	1.48	1.35
24	c	511	CLA	O2D-CGD	5.18	1.45	1.33
24	C	508	CLA	C1D-ND	5.17	1.44	1.37
24	A	406	CLA	C3C-C2C	5.17	1.47	1.36
24	C	503	CLA	CHC-C1C	5.17	1.48	1.35
24	C	503	CLA	C1D-ND	5.17	1.44	1.37
24	C	511	CLA	C1D-ND	5.17	1.44	1.37
24	c	506	CLA	O2D-CGD	5.17	1.45	1.33
24	B	603	CLA	C3C-C2C	5.17	1.47	1.36
24	b	612	CLA	C3C-C2C	5.16	1.47	1.36
24	c	507	CLA	C3C-C2C	5.16	1.47	1.36
24	c	513	CLA	C3C-C2C	5.16	1.47	1.36
24	B	617	CLA	O2D-CGD	5.15	1.45	1.33
24	a	407	CLA	C3C-C2C	5.15	1.47	1.36
24	B	615	CLA	CHC-C1C	5.15	1.48	1.35
24	b	610	CLA	C3B-C2B	5.15	1.47	1.40
24	b	615	CLA	CHC-C1C	5.14	1.48	1.35
24	B	613	CLA	C3C-C2C	5.14	1.47	1.36
24	b	618	CLA	O2D-CGD	5.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	CHC-C1C	5.14	1.48	1.35
24	C	510	CLA	C1D-ND	5.14	1.44	1.37
24	b	621	CLA	O2D-CGD	5.14	1.45	1.33
24	c	510	CLA	CHC-C1C	5.14	1.48	1.35
24	C	507	CLA	C1D-ND	5.14	1.44	1.37
24	d	401	CLA	C3C-C2C	5.13	1.47	1.36
24	C	512	CLA	C3C-C2C	5.13	1.47	1.36
24	b	616	CLA	C1D-ND	5.13	1.44	1.37
24	b	606	CLA	CHC-C1C	5.12	1.48	1.35
24	c	508	CLA	C3C-C2C	5.12	1.47	1.36
24	c	515	CLA	O2D-CGD	5.12	1.45	1.33
24	b	618	CLA	C1D-ND	5.11	1.44	1.37
24	b	616	CLA	C3C-C2C	5.11	1.47	1.36
24	B	614	CLA	C3C-C2C	5.10	1.47	1.36
24	A	405	CLA	CHC-C1C	5.10	1.48	1.35
24	B	607	CLA	C3C-C2C	5.10	1.47	1.36
24	d	404	CLA	CHC-C1C	5.09	1.48	1.35
24	b	613	CLA	O2D-CGD	5.09	1.45	1.33
24	b	611	CLA	C1D-ND	5.08	1.44	1.37
24	D	404	CLA	CHC-C1C	5.08	1.48	1.35
24	B	607	CLA	O2D-CGD	5.08	1.45	1.33
24	a	406	CLA	O2D-CGD	5.08	1.45	1.33
24	A	406	CLA	CHC-C1C	5.08	1.48	1.35
24	B	617	CLA	C3C-C2C	5.07	1.47	1.36
24	b	621	CLA	C3C-C2C	5.07	1.47	1.36
24	B	610	CLA	C1D-ND	5.07	1.44	1.37
24	C	505	CLA	CHC-C1C	5.07	1.48	1.35
24	C	507	CLA	O2D-CGD	5.06	1.45	1.33
25	a	408	PHO	O2D-CGD	5.06	1.45	1.33
24	b	611	CLA	C3C-C2C	5.06	1.47	1.36
24	B	615	CLA	C3C-C2C	5.06	1.47	1.36
24	c	507	CLA	CHC-C1C	5.06	1.47	1.35
24	B	616	CLA	O2D-CGD	5.06	1.45	1.33
24	C	508	CLA	CHC-C1C	5.05	1.47	1.35
24	B	612	CLA	CHC-C1C	5.05	1.47	1.35
24	C	506	CLA	CHC-C1C	5.05	1.47	1.35
24	c	512	CLA	O2D-CGD	5.05	1.45	1.33
24	c	510	CLA	C1D-ND	5.05	1.44	1.37
24	c	512	CLA	CHC-C1C	5.04	1.47	1.35
24	B	605	CLA	CHC-C1C	5.04	1.47	1.35
26	c	526	BCR	C23-C22	-5.04	1.35	1.45
24	b	609	CLA	O2D-CGD	5.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	515	CLA	C1D-ND	5.04	1.44	1.37
24	b	607	CLA	O2D-CGD	5.04	1.45	1.33
24	B	603	CLA	CHC-C1C	5.03	1.47	1.35
24	B	606	CLA	C3C-C2C	5.03	1.47	1.36
24	C	512	CLA	CHC-C1C	5.03	1.47	1.35
24	b	610	CLA	C3C-C2C	5.02	1.47	1.36
24	B	607	CLA	CHC-C1C	5.02	1.47	1.35
24	c	514	CLA	O2D-CGD	5.02	1.45	1.33
24	b	610	CLA	CHC-C1C	5.02	1.47	1.35
24	C	508	CLA	C3C-C2C	5.02	1.47	1.36
24	c	513	CLA	O2D-CGD	5.01	1.45	1.33
24	a	409	CLA	C1D-ND	5.00	1.43	1.37
24	C	514	CLA	CHC-C1C	5.00	1.47	1.35
24	B	612	CLA	C1D-ND	5.00	1.43	1.37
24	B	609	CLA	CHC-C1C	4.99	1.47	1.35
24	b	613	CLA	C1D-ND	4.98	1.43	1.37
24	C	512	CLA	O2D-CGD	4.98	1.45	1.33
24	c	511	CLA	CHC-C1C	4.98	1.47	1.35
24	C	509	CLA	O2D-CGD	4.98	1.45	1.33
24	b	616	CLA	O2D-CGD	4.98	1.45	1.33
25	d	403	PHO	O2D-CGD	4.98	1.45	1.33
24	C	504	CLA	CHC-C1C	4.98	1.47	1.35
24	C	502	CLA	C3C-C2C	4.98	1.47	1.36
24	B	604	CLA	CHC-C1C	4.97	1.47	1.35
24	C	513	CLA	CHC-C1C	4.97	1.47	1.35
24	C	514	CLA	C1D-ND	4.97	1.43	1.37
24	A	405	CLA	C3C-C2C	4.97	1.47	1.36
24	b	617	CLA	O2D-CGD	4.97	1.45	1.33
24	B	602	CLA	C1D-ND	4.97	1.43	1.37
24	A	406	CLA	O2D-CGD	4.97	1.45	1.33
24	c	504	CLA	CHC-C1C	4.97	1.47	1.35
24	B	615	CLA	O2D-CGD	4.97	1.45	1.33
24	c	506	CLA	CHC-C1C	4.96	1.47	1.35
24	c	513	CLA	CHC-C1C	4.96	1.47	1.35
24	c	503	CLA	O2D-CGD	4.96	1.45	1.33
24	b	620	CLA	O2D-CGD	4.95	1.45	1.33
24	B	604	CLA	O2D-CGD	4.94	1.45	1.33
24	a	409	CLA	O2D-CGD	4.94	1.45	1.33
24	d	404	CLA	C3C-C2C	4.94	1.47	1.36
24	C	509	CLA	CHC-C1C	4.93	1.47	1.35
24	B	608	CLA	CHC-C1C	4.93	1.47	1.35
24	B	606	CLA	C1D-ND	4.92	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C3C-C2C	4.92	1.47	1.36
24	A	409	CLA	O2D-CGD	4.92	1.45	1.33
24	d	404	CLA	O2D-CGD	4.92	1.45	1.33
24	b	613	CLA	CHC-C1C	4.92	1.47	1.35
24	c	509	CLA	CHC-C1C	4.92	1.47	1.35
25	a	408	PHO	C3D-C2D	4.92	1.48	1.39
24	C	506	CLA	O2D-CGD	4.90	1.45	1.33
24	B	604	CLA	C1D-ND	4.90	1.43	1.37
24	b	619	CLA	CHC-C1C	4.89	1.47	1.35
24	C	514	CLA	C3C-C2C	4.89	1.47	1.36
24	B	614	CLA	O2D-CGD	4.89	1.45	1.33
24	b	607	CLA	C1D-ND	4.89	1.43	1.37
24	C	505	CLA	C1D-ND	4.89	1.43	1.37
24	B	611	CLA	CHC-C1C	4.89	1.47	1.35
24	B	609	CLA	O2D-CGD	4.88	1.45	1.33
24	b	620	CLA	CHC-C1C	4.88	1.47	1.35
24	C	513	CLA	O2D-CGD	4.88	1.45	1.33
24	b	619	CLA	O2D-CGD	4.88	1.45	1.33
24	d	401	CLA	C1D-ND	4.88	1.43	1.37
24	b	611	CLA	O2D-CGD	4.88	1.45	1.33
24	B	616	CLA	C3B-C2B	4.88	1.47	1.40
24	D	401	CLA	CHC-C1C	4.87	1.47	1.35
24	c	513	CLA	C1D-ND	4.87	1.43	1.37
24	B	614	CLA	C1D-ND	4.87	1.43	1.37
24	b	621	CLA	CHC-C1C	4.87	1.47	1.35
24	c	509	CLA	O2D-CGD	4.87	1.45	1.33
24	d	404	CLA	C1D-ND	4.86	1.43	1.37
24	B	611	CLA	C1D-ND	4.86	1.43	1.37
24	C	502	CLA	CHC-C1C	4.86	1.47	1.35
24	b	619	CLA	C3C-C2C	4.86	1.47	1.36
24	B	603	CLA	O2D-CGD	4.86	1.45	1.33
24	D	401	CLA	O2D-CGD	4.85	1.45	1.33
24	c	508	CLA	CHC-C1C	4.85	1.47	1.35
24	b	612	CLA	CHC-C1C	4.85	1.47	1.35
24	B	613	CLA	O2D-CGD	4.85	1.45	1.33
24	c	503	CLA	C1D-ND	4.84	1.43	1.37
24	c	507	CLA	C3B-C2B	4.84	1.47	1.40
24	C	511	CLA	CHC-C1C	4.84	1.47	1.35
26	C	515	BCR	C23-C22	-4.84	1.35	1.45
24	b	608	CLA	O2D-CGD	4.83	1.45	1.33
24	C	514	CLA	O2D-CGD	4.83	1.45	1.33
24	b	612	CLA	O2D-CGD	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C3C-C2C	4.83	1.47	1.36
24	c	503	CLA	CHC-C1C	4.83	1.47	1.35
24	C	510	CLA	CHC-C1C	4.83	1.47	1.35
24	C	508	CLA	O2D-CGD	4.82	1.45	1.33
24	b	609	CLA	CHC-C1C	4.82	1.47	1.35
24	c	505	CLA	O2D-CGD	4.82	1.45	1.33
26	d	405	BCR	C23-C22	-4.82	1.35	1.45
25	A	407	PHO	O2D-CGD	4.82	1.45	1.33
24	d	402	CLA	C1D-ND	4.82	1.43	1.37
26	y	101	BCR	C23-C22	-4.82	1.35	1.45
24	D	403	CLA	CHC-C1C	4.81	1.47	1.35
24	D	401	CLA	C1D-ND	4.81	1.43	1.37
24	c	508	CLA	O2D-CGD	4.80	1.44	1.33
24	D	404	CLA	O2D-CGD	4.80	1.44	1.33
24	C	507	CLA	CHC-C1C	4.80	1.47	1.35
24	b	618	CLA	CHC-C1C	4.79	1.47	1.35
24	B	617	CLA	CHC-C1C	4.79	1.47	1.35
24	a	409	CLA	CHC-C1C	4.79	1.47	1.35
24	B	614	CLA	CHC-C1C	4.79	1.47	1.35
26	C	516	BCR	C23-C22	-4.79	1.35	1.45
24	b	614	CLA	CHC-C1C	4.78	1.47	1.35
24	B	616	CLA	C3C-C2C	4.77	1.46	1.36
24	A	405	CLA	O2D-CGD	4.76	1.44	1.33
24	b	619	CLA	C1D-ND	4.75	1.43	1.37
24	C	510	CLA	CHD-C1D	4.75	1.47	1.38
24	a	406	CLA	CHC-C1C	4.74	1.47	1.35
24	C	503	CLA	O2D-CGD	4.73	1.44	1.33
24	d	402	CLA	CHC-C1C	4.73	1.47	1.35
24	C	502	CLA	O2D-CGD	4.72	1.44	1.33
26	B	620	BCR	C23-C22	-4.72	1.35	1.45
24	c	510	CLA	O2D-CGD	4.72	1.44	1.33
24	A	405	CLA	C1D-ND	4.72	1.43	1.37
24	c	511	CLA	CHD-C1D	4.72	1.47	1.38
24	C	509	CLA	CHD-C1D	4.71	1.47	1.38
25	A	408	PHO	O2D-CGD	4.70	1.44	1.33
24	C	509	CLA	C1D-ND	4.70	1.43	1.37
24	C	506	CLA	C1D-ND	4.70	1.43	1.37
24	C	511	CLA	O2D-CGD	4.70	1.44	1.33
24	d	402	CLA	O2A-CGA	4.69	1.47	1.33
24	c	512	CLA	C1D-ND	4.69	1.43	1.37
26	b	624	BCR	C23-C22	-4.68	1.35	1.45
24	B	611	CLA	O2D-CGD	4.68	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	O2D-CGD	4.68	1.44	1.33
24	c	504	CLA	O2D-CGD	4.67	1.44	1.33
24	B	612	CLA	O2D-CGD	4.67	1.44	1.33
24	c	509	CLA	C1D-ND	4.66	1.43	1.37
24	C	513	CLA	C1D-ND	4.66	1.43	1.37
24	c	514	CLA	C1D-ND	4.66	1.43	1.37
26	k	103	BCR	C23-C22	-4.65	1.35	1.45
26	D	405	BCR	C23-C22	-4.65	1.35	1.45
24	D	403	CLA	C1D-ND	4.65	1.43	1.37
24	b	621	CLA	CHD-C1D	4.65	1.47	1.38
24	c	507	CLA	O2D-CGD	4.64	1.44	1.33
24	C	505	CLA	O2D-CGD	4.64	1.44	1.33
26	a	410	BCR	C23-C22	-4.63	1.36	1.45
24	d	402	CLA	O2D-CGD	4.63	1.44	1.33
26	h	101	BCR	C23-C22	-4.62	1.36	1.45
24	B	606	CLA	CHC-C1C	4.62	1.46	1.35
24	c	504	CLA	C1D-ND	4.61	1.43	1.37
24	c	507	CLA	C1D-ND	4.61	1.43	1.37
24	D	403	CLA	O2A-CGA	4.61	1.46	1.33
35	B	622	HTG	C1'-S1	-4.61	1.75	1.81
24	B	605	CLA	C3C-C2C	4.61	1.46	1.36
24	B	613	CLA	CHD-C1D	4.60	1.47	1.38
24	d	401	CLA	O2D-CGD	4.60	1.44	1.33
24	B	615	CLA	C1D-ND	4.59	1.43	1.37
24	C	512	CLA	C1D-ND	4.59	1.43	1.37
26	T	102	BCR	C23-C22	-4.57	1.36	1.45
24	a	407	CLA	CHD-C1D	4.57	1.47	1.38
25	A	408	PHO	OBD-CAD	4.57	1.28	1.22
24	b	614	CLA	CHD-C1D	4.57	1.47	1.38
24	b	609	CLA	C3C-C2C	4.56	1.46	1.36
24	B	610	CLA	O2D-CGD	4.54	1.44	1.33
34	z	101	LMG	O8-C28	4.54	1.46	1.33
24	b	613	CLA	O2A-CGA	4.53	1.46	1.33
24	D	404	CLA	C1D-ND	4.53	1.43	1.37
24	B	616	CLA	O2A-CGA	4.52	1.46	1.33
26	c	516	BCR	C23-C22	-4.52	1.36	1.45
24	d	401	CLA	CHC-C1C	4.51	1.46	1.35
26	b	623	BCR	C23-C22	-4.50	1.36	1.45
24	b	613	CLA	CHD-C1D	4.50	1.47	1.38
26	t	101	BCR	C23-C22	-4.49	1.36	1.45
24	b	615	CLA	O2D-CGD	4.49	1.44	1.33
26	H	101	BCR	C23-C22	-4.49	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	OBD-CAD	4.48	1.30	1.22
26	Y	101	BCR	C23-C22	-4.48	1.36	1.45
36	D	407	DGD	O1G-C1A	4.47	1.46	1.33
24	C	510	CLA	O2A-CGA	4.47	1.46	1.33
24	b	615	CLA	C1D-ND	4.46	1.43	1.37
24	B	608	CLA	O2D-CGD	4.46	1.44	1.33
27	A	416	SQD	O48-C23	4.46	1.46	1.33
24	B	602	CLA	O2A-CGA	4.44	1.46	1.33
24	b	617	CLA	C1D-ND	4.43	1.43	1.37
24	c	505	CLA	CHD-C1D	4.43	1.47	1.38
36	d	407	DGD	O2G-C1B	4.43	1.46	1.34
24	B	609	CLA	CHD-C1D	4.42	1.47	1.38
24	c	510	CLA	O2A-CGA	4.42	1.46	1.33
26	b	622	BCR	C23-C22	-4.42	1.36	1.45
24	D	403	CLA	CHD-C1D	4.42	1.47	1.38
24	B	607	CLA	CHD-C1D	4.42	1.47	1.38
24	b	615	CLA	CHD-C1D	4.41	1.47	1.38
25	a	408	PHO	OBD-CAD	4.41	1.28	1.22
34	C	501	LMG	O7-C10	4.41	1.46	1.34
27	f	101	SQD	O47-C7	4.41	1.46	1.34
34	C	520	LMG	O8-C28	4.40	1.46	1.33
27	a	402	SQD	O48-C23	4.40	1.46	1.33
24	c	506	CLA	C1D-ND	4.40	1.43	1.37
24	D	403	CLA	O2D-CGD	4.40	1.43	1.33
24	c	515	CLA	CHD-C1D	4.40	1.46	1.38
24	A	409	CLA	C1D-ND	4.40	1.43	1.37
24	a	407	CLA	O2D-CGD	4.39	1.43	1.33
36	D	407	DGD	O2G-C1B	4.39	1.46	1.34
24	a	407	CLA	O2A-CGA	4.39	1.46	1.33
24	a	409	CLA	O2A-CGA	4.39	1.46	1.33
26	B	618	BCR	C23-C22	-4.39	1.36	1.45
24	c	509	CLA	O2A-CGA	4.38	1.46	1.33
37	e	101	LHG	O8-C23	4.38	1.46	1.33
24	A	406	CLA	CHD-C1D	4.38	1.46	1.38
24	B	602	CLA	CHD-C1D	4.37	1.46	1.38
24	c	507	CLA	CHD-C1D	4.37	1.46	1.38
27	F	101	SQD	O47-C7	4.37	1.46	1.34
26	K	101	BCR	C23-C22	-4.36	1.36	1.45
24	b	606	CLA	CHD-C1D	4.36	1.46	1.38
34	C	521	LMG	O7-C10	4.35	1.46	1.34
26	A	410	BCR	C23-C22	-4.35	1.36	1.45
24	c	508	CLA	CHD-C1D	4.34	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402	CLA	CHD-C1D	4.34	1.46	1.38
24	B	608	CLA	C1D-ND	4.33	1.43	1.37
24	c	512	CLA	CHD-C1D	4.33	1.46	1.38
26	B	619	BCR	C23-C22	-4.33	1.36	1.45
34	c	521	LMG	O7-C10	4.32	1.46	1.34
24	B	603	CLA	CHD-C1D	4.32	1.46	1.38
24	c	513	CLA	CHD-C1D	4.32	1.46	1.38
24	b	610	CLA	O2D-CGD	4.32	1.43	1.33
24	B	606	CLA	O2A-CGA	4.32	1.46	1.33
24	C	507	CLA	CHD-C1D	4.32	1.46	1.38
24	c	510	CLA	CHD-C1D	4.31	1.46	1.38
24	C	513	CLA	O2A-CGA	4.31	1.45	1.33
24	B	603	CLA	C1D-ND	4.31	1.43	1.37
36	d	407	DGD	O1G-C1A	4.31	1.45	1.33
24	C	506	CLA	CHD-C1D	4.30	1.46	1.38
24	B	604	CLA	O2A-CGA	4.30	1.45	1.33
24	C	502	CLA	C1D-ND	4.29	1.43	1.37
24	C	508	CLA	O2A-CGA	4.29	1.45	1.33
24	C	511	CLA	CHD-C1D	4.29	1.46	1.38
24	b	606	CLA	O2A-CGA	4.29	1.45	1.33
37	E	101	LHG	O8-C23	4.29	1.45	1.33
27	b	601	SQD	O47-C7	4.29	1.46	1.34
24	C	503	CLA	CHD-C1D	4.28	1.46	1.38
24	D	401	CLA	OBD-CAD	4.28	1.29	1.22
24	C	505	CLA	CHD-C1D	4.28	1.46	1.38
24	c	515	CLA	O2A-CGA	4.28	1.45	1.33
24	b	617	CLA	O2A-CGA	4.28	1.45	1.33
36	c	519	DGD	O1G-C1A	4.27	1.45	1.33
24	B	617	CLA	C1D-ND	4.27	1.43	1.37
24	c	514	CLA	O2A-CGA	4.26	1.45	1.33
24	d	401	CLA	O2A-CGA	4.26	1.45	1.33
34	C	501	LMG	O8-C28	4.26	1.45	1.33
24	c	503	CLA	O2A-CGA	4.26	1.45	1.33
24	c	504	CLA	CHD-C1D	4.26	1.46	1.38
34	c	520	LMG	O8-C28	4.26	1.45	1.33
36	C	518	DGD	O1G-C1A	4.25	1.45	1.33
24	b	617	CLA	CHD-C1D	4.25	1.46	1.38
24	C	502	CLA	O2A-CGA	4.25	1.45	1.33
24	D	404	CLA	CHD-C1D	4.25	1.46	1.38
24	A	406	CLA	CHD-C4C	4.25	1.48	1.39
24	c	508	CLA	O2A-CGA	4.25	1.45	1.33
24	B	612	CLA	CHD-C1D	4.24	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	OBD-CAD	4.24	1.29	1.22
24	b	607	CLA	CHD-C1D	4.24	1.46	1.38
24	B	608	CLA	O2A-CGA	4.23	1.45	1.33
24	b	607	CLA	C3D-C2D	4.23	1.50	1.39
24	b	616	CLA	CHD-C1D	4.23	1.46	1.38
24	b	619	CLA	CHD-C1D	4.23	1.46	1.38
24	B	605	CLA	O2D-CGD	4.23	1.43	1.33
24	a	409	CLA	CHD-C1D	4.23	1.46	1.38
24	B	609	CLA	O2A-CGA	4.22	1.45	1.33
24	c	503	CLA	CHD-C1D	4.22	1.46	1.38
24	b	612	CLA	CHD-C1D	4.22	1.46	1.38
25	d	403	PHO	OBD-CAD	4.22	1.28	1.22
24	B	608	CLA	OBD-CAD	4.22	1.29	1.22
24	B	614	CLA	CHD-C1D	4.21	1.46	1.38
34	Z	101	LMG	O7-C10	4.21	1.46	1.34
24	b	619	CLA	CHD-C4C	4.21	1.48	1.39
27	A	416	SQD	O47-C7	4.21	1.46	1.34
34	C	521	LMG	O8-C28	4.21	1.45	1.33
24	d	404	CLA	CHD-C1D	4.20	1.46	1.38
34	c	521	LMG	O8-C28	4.20	1.45	1.33
24	C	507	CLA	O2A-CGA	4.20	1.45	1.33
24	C	509	CLA	O2A-CGA	4.20	1.45	1.33
24	c	504	CLA	O2A-CGA	4.19	1.45	1.33
24	C	506	CLA	O2A-CGA	4.19	1.45	1.33
24	b	616	CLA	O2A-CGA	4.19	1.45	1.33
40	v	202	HEC	CBC-CAC	-4.18	1.33	1.49
27	f	101	SQD	O48-C23	4.18	1.45	1.33
37	e	101	LHG	O7-C7	4.18	1.46	1.34
24	C	514	CLA	O2A-CGA	4.18	1.45	1.33
24	B	610	CLA	O2A-CGA	4.18	1.45	1.33
34	b	625	LMG	O8-C28	4.17	1.45	1.33
27	F	101	SQD	O48-C23	4.17	1.45	1.33
24	a	406	CLA	CHD-C1D	4.17	1.46	1.38
24	d	401	CLA	CHD-C1D	4.16	1.46	1.38
24	c	511	CLA	O2A-CGA	4.16	1.45	1.33
34	z	101	LMG	O7-C10	4.16	1.46	1.34
24	C	504	CLA	O2A-CGA	4.16	1.45	1.33
24	c	512	CLA	O2A-CGA	4.16	1.45	1.33
24	B	617	CLA	CHD-C1D	4.16	1.46	1.38
24	b	608	CLA	CHD-C1D	4.16	1.46	1.38
24	b	620	CLA	CHD-C1D	4.16	1.46	1.38
36	c	518	DGD	O1G-C1A	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	CHD-C1D	4.16	1.46	1.38
37	l	102	LHG	O8-C23	4.16	1.45	1.33
24	B	609	CLA	C3D-C2D	4.15	1.50	1.39
37	D	410	LHG	O7-C7	4.15	1.46	1.34
24	d	404	CLA	O2A-CGA	4.15	1.45	1.33
24	b	610	CLA	O2A-CGA	4.15	1.45	1.33
24	b	614	CLA	O2A-CGA	4.14	1.45	1.33
27	l	101	SQD	O47-C7	4.14	1.46	1.34
24	C	503	CLA	C3D-C2D	4.14	1.50	1.39
24	c	511	CLA	CHD-C4C	4.14	1.48	1.39
24	b	619	CLA	O2A-CGA	4.14	1.45	1.33
24	B	605	CLA	CHD-C1D	4.14	1.46	1.38
24	B	617	CLA	O2A-CGA	4.13	1.45	1.33
24	b	621	CLA	O2A-CGA	4.13	1.45	1.33
40	V	203	HEC	CBC-CAC	-4.13	1.34	1.49
24	c	513	CLA	CHD-C4C	4.12	1.48	1.39
24	b	609	CLA	O2A-CGA	4.12	1.45	1.33
37	d	409	LHG	O8-C23	4.12	1.45	1.33
24	C	505	CLA	CHD-C4C	4.12	1.48	1.39
24	c	515	CLA	CHD-C4C	4.12	1.48	1.39
24	C	512	CLA	O2A-CGA	4.11	1.45	1.33
24	d	401	CLA	OBD-CAD	4.11	1.29	1.22
24	b	608	CLA	O2A-CGA	4.11	1.45	1.33
37	E	101	LHG	O7-C7	4.11	1.45	1.34
24	a	407	CLA	CHD-C4C	4.11	1.48	1.39
37	d	410	LHG	O8-C23	4.11	1.45	1.33
24	B	611	CLA	CHD-C1D	4.10	1.46	1.38
24	b	610	CLA	CHD-C1D	4.10	1.46	1.38
24	C	505	CLA	O2A-CGA	4.10	1.45	1.33
36	H	102	DGD	O2G-C1B	4.10	1.45	1.34
24	c	514	CLA	CHD-C1D	4.09	1.46	1.38
24	C	508	CLA	CHD-C1D	4.09	1.46	1.38
24	b	616	CLA	C3D-C2D	4.09	1.50	1.39
24	C	513	CLA	CHD-C1D	4.09	1.46	1.38
24	C	503	CLA	O2A-CGA	4.09	1.45	1.33
24	b	612	CLA	C1D-ND	4.08	1.42	1.37
24	C	514	CLA	OBD-CAD	4.08	1.29	1.22
24	c	508	CLA	CHD-C4C	4.08	1.48	1.39
25	d	403	PHO	O2A-CGA	4.08	1.45	1.33
24	d	402	CLA	CHD-C4C	4.08	1.48	1.39
24	C	507	CLA	C3D-C2D	4.08	1.50	1.39
24	d	401	CLA	C3D-C2D	4.07	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	O2A-CGA	4.07	1.45	1.33
36	h	102	DGD	O1G-C1A	4.07	1.45	1.33
24	B	607	CLA	O2A-CGA	4.07	1.45	1.33
37	l	102	LHG	O7-C7	4.07	1.45	1.34
34	c	501	LMG	O8-C28	4.07	1.45	1.33
24	B	616	CLA	C3D-C2D	4.07	1.50	1.39
27	b	601	SQD	O48-C23	4.07	1.45	1.33
34	B	621	LMG	O8-C28	4.07	1.45	1.33
24	C	514	CLA	CHD-C1D	4.07	1.46	1.38
24	b	621	CLA	CHD-C4C	4.07	1.48	1.39
27	a	402	SQD	O47-C7	4.06	1.45	1.34
34	C	520	LMG	O7-C10	4.06	1.45	1.34
24	D	401	CLA	O2A-CGA	4.06	1.45	1.33
34	c	520	LMG	O7-C10	4.06	1.45	1.34
24	c	507	CLA	CHD-C4C	4.06	1.48	1.39
24	C	512	CLA	CHD-C4C	4.06	1.48	1.39
24	C	511	CLA	O2A-CGA	4.06	1.45	1.33
36	C	517	DGD	O2G-C1B	4.05	1.45	1.34
24	B	613	CLA	O2A-CGA	4.05	1.45	1.33
24	A	409	CLA	C3D-C2D	4.05	1.50	1.39
34	B	621	LMG	O7-C10	4.05	1.45	1.34
35	d	411	HTG	C1'-S1	-4.05	1.76	1.81
24	C	509	CLA	C3D-C2D	4.05	1.50	1.39
25	a	408	PHO	O2A-CGA	4.05	1.45	1.33
24	b	611	CLA	CHD-C1D	4.05	1.46	1.38
24	B	616	CLA	CHD-C1D	4.04	1.46	1.38
24	B	611	CLA	O2A-CGA	4.04	1.45	1.33
24	b	620	CLA	OBD-CAD	4.04	1.29	1.22
27	l	101	SQD	O48-C23	4.03	1.45	1.33
24	b	611	CLA	O2A-CGA	4.03	1.45	1.33
24	D	401	CLA	CHD-C1D	4.03	1.46	1.38
24	B	617	CLA	OBD-CAD	4.03	1.29	1.22
24	D	401	CLA	C3D-C2D	4.03	1.50	1.39
24	c	506	CLA	O2A-CGA	4.03	1.45	1.33
24	b	606	CLA	CHD-C4C	4.03	1.48	1.39
24	c	511	CLA	OBD-CAD	4.03	1.29	1.22
24	c	510	CLA	C3D-C2D	4.03	1.50	1.39
35	b	603	HTG	C1'-S1	-4.03	1.76	1.81
24	b	620	CLA	C3D-C2D	4.02	1.50	1.39
24	B	610	CLA	OBD-CAD	4.01	1.29	1.22
24	c	514	CLA	CHD-C4C	4.00	1.48	1.39
24	B	606	CLA	CHD-C1D	4.00	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C3D-C2D	4.00	1.50	1.39
24	b	620	CLA	O2A-CGA	3.99	1.45	1.33
24	b	608	CLA	CHD-C4C	3.98	1.48	1.39
24	c	504	CLA	C3D-C2D	3.98	1.50	1.39
24	c	507	CLA	OBD-CAD	3.98	1.29	1.22
24	c	513	CLA	O2A-CGA	3.98	1.45	1.33
24	B	604	CLA	CHD-C1D	3.97	1.46	1.38
24	A	405	CLA	C3D-C2D	3.97	1.50	1.39
24	B	610	CLA	CHD-C1D	3.97	1.46	1.38
24	c	505	CLA	O2A-CGA	3.97	1.44	1.33
24	B	612	CLA	O2A-CGA	3.97	1.44	1.33
24	C	502	CLA	C3D-C2D	3.96	1.49	1.39
36	c	517	DGD	O2G-C1B	3.96	1.45	1.34
36	c	519	DGD	O2G-C1B	3.96	1.45	1.34
40	v	202	HEC	CBB-CAB	-3.96	1.34	1.49
34	j	101	LMG	O8-C28	3.95	1.44	1.33
24	C	503	CLA	CHD-C4C	3.95	1.48	1.39
24	C	509	CLA	CHD-C4C	3.95	1.48	1.39
24	B	614	CLA	O2A-CGA	3.95	1.44	1.33
36	H	102	DGD	O1G-C1A	3.95	1.44	1.33
24	C	510	CLA	OBD-CAD	3.95	1.29	1.22
37	d	410	LHG	O7-C7	3.95	1.45	1.34
24	C	504	CLA	CHD-C1D	3.95	1.46	1.38
27	a	411	SQD	O48-C23	3.95	1.44	1.33
25	A	407	PHO	C3C-C2C	3.94	1.49	1.37
24	c	506	CLA	CHD-C1D	3.94	1.46	1.38
24	c	504	CLA	CHD-C4C	3.94	1.48	1.39
37	D	410	LHG	O8-C23	3.94	1.44	1.33
24	C	511	CLA	CHD-C4C	3.93	1.48	1.39
25	a	408	PHO	C3C-C2C	3.93	1.49	1.37
24	C	510	CLA	CHD-C4C	3.93	1.48	1.39
35	O	303	HTG	C1'-S1	-3.93	1.76	1.81
24	a	406	CLA	CHD-C4C	3.93	1.48	1.39
24	b	619	CLA	C3D-C2D	3.93	1.49	1.39
24	C	511	CLA	C3D-C2D	3.92	1.49	1.39
24	d	404	CLA	CHD-C4C	3.92	1.48	1.39
24	b	615	CLA	C3D-C2D	3.92	1.49	1.39
36	C	518	DGD	O2G-C1B	3.92	1.45	1.34
24	A	409	CLA	CHD-C1D	3.92	1.46	1.38
24	C	512	CLA	CHD-C1D	3.91	1.46	1.38
24	B	605	CLA	O2A-CGA	3.91	1.44	1.33
24	b	606	CLA	C3D-C2D	3.91	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	411	SQD	O47-C7	3.91	1.45	1.34
24	C	510	CLA	C3D-C2D	3.90	1.49	1.39
34	j	101	LMG	O7-C10	3.90	1.45	1.34
24	b	614	CLA	CHD-C4C	3.89	1.48	1.39
24	B	613	CLA	C1D-ND	3.89	1.42	1.37
27	A	411	SQD	O47-C7	3.89	1.45	1.34
37	d	408	LHG	O8-C23	3.89	1.44	1.33
24	a	409	CLA	CHD-C4C	3.89	1.48	1.39
24	D	404	CLA	O2A-CGA	3.88	1.44	1.33
24	c	506	CLA	C3D-C2D	3.88	1.49	1.39
24	b	615	CLA	CHD-C4C	3.88	1.48	1.39
25	A	407	PHO	O2A-CGA	3.88	1.44	1.33
24	b	615	CLA	O2A-CGA	3.88	1.44	1.33
24	C	513	CLA	C3D-C2D	3.88	1.49	1.39
24	B	611	CLA	CHD-C4C	3.88	1.48	1.39
24	b	607	CLA	O2A-CGA	3.87	1.44	1.33
24	c	512	CLA	CHD-C4C	3.87	1.48	1.39
37	L	101	LHG	O8-C23	3.87	1.44	1.33
24	B	608	CLA	CHD-C1D	3.87	1.45	1.38
24	C	505	CLA	C3D-C2D	3.86	1.49	1.39
24	c	506	CLA	OBD-CAD	3.86	1.29	1.22
24	A	409	CLA	O2A-CGA	3.86	1.44	1.33
24	B	607	CLA	C3D-C2D	3.86	1.49	1.39
24	D	403	CLA	CHD-C4C	3.85	1.48	1.39
24	C	504	CLA	OBD-CAD	3.85	1.29	1.22
27	A	411	SQD	O48-C23	3.85	1.44	1.33
24	c	514	CLA	C3D-C2D	3.85	1.49	1.39
36	C	519	DGD	O1G-C1A	3.85	1.44	1.33
24	b	612	CLA	C3D-C2D	3.85	1.49	1.39
35	b	628	HTG	C1'-S1	-3.85	1.76	1.81
24	A	406	CLA	C3D-C2D	3.83	1.49	1.39
24	b	616	CLA	CHD-C4C	3.83	1.48	1.39
24	C	508	CLA	CHD-C4C	3.83	1.48	1.39
24	B	611	CLA	C3D-C2D	3.83	1.49	1.39
24	b	610	CLA	CHD-C4C	3.83	1.48	1.39
24	A	406	CLA	O2A-CGA	3.83	1.44	1.33
24	B	603	CLA	OBD-CAD	3.82	1.29	1.22
24	B	604	CLA	C3D-C2D	3.82	1.49	1.39
24	B	615	CLA	O2A-CGA	3.82	1.44	1.33
36	h	102	DGD	O2G-C1B	3.81	1.45	1.34
24	B	602	CLA	C3D-C2D	3.81	1.49	1.39
24	b	615	CLA	OBD-CAD	3.81	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	CHD-C4C	3.81	1.47	1.39
24	b	621	CLA	C3D-C2D	3.81	1.49	1.39
24	b	607	CLA	OBD-CAD	3.80	1.29	1.22
24	C	504	CLA	C3D-C2D	3.80	1.49	1.39
24	b	610	CLA	OBD-CAD	3.80	1.29	1.22
24	B	614	CLA	CHD-C4C	3.80	1.47	1.39
24	C	508	CLA	OBD-CAD	3.80	1.29	1.22
36	c	517	DGD	O1G-C1A	3.80	1.44	1.33
24	c	515	CLA	C3D-C2D	3.80	1.49	1.39
24	C	507	CLA	CHD-C4C	3.80	1.47	1.39
24	C	506	CLA	CHD-C4C	3.80	1.47	1.39
24	d	402	CLA	C3D-C2D	3.80	1.49	1.39
24	c	510	CLA	OBD-CAD	3.79	1.29	1.22
24	c	515	CLA	OBD-CAD	3.79	1.29	1.22
24	c	509	CLA	C3D-C2D	3.79	1.49	1.39
24	b	614	CLA	C3D-C2D	3.79	1.49	1.39
24	A	409	CLA	OBD-CAD	3.79	1.29	1.22
24	A	409	CLA	CHD-C4C	3.78	1.47	1.39
36	C	517	DGD	O1G-C1A	3.78	1.44	1.33
24	B	612	CLA	CHD-C4C	3.78	1.47	1.39
24	c	511	CLA	C3D-C2D	3.77	1.49	1.39
24	c	505	CLA	C3D-C2D	3.77	1.49	1.39
24	b	620	CLA	CHD-C4C	3.77	1.47	1.39
24	B	615	CLA	CHD-C4C	3.77	1.47	1.39
24	B	602	CLA	CHD-C4C	3.76	1.47	1.39
24	a	409	CLA	C3D-C2D	3.76	1.49	1.39
24	b	611	CLA	C3D-C2D	3.75	1.49	1.39
24	B	609	CLA	CHD-C4C	3.75	1.47	1.39
24	C	514	CLA	CHD-C4C	3.75	1.47	1.39
34	c	501	LMG	O7-C10	3.75	1.44	1.34
24	b	613	CLA	C3D-C2D	3.75	1.49	1.39
24	b	609	CLA	CHD-C1D	3.75	1.45	1.38
24	b	611	CLA	CHD-C4C	3.75	1.47	1.39
24	D	401	CLA	CHD-C4C	3.75	1.47	1.39
24	a	407	CLA	C3D-C2D	3.74	1.49	1.39
24	c	508	CLA	C3D-C2D	3.74	1.49	1.39
24	B	610	CLA	C3D-C2D	3.74	1.49	1.39
24	C	505	CLA	OBD-CAD	3.74	1.28	1.22
24	C	514	CLA	C3D-C2D	3.74	1.49	1.39
24	d	404	CLA	C3D-C2D	3.73	1.49	1.39
24	b	609	CLA	OBD-CAD	3.73	1.28	1.22
24	D	404	CLA	C3D-C2D	3.73	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C3D-C2D	3.73	1.49	1.39
34	J	101	LMG	O7-C10	3.73	1.44	1.34
24	B	615	CLA	OBD-CAD	3.73	1.28	1.22
24	C	513	CLA	CHD-C4C	3.72	1.47	1.39
24	c	507	CLA	O2A-CGA	3.72	1.44	1.33
24	a	406	CLA	C3D-C2D	3.72	1.49	1.39
24	b	618	CLA	C3D-C2D	3.72	1.49	1.39
24	C	504	CLA	CHD-C4C	3.72	1.47	1.39
36	c	518	DGD	O2G-C1B	3.72	1.44	1.34
37	L	101	LHG	O7-C7	3.72	1.44	1.34
24	B	606	CLA	CHD-C4C	3.71	1.47	1.39
34	J	101	LMG	O8-C28	3.71	1.44	1.33
24	c	513	CLA	OBD-CAD	3.71	1.28	1.22
35	B	624	HTG	C1'-S1	-3.71	1.76	1.81
38	e	102	HEM	C4D-ND	-3.70	1.33	1.40
24	B	608	CLA	C3D-C2D	3.70	1.49	1.39
24	b	607	CLA	CHD-C4C	3.70	1.47	1.39
24	c	510	CLA	CHD-C4C	3.70	1.47	1.39
24	b	612	CLA	O2A-CGA	3.70	1.44	1.33
24	A	405	CLA	O2A-CGA	3.69	1.44	1.33
34	b	625	LMG	O7-C10	3.69	1.44	1.34
24	D	404	CLA	OBD-CAD	3.69	1.28	1.22
24	B	610	CLA	CHD-C4C	3.69	1.47	1.39
24	D	403	CLA	C3D-C2D	3.69	1.49	1.39
24	B	614	CLA	C3D-C2D	3.69	1.49	1.39
24	C	511	CLA	OBD-CAD	3.69	1.28	1.22
24	B	608	CLA	CHD-C4C	3.69	1.47	1.39
24	c	505	CLA	CHD-C4C	3.69	1.47	1.39
25	A	408	PHO	C3C-C2C	3.68	1.48	1.37
25	A	408	PHO	O2A-CGA	3.68	1.44	1.33
24	B	616	CLA	CHD-C4C	3.68	1.47	1.39
24	D	403	CLA	OBD-CAD	3.68	1.28	1.22
24	B	603	CLA	O2A-CGA	3.68	1.44	1.33
24	b	609	CLA	C3D-C2D	3.67	1.49	1.39
25	d	403	PHO	C3C-C2C	3.67	1.48	1.37
24	B	603	CLA	CHD-C4C	3.67	1.47	1.39
35	c	523	HTG	C1'-S1	-3.66	1.76	1.81
37	D	408	LHG	O8-C23	3.66	1.44	1.33
24	C	512	CLA	C3D-C2D	3.66	1.49	1.39
24	c	509	CLA	CHD-C1D	3.65	1.45	1.38
24	a	407	CLA	OBD-CAD	3.65	1.28	1.22
24	B	604	CLA	CHD-C4C	3.65	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	OBD-CAD	3.65	1.28	1.22
24	c	503	CLA	CHD-C4C	3.64	1.47	1.39
24	B	616	CLA	OBD-CAD	3.64	1.28	1.22
24	c	503	CLA	OBD-CAD	3.64	1.28	1.22
24	c	509	CLA	CHD-C4C	3.64	1.47	1.39
24	B	617	CLA	CHD-C4C	3.63	1.47	1.39
40	V	203	HEC	CBB-CAB	-3.62	1.35	1.49
38	E	103	HEM	C4D-ND	-3.62	1.34	1.40
24	B	613	CLA	C3D-C2D	3.62	1.49	1.39
24	C	512	CLA	OBD-CAD	3.62	1.28	1.22
24	B	607	CLA	CHD-C4C	3.62	1.47	1.39
24	C	506	CLA	C3D-C2D	3.61	1.49	1.39
24	A	405	CLA	OBD-CAD	3.61	1.28	1.22
37	d	409	LHG	O7-C7	3.61	1.44	1.34
24	c	513	CLA	C3D-C2D	3.60	1.49	1.39
24	b	618	CLA	CHD-C4C	3.60	1.47	1.39
24	B	614	CLA	OBD-CAD	3.59	1.28	1.22
36	C	519	DGD	O2G-C1B	3.59	1.44	1.34
35	B	631	HTG	C1'-S1	-3.59	1.76	1.81
24	B	606	CLA	C3D-C2D	3.59	1.48	1.39
24	B	612	CLA	OBD-CAD	3.59	1.28	1.22
24	B	613	CLA	CHD-C4C	3.58	1.47	1.39
35	D	411	HTG	C1'-S1	-3.58	1.76	1.81
24	A	405	CLA	CHD-C1D	3.58	1.45	1.38
25	A	408	PHO	CHA-CBD	-3.58	1.48	1.52
24	c	512	CLA	C3D-C2D	3.58	1.48	1.39
24	b	610	CLA	C3D-C2D	3.57	1.48	1.39
24	C	502	CLA	OBD-CAD	3.57	1.28	1.22
24	b	613	CLA	OBD-CAD	3.57	1.28	1.22
24	b	618	CLA	CHD-C1D	3.57	1.45	1.38
24	d	401	CLA	CHD-C4C	3.55	1.47	1.39
24	B	617	CLA	C3D-C2D	3.55	1.48	1.39
24	b	608	CLA	OBD-CAD	3.55	1.28	1.22
24	a	406	CLA	O2A-CGA	3.53	1.43	1.33
24	A	405	CLA	CHD-C4C	3.53	1.47	1.39
24	C	508	CLA	C3D-C2D	3.53	1.48	1.39
24	B	615	CLA	C3D-C2D	3.53	1.48	1.39
24	b	619	CLA	OBD-CAD	3.53	1.28	1.22
35	C	523	HTG	C1'-S1	-3.52	1.76	1.81
24	b	621	CLA	OBD-CAD	3.52	1.28	1.22
24	D	404	CLA	CHD-C4C	3.52	1.47	1.39
24	c	506	CLA	CHD-C4C	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	C3D-C2D	3.52	1.48	1.39
24	b	611	CLA	OBD-CAD	3.52	1.28	1.22
24	B	615	CLA	CHD-C1D	3.52	1.45	1.38
37	D	409	LHG	O8-C23	3.52	1.43	1.33
24	b	608	CLA	C3D-C2D	3.52	1.48	1.39
35	b	604	HTG	C1'-S1	-3.51	1.76	1.81
24	B	604	CLA	OBD-CAD	3.51	1.28	1.22
24	b	617	CLA	C3D-C2D	3.51	1.48	1.39
35	B	630	HTG	C1'-S1	-3.50	1.77	1.81
24	c	514	CLA	OBD-CAD	3.50	1.28	1.22
24	C	502	CLA	CHD-C4C	3.49	1.47	1.39
24	b	616	CLA	OBD-CAD	3.49	1.28	1.22
24	a	406	CLA	OBD-CAD	3.49	1.28	1.22
24	a	409	CLA	OBD-CAD	3.48	1.28	1.22
24	b	609	CLA	C1C-C2C	3.48	1.51	1.44
24	b	617	CLA	OBD-CAD	3.48	1.28	1.22
37	D	409	LHG	O7-C7	3.47	1.44	1.34
38	E	103	HEM	C1B-NB	-3.47	1.34	1.40
24	d	404	CLA	OBD-CAD	3.46	1.28	1.22
24	B	611	CLA	OBD-CAD	3.46	1.28	1.22
24	B	605	CLA	CHD-C4C	3.44	1.47	1.39
37	D	408	LHG	O7-C7	3.44	1.44	1.34
35	C	522	HTG	C1'-S1	-3.41	1.77	1.81
24	c	504	CLA	OBD-CAD	3.40	1.28	1.22
24	c	507	CLA	C3D-C2D	3.40	1.48	1.39
24	c	512	CLA	OBD-CAD	3.40	1.28	1.22
24	B	607	CLA	OBD-CAD	3.40	1.28	1.22
24	b	618	CLA	OBD-CAD	3.40	1.28	1.22
24	b	609	CLA	CHD-C4C	3.38	1.47	1.39
40	v	202	HEC	C2B-C3B	-3.38	1.37	1.40
37	d	408	LHG	O7-C7	3.38	1.43	1.34
40	v	202	HEC	C4B-C3B	3.37	1.49	1.43
35	V	204	HTG	C1'-S1	-3.37	1.77	1.81
24	c	509	CLA	OBD-CAD	3.37	1.28	1.22
24	C	513	CLA	OBD-CAD	3.35	1.28	1.22
35	c	522	HTG	C1'-S1	-3.34	1.77	1.81
24	b	612	CLA	OBD-CAD	3.34	1.28	1.22
24	c	505	CLA	OBD-CAD	3.33	1.28	1.22
24	b	617	CLA	CHD-C4C	3.32	1.46	1.39
35	B	623	HTG	C1'-S1	-3.32	1.77	1.81
24	c	508	CLA	OBD-CAD	3.32	1.28	1.22
24	b	612	CLA	CHD-C4C	3.31	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	OBD-CAD	3.31	1.28	1.22
38	e	102	HEM	C1B-NB	-3.30	1.34	1.40
24	B	609	CLA	OBD-CAD	3.28	1.28	1.22
40	V	203	HEC	C4B-C3B	3.28	1.49	1.43
24	B	606	CLA	OBD-CAD	3.28	1.28	1.22
24	b	606	CLA	OBD-CAD	3.27	1.28	1.22
24	C	507	CLA	OBD-CAD	3.23	1.28	1.22
24	B	613	CLA	OBD-CAD	3.22	1.28	1.22
24	c	510	CLA	C1C-C2C	3.21	1.50	1.44
35	b	627	HTG	C1'-S1	-3.20	1.77	1.81
24	B	602	CLA	OBD-CAD	3.17	1.27	1.22
25	a	408	PHO	CHA-CBD	-3.14	1.48	1.52
24	B	605	CLA	C3D-C2D	3.12	1.47	1.39
24	A	405	CLA	C4C-C3C	3.10	1.50	1.45
24	C	509	CLA	OBD-CAD	3.08	1.27	1.22
38	e	102	HEM	FE-NB	3.07	2.12	1.96
24	c	507	CLA	C4C-C3C	3.07	1.50	1.45
24	B	613	CLA	C4C-C3C	3.07	1.50	1.45
24	b	615	CLA	C1C-C2C	3.05	1.50	1.44
24	B	614	CLA	C4C-C3C	3.03	1.50	1.45
24	B	607	CLA	C1C-C2C	3.02	1.50	1.44
24	d	402	CLA	OBD-CAD	2.99	1.27	1.22
24	B	604	CLA	C1C-C2C	2.99	1.50	1.44
24	C	509	CLA	C4C-C3C	2.98	1.50	1.45
24	C	510	CLA	C4C-C3C	2.98	1.50	1.45
24	C	506	CLA	C4C-C3C	2.96	1.50	1.45
24	c	509	CLA	C4D-CHA	2.96	1.48	1.38
24	D	403	CLA	C1C-C2C	2.95	1.50	1.44
24	a	406	CLA	C4C-C3C	2.95	1.50	1.45
24	b	621	CLA	C4C-C3C	2.95	1.50	1.45
24	D	401	CLA	C4D-CHA	2.94	1.48	1.38
24	c	506	CLA	C1C-C2C	2.94	1.50	1.44
24	b	608	CLA	C1C-C2C	2.93	1.50	1.44
27	A	416	SQD	C6-S	-2.93	1.66	1.77
24	c	512	CLA	C1B-CHB	2.91	1.49	1.41
27	a	402	SQD	C6-S	-2.91	1.66	1.77
27	A	411	SQD	C6-S	-2.91	1.66	1.77
27	f	101	SQD	C6-S	-2.90	1.66	1.77
40	V	203	HEC	C2B-C3B	-2.90	1.37	1.40
24	D	403	CLA	C4C-C3C	2.89	1.50	1.45
24	b	615	CLA	C4C-C3C	2.88	1.50	1.45
24	c	505	CLA	C1C-C2C	2.86	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	C1B-CHB	2.86	1.48	1.41
24	D	404	CLA	C1C-C2C	2.86	1.50	1.44
24	b	618	CLA	C1C-C2C	2.85	1.50	1.44
24	d	404	CLA	C1C-C2C	2.84	1.50	1.44
24	D	401	CLA	C4C-C3C	2.84	1.49	1.45
24	C	512	CLA	C4D-CHA	2.84	1.48	1.38
24	b	611	CLA	C1C-C2C	2.83	1.50	1.44
24	C	503	CLA	C4C-C3C	2.83	1.49	1.45
24	b	609	CLA	C4C-C3C	2.82	1.49	1.45
24	A	405	CLA	C1C-C2C	2.82	1.50	1.44
24	D	403	CLA	C1B-CHB	2.82	1.48	1.41
24	B	611	CLA	C4B-CHC	2.81	1.48	1.41
24	c	506	CLA	C4D-CHA	2.80	1.48	1.38
24	B	605	CLA	OBD-CAD	2.80	1.27	1.22
24	C	508	CLA	C1C-C2C	2.80	1.50	1.44
24	b	620	CLA	C4D-CHA	2.78	1.48	1.38
24	C	505	CLA	C4C-C3C	2.78	1.49	1.45
24	B	614	CLA	C4D-CHA	2.78	1.48	1.38
24	B	608	CLA	C1B-CHB	2.78	1.48	1.41
25	A	407	PHO	CHA-CBD	-2.78	1.49	1.52
24	C	503	CLA	C1C-C2C	2.78	1.49	1.44
24	c	503	CLA	C1B-CHB	2.76	1.48	1.41
24	b	619	CLA	C4C-C3C	2.76	1.49	1.45
24	A	409	CLA	C4B-CHC	2.76	1.48	1.41
24	C	513	CLA	C1C-C2C	2.76	1.49	1.44
24	c	512	CLA	C1C-C2C	2.75	1.49	1.44
24	b	609	CLA	C4B-CHC	2.75	1.48	1.41
24	B	612	CLA	C1C-C2C	2.75	1.49	1.44
24	b	609	CLA	C4D-CHA	2.74	1.48	1.38
24	a	407	CLA	C4D-CHA	2.74	1.48	1.38
24	B	607	CLA	C4D-CHA	2.74	1.48	1.38
24	a	406	CLA	C4D-CHA	2.74	1.48	1.38
24	c	507	CLA	C1C-C2C	2.73	1.49	1.44
24	a	406	CLA	C1B-CHB	2.72	1.48	1.41
27	a	411	SQD	C6-S	-2.72	1.67	1.77
24	A	405	CLA	C4D-CHA	2.72	1.48	1.38
24	b	621	CLA	C4D-CHA	2.72	1.48	1.38
24	C	510	CLA	C1B-CHB	2.72	1.48	1.41
24	c	513	CLA	C4D-CHA	2.71	1.48	1.38
24	C	502	CLA	C1C-C2C	2.71	1.49	1.44
24	b	610	CLA	C4D-CHA	2.71	1.48	1.38
24	C	503	CLA	C4D-CHA	2.71	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C1B-CHB	2.70	1.48	1.41
24	b	615	CLA	C1B-CHB	2.70	1.48	1.41
24	c	503	CLA	C4C-C3C	2.70	1.49	1.45
24	B	608	CLA	C4B-CHC	2.70	1.48	1.41
24	B	603	CLA	C4C-C3C	2.69	1.49	1.45
24	c	511	CLA	C4D-CHA	2.69	1.48	1.38
24	B	616	CLA	C4D-CHA	2.69	1.48	1.38
24	b	618	CLA	C1B-CHB	2.68	1.48	1.41
24	b	609	CLA	C1B-CHB	2.68	1.48	1.41
24	B	609	CLA	C4D-CHA	2.68	1.47	1.38
24	C	508	CLA	C4D-CHA	2.68	1.47	1.38
24	c	515	CLA	C4C-C3C	2.68	1.49	1.45
24	C	507	CLA	C1B-CHB	2.68	1.48	1.41
24	b	611	CLA	C4D-CHA	2.68	1.47	1.38
24	C	510	CLA	C1C-C2C	2.67	1.49	1.44
24	C	503	CLA	C1B-CHB	2.67	1.48	1.41
24	c	510	CLA	C4D-CHA	2.67	1.47	1.38
24	B	611	CLA	C4C-C3C	2.67	1.49	1.45
24	b	613	CLA	C4D-CHA	2.67	1.47	1.38
24	A	406	CLA	C1B-CHB	2.67	1.48	1.41
24	c	510	CLA	C4C-C3C	2.66	1.49	1.45
38	E	103	HEM	FE-NB	2.66	2.10	1.96
24	b	617	CLA	C1B-CHB	2.66	1.48	1.41
24	c	503	CLA	C4D-CHA	2.66	1.47	1.38
24	b	619	CLA	C4D-CHA	2.66	1.47	1.38
24	b	610	CLA	C1C-C2C	2.65	1.49	1.44
24	B	608	CLA	C4D-CHA	2.65	1.47	1.38
24	b	615	CLA	C4D-CHA	2.65	1.47	1.38
24	b	617	CLA	C1C-C2C	2.65	1.49	1.44
24	A	409	CLA	C1C-C2C	2.65	1.49	1.44
24	d	402	CLA	C1C-C2C	2.65	1.49	1.44
24	C	507	CLA	C4D-CHA	2.64	1.47	1.38
24	B	605	CLA	C1B-CHB	2.64	1.48	1.41
24	B	614	CLA	C1C-C2C	2.64	1.49	1.44
24	B	602	CLA	C4D-CHA	2.64	1.47	1.38
24	d	402	CLA	C4D-CHA	2.64	1.47	1.38
24	A	405	CLA	C1B-CHB	2.64	1.48	1.41
24	b	616	CLA	C4D-CHA	2.64	1.47	1.38
24	c	513	CLA	C1B-CHB	2.64	1.48	1.41
24	B	617	CLA	C1B-CHB	2.64	1.48	1.41
24	C	513	CLA	C4D-CHA	2.64	1.47	1.38
24	B	612	CLA	C4D-CHA	2.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	C1C-C2C	2.63	1.49	1.44
24	c	512	CLA	C4D-CHA	2.63	1.47	1.38
32	a	416	PL9	C6-C5	2.63	1.49	1.35
24	C	510	CLA	C4D-CHA	2.63	1.47	1.38
34	Z	101	LMG	O8-C28	2.63	1.46	1.33
24	a	409	CLA	C4D-CHA	2.63	1.47	1.38
24	C	504	CLA	C4C-C3C	2.63	1.49	1.45
24	C	505	CLA	C4D-CHA	2.63	1.47	1.38
24	C	511	CLA	C4D-CHA	2.62	1.47	1.38
24	B	603	CLA	C1C-C2C	2.62	1.49	1.44
24	C	504	CLA	C1C-C2C	2.62	1.49	1.44
24	c	507	CLA	C4D-CHA	2.62	1.47	1.38
24	b	621	CLA	C1B-CHB	2.61	1.48	1.41
24	B	613	CLA	C4D-CHA	2.61	1.47	1.38
24	c	509	CLA	C1C-C2C	2.61	1.49	1.44
24	c	514	CLA	C4C-C3C	2.61	1.49	1.45
24	c	510	CLA	C4B-CHC	2.61	1.48	1.41
24	C	509	CLA	C4D-CHA	2.60	1.47	1.38
24	c	511	CLA	C1C-C2C	2.60	1.49	1.44
24	C	502	CLA	C4D-CHA	2.60	1.47	1.38
24	B	611	CLA	C4D-CHA	2.60	1.47	1.38
24	C	508	CLA	C4B-CHC	2.60	1.48	1.41
24	b	614	CLA	C1B-CHB	2.60	1.48	1.41
27	b	601	SQD	C6-S	-2.60	1.67	1.77
24	C	511	CLA	C1C-C2C	2.60	1.49	1.44
24	C	502	CLA	C4C-C3C	2.60	1.49	1.45
24	d	402	CLA	C1B-NB	-2.60	1.32	1.35
24	c	509	CLA	C1B-CHB	2.60	1.48	1.41
24	C	511	CLA	C1B-CHB	2.60	1.48	1.41
24	b	616	CLA	C1B-CHB	2.60	1.48	1.41
24	d	401	CLA	C1B-CHB	2.60	1.48	1.41
24	b	615	CLA	C4B-CHC	2.59	1.48	1.41
24	C	514	CLA	C1B-CHB	2.59	1.48	1.41
24	c	514	CLA	C1C-C2C	2.59	1.49	1.44
24	c	504	CLA	C4D-CHA	2.59	1.47	1.38
35	D	411	HTG	C1-S1	-2.59	1.76	1.80
24	d	404	CLA	C4B-CHC	2.59	1.48	1.41
24	b	614	CLA	C4C-C3C	2.58	1.49	1.45
24	B	608	CLA	C4C-C3C	2.58	1.49	1.45
24	B	613	CLA	C1C-C2C	2.58	1.49	1.44
24	C	506	CLA	C1B-CHB	2.58	1.48	1.41
24	C	509	CLA	C1C-C2C	2.58	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C1B-CHB	2.58	1.48	1.41
24	b	618	CLA	C4C-C3C	2.58	1.49	1.45
24	b	608	CLA	C4D-CHA	2.58	1.47	1.38
24	B	605	CLA	C4D-CHA	2.58	1.47	1.38
24	b	618	CLA	C4D-CHA	2.58	1.47	1.38
24	b	607	CLA	C1C-C2C	2.58	1.49	1.44
24	c	508	CLA	C4D-CHA	2.58	1.47	1.38
24	d	404	CLA	C4D-CHA	2.58	1.47	1.38
24	a	409	CLA	C4C-C3C	2.57	1.49	1.45
24	a	407	CLA	C1C-C2C	2.57	1.49	1.44
24	c	505	CLA	C4B-CHC	2.57	1.48	1.41
25	d	403	PHO	CHA-CBD	-2.57	1.49	1.52
32	A	419	PL9	C6-C5	2.57	1.48	1.35
24	b	613	CLA	C4B-CHC	2.57	1.48	1.41
24	c	506	CLA	C4C-C3C	2.57	1.49	1.45
24	b	606	CLA	C4D-CHA	2.56	1.47	1.38
24	B	613	CLA	C1B-CHB	2.56	1.48	1.41
24	b	617	CLA	C4D-CHA	2.56	1.47	1.38
24	C	512	CLA	C1B-CHB	2.56	1.48	1.41
32	d	406	PL9	C6-C5	2.55	1.48	1.35
24	c	504	CLA	C1B-CHB	2.55	1.48	1.41
24	B	612	CLA	C4B-CHC	2.55	1.48	1.41
24	d	404	CLA	C1B-NB	-2.55	1.32	1.35
24	B	617	CLA	C4D-CHA	2.55	1.47	1.38
24	b	611	CLA	C4B-CHC	2.54	1.48	1.41
24	c	511	CLA	C4C-C3C	2.54	1.49	1.45
24	C	513	CLA	C4C-C3C	2.54	1.49	1.45
24	c	515	CLA	C4D-CHA	2.54	1.47	1.38
24	D	403	CLA	C3D-C4D	-2.54	1.38	1.44
24	D	404	CLA	C4D-CHA	2.54	1.47	1.38
24	B	612	CLA	C4C-C3C	2.54	1.49	1.45
24	b	616	CLA	C4B-CHC	2.54	1.48	1.41
24	B	609	CLA	C1C-C2C	2.53	1.49	1.44
24	B	603	CLA	C4D-CHA	2.53	1.47	1.38
24	b	607	CLA	C4C-C3C	2.53	1.49	1.45
24	B	602	CLA	C1C-C2C	2.53	1.49	1.44
24	B	616	CLA	C4C-C3C	2.53	1.49	1.45
24	b	610	CLA	C4B-CHC	2.53	1.48	1.41
24	b	617	CLA	C4B-CHC	2.52	1.48	1.41
24	B	615	CLA	C4D-CHA	2.52	1.47	1.38
24	C	506	CLA	C4D-CHA	2.52	1.47	1.38
24	C	504	CLA	C4D-CHA	2.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C1C-C2C	2.52	1.49	1.44
24	B	605	CLA	C1C-C2C	2.51	1.49	1.44
24	c	514	CLA	C4B-CHC	2.51	1.48	1.41
24	b	608	CLA	C4B-CHC	2.51	1.48	1.41
32	D	406	PL9	C6-C5	2.51	1.48	1.35
24	b	613	CLA	C4C-C3C	2.51	1.49	1.45
24	D	401	CLA	C1C-C2C	2.51	1.49	1.44
24	B	613	CLA	C3D-C4D	-2.51	1.38	1.44
24	B	604	CLA	C4D-CHA	2.50	1.47	1.38
36	H	102	DGD	O5D-C1E	2.50	1.44	1.40
24	C	506	CLA	C1C-C2C	2.50	1.49	1.44
24	b	606	CLA	C1C-C2C	2.50	1.49	1.44
24	B	614	CLA	C1B-CHB	2.49	1.47	1.41
24	B	604	CLA	C1B-CHB	2.49	1.47	1.41
24	D	403	CLA	C4D-CHA	2.49	1.47	1.38
24	d	402	CLA	C4C-C3C	2.49	1.49	1.45
24	b	612	CLA	C4D-CHA	2.49	1.47	1.38
24	B	606	CLA	C4D-CHA	2.49	1.47	1.38
24	a	407	CLA	C4B-CHC	2.49	1.47	1.41
24	B	602	CLA	C4B-CHC	2.48	1.47	1.41
24	B	609	CLA	C4C-C3C	2.48	1.49	1.45
24	B	608	CLA	C1C-C2C	2.48	1.49	1.44
24	b	612	CLA	C1C-C2C	2.48	1.49	1.44
24	B	611	CLA	C1B-CHB	2.48	1.47	1.41
24	b	606	CLA	C4B-CHC	2.48	1.47	1.41
24	C	503	CLA	C4B-CHC	2.48	1.47	1.41
24	d	402	CLA	C1B-CHB	2.48	1.47	1.41
24	C	511	CLA	C4B-CHC	2.47	1.47	1.41
27	l	101	SQD	C6-S	-2.47	1.68	1.77
24	C	505	CLA	C1C-C2C	2.47	1.49	1.44
24	c	511	CLA	C1B-CHB	2.47	1.47	1.41
24	c	513	CLA	C4C-C3C	2.47	1.49	1.45
24	c	509	CLA	C4C-C3C	2.47	1.49	1.45
24	c	515	CLA	C1C-C2C	2.47	1.49	1.44
35	C	522	HTG	C1-S1	-2.47	1.76	1.80
24	c	514	CLA	C4D-CHA	2.46	1.47	1.38
24	c	505	CLA	C4D-CHA	2.46	1.47	1.38
36	h	102	DGD	O5D-C1E	2.46	1.44	1.40
24	c	507	CLA	C3D-C4D	-2.46	1.38	1.44
24	b	607	CLA	C4B-CHC	2.46	1.47	1.41
24	d	404	CLA	C4C-C3C	2.46	1.49	1.45
24	B	606	CLA	C1B-CHB	2.46	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	C4B-CHC	2.45	1.47	1.41
24	C	510	CLA	C4B-CHC	2.45	1.47	1.41
24	c	505	CLA	C1B-CHB	2.45	1.47	1.41
24	C	507	CLA	C4C-C3C	2.45	1.49	1.45
24	a	407	CLA	C4C-C3C	2.45	1.49	1.45
24	b	620	CLA	C4C-C3C	2.45	1.49	1.45
35	c	522	HTG	C1-S1	-2.45	1.77	1.80
24	A	409	CLA	C4D-CHA	2.45	1.47	1.38
24	c	511	CLA	C3D-C4D	-2.44	1.38	1.44
24	b	606	CLA	C1B-CHB	2.44	1.47	1.41
24	c	508	CLA	C3D-C4D	-2.43	1.38	1.44
24	C	512	CLA	C4C-C3C	2.43	1.49	1.45
24	b	608	CLA	C1B-CHB	2.43	1.47	1.41
24	a	407	CLA	C3D-C4D	-2.43	1.38	1.44
24	B	615	CLA	C1C-C2C	2.43	1.49	1.44
24	a	409	CLA	C1C-NC	-2.43	1.34	1.37
24	d	401	CLA	C4D-CHA	2.43	1.47	1.38
24	B	610	CLA	C4D-CHA	2.43	1.47	1.38
24	b	610	CLA	C4C-C3C	2.43	1.49	1.45
24	b	614	CLA	C4D-CHA	2.42	1.47	1.38
24	b	607	CLA	C1B-CHB	2.42	1.47	1.41
24	B	615	CLA	C3D-C4D	-2.42	1.38	1.44
24	c	508	CLA	C4C-C3C	2.42	1.49	1.45
24	c	512	CLA	C4B-CHC	2.41	1.47	1.41
24	C	503	CLA	C3D-C4D	-2.41	1.38	1.44
24	B	602	CLA	C3D-C4D	-2.41	1.38	1.44
24	C	514	CLA	C4D-CHA	2.41	1.47	1.38
24	c	511	CLA	C4B-CHC	2.41	1.47	1.41
24	c	507	CLA	C1B-CHB	2.41	1.47	1.41
24	B	616	CLA	C1B-CHB	2.40	1.47	1.41
35	b	628	HTG	C1-S1	-2.40	1.77	1.80
24	c	507	CLA	C4B-CHC	2.40	1.47	1.41
24	C	504	CLA	C4B-CHC	2.39	1.47	1.41
24	D	404	CLA	C4B-CHC	2.39	1.47	1.41
24	A	409	CLA	C1B-CHB	2.39	1.47	1.41
24	c	515	CLA	C4B-CHC	2.39	1.47	1.41
24	D	403	CLA	C4B-CHC	2.39	1.47	1.41
27	F	101	SQD	C6-S	-2.39	1.68	1.77
24	B	605	CLA	C4B-CHC	2.39	1.47	1.41
30	M	101	LMT	O1'-C1'	2.39	1.44	1.40
24	c	510	CLA	C1B-CHB	2.38	1.47	1.41
24	C	507	CLA	C1C-C2C	2.38	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	C4B-CHC	2.38	1.47	1.41
24	a	409	CLA	C1C-C2C	2.38	1.49	1.44
24	b	613	CLA	C3D-C4D	-2.37	1.38	1.44
24	B	607	CLA	C1B-CHB	2.37	1.47	1.41
24	c	503	CLA	C1C-C2C	2.37	1.49	1.44
24	B	605	CLA	C4C-C3C	2.37	1.49	1.45
24	b	608	CLA	C4C-C3C	2.37	1.49	1.45
24	B	614	CLA	C4B-CHC	2.36	1.47	1.41
24	B	605	CLA	C3D-C4D	-2.36	1.38	1.44
24	c	505	CLA	C4C-C3C	2.36	1.49	1.45
24	B	610	CLA	C4B-CHC	2.36	1.47	1.41
35	c	523	HTG	C1-S1	-2.36	1.77	1.80
24	C	506	CLA	C4B-CHC	2.36	1.47	1.41
24	B	604	CLA	C4B-CHC	2.36	1.47	1.41
24	C	504	CLA	C3D-C4D	-2.35	1.38	1.44
24	c	514	CLA	C3D-C4D	-2.35	1.38	1.44
24	C	504	CLA	C1B-CHB	2.35	1.47	1.41
24	B	617	CLA	C4C-C3C	2.35	1.49	1.45
24	b	607	CLA	C4D-CHA	2.35	1.46	1.38
24	d	401	CLA	C4C-C3C	2.35	1.49	1.45
24	C	506	CLA	C3D-C4D	-2.35	1.38	1.44
24	C	510	CLA	C3D-C4D	-2.35	1.38	1.44
24	B	611	CLA	C1C-C2C	2.35	1.49	1.44
24	B	612	CLA	C3D-C4D	-2.35	1.38	1.44
24	C	512	CLA	C1C-C2C	2.35	1.49	1.44
35	B	631	HTG	C1-S1	-2.35	1.77	1.80
24	b	612	CLA	C4B-CHC	2.35	1.47	1.41
24	A	409	CLA	C4C-C3C	2.35	1.49	1.45
24	C	511	CLA	C4C-C3C	2.34	1.49	1.45
24	D	401	CLA	C3D-C4D	-2.34	1.38	1.44
24	b	616	CLA	C3D-C4D	-2.34	1.38	1.44
24	A	406	CLA	C4D-CHA	2.34	1.46	1.38
35	d	411	HTG	C1-S1	-2.34	1.77	1.80
24	b	613	CLA	C1B-CHB	2.33	1.47	1.41
24	C	502	CLA	C1B-CHB	2.33	1.47	1.41
24	a	406	CLA	C1C-C2C	2.33	1.49	1.44
24	B	602	CLA	C4C-C3C	2.33	1.49	1.45
35	V	204	HTG	C1-S1	-2.32	1.77	1.80
24	c	504	CLA	C4C-C3C	2.32	1.49	1.45
24	C	508	CLA	C4C-C3C	2.32	1.49	1.45
24	d	404	CLA	C1B-CHB	2.32	1.47	1.41
24	b	617	CLA	C3D-C4D	-2.32	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C1B-CHB	2.31	1.47	1.41
24	B	616	CLA	C1C-C2C	2.31	1.49	1.44
24	b	614	CLA	C1C-C2C	2.31	1.49	1.44
24	c	506	CLA	C3D-C4D	-2.31	1.39	1.44
24	b	612	CLA	C1B-CHB	2.31	1.47	1.41
24	C	508	CLA	C1B-CHB	2.30	1.47	1.41
24	A	405	CLA	C4B-CHC	2.30	1.47	1.41
24	b	616	CLA	C1C-C2C	2.30	1.49	1.44
24	c	504	CLA	C1C-C2C	2.30	1.49	1.44
24	B	607	CLA	C4C-C3C	2.29	1.49	1.45
24	b	611	CLA	C1B-CHB	2.29	1.47	1.41
30	m	103	LMT	O1'-C1'	2.29	1.44	1.40
24	d	402	CLA	C4B-CHC	2.29	1.47	1.41
24	C	509	CLA	C3D-C4D	-2.29	1.39	1.44
24	b	610	CLA	C3D-C4D	-2.29	1.39	1.44
24	B	608	CLA	C3D-C4D	-2.28	1.39	1.44
24	b	620	CLA	C4B-CHC	2.28	1.47	1.41
24	B	611	CLA	C3D-C4D	-2.28	1.39	1.44
24	B	604	CLA	C3D-C4D	-2.28	1.39	1.44
24	B	610	CLA	C3D-C4D	-2.28	1.39	1.44
24	c	509	CLA	C4B-CHC	2.28	1.47	1.41
24	B	616	CLA	C4B-CHC	2.28	1.47	1.41
24	A	406	CLA	C4C-C3C	2.28	1.49	1.45
24	B	603	CLA	C1B-CHB	2.28	1.47	1.41
24	b	608	CLA	C3D-C4D	-2.28	1.39	1.44
24	b	616	CLA	C4C-C3C	2.28	1.49	1.45
24	a	407	CLA	C1B-CHB	2.27	1.47	1.41
24	c	508	CLA	C1B-CHB	2.27	1.47	1.41
24	A	405	CLA	MG-ND	-2.27	2.01	2.05
24	d	404	CLA	C3D-C4D	-2.27	1.39	1.44
24	B	606	CLA	C4C-C3C	2.27	1.49	1.45
24	C	509	CLA	C4B-CHC	2.27	1.47	1.41
24	C	513	CLA	C1B-CHB	2.27	1.47	1.41
24	b	610	CLA	C1B-CHB	2.27	1.47	1.41
24	D	404	CLA	C4C-C3C	2.26	1.48	1.45
24	b	617	CLA	C4C-C3C	2.26	1.48	1.45
24	C	507	CLA	C3D-C4D	-2.26	1.39	1.44
24	c	514	CLA	C1B-CHB	2.26	1.47	1.41
24	a	409	CLA	C1B-CHB	2.26	1.47	1.41
24	c	513	CLA	C3D-C4D	-2.25	1.39	1.44
24	B	609	CLA	C3D-C4D	-2.25	1.39	1.44
24	B	613	CLA	C4B-CHC	2.25	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	C4B-CHC	2.25	1.47	1.41
24	C	514	CLA	C4B-CHC	2.25	1.47	1.41
24	C	511	CLA	C3D-C4D	-2.25	1.39	1.44
24	b	621	CLA	C1C-C2C	2.24	1.48	1.44
24	c	504	CLA	C3D-C4D	-2.24	1.39	1.44
24	D	404	CLA	C1B-CHB	2.24	1.47	1.41
24	C	514	CLA	C1C-C2C	2.24	1.48	1.44
24	B	604	CLA	C4C-C3C	2.24	1.48	1.45
24	b	620	CLA	C1B-CHB	2.24	1.47	1.41
24	d	402	CLA	C3D-C4D	-2.24	1.39	1.44
24	B	603	CLA	C4B-CHC	2.24	1.47	1.41
36	D	407	DGD	O3G-C1D	2.24	1.44	1.40
24	C	502	CLA	C4B-CHC	2.24	1.47	1.41
24	C	514	CLA	C4C-C3C	2.24	1.48	1.45
24	C	508	CLA	C3D-C4D	-2.23	1.39	1.44
24	c	506	CLA	C1B-CHB	2.23	1.47	1.41
24	b	614	CLA	C4B-CHC	2.23	1.47	1.41
32	a	416	PL9	C2-C3	2.23	1.40	1.34
24	B	602	CLA	C1B-CHB	2.23	1.47	1.41
24	b	606	CLA	C3D-C4D	-2.23	1.39	1.44
24	C	502	CLA	C3D-C4D	-2.22	1.39	1.44
38	e	102	HEM	CHB-C1B	2.22	1.40	1.35
24	B	616	CLA	C3D-C4D	-2.22	1.39	1.44
38	e	102	HEM	C3B-C4B	2.21	1.49	1.44
24	b	611	CLA	C4C-C3C	2.21	1.48	1.45
24	a	406	CLA	C3D-C4D	-2.21	1.39	1.44
24	b	618	CLA	C4B-CHC	2.21	1.47	1.41
24	c	515	CLA	C3D-C4D	-2.21	1.39	1.44
24	d	404	CLA	C1D-C2D	2.20	1.49	1.45
24	b	619	CLA	C1B-CHB	2.20	1.47	1.41
24	C	505	CLA	C3D-C4D	-2.20	1.39	1.44
24	B	609	CLA	C1B-CHB	2.20	1.47	1.41
35	b	604	HTG	C1-S1	-2.20	1.77	1.80
24	c	505	CLA	C3D-C4D	-2.20	1.39	1.44
24	B	617	CLA	C3D-C4D	-2.19	1.39	1.44
24	b	612	CLA	C3D-C4D	-2.19	1.39	1.44
24	b	609	CLA	MG-NA	2.19	2.11	2.06
24	B	610	CLA	C1C-C2C	2.19	1.48	1.44
24	C	513	CLA	C3D-C4D	-2.19	1.39	1.44
24	B	612	CLA	C1B-CHB	2.19	1.47	1.41
24	c	506	CLA	C4B-CHC	2.19	1.47	1.41
24	c	515	CLA	C1D-C2D	2.17	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	CLA	C1B-CHB	2.17	1.47	1.41
32	D	406	PL9	C2-C3	2.17	1.40	1.34
24	D	401	CLA	C4B-CHC	2.16	1.47	1.41
24	A	406	CLA	C3D-C4D	-2.16	1.39	1.44
24	C	505	CLA	C4B-CHC	2.16	1.47	1.41
24	c	510	CLA	C3D-C4D	-2.16	1.39	1.44
24	B	617	CLA	C1C-NC	-2.16	1.34	1.37
24	c	508	CLA	C1C-C2C	2.16	1.48	1.44
24	c	508	CLA	C1B-NB	-2.16	1.33	1.35
38	E	103	HEM	C1D-ND	-2.16	1.34	1.38
24	b	609	CLA	MG-ND	-2.15	2.01	2.05
24	b	620	CLA	C1C-C2C	2.14	1.48	1.44
24	c	512	CLA	C4C-C3C	2.14	1.48	1.45
24	C	512	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	613	CLA	MG-NA	2.14	2.11	2.06
24	c	503	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	615	CLA	C4B-CHC	2.13	1.46	1.41
24	B	616	CLA	C1C-NC	-2.13	1.34	1.37
24	B	615	CLA	C1B-NB	-2.13	1.33	1.35
24	c	515	CLA	C1B-CHB	2.12	1.46	1.41
24	b	619	CLA	C3D-C4D	-2.12	1.39	1.44
24	c	503	CLA	C4B-CHC	2.12	1.46	1.41
24	b	615	CLA	C3D-C4D	-2.11	1.39	1.44
24	c	513	CLA	C4B-CHC	2.11	1.46	1.41
24	b	619	CLA	C4B-CHC	2.11	1.46	1.41
24	B	606	CLA	C3D-C4D	-2.11	1.39	1.44
24	c	504	CLA	C4B-CHC	2.10	1.46	1.41
24	b	619	CLA	C1C-C2C	2.10	1.48	1.44
24	B	617	CLA	C1C-C2C	2.10	1.48	1.44
35	C	523	HTG	C1-S1	-2.09	1.77	1.80
24	b	607	CLA	C3D-C4D	-2.09	1.39	1.44
24	B	605	CLA	MG-NA	2.09	2.11	2.06
24	c	508	CLA	C4B-CHC	2.08	1.46	1.41
24	B	615	CLA	C4C-C3C	2.08	1.48	1.45
24	B	603	CLA	C3D-C4D	-2.08	1.39	1.44
24	B	603	CLA	C1C-NC	-2.08	1.34	1.37
35	b	603	HTG	C1-S1	-2.08	1.77	1.80
24	A	405	CLA	MG-NA	2.08	2.11	2.06
24	a	406	CLA	C4B-CHC	2.08	1.46	1.41
24	b	621	CLA	C3D-C4D	-2.08	1.39	1.44
24	b	617	CLA	C1C-NC	-2.08	1.34	1.37
35	B	624	HTG	C1-S1	-2.07	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C3A-C2A	-2.06	1.52	1.54
38	E	103	HEM	CHB-C1B	2.06	1.40	1.35
24	C	512	CLA	C4B-CHC	2.06	1.46	1.41
24	C	514	CLA	C3D-C4D	-2.05	1.39	1.44
24	b	606	CLA	C4C-C3C	2.05	1.48	1.45
36	D	407	DGD	O5D-C1E	2.05	1.43	1.40
24	b	620	CLA	C3D-C4D	-2.05	1.39	1.44
24	B	605	CLA	MG-ND	-2.05	2.01	2.05
24	b	621	CLA	C4B-CHC	2.05	1.46	1.41
35	B	630	HTG	C1-S1	-2.05	1.77	1.80
24	b	618	CLA	C3D-C4D	-2.04	1.39	1.44
26	b	622	BCR	C19-C18	2.04	1.50	1.45
24	b	611	CLA	C3D-C4D	-2.04	1.39	1.44
24	b	609	CLA	C3D-C4D	-2.03	1.39	1.44
38	e	102	HEM	C1D-ND	-2.03	1.34	1.38
36	d	407	DGD	O5D-C1E	2.03	1.43	1.40
24	B	609	CLA	C4B-CHC	2.03	1.46	1.41
24	B	607	CLA	C1B-NB	-2.03	1.33	1.35
24	C	507	CLA	C4B-CHC	2.02	1.46	1.41
24	a	409	CLA	C4B-CHC	2.02	1.46	1.41
24	B	603	CLA	C1B-NB	-2.02	1.33	1.35
24	A	409	CLA	C3D-C4D	-2.02	1.39	1.44
24	A	406	CLA	C1C-C2C	2.02	1.48	1.44
24	D	403	CLA	C1C-NC	-2.01	1.34	1.37
34	j	101	LMG	O1-C1	2.01	1.43	1.40
24	b	621	CLA	C1C-NC	-2.01	1.34	1.37

