Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 08:20 PM JST

PDB ID	:	5ZZN
Title	:	Crystal structure of photosystem II from an SQDG-deficient mutant of Thermosynechococcus elongatus
Authors	:	Nakajima, Y.; Umena, Y.; Nagao, R.; Endo, K.; Kobayashi, K.; Akita, F.; Suga, M.; Wada, H.; Noguchi, T.; Shen, J.R.
Deposited on	:	2018-06-03
Resolution	:	2.10 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:

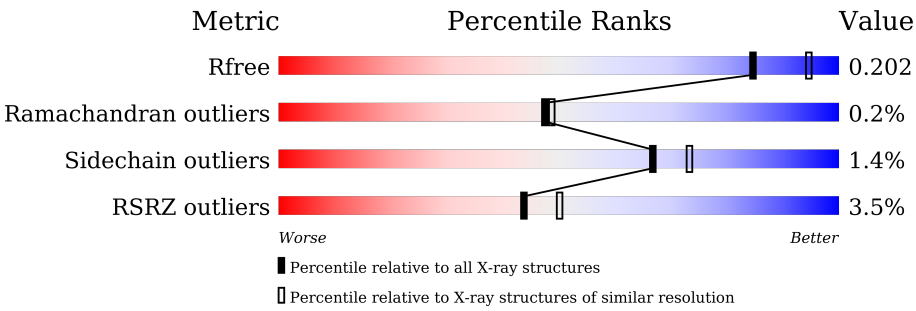
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.10 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	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	334	% 99%
1	a	334	% 98%
2	B	505	2% 99%
2	b	505	5% 97%
3	C	455	% 97%
3	c	455	2% 97%

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Mol	Chain	Length	Quality of chain
4	D	342	%, 98%
4	d	342	2%, 99%
5	E	81	9%, 95%
5	e	81	11%, 98%
6	F	34	12%, 94%, 6%
6	f	34	3%, 94%, 6%
7	H	63	3%, 98%
7	h	63	6%, 97%
8	I	37	3%, 92%, 5%
8	i	37	5%, 97%
9	J	40	8%, 92%, 8%
9	j	40	2%, 100%
10	K	37	100%
10	k	37	95%, 5%
11	L	36	8%, 94%, 6%
11	l	36	6%, 94%
12	M	34	3%, 94%
12	m	34	6%, 94%, 6%
13	O	243	4%, 98%
13	o	243	8%, 97%
14	T	30	3%, 90%, 10%
14	t	30	3%, 93%, 7%
15	U	97	2%, 96%
15	u	97	%, 96%
16	V	137	99%

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Mol	Chain	Length	Quality of chain
16	v	137	4% 100%
17	Y	29	10% 93% 7%
17	y	29	17% 93% 7%
18	X	39	10% 97%
18	x	39	10% 95%
19	Z	62	15% 97%
19	z	62	19% 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
22	CLA	A	404	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	D	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	D	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	409	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	-
22	CLA	b	620	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
28	LMT	C	520	X	-	-	-
28	LMT	z	101	X	-	-	-
32	HTG	B	624	-	-	-	X
32	HTG	U	203	-	-	-	X

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 53800 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 II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2626	1717	432	462	15	0	2	0
1	a	334	2629	1721	433	460	15	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	4009	2626	671	699	13	0	5	0
2	b	504	3988	2616	661	698	13	0	4	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	3526	2303	592	617	14	0	5	0
3	c	455	3531	2311	591	615	14	0	2	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	2746	1818	449	467	12	0	3	0
4	d	342	2738	1813	448	464	13	0	2	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	80	665	433	106	126	0	2	0
5	e	81	649	425	105	119	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	274	187	45	41	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	63	509	339	84	84	2	0	1	0
7	h	63	506	337	81	86	2	0	1	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	35	284	193	44	46	1	0	0	0
8	i	37	294	199	47	47	1	0	0	1