All (2520) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	615	CLA	C1D-ND-C4D	-10.22	99.08	106.33
24	b	610	CLA	C1D-ND-C4D	-10.12	99.15	106.33
24	B	610	CLA	C1D-ND-C4D	-10.04	99.20	106.33
24	A	409	CLA	C1D-ND-C4D	-9.95	99.27	106.33
24	B	606	CLA	C1D-ND-C4D	-9.75	99.41	106.33
24	C	514	CLA	C1D-ND-C4D	-9.61	99.51	106.33
24	c	514	CLA	C1D-ND-C4D	-9.57	99.53	106.33
24	C	504	CLA	C1D-ND-C4D	-9.54	99.56	106.33
24	A	406	CLA	C1D-ND-C4D	-9.53	99.57	106.33
24	C	512	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	B	604	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	c	512	CLA	C1D-ND-C4D	-9.51	99.58	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	C1D-ND-C4D	-9.43	99.63	106.33
24	D	404	CLA	C1D-ND-C4D	-9.40	99.66	106.33
24	c	513	CLA	C1D-ND-C4D	-9.40	99.66	106.33
24	c	505	CLA	C1D-ND-C4D	-9.36	99.69	106.33
24	b	611	CLA	C1D-ND-C4D	-9.32	99.72	106.33
24	a	409	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	c	515	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	B	605	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	c	503	CLA	C1D-ND-C4D	-9.28	99.74	106.33
24	d	404	CLA	C1D-ND-C4D	-9.28	99.75	106.33
24	b	607	CLA	C1D-ND-C4D	-9.26	99.75	106.33
24	b	616	CLA	C1D-ND-C4D	-9.25	99.76	106.33
24	c	510	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	b	614	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	B	603	CLA	C1D-ND-C4D	-9.15	99.83	106.33
24	b	606	CLA	C1D-ND-C4D	-9.13	99.85	106.33
24	B	615	CLA	C2D-C1D-ND	9.11	116.82	110.10
24	a	407	CLA	C1D-ND-C4D	-9.07	99.89	106.33
24	c	509	CLA	C1D-ND-C4D	-9.05	99.90	106.33
24	C	509	CLA	C1D-ND-C4D	-9.05	99.90	106.33
24	b	618	CLA	C1D-ND-C4D	-9.05	99.91	106.33
24	b	620	CLA	C1D-ND-C4D	-9.04	99.92	106.33
24	b	619	CLA	C1D-ND-C4D	-9.02	99.93	106.33
24	B	602	CLA	C1D-ND-C4D	-9.01	99.93	106.33
24	b	610	CLA	C2D-C1D-ND	9.00	116.74	110.10
24	B	609	CLA	C1D-ND-C4D	-8.99	99.95	106.33
24	B	617	CLA	C1D-ND-C4D	-8.97	99.96	106.33
24	A	409	CLA	C2D-C1D-ND	8.95	116.70	110.10
24	C	505	CLA	C1D-ND-C4D	-8.92	100.00	106.33
24	b	617	CLA	C1D-ND-C4D	-8.92	100.00	106.33
24	c	506	CLA	C1D-ND-C4D	-8.88	100.03	106.33
24	c	509	CLA	C2D-C1D-ND	8.87	116.64	110.10
24	b	615	CLA	C1D-ND-C4D	-8.84	100.06	106.33
24	b	608	CLA	C1D-ND-C4D	-8.83	100.06	106.33
24	b	613	CLA	C1D-ND-C4D	-8.82	100.07	106.33
24	B	607	CLA	C1D-ND-C4D	-8.80	100.09	106.33
24	C	510	CLA	C1D-ND-C4D	-8.77	100.11	106.33
24	C	512	CLA	C2D-C1D-ND	8.75	116.55	110.10
24	c	510	CLA	C2D-C1D-ND	8.71	116.52	110.10
24	c	511	CLA	C1D-ND-C4D	-8.71	100.15	106.33
24	B	610	CLA	C2D-C1D-ND	8.67	116.50	110.10
24	C	513	CLA	C1D-ND-C4D	-8.65	100.19	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	406	CLA	C1D-ND-C4D	-8.65	100.19	106.33
24	C	508	CLA	C1D-ND-C4D	-8.64	100.20	106.33
24	c	503	CLA	C2D-C1D-ND	8.62	116.45	110.10
24	C	511	CLA	C1D-ND-C4D	-8.61	100.22	106.33
24	B	611	CLA	C1D-ND-C4D	-8.59	100.23	106.33
24	b	618	CLA	C2D-C1D-ND	8.59	116.44	110.10
24	b	621	CLA	C1D-ND-C4D	-8.58	100.24	106.33
24	d	401	CLA	C1D-ND-C4D	-8.57	100.24	106.33
24	c	506	CLA	C2D-C1D-ND	8.57	116.42	110.10
24	b	616	CLA	C2D-C1D-ND	8.57	116.42	110.10
24	c	514	CLA	C2D-C1D-ND	8.56	116.41	110.10
24	B	605	CLA	C2D-C1D-ND	8.51	116.37	110.10
24	B	607	CLA	C2D-C1D-ND	8.50	116.37	110.10
24	b	619	CLA	C2D-C1D-ND	8.49	116.36	110.10
24	C	507	CLA	C1D-ND-C4D	-8.48	100.31	106.33
24	c	505	CLA	C2D-C1D-ND	8.47	116.35	110.10
24	B	614	CLA	C1D-ND-C4D	-8.43	100.35	106.33
24	C	503	CLA	C1D-ND-C4D	-8.41	100.36	106.33
24	b	611	CLA	C2D-C1D-ND	8.40	116.29	110.10
24	B	608	CLA	C1D-ND-C4D	-8.40	100.37	106.33
24	D	401	CLA	C1D-ND-C4D	-8.38	100.38	106.33
24	c	508	CLA	C1D-ND-C4D	-8.37	100.39	106.33
24	C	508	CLA	C2D-C1D-ND	8.36	116.27	110.10
24	B	606	CLA	C2D-C1D-ND	8.36	116.26	110.10
24	b	615	CLA	C2D-C1D-ND	8.36	116.26	110.10
24	b	612	CLA	C1D-ND-C4D	-8.33	100.42	106.33
24	C	502	CLA	C1D-ND-C4D	-8.33	100.42	106.33
24	B	612	CLA	C2D-C1D-ND	8.32	116.23	110.10
24	D	404	CLA	C2D-C1D-ND	8.32	116.23	110.10
24	B	616	CLA	C2D-C1D-ND	8.31	116.23	110.10
24	c	504	CLA	C1D-ND-C4D	-8.29	100.44	106.33
24	B	614	CLA	C2D-C1D-ND	8.26	116.19	110.10
24	d	402	CLA	C4A-NA-C1A	-8.26	102.99	106.71
24	B	616	CLA	C1D-ND-C4D	-8.25	100.47	106.33
24	b	612	CLA	C2D-C1D-ND	8.24	116.18	110.10
24	D	403	CLA	C1D-ND-C4D	-8.24	100.48	106.33
24	b	609	CLA	C2D-C1D-ND	8.24	116.17	110.10
24	C	514	CLA	C2D-C1D-ND	8.23	116.17	110.10
24	C	506	CLA	C1D-ND-C4D	-8.21	100.50	106.33
24	B	604	CLA	C2D-C1D-ND	8.17	116.12	110.10
24	B	608	CLA	C2D-C1D-ND	8.16	116.12	110.10
24	b	607	CLA	C2D-C1D-ND	8.16	116.12	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	408	PHO	O2D-CGD-CBD	8.16	121.33	111.00
24	b	609	CLA	C1D-ND-C4D	-8.14	100.55	106.33
24	B	609	CLA	C2D-C1D-ND	8.12	116.09	110.10
24	C	513	CLA	C2D-C1D-ND	8.09	116.06	110.10
24	A	405	CLA	C4A-NA-C1A	-8.07	103.08	106.71
24	b	614	CLA	C2D-C1D-ND	8.05	116.04	110.10
24	B	603	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	B	617	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	d	404	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	b	620	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	a	407	CLA	C2D-C1D-ND	8.03	116.02	110.10
24	c	507	CLA	C1D-ND-C4D	-8.03	100.63	106.33
24	B	611	CLA	C2D-C1D-ND	8.00	116.00	110.10
24	c	512	CLA	C2D-C1D-ND	7.99	115.99	110.10
24	d	401	CLA	C2D-C1D-ND	7.97	115.98	110.10
24	C	504	CLA	C2D-C1D-ND	7.97	115.98	110.10
24	d	402	CLA	C1D-ND-C4D	-7.95	100.69	106.33
24	a	409	CLA	C2D-C1D-ND	7.93	115.95	110.10
24	C	502	CLA	C2D-C1D-ND	7.91	115.93	110.10
24	C	505	CLA	C2D-C1D-ND	7.90	115.92	110.10
24	C	509	CLA	C2D-C1D-ND	7.88	115.91	110.10
24	B	602	CLA	C2D-C1D-ND	7.87	115.91	110.10
24	C	507	CLA	C2D-C1D-ND	7.87	115.90	110.10
24	C	511	CLA	C2D-C1D-ND	7.79	115.84	110.10
24	D	401	CLA	C2D-C1D-ND	7.79	115.84	110.10
24	B	613	CLA	C1D-ND-C4D	-7.76	100.83	106.33
24	b	617	CLA	C2D-C1D-ND	7.72	115.79	110.10
24	c	513	CLA	C2D-C1D-ND	7.69	115.77	110.10
24	a	406	CLA	C2D-C1D-ND	7.68	115.76	110.10
24	c	515	CLA	C2D-C1D-ND	7.67	115.76	110.10
24	A	405	CLA	C1D-ND-C4D	-7.65	100.90	106.33
25	d	403	PHO	O2D-CGD-CBD	7.65	120.69	111.00
24	A	405	CLA	C2D-C1D-ND	7.64	115.73	110.10
24	c	504	CLA	C2D-C1D-ND	7.63	115.73	110.10
24	b	606	CLA	C2D-C1D-ND	7.60	115.71	110.10
24	b	621	CLA	C2D-C1D-ND	7.59	115.70	110.10
24	D	403	CLA	C2D-C1D-ND	7.56	115.68	110.10
24	C	503	CLA	C2D-C1D-ND	7.42	115.57	110.10
24	b	608	CLA	C2D-C1D-ND	7.38	115.54	110.10
24	A	406	CLA	C2D-C1D-ND	7.27	115.47	110.10
24	c	508	CLA	C2D-C1D-ND	7.27	115.46	110.10
24	b	613	CLA	C2D-C1D-ND	7.21	115.42	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	CMD-C2D-C1D	7.21	137.42	124.71
24	C	510	CLA	C2D-C1D-ND	7.20	115.41	110.10
24	B	612	CLA	C4A-NA-C1A	-7.20	103.47	106.71
24	B	616	CLA	C4A-NA-C1A	-7.19	103.47	106.71
24	b	609	CLA	CMD-C2D-C1D	7.14	137.29	124.71
24	B	607	CLA	C4A-NA-C1A	-7.09	103.52	106.71
24	D	403	CLA	C4A-NA-C1A	-7.07	103.53	106.71
24	c	511	CLA	C2D-C1D-ND	7.03	115.28	110.10
24	b	620	CLA	C4A-NA-C1A	-7.01	103.55	106.71
24	C	508	CLA	CMD-C2D-C1D	6.93	136.93	124.71
24	B	613	CLA	C2D-C1D-ND	6.90	115.19	110.10
24	c	505	CLA	C4A-NA-C1A	-6.90	103.61	106.71
24	d	404	CLA	CMD-C2D-C1D	6.86	136.81	124.71
24	D	403	CLA	CMD-C2D-C1D	6.85	136.79	124.71
24	B	615	CLA	CMD-C2D-C1D	6.85	136.79	124.71
24	b	610	CLA	CMD-C2D-C1D	6.81	136.72	124.71
24	c	507	CLA	C4A-NA-C1A	-6.75	103.67	106.71
24	C	504	CLA	C4A-NA-C1A	-6.71	103.69	106.71
24	A	405	CLA	C2C-C1C-NC	6.67	116.22	109.97
24	b	616	CLA	CHD-C4C-C3C	-6.64	115.08	124.84
24	b	607	CLA	C4A-NA-C1A	-6.64	103.72	106.71
24	B	610	CLA	CHD-C4C-C3C	-6.63	115.09	124.84
24	a	406	CLA	C2C-C1C-NC	6.62	116.17	109.97
24	b	618	CLA	CHD-C4C-C3C	-6.60	115.14	124.84
25	A	407	PHO	O2D-CGD-CBD	6.60	119.36	111.00
24	d	402	CLA	C2D-C1D-ND	6.59	114.96	110.10
24	d	404	CLA	C4A-NA-C1A	-6.58	103.75	106.71
24	b	606	CLA	CMD-C2D-C1D	6.58	136.31	124.71
24	C	506	CLA	C2D-C1D-ND	6.57	114.95	110.10
24	B	603	CLA	C4A-NA-C1A	-6.57	103.75	106.71
24	c	515	CLA	CHD-C1D-ND	-6.56	118.42	124.45
24	d	404	CLA	CHD-C1D-ND	-6.53	118.45	124.45
24	C	509	CLA	C4A-NA-C1A	-6.53	103.77	106.71
25	A	408	PHO	O2D-CGD-CBD	6.52	119.25	111.00
24	b	612	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
24	c	515	CLA	CMD-C2D-C1D	6.47	136.12	124.71
35	b	628	HTG	C1'-S1-C1	6.47	112.19	100.09
24	c	511	CLA	CMD-C2D-C1D	6.47	136.11	124.71
24	b	608	CLA	C4A-NA-C1A	-6.46	103.80	106.71
24	B	614	CLA	C2C-C1C-NC	6.45	116.02	109.97
24	C	508	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
24	B	607	CLA	CHD-C4C-C3C	-6.44	115.37	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	CMD-C2D-C1D	6.44	136.07	124.71
24	D	401	CLA	CMD-C2D-C1D	6.43	136.05	124.71
24	B	602	CLA	CMD-C2D-C1D	6.43	136.05	124.71
24	b	613	CLA	CMD-C2D-C1D	6.43	136.04	124.71
24	b	610	CLA	CHD-C4C-C3C	-6.42	115.40	124.84
24	c	508	CLA	CMD-C2D-C1D	6.42	136.02	124.71
24	a	407	CLA	CMD-C2D-C1D	6.40	135.99	124.71
24	B	602	CLA	C4A-NA-C1A	-6.39	103.83	106.71
24	C	512	CLA	CMD-C2D-C1D	6.38	135.96	124.71
24	B	606	CLA	C4A-NA-C1A	-6.37	103.84	106.71
24	B	613	CLA	C4A-NA-C1A	-6.37	103.84	106.71
24	a	406	CLA	CMD-C2D-C1D	6.37	135.94	124.71
24	A	409	CLA	CHD-C4C-C3C	-6.36	115.49	124.84
24	A	406	CLA	CMD-C2D-C1D	6.36	135.92	124.71
24	C	504	CLA	CMD-C2D-C1D	6.35	135.91	124.71
24	D	401	CLA	C2C-C1C-NC	6.35	115.92	109.97
24	d	401	CLA	C2C-C1C-NC	6.35	115.92	109.97
24	B	605	CLA	C2C-C1C-NC	6.34	115.91	109.97
24	B	605	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
24	b	606	CLA	CHD-C4C-C3C	-6.30	115.57	124.84
24	c	505	CLA	CMD-C2D-C1D	6.29	135.79	124.71
24	B	606	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
24	c	510	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
24	B	615	CLA	CHD-C1D-ND	-6.28	118.69	124.45
24	C	505	CLA	CHD-C1D-ND	-6.28	118.69	124.45
24	b	608	CLA	CMD-C2D-C1D	6.26	135.75	124.71
24	b	610	CLA	CHD-C1D-ND	-6.26	118.70	124.45
24	B	604	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
24	c	506	CLA	CHD-C1D-ND	-6.25	118.71	124.45
24	B	617	CLA	O2D-CGD-CBD	6.24	122.35	111.27
24	C	510	CLA	O2D-CGD-CBD	6.23	122.34	111.27
24	b	606	CLA	CHD-C1D-ND	-6.23	118.73	124.45
24	C	510	CLA	CMD-C2D-C1D	6.22	135.68	124.71
24	b	609	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	b	618	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	D	403	CLA	C2C-C1C-NC	6.19	115.77	109.97
24	D	403	CLA	CHD-C1D-ND	-6.19	118.77	124.45
24	B	609	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
24	b	611	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
24	d	402	CLA	C2C-C1C-NC	6.17	115.75	109.97
24	b	619	CLA	C2C-C1C-NC	6.17	115.75	109.97
24	C	505	CLA	CMD-C2D-C1D	6.15	135.56	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	C2C-C1C-NC	6.15	115.73	109.97
24	d	402	CLA	CMD-C2D-C1D	6.14	135.54	124.71
24	c	505	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
24	c	509	CLA	CHD-C4C-C3C	-6.11	115.85	124.84
24	b	618	CLA	CMD-C2D-C1D	6.11	135.48	124.71
24	B	612	CLA	CHD-C4C-C3C	-6.10	115.88	124.84
24	b	609	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
24	c	514	CLA	CHD-C1D-ND	-6.09	118.86	124.45
35	d	411	HTG	C1'-S1-C1	6.08	111.46	100.09
24	b	614	CLA	C2C-C1C-NC	6.07	115.66	109.97
24	C	504	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
24	d	401	CLA	CHD-C1D-ND	-6.06	118.89	124.45
24	b	611	CLA	CMD-C2D-C1D	6.06	135.39	124.71
24	C	506	CLA	CMD-C2D-C1D	6.05	135.37	124.71
24	b	614	CLA	C4A-NA-C1A	-6.05	103.99	106.71
24	C	512	CLA	CHD-C1D-ND	-6.04	118.90	124.45
24	b	608	CLA	O2D-CGD-CBD	6.03	121.99	111.27
24	A	409	CLA	CHD-C1D-ND	-6.02	118.92	124.45
24	c	512	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
24	b	621	CLA	C2C-C1C-NC	6.02	115.61	109.97
24	b	617	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
24	C	506	CLA	C2C-C1C-NC	6.02	115.61	109.97
24	c	507	CLA	CMD-C2D-C1D	6.01	135.31	124.71
24	C	507	CLA	C2C-C1C-NC	6.01	115.60	109.97
24	B	614	CLA	CMD-C2D-C1D	6.00	135.30	124.71
24	d	404	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
24	c	509	CLA	O2D-CGD-CBD	6.00	121.94	111.27
24	D	404	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
24	B	603	CLA	CMD-C2D-C1D	5.99	135.28	124.71
24	b	607	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
24	c	507	CLA	C2D-C1D-ND	5.98	114.51	110.10
24	c	509	CLA	C2C-C1C-NC	5.97	115.57	109.97
24	c	503	CLA	C2C-C1C-NC	5.97	115.56	109.97
24	B	602	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
24	B	609	CLA	C2C-C1C-NC	5.97	115.56	109.97
24	c	503	CLA	CMD-C2D-C1D	5.96	135.21	124.71
24	b	615	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
24	C	511	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
24	c	513	CLA	CMD-C2D-C1D	5.95	135.20	124.71
24	C	509	CLA	C2C-C1C-NC	5.94	115.54	109.97
24	b	613	CLA	C4A-NA-C1A	-5.93	104.04	106.71
24	c	514	CLA	CMD-C2D-C1D	5.93	135.16	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	C2C-C1C-NC	5.92	115.52	109.97
35	B	624	HTG	C1'-S1-C1	5.92	111.17	100.09
24	D	401	CLA	CHD-C1D-ND	-5.91	119.03	124.45
24	c	507	CLA	O2D-CGD-CBD	5.90	121.76	111.27
24	A	406	CLA	CHD-C1D-ND	-5.90	119.03	124.45
24	b	612	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	B	602	CLA	CHD-C1D-ND	-5.90	119.04	124.45
24	D	404	CLA	CMD-C2D-C1D	5.89	135.10	124.71
24	b	609	CLA	C4A-NA-C1A	-5.89	104.06	106.71
24	c	506	CLA	CMD-C2D-C1D	5.89	135.09	124.71
24	b	621	CLA	CMD-C2D-C1D	5.89	135.09	124.71
24	B	611	CLA	CMD-C2D-C1D	5.89	135.09	124.71
24	C	505	CLA	C2C-C1C-NC	5.88	115.48	109.97
24	B	603	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
24	a	409	CLA	C2C-C1C-NC	5.86	115.46	109.97
24	c	507	CLA	C2C-C1C-NC	5.85	115.46	109.97
24	B	615	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	a	407	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
24	a	407	CLA	C4A-NA-C1A	-5.84	104.08	106.71
24	B	613	CLA	CMD-C2D-C1D	5.83	134.99	124.71
24	B	617	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
24	b	620	CLA	CHD-C1D-ND	-5.83	119.10	124.45
24	C	503	CLA	CHD-C4C-C3C	-5.83	116.28	124.84
24	B	616	CLA	CHD-C4C-C3C	-5.83	116.28	124.84
24	C	511	CLA	CMD-C2D-C1D	5.82	134.98	124.71
35	c	522	HTG	C1'-S1-C1	5.82	110.97	100.09
24	C	512	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	C	513	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	b	611	CLA	C4A-NA-C1A	-5.81	104.09	106.71
24	b	614	CLA	CMD-C2D-C1D	5.80	134.94	124.71
24	d	401	CLA	CMD-C2D-C1D	5.80	134.94	124.71
24	C	504	CLA	C2C-C1C-NC	5.78	115.39	109.97
24	C	507	CLA	CMD-C2D-C1D	5.78	134.90	124.71
24	B	615	CLA	C4A-NA-C1A	-5.78	104.11	106.71
24	b	609	CLA	O2D-CGD-CBD	5.77	121.52	111.27
24	A	405	CLA	CMD-C2D-C1D	5.76	134.87	124.71
24	C	513	CLA	C4A-NA-C1A	-5.76	104.11	106.71
24	c	511	CLA	O2D-CGD-CBD	5.75	121.49	111.27
24	B	616	CLA	CMD-C2D-C1D	5.75	134.85	124.71
24	c	508	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	c	512	CLA	CMD-C2D-C1D	5.74	134.84	124.71
24	B	607	CLA	O2D-CGD-CBD	5.74	121.47	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	CLA	C4A-NA-C1A	-5.74	104.13	106.71
24	C	510	CLA	C2C-C1C-NC	5.73	115.34	109.97
24	c	514	CLA	O2D-CGD-CBD	5.73	121.45	111.27
24	b	607	CLA	O2D-CGD-CBD	5.73	121.45	111.27
24	B	605	CLA	CHD-C1D-ND	-5.73	119.19	124.45
24	D	403	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
24	c	513	CLA	C2C-C1C-NC	5.72	115.33	109.97
24	B	605	CLA	C4A-NA-C1A	-5.72	104.13	106.71
24	b	620	CLA	CMD-C2D-C1D	5.72	134.79	124.71
24	B	614	CLA	CHD-C1D-ND	-5.71	119.21	124.45
24	B	608	CLA	C4A-NA-C1A	-5.71	104.14	106.71
24	C	503	CLA	C4A-NA-C1A	-5.71	104.14	106.71
24	b	613	CLA	CHD-C1D-ND	-5.70	119.22	124.45
24	a	407	CLA	CHD-C1D-ND	-5.70	119.22	124.45
24	D	404	CLA	CHD-C1D-ND	-5.69	119.22	124.45
24	b	611	CLA	CHD-C1D-ND	-5.69	119.22	124.45
24	C	506	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
24	b	614	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
24	C	505	CLA	O2D-CGD-CBD	5.67	121.34	111.27
24	b	610	CLA	C2C-C1C-NC	5.67	115.28	109.97
24	B	611	CLA	C2C-C1C-NC	5.67	115.28	109.97
24	B	614	CLA	C4A-NA-C1A	-5.67	104.16	106.71
24	c	511	CLA	C2C-C1C-NC	5.66	115.28	109.97
24	B	603	CLA	CHD-C1D-ND	-5.66	119.25	124.45
24	B	604	CLA	C2C-C1C-NC	5.65	115.27	109.97
24	c	503	CLA	O2D-CGD-CBD	5.65	121.31	111.27
24	c	504	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
24	C	502	CLA	CMD-C2D-C1D	5.65	134.66	124.71
24	c	506	CLA	C2C-C1C-NC	5.65	115.26	109.97
24	b	620	CLA	C2C-C1C-NC	5.64	115.25	109.97
24	B	606	CLA	O2D-CGD-CBD	5.64	121.29	111.27
24	C	503	CLA	C2C-C1C-NC	5.64	115.25	109.97
24	B	606	CLA	CHD-C1D-ND	-5.64	119.28	124.45
24	b	616	CLA	CMD-C2D-C1D	5.64	134.65	124.71
24	c	513	CLA	CHD-C1D-ND	-5.63	119.28	124.45
24	c	512	CLA	CHD-C1D-ND	-5.63	119.28	124.45
24	B	611	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
24	B	616	CLA	C2C-C1C-NC	5.62	115.24	109.97
24	b	609	CLA	CHD-C1D-ND	-5.62	119.29	124.45
24	B	611	CLA	CHD-C1D-ND	-5.62	119.29	124.45
24	b	612	CLA	CMD-C2D-C1D	5.60	134.59	124.71
24	b	613	CLA	C2C-C1C-NC	5.60	115.22	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	616	CLA	C2C-C1C-NC	5.59	115.21	109.97
24	C	513	CLA	C2C-C1C-NC	5.59	115.21	109.97
24	B	608	CLA	CMD-C2D-C1D	5.59	134.56	124.71
24	B	607	CLA	CMD-C2D-C1D	5.59	134.56	124.71
24	C	508	CLA	CHD-C1D-ND	-5.58	119.32	124.45
24	C	502	CLA	C2C-C1C-NC	5.58	115.20	109.97
24	B	606	CLA	CMD-C2D-C1D	5.58	134.55	124.71
24	C	507	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
24	C	514	CLA	CMD-C2D-C1D	5.57	134.54	124.71
24	C	504	CLA	CHD-C1D-ND	-5.56	119.34	124.45
24	C	506	CLA	O2D-CGD-CBD	5.55	121.14	111.27
24	B	608	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
24	a	409	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
27	A	411	SQD	O6-C1-C2	5.55	116.97	108.30
24	B	613	CLA	C2C-C1C-NC	5.55	115.17	109.97
24	b	608	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
24	c	513	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
24	c	504	CLA	C2C-C1C-NC	5.53	115.16	109.97
24	B	617	CLA	C2C-C1C-NC	5.53	115.15	109.97
24	B	610	CLA	CHD-C1D-ND	-5.52	119.38	124.45
24	c	509	CLA	CMD-C2D-C1D	5.52	134.44	124.71
24	c	514	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
24	b	615	CLA	C2C-C1C-NC	5.52	115.14	109.97
24	C	510	CLA	CHD-C1D-ND	-5.52	119.38	124.45
24	c	503	CLA	CHD-C4C-C3C	-5.51	116.73	124.84
24	d	402	CLA	CHD-C1D-ND	-5.51	119.39	124.45
24	c	506	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
24	B	617	CLA	CMD-C2D-C1D	5.51	134.43	124.71
24	b	620	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
24	C	512	CLA	C2C-C1C-NC	5.50	115.13	109.97
24	b	619	CLA	C1-C2-C3	-5.50	116.53	126.04
24	c	511	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
24	B	612	CLA	CHD-C1D-ND	-5.49	119.41	124.45
24	c	503	CLA	CHD-C1D-ND	-5.49	119.41	124.45
24	C	514	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
24	c	508	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
24	b	619	CLA	CHD-C1D-ND	-5.48	119.41	124.45
24	C	514	CLA	CHD-C1D-ND	-5.48	119.42	124.45
24	C	509	CLA	CHD-C1D-ND	-5.48	119.42	124.45
24	C	507	CLA	CHD-C1D-ND	-5.47	119.42	124.45
24	C	511	CLA	C2C-C1C-NC	5.47	115.10	109.97
24	c	515	CLA	C2C-C1C-NC	5.46	115.09	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	CMD-C2D-C1D	5.46	134.34	124.71
24	C	510	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
24	C	502	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
24	c	515	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
24	B	607	CLA	C2C-C1C-NC	5.46	115.09	109.97
24	b	619	CLA	O2D-CGD-CBD	5.46	120.96	111.27
24	a	406	CLA	C4A-NA-C1A	-5.46	104.25	106.71
24	c	508	CLA	CHD-C1D-ND	-5.45	119.45	124.45
24	B	603	CLA	C2C-C1C-NC	5.45	115.07	109.97
38	E	103	HEM	CAD-CBD-CGD	5.41	125.25	113.60
24	b	612	CLA	C3C-C4C-NC	5.41	116.64	110.57
24	b	621	CLA	C4A-NA-C1A	-5.40	104.28	106.71
24	C	508	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	C	513	CLA	O2D-CGD-CBD	5.40	120.86	111.27
24	A	406	CLA	C2C-C1C-NC	5.39	115.03	109.97
24	B	609	CLA	C4A-NA-C1A	-5.39	104.28	106.71
24	C	503	CLA	CMD-C2D-C1D	5.39	134.21	124.71
24	c	504	CLA	CHD-C1D-ND	-5.39	119.50	124.45
24	b	613	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
24	c	504	CLA	O2D-CGD-CBD	5.38	120.83	111.27
24	B	615	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	c	505	CLA	CHD-C1D-ND	-5.37	119.52	124.45
24	C	502	CLA	O2D-CGD-CBD	5.37	120.81	111.27
24	b	606	CLA	C4A-NA-C1A	-5.36	104.30	106.71
24	C	514	CLA	C2C-C1C-NC	5.36	115.00	109.97
24	c	510	CLA	C2C-C1C-NC	5.36	114.99	109.97
24	c	504	CLA	CMD-C2D-C1D	5.35	134.15	124.71
24	B	612	CLA	C2C-C1C-NC	5.34	114.98	109.97
27	b	601	SQD	O6-C1-C2	5.34	116.64	108.30
24	c	510	CLA	O2D-CGD-CBD	5.34	120.75	111.27
24	b	619	CLA	CMD-C2D-C1D	5.34	134.12	124.71
24	C	509	CLA	O2D-CGD-CBD	5.33	120.73	111.27
24	a	406	CLA	CHD-C1D-ND	-5.32	119.56	124.45
24	c	509	CLA	CHD-C1D-ND	-5.32	119.56	124.45
24	b	614	CLA	CHD-C1D-ND	-5.32	119.56	124.45
24	b	611	CLA	O2D-CGD-CBD	5.31	120.71	111.27
24	C	508	CLA	C4A-NA-C1A	-5.31	104.32	106.71
24	a	409	CLA	CMD-C2D-C1D	5.31	134.06	124.71
24	B	615	CLA	O2D-CGD-CBD	5.30	120.69	111.27
24	b	608	CLA	CHD-C1D-ND	-5.30	119.58	124.45
24	C	508	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
24	c	514	CLA	C4A-NA-C1A	-5.29	104.33	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	609	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
24	D	404	CLA	O2D-CGD-CBD	5.28	120.65	111.27
24	B	604	CLA	CMD-C2D-C1D	5.28	134.01	124.71
24	C	513	CLA	CMD-C2D-C1D	5.27	134.01	124.71
24	B	610	CLA	C4A-NA-C1A	-5.27	104.33	106.71
24	C	502	CLA	CHD-C1D-ND	-5.27	119.61	124.45
24	b	621	CLA	CHD-C1D-ND	-5.26	119.62	124.45
35	B	631	HTG	C1'-S1-C1	5.26	109.93	100.09
24	c	510	CLA	C4A-NA-C1A	-5.26	104.34	106.71
24	B	608	CLA	CHD-C1D-ND	-5.25	119.63	124.45
24	B	602	CLA	C2C-C1C-NC	5.24	114.88	109.97
24	c	512	CLA	C2C-C1C-NC	5.24	114.88	109.97
24	b	606	CLA	O2D-CGD-CBD	5.24	120.58	111.27
24	B	602	CLA	O2D-CGD-CBD	5.24	120.58	111.27
24	C	509	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
24	c	511	CLA	C4A-NA-C1A	-5.24	104.35	106.71
24	d	402	CLA	O2D-CGD-CBD	5.24	120.57	111.27
24	b	607	CLA	CHD-C1D-ND	-5.24	119.64	124.45
24	d	402	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
24	C	511	CLA	C4A-NA-C1A	-5.22	104.36	106.71
24	c	507	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
24	b	618	CLA	C1-C2-C3	-5.20	117.04	126.04
24	B	605	CLA	O2D-CGD-CBD	5.20	120.50	111.27
24	b	608	CLA	C2C-C1C-NC	5.20	114.84	109.97
24	b	616	CLA	O2D-CGD-CBD	5.19	120.50	111.27
24	B	604	CLA	CHD-C1D-ND	-5.19	119.69	124.45
24	b	610	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
24	c	505	CLA	C2C-C1C-NC	5.18	114.83	109.97
24	B	615	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
24	b	609	CLA	C3C-C4C-NC	5.18	116.38	110.57
24	B	614	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
24	B	616	CLA	CHD-C1D-ND	-5.17	119.70	124.45
24	C	511	CLA	O2D-CGD-CBD	5.17	120.45	111.27
24	A	405	CLA	C3C-C4C-NC	5.16	116.36	110.57
24	b	621	CLA	O2D-CGD-CBD	5.16	120.43	111.27
24	B	607	CLA	CHD-C1D-ND	-5.15	119.72	124.45
24	A	409	CLA	C2C-C1C-NC	5.14	114.79	109.97
24	b	615	CLA	CMD-C2D-C1D	5.14	133.78	124.71
24	D	403	CLA	C3C-C4C-NC	5.14	116.34	110.57
24	B	616	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
24	B	604	CLA	O2D-CGD-CBD	5.13	120.39	111.27
24	B	610	CLA	C2C-C1C-NC	5.13	114.78	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	406	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
24	d	404	CLA	C2C-C1C-NC	5.13	114.78	109.97
24	b	617	CLA	C3C-C4C-NC	5.12	116.32	110.57
35	c	523	HTG	C1'-S1-C1	5.12	109.67	100.09
24	C	511	CLA	CHD-C1D-ND	-5.11	119.75	124.45
24	c	514	CLA	C2C-C1C-NC	5.11	114.76	109.97
24	b	619	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
24	b	618	CLA	C3C-C4C-NC	5.10	116.29	110.57
24	b	607	CLA	C2C-C1C-NC	5.09	114.74	109.97
24	a	407	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
24	D	404	CLA	C4A-NA-C1A	-5.07	104.42	106.71
24	d	401	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
24	b	613	CLA	O2D-CGD-CBD	5.07	120.28	111.27
24	a	409	CLA	CHD-C1D-ND	-5.07	119.80	124.45
24	b	616	CLA	CHD-C1D-ND	-5.07	119.80	124.45
24	a	407	CLA	C2C-C1C-NC	5.06	114.71	109.97
38	e	102	HEM	CBA-CAA-C2A	-5.06	103.99	112.62
24	B	605	CLA	C3C-C4C-NC	5.05	116.24	110.57
24	B	604	CLA	C3C-C4C-NC	5.05	116.23	110.57
24	b	606	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	b	616	CLA	C4A-NA-C1A	-5.04	104.44	106.71
24	b	621	CLA	CHD-C4C-C3C	-5.04	117.44	124.84
25	d	403	PHO	C1-C2-C3	-5.03	117.34	126.04
24	B	617	CLA	CHD-C1D-ND	-5.03	119.83	124.45
24	B	611	CLA	O2D-CGD-CBD	5.02	120.19	111.27
24	c	506	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	C	503	CLA	O2D-CGD-CBD	5.01	120.17	111.27
24	B	613	CLA	O2D-CGD-CBD	5.01	120.16	111.27
24	c	509	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	D	404	CLA	C2C-C1C-NC	4.99	114.65	109.97
24	b	612	CLA	CHD-C1D-ND	-4.99	119.87	124.45
24	B	613	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
24	A	405	CLA	CHD-C4C-C3C	-4.98	117.51	124.84
24	B	611	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
24	c	509	CLA	C3C-C4C-NC	4.98	116.16	110.57
24	C	513	CLA	CHD-C1D-ND	-4.97	119.88	124.45
26	D	405	BCR	C24-C23-C22	-4.97	118.73	126.23
24	c	503	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
24	B	605	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	b	611	CLA	C2C-C1C-NC	4.96	114.62	109.97
24	b	617	CLA	C4A-NA-C1A	-4.96	104.48	106.71
24	b	617	CLA	O2D-CGD-CBD	4.96	120.08	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
24	c	506	CLA	C4A-NA-C1A	-4.96	104.48	106.71
24	c	511	CLA	CHD-C1D-ND	-4.96	119.90	124.45
24	c	508	CLA	C4A-NA-C1A	-4.95	104.48	106.71
24	b	616	CLA	C3C-C4C-NC	4.93	116.10	110.57
24	b	618	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	b	601	SQD	O47-C7-C8	4.93	122.13	111.50
24	C	512	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
24	C	503	CLA	CHD-C1D-ND	-4.93	119.92	124.45
24	c	515	CLA	C4A-NA-C1A	-4.93	104.49	106.71
24	c	505	CLA	O2D-CGD-CBD	4.93	120.03	111.27
35	b	603	HTG	C1'-S1-C1	4.93	109.30	100.09
24	b	617	CLA	CMD-C2D-C1D	4.92	133.39	124.71
24	c	512	CLA	O2D-CGD-CBD	4.92	120.01	111.27
24	C	509	CLA	CMD-C2D-C1D	4.92	133.38	124.71
24	B	607	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
24	B	609	CLA	CHD-C1D-ND	-4.91	119.94	124.45
24	b	607	CLA	CMD-C2D-C1D	4.91	133.36	124.71
24	A	409	CLA	CMD-C2D-C1D	4.91	133.36	124.71
24	C	506	CLA	C4A-NA-C1A	-4.90	104.50	106.71
24	c	510	CLA	C3C-C4C-NC	4.90	116.06	110.57
24	D	401	CLA	CHD-C4C-C3C	-4.89	117.65	124.84
24	b	614	CLA	O2D-CGD-CBD	4.89	119.96	111.27
27	f	101	SQD	O47-C7-C8	4.89	122.03	111.50
24	d	404	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
24	B	609	CLA	CMD-C2D-C1D	4.88	133.32	124.71
24	B	613	CLA	C3C-C4C-NC	4.88	116.05	110.57
24	c	510	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
36	D	407	DGD	O2G-C1B-C2B	4.87	122.00	111.50
24	a	406	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
24	D	401	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
24	D	401	CLA	C1C-C2C-C3C	-4.86	101.84	106.96
24	c	503	CLA	C4A-NA-C1A	-4.86	104.52	106.71
35	B	630	HTG	C1'-S1-C1	4.85	109.17	100.09
24	b	619	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
24	c	505	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
24	B	608	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
35	C	522	HTG	C1'-S1-C1	4.84	109.15	100.09
24	b	616	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
35	C	523	HTG	C1-O5-C5	4.83	121.49	112.58
27	a	411	SQD	O47-C7-C8	4.81	121.87	111.50
24	b	615	CLA	C4A-NA-C1A	-4.80	104.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
24	C	505	CLA	CHD-C4C-C3C	-4.80	117.79	124.84
24	b	615	CLA	CHD-C1D-ND	-4.79	120.05	124.45
24	B	606	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	A	409	CLA	C3D-C4D-ND	4.79	117.98	110.24
24	C	507	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
24	B	614	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
24	B	607	CLA	C3C-C4C-NC	4.78	115.93	110.57
24	C	502	CLA	C4A-NA-C1A	-4.78	104.56	106.71
24	B	603	CLA	O2D-CGD-CBD	4.77	119.75	111.27
24	a	409	CLA	O2D-CGD-CBD	4.76	119.73	111.27
24	A	406	CLA	C3D-C4D-ND	4.76	117.94	110.24
27	a	411	SQD	O6-C1-C2	4.76	115.73	108.30
24	a	406	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
24	b	617	CLA	C2C-C1C-NC	4.74	114.42	109.97
24	C	505	CLA	C4A-NA-C1A	-4.73	104.58	106.71
24	b	621	CLA	C3B-C4B-NB	4.73	115.33	109.21
24	d	401	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	c	514	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	C	508	CLA	O2D-CGD-CBD	4.71	119.63	111.27
24	c	506	CLA	O2D-CGD-CBD	4.69	119.61	111.27
24	B	602	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
24	C	505	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
34	c	521	LMG	O7-C10-C11	4.69	121.60	111.50
24	C	504	CLA	C3C-C4C-NC	4.68	115.82	110.57
24	b	611	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
24	c	505	CLA	C3C-C4C-NC	4.68	115.82	110.57
35	C	523	HTG	C1'-S1-C1	4.68	108.84	100.09
24	c	508	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
24	b	620	CLA	O2D-CGD-CBD	4.67	119.57	111.27
38	e	102	HEM	CAD-CBD-CGD	4.67	123.65	113.60
24	C	502	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
38	E	103	HEM	CHC-C4B-NB	4.67	129.50	124.43
34	C	521	LMG	O7-C10-C11	4.67	121.56	111.50
24	b	611	CLA	C3C-C4C-NC	4.67	115.80	110.57
24	d	401	CLA	C3B-C4B-NB	4.66	115.24	109.21
24	B	611	CLA	C3C-C4C-NC	4.66	115.80	110.57
24	B	609	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
24	C	513	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	613	CLA	CHD-C1D-ND	-4.65	120.18	124.45
24	c	504	CLA	C4A-NA-C1A	-4.65	104.62	106.71
24	b	621	CLA	C3D-C2D-C1D	-4.64	99.49	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	B	624	HTG	O5-C1-C2	4.64	116.15	110.31
24	B	606	CLA	C3C-C4C-NC	4.64	115.77	110.57
24	B	612	CLA	C3D-C2D-C1D	-4.64	99.51	105.83
24	b	610	CLA	C4A-NA-C1A	-4.63	104.62	106.71
24	b	612	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	b	615	CLA	C3C-C4C-NC	4.63	115.77	110.57
24	C	508	CLA	C3C-C4C-NC	4.63	115.76	110.57
24	c	510	CLA	CMD-C2D-C1D	4.62	132.86	124.71
24	c	510	CLA	CHD-C1D-ND	-4.62	120.21	124.45
24	D	403	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
24	b	614	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	c	507	CLA	C3C-C4C-NC	4.60	115.73	110.57
24	B	606	CLA	C3D-C4D-ND	4.59	117.67	110.24
34	C	501	LMG	O7-C10-C11	4.59	121.39	111.50
24	c	512	CLA	C3D-C4D-ND	4.59	117.66	110.24
24	B	610	CLA	O2D-CGD-CBD	4.58	119.42	111.27
24	B	615	CLA	C3D-C4D-ND	4.58	117.64	110.24
24	A	409	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
26	D	405	BCR	C7-C8-C9	-4.57	119.33	126.23
24	d	402	CLA	C3C-C4C-NC	4.57	115.69	110.57
26	y	101	BCR	C33-C5-C6	-4.56	119.40	124.53
24	b	620	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	b	607	CLA	C3C-C4C-NC	4.55	115.68	110.57
27	F	101	SQD	O6-C1-C2	4.55	115.41	108.30
24	B	617	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	C	503	CLA	C3C-C4C-NC	4.53	115.65	110.57
24	a	407	CLA	O2D-CGD-CBD	4.52	119.31	111.27
24	b	607	CLA	C3D-C4D-ND	4.52	117.55	110.24
24	C	506	CLA	C3C-C4C-NC	4.52	115.64	110.57
24	C	506	CLA	CHD-C1D-ND	-4.52	120.30	124.45
24	C	514	CLA	C3D-C4D-ND	4.52	117.55	110.24
24	B	612	CLA	O2D-CGD-CBD	4.52	119.30	111.27
24	B	609	CLA	C3C-C4C-NC	4.51	115.63	110.57
24	C	507	CLA	O2D-CGD-CBD	4.51	119.28	111.27
24	B	617	CLA	C4A-NA-C1A	-4.51	104.68	106.71
24	b	615	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
24	D	404	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
24	C	504	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	c	507	CLA	CHD-C1D-ND	-4.50	120.32	124.45
24	B	610	CLA	C3D-C4D-ND	4.50	117.51	110.24
24	C	514	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	B	616	CLA	C3C-C4C-NC	4.49	115.61	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	602	LMT	C1'-O5'-C5'	4.49	122.50	113.69
24	C	511	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
24	b	612	CLA	O2D-CGD-CBD	4.47	119.22	111.27
24	b	617	CLA	CHD-C1D-ND	-4.47	120.34	124.45
24	A	405	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	b	612	CLA	C4A-NA-C1A	-4.47	104.70	106.71
24	B	604	CLA	C3D-C4D-ND	4.46	117.46	110.24
24	D	401	CLA	O2D-CGD-CBD	4.46	119.20	111.27
24	b	609	CLA	C1C-C2C-C3C	-4.46	102.26	106.96
27	l	101	SQD	O47-C7-C8	4.45	121.10	111.50
24	c	515	CLA	C3D-C4D-ND	4.45	117.44	110.24
24	A	405	CLA	CHD-C1D-ND	-4.45	120.36	124.45
24	D	404	CLA	C3C-C4C-NC	4.45	115.56	110.57
24	D	404	CLA	C3D-C4D-ND	4.45	117.43	110.24
24	b	615	CLA	O2D-CGD-CBD	4.44	119.16	111.27
24	b	606	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	c	515	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	B	612	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	A	406	CLA	C4A-NA-C1A	-4.44	104.71	106.71
24	B	613	CLA	CAC-C3C-C4C	4.44	130.57	124.81
24	C	503	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
35	B	622	HTG	C1'-S1-C1	4.43	108.38	100.09
24	C	514	CLA	CAC-C3C-C4C	4.43	130.55	124.81
24	C	509	CLA	C3D-C4D-ND	4.42	117.39	110.24
24	A	406	CLA	O2D-CGD-CBD	4.41	119.11	111.27
24	C	504	CLA	C3D-C4D-ND	4.41	117.38	110.24
24	B	617	CLA	C3B-C4B-NB	4.41	114.91	109.21
24	B	603	CLA	C3C-C4C-NC	4.41	115.52	110.57
24	B	617	CLA	C3C-C4C-NC	4.41	115.51	110.57
24	B	604	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
24	d	404	CLA	C3C-C4C-NC	4.40	115.51	110.57
24	B	610	CLA	C3C-C4C-NC	4.40	115.51	110.57
36	d	407	DGD	O2G-C1B-C2B	4.39	120.97	111.50
24	B	604	CLA	C4A-NA-C1A	-4.39	104.73	106.71
24	a	409	CLA	C3D-C4D-ND	4.39	117.34	110.24
24	C	512	CLA	C4A-NA-C1A	-4.39	104.73	106.71
24	d	404	CLA	C3D-C4D-ND	4.39	117.34	110.24
24	C	502	CLA	C3C-C4C-NC	4.39	115.49	110.57
27	A	411	SQD	O47-C7-C8	4.38	120.95	111.50
24	c	511	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
24	A	405	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
24	b	610	CLA	O2D-CGD-CBD	4.37	119.04	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	607	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	C	514	CLA	C4A-NA-C1A	-4.36	104.75	106.71
24	c	505	CLA	C1D-CHD-C4C	-4.35	116.68	126.06
24	B	608	CLA	C3C-C4C-NC	4.34	115.44	110.57
24	c	514	CLA	C3D-C4D-ND	4.34	117.25	110.24
24	B	603	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
25	A	408	PHO	C1-C2-C3	-4.33	118.55	126.04
24	A	409	CLA	C3C-C4C-NC	4.33	115.43	110.57
24	B	614	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
24	C	509	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
24	B	603	CLA	C3D-C4D-ND	4.33	117.24	110.24
24	b	613	CLA	C3D-C4D-ND	4.33	117.23	110.24
24	c	504	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
24	b	606	CLA	C3D-C4D-ND	4.32	117.23	110.24
26	Y	101	BCR	C33-C5-C6	-4.32	119.68	124.53
24	b	610	CLA	C3D-C4D-ND	4.32	117.22	110.24
36	C	517	DGD	O2G-C1B-C2B	4.32	120.81	111.50
24	c	513	CLA	C3D-C4D-ND	4.31	117.21	110.24
38	e	102	HEM	CHC-C4B-NB	4.31	129.11	124.43
24	b	618	CLA	C4A-NA-C1A	-4.31	104.77	106.71
26	k	103	BCR	C24-C23-C22	-4.30	119.73	126.23
24	B	607	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
24	B	605	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
24	c	507	CLA	CAC-C3C-C4C	4.29	130.38	124.81
24	d	401	CLA	C3D-C4D-ND	4.29	117.18	110.24
24	b	608	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
24	B	602	CLA	C3C-C4C-NC	4.28	115.37	110.57
24	A	409	CLA	C4A-NA-C1A	-4.28	104.78	106.71
24	C	505	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
24	b	613	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
24	b	610	CLA	C3C-C4C-NC	4.28	115.37	110.57
24	B	612	CLA	C3D-C4D-ND	4.27	117.14	110.24
24	b	610	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
24	C	505	CLA	C3D-C4D-ND	4.26	117.14	110.24
24	B	614	CLA	C3C-C4C-NC	4.26	115.35	110.57
32	A	419	PL9	C32-C33-C34	-4.25	117.42	127.66
24	b	608	CLA	C1D-CHD-C4C	-4.25	116.89	126.06
24	C	510	CLA	C3C-C4C-NC	4.25	115.34	110.57
24	C	514	CLA	C3C-C4C-NC	4.25	115.34	110.57
24	C	513	CLA	C3C-C4C-NC	4.25	115.33	110.57
24	B	609	CLA	C3D-C4D-ND	4.25	117.11	110.24
26	b	622	BCR	C33-C5-C6	-4.24	119.77	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	O2D-CGD-CBD	4.23	118.79	111.27
24	c	512	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
24	c	506	CLA	C3C-C4C-NC	4.23	115.31	110.57
24	C	510	CLA	C3D-C4D-ND	4.23	117.07	110.24
24	c	510	CLA	C3D-C4D-ND	4.22	117.07	110.24
24	c	504	CLA	C3C-C4C-NC	4.22	115.31	110.57
24	c	503	CLA	O2D-CGD-O1D	-4.21	115.60	123.84
26	D	405	BCR	C38-C26-C25	-4.21	119.80	124.53
24	C	512	CLA	C3C-C4C-NC	4.21	115.29	110.57
24	a	406	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
24	b	619	CLA	C4A-NA-C1A	-4.21	104.81	106.71
24	b	614	CLA	C3D-C4D-ND	4.20	117.04	110.24
24	a	409	CLA	C3C-C4C-NC	4.20	115.28	110.57
24	C	514	CLA	O2D-CGD-CBD	4.20	118.72	111.27
24	B	602	CLA	C3D-C4D-ND	4.19	117.02	110.24
24	d	401	CLA	O2D-CGD-CBD	4.19	118.72	111.27
24	d	401	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
24	C	511	CLA	C3C-C4C-NC	4.18	115.26	110.57
24	c	511	CLA	C1D-CHD-C4C	-4.18	117.04	126.06
24	C	504	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
24	a	407	CLA	C3D-C4D-ND	4.18	116.99	110.24
24	C	510	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
24	b	619	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
24	c	513	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
24	C	512	CLA	C3D-C4D-ND	4.16	116.97	110.24
24	B	613	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
24	B	608	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
24	c	512	CLA	C3C-C4C-NC	4.15	115.23	110.57
24	c	513	CLA	C4A-NA-C1A	-4.15	104.84	106.71
24	b	619	CLA	C3D-C4D-ND	4.15	116.95	110.24
24	b	611	CLA	C3D-C4D-ND	4.15	116.95	110.24
26	d	405	BCR	C38-C26-C25	-4.15	119.87	124.53
24	b	620	CLA	C3D-C4D-ND	4.15	116.94	110.24
27	a	402	SQD	O47-C7-C8	4.14	120.43	111.50
24	C	503	CLA	C3D-C4D-ND	4.14	116.94	110.24
24	b	613	CLA	C3C-C4C-NC	4.14	115.21	110.57
24	a	409	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
24	b	606	CLA	C3C-C4C-NC	4.14	115.21	110.57
24	a	409	CLA	C3B-C4B-NB	4.13	114.55	109.21
24	b	617	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
24	c	514	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
24	c	503	CLA	C3C-C4C-NC	4.13	115.20	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
24	C	510	CLA	O2D-CGD-O1D	-4.13	115.77	123.84
24	C	509	CLA	C3C-C4C-NC	4.12	115.20	110.57
24	B	617	CLA	C3D-C4D-ND	4.12	116.91	110.24
24	c	505	CLA	C3D-C4D-ND	4.12	116.90	110.24
24	A	406	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
24	C	503	CLA	O2D-CGD-O1D	-4.12	115.79	123.84
26	y	101	BCR	C15-C14-C13	-4.11	121.44	127.31
24	c	503	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
27	b	601	SQD	O7-S-C6	4.10	111.81	106.94
24	b	620	CLA	C3C-C4C-NC	4.10	115.17	110.57
24	b	615	CLA	C3D-C4D-ND	4.10	116.87	110.24
24	b	614	CLA	C3C-C4C-NC	4.09	115.16	110.57
24	b	617	CLA	C3D-C4D-ND	4.09	116.85	110.24
24	C	507	CLA	C4A-NA-C1A	-4.08	104.87	106.71
24	c	511	CLA	C3D-C4D-ND	4.08	116.84	110.24
24	b	616	CLA	C3D-C4D-ND	4.07	116.83	110.24
26	d	405	BCR	C15-C14-C13	-4.07	121.50	127.31
26	H	101	BCR	C38-C26-C25	-4.07	119.96	124.53
24	B	606	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	b	614	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	b	608	CLA	C3C-C4C-NC	4.06	115.12	110.57
24	b	610	CLA	O2D-CGD-O1D	-4.06	115.91	123.84
24	b	618	CLA	C3B-C4B-NB	4.05	114.45	109.21
24	c	513	CLA	O2D-CGD-CBD	4.05	118.47	111.27
24	b	621	CLA	C3D-C4D-ND	4.05	116.79	110.24
26	c	516	BCR	C7-C8-C9	-4.05	120.12	126.23
24	C	513	CLA	C3D-C4D-ND	4.05	116.78	110.24
24	C	507	CLA	C3C-C4C-NC	4.05	115.11	110.57
24	A	406	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
24	c	506	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
24	b	616	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
24	b	607	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
24	C	505	CLA	CAC-C3C-C4C	4.03	130.04	124.81
24	d	401	CLA	C3C-C4C-NC	4.03	115.09	110.57
24	d	402	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
24	c	507	CLA	C3D-C4D-ND	4.03	116.76	110.24
24	B	610	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
24	D	401	CLA	C3B-C4B-NB	4.03	114.42	109.21
24	c	512	CLA	C3B-C4B-NB	4.03	114.42	109.21
24	b	608	CLA	C3D-C4D-ND	4.02	116.75	110.24
24	d	402	CLA	C3D-C4D-ND	4.02	116.74	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	506	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	c	515	CLA	O2D-CGD-CBD	4.02	118.41	111.27
24	d	402	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
24	c	511	CLA	C3C-C4C-NC	4.01	115.07	110.57
24	C	502	CLA	C3D-C4D-ND	4.01	116.73	110.24
24	a	409	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
24	B	613	CLA	C3B-C4B-NB	4.01	114.39	109.21
24	D	401	CLA	C3D-C4D-ND	4.01	116.72	110.24
24	B	615	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
24	b	621	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	C	506	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
24	c	513	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
24	c	506	CLA	C3D-C4D-ND	4.00	116.71	110.24
24	c	515	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	C	507	CLA	C3D-C4D-ND	4.00	116.70	110.24
27	F	101	SQD	O47-C7-C8	3.99	120.11	111.50
24	c	511	CLA	C3B-C4B-NB	3.99	114.37	109.21
24	C	511	CLA	C3D-C4D-ND	3.98	116.68	110.24
26	C	516	BCR	C7-C8-C9	-3.97	120.24	126.23
24	a	407	CLA	C3C-C4C-NC	3.97	115.02	110.57
24	B	605	CLA	CMC-C2C-C1C	3.97	131.08	125.04
24	B	609	CLA	O2D-CGD-CBD	3.97	118.32	111.27
24	b	618	CLA	C1C-C2C-C3C	-3.97	102.79	106.96
36	c	518	DGD	O2G-C1B-C2B	3.96	120.04	111.50
24	B	609	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
24	a	406	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
24	B	607	CLA	CMC-C2C-C1C	3.96	131.06	125.04
34	c	501	LMG	O7-C10-C11	3.95	120.02	111.50
26	C	515	BCR	C33-C5-C6	-3.95	120.09	124.53
24	c	509	CLA	C3D-C4D-ND	3.95	116.63	110.24
24	C	511	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
24	c	508	CLA	C3D-C4D-ND	3.95	116.62	110.24
24	B	606	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
24	B	615	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	c	504	CLA	C3D-C4D-ND	3.93	116.60	110.24
24	c	508	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
24	c	503	CLA	C3D-C4D-ND	3.93	116.59	110.24
24	c	508	CLA	C3C-C4C-NC	3.92	114.97	110.57
24	B	609	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
37	E	101	LHG	O7-C7-C8	3.92	119.95	111.50
26	d	405	BCR	C7-C8-C9	-3.92	120.31	126.23
24	C	505	CLA	C3B-C4B-NB	3.92	114.27	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	C3D-C4D-ND	3.92	116.57	110.24
24	a	406	CLA	C3C-C4C-NC	3.91	114.96	110.57
24	b	617	CLA	C4C-C3C-C2C	-3.91	101.20	106.90
24	C	513	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
24	B	604	CLA	C1D-CHD-C4C	-3.90	117.63	126.06
34	Z	101	LMG	O7-C10-C11	3.90	119.92	111.50
24	c	509	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
24	C	508	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
34	C	520	LMG	O8-C28-C29	3.90	124.15	111.91
24	b	619	CLA	C3C-C4C-NC	3.90	114.95	110.57
24	C	512	CLA	O2D-CGD-CBD	3.90	118.20	111.27
24	c	508	CLA	C3B-C4B-NB	3.90	114.25	109.21
36	C	518	DGD	O2G-C1B-C2B	3.89	119.89	111.50
24	d	401	CLA	C4A-NA-C1A	-3.89	104.96	106.71
24	B	611	CLA	C3D-C4D-ND	3.89	116.53	110.24
34	c	501	LMG	C7-O1-C1	-3.89	106.15	113.74
24	b	608	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
24	a	407	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
35	B	623	HTG	C1'-S1-C1	3.87	107.33	100.09
24	a	406	CLA	CAC-C3C-C4C	3.87	129.83	124.81
24	b	612	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
27	l	101	SQD	O6-C1-C2	3.86	114.33	108.30
24	d	402	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
24	A	409	CLA	C1C-C2C-C3C	-3.85	102.90	106.96
24	c	504	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
32	a	416	PL9	C15-C14-C16	3.85	121.75	115.27
24	b	611	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
24	D	403	CLA	O2D-CGD-CBD	3.84	118.09	111.27
24	b	613	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	B	613	CLA	C3D-C4D-ND	3.83	116.44	110.24
37	d	409	LHG	O7-C7-C8	3.82	119.74	111.50
27	b	601	SQD	C3-C4-C5	3.82	117.06	110.24
24	C	504	CLA	O2D-CGD-CBD	3.82	118.06	111.27
26	c	526	BCR	C33-C5-C6	-3.82	120.24	124.53
35	b	604	HTG	C1'-S1-C1	3.82	107.23	100.09
24	C	509	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
24	b	606	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
26	B	618	BCR	C33-C5-C6	-3.81	120.25	124.53
26	C	515	BCR	C7-C8-C9	-3.81	120.48	126.23
26	d	405	BCR	C33-C5-C6	-3.81	120.25	124.53
24	A	406	CLA	C3B-C4B-NB	3.80	114.13	109.21
24	d	402	CLA	C3B-C4B-NB	3.80	114.13	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	C3B-C4B-NB	3.80	114.13	109.21
24	b	611	CLA	CMC-C2C-C1C	3.80	130.83	125.04
24	B	604	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
37	D	409	LHG	O7-C7-C8	3.80	119.69	111.50
24	a	406	CLA	C3D-C4D-ND	3.80	116.38	110.24
24	c	513	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
24	D	403	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	c	510	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	b	619	CLA	C3B-C4B-NB	3.79	114.11	109.21
24	B	615	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
24	C	512	CLA	C3B-C4B-NB	3.78	114.10	109.21
24	B	612	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
34	Z	101	LMG	C1-C2-C3	3.78	117.87	110.00
36	D	407	DGD	C4D-C3D-C2D	3.78	117.42	110.82
24	c	513	CLA	C3B-C4B-NB	3.78	114.09	109.21
24	c	510	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
24	c	512	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	b	612	CLA	C3B-C4B-NB	3.76	114.08	109.21
24	B	607	CLA	C3D-C4D-ND	3.76	116.32	110.24
35	b	627	HTG	C1'-S1-C1	3.76	107.12	100.09
24	D	403	CLA	C3D-C4D-ND	3.76	116.31	110.24
24	b	618	CLA	C1D-CHD-C4C	-3.76	117.96	126.06
24	B	614	CLA	C3B-C4B-NB	3.75	114.06	109.21
24	C	509	CLA	C3B-C4B-NB	3.75	114.06	109.21
24	b	610	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
24	D	403	CLA	C3B-C4B-NB	3.75	114.06	109.21
24	B	617	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
24	b	609	CLA	CMC-C2C-C1C	3.75	130.75	125.04
24	a	406	CLA	C3B-C4B-NB	3.74	114.05	109.21
26	K	101	BCR	C33-C5-C6	-3.74	120.32	124.53
24	C	510	CLA	C4A-NA-C1A	-3.74	105.02	106.71
24	C	505	CLA	CMC-C2C-C1C	3.74	130.73	125.04
24	b	608	CLA	O2A-CGA-O1A	-3.74	114.16	123.59
24	C	514	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
24	b	620	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
24	B	603	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
24	C	511	CLA	C3B-C4B-NB	3.73	114.03	109.21
24	b	608	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
24	C	502	CLA	CAC-C3C-C4C	3.73	129.65	124.81
24	A	406	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
24	C	513	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
24	c	504	CLA	C1C-C2C-C3C	-3.72	103.04	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
24	b	615	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
24	c	511	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
24	c	512	CLA	C4A-NA-C1A	-3.72	105.03	106.71
24	B	612	CLA	C1-C2-C3	-3.72	119.61	126.04
24	b	612	CLA	C3D-C4D-ND	3.72	116.25	110.24
26	T	102	BCR	C33-C5-C6	-3.72	120.35	124.53
36	c	517	DGD	O2G-C1B-C2B	3.72	119.51	111.50
24	B	608	CLA	C3D-C4D-ND	3.71	116.24	110.24
37	e	101	LHG	O7-C7-C8	3.71	119.50	111.50
26	D	405	BCR	C33-C5-C6	-3.71	120.37	124.53
24	C	512	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
24	c	508	CLA	O2D-CGD-CBD	3.70	117.85	111.27
24	B	602	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
24	D	401	CLA	CAA-C2A-C3A	-3.70	102.65	112.78
34	J	101	LMG	O7-C10-C11	3.70	119.47	111.50
38	e	102	HEM	CHD-C1D-ND	3.70	128.45	124.43
24	B	614	CLA	C3D-C4D-ND	3.70	116.22	110.24
24	C	503	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
24	b	620	CLA	C3B-C4B-NB	3.69	113.98	109.21
24	B	605	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
24	b	612	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
35	V	204	HTG	C1'-S1-C1	3.68	106.98	100.09
24	B	613	CLA	C4C-C3C-C2C	-3.68	101.53	106.90
24	c	515	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
24	C	510	CLA	C1-C2-C3	-3.68	119.67	126.04
32	A	419	PL9	C27-C28-C29	-3.68	118.80	127.66
34	C	520	LMG	O7-C10-C11	3.67	119.42	111.50
24	C	507	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
24	B	607	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
24	A	405	CLA	CMB-C2B-C3B	3.67	131.54	124.68
24	C	512	CLA	C1-O2A-CGA	3.67	126.07	116.44
24	b	621	CLA	CAC-C3C-C4C	3.67	129.57	124.81
24	C	508	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
24	c	511	CLA	CAC-C3C-C4C	3.66	129.56	124.81
24	c	511	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
32	D	406	PL9	C40-C39-C41	3.66	121.42	115.27
24	B	616	CLA	O2D-CGD-CBD	3.65	117.76	111.27
24	B	610	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	B	611	CLA	CAC-C3C-C4C	3.65	129.55	124.81
27	A	416	SQD	O47-C7-C8	3.65	119.37	111.50
24	b	620	CLA	C1C-C2C-C3C	-3.65	103.12	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	515	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
24	C	502	CLA	O2D-CGD-O1D	-3.64	116.71	123.84
24	B	614	CLA	C1-C2-C3	-3.64	119.75	126.04
24	b	621	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
24	b	606	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	D	403	CLA	C1-C2-C3	-3.64	119.75	126.04
24	C	511	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	b	619	CLA	CAC-C3C-C4C	3.63	129.53	124.81
24	C	509	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
24	D	404	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
24	c	506	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
32	a	416	PL9	C22-C23-C24	-3.63	118.92	127.66
34	B	621	LMG	O7-C10-C11	3.63	119.32	111.50
24	c	511	CLA	C1-C2-C3	-3.62	119.78	126.04
24	C	510	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	a	409	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	B	609	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	C	510	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	c	507	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
24	A	406	CLA	CBC-CAC-C3C	-3.61	102.47	112.43
24	C	506	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	b	615	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
38	E	103	HEM	C1B-NB-C4B	3.61	108.80	105.07
24	d	402	CLA	O2A-CGA-CBA	3.61	123.22	111.91
26	d	405	BCR	C24-C23-C22	-3.60	120.79	126.23
24	B	615	CLA	C4-C3-C5	3.60	121.33	115.27
24	C	503	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
27	a	411	SQD	C1-O5-C5	-3.60	106.62	113.69
34	c	501	LMG	C8-O7-C10	-3.60	108.93	117.79
24	d	401	CLA	CHC-C1C-C2C	-3.60	116.77	126.72
24	C	502	CLA	C1C-C2C-C3C	-3.60	103.18	106.96
24	C	505	CLA	C3C-C4C-NC	3.58	114.59	110.57
24	c	503	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
24	C	505	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
24	A	409	CLA	O2D-CGD-CBD	3.58	117.62	111.27
24	B	602	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
32	a	416	PL9	C17-C18-C19	-3.57	119.06	127.66
24	C	504	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
34	z	101	LMG	O7-C10-C11	3.57	119.19	111.50
24	c	512	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
24	B	604	CLA	C3B-C4B-NB	3.56	113.82	109.21
24	c	507	CLA	C1D-CHD-C4C	-3.56	118.38	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	410	LHG	O7-C7-C8	3.56	119.17	111.50
24	a	409	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
24	B	617	CLA	CAC-C3C-C4C	3.55	129.42	124.81
24	C	505	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
35	b	628	HTG	O5-C1-C2	3.55	114.78	110.31
24	c	508	CLA	CAC-C3C-C4C	3.55	129.41	124.81
24	b	619	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
24	a	409	CLA	C4A-NA-C1A	-3.55	105.11	106.71
24	c	506	CLA	C3B-C4B-NB	3.54	113.79	109.21
24	c	508	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
24	B	615	CLA	O2A-CGA-O1A	-3.54	114.67	123.59
24	D	404	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
24	A	409	CLA	C4-C3-C5	3.53	121.21	115.27
32	A	419	PL9	C22-C23-C24	-3.53	119.17	127.66
24	D	403	CLA	CED-O2D-CGD	3.53	123.91	115.94
24	b	620	CLA	C4-C3-C5	3.53	121.20	115.27
24	c	504	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
25	A	407	PHO	C1-C2-C3	-3.52	119.95	126.04
26	h	101	BCR	C38-C26-C25	-3.52	120.57	124.53
24	C	506	CLA	C3D-C2D-C1D	-3.52	101.02	105.83
24	B	616	CLA	C3D-C4D-ND	3.52	115.93	110.24
24	B	608	CLA	CMC-C2C-C1C	3.52	130.40	125.04
24	C	508	CLA	CMC-C2C-C1C	3.52	130.40	125.04
24	d	404	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
24	c	506	CLA	C4-C3-C5	3.51	121.17	115.27
24	d	404	CLA	CMC-C2C-C1C	3.51	130.38	125.04
27	l	101	SQD	O7-S-C6	3.51	111.11	106.94
24	b	611	CLA	CAC-C3C-C4C	3.51	129.36	124.81
32	a	416	PL9	C32-C33-C34	-3.51	119.22	127.66
27	f	101	SQD	C1-O5-C5	3.50	120.57	113.69
24	b	608	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
36	D	407	DGD	C1D-C2D-C3D	3.50	117.28	110.00
24	b	608	CLA	C3B-C4B-NB	3.50	113.73	109.21
24	B	615	CLA	CAC-C3C-C4C	3.49	129.34	124.81
24	D	404	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
24	A	405	CLA	C3D-C4D-ND	3.49	115.88	110.24
24	C	508	CLA	C3D-C4D-ND	3.49	115.88	110.24
37	l	102	LHG	O7-C7-C8	3.49	119.02	111.50
24	b	614	CLA	C3B-C4B-NB	3.49	113.72	109.21
24	C	506	CLA	CAC-C3C-C4C	3.49	129.33	124.81
24	a	407	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
24	d	404	CLA	C3B-C4B-NB	3.48	113.71	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	403	PHO	O2D-CGD-O1D	-3.48	117.04	123.84
24	C	512	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
24	B	612	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
24	B	616	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
24	B	617	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
24	c	514	CLA	CBC-CAC-C3C	-3.47	102.86	112.43
24	b	607	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
37	D	410	LHG	O7-C7-C8	3.47	118.98	111.50
24	A	405	CLA	CAC-C3C-C4C	3.47	129.31	124.81
24	c	510	CLA	O2D-CGD-O1D	-3.46	117.06	123.84
37	L	101	LHG	O7-C7-C8	3.46	118.95	111.50
24	C	504	CLA	C3B-C4B-NB	3.46	113.68	109.21
34	c	520	LMG	O7-C10-C11	3.46	118.95	111.50
24	C	506	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
24	b	607	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
24	b	613	CLA	C1-C2-C3	-3.44	120.09	126.04
24	b	619	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
26	B	620	BCR	C38-C26-C25	-3.44	120.66	124.53
24	c	509	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
24	c	514	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
37	D	408	LHG	O7-C7-C8	3.43	118.90	111.50
24	D	404	CLA	C3B-C4B-NB	3.43	113.65	109.21
24	D	403	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
24	B	603	CLA	C3B-C4B-NB	3.43	113.65	109.21
26	t	101	BCR	C33-C5-C6	-3.43	120.68	124.53
24	B	615	CLA	C3B-C4B-NB	3.43	113.64	109.21
24	b	619	CLA	CHC-C1C-C2C	-3.42	117.25	126.72
24	b	620	CLA	C1D-CHD-C4C	-3.42	118.67	126.06
24	B	611	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
24	d	404	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
27	A	411	SQD	O8-S-C6	3.42	111.18	105.74
24	c	515	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	B	605	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	C	510	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
25	A	408	PHO	C1A-C2A-C3A	-3.41	99.59	102.84
24	b	608	CLA	C4-C3-C5	3.41	121.01	115.27
24	c	505	CLA	CMC-C2C-C1C	3.41	130.23	125.04
25	d	403	PHO	CMB-C2B-C3B	3.41	131.06	124.68
26	b	622	BCR	C7-C8-C9	-3.41	121.08	126.23
24	b	617	CLA	C4-C3-C5	3.41	121.00	115.27
24	a	406	CLA	CHC-C1C-C2C	-3.41	117.30	126.72
24	B	606	CLA	CMC-C2C-C1C	3.41	130.23	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	603	CLA	CAA-C2A-C3A	-3.41	103.45	112.78
32	A	419	PL9	C37-C38-C39	-3.40	119.46	127.66
24	B	603	CLA	C4-C3-C5	3.40	121.00	115.27
24	B	605	CLA	C3D-C4D-ND	3.40	115.73	110.24
24	b	611	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
24	c	507	CLA	C3D-C2D-C1D	-3.39	101.20	105.83
24	d	404	CLA	O2D-CGD-CBD	3.39	117.30	111.27
24	b	621	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
36	h	102	DGD	O2G-C1B-C2B	3.39	118.81	111.50
24	b	617	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
24	B	603	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
24	B	612	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
26	C	515	BCR	C38-C26-C25	-3.38	120.73	124.53
24	C	502	CLA	C3B-C4B-NB	3.38	113.58	109.21
24	c	514	CLA	C3C-C4C-NC	3.38	114.36	110.57
24	D	401	CLA	CHC-C1C-C2C	-3.38	117.38	126.72
26	Y	101	BCR	C38-C26-C25	-3.38	120.74	124.53
25	A	408	PHO	C4-C3-C5	3.37	120.94	115.27
24	C	502	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
24	c	505	CLA	C4-C3-C5	3.37	120.94	115.27
24	C	514	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
24	b	616	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
24	c	505	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
24	C	513	CLA	C3B-C4B-NB	3.37	113.56	109.21
24	b	620	CLA	CAC-C3C-C4C	3.36	129.17	124.81
30	I	102	LMT	O1B-C4'-C3'	3.36	116.21	107.28
24	c	513	CLA	C3C-C4C-NC	3.36	114.33	110.57
27	f	101	SQD	O7-S-C6	3.35	110.92	106.94
32	a	416	PL9	C37-C38-C39	-3.35	119.60	127.66
24	B	616	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
24	B	616	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
24	D	401	CLA	CAC-C3C-C4C	3.34	129.15	124.81
24	D	401	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
24	c	503	CLA	C3B-C4B-NB	3.34	113.52	109.21
24	a	406	CLA	O2A-CGA-O1A	-3.34	115.17	123.59
24	B	615	CLA	CMC-C2C-C1C	3.34	130.12	125.04
24	B	615	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
24	b	618	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
24	B	611	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
24	c	504	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	c	504	CLA	C1-C2-C3	-3.33	120.28	126.04
24	B	612	CLA	C3B-C4B-NB	3.33	113.52	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	416	PL9	C7-C8-C9	-3.33	121.25	126.79
24	b	621	CLA	O2A-CGA-CBA	3.33	122.36	111.91
26	c	516	BCR	C38-C26-C25	-3.33	120.79	124.53
24	c	505	CLA	CAC-C3C-C4C	3.32	129.12	124.81
24	C	509	CLA	O2A-CGA-O1A	-3.32	115.21	123.59
24	C	514	CLA	CMC-C2C-C1C	3.32	130.10	125.04
24	b	607	CLA	CAA-C2A-C3A	-3.32	103.69	112.78
24	B	603	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
24	C	506	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	b	607	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	d	402	CLA	C1-C2-C3	-3.32	120.31	126.04
24	A	405	CLA	CAA-C2A-C3A	-3.32	103.70	112.78
24	B	604	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
24	c	507	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
24	c	513	CLA	C4-C3-C5	3.31	120.84	115.27
24	b	612	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
24	a	409	CLA	C1-C2-C3	-3.31	120.32	126.04
24	C	514	CLA	C3B-C4B-NB	3.30	113.48	109.21
38	e	102	HEM	C1B-NB-C4B	3.30	108.49	105.07
24	a	409	CLA	C4C-C3C-C2C	-3.30	102.08	106.90
24	b	621	CLA	CHC-C1C-C2C	-3.30	117.60	126.72
24	b	616	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
25	a	408	PHO	O1D-CGD-CBD	-3.29	119.25	124.74
24	B	616	CLA	C3B-C4B-NB	3.29	113.47	109.21
24	d	401	CLA	CMA-C3A-C2A	-3.29	100.55	113.83
36	D	407	DGD	C1E-O6E-C5E	3.29	120.15	113.69
24	A	405	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
24	b	617	CLA	C3B-C4B-NB	3.29	113.46	109.21
24	B	610	CLA	CHD-C4C-NC	3.29	129.38	124.20
24	c	513	CLA	CAC-C3C-C4C	3.29	129.07	124.81
24	c	510	CLA	CMB-C2B-C3B	3.28	130.82	124.68
24	c	507	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
24	C	506	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
24	B	611	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
36	D	407	DGD	C3D-C4D-C5D	3.28	116.09	110.24
32	A	419	PL9	C10-C9-C11	3.28	120.78	115.27
32	A	419	PL9	C15-C14-C16	3.27	120.77	115.27
37	D	408	LHG	O8-C23-O10	-3.27	115.34	123.59
24	B	617	CLA	CHC-C1C-C2C	-3.26	117.69	126.72
24	b	610	CLA	CMC-C2C-C1C	3.26	130.00	125.04
25	d	403	PHO	C4-C3-C5	3.26	120.76	115.27
24	b	618	CLA	O2D-CGD-CBD	3.26	117.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	CAA-C2A-C3A	-3.26	103.86	112.78
24	B	604	CLA	CMC-C2C-C1C	3.26	130.00	125.04
27	a	411	SQD	O8-S-C6	3.26	110.93	105.74
27	a	402	SQD	O48-C23-C24	3.26	122.13	111.91
24	B	612	CLA	CAC-C3C-C4C	3.25	129.03	124.81
27	a	411	SQD	C1-C2-C3	-3.25	103.23	110.00
24	a	409	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
36	C	519	DGD	O3G-C3G-C2G	-3.25	103.07	110.90
32	D	406	PL9	C42-C43-C44	-3.24	119.85	127.66
24	b	611	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	b	608	CLA	CMC-C2C-C1C	3.24	129.98	125.04
24	c	508	CLA	CHC-C1C-C2C	-3.24	117.75	126.72
24	B	607	CLA	C3B-C4B-NB	3.24	113.40	109.21
24	C	512	CLA	CAC-C3C-C4C	3.24	129.02	124.81
24	D	401	CLA	C3C-C4C-NC	3.24	114.20	110.57
24	B	606	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	c	509	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
24	A	409	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
24	C	504	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
24	b	612	CLA	CMC-C2C-C1C	3.23	129.95	125.04
24	b	615	CLA	C3B-C4B-NB	3.22	113.38	109.21
24	c	513	CLA	CHC-C1C-C2C	-3.22	117.80	126.72
34	j	101	LMG	O7-C10-C11	3.22	118.44	111.50
24	b	613	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
24	C	509	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
25	A	408	PHO	CMB-C2B-C3B	3.22	130.70	124.68
24	C	503	CLA	O2A-CGA-O1A	-3.22	115.47	123.59
24	b	621	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
38	E	103	HEM	CBA-CAA-C2A	-3.22	107.13	112.62
26	C	516	BCR	C24-C23-C22	-3.22	121.38	126.23
24	C	514	CLA	C1-C2-C3	-3.21	120.48	126.04
27	F	101	SQD	O7-S-C6	3.21	110.76	106.94
24	b	616	CLA	C3B-C4B-NB	3.21	113.36	109.21
32	a	416	PL9	C20-C19-C21	3.21	120.67	115.27
24	a	406	CLA	O2A-CGA-CBA	3.21	121.98	111.91
24	b	610	CLA	O2A-CGA-O1A	-3.21	115.49	123.59
24	C	509	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
24	b	614	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
25	A	407	PHO	C1A-C2A-C3A	-3.20	99.79	102.84
24	b	610	CLA	C3B-C4B-NB	3.20	113.35	109.21
24	b	615	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
38	E	103	HEM	CHB-C1B-NB	3.20	128.34	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	402	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
24	c	506	CLA	CAC-C3C-C4C	3.20	128.96	124.81
24	b	608	CLA	O2A-CGA-CBA	3.20	121.94	111.91
24	b	610	CLA	CHD-C4C-NC	3.19	129.24	124.20
24	C	511	CLA	C1-C2-C3	-3.19	120.52	126.04
24	C	513	CLA	CMB-C2B-C3B	3.19	130.65	124.68
24	B	614	CLA	CHC-C1C-C2C	-3.19	117.90	126.72
24	A	405	CLA	O2D-CGD-CBD	3.19	116.93	111.27
24	b	615	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
24	c	515	CLA	CAC-C3C-C4C	3.19	128.94	124.81
24	b	617	CLA	C1-C2-C3	-3.19	120.53	126.04
32	a	416	PL9	C30-C29-C31	3.19	120.63	115.27
24	b	609	CLA	C3D-C4D-ND	3.18	115.39	110.24
24	B	610	CLA	C3B-C4B-NB	3.18	113.33	109.21
24	C	507	CLA	CAC-C3C-C4C	3.18	128.94	124.81
24	B	602	CLA	CMB-C2B-C3B	3.18	130.63	124.68
24	B	608	CLA	C3B-C4B-NB	3.18	113.32	109.21
24	c	507	CLA	C3B-C4B-NB	3.18	113.32	109.21
24	b	606	CLA	CHD-C4C-NC	3.18	129.22	124.20
24	D	404	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
24	B	613	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	B	614	CLA	CED-O2D-CGD	3.18	123.13	115.94
32	A	419	PL9	C7-C8-C9	-3.18	121.50	126.79
32	a	416	PL9	C10-C9-C11	3.18	120.61	115.27
24	b	607	CLA	CAC-C3C-C4C	3.18	128.93	124.81
24	c	510	CLA	C3B-C4B-NB	3.17	113.31	109.21
24	c	509	CLA	CAC-C3C-C4C	3.17	128.93	124.81
24	D	401	CLA	CBC-CAC-C3C	-3.17	103.68	112.43
24	B	608	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
24	C	512	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
32	a	416	PL9	C27-C28-C29	-3.16	120.05	127.66
24	c	512	CLA	CMC-C2C-C1C	3.16	129.85	125.04
24	B	603	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
26	d	405	BCR	C3-C4-C5	-3.16	108.44	114.08
24	A	406	CLA	CAA-C2A-C3A	-3.16	104.14	112.78
24	C	509	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	C	502	CLA	CMC-C2C-C1C	3.15	129.84	125.04
24	B	606	CLA	C3B-C4B-NB	3.15	113.28	109.21
24	B	614	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	B	605	CLA	C1-C2-C3	-3.15	120.59	126.04
24	D	401	CLA	C4A-NA-C1A	-3.15	105.29	106.71
24	B	603	CLA	CMB-C2B-C3B	3.15	130.57	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	405	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
27	a	411	SQD	C45-O47-C7	-3.15	110.04	117.79
27	A	416	SQD	O48-C23-C24	3.15	121.78	111.91
24	b	617	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
32	a	416	PL9	C42-C43-C44	-3.14	120.11	127.66
24	B	611	CLA	C1D-CHD-C4C	-3.13	119.30	126.06
24	a	407	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
24	B	612	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
24	C	512	CLA	C4-C3-C5	3.13	120.53	115.27
24	c	509	CLA	C4A-NA-C1A	-3.13	105.30	106.71
24	b	613	CLA	O2A-CGA-CBA	3.13	121.72	111.91
24	B	611	CLA	C1-C2-C3	-3.13	120.64	126.04
26	k	103	BCR	C33-C5-C6	-3.13	121.02	124.53
27	b	601	SQD	O48-C23-C24	3.12	121.71	111.91
24	b	613	CLA	C3B-C4B-NB	3.12	113.25	109.21
24	C	507	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
24	a	407	CLA	CAA-C2A-C3A	-3.12	104.23	112.78
24	c	509	CLA	C3B-C4B-NB	3.12	113.25	109.21
24	b	609	CLA	CAC-C3C-C4C	3.12	128.86	124.81
24	B	610	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
24	A	405	CLA	C3B-C4B-NB	3.12	113.24	109.21
32	A	419	PL9	C20-C19-C21	3.12	120.51	115.27
36	H	102	DGD	O2G-C1B-C2B	3.11	118.21	111.50
24	a	406	CLA	CAA-C2A-C3A	-3.11	104.26	112.78
24	B	603	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
24	c	505	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
30	I	102	LMT	C1B-O5B-C5B	3.11	119.79	113.69
24	d	404	CLA	CAC-C3C-C4C	3.11	128.84	124.81
24	B	602	CLA	C3B-C4B-NB	3.10	113.22	109.21
26	H	101	BCR	C7-C8-C9	-3.10	121.55	126.23
37	e	101	LHG	O8-C23-C24	3.10	121.64	111.91
24	C	503	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	c	506	CLA	CMC-C2C-C1C	3.10	129.76	125.04
24	C	510	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	B	617	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	b	610	CLA	C4-C3-C5	3.10	120.48	115.27
34	Z	101	LMG	C7-O1-C1	-3.10	107.69	113.74
24	B	605	CLA	O2A-CGA-O1A	-3.10	115.78	123.59
24	A	409	CLA	CHD-C4C-NC	3.10	129.08	124.20
24	B	602	CLA	C4C-C3C-C2C	-3.10	102.39	106.90
24	a	409	CLA	CAC-C3C-C4C	3.09	128.82	124.81
24	d	401	CLA	C1D-CHD-C4C	-3.09	119.39	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	609	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
24	C	514	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
24	A	406	CLA	CMB-C2B-C3B	3.08	130.45	124.68
24	D	403	CLA	O2A-CGA-CBA	3.08	121.58	111.91
24	c	508	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
24	a	409	CLA	C4-C3-C5	3.08	120.45	115.27
27	A	411	SQD	C1-C2-C3	-3.08	103.58	110.00
32	a	416	PL9	C7-C3-C4	3.08	119.38	116.88
24	B	609	CLA	CMA-C3A-C4A	-3.07	103.51	111.77
24	B	617	CLA	C1C-C2C-C3C	-3.07	103.72	106.96
24	b	612	CLA	CAA-C2A-C3A	-3.07	104.37	112.78
24	b	618	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
24	a	407	CLA	CAC-C3C-C4C	3.07	128.79	124.81
35	C	523	HTG	O5-C5-C4	3.07	115.26	109.69
24	c	504	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
24	B	613	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
24	C	511	CLA	CMC-C2C-C1C	3.06	129.71	125.04
37	d	408	LHG	O7-C7-C8	3.06	118.11	111.50
24	C	502	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
24	b	620	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
24	c	504	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
24	c	510	CLA	C4C-C3C-C2C	-3.05	102.44	106.90
24	B	616	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
24	c	513	CLA	C1-C2-C3	-3.05	120.77	126.04
24	b	620	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
24	b	616	CLA	CAC-C3C-C4C	3.05	128.76	124.81
24	A	409	CLA	CMC-C2C-C1C	3.05	129.68	125.04
24	A	406	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
24	B	615	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
24	D	403	CLA	CMC-C2C-C1C	3.04	129.68	125.04
26	K	101	BCR	C20-C21-C22	-3.04	122.97	127.31
24	B	609	CLA	CMB-C2B-C3B	3.04	130.37	124.68
24	b	611	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
24	C	508	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
26	k	103	BCR	C38-C26-C25	-3.04	121.11	124.53
24	B	613	CLA	C1D-CHD-C4C	-3.04	119.50	126.06
24	B	615	CLA	O2A-CGA-CBA	3.04	121.44	111.91
24	C	506	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
35	O	303	HTG	C1'-S1-C1	3.04	105.77	100.09
24	c	512	CLA	C4-C3-C5	3.04	120.38	115.27
35	B	624	HTG	C1-C2-C3	3.04	116.58	110.59
27	A	411	SQD	C45-O47-C7	-3.04	110.32	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
26	c	526	BCR	C15-C14-C13	-3.03	122.98	127.31
24	c	513	CLA	CHD-C4C-NC	3.03	128.97	124.20
26	A	410	BCR	C33-C5-C6	-3.03	121.13	124.53
24	A	406	CLA	CAC-C3C-C4C	3.03	128.74	124.81
24	B	607	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
24	b	616	CLA	C1-C2-C3	-3.02	120.82	126.04
32	A	419	PL9	C42-C43-C44	-3.02	120.39	127.66
34	Z	101	LMG	O6-C1-C2	3.02	116.74	110.35
24	b	608	CLA	CAC-C3C-C4C	3.02	128.73	124.81
24	D	403	CLA	CAC-C3C-C4C	3.02	128.72	124.81
24	B	616	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
24	c	514	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
24	C	514	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	D	404	CLA	CAC-C3C-C4C	3.01	128.72	124.81
24	B	611	CLA	CAA-C2A-C3A	-3.01	104.53	112.78
24	b	607	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
24	A	406	CLA	C3C-C4C-NC	3.01	113.94	110.57
24	C	507	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
24	b	606	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
24	c	513	CLA	CMC-C2C-C1C	3.00	129.62	125.04
30	I	102	LMT	C1'-O5'-C5'	3.00	119.59	113.69
24	C	512	CLA	CHC-C1C-C2C	-3.00	118.41	126.72
32	d	406	PL9	C10-C9-C11	3.00	120.32	115.27
24	b	617	CLA	C2A-C1A-CHA	-3.00	118.61	123.86
24	B	608	CLA	C4-C3-C5	3.00	120.32	115.27
24	C	510	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
24	b	613	CLA	CAC-C3C-C4C	3.00	128.70	124.81
24	b	616	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
24	B	610	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
24	c	503	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
24	d	402	CLA	O2A-CGA-O1A	-2.99	116.05	123.59
24	b	609	CLA	C3B-C4B-NB	2.99	113.08	109.21
24	c	508	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	b	607	CLA	C4-C3-C5	2.99	120.30	115.27
24	b	609	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
24	D	401	CLA	O2A-CGA-O1A	-2.99	116.06	123.59
24	b	614	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
24	c	514	CLA	CHD-C4C-NC	2.98	128.91	124.20
32	d	406	PL9	C40-C39-C41	2.98	120.29	115.27
26	c	516	BCR	C31-C1-C6	-2.98	105.46	110.30
34	b	625	LMG	O8-C28-C29	2.98	121.26	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	612	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
24	c	509	CLA	CMC-C2C-C1C	2.98	129.57	125.04
32	A	419	PL9	C25-C24-C26	2.98	120.28	115.27
24	d	402	CLA	C4-C3-C5	2.97	120.28	115.27
24	B	611	CLA	O2A-CGA-CBA	2.97	121.24	111.91
26	A	410	BCR	C15-C14-C13	-2.97	123.07	127.31
24	B	610	CLA	C1-C2-C3	-2.97	120.90	126.04
37	D	408	LHG	O8-C23-C24	2.97	121.23	111.91
24	c	514	CLA	C3B-C4B-NB	2.97	113.05	109.21
24	C	503	CLA	C1-C2-C3	-2.97	120.91	126.04
24	d	402	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	b	611	CLA	C3B-C4B-NB	2.97	113.05	109.21
24	d	404	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	A	405	CLA	CAA-C2A-C1A	-2.97	102.25	111.97
24	B	609	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
24	C	508	CLA	CHD-C4C-NC	2.96	128.87	124.20
24	c	505	CLA	C3B-C4B-NB	2.96	113.04	109.21
24	A	406	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
27	f	101	SQD	O5-C5-C4	2.96	115.07	109.69
27	b	601	SQD	C44-O6-C1	-2.96	107.96	113.74
24	c	511	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
24	c	515	CLA	CMC-C2C-C1C	2.96	129.54	125.04
24	C	507	CLA	C4-C3-C5	2.95	120.24	115.27
26	D	405	BCR	C28-C27-C26	-2.95	108.81	114.08
24	d	404	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
37	D	409	LHG	O8-C23-O10	-2.95	116.16	123.59
24	d	402	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
24	c	503	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	B	610	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
24	C	511	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
32	D	406	PL9	C53-C6-C1	2.94	121.00	114.99
26	B	620	BCR	C24-C23-C22	-2.94	121.80	126.23
24	a	407	CLA	CBC-CAC-C3C	-2.93	104.34	112.43
24	d	401	CLA	C2A-C1A-CHA	-2.93	118.73	123.86
24	b	606	CLA	C4-C3-C5	2.93	120.20	115.27
24	B	607	CLA	C1-O2A-CGA	2.93	124.13	116.44
24	B	605	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
36	c	519	DGD	O2G-C1B-C2B	2.93	117.81	111.50
24	b	615	CLA	CAC-C3C-C4C	2.93	128.61	124.81
24	d	402	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
24	b	613	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	d	404	CLA	C4-C3-C5	2.93	120.19	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	409	CLA	C2A-C1A-CHA	-2.93	118.74	123.86
24	c	511	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	b	614	CLA	CMC-C2C-C1C	2.92	129.49	125.04
36	c	519	DGD	O1G-C1A-C2A	2.92	121.09	111.91
24	C	507	CLA	CAA-C2A-C3A	-2.92	104.77	112.78
24	b	606	CLA	C3B-C4B-NB	2.92	112.99	109.21
26	Y	101	BCR	C15-C14-C13	-2.92	123.14	127.31
24	b	616	CLA	CHD-C4C-NC	2.92	128.81	124.20
27	A	411	SQD	C44-O6-C1	-2.92	108.03	113.74
25	A	407	PHO	CMA-C3A-C4A	-2.92	107.98	114.38
24	A	405	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
24	B	604	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
24	B	612	CLA	CMC-C2C-C1C	2.92	129.49	125.04
24	B	606	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	C	504	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
24	c	509	CLA	CHC-C1C-C2C	-2.92	118.66	126.72
24	B	614	CLA	C4-C3-C5	2.92	120.18	115.27
24	C	502	CLA	CBC-CAC-C3C	-2.91	104.39	112.43
27	l	101	SQD	O8-S-C6	2.91	110.39	105.74
24	c	515	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	C	514	CLA	C4-C3-C5	2.91	120.17	115.27
24	B	611	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
26	Y	101	BCR	C16-C17-C18	-2.91	123.15	127.31
24	c	509	CLA	O2A-CGA-CBA	2.91	121.05	111.91
26	B	619	BCR	C29-C30-C25	2.91	114.96	110.48
24	B	613	CLA	CMB-C2B-C3B	2.91	130.12	124.68
24	B	607	CLA	C4-C3-C5	2.91	120.17	115.27
24	A	405	CLA	CMC-C2C-C1C	2.91	129.47	125.04
24	c	512	CLA	CHD-C4C-NC	2.91	128.79	124.20
24	b	616	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
32	d	406	PL9	C7-C8-C9	-2.91	121.95	126.79
24	c	506	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
24	A	409	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	c	503	CLA	CAC-C3C-C4C	2.91	128.58	124.81
32	A	419	PL9	C53-C6-C1	2.90	120.93	114.99
24	C	513	CLA	C1-C2-C3	-2.90	121.02	126.04
24	A	409	CLA	C3B-C4B-NB	2.89	112.95	109.21
24	B	608	CLA	C1-O2A-CGA	2.89	124.03	116.44
27	A	411	SQD	C1-O5-C5	-2.89	108.01	113.69
24	C	508	CLA	C4-C3-C5	2.89	120.14	115.27
24	d	401	CLA	CAC-C3C-C4C	2.89	128.56	124.81
24	C	511	CLA	C4-C3-C5	2.89	120.13	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
24	A	406	CLA	CHD-C4C-NC	2.89	128.76	124.20
24	B	604	CLA	C4-C3-C5	2.89	120.13	115.27
24	B	607	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
26	C	515	BCR	C16-C17-C18	-2.88	123.19	127.31
24	B	612	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
24	b	610	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
24	c	515	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
26	b	624	BCR	C38-C26-C25	-2.88	121.29	124.53
24	B	608	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
24	a	407	CLA	C3B-C4B-NB	2.88	112.93	109.21
24	b	608	CLA	CMA-C3A-C2A	-2.88	102.21	113.83
24	B	615	CLA	CHD-C4C-NC	2.88	128.74	124.20
24	b	615	CLA	O2A-CGA-CBA	2.88	120.94	111.91
24	b	609	CLA	C1-C2-C3	-2.87	121.07	126.04
24	a	407	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
26	K	101	BCR	C37-C22-C21	-2.87	118.90	122.92
24	C	513	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
24	b	619	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	A	406	CLA	C1-C2-C3	-2.87	121.08	126.04
24	C	511	CLA	CAC-C3C-C4C	2.87	128.53	124.81
24	b	617	CLA	O2A-CGA-CBA	2.87	120.91	111.91
24	b	607	CLA	C1-C2-C3	-2.87	121.08	126.04
24	a	407	CLA	CHD-C4C-NC	2.87	128.72	124.20
32	d	406	PL9	C7-C3-C4	-2.86	114.55	116.88
24	C	508	CLA	CAC-C3C-C4C	2.86	128.53	124.81
24	c	515	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
24	A	406	CLA	C4-C3-C5	2.86	120.08	115.27
24	C	503	CLA	C3B-C4B-NB	2.86	112.91	109.21
36	c	518	DGD	C2G-O2G-C1B	-2.86	110.75	117.79
24	c	514	CLA	O2A-CGA-CBA	2.86	120.88	111.91
26	y	101	BCR	C28-C27-C26	-2.86	108.97	114.08
32	d	406	PL9	C53-C6-C1	2.86	120.83	114.99
24	d	401	CLA	C4C-C3C-C2C	-2.86	102.74	106.90
24	c	512	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
26	b	622	BCR	C15-C14-C13	-2.85	123.24	127.31
24	B	607	CLA	CHD-C4C-NC	2.85	128.70	124.20
24	b	606	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	b	609	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
24	b	608	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
24	d	401	CLA	CAA-C2A-C3A	-2.85	104.99	112.78
24	D	404	CLA	CHC-C1C-C2C	-2.84	118.86	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	CMA-C3A-C4A	-2.84	104.14	111.77
26	h	101	BCR	C16-C17-C18	-2.84	123.25	127.31
24	B	606	CLA	CAC-C3C-C4C	2.84	128.49	124.81
24	B	605	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
24	B	613	CLA	CMC-C2C-C1C	2.84	129.36	125.04
27	a	411	SQD	C44-O6-C1	-2.84	108.20	113.74
24	D	401	CLA	CMB-C2B-C3B	2.84	129.98	124.68
32	a	416	PL9	C53-C6-C1	2.83	120.78	114.99
24	C	507	CLA	CBC-CAC-C3C	-2.83	104.63	112.43
25	d	403	PHO	C1A-C2A-C3A	-2.83	100.15	102.84
30	A	417	LMT	O5'-C5'-C4'	2.83	115.72	109.75
24	b	609	CLA	O1D-CGD-CBD	-2.83	118.70	124.48
24	B	614	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
24	C	507	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
40	V	203	HEC	CMB-C2B-C1B	-2.82	124.12	128.46
26	b	624	BCR	C37-C22-C23	2.82	122.53	118.08
24	C	505	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
37	L	101	LHG	O8-C23-C24	2.82	120.77	111.91
24	B	607	CLA	CAC-C3C-C4C	2.82	128.47	124.81
24	B	605	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
26	T	102	BCR	C29-C28-C27	-2.82	105.07	111.38
24	B	611	CLA	C3B-C4B-NB	2.82	112.86	109.21
38	E	103	HEM	CBD-CAD-C3D	-2.82	104.79	112.63
24	a	407	CLA	O2A-CGA-CBA	2.82	120.76	111.91
24	C	511	CLA	CHD-C4C-NC	2.82	128.65	124.20
37	d	410	LHG	O8-C23-C24	2.82	120.75	111.91
24	c	512	CLA	CBC-CAC-C3C	-2.82	104.66	112.43
27	F	101	SQD	O9-S-C6	2.82	110.29	106.94
34	Z	101	LMG	C4-C3-C2	2.82	115.74	110.82
24	B	616	CLA	CAC-C3C-C4C	2.82	128.46	124.81
24	b	613	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	b	616	CLA	CMC-C2C-C1C	2.81	129.32	125.04
24	c	513	CLA	CMB-C2B-C3B	2.81	129.94	124.68
25	A	407	PHO	O1D-CGD-CBD	-2.81	120.06	124.74
24	B	606	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
36	c	517	DGD	C2G-O2G-C1B	-2.81	110.88	117.79
24	C	510	CLA	CAC-C3C-C4C	2.81	128.45	124.81
25	A	408	PHO	O2D-CGD-O1D	-2.81	118.35	123.84
24	C	504	CLA	C4-C3-C5	2.80	119.99	115.27
27	b	601	SQD	O47-C7-O49	-2.80	116.93	123.70
24	b	608	CLA	CMB-C2B-C3B	2.80	129.92	124.68
24	b	617	CLA	CAC-C3C-C4C	2.80	128.44	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	606	CLA	O2A-CGA-CBA	2.80	120.70	111.91
24	b	606	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
24	D	403	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
24	B	615	CLA	CBC-CAC-C3C	-2.80	104.72	112.43
32	A	419	PL9	C8-C7-C3	2.80	119.89	111.98
24	B	606	CLA	CHD-C4C-NC	2.80	128.61	124.20
24	C	503	CLA	O2A-CGA-CBA	2.80	120.69	111.91
24	c	514	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
24	a	407	CLA	C1-C2-C3	-2.79	121.21	126.04
24	C	509	CLA	O2A-CGA-CBA	2.79	120.68	111.91
24	b	613	CLA	CMC-C2C-C1C	2.79	129.29	125.04
24	B	608	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
24	b	615	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
24	c	503	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
24	C	509	CLA	C1-C2-C3	-2.79	121.22	126.04
24	B	605	CLA	C4-C3-C5	2.79	119.97	115.27
24	B	609	CLA	CHD-C4C-NC	2.79	128.60	124.20
25	a	408	PHO	CMA-C3A-C4A	-2.79	108.27	114.38
24	C	513	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
24	C	513	CLA	C4-C3-C5	2.79	119.96	115.27
24	c	509	CLA	C4-C3-C5	2.79	119.96	115.27
38	E	103	HEM	CMD-C2D-C1D	2.78	129.28	125.04
24	C	503	CLA	CAC-C3C-C4C	2.78	128.42	124.81
24	a	406	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
24	b	612	CLA	C4-C3-C5	2.78	119.95	115.27
24	B	604	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
34	z	101	LMG	O8-C28-C29	2.78	120.63	111.91
24	b	618	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	c	508	CLA	CBC-CAC-C3C	-2.77	104.78	112.43
26	h	101	BCR	C11-C10-C9	-2.77	123.35	127.31
24	a	406	CLA	CAA-C2A-C1A	-2.77	102.89	111.97
24	B	615	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
24	B	608	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
24	B	612	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	c	509	CLA	O2A-CGA-O1A	-2.77	116.60	123.59
24	C	513	CLA	CMC-C2C-C1C	2.77	129.26	125.04
24	B	604	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
24	b	617	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
24	a	409	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
37	d	408	LHG	O8-C23-C24	2.77	120.59	111.91
24	a	407	CLA	CMC-C2C-C1C	2.77	129.25	125.04
24	c	508	CLA	CMB-C2B-C3B	2.76	129.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	602	CLA	CHD-C4C-NC	2.76	128.56	124.20
24	b	619	CLA	O2A-CGA-CBA	2.76	120.58	111.91
27	F	101	SQD	C3-C4-C5	2.76	115.17	110.24
24	C	514	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
24	b	612	CLA	CAC-C3C-C4C	2.76	128.40	124.81
24	B	602	CLA	O2A-CGA-CBA	2.76	120.58	111.91
24	c	506	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
24	C	502	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
26	T	102	BCR	C2-C1-C6	2.76	114.73	110.48
34	j	101	LMG	O8-C28-O10	-2.76	116.63	123.59
24	C	503	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
34	b	625	LMG	O7-C10-C11	2.75	117.44	111.50
24	b	616	CLA	C2A-C1A-CHA	-2.75	119.04	123.86
24	B	608	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
26	c	516	BCR	C15-C14-C13	-2.75	123.38	127.31
24	B	606	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
24	b	618	CLA	C4-C3-C5	2.75	119.90	115.27
26	y	101	BCR	C16-C17-C18	-2.75	123.39	127.31
24	B	602	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
24	b	621	CLA	C1-C2-C3	-2.75	121.29	126.04
24	C	502	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
24	C	504	CLA	CAC-C3C-C4C	2.74	128.37	124.81
24	c	514	CLA	CMC-C2C-C1C	2.74	129.22	125.04
24	b	614	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
32	a	416	PL9	C25-C24-C26	2.74	119.88	115.27
37	D	410	LHG	O8-C23-C24	2.74	120.51	111.91
24	B	611	CLA	C4-C3-C5	2.74	119.88	115.27
24	c	513	CLA	CBC-CAC-C3C	-2.74	104.89	112.43
37	L	101	LHG	C6-C5-C4	-2.74	105.32	111.79
24	A	409	CLA	CAA-C2A-C3A	-2.73	105.29	112.78
24	C	514	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
24	b	610	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
24	B	604	CLA	CMB-C2B-C3B	2.73	129.79	124.68
24	C	503	CLA	CMC-C2C-C1C	2.73	129.20	125.04
24	B	613	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
27	f	101	SQD	O48-C23-C24	2.73	120.47	111.91
24	b	610	CLA	OBD-CAD-C3D	-2.73	121.96	128.52
27	A	416	SQD	C3-C4-C5	2.73	115.10	110.24
26	D	405	BCR	C15-C14-C13	-2.73	123.42	127.31
24	B	609	CLA	O2A-CGA-CBA	2.73	120.46	111.91
24	C	511	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
24	b	607	CLA	CHC-C1C-C2C	-2.72	119.19	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	613	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
24	c	512	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
24	b	610	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
26	Y	101	BCR	C37-C22-C23	2.72	122.36	118.08
24	D	404	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
24	b	611	CLA	CMB-C2B-C3B	2.72	129.77	124.68
24	B	602	CLA	C1-C2-C3	-2.72	121.34	126.04
36	C	517	DGD	O1G-C1A-O1A	-2.72	116.74	123.59
24	c	510	CLA	CMC-C2C-C1C	2.71	129.17	125.04
24	A	405	CLA	CHC-C1C-C2C	-2.71	119.21	126.72
24	b	606	CLA	C2A-C1A-CHA	-2.71	119.11	123.86
26	b	623	BCR	C38-C26-C25	-2.71	121.48	124.53
26	K	101	BCR	C24-C23-C22	-2.71	122.14	126.23
32	d	406	PL9	C37-C38-C39	-2.71	121.13	127.66
26	B	620	BCR	C2-C1-C6	2.71	114.65	110.48
36	c	517	DGD	O1G-C1A-O1A	-2.71	116.75	123.59
24	d	404	CLA	CHD-C4C-NC	2.71	128.47	124.20
36	C	518	DGD	O1G-C1A-C2A	2.71	120.41	111.91
37	E	101	LHG	C5-O7-C7	-2.71	111.12	117.79
32	A	419	PL9	C45-C44-C46	2.71	119.82	115.27
27	a	411	SQD	O48-C23-C24	2.71	120.40	111.91
24	B	604	CLA	O2A-CGA-CBA	2.71	120.40	111.91
34	z	101	LMG	O6-C5-C4	2.70	114.60	109.69
24	c	515	CLA	C1-C2-C3	-2.70	121.37	126.04
38	e	102	HEM	C4D-ND-C1D	2.70	107.86	105.07
25	a	408	PHO	CMB-C2B-C3B	2.70	129.73	124.68
26	B	620	BCR	C28-C27-C26	-2.70	109.26	114.08
26	T	102	BCR	C28-C27-C26	-2.70	109.26	114.08
24	b	619	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
24	C	511	CLA	CMB-C2B-C3B	2.70	129.72	124.68
24	C	503	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
32	d	406	PL9	C15-C14-C16	2.70	119.81	115.27
26	c	526	BCR	C7-C8-C9	-2.70	122.16	126.23
25	a	408	PHO	C1-O2A-CGA	2.70	123.52	116.44
24	C	510	CLA	C4-C3-C5	2.69	119.80	115.27
24	b	613	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
24	b	611	CLA	CHD-C4C-NC	2.69	128.44	124.20
27	F	101	SQD	C1-C2-C3	-2.69	104.39	110.00
27	A	411	SQD	O48-C23-C24	2.69	120.34	111.91
26	K	101	BCR	C7-C8-C9	-2.69	122.17	126.23
32	A	419	PL9	C35-C34-C36	2.69	119.79	115.27
30	m	102	LMT	C1'-O5'-C5'	-2.69	108.41	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	405	BCR	C28-C27-C26	-2.69	109.28	114.08
24	B	612	CLA	C4-C3-C5	2.69	119.79	115.27
36	h	102	DGD	O1G-C1A-C2A	2.69	120.33	111.91
24	b	612	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
24	a	407	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
24	c	505	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
24	B	615	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	c	509	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	C	507	CLA	C1-C2-C3	-2.68	121.41	126.04
27	A	411	SQD	O9-S-C6	2.68	110.12	106.94
24	B	604	CLA	CAC-C3C-C4C	2.68	128.29	124.81
24	c	510	CLA	C1-C2-C3	-2.68	121.41	126.04
24	b	609	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
24	D	403	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	B	614	CLA	C1D-CHD-C4C	-2.68	120.28	126.06
24	D	404	CLA	CHD-C4C-NC	2.68	128.42	124.20
24	c	505	CLA	O2A-CGA-CBA	2.68	120.31	111.91
24	C	508	CLA	CBC-CAC-C3C	-2.68	105.05	112.43
24	A	405	CLA	CMA-C3A-C2A	-2.67	103.04	113.83
24	c	504	CLA	O2A-CGA-CBA	2.67	120.30	111.91
27	b	601	SQD	C1-C2-C3	-2.67	104.43	110.00
35	b	628	HTG	C1-O5-C5	2.67	117.51	112.58
24	c	510	CLA	C4-C3-C5	2.67	119.77	115.27
32	D	406	PL9	C25-C24-C26	2.67	119.76	115.27
24	B	616	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
24	B	614	CLA	O2A-CGA-CBA	2.67	120.28	111.91
24	d	401	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
27	a	411	SQD	O47-C7-O49	-2.67	117.26	123.70
24	B	606	CLA	C4-C3-C5	2.67	119.75	115.27
24	B	608	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
24	b	611	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
24	b	618	CLA	O2A-CGA-CBA	2.66	120.26	111.91
24	C	512	CLA	CHD-C4C-NC	2.66	128.40	124.20
27	A	411	SQD	O48-C23-O10	-2.66	116.87	123.59
24	C	509	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
24	b	609	CLA	O2A-CGA-CBA	2.66	120.26	111.91
24	B	615	CLA	CMB-C2B-C3B	2.66	129.65	124.68
24	c	511	CLA	CMB-C2B-C3B	2.66	129.65	124.68
24	B	608	CLA	CAC-C3C-C4C	2.65	128.25	124.81
26	B	618	BCR	C7-C8-C9	-2.65	122.23	126.23
24	b	613	CLA	C2A-C1A-CHA	-2.64	119.23	123.86
32	a	416	PL9	C40-C39-C41	2.64	119.72	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	l	101	SQD	O48-C23-C24	2.64	120.20	111.91
35	D	411	HTG	C1'-S1-C1	2.64	105.03	100.09
24	C	513	CLA	CHD-C4C-NC	2.64	128.36	124.20
24	c	510	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
37	d	408	LHG	O8-C23-O10	-2.64	116.94	123.59
24	D	404	CLA	C4-C3-C5	2.63	119.70	115.27
24	D	403	CLA	C1D-CHD-C4C	-2.63	120.38	126.06
24	c	515	CLA	O2A-CGA-CBA	2.63	120.16	111.91
24	B	607	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
24	B	605	CLA	CAC-C3C-C4C	2.63	128.22	124.81
30	b	602	LMT	O5'-C5'-C4'	2.63	115.29	109.75
24	b	614	CLA	C1-C2-C3	-2.63	121.50	126.04
24	c	504	CLA	CAC-C3C-C4C	2.63	128.22	124.81
24	c	505	CLA	CHD-C4C-NC	2.63	128.34	124.20
30	m	103	LMT	C1-O1'-C1'	-2.63	109.48	113.84
30	I	102	LMT	C2'-C3'-C4'	-2.63	103.69	109.68
24	D	401	CLA	CMA-C3A-C2A	-2.62	103.24	113.83
24	C	510	CLA	CMB-C2B-C3B	2.62	129.59	124.68
24	A	409	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
24	b	611	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
24	b	614	CLA	CHD-C4C-NC	2.62	128.34	124.20
24	b	608	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
24	d	404	CLA	CMB-C2B-C3B	2.62	129.58	124.68
24	B	605	CLA	O2A-CGA-CBA	2.62	120.12	111.91
24	c	515	CLA	CMB-C2B-C3B	2.62	129.57	124.68
24	D	401	CLA	CMA-C3A-C4A	-2.62	104.74	111.77
24	c	507	CLA	CMC-C2C-C1C	2.61	129.02	125.04
32	d	406	PL9	C20-C19-C21	2.61	119.67	115.27
24	c	510	CLA	CHD-C4C-NC	2.61	128.32	124.20
24	B	617	CLA	CMB-C2B-C3B	2.61	129.57	124.68
34	C	521	LMG	C8-O7-C10	-2.61	111.36	117.79
34	c	521	LMG	O8-C28-C29	2.61	120.10	111.91
24	c	511	CLA	O2A-CGA-CBA	2.61	120.10	111.91
26	c	516	BCR	C3-C4-C5	-2.61	109.42	114.08
24	a	407	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
32	D	406	PL9	C15-C14-C16	2.61	119.66	115.27
24	c	508	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
24	b	619	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
24	C	513	CLA	O2A-CGA-CBA	2.61	120.09	111.91
35	V	204	HTG	C1-C2-C3	-2.61	105.44	110.59
24	c	512	CLA	C1-C2-C3	-2.61	121.53	126.04
24	a	409	CLA	CHB-C4A-NA	2.61	128.12	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	407	PHO	CMC-C2C-C3C	2.61	129.85	124.94
24	C	508	CLA	CMB-C2B-C3B	2.61	129.55	124.68
34	C	521	LMG	O8-C28-C29	2.61	120.08	111.91
35	b	627	HTG	C1-O5-C5	2.61	117.39	112.58
24	b	618	CLA	CAC-C3C-C4C	2.61	128.19	124.81
24	B	608	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
24	B	609	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
24	c	508	CLA	CED-O2D-CGD	2.60	121.82	115.94
24	b	619	CLA	C4-C3-C5	2.60	119.65	115.27
24	C	511	CLA	O1D-CGD-CBD	-2.60	119.16	124.48
24	b	614	CLA	CAC-C3C-C4C	2.60	128.18	124.81
36	c	517	DGD	O1G-C1A-C2A	2.60	120.06	111.91
24	C	513	CLA	CAC-C3C-C4C	2.60	128.18	124.81
24	B	608	CLA	O2A-CGA-CBA	2.60	120.06	111.91
24	B	607	CLA	C1-C2-C3	-2.60	121.55	126.04
24	b	610	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
24	d	404	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
32	A	419	PL9	C30-C29-C31	2.59	119.63	115.27
24	C	507	CLA	O2A-CGA-CBA	2.59	120.04	111.91
27	F	101	SQD	O48-C23-C24	2.59	120.04	111.91
37	D	409	LHG	C5-O7-C7	-2.59	111.41	117.79
24	b	607	CLA	CHD-C4C-NC	2.59	128.28	124.20
24	d	404	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
36	C	518	DGD	O2G-C1B-O1B	-2.59	117.44	123.70
24	a	406	CLA	O2D-CGD-CBD	2.59	115.87	111.27
24	b	608	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
24	b	619	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
38	e	102	HEM	CBD-CAD-C3D	-2.59	105.44	112.63
40	v	202	HEC	O2A-CGA-O1A	-2.59	116.85	123.30
24	d	402	CLA	CMB-C2B-C3B	2.59	129.52	124.68
24	B	617	CLA	C1-O2A-CGA	2.59	123.23	116.44
24	C	504	CLA	C1-C2-C3	-2.58	121.57	126.04
25	A	408	PHO	O2A-CGA-O1A	-2.58	117.07	123.59
37	E	101	LHG	O8-C23-C24	2.58	120.02	111.91
24	C	510	CLA	C1-O2A-CGA	2.58	123.22	116.44
26	a	410	BCR	C15-C14-C13	-2.58	123.62	127.31
26	c	526	BCR	C11-C10-C9	-2.58	123.63	127.31
24	b	617	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
24	B	603	CLA	CHD-C4C-NC	2.58	128.27	124.20
24	c	505	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
34	z	101	LMG	C3-C4-C5	2.58	114.83	110.24
24	B	603	CLA	CBC-CAC-C3C	-2.58	105.33	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	406	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
24	d	402	CLA	CAC-C3C-C4C	2.57	128.15	124.81
24	C	505	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
24	C	513	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
24	c	503	CLA	O2A-CGA-CBA	2.57	119.97	111.91
24	A	409	CLA	C1-C2-C3	-2.57	121.60	126.04
24	b	615	CLA	CMC-C2C-C1C	2.57	128.95	125.04
24	B	612	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
24	C	504	CLA	CHD-C4C-NC	2.57	128.25	124.20
24	c	508	CLA	CHD-C4C-NC	2.57	128.25	124.20
25	a	408	PHO	C1A-C2A-C3A	-2.56	100.40	102.84
24	b	613	CLA	CMB-C2B-C3B	2.56	129.47	124.68
24	C	507	CLA	CHD-C4C-NC	2.56	128.24	124.20
24	A	406	CLA	CMC-C2C-C1C	2.56	128.94	125.04
24	B	610	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
24	C	509	CLA	CMB-C2B-C3B	2.56	129.46	124.68
26	h	101	BCR	C10-C11-C12	-2.55	115.24	123.22
26	B	620	BCR	C36-C18-C17	-2.55	119.35	122.92
26	A	410	BCR	C7-C8-C9	-2.55	122.38	126.23
24	B	602	CLA	C4-C3-C5	2.55	119.57	115.27
24	C	505	CLA	C4-C3-C5	2.55	119.56	115.27
24	C	511	CLA	C1-O2A-CGA	2.55	123.14	116.44
24	b	610	CLA	O2A-CGA-CBA	2.55	119.92	111.91
24	B	607	CLA	CHC-C1C-C2C	-2.55	119.66	126.72
24	d	401	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
24	D	403	CLA	CMA-C3A-C2A	-2.55	103.54	113.83
24	D	404	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
36	D	407	DGD	O1G-C1A-C2A	2.55	119.90	111.91
26	B	619	BCR	C28-C27-C26	-2.55	109.53	114.08
24	B	617	CLA	CHD-C4C-NC	2.55	128.22	124.20
24	a	406	CLA	CMA-C3A-C4A	-2.54	104.93	111.77
35	V	204	HTG	O5-C1-C2	-2.54	107.11	110.31
32	a	416	PL9	C35-C34-C36	2.54	119.55	115.27
24	b	621	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
26	D	405	BCR	C37-C22-C23	2.54	122.08	118.08
26	c	526	BCR	C20-C21-C22	-2.54	123.69	127.31
24	c	505	CLA	C1-C2-C3	-2.54	121.65	126.04
24	c	514	CLA	C1-C2-C3	-2.54	121.66	126.04
26	H	101	BCR	C29-C30-C25	2.53	114.38	110.48
24	d	402	CLA	CMC-C2C-C1C	2.53	128.90	125.04
24	b	619	CLA	CBC-CAC-C3C	-2.53	105.44	112.43
24	B	602	CLA	CAC-C3C-C4C	2.53	128.10	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	CHD-C4C-NC	2.53	128.20	124.20
30	a	417	LMT	C1-O1'-C1'	-2.53	109.64	113.84
24	c	514	CLA	CBA-CAA-C2A	-2.53	106.39	113.86
24	B	609	CLA	CMC-C2C-C1C	2.53	128.89	125.04
24	b	608	CLA	CHD-C4C-NC	2.53	128.19	124.20
24	c	507	CLA	C1-O2A-CGA	2.53	123.08	116.44
26	t	101	BCR	C11-C10-C9	-2.53	123.70	127.31
24	c	512	CLA	CMB-C2B-C3B	2.53	129.41	124.68
32	d	406	PL9	C8-C7-C3	2.53	119.12	111.98
26	C	516	BCR	C33-C5-C6	-2.52	121.70	124.53
24	A	409	CLA	O2A-CGA-CBA	2.52	119.82	111.91
37	D	409	LHG	O8-C23-C24	2.52	119.81	111.91
24	C	504	CLA	CMB-C2B-C3B	2.52	129.39	124.68
24	C	505	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
24	c	513	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
24	c	511	CLA	CHD-C4C-NC	2.52	128.17	124.20
26	c	526	BCR	C38-C26-C25	-2.52	121.70	124.53
30	A	417	LMT	C1'-O5'-C5'	2.51	118.62	113.69
38	e	102	HEM	CHB-C1B-NB	2.51	127.48	124.38
24	c	504	CLA	CHD-C4C-NC	2.51	128.16	124.20
24	c	512	CLA	O2A-CGA-CBA	2.51	119.79	111.91
24	C	509	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
24	B	611	CLA	CMA-C3A-C4A	-2.51	105.03	111.77
24	A	409	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
30	m	103	LMT	O5B-C5B-C4B	2.51	114.25	109.69
24	c	510	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
24	A	405	CLA	CMA-C3A-C4A	-2.51	105.04	111.77
24	b	611	CLA	C1-C2-C3	-2.51	121.71	126.04
26	c	526	BCR	C24-C23-C22	-2.50	122.45	126.23
38	E	103	HEM	C4B-C3B-C2B	-2.50	105.13	107.11
37	D	409	LHG	O7-C7-O9	-2.50	117.65	123.70
24	d	402	CLA	CMA-C3A-C2A	-2.50	103.73	113.83
24	c	511	CLA	CMC-C2C-C1C	2.50	128.85	125.04
32	d	406	PL9	C42-C43-C44	-2.50	121.63	127.66
24	b	615	CLA	CHD-C4C-NC	2.50	128.15	124.20
24	D	401	CLA	CHD-C4C-NC	2.50	128.15	124.20
34	c	501	LMG	O8-C28-C29	2.50	119.75	111.91
24	B	607	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
24	b	614	CLA	C4-C3-C5	2.50	119.47	115.27
24	b	606	CLA	CMB-C2B-C3B	2.50	129.35	124.68
40	V	203	HEC	CBA-CAA-C2A	-2.50	108.40	112.60
24	C	507	CLA	CMC-C2C-C1C	2.50	128.84	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	611	CLA	C4-C3-C5	2.49	119.46	115.27
24	d	401	CLA	CAA-CBA-CGA	2.49	120.53	113.25
24	B	603	CLA	CAA-CBA-CGA	-2.49	105.97	113.25
24	b	619	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
24	A	405	CLA	O2A-CGA-CBA	2.49	119.72	111.91
27	a	402	SQD	O9-S-C6	2.49	109.90	106.94
24	D	401	CLA	CMC-C2C-C1C	2.49	128.83	125.04
26	T	102	BCR	C1-C6-C7	2.49	122.81	115.78
24	B	604	CLA	CHD-C4C-NC	2.49	128.12	124.20
24	c	515	CLA	CHD-C4C-NC	2.49	128.12	124.20
24	D	403	CLA	C2A-C1A-CHA	-2.48	119.51	123.86
24	B	610	CLA	CBC-CAC-C3C	-2.48	105.58	112.43
24	b	607	CLA	O2A-CGA-CBA	2.48	119.70	111.91
24	D	404	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
24	C	504	CLA	O2A-CGA-CBA	2.48	119.70	111.91
26	a	410	BCR	C34-C9-C10	-2.48	119.44	122.92
26	B	620	BCR	C3-C4-C5	-2.48	109.64	114.08
24	c	503	CLA	OBD-CAD-C3D	-2.48	122.55	128.52
32	D	406	PL9	C7-C8-C9	-2.48	122.66	126.79
24	b	607	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
34	c	520	LMG	O8-C28-C29	2.48	119.68	111.91
38	E	103	HEM	O2A-CGA-CBA	2.48	121.99	114.03
24	C	508	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
24	b	612	CLA	CAA-CBA-CGA	2.48	120.49	113.25
24	c	514	CLA	C4-C3-C5	2.48	119.44	115.27
24	B	602	CLA	CMC-C2C-C1C	2.48	128.81	125.04
37	d	409	LHG	O8-C23-C24	2.48	119.68	111.91
24	B	611	CLA	CMB-C2B-C3B	2.48	129.31	124.68
24	B	616	CLA	CHD-C4C-NC	2.47	128.10	124.20
32	A	419	PL9	C7-C3-C4	2.47	118.89	116.88
24	c	511	CLA	C4-C3-C5	2.47	119.43	115.27
24	C	508	CLA	C3B-C4B-NB	2.47	112.40	109.21
24	C	504	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
24	c	510	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
26	d	405	BCR	C37-C22-C23	2.47	121.97	118.08
24	c	505	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
24	c	509	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
24	A	406	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
34	c	501	LMG	O7-C10-O9	-2.46	117.75	123.70
27	b	601	SQD	O48-C23-O10	-2.46	117.38	123.59
24	b	621	CLA	CMB-C2B-C3B	2.46	129.28	124.68
24	c	512	CLA	CAC-C3C-C4C	2.46	128.00	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	620	CLA	CHD-C4C-NC	2.46	128.08	124.20
24	B	614	CLA	CMB-C2B-C3B	2.46	129.28	124.68
24	B	616	CLA	C1-O2A-CGA	2.46	122.89	116.44
24	C	503	CLA	CHD-C4C-NC	2.46	128.08	124.20
24	a	407	CLA	C4-C3-C5	2.46	119.41	115.27
24	C	506	CLA	CMC-C2C-C1C	2.46	128.78	125.04
24	A	406	CLA	CMA-C3A-C2A	-2.45	103.93	113.83
24	b	607	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
34	C	501	LMG	O8-C28-C29	2.45	119.61	111.91
24	c	513	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
24	C	514	CLA	O2A-CGA-CBA	2.45	119.61	111.91
24	a	409	CLA	O2A-CGA-CBA	2.45	119.61	111.91
24	c	513	CLA	O2A-CGA-CBA	2.45	119.60	111.91
24	c	503	CLA	CHD-C4C-NC	2.45	128.06	124.20
32	D	406	PL9	C37-C38-C39	-2.45	121.77	127.66
26	B	620	BCR	C15-C14-C13	-2.45	123.82	127.31
24	b	615	CLA	C1-C2-C3	-2.45	121.81	126.04
24	C	512	CLA	CMC-C2C-C1C	2.45	128.76	125.04
24	B	604	CLA	CHC-C1C-C2C	-2.44	119.96	126.72
24	c	515	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
24	C	508	CLA	O2A-CGA-CBA	2.44	119.56	111.91
24	b	612	CLA	CHD-C4C-NC	2.44	128.05	124.20
26	K	101	BCR	C2-C1-C6	2.44	114.23	110.48
24	b	615	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
24	b	613	CLA	CMA-C3A-C2A	-2.44	104.00	113.83
24	A	409	CLA	CMA-C3A-C2A	-2.44	104.00	113.83
40	V	203	HEC	CMB-C2B-C3B	2.44	128.69	125.82
24	c	510	CLA	CAC-C3C-C4C	2.44	127.97	124.81
26	h	101	BCR	C7-C8-C9	-2.44	122.55	126.23
25	d	403	PHO	O2A-CGA-CBA	2.43	119.55	111.91
27	l	101	SQD	C1-O5-C5	-2.43	108.91	113.69
24	a	409	CLA	CHD-C4C-NC	2.43	128.04	124.20
24	B	603	CLA	CAC-C3C-C4C	2.43	127.97	124.81
24	D	401	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
36	d	407	DGD	O6E-C5E-C4E	2.43	114.11	109.69
24	d	404	CLA	CGD-CBD-CAD	-2.43	102.86	110.73
26	b	624	BCR	C2-C1-C6	2.43	114.22	110.48
24	c	503	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
26	t	101	BCR	C15-C16-C17	-2.43	118.49	123.47
24	b	612	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
27	l	101	SQD	O9-S-C6	2.43	109.83	106.94
24	B	608	CLA	O2A-CGA-O1A	-2.43	117.46	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	410	LHG	O8-C23-O10	-2.43	117.46	123.59
24	c	508	CLA	O2A-CGA-CBA	2.43	119.53	111.91
38	e	102	HEM	CHA-C4D-ND	2.43	127.38	124.38
26	B	618	BCR	C34-C9-C10	-2.43	119.52	122.92
24	B	607	CLA	CMB-C2B-C3B	2.43	129.22	124.68
25	A	407	PHO	CMB-C2B-C3B	2.43	129.22	124.68
26	t	101	BCR	C1-C6-C7	2.43	122.64	115.78
24	C	514	CLA	CAA-C2A-C3A	-2.43	106.14	112.78
24	C	506	CLA	C4-C3-C5	2.42	119.35	115.27
36	h	102	DGD	O1G-C1A-O1A	-2.42	117.48	123.59
24	b	611	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
26	t	101	BCR	C2-C1-C6	2.42	114.21	110.48
24	b	612	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
24	b	617	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
24	d	404	CLA	O2A-CGA-CBA	2.42	119.49	111.91
24	B	603	CLA	C1-C2-C3	-2.41	121.87	126.04
26	B	618	BCR	C11-C10-C9	-2.41	123.87	127.31
37	d	408	LHG	O7-C7-O9	-2.41	117.88	123.70
26	A	410	BCR	C37-C22-C21	-2.41	119.55	122.92
24	a	406	CLA	CMA-C3A-C2A	-2.41	104.11	113.83
24	D	401	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	b	607	CLA	CMB-C2B-C3B	2.41	129.18	124.68
24	C	502	CLA	O2A-CGA-CBA	2.41	119.46	111.91
24	B	616	CLA	C4-C3-C5	2.41	119.32	115.27
30	a	401	LMT	O5'-C5'-C4'	2.41	114.83	109.75
24	B	613	CLA	C4-C3-C5	2.41	119.32	115.27
25	A	408	PHO	CMD-C2D-C3D	2.41	129.18	124.68
24	b	614	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
24	B	605	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
32	d	406	PL9	O1-C4-C3	-2.40	118.08	120.72
26	B	620	BCR	C7-C8-C9	-2.40	122.61	126.23
24	d	404	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
24	b	607	CLA	CMA-C3A-C4A	-2.40	105.32	111.77
24	c	509	CLA	CHD-C4C-NC	2.40	127.98	124.20
36	c	517	DGD	O3G-C3G-C2G	-2.40	105.11	110.90
24	B	606	CLA	C1-O2A-CGA	2.40	122.73	116.44
30	m	103	LMT	C1B-O5B-C5B	2.40	118.39	113.69
24	C	513	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
24	D	404	CLA	O2A-CGA-CBA	2.39	119.41	111.91
26	D	405	BCR	C10-C11-C12	-2.39	115.75	123.22
26	d	405	BCR	C29-C30-C25	2.39	114.16	110.48
26	a	410	BCR	C33-C5-C6	-2.39	121.84	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	603	CLA	CMA-C3A-C4A	-2.39	105.35	111.77
38	E	103	HEM	C4D-ND-C1D	2.39	107.54	105.07
24	c	508	CLA	CGD-CBD-CAD	-2.39	103.00	110.73
24	a	407	CLA	OBD-CAD-C3D	-2.39	122.78	128.52
25	A	407	PHO	CBA-CAA-C2A	-2.39	106.84	113.81
26	H	101	BCR	C37-C22-C21	-2.39	119.58	122.92
34	c	521	LMG	C8-O7-C10	-2.39	111.92	117.79
24	c	512	CLA	O1D-CGD-CBD	-2.39	119.60	124.48
37	d	410	LHG	O8-C23-O10	-2.38	117.58	123.59
24	A	409	CLA	CMB-C2B-C3B	2.38	129.14	124.68
24	C	503	CLA	C4-C3-C5	2.38	119.28	115.27
26	C	516	BCR	C3-C4-C5	-2.38	109.82	114.08
24	b	620	CLA	CMC-C2C-C1C	2.38	128.67	125.04
24	B	612	CLA	O2A-CGA-CBA	2.38	119.38	111.91
35	b	627	HTG	C1-C2-C3	2.38	115.29	110.59
24	C	502	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
24	A	406	CLA	O2A-CGA-CBA	2.38	119.37	111.91
24	C	513	CLA	C1-O2A-CGA	2.38	122.68	116.44
37	l	102	LHG	O8-C23-C24	2.38	119.36	111.91
36	D	407	DGD	O6E-C5E-C4E	2.37	114.01	109.69
24	B	602	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	C	512	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	c	505	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
24	c	515	CLA	C4-C3-C5	2.37	119.26	115.27
24	B	614	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
30	m	103	LMT	O1'-C1'-C2'	2.37	112.01	108.30
24	b	615	CLA	CMB-C2B-C3B	2.37	129.12	124.68
24	B	608	CLA	CMB-C2B-C3B	2.37	129.11	124.68
36	c	518	DGD	O1G-C1A-C2A	2.37	119.35	111.91
24	c	503	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	c	514	CLA	C4C-C3C-C2C	-2.37	103.45	106.90
24	b	613	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
24	b	616	CLA	C4-C3-C5	2.37	119.25	115.27
24	C	504	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
36	C	519	DGD	O2G-C1B-C2B	2.37	116.60	111.50
24	b	617	CLA	OBD-CAD-C3D	-2.37	122.83	128.52
24	c	506	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
24	b	615	CLA	CMA-C3A-C4A	-2.36	105.42	111.77
24	b	609	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
24	b	609	CLA	C4-C3-C5	2.36	119.25	115.27
24	c	506	CLA	CHD-C4C-NC	2.36	127.93	124.20
32	D	406	PL9	C12-C13-C14	-2.36	121.97	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	401	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
24	B	614	CLA	O2D-CGD-CBD	2.36	115.46	111.27
24	c	503	CLA	CMC-C2C-C1C	2.36	128.63	125.04
24	A	409	CLA	CMA-C3A-C4A	-2.36	105.44	111.77
24	c	513	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
26	A	410	BCR	C38-C26-C25	-2.35	121.88	124.53
24	B	609	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
24	c	503	CLA	C4-C3-C5	2.35	119.23	115.27
36	d	407	DGD	O1G-C1A-C2A	2.35	119.28	111.91
30	D	402	LMT	O1B-C4'-C3'	2.35	113.52	107.28
24	C	505	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
36	H	102	DGD	O1G-C1A-O1A	-2.35	117.67	123.59
35	C	522	HTG	O5-C1-C2	2.35	113.26	110.31
26	D	405	BCR	C30-C25-C24	2.35	122.41	115.78
26	C	516	BCR	C21-C20-C19	-2.35	115.90	123.22
37	D	408	LHG	O7-C7-O9	-2.34	118.03	123.70
27	A	411	SQD	O47-C7-O49	-2.34	118.04	123.70
27	a	402	SQD	O48-C23-O10	-2.34	117.68	123.59
36	C	518	DGD	O1G-C1A-O1A	-2.34	117.68	123.59
24	B	606	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
34	J	101	LMG	O8-C28-O10	-2.34	117.68	123.59
24	c	505	CLA	C2A-C1A-CHA	-2.34	119.76	123.86
27	a	402	SQD	O8-S-C6	2.34	109.47	105.74
24	C	514	CLA	CHD-C4C-NC	2.34	127.89	124.20
27	f	101	SQD	O47-C7-O49	-2.34	118.05	123.70
26	a	410	BCR	C35-C13-C14	-2.33	119.65	122.92
24	c	514	CLA	CED-O2D-CGD	2.33	121.22	115.94
24	B	608	CLA	CHD-C4C-NC	2.33	127.88	124.20
24	C	507	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
32	d	406	PL9	C22-C23-C24	-2.33	122.04	127.66
24	b	614	CLA	C1-O2A-CGA	2.33	122.56	116.44
24	B	610	CLA	C4-C3-C5	2.33	119.19	115.27
24	B	616	CLA	CED-O2D-CGD	2.33	121.21	115.94
26	B	620	BCR	C16-C17-C18	-2.33	123.99	127.31
26	y	101	BCR	C10-C11-C12	-2.33	115.95	123.22
35	c	522	HTG	C1-O5-C5	2.33	116.87	112.58
24	B	608	CLA	OBD-CAD-C3D	-2.33	122.92	128.52
24	c	514	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
24	c	511	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
24	B	616	CLA	C11-C10-C8	-2.33	108.40	115.92
24	d	401	CLA	O2A-CGA-CBA	2.33	119.21	111.91
24	C	506	CLA	CHD-C4C-NC	2.33	127.87	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	409	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
24	c	506	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
24	c	508	CLA	C4-C3-C5	2.32	119.18	115.27
26	C	516	BCR	C11-C10-C9	-2.32	124.00	127.31
24	B	609	CLA	C1-C2-C3	-2.32	122.03	126.04
24	C	505	CLA	C1-O2A-CGA	2.32	122.53	116.44
36	C	517	DGD	O1G-C1A-C2A	2.32	119.19	111.91
27	A	416	SQD	O5-C5-C4	2.32	113.91	109.69
24	b	613	CLA	CHD-C4C-NC	2.32	127.86	124.20
30	a	401	LMT	C1'-O5'-C5'	2.32	118.24	113.69
24	A	406	CLA	CAA-CBA-CGA	2.32	120.02	113.25
27	F	101	SQD	C44-O6-C1	-2.31	109.22	113.74
24	C	510	CLA	CHD-C4C-NC	2.31	127.85	124.20
24	b	616	CLA	O2A-CGA-CBA	2.31	119.17	111.91
34	B	621	LMG	O8-C28-C29	2.31	119.16	111.91
24	b	620	CLA	C11-C10-C8	-2.31	108.45	115.92
32	d	406	PL9	C35-C34-C36	2.31	119.16	115.27
24	C	508	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
26	T	102	BCR	C35-C13-C12	2.31	121.72	118.08
26	a	410	BCR	C37-C22-C21	-2.31	119.69	122.92
25	d	403	PHO	CMA-C3A-C4A	-2.31	109.32	114.38
35	B	622	HTG	C1-O5-C5	2.30	116.83	112.58
24	B	617	CLA	O2A-CGA-CBA	2.30	119.14	111.91
24	b	620	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
26	h	101	BCR	C31-C1-C6	-2.30	106.57	110.30
26	Y	101	BCR	C10-C11-C12	-2.30	116.04	123.22
24	B	614	CLA	CMC-C2C-C1C	2.30	128.54	125.04
24	a	409	CLA	CMA-C3A-C4A	-2.30	105.59	111.77
36	h	102	DGD	O4D-C4D-C3D	-2.30	105.04	110.35
37	d	409	LHG	C5-O7-C7	-2.30	112.13	117.79
24	b	613	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
40	V	203	HEC	O2D-CGD-CBD	2.30	121.41	114.03
24	C	503	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
24	c	510	CLA	O2A-CGA-CBA	2.30	119.11	111.91
24	B	611	CLA	CMC-C2C-C1C	2.29	128.53	125.04
34	C	520	LMG	O8-C28-O10	-2.29	117.81	123.59
24	C	504	CLA	CMC-C2C-C1C	2.29	128.53	125.04
24	b	613	CLA	C11-C10-C8	-2.29	108.52	115.92
26	b	624	BCR	C16-C17-C18	-2.29	124.04	127.31
24	c	514	CLA	CHB-C4A-NA	2.29	127.68	124.51
35	B	623	HTG	C1-C2-C3	2.29	115.11	110.59
36	h	102	DGD	O2G-C1B-O1B	-2.29	118.17	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	601	SQD	O9-S-C6	2.29	109.66	106.94
24	b	621	CLA	O1D-CGD-CBD	-2.29	119.81	124.48
36	H	102	DGD	O1G-C1A-C2A	2.28	119.08	111.91
24	c	504	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	c	512	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	B	606	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
24	C	507	CLA	CMB-C2B-C3B	2.28	128.94	124.68
27	a	411	SQD	O9-S-C6	2.28	109.65	106.94
24	A	406	CLA	CED-O2D-CGD	2.28	121.09	115.94
24	A	409	CLA	CHB-C4A-NA	2.28	127.66	124.51
26	D	405	BCR	C37-C22-C21	-2.28	119.73	122.92
26	h	101	BCR	C29-C30-C25	2.28	113.98	110.48
24	D	404	CLA	CMC-C2C-C1C	2.28	128.50	125.04
24	a	409	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
24	b	614	CLA	CGD-CBD-CAD	-2.27	103.37	110.73
40	v	202	HEC	CBA-CAA-C2A	-2.27	108.77	112.60
24	A	406	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
40	v	202	HEC	O2A-CGA-CBA	2.27	121.33	114.03
24	C	508	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
26	Y	101	BCR	C40-C30-C25	-2.27	106.62	110.30
24	C	510	CLA	O2A-CGA-CBA	2.27	119.03	111.91
34	Z	101	LMG	C9-C8-C7	-2.27	106.42	111.79
25	a	408	PHO	O2D-CGD-O1D	-2.26	119.41	123.84
26	b	623	BCR	C37-C22-C21	-2.26	119.75	122.92
24	b	607	CLA	C1-O2A-CGA	2.26	122.38	116.44
24	b	608	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
24	a	406	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
24	B	611	CLA	OBD-CAD-C3D	-2.26	123.08	128.52
24	b	618	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
25	A	408	PHO	O2A-CGA-CBA	2.26	118.99	111.91
24	b	613	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
24	B	617	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
24	C	510	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	D	401	CLA	C1-C2-C3	-2.25	122.15	126.04
26	b	624	BCR	C3-C4-C5	-2.25	110.06	114.08
24	C	505	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
34	B	621	LMG	C9-C8-C7	-2.25	106.47	111.79
27	f	101	SQD	O9-S-C6	2.25	109.61	106.94
27	F	101	SQD	C1-O5-C5	-2.25	109.27	113.69
24	C	506	CLA	O2A-CGA-CBA	2.25	118.97	111.91
24	B	602	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
24	b	619	CLA	C4-C3-C2	-2.25	117.92	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	T	102	BCR	C29-C30-C25	2.24	113.94	110.48
35	B	631	HTG	C1-O5-C5	2.24	116.72	112.58
24	D	401	CLA	O2A-CGA-CBA	2.24	118.94	111.91
26	c	526	BCR	C2-C1-C6	2.24	113.93	110.48
32	a	416	PL9	C45-C44-C46	2.24	119.04	115.27
24	b	609	CLA	CHD-C4C-NC	2.24	127.73	124.20
24	b	618	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
26	T	102	BCR	C7-C6-C5	-2.24	116.05	121.46
36	D	407	DGD	O6D-C5D-C6D	2.24	111.18	106.67
24	b	618	CLA	CMC-C2C-C1C	2.24	128.44	125.04
26	b	622	BCR	C29-C30-C25	2.23	113.92	110.48
26	d	405	BCR	C29-C28-C27	-2.23	106.39	111.38
24	C	502	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
30	A	417	LMT	C1B-O1B-C4'	-2.23	112.44	117.96
24	a	406	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
32	D	406	PL9	C27-C28-C29	-2.23	122.29	127.66
26	B	620	BCR	C34-C9-C8	2.23	121.59	118.08
24	B	610	CLA	O2A-CGA-CBA	2.23	118.90	111.91
24	B	616	CLA	CHA-C1A-NA	-2.23	121.29	126.40
24	c	511	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
24	B	603	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
24	A	406	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
32	D	406	PL9	C40-C39-C38	-2.23	117.97	123.68
24	b	611	CLA	O2A-CGA-CBA	2.22	118.89	111.91
26	a	410	BCR	C38-C26-C25	-2.22	122.03	124.53
36	d	407	DGD	O5D-C1E-C2E	2.22	111.78	108.30
24	b	612	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
24	c	515	CLA	CHB-C4A-NA	2.22	127.59	124.51
34	B	621	LMG	C30-C29-C28	-2.22	105.54	113.62
24	b	614	CLA	O2A-CGA-CBA	2.22	118.88	111.91
26	k	103	BCR	C11-C10-C9	-2.22	124.14	127.31
24	b	619	CLA	CHD-C4C-NC	2.22	127.70	124.20
24	B	610	CLA	CMB-C2B-C1B	2.22	131.88	128.46
30	b	602	LMT	O5'-C1'-C2'	2.22	115.05	110.35
32	A	419	PL9	C35-C34-C33	-2.22	117.98	123.68
24	b	608	CLA	C7-C6-C5	-2.22	107.33	113.36
24	b	614	CLA	CED-O2D-CGD	2.22	120.95	115.94
24	B	604	CLA	CED-O2D-CGD	2.22	120.95	115.94
24	D	404	CLA	CMA-C3A-C2A	-2.22	104.89	113.83
26	b	623	BCR	C29-C30-C25	2.22	113.89	110.48
34	j	101	LMG	O8-C28-C29	2.21	118.86	111.91
24	b	616	CLA	O2A-CGA-O1A	-2.21	118.00	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	405	BCR	C16-C17-C18	-2.21	124.15	127.31
26	K	101	BCR	C29-C30-C25	2.21	113.89	110.48
24	c	506	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
24	C	502	CLA	CHD-C4C-NC	2.21	127.69	124.20
24	a	407	CLA	CHB-C4A-NA	2.21	127.57	124.51
38	E	103	HEM	CHA-C4D-ND	2.21	127.11	124.38
24	b	617	CLA	CHD-C4C-NC	2.21	127.69	124.20
24	B	608	CLA	C1-C2-C3	-2.21	122.22	126.04
34	c	501	LMG	O1-C1-C2	2.21	111.75	108.30
24	b	611	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
24	C	513	CLA	CED-O2D-CGD	2.21	120.94	115.94
27	A	416	SQD	O48-C23-O10	-2.21	118.02	123.59
24	C	508	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
24	b	606	CLA	CMC-C2C-C1C	2.20	128.39	125.04
26	K	101	BCR	C11-C10-C9	-2.20	124.17	127.31
24	B	603	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
37	L	101	LHG	O8-C23-O10	-2.20	118.04	123.59
26	D	405	BCR	C29-C28-C27	-2.20	106.46	111.38
25	A	408	PHO	C4A-C3A-C2A	-2.20	100.75	102.84
24	b	614	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
24	C	513	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
34	J	101	LMG	C9-C8-C7	-2.20	106.59	111.79
24	C	509	CLA	CHD-C4C-NC	2.20	127.66	124.20
24	d	401	CLA	CMB-C2B-C3B	2.20	128.78	124.68
24	C	511	CLA	O2A-CGA-CBA	2.19	118.79	111.91
24	B	610	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	D	404	CLA	CMB-C2B-C3B	2.19	128.78	124.68
24	C	510	CLA	CMC-C2C-C1C	2.19	128.37	125.04
24	b	607	CLA	CMC-C2C-C1C	2.19	128.37	125.04
26	y	101	BCR	C35-C13-C14	-2.19	119.86	122.92
27	a	402	SQD	C45-O47-C7	-2.19	112.41	117.79
24	c	506	CLA	O2A-CGA-CBA	2.19	118.77	111.91
24	d	404	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
24	D	403	CLA	CBC-CAC-C3C	-2.18	106.41	112.43
24	b	612	CLA	C1-O2A-CGA	2.18	122.17	116.44
24	D	401	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
26	T	102	BCR	C21-C20-C19	-2.18	116.41	123.22
35	B	622	HTG	O5-C1-C2	2.18	113.06	110.31
24	B	611	CLA	CHD-C4C-NC	2.18	127.64	124.20
37	d	409	LHG	O8-C23-O10	-2.18	118.10	123.59
24	C	506	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
34	c	521	LMG	O7-C10-O9	-2.18	118.44	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	BCR	C10-C11-C12	-2.17	116.44	123.22
26	y	101	BCR	C21-C20-C19	-2.17	116.44	123.22
24	c	503	CLA	C1-O2A-CGA	2.17	122.14	116.44
26	t	101	BCR	C21-C20-C19	-2.17	116.45	123.22
35	c	523	HTG	C1-O5-C5	2.17	116.58	112.58
24	c	508	CLA	CMC-C2C-C1C	2.17	128.34	125.04
24	C	505	CLA	CHD-C4C-NC	2.17	127.62	124.20
26	T	102	BCR	C19-C18-C17	-2.17	115.62	118.94
36	h	102	DGD	C3G-O3G-C1D	-2.16	109.51	113.74
24	c	506	CLA	CMB-C2B-C3B	2.16	128.73	124.68
36	d	407	DGD	C1E-O6E-C5E	2.16	117.93	113.69
24	b	606	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
24	b	616	CLA	OBD-CAD-C3D	-2.16	123.32	128.52
26	Y	101	BCR	C21-C20-C19	-2.16	116.48	123.22
24	B	604	CLA	CAA-CBA-CGA	2.16	119.56	113.25
24	c	504	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
37	L	101	LHG	O7-C7-O9	-2.16	118.48	123.70
24	b	607	CLA	CMA-C3A-C2A	-2.16	105.12	113.83
37	d	408	LHG	C5-O7-C7	-2.16	112.48	117.79
24	C	514	CLA	CHB-C4A-NA	2.16	127.49	124.51
24	c	510	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
26	c	516	BCR	C28-C27-C26	-2.15	110.23	114.08
24	b	621	CLA	CED-O2D-CGD	2.15	120.81	115.94
24	b	618	CLA	CED-O2D-CGD	2.15	120.80	115.94
32	D	406	PL9	C20-C19-C21	2.15	118.89	115.27
24	B	607	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
24	c	515	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
27	l	101	SQD	O47-C7-O49	-2.15	118.51	123.70
24	B	613	CLA	C11-C10-C8	-2.15	108.97	115.92
24	C	513	CLA	CBA-CAA-C2A	-2.15	107.52	113.86
26	c	526	BCR	C16-C17-C18	-2.15	124.24	127.31
26	a	410	BCR	C40-C30-C25	-2.15	106.82	110.30
37	d	409	LHG	O7-C7-O9	-2.15	118.51	123.70
24	B	602	CLA	C2A-C1A-CHA	-2.15	120.11	123.86
24	C	514	CLA	CBC-CAC-C3C	-2.15	106.52	112.43
24	B	610	CLA	CGD-CBD-CAD	-2.15	103.78	110.73
38	E	103	HEM	O2D-CGD-CBD	2.14	120.92	114.03
24	B	615	CLA	CED-O2D-CGD	2.14	120.79	115.94
38	e	102	HEM	C4B-C3B-C2B	-2.14	105.41	107.11
30	D	402	LMT	O5'-C5'-C4'	2.14	114.26	109.75
24	C	508	CLA	C11-C12-C13	-2.14	109.01	115.92
35	b	604	HTG	O5-C1-C2	2.14	113.00	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	619	BCR	C2-C1-C6	2.14	113.77	110.48
24	b	609	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
36	C	518	DGD	O6D-C1D-O3G	-2.14	104.91	109.97
24	b	619	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	a	409	CLA	CED-O2D-CGD	2.14	120.77	115.94
26	c	516	BCR	C35-C13-C14	-2.14	119.93	122.92
26	c	516	BCR	C2-C1-C6	2.14	113.77	110.48
24	C	511	CLA	CMA-C3A-C4A	-2.13	106.03	111.77
32	D	406	PL9	C15-C14-C13	-2.13	118.20	123.68
34	C	520	LMG	O6-C5-C6	2.13	111.74	106.44
32	D	406	PL9	C10-C9-C11	2.13	118.86	115.27
24	b	610	CLA	CMB-C2B-C1B	2.13	131.74	128.46
24	B	604	CLA	C1-O2A-CGA	2.13	122.04	116.44
24	B	616	CLA	OBD-CAD-C3D	-2.13	123.39	128.52
24	D	401	CLA	CAA-CBA-CGA	2.13	119.48	113.25
26	y	101	BCR	C24-C23-C22	-2.13	123.02	126.23
24	A	405	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
26	c	516	BCR	C33-C5-C6	-2.13	122.14	124.53
26	h	101	BCR	C36-C18-C17	-2.13	119.94	122.92
24	B	617	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
26	K	101	BCR	C16-C17-C18	-2.12	124.28	127.31
24	C	509	CLA	C4-C3-C5	2.12	118.84	115.27
26	C	515	BCR	C15-C14-C13	-2.12	124.28	127.31
32	a	416	PL9	C51-C49-C50	2.12	119.29	114.60
24	B	612	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
36	C	517	DGD	O6D-C5D-C6D	2.12	110.94	106.67
24	b	610	CLA	CAC-C3C-C4C	2.12	127.56	124.81
35	C	523	HTG	O5-C1-C2	2.11	112.97	110.31
24	b	620	CLA	C1-C2-C3	-2.11	122.39	126.04
32	A	419	PL9	C40-C39-C41	2.11	118.83	115.27
34	C	521	LMG	O7-C10-O9	-2.11	118.60	123.70
24	B	611	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
24	B	616	CLA	O2A-CGA-CBA	2.11	118.53	111.91
24	b	621	CLA	C4-C3-C5	2.11	118.82	115.27
24	c	515	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
34	c	521	LMG	O8-C28-O10	-2.11	118.27	123.59
24	B	613	CLA	O2A-CGA-CBA	2.11	118.52	111.91
27	A	416	SQD	O9-S-C6	2.11	109.44	106.94
36	c	519	DGD	O1G-C1A-O1A	-2.11	118.28	123.59
24	c	506	CLA	C1-O2A-CGA	2.10	121.97	116.44
35	C	523	HTG	C1-C2-C3	-2.10	106.43	110.59
24	D	403	CLA	O2A-CGA-O1A	-2.10	118.28	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	508	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
24	d	401	CLA	CHD-C4C-NC	2.10	127.52	124.20
26	y	101	BCR	C1-C6-C7	2.10	121.73	115.78
35	D	411	HTG	O5-C1-C2	2.10	112.96	110.31
24	C	507	CLA	CGD-CBD-CAD	-2.10	103.93	110.73
30	m	102	LMT	C3'-C4'-C5'	-2.10	106.11	110.93
24	c	514	CLA	CMA-C3A-C4A	-2.10	106.12	111.77
24	b	611	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
35	B	624	HTG	C1-O5-C5	2.10	116.45	112.58
25	A	407	PHO	C4A-C3A-C2A	-2.10	100.84	102.84
34	J	101	LMG	C7-O1-C1	-2.10	109.64	113.74
24	a	406	CLA	CMB-C2B-C3B	2.10	128.60	124.68
24	B	609	CLA	C1-O2A-CGA	2.09	121.94	116.44
24	b	621	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
26	B	620	BCR	C2-C3-C4	-2.09	106.70	111.38
24	B	611	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
36	D	407	DGD	O2G-C1B-O1B	-2.09	118.64	123.70
27	a	411	SQD	O48-C23-O10	-2.09	118.31	123.59
24	b	621	CLA	CHD-C4C-NC	2.09	127.50	124.20
24	B	614	CLA	CMA-C3A-C4A	-2.09	106.15	111.77
27	A	416	SQD	O8-S-C6	2.09	109.07	105.74
24	B	615	CLA	C1-C2-C3	-2.09	122.43	126.04
38	E	103	HEM	C3C-C4C-NC	-2.09	107.00	110.94
26	b	624	BCR	C10-C11-C12	-2.09	116.70	123.22
24	a	409	CLA	CMA-C3A-C2A	-2.09	105.40	113.83
26	D	405	BCR	C29-C30-C25	2.09	113.70	110.48
25	d	403	PHO	C4-C3-C2	-2.09	118.32	123.68
24	c	512	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
24	D	404	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
26	b	624	BCR	C15-C14-C13	-2.09	124.33	127.31
24	B	602	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
24	C	511	CLA	C6-C7-C8	-2.08	109.18	115.92
34	C	520	LMG	C30-C29-C28	-2.08	106.04	113.62
24	b	620	CLA	CHA-C1A-NA	-2.08	121.63	126.40
35	B	623	HTG	C1-O5-C5	2.08	116.42	112.58
34	C	521	LMG	O6-C5-C6	2.08	111.61	106.44
26	H	101	BCR	C24-C23-C22	-2.08	123.09	126.23
24	c	512	CLA	CHB-C4A-NA	2.08	127.39	124.51
34	b	625	LMG	O7-C10-O9	-2.08	118.67	123.70
26	K	101	BCR	C31-C1-C6	-2.08	106.93	110.30
24	c	510	CLA	C1-O2A-CGA	2.08	121.89	116.44
24	B	605	CLA	CHA-C1A-NA	-2.08	121.64	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	611	CLA	CHB-C4A-NA	2.08	127.38	124.51
24	A	405	CLA	CAA-CBA-CGA	-2.08	107.19	113.25
24	B	609	CLA	CHB-C4A-NA	2.08	127.38	124.51
24	b	613	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
32	D	406	PL9	C51-C49-C50	2.07	119.19	114.60
24	B	614	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
24	a	406	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
26	b	623	BCR	C3-C4-C5	-2.07	110.37	114.08
24	C	503	CLA	C16-C15-C13	-2.07	109.22	115.92
24	B	607	CLA	C6-C7-C8	-2.07	109.22	115.92
24	D	403	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
24	c	510	CLA	CHB-C4A-NA	2.07	127.38	124.51
24	b	609	CLA	CHA-C1A-NA	-2.07	121.65	126.40
24	b	610	CLA	C5-C3-C2	-2.07	116.93	121.12
24	C	504	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
24	C	508	CLA	CHA-C1A-NA	-2.07	121.66	126.40
37	l	102	LHG	C6-C5-C4	-2.06	106.90	111.79
24	B	606	CLA	CMB-C2B-C1B	2.06	131.64	128.46
24	B	602	CLA	CHB-C4A-NA	2.06	127.36	124.51
24	c	503	CLA	C1-C2-C3	-2.06	122.48	126.04
26	C	516	BCR	C40-C30-C25	-2.06	106.95	110.30
24	B	616	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
26	t	101	BCR	C35-C13-C12	2.06	121.32	118.08
24	B	604	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
34	C	501	LMG	O7-C10-O9	-2.06	118.72	123.70
34	b	625	LMG	O8-C28-O10	-2.06	118.39	123.59
24	C	505	CLA	C1-C2-C3	-2.06	122.48	126.04
24	B	603	CLA	CMA-C3A-C2A	-2.06	105.53	113.83
30	a	401	LMT	O5B-C5B-C4B	2.06	113.43	109.69
24	B	614	CLA	CMA-C3A-C2A	-2.06	105.53	113.83
26	y	101	BCR	C40-C30-C25	-2.06	106.96	110.30
24	c	508	CLA	CHB-C4A-NA	2.06	127.35	124.51
24	C	512	CLA	O2A-C1-C2	-2.05	103.23	108.64
24	C	513	CLA	CHB-C4A-NA	2.05	127.35	124.51
24	D	404	CLA	CGD-CBD-CAD	-2.05	104.08	110.73
24	b	608	CLA	C5-C3-C2	-2.05	116.96	121.12
24	B	609	CLA	CAC-C3C-C4C	2.05	127.47	124.81
26	B	620	BCR	C23-C24-C25	-2.05	121.44	127.20
32	D	406	PL9	C22-C23-C24	-2.05	122.73	127.66
24	C	510	CLA	C16-C15-C13	-2.05	109.31	115.92
24	C	510	CLA	C4-C3-C2	-2.05	118.43	123.68
24	C	507	CLA	C2A-C1A-CHA	-2.05	120.28	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	417	LMT	C1B-O1B-C4'	-2.05	112.90	117.96
26	d	405	BCR	C40-C30-C25	-2.05	106.98	110.30
24	c	509	CLA	CAA-C2A-C1A	2.04	118.68	111.97
36	h	102	DGD	C6D-C5D-C4D	2.04	116.36	112.09
24	B	604	CLA	C1B-CHB-C4A	-2.04	126.07	130.12
24	d	402	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
24	b	612	CLA	O2A-CGA-CBA	2.04	118.32	111.91
25	d	403	PHO	O2A-CGA-O1A	-2.04	118.43	123.59
24	B	606	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
24	d	401	CLA	CHC-C1C-NC	2.04	127.30	124.20
26	A	410	BCR	C8-C7-C6	-2.04	121.47	127.20
24	b	607	CLA	C1B-CHB-C4A	-2.04	126.07	130.12
24	B	617	CLA	C4-C3-C5	2.04	118.70	115.27
24	C	513	CLA	CMA-C3A-C4A	-2.04	106.29	111.77
24	A	405	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
35	b	627	HTG	O5-C1-C2	2.04	112.88	110.31
24	B	617	CLA	O2A-C1-C2	2.04	113.99	108.64
26	t	101	BCR	C7-C6-C5	-2.04	116.53	121.46
24	c	515	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
27	l	101	SQD	C45-O47-C7	-2.04	112.78	117.79
30	D	402	LMT	C3B-C4B-C5B	2.04	113.87	110.24
24	b	615	CLA	C4-C3-C5	2.04	118.70	115.27
25	d	403	PHO	C4A-C3A-C2A	-2.04	100.90	102.84
24	B	614	CLA	CHA-C1A-NA	-2.03	121.74	126.40
24	B	609	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	B	614	CLA	CHD-C4C-NC	2.03	127.41	124.20
26	d	405	BCR	C38-C26-C27	2.03	117.52	113.62
26	b	623	BCR	C11-C12-C13	-2.03	120.71	126.42
26	B	618	BCR	C21-C20-C19	-2.03	116.88	123.22
36	c	517	DGD	O2G-C1B-O1B	-2.03	118.80	123.70
24	B	606	CLA	CED-O2D-CGD	2.03	120.53	115.94
26	k	103	BCR	C20-C21-C22	-2.03	124.41	127.31
24	c	504	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	a	407	CLA	CAA-CBA-CGA	2.03	119.18	113.25
24	c	506	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
24	b	607	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
24	A	405	CLA	O2A-C1-C2	2.03	113.96	108.64
25	a	408	PHO	CED-O2D-CGD	2.03	120.52	115.94
24	B	614	CLA	C2A-C1A-CHA	-2.03	120.32	123.86
24	C	512	CLA	C11-C10-C8	-2.03	109.37	115.92
26	T	102	BCR	C36-C18-C19	2.03	121.27	118.08
24	b	616	CLA	CBC-CAC-C3C	-2.02	106.85	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	512	CLA	C1-O2A-CGA	2.02	121.75	116.44
24	D	401	CLA	OBD-CAD-C3D	-2.02	123.65	128.52
32	A	419	PL9	C25-C24-C23	-2.02	118.49	123.68
24	b	621	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
38	e	102	HEM	O2D-CGD-CBD	2.02	120.52	114.03
24	c	507	CLA	CHA-C1A-NA	-2.02	121.78	126.40
26	C	516	BCR	C15-C16-C17	-2.02	119.34	123.47
32	d	406	PL9	C12-C13-C14	-2.02	122.80	127.66
40	v	202	HEC	O2D-CGD-CBD	2.02	120.51	114.03
26	c	526	BCR	C21-C20-C19	-2.02	116.92	123.22
26	K	101	BCR	C38-C26-C25	-2.02	122.27	124.53
24	c	508	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
24	C	511	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
24	c	504	CLA	CMC-C2C-C1C	2.01	128.10	125.04
24	b	615	CLA	CHB-C4A-NA	2.01	127.29	124.51
26	A	410	BCR	C36-C18-C17	-2.01	120.11	122.92
36	d	407	DGD	O6D-C5D-C6D	2.01	110.72	106.67
36	C	519	DGD	O1G-C1A-C2A	2.01	118.22	111.91
38	E	103	HEM	O2D-CGD-O1D	-2.01	118.29	123.30
26	b	624	BCR	C21-C20-C19	-2.01	116.95	123.22
37	e	101	LHG	O8-C23-O10	-2.01	118.53	123.59
32	D	406	PL9	C31-C32-C33	-2.01	105.29	111.88
26	a	410	BCR	C20-C21-C22	-2.01	124.45	127.31
24	B	614	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	c	514	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
24	c	508	CLA	C2A-C1A-CHA	-2.00	120.35	123.86
24	b	617	CLA	CHB-C4A-NA	2.00	127.28	124.51
35	D	411	HTG	O5-C1-S1	-2.00	105.04	109.82
34	Z	101	LMG	C9-O8-C28	2.00	122.13	117.10
24	b	617	CLA	C4D-CHA-C1A	-2.00	118.81	121.25

All (59) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	608	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	B	617	CLA	ND
24	C	502	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	D	401	CLA	ND
24	D	403	CLA	ND
24	D	404	CLA	ND
24	a	406	CLA	ND
24	a	409	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	609	CLA	ND
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	b	618	CLA	ND
24	b	619	CLA	ND
24	b	620	CLA	ND
24	b	621	CLA	ND
24	c	503	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND

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Mol	Chain	Res	Type	Atom
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	c	514	CLA	ND
24	d	401	CLA	ND
24	d	402	CLA	ND
24	d	404	CLA	ND

All (1188) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2-C3-C5-C6
24	B	615	CLA	C4-C3-C5-C6
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	508	CLA	C2-C3-C5-C6
24	C	508	CLA	C4-C3-C5-C6
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	D	401	CLA	CHA-CBD-CGD-O1D
24	D	401	CLA	CHA-CBD-CGD-O2D
24	b	610	CLA	C2-C3-C5-C6
24	b	610	CLA	C4-C3-C5-C6
24	b	611	CLA	CHA-CBD-CGD-O1D
24	b	611	CLA	CHA-CBD-CGD-O2D
24	b	619	CLA	CHA-CBD-CGD-O1D
24	b	619	CLA	CHA-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O1D
24	b	619	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
26	B	618	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	D	405	BCR	C37-C22-C23-C24
26	D	405	BCR	C23-C24-C25-C30
26	Y	101	BCR	C21-C22-C23-C24
26	Y	101	BCR	C37-C22-C23-C24
26	d	405	BCR	C37-C22-C23-C24
26	d	405	BCR	C23-C24-C25-C30
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
27	A	411	SQD	C5-C6-S-O8
27	A	416	SQD	O6-C44-C45-O47
27	F	101	SQD	C8-C7-O47-C45
27	a	402	SQD	O6-C44-C45-O47
27	b	601	SQD	O5-C1-O6-C44
27	b	601	SQD	O49-C7-O47-C45
27	b	601	SQD	C5-C6-S-O7
27	b	601	SQD	C5-C6-S-O8
27	b	601	SQD	C5-C6-S-O9
27	f	101	SQD	O49-C7-O47-C45
27	f	101	SQD	C8-C7-O47-C45
27	f	101	SQD	C5-C6-S-O7
27	f	101	SQD	C5-C6-S-O8
27	f	101	SQD	C5-C6-S-O9
27	l	101	SQD	O49-C7-O47-C45
28	A	414	GOL	O1-C1-C2-C3
28	B	626	GOL	O1-C1-C2-C3
28	B	627	GOL	O1-C1-C2-C3
28	C	524	GOL	O1-C1-C2-C3
28	F	103	GOL	O1-C1-C2-C3
28	O	302	GOL	O1-C1-C2-C3
28	T	101	GOL	O1-C1-C2-C3
28	T	103	GOL	O1-C1-C2-C3
28	V	205	GOL	O1-C1-C2-C3
28	V	205	GOL	C1-C2-C3-O3
28	V	208	GOL	O1-C1-C2-C3
28	a	412	GOL	C1-C2-C3-O3
28	b	631	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
28	v	203	GOL	C1-C2-C3-O3
28	v	204	GOL	O1-C1-C2-C3
28	v	205	GOL	O1-C1-C2-C3
30	B	634	LMT	C2'-C1'-O1'-C1
30	B	634	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
30	E	102	LMT	C2'-C1'-O1'-C1
30	E	102	LMT	O5'-C1'-O1'-C1
30	I	102	LMT	C2'-C1'-O1'-C1
30	I	102	LMT	O5'-C1'-O1'-C1
30	M	101	LMT	O5'-C1'-O1'-C1
30	a	401	LMT	C2'-C1'-O1'-C1
30	a	401	LMT	O5'-C1'-O1'-C1
30	a	417	LMT	C2'-C1'-O1'-C1
30	b	602	LMT	C2'-C1'-O1'-C1
30	b	602	LMT	O5'-C1'-O1'-C1
30	b	626	LMT	C2'-C1'-O1'-C1
30	b	626	LMT	O5'-C1'-O1'-C1
30	f	102	LMT	C2'-C1'-O1'-C1
30	f	102	LMT	O5'-C1'-O1'-C1
32	a	416	PL9	C18-C19-C21-C22
32	a	416	PL9	C20-C19-C21-C22
32	a	416	PL9	C28-C29-C31-C32
32	a	416	PL9	C30-C29-C31-C32
34	C	501	LMG	O9-C10-O7-C8
34	C	501	LMG	C11-C10-O7-C8
34	Z	101	LMG	C2-C1-O1-C7
34	Z	101	LMG	O6-C1-O1-C7
34	Z	101	LMG	O9-C10-O7-C8
34	z	101	LMG	O9-C10-O7-C8
35	B	623	HTG	C2'-C1'-S1-C1
35	C	522	HTG	C2'-C1'-S1-C1
35	V	204	HTG	C2-C1-S1-C1'
35	V	204	HTG	O5-C1-S1-C1'
36	D	407	DGD	O1B-C1B-O2G-C2G
36	D	407	DGD	C2D-C1D-O3G-C3G
36	D	407	DGD	O6D-C1D-O3G-C3G
36	D	407	DGD	C2E-C1E-O5D-C6D
36	D	407	DGD	O6E-C1E-O5D-C6D
36	d	407	DGD	O1B-C1B-O2G-C2G
36	d	407	DGD	C2E-C1E-O5D-C6D
36	d	407	DGD	O6E-C1E-O5D-C6D
37	D	409	LHG	C3-O3-P-O6
37	D	409	LHG	C4-O6-P-O4
37	E	101	LHG	C4-O6-P-O3
37	E	101	LHG	C4-O6-P-O5
37	E	101	LHG	O10-C23-O8-C6
37	E	101	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
37	L	101	LHG	C4-O6-P-O4
37	d	409	LHG	O2-C2-C3-O3
37	d	409	LHG	C3-O3-P-O4
37	d	409	LHG	C4-O6-P-O4
37	e	101	LHG	C4-O6-P-O5
37	e	101	LHG	O7-C5-C6-O8
37	l	102	LHG	C4-O6-P-O3
37	l	102	LHG	C4-O6-P-O4
37	l	102	LHG	C4-O6-P-O5
37	e	101	LHG	O10-C23-O8-C6
27	F	101	SQD	O49-C7-O47-C45
27	F	101	SQD	C24-C23-O48-C46
27	b	601	SQD	C8-C7-O47-C45
27	l	101	SQD	C8-C7-O47-C45
34	Z	101	LMG	C11-C10-O7-C8
34	z	101	LMG	C11-C10-O7-C8
36	D	407	DGD	C2B-C1B-O2G-C2G
36	d	407	DGD	C2B-C1B-O2G-C2G
32	a	416	PL9	C25-C24-C26-C27
37	e	101	LHG	C24-C23-O8-C6
30	M	101	LMT	O5'-C5'-C6'-O6'
34	Z	101	LMG	C4-C5-C6-O5
30	I	102	LMT	O5B-C5B-C6B-O6B
24	b	619	CLA	C3-C5-C6-C7
24	b	621	CLA	C3-C5-C6-C7
27	F	101	SQD	O10-C23-O48-C46
34	Z	101	LMG	O6-C5-C6-O5
30	M	101	LMT	C4'-C5'-C6'-O6'
27	b	601	SQD	C31-C32-C33-C34
30	I	102	LMT	C3'-C4'-O1B-C1B
34	C	521	LMG	O6-C5-C6-O5
35	C	522	HTG	S1-C1'-C2'-C3'
37	d	410	LHG	C30-C31-C32-C33
30	D	402	LMT	O5B-C5B-C6B-O6B
24	B	617	CLA	C4-C3-C5-C6
24	b	619	CLA	C4-C3-C5-C6
32	A	419	PL9	C25-C24-C26-C27
32	a	416	PL9	C15-C14-C16-C17
24	B	617	CLA	C2-C3-C5-C6
24	b	619	CLA	C2-C3-C5-C6
32	A	419	PL9	C23-C24-C26-C27
32	a	416	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
32	a	416	PL9	C23-C24-C26-C27
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	611	CLA	C2A-CAA-CBA-CGA
30	a	417	LMT	O5'-C1'-O1'-C1
36	c	518	DGD	C3B-C4B-C5B-C6B
35	C	523	HTG	O5-C5-C6-O6
37	d	409	LHG	C1-C2-C3-O3
24	C	507	CLA	C3-C5-C6-C7
24	c	508	CLA	C15-C16-C17-C18
24	b	608	CLA	CBD-CGD-O2D-CED
36	d	407	DGD	C2D-C1D-O3G-C3G
36	d	407	DGD	C2A-C1A-O1G-C1G
24	B	603	CLA	C14-C13-C15-C16
24	d	401	CLA	CBD-CGD-O2D-CED
26	B	620	BCR	C7-C8-C9-C34
26	d	405	BCR	C7-C8-C9-C34
26	D	405	BCR	C21-C22-C23-C24
26	d	405	BCR	C21-C22-C23-C24
30	D	402	LMT	C4B-C5B-C6B-O6B
24	C	510	CLA	C8-C10-C11-C12
24	c	514	CLA	C10-C11-C12-C13
24	B	603	CLA	C15-C16-C17-C18
24	b	609	CLA	C15-C16-C17-C18
24	b	621	CLA	C10-C11-C12-C13
35	b	628	HTG	C1'-C2'-C3'-C4'
24	B	615	CLA	C10-C11-C12-C13
24	b	620	CLA	C10-C11-C12-C13
28	V	206	GOL	O1-C1-C2-O2
28	b	629	GOL	O2-C2-C3-O3
28	b	631	GOL	O1-C1-C2-O2
28	b	633	GOL	O1-C1-C2-O2
27	F	101	SQD	C23-C24-C25-C26
27	l	101	SQD	C7-C8-C9-C10
34	C	521	LMG	C28-C29-C30-C31
24	C	510	CLA	C2-C1-O2A-CGA
24	b	606	CLA	C2-C1-O2A-CGA
24	B	612	CLA	C15-C16-C17-C18
24	b	606	CLA	C10-C11-C12-C13
24	b	618	CLA	C8-C10-C11-C12
36	C	518	DGD	C1B-C2B-C3B-C4B
24	B	614	CLA	C11-C10-C8-C7
24	B	605	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	b	606	CLA	C8-C10-C11-C12
27	f	101	SQD	C31-C32-C33-C34
36	d	407	DGD	O6D-C1D-O3G-C3G
24	A	409	CLA	C15-C16-C17-C18
24	B	614	CLA	C8-C10-C11-C12
32	D	406	PL9	C39-C41-C42-C43
32	a	416	PL9	C9-C11-C12-C13
32	a	416	PL9	C14-C16-C17-C18
30	E	102	LMT	O1'-C1-C2-C3
30	M	101	LMT	O1'-C1-C2-C3
36	D	407	DGD	C1A-C2A-C3A-C4A
36	C	519	DGD	C6B-C7B-C8B-C9B
24	B	602	CLA	C3-C5-C6-C7
24	B	617	CLA	C3-C5-C6-C7
24	b	608	CLA	C5-C6-C7-C8
37	d	408	LHG	C24-C23-O8-C6
36	d	407	DGD	O1A-C1A-O1G-C1G
24	c	512	CLA	C8-C10-C11-C12
24	B	614	CLA	C15-C16-C17-C18
24	B	616	CLA	C10-C11-C12-C13
24	c	511	CLA	C13-C15-C16-C17
37	L	101	LHG	C4-O6-P-O3
37	d	409	LHG	C3-O3-P-O6
37	e	101	LHG	C3-O3-P-O6
35	B	623	HTG	C1'-C2'-C3'-C4'
24	A	409	CLA	C8-C10-C11-C12
24	B	614	CLA	C13-C15-C16-C17
24	b	619	CLA	C15-C16-C17-C18
30	a	401	LMT	C4B-C5B-C6B-O6B
37	D	410	LHG	C30-C31-C32-C33
24	a	406	CLA	C2C-C3C-CAC-CBC
24	b	611	CLA	C3-C5-C6-C7
30	D	402	LMT	C5'-C4'-O1B-C1B
30	I	102	LMT	C4B-C5B-C6B-O6B
34	J	101	LMG	C35-C36-C37-C38
37	E	101	LHG	C8-C7-O7-C5
27	a	402	SQD	C16-C17-C18-C19
35	B	623	HTG	C2'-C3'-C4'-C5'
36	C	517	DGD	CBA-CCA-CDA-CEA
36	C	517	DGD	C4B-C5B-C6B-C7B
36	C	517	DGD	C5B-C6B-C7B-C8B
36	D	407	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
36	c	517	DGD	C5A-C6A-C7A-C8A
37	d	410	LHG	C9-C10-C11-C12
37	d	410	LHG	C13-C14-C15-C16
24	b	620	CLA	C16-C17-C18-C20
36	h	102	DGD	C6A-C7A-C8A-C9A
37	d	410	LHG	C29-C30-C31-C32
37	E	101	LHG	O9-C7-O7-C5
27	f	101	SQD	C7-C8-C9-C10
34	B	621	LMG	C36-C37-C38-C39
34	C	521	LMG	C17-C18-C19-C20
34	b	625	LMG	C16-C17-C18-C19
30	E	102	LMT	C4-C5-C6-C7
34	C	520	LMG	C38-C39-C40-C41
36	H	102	DGD	C7A-C8A-C9A-CAA
27	F	101	SQD	C28-C29-C30-C31
37	D	408	LHG	C30-C31-C32-C33
27	a	411	SQD	C7-C8-C9-C10
34	C	501	LMG	C2-C1-O1-C7
36	c	518	DGD	C2E-C1E-O5D-C6D
27	b	601	SQD	C17-C18-C19-C20
27	f	101	SQD	C25-C26-C27-C28
36	d	407	DGD	C4B-C5B-C6B-C7B
37	d	408	LHG	O10-C23-O8-C6
24	C	502	CLA	C16-C17-C18-C19
32	d	406	PL9	C15-C14-C16-C17
27	b	601	SQD	C11-C10-C9-C8
36	D	407	DGD	C4A-C5A-C6A-C7A
36	d	407	DGD	C8B-C9B-CAB-CBB
37	l	102	LHG	C14-C15-C16-C17
32	d	406	PL9	C13-C14-C16-C17
24	A	406	CLA	C6-C7-C8-C9
24	C	511	CLA	C6-C7-C8-C9
24	c	508	CLA	C14-C13-C15-C16
36	C	517	DGD	O6D-C5D-C6D-O5D
34	C	520	LMG	C10-C11-C12-C13
27	l	101	SQD	C28-C29-C30-C31
30	B	634	LMT	C2-C3-C4-C5
30	b	602	LMT	C3-C4-C5-C6
34	C	521	LMG	C16-C17-C18-C19
36	C	518	DGD	C4B-C5B-C6B-C7B
36	c	518	DGD	C5A-C6A-C7A-C8A
36	c	518	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
37	d	410	LHG	C10-C11-C12-C13
28	A	413	GOL	C1-C2-C3-O3
28	B	625	GOL	C1-C2-C3-O3
28	B	628	GOL	O1-C1-C2-C3
28	B	635	GOL	O1-C1-C2-C3
28	V	206	GOL	O1-C1-C2-C3
28	a	413	GOL	C1-C2-C3-O3
28	b	629	GOL	C1-C2-C3-O3
28	b	632	GOL	C1-C2-C3-O3
28	b	633	GOL	O1-C1-C2-C3
28	c	527	GOL	O1-C1-C2-C3
28	f	104	GOL	C1-C2-C3-O3
24	c	514	CLA	C3-C5-C6-C7
24	b	611	CLA	C13-C15-C16-C17
36	C	519	DGD	CBA-CCA-CDA-CEA
27	a	402	SQD	C10-C11-C12-C13
30	B	634	LMT	C3-C4-C5-C6
30	D	402	LMT	C3'-C4'-O1B-C1B
34	b	625	LMG	C30-C31-C32-C33
34	c	501	LMG	C12-C13-C14-C15
36	C	518	DGD	C5A-C6A-C7A-C8A
36	h	102	DGD	C7A-C8A-C9A-CAA
37	D	410	LHG	C31-C32-C33-C34
30	m	103	LMT	O5B-C5B-C6B-O6B
24	b	620	CLA	C16-C17-C18-C19
34	C	501	LMG	O6-C1-O1-C7
32	d	406	PL9	C39-C41-C42-C43
27	a	402	SQD	C17-C18-C19-C20
27	a	402	SQD	C25-C26-C27-C28
27	a	402	SQD	C34-C35-C36-C37
27	l	101	SQD	C29-C30-C31-C32
34	Z	101	LMG	C19-C20-C21-C22
37	E	101	LHG	C9-C10-C11-C12
30	I	102	LMT	C5-C6-C7-C8
34	c	501	LMG	C16-C17-C18-C19
36	h	102	DGD	C5B-C6B-C7B-C8B
27	l	101	SQD	C31-C32-C33-C34
37	d	410	LHG	C15-C16-C17-C18
24	B	617	CLA	C8-C10-C11-C12
30	M	101	LMT	C2-C1-O1'-C1'
34	C	521	LMG	C15-C16-C17-C18
34	J	101	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
36	H	102	DGD	CCA-CDA-CEA-CFA
36	c	517	DGD	O6D-C5D-C6D-O5D
30	m	103	LMT	C11-C10-C9-C8
36	H	102	DGD	CBA-CCA-CDA-CEA
24	b	606	CLA	CBA-CGA-O2A-C1
24	c	512	CLA	C2-C3-C5-C6
28	A	414	GOL	O1-C1-C2-O2
28	B	625	GOL	O2-C2-C3-O3
28	B	626	GOL	O1-C1-C2-O2
28	B	627	GOL	O1-C1-C2-O2
28	B	635	GOL	O1-C1-C2-O2
28	F	103	GOL	O1-C1-C2-O2
28	T	103	GOL	O1-C1-C2-O2
28	V	205	GOL	O1-C1-C2-O2
28	V	208	GOL	O1-C1-C2-O2
28	a	412	GOL	O2-C2-C3-O3
28	v	205	GOL	O1-C1-C2-O2
24	C	508	CLA	C5-C6-C7-C8
37	l	102	LHG	C31-C32-C33-C34
24	d	401	CLA	C2C-C3C-CAC-CBC
34	b	625	LMG	C17-C18-C19-C20
34	z	101	LMG	C12-C13-C14-C15
36	C	518	DGD	CAB-CBB-CCB-CDB
24	B	617	CLA	C2-C1-O2A-CGA
36	d	407	DGD	C4A-C5A-C6A-C7A
36	d	407	DGD	CCB-CDB-CEB-CFB
30	I	102	LMT	C6-C7-C8-C9
37	L	101	LHG	C34-C35-C36-C37
26	B	618	BCR	C5-C6-C7-C8
26	B	620	BCR	C5-C6-C7-C8
26	D	405	BCR	C23-C24-C25-C26
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	b	622	BCR	C1-C6-C7-C8
26	b	622	BCR	C5-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C26
34	c	501	LMG	C30-C31-C32-C33
24	B	602	CLA	C10-C11-C12-C13
34	b	625	LMG	C11-C10-O7-C8
27	l	101	SQD	C26-C27-C28-C29
37	d	410	LHG	C12-C13-C14-C15
36	C	518	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
30	A	417	LMT	O1'-C1-C2-C3
34	z	101	LMG	C16-C17-C18-C19
36	c	519	DGD	C2B-C3B-C4B-C5B
24	b	619	CLA	C13-C15-C16-C17
27	f	101	SQD	C34-C35-C36-C37
36	c	517	DGD	C6A-C7A-C8A-C9A
24	B	606	CLA	C4-C3-C5-C6
24	c	512	CLA	C4-C3-C5-C6
24	B	610	CLA	C2-C3-C5-C6
24	C	506	CLA	C11-C12-C13-C15
24	C	513	CLA	C11-C10-C8-C7
24	D	404	CLA	C11-C10-C8-C7
24	b	619	CLA	C12-C13-C15-C16
24	c	508	CLA	C12-C13-C15-C16
24	b	606	CLA	O1A-CGA-O2A-C1
36	C	517	DGD	C7A-C8A-C9A-CAA
37	e	101	LHG	C7-C8-C9-C10
24	c	514	CLA	CBA-CGA-O2A-C1
37	L	101	LHG	C12-C13-C14-C15
27	a	402	SQD	C31-C32-C33-C34
30	a	401	LMT	C2-C3-C4-C5
34	j	101	LMG	C36-C37-C38-C39
27	A	416	SQD	C28-C29-C30-C31
37	d	410	LHG	C28-C29-C30-C31
27	l	101	SQD	C23-C24-C25-C26
34	C	501	LMG	C10-C11-C12-C13
34	C	520	LMG	C28-C29-C30-C31
35	B	630	HTG	C2'-C3'-C4'-C5'
35	O	303	HTG	C2'-C3'-C4'-C5'
36	C	517	DGD	C3B-C4B-C5B-C6B
34	C	501	LMG	C36-C37-C38-C39
34	b	625	LMG	C14-C15-C16-C17
24	c	513	CLA	CBA-CGA-O2A-C1
24	c	504	CLA	C16-C17-C18-C20
36	c	518	DGD	O6E-C1E-O5D-C6D
30	I	102	LMT	C3-C4-C5-C6
34	b	625	LMG	C18-C19-C20-C21
34	c	501	LMG	C13-C14-C15-C16
34	C	520	LMG	C11-C10-O7-C8
34	c	501	LMG	C11-C10-O7-C8
37	l	102	LHG	C30-C31-C32-C33
24	d	401	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
34	j	101	LMG	C14-C15-C16-C17
34	C	520	LMG	O9-C10-O7-C8
37	D	408	LHG	C23-C24-C25-C26
34	C	501	LMG	C14-C15-C16-C17
34	C	501	LMG	C13-C14-C15-C16
37	D	408	LHG	C29-C30-C31-C32
37	e	101	LHG	C14-C15-C16-C17
24	C	502	CLA	C16-C17-C18-C20
27	A	411	SQD	C10-C11-C12-C13
36	C	518	DGD	CAA-CBA-CCA-CDA
36	c	517	DGD	C2A-C3A-C4A-C5A
36	c	517	DGD	O6E-C5E-C6E-O5E
24	D	404	CLA	C4-C3-C5-C6
24	B	606	CLA	C2-C3-C5-C6
25	A	407	PHO	C2-C3-C5-C6
32	A	419	PL9	C4-C3-C7-C8
32	a	416	PL9	C4-C3-C7-C8
36	c	519	DGD	CBA-CCA-CDA-CEA
37	d	410	LHG	C31-C32-C33-C34
37	e	101	LHG	C13-C14-C15-C16
24	B	614	CLA	C11-C10-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	C	513	CLA	C11-C10-C8-C9
30	D	402	LMT	C6-C7-C8-C9
37	D	410	LHG	C32-C33-C34-C35
34	J	101	LMG	O6-C5-C6-O5
35	d	411	HTG	C4-C5-C6-O6
30	a	401	LMT	C7-C8-C9-C10
37	D	410	LHG	C10-C11-C12-C13
24	c	513	CLA	O1A-CGA-O2A-C1
24	c	514	CLA	O1A-CGA-O2A-C1
24	C	512	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
34	b	625	LMG	O9-C10-O7-C8
27	A	416	SQD	C18-C19-C20-C21
30	a	401	LMT	C5-C6-C7-C8
36	D	407	DGD	C9B-CAB-CBB-CCB
24	b	618	CLA	C10-C11-C12-C13
24	a	409	CLA	C13-C15-C16-C17
24	c	511	CLA	C8-C10-C11-C12
37	l	102	LHG	O6-C4-C5-C6
35	b	627	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
36	h	102	DGD	C2B-C3B-C4B-C5B
24	B	602	CLA	CBA-CGA-O2A-C1
34	c	501	LMG	O9-C10-O7-C8
24	d	404	CLA	C4-C3-C5-C6
27	b	601	SQD	C28-C29-C30-C31
36	C	518	DGD	C9A-CAA-CBA-CCA
34	C	501	LMG	C28-C29-C30-C31
37	D	410	LHG	C28-C29-C30-C31
36	C	517	DGD	O6E-C5E-C6E-O5E
24	b	606	CLA	C3-C5-C6-C7
27	A	416	SQD	O6-C44-C45-C46
27	b	601	SQD	C44-C45-C46-O48
27	f	101	SQD	C44-C45-C46-O48
34	C	501	LMG	O1-C7-C8-C9
36	c	518	DGD	C4B-C5B-C6B-C7B
36	d	407	DGD	O1G-C1G-C2G-C3G
37	L	101	LHG	C13-C14-C15-C16
37	d	408	LHG	C29-C30-C31-C32
37	e	101	LHG	C4-C5-C6-O8
37	l	102	LHG	C25-C26-C27-C28
30	a	401	LMT	O5B-C5B-C6B-O6B
34	j	101	LMG	O6-C5-C6-O5
24	c	505	CLA	C8-C10-C11-C12
37	l	102	LHG	C13-C14-C15-C16
36	C	518	DGD	C2G-C3G-O3G-C1D
36	C	518	DGD	C5D-C6D-O5D-C1E
36	c	518	DGD	C2G-C3G-O3G-C1D
36	c	518	DGD	C5D-C6D-O5D-C1E
34	C	520	LMG	C39-C40-C41-C42
30	M	102	LMT	O5'-C5'-C6'-O6'
36	c	517	DGD	C4D-C5D-C6D-O5D
34	C	521	LMG	C18-C19-C20-C21
27	a	411	SQD	C10-C11-C12-C13
28	C	524	GOL	O1-C1-C2-O2
28	T	101	GOL	O1-C1-C2-O2
28	a	413	GOL	O2-C2-C3-O3
28	v	203	GOL	O1-C1-C2-O2
28	v	204	GOL	O1-C1-C2-O2
35	V	204	HTG	C2'-C3'-C4'-C5'
24	d	401	CLA	O1D-CGD-O2D-CED
24	a	409	CLA	C10-C11-C12-C13
24	B	610	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C4-C3-C5-C6
24	C	511	CLA	C4-C3-C5-C6
25	A	407	PHO	C4-C3-C5-C6
27	A	411	SQD	C15-C16-C17-C18
34	j	101	LMG	C38-C39-C40-C41
36	C	518	DGD	C3B-C4B-C5B-C6B
30	E	102	LMT	C4'-C5'-C6'-O6'
27	F	101	SQD	C46-C45-O47-C7
35	b	628	HTG	O5-C5-C6-O6
24	b	613	CLA	C13-C15-C16-C17
35	B	623	HTG	C4'-C5'-C6'-C7'
24	B	615	CLA	C3-C5-C6-C7
27	a	411	SQD	C15-C16-C17-C18
37	d	410	LHG	C35-C36-C37-C38
34	c	521	LMG	C40-C41-C42-C43
24	c	504	CLA	C16-C17-C18-C19
36	C	518	DGD	C8B-C9B-CAB-CBB
36	c	519	DGD	C4A-C5A-C6A-C7A
24	B	602	CLA	O1A-CGA-O2A-C1
30	I	102	LMT	C4-C5-C6-C7
37	E	101	LHG	C10-C11-C12-C13
37	d	409	LHG	C32-C33-C34-C35
36	C	517	DGD	C4D-C5D-C6D-O5D
27	a	402	SQD	C7-C8-C9-C10
24	b	609	CLA	C10-C11-C12-C13
36	C	518	DGD	C2E-C1E-O5D-C6D
30	a	401	LMT	C6-C7-C8-C9
36	H	102	DGD	O2G-C1B-C2B-C3B
36	c	518	DGD	CCA-CDA-CEA-CFA
36	c	517	DGD	C4B-C5B-C6B-C7B
24	A	409	CLA	C11-C10-C8-C7
24	B	616	CLA	C11-C10-C8-C7
24	B	616	CLA	C12-C13-C15-C16
24	C	511	CLA	C2-C3-C5-C6
24	b	618	CLA	C11-C12-C13-C15
24	b	619	CLA	C11-C12-C13-C15
24	c	508	CLA	C11-C10-C8-C7
36	d	407	DGD	CDB-CEB-CFB-CGB
37	L	101	LHG	C32-C33-C34-C35
24	B	602	CLA	C11-C10-C8-C9
24	B	615	CLA	C6-C7-C8-C9
24	B	615	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C14-C13-C15-C16
24	B	616	CLA	C14-C13-C15-C16
24	D	404	CLA	C11-C10-C8-C9
24	b	606	CLA	C6-C7-C8-C9
24	b	619	CLA	C11-C12-C13-C14
24	c	508	CLA	C11-C10-C8-C9
24	c	511	CLA	C14-C13-C15-C16
24	c	513	CLA	CBD-CGD-O2D-CED
27	l	101	SQD	C11-C10-C9-C8
34	J	101	LMG	C16-C17-C18-C19
36	C	517	DGD	CAA-CBA-CCA-CDA
37	D	409	LHG	C32-C33-C34-C35
24	b	621	CLA	CBA-CGA-O2A-C1
24	C	503	CLA	C16-C17-C18-C20
35	b	627	HTG	C2'-C3'-C4'-C5'
36	h	102	DGD	CDA-CEA-CFA-CGA
27	b	601	SQD	C9-C10-C11-C12
36	c	519	DGD	C3B-C4B-C5B-C6B
24	c	515	CLA	C10-C11-C12-C13
24	A	409	CLA	CBA-CGA-O2A-C1
27	l	101	SQD	C12-C13-C14-C15
37	e	101	LHG	O6-C4-C5-C6
37	e	101	LHG	C11-C12-C13-C14
32	A	419	PL9	C30-C29-C31-C32
24	B	616	CLA	C2-C3-C5-C6
36	c	517	DGD	CBB-CCB-CDB-CEB
27	a	411	SQD	C11-C12-C13-C14
34	c	501	LMG	C29-C30-C31-C32
24	a	406	CLA	C4C-C3C-CAC-CBC
27	a	402	SQD	C26-C27-C28-C29
24	C	513	CLA	CBA-CGA-O2A-C1
24	B	602	CLA	C3A-C2A-CAA-CBA
34	B	621	LMG	C32-C33-C34-C35
36	H	102	DGD	C5B-C6B-C7B-C8B
36	c	518	DGD	CAA-CBA-CCA-CDA
34	Z	101	LMG	C14-C15-C16-C17
34	j	101	LMG	C13-C14-C15-C16
37	E	101	LHG	C25-C26-C27-C28
24	b	616	CLA	C15-C16-C17-C18
27	l	101	SQD	C44-C45-C46-O48
34	Z	101	LMG	C7-C8-C9-O8
36	D	407	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
37	E	101	LHG	C4-C5-C6-O8
34	c	501	LMG	C19-C20-C21-C22
34	c	521	LMG	C38-C39-C40-C41
34	J	101	LMG	C17-C18-C19-C20
36	c	518	DGD	C8A-C9A-CAA-CBA
34	c	501	LMG	C34-C35-C36-C37
34	c	521	LMG	C30-C31-C32-C33
36	h	102	DGD	C9B-CAB-CBB-CCB
27	A	416	SQD	C23-C24-C25-C26
34	b	625	LMG	C28-C29-C30-C31
24	b	608	CLA	O1D-CGD-O2D-CED
28	A	413	GOL	O2-C2-C3-O3
28	B	628	GOL	O1-C1-C2-O2
28	O	302	GOL	O1-C1-C2-O2
28	V	205	GOL	O2-C2-C3-O3
28	v	203	GOL	O2-C2-C3-O3
37	L	101	LHG	C14-C15-C16-C17
37	l	102	LHG	O6-C4-C5-O7
30	b	626	LMT	C1-C2-C3-C4
30	b	626	LMT	C3'-C4'-O1B-C1B
24	A	409	CLA	O1A-CGA-O2A-C1
34	B	621	LMG	C28-C29-C30-C31
36	C	517	DGD	CDA-CEA-CFA-CGA
36	c	517	DGD	C4A-C5A-C6A-C7A
24	a	409	CLA	C8-C10-C11-C12
36	d	407	DGD	C9A-CAA-CBA-CCA
37	E	101	LHG	C17-C18-C19-C20
27	l	101	SQD	O47-C45-C46-O48
34	C	501	LMG	O1-C7-C8-O7
37	E	101	LHG	O7-C5-C6-O8
36	H	102	DGD	CBB-CCB-CDB-CEB
34	z	101	LMG	C11-C12-C13-C14
36	c	518	DGD	C4A-C5A-C6A-C7A
30	E	102	LMT	C5-C6-C7-C8
24	C	510	CLA	C10-C11-C12-C13
24	A	409	CLA	C14-C13-C15-C16
24	C	505	CLA	C14-C13-C15-C16
24	C	507	CLA	C6-C7-C8-C9
24	C	507	CLA	C11-C12-C13-C14
24	b	607	CLA	C14-C13-C15-C16
24	c	507	CLA	C11-C12-C13-C14
24	c	514	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
34	C	501	LMG	C11-C12-C13-C14
24	B	617	CLA	C5-C6-C7-C8
24	C	511	CLA	C8-C10-C11-C12
30	m	103	LMT	C1-C2-C3-C4
24	C	514	CLA	C16-C17-C18-C19
30	f	102	LMT	C4'-C5'-C6'-O6'
30	E	102	LMT	C2-C3-C4-C5
26	B	620	BCR	C7-C8-C9-C10
26	d	405	BCR	C7-C8-C9-C10
24	c	506	CLA	C15-C16-C17-C18
24	b	616	CLA	C13-C15-C16-C17
24	B	616	CLA	C8-C10-C11-C12
24	B	603	CLA	C12-C13-C15-C16
24	B	612	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C15
24	B	615	CLA	C12-C13-C15-C16
24	C	505	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C15
24	b	606	CLA	C6-C7-C8-C10
24	b	621	CLA	C11-C12-C13-C15
24	c	511	CLA	C12-C13-C15-C16
32	A	419	PL9	C28-C29-C31-C32
24	b	621	CLA	O1A-CGA-O2A-C1
36	D	407	DGD	C2A-C3A-C4A-C5A
27	f	101	SQD	C32-C33-C34-C35
27	A	411	SQD	C16-C17-C18-C19
30	B	634	LMT	C11-C10-C9-C8
34	B	621	LMG	C16-C17-C18-C19
24	d	401	CLA	C4C-C3C-CAC-CBC
24	b	612	CLA	C3-C5-C6-C7
30	I	102	LMT	C5'-C4'-O1B-C1B
24	c	511	CLA	C10-C11-C12-C13
27	a	402	SQD	C30-C31-C32-C33
30	E	102	LMT	C3-C4-C5-C6
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	511	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	b	618	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	c	503	CLA	CAD-CBD-CGD-O2D
24	c	514	CLA	CAD-CBD-CGD-O2D
24	c	515	CLA	CAD-CBD-CGD-O2D
24	d	404	CLA	CAD-CBD-CGD-O2D
34	c	501	LMG	C20-C21-C22-C23
24	B	602	CLA	C8-C10-C11-C12
24	C	507	CLA	C5-C6-C7-C8
36	H	102	DGD	CDB-CEB-CFB-CGB
24	c	505	CLA	CBD-CGD-O2D-CED
34	z	101	LMG	O6-C1-O1-C7
36	C	518	DGD	O6E-C1E-O5D-C6D
24	C	509	CLA	C13-C15-C16-C17
25	d	403	PHO	C2C-C3C-CAC-CBC
27	F	101	SQD	C44-C45-C46-O48
27	a	402	SQD	O6-C44-C45-C46
37	D	410	LHG	C2-C3-O3-P
37	d	410	LHG	C2-C3-O3-P
24	c	514	CLA	CBD-CGD-O2D-CED
37	D	410	LHG	C34-C35-C36-C37
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	512	CLA	O1A-CGA-O2A-C1
30	f	102	LMT	C9-C10-C11-C12
27	F	101	SQD	O47-C45-C46-O48
34	Z	101	LMG	O7-C8-C9-O8
24	c	511	CLA	C16-C17-C18-C19
28	a	413	GOL	O1-C1-C2-O2
28	c	527	GOL	O1-C1-C2-O2
28	f	104	GOL	O2-C2-C3-O3
34	j	101	LMG	C29-C30-C31-C32
24	b	621	CLA	C4-C3-C5-C6
24	b	621	CLA	C2-C3-C5-C6
27	b	601	SQD	C13-C14-C15-C16
27	A	416	SQD	C5-C6-S-O8
24	B	602	CLA	C2A-CAA-CBA-CGA
24	c	512	CLA	CBA-CGA-O2A-C1
34	j	101	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	l	101	SQD	C15-C16-C17-C18
36	D	407	DGD	CCA-CDA-CEA-CFA
24	C	507	CLA	C1A-C2A-CAA-CBA
37	D	409	LHG	C4-O6-P-O3
37	d	409	LHG	C4-O6-P-O3
37	l	102	LHG	C10-C11-C12-C13
34	b	625	LMG	C15-C16-C17-C18
24	D	404	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
36	C	518	DGD	C8A-C9A-CAA-CBA
32	a	416	PL9	C3-C7-C8-C9
37	D	409	LHG	C3-O3-P-O4
37	D	409	LHG	C4-O6-P-O5
37	L	101	LHG	C4-O6-P-O5
37	e	101	LHG	C3-O3-P-O5
27	A	416	SQD	C17-C18-C19-C20
36	H	102	DGD	CDA-CEA-CFA-CGA
34	C	520	LMG	C16-C17-C18-C19
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	b	606	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
27	A	411	SQD	C5-C6-S-O7
36	c	519	DGD	C1B-C2B-C3B-C4B
30	M	101	LMT	C2-C3-C4-C5
34	c	501	LMG	C22-C23-C24-C25
34	Z	101	LMG	C12-C13-C14-C15
24	c	513	CLA	O1D-CGD-O2D-CED
27	A	411	SQD	C17-C18-C19-C20
36	d	407	DGD	C5A-C6A-C7A-C8A
24	b	614	CLA	C4-C3-C5-C6
24	A	406	CLA	C12-C13-C15-C16
24	C	502	CLA	C12-C13-C15-C16
24	b	611	CLA	C12-C13-C15-C16
37	e	101	LHG	O6-C4-C5-O7
34	z	101	LMG	C18-C19-C20-C21
34	j	101	LMG	C28-C29-C30-C31
36	c	517	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
36	h	102	DGD	C9A-CAA-CBA-CCA
24	C	514	CLA	C16-C17-C18-C20
34	C	521	LMG	C4-C5-C6-O5
24	B	602	CLA	CAA-CBA-CGA-O2A
24	a	409	CLA	O1A-CGA-O2A-C1
27	b	601	SQD	O47-C45-C46-O48
36	d	407	DGD	O1G-C1G-C2G-O2G
34	C	521	LMG	C8-C7-O1-C1
27	A	416	SQD	C19-C20-C21-C22
24	d	404	CLA	C2-C3-C5-C6
37	D	410	LHG	C33-C34-C35-C36
24	B	612	CLA	C14-C13-C15-C16
24	b	621	CLA	C11-C12-C13-C14
27	l	101	SQD	C32-C33-C34-C35
35	b	627	HTG	C3'-C4'-C5'-C6'
30	A	417	LMT	O5'-C1'-O1'-C1
27	b	601	SQD	C18-C19-C20-C21
30	f	102	LMT	C4-C5-C6-C7
36	h	102	DGD	O2G-C1B-C2B-C3B
34	j	101	LMG	C20-C21-C22-C23
34	C	521	LMG	C30-C31-C32-C33
34	c	521	LMG	C29-C30-C31-C32
34	b	625	LMG	C19-C20-C21-C22
34	B	621	LMG	O8-C28-C29-C30
24	B	604	CLA	C5-C6-C7-C8
24	A	406	CLA	C13-C15-C16-C17
30	E	102	LMT	C1-C2-C3-C4
37	e	101	LHG	O8-C23-C24-C25
37	e	101	LHG	C26-C27-C28-C29
36	C	518	DGD	CBB-CCB-CDB-CEB
24	C	510	CLA	C3-C5-C6-C7
34	j	101	LMG	C40-C41-C42-C43
27	b	601	SQD	C46-C45-O47-C7
27	l	101	SQD	C46-C45-O47-C7
24	B	611	CLA	C2A-CAA-CBA-CGA
24	b	615	CLA	C2A-CAA-CBA-CGA
24	c	514	CLA	C15-C16-C17-C18
24	c	511	CLA	C2-C1-O2A-CGA
24	c	514	CLA	C2-C1-O2A-CGA
24	c	515	CLA	C2-C1-O2A-CGA
30	m	103	LMT	C9-C10-C11-C12
34	b	625	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
37	D	410	LHG	O10-C23-O8-C6
24	C	506	CLA	C16-C17-C18-C19
34	c	520	LMG	C28-C29-C30-C31
24	b	606	CLA	C4-C3-C5-C6
34	j	101	LMG	C30-C31-C32-C33
26	C	515	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	c	516	BCR	C23-C24-C25-C30
30	b	602	LMT	O1'-C1-C2-C3
27	b	601	SQD	C24-C25-C26-C27
36	c	519	DGD	C7B-C8B-C9B-CAB
34	b	625	LMG	C29-C28-O8-C9
34	C	521	LMG	C29-C30-C31-C32
30	D	402	LMT	O5'-C1'-O1'-C1
30	M	102	LMT	O5'-C1'-O1'-C1
36	C	517	DGD	O6E-C1E-O5D-C6D
34	J	101	LMG	C10-C11-C12-C13
24	c	508	CLA	C10-C11-C12-C13
27	f	101	SQD	O47-C45-C46-O48
24	B	602	CLA	C15-C16-C17-C18
37	e	101	LHG	C4-O6-P-O3
36	d	407	DGD	C5B-C6B-C7B-C8B
24	C	504	CLA	C5-C6-C7-C8
36	c	518	DGD	C9A-CAA-CBA-CCA
24	C	503	CLA	C16-C17-C18-C19
24	a	409	CLA	CBA-CGA-O2A-C1
24	a	409	CLA	C4-C3-C5-C6
34	C	520	LMG	C18-C19-C20-C21
35	c	522	HTG	C3'-C4'-C5'-C6'
24	C	507	CLA	C6-C7-C8-C10
24	C	511	CLA	C6-C7-C8-C10
24	b	607	CLA	C12-C13-C15-C16
36	c	519	DGD	C8B-C9B-CAB-CBB
37	E	101	LHG	C26-C27-C28-C29
24	A	409	CLA	C11-C10-C8-C9
24	B	616	CLA	C11-C10-C8-C9
24	b	611	CLA	C14-C13-C15-C16
26	h	101	BCR	C9-C10-C11-C12
37	d	408	LHG	C30-C31-C32-C33
27	F	101	SQD	C26-C27-C28-C29
37	D	408	LHG	C26-C27-C28-C29
37	l	102	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	c	519	DGD	O1A-C1A-O1G-C1G
34	C	521	LMG	O9-C10-O7-C8
24	D	401	CLA	C15-C16-C17-C18
32	a	416	PL9	C12-C11-C9-C10
37	e	101	LHG	C23-C24-C25-C26
30	m	102	LMT	O5'-C5'-C6'-O6'
34	C	520	LMG	C21-C22-C23-C24
27	l	101	SQD	C24-C23-O48-C46
36	c	519	DGD	C2A-C1A-O1G-C1G
37	D	410	LHG	C24-C23-O8-C6
32	A	419	PL9	C2-C3-C7-C8
37	D	410	LHG	C15-C16-C17-C18
24	b	606	CLA	CAA-CBA-CGA-O2A
24	c	505	CLA	O1D-CGD-O2D-CED
27	l	101	SQD	C9-C10-C11-C12
24	C	503	CLA	CBD-CGD-O2D-CED
34	B	621	LMG	C10-C11-C12-C13
27	l	101	SQD	C13-C14-C15-C16
27	A	416	SQD	O5-C1-O6-C44
24	B	615	CLA	C5-C6-C7-C8
34	z	101	LMG	C15-C16-C17-C18
37	L	101	LHG	O6-C4-C5-C6
34	C	521	LMG	C39-C40-C41-C42
38	E	103	HEM	CAD-CBD-CGD-O1D
36	D	407	DGD	C3A-C4A-C5A-C6A
24	b	615	CLA	C16-C17-C18-C19
34	C	501	LMG	O8-C28-C29-C30
34	C	501	LMG	C15-C16-C17-C18
36	C	519	DGD	CBB-CCB-CDB-CEB
36	c	519	DGD	C6A-C7A-C8A-C9A
38	e	102	HEM	CAA-CBA-CGA-O1A
24	C	508	CLA	CBD-CGD-O2D-CED
27	F	101	SQD	C30-C31-C32-C33
27	a	402	SQD	C18-C19-C20-C21
34	J	101	LMG	C20-C21-C22-C23
24	B	602	CLA	C2-C1-O2A-CGA
24	b	613	CLA	C2-C1-O2A-CGA
24	d	402	CLA	C2-C1-O2A-CGA
24	b	610	CLA	C10-C11-C12-C13
37	D	410	LHG	C24-C25-C26-C27
36	C	517	DGD	C2E-C1E-O5D-C6D
36	c	517	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
24	C	502	CLA	C2A-CAA-CBA-CGA
27	f	101	SQD	O6-C44-C45-O47
30	b	602	LMT	C7-C8-C9-C10
37	D	408	LHG	C32-C33-C34-C35
24	D	401	CLA	C2C-C3C-CAC-CBC
30	f	102	LMT	C2-C3-C4-C5
36	C	517	DGD	C5A-C6A-C7A-C8A
37	d	408	LHG	C32-C33-C34-C35
24	B	614	CLA	C11-C12-C13-C14
24	C	502	CLA	C11-C12-C13-C14
24	C	513	CLA	C14-C13-C15-C16
24	b	610	CLA	C11-C10-C8-C9
24	b	615	CLA	C11-C12-C13-C14
24	c	506	CLA	C11-C12-C13-C14
24	b	615	CLA	C16-C17-C18-C20
27	A	416	SQD	C34-C35-C36-C37
27	a	411	SQD	C12-C13-C14-C15
34	C	520	LMG	C11-C12-C13-C14
38	e	102	HEM	CAA-CBA-CGA-O2A
24	a	409	CLA	C15-C16-C17-C18
36	C	518	DGD	C7B-C8B-C9B-CAB
30	m	103	LMT	C4-C5-C6-C7
34	c	520	LMG	C7-C8-C9-O8
34	z	101	LMG	C7-C8-C9-O8
24	c	511	CLA	C16-C17-C18-C20
36	c	517	DGD	O6E-C1E-O5D-C6D
26	D	405	BCR	C7-C8-C9-C34
34	c	520	LMG	C4-C5-C6-O5
24	c	503	CLA	CBD-CGD-O2D-CED
36	H	102	DGD	C6B-C7B-C8B-C9B
40	V	203	HEC	CAD-CBD-CGD-O2D
34	C	501	LMG	C37-C38-C39-C40
37	D	409	LHG	C26-C27-C28-C29
24	A	406	CLA	C6-C7-C8-C10
24	D	403	CLA	C12-C13-C15-C16
24	c	507	CLA	C11-C12-C13-C15
34	b	625	LMG	C37-C38-C39-C40
24	D	404	CLA	C8-C10-C11-C12
34	c	501	LMG	C10-C11-C12-C13
38	E	103	HEM	CAD-CBD-CGD-O2D
36	C	518	DGD	C4A-C5A-C6A-C7A
26	H	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	A	416	SQD	C15-C16-C17-C18
36	C	519	DGD	C2A-C3A-C4A-C5A
30	m	102	LMT	C3-C4-C5-C6
34	Z	101	LMG	C11-C12-C13-C14
40	V	203	HEC	CAD-CBD-CGD-O1D
27	b	601	SQD	C27-C28-C29-C30
35	B	622	HTG	S1-C1'-C2'-C3'
24	A	409	CLA	C3-C5-C6-C7
24	C	508	CLA	C2A-CAA-CBA-CGA
28	f	104	GOL	O1-C1-C2-O2
30	b	602	LMT	C4-C5-C6-C7
24	c	514	CLA	O1D-CGD-O2D-CED
37	D	408	LHG	C11-C12-C13-C14
30	b	626	LMT	C6-C7-C8-C9
24	C	508	CLA	C16-C17-C18-C19
27	a	402	SQD	C28-C29-C30-C31
34	b	625	LMG	C20-C21-C22-C23
36	d	407	DGD	C1B-C2B-C3B-C4B
30	M	102	LMT	C5-C6-C7-C8
34	C	501	LMG	C16-C17-C18-C19
27	l	101	SQD	O10-C23-O48-C46
37	d	410	LHG	C33-C34-C35-C36
34	c	521	LMG	C28-C29-C30-C31
27	a	411	SQD	O6-C44-C45-O47
36	D	407	DGD	O2G-C2G-C3G-O3G
37	d	408	LHG	C23-C24-C25-C26
35	d	411	HTG	O5-C5-C6-O6
24	C	503	CLA	O1D-CGD-O2D-CED
36	c	518	DGD	C1A-C2A-C3A-C4A
37	E	101	LHG	C18-C19-C20-C21
27	a	402	SQD	C35-C36-C37-C38
32	a	416	PL9	C45-C44-C46-C47
24	b	618	CLA	C2-C1-O2A-CGA
24	b	619	CLA	C2-C1-O2A-CGA
24	a	409	CLA	C2-C3-C5-C6
24	b	620	CLA	C13-C15-C16-C17
27	A	416	SQD	C11-C12-C13-C14
34	b	625	LMG	C29-C30-C31-C32
32	a	416	PL9	C2-C3-C7-C8
27	a	402	SQD	O10-C23-O48-C46
35	B	631	HTG	S1-C1'-C2'-C3'
35	O	303	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
24	c	503	CLA	C2A-CAA-CBA-CGA
36	D	407	DGD	CAA-CBA-CCA-CDA
26	B	620	BCR	C1-C6-C7-C8
26	B	620	BCR	C23-C24-C25-C30
26	C	516	BCR	C1-C6-C7-C8
26	c	516	BCR	C1-C6-C7-C8
26	c	516	BCR	C5-C6-C7-C8
26	c	516	BCR	C23-C24-C25-C26
26	c	526	BCR	C1-C6-C7-C8
26	k	103	BCR	C1-C6-C7-C8
24	C	502	CLA	C15-C16-C17-C18
37	d	409	LHG	C11-C10-C9-C8
34	c	501	LMG	O8-C28-C29-C30
38	e	102	HEM	CAD-CBD-CGD-O1D
28	T	103	GOL	C1-C2-C3-O3
28	a	413	GOL	O1-C1-C2-C3
24	B	613	CLA	O1A-CGA-O2A-C1
24	B	614	CLA	C10-C11-C12-C13
24	b	606	CLA	C2-C3-C5-C6
34	C	520	LMG	C31-C32-C33-C34
30	M	101	LMT	C1-C2-C3-C4
24	B	609	CLA	C16-C17-C18-C19
24	A	409	CLA	C10-C11-C12-C13
24	b	615	CLA	C15-C16-C17-C18
24	b	617	CLA	C8-C10-C11-C12
30	b	626	LMT	C5-C6-C7-C8
37	l	102	LHG	C17-C18-C19-C20
40	v	202	HEC	CAD-CBD-CGD-O2D
34	c	520	LMG	C39-C40-C41-C42
36	C	518	DGD	C4E-C5E-C6E-O5E
30	m	103	LMT	C5-C6-C7-C8
24	C	505	CLA	C4-C3-C5-C6
24	A	409	CLA	C11-C12-C13-C15
24	A	409	CLA	C12-C13-C15-C16
24	B	602	CLA	C11-C10-C8-C7
24	C	513	CLA	C12-C13-C15-C16
27	a	402	SQD	C24-C23-O48-C46
27	b	601	SQD	C19-C20-C21-C22
37	e	101	LHG	C15-C16-C17-C18
28	A	412	GOL	O1-C1-C2-O2
28	b	632	GOL	O2-C2-C3-O3
27	A	416	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
30	D	402	LMT	C2'-C1'-O1'-C1
37	D	408	LHG	C17-C18-C19-C20
36	c	519	DGD	O1G-C1A-C2A-C3A
24	a	409	CLA	C16-C17-C18-C20
35	D	411	HTG	C2'-C1'-S1-C1
35	b	604	HTG	O5-C1-S1-C1'
34	C	521	LMG	C11-C12-C13-C14
24	c	515	CLA	C4-C3-C5-C6
37	E	101	LHG	C7-C8-C9-C10
24	A	406	CLA	C14-C13-C15-C16
24	C	502	CLA	C14-C13-C15-C16
24	C	513	CLA	C6-C7-C8-C9
24	b	617	CLA	C11-C10-C8-C9
24	C	511	CLA	O1A-CGA-O2A-C1
27	f	101	SQD	C24-C25-C26-C27
24	B	608	CLA	C3A-C2A-CAA-CBA
24	b	612	CLA	C3A-C2A-CAA-CBA
24	C	513	CLA	CAA-CBA-CGA-O2A
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	514	CLA	CAD-CBD-CGD-O2D
24	b	609	CLA	CAD-CBD-CGD-O2D
24	b	621	CLA	CAD-CBD-CGD-O2D
24	c	505	CLA	CAD-CBD-CGD-O2D
25	A	407	PHO	CAD-CBD-CGD-O2D
34	z	101	LMG	C17-C18-C19-C20
37	l	102	LHG	C12-C13-C14-C15
24	B	607	CLA	C10-C11-C12-C13
24	B	614	CLA	C2-C1-O2A-CGA
37	d	408	LHG	C11-C10-C9-C8
30	D	402	LMT	C4'-C5'-C6'-O6'
36	C	519	DGD	C8A-C9A-CAA-CBA
24	b	608	CLA	C4-C3-C5-C6
24	c	506	CLA	C4-C3-C5-C6
34	B	621	LMG	C17-C18-C19-C20
36	c	518	DGD	C7A-C8A-C9A-CAA
36	H	102	DGD	O1B-C1B-C2B-C3B
27	l	101	SQD	O5-C1-O6-C44
24	c	514	CLA	CAA-CBA-CGA-O2A
27	f	101	SQD	O47-C7-C8-C9
36	D	407	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
25	A	408	PHO	C2C-C3C-CAC-CBC
24	D	403	CLA	O2A-C1-C2-C3
25	a	408	PHO	O2A-C1-C2-C3
30	D	402	LMT	C7-C8-C9-C10
34	c	521	LMG	C31-C32-C33-C34
37	L	101	LHG	C27-C28-C29-C30
37	l	102	LHG	C27-C28-C29-C30
40	v	202	HEC	CAD-CBD-CGD-O1D
34	j	101	LMG	C19-C20-C21-C22
24	C	504	CLA	C10-C11-C12-C13
24	B	608	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	c	506	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O2D
24	c	512	CLA	CHA-CBD-CGD-O2D
24	d	401	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O2D
36	C	517	DGD	C2A-C3A-C4A-C5A
37	D	410	LHG	C29-C30-C31-C32
27	A	411	SQD	C32-C33-C34-C35
36	d	407	DGD	O2G-C2G-C3G-O3G
30	b	602	LMT	C6-C7-C8-C9
24	B	603	CLA	C8-C10-C11-C12
24	B	608	CLA	C3-C5-C6-C7
38	e	102	HEM	CAD-CBD-CGD-O2D
24	D	401	CLA	C4C-C3C-CAC-CBC
37	D	410	LHG	C25-C26-C27-C28
25	d	403	PHO	CHA-CBD-CGD-O2D
28	c	525	GOL	O2-C2-C3-O3
34	b	625	LMG	O8-C28-C29-C30
24	B	617	CLA	C11-C10-C8-C7
24	C	508	CLA	C11-C10-C8-C7
34	b	625	LMG	C36-C37-C38-C39
24	B	604	CLA	C6-C7-C8-C9
24	B	605	CLA	C6-C7-C8-C9
24	a	407	CLA	C6-C7-C8-C9
37	D	409	LHG	C14-C15-C16-C17
27	A	416	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	A	411	SQD	O47-C7-C8-C9
34	z	101	LMG	C13-C14-C15-C16
34	C	521	LMG	C11-C10-O7-C8
37	E	101	LHG	O7-C7-C8-C9
24	B	613	CLA	CBA-CGA-O2A-C1
27	b	601	SQD	C29-C30-C31-C32
28	A	412	GOL	O1-C1-C2-C3
32	a	416	PL9	C43-C44-C46-C47
24	c	514	CLA	CAA-CBA-CGA-O1A
34	c	501	LMG	C11-C12-C13-C14
24	C	511	CLA	CBA-CGA-O2A-C1
30	M	101	LMT	C9-C10-C11-C12
24	c	513	CLA	C1A-C2A-CAA-CBA
24	C	508	CLA	C16-C17-C18-C20
35	B	623	HTG	C4-C5-C6-O6
24	b	621	CLA	C2-C1-O2A-CGA
37	d	409	LHG	C31-C32-C33-C34
36	c	519	DGD	O1A-C1A-C2A-C3A
24	A	405	CLA	C2C-C3C-CAC-CBC
34	C	520	LMG	O7-C10-C11-C12
24	C	504	CLA	C15-C16-C17-C18
24	d	404	CLA	C3-C5-C6-C7
27	a	411	SQD	C32-C33-C34-C35
30	A	417	LMT	C2'-C1'-O1'-C1
30	M	102	LMT	C2'-C1'-O1'-C1
37	d	409	LHG	C4-O6-P-O5
30	f	102	LMT	C2B-C1B-O1B-C4'
37	E	101	LHG	O9-C7-C8-C9
26	C	516	BCR	C5-C6-C7-C8
25	a	408	PHO	C8-C10-C11-C12
24	C	513	CLA	CAA-CBA-CGA-O1A
24	B	603	CLA	C2A-CAA-CBA-CGA
27	A	411	SQD	O49-C7-C8-C9
27	f	101	SQD	O49-C7-C8-C9
27	A	416	SQD	C33-C34-C35-C36
32	A	419	PL9	C46-C47-C48-C49
24	B	608	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	a	407	CLA	CAD-CBD-CGD-O1D
24	b	612	CLA	CAD-CBD-CGD-O1D
24	c	508	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	A	411	SQD	C5-C6-S-O9
27	A	416	SQD	C5-C6-S-O7
27	A	416	SQD	C5-C6-S-O9
34	b	625	LMG	O10-C28-C29-C30
30	a	401	LMT	C3-C4-C5-C6
24	B	617	CLA	C11-C10-C8-C9
24	C	508	CLA	C11-C10-C8-C9
24	a	409	CLA	C11-C12-C13-C14
24	b	608	CLA	C6-C7-C8-C9
24	b	619	CLA	C14-C13-C15-C16
24	d	404	CLA	C14-C13-C15-C16
27	a	402	SQD	C15-C16-C17-C18
24	C	502	CLA	C13-C15-C16-C17
24	C	506	CLA	CAA-CBA-CGA-O2A
37	L	101	LHG	O7-C7-C8-C9
37	d	408	LHG	O8-C23-C24-C25
37	l	102	LHG	O7-C7-C8-C9
37	l	102	LHG	C29-C30-C31-C32
37	d	409	LHG	C14-C15-C16-C17
34	J	101	LMG	O7-C10-C11-C12
37	D	408	LHG	O8-C23-C24-C25
34	C	520	LMG	O9-C10-C11-C12
32	A	419	PL9	C45-C44-C46-C47
30	M	102	LMT	C4'-C5'-C6'-O6'
24	B	605	CLA	C6-C7-C8-C10
24	a	407	CLA	C6-C7-C8-C10
24	a	409	CLA	C11-C12-C13-C15
24	b	608	CLA	C2-C3-C5-C6
24	b	608	CLA	C6-C7-C8-C10
24	b	611	CLA	C11-C12-C13-C15
24	b	617	CLA	C11-C10-C8-C7
24	c	506	CLA	C2-C3-C5-C6
24	c	509	CLA	C11-C10-C8-C7
24	d	404	CLA	C12-C13-C15-C16
32	a	416	PL9	C12-C11-C9-C8
35	c	523	HTG	C2-C1-S1-C1'
37	l	102	LHG	O9-C7-C8-C9
27	F	101	SQD	C33-C34-C35-C36
27	a	411	SQD	C31-C32-C33-C34
36	h	102	DGD	C6B-C7B-C8B-C9B
37	D	409	LHG	C16-C17-C18-C19
24	b	618	CLA	CAA-CBA-CGA-O2A

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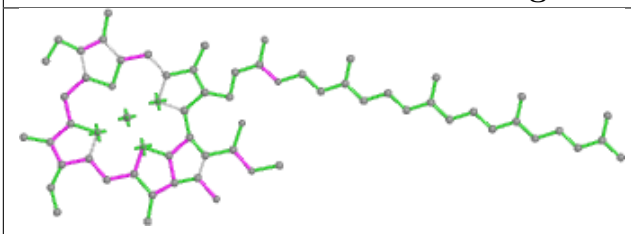
Mol	Chain	Res	Type	Atoms
24	c	507	CLA	CAA-CBA-CGA-O2A
34	z	101	LMG	O7-C10-C11-C12
36	C	518	DGD	O2G-C1B-C2B-C3B
37	E	101	LHG	O8-C23-C24-C25
26	C	516	BCR	C7-C8-C9-C10
26	D	405	BCR	C7-C8-C9-C10
37	L	101	LHG	O9-C7-C8-C9
34	J	101	LMG	C12-C13-C14-C15
36	H	102	DGD	C9A-CAA-CBA-CCA
30	m	102	LMT	C2-C1-O1'-C1'
24	B	614	CLA	CAA-CBA-CGA-O2A
24	c	512	CLA	CAA-CBA-CGA-O2A
27	a	411	SQD	O47-C7-C8-C9
37	d	410	LHG	O8-C23-C24-C25
27	A	411	SQD	C26-C27-C28-C29
24	C	506	CLA	CAA-CBA-CGA-O1A
37	d	408	LHG	O10-C23-C24-C25
25	d	403	PHO	C8-C10-C11-C12
34	z	101	LMG	O9-C10-C11-C12
37	D	408	LHG	O10-C23-C24-C25
37	E	101	LHG	C24-C25-C26-C27
24	B	611	CLA	C8-C10-C11-C12
24	a	406	CLA	C13-C15-C16-C17
37	E	101	LHG	O10-C23-C24-C25
34	c	520	LMG	O7-C10-C11-C12

There are no ring outliers.

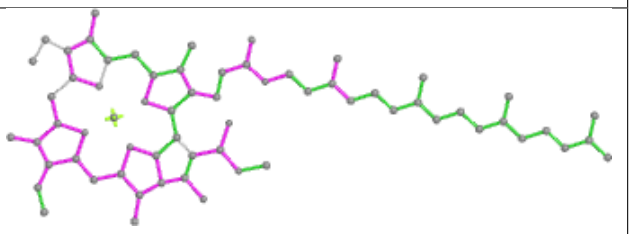
No monomer is involved in short contacts.

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.

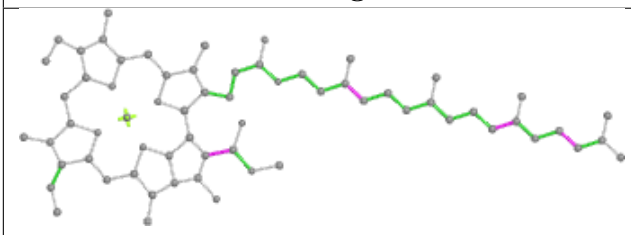
Ligand CLA c 506



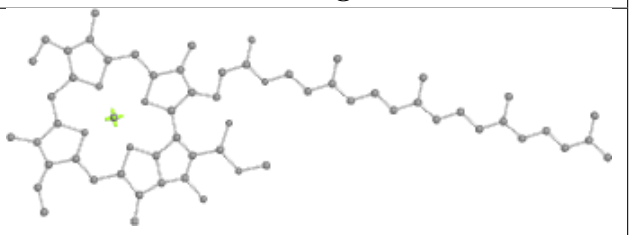
Bond lengths



Bond angles

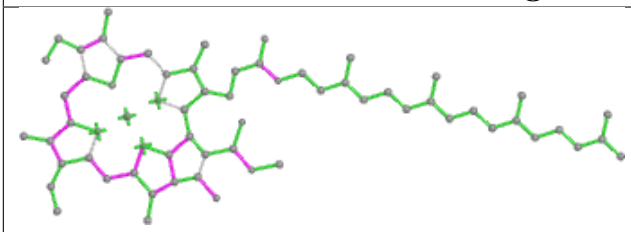


Torsions

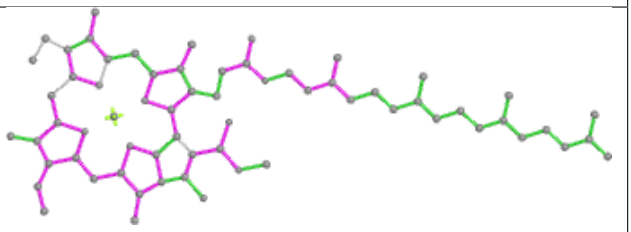


Rings

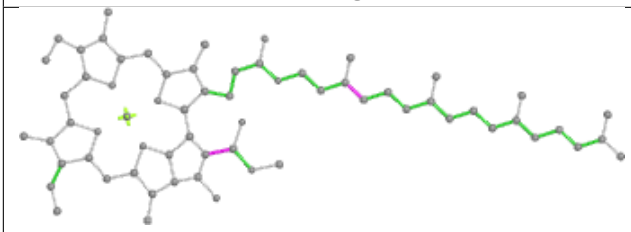
Ligand CLA B 610



Bond lengths



Bond angles



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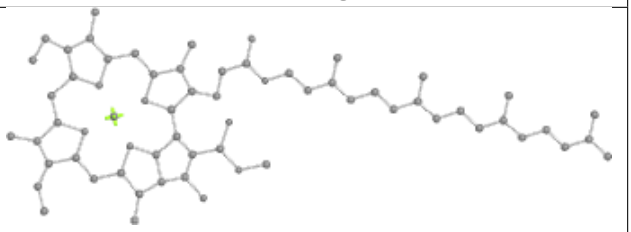
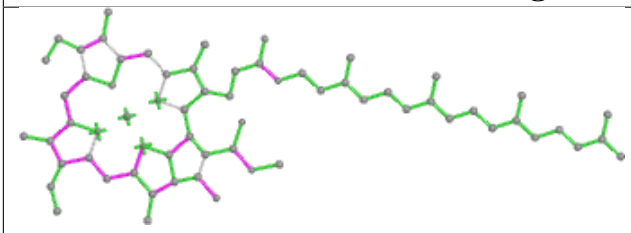
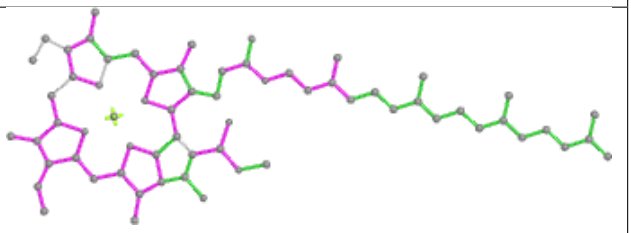


Rings

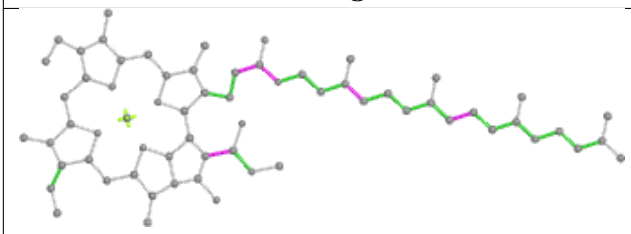
Ligand CLA c 512



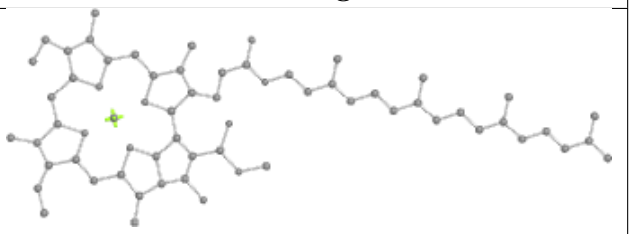
Bond lengths



Bond angles



Torsions



Rings

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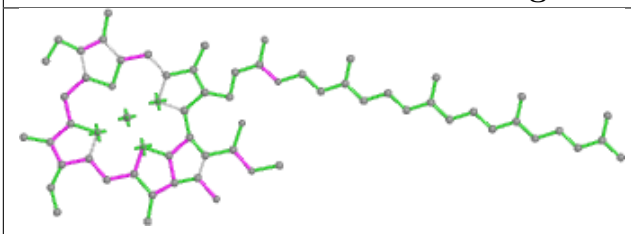

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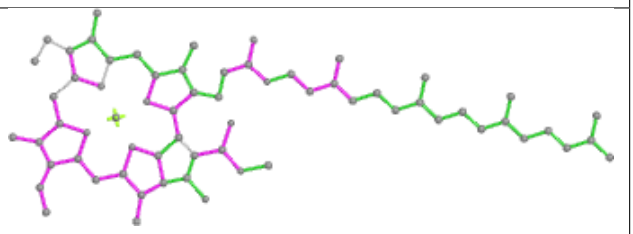
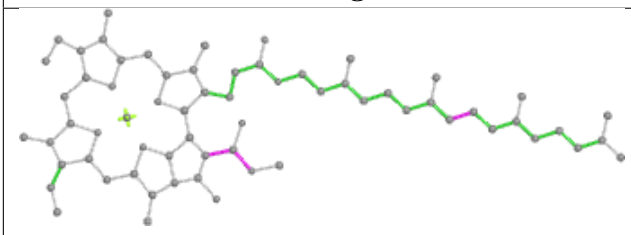
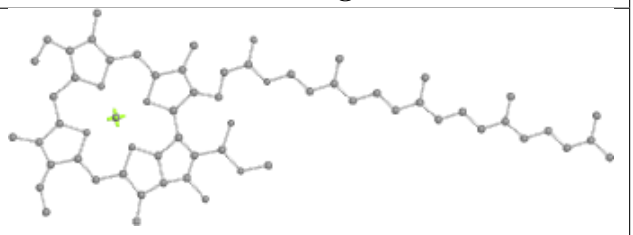


Bond angles



Torsions



Rings

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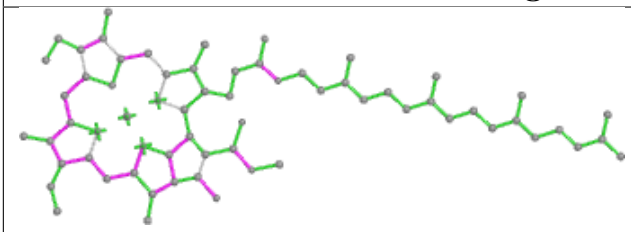

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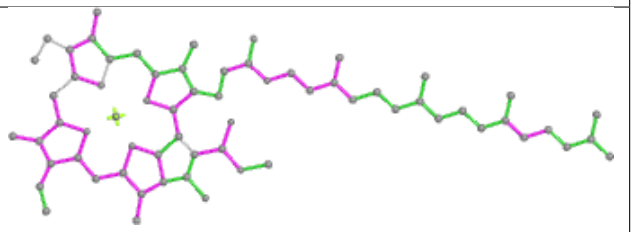

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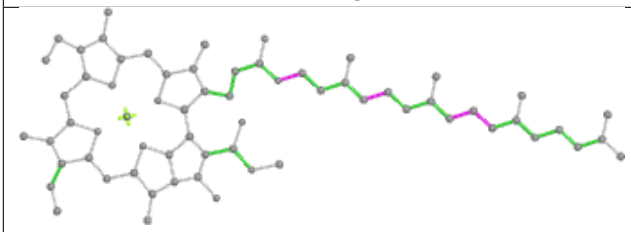

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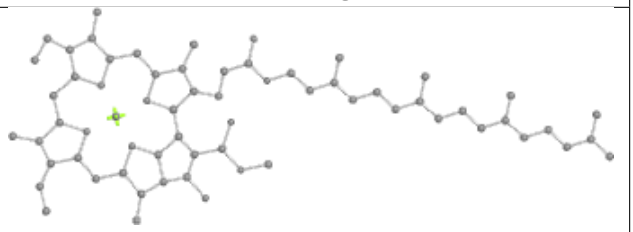

Rings

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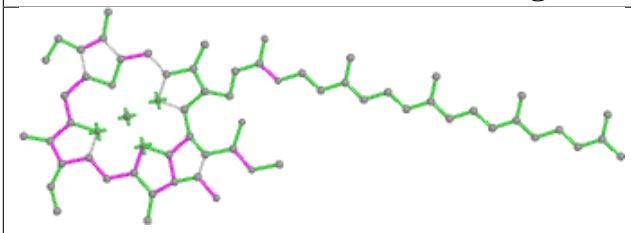

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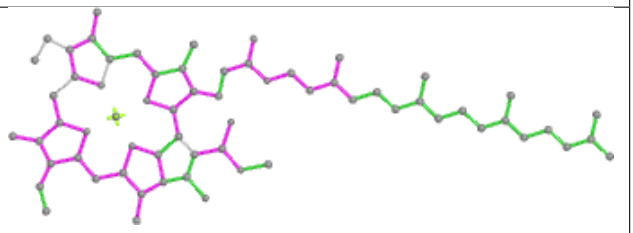

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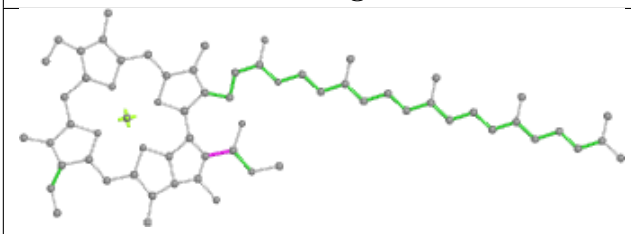

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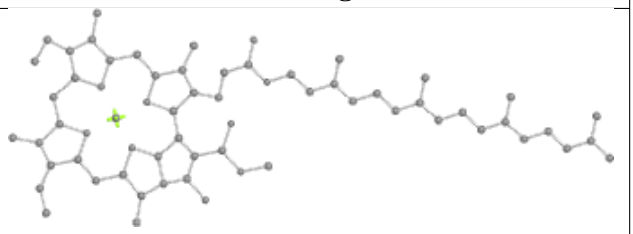

Rings

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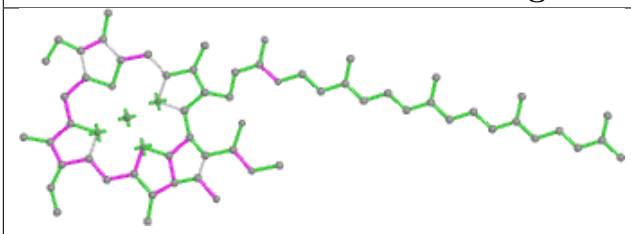

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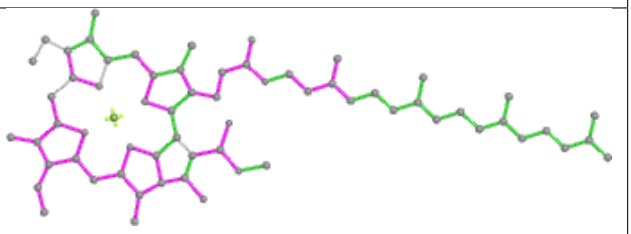

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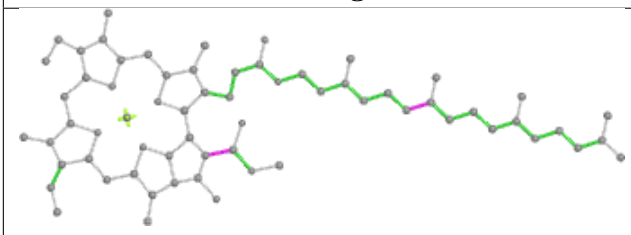

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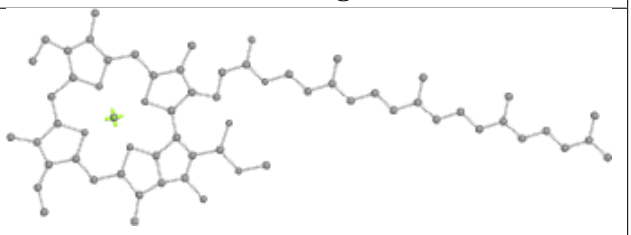
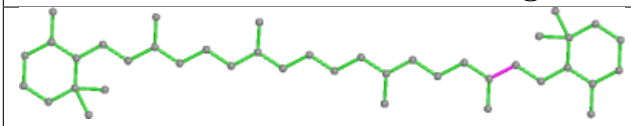


Rings

Ligand BCR A 410



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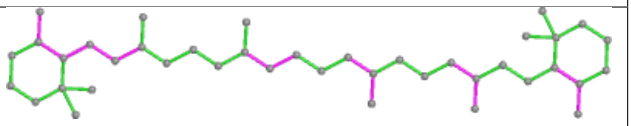
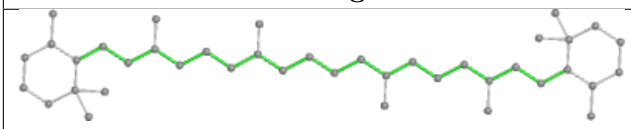


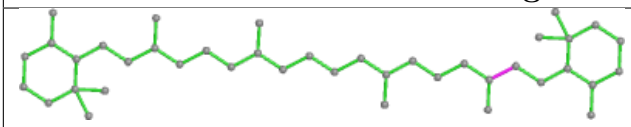
Bond angles



Torsions

Rings

Ligand BCR T 102



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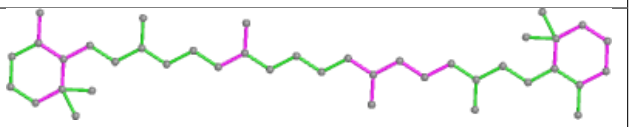
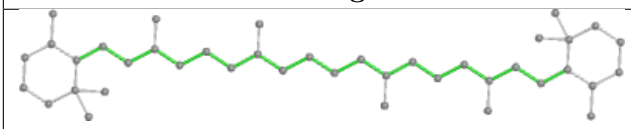


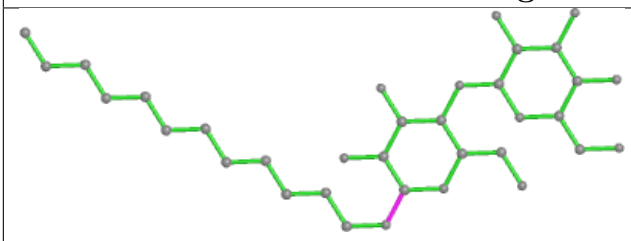
Bond angles



Torsions

Rings

Ligand LMT M 101



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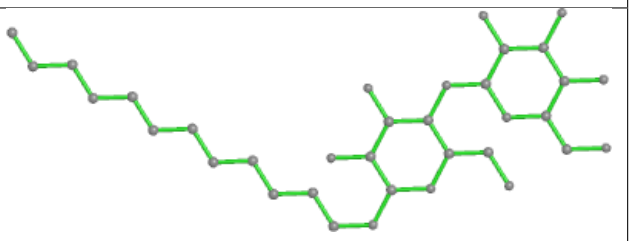

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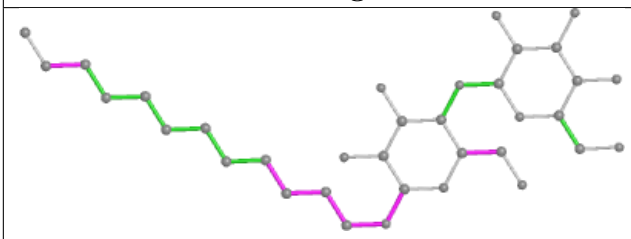
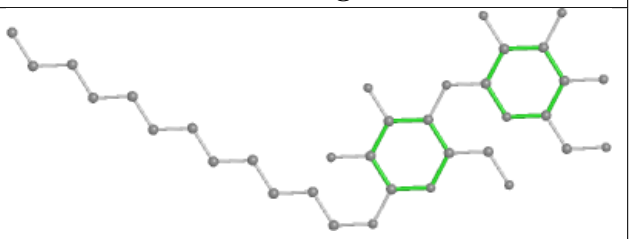
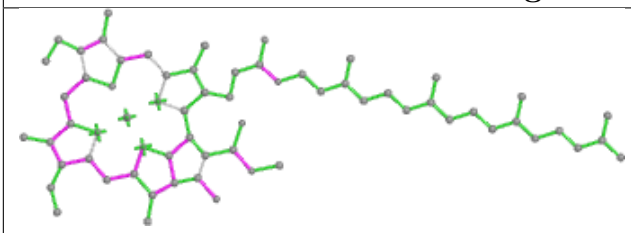


Torsions

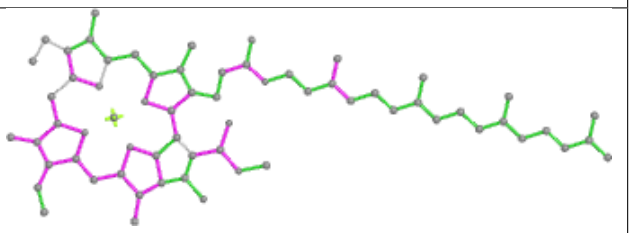


Rings

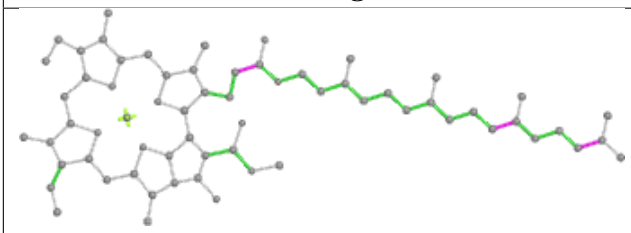
Ligand CLA C 506



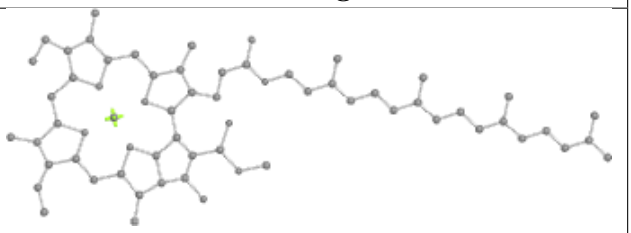
Bond lengths



Bond angles

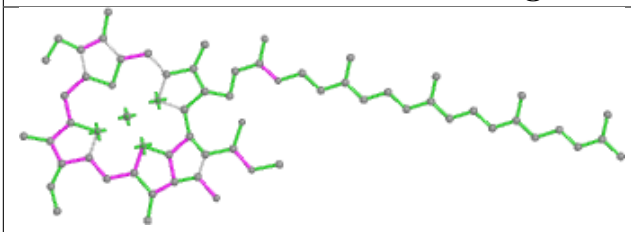


Torsions

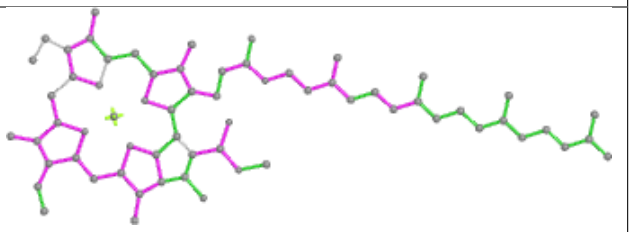


Rings

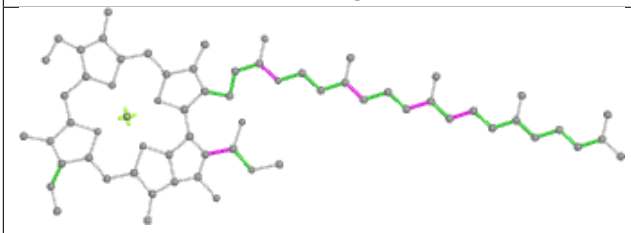
Ligand CLA C 511



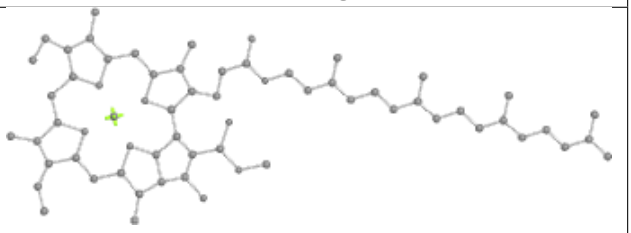
Bond lengths



Bond angles

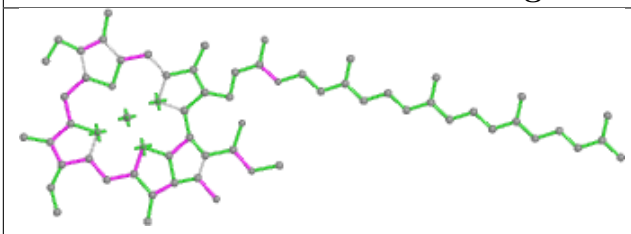


Torsions



Rings

Ligand CLA B 614



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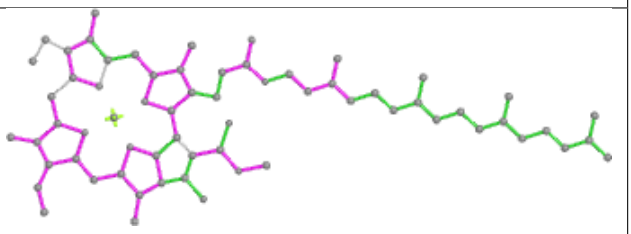
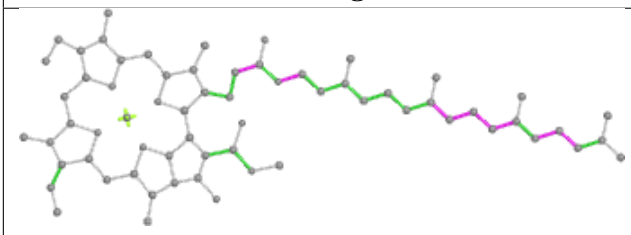
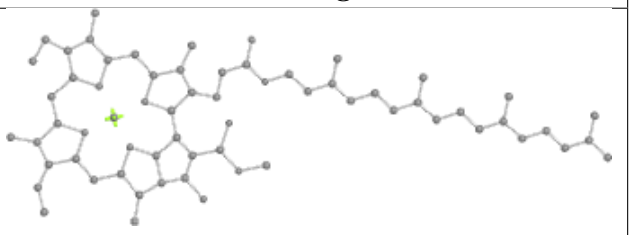


Bond angles

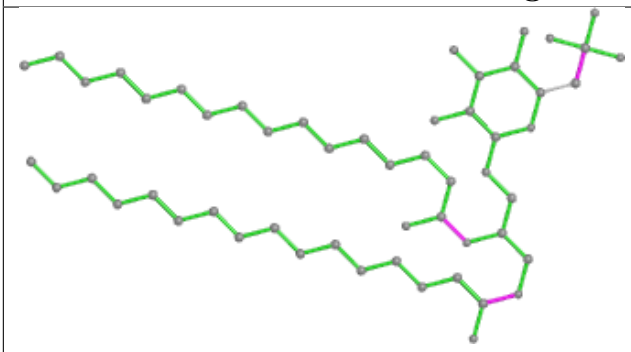


Torsions



Rings

Ligand SQD A 416



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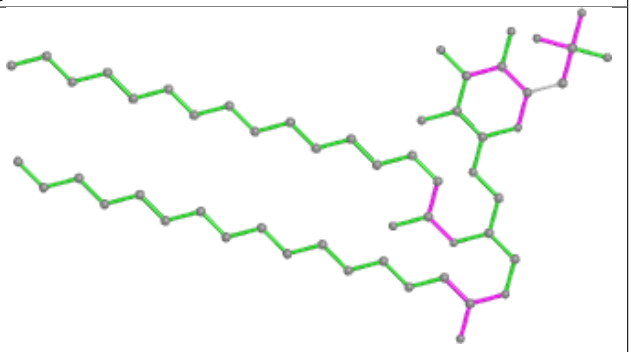
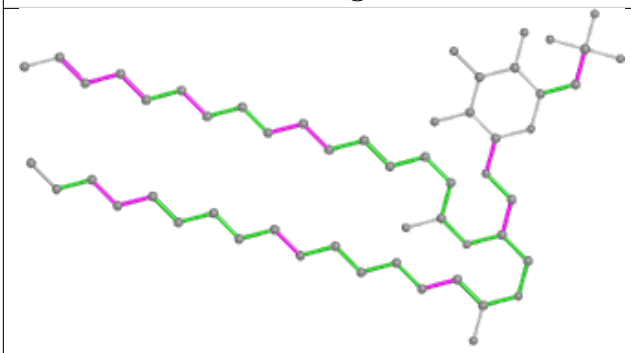


Bond angles



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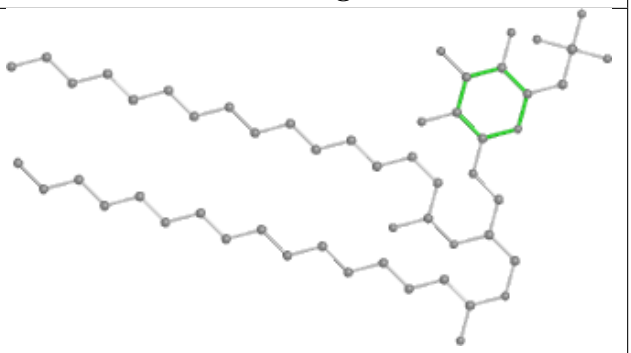
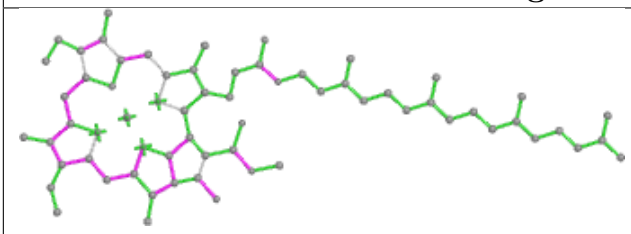


Rings

Ligand CLA b 613



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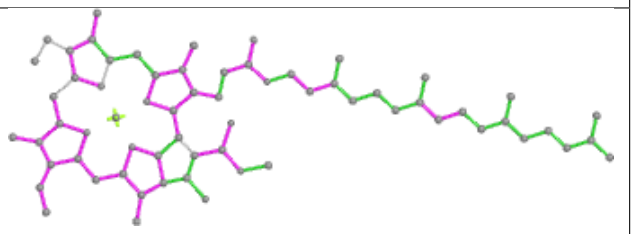
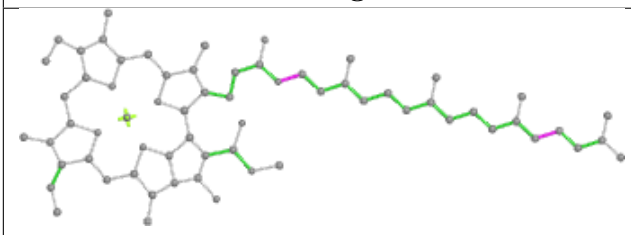


Bond angles



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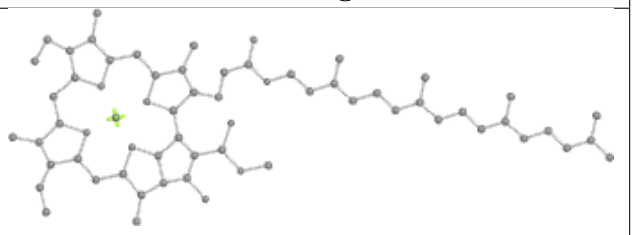
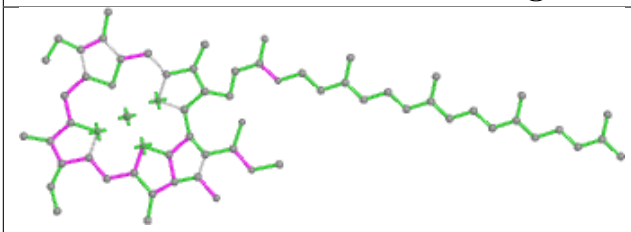
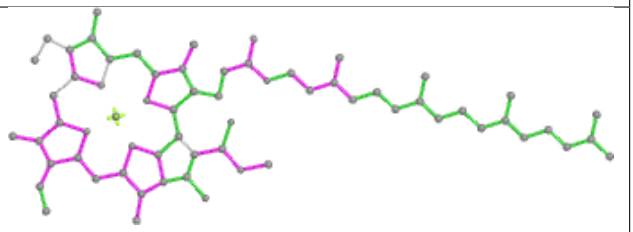


Rings

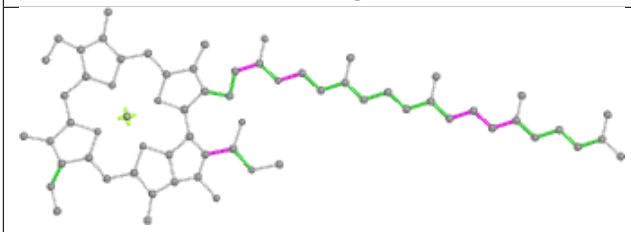
Ligand CLA b 618



Bond lengths



Bond angles



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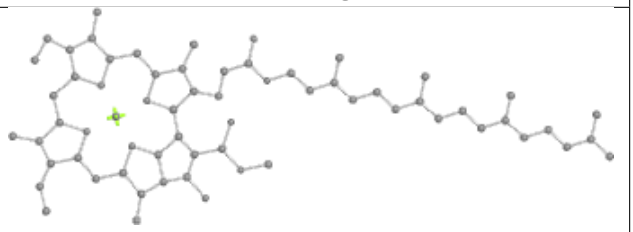
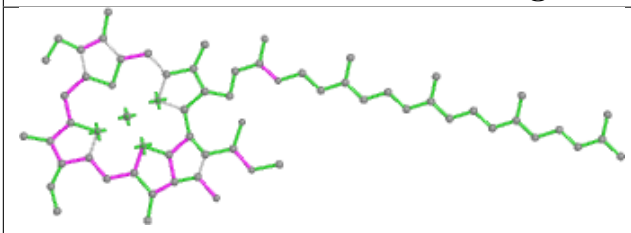


Rings

Ligand CLA c 503



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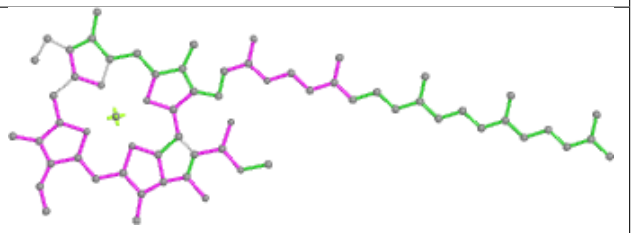
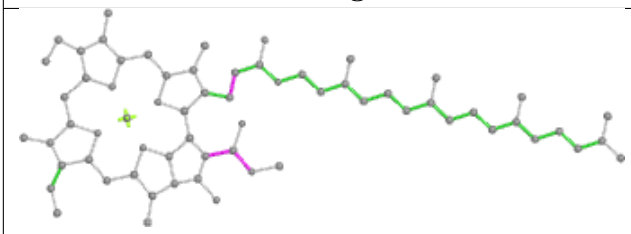


Bond angles



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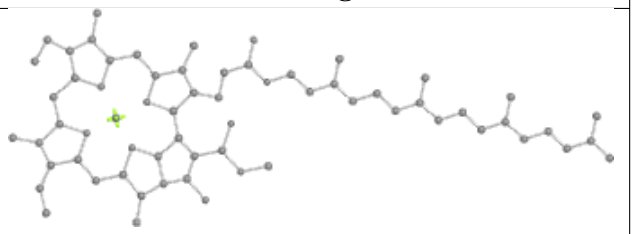
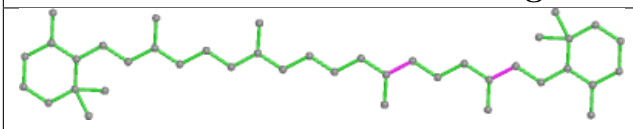


Rings

Ligand BCR b 622



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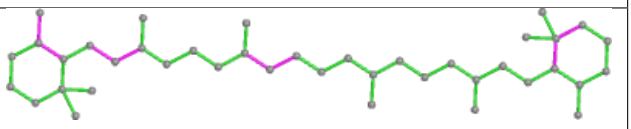
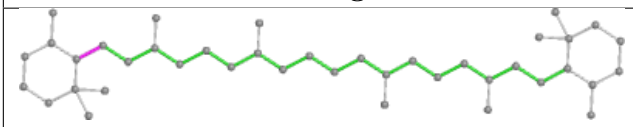


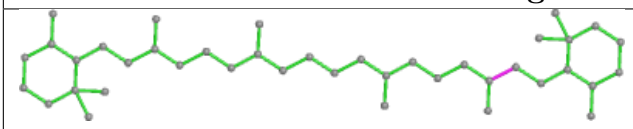
Bond angles



Torsions

Rings

Ligand BCR c 526



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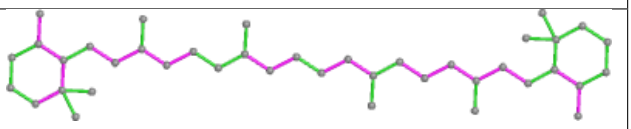
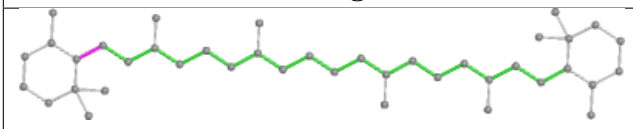
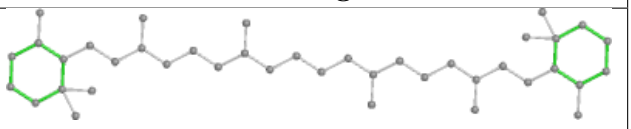


Bond angles

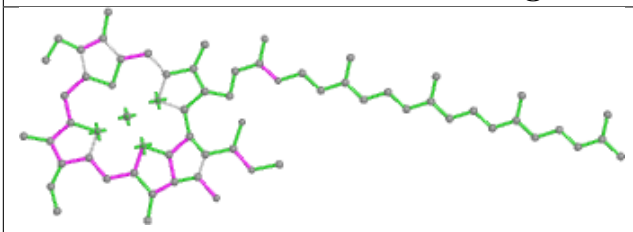


Torsions



Rings

Ligand CLA C 503



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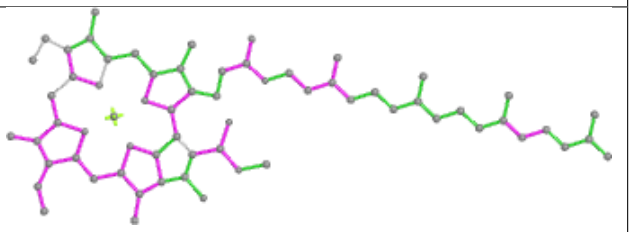
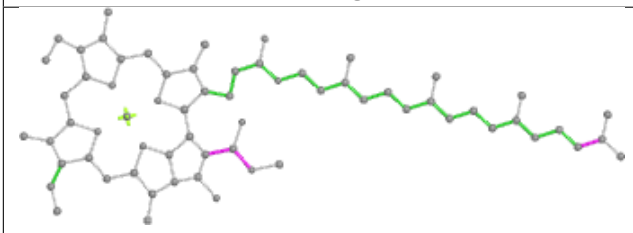


Bond angles



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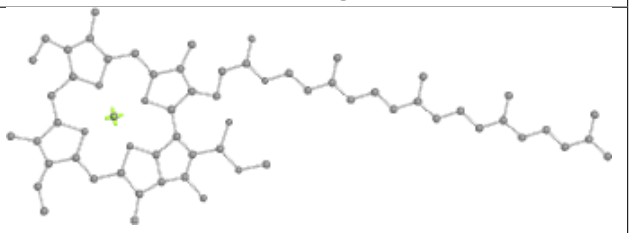
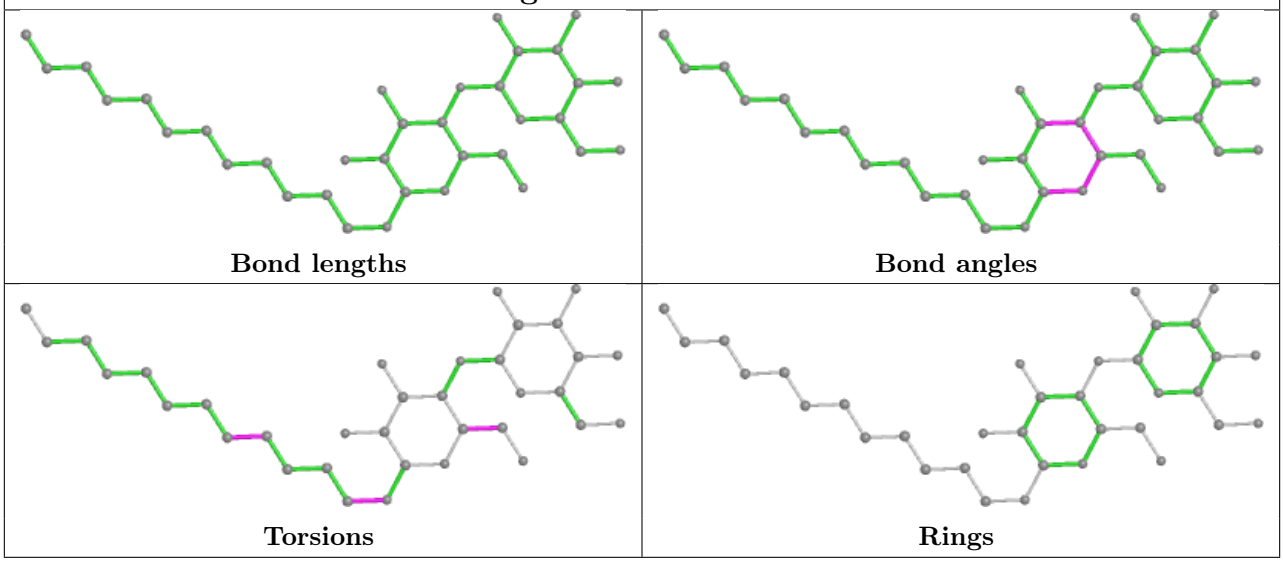
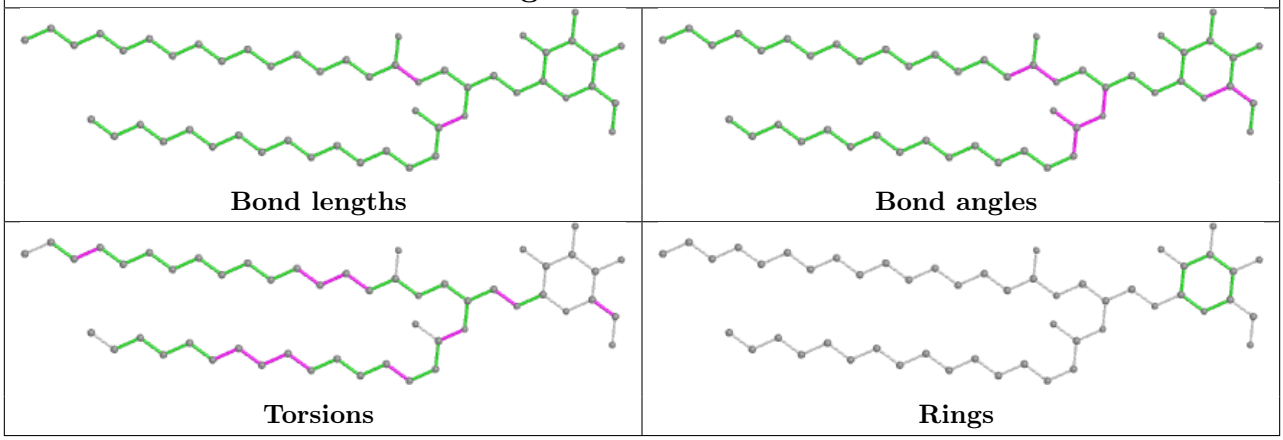


Rings

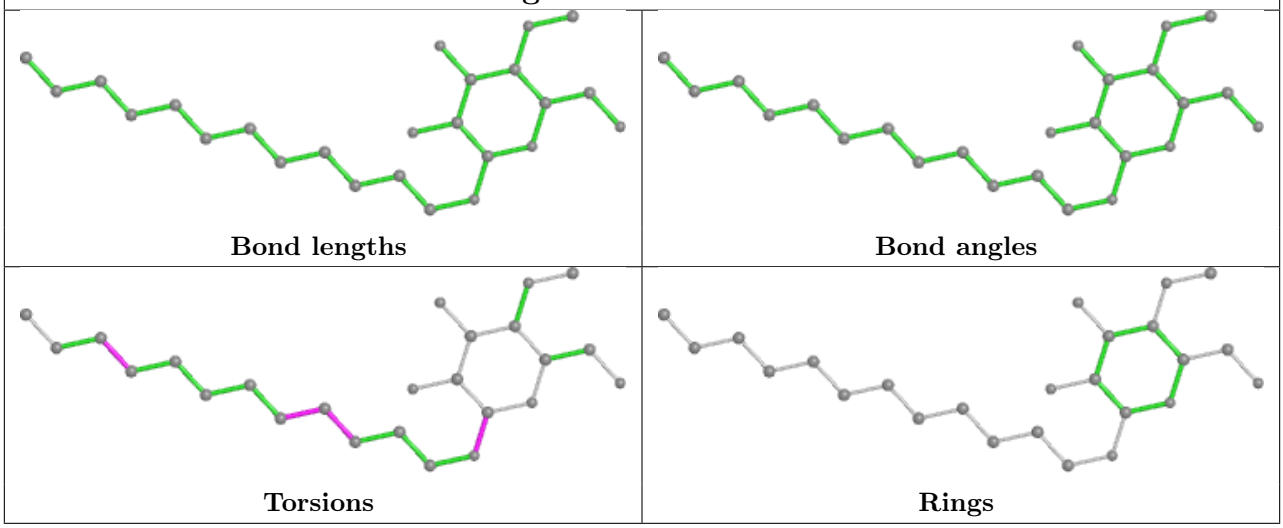
Ligand LMT m 102



Ligand LMG C 521



Ligand LMT B 634



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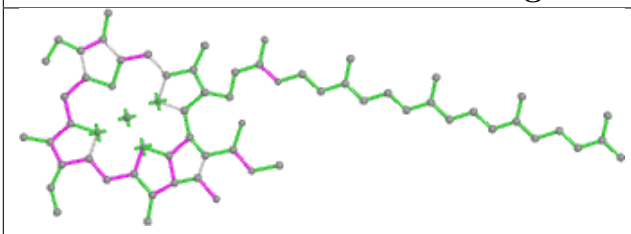
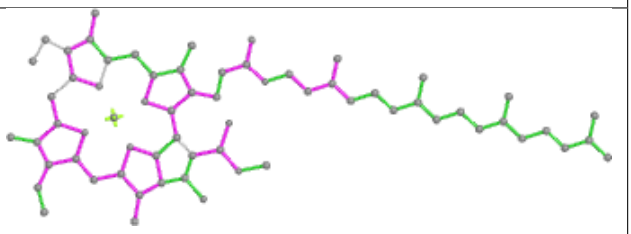
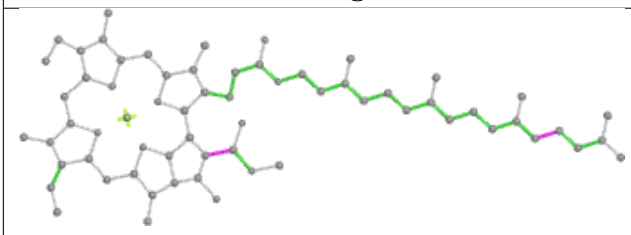


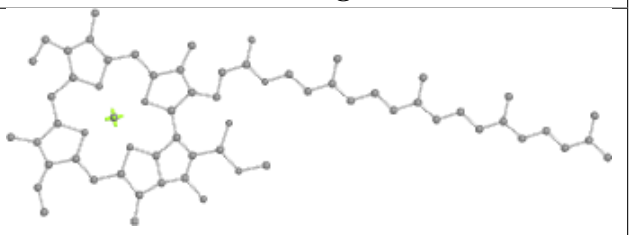
Bond lengths



Bond angles

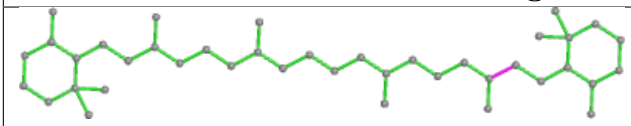


Torsions

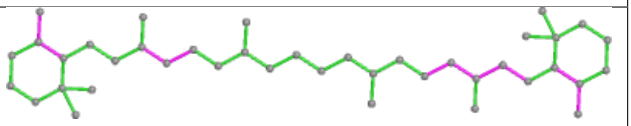


Rings

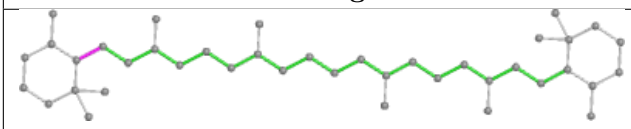
Ligand BCR k 103



Bond lengths



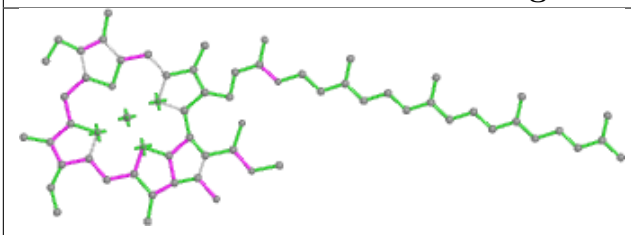
Bond angles



Torsions

Rings

Ligand CLA c 514



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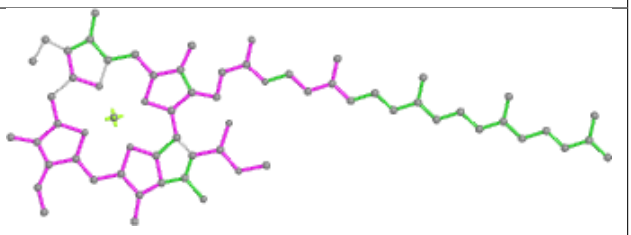
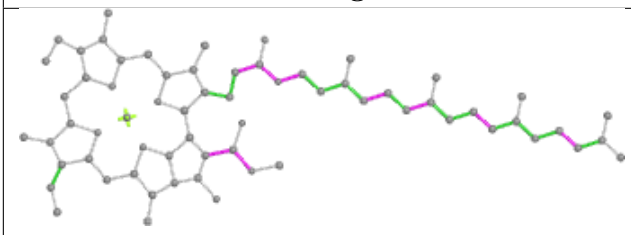
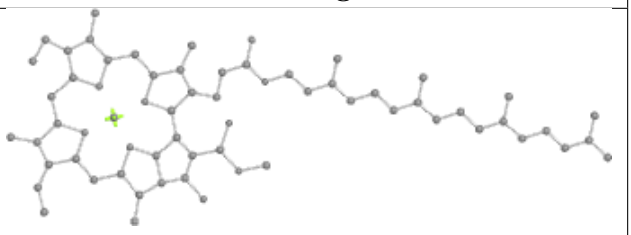


Bond angles

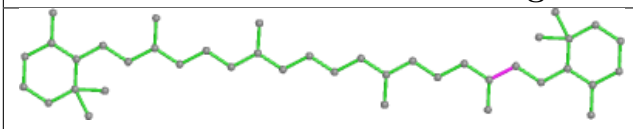


Torsions

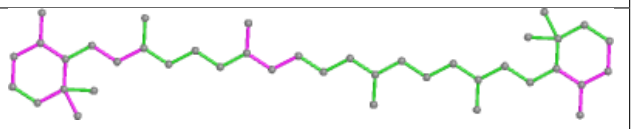


Rings

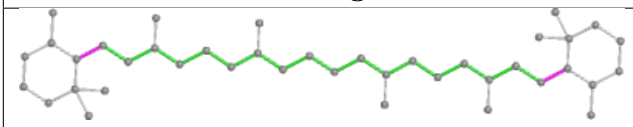
Ligand BCR c 516



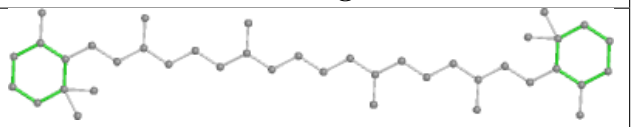
Bond lengths



Bond angles

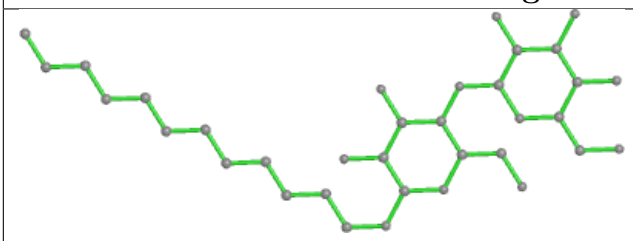


Torsions



Rings

Ligand LMT E 102



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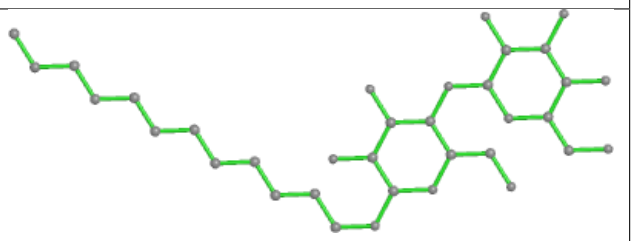
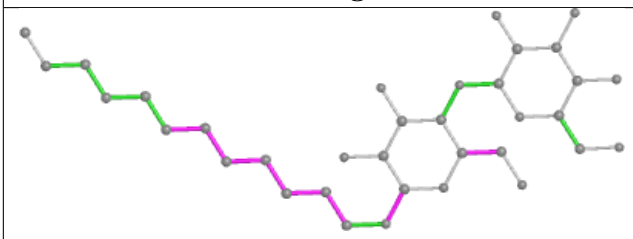


Bond angles



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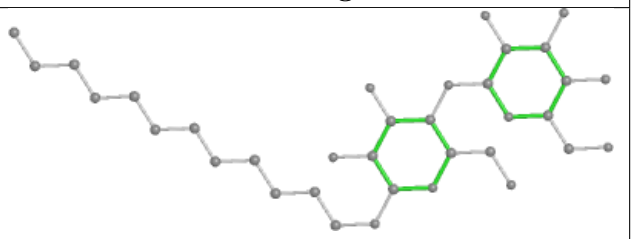
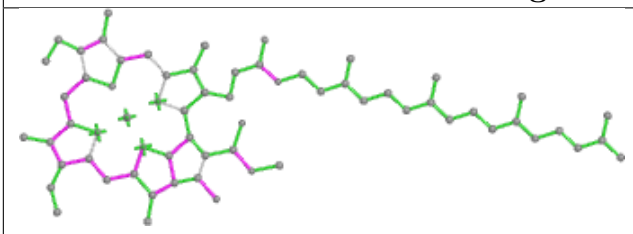


Rings

Ligand CLA c 504



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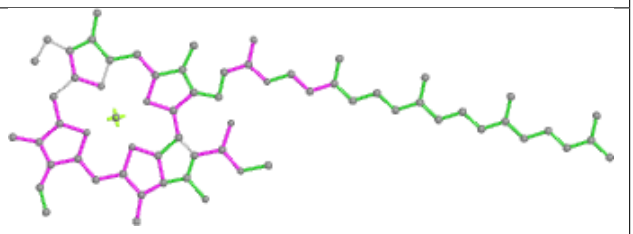
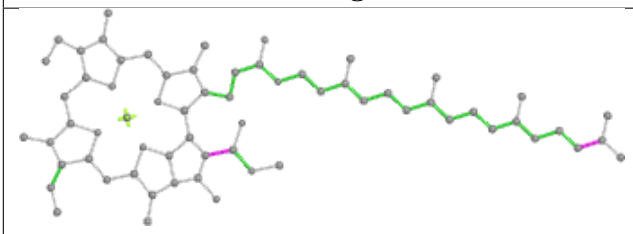
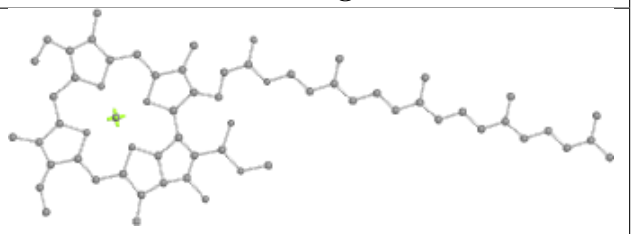


Bond angles

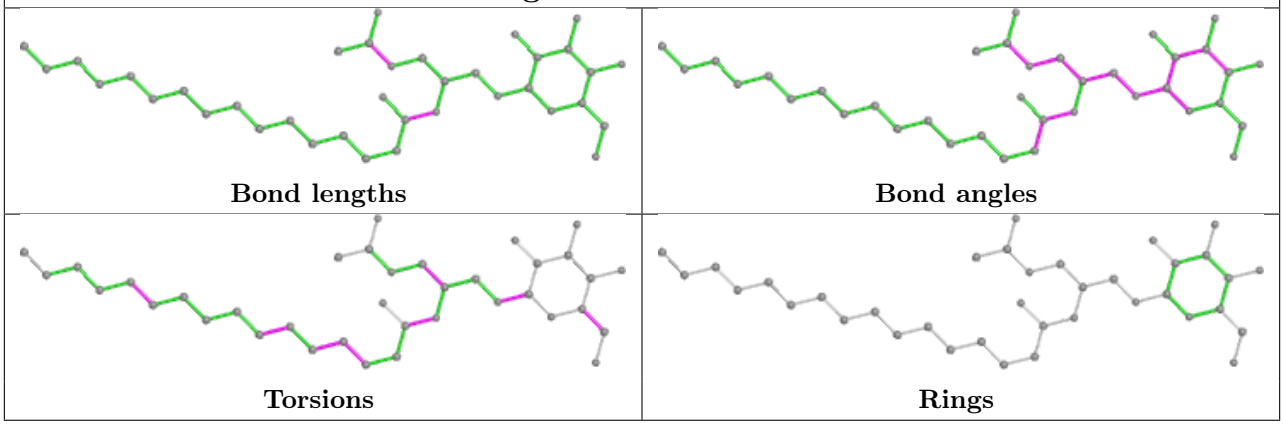


Torsions

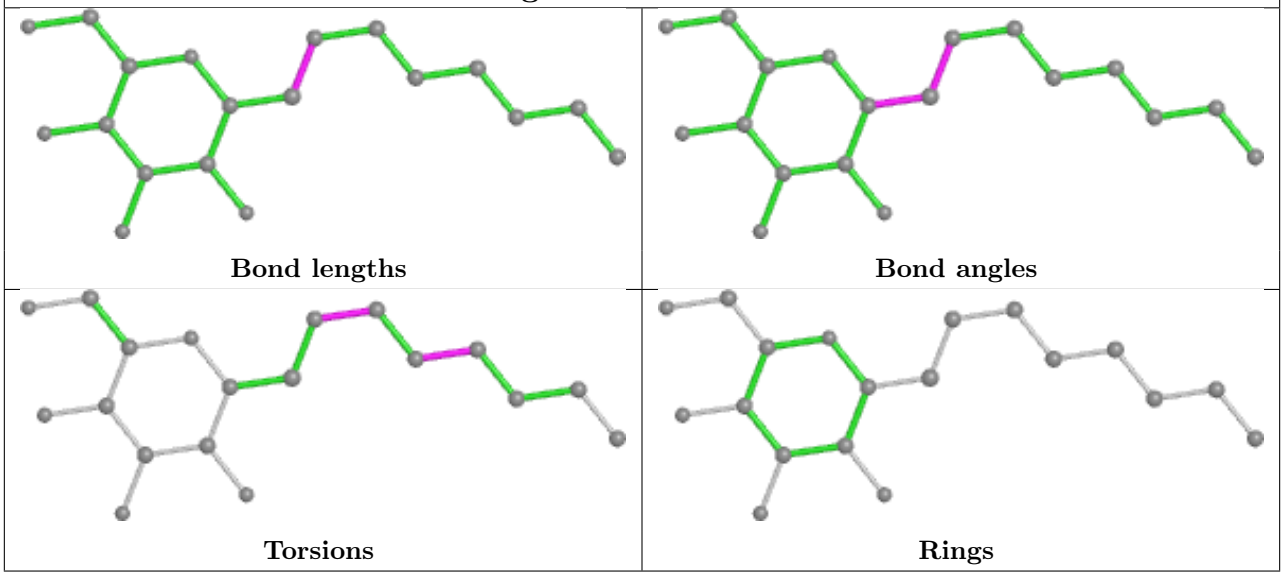


Rings

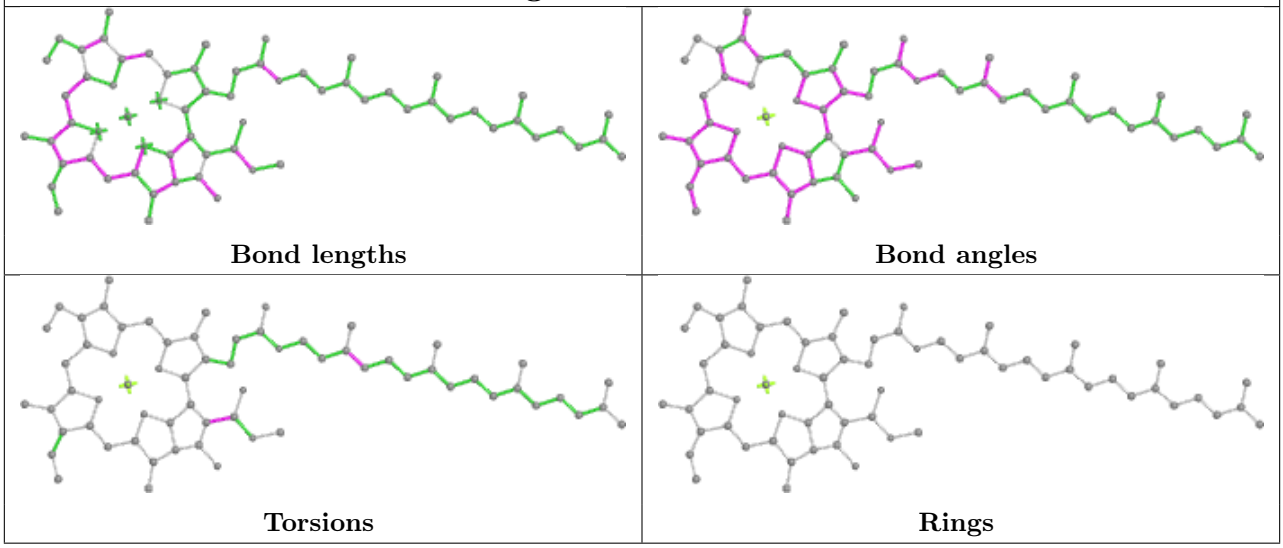
Ligand LMG Z 101



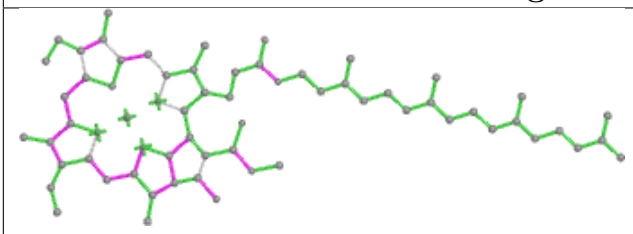
Ligand HTG O 303



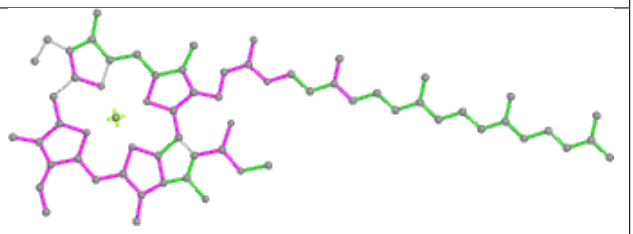
Ligand CLA B 606



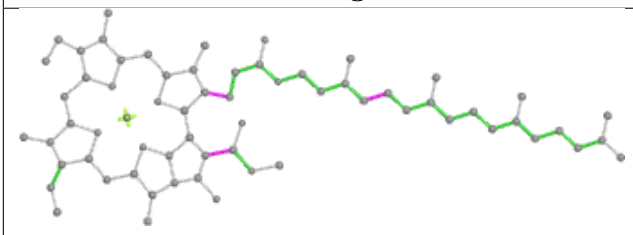
Ligand CLA b 612



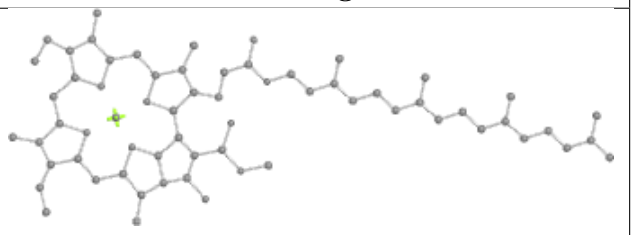
Bond lengths



Bond angles

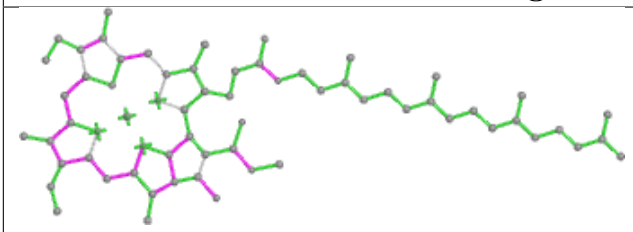


Torsions



Rings

Ligand CLA b 611



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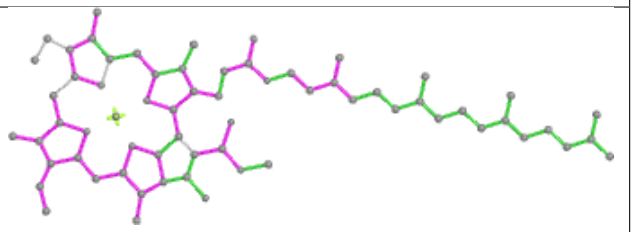
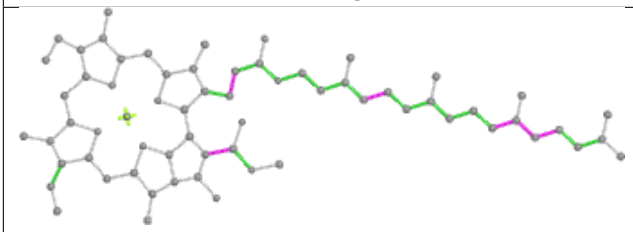


Bond angles



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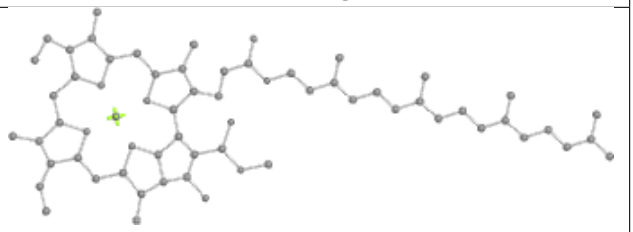

Rings

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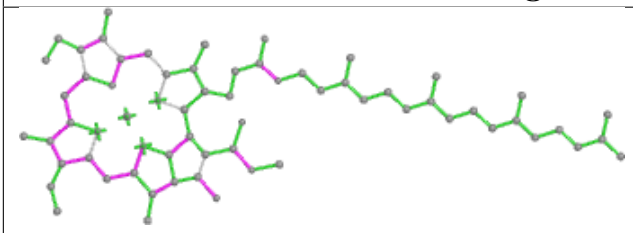
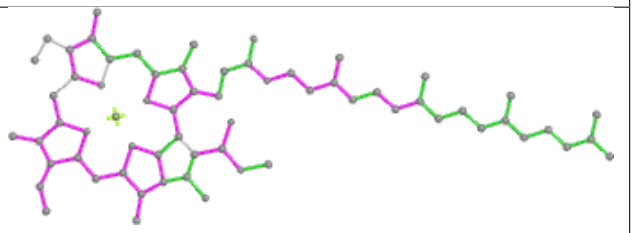
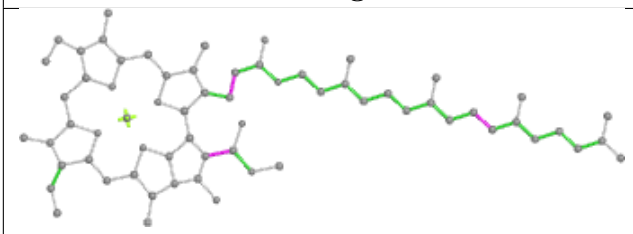


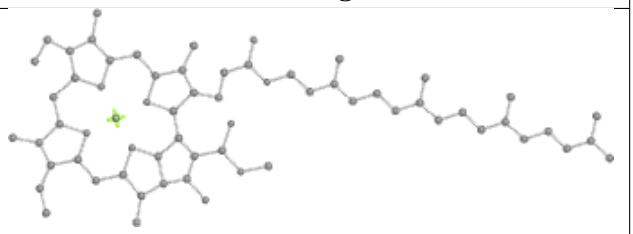
Bond lengths



Bond angles

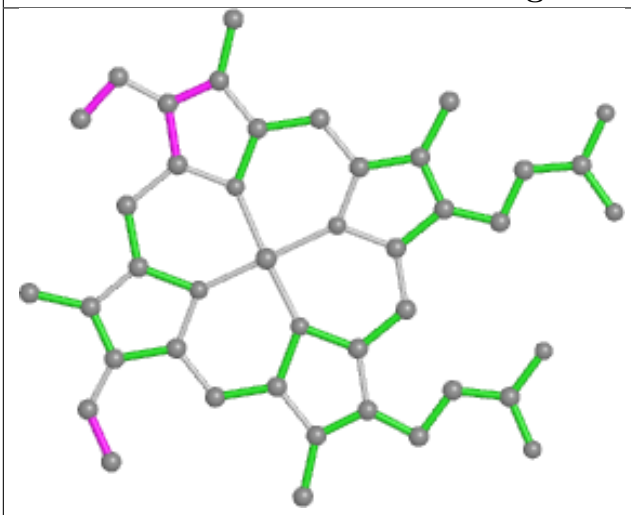


Torsions



Rings

Ligand HEC v 202



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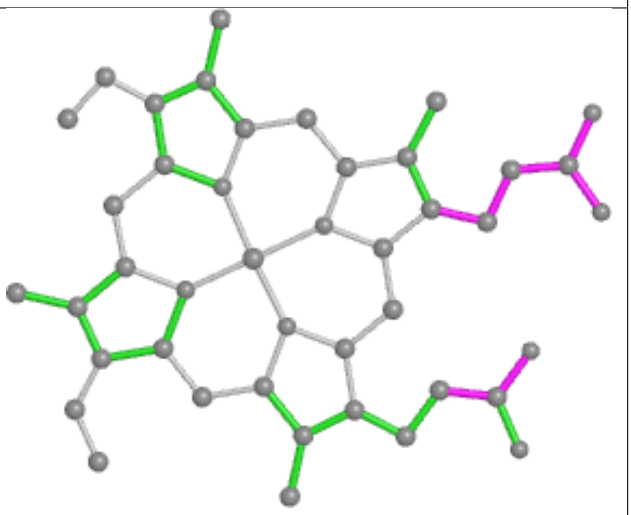
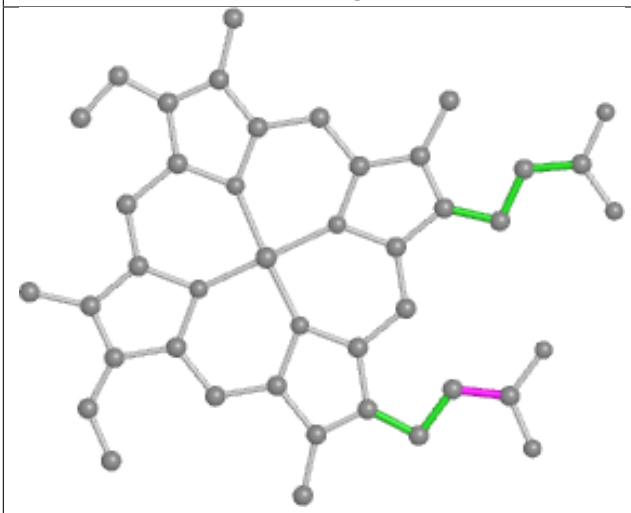


Bond angles



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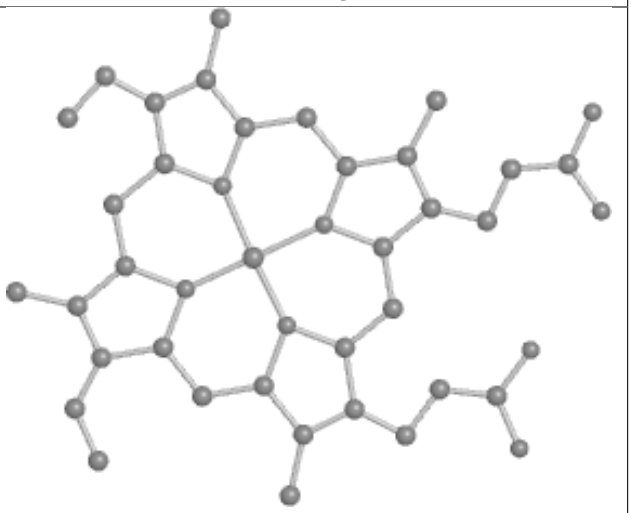
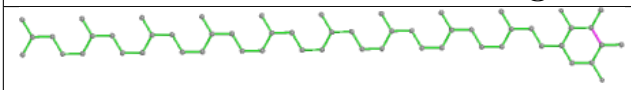


Rings

Ligand PL9 A 419



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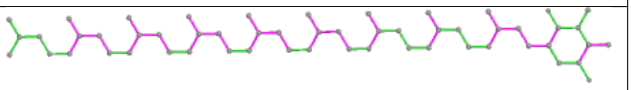
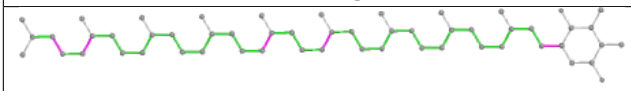
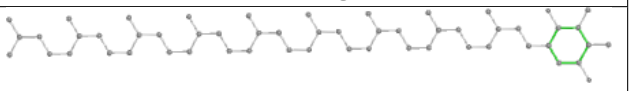


Bond angles

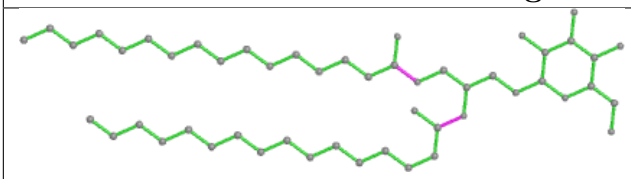


Torsions



Rings

Ligand LMG c 520



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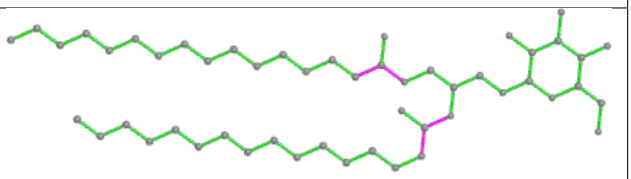
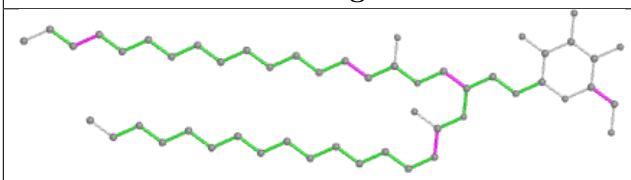


Bond angles



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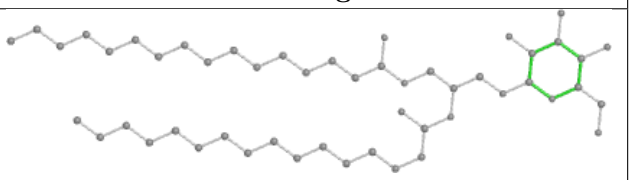
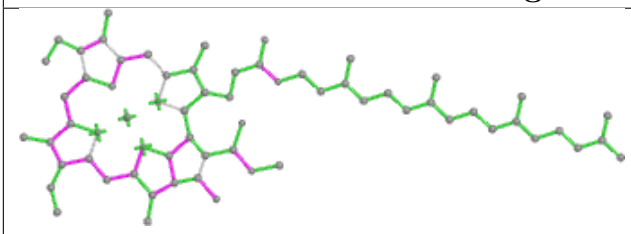


Rings

Ligand CLA B 615



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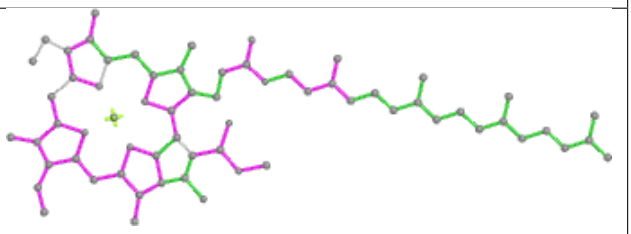
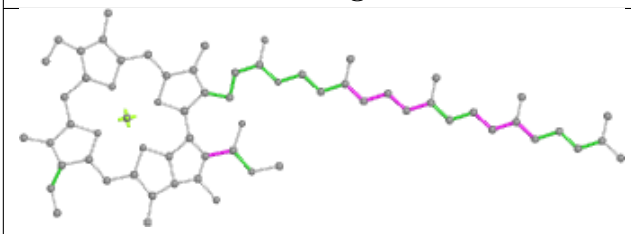
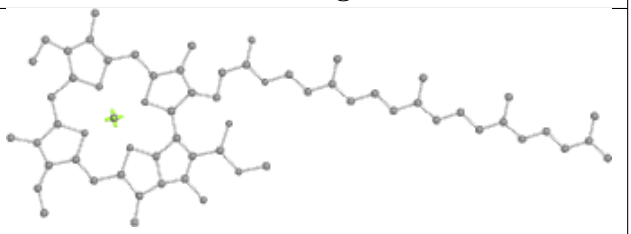


Bond angles

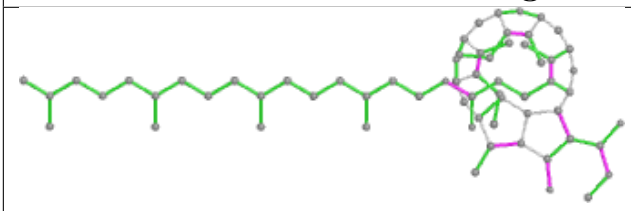


Torsions



Rings

Ligand PHO A 408



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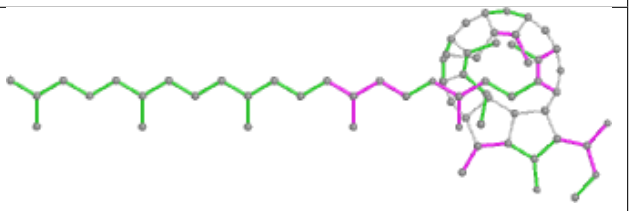
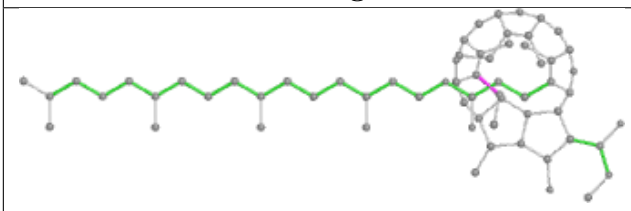
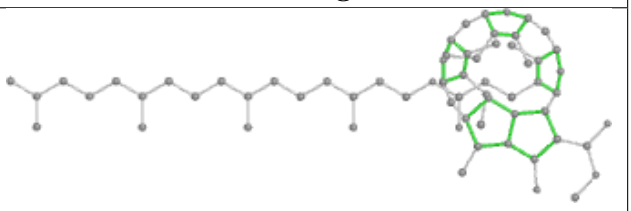


Bond angles

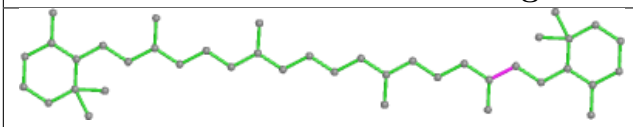


Torsions



Rings

Ligand BCR K 101



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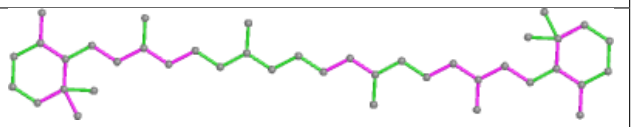
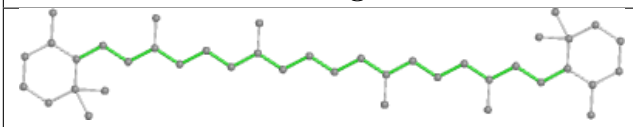


Bond angles



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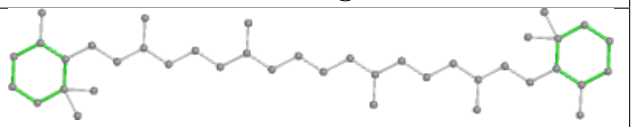
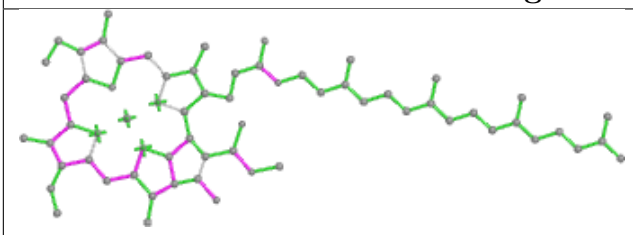
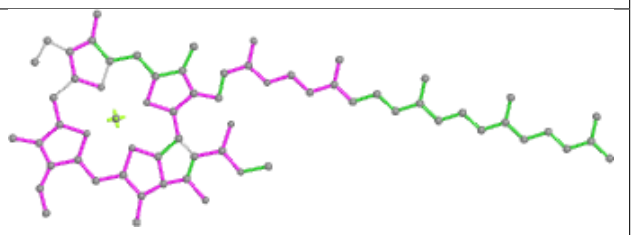


Rings

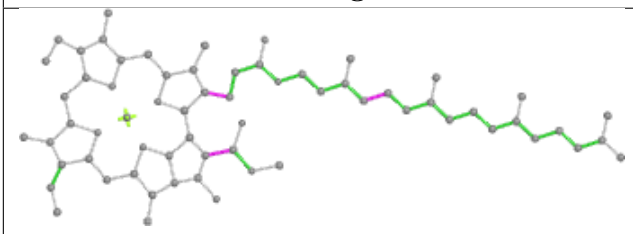
Ligand CLA B 608



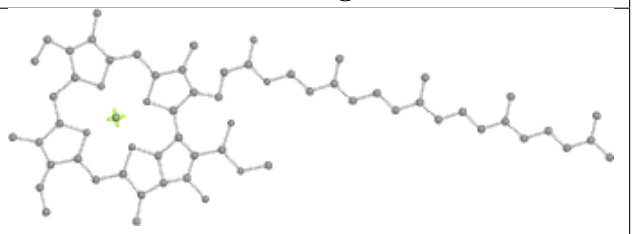
Bond lengths



Bond angles

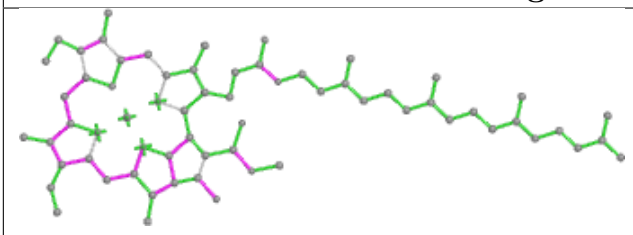


Torsions

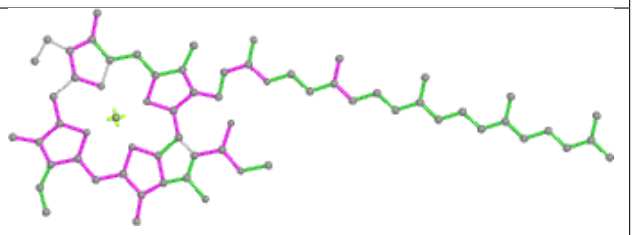


Rings

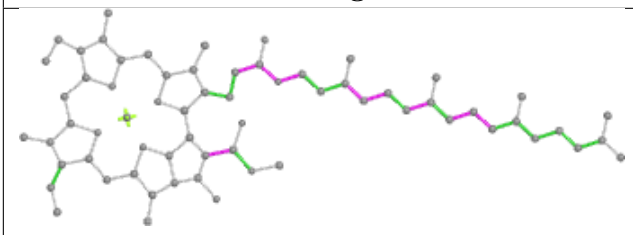
Ligand CLA b 606



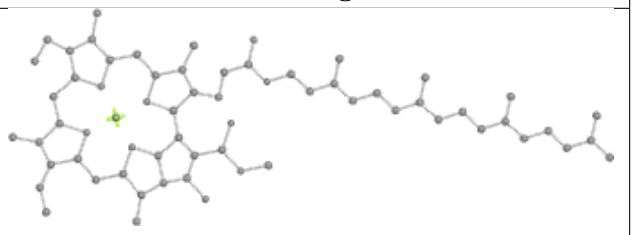
Bond lengths



Bond angles

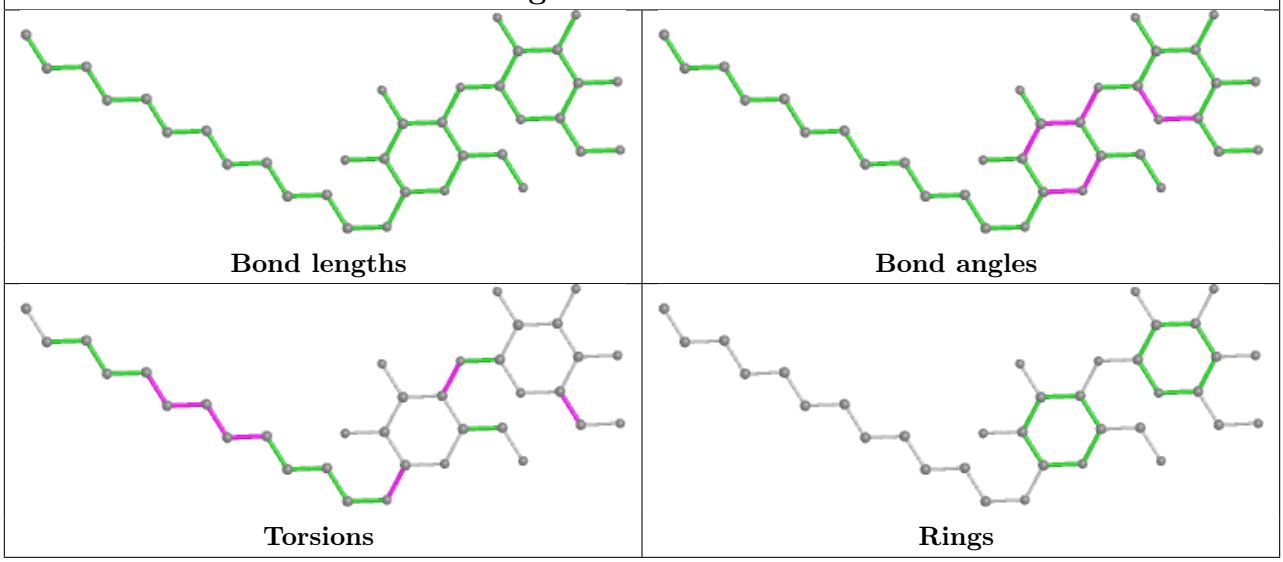


Torsions

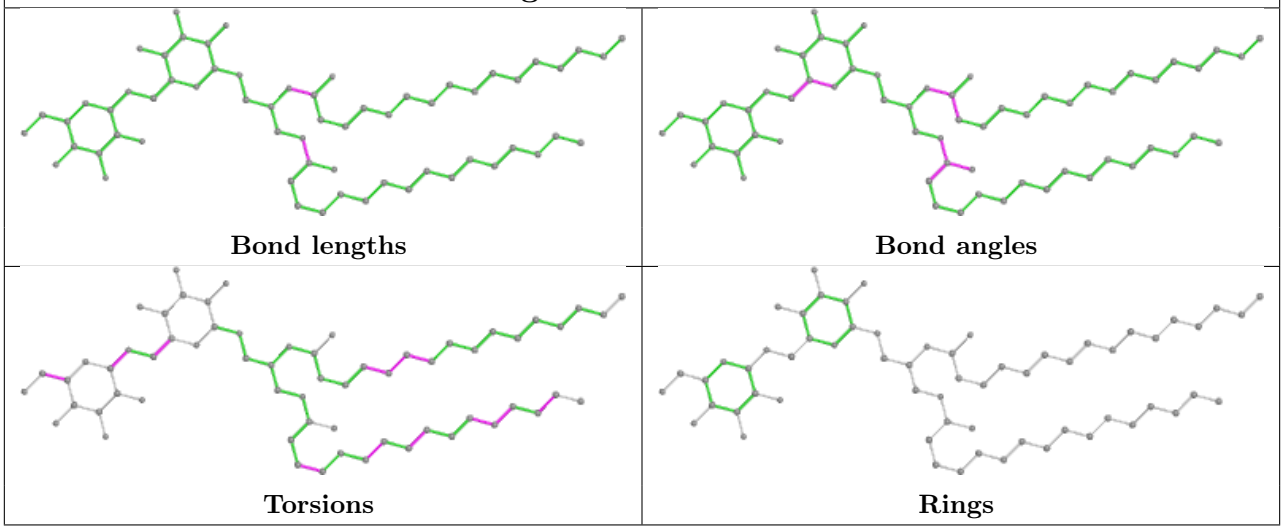


Rings

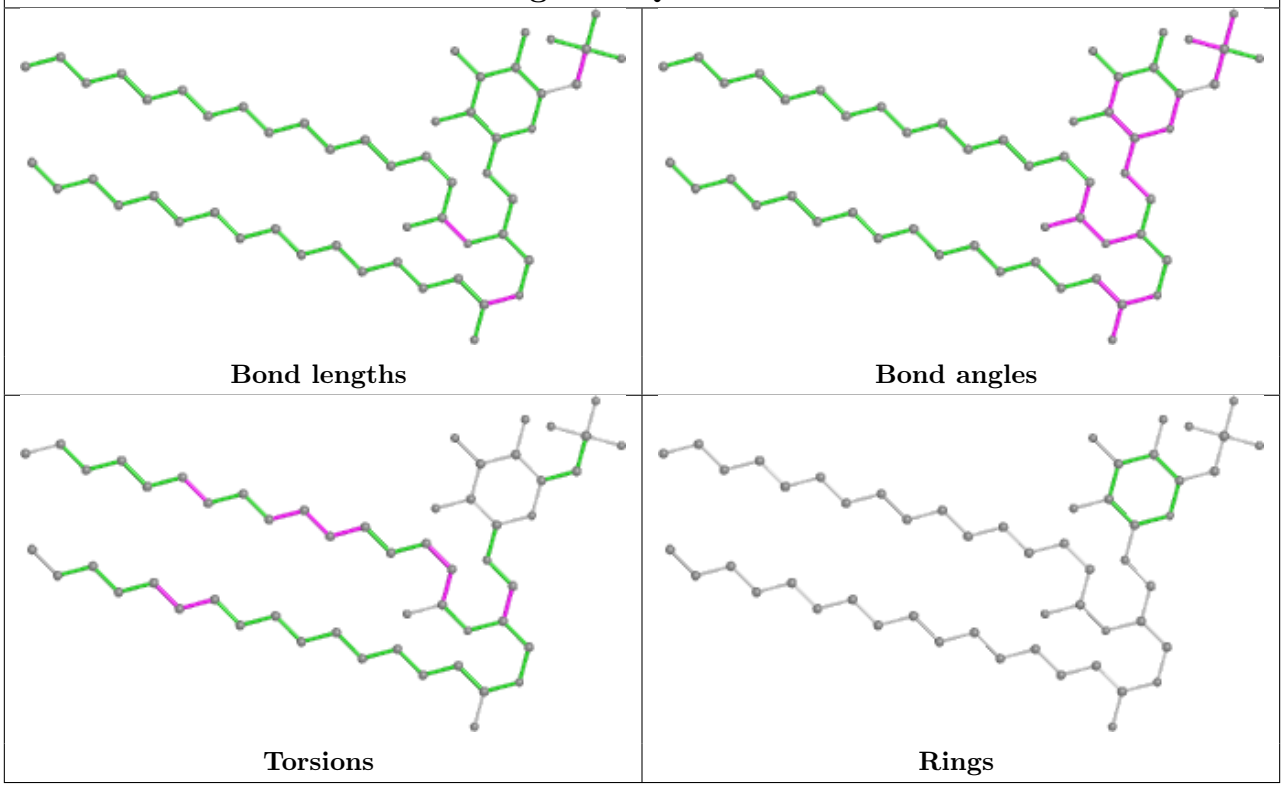
Ligand LMT I 102



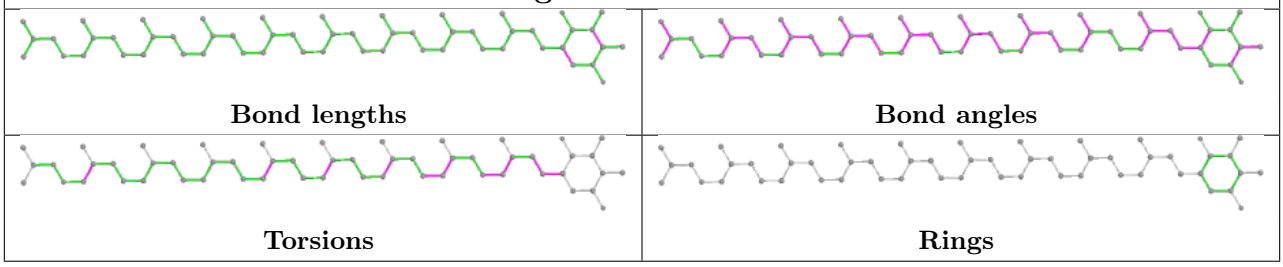
Ligand DGD C 517



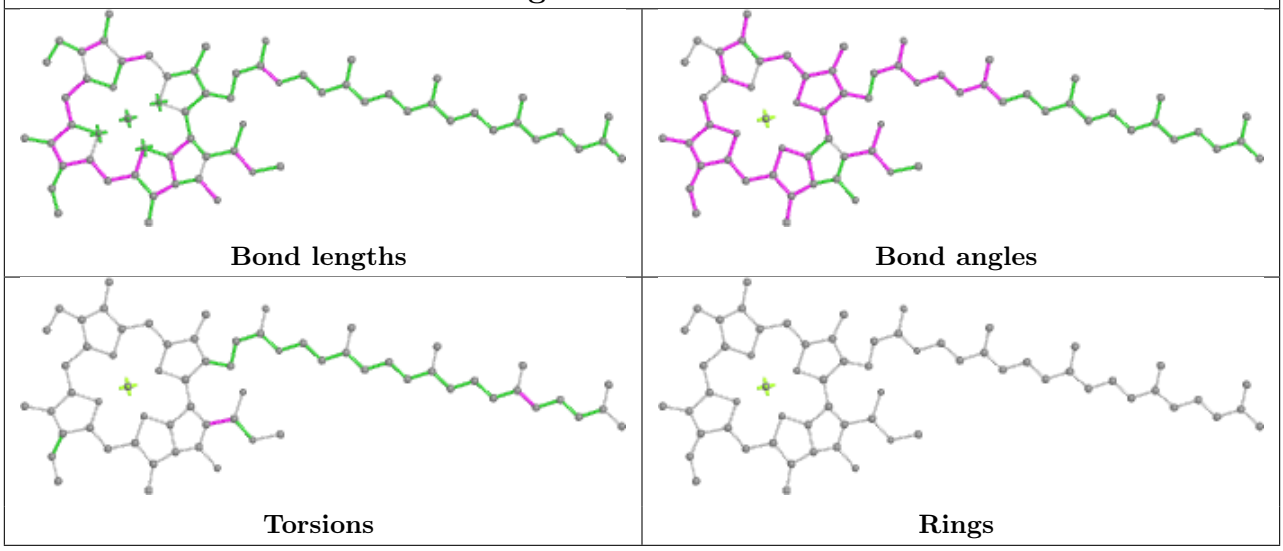
Ligand SQD a 411



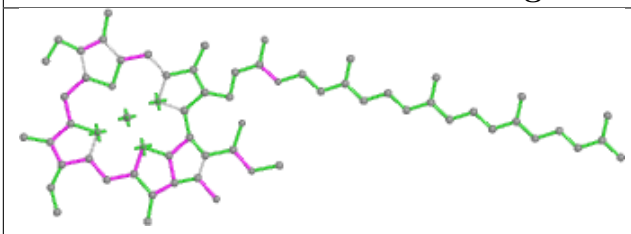
Ligand PL9 a 416



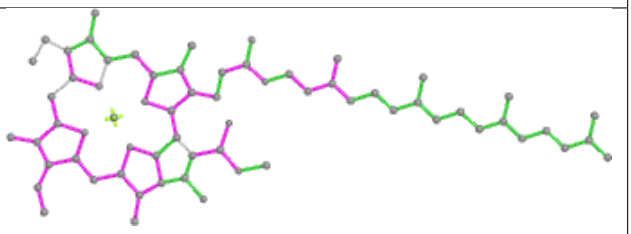
Ligand CLA b 607



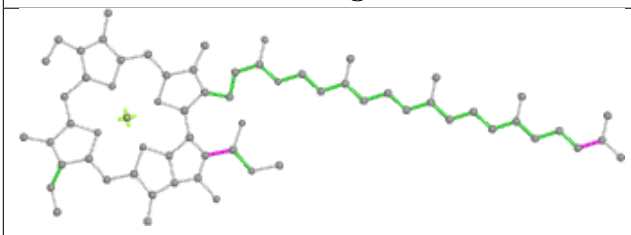
Ligand CLA C 514



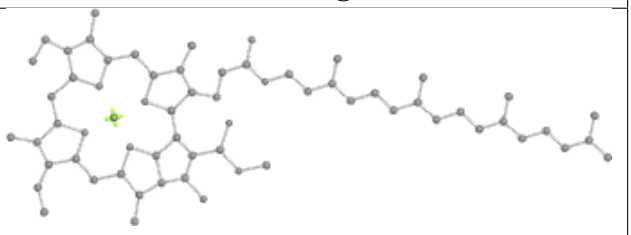
Bond lengths



Bond angles

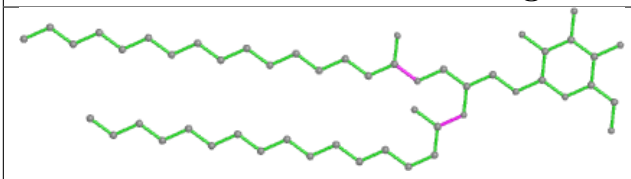


Torsions

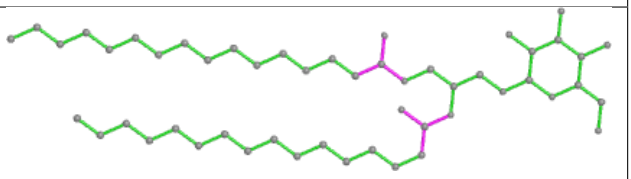


Rings

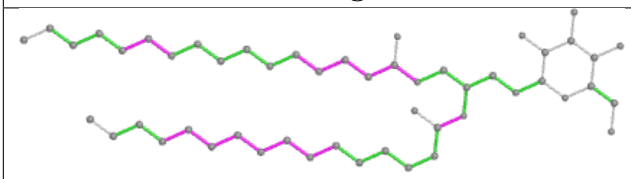
Ligand LMG b 625



Bond lengths



Bond angles



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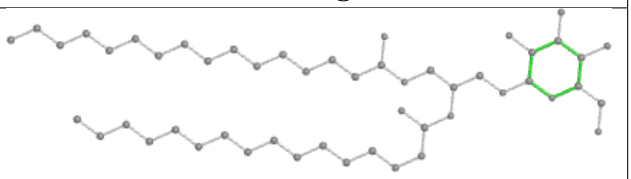
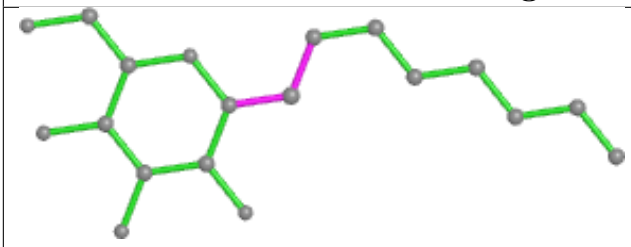
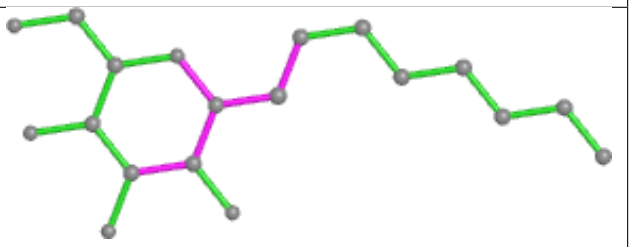