- 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	37	262	177	41	43	1	0	0	0
9	j	40	279	187	44	47	1	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	296	206	43	47	0	1	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	k	37	285	199	42	44	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			
11	L	36	292	196	45	51	0	1	0
11	l	35	296	200	45	51	0	2	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	33	264	177	38	48	1	0	1	0
12	m	34	269	180	39	49	1	0	1	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	1876	1172	315	385	4	0	4	0
13	o	243	1876	1174	311	385	6	0	6	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	259	181	36	40	2	0	0	0
14	t	30	259	181	36	40	2	0	0	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	785	497	133	155	0	1	0
15	u	97	783	496	130	157	0	1	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	1083	685	183	211	4	0	2	0
16	v	137	1063	672	178	209	4	0	1	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	217	144	35	34	4	0	1	0
17	y	29	209	136	37	33	3	0	0	0

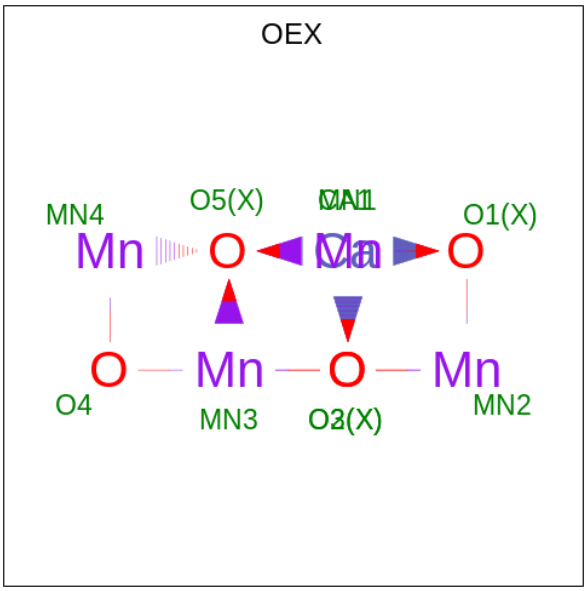
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	X	39	292	196	47	49	0	1	0
18	x	38	289	194	46	49	0	1	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	465	321	67	75	2	0	0	0
19	z	62	459	318	67	72	2	0	0	0

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).

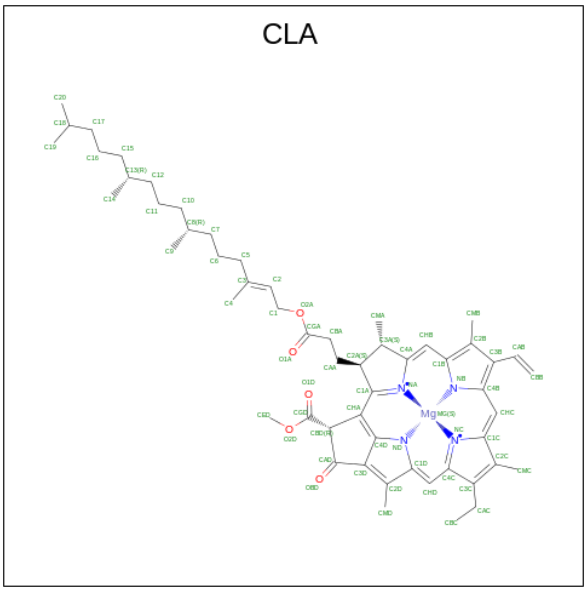


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
20	A	1	10	1	4	5	0	0
20	a	1	10	1	4	5	0	0

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
21	A	2	2	2	0	0
21	a	2	2	2	0	0
21	v	1	1	1	0	0

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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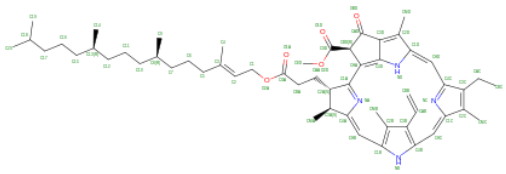
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
22	c	1	65	55	1	4	5	0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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).