Rings

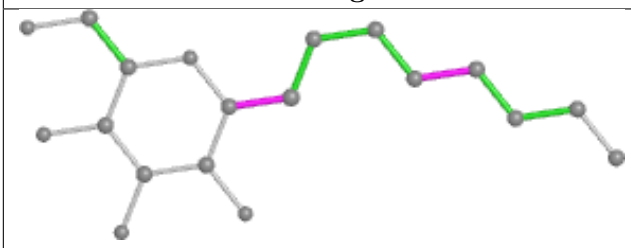
Ligand HTG V 204



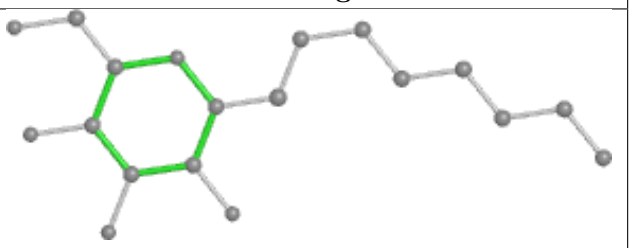
Bond lengths



Bond angles

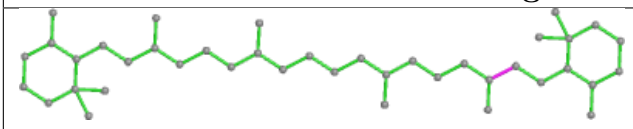


Torsions

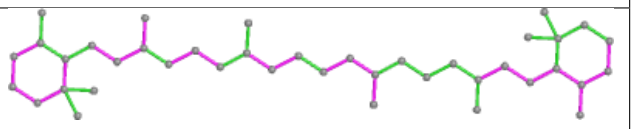


Rings

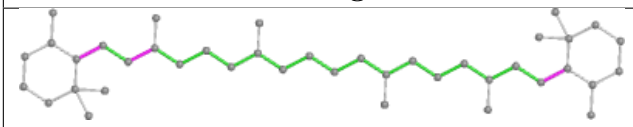
Ligand BCR B 620



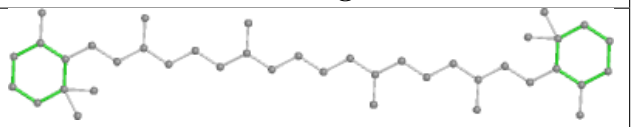
Bond lengths



Bond angles

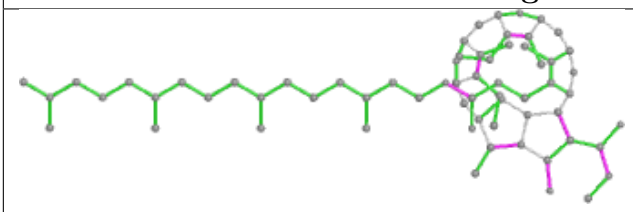


Torsions

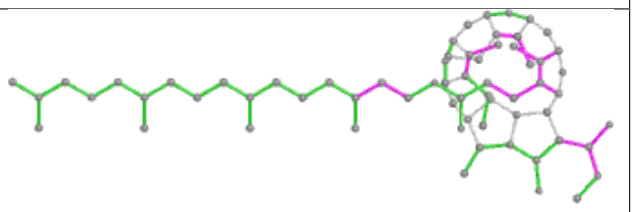


Rings

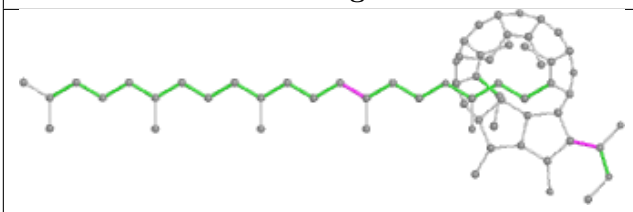
Ligand PHO A 407



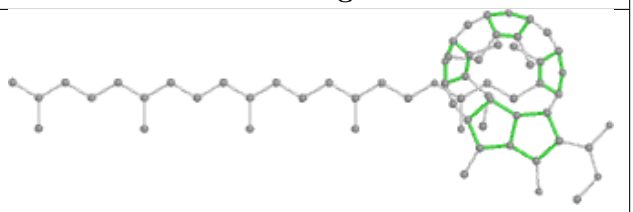
Bond lengths



Bond angles

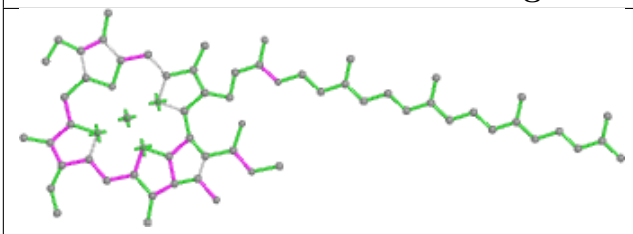


Torsions

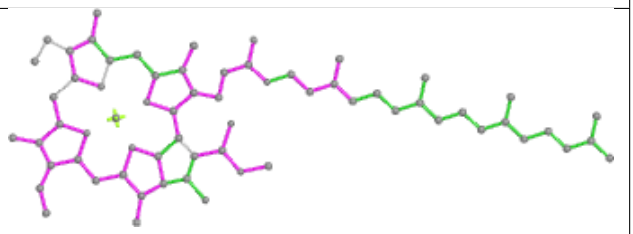


Rings

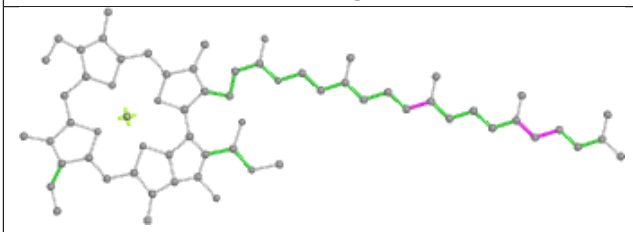
Ligand CLA A 406



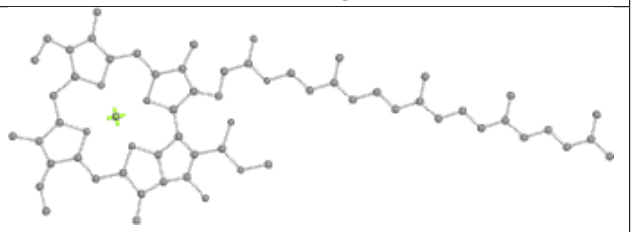
Bond lengths



Bond angles

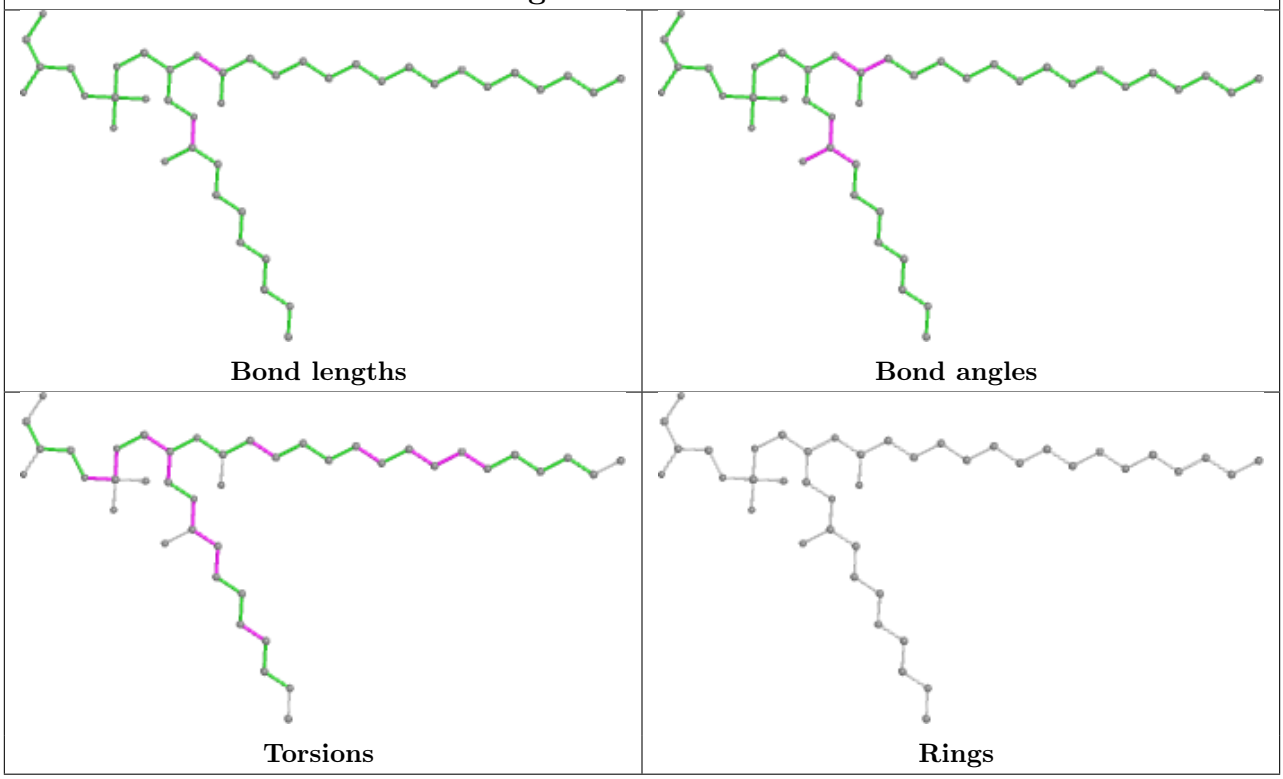


Torsions

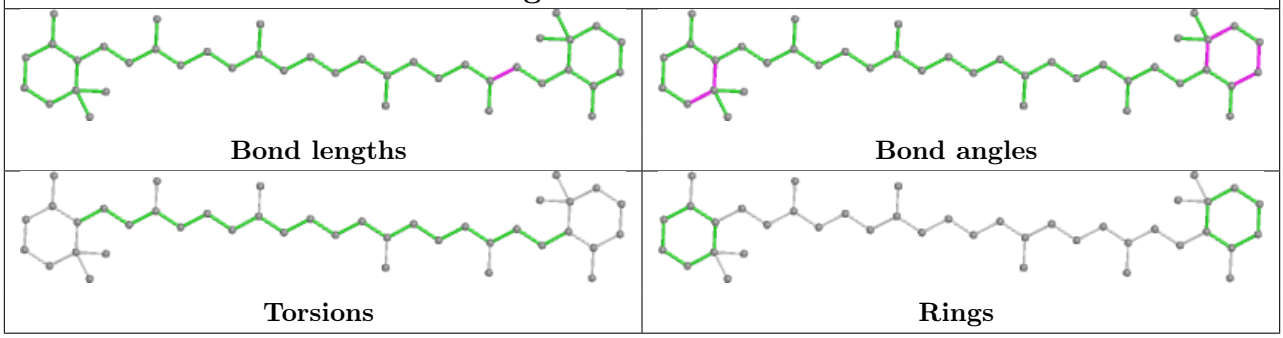


Rings

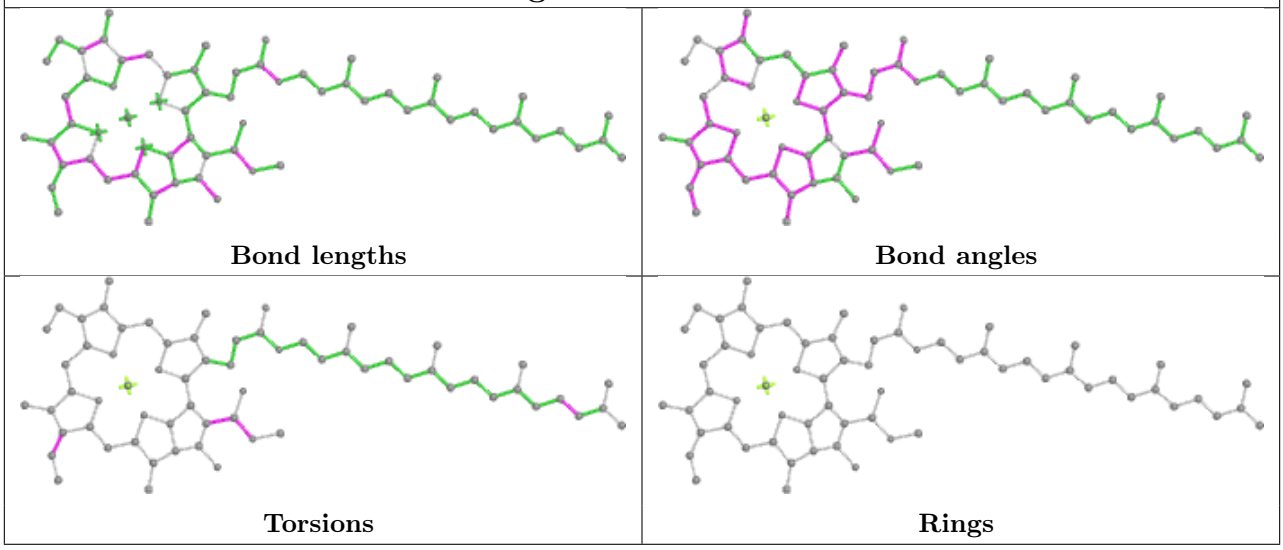
Ligand LHG e 101



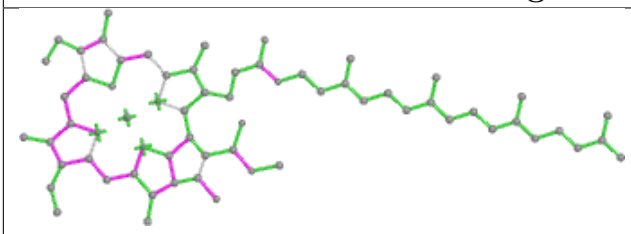
Ligand BCR B 619



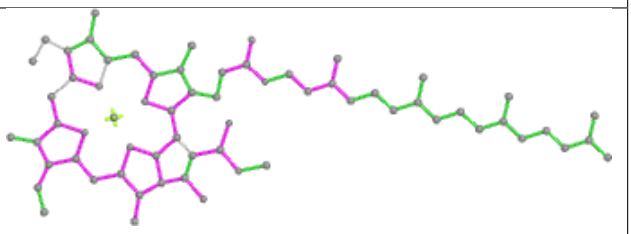
Ligand CLA d 401



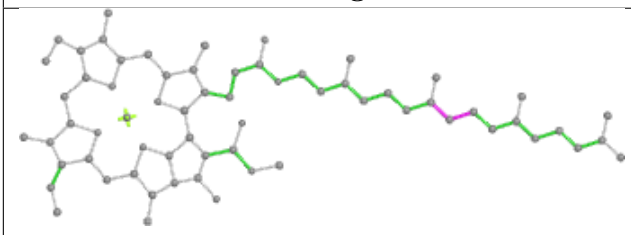
Ligand CLA b 617



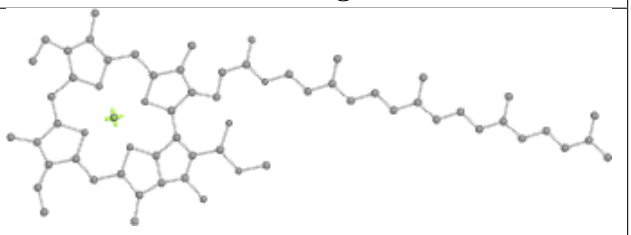
Bond lengths



Bond angles

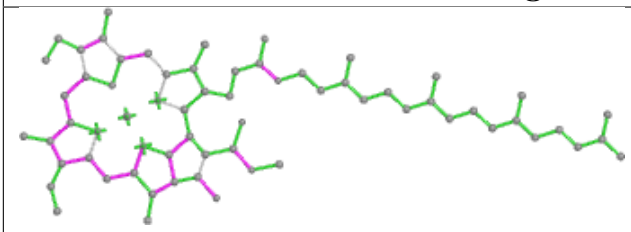


Torsions

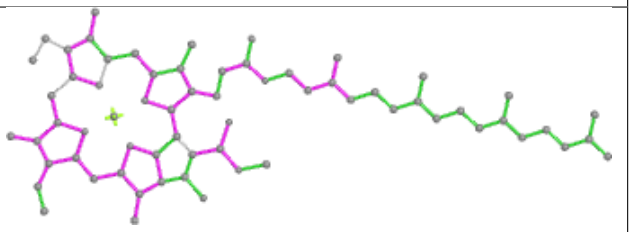


Rings

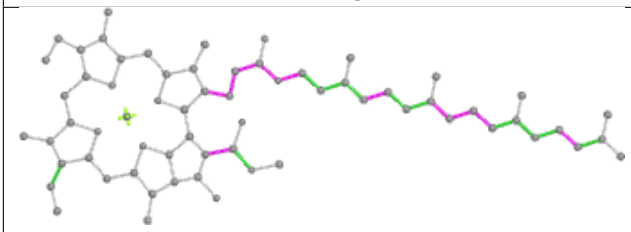
Ligand CLA B 602



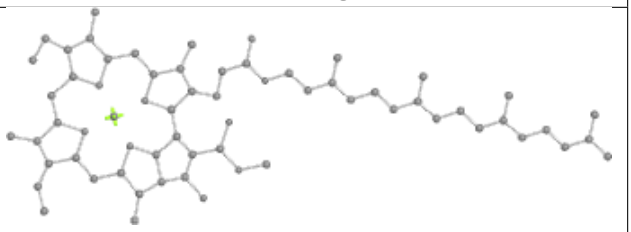
Bond lengths



Bond angles

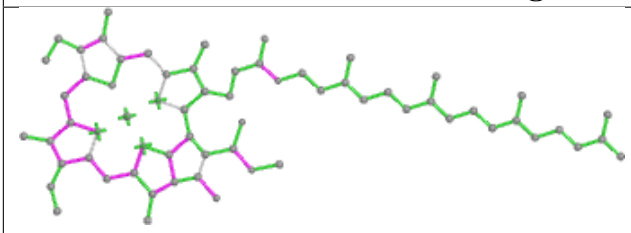


Torsions

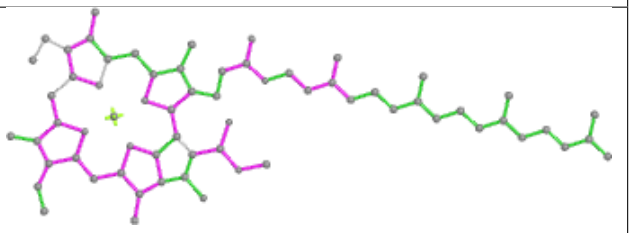


Rings

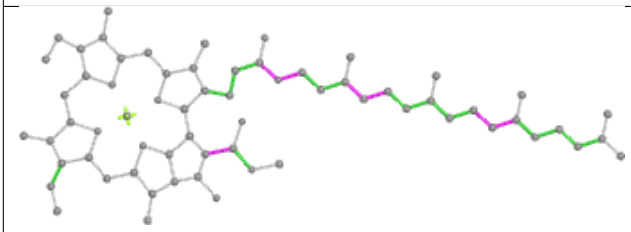
Ligand CLA b 621



Bond lengths



Bond angles



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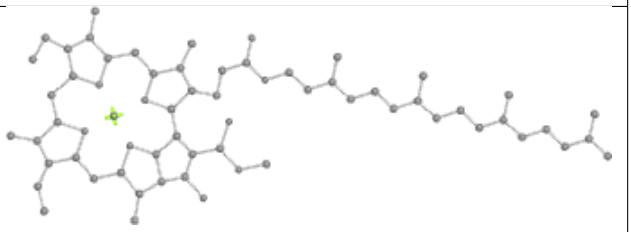
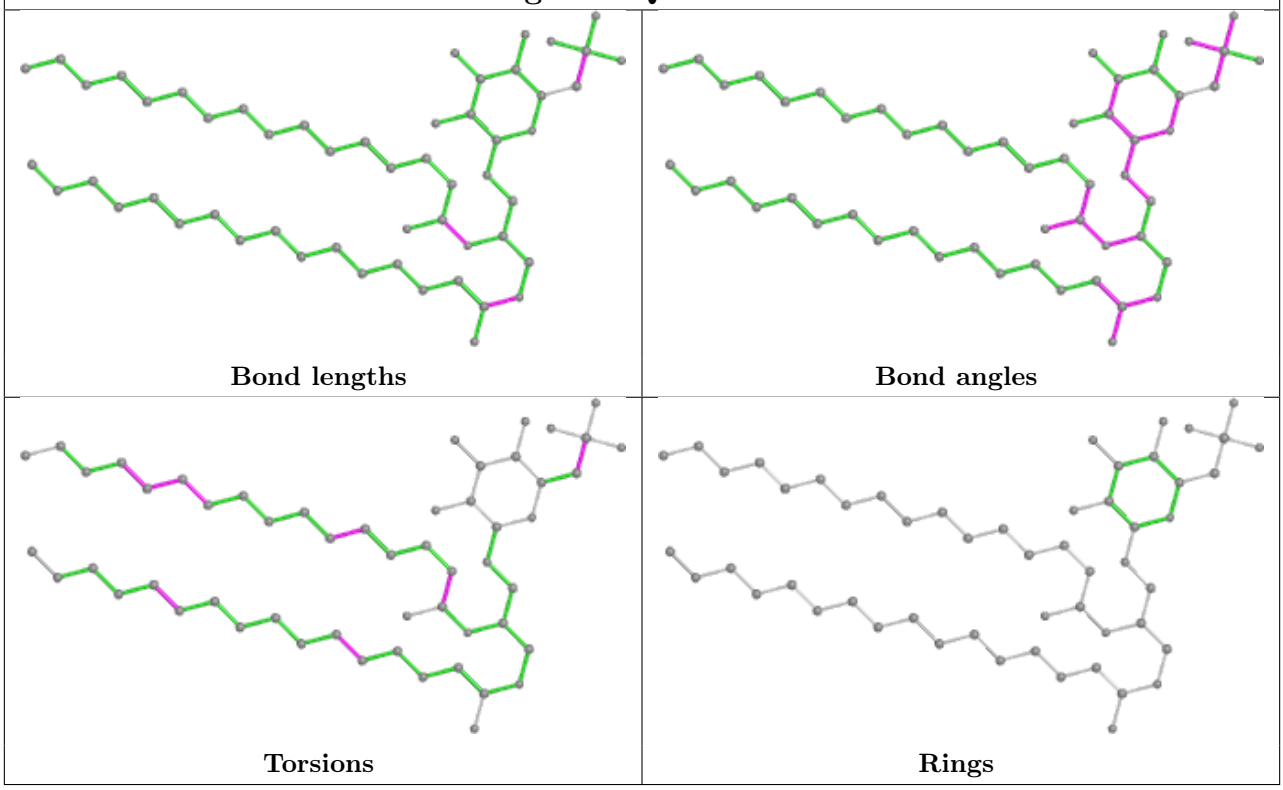
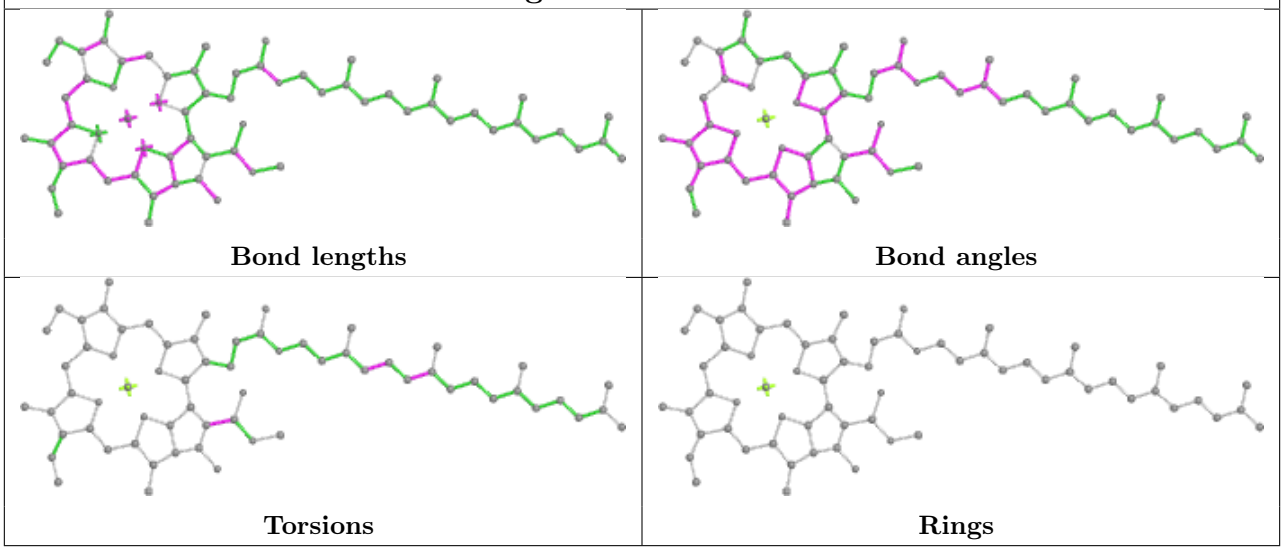


Rings

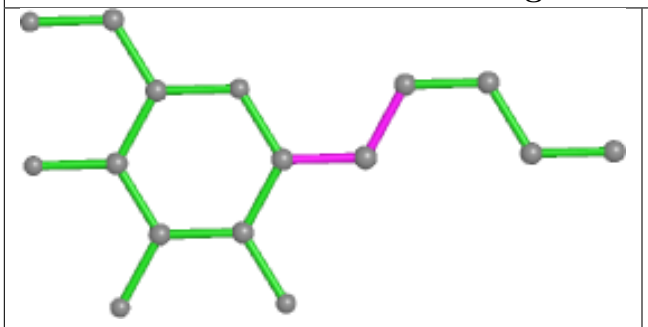
Ligand SQD A 411



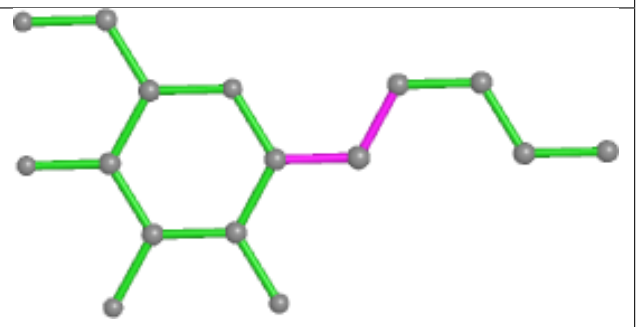
Ligand CLA B 605



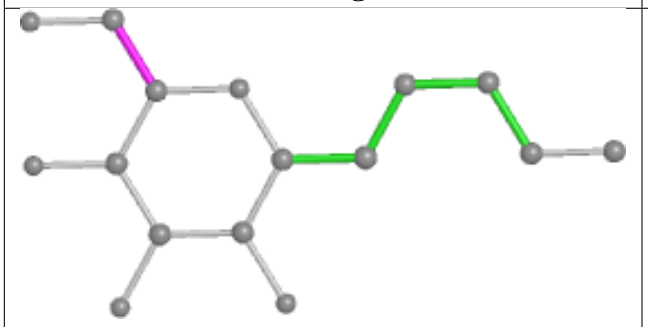
Ligand HTG d 411



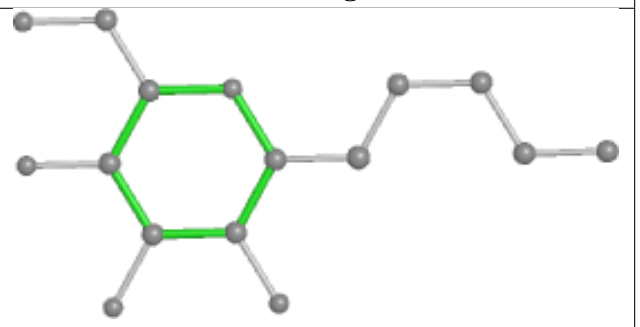
Bond lengths



Bond angles

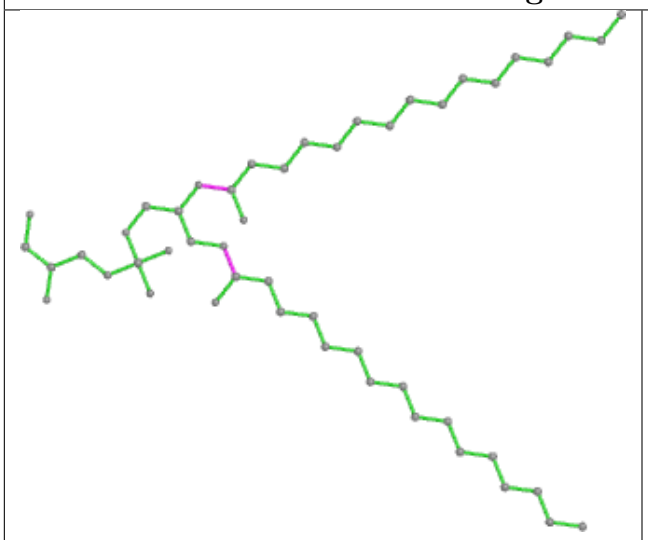


Torsions



Rings

Ligand LHG L 101



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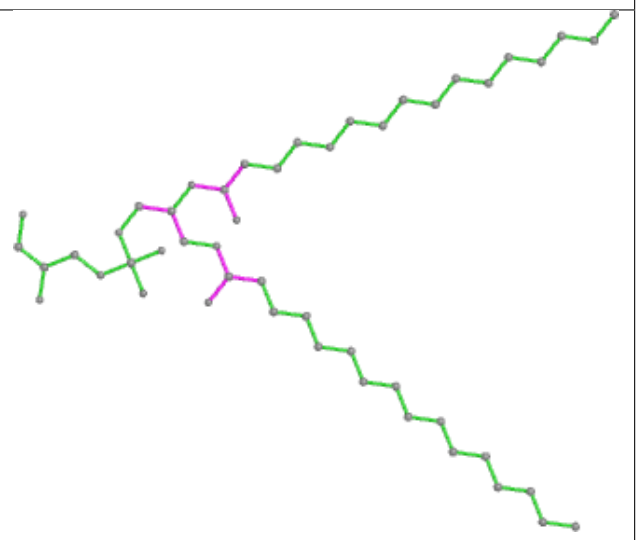
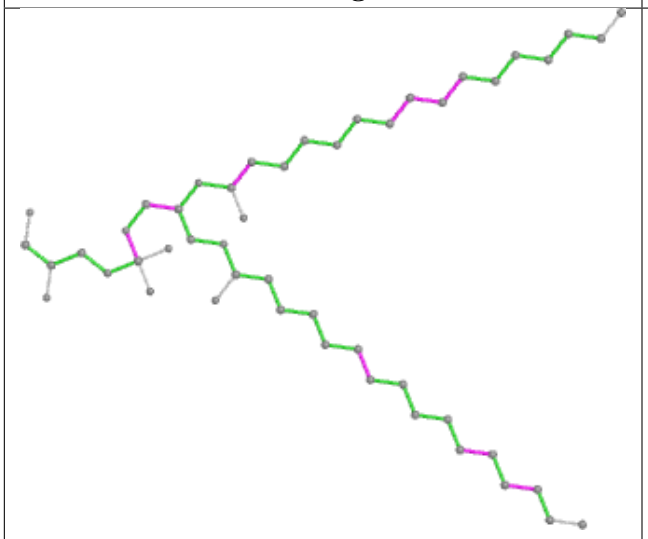
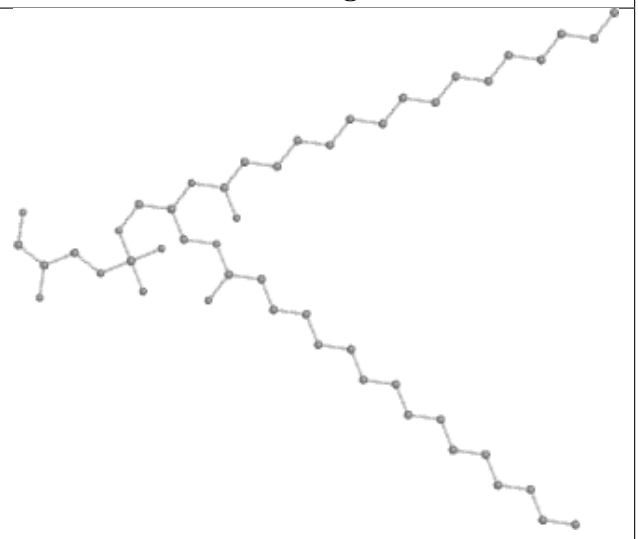


Bond angles

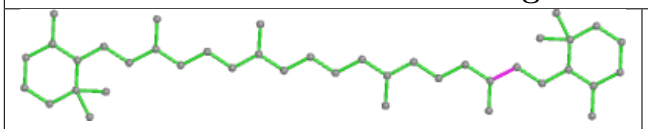


Torsions



Rings

Ligand BCR H 101



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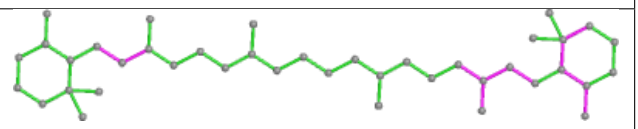
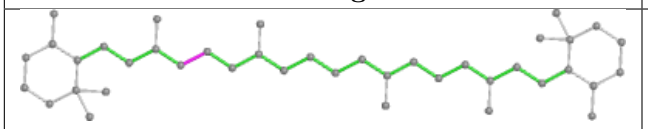
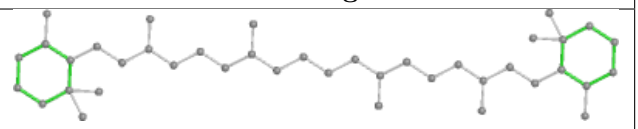


Bond angles

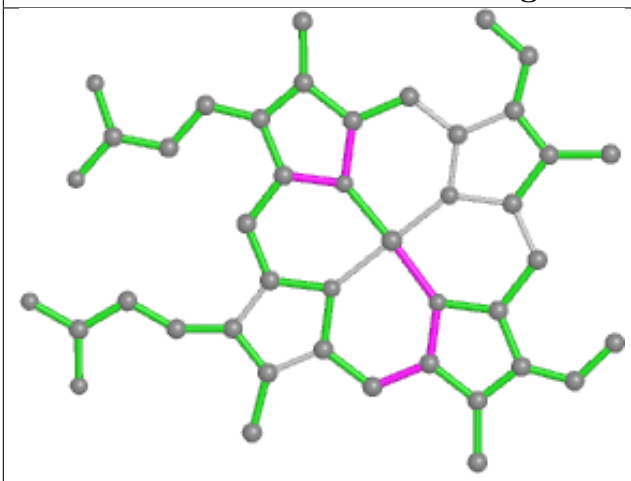


Torsions



Rings

Ligand HEM E 103



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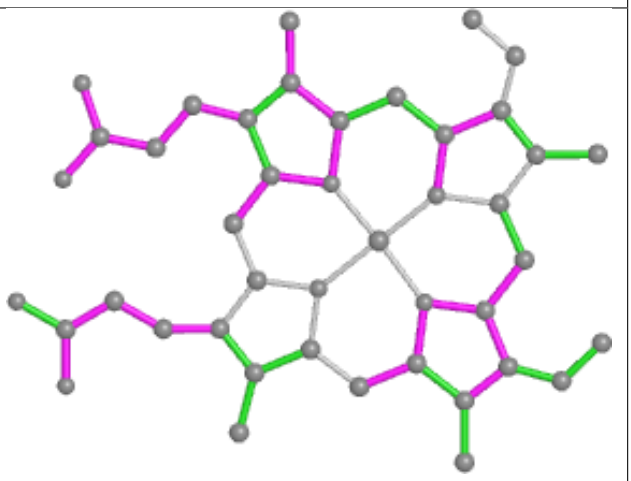
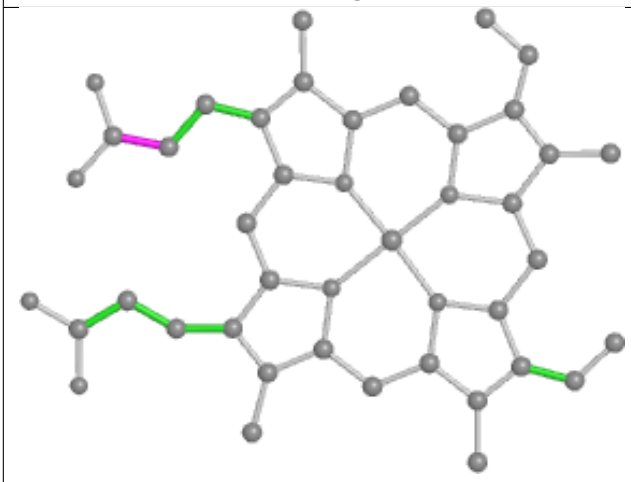


Bond angles



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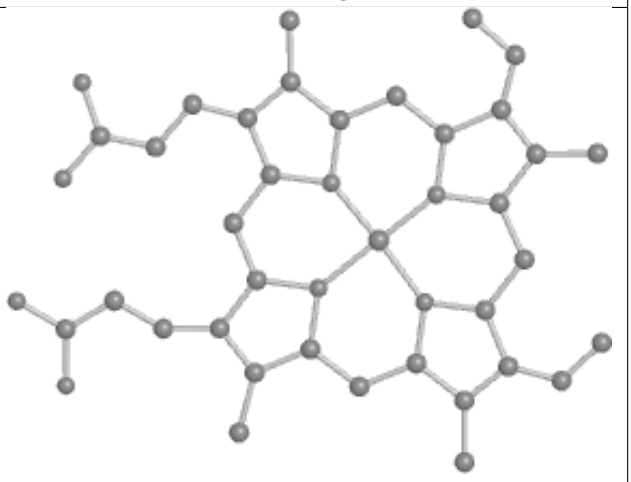
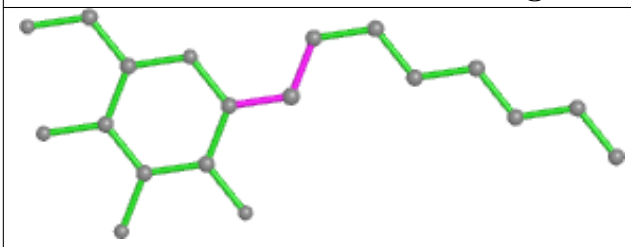


Rings

Ligand HTG c 523



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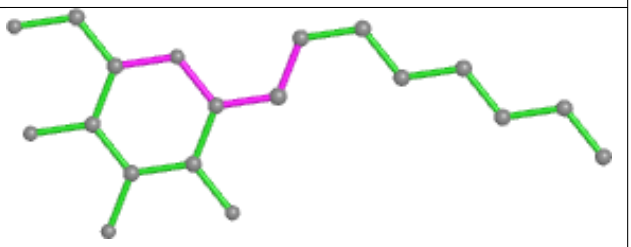
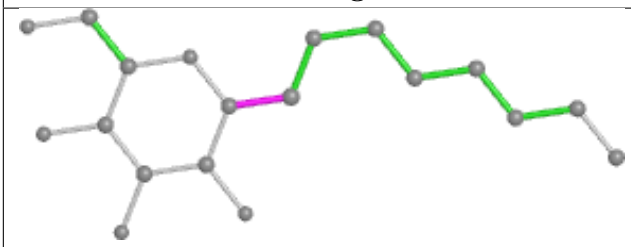


Bond angles



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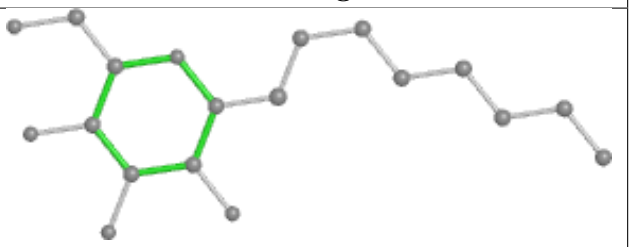
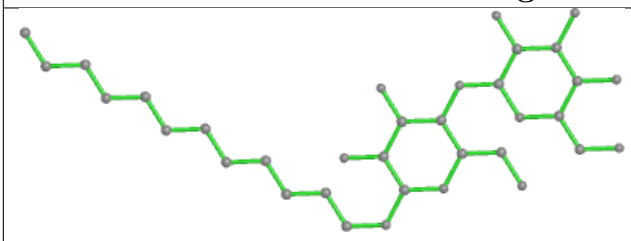


Rings

Ligand LMT M 102



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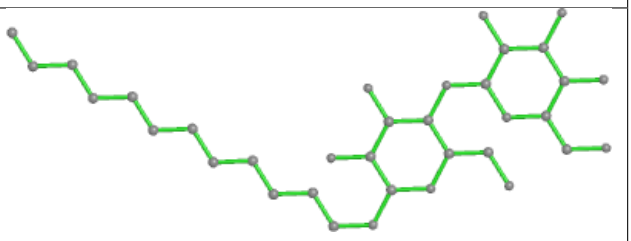
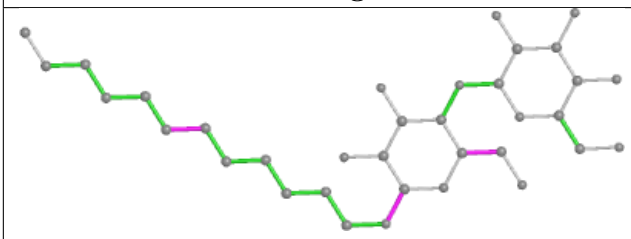


Bond angles



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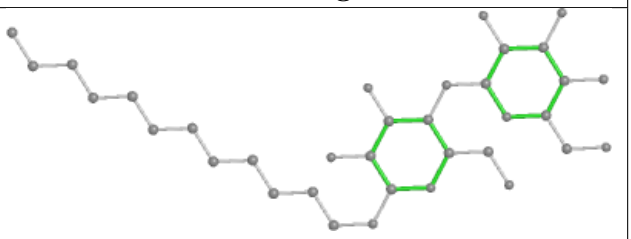
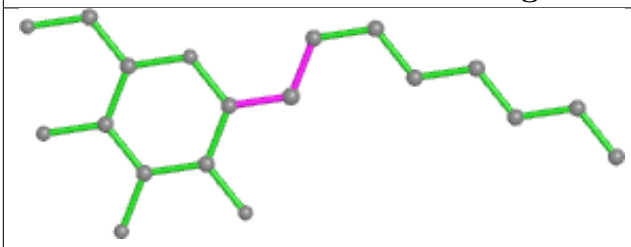


Rings

Ligand HTG C 522



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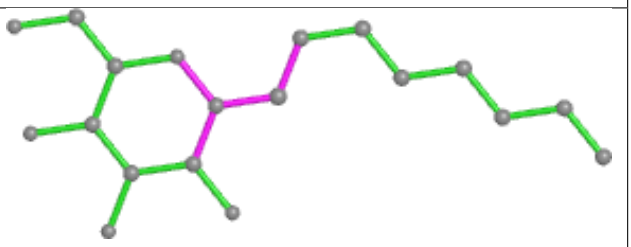
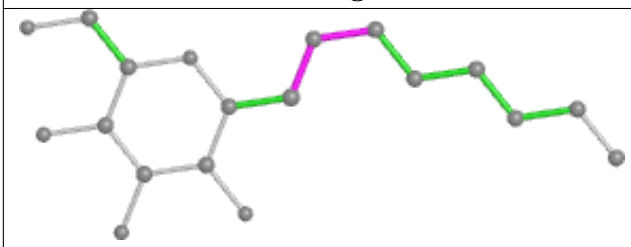


Bond angles



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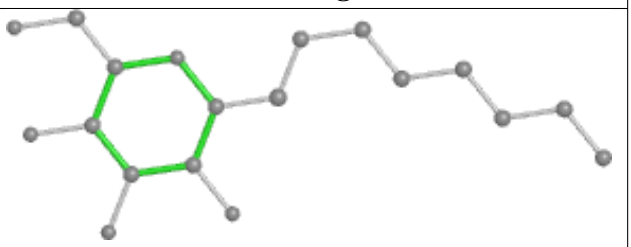
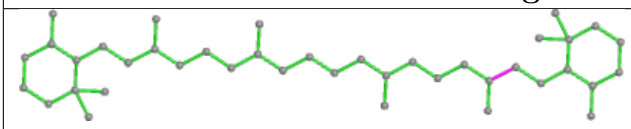


Rings

Ligand BCR C 516



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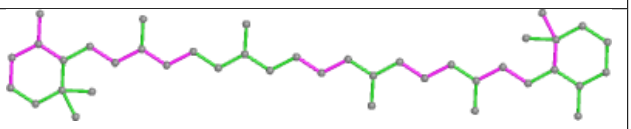
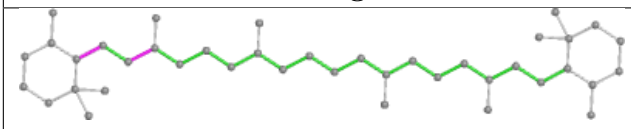


Bond angles



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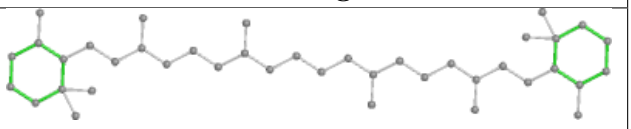
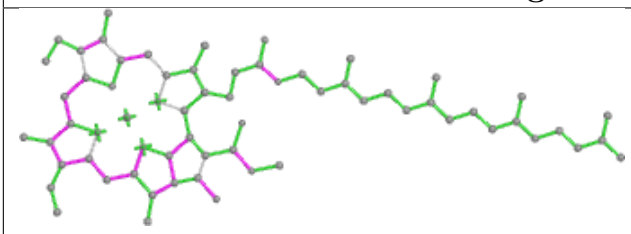


Rings

Ligand CLA b 608



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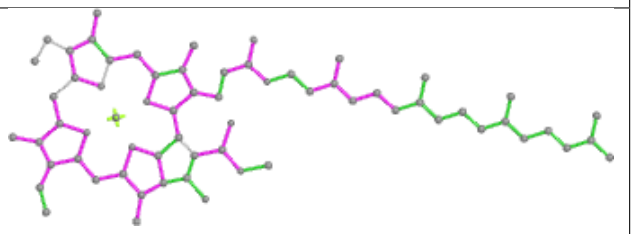
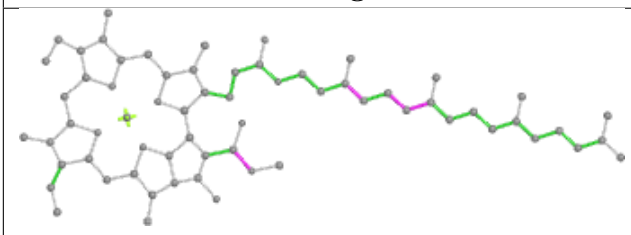


Bond angles



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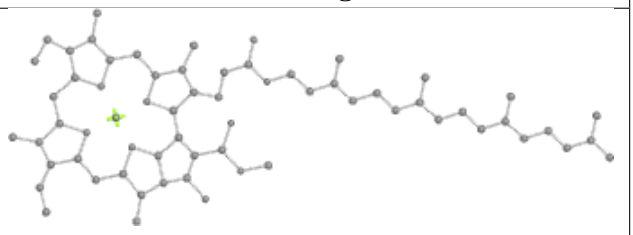
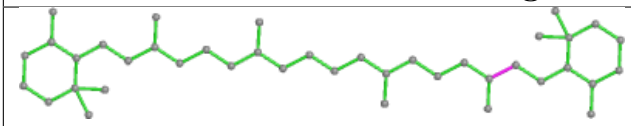


Rings

Ligand BCR Y 101



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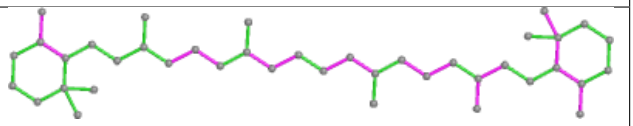
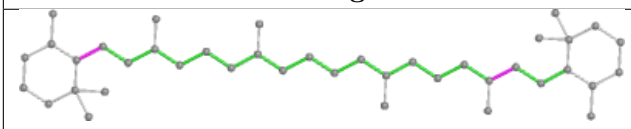


Bond angles



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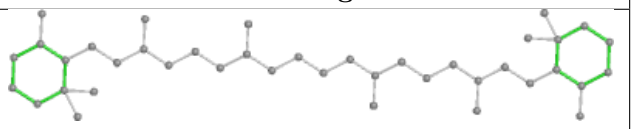
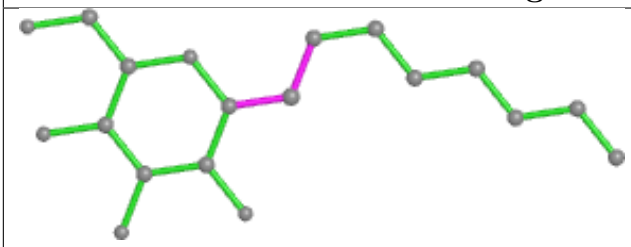


Rings

Ligand HTG c 522



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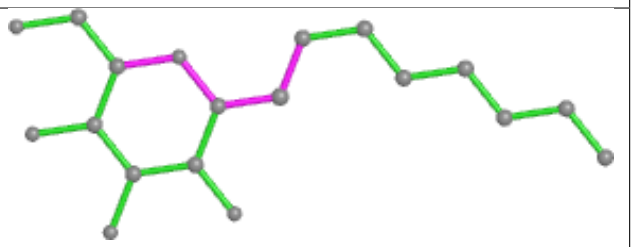
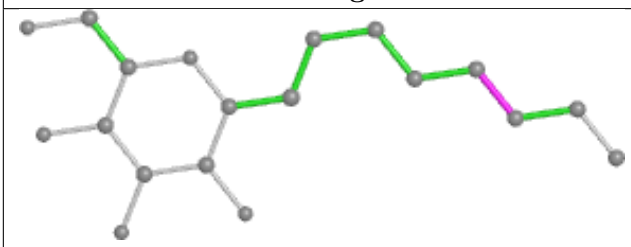


Bond angles



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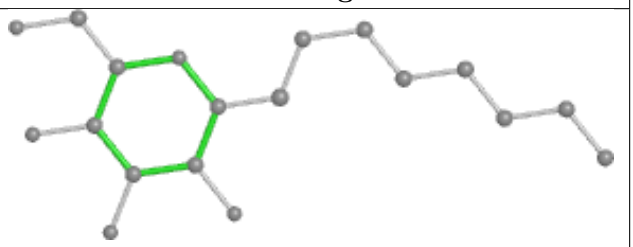
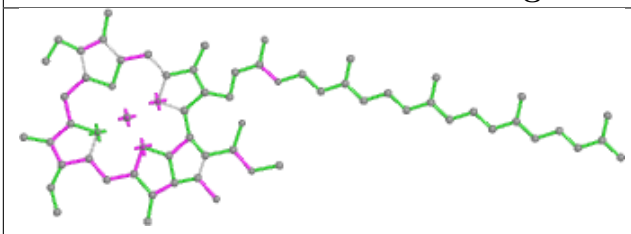


Rings

Ligand CLA A 405



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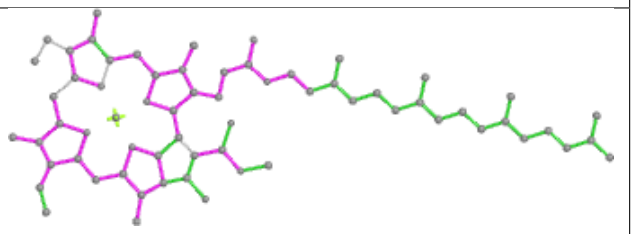
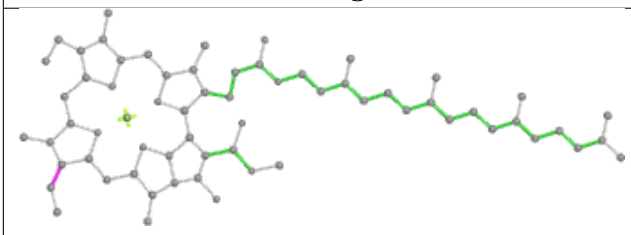


Bond angles



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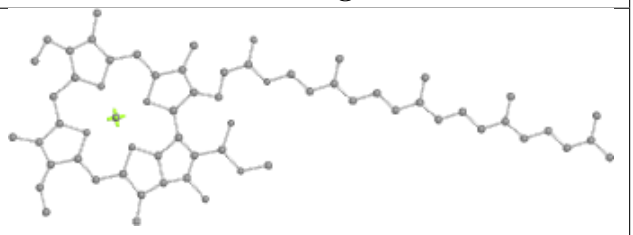
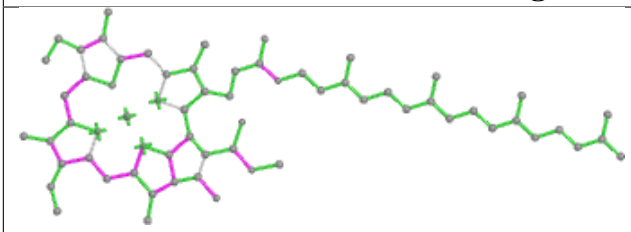


Rings

Ligand CLA c 513



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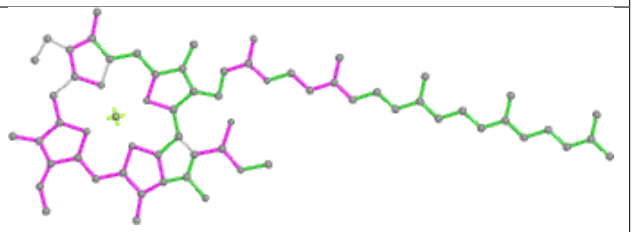
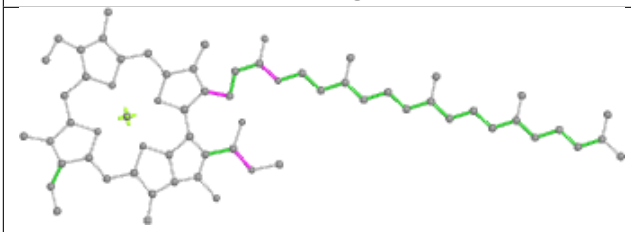


Bond angles



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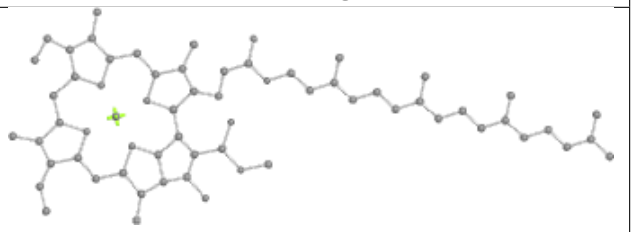
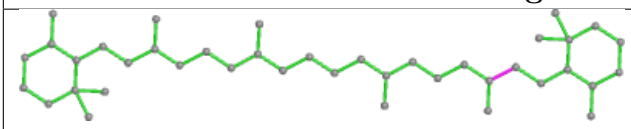
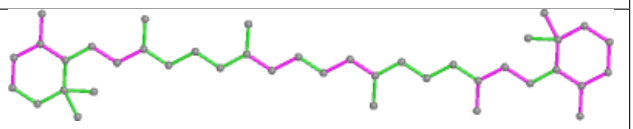


Rings

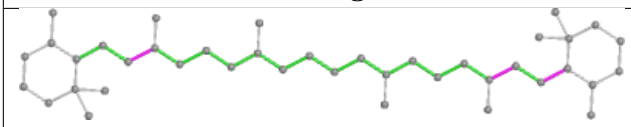
Ligand BCR d 405



Bond lengths



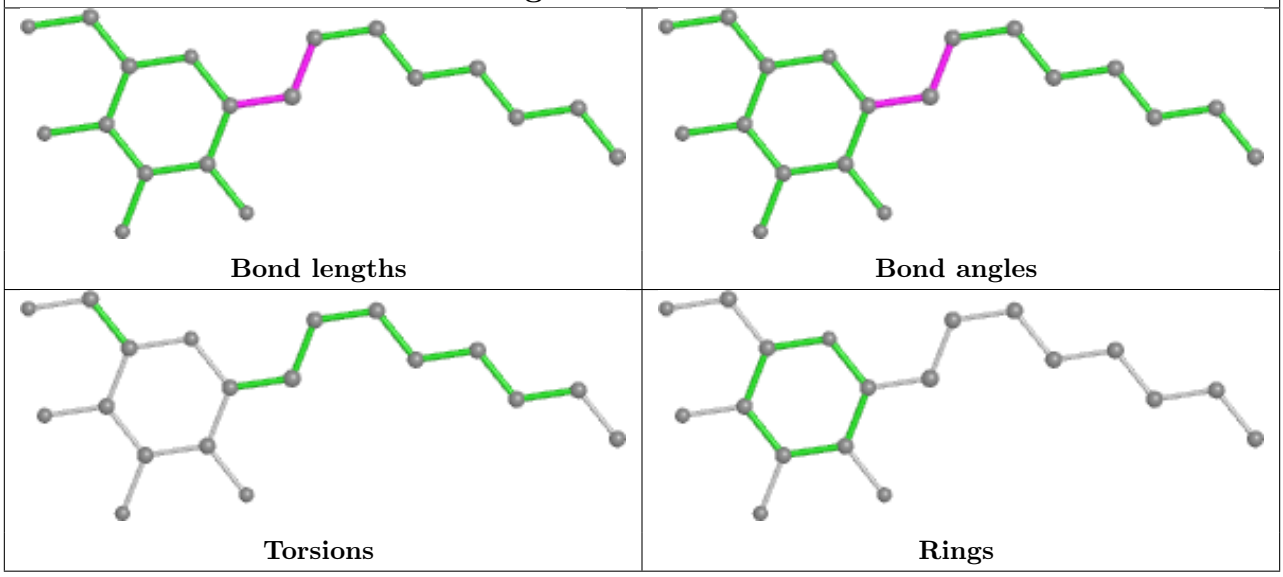
Bond angles



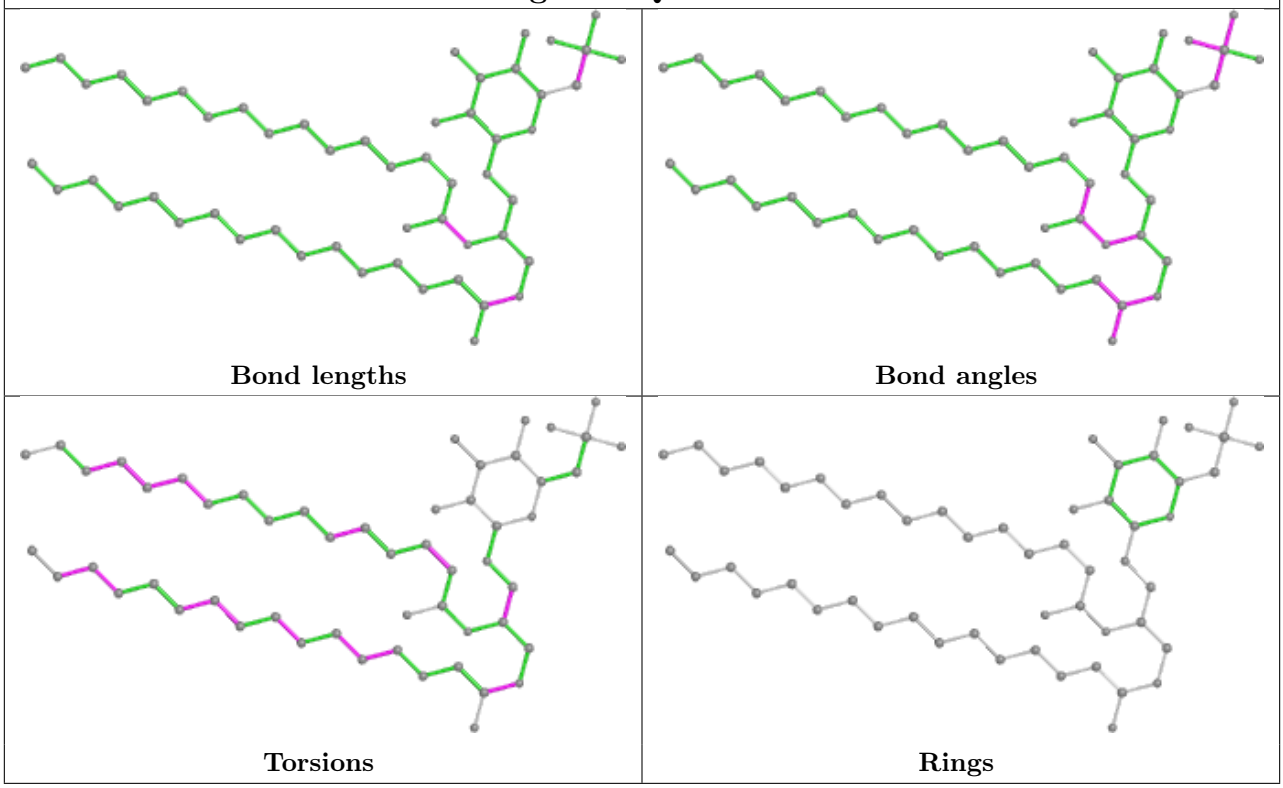
Torsions

Rings

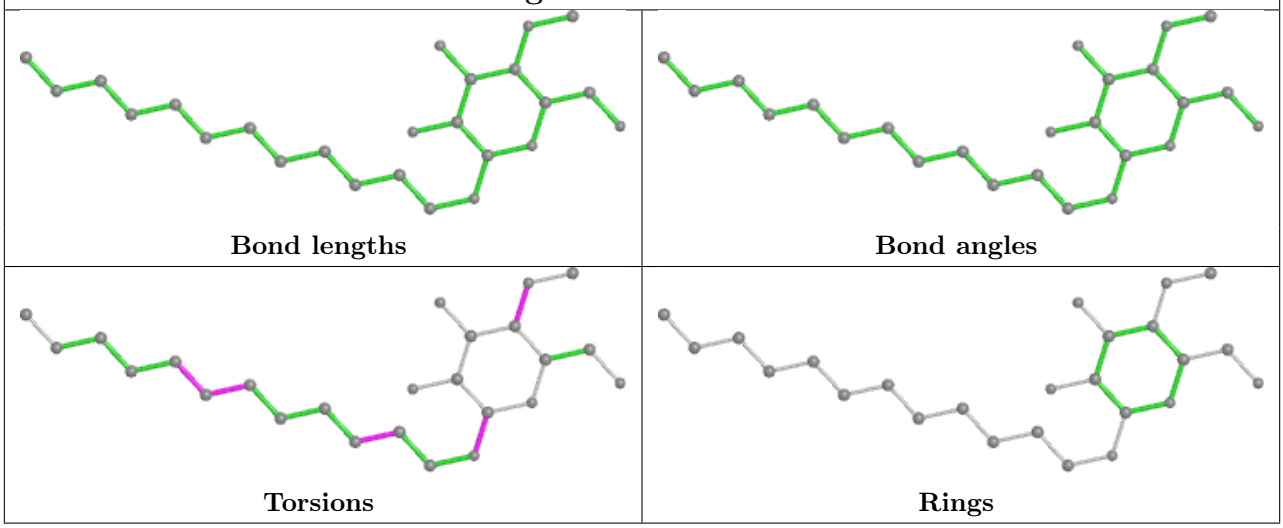
Ligand HTG b 603



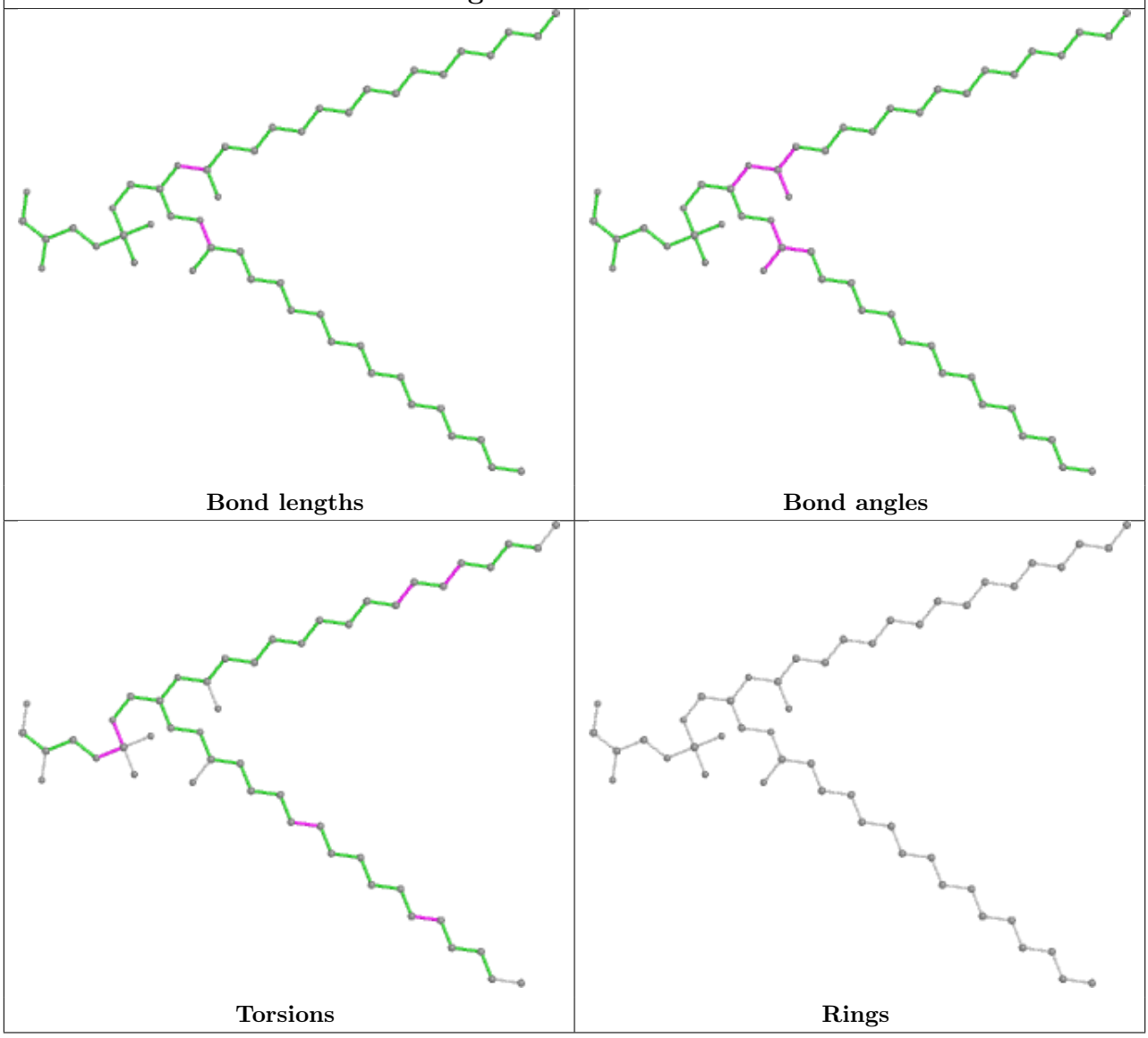
Ligand SQD a 402



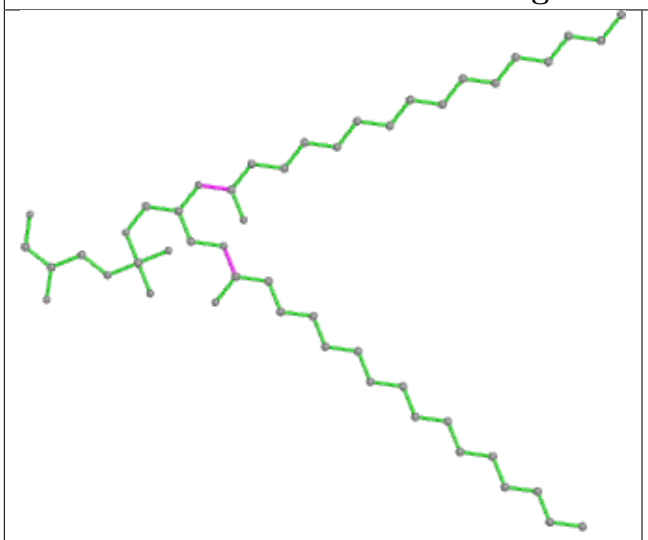
Ligand LMT b 626



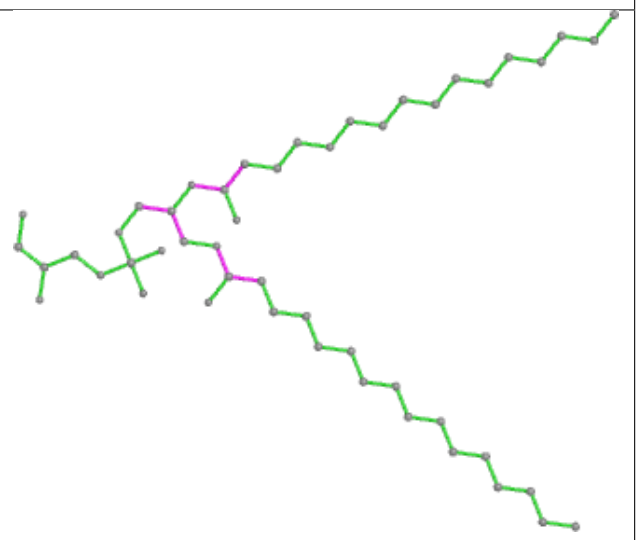
Ligand LHG D 409



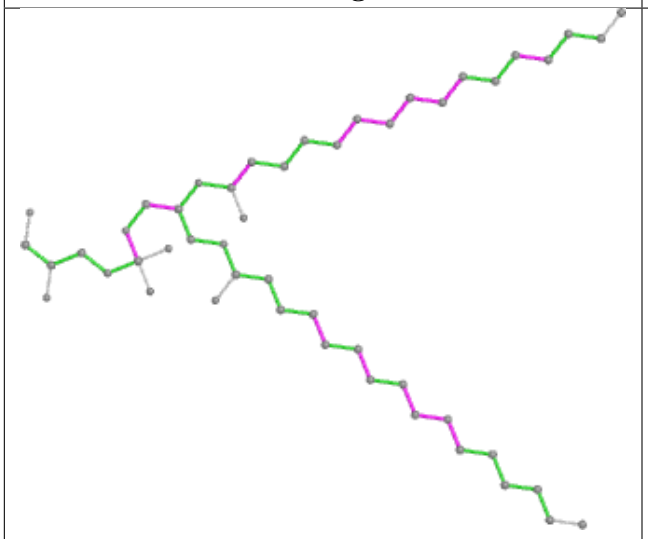
Ligand LHG l 102



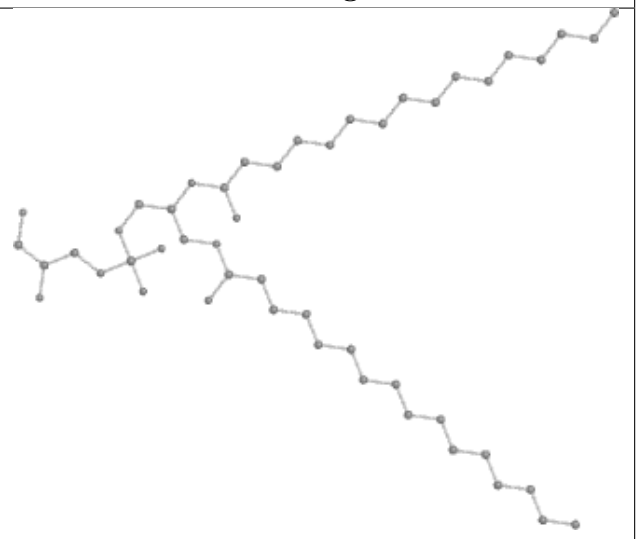
Bond lengths



Bond angles

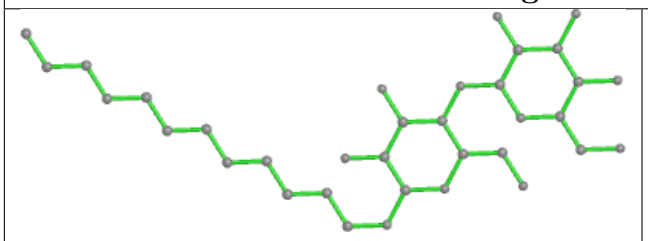


Torsions



Rings

Ligand LMT D 402



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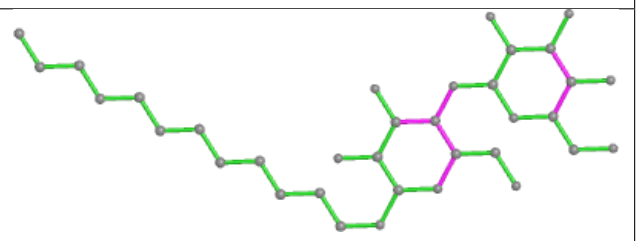
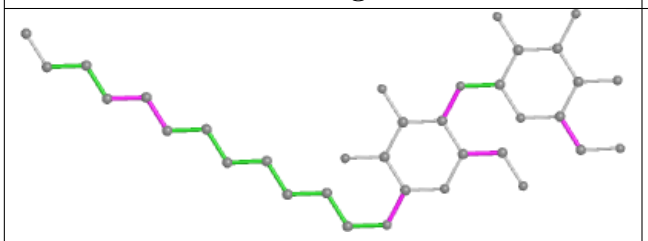


Bond angles



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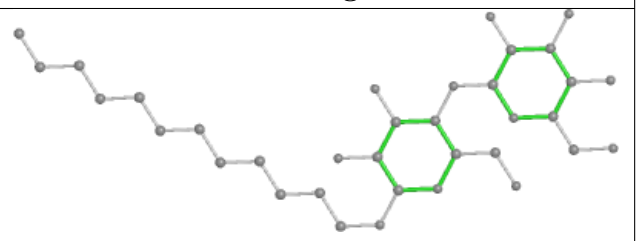
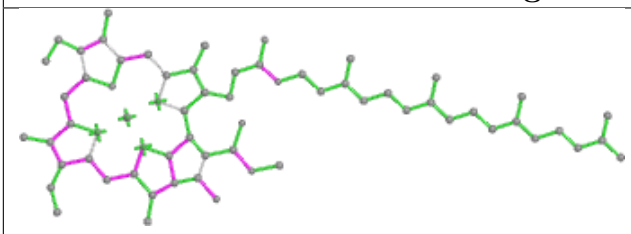


Rings

Ligand CLA A 409



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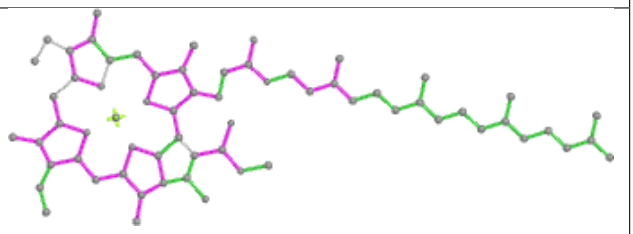
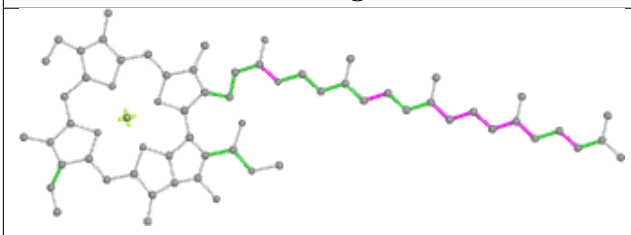
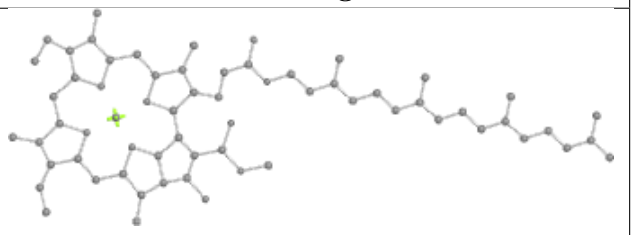


Bond angles

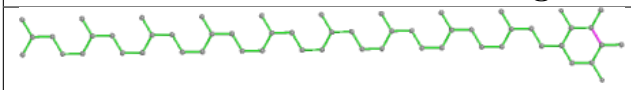


Torsions

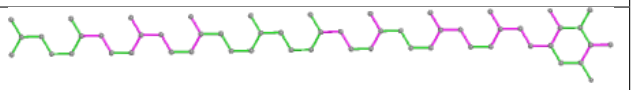


Rings

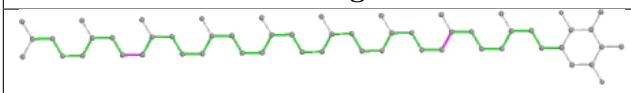
Ligand PL9 d 406



Bond lengths



Bond angles



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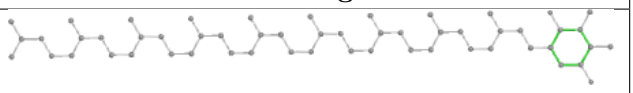
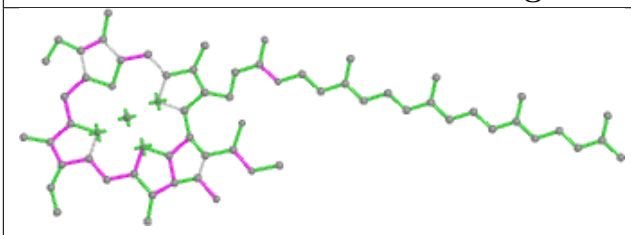
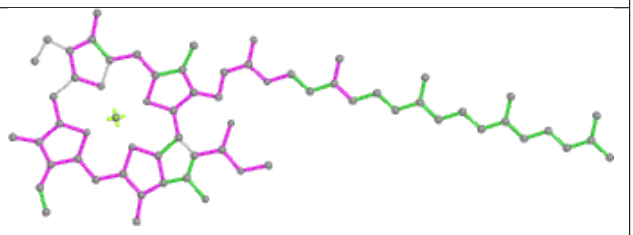


Rings

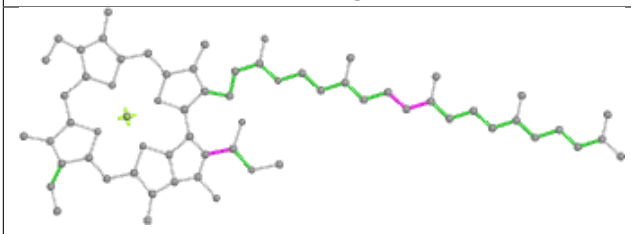
Ligand CLA B 604



Bond lengths



Bond angles



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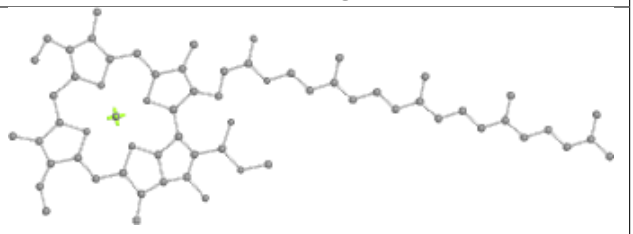
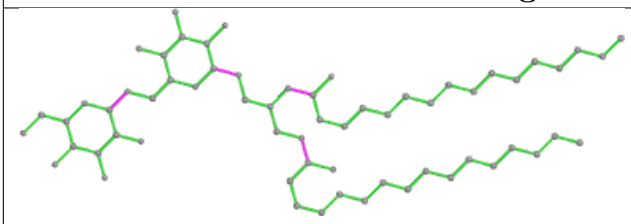


Rings

Ligand DGD D 407



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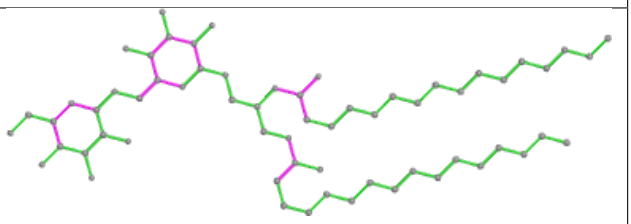
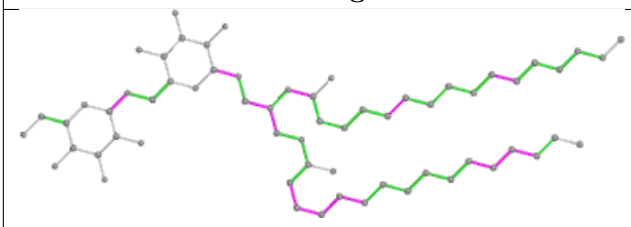


Bond angles



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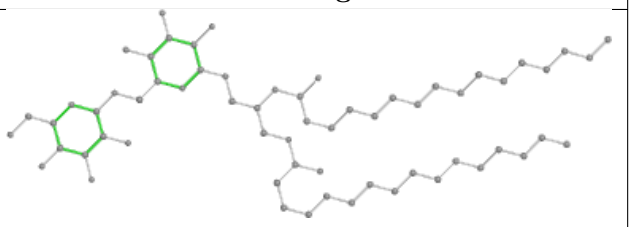
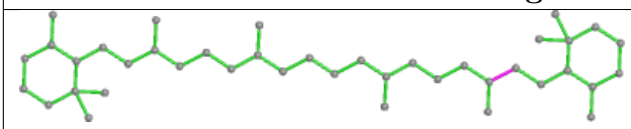


Rings

Ligand BCR h 101



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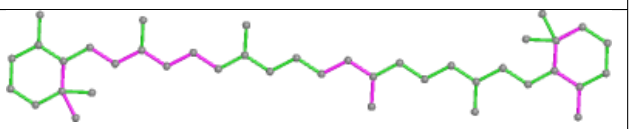
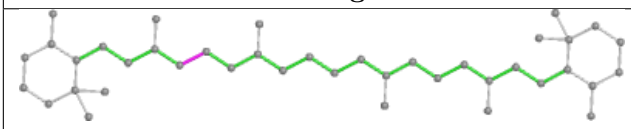
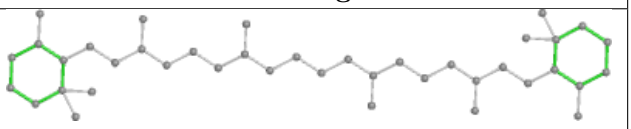


Bond angles

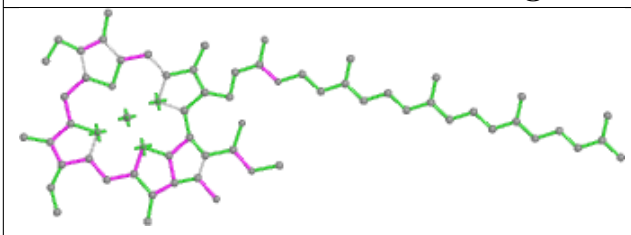


Torsions



Rings

Ligand CLA C 504



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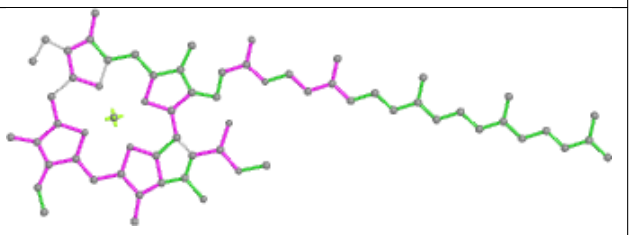
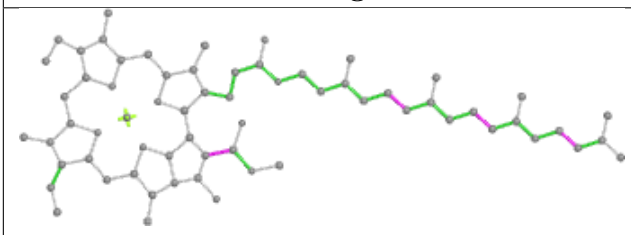
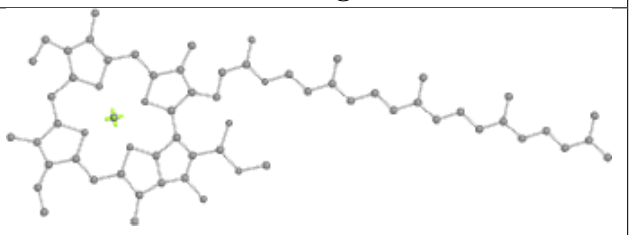


Bond angles

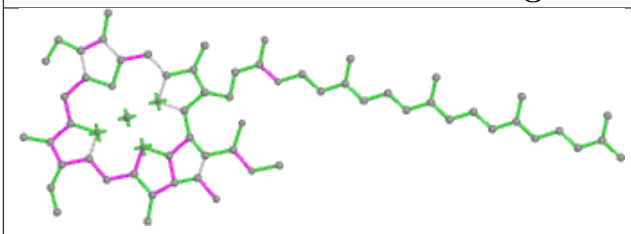


Torsions



Rings

Ligand CLA B 612



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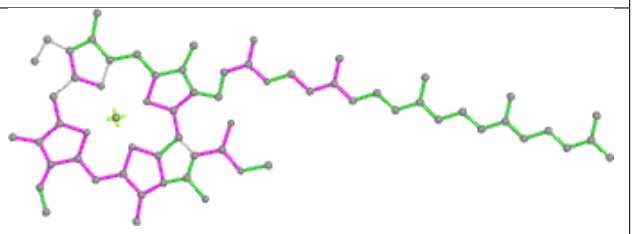
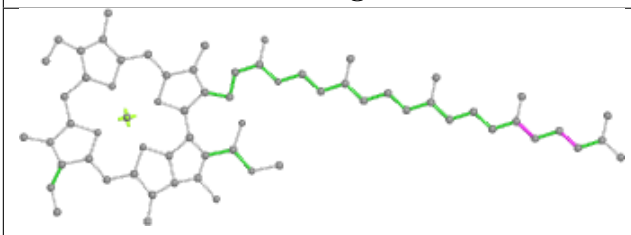


Bond angles



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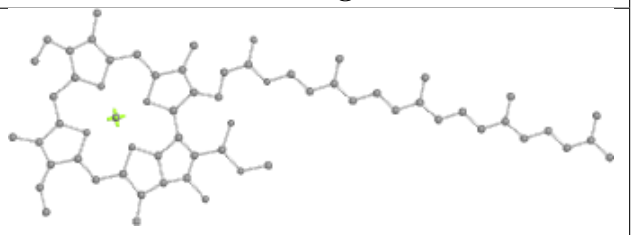
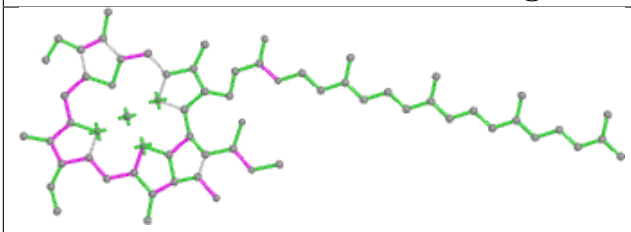


Rings

Ligand CLA D 404



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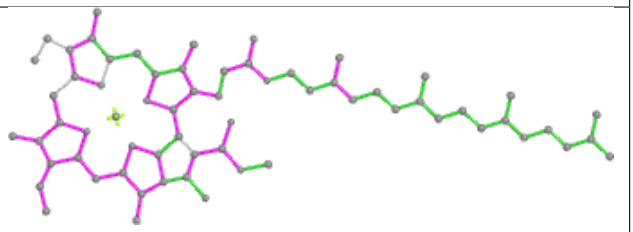
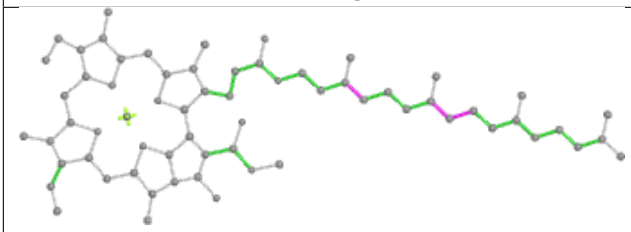


Bond angles



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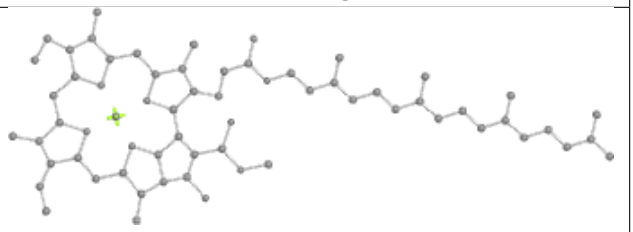
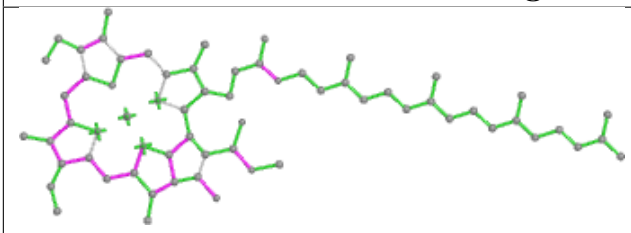


Rings

Ligand CLA C 507



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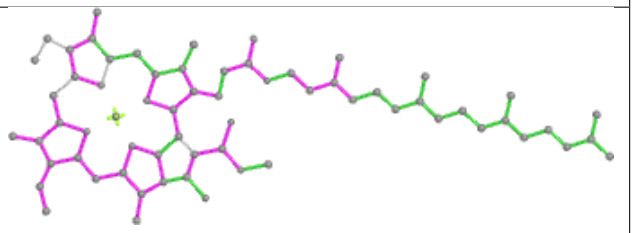
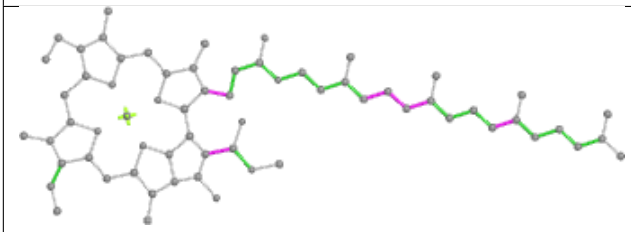
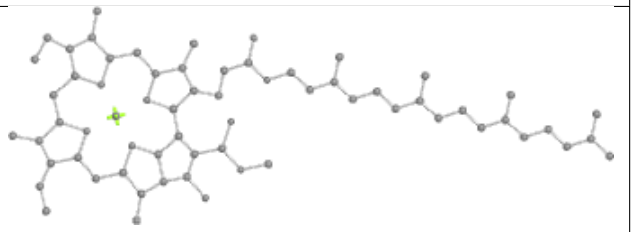


Bond angles

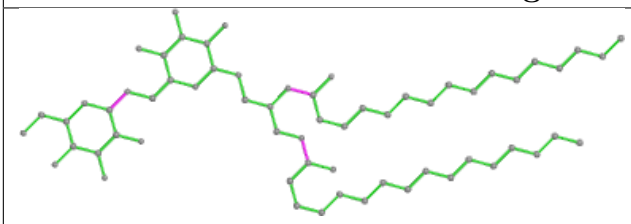


Torsions



Rings

Ligand DGD d 407



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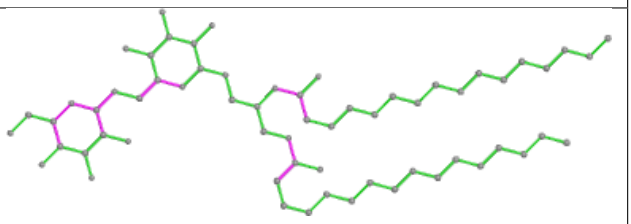
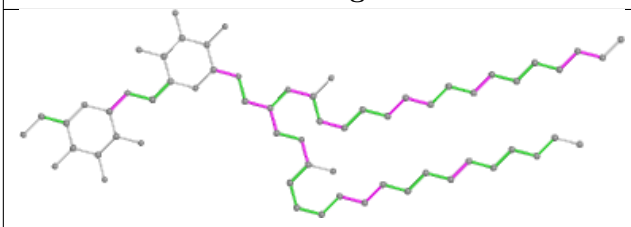


Bond angles



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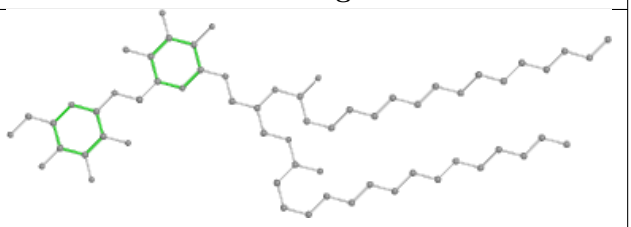
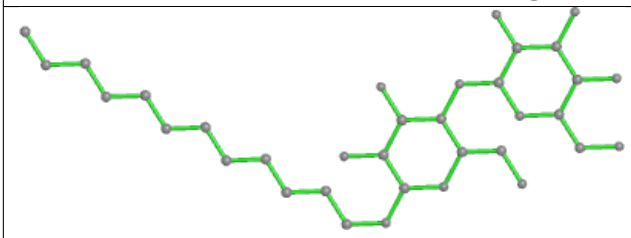


Rings

Ligand LMT a 417



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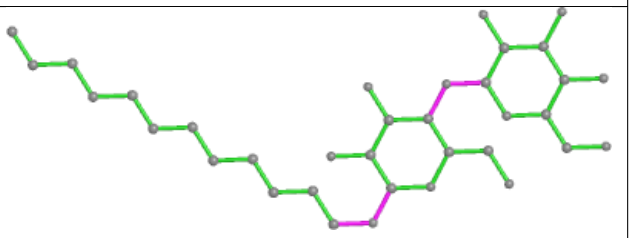
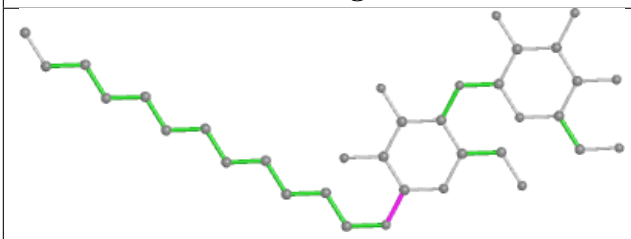
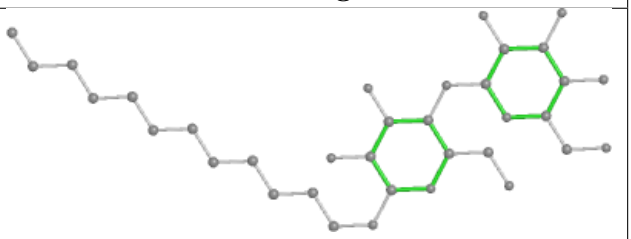


Bond angles

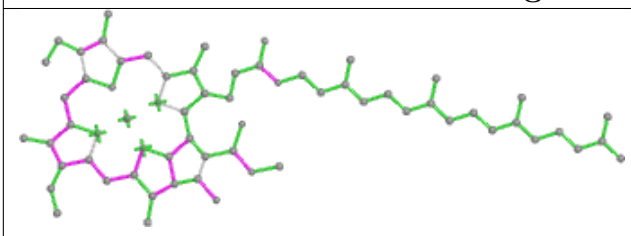


Torsions

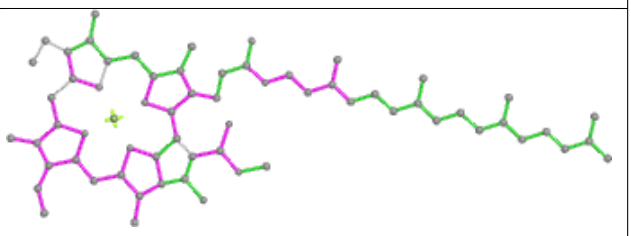


Rings

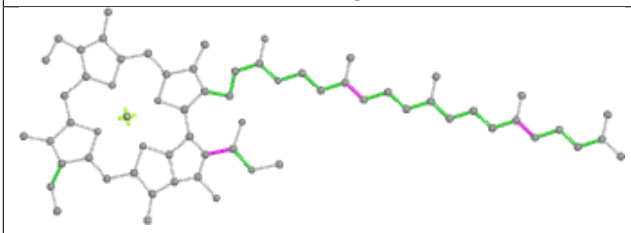
Ligand CLA C 505



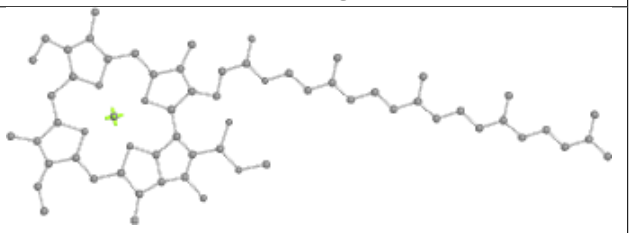
Bond lengths



Bond angles

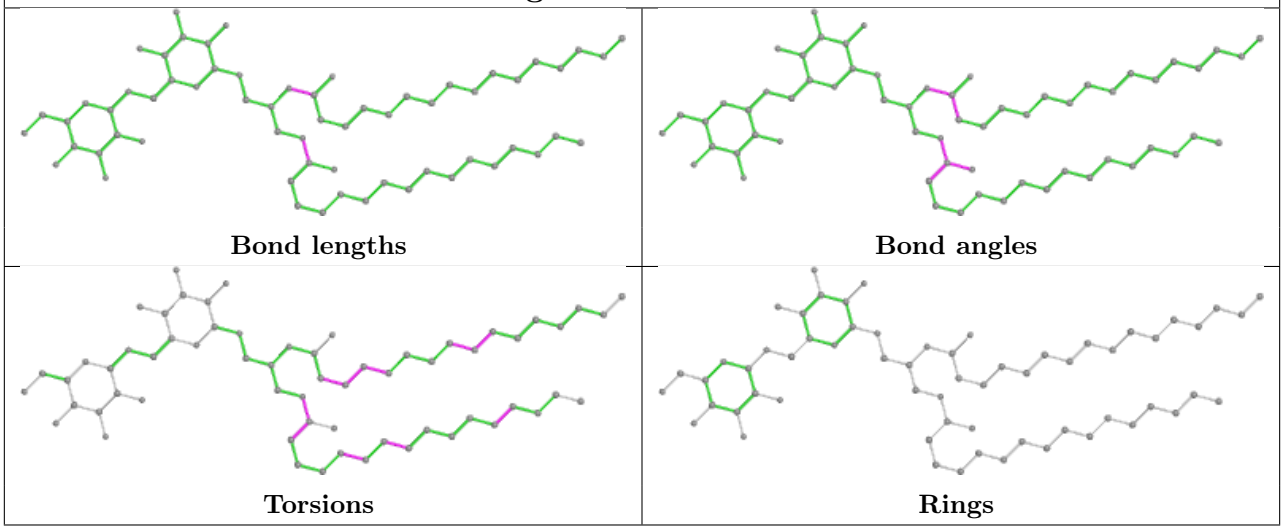


Torsions

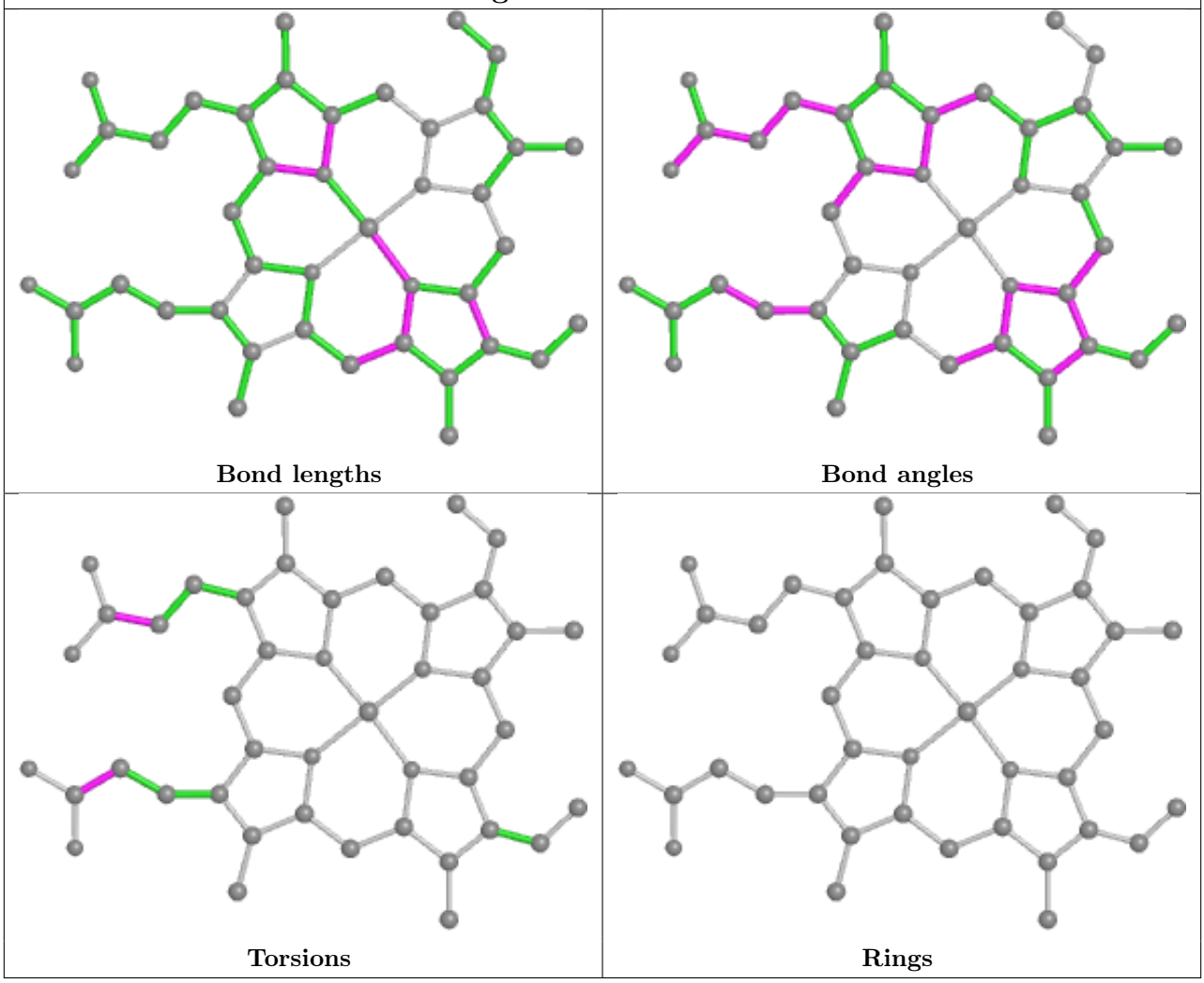


Rings

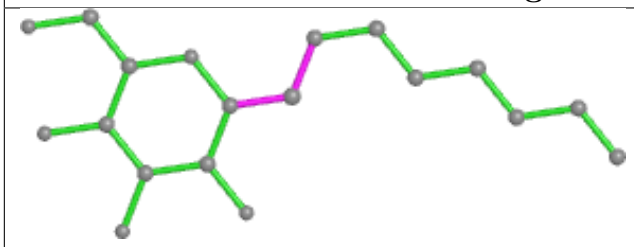
Ligand DGD c 519



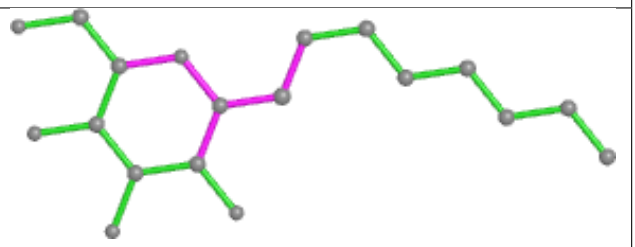
Ligand HEM e 102



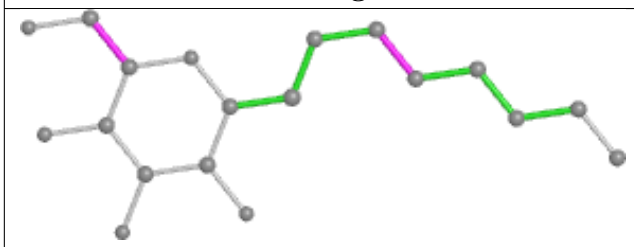
Ligand HTG b 628



Bond lengths



Bond angles



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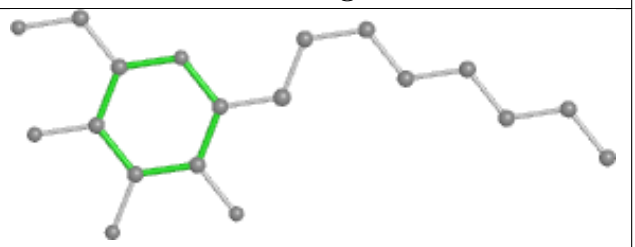
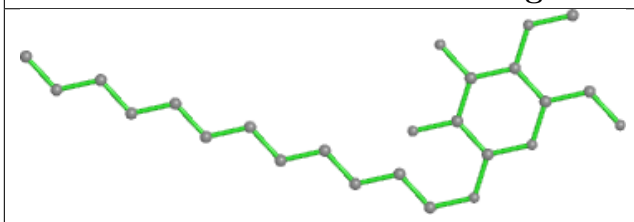


Rings

Ligand LMT b 602



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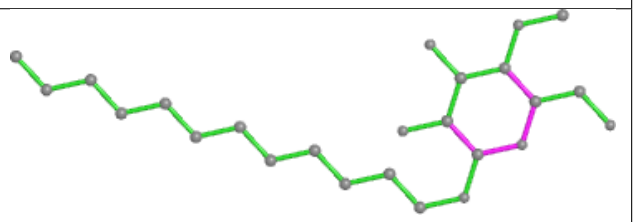
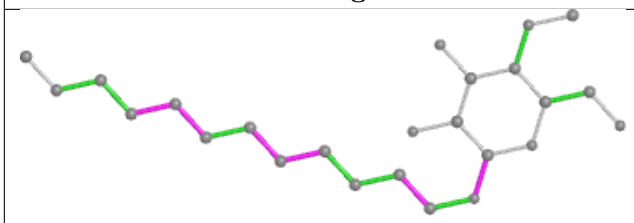


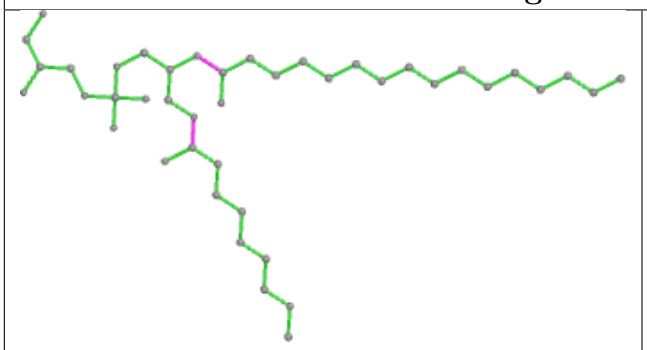
Bond angles



Torsions

Rings

Ligand LHG E 101



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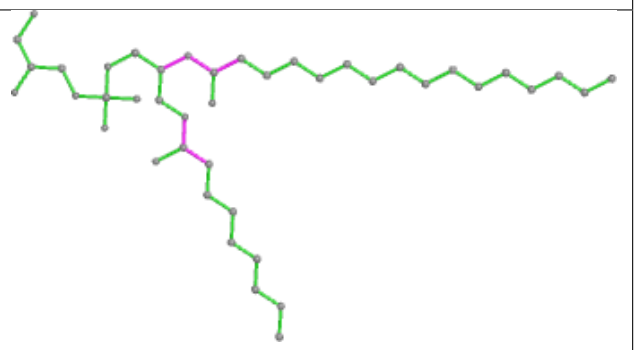
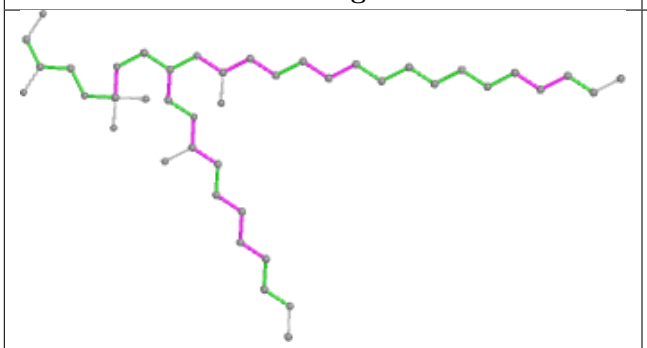


Bond angles



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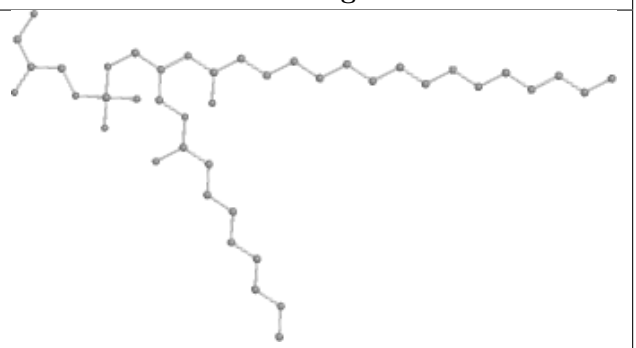
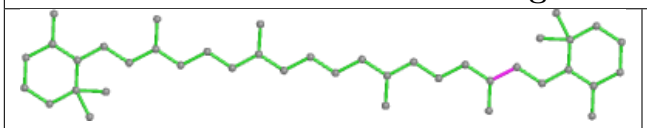


Rings

Ligand BCR t 101



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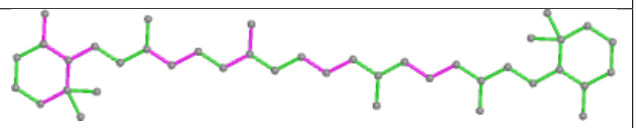
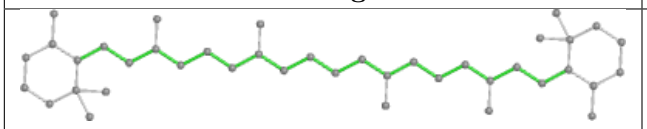


Bond angles



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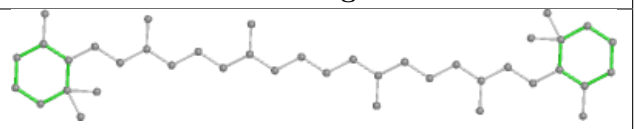
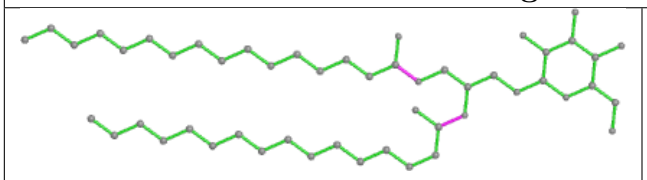
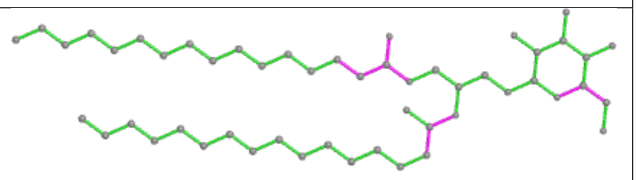


Rings

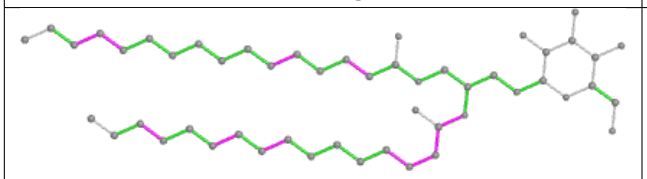
Ligand LMG C 520



Bond lengths



Bond angles



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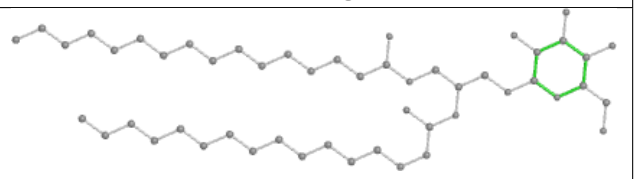
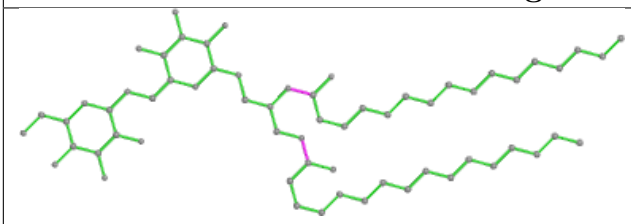


Rings

Ligand DGD c 518



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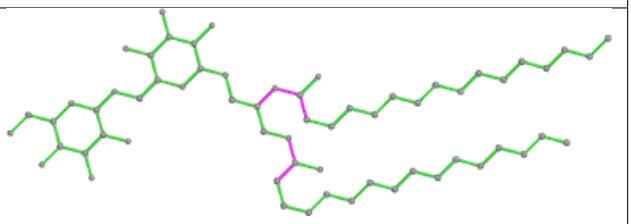
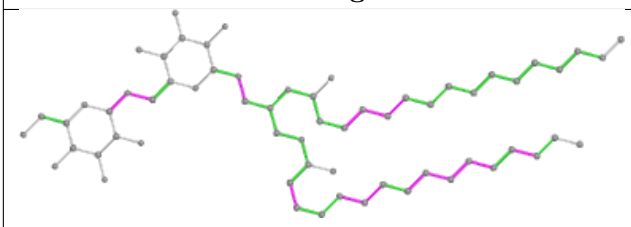
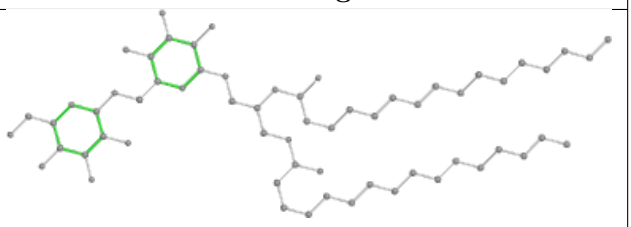


Bond angles

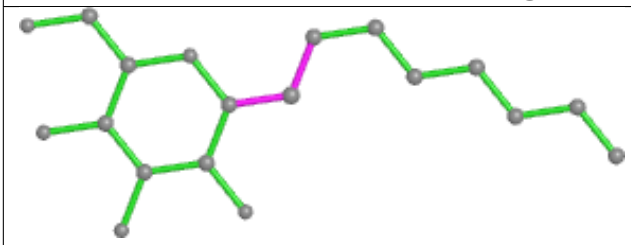


Torsions

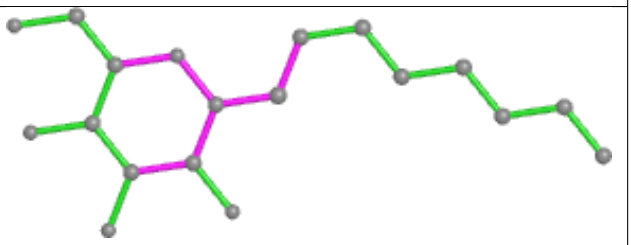


Rings

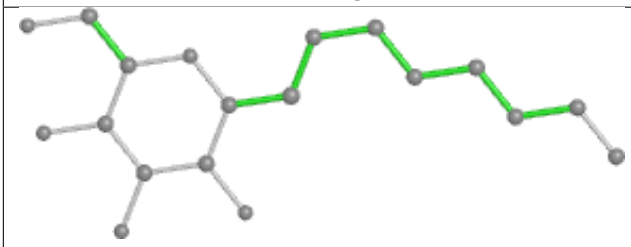
Ligand HTG B 624



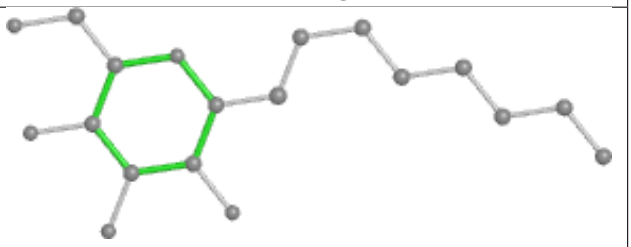
Bond lengths



Bond angles

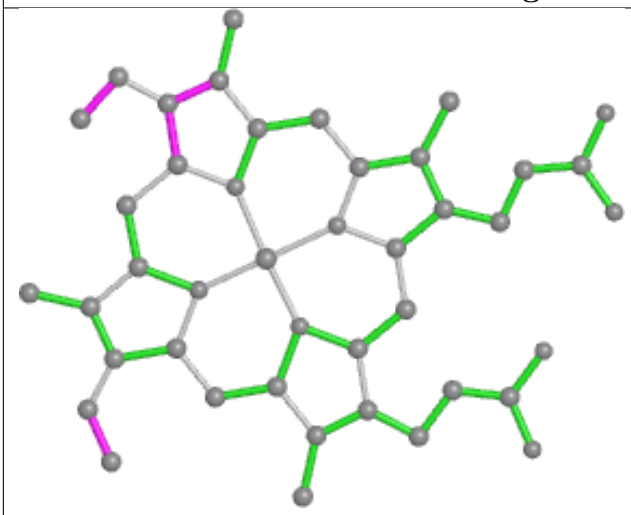


Torsions



Rings

Ligand HEC V 203



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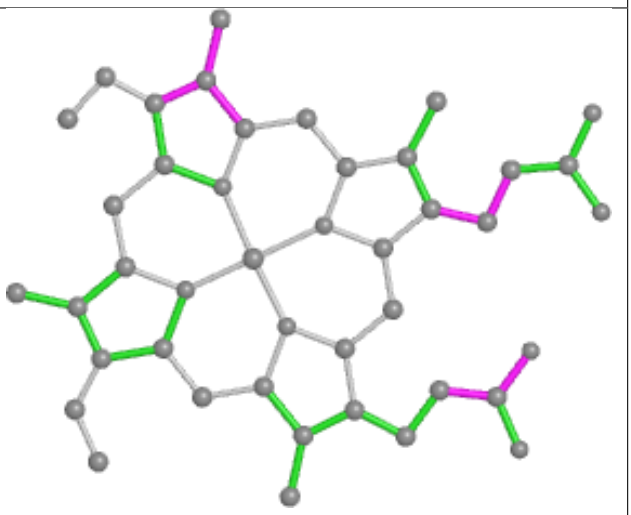
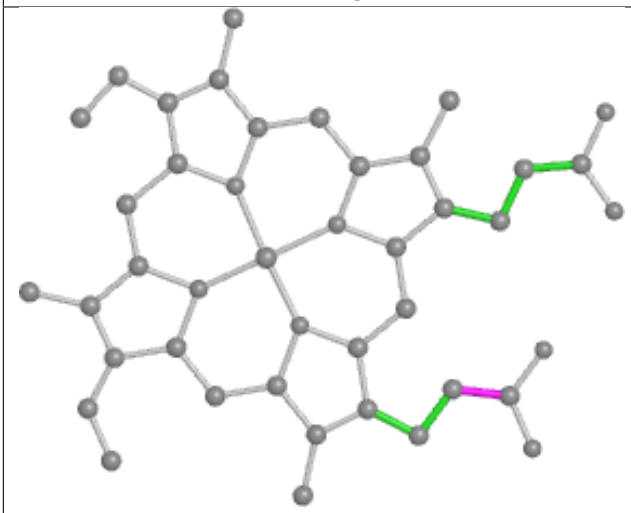
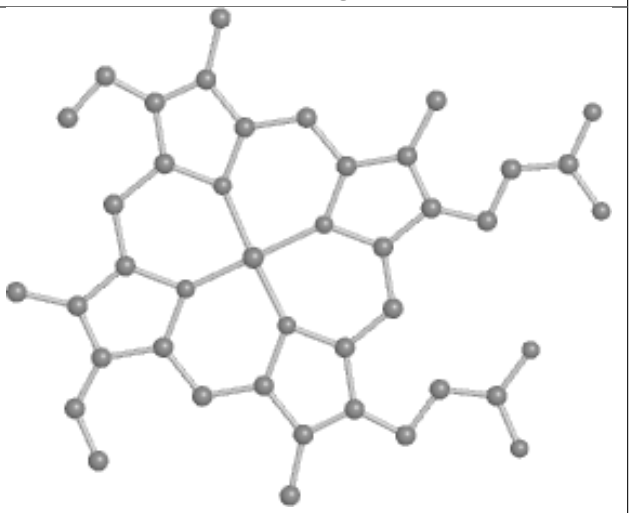


Bond angles

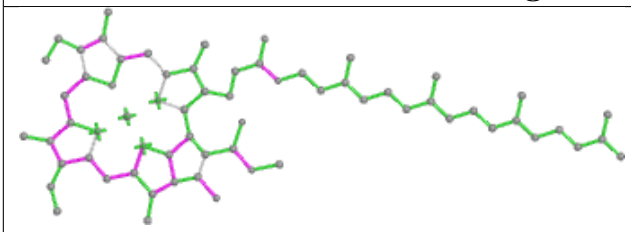


Torsions



Rings

Ligand CLA B 611



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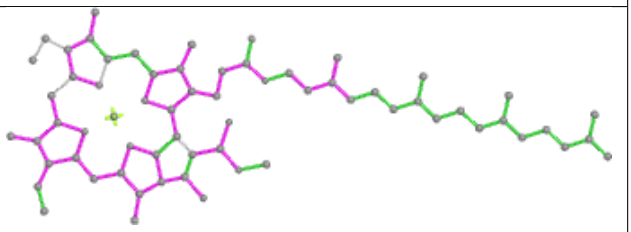
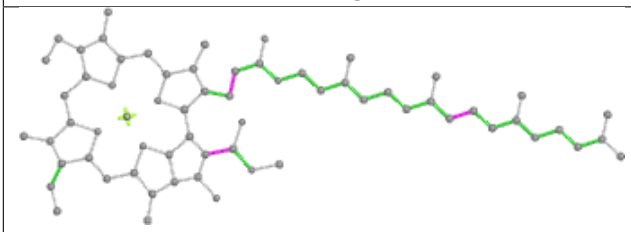
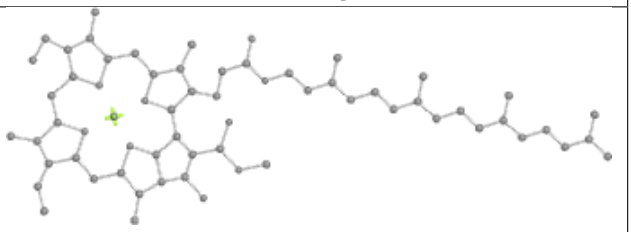


Bond angles

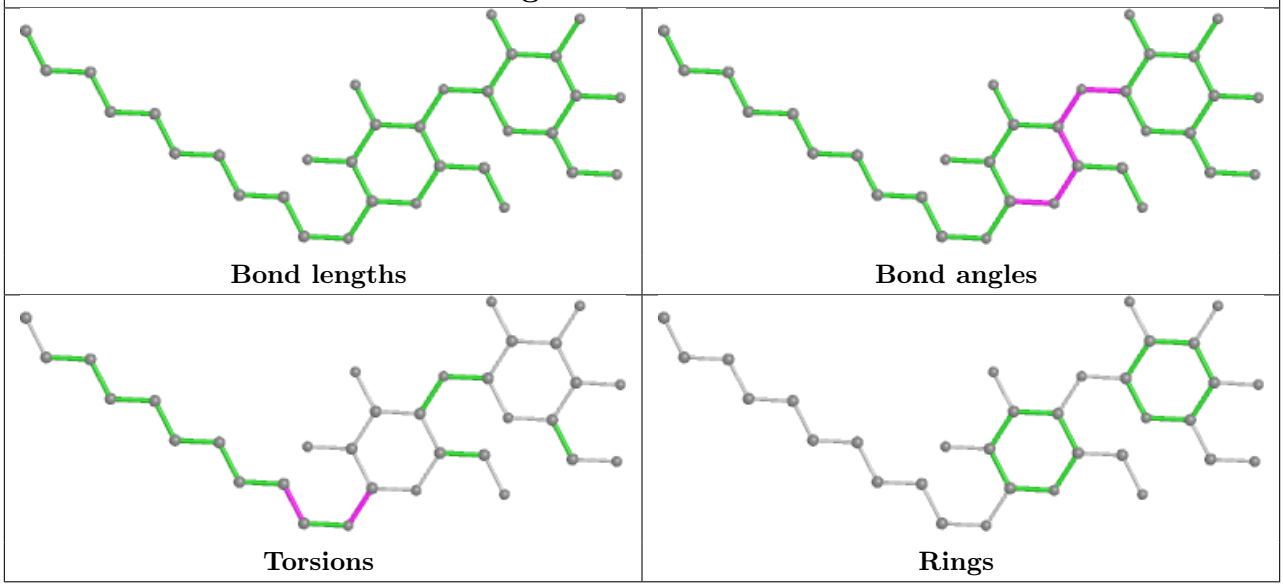


Torsions

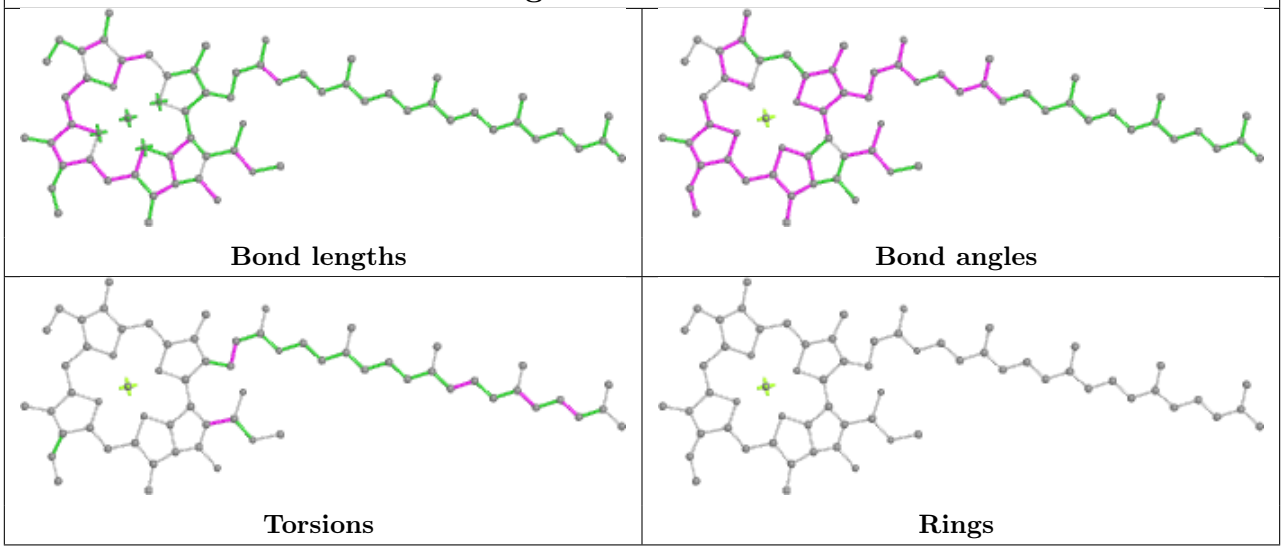


Rings

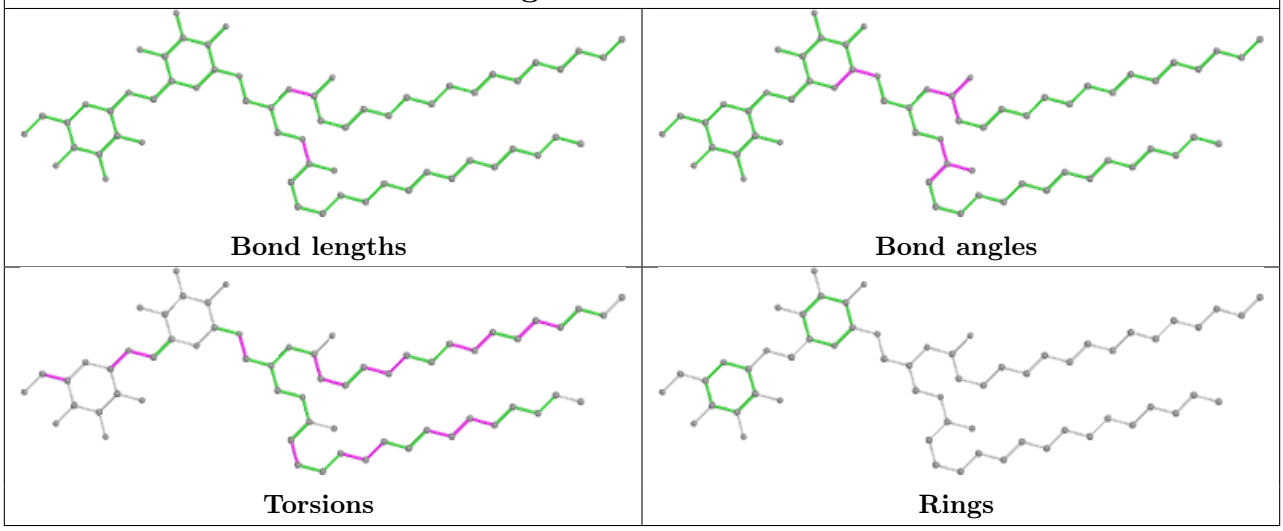
Ligand LMT A 417



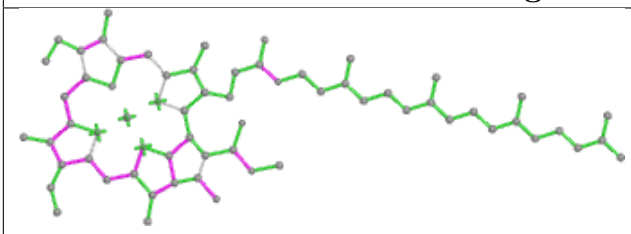
Ligand CLA B 603



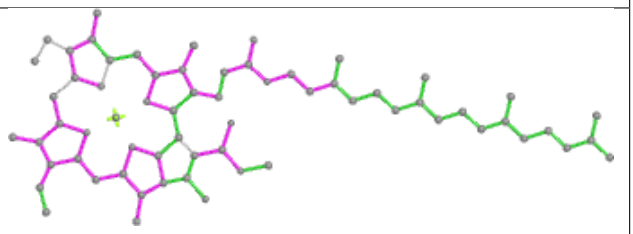
Ligand DGD C 518



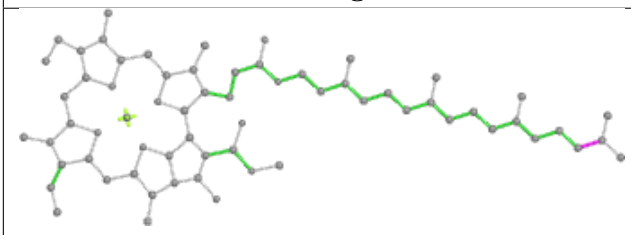
Ligand CLA B 609



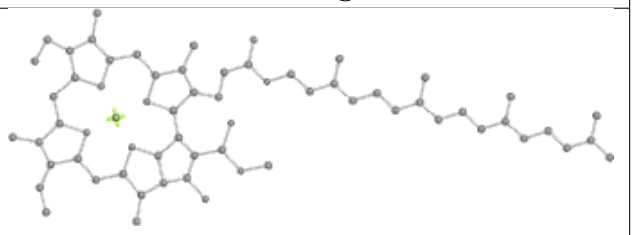
Bond lengths



Bond angles

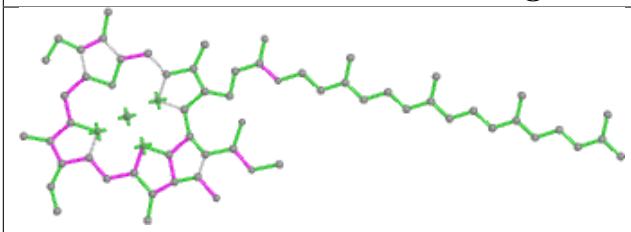


Torsions

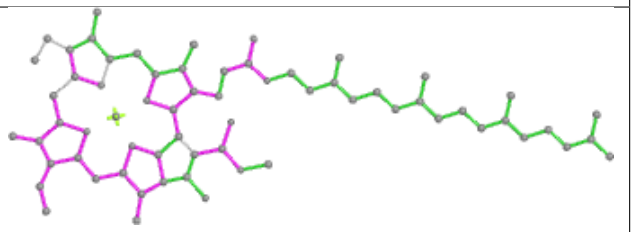


Rings

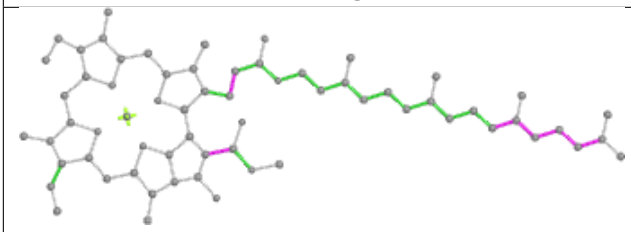
Ligand CLA C 502



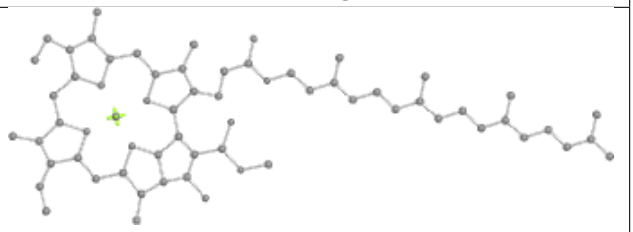
Bond lengths



Bond angles

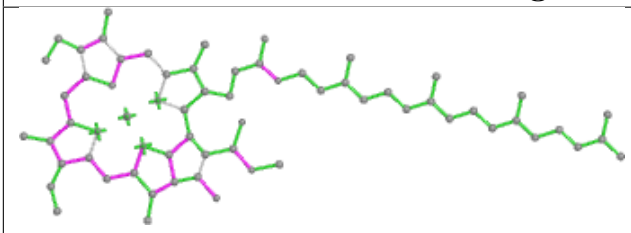


Torsions

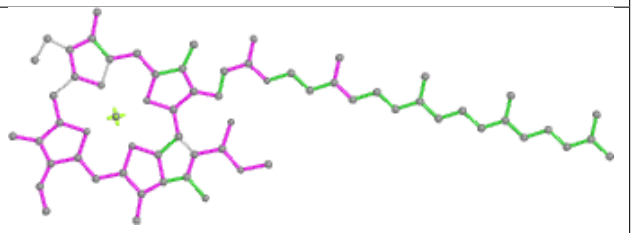


Rings

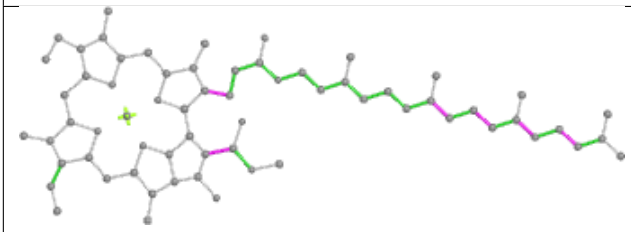
Ligand CLA c 508



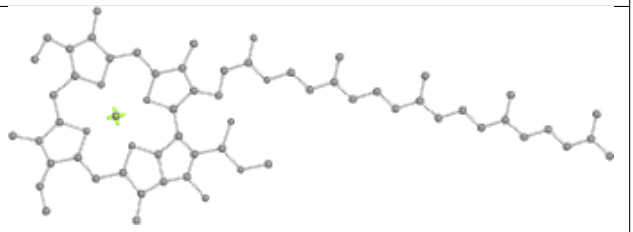
Bond lengths



Bond angles

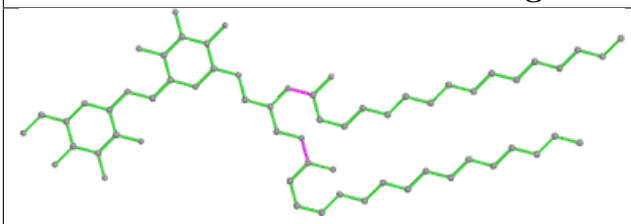


Torsions



Rings

Ligand DGD c 517



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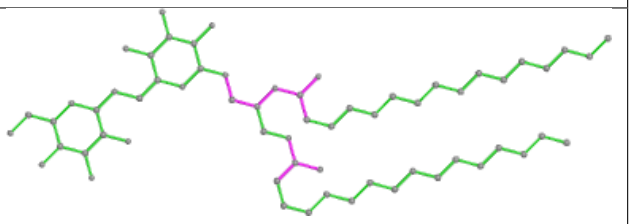
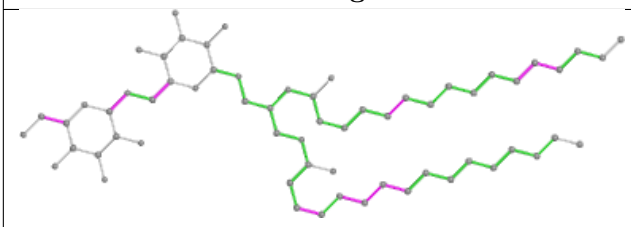


Bond angles



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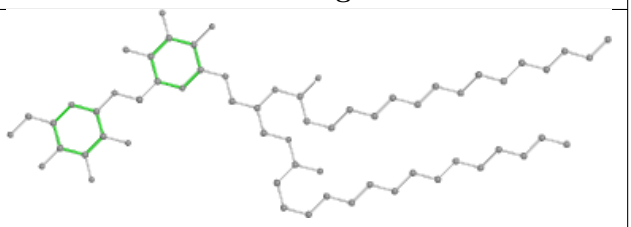
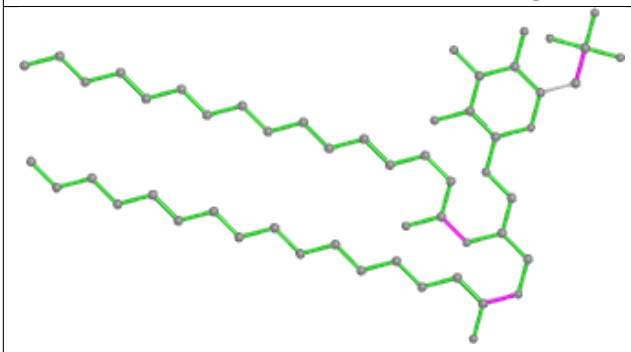


Rings

Ligand SQD b 601



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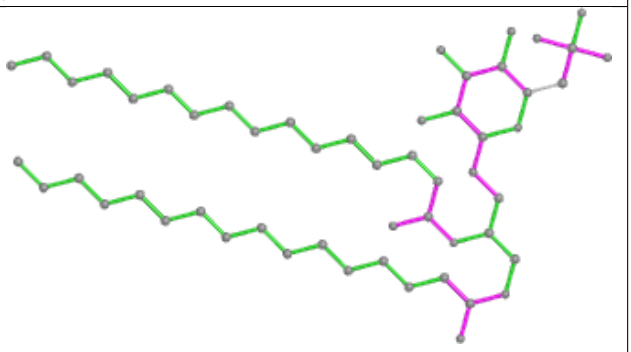
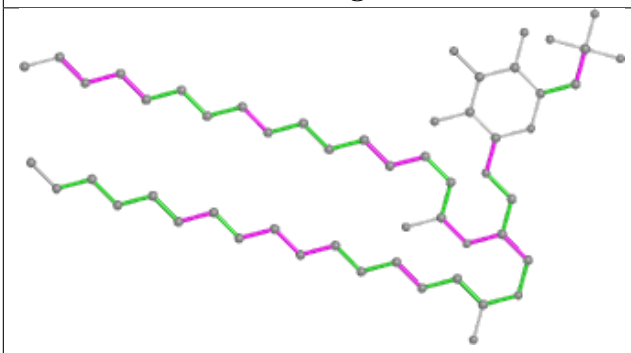


Bond angles



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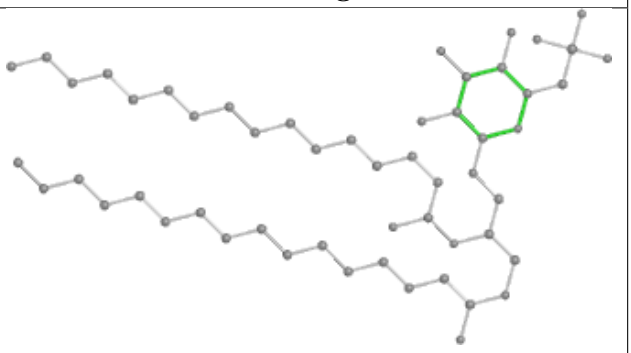
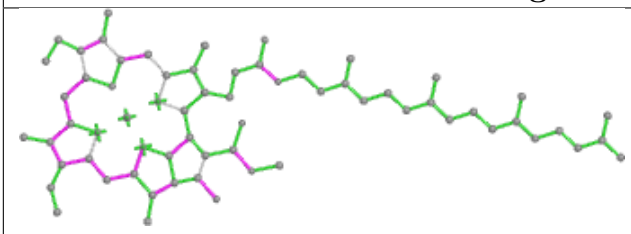


Rings

Ligand CLA c 509



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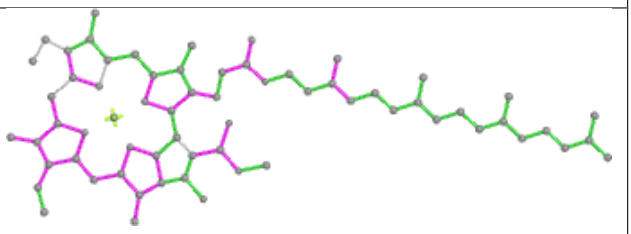
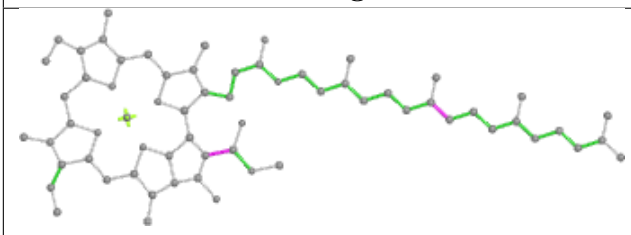


Bond angles



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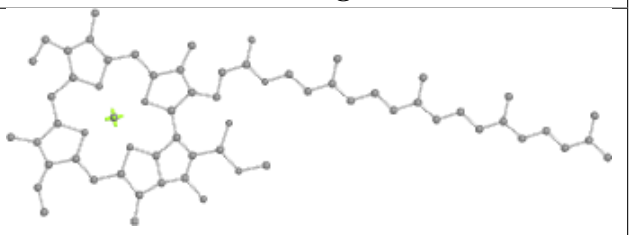
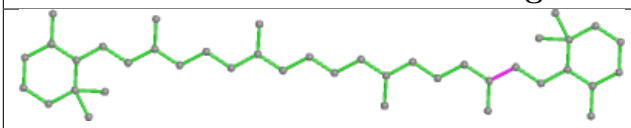


Rings

Ligand BCR b 624



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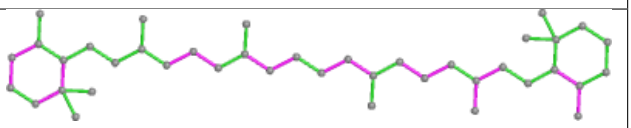
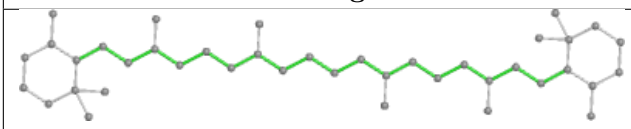


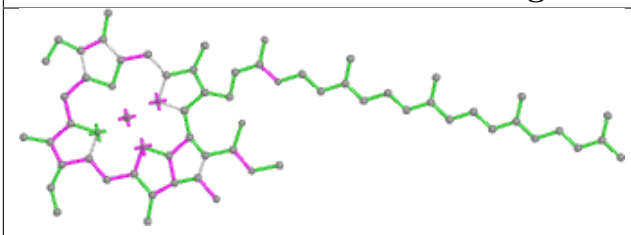
Bond angles



Torsions

Rings

Ligand CLA b 609



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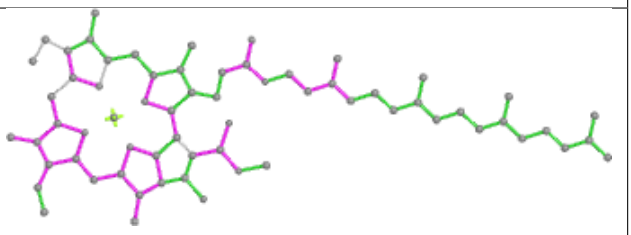
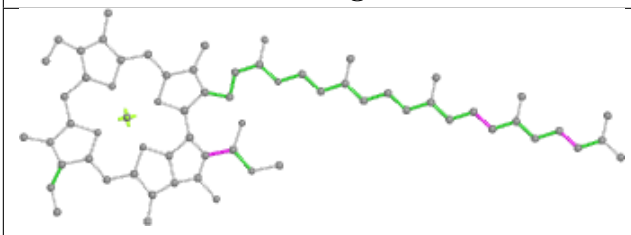
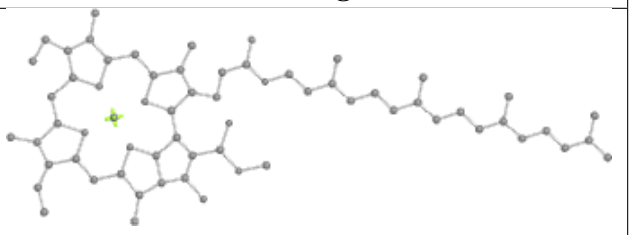


Bond angles

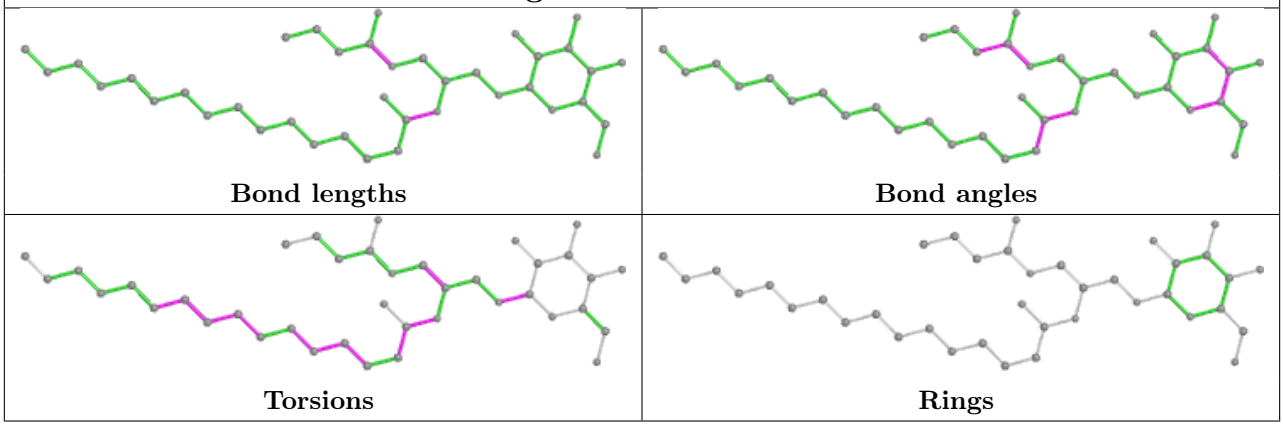


Torsions



Rings

Ligand LMG z 101



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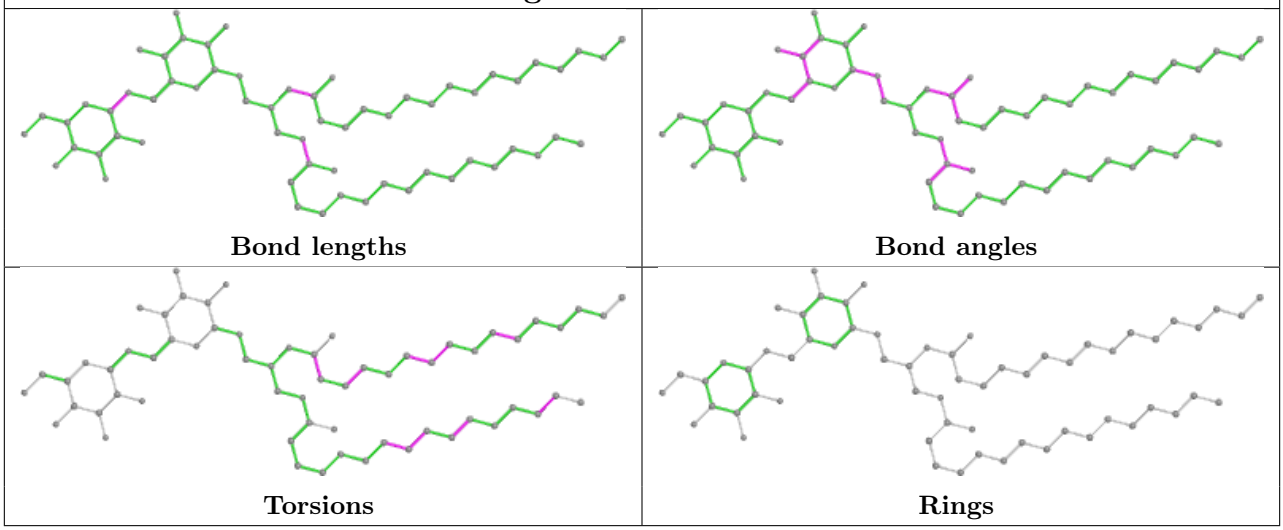

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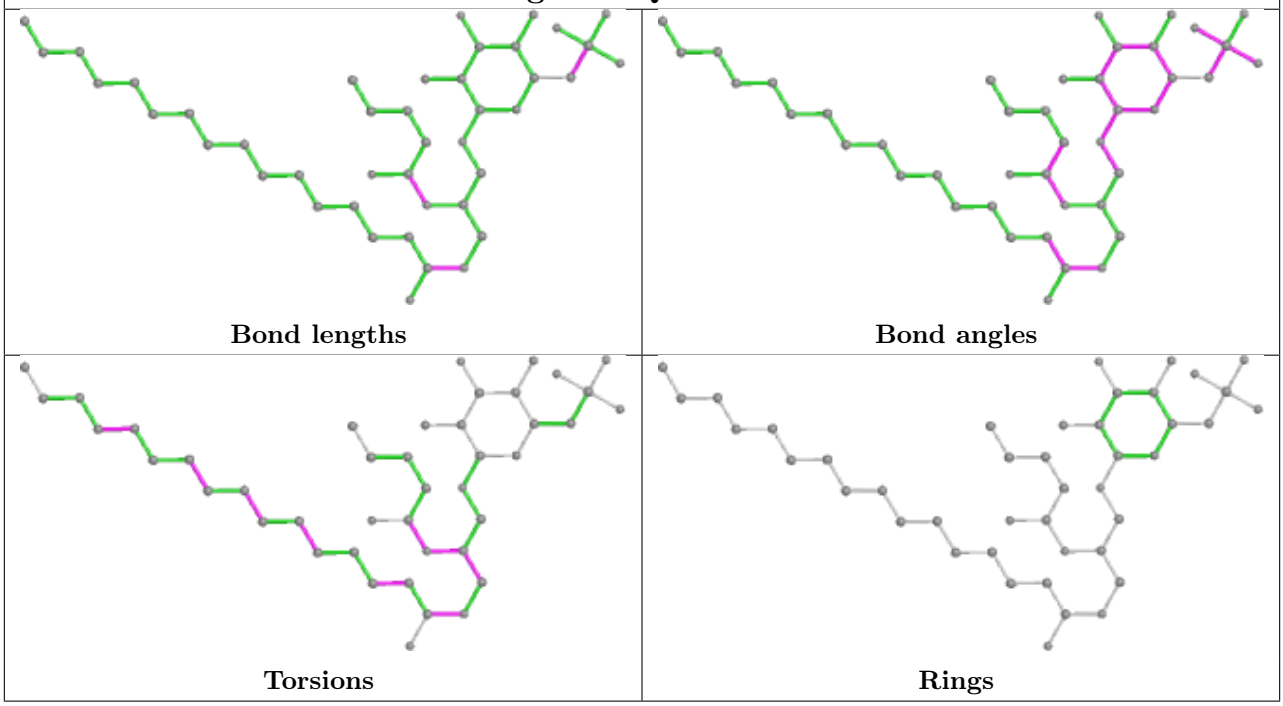
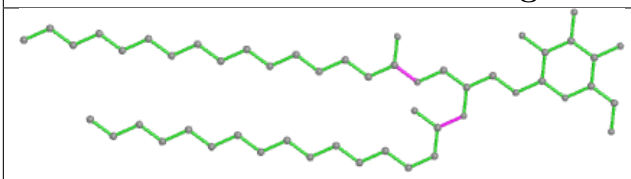
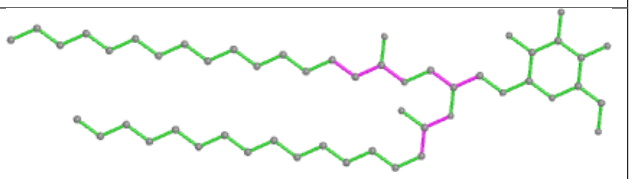


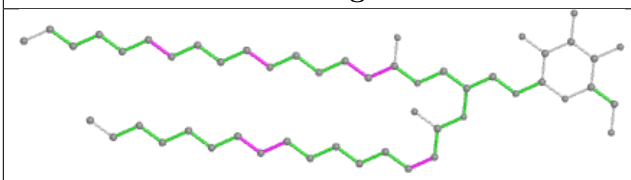
Ligand LMG B 621



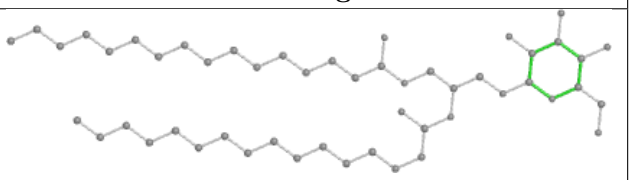
Bond lengths



Bond angles

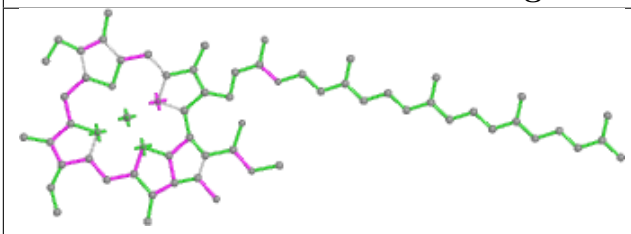


Torsions

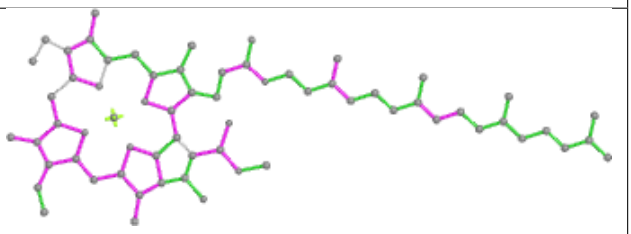


Rings

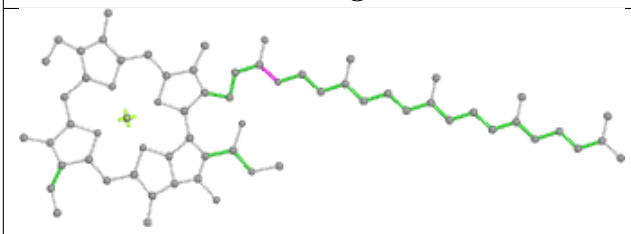
Ligand CLA B 613



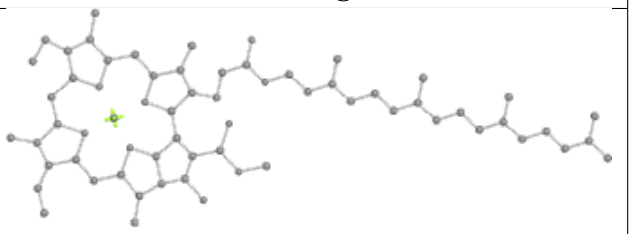
Bond lengths



Bond angles

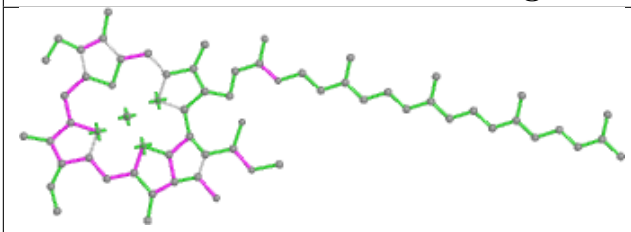


Torsions



Rings

Ligand CLA D 403



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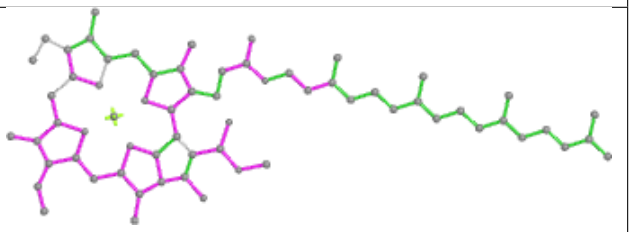
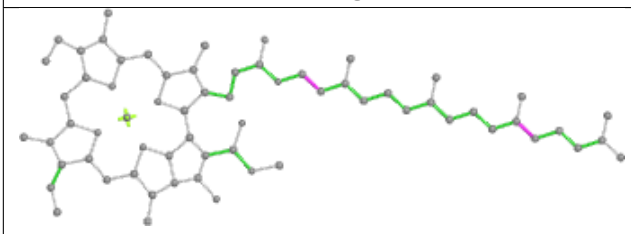


Bond angles



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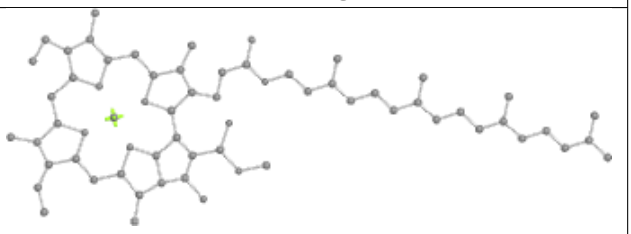
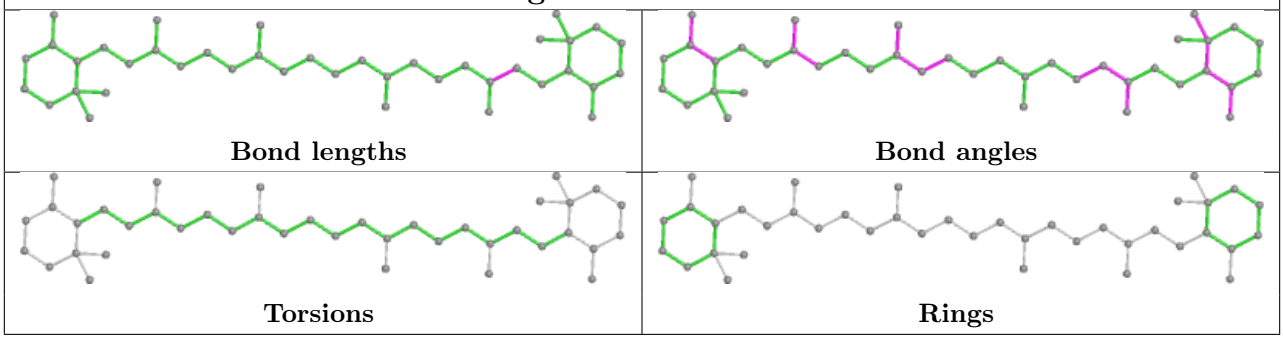


Rings

Ligand BCR a 410



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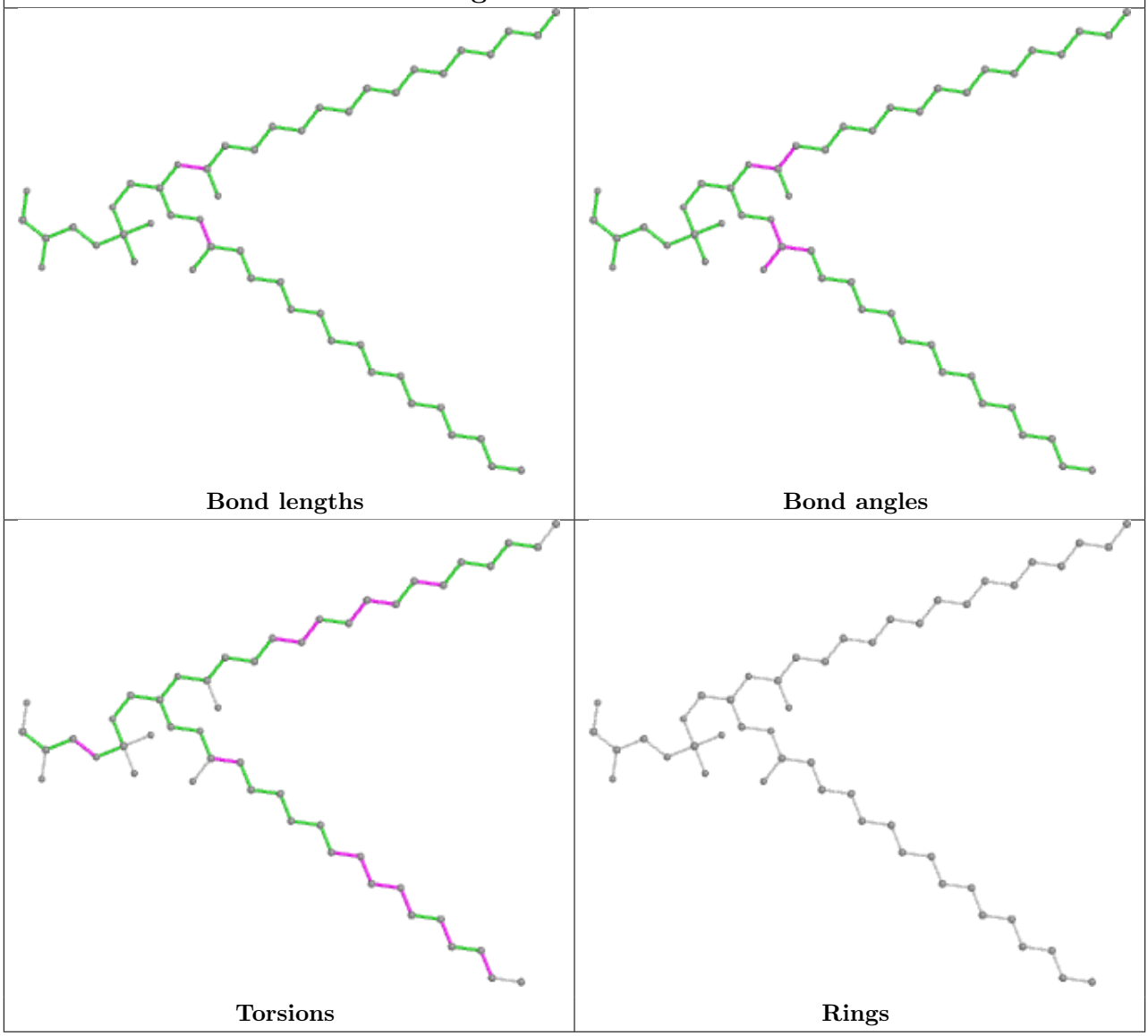
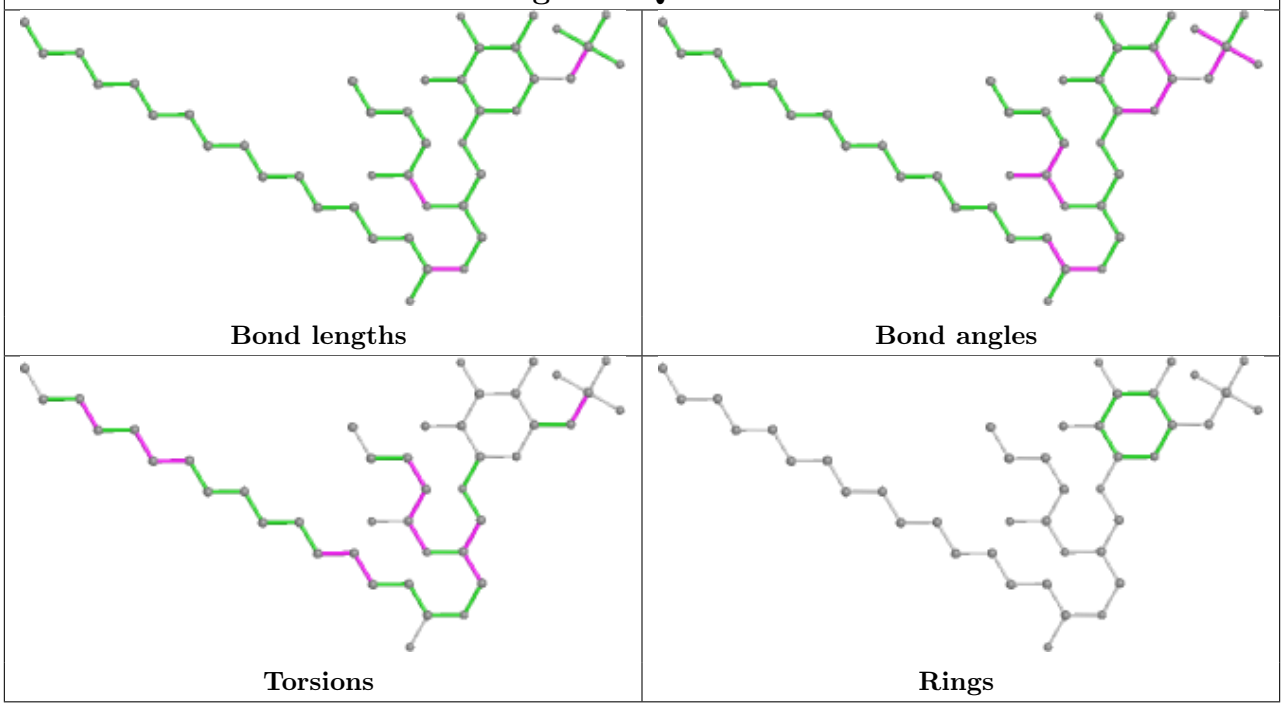
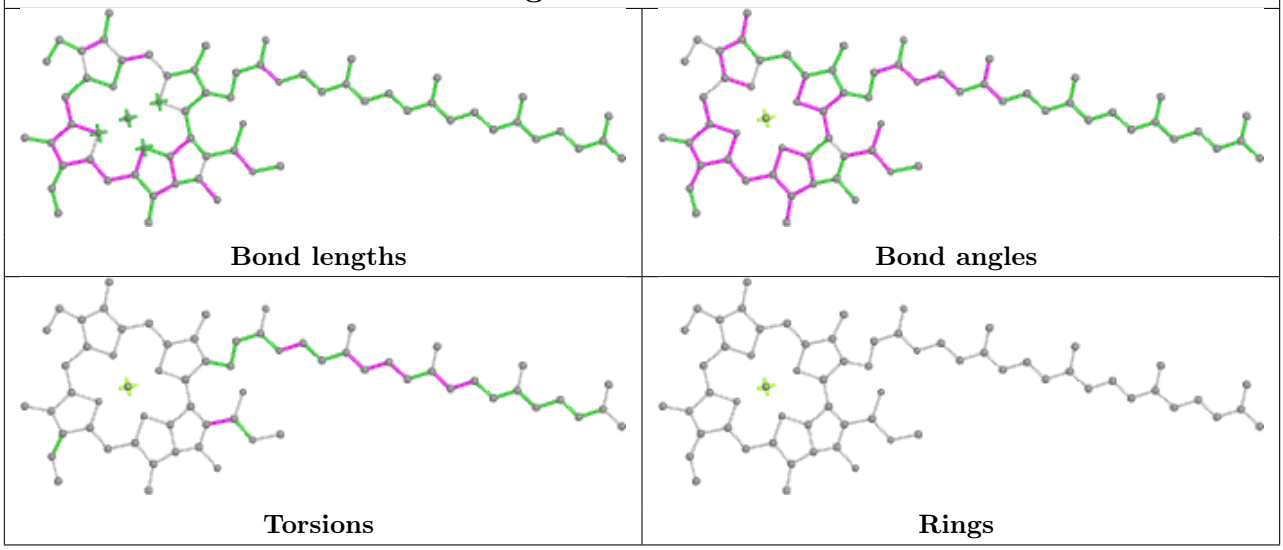


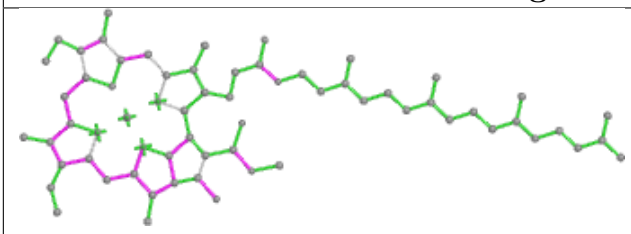
Ligand SQD f 101



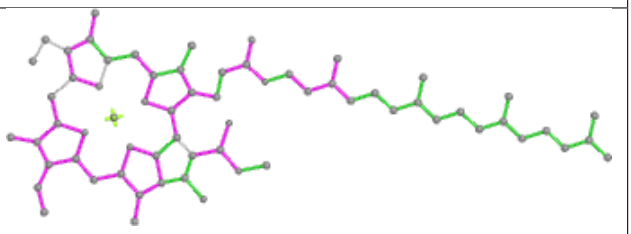
Ligand CLA B 617



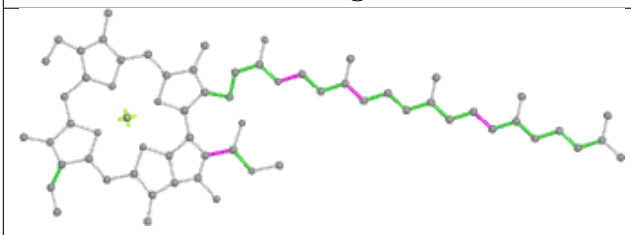
Ligand CLA c 515



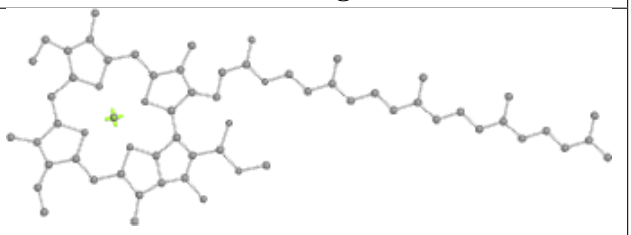
Bond lengths



Bond angles

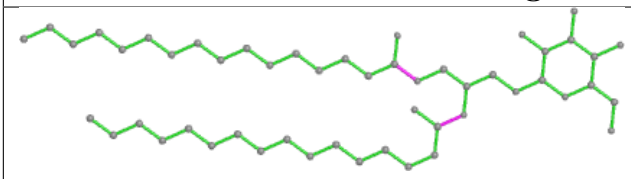


Torsions



Rings

Ligand LMG c 501



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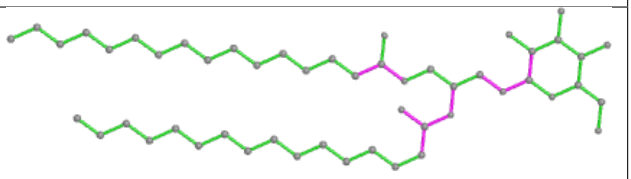
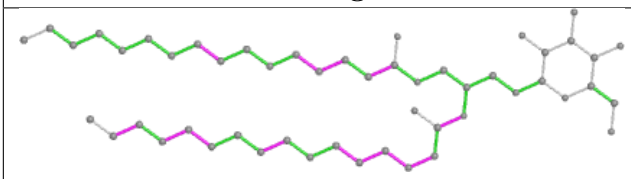
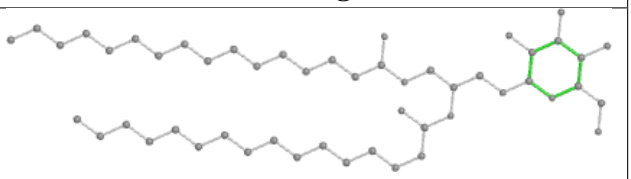


Bond angles

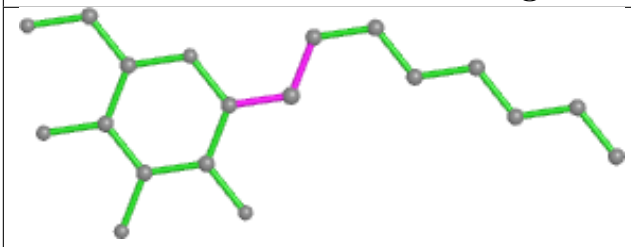


Torsions

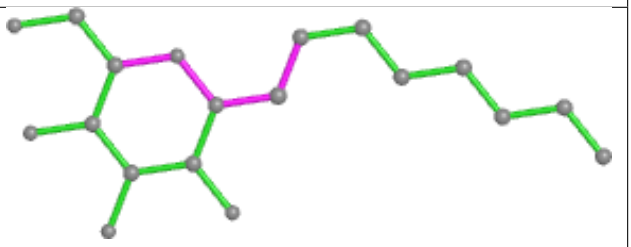


Rings

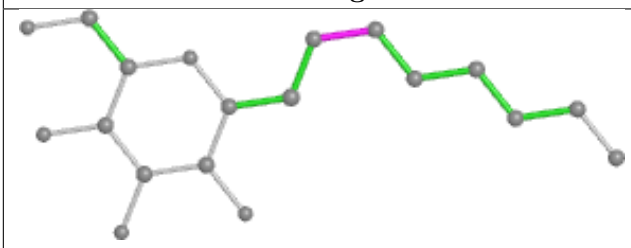
Ligand HTG B 631



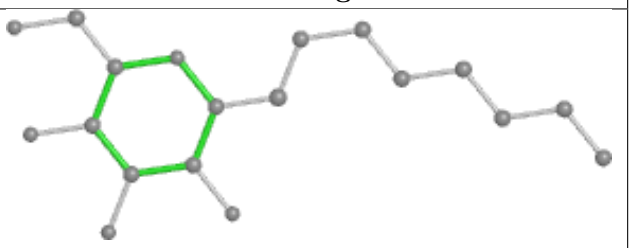
Bond lengths



Bond angles

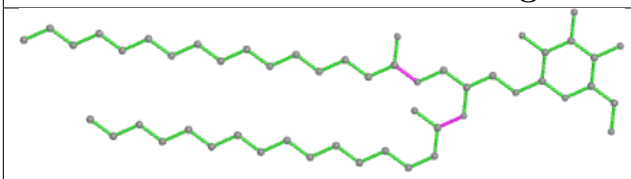


Torsions

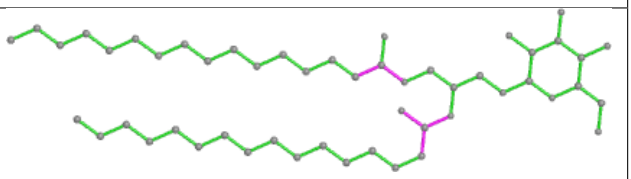


Rings

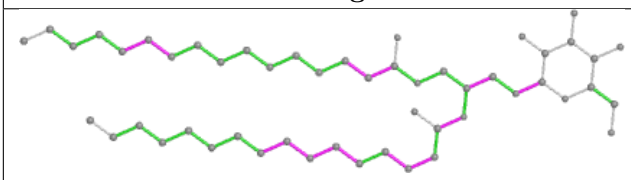
Ligand LMG C 501



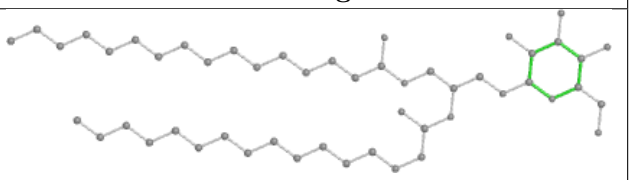
Bond lengths



Bond angles

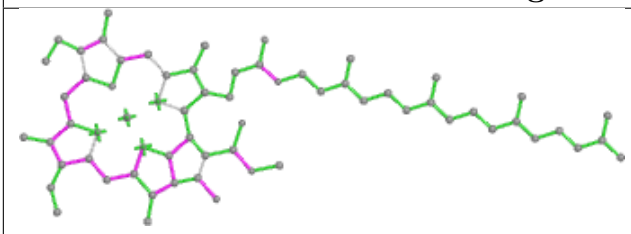


Torsions

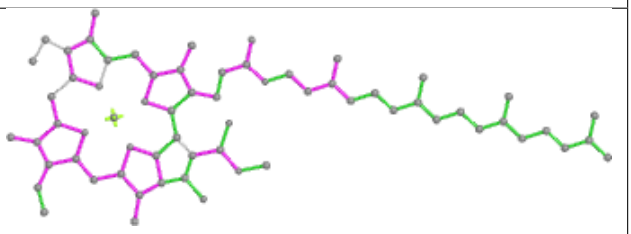


Rings

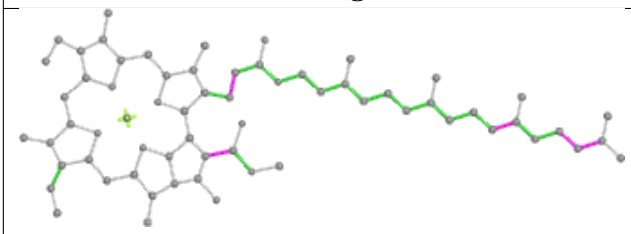
Ligand CLA b 615



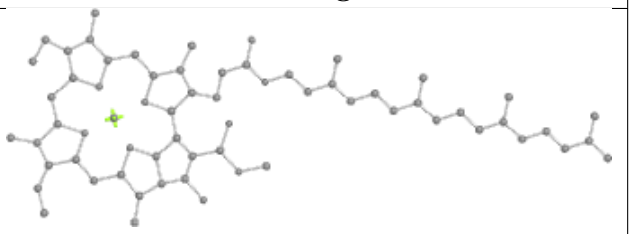
Bond lengths



Bond angles

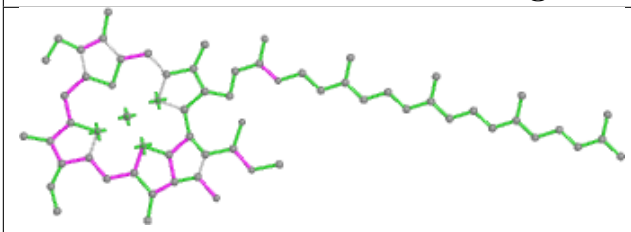


Torsions

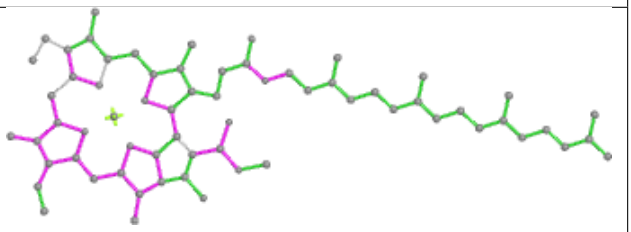


Rings

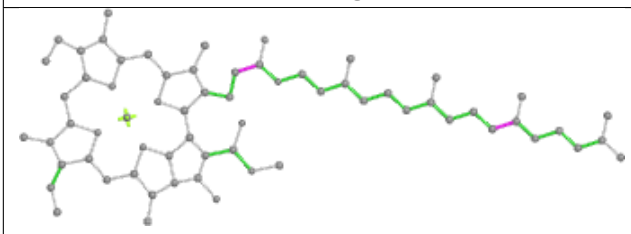
Ligand CLA c 507



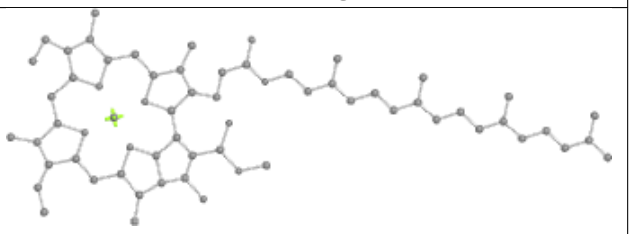
Bond lengths



Bond angles

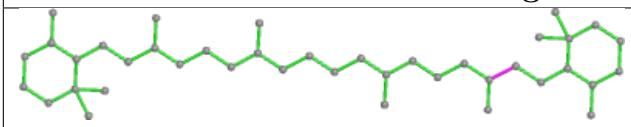


Torsions

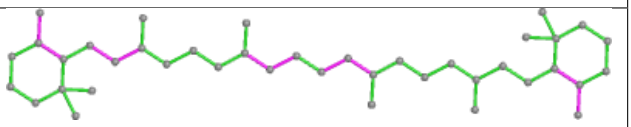


Rings

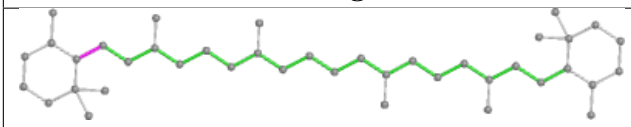
Ligand BCR C 515



Bond lengths



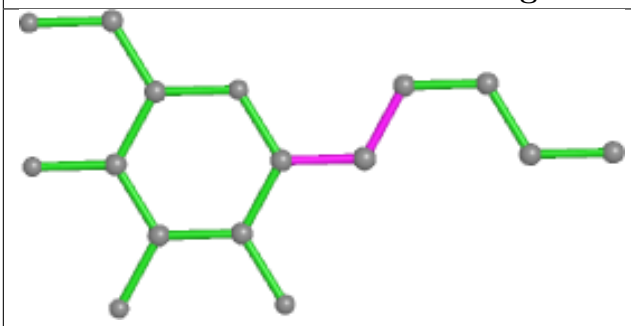
Bond angles



Torsions

Rings

Ligand HTG D 411



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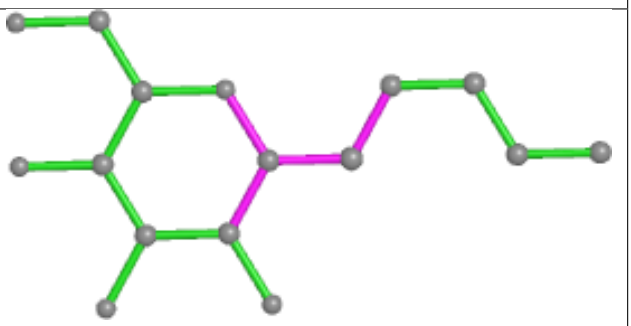
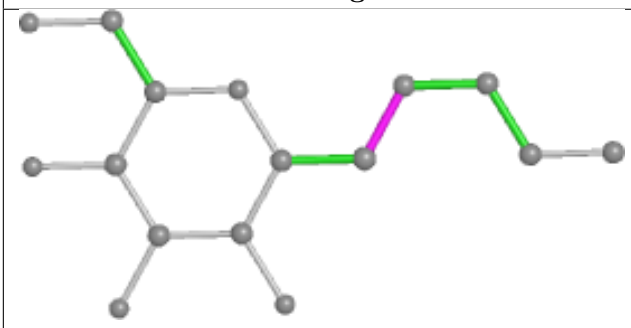
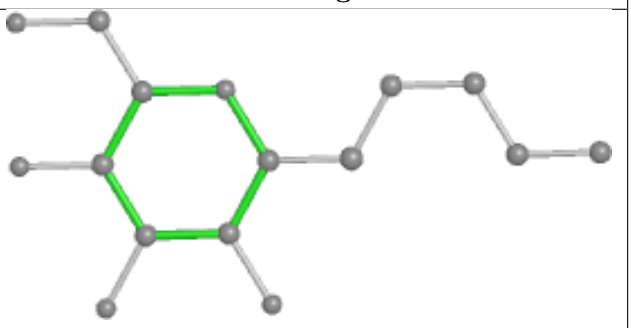


Bond angles

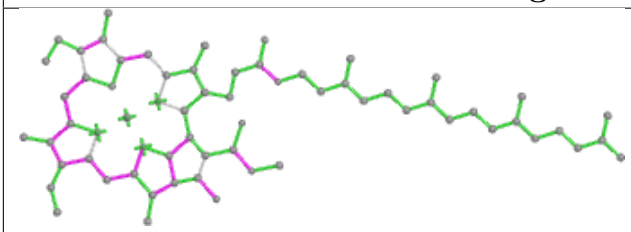


Torsions

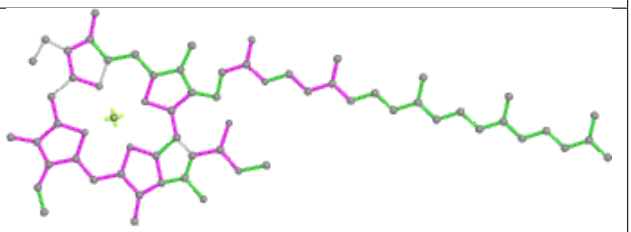


Rings

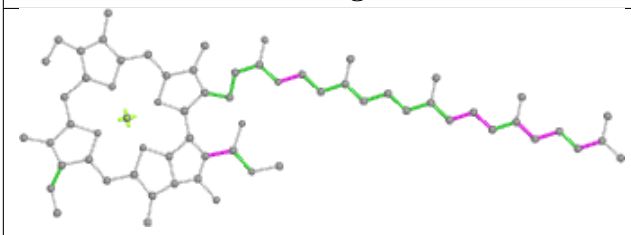
Ligand CLA c 511



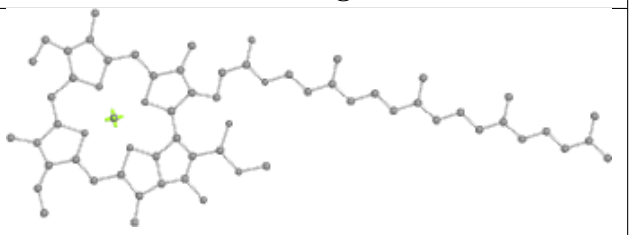
Bond lengths



Bond angles

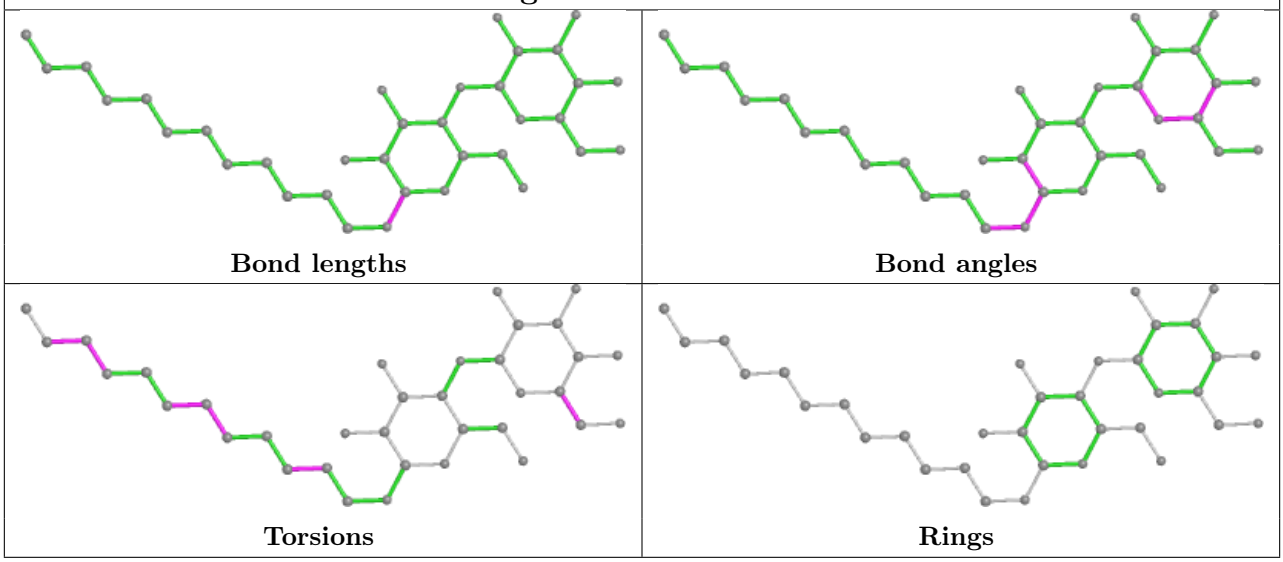


Torsions

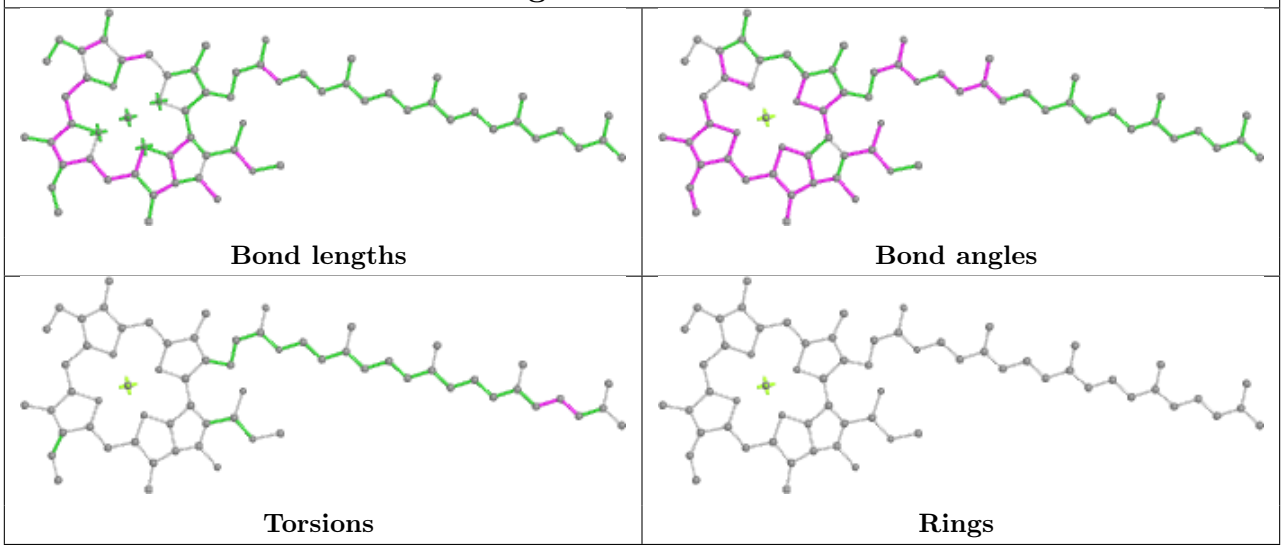


Rings

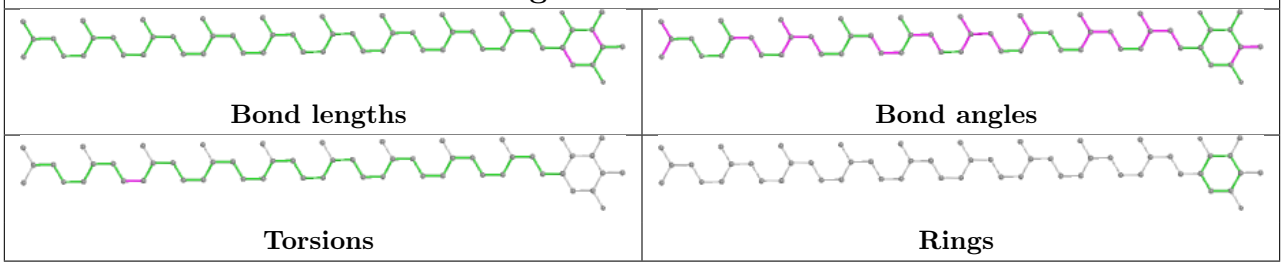
Ligand LMT m 103



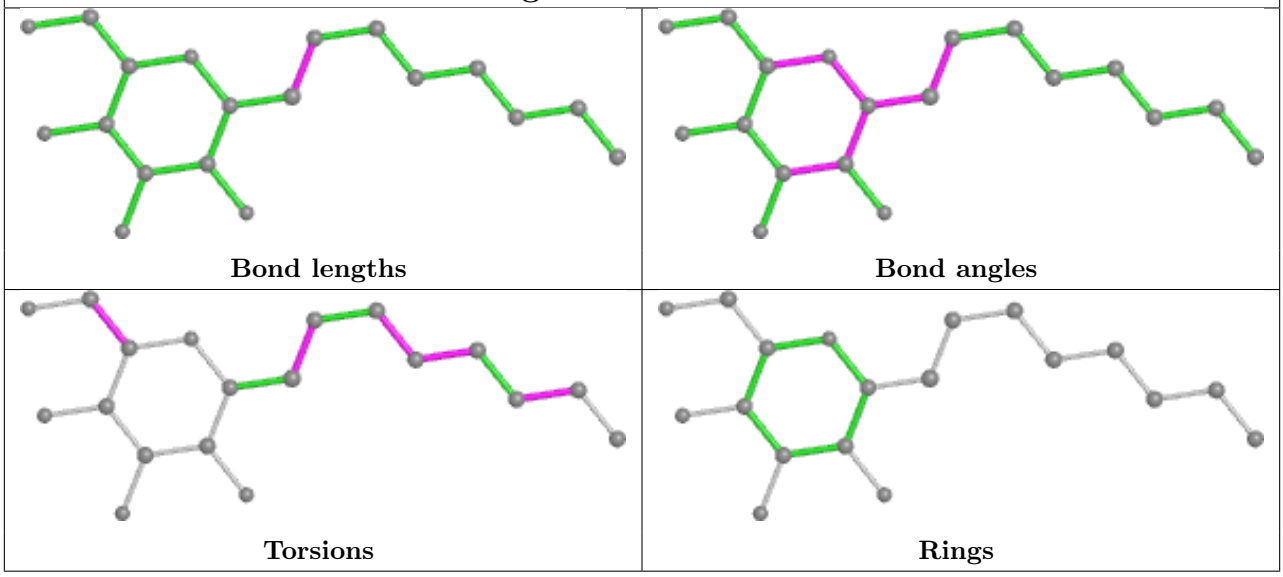
Ligand CLA b 616



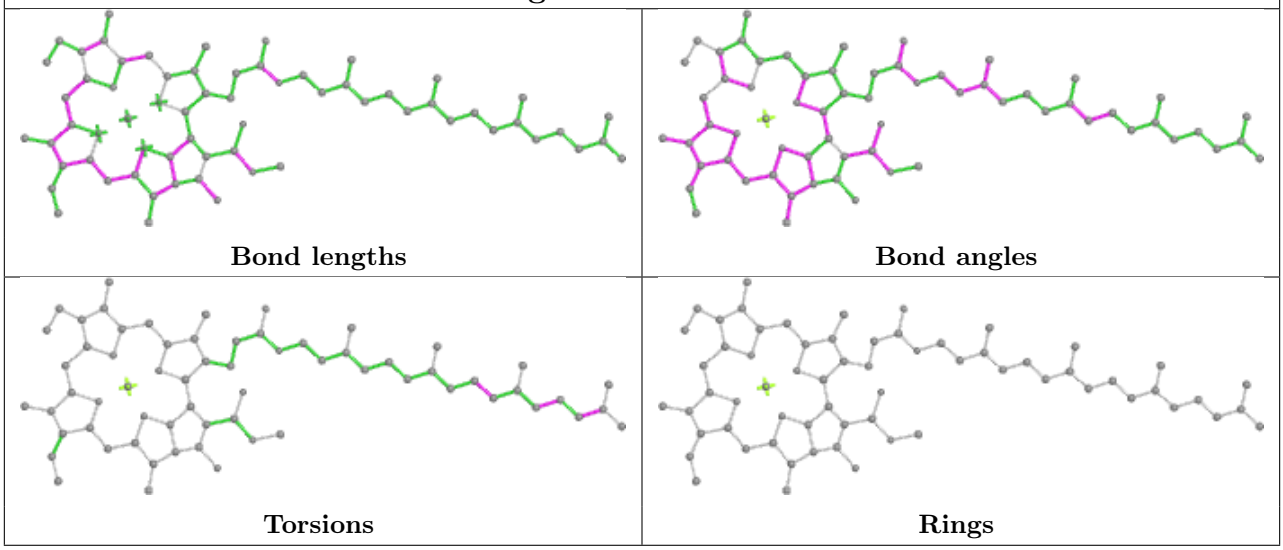
Ligand PL9 D 406



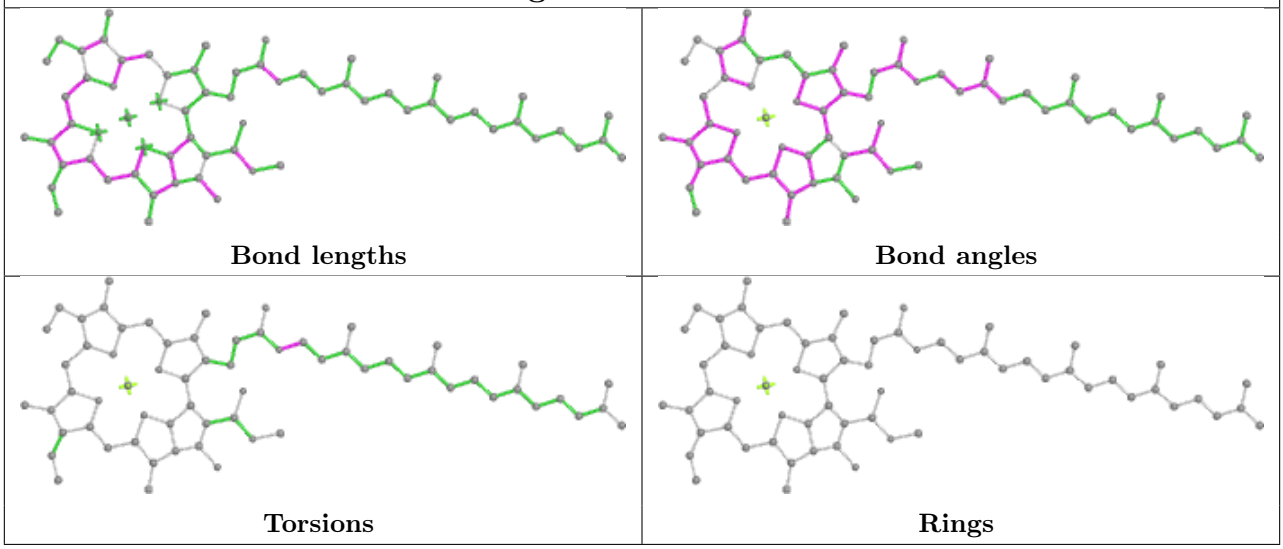
Ligand HTG B 623



Ligand CLA b 620



Ligand CLA d 402



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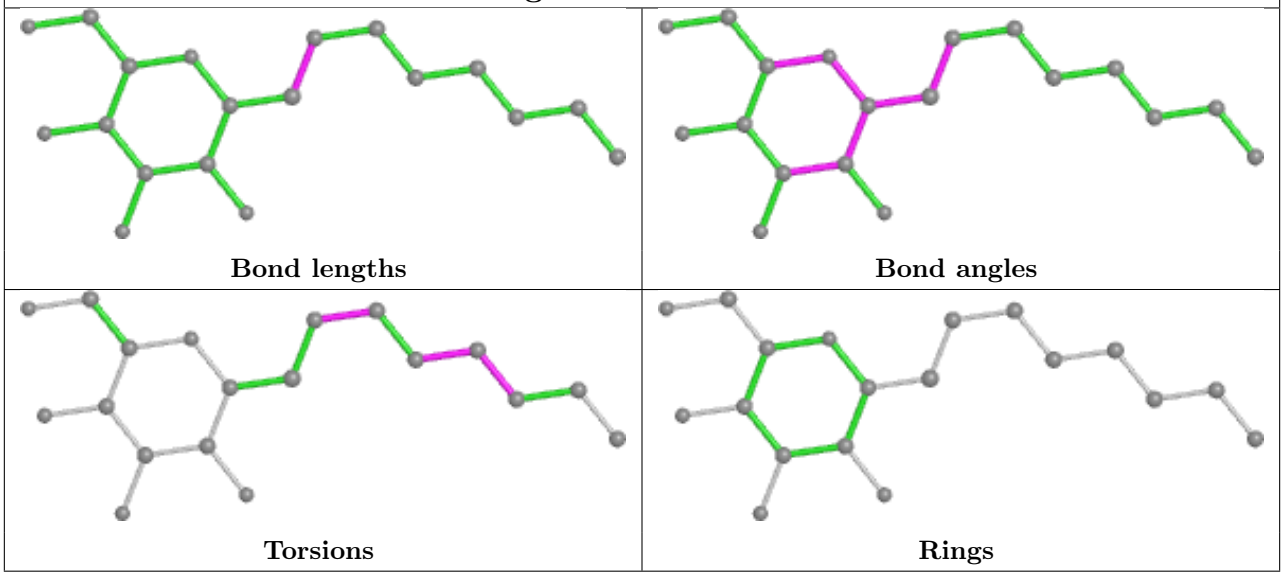
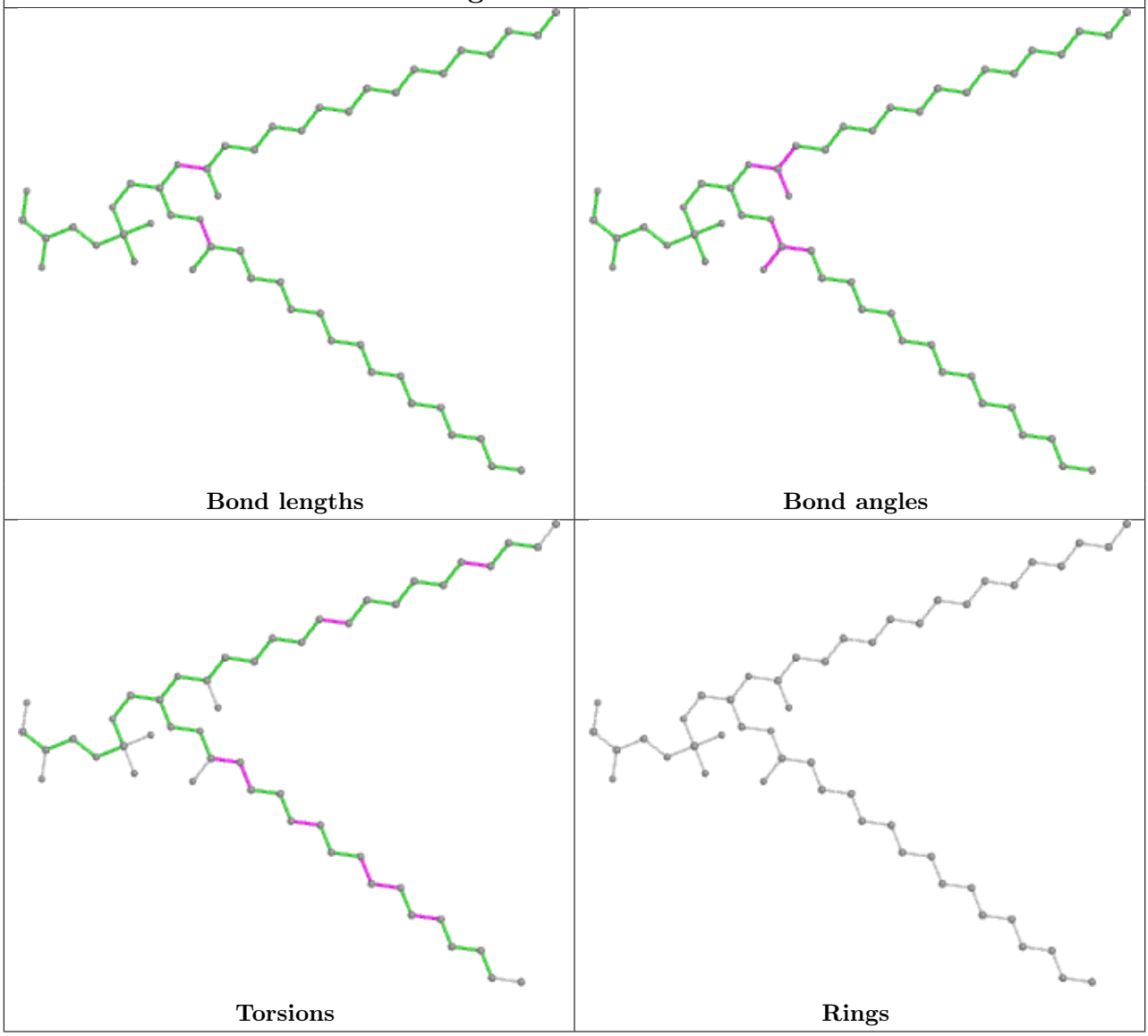
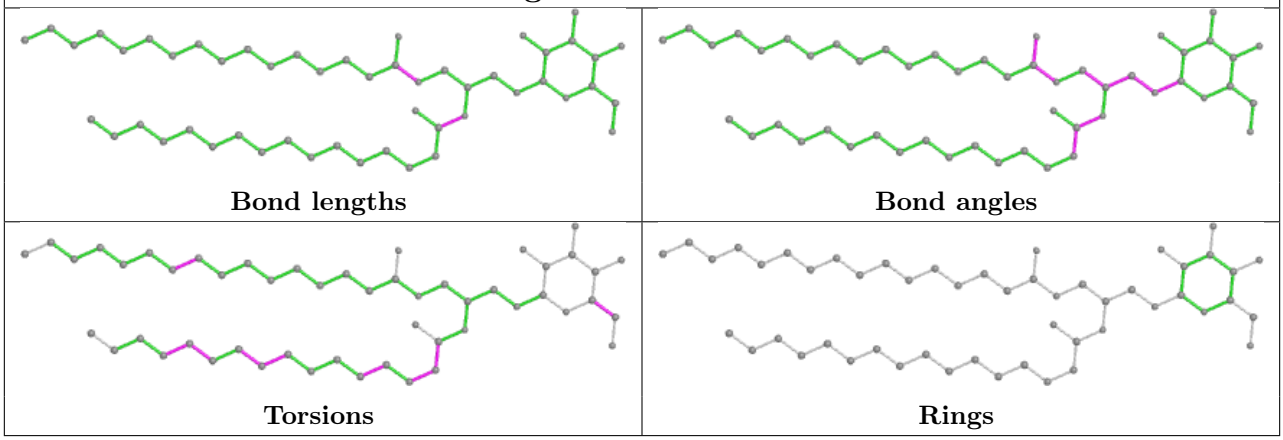


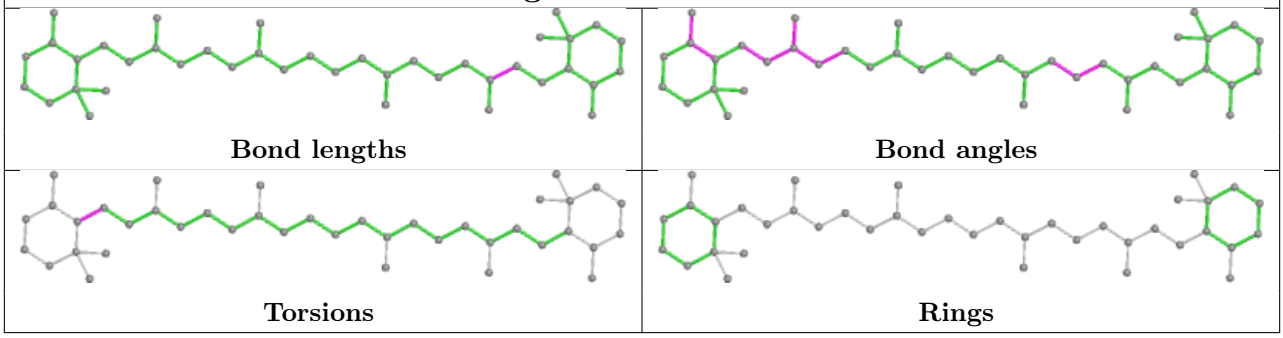
Ligand LHG D 408



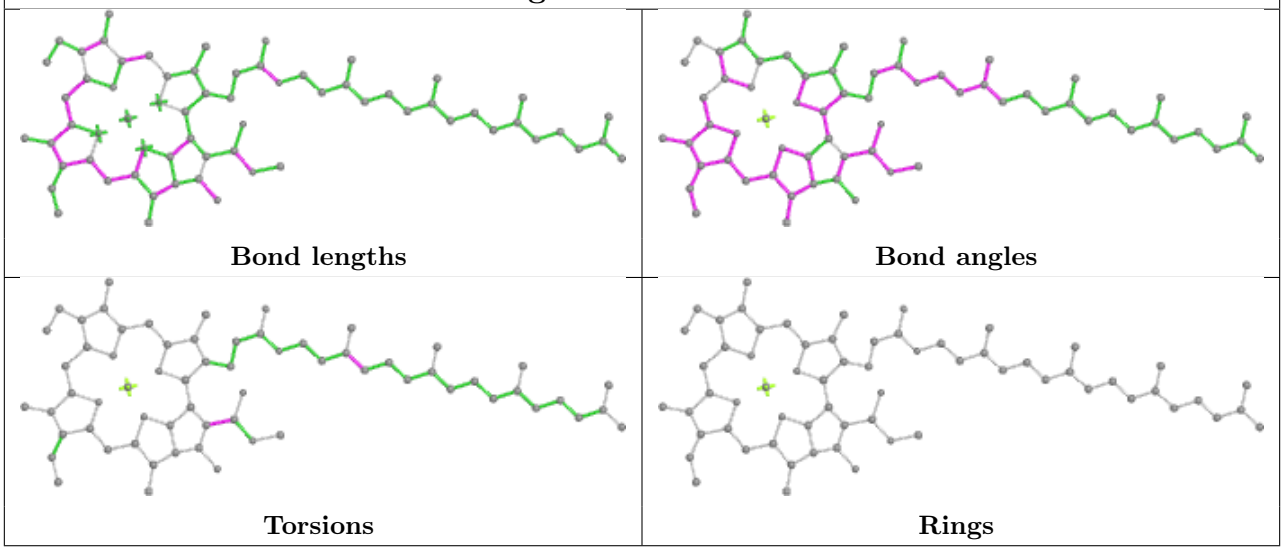
Ligand LMG J 101



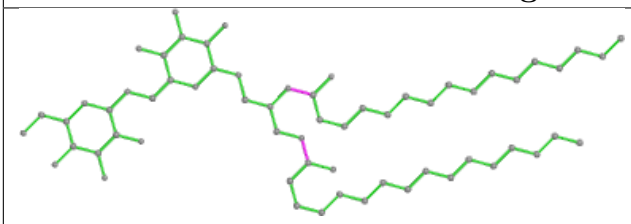
Ligand BCR B 618



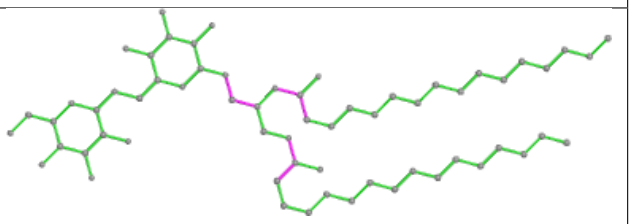
Ligand CLA b 614



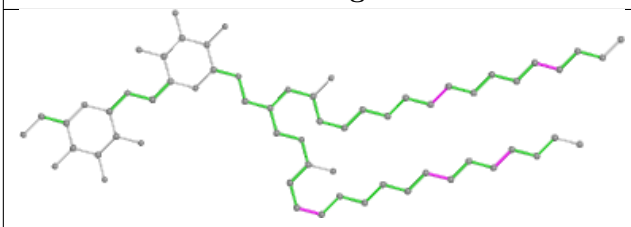
Ligand DGD C 519



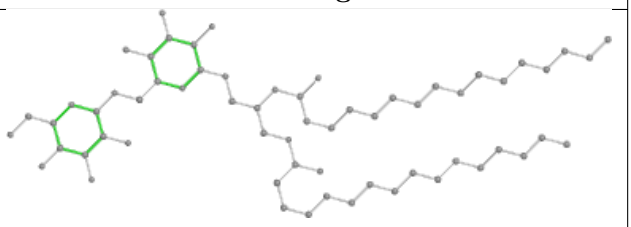
Bond lengths



Bond angles

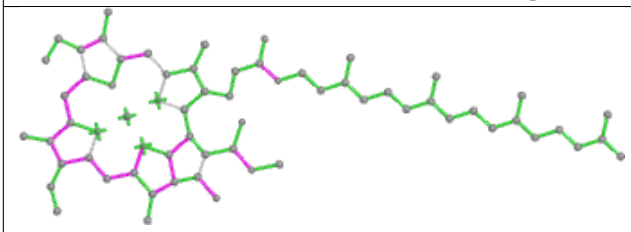


Torsions



Rings

Ligand CLA C 512



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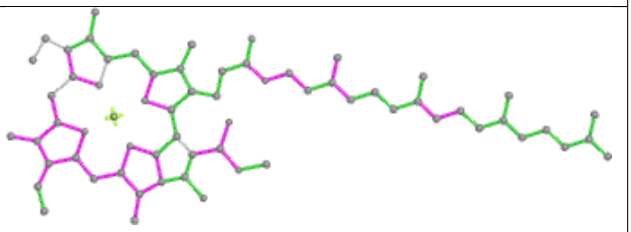
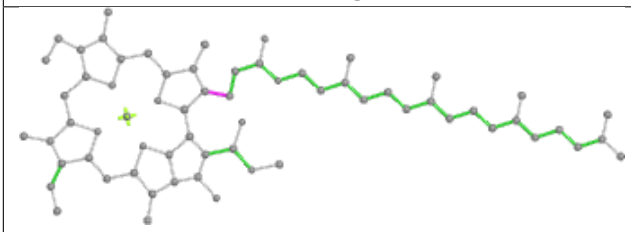
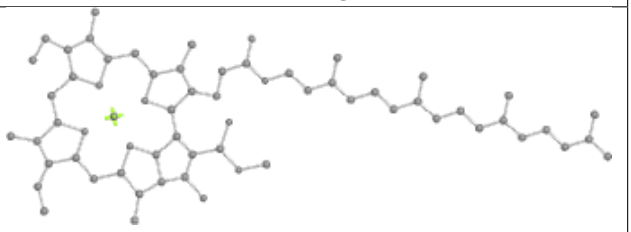


Bond angles

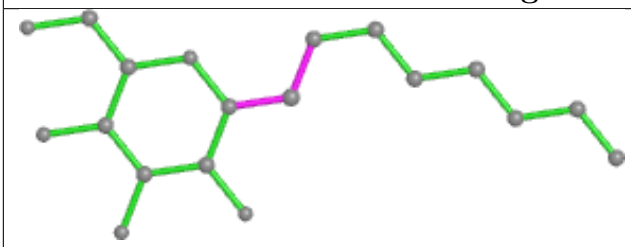


Torsions

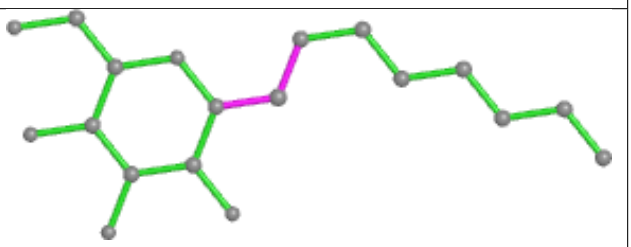


Rings

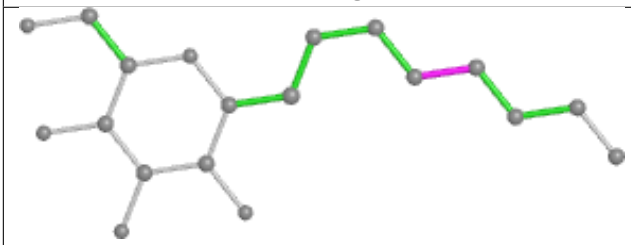
Ligand HTG B 630



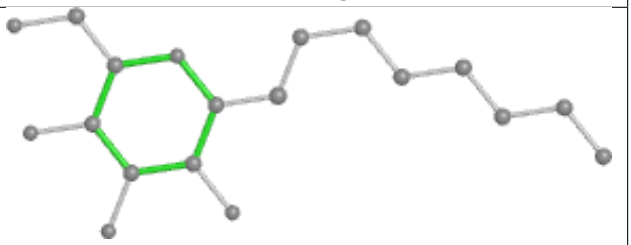
Bond lengths



Bond angles

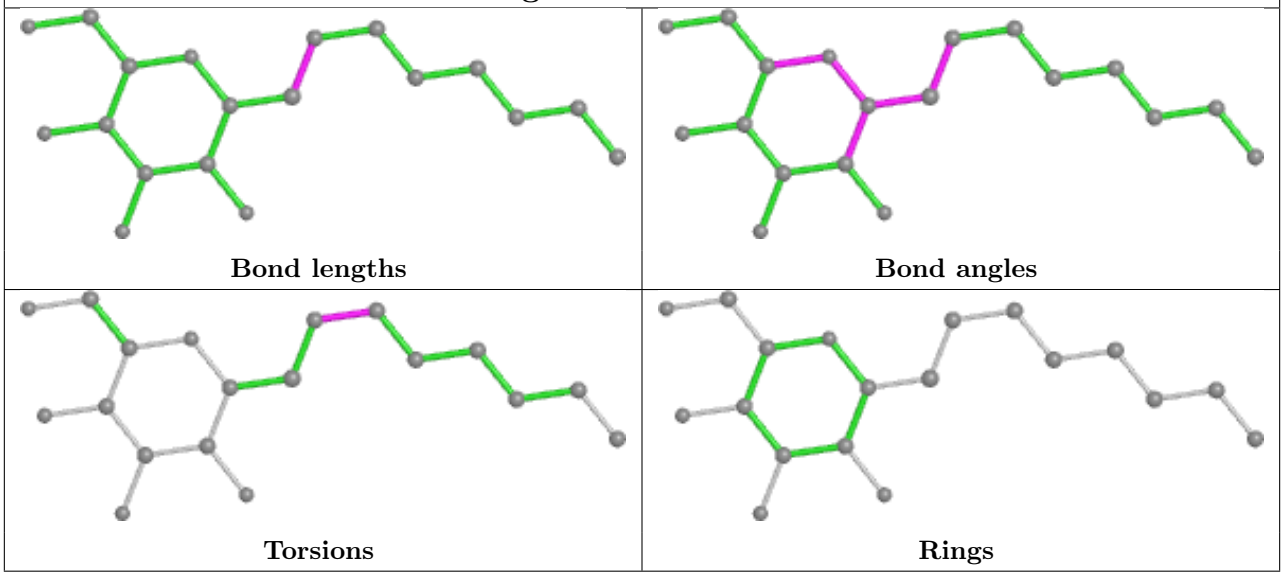


Torsions

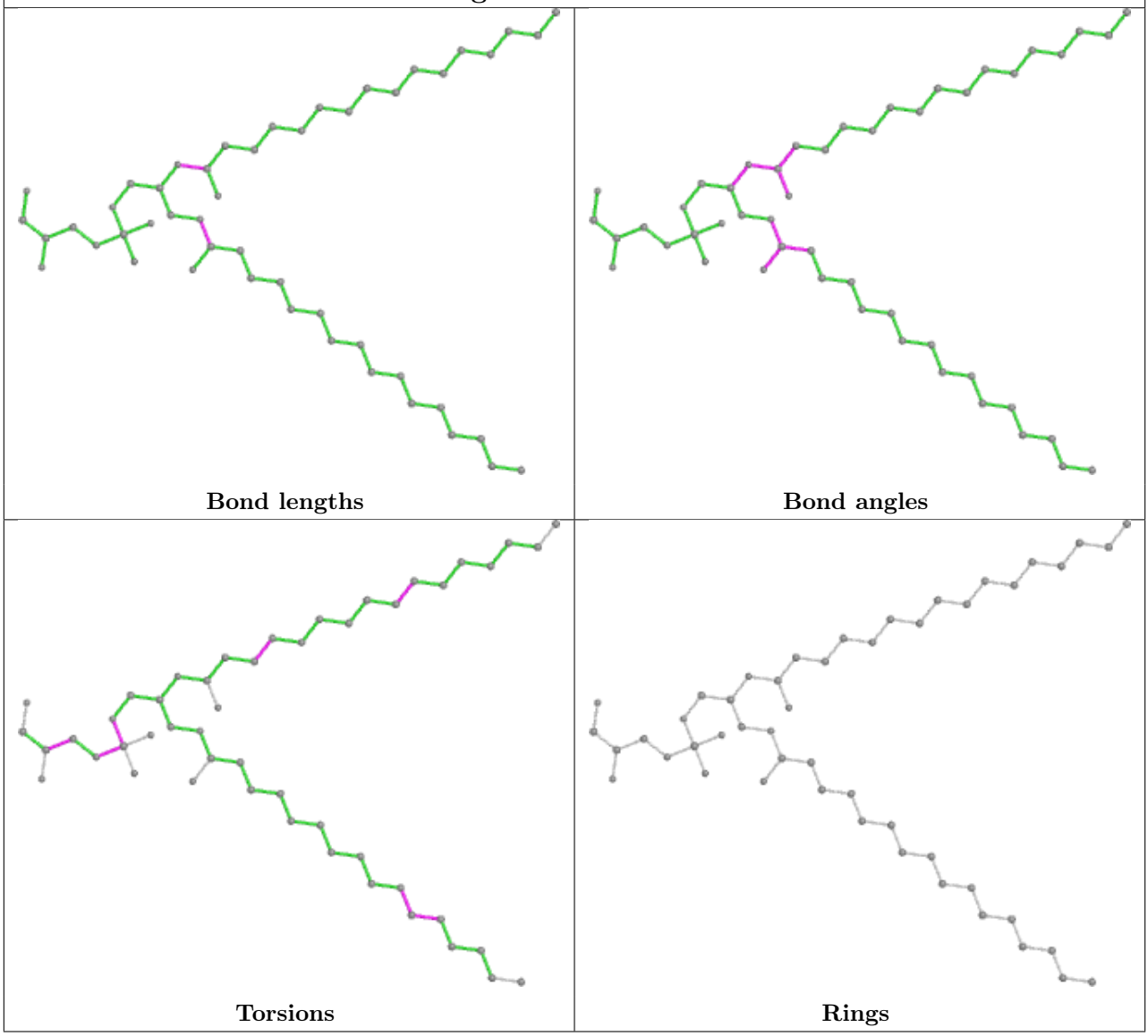


Rings

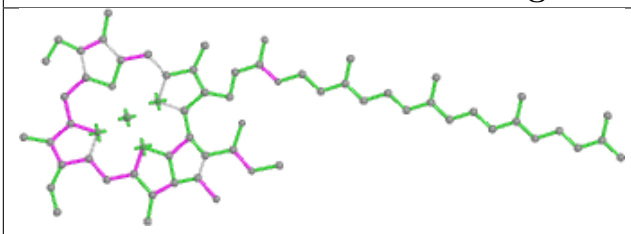
Ligand HTG B 622



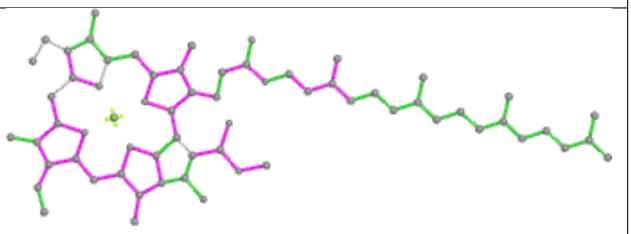
Ligand LHG d 409



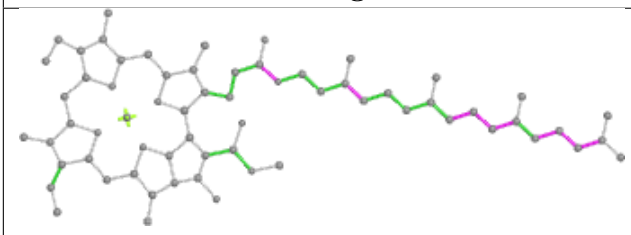
Ligand CLA a 409



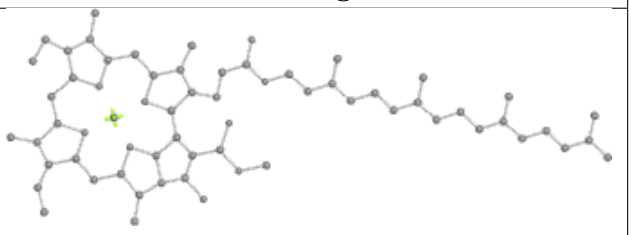
Bond lengths



Bond angles

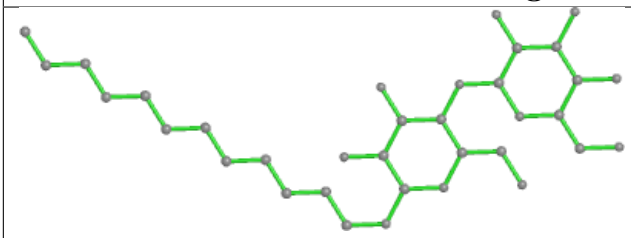


Torsions

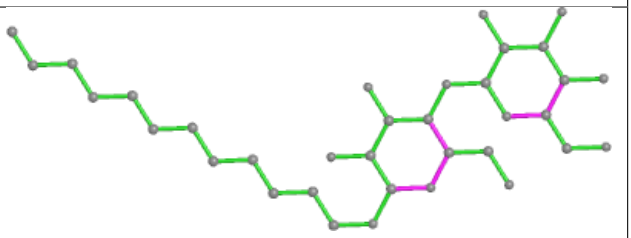


Rings

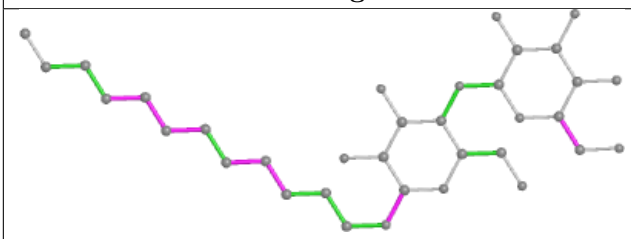
Ligand LMT a 401



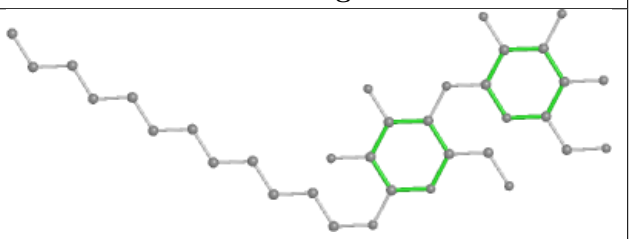
Bond lengths



Bond angles

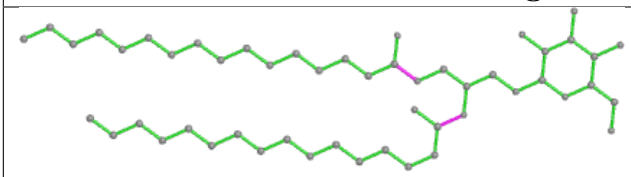


Torsions



Rings

Ligand LMG c 521



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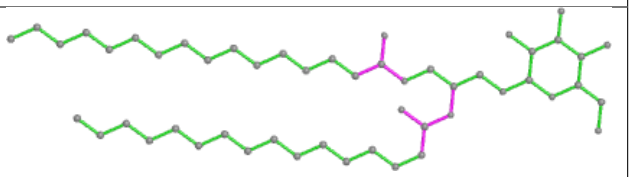
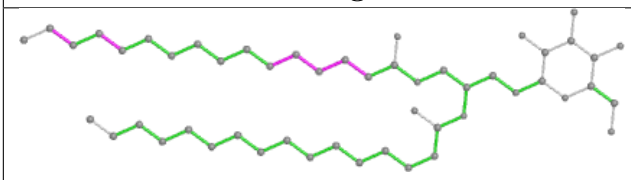
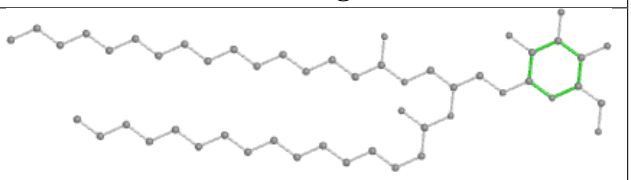


Bond angles

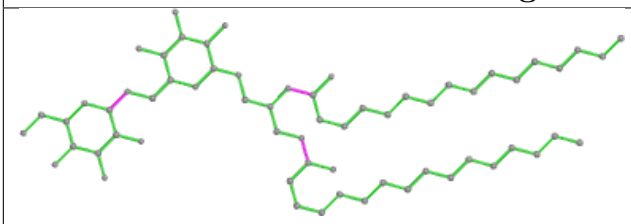


Torsions



Rings

Ligand DGD H 102



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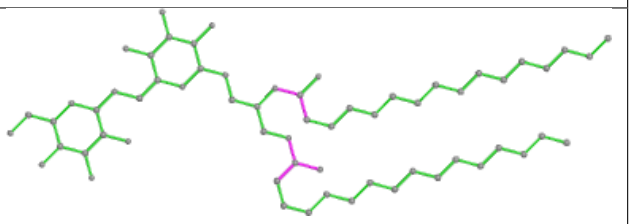
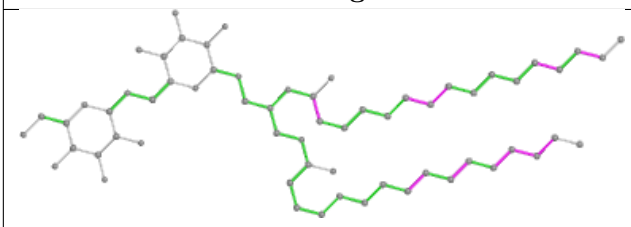


Bond angles



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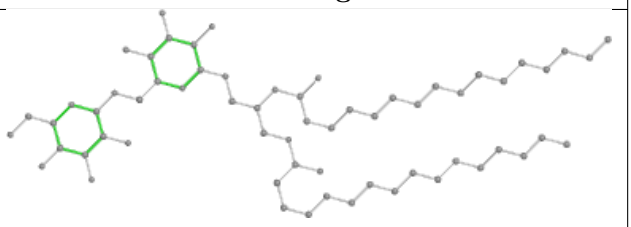
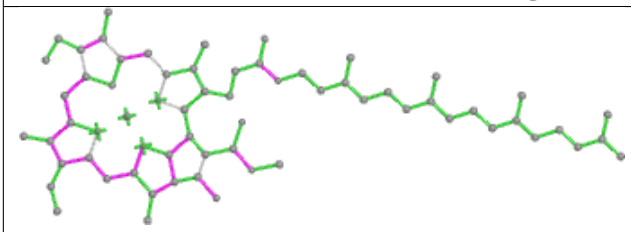


Rings

Ligand CLA C 508



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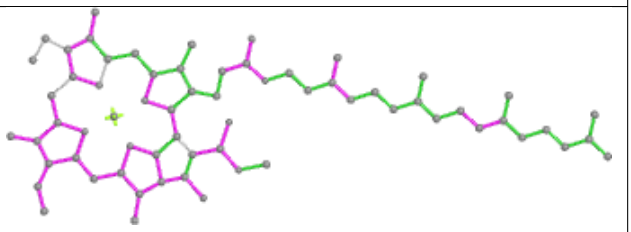
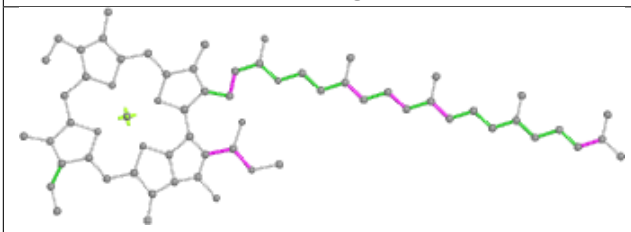


Bond angles



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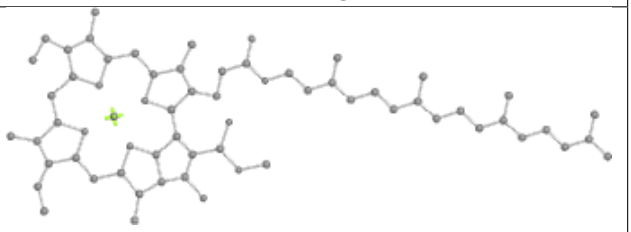
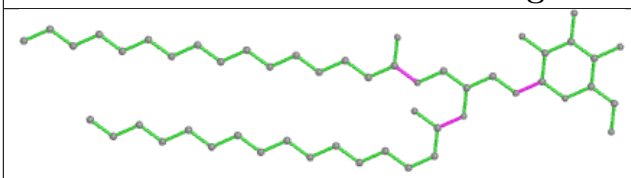


Rings

Ligand LMG j 101



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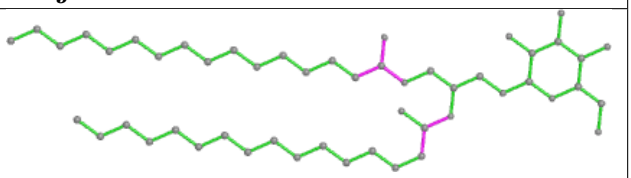
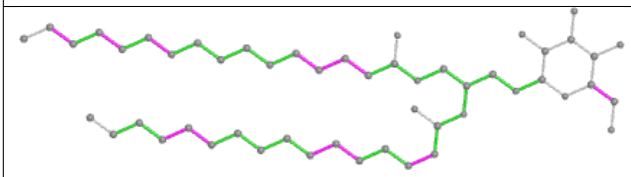


Bond angles



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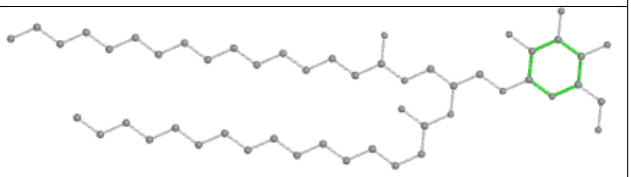
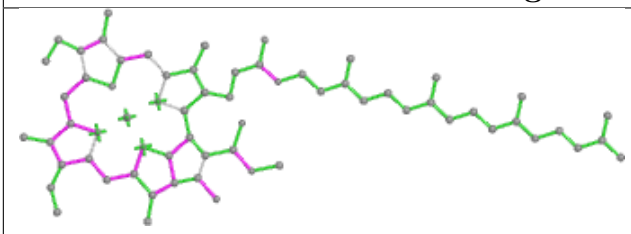


Rings

Ligand CLA B 616



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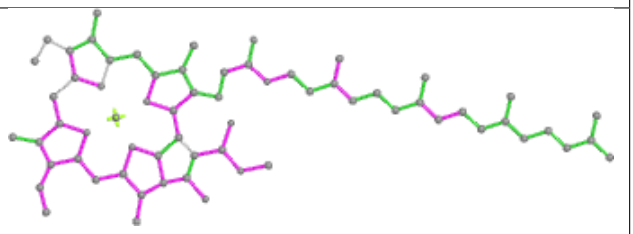
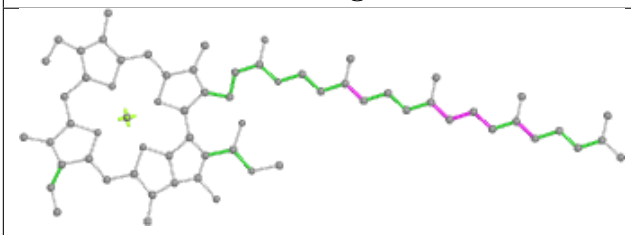


Bond angles



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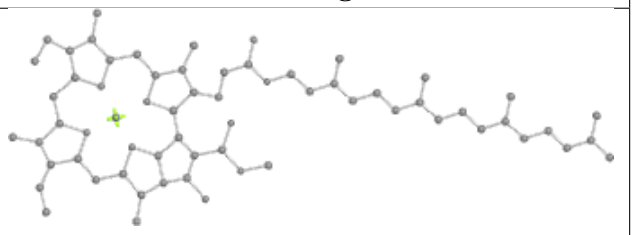
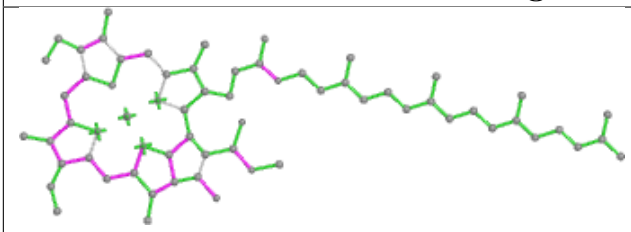


Rings

Ligand CLA b 619



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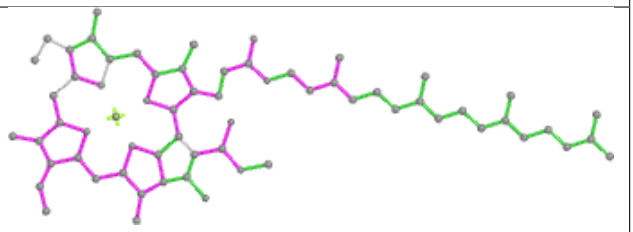
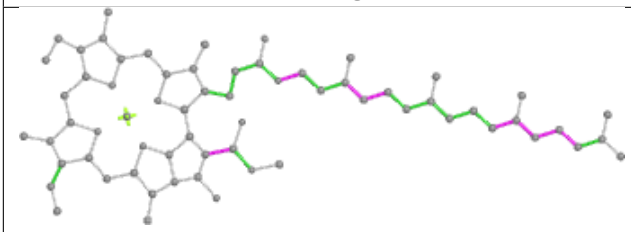
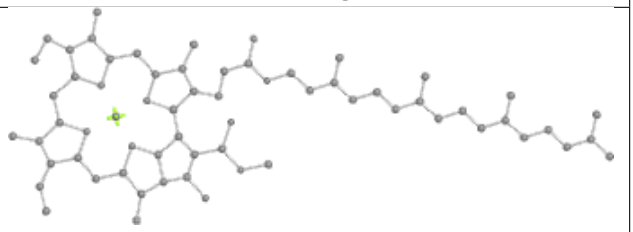


Bond angles

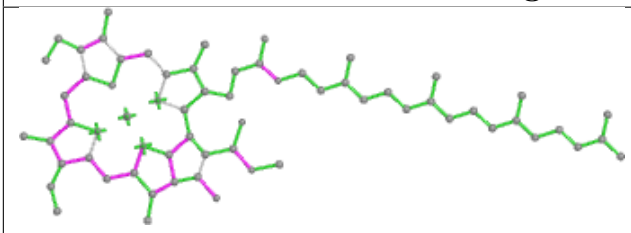


Torsions



Rings

Ligand CLA D 401



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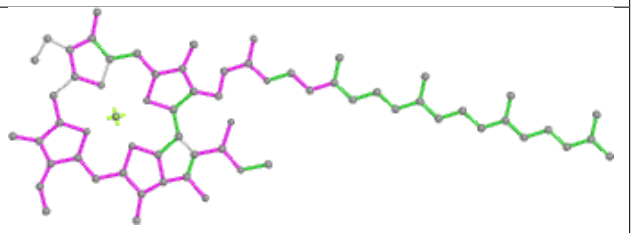
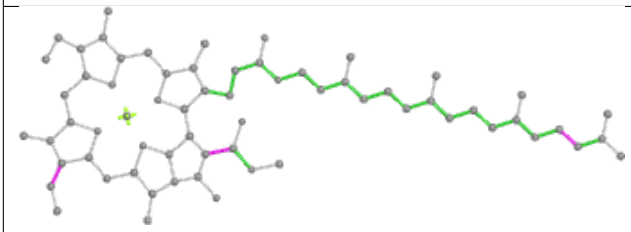


Bond angles



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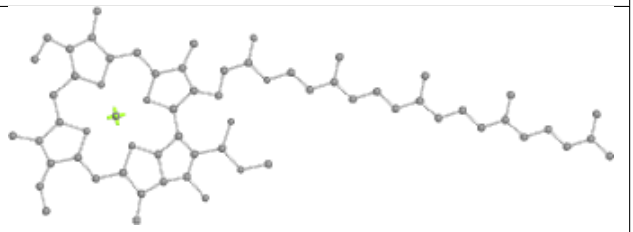
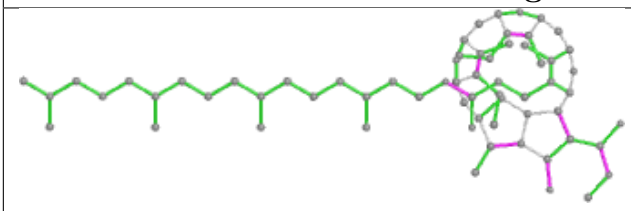


Rings

Ligand PHO d 403



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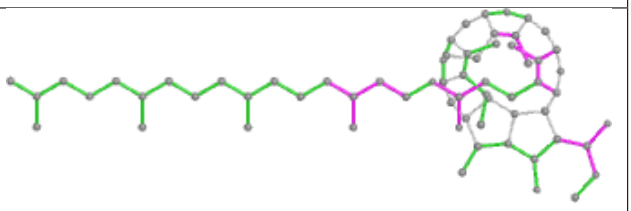
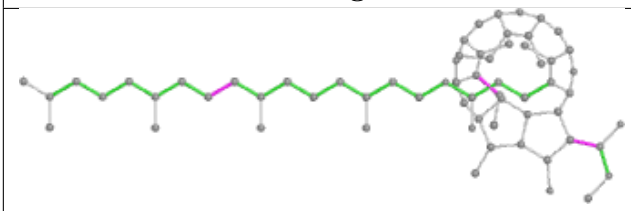


Bond angles



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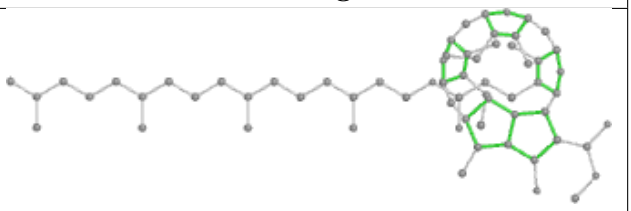
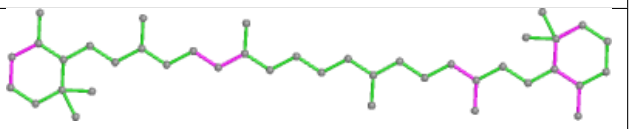


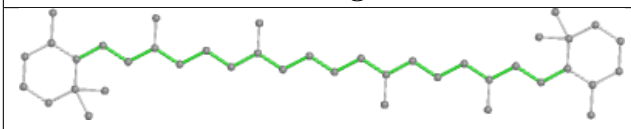
Rings

Ligand BCR b 623

Bond lengths



Bond angles



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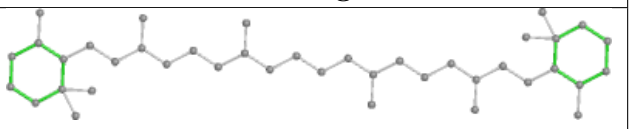
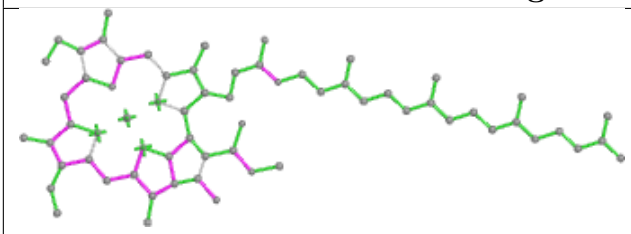


Rings

Ligand CLA d 404



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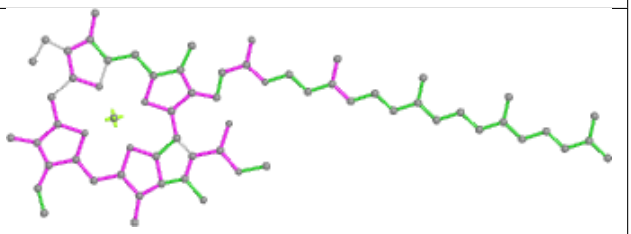
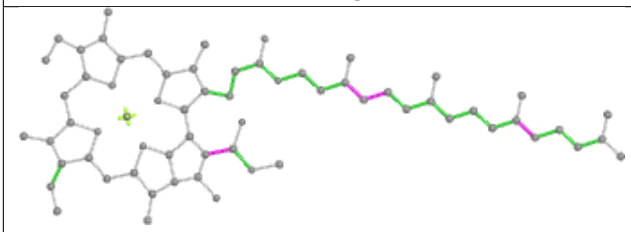


Bond angles



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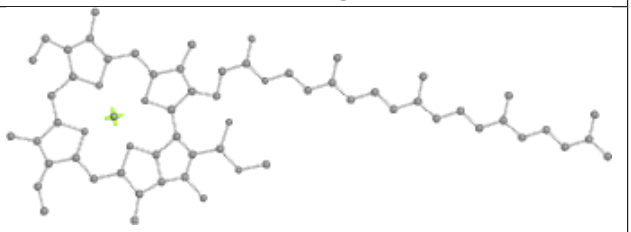
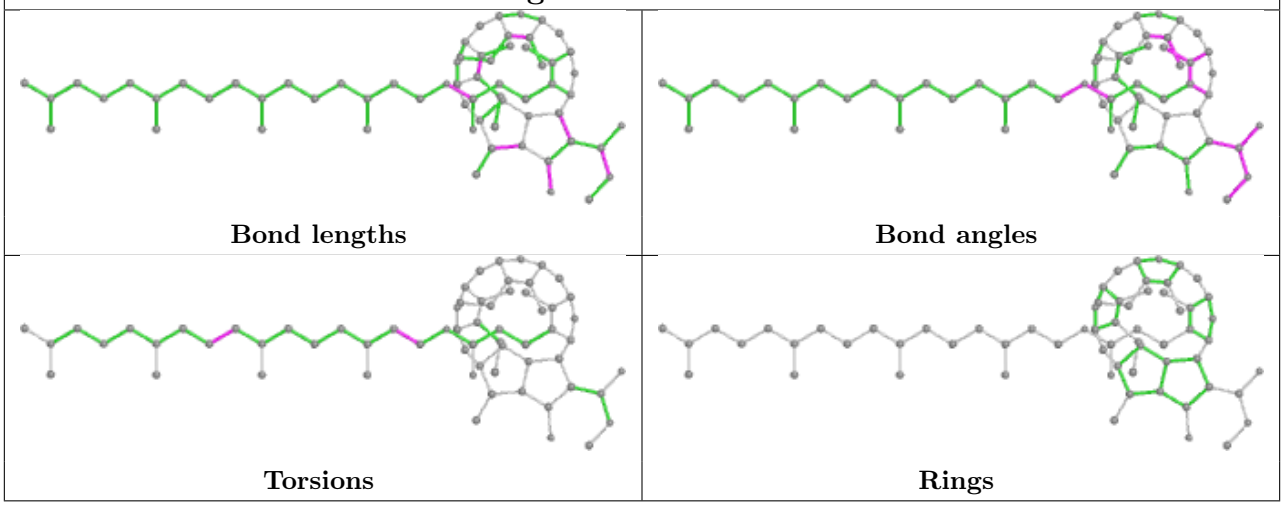
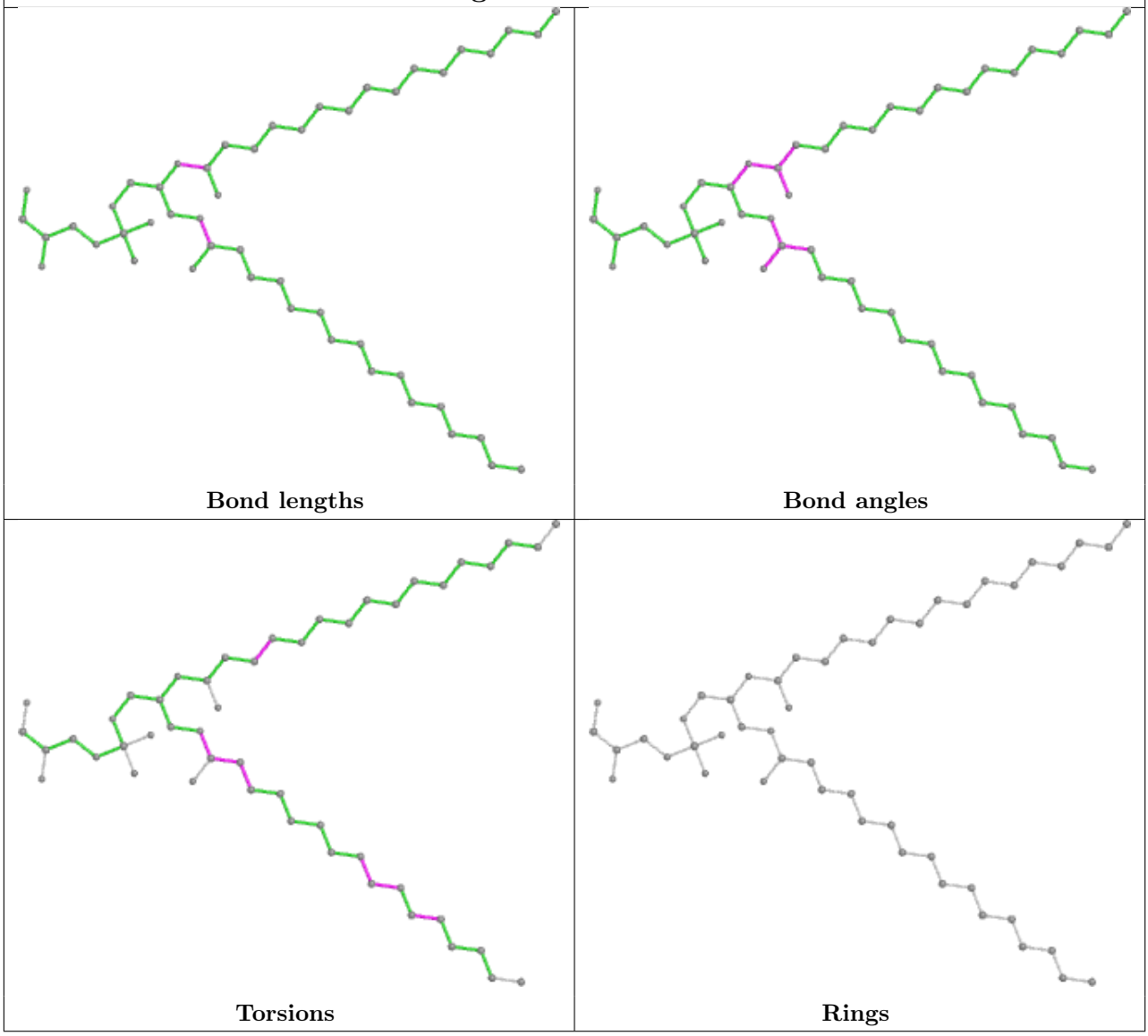


Rings

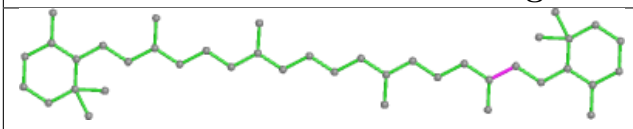
Ligand PHO a 408



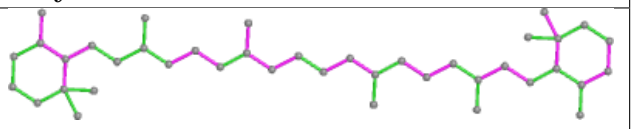
Ligand LHG d 408



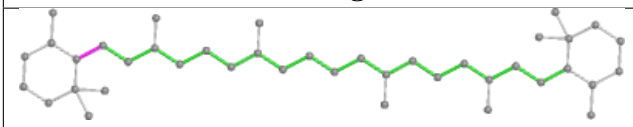
Ligand BCR y 101



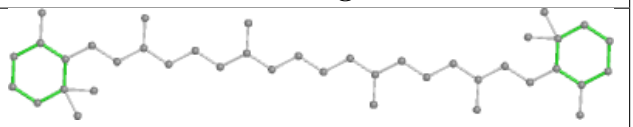
Bond lengths



Bond angles

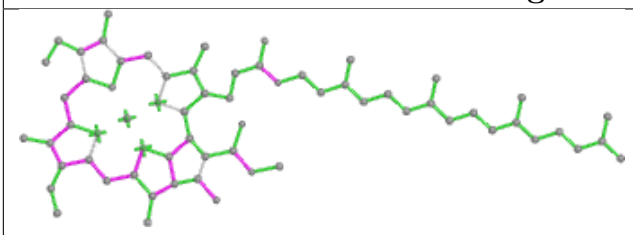


Torsions

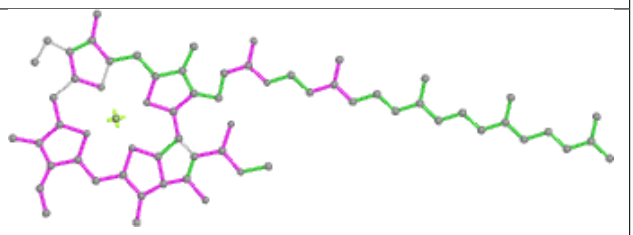


Rings

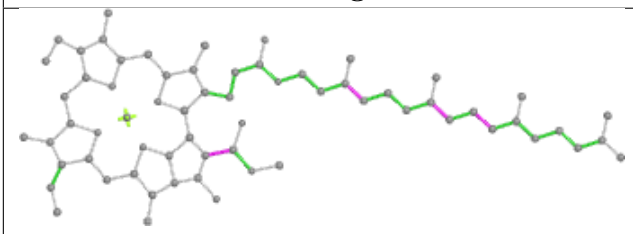
Ligand CLA b 610



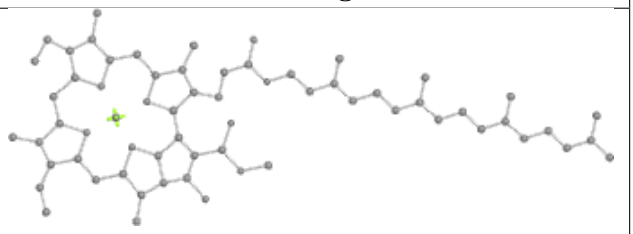
Bond lengths



Bond angles

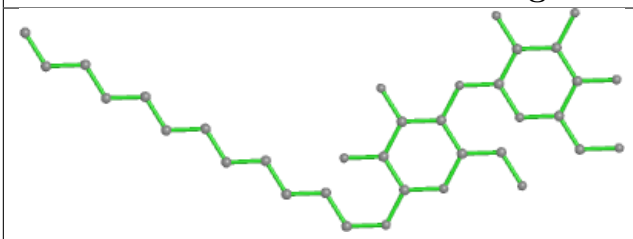


Torsions

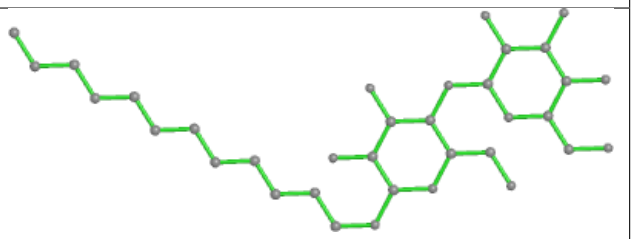


Rings

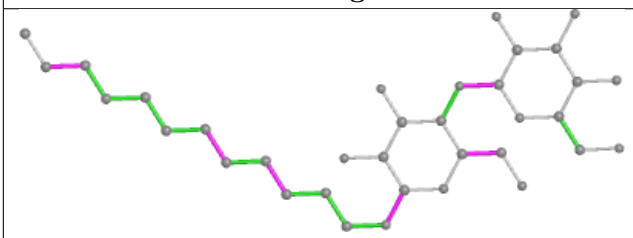
Ligand LMT f 102



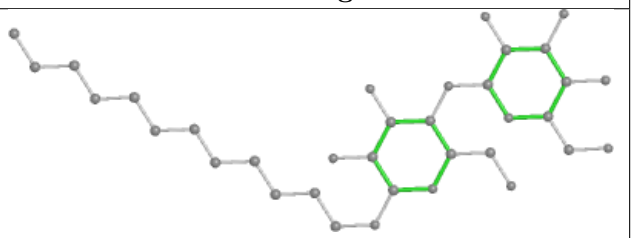
Bond lengths



Bond angles

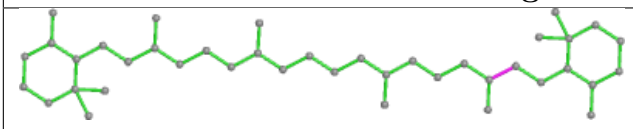


Torsions

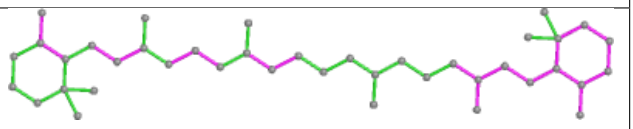


Rings

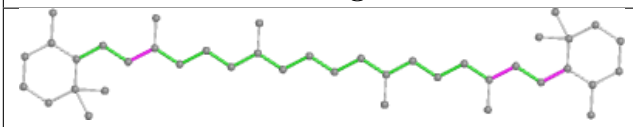
Ligand BCR D 405



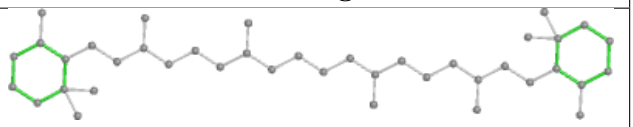
Bond lengths



Bond angles

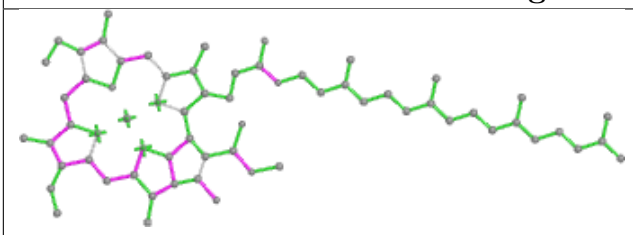


Torsions

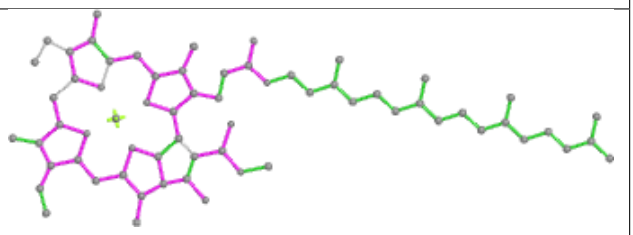


Rings

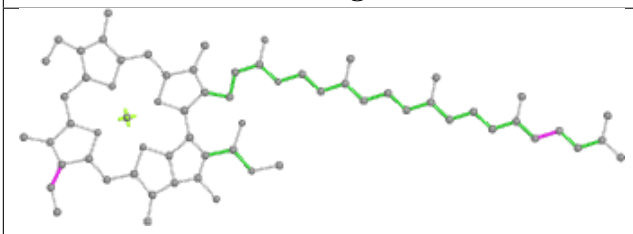
Ligand CLA a 406



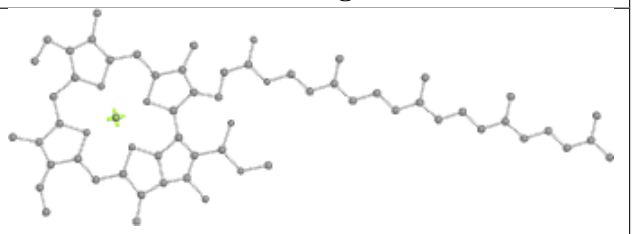
Bond lengths



Bond angles

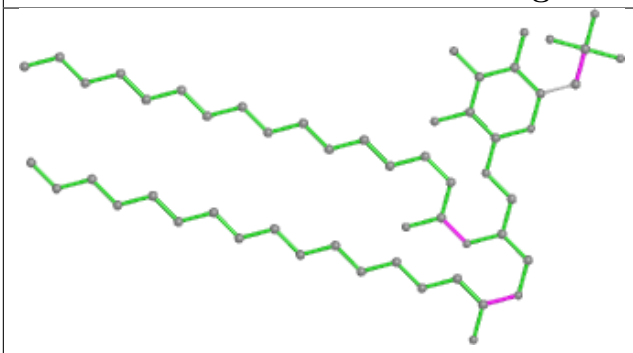


Torsions

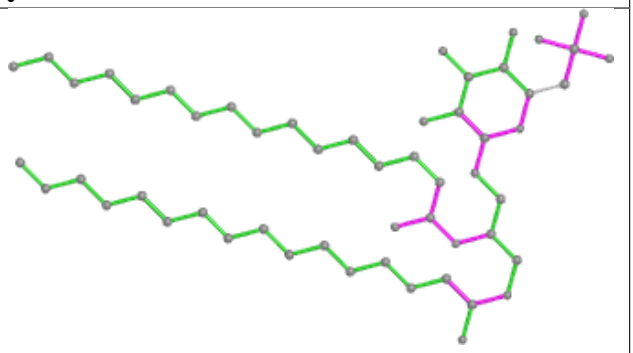


Rings

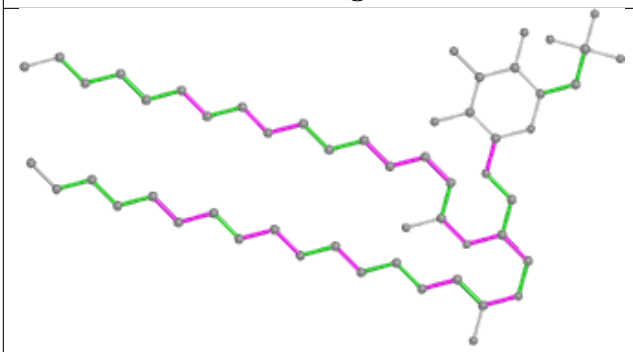
Ligand SQD l 101



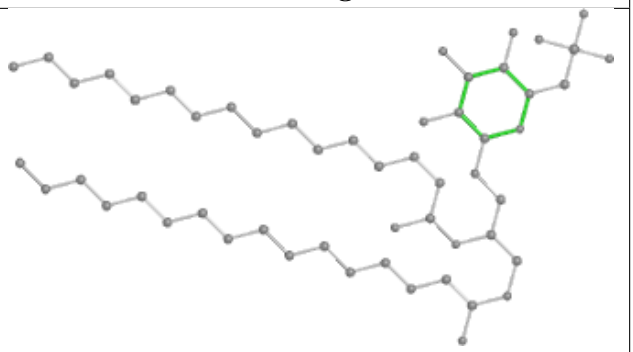
Bond lengths



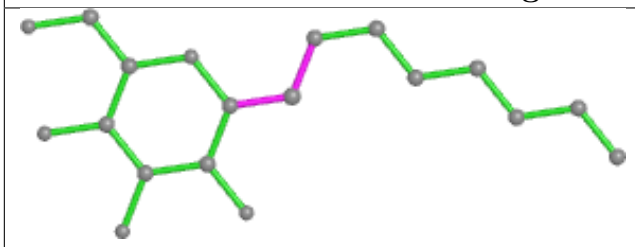
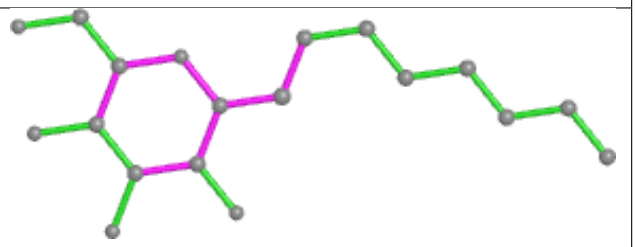
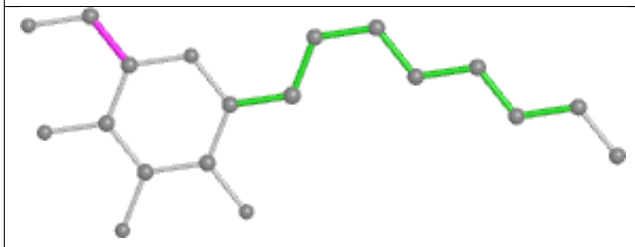
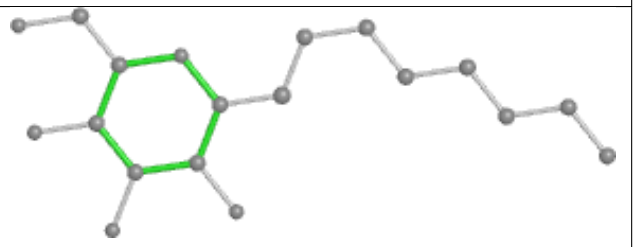
Bond angles

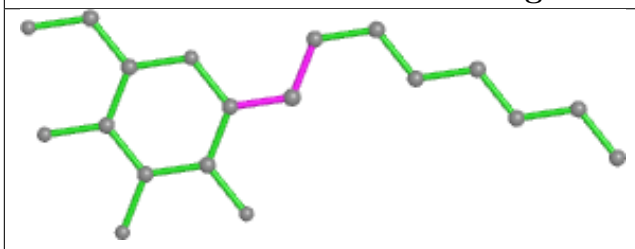
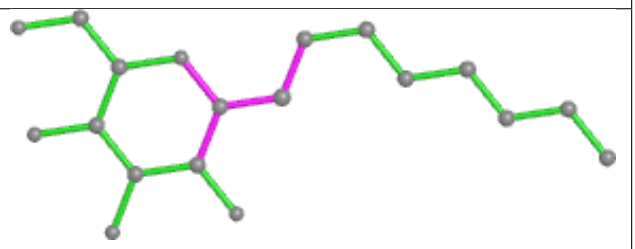
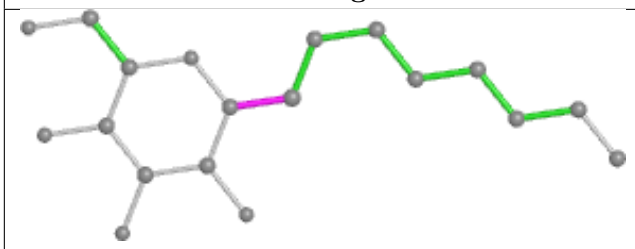
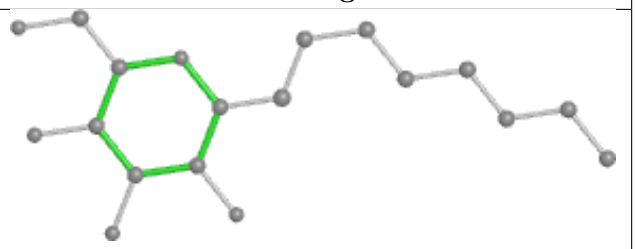