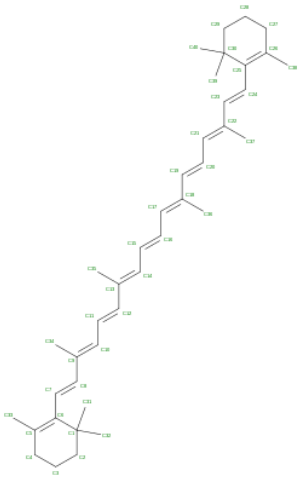
PHO



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

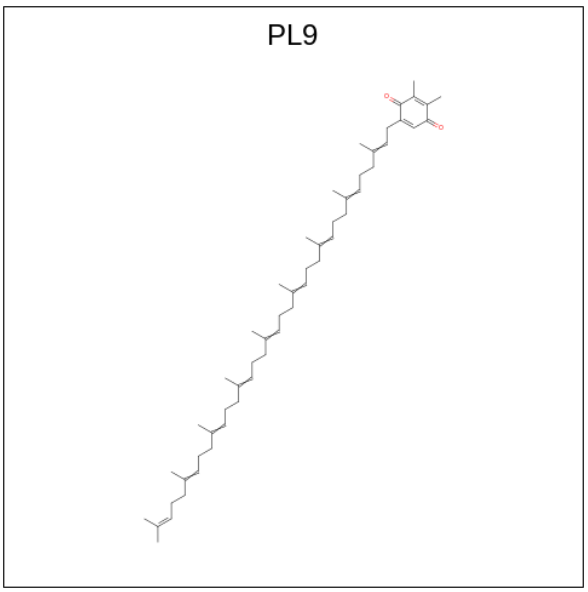
BCR



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

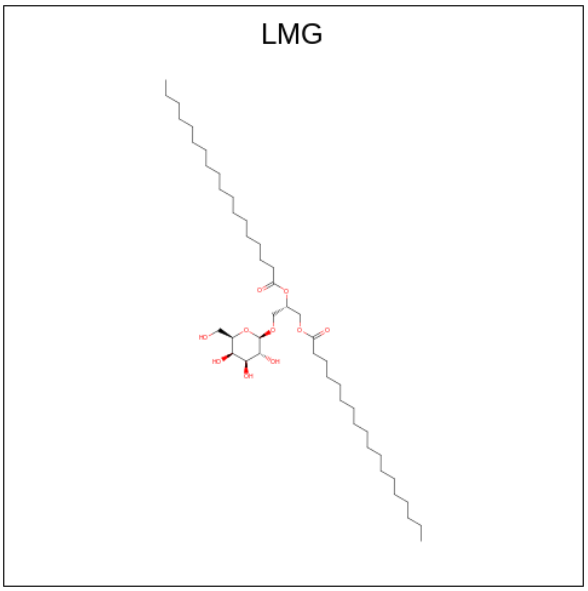
- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

$C_{53}H_{80}O_2$).



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

- Molecule 26 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		
26	A	1	51	41	10	0	0
26	B	1	51	41	10	0	0
26	C	1	49	39	10	0	0
26	C	1	48	38	10	0	0
26	D	1	47	37	10	0	0
26	a	1	51	41	10	0	0
26	b	1	49	39	10	0	0
26	c	1	38	28	10	0	0
26	c	1	51	41	10	0	0
26	d	1	47	37	10	0	0

- Molecule 27 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
27	A	5	119	104	15	0	0
27	B	5	127	117	10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	2	Total C O 35 30 5	0	0
27	D	1	Total C 16 16	0	0
27	E	2	Total C 29 29	0	0
27	H	2	Total C 14 14	0	0
27	I	4	Total C 59 59	0	0
27	J	1	Total C 16 16	0	0
27	K	1	Total C 10 10	0	0
27	T	1	Total C 13 13	0	0
27	U	1	Total C 14 14	0	0
27	X	1	Total C 16 16	0	0
27	Z	1	Total C 6 6	0	0
27	a	4	Total C O 96 86 10	0	0
27	b	4	Total C O 108 98 10	0	0
27	c	3	Total C O 53 48 5	0	0
27	d	2	Total C O 52 47 5	0	0
27	e	2	Total C 19 19	0	0
27	h	1	Total C 8 8	0	0
27	i	4	Total C 60 60	0	0
27	j	2	Total C O 49 44 5	0	0
27	t	1	Total C 16 16	0	0
27	u	1	Total C 13 13	0	0