Torsions

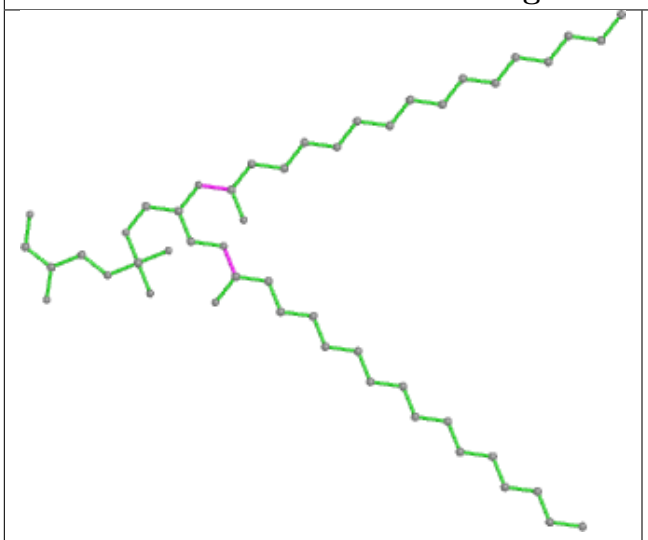


Rings

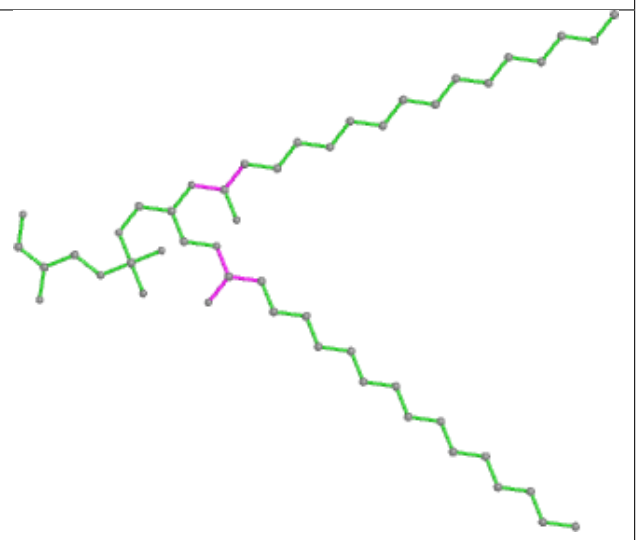
Ligand HTG C 523	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HTG b 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

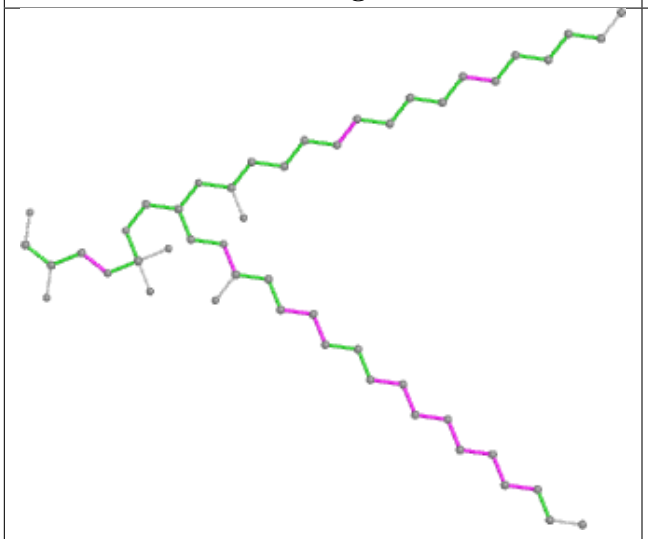
Ligand LHG D 410



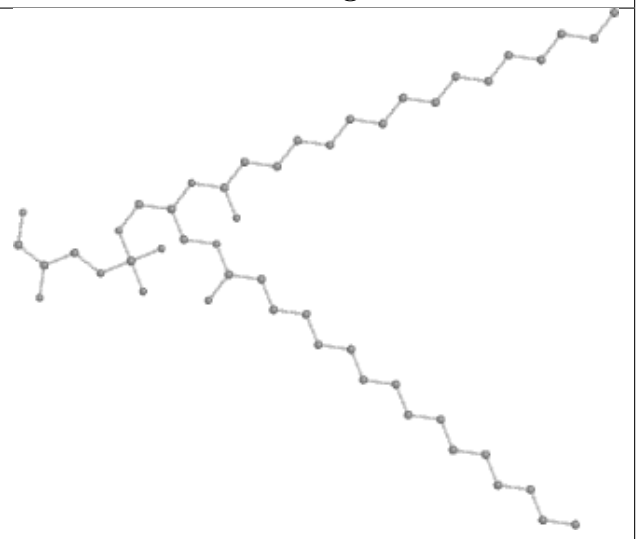
Bond lengths



Bond angles

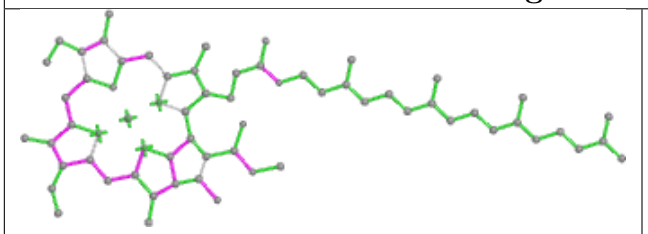


Torsions

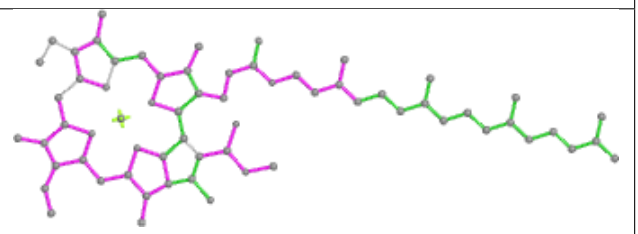


Rings

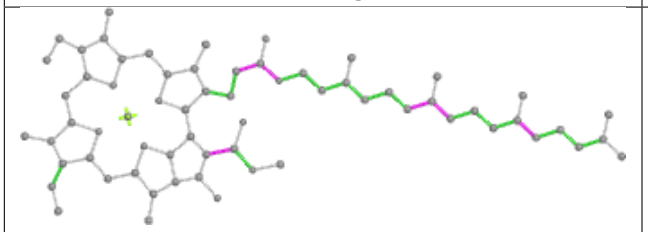
Ligand CLA C 513



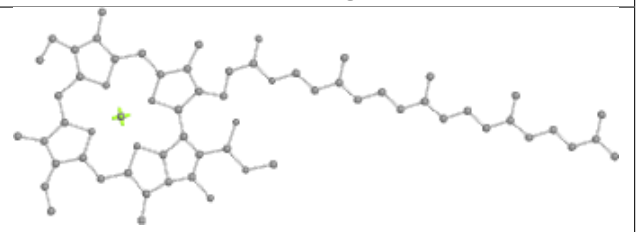
Bond lengths



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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	0.67	44 (13%)	3	5	16, 23, 42, 79	0
1	a	334/344 (97%)	0.83	59 (17%)	1	1	17, 25, 48, 82	0
2	B	504/505 (99%)	0.27	42 (8%)	11	17	18, 27, 52, 90	0
2	b	504/505 (99%)	0.46	50 (9%)	7	12	19, 29, 60, 108	0
3	C	451/455 (99%)	0.24	28 (6%)	20	29	20, 32, 49, 89	0
3	c	455/455 (100%)	0.43	38 (8%)	11	17	23, 35, 50, 87	0
4	D	342/342 (100%)	0.88	63 (18%)	1	1	15, 24, 40, 114	0
4	d	341/342 (99%)	0.59	39 (11%)	5	8	18, 26, 42, 90	0
5	E	81/84 (96%)	1.20	15 (18%)	1	1	27, 40, 68, 97	0
5	e	81/84 (96%)	1.09	15 (18%)	1	1	32, 45, 77, 97	0
6	F	34/44 (77%)	0.35	6 (17%)	1	1	26, 35, 56, 64	0
6	f	32/44 (72%)	0.40	4 (12%)	3	6	31, 37, 84, 99	0
7	H	65/65 (100%)	0.34	3 (4%)	32	42	24, 34, 52, 97	0
7	h	65/65 (100%)	0.55	6 (9%)	9	14	28, 37, 58, 113	0
8	I	37/38 (97%)	0.83	5 (13%)	3	5	30, 34, 91, 101	0
8	i	37/38 (97%)	0.73	5 (13%)	3	5	29, 34, 79, 102	0
9	J	38/39 (97%)	0.73	8 (21%)	1	1	26, 38, 85, 109	0
9	j	38/39 (97%)	0.25	3 (7%)	12	19	30, 41, 84, 85	0
10	K	37/37 (100%)	0.16	0	100	100	31, 38, 55, 64	0
10	k	37/37 (100%)	0.86	8 (21%)	0	1	33, 42, 56, 66	0
11	L	37/37 (100%)	1.17	11 (29%)	0	0	16, 20, 66, 91	0
11	l	37/37 (100%)	1.04	6 (16%)	1	2	17, 21, 61, 91	0
12	M	33/36 (91%)	0.89	6 (18%)	1	1	18, 23, 44, 100	0
12	m	33/36 (91%)	0.76	5 (15%)	2	3	19, 23, 44, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.38	21 (8%)	10	16	16, 34, 65, 113	0
13	o	243/244 (99%)	0.89	52 (21%)	0	1	18, 35, 75, 122	0
14	T	29/31 (93%)	0.98	4 (13%)	2	4	17, 23, 48, 85	0
14	t	29/31 (93%)	0.55	2 (6%)	16	25	17, 23, 49, 85	0
15	U	97/104 (93%)	0.26	5 (5%)	27	37	22, 33, 53, 85	0
15	u	97/104 (93%)	-0.11	0	100	100	25, 34, 51, 85	0
16	V	137/137 (100%)	-0.03	0	100	100	23, 33, 54, 70	0
16	v	137/137 (100%)	0.49	13 (9%)	8	13	26, 38, 57, 72	0
17	Y	29/30 (96%)	2.05	9 (31%)	0	0	38, 50, 91, 107	0
17	y	29/30 (96%)	1.91	9 (31%)	0	0	40, 54, 91, 107	0
18	X	39/40 (97%)	0.77	8 (20%)	1	1	32, 42, 80, 92	0
18	x	39/40 (97%)	1.59	11 (28%)	0	0	35, 45, 93, 96	0
19	Z	62/62 (100%)	1.28	18 (29%)	0	0	40, 52, 87, 98	0
19	z	62/62 (100%)	2.95	36 (58%)	0	0	44, 53, 87, 98	0
20	R	34/34 (100%)	9.29	34 (100%)	0	0	69, 93, 111, 118	0
All	All	5293/5382 (98%)	0.65	691 (13%)	3	5	15, 31, 63, 122	0

All (691) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	18.4
20	R	6	LEU	14.1
20	R	14	LEU	13.2
20	R	31	VAL	13.0
20	R	20	VAL	12.0
17	Y	18	VAL	11.4
20	R	19	ALA	11.1
20	R	25	PRO	11.0
20	R	16	ALA	11.0
20	R	5	VAL	10.6
20	R	27	ALA	10.4
19	z	3	ILE	10.4
20	R	23	ILE	10.2
20	R	32	GLN	10.2
18	x	38	GLN	9.8
19	z	62	VAL	9.7
17	Y	19	ILE	9.5

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Mol	Chain	Res	Type	RSRZ
20	R	15	ALA	9.5
8	i	37	LEU	9.5
20	R	34	LEU	9.4
19	z	5	PHE	9.3
20	R	13	LEU	9.3
20	R	21	ARG	9.2
20	R	24	LEU	9.2
17	y	19	ILE	9.2
20	R	26	TYR	9.1
7	h	65	LEU	8.8
20	R	10	LEU	8.8
20	R	9	LEU	8.7
17	y	18	VAL	8.3
20	R	22	ASN	8.3
20	R	29	LYS	8.3
20	R	7	VAL	8.2
4	D	11	GLU	8.1
1	A	11	ALA	8.0
18	x	2	THR	8.0
20	R	12	VAL	8.0
8	I	38	GLU	7.9
20	R	28	VAL	7.9
20	R	17	GLY	7.7
2	b	495	PHE	7.7
8	I	37	LEU	7.6
19	z	4	LEU	7.6
20	R	3	TRP	7.6
18	x	37	VAL	7.5
19	z	60	PHE	7.4
20	R	30	GLN	7.4
7	H	65	LEU	7.4
20	R	11	PRO	7.1
20	R	35	LEU	7.1
17	Y	22	LEU	7.0
2	B	85	GLY	6.9
19	Z	62	VAL	6.9
1	a	11	ALA	6.6
19	z	42	LEU	6.4
2	b	491	VAL	6.4
20	R	33	LYS	6.3
19	z	61	VAL	6.3
2	b	486	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
13	O	60	ARG	6.2
5	e	5	THR	6.2
17	y	20	ALA	6.2
19	Z	3	ILE	6.2
13	o	246	ALA	6.1
2	b	504	THR	6.1
18	x	34	ILE	6.1
2	b	499	VAL	6.0
13	o	36	GLN	6.0
19	z	7	LEU	6.0
10	k	18	PHE	5.9
2	b	293	ALA	5.8
2	b	496	TYR	5.8
17	Y	20	ALA	5.7
5	E	84	LYS	5.5
6	f	14	PRO	5.5
1	A	13	LEU	5.5
2	B	494	GLY	5.5
6	f	15	ILE	5.4
13	o	35	SER	5.4
6	F	16	PHE	5.3
2	B	495	PHE	5.3
18	x	40	SER	5.3
2	b	493	TRP	5.3
19	Z	31	GLN	5.3
4	D	12	ARG	5.3
2	b	487	SER	5.3
5	E	17	VAL	5.3
5	e	6	GLY	5.2
9	J	2	SER	5.2
7	H	66	GLY	5.1
19	z	33	TRP	5.1
2	b	494	GLY	5.1
19	z	41	PHE	5.1
17	y	22	LEU	5.1
2	b	505	ARG	5.1
5	e	4	THR	5.1
16	v	17	LYS	5.0
8	I	36	ASP	5.0
2	b	295	GLY	5.0
19	Z	36	SER	5.0
3	c	146	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
11	l	1	MET	5.0
5	E	21	VAL	4.9
7	H	64	ALA	4.9
3	c	143	TYR	4.8
2	b	85	GLY	4.8
18	x	39	ARG	4.8
19	Z	7	LEU	4.8
19	z	39	LEU	4.8
13	o	25	THR	4.8
20	R	2	ASP	4.8
18	X	40	SER	4.8
5	E	6	GLY	4.7
7	h	66	GLY	4.7
13	o	56	PRO	4.7
13	o	59	LYS	4.7
19	z	2	THR	4.6
13	o	34	SER	4.6
20	R	8	VAL	4.6
13	o	23	ASP	4.6
2	B	297	THR	4.6
13	o	133	VAL	4.6
6	f	16	PHE	4.6
19	Z	35	ARG	4.6
5	e	25	ILE	4.6
6	F	15	ILE	4.6
2	b	497	GLN	4.6
4	D	201	VAL	4.6
19	Z	33	TRP	4.5
9	J	3	GLU	4.5
4	d	182	LEU	4.5
2	b	86	ILE	4.5
13	o	61	GLN	4.5
2	b	502	VAL	4.5
10	k	12	PRO	4.5
8	i	34	ARG	4.4
2	B	486	LEU	4.4
3	c	147	PHE	4.4
19	z	9	LEU	4.4
2	b	294	SER	4.4
4	d	179	PHE	4.3
13	o	87	VAL	4.3
2	b	84	THR	4.3

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Mol	Chain	Res	Type	RSRZ
13	o	27	ARG	4.3
20	R	4	ARG	4.3
4	D	156	VAL	4.3
1	a	290	ILE	4.2
17	Y	21	GLN	4.2
8	i	38	GLU	4.2
1	a	193	LEU	4.2
18	X	37	VAL	4.2
13	O	58	ASN	4.2
13	o	58	ASN	4.2
2	b	485	GLU	4.1
18	X	2	THR	4.1
13	o	26	ALA	4.1
13	o	32	ILE	4.1
19	z	1	MET	4.1
13	o	4	THR	4.1
19	z	35	ARG	4.1
13	O	25	THR	4.1
17	Y	25	ILE	4.0
8	i	36	ASP	4.0
2	b	126	PRO	4.0
19	z	53	VAL	4.0
1	A	200	LEU	4.0
4	D	279	LEU	4.0
19	z	59	PHE	4.0
2	B	86[A]	ILE	3.9
1	a	288	LEU	3.9
1	a	184	ILE	3.9
1	A	288	LEU	3.9
13	o	38	TYR	3.9
1	a	197	PHE	3.9
1	a	280	VAL	3.9
2	B	84	THR	3.9
14	t	29	ILE	3.9
4	D	153	PHE	3.8
4	D	191	TRP	3.8
3	C	432	VAL	3.8
2	b	490	GLN	3.8
12	M	33	GLN	3.8
1	a	297	LEU	3.8
3	c	134	ILE	3.8
13	o	37	THR	3.8

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Mol	Chain	Res	Type	RSRZ
13	O	27	ARG	3.8
4	D	205	LEU	3.8
13	o	208	THR	3.7
12	m	34	LYS	3.7
4	D	289	LEU	3.7
15	U	8	GLU	3.7
19	Z	32	ASP	3.7
13	o	60	ARG	3.7
15	U	79	LEU	3.7
17	y	41	VAL	3.7
1	A	285	PHE	3.7
1	a	200	LEU	3.7
1	a	285	PHE	3.7
3	C	257	PHE	3.7
19	Z	4	LEU	3.7
2	b	127	ARG	3.7
13	o	33	ASP	3.6
1	a	192	ILE	3.6
4	D	238	THR	3.6
14	T	30	THR	3.6
4	D	280	TRP	3.6
13	O	62	GLU	3.6
4	d	12	ARG	3.6
4	D	150	ILE	3.6
5	E	4	THR	3.6
13	O	56	PRO	3.6
2	B	489	GLU	3.6
19	z	25	VAL	3.6
19	z	32	ASP	3.5
14	T	9	ILE	3.5
2	b	129	GLY	3.5
2	b	484	PRO	3.5
2	b	297	THR	3.5
4	D	196	PHE	3.5
13	O	59	LYS	3.5
3	c	21	ILE	3.5
2	b	290	ALA	3.5
4	D	152	VAL	3.5
18	X	38	GLN	3.5
4	D	149	PRO	3.4
17	y	21	GLN	3.4
4	d	196	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
11	L	31	PHE	3.4
11	L	2	GLU	3.4
2	b	500	GLY	3.4
3	c	145	SER	3.4
1	A	202	VAL	3.4
4	D	286	VAL	3.4
19	z	58	ASN	3.4
3	C	262	ARG	3.4
13	o	132	ASN	3.4
3	c	432	VAL	3.4
4	d	14	TRP	3.4
1	A	287	ALA	3.4
17	y	25	ILE	3.4
1	a	161	TYR	3.4
1	A	197	PHE	3.4
5	e	59	GLU	3.4
13	o	62	GLU	3.4
2	B	298	LEU	3.4
4	D	276	VAL	3.4
4	D	293	LEU	3.4
13	o	89	SER	3.3
19	z	30	PRO	3.3
2	b	296	ALA	3.3
19	z	6	GLN	3.3
1	a	163	ILE	3.3
18	X	31	ILE	3.3
2	B	461	LEU	3.3
9	J	6	ARG	3.3
11	l	2	GLU	3.3
1	a	202	VAL	3.3
2	b	292	LEU	3.3
5	e	84	LYS	3.3
6	F	14	PRO	3.3
19	Z	60	PHE	3.2
4	D	204	VAL	3.2
1	A	230	THR	3.2
1	A	290	ILE	3.2
16	v	19	ILE	3.2
2	B	457	VAL	3.2
2	b	488	PRO	3.2
16	v	110	LYS	3.2
1	a	157	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	253	LEU	3.2
16	v	107	LEU	3.2
4	D	160	TYR	3.2
11	l	3	PRO	3.2
1	A	186	PHE	3.2
3	c	257	PHE	3.2
9	J	5	GLY	3.2
10	k	14	ALA	3.2
4	D	175	VAL	3.2
18	x	36	LYS	3.2
3	c	259	TRP	3.2
17	Y	43	ARG	3.2
13	O	28	GLY	3.2
19	Z	61	VAL	3.2
13	o	91	GLY	3.1
13	o	211	ILE	3.1
3	C	436	PHE	3.1
6	F	18	VAL	3.1
19	z	31	GLN	3.1
4	D	148	ALA	3.1
1	A	278	TRP	3.1
1	A	193	LEU	3.1
11	L	29	LEU	3.1
19	z	40	ILE	3.1
13	o	24	ASP	3.1
19	Z	1	MET	3.1
13	O	61	GLN	3.1
2	b	501	ASP	3.1
19	Z	39	LEU	3.1
19	Z	42	LEU	3.1
15	U	70	ARG	3.1
13	o	135	SER	3.0
5	e	21	VAL	3.0
12	M	16[A]	LEU	3.0
14	T	13	ILE	3.0
2	B	496	TYR	3.0
3	C	143	TYR	3.0
4	D	275	PRO	3.0
5	E	5	THR	3.0
19	Z	34	ASP	3.0
10	k	17	ILE	3.0
13	o	126	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	293	ALA	3.0
3	C	260	ALA	3.0
4	D	182	LEU	3.0
4	d	148	ALA	3.0
4	d	283	ALA	3.0
1	A	321	ILE	3.0
4	d	184	PHE	3.0
1	A	12	ASN	3.0
2	b	125	ASP	3.0
9	J	24	VAL	3.0
4	d	205	LEU	3.0
13	O	93	LEU	3.0
1	a	182	PHE	3.0
3	C	431	PHE	3.0
2	B	504	THR	3.0
4	D	278	GLY	3.0
2	B	487	SER	3.0
19	z	29	SER	3.0
2	B	499	VAL	3.0
4	d	175	VAL	3.0
4	d	201	VAL	3.0
2	b	298	LEU	2.9
4	d	178	ILE	2.9
4	d	325	ILE	2.9
19	z	38	GLN	2.9
3	C	145[A]	SER	2.9
3	c	20	SER	2.9
5	E	19	TYR	2.9
8	I	34	ARG	2.9
4	d	185	PHE	2.9
3	c	144	SER	2.9
16	v	26	TYR	2.9
3	c	411	ALA	2.9
8	I	35	LYS	2.9
2	b	489	GLU	2.9
13	o	134	THR	2.9
11	L	1	MET	2.9
11	l	31	PHE	2.9
4	D	202	ALA	2.9
13	o	130	GLN	2.9
2	B	488	PRO	2.9
2	b	492	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
18	X	34	ILE	2.9
13	O	26	ALA	2.9
4	d	156	VAL	2.9
1	a	186	PHE	2.9
13	o	131	PRO	2.8
1	a	284	TRP	2.8
2	B	460	LEU	2.8
4	D	200	GLY	2.8
3	c	142	GLU	2.8
1	a	286	ALA	2.8
5	E	22	ILE	2.8
2	b	503	THR	2.8
1	A	196	PRO	2.8
10	k	13	GLU	2.8
1	a	205	VAL	2.8
1	a	293	MET	2.8
4	D	193	LEU	2.8
18	x	30	ALA	2.8
1	A	77	ILE	2.8
9	J	7	ILE	2.8
1	a	295	PHE	2.8
4	d	187	GLY	2.8
19	z	49	ALA	2.8
1	A	192	ILE	2.8
1	a	235	TYR	2.8
1	A	283	VAL	2.8
1	A	297	LEU	2.8
4	D	122	LEU	2.8
4	D	183	LEU	2.8
7	h	22	ALA	2.8
13	o	22	LEU	2.8
18	x	3	ILE	2.8
4	D	146	PHE	2.8
4	D	119	ALA	2.7
2	B	295	GLY	2.7
5	E	83	LEU	2.7
1	a	194	MET	2.7
3	c	425	TRP	2.7
4	d	280	TRP	2.7
1	a	299	GLY	2.7
9	j	6	ARG	2.7
1	a	326	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
4	d	183	LEU	2.7
11	l	25	LEU	2.7
1	A	176	ILE	2.7
4	D	325	ILE	2.7
5	e	61	ARG	2.7
13	O	65	PHE	2.7
3	c	428	THR	2.7
19	z	56	VAL	2.7
11	L	23	LEU	2.7
11	l	27	LEU	2.7
19	z	57	LEU	2.7
4	D	199	MET	2.7
13	o	209	GLY	2.7
2	B	503	THR	2.7
13	o	140	THR	2.7
5	E	20	TRP	2.7
2	B	502	VAL	2.7
4	D	154	VAL	2.7
2	b	483	ASP	2.7
1	a	282	GLY	2.7
4	D	192	THR	2.7
2	b	291	SER	2.7
4	D	290	ALA	2.7
13	o	139	SER	2.7
2	B	462	PHE	2.7
2	B	464	PHE	2.7
2	b	123	PHE	2.7
3	C	259	TRP	2.7
3	C	407	VAL	2.7
12	M	34	LYS	2.7
3	c	426	LEU	2.7
13	o	63	ALA	2.6
1	A	205	VAL	2.6
4	D	281	MET	2.6
1	A	210	LEU	2.6
3	c	404	LEU	2.6
9	j	2	SER	2.6
16	v	106	ASN	2.6
3	c	410	VAL	2.6
4	D	277	THR	2.6
4	d	209	LEU	2.6
11	L	30	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
13	o	21	THR	2.6
2	B	459	ALA	2.6
1	a	195	HIS	2.6
4	D	284	ILE	2.6
13	o	30	TYR	2.6
13	o	64	GLU	2.6
17	y	23	THR	2.6
4	d	279	LEU	2.6
1	A	203	ALA	2.6
16	v	16	GLY	2.6
17	Y	30	ILE	2.6
1	a	180	PHE	2.6
1	a	330	VAL	2.6
3	c	155	ASN	2.6
2	B	165	GLY	2.6
3	C	23	ALA	2.6
19	z	10	ALA	2.6
1	A	184	ILE	2.6
19	z	14	ILE	2.6
3	C	255	THR	2.6
19	Z	2	THR	2.6
1	a	281	VAL	2.6
2	b	457	VAL	2.6
5	e	79	PHE	2.5
3	c	433	LEU	2.5
4	D	116	LEU	2.5
4	D	283	ALA	2.5
13	o	57	LYS	2.5
1	a	279	PRO	2.5
5	E	81	GLU	2.5
1	A	185	VAL	2.5
4	D	274	VAL	2.5
4	D	287	VAL	2.5
1	A	182	PHE	2.5
4	d	188	PHE	2.5
1	a	287	ALA	2.5
3	C	404	LEU	2.5
3	c	140	LEU	2.5
5	E	73	LYS	2.5
13	O	136	ILE	2.5
4	d	152	VAL	2.5
2	B	456	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	c	163	PHE	2.5
4	d	289	LEU	2.5
4	d	321	LEU	2.5
14	t	30	THR	2.5
16	v	108	THR	2.5
2	b	413	ASP	2.5
4	D	159	ILE	2.5
7	h	6	TRP	2.5
19	z	18	VAL	2.5
18	X	39	ARG	2.5
3	C	181	PHE	2.5
4	d	281	MET	2.5
9	J	4	GLY	2.5
16	v	95	LEU	2.5
3	c	429	SER	2.5
1	a	321	ILE	2.5
4	d	159	ILE	2.5
1	a	324	ALA	2.5
2	B	296	ALA	2.5
1	A	201	GLY	2.5
18	x	8	LYS	2.5
3	c	201	ASN	2.5
13	o	245	PRO	2.4
5	E	72	ALA	2.4
13	o	243	ILE	2.4
13	O	133	VAL	2.4
3	C	425	TRP	2.4
13	O	88	ASN	2.4
1	A	180	PHE	2.4
1	A	300	PHE	2.4
2	B	479	PHE	2.4
3	c	431	PHE	2.4
4	D	181	PHE	2.4
4	d	193	LEU	2.4
13	o	142	PHE	2.4
19	Z	30	PRO	2.4
4	D	203	GLY	2.4
7	h	64	ALA	2.4
1	A	160	ILE	2.4
13	o	136	ILE	2.4
1	A	281	VAL	2.4
1	a	185	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
13	O	137	THR	2.4
12	m	33	GLN	2.4
4	D	184	PHE	2.4
10	k	21	LEU	2.4
8	i	35	LYS	2.4
7	h	23	PRO	2.4
1	A	284	TRP	2.4
1	a	191	ASN	2.4
12	m	13	LEU	2.4
2	B	453	PHE	2.4
4	D	185	PHE	2.4
12	M	14	PHE	2.4
12	m	14	PHE	2.4
1	a	203	ALA	2.4
4	d	329	MET	2.4
3	c	200	THR	2.4
13	O	138	THR	2.4
1	A	16	ARG	2.4
1	A	282	GLY	2.4
1	a	190	HIS	2.4
4	d	284	ILE	2.4
4	d	74	LEU	2.4
2	B	463	PHE	2.4
2	b	302	TRP	2.4
3	C	435	PHE	2.4
4	D	170	ALA	2.4
2	b	124	ARG	2.4
3	C	428	THR	2.4
2	B	408	GLY	2.4
16	v	15	GLU	2.4
16	v	86	GLN	2.4
13	o	66	VAL	2.4
2	B	127	ARG	2.3
2	B	402	TYR	2.3
1	a	278	TRP	2.3
19	Z	38	GLN	2.3
5	e	36	LEU	2.3
5	e	26	THR	2.3
6	F	13	TYR	2.3
3	c	207	ARG	2.3
4	d	328	TRP	2.3
15	U	73	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	c	434	ALA	2.3
2	B	324	LEU	2.3
3	C	261	ARG	2.3
2	b	363	PHE	2.3
1	A	188	ALA	2.3
1	A	324	ALA	2.3
4	D	158	LEU	2.3
13	o	199	LEU	2.3
13	O	30	TYR	2.3
1	a	300	PHE	2.3
1	A	198	HIS	2.3
2	B	505	ARG	2.3
13	o	141	ASP	2.3
3	c	166	ILE	2.3
1	a	341	LEU	2.3
4	D	291	LEU	2.3
13	O	24	ASP	2.3
2	B	497	GLN	2.2
5	e	17	VAL	2.2
6	F	17	THR	2.2
2	b	460	LEU	2.2
3	c	253	LEU	2.2
3	c	401	LEU	2.2
11	L	27	LEU	2.2
13	o	239	PHE	2.2
1	a	172	MET	2.2
16	v	18	THR	2.2
1	a	188	ALA	2.2
13	o	202	ALA	2.2
1	a	283	VAL	2.2
11	L	24[A]	ILE	2.2
3	C	433	LEU	2.2
10	k	10	LYS	2.2
13	o	194	LYS	2.2
4	D	195	PRO	2.2
1	A	211	PHE	2.2
1	a	206	PHE	2.2
2	B	325	PHE	2.2
11	L	35	PHE	2.2
18	x	35	ASP	2.2
4	D	197	HIS	2.2
4	D	174	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
13	O	87	VAL	2.2
1	a	224	ILE	2.2
18	X	3	ILE	2.2
17	y	43	ARG	2.2
19	z	47	TRP	2.2
4	D	198	MET	2.2
9	J	28	PHE	2.2
13	o	95	PHE	2.2
1	a	298	ASN	2.2
4	D	76	VAL	2.2
4	d	204	VAL	2.2
1	a	160	ILE	2.2
1	a	13	LEU	2.2
4	d	202	ALA	2.2
17	Y	26	ALA	2.2
3	C	152	LYS	2.2
5	E	46	VAL	2.2
12	M	17	VAL	2.2
1	a	291	SER	2.1
1	a	176	ILE	2.1
1	a	210	LEU	2.1
3	C	426	LEU	2.1
3	C	453	ALA	2.1
1	A	206	PHE	2.1
1	A	249	VAL	2.1
15	U	59	GLU	2.1
19	z	54	VAL	2.1
1	a	292	THR	2.1
16	v	12	LEU	2.1
1	a	243	GLU	2.1
4	d	296	TYR	2.1
14	T	8	PHE	2.1
3	C	155	ASN	2.1
2	B	500	GLY	2.1
3	C	401	LEU	2.1
4	D	151	ALA	2.1
4	d	237	PRO	2.1
19	z	34	ASP	2.1
3	c	193	GLY	2.1
4	D	13	GLY	2.1
12	M	15	VAL	2.1
1	A	286	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	291	SER	2.1
13	O	63	ALA	2.1
2	B	490	GLN	2.1
3	c	184	GLY	2.1
2	B	349	LYS	2.1
2	b	498	LYS	2.1
2	B	302	TRP	2.1
3	c	436	PHE	2.1
4	D	273	PHE	2.1
4	d	181	PHE	2.1
4	d	191	TRP	2.1
5	e	37	PHE	2.1
1	A	153	SER	2.1
2	b	304	ALA	2.1
3	c	141	GLU	2.1
4	d	212	ALA	2.1
3	C	256	PRO	2.1
11	L	3	PRO	2.1
6	f	17	THR	2.0
1	a	229	GLU	2.0
2	b	402	TYR	2.0
5	E	59	GLU	2.0
4	D	282	SER	2.0
4	D	188	PHE	2.0
19	z	20	VAL	2.0
1	a	156	ALA	2.0
4	d	195	PRO	2.0
3	c	183	GLY	2.0
1	A	78	ILE	2.0
1	a	78	ILE	2.0
4	D	321	LEU	2.0
11	L	25	LEU	2.0
12	m	9	ILE	2.0
1	a	228	THR	2.0
3	c	262	ARG	2.0
3	C	284	PHE	2.0
3	C	434	ALA	2.0
3	c	112	PHE	2.0
5	e	7	GLU	2.0
9	j	5	GLY	2.0
2	b	223	GLN	2.0
2	b	120	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
10	k	11	LEU	2.0
5	e	81	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	FME	j	1	10/11	0.76	0.35	53,71,94,136	0
12	FME	m	1	10/11	0.93	0.15	25,31,61,62	0
14	FME	t	1	10/11	0.95	0.11	13,22,33,65	0
14	FME	T	1	10/11	0.96	0.15	21,27,45,56	0
12	FME	M	1	10/11	0.96	0.14	23,34,56,61	0
8	FME	i	1	10/11	0.97	0.15	23,34,37,42	0
8	FME	I	1	10/11	0.97	0.11	22,34,37,40	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	GOL	B	635	6/6	0.22	0.43	82,91,97,98	0
36	DGD	D	407	62/66	0.51	0.49	44,89,114,119	0
29	UNL	k	102	10/-	0.58	0.61	54,83,94,102	0
36	DGD	d	407	62/66	0.59	0.44	41,88,117,122	0
29	UNL	j	103	10/-	0.60	0.32	44,61,67,73	0
30	LMT	f	102	35/35	0.60	0.36	56,83,109,113	0
30	LMT	E	102	35/35	0.61	0.34	43,81,105,107	0
35	HTG	b	628	19/19	0.61	0.31	48,90,106,124	0
29	UNL	A	415	28/-	0.62	0.30	55,65,84,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	LMG	Z	101	37/55	0.62	0.32	32,81,104,105	0
35	HTG	b	604	19/19	0.62	0.19	50,80,106,112	0
29	UNL	a	414	30/-	0.64	0.28	45,65,86,89	0
30	LMT	m	103	35/35	0.65	0.27	30,60,86,90	0
29	UNL	C	526	34/-	0.65	0.34	46,71,82,84	0
29	UNL	b	634	33/-	0.65	0.26	42,71,112,116	0
30	LMT	M	101	35/35	0.66	0.28	35,60,79,85	0
33	CA	b	605	1/1	0.67	0.14	95,95,95,95	0
35	HTG	d	411	16/19	0.67	0.27	54,73,84,87	0
28	GOL	O	302	6/6	0.68	0.18	52,61,64,70	0
27	SQD	l	101	54/54	0.68	0.25	31,67,98,101	0
32	PL9	A	419	55/55	0.69	0.29	38,66,87,92	0
30	LMT	b	626	25/35	0.69	0.29	33,67,110,115	0
28	GOL	T	103	6/6	0.69	0.31	63,76,80,81	0
30	LMT	D	402	35/35	0.69	0.25	32,75,96,97	0
35	HTG	D	411	16/19	0.70	0.24	38,100,111,113	0
29	UNL	k	101	32/-	0.70	0.38	42,75,105,108	0
30	LMT	m	102	35/35	0.70	0.22	16,51,73,79	0
37	LHG	E	101	42/49	0.70	0.25	38,73,93,103	0
35	HTG	B	624	19/19	0.71	0.36	38,95,102,121	0
29	UNL	J	103	10/-	0.71	0.44	38,53,73,75	0
34	LMG	z	101	39/55	0.72	0.39	47,74,94,101	0
27	SQD	b	601	54/54	0.73	0.23	36,58,91,95	0
29	UNL	i	101	40/-	0.73	0.24	36,64,96,108	0
29	UNL	B	632	33/-	0.74	0.24	32,70,105,113	0
37	LHG	e	101	42/49	0.74	0.23	49,87,117,128	0
28	GOL	v	203	6/6	0.75	0.29	50,69,71,78	0
30	LMT	I	102	35/35	0.75	0.34	59,81,95,100	0
32	PL9	a	416	55/55	0.75	0.27	50,76,94,95	0
29	UNL	I	101	40/-	0.76	0.29	27,63,114,119	0
33	CA	B	601	1/1	0.76	0.09	79,79,79,79	0
35	HTG	B	631	19/19	0.76	0.21	25,84,104,120	0
35	HTG	C	523	19/19	0.76	0.28	46,75,97,109	0
27	SQD	a	402	54/54	0.76	0.23	34,61,79,100	0
29	UNL	x	101	10/-	0.76	0.17	35,44,57,58	0
30	LMT	a	417	35/35	0.77	0.41	52,76,90,94	0
34	LMG	C	520	51/55	0.77	0.28	26,61,82,87	0
28	GOL	t	102	6/6	0.77	0.33	29,60,65,69	0
34	LMG	c	521	51/55	0.77	0.28	35,79,91,98	0
28	GOL	A	414	6/6	0.78	0.19	40,60,69,70	0
30	LMT	B	634	25/35	0.78	0.27	32,63,105,111	0
30	LMT	M	102	35/35	0.78	0.20	22,50,66,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	LMT	b	602	25/35	0.79	0.30	22,63,102,106	0
34	LMG	C	521	51/55	0.79	0.23	31,74,90,96	0
29	UNL	d	413	36/-	0.80	0.19	35,58,94,99	0
34	LMG	c	501	51/55	0.80	0.21	39,60,77,85	0
27	SQD	A	416	54/54	0.80	0.18	28,52,75,76	0
28	GOL	V	205	6/6	0.80	0.39	37,54,59,72	0
28	GOL	a	413	6/6	0.80	0.22	38,67,69,71	0
29	UNL	D	413	40/-	0.81	0.20	33,55,105,108	0
28	GOL	b	632	6/6	0.81	0.29	40,46,68,69	0
30	LMT	a	401	35/35	0.82	0.19	28,61,79,86	0
35	HTG	c	523	19/19	0.83	0.32	60,84,93,98	0
27	SQD	f	101	43/54	0.83	0.30	55,82,109,117	0
34	LMG	B	621	51/55	0.83	0.25	20,35,52,64	0
28	GOL	v	204	6/6	0.84	0.20	47,64,70,92	0
34	LMG	c	520	51/55	0.84	0.22	33,63,86,88	0
29	UNL	d	412	17/-	0.84	0.16	31,48,79,85	0
34	LMG	C	501	51/55	0.84	0.19	37,54,74,82	0
28	GOL	B	627	6/6	0.85	0.22	31,35,43,44	0
29	UNL	M	103	10/-	0.85	0.18	34,42,59,64	0
35	HTG	B	623	19/19	0.85	0.16	29,42,64,71	0
29	UNL	X	101	10/-	0.85	0.15	29,37,41,42	0
30	LMT	A	417	33/35	0.85	0.19	27,65,78,85	0
35	HTG	c	522	19/19	0.86	0.17	63,69,80,85	0
35	HTG	B	630	19/19	0.86	0.17	30,54,78,81	0
24	CLA	c	515	65/65	0.86	0.27	37,51,79,88	0
28	GOL	A	413	6/6	0.86	0.19	35,38,41,42	0
36	DGD	H	102	62/66	0.86	0.19	20,29,42,58	0
28	GOL	V	208	6/6	0.86	0.26	41,56,62,63	0
26	BCR	k	103	40/40	0.86	0.17	32,40,48,52	0
29	UNL	m	101	10/-	0.86	0.26	37,51,60,62	0
28	GOL	V	206	6/6	0.87	0.20	21,38,44,48	0
26	BCR	h	101	40/40	0.87	0.12	27,35,46,49	0
36	DGD	h	102	62/66	0.87	0.17	23,35,52,69	0
26	BCR	d	405	40/40	0.87	0.16	29,35,63,64	0
34	LMG	b	625	51/55	0.87	0.28	24,39,59,71	0
35	HTG	V	204	19/19	0.88	0.26	40,65,99,175	0
28	GOL	C	524	6/6	0.88	0.21	39,45,57,60	0
26	BCR	H	101	40/40	0.88	0.13	21,32,48,52	0
33	CA	F	102	1/1	0.88	0.14	72,72,72,72	0
28	GOL	B	628	6/6	0.88	0.22	35,46,67,70	0
27	SQD	F	101	43/54	0.88	0.30	39,70,96,105	0
28	GOL	T	101	6/6	0.89	0.18	35,60,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	GOL	c	527	6/6	0.89	0.21	36,57,61,63	0
33	CA	f	103	1/1	0.89	0.12	72,72,72,72	0
35	HTG	b	627	19/19	0.89	0.23	27,44,80,80	0
24	CLA	b	614	65/65	0.89	0.12	24,31,41,50	0
32	PL9	d	406	55/55	0.89	0.21	16,23,35,47	0
37	LHG	d	408	49/49	0.89	0.23	26,34,46,50	0
24	CLA	c	505	65/65	0.89	0.13	29,35,46,60	0
28	GOL	B	626	6/6	0.90	0.21	32,37,40,59	0
26	BCR	Y	101	40/40	0.90	0.12	28,35,49,50	0
26	BCR	c	526	40/40	0.90	0.16	39,48,59,63	0
34	LMG	j	101	51/55	0.90	0.19	26,39,70,82	0
28	GOL	b	631	6/6	0.90	0.11	39,46,48,60	0
27	SQD	a	411	54/54	0.90	0.22	32,56,75,78	0
28	GOL	c	525	6/6	0.90	0.24	43,46,61,62	0
24	CLA	c	514	65/65	0.90	0.18	34,43,67,76	0
36	DGD	c	518	62/66	0.90	0.19	24,35,79,94	0
24	CLA	C	509	65/65	0.90	0.16	21,29,78,80	0
26	BCR	B	619	40/40	0.90	0.17	17,25,44,46	0
37	LHG	D	408	49/49	0.90	0.25	16,31,43,54	0
27	SQD	A	411	54/54	0.90	0.21	26,51,71,78	0
24	CLA	c	506	65/65	0.90	0.17	26,33,51,61	0
35	HTG	b	603	19/19	0.90	0.14	34,44,64,67	0
37	LHG	l	102	49/49	0.90	0.19	19,30,48,57	0
24	CLA	B	610	65/65	0.91	0.12	19,26,36,40	0
28	GOL	F	103	6/6	0.91	0.18	52,59,65,68	0
26	BCR	T	102	40/40	0.91	0.16	14,28,36,42	0
24	CLA	B	603	65/65	0.91	0.12	18,25,32,38	0
26	BCR	b	622	40/40	0.91	0.18	16,26,33,36	0
26	BCR	b	623	40/40	0.91	0.21	15,27,40,46	0
29	UNL	D	412	17/-	0.91	0.16	24,45,74,78	0
32	PL9	D	406	55/55	0.91	0.24	14,23,36,43	0
26	BCR	c	516	40/40	0.91	0.12	29,36,47,57	0
24	CLA	c	507	65/65	0.91	0.12	22,31,52,62	0
28	GOL	a	412	6/6	0.91	0.16	22,37,41,45	0
24	CLA	c	513	65/65	0.91	0.13	30,39,50,54	0
24	CLA	C	514	65/65	0.91	0.16	32,42,69,72	0
35	HTG	C	522	19/19	0.91	0.18	53,65,89,95	0
24	CLA	B	604	65/65	0.91	0.12	18,25,32,40	0
24	CLA	b	620	65/65	0.91	0.12	22,31,51,74	0
26	BCR	D	405	40/40	0.91	0.14	22,31,61,77	0
28	GOL	b	630	6/6	0.92	0.16	37,48,50,52	0
24	CLA	b	607	65/65	0.92	0.12	23,30,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	GOL	B	625	6/6	0.92	0.14	28,43,48,55	0
24	CLA	B	612	65/65	0.92	0.17	15,21,37,41	0
26	BCR	C	515	40/40	0.92	0.11	31,42,49,53	0
28	GOL	f	104	6/6	0.92	0.22	45,51,59,61	0
26	BCR	t	101	40/40	0.92	0.12	15,24,45,49	0
28	GOL	B	633	6/6	0.92	0.10	27,36,40,41	0
26	BCR	y	101	40/40	0.92	0.12	31,40,53,60	0
24	CLA	B	615	65/65	0.92	0.14	15,24,67,78	0
24	CLA	b	621	65/65	0.92	0.15	21,35,82,84	0
24	CLA	C	504	65/65	0.92	0.11	24,33,42,48	0
34	LMG	J	101	51/55	0.92	0.22	20,37,78,86	0
36	DGD	C	518	62/66	0.92	0.23	22,32,76,92	0
24	CLA	C	505	65/65	0.92	0.21	22,29,59,77	0
24	CLA	C	507	65/65	0.92	0.16	28,42,81,88	0
28	GOL	V	201	6/6	0.92	0.11	27,29,40,41	0
36	DGD	c	519	62/66	0.92	0.20	26,34,65,72	0
24	CLA	c	509	65/65	0.92	0.12	27,34,49,58	0
26	BCR	b	624	40/40	0.92	0.10	20,32,46,52	0
24	CLA	B	608	65/65	0.92	0.18	13,20,31,35	0
28	GOL	A	412	6/6	0.92	0.10	29,31,34,37	0
35	HTG	B	622	19/19	0.92	0.11	26,30,44,56	0
24	CLA	B	602	65/65	0.92	0.16	24,39,82,104	0
28	GOL	b	629	6/6	0.92	0.13	32,40,48,57	0
28	GOL	v	201	6/6	0.93	0.13	31,40,49,50	0
24	CLA	b	612	65/65	0.93	0.21	14,23,30,36	0
24	CLA	c	510	65/65	0.93	0.16	24,31,70,87	0
28	GOL	v	205	6/6	0.93	0.17	25,39,52,58	0
24	CLA	c	512	65/65	0.93	0.17	26,32,44,59	0
24	CLA	C	511	65/65	0.93	0.15	23,29,41,62	0
36	DGD	C	519	62/66	0.93	0.23	20,30,58,63	0
24	CLA	b	616	65/65	0.93	0.13	18,26,38,52	0
24	CLA	b	619	65/65	0.93	0.14	15,25,72,77	0
36	DGD	c	517	62/66	0.93	0.17	23,32,68,76	0
26	BCR	B	618	40/40	0.93	0.16	15,23,33,41	0
24	CLA	C	512	65/65	0.93	0.11	26,32,41,48	0
24	CLA	C	513	65/65	0.93	0.12	29,42,67,74	0
24	CLA	c	503	65/65	0.93	0.11	29,34,45,54	0
24	CLA	B	607	65/65	0.93	0.11	18,26,51,75	0
26	BCR	K	101	40/40	0.93	0.12	27,33,42,47	0
37	LHG	L	101	49/49	0.93	0.23	15,29,47,58	0
24	CLA	b	606	65/65	0.93	0.18	30,46,82,98	0
37	LHG	d	409	49/49	0.93	0.14	17,26,39,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	C	502	65/65	0.93	0.11	25,32,47,58	0
24	CLA	c	508	65/65	0.93	0.12	30,41,65,70	0
33	CA	o	301	1/1	0.94	0.07	62,62,62,62	0
24	CLA	a	407	65/65	0.94	0.26	19,25,72,79	0
24	CLA	a	409	65/65	0.94	0.12	20,27,83,88	0
26	BCR	C	516	40/40	0.94	0.09	25,34,43,46	0
24	CLA	C	508	65/65	0.94	0.11	25,35,48,57	0
24	CLA	c	504	65/65	0.94	0.14	26,32,45,55	0
24	CLA	B	605	65/65	0.94	0.14	15,22,51,63	0
36	DGD	C	517	62/66	0.94	0.14	22,33,75,83	0
28	GOL	V	207	6/6	0.94	0.21	35,38,41,44	0
24	CLA	b	608	65/65	0.94	0.10	22,29,38,42	0
24	CLA	b	611	65/65	0.94	0.10	19,31,58,74	0
26	BCR	a	410	40/40	0.94	0.09	16,24,31,33	0
24	CLA	C	503	65/65	0.94	0.12	22,28,40,51	0
24	CLA	b	613	65/65	0.94	0.11	22,29,38,42	0
24	CLA	A	405	65/65	0.94	0.26	15,18,26,50	0
24	CLA	b	615	65/65	0.94	0.11	21,28,39,46	0
24	CLA	B	614	65/65	0.94	0.17	14,22,45,52	0
24	CLA	b	617	65/65	0.94	0.11	18,26,36,50	0
37	LHG	D	409	49/49	0.94	0.18	17,27,48,60	0
37	LHG	D	410	49/49	0.94	0.18	20,33,91,95	0
28	GOL	B	629	6/6	0.94	0.25	24,40,61,78	0
24	CLA	b	618	65/65	0.94	0.18	15,23,48,56	0
24	CLA	d	404	65/65	0.94	0.12	27,34,74,81	0
25	PHO	d	403	64/64	0.94	0.20	20,25,34,38	0
37	LHG	d	410	49/49	0.94	0.18	23,35,85,104	0
35	HTG	O	303	19/19	0.94	0.09	24,32,47,48	0
22	CL	u	201	1/1	0.94	0.05	63,63,63,63	0
38	HEM	e	102	43/43	0.94	0.18	38,48,65,84	0
26	BCR	A	410	40/40	0.95	0.10	16,26,33,35	0
24	CLA	B	611	65/65	0.95	0.12	19,26,36,39	0
24	CLA	C	506	65/65	0.95	0.10	21,29,45,53	0
26	BCR	B	620	40/40	0.95	0.10	22,29,42,47	0
24	CLA	A	409	65/65	0.95	0.12	18,27,83,92	0
24	CLA	b	609	65/65	0.95	0.15	16,25,56,66	0
24	CLA	b	610	65/65	0.95	0.11	18,24,37,42	0
24	CLA	B	613	65/65	0.95	0.11	15,23,32,35	0
24	CLA	B	606	65/65	0.95	0.09	16,22,34,38	0
24	CLA	C	510	65/65	0.95	0.11	25,32,51,57	0
23	BCT	a	418	4/4	0.95	0.17	30,33,42,44	0
24	CLA	c	511	65/65	0.95	0.10	29,36,49,55	0

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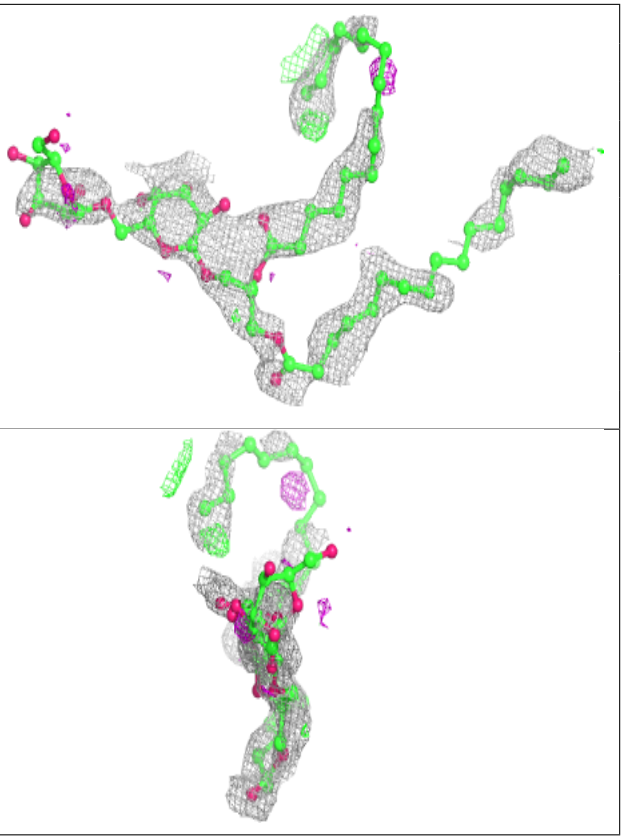
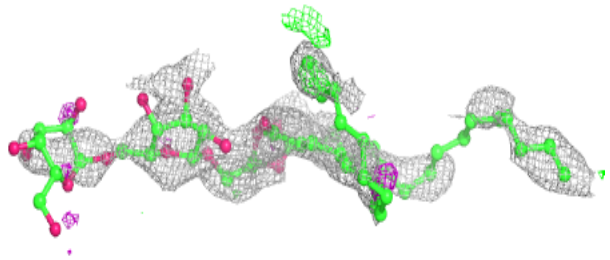
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	616	65/65	0.95	0.11	19,28,48,60	0
24	CLA	B	617	65/65	0.95	0.17	19,28,88,91	0
28	GOL	b	633	6/6	0.95	0.29	32,54,63,71	0
22	CL	V	202	1/1	0.95	0.05	63,63,63,63	0
24	CLA	D	404	65/65	0.95	0.12	21,28,73,84	0
24	CLA	B	609	65/65	0.95	0.14	17,22,32,36	0
25	PHO	A	407	64/64	0.95	0.18	15,18,23,28	0
25	PHO	A	408	64/64	0.95	0.26	16,22,30,32	0
25	PHO	a	408	64/64	0.95	0.18	16,21,29,37	0
28	GOL	C	525	6/6	0.95	0.13	20,24,26,27	0
24	CLA	A	406	65/65	0.95	0.26	15,19,84,88	0
24	CLA	a	406	65/65	0.96	0.24	17,20,35,51	0
24	CLA	D	401	65/65	0.96	0.24	13,18,30,32	0
24	CLA	D	403	65/65	0.96	0.28	14,19,36,42	0
33	CA	c	502	1/1	0.96	0.04	44,44,44,44	0
23	BCT	A	404	4/4	0.96	0.10	27,30,39,40	0
24	CLA	d	401	65/65	0.96	0.21	16,19,26,42	0
38	HEM	E	103	43/43	0.96	0.17	27,38,50,56	0
24	CLA	d	402	65/65	0.96	0.24	18,22,38,46	0
33	CA	O	301	1/1	0.97	0.05	56,56,56,56	0
39	MG	J	102	1/1	0.97	0.04	28,28,28,28	0
40	HEC	V	203	43/43	0.97	0.08	23,26,31,36	0
40	HEC	v	202	43/43	0.97	0.10	29,33,40,48	0
39	MG	j	102	1/1	0.98	0.16	34,34,34,34	0
22	CL	A	403	1/1	0.98	0.07	23,23,23,23	0
28	GOL	c	524	6/6	0.98	0.15	25,28,30,34	0
21	FE2	A	401	1/1	0.99	0.10	27,27,27,27	0
21	FE2	a	403	1/1	0.99	0.11	30,30,30,30	0
22	CL	a	405	1/1	0.99	0.12	26,26,26,26	0
22	CL	A	402	1/1	0.99	0.10	19,19,19,19	0
31	OEX	A	418	10/10	0.99	0.09	16,23,28,32	0
31	OEX	a	415	10/10	0.99	0.11	20,24,35,37	0
22	CL	a	404	1/1	1.00	0.10	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DGD D 407:

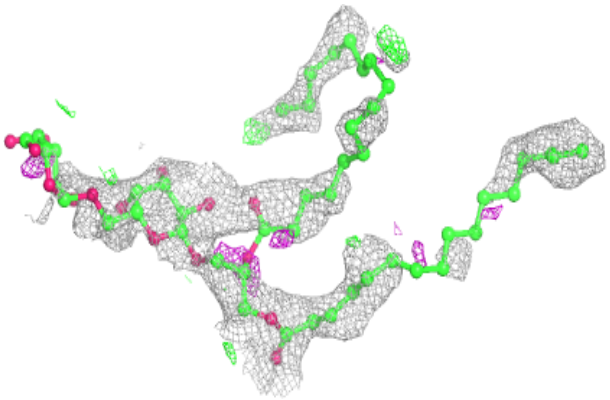
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

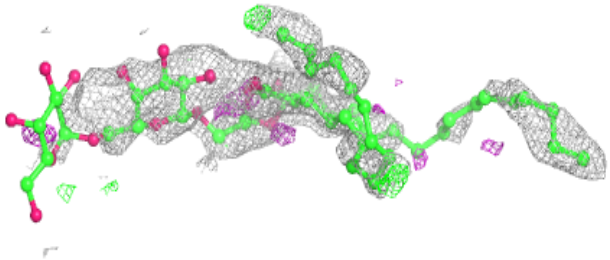


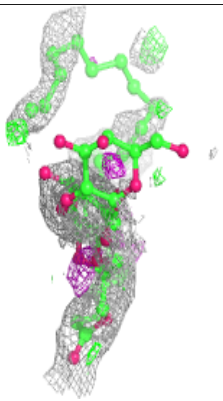


Electron density around DGD d 407:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

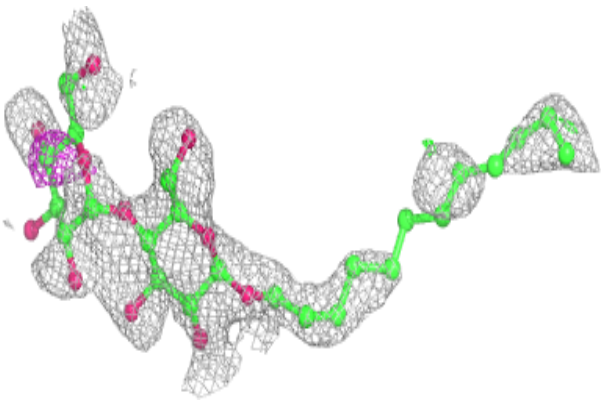


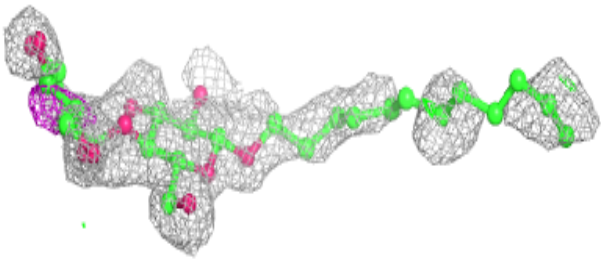


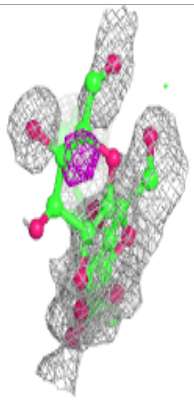


Electron density around LMT f 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

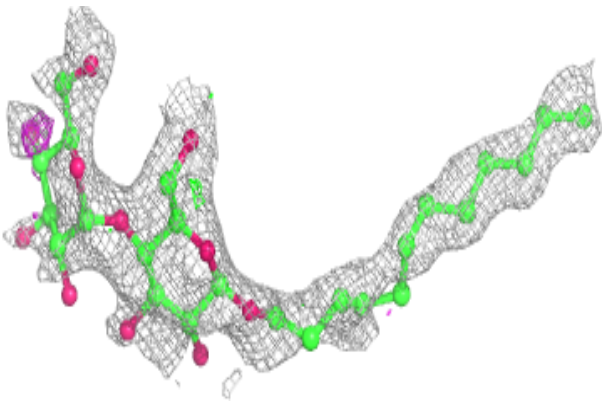


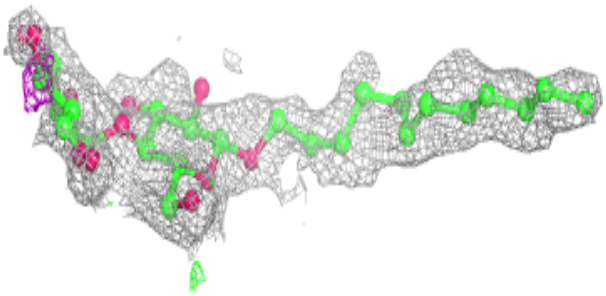


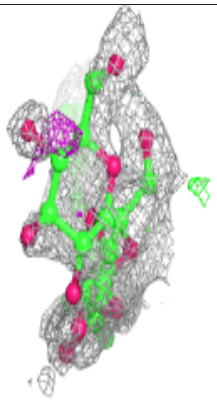


Electron density around LMT E 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

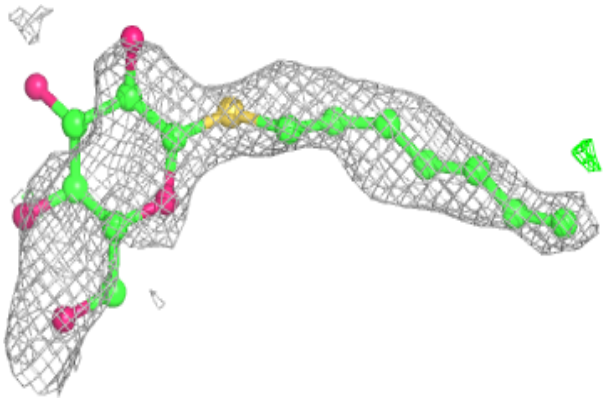


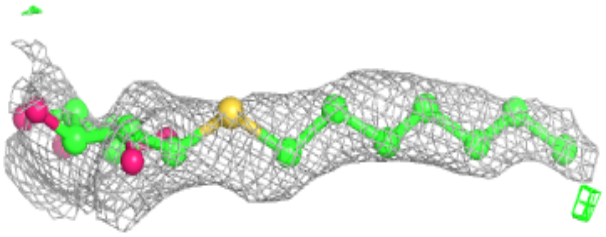


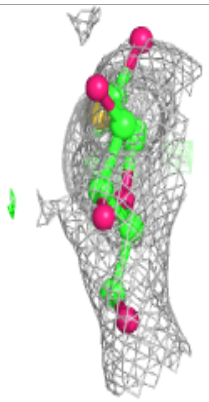


Electron density around HTG b 628:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

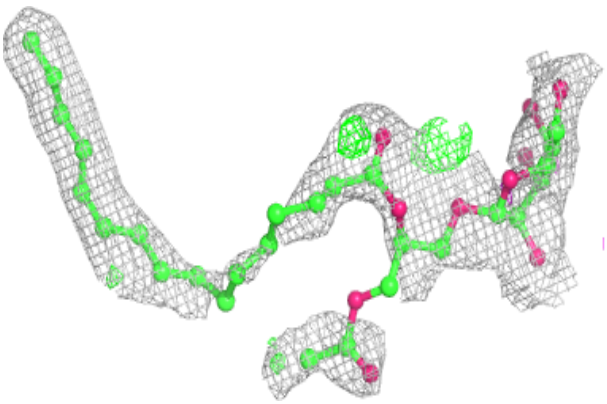


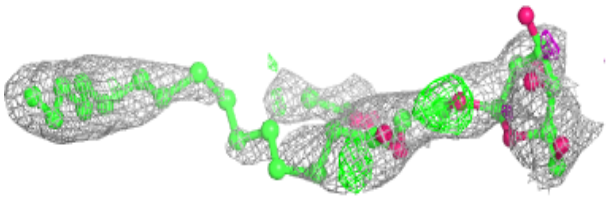


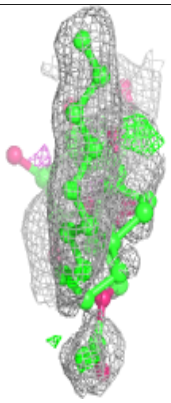


Electron density around LMG Z 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

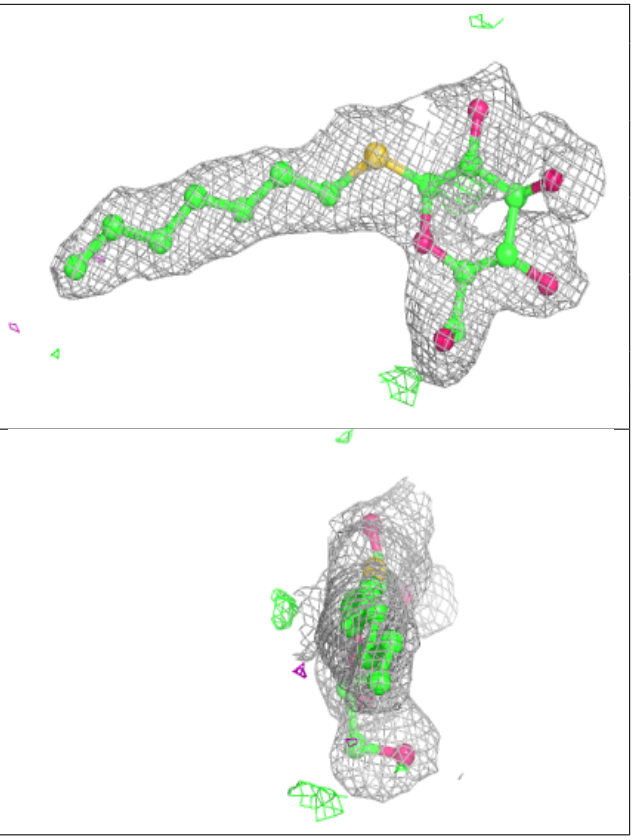


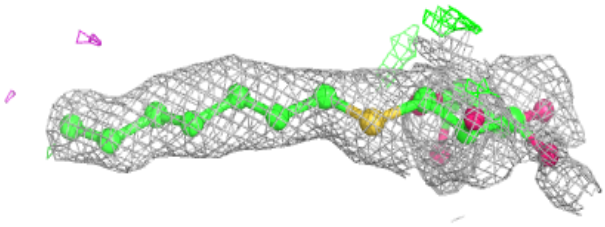




Electron density around HTG b 604:

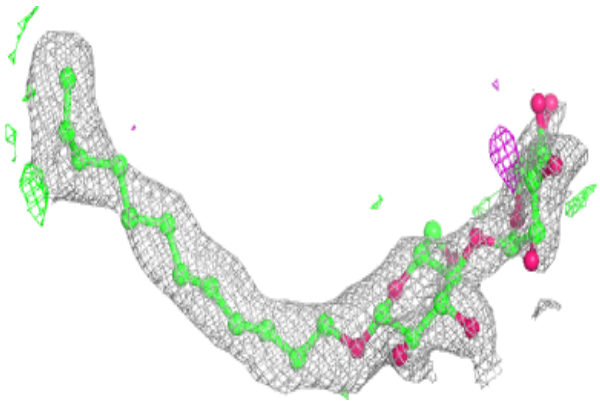
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

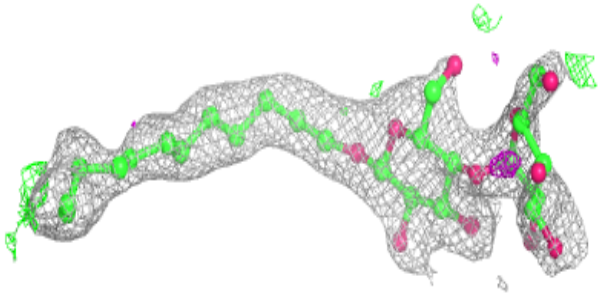


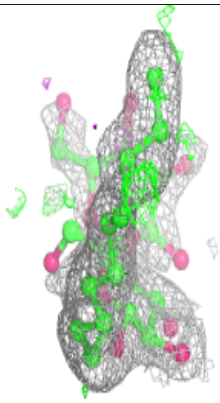


Electron density around LMT m 103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

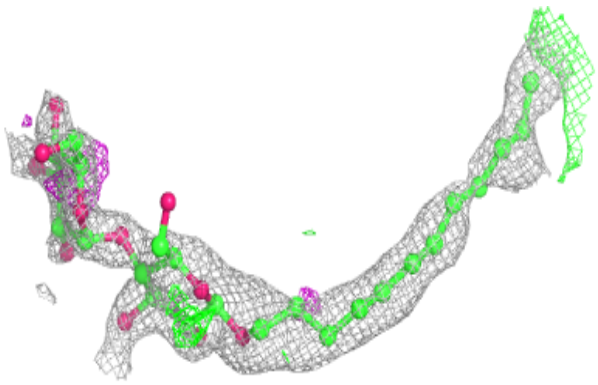


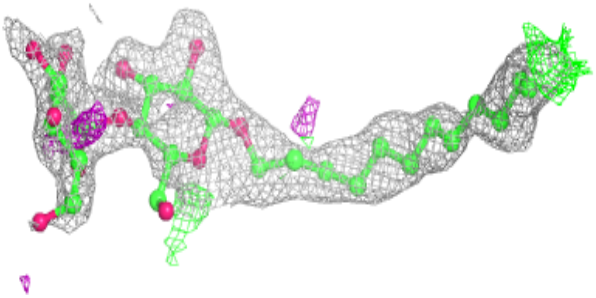


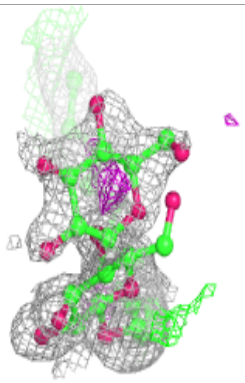


Electron density around LMT M 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

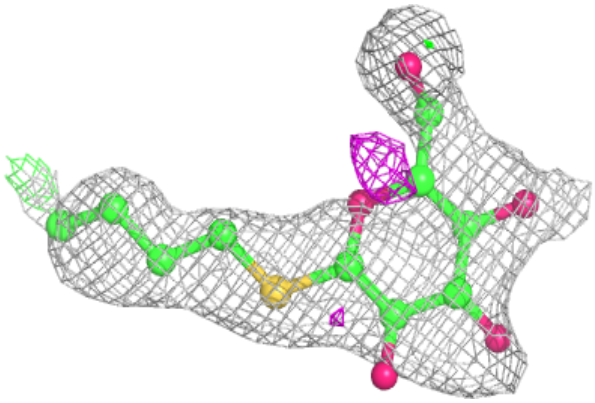


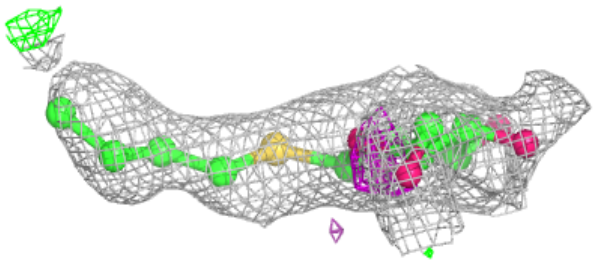


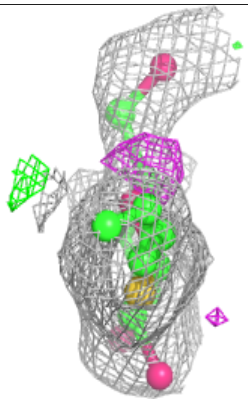


Electron density around HTG d 411:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

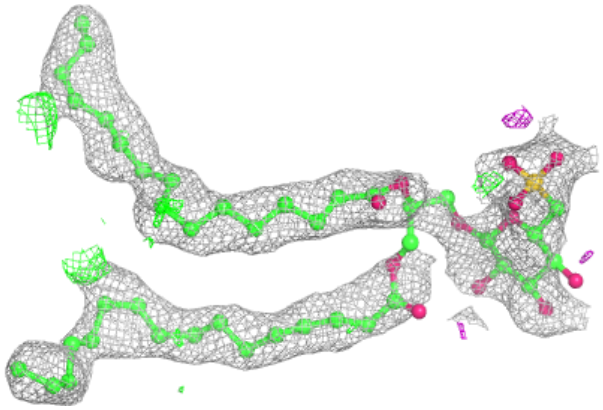


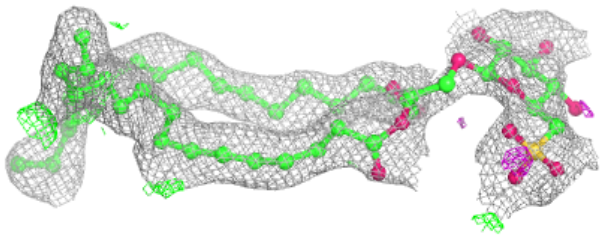


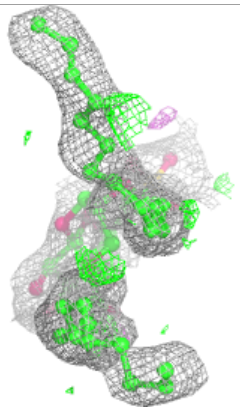


Electron density around SQD l 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

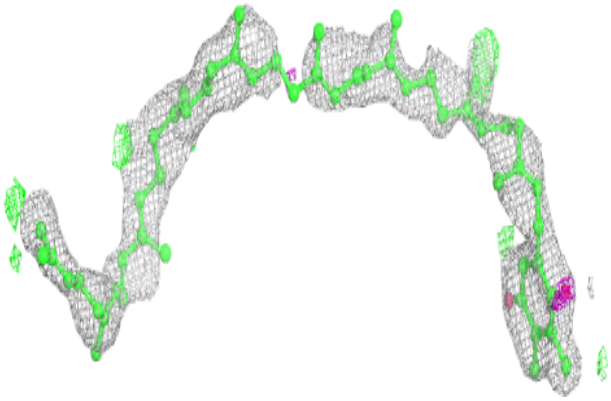


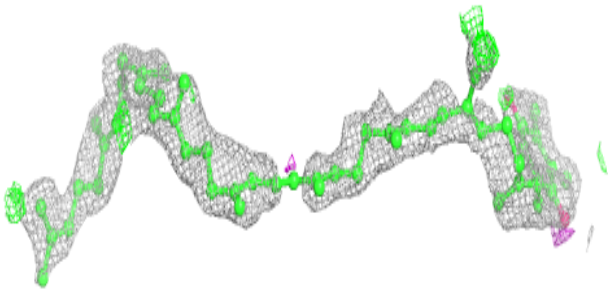


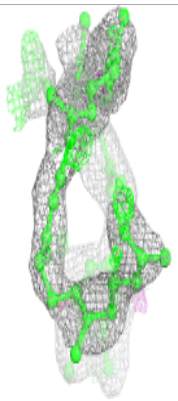


Electron density around PL9 A 419:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

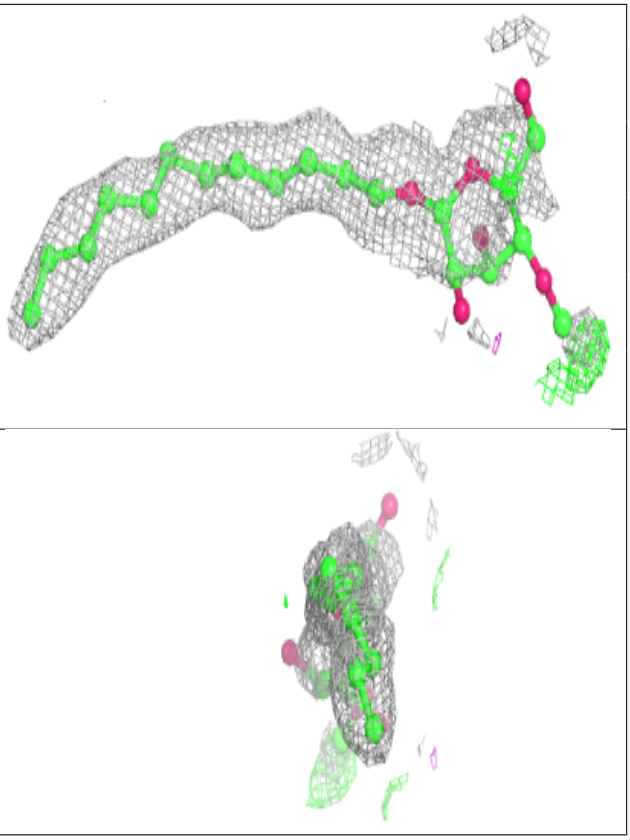






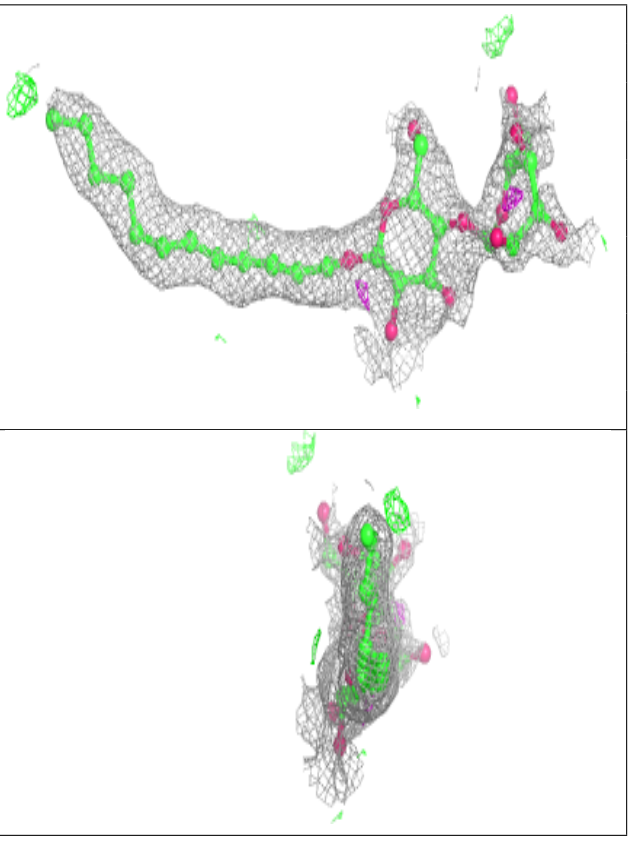
Electron density around LMT b 626:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



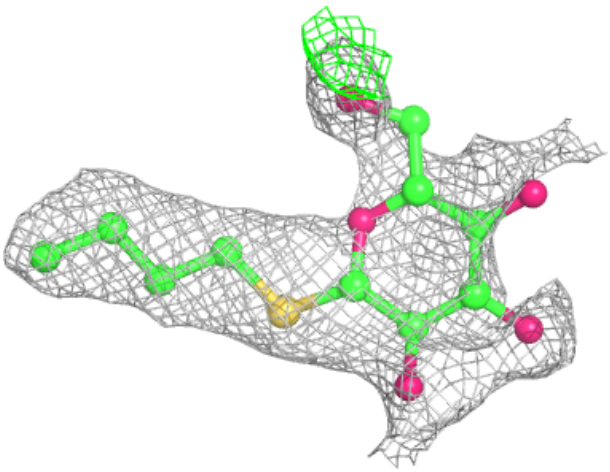
Electron density around LMT D 402:

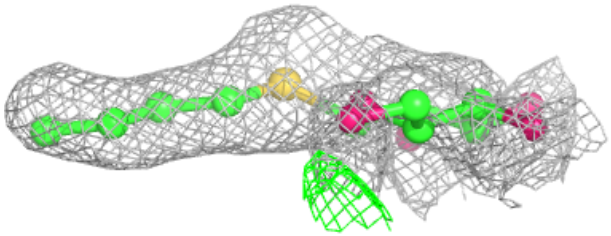
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

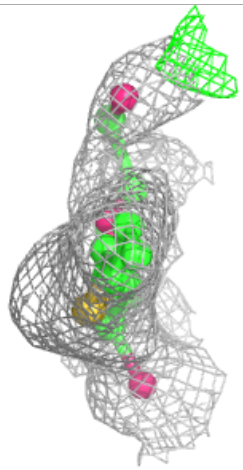


Electron density around HTG D 411:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

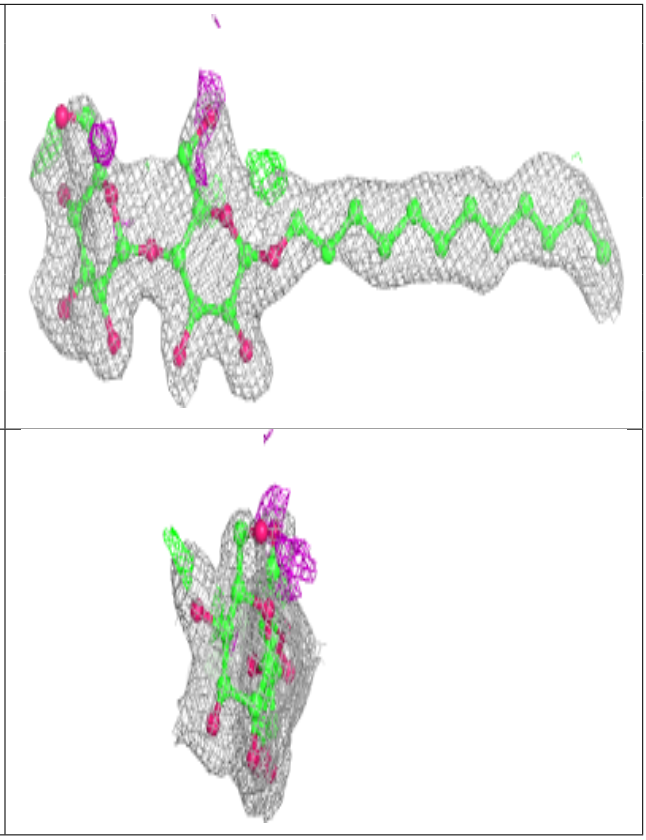






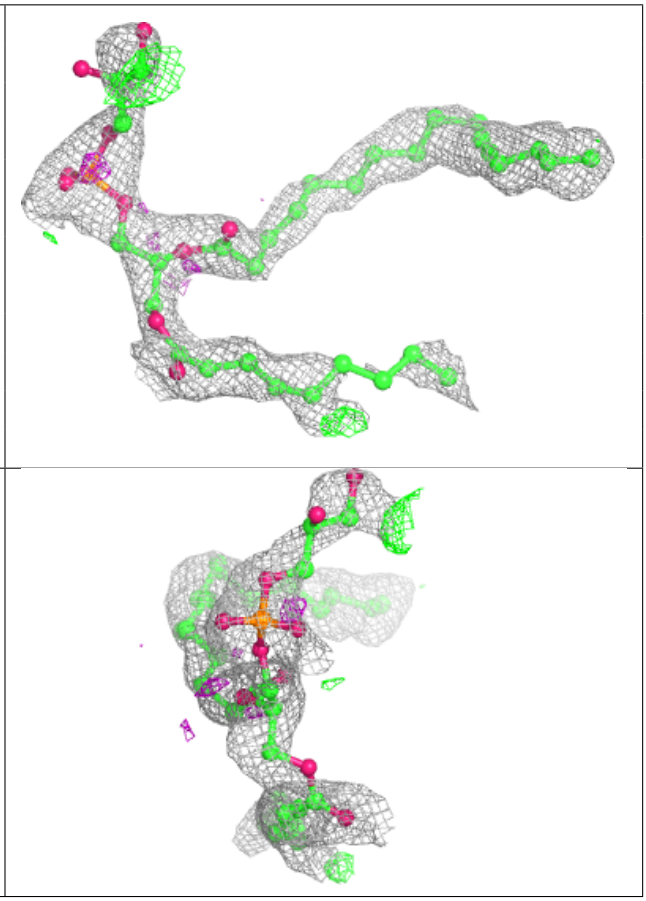
Electron density around LMT m 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



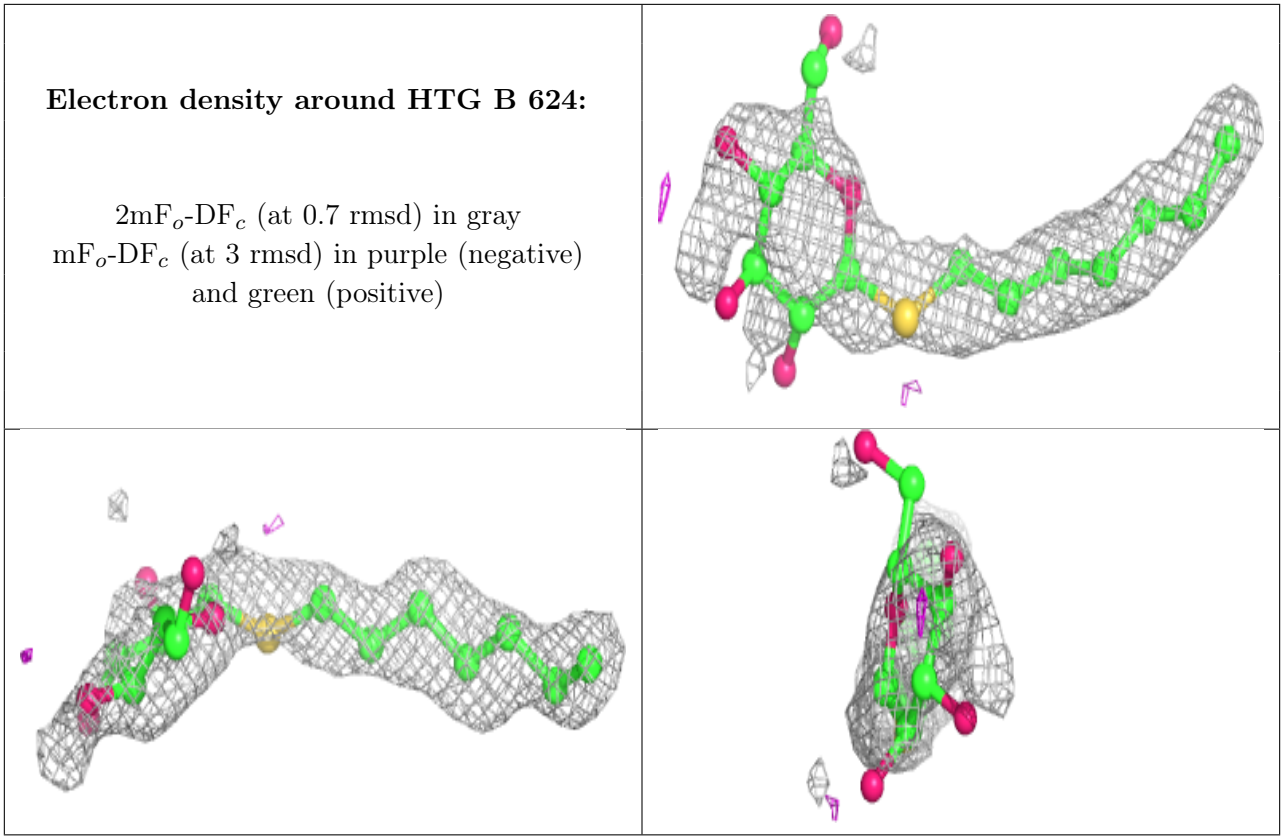
Electron density around LHG E 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



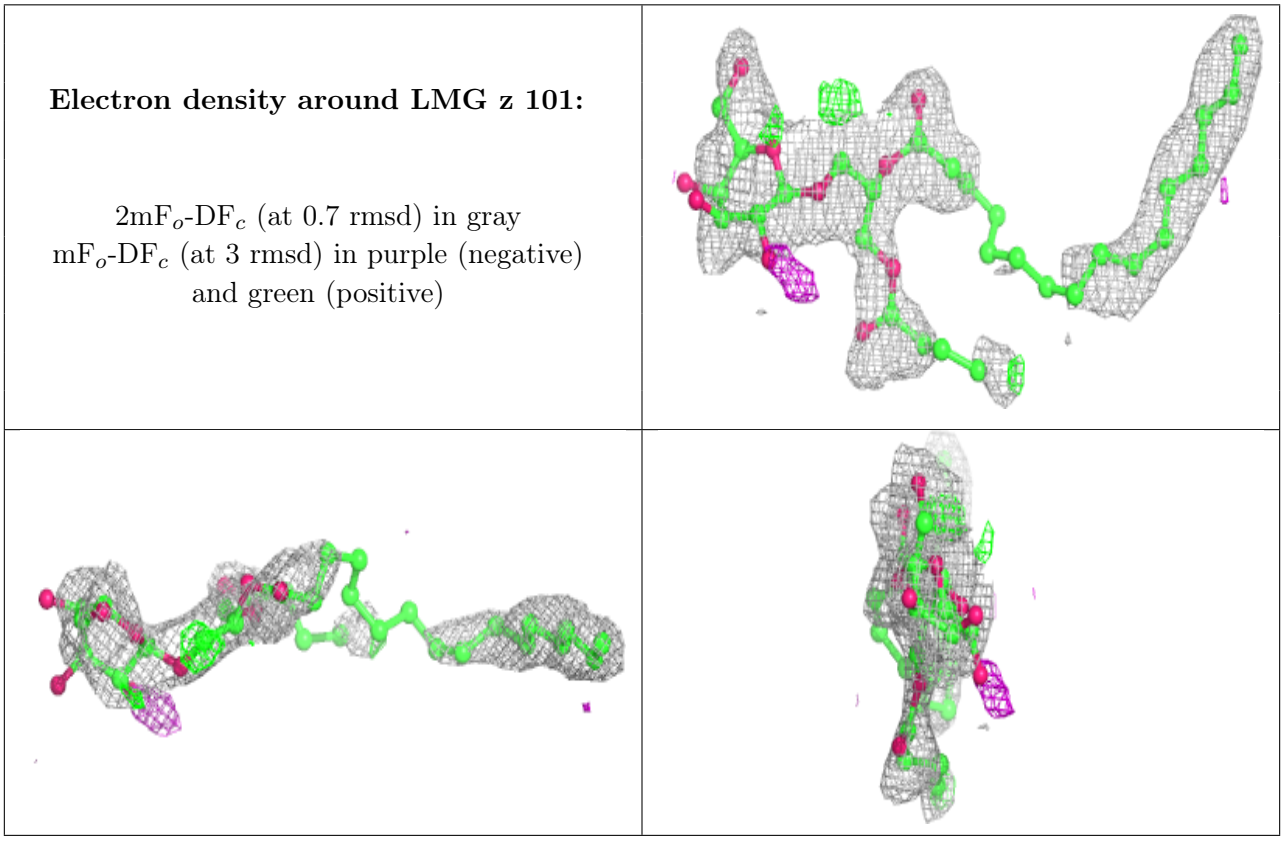
Electron density around HTG B 624:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



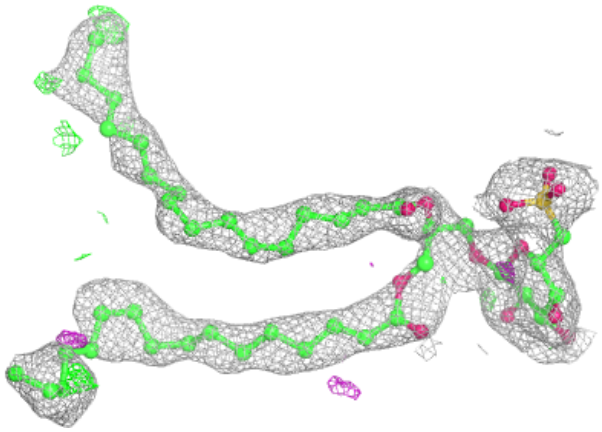
Electron density around LMG z 101:

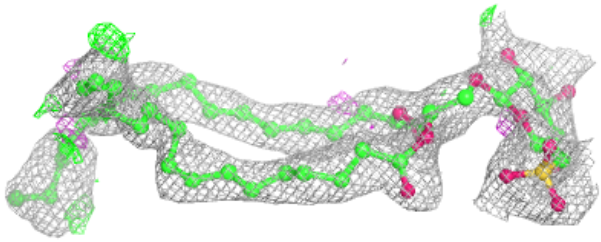
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

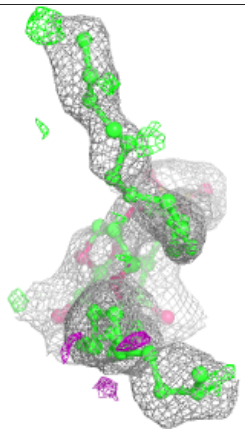


Electron density around SQD b 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

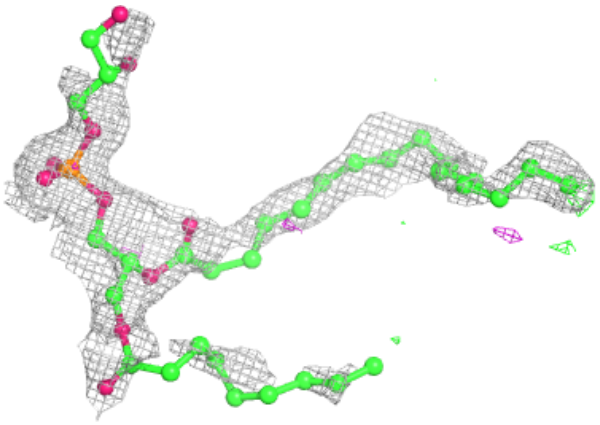


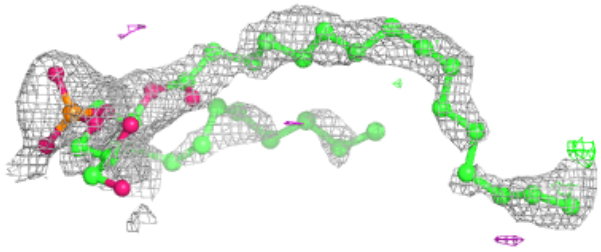


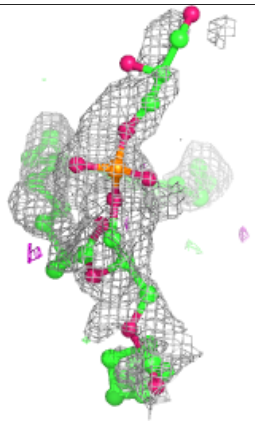


Electron density around LHG e 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

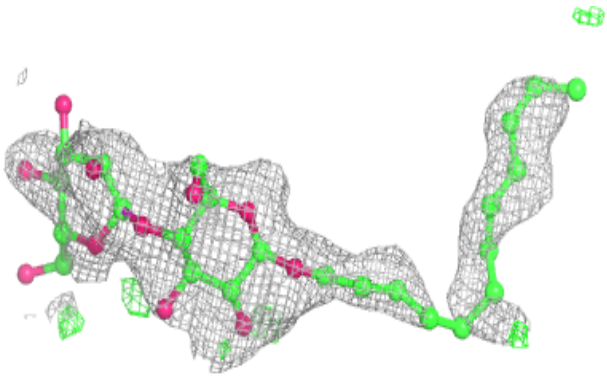


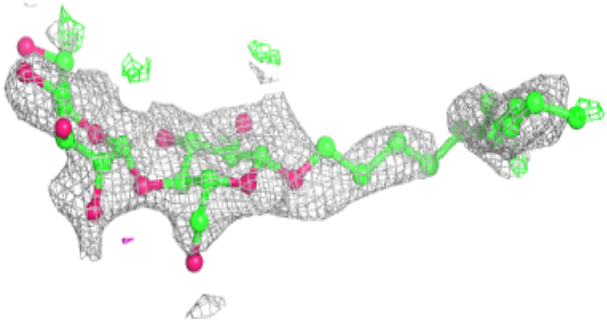


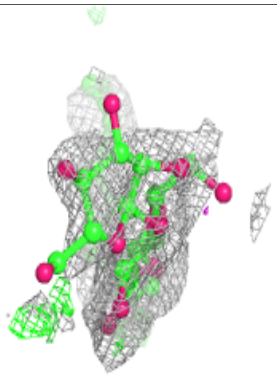


Electron density around LMT I 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

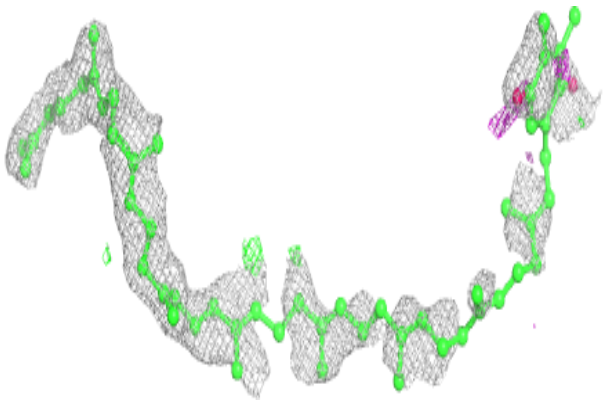


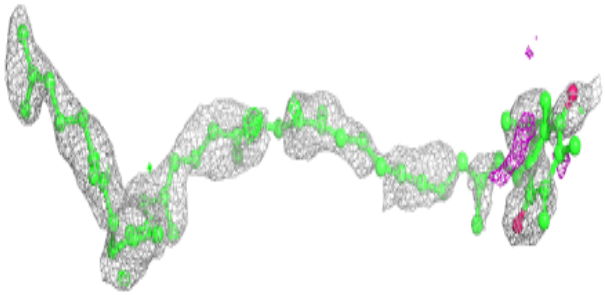


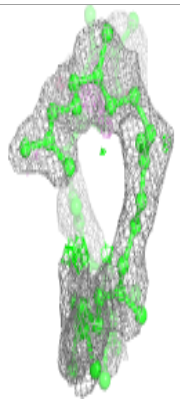


Electron density around PL9 a 416:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

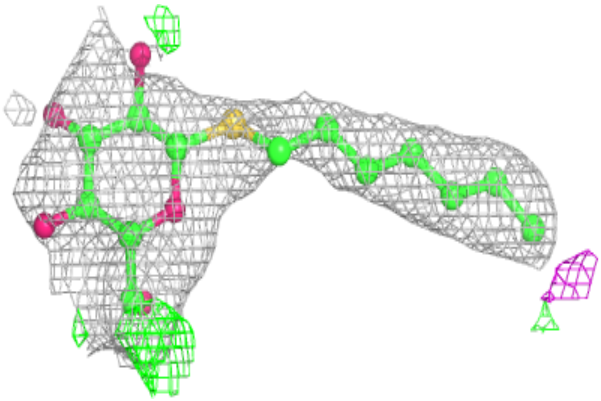


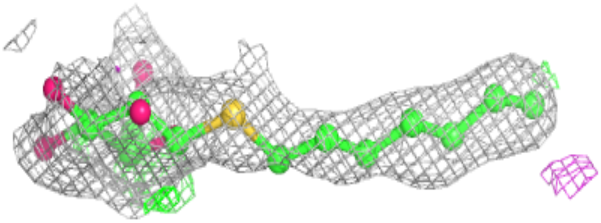


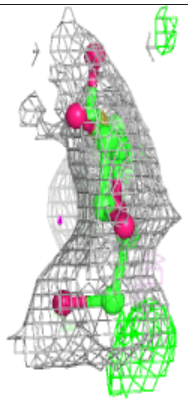


Electron density around HTG B 631:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

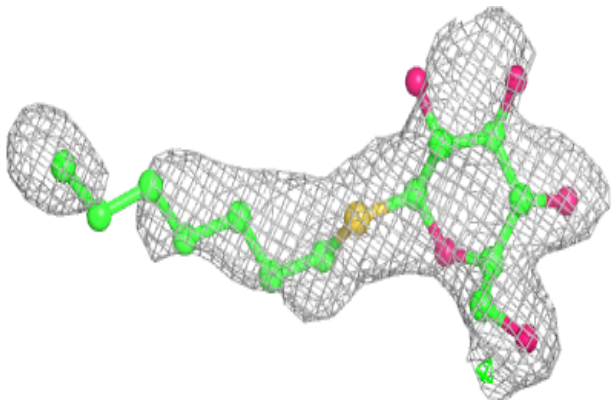


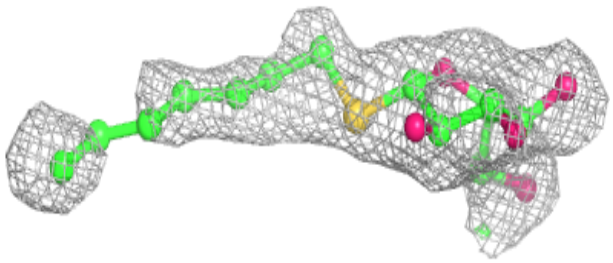


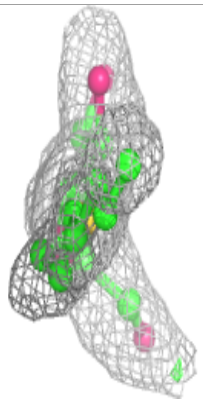


Electron density around HTG C 523:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

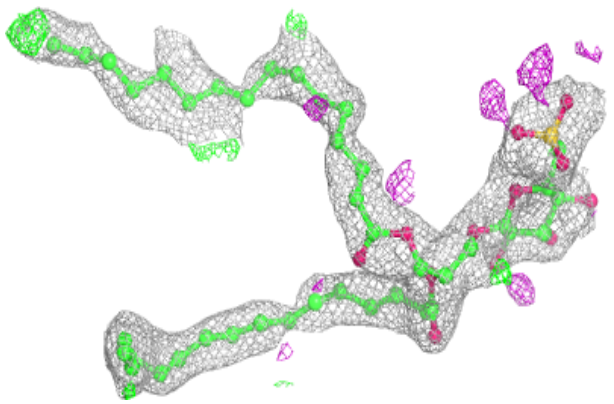


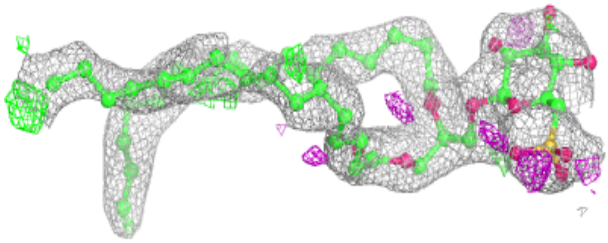


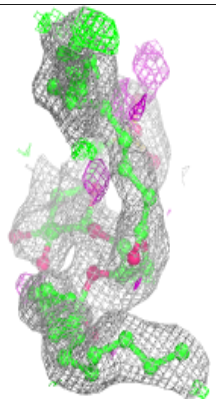


Electron density around SQD a 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

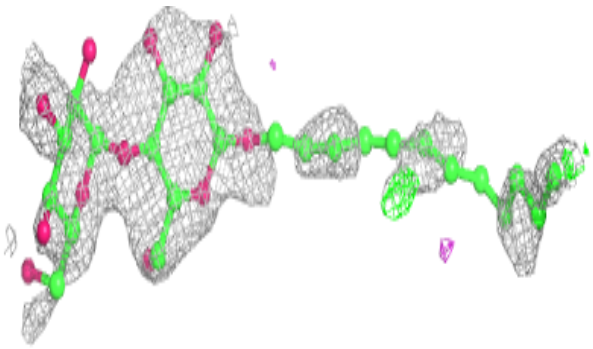


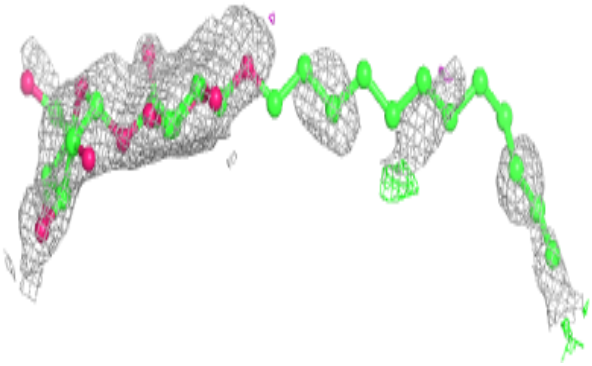


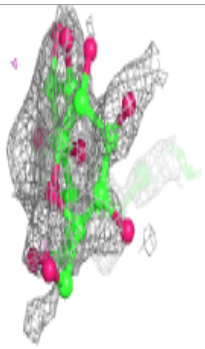


Electron density around LMT a 417:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

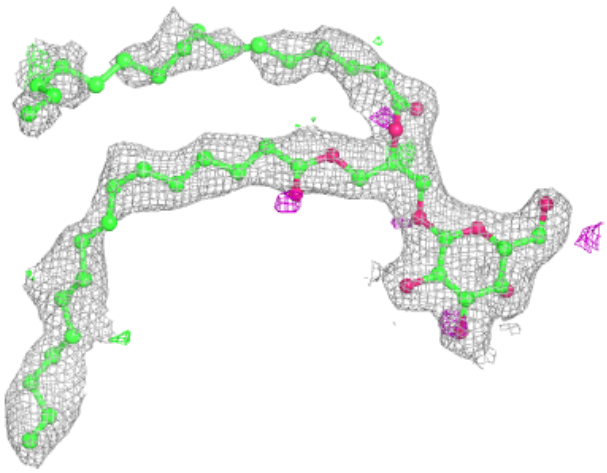


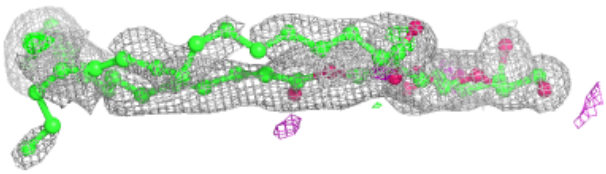


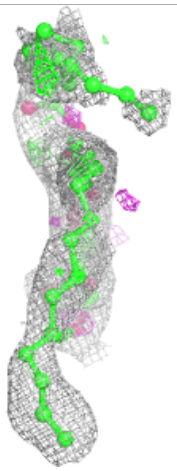


Electron density around LMG C 520:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

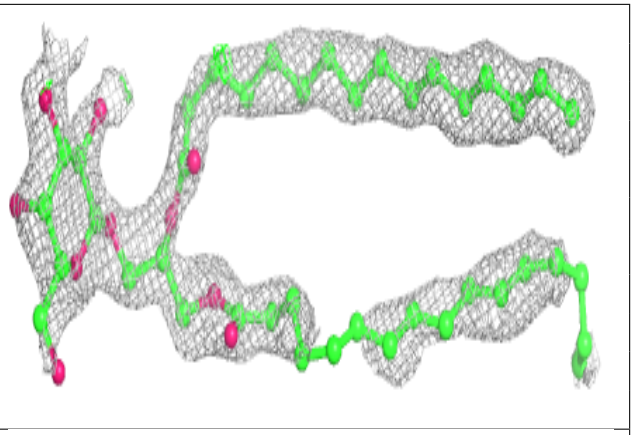


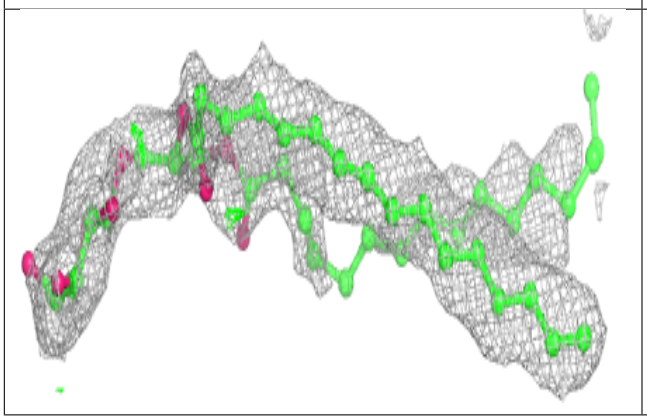


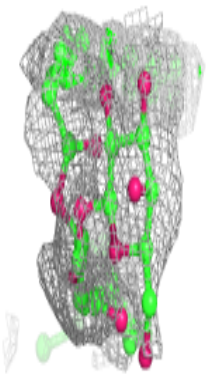


Electron density around LMG c 521:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

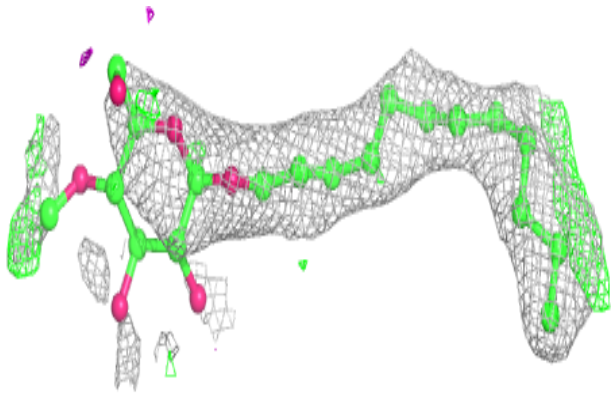


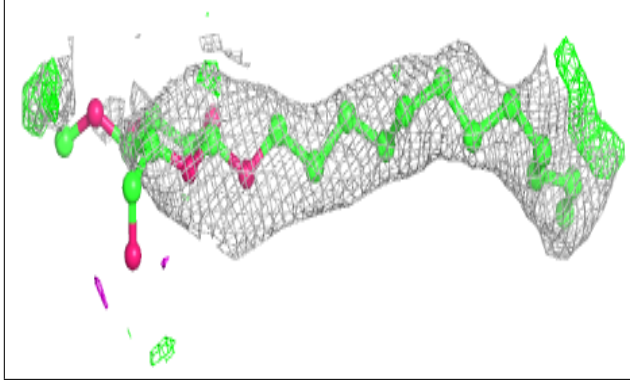


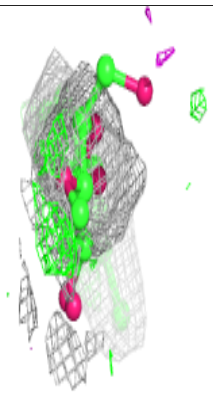


Electron density around LMT B 634:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

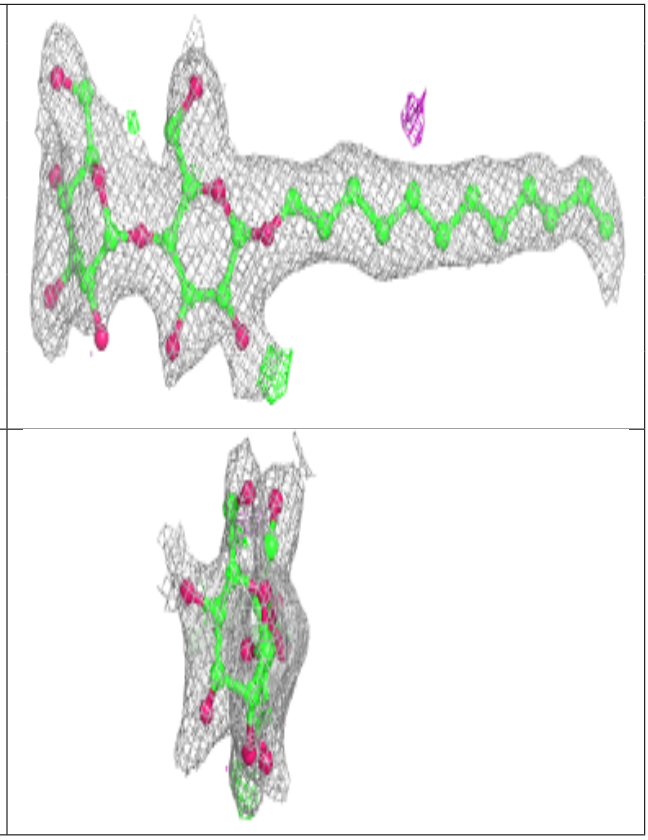






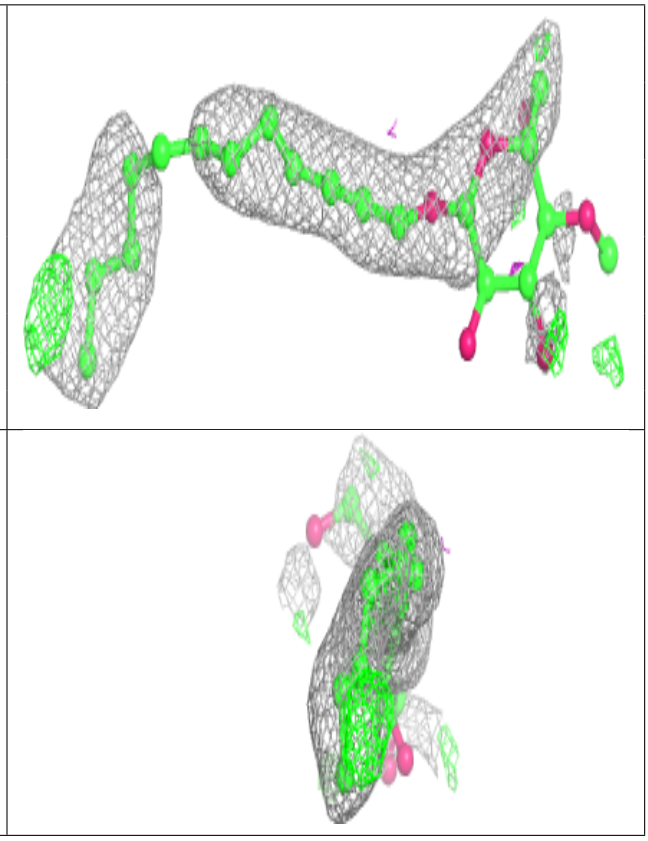
Electron density around LMT M 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



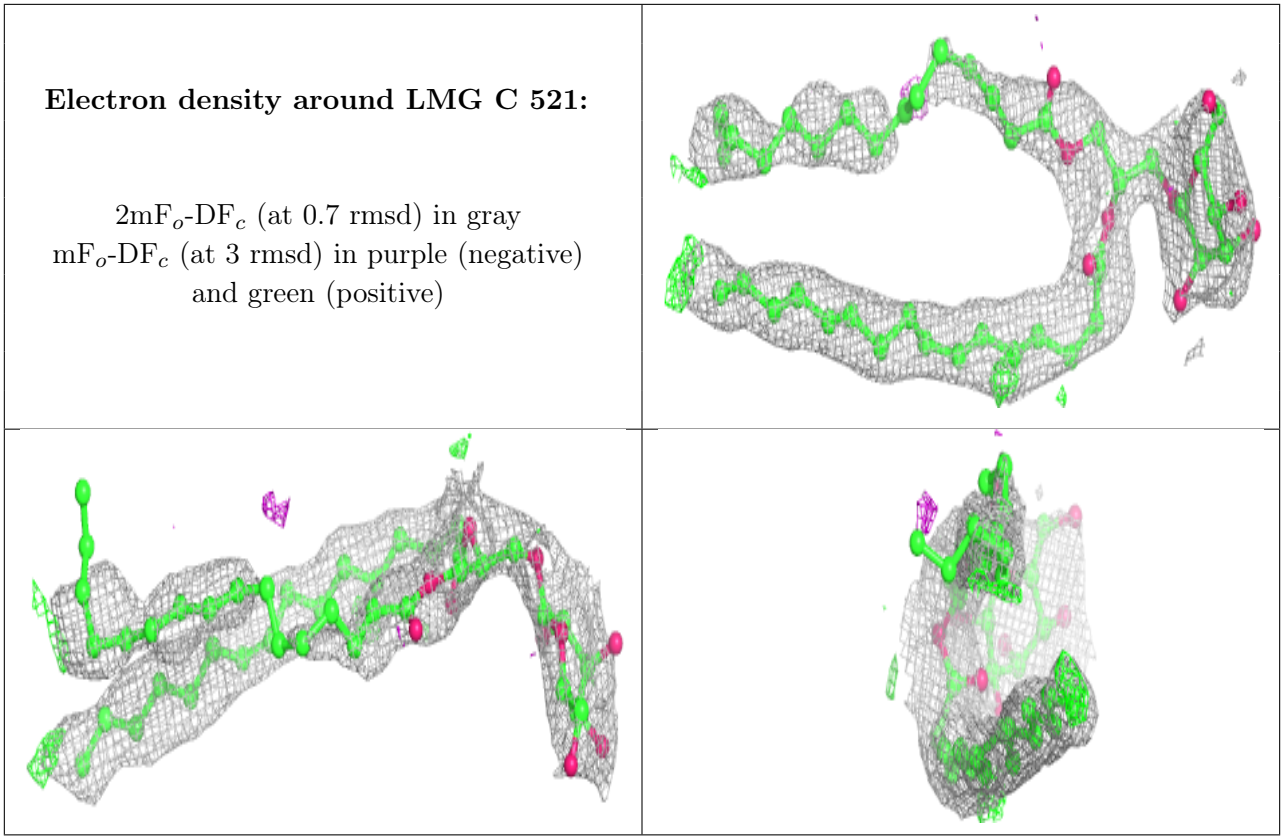
Electron density around LMT b 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



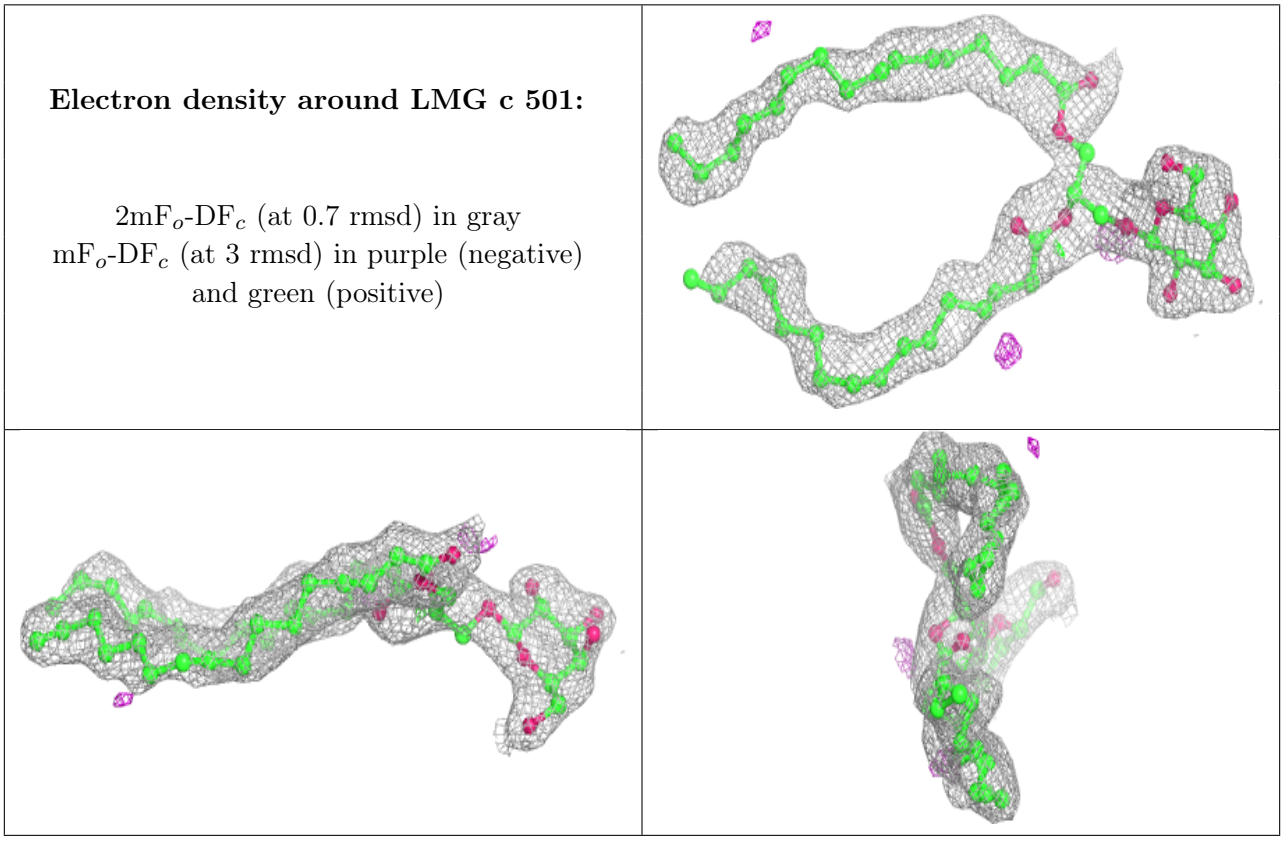
Electron density around LMG C 521:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



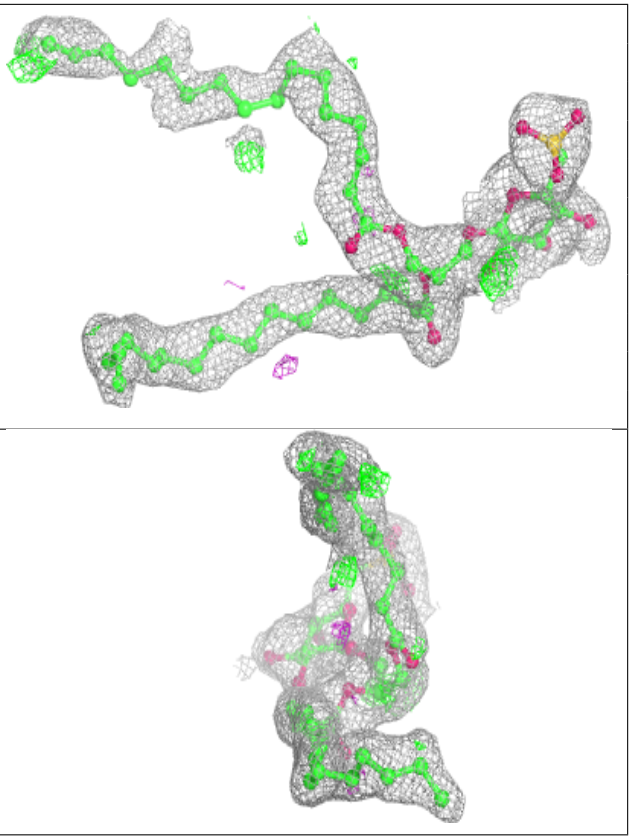
Electron density around LMG c 501:

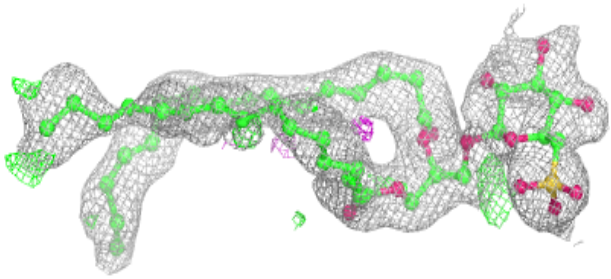
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD A 416:

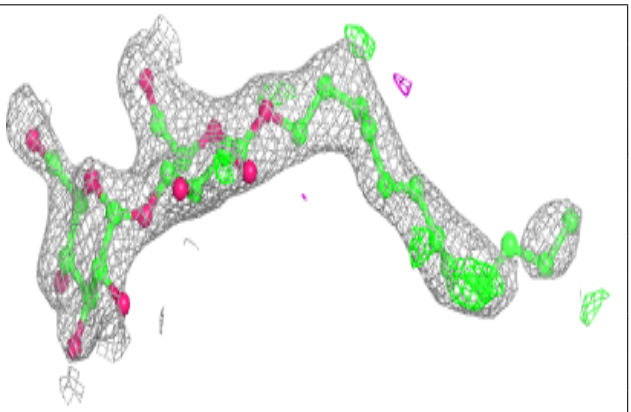
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

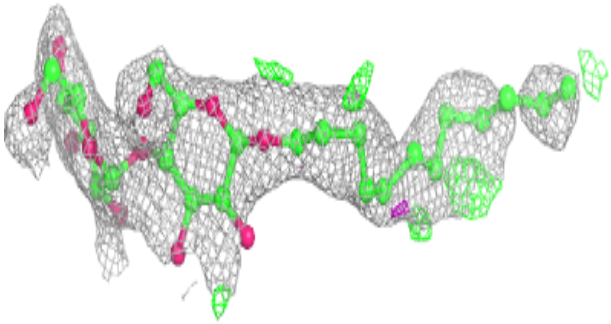


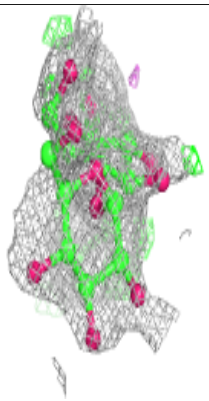


Electron density around LMT a 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

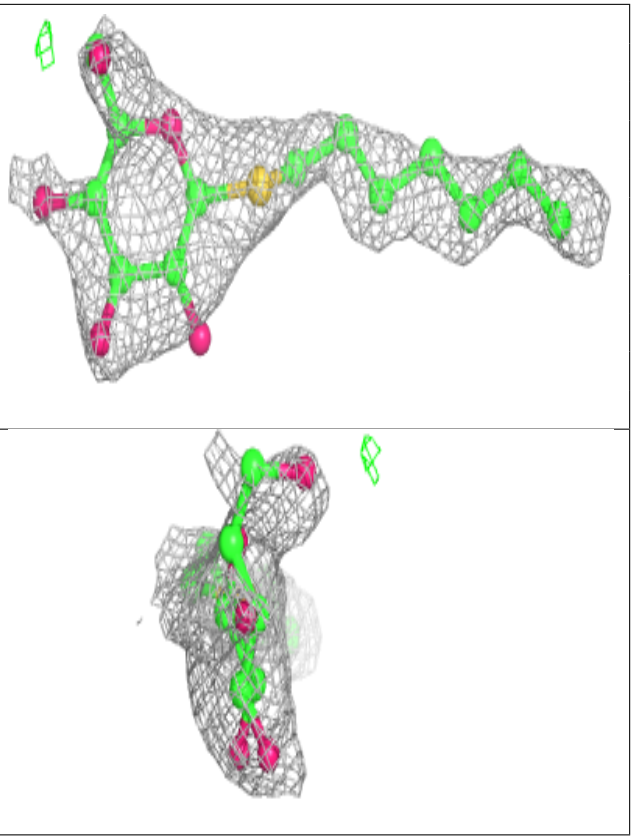






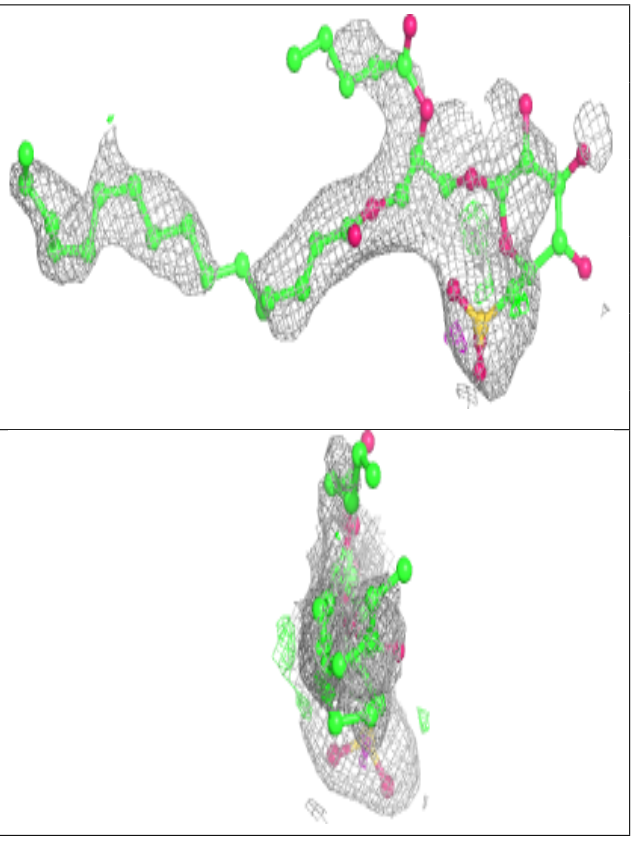
Electron density around HTG c 523:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



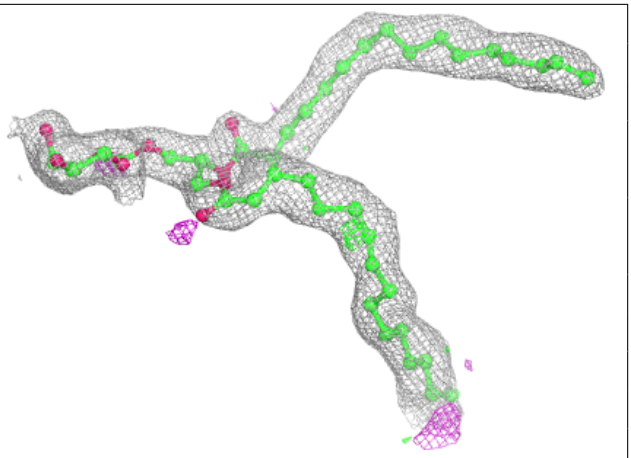
Electron density around SQD f 101:

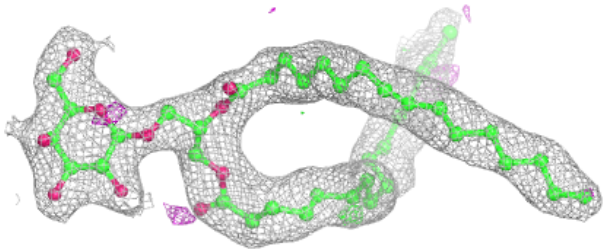
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

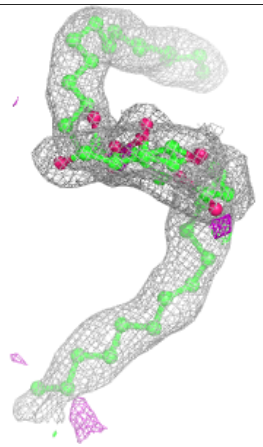


Electron density around LMG B 621:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

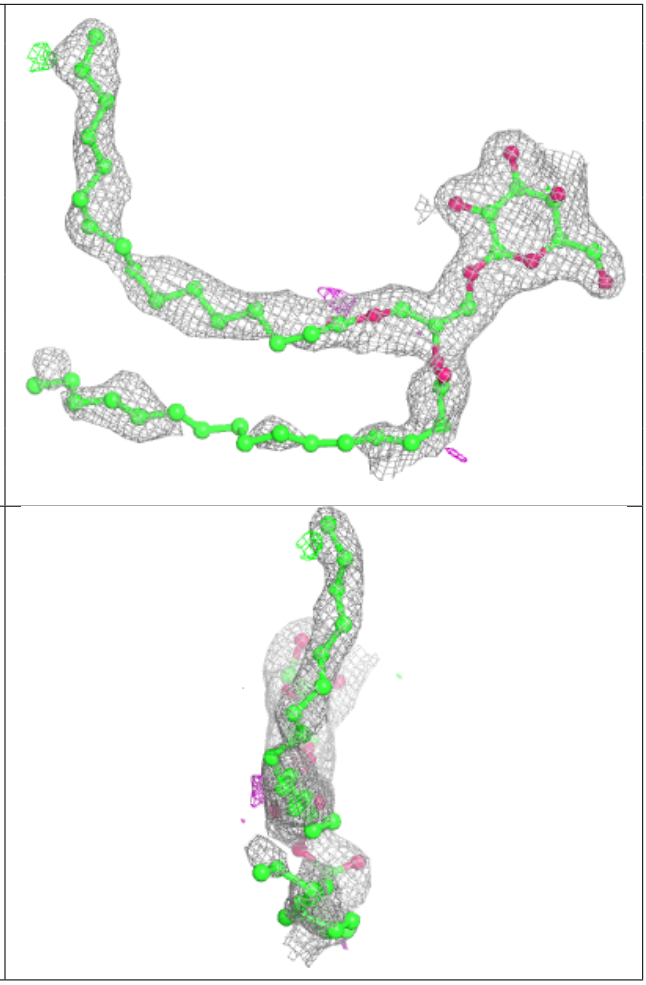






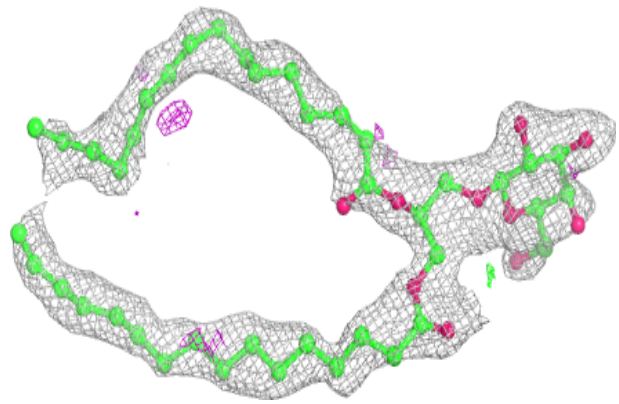
Electron density around LMG c 520:

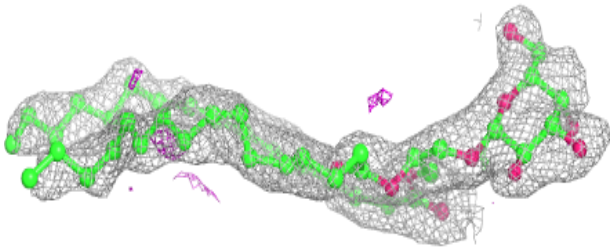
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

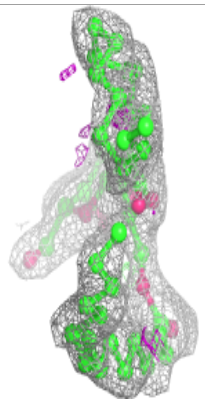


Electron density around LMG C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

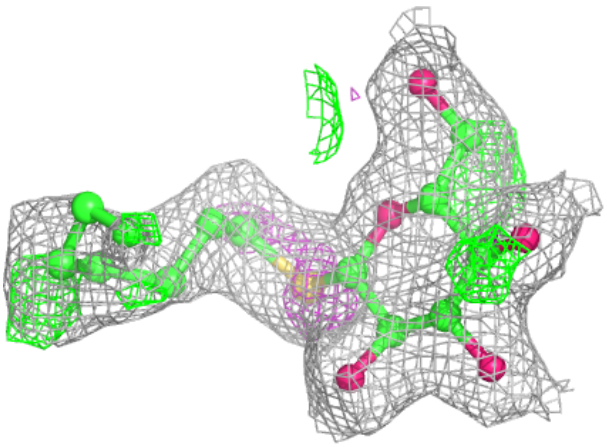


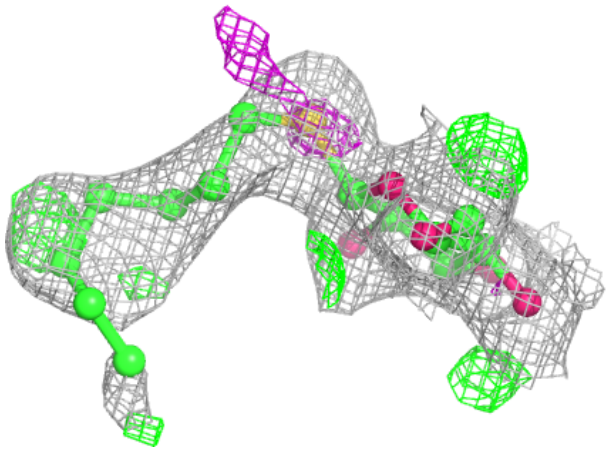


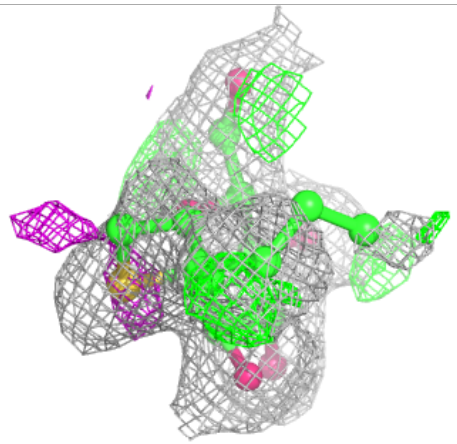


Electron density around HTG B 623:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

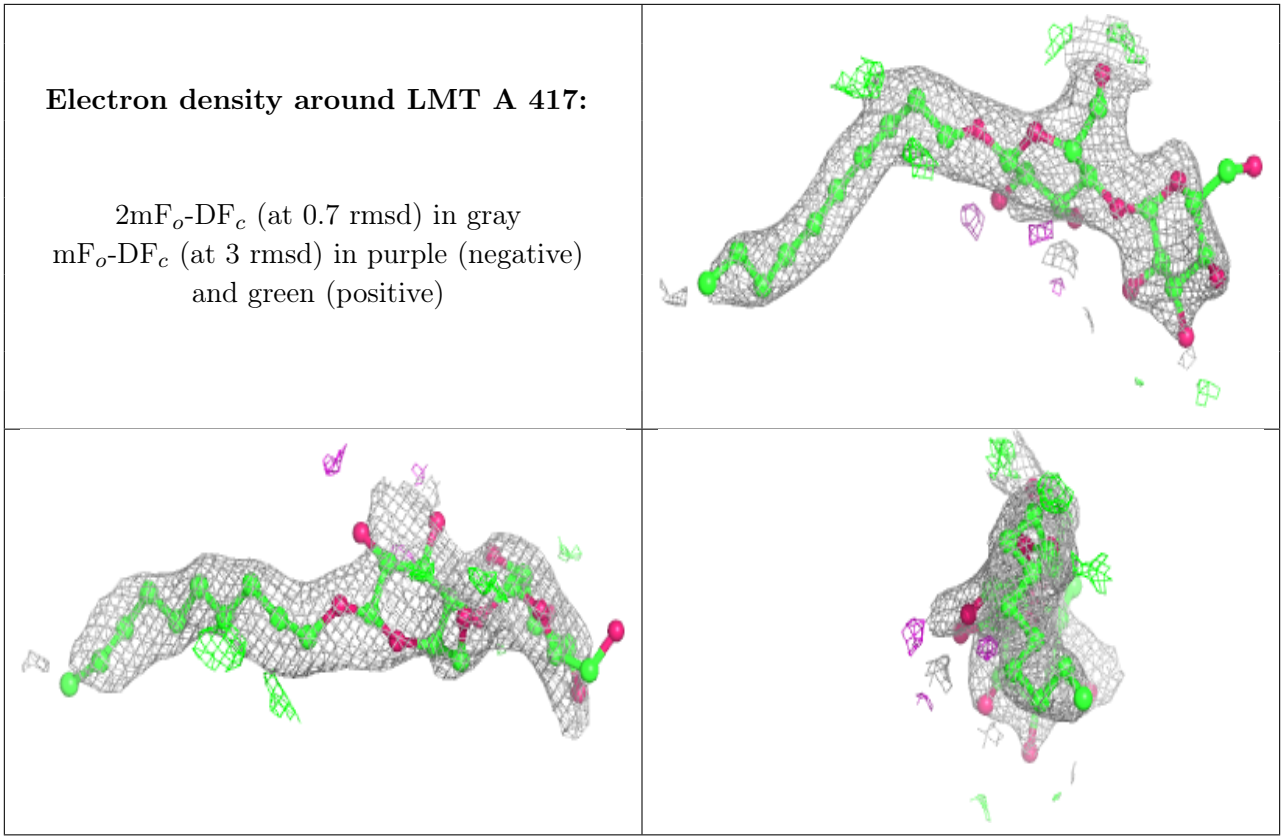






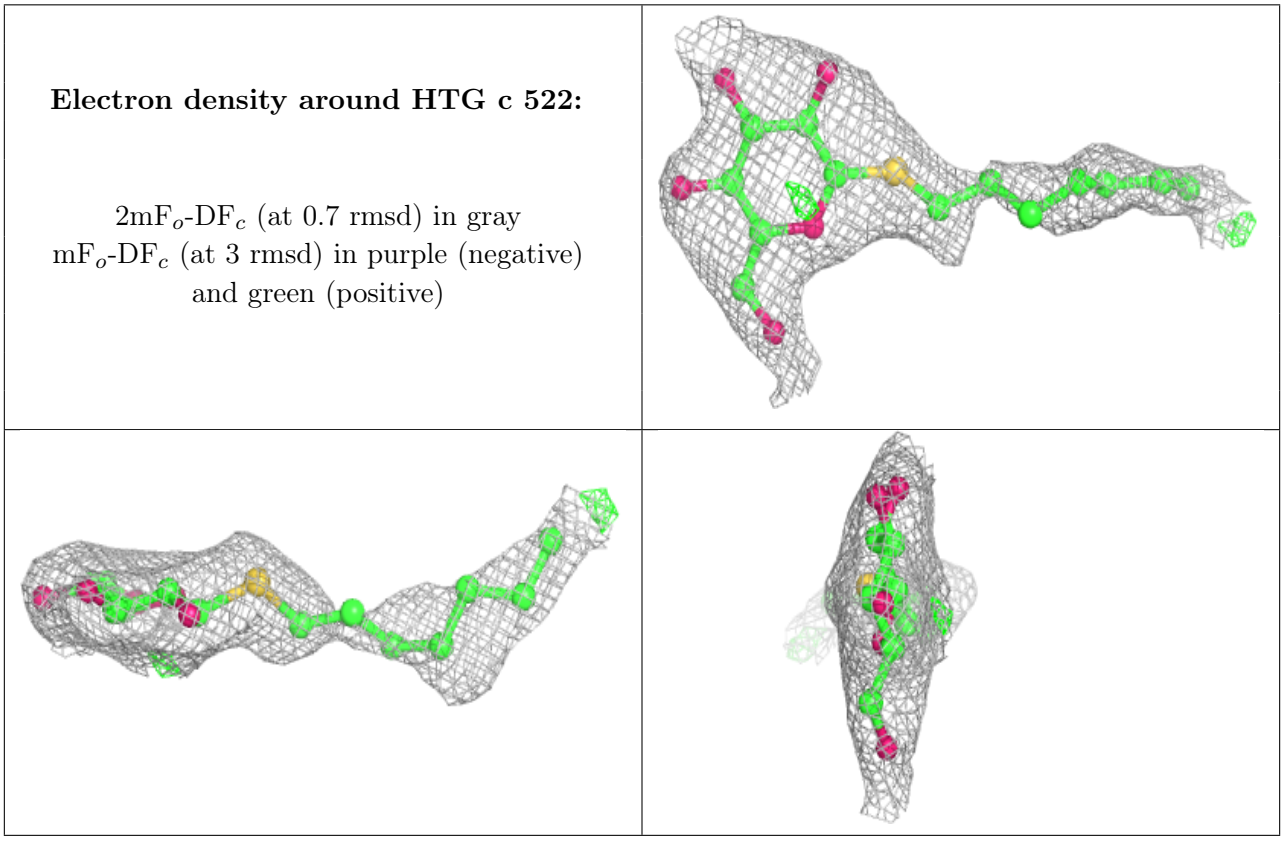
Electron density around LMT A 417:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



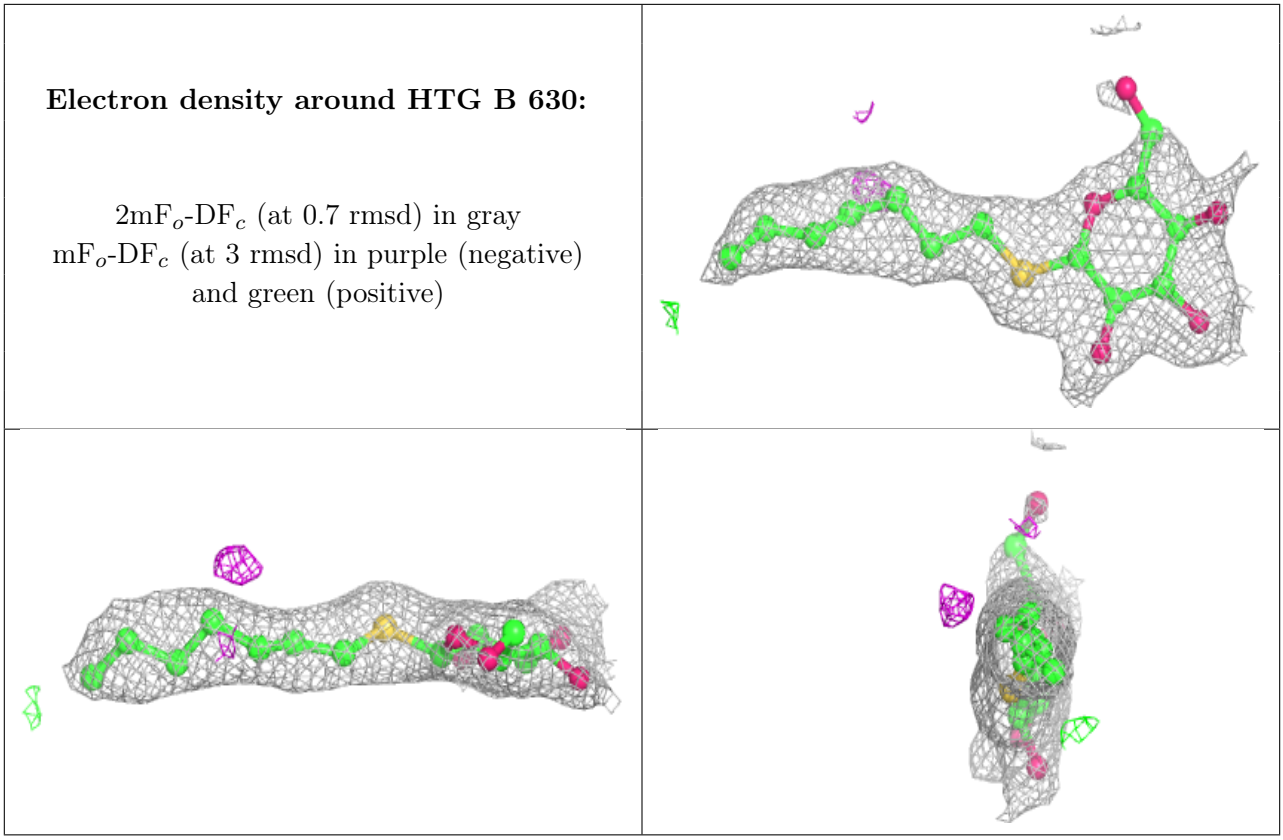
Electron density around HTG c 522:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



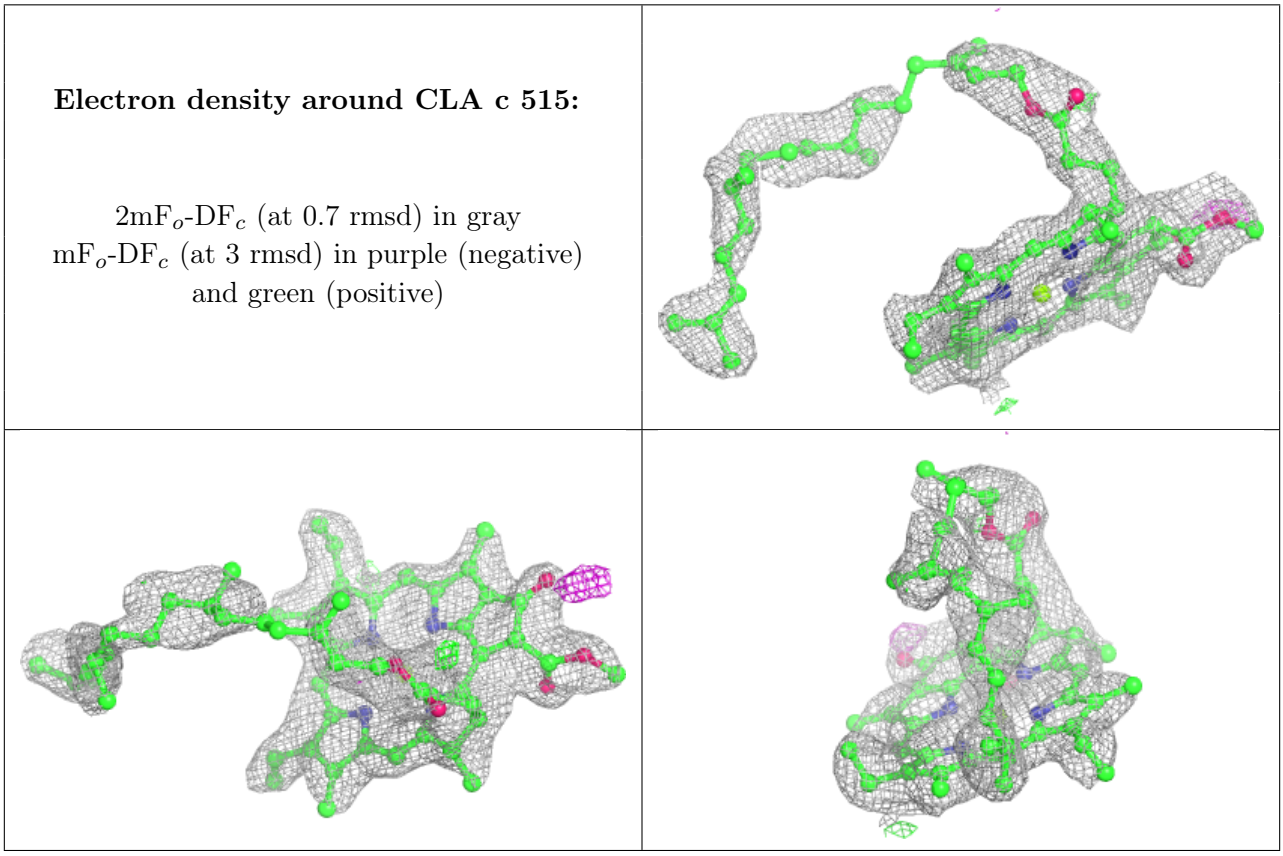
Electron density around HTG B 630:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



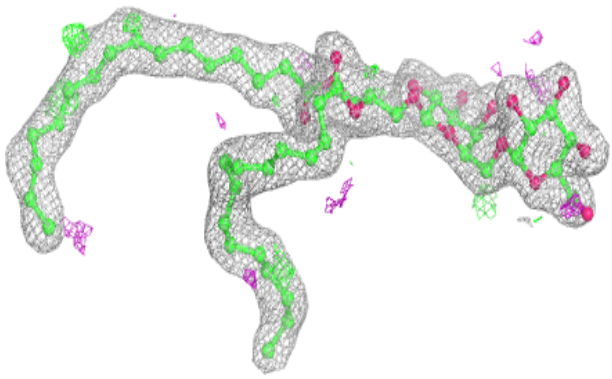
Electron density around CLA c 515:

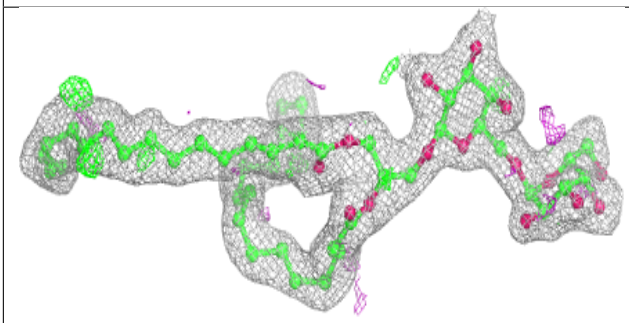
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

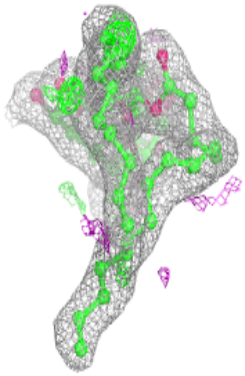


Electron density around DGD H 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

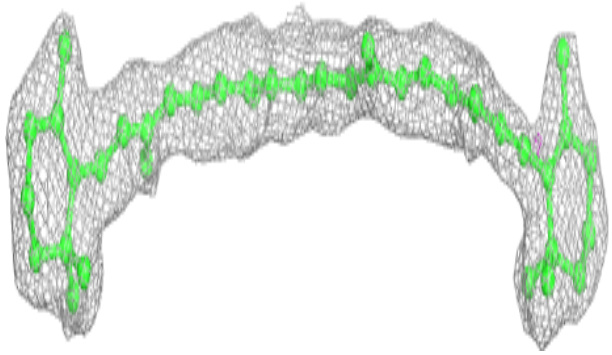


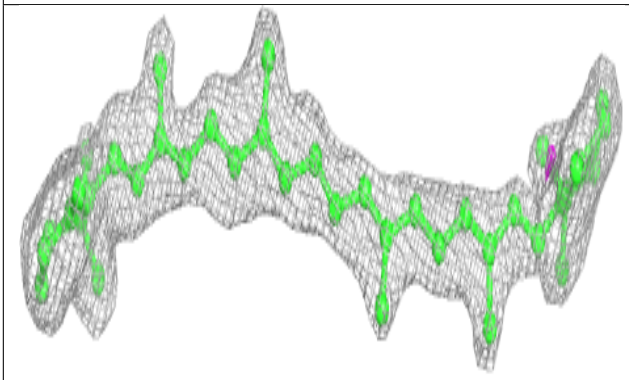


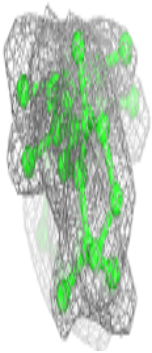


Electron density around BCR k 103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

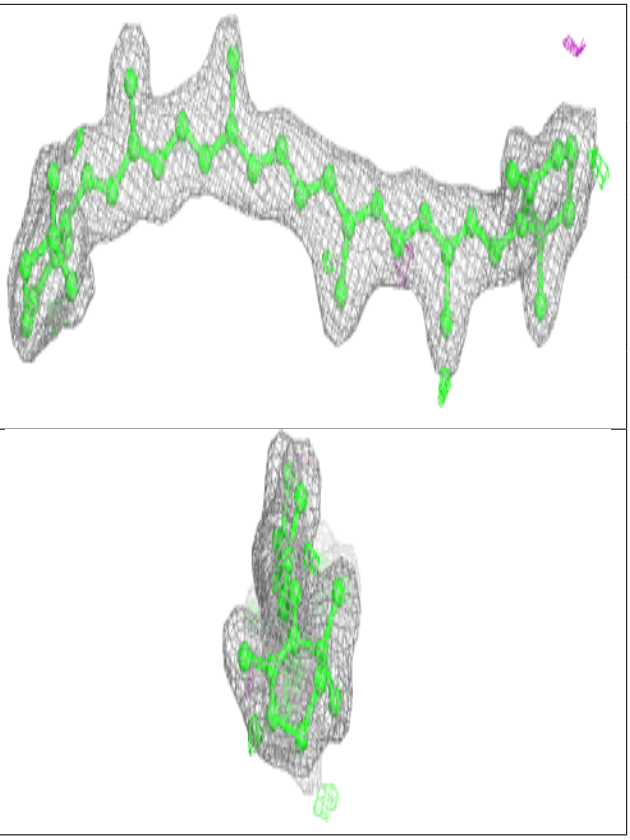






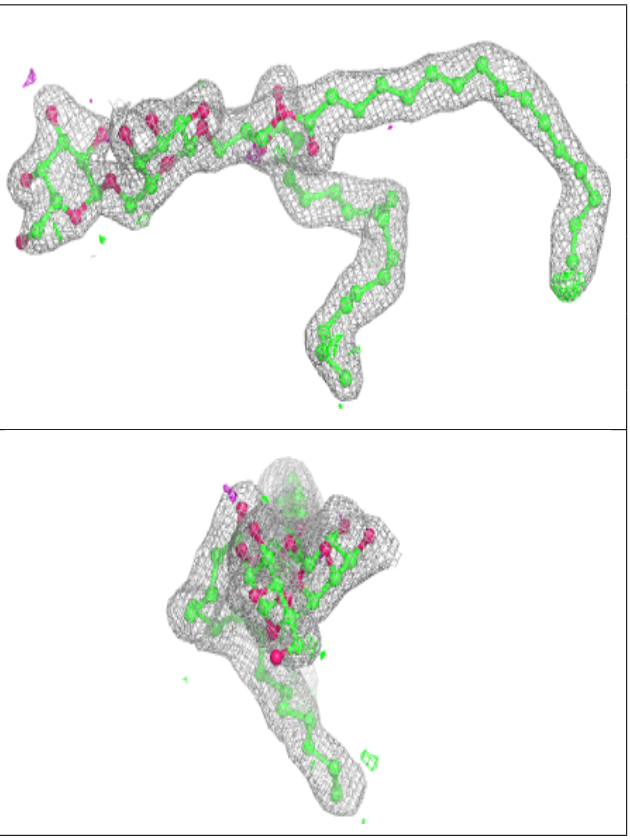
Electron density around BCR h 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



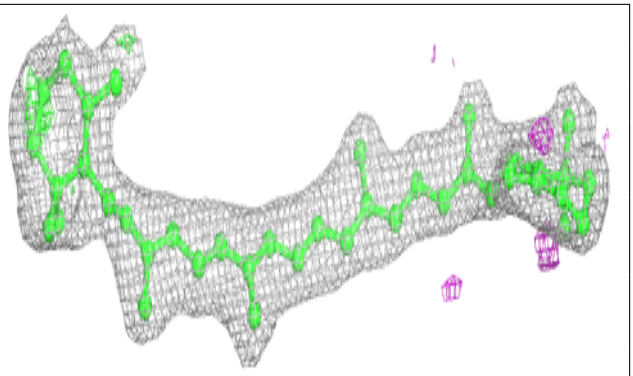
Electron density around DGD h 102:

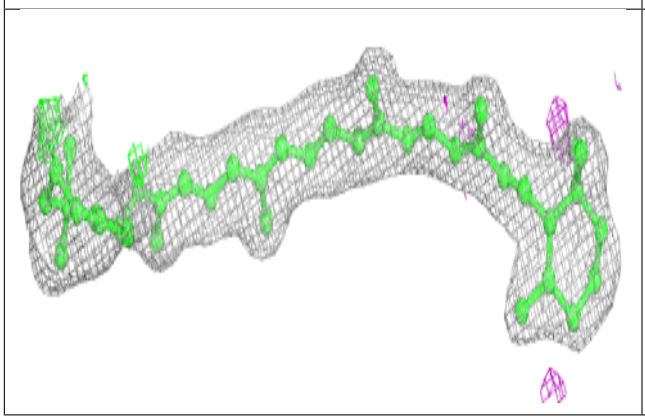
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

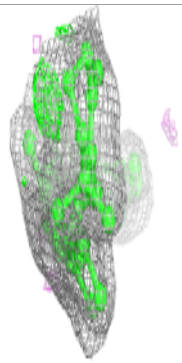


Electron density around BCR d 405:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

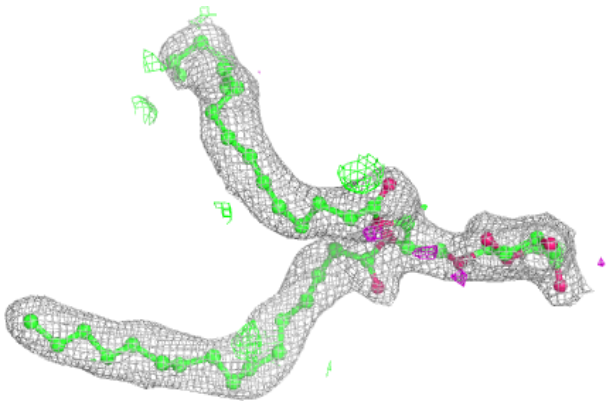


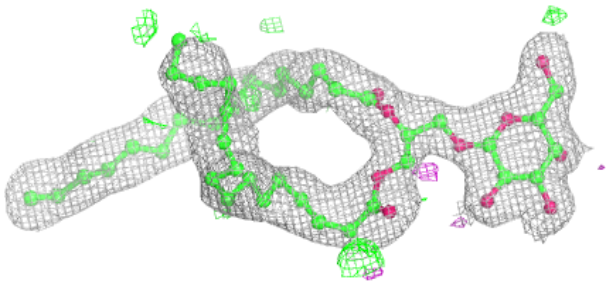


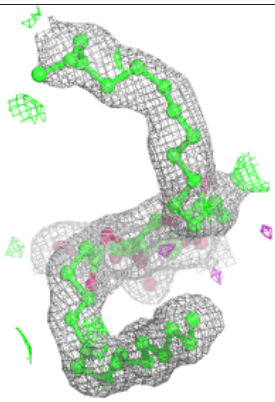


Electron density around LMG b 625:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

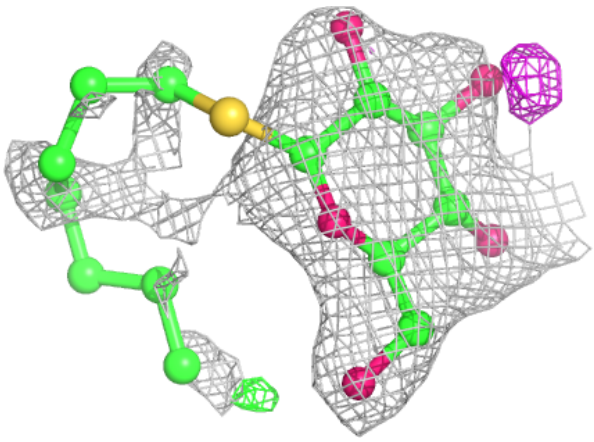


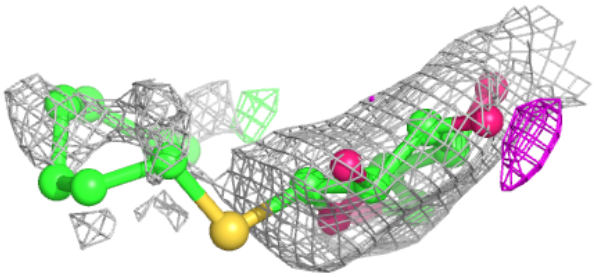


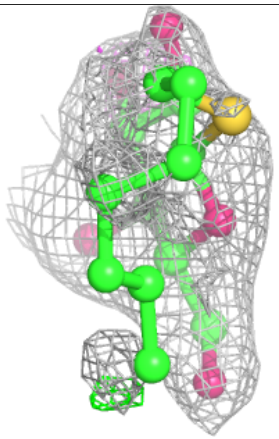


Electron density around HTG V 204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

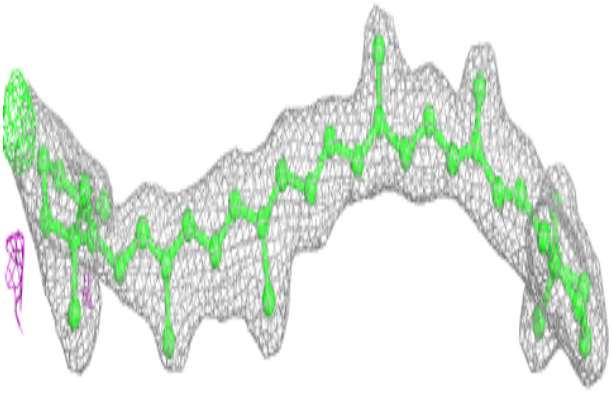


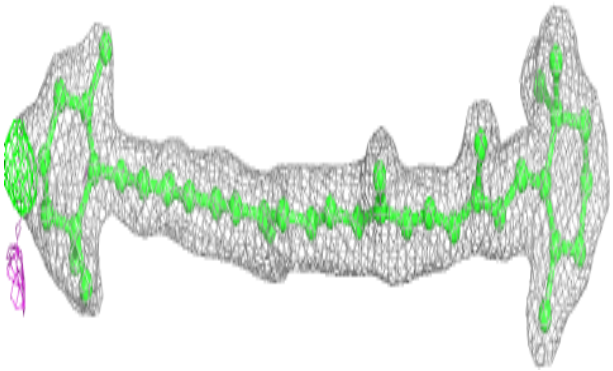


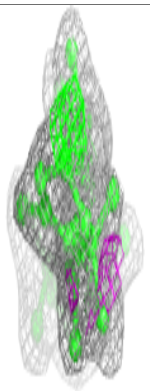


Electron density around BCR H 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

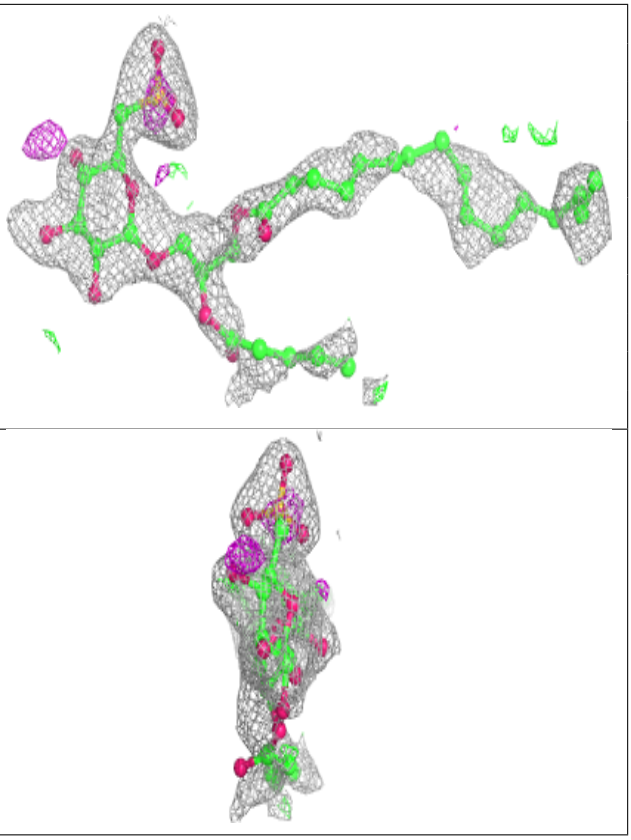






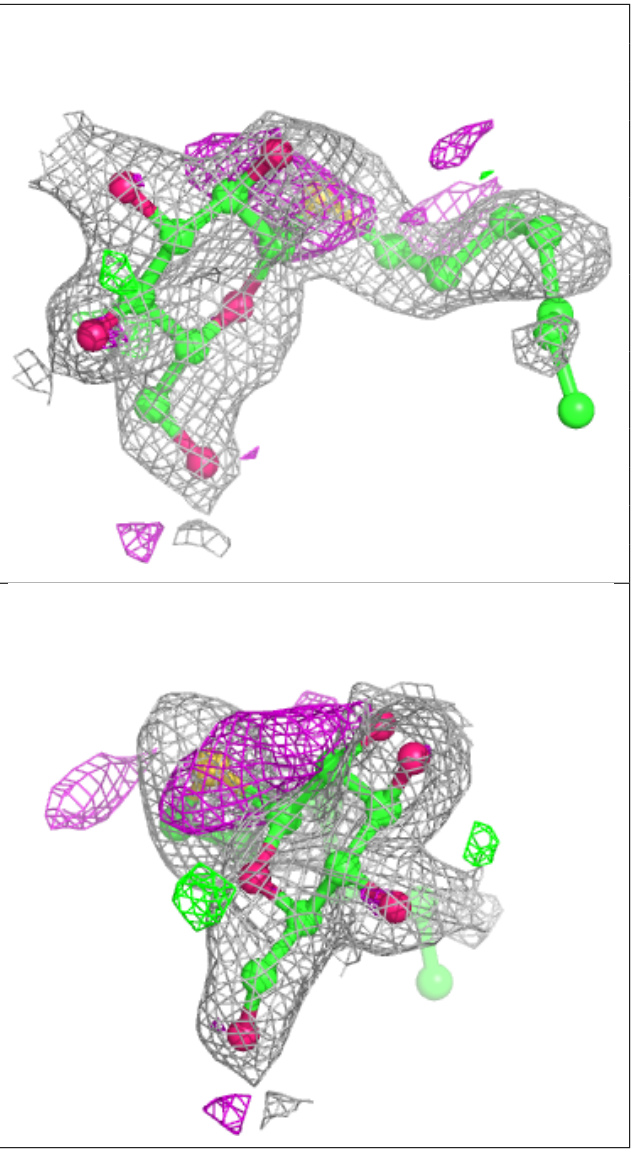
Electron density around SQD F 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



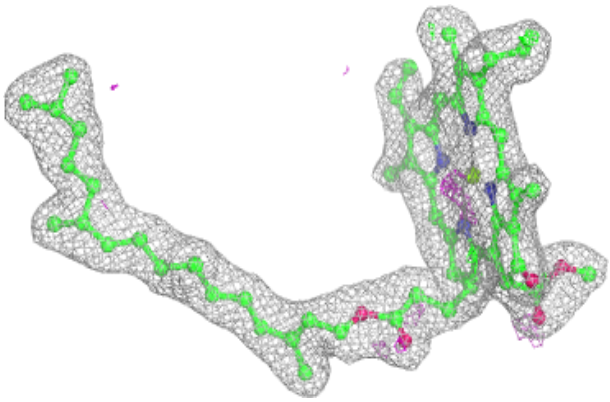
Electron density around HTG b 627:

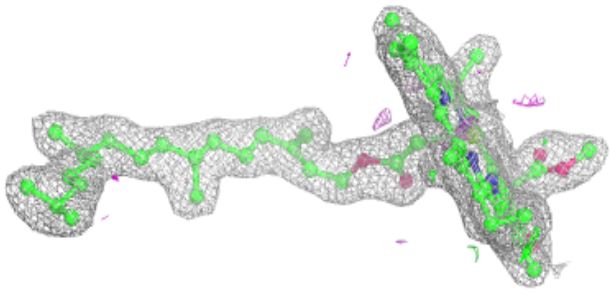
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

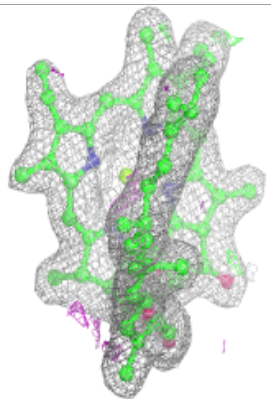


Electron density around CLA b 614:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

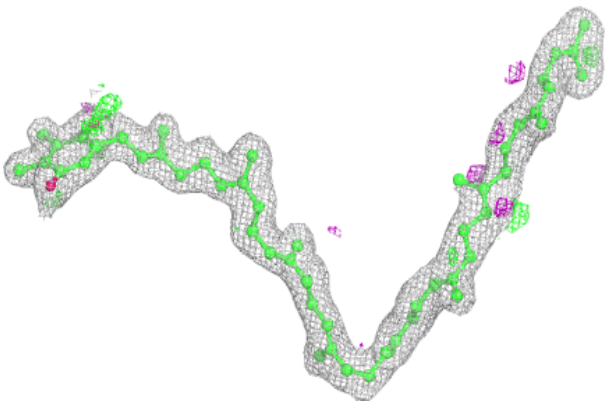


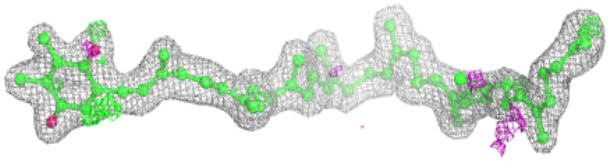




Electron density around PL9 d 406:

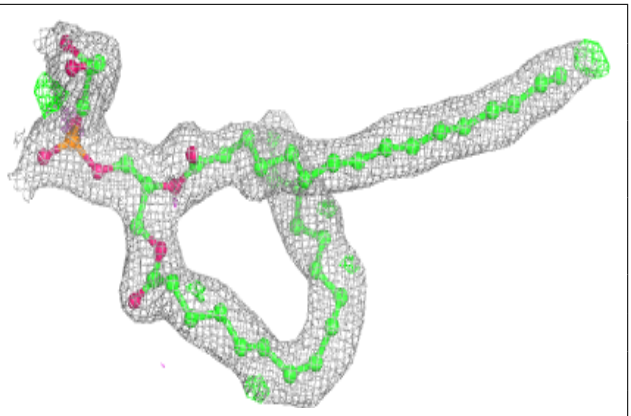
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

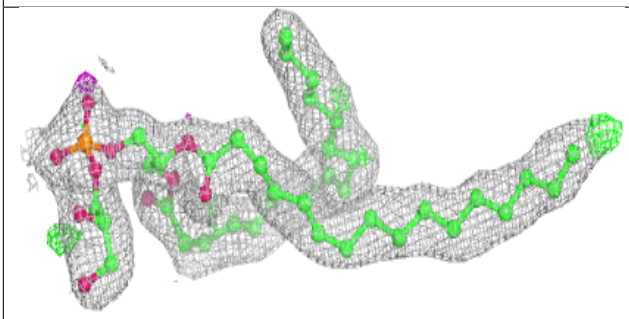


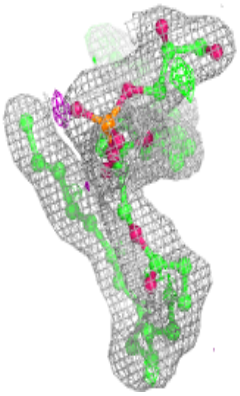


Electron density around LHG d 408:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

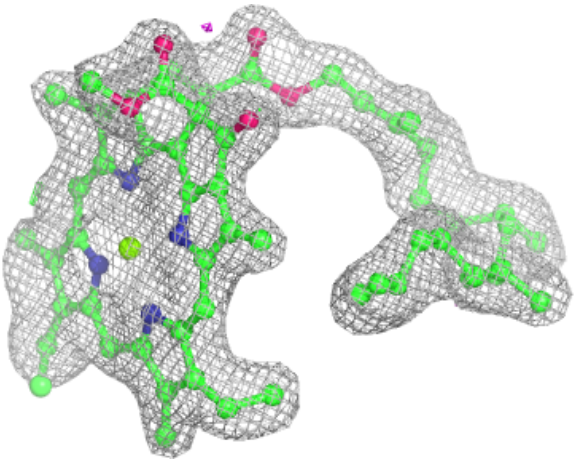


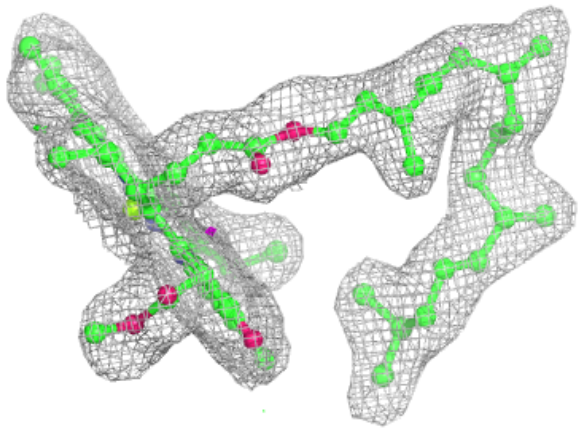


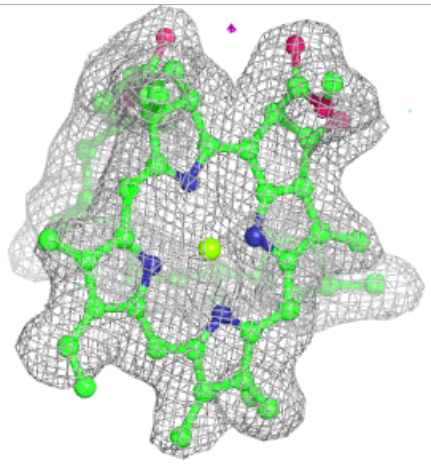


Electron density around CLA c 505:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

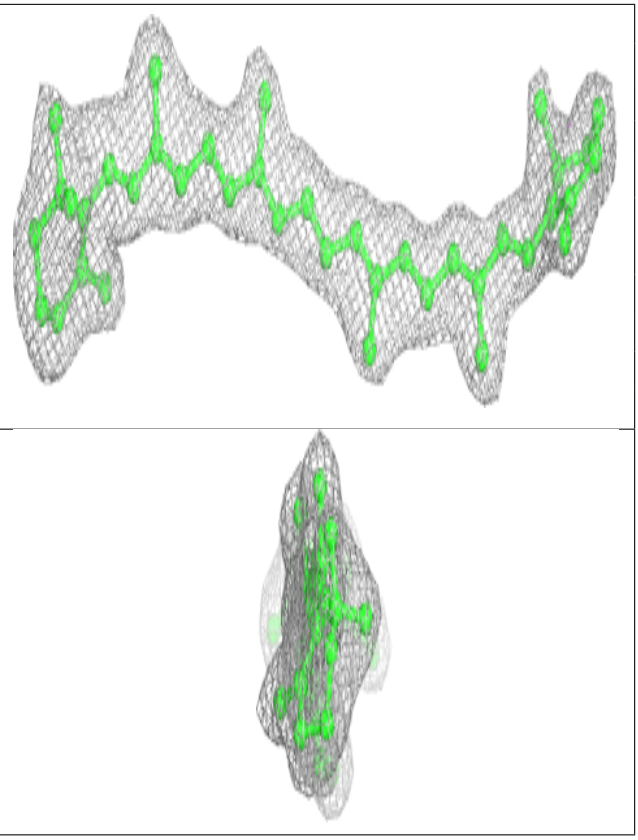






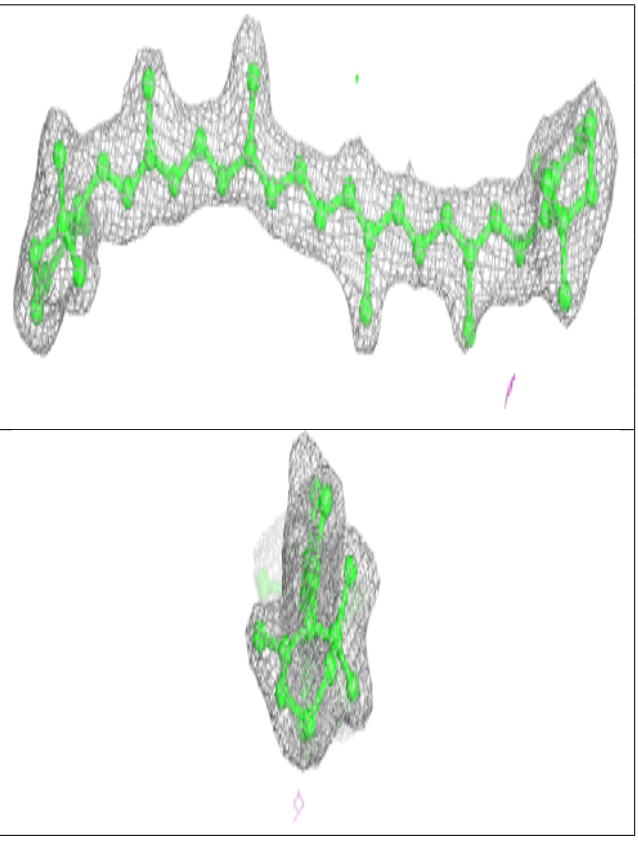
Electron density around BCR Y 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



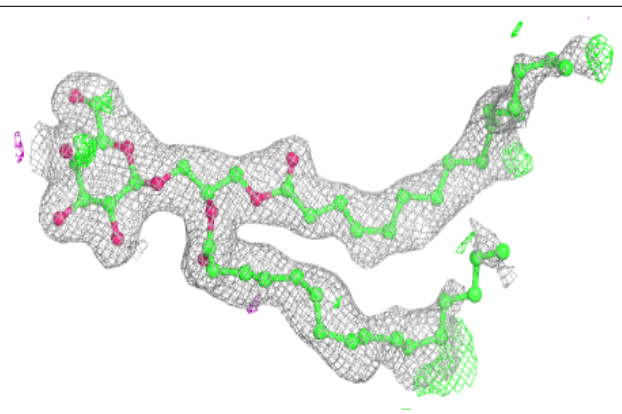
Electron density around BCR c 526:

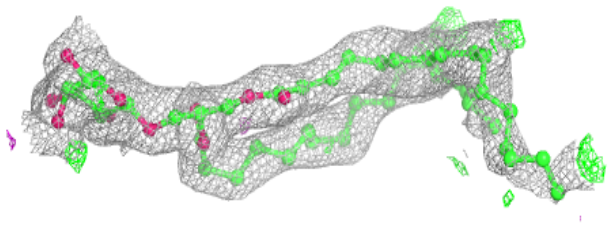
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

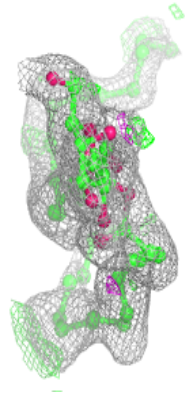


Electron density around LMG j 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

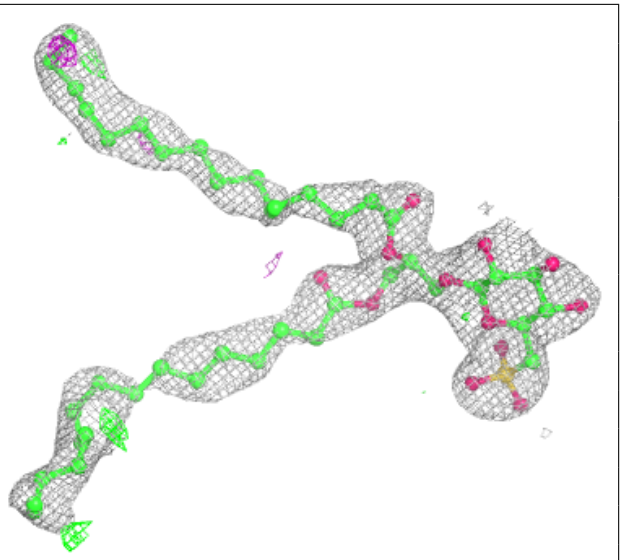


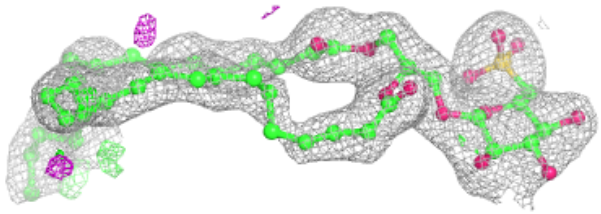


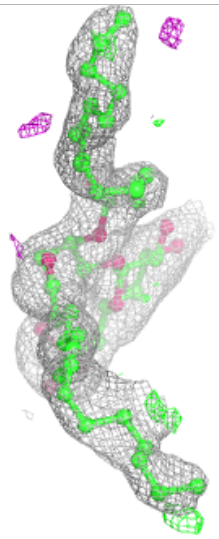


Electron density around SQD a 411:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

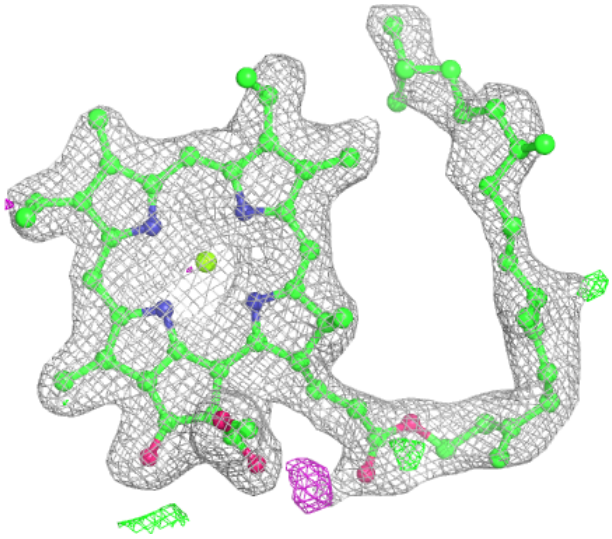


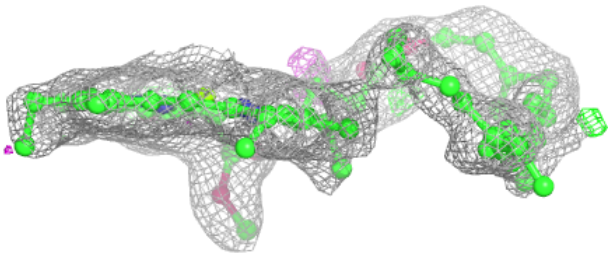


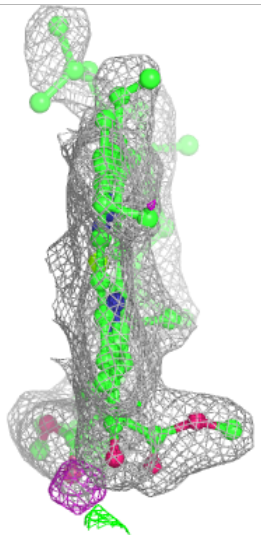


Electron density around CLA c 514:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

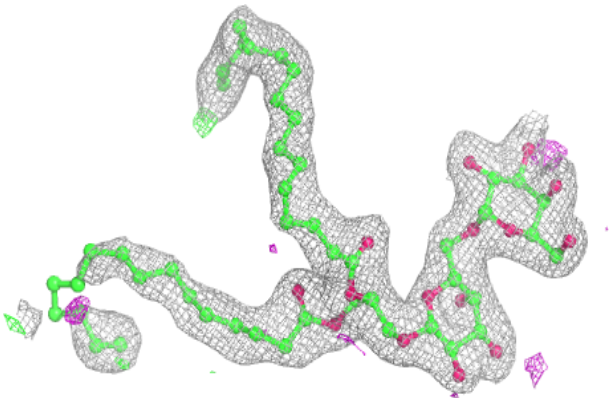


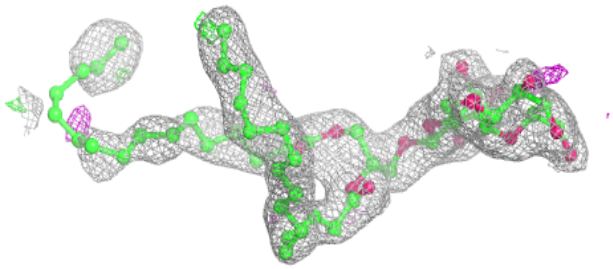


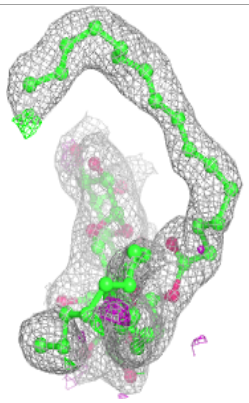


Electron density around DGD c 518:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

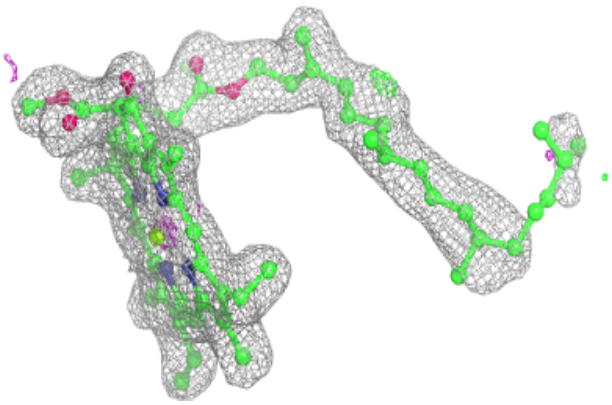


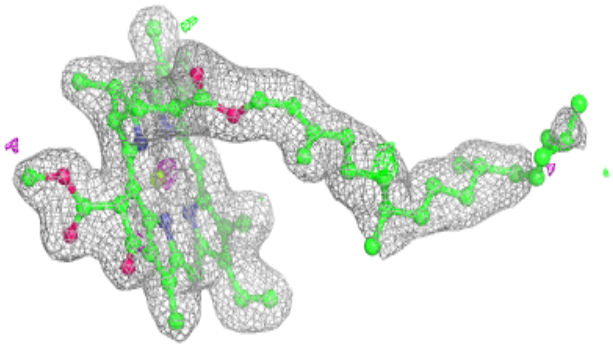


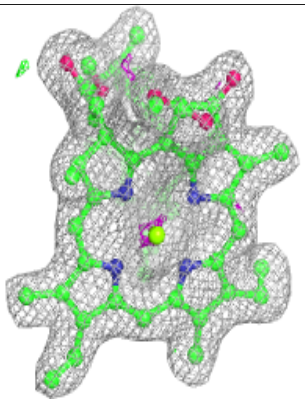


Electron density around CLA C 509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

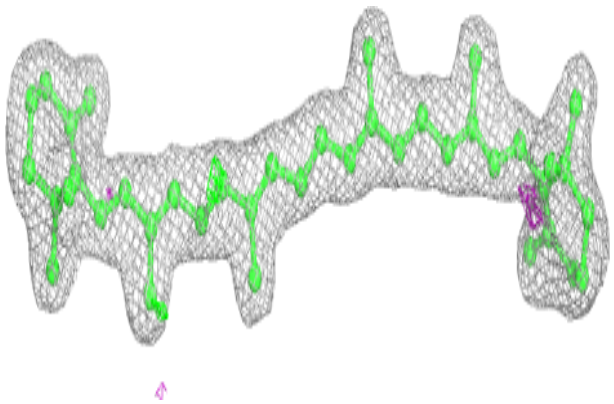


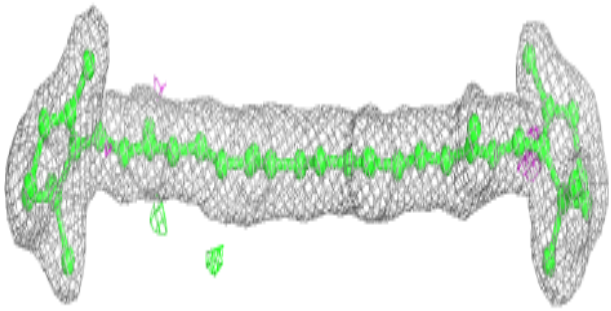


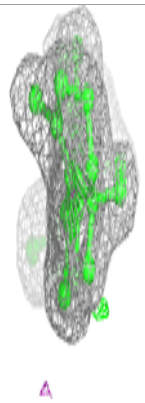


Electron density around BCR B 619:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

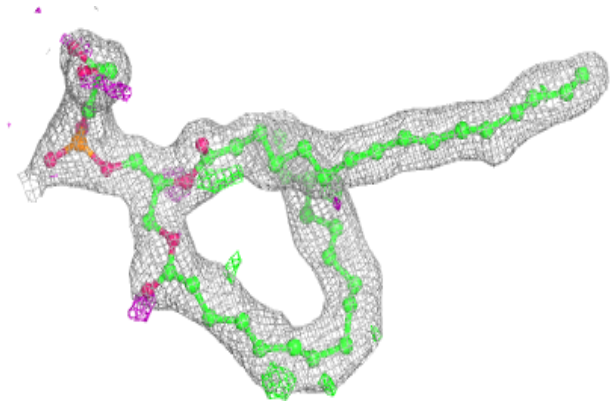


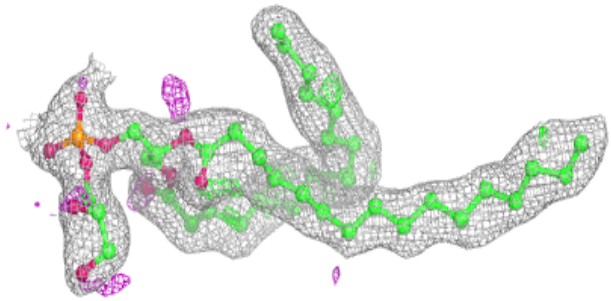


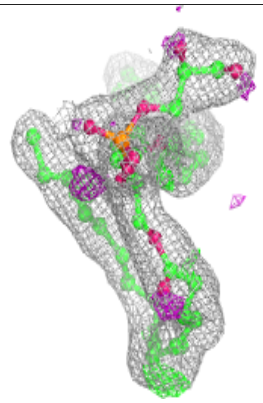


Electron density around LHG D 408:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

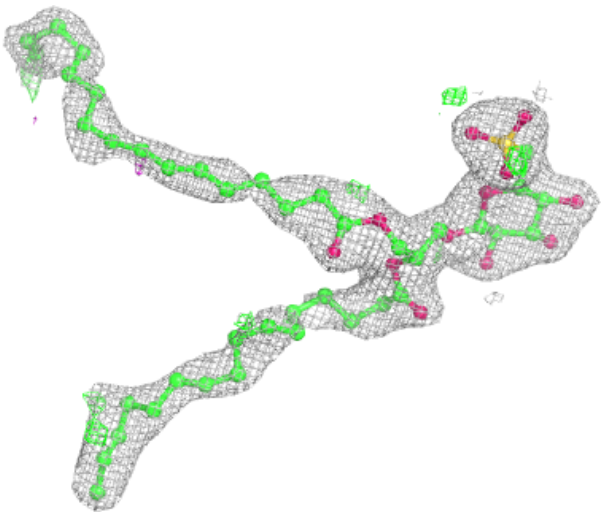


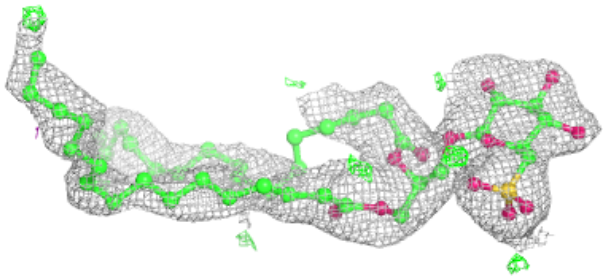


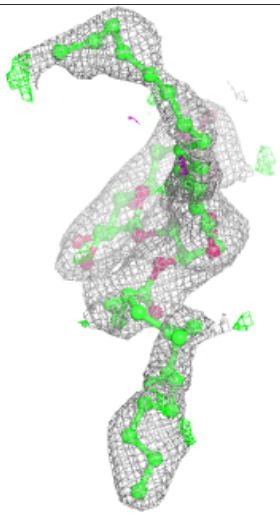


Electron density around SQD A 411:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

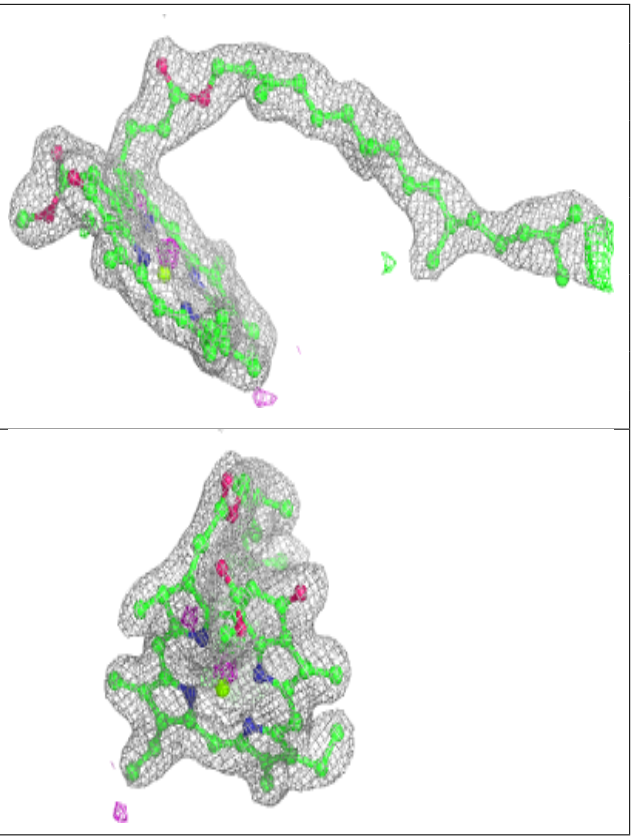






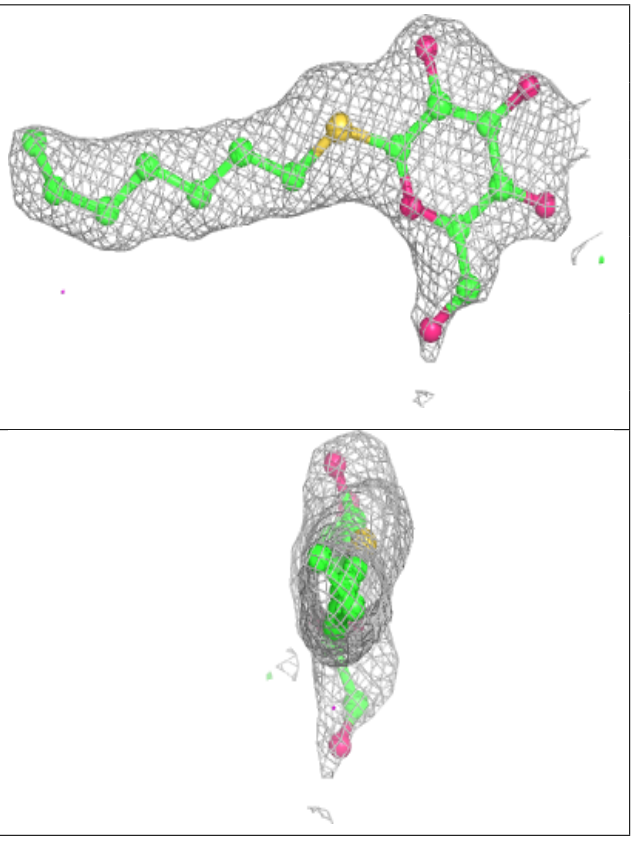
Electron density around CLA c 506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



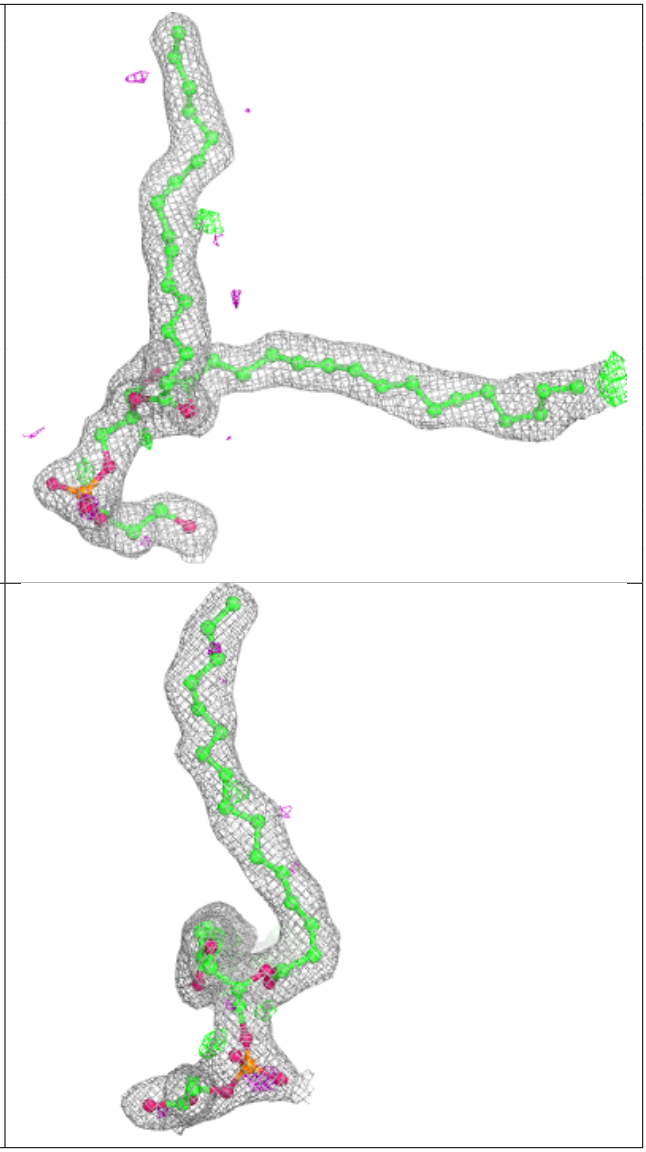
Electron density around HTG b 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



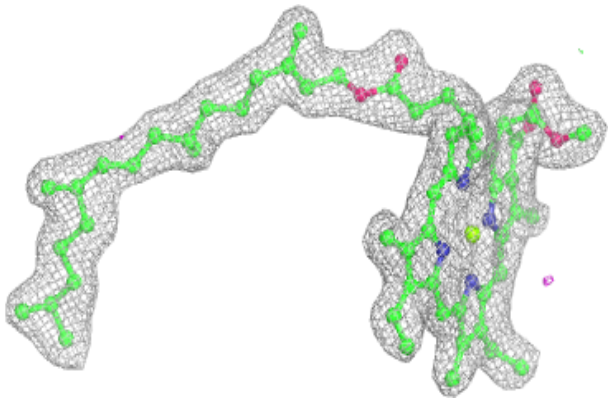
Electron density around LHG l 102:

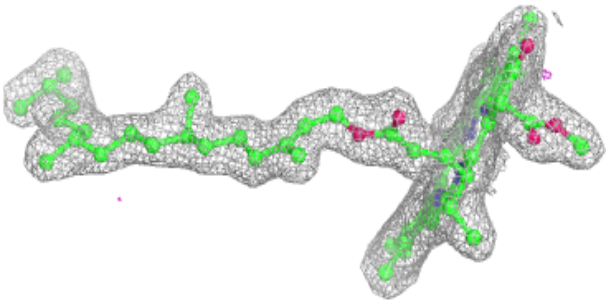
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

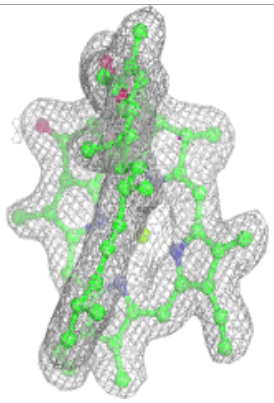


Electron density around CLA B 610:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

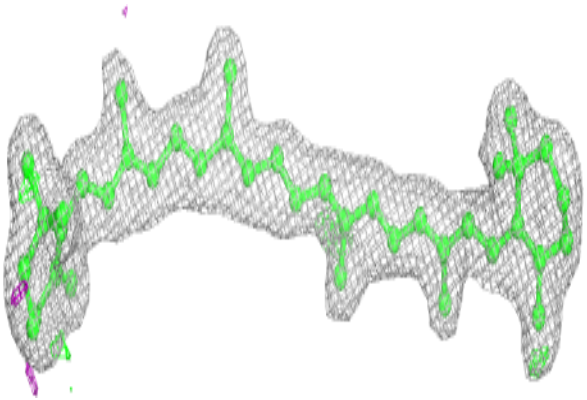


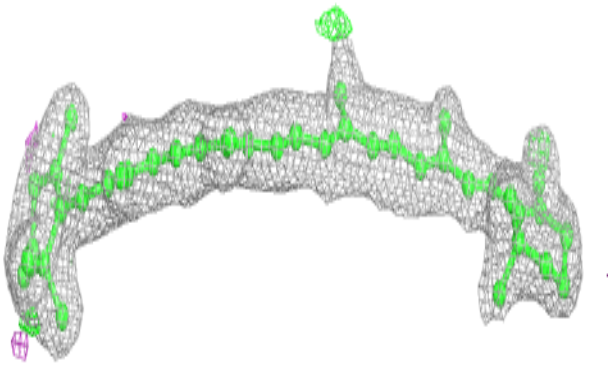


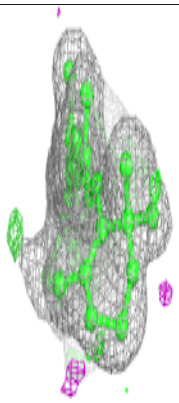


Electron density around BCR T 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

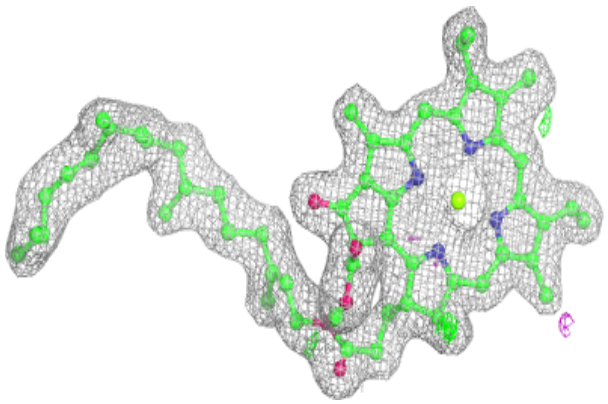


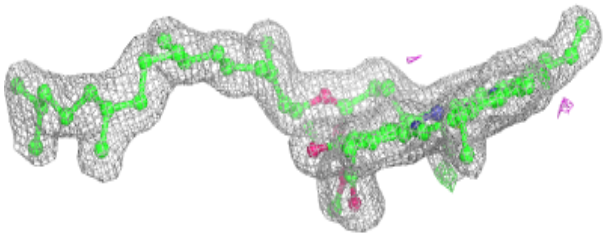


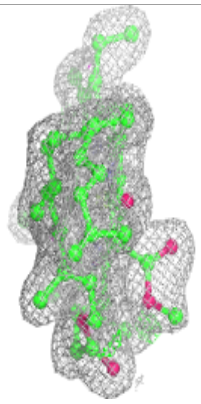


Electron density around CLA B 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

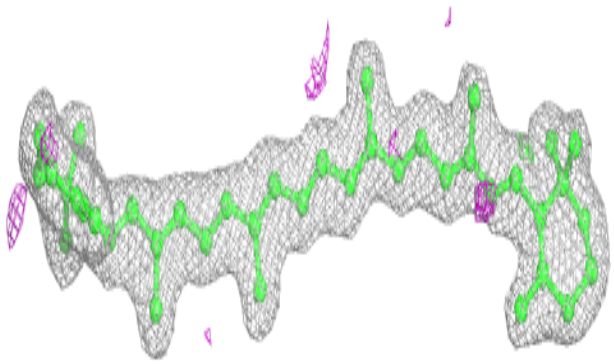


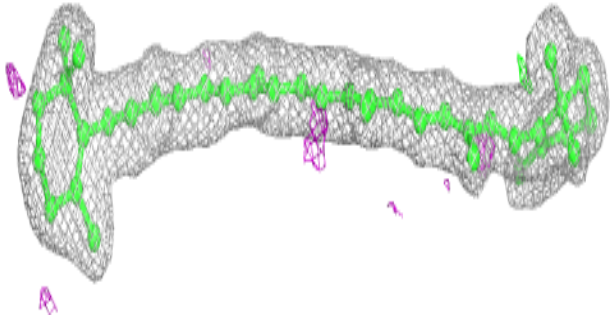


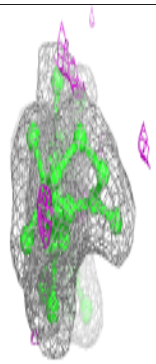


Electron density around BCR b 622:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

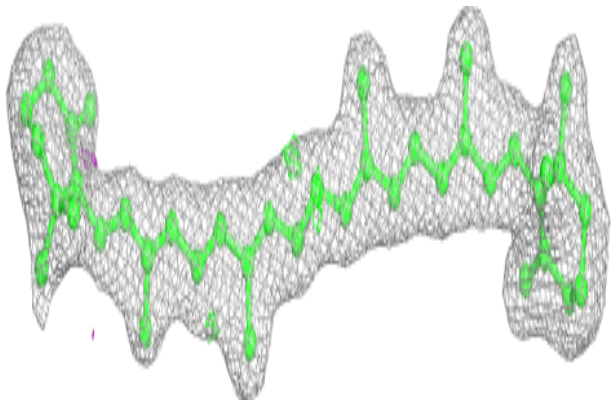


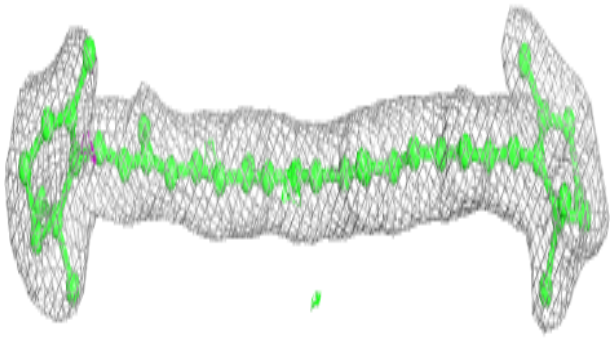


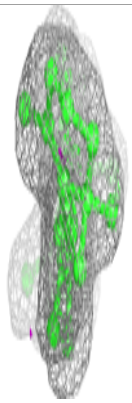


Electron density around BCR b 623:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

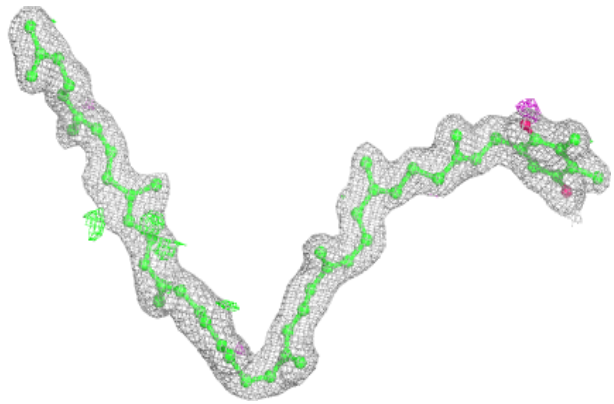


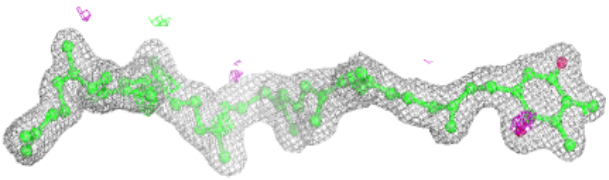


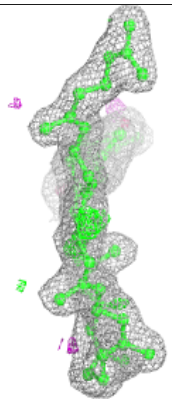


Electron density around PL9 D 406:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

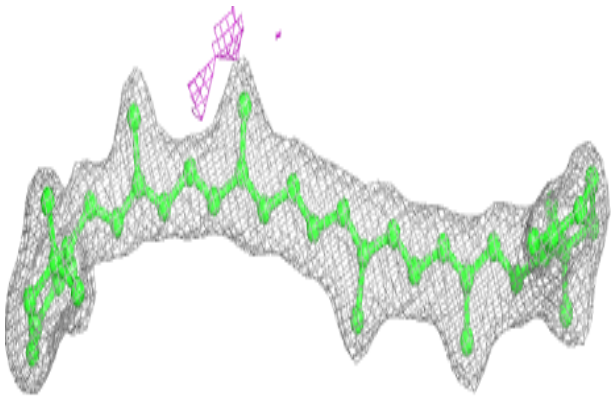


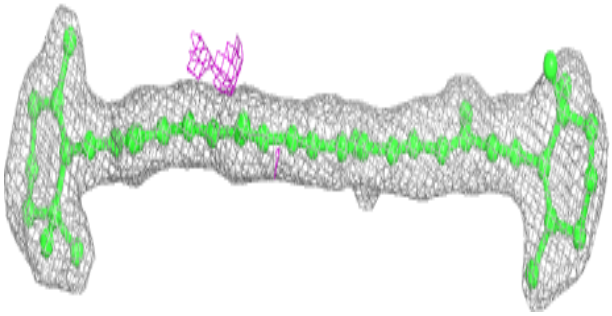


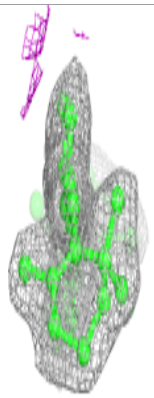


Electron density around BCR c 516:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

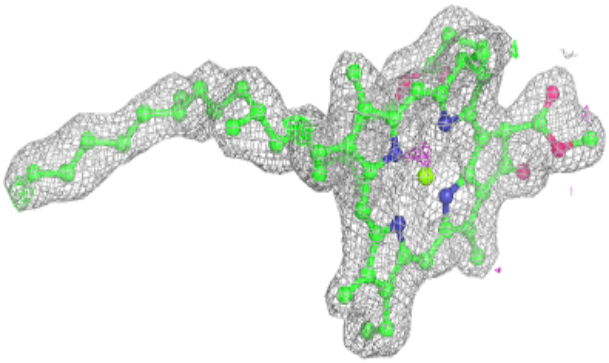


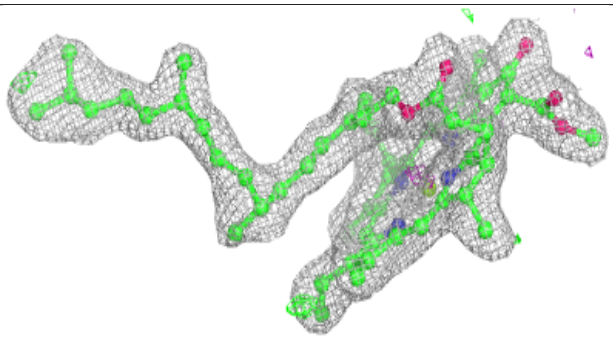


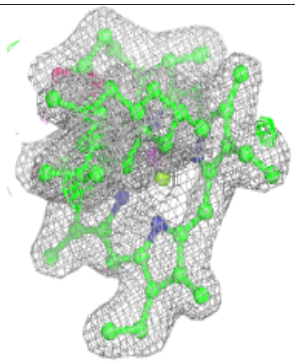


Electron density around CLA c 507:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

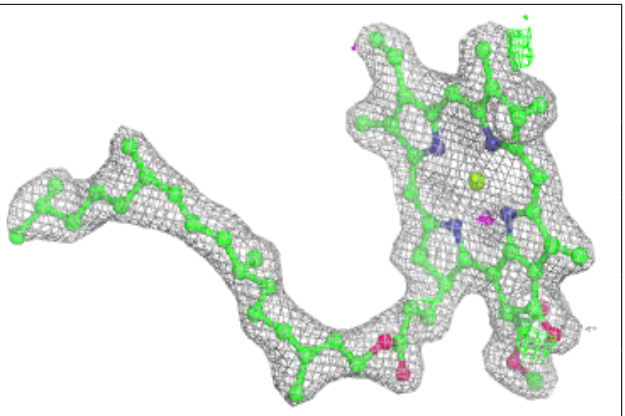


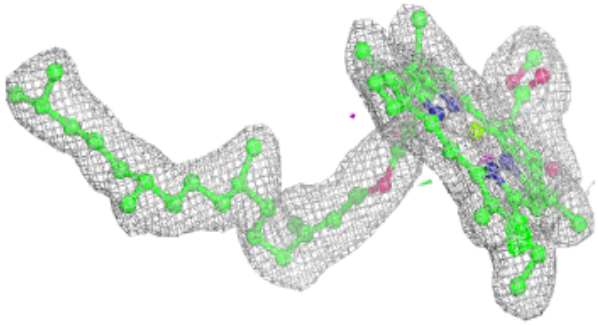


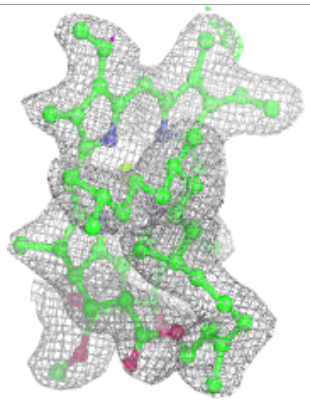


Electron density around CLA c 513:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

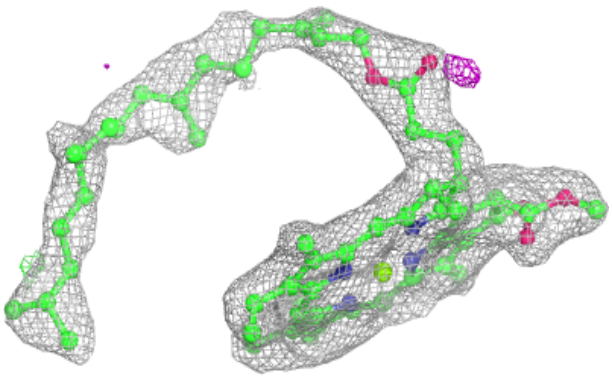


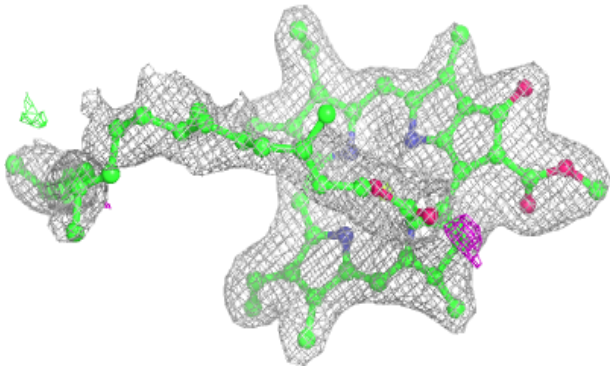


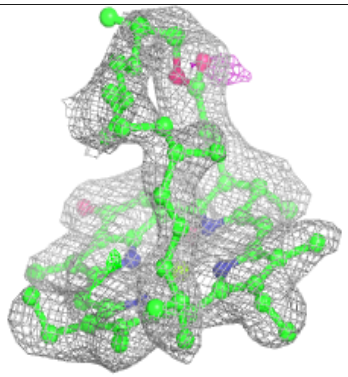


Electron density around CLA C 514:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

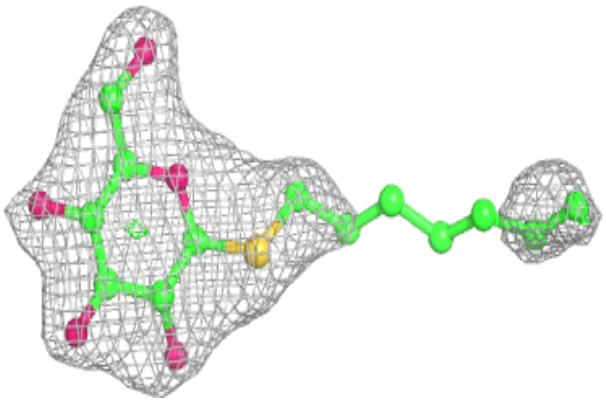


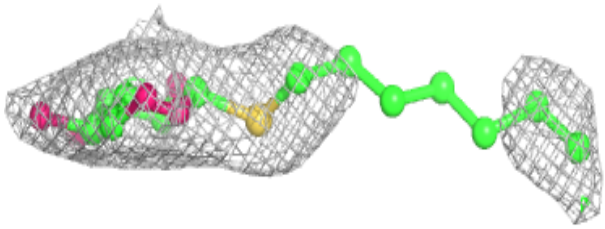


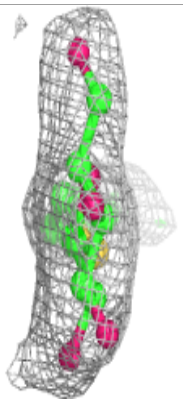


Electron density around HTG C 522:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

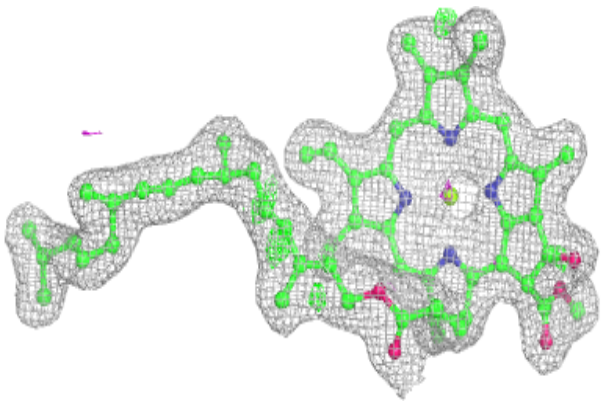


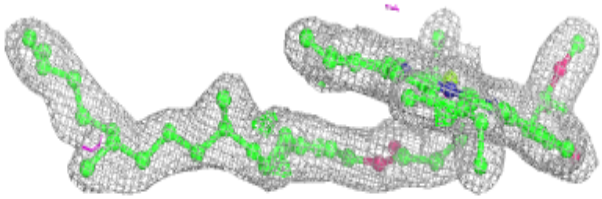


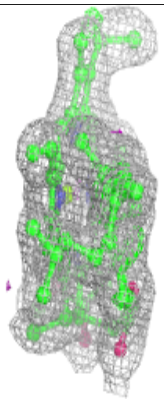


Electron density around CLA B 604:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

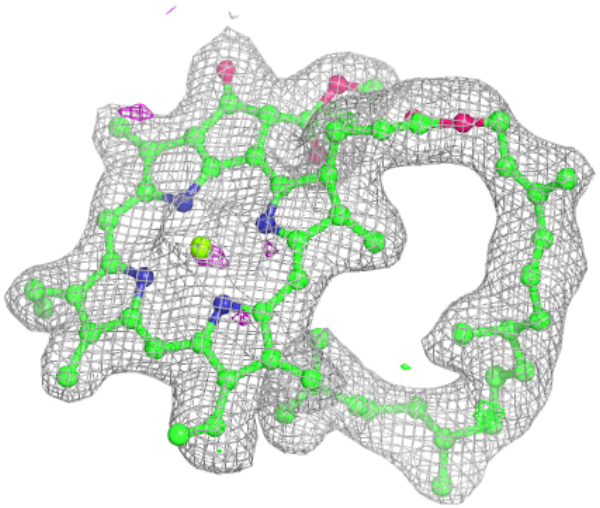


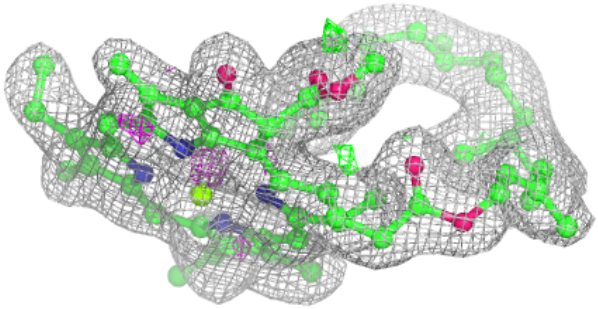




Electron density around CLA b 620:

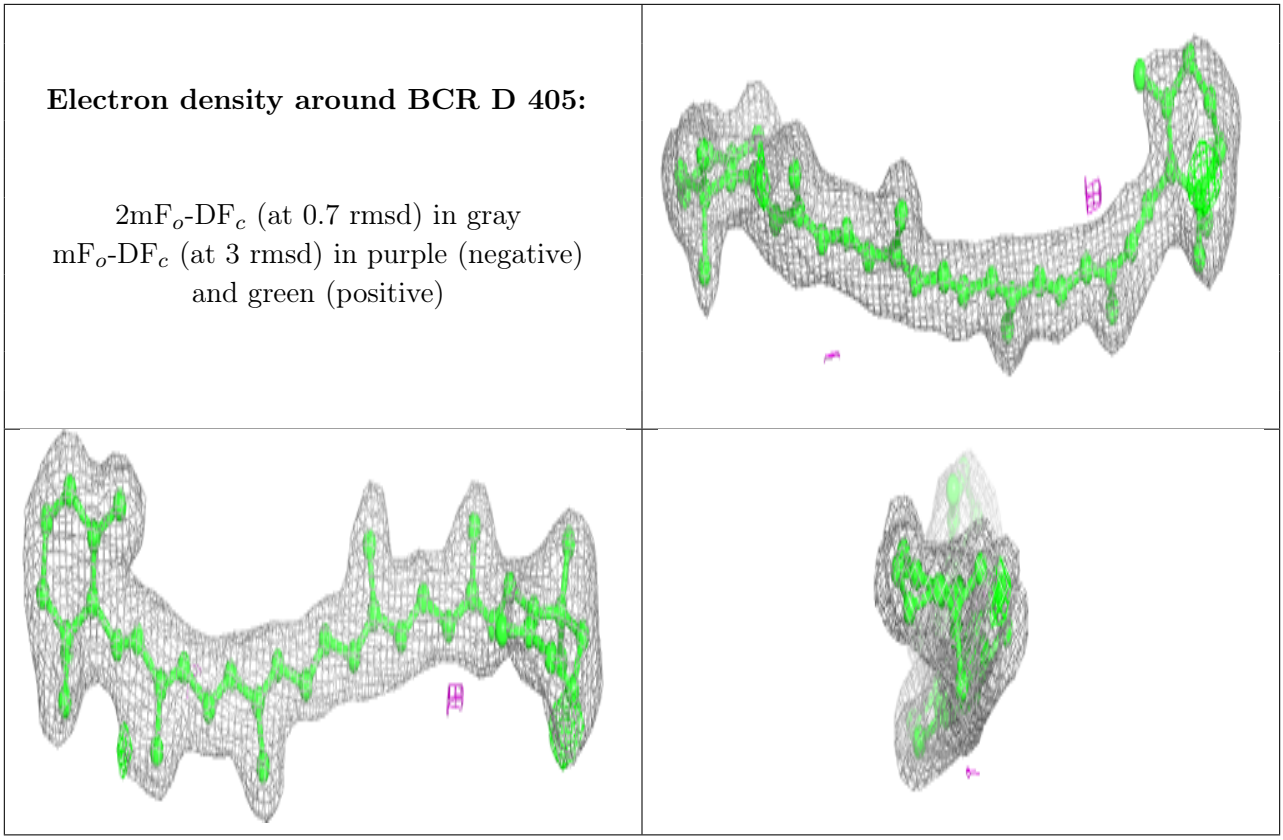
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





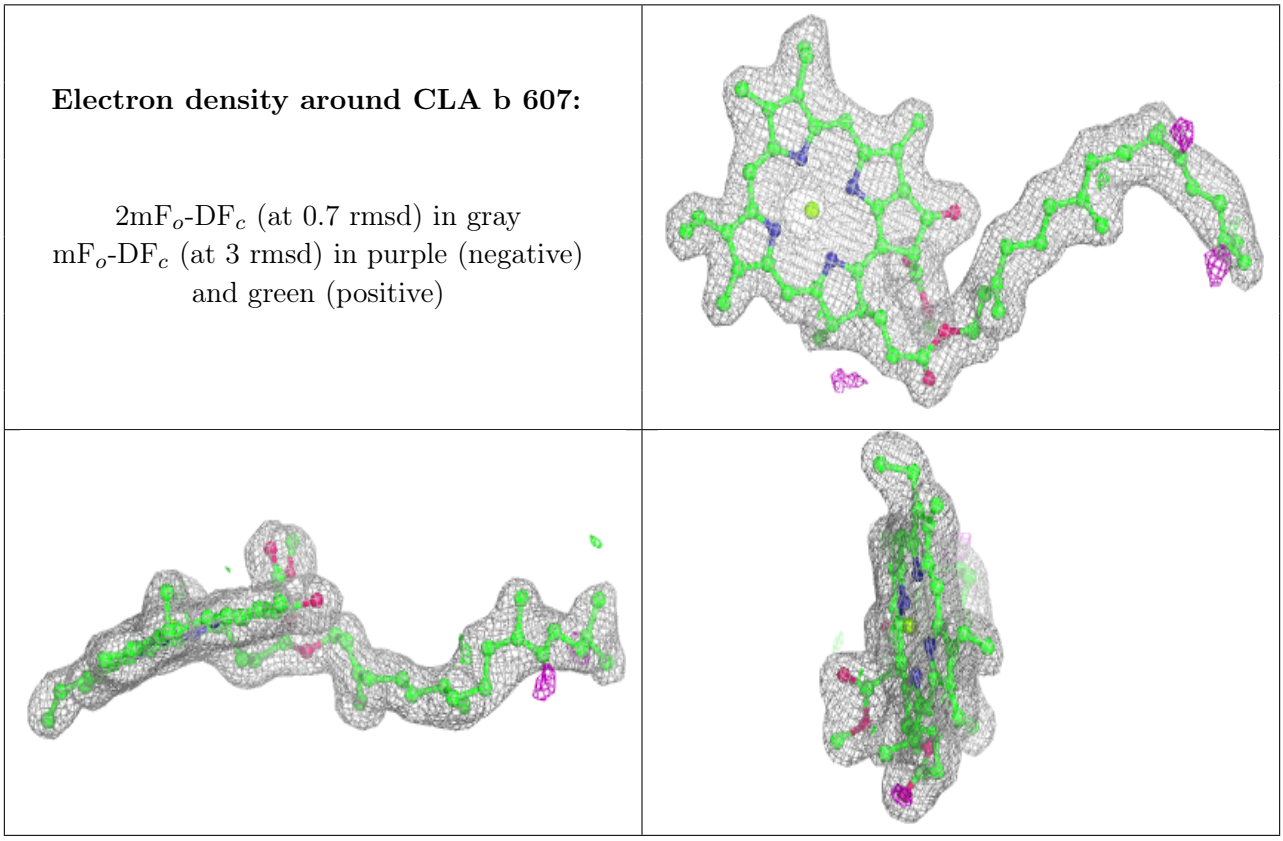
Electron density around BCR D 405:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



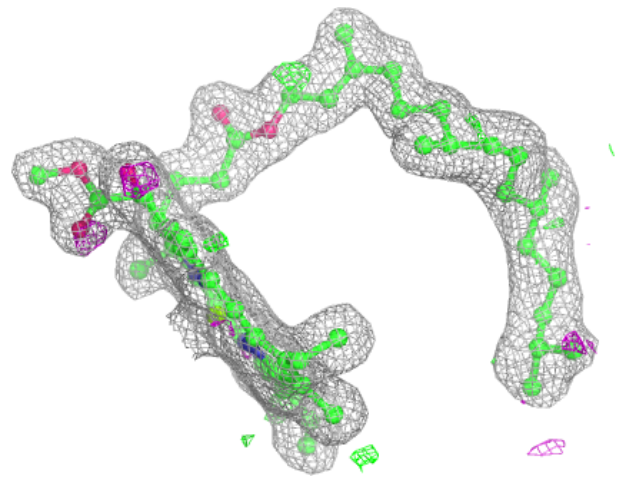
Electron density around CLA b 607:

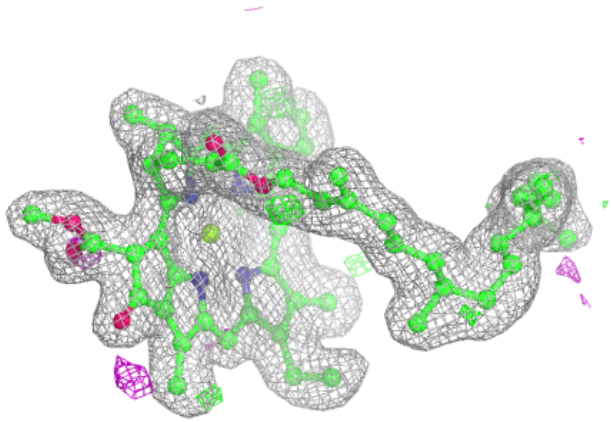
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

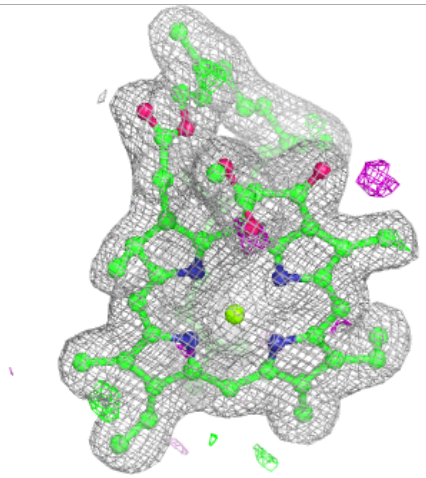


Electron density around CLA B 612:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

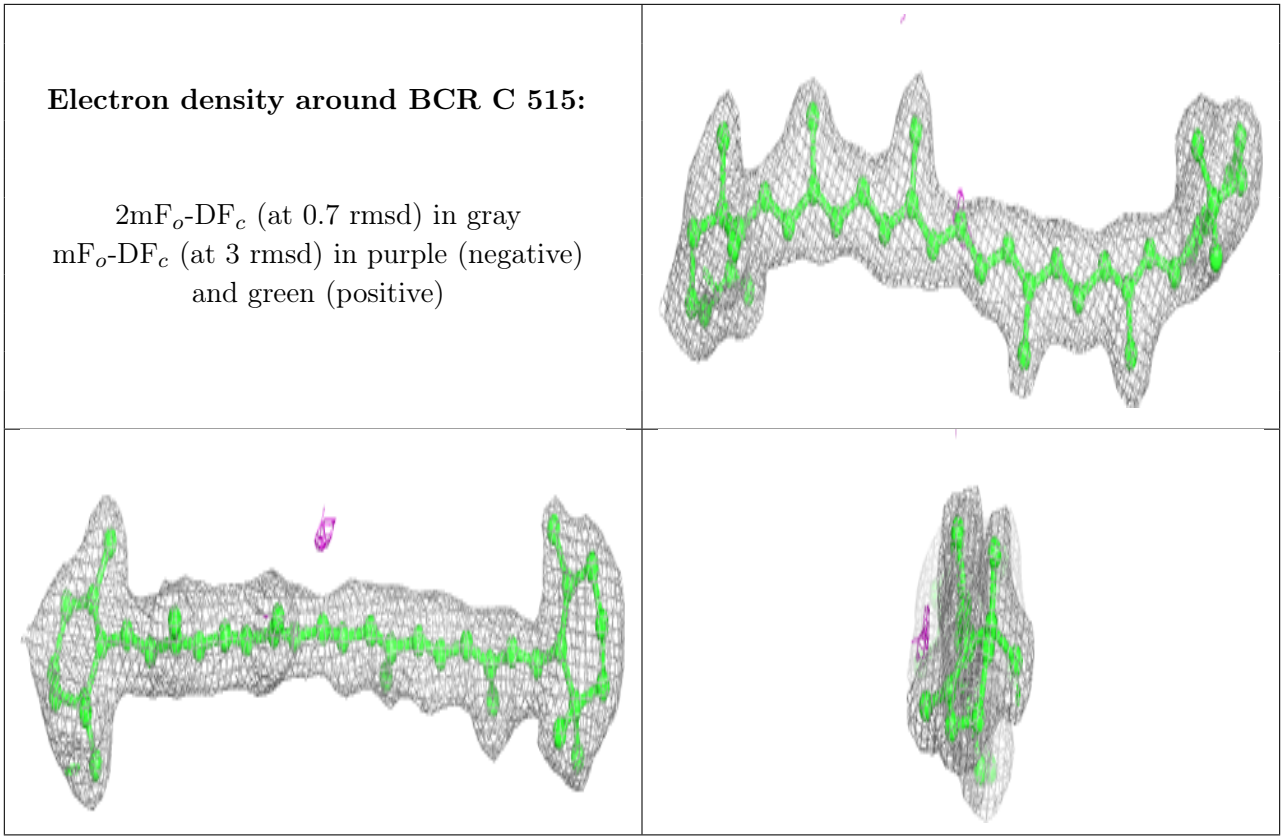






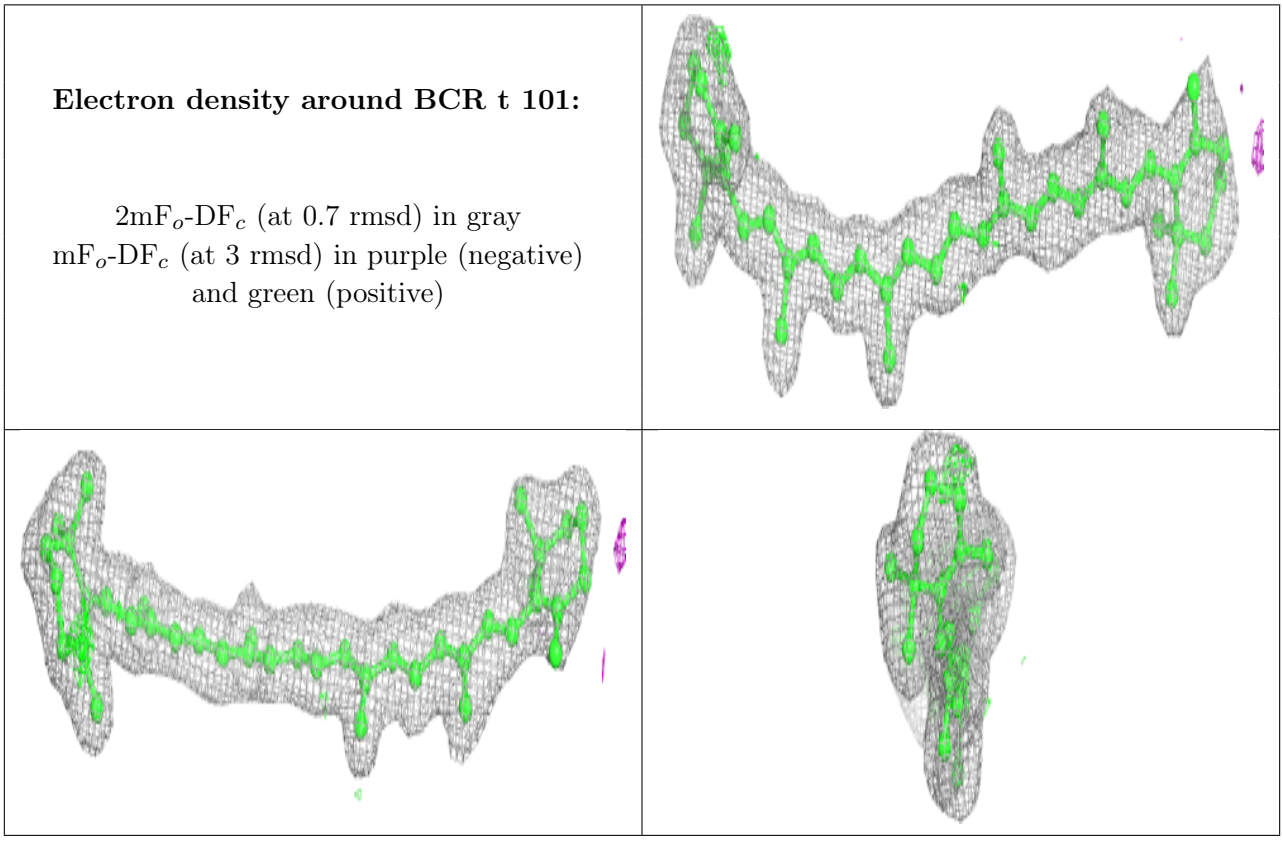
Electron density around BCR C 515:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



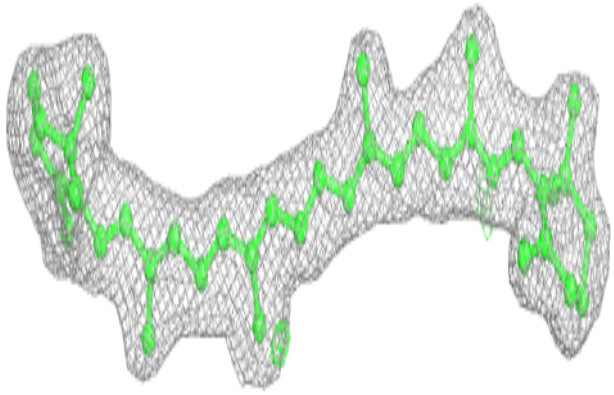
Electron density around BCR t 101:

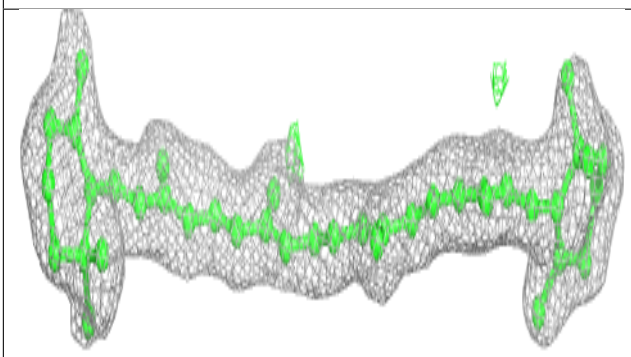
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

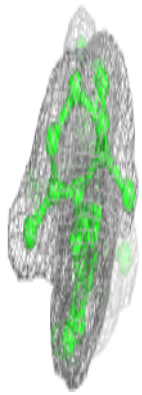


Electron density around BCR y 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

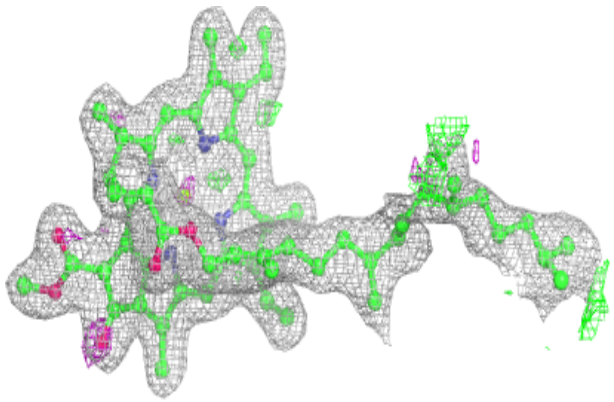


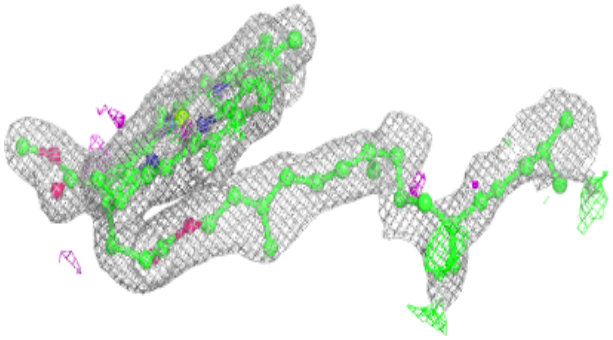


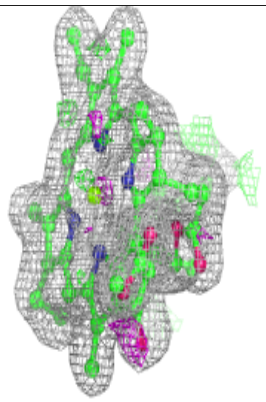


Electron density around CLA B 615:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

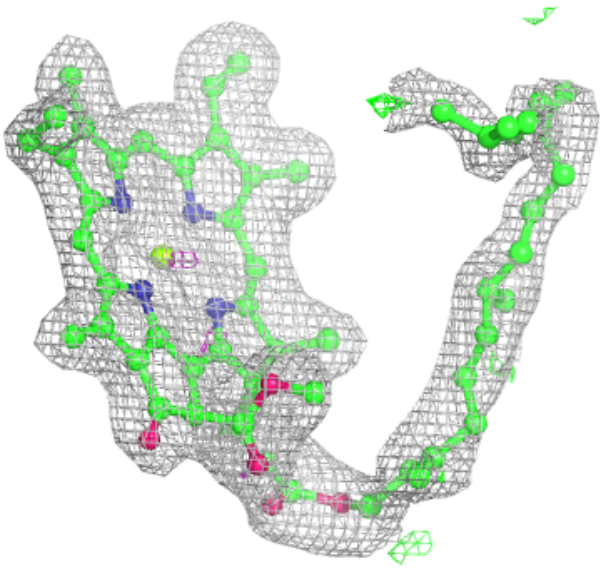


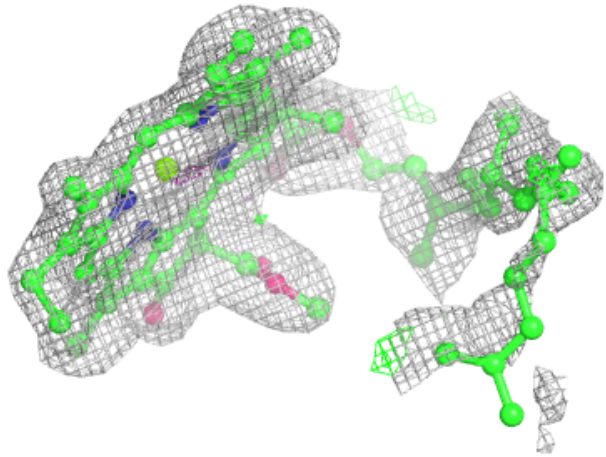


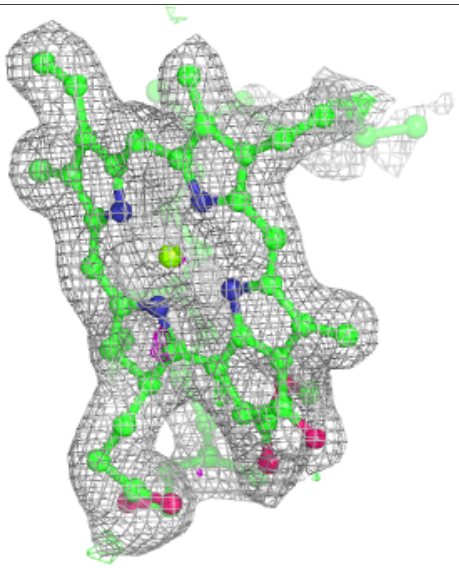


Electron density around CLA b 621:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

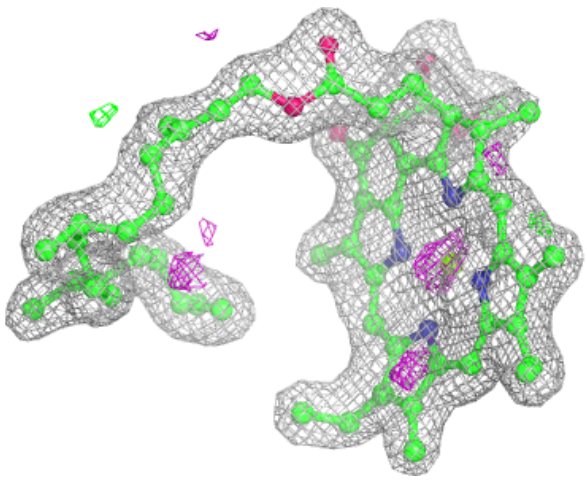


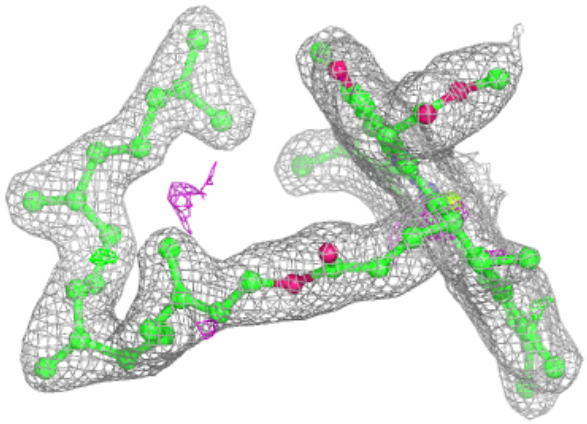


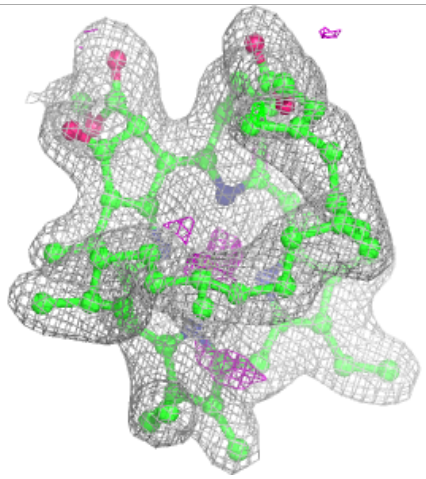


Electron density around CLA C 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

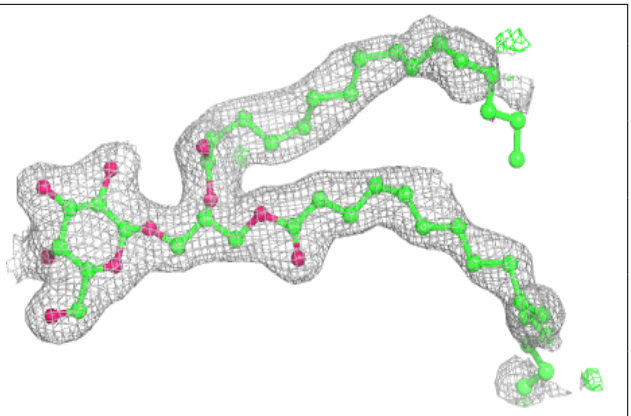


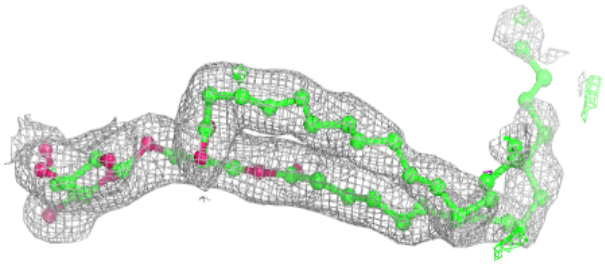


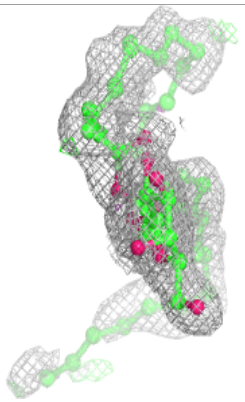


Electron density around LMG J 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

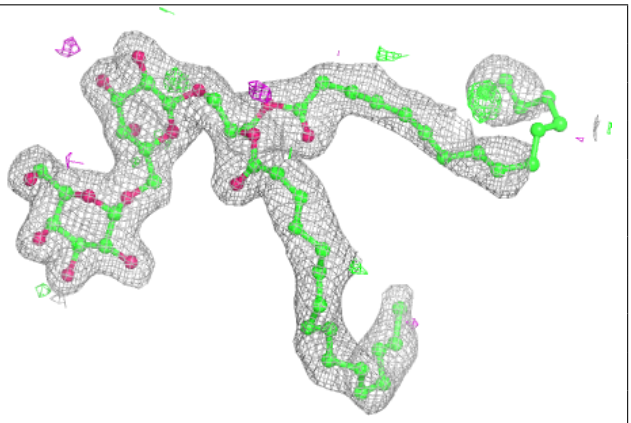


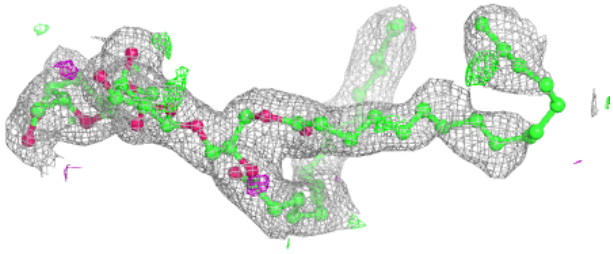


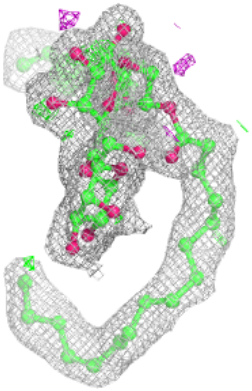


Electron density around DGD C 518:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

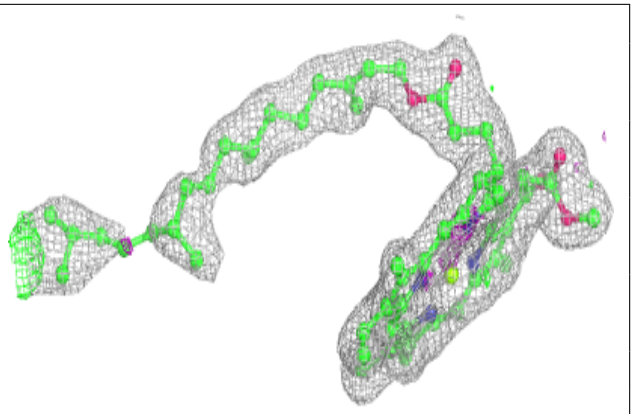


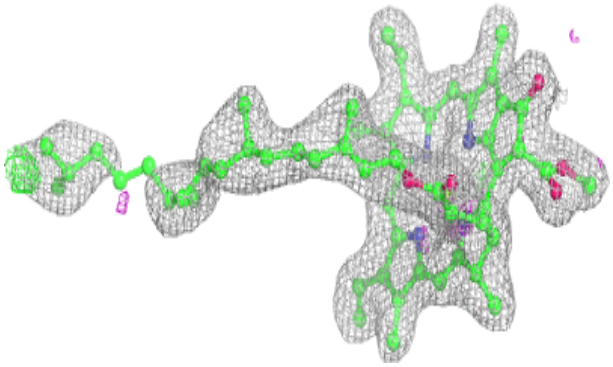


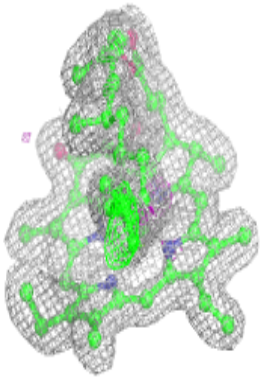


Electron density around CLA C 505:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

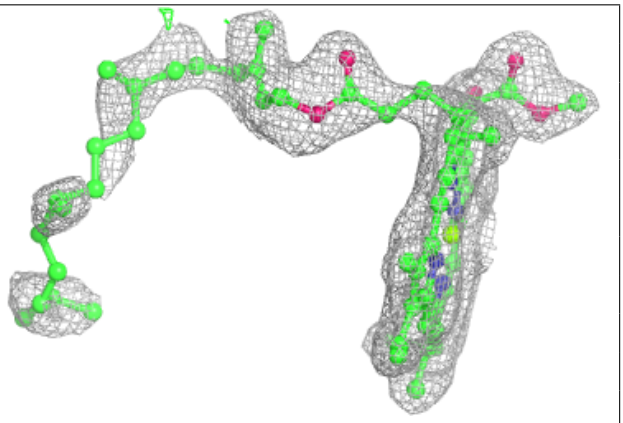


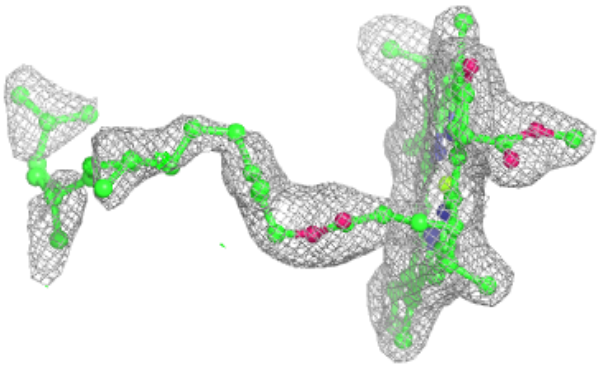


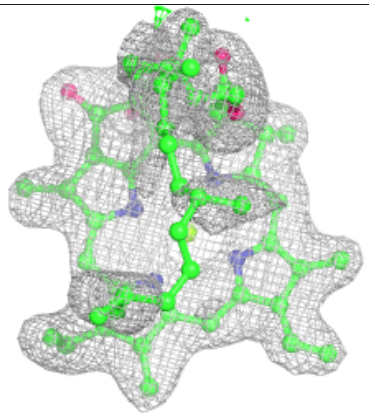


Electron density around CLA C 507:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

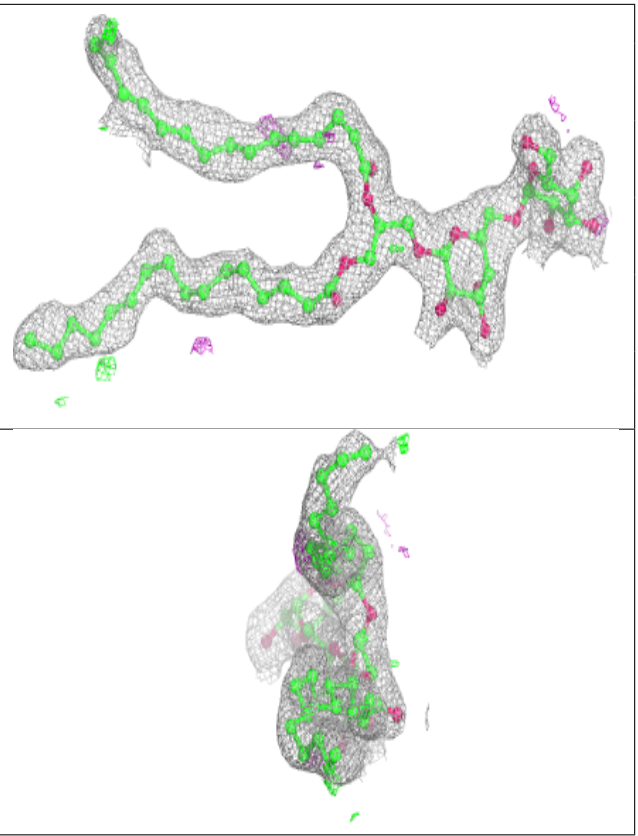


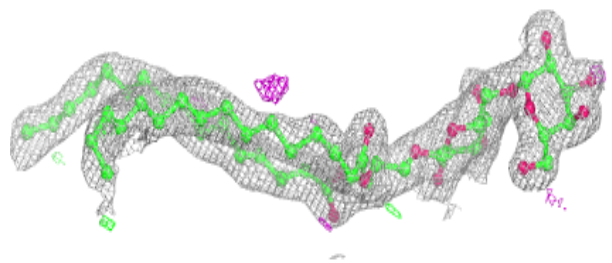




Electron density around DGD c 519:

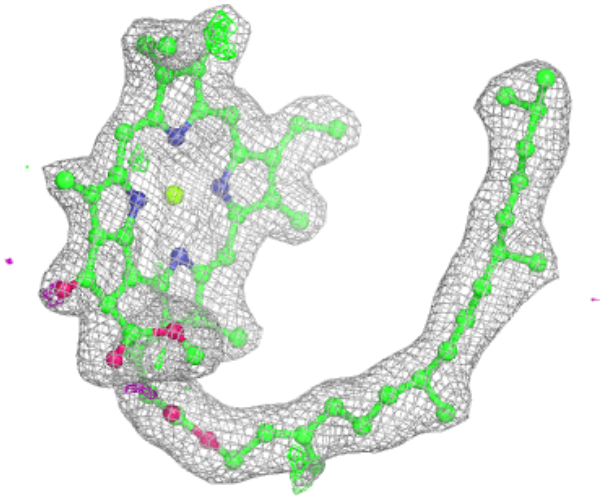
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

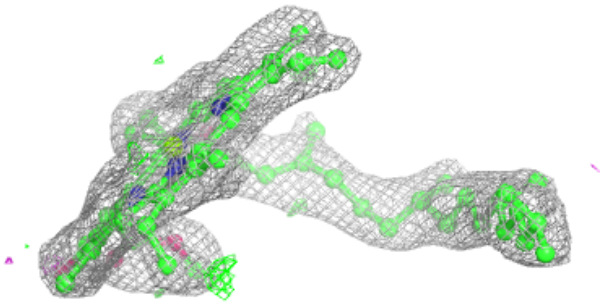


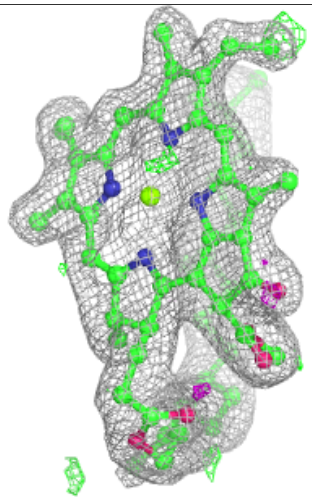


Electron density around CLA c 509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

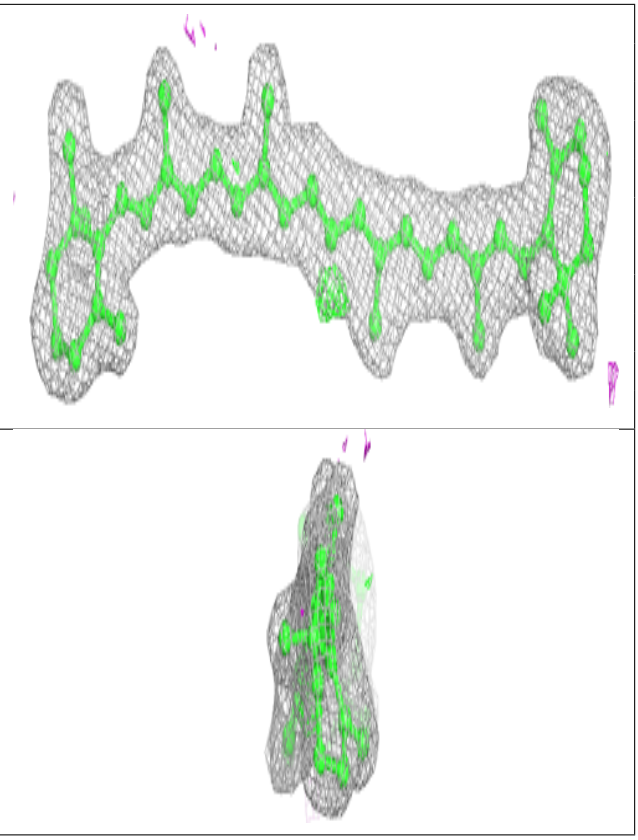






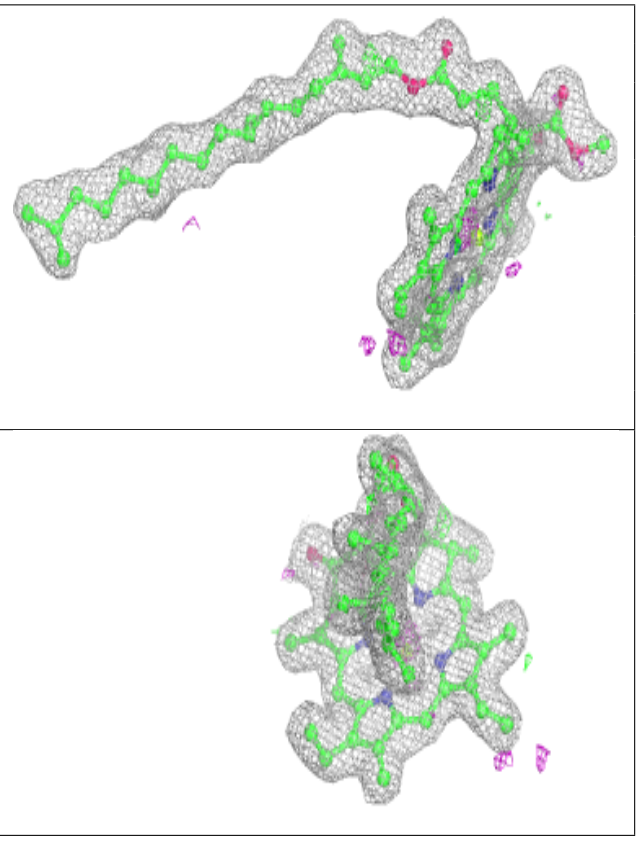
Electron density around BCR b 624:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



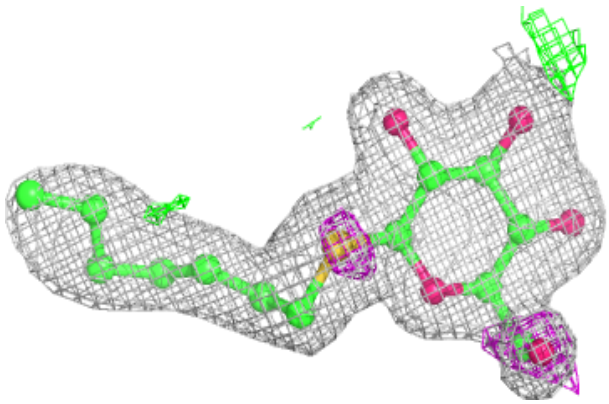
Electron density around CLA B 608:

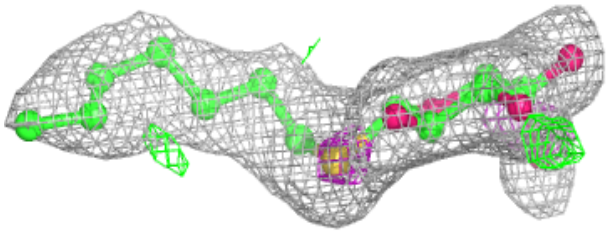
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

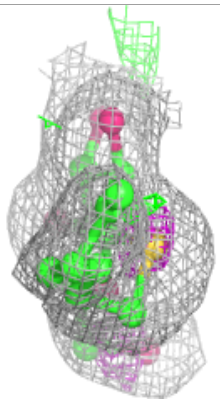


Electron density around HTG B 622:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

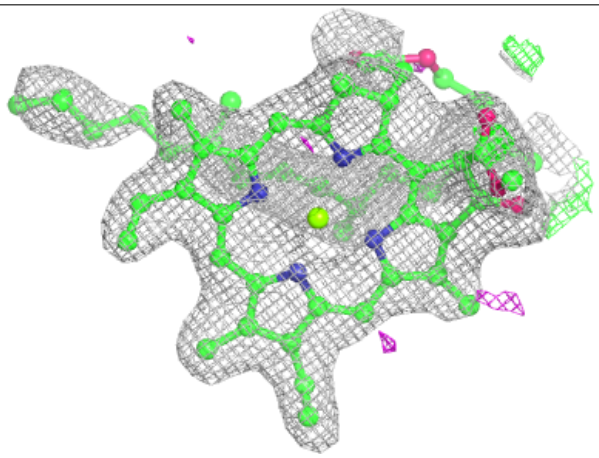


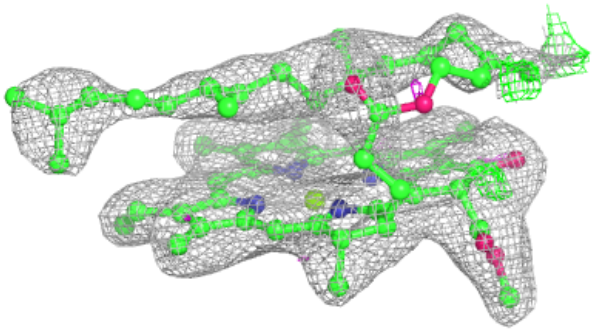


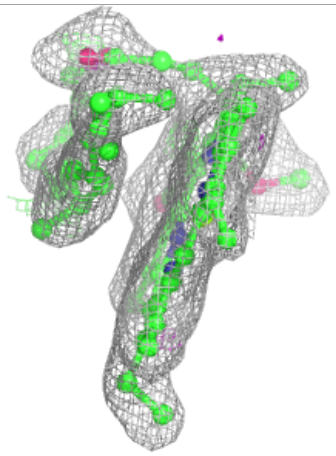


Electron density around CLA B 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

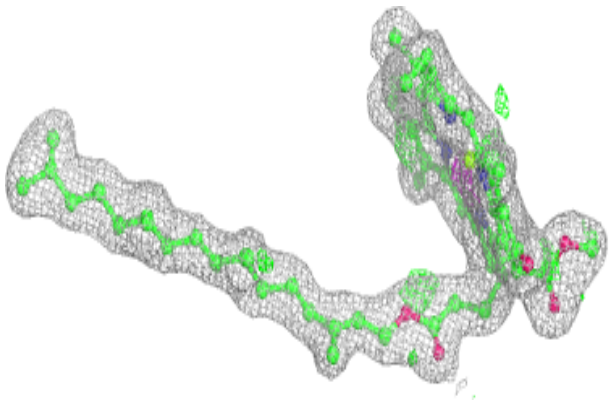


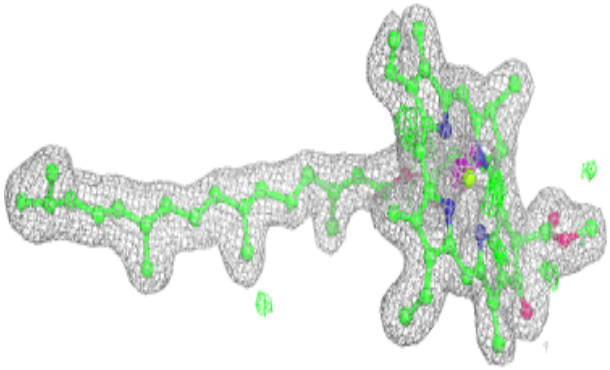


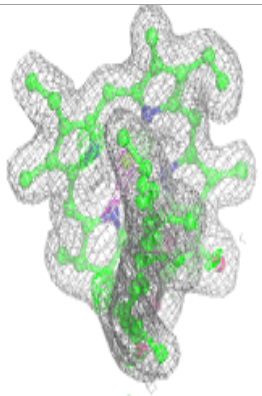


Electron density around CLA b 612:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

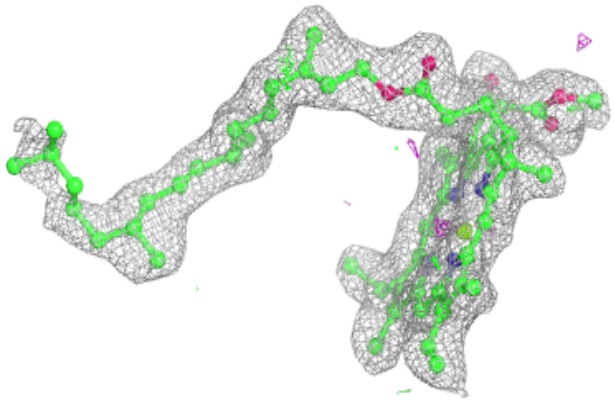


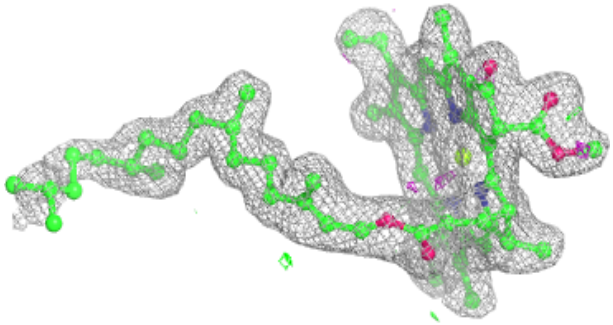


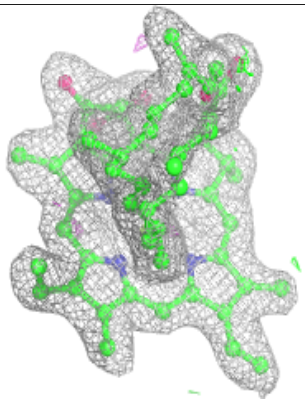


Electron density around CLA c 510:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

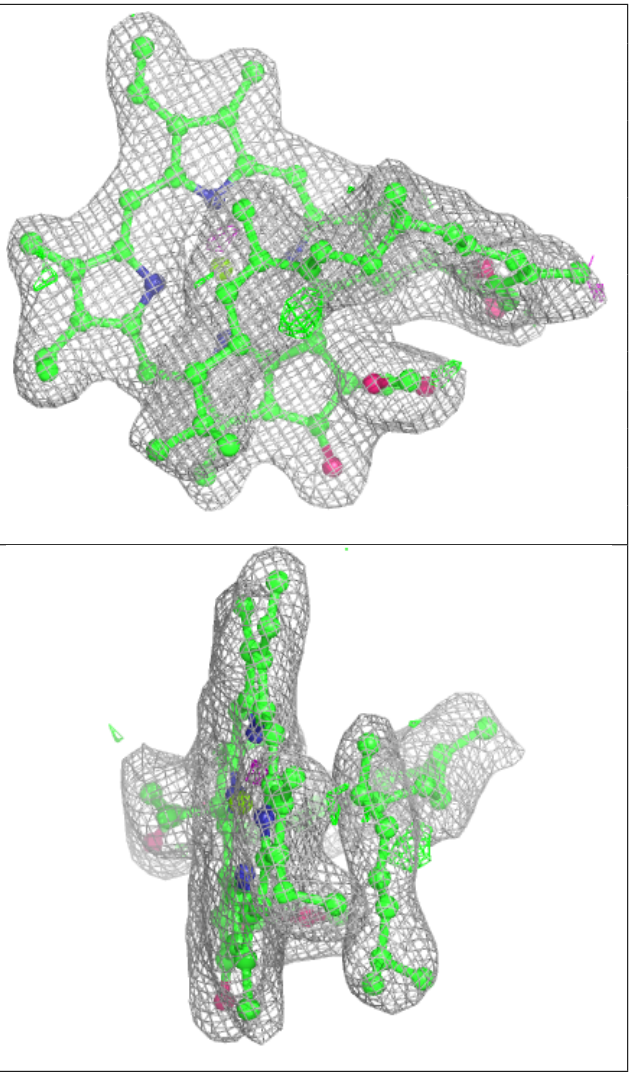






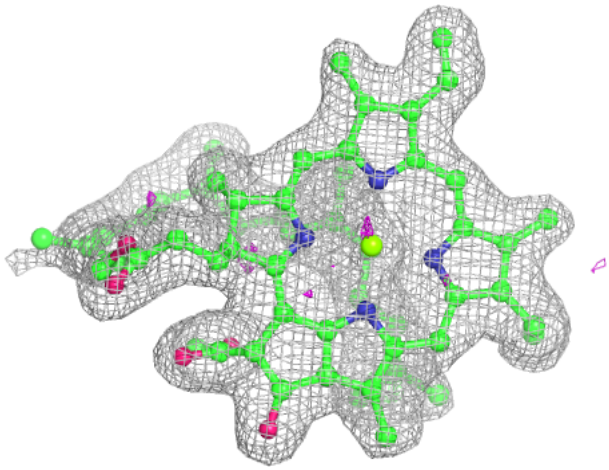
Electron density around CLA c 512:

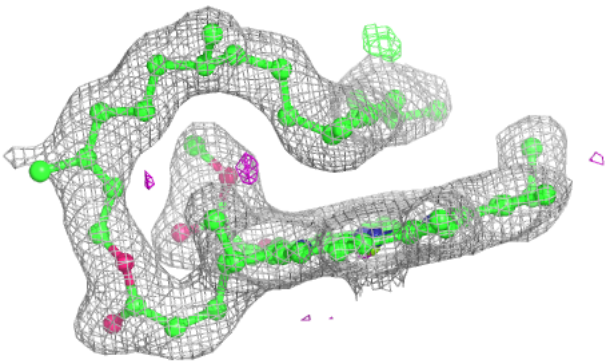
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

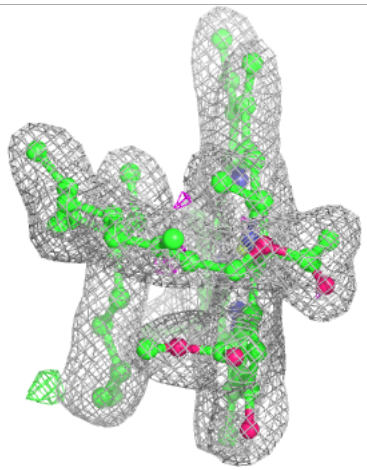


Electron density around CLA C 511:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

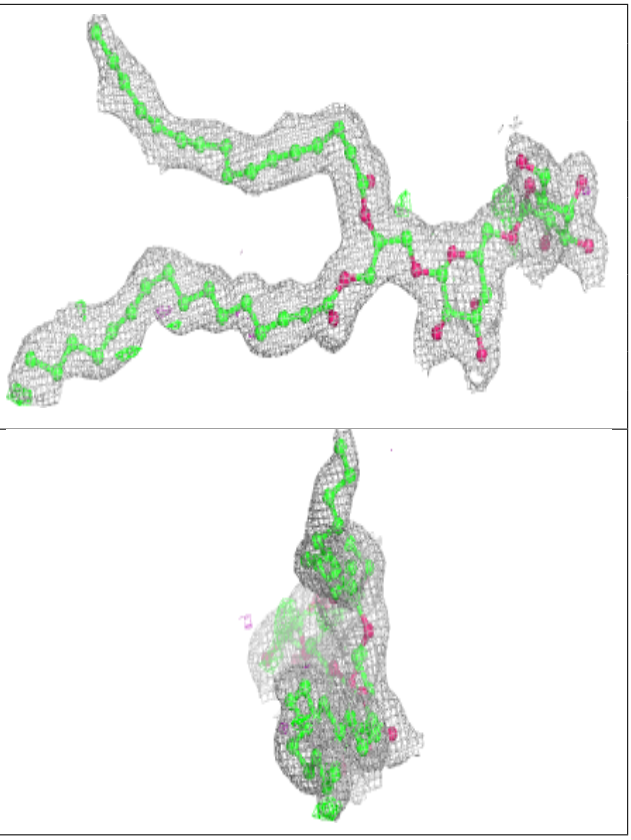






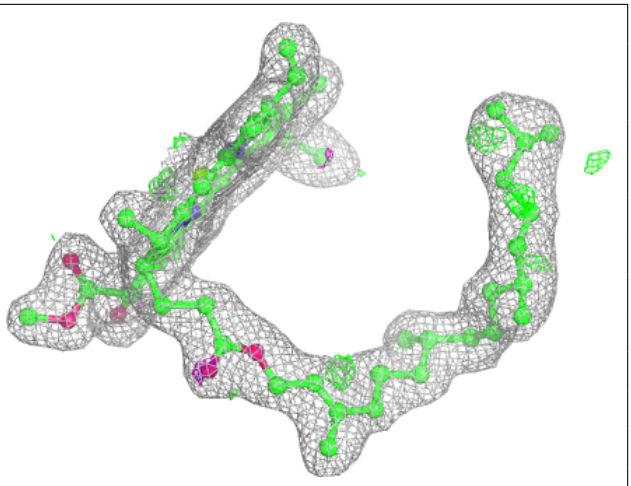
Electron density around DGD C 519:

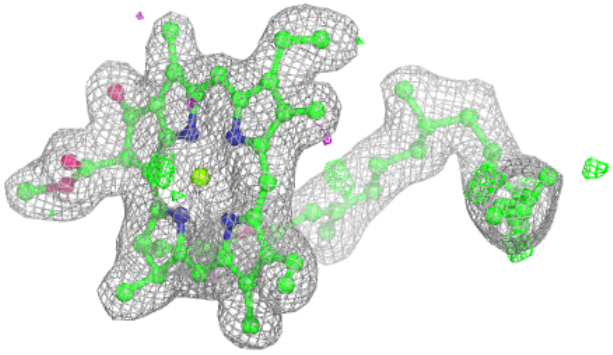
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

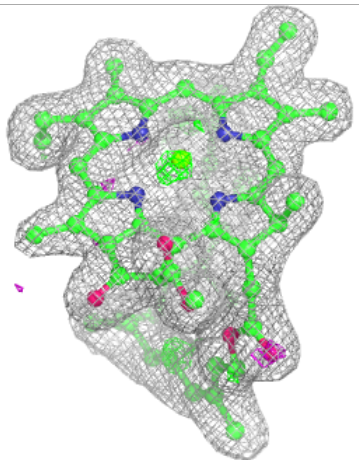


Electron density around CLA b 616:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

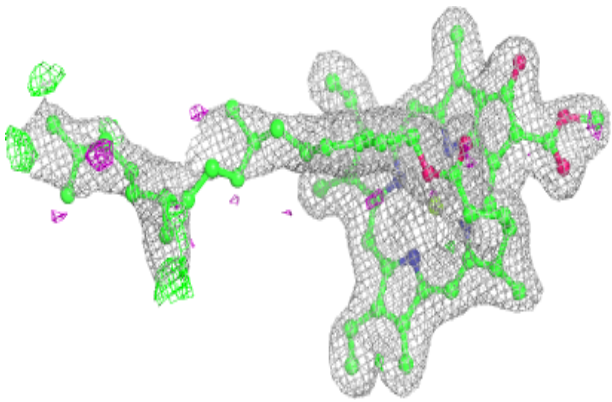


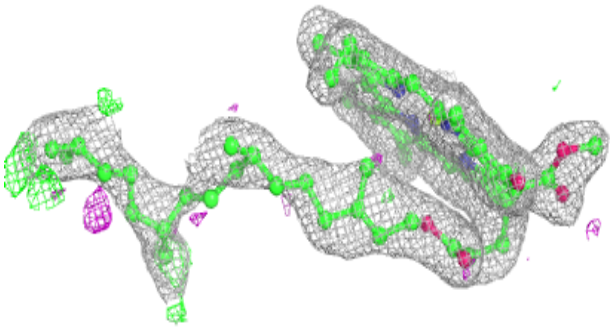


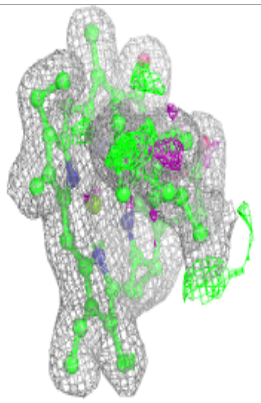


Electron density around CLA b 619:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

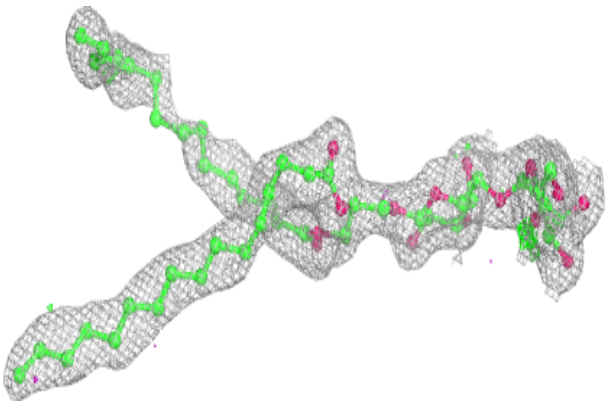


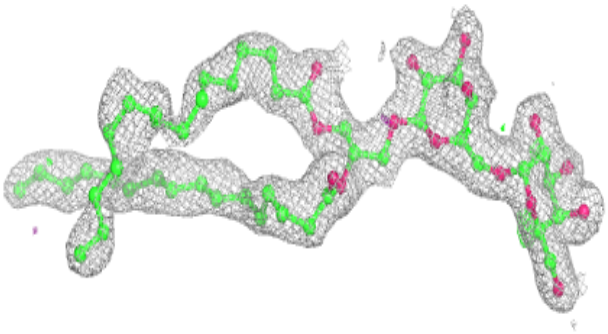


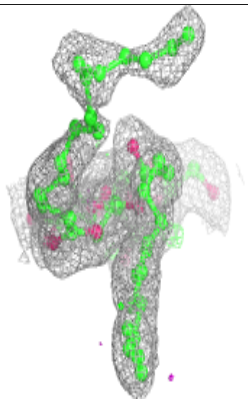


Electron density around DGD c 517:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

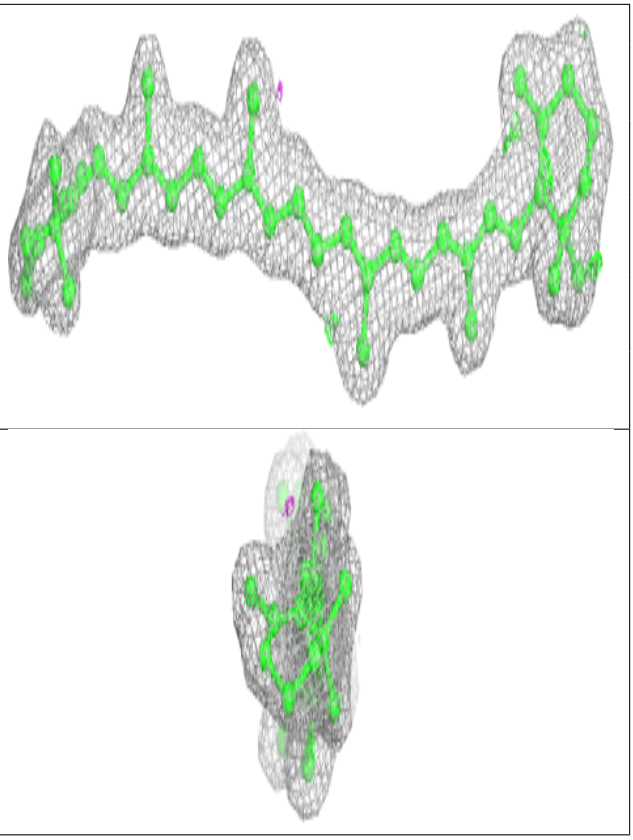






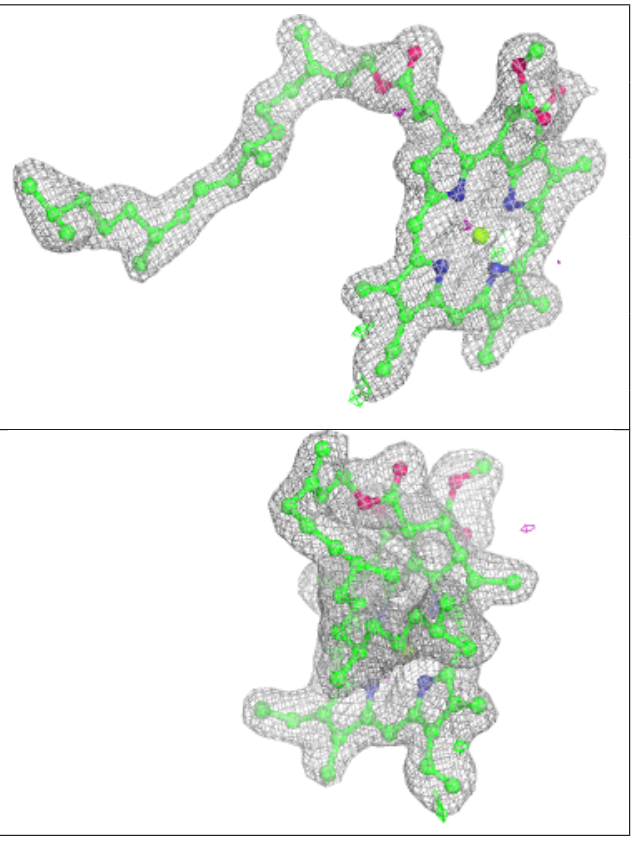
Electron density around BCR B 618:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



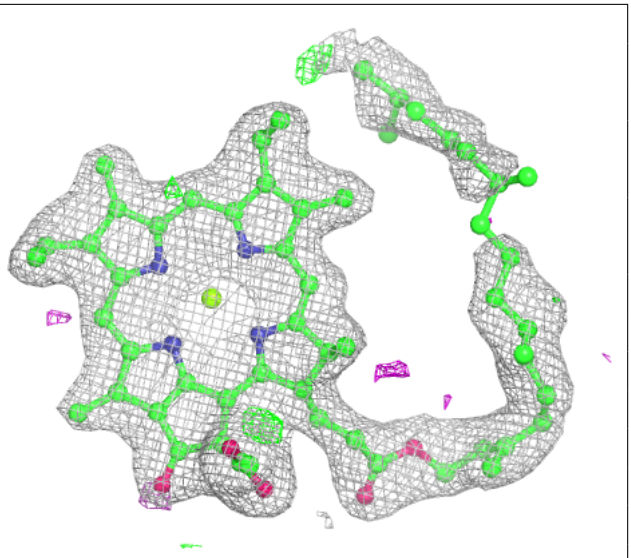
Electron density around CLA C 512:

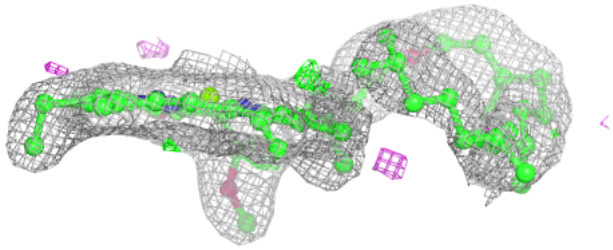
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

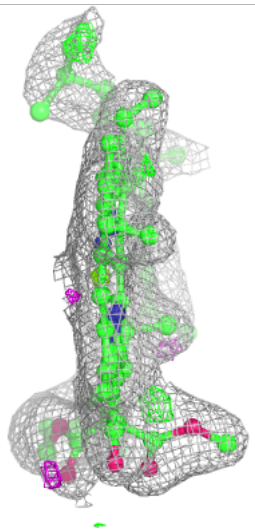


Electron density around CLA C 513:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

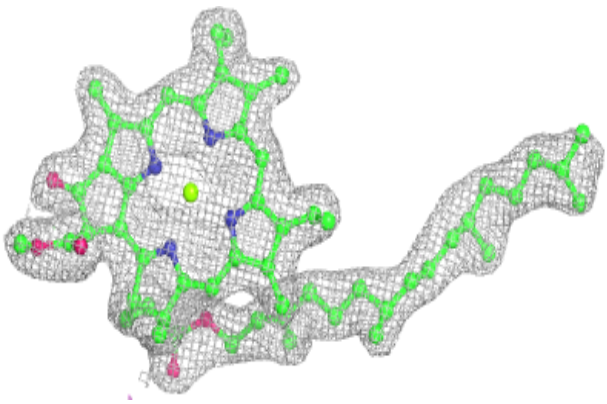


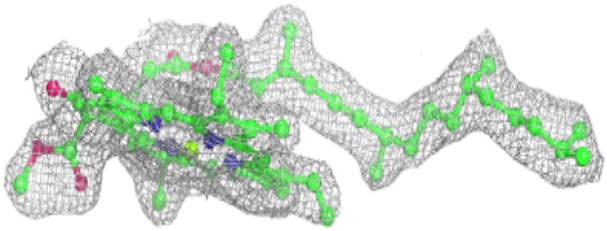


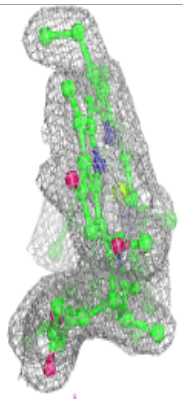


Electron density around CLA c 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

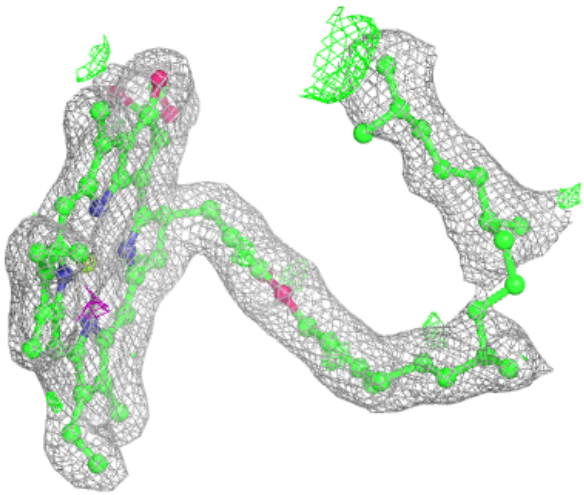


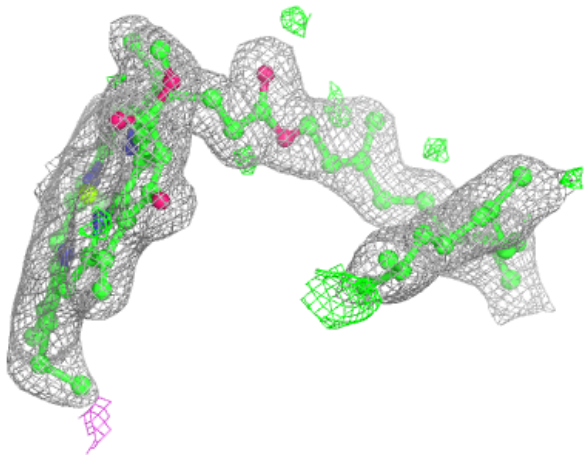


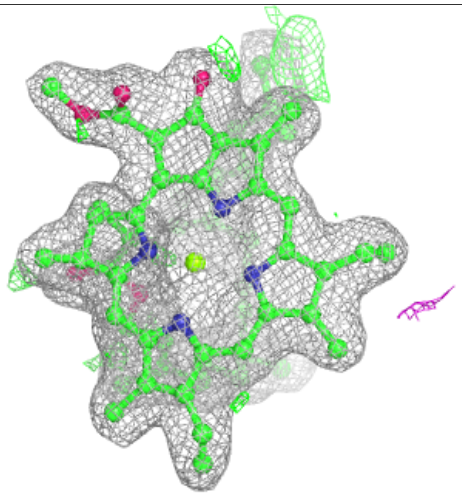


Electron density around CLA B 607:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

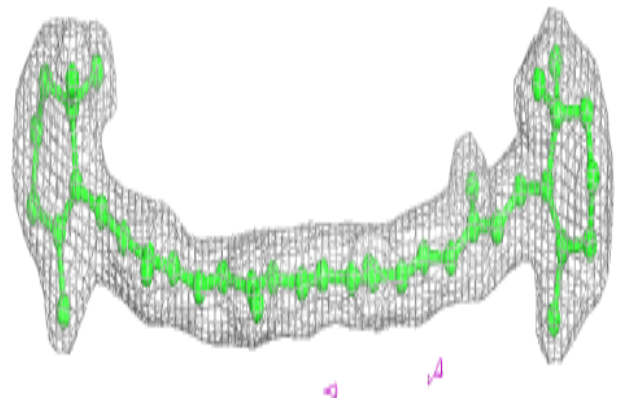


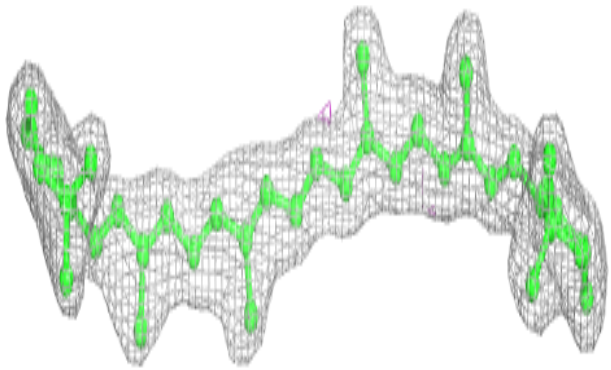


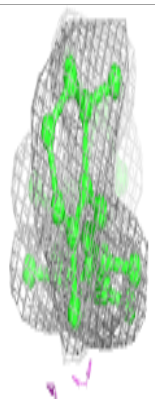


Electron density around BCR K 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

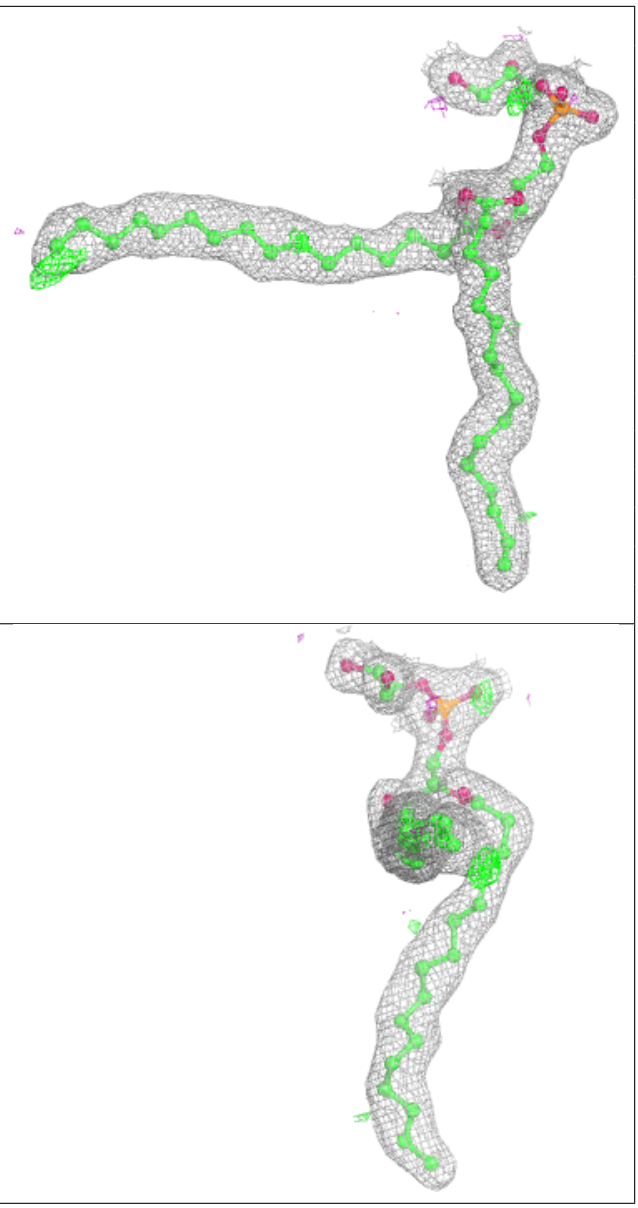






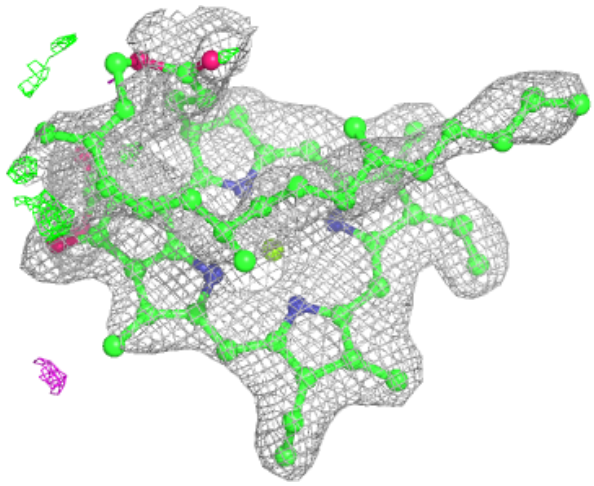
Electron density around LHG L 101:

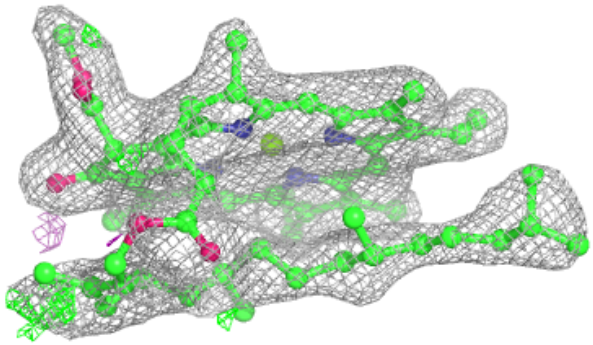
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

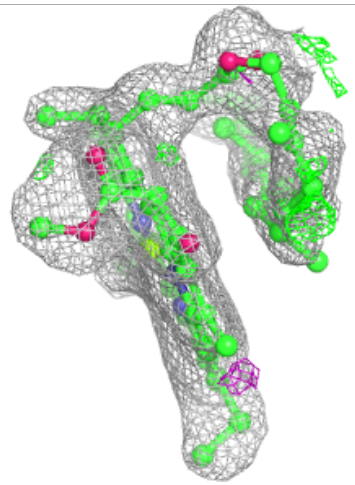


Electron density around CLA b 606:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

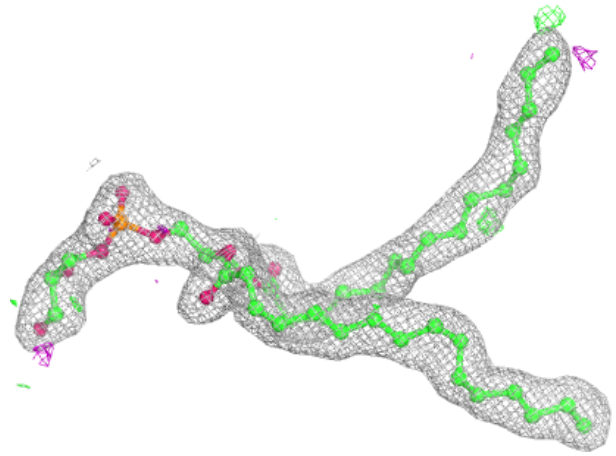


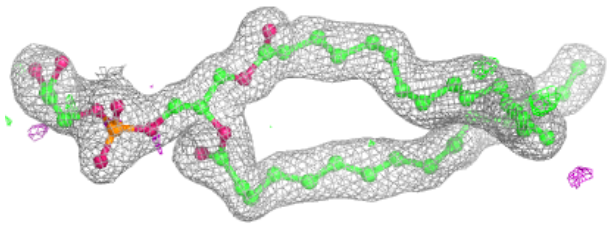


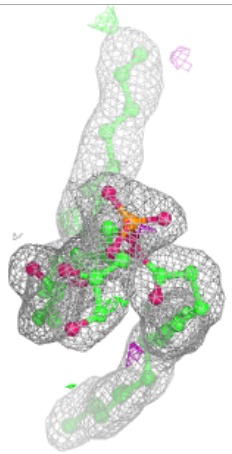


Electron density around LHG d 409:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

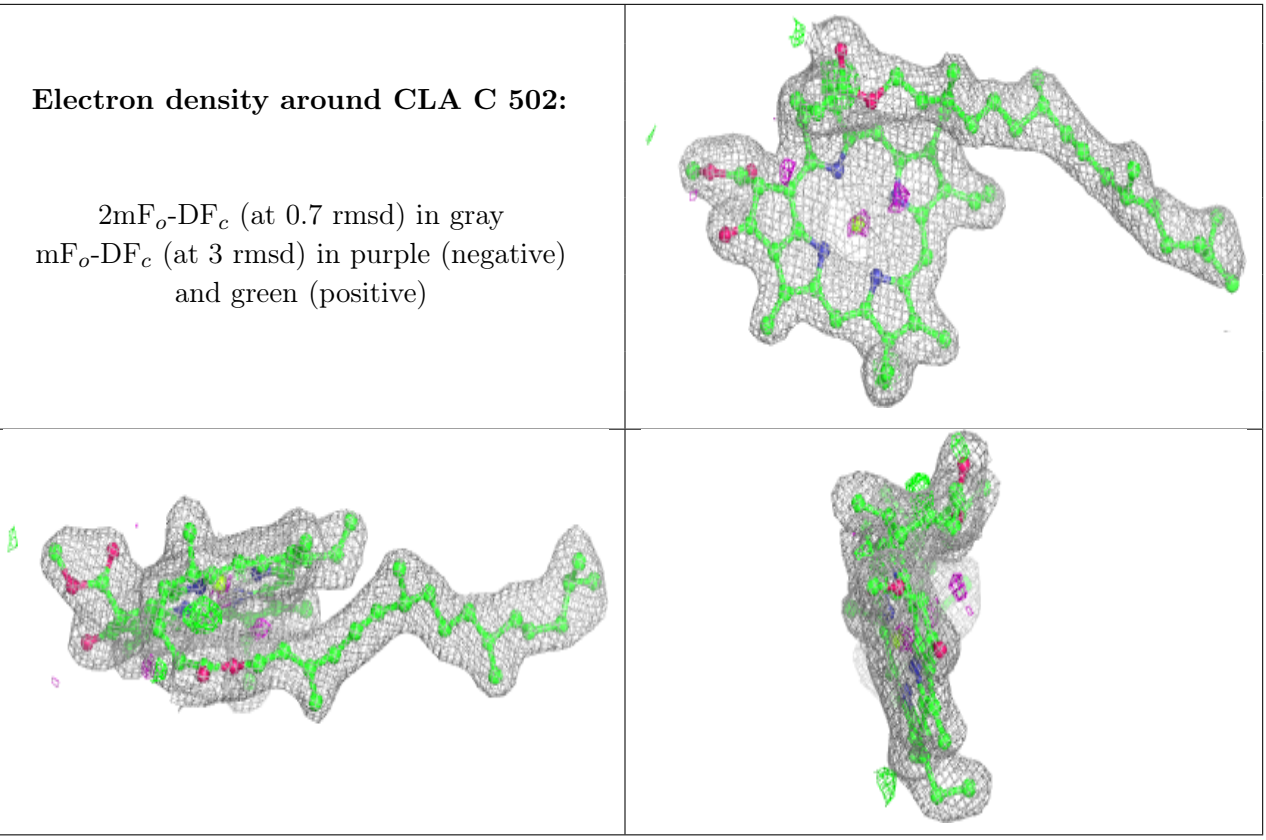






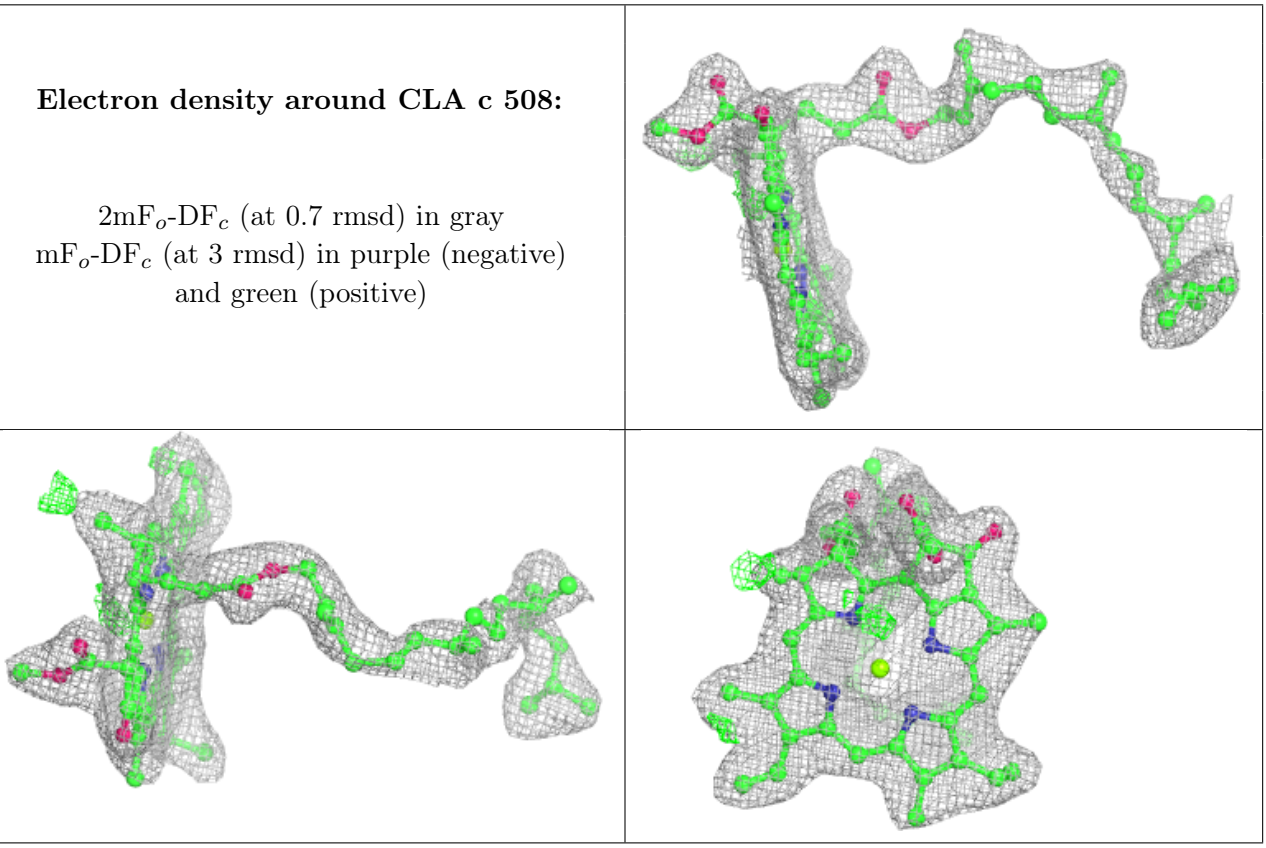
Electron density around CLA C 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



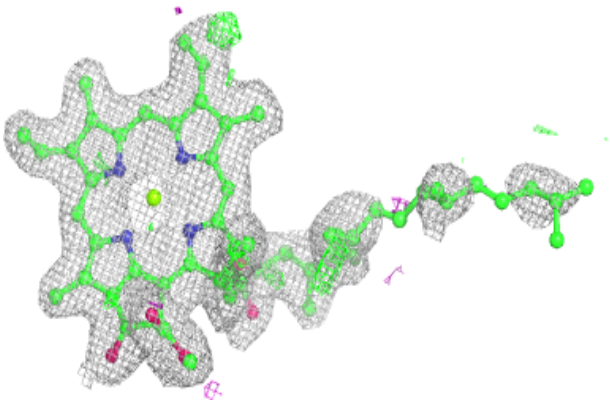
Electron density around CLA c 508:

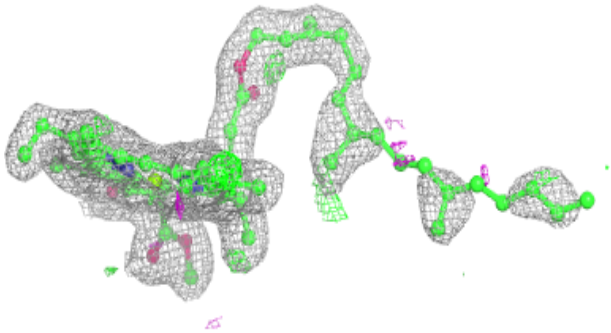
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

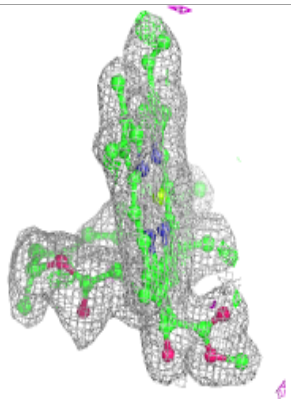


Electron density around CLA a 407:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

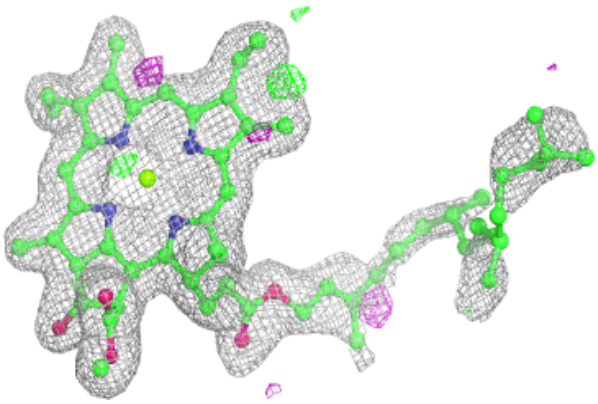


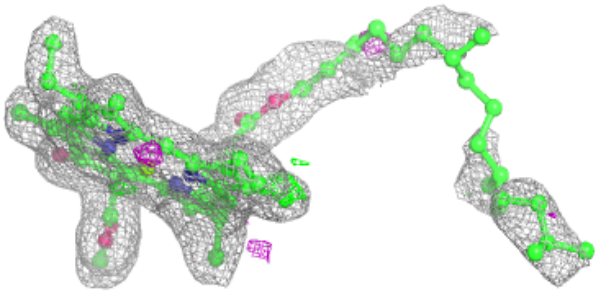


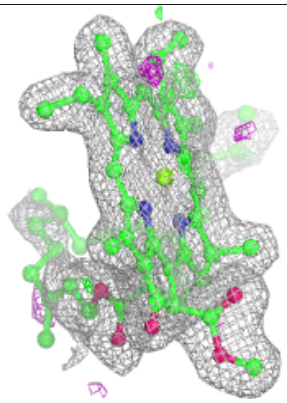


Electron density around CLA a 409:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

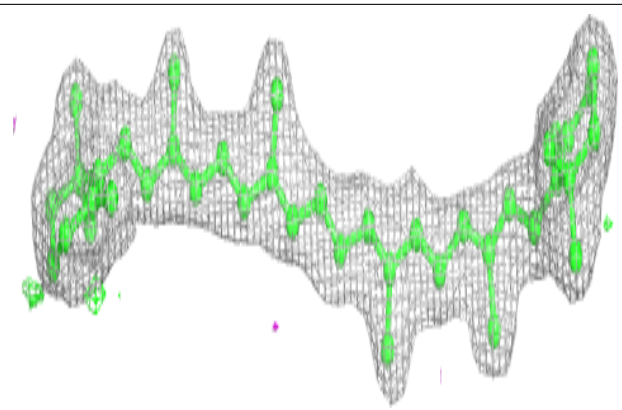


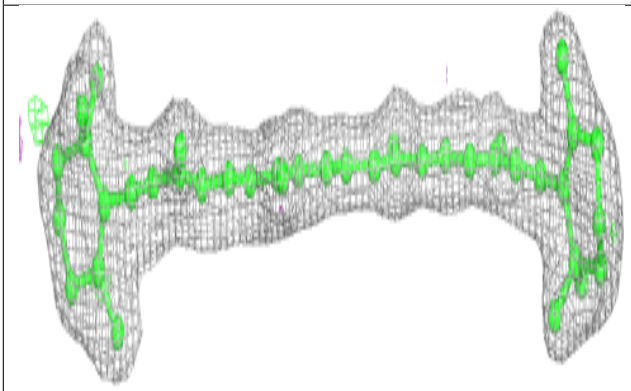


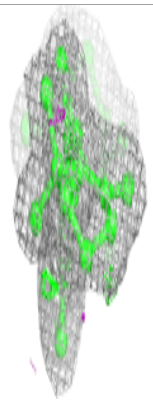


Electron density around BCR C 516:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

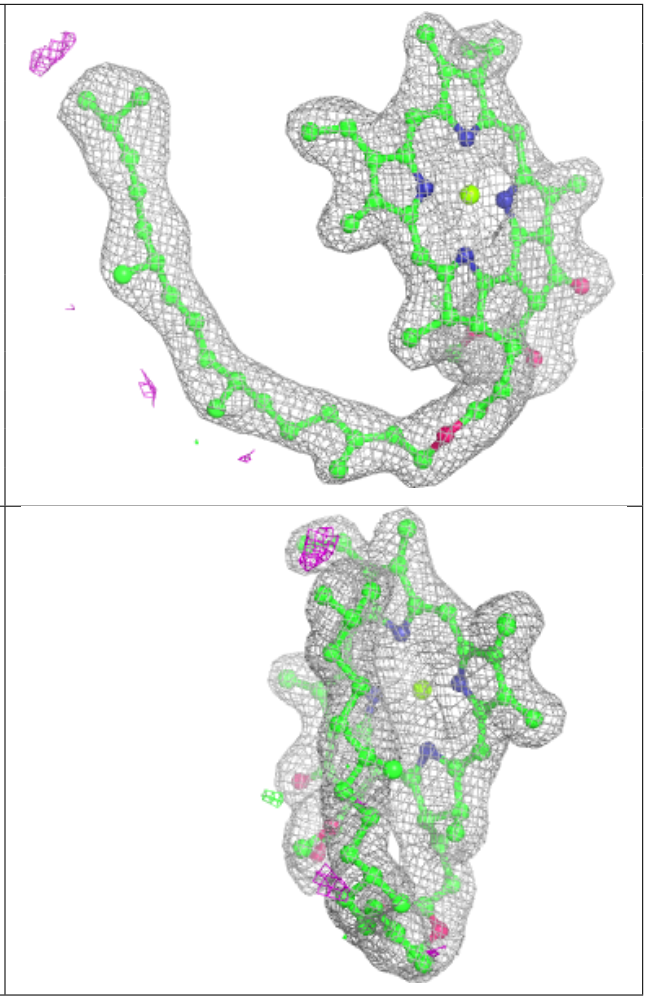






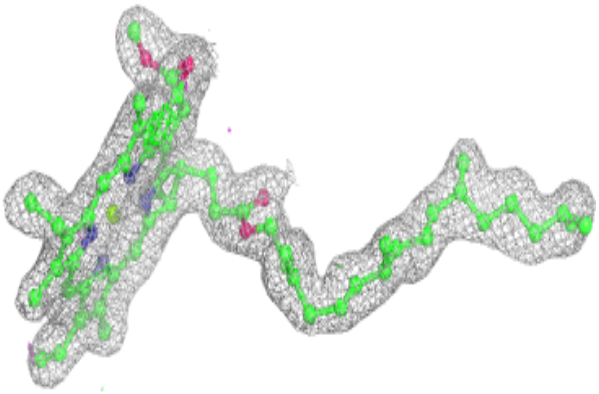
Electron density around CLA C 508:

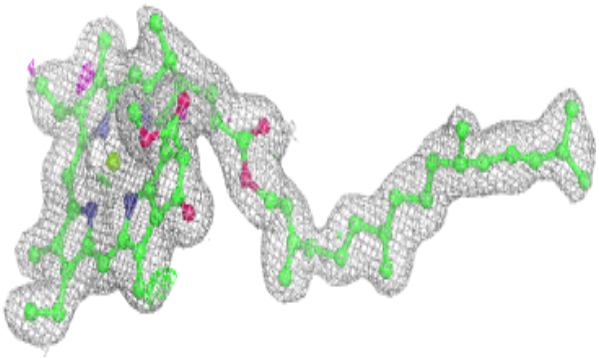
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

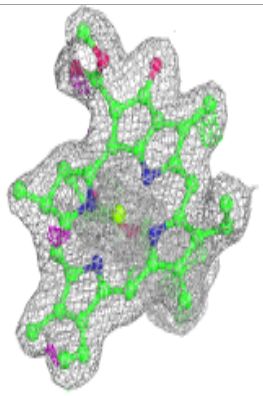


Electron density around CLA c 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

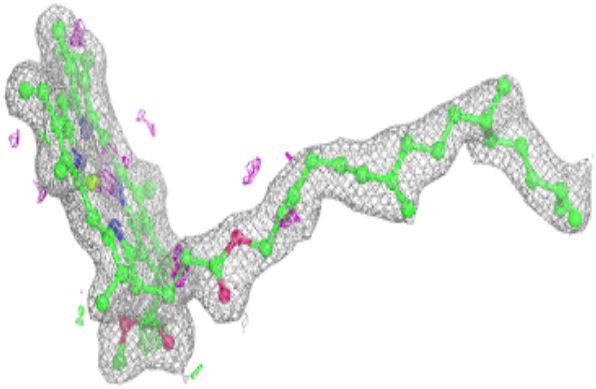


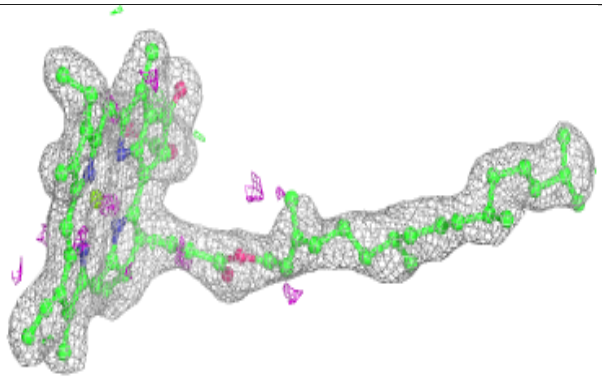


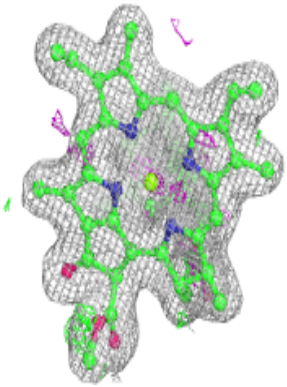


Electron density around CLA B 605:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

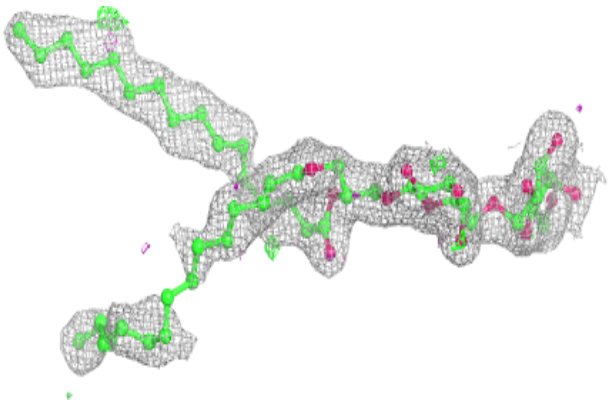


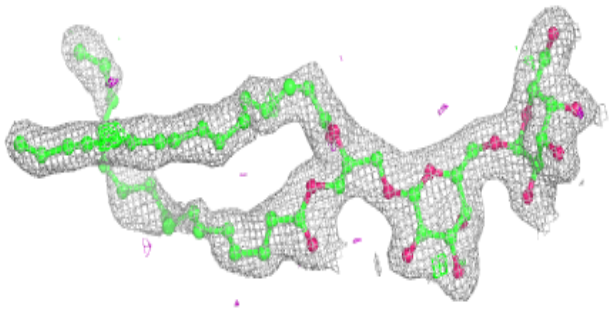


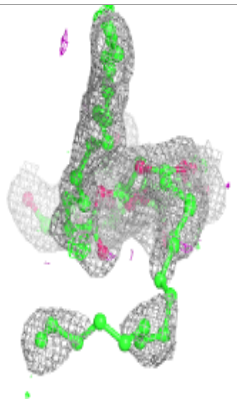


Electron density around DGD C 517:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

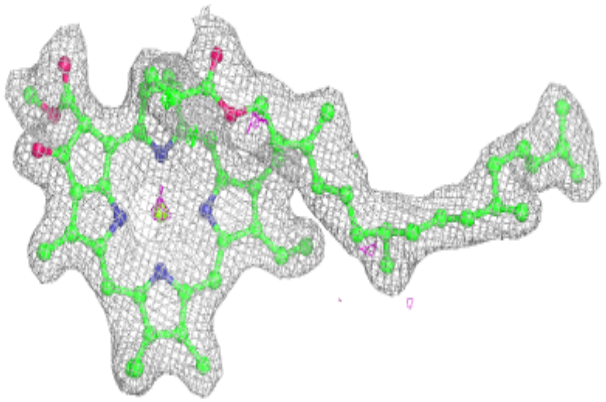


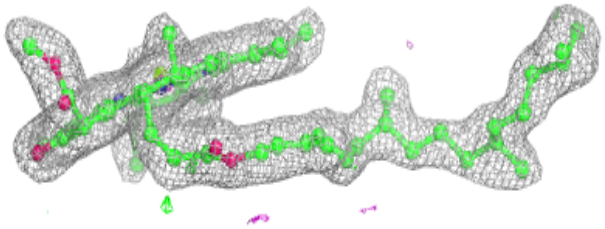


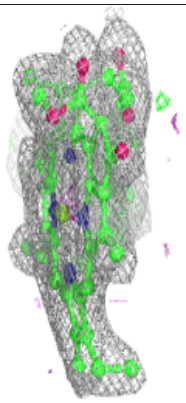


Electron density around CLA b 608:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

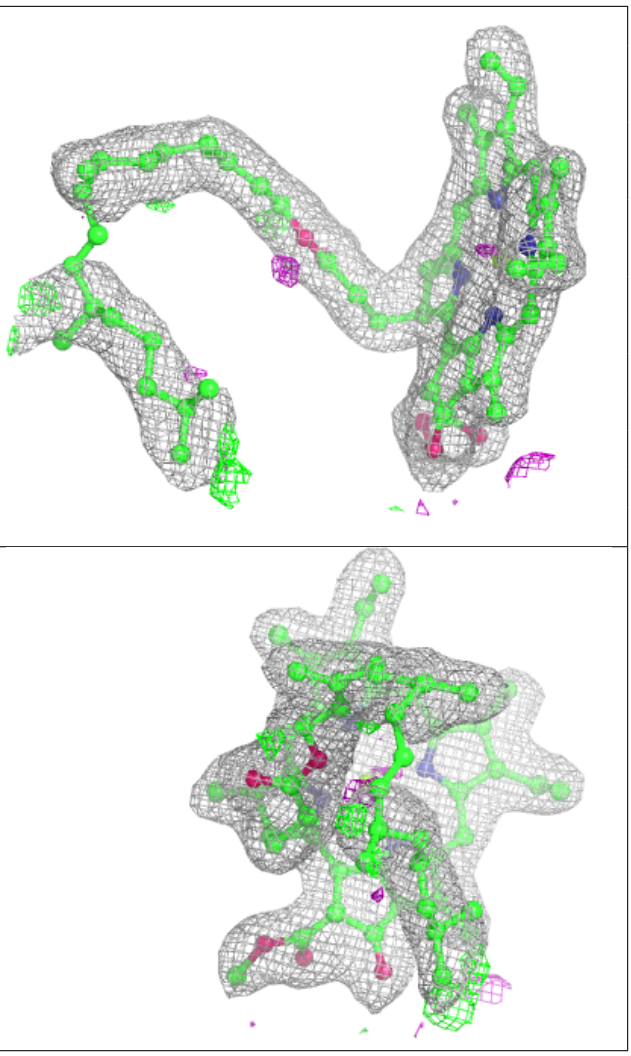






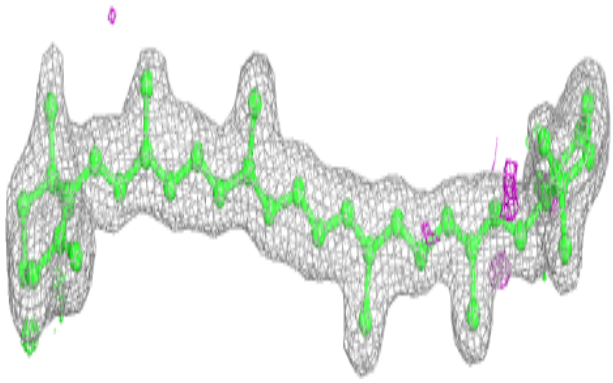
Electron density around CLA b 611:

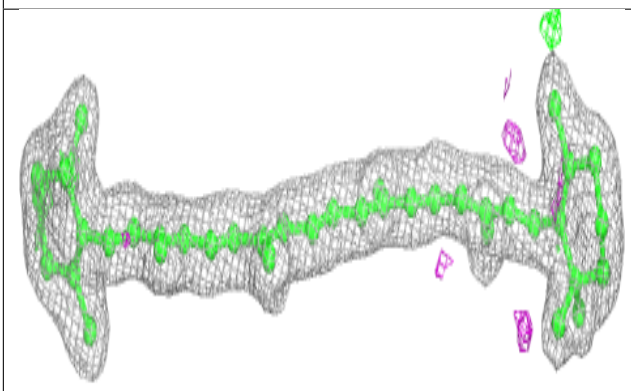
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

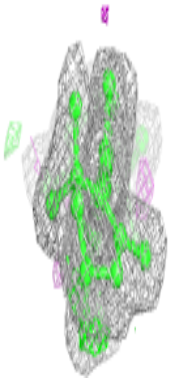


Electron density around BCR a 410:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

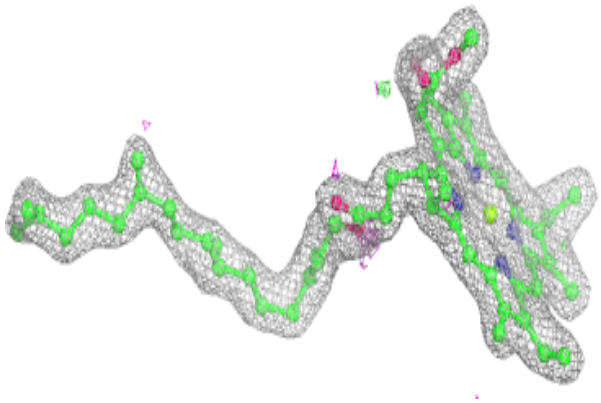


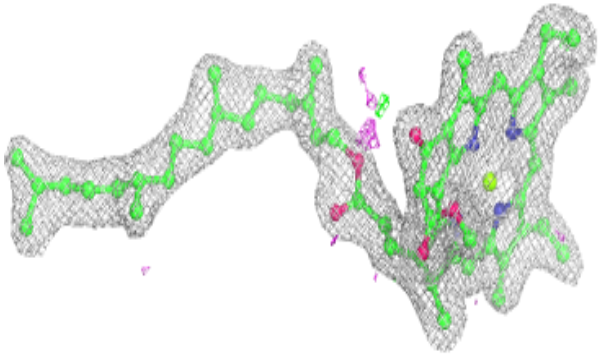


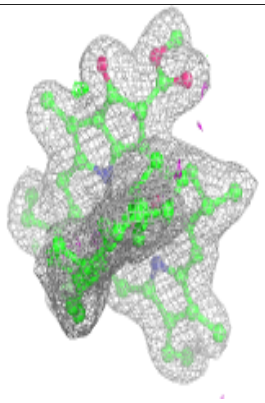


Electron density around CLA C 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

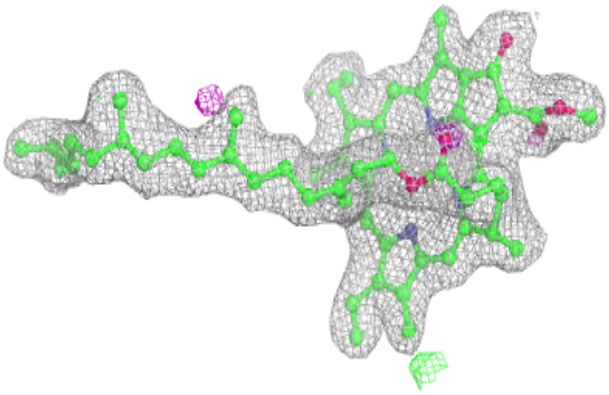


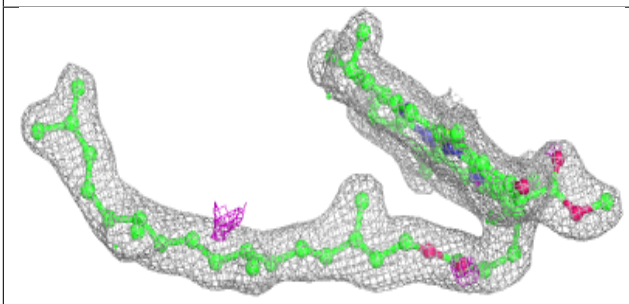


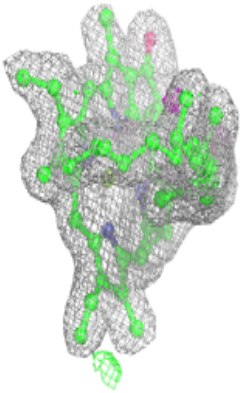


Electron density around CLA b 613:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

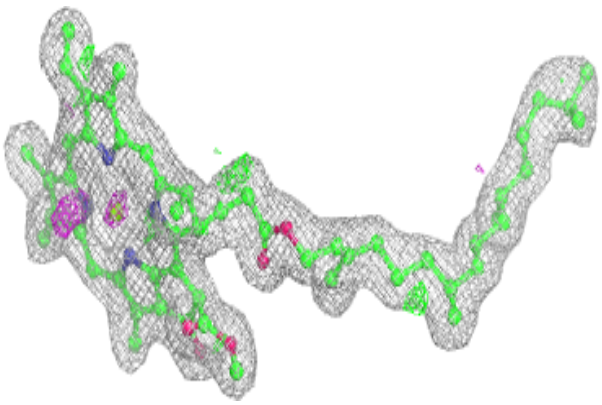


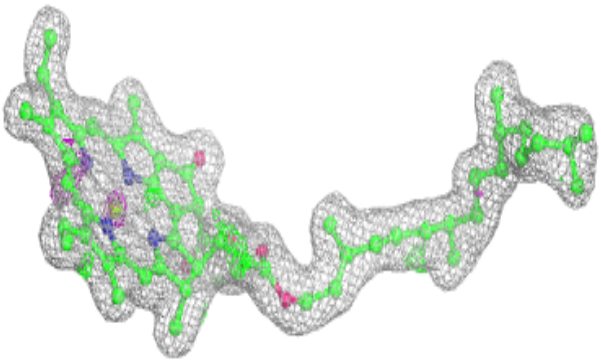




Electron density around CLA A 405:

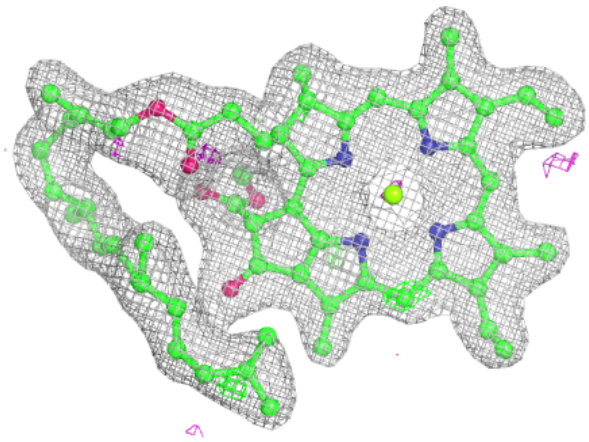
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

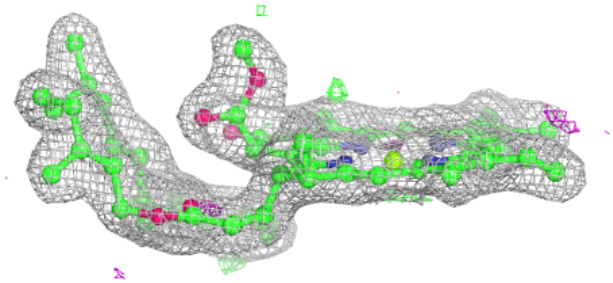


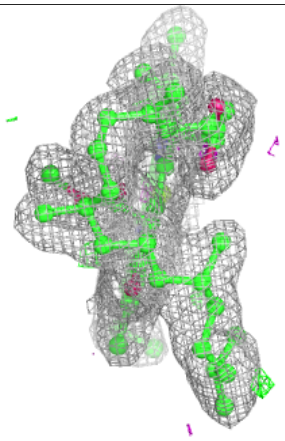


Electron density around CLA b 615:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

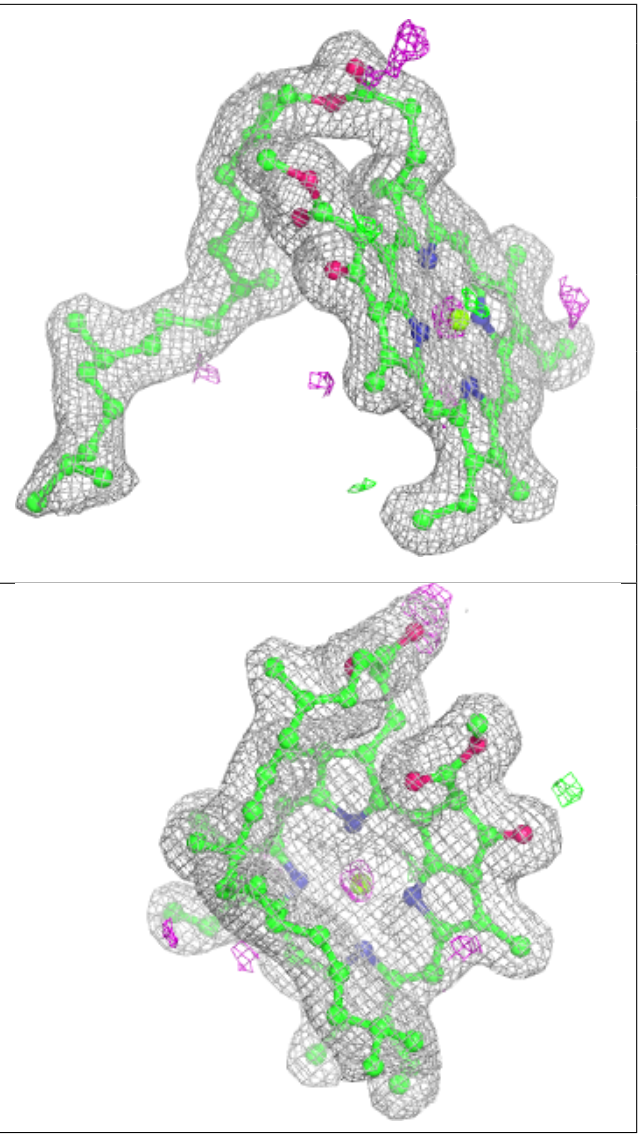






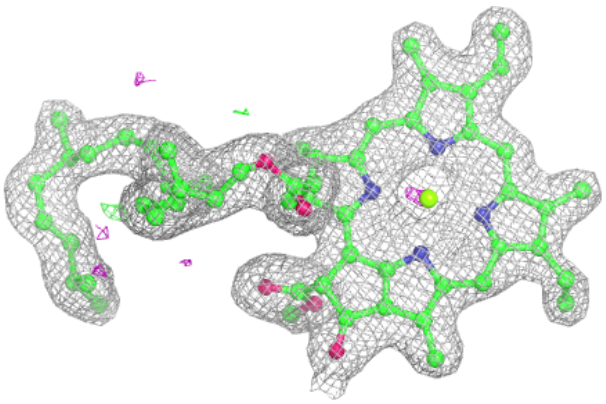
Electron density around CLA B 614:

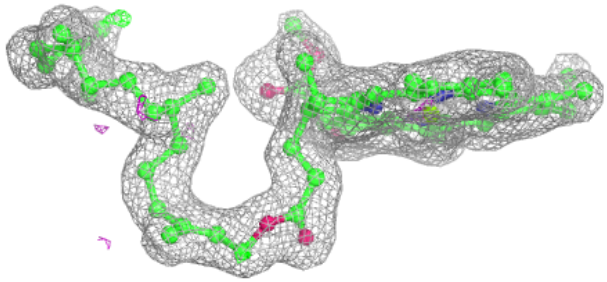
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

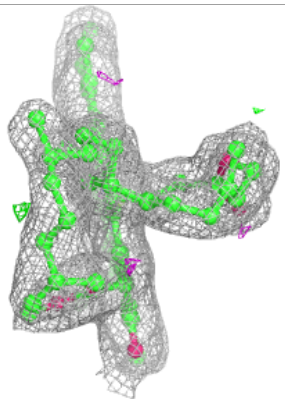


Electron density around CLA b 617:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

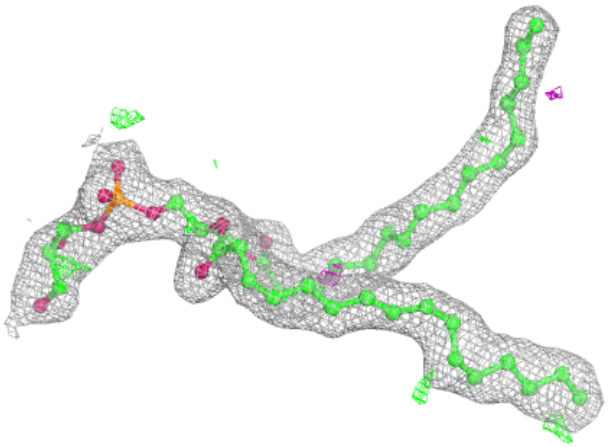


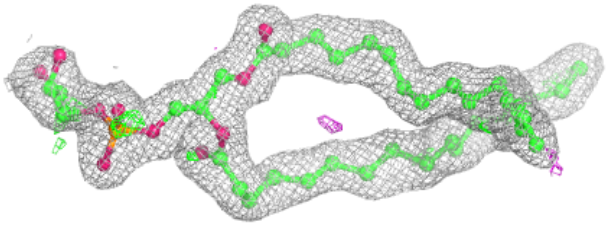


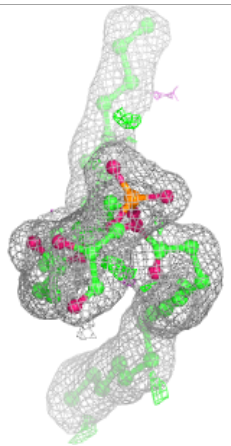


Electron density around LHG D 409:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

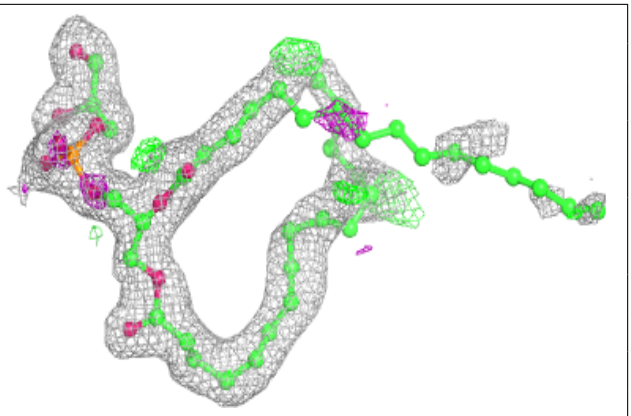


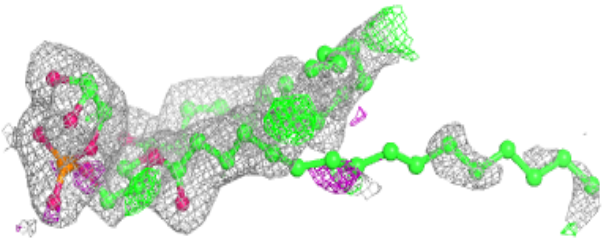


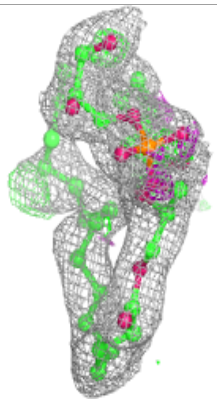


Electron density around LHG D 410:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

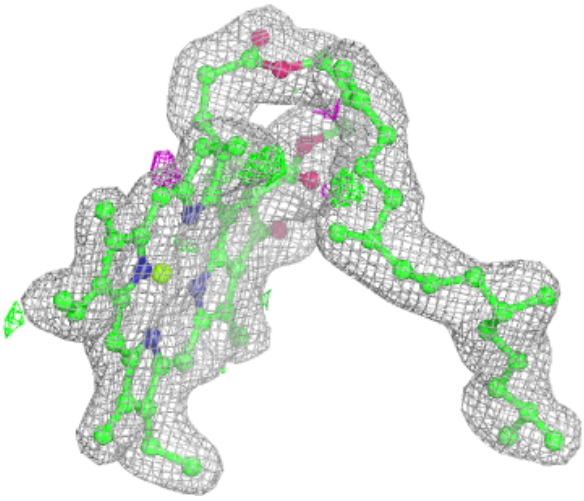


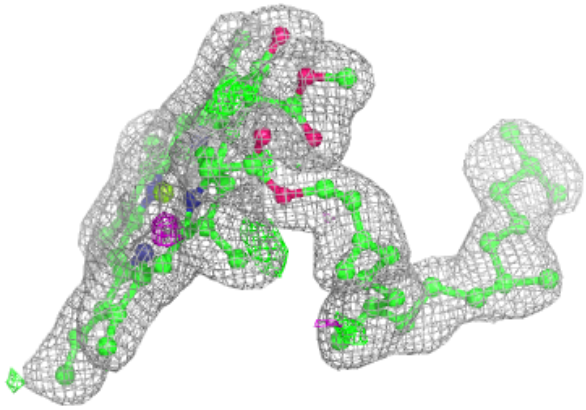


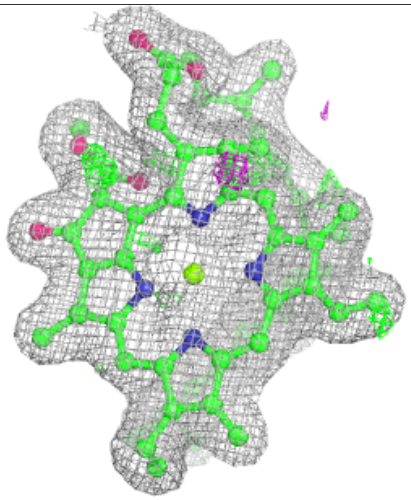


Electron density around CLA b 618:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

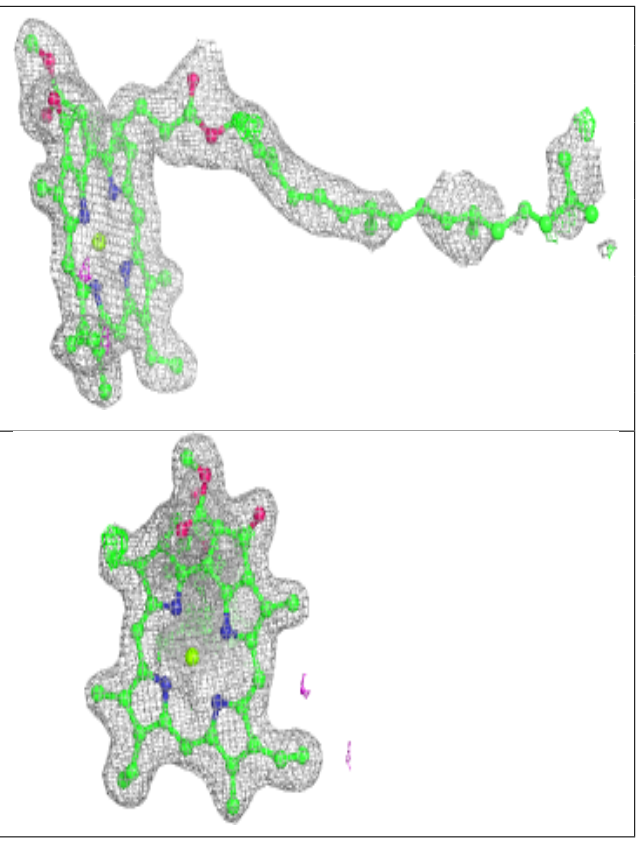






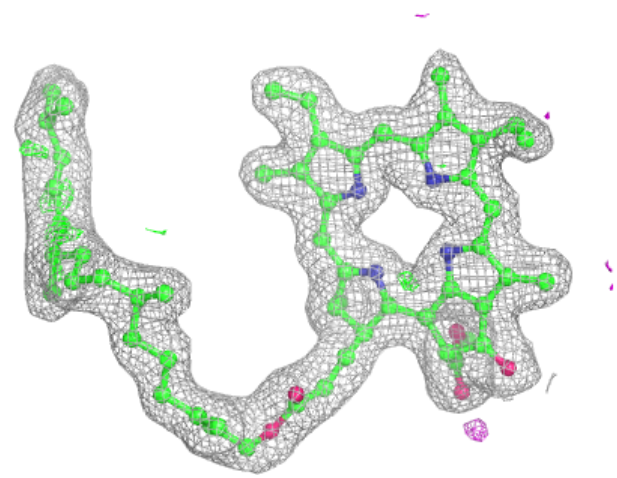
Electron density around CLA d 404:

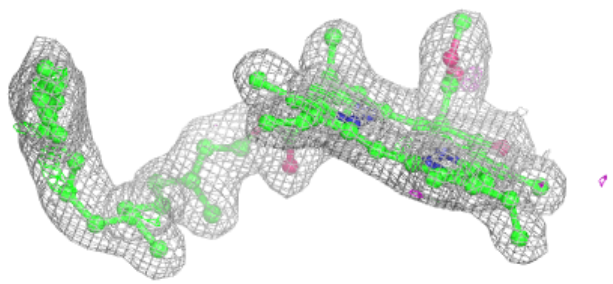
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

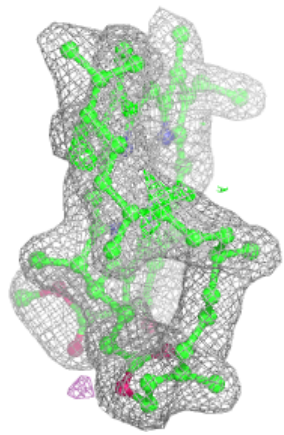


Electron density around PHO d 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

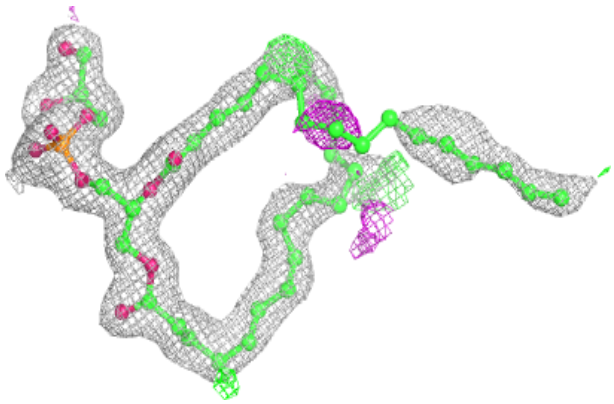


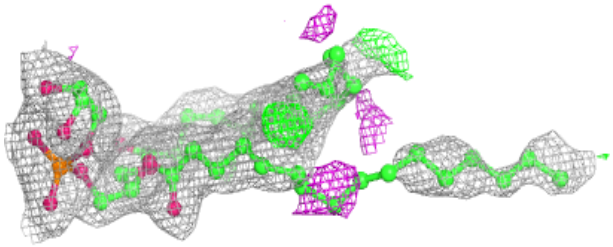


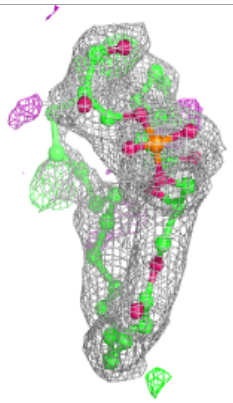


Electron density around LHG d 410:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

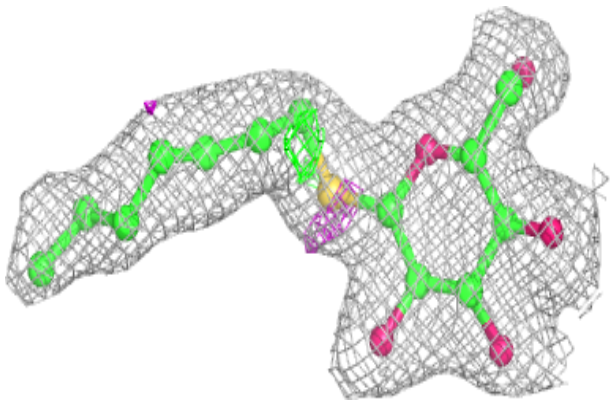


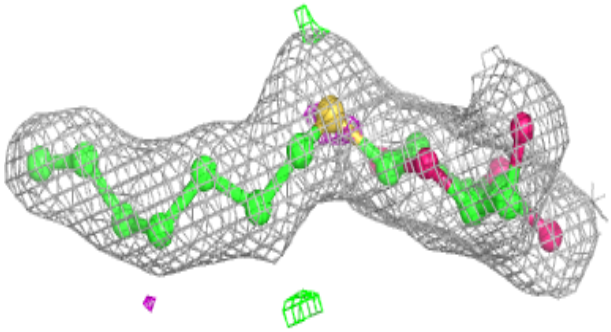


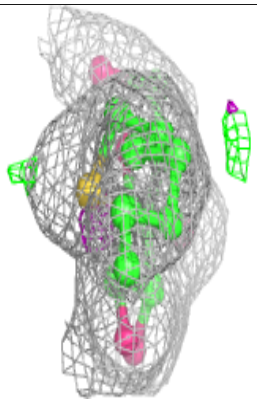


Electron density around HTG O 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

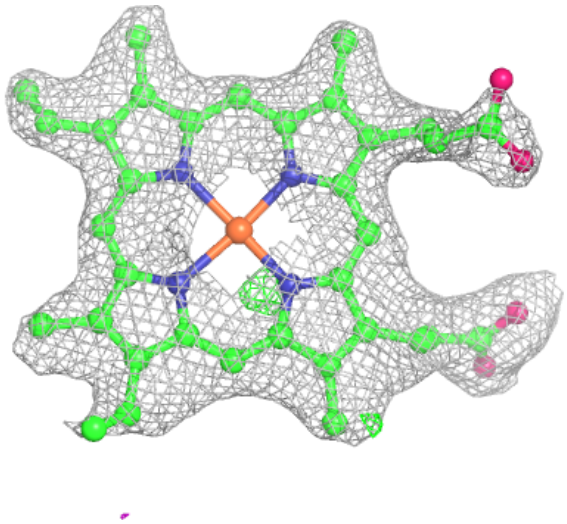


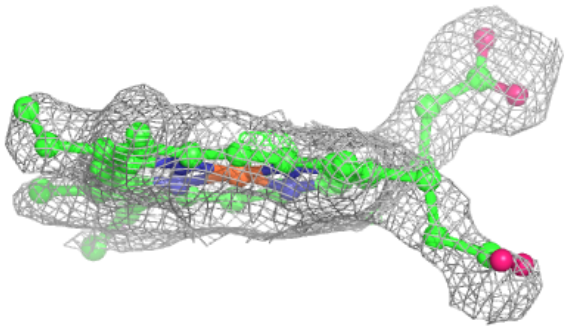


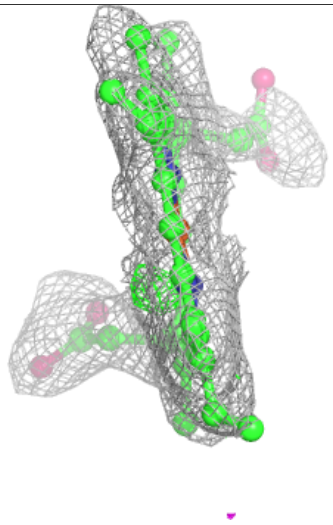


Electron density around HEM e 102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

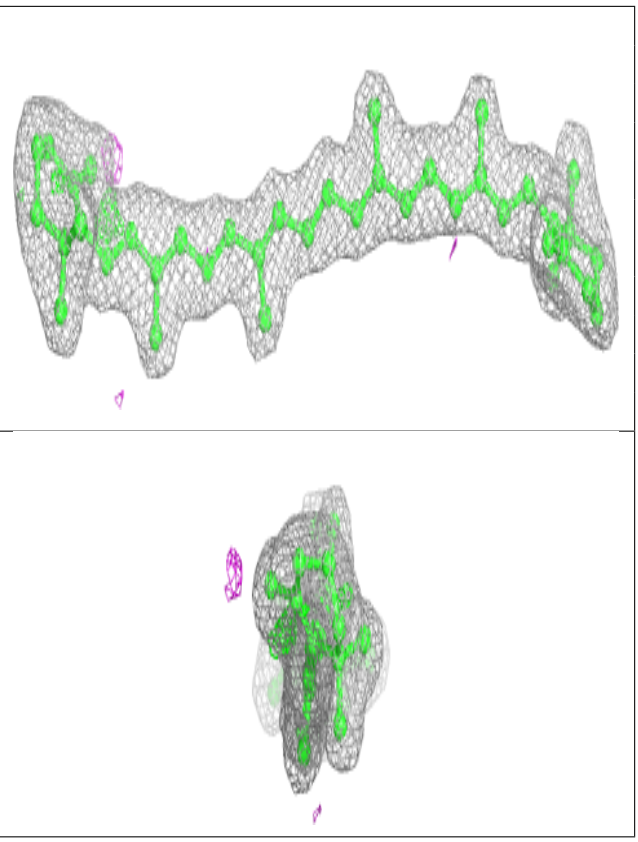






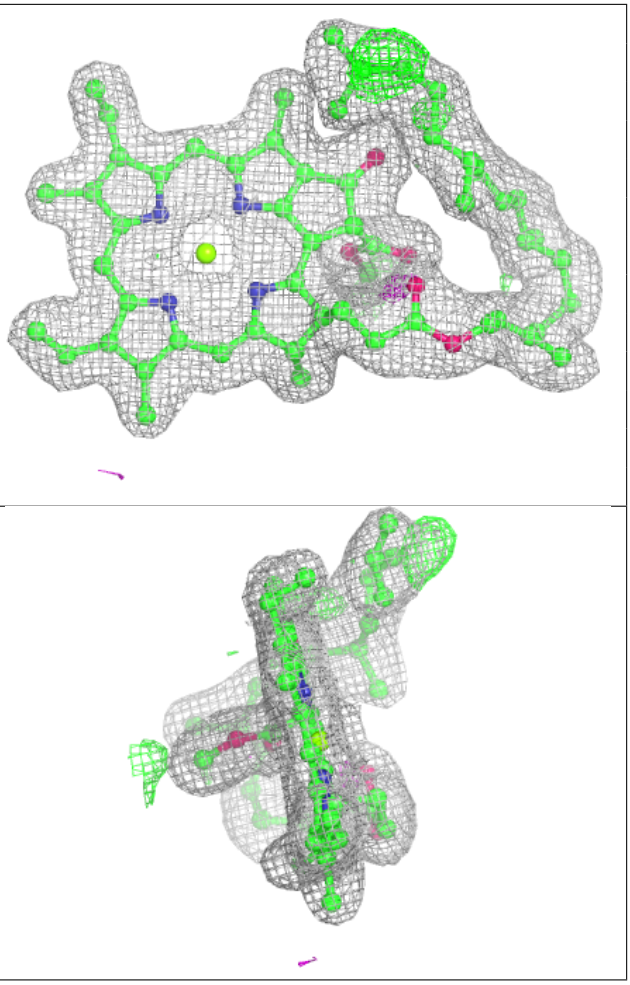
Electron density around BCR A 410:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



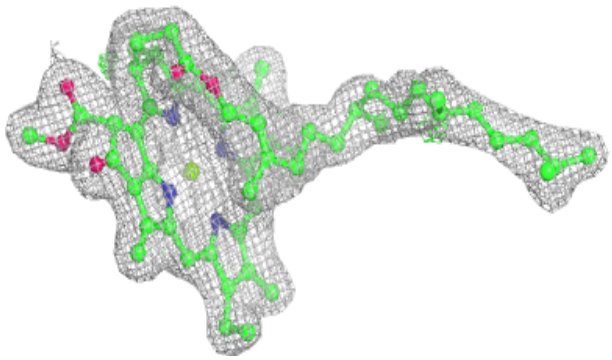
Electron density around CLA B 611:

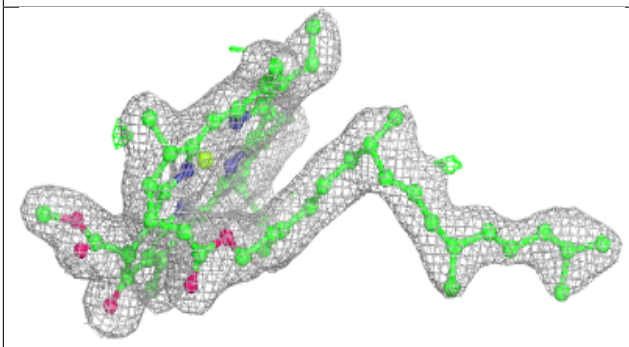
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

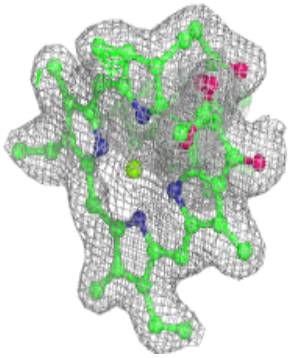


Electron density around CLA C 506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

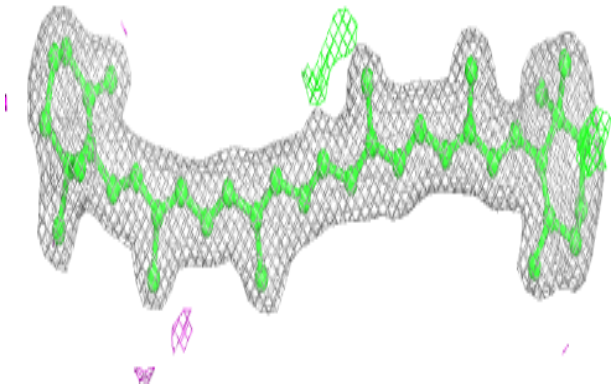


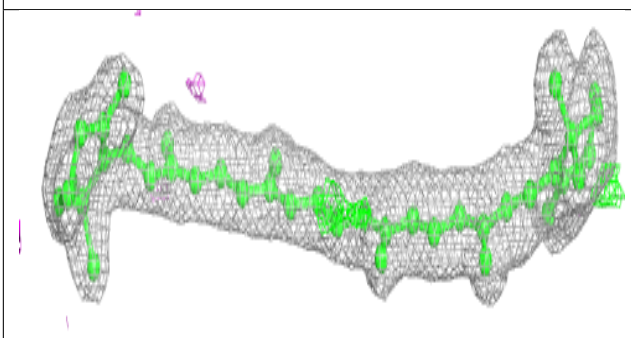


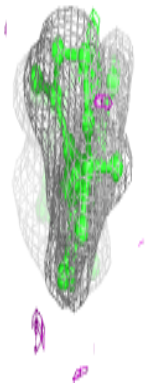


Electron density around BCR B 620:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

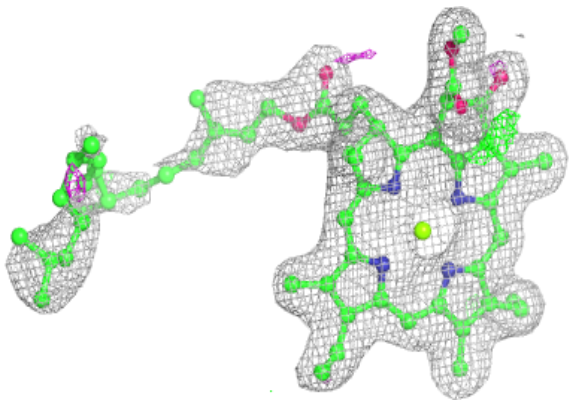


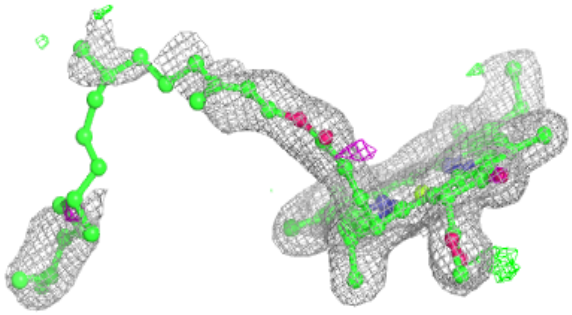


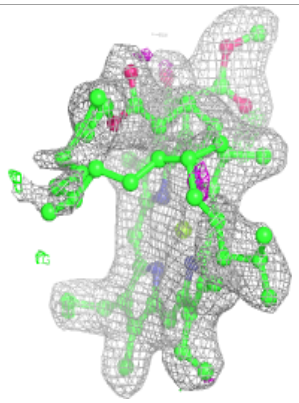


Electron density around CLA A 409:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

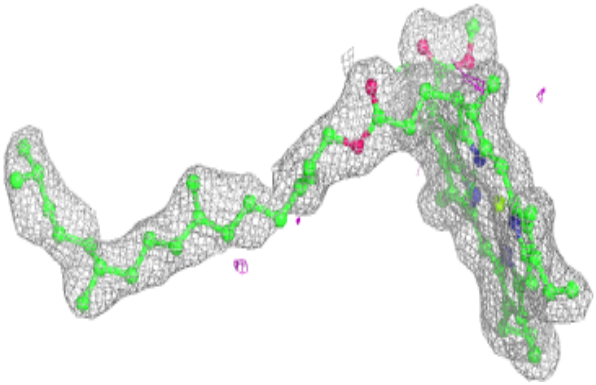


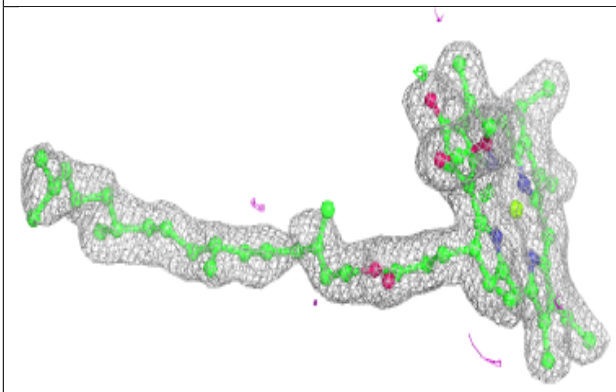


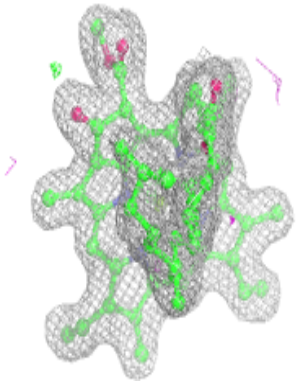


Electron density around CLA b 609:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

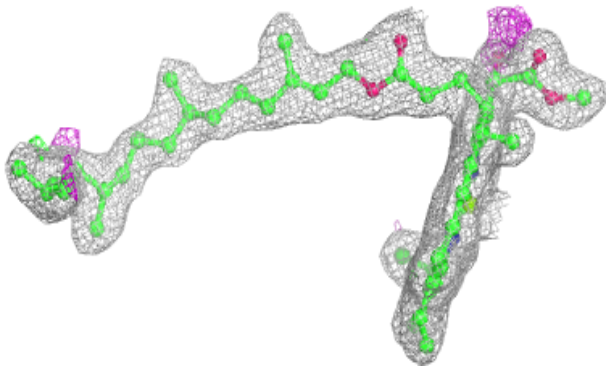


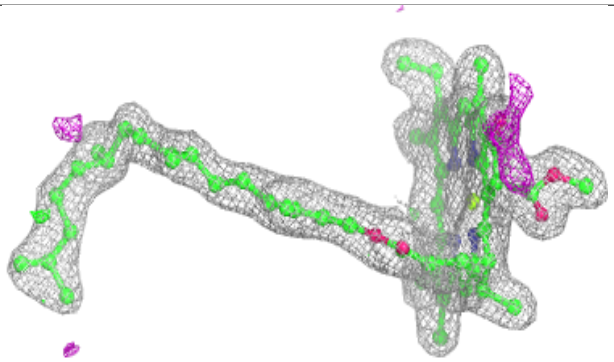


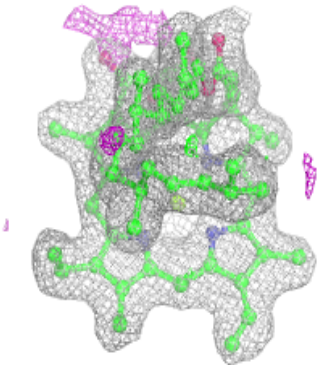


Electron density around CLA b 610:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

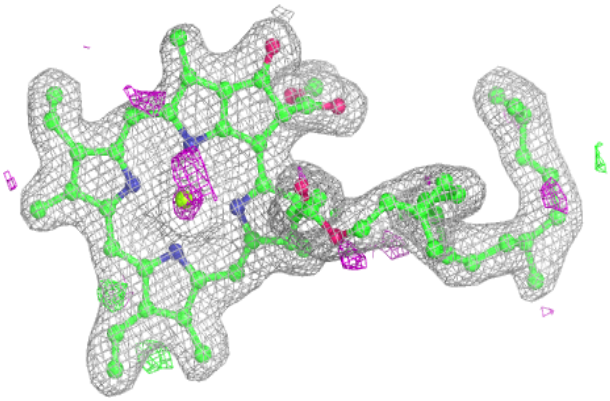


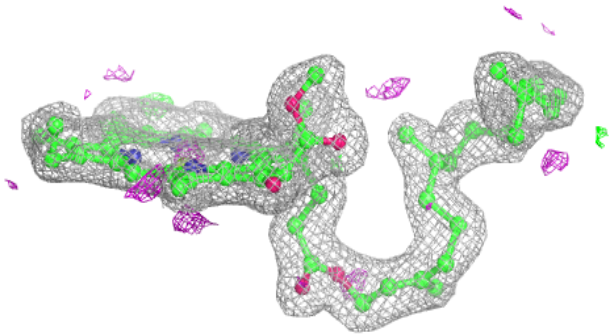


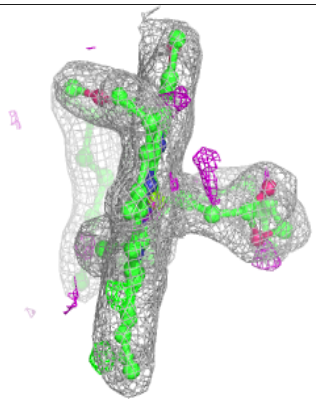


Electron density around CLA B 613:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

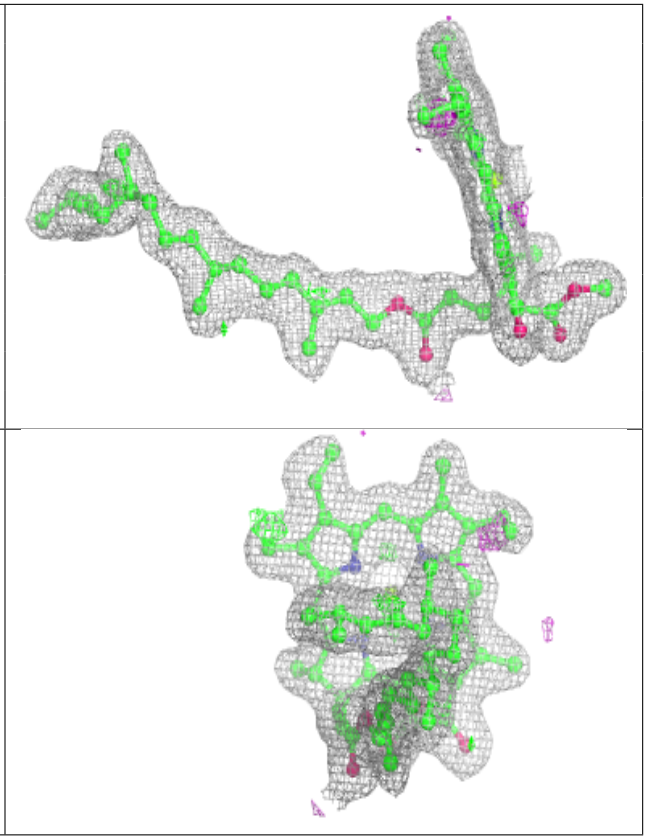






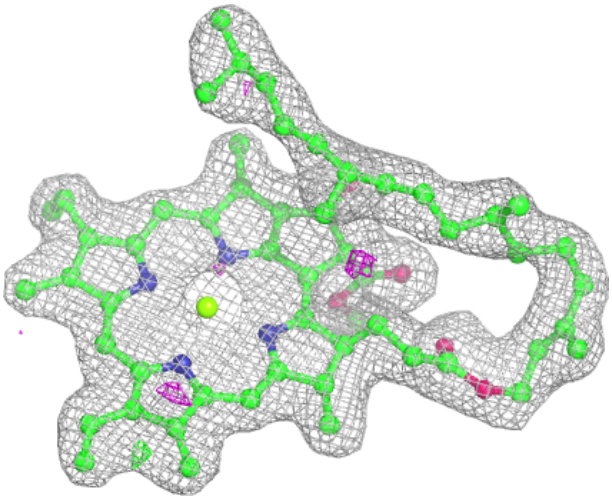
Electron density around CLA B 606:

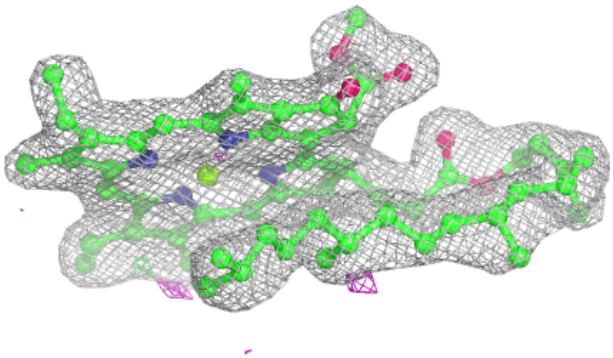
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 510:

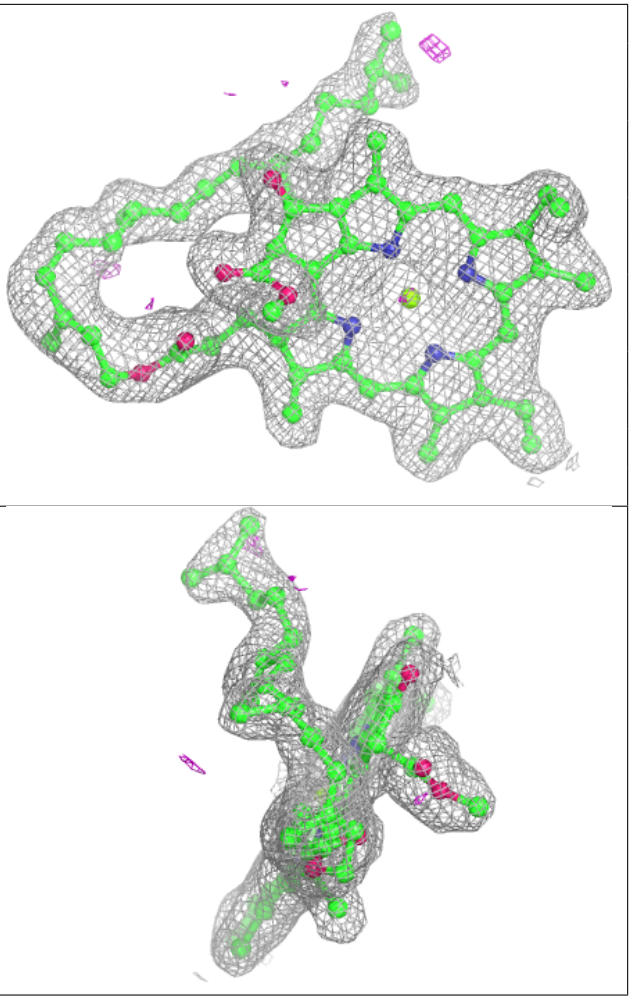
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





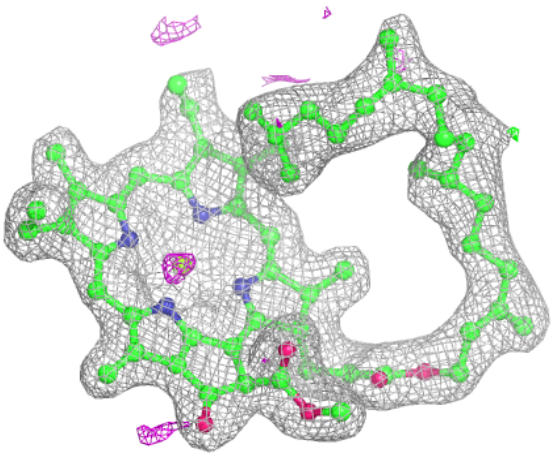
Electron density around CLA c 511:

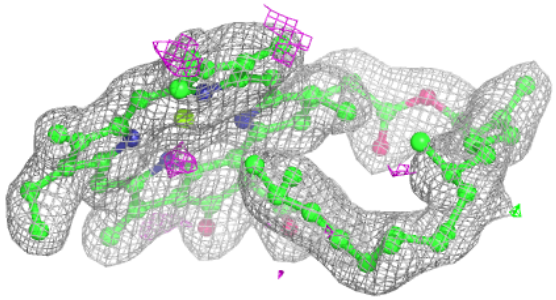
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

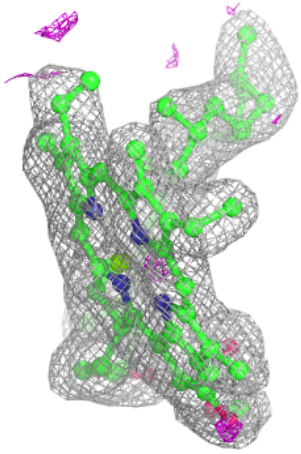


Electron density around CLA B 616:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

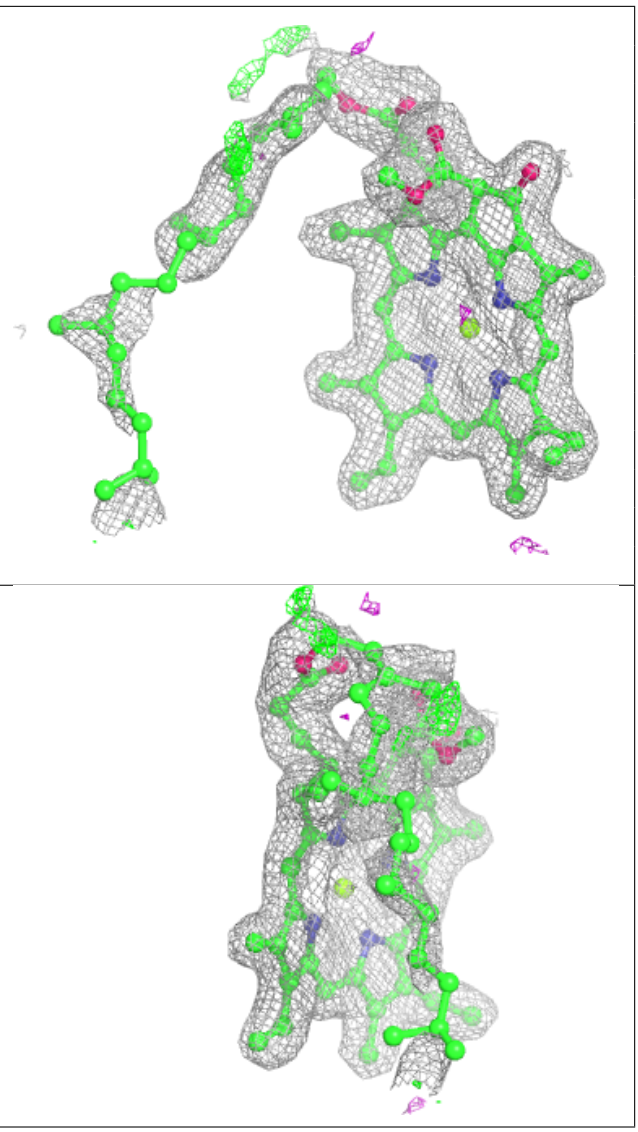






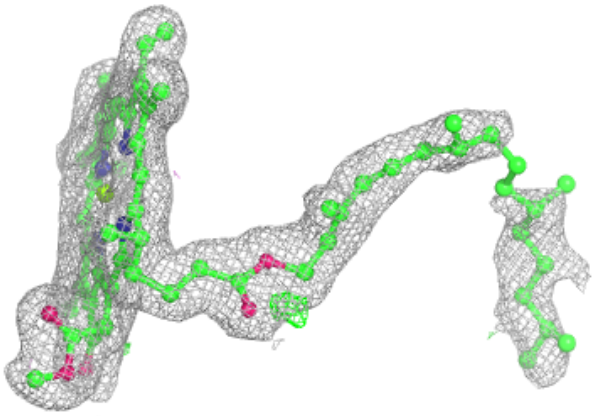
Electron density around CLA B 617:

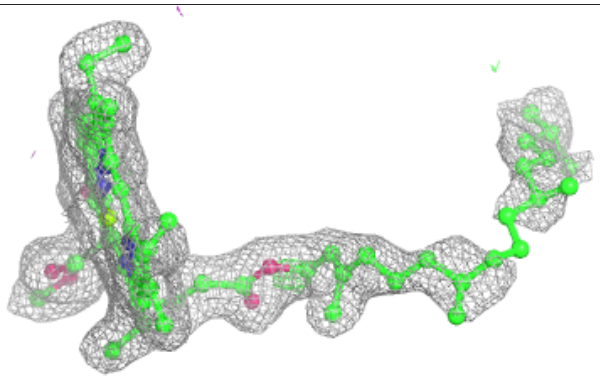
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

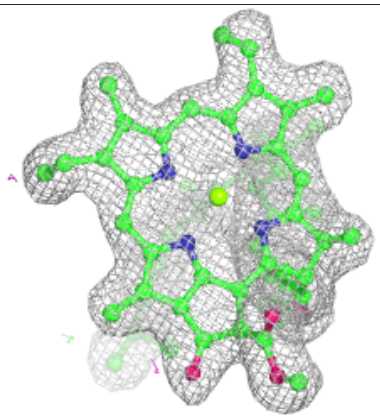


Electron density around CLA D 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

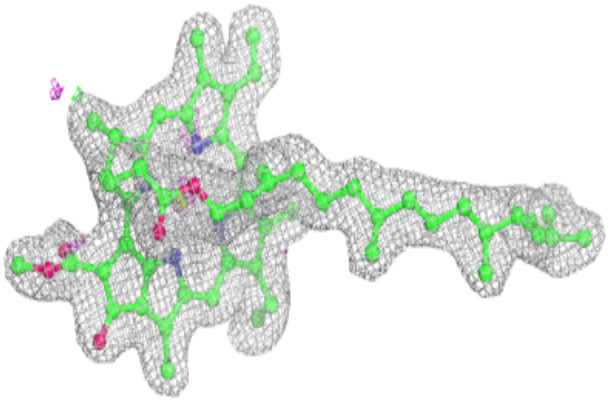


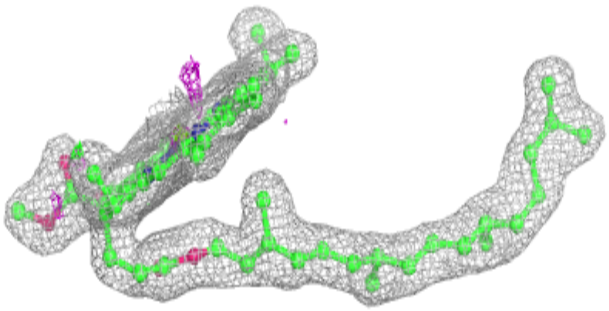


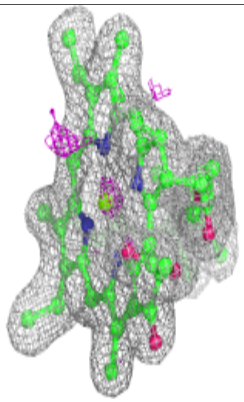


Electron density around CLA B 609:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

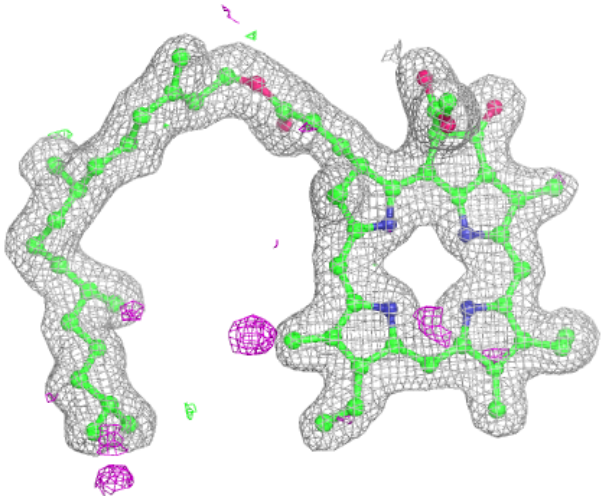


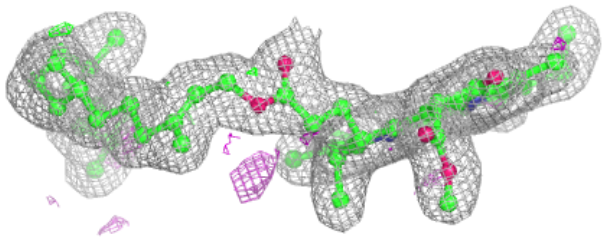




Electron density around PHO A 407:

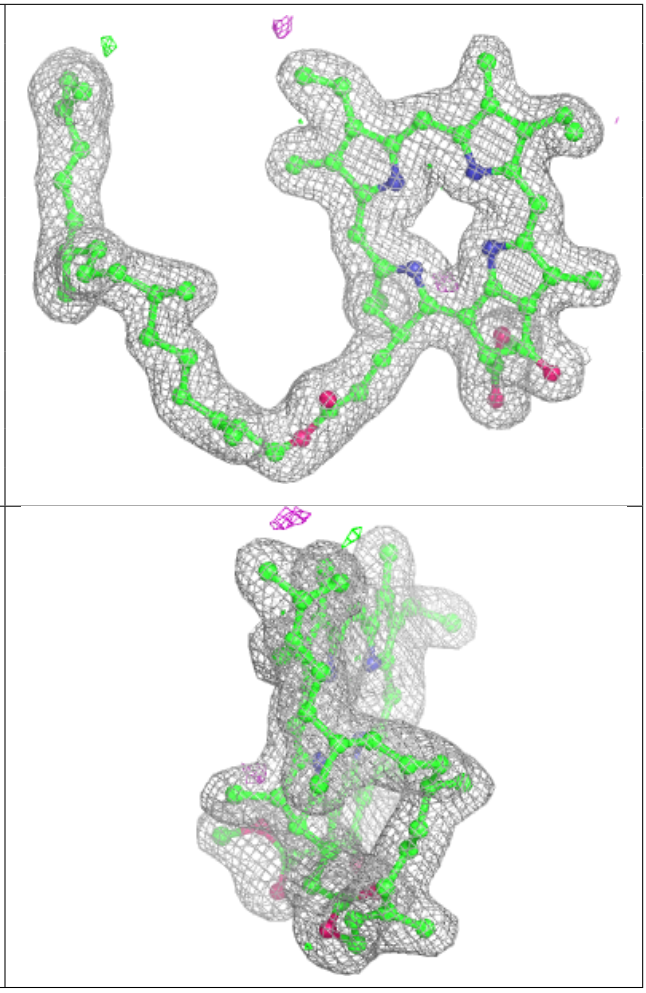
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





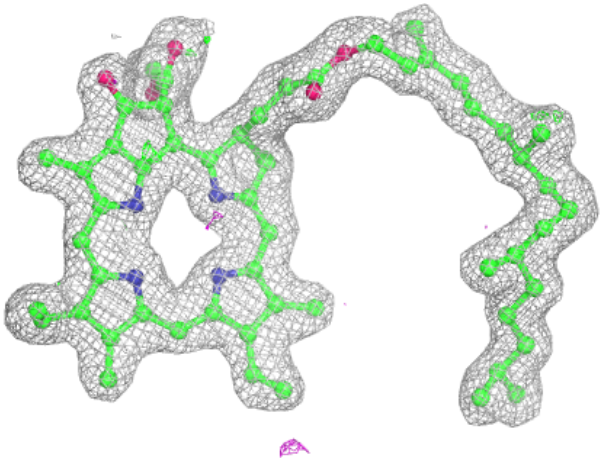
Electron density around PHO A 408:

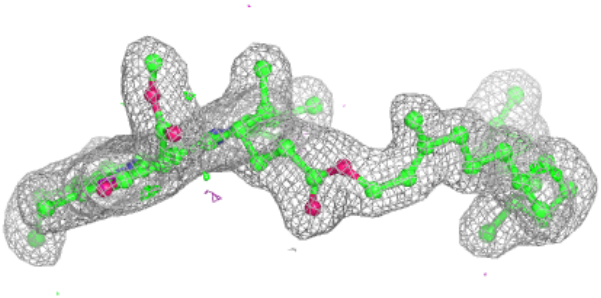
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

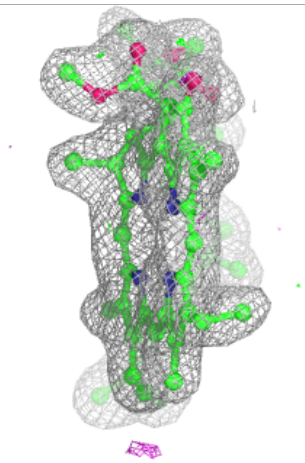


Electron density around PHO a 408:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

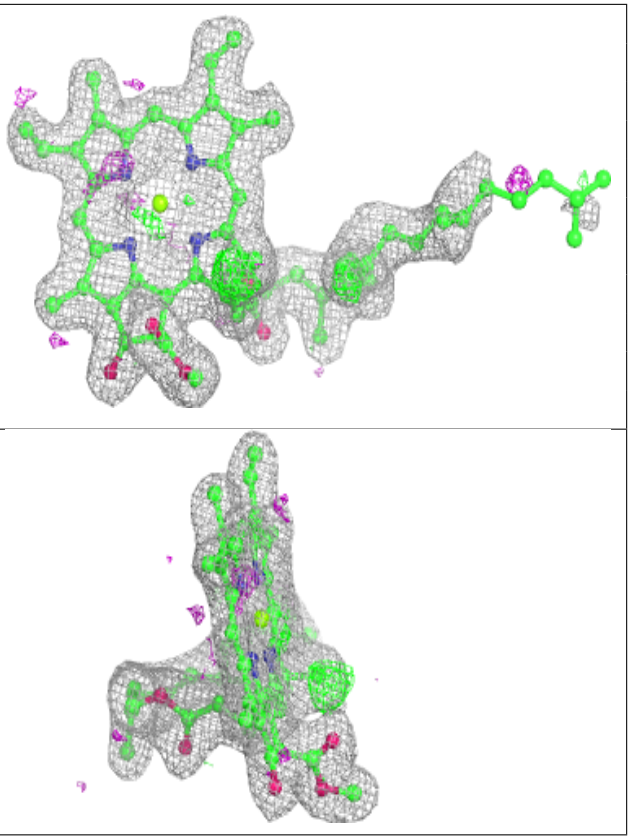






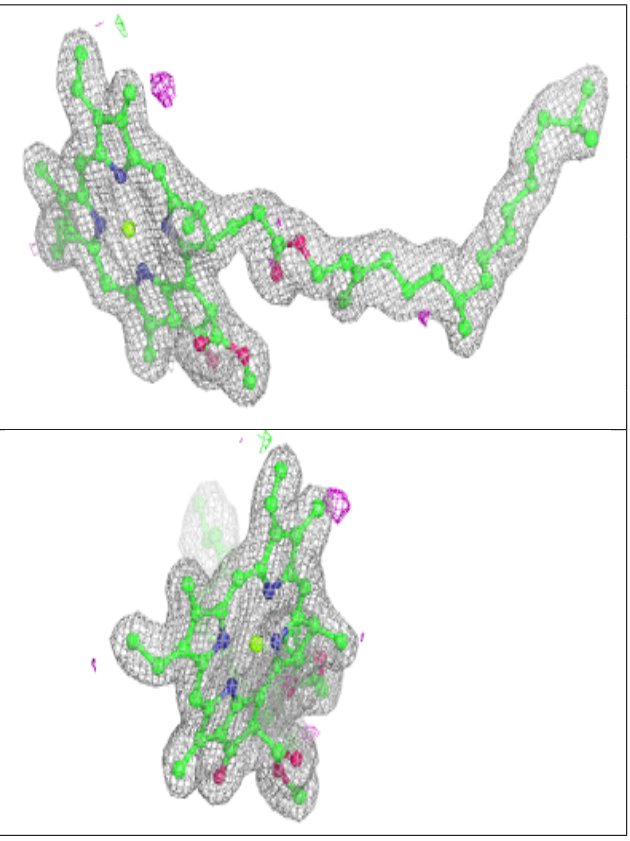
Electron density around CLA A 406:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



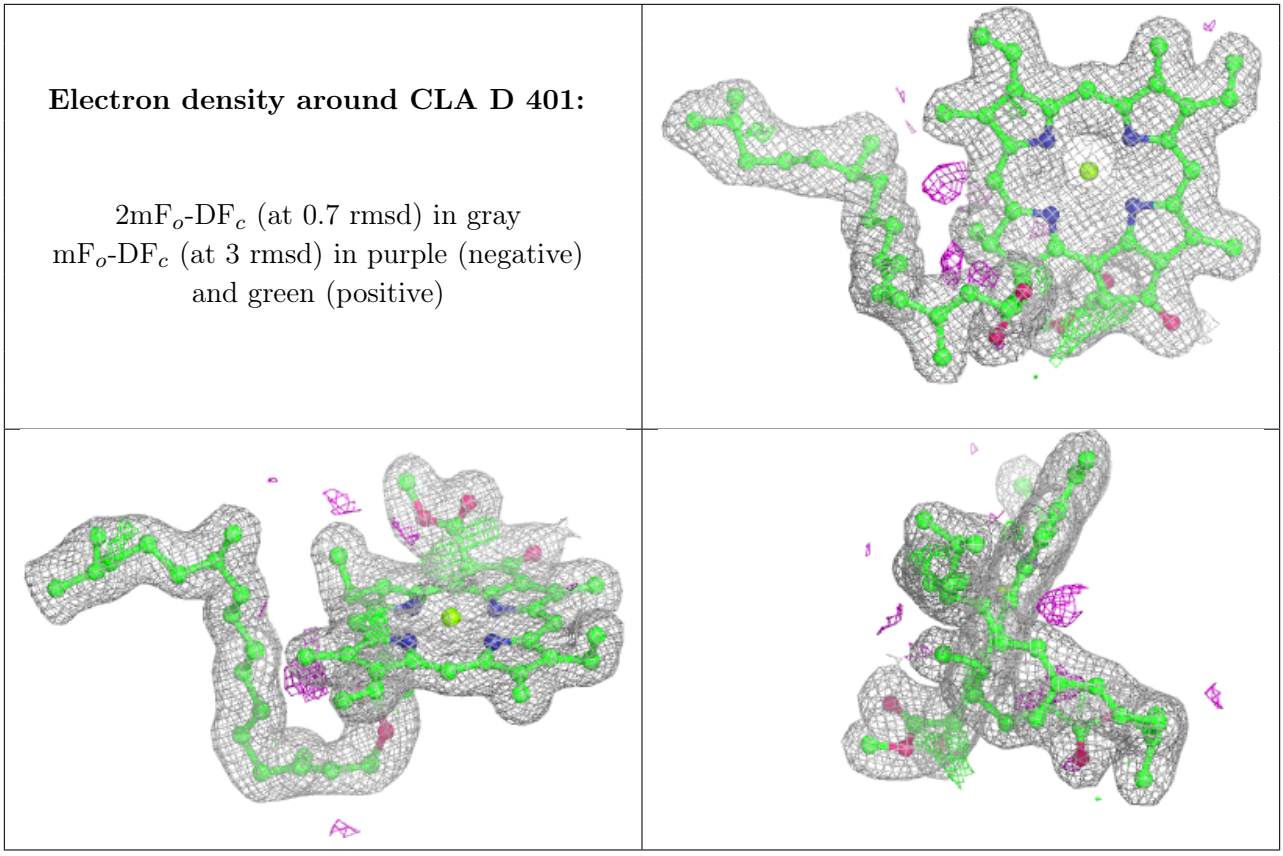
Electron density around CLA a 406:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



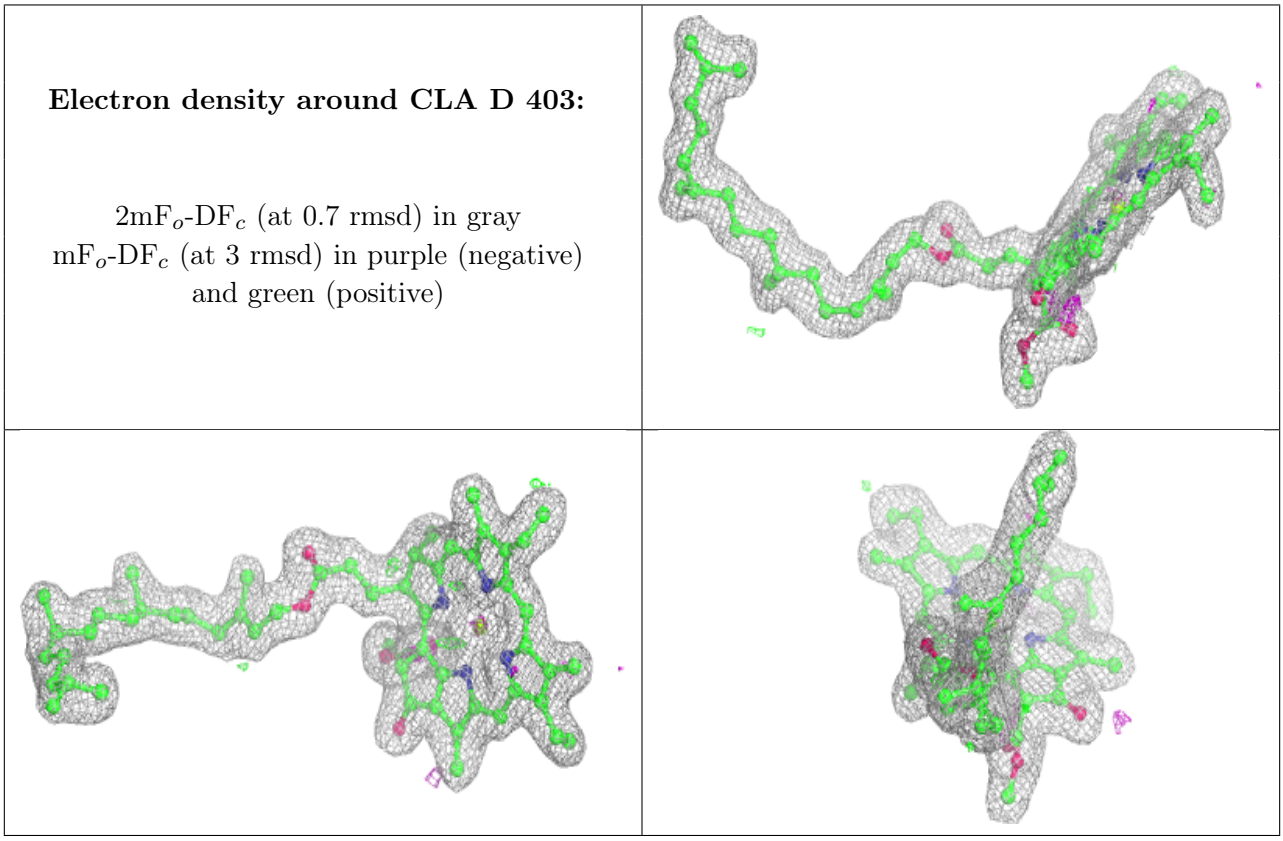
Electron density around CLA D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



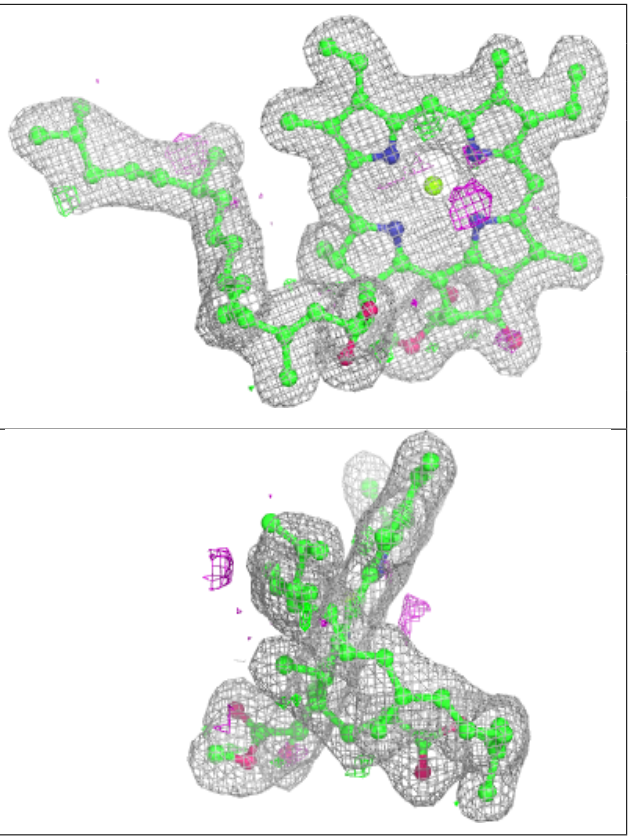
Electron density around CLA D 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



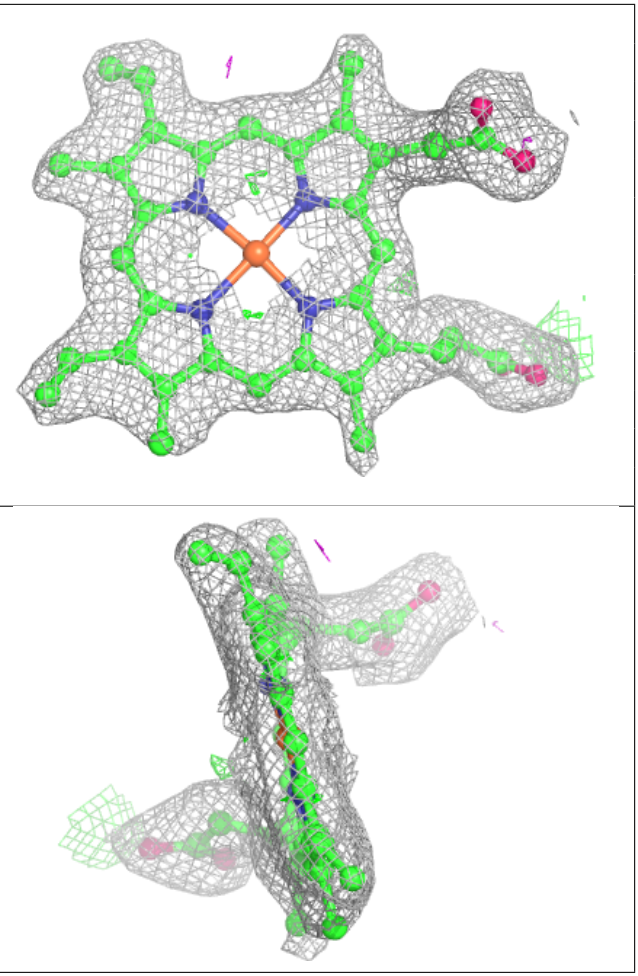
Electron density around CLA d 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



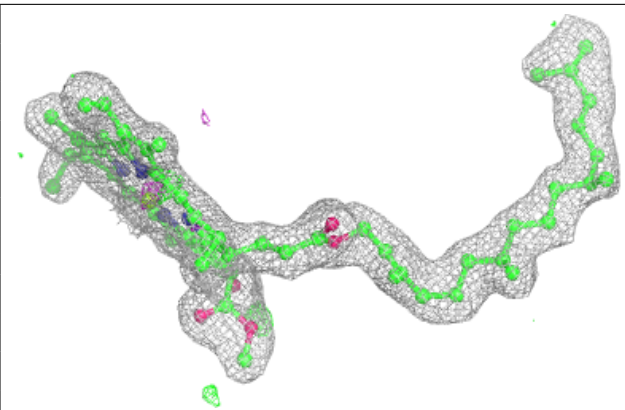
Electron density around HEM E 103:

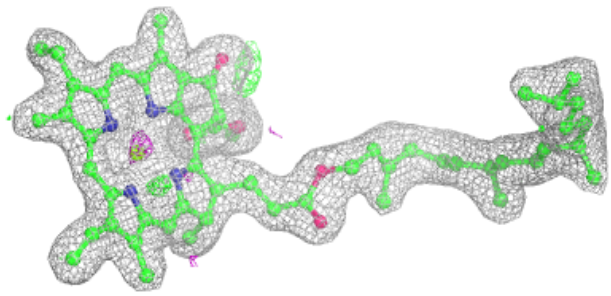
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

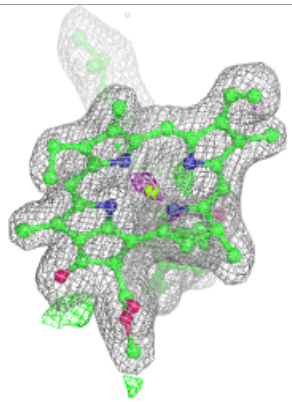


Electron density around CLA d 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

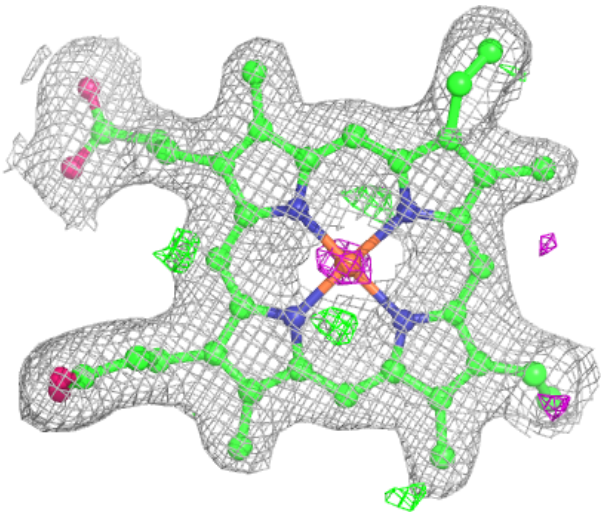


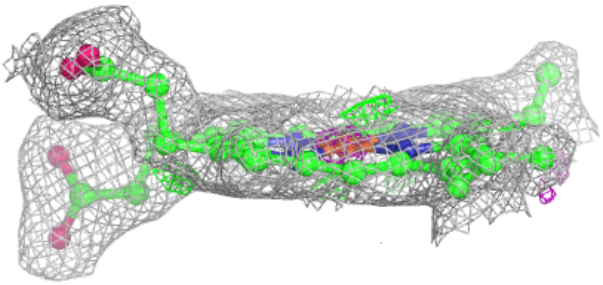


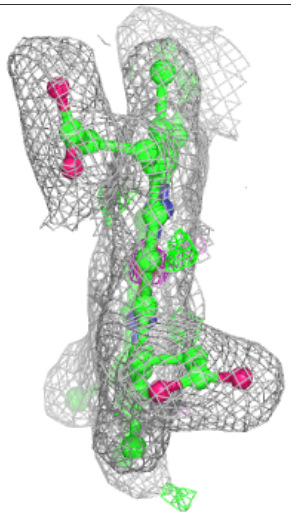


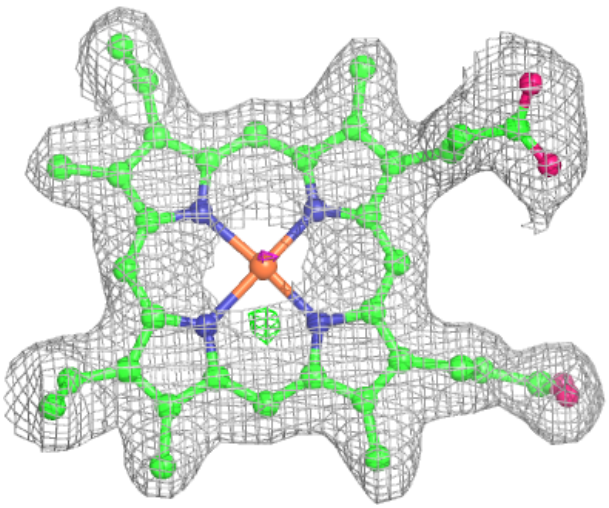
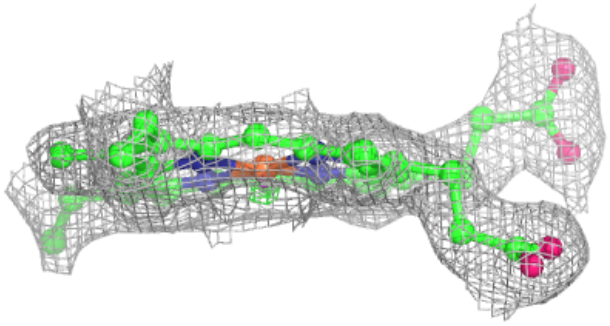
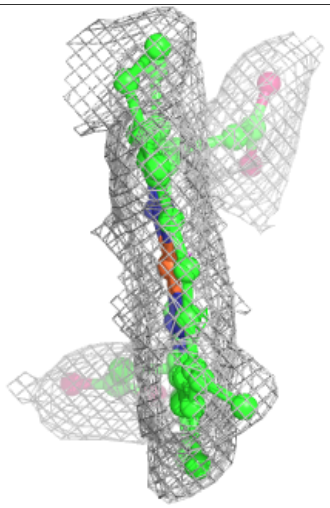
Electron density around HEC V 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC v 202: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.