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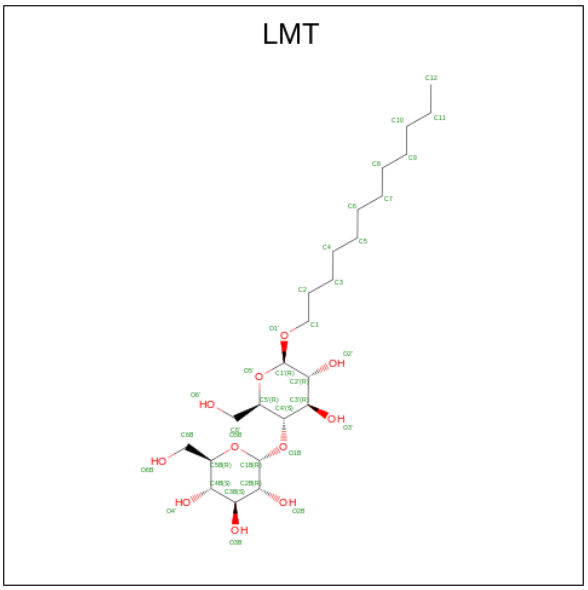
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	x	1	Total C 16 16	0	0

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 35 24 11	0	0
28	B	1	Total C O 35 24 11	0	0
28	C	1	Total C O 35 24 11	0	0
28	F	1	Total C O 24 18 6	0	0
28	J	1	Total C O 24 18 6	0	0
28	M	1	Total C O 35 24 11	0	0
28	M	1	Total C O 24 18 6	0	0
28	T	1	Total C O 24 18 6	0	0
28	Z	1	Total C O 35 24 11	0	0
28	a	1	Total C O 35 24 11	0	0

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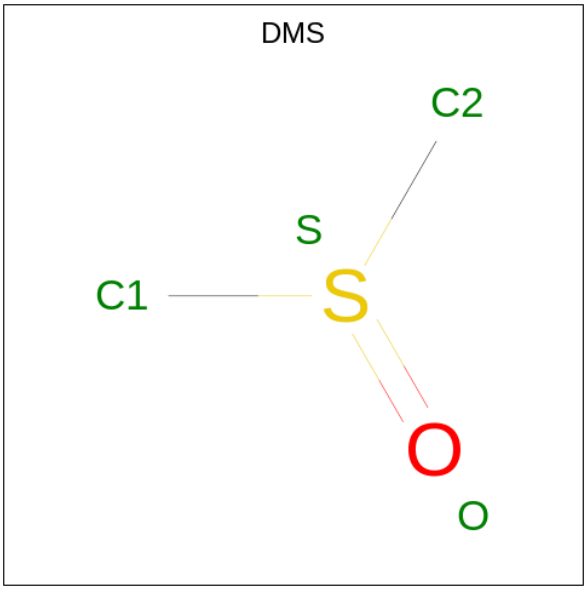
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
28	b	1	25	19	6		0	0
			Total	C	O			
28	c	1	35	24	11		0	0
			Total	C	O			
28	j	1	23	18	5		0	0
			Total	C	O			
28	l	1	24	18	6		0	0
			Total	C	O			
28	m	1	35	24	11		0	0
			Total	C	O			
28	m	1	25	18	7		0	0
			Total	C	O			
28	m	1	23	18	5		0	0
			Total	C	O			
28	t	1	24	18	6		0	0
			Total	C	O			
28	z	1	32	21	11		0	0

- Molecule 29 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	A	1	4	2	1	1	0	0
			Total	C	O	S		
29	A	1	4	2	1	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	A	1	4	2	1	1	0	0
			Total	C	O	S		
29	A	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	B	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	C	1	4	2	1	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	C	1	4	2	1	1	0	0
			Total	C	O	S		
29	D	1	4	2	1	1	0	0
			Total	C	O	S		
29	D	1	4	2	1	1	0	0
			Total	C	O	S		
29	D	1	4	2	1	1	0	0
			Total	C	O	S		
29	D	1	4	2	1	1	0	0
			Total	C	O	S		
29	D	1	4	2	1	1	0	0
			Total	C	O	S		
29	E	1	4	2	1	1	0	0
			Total	C	O	S		
29	I	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	O	1	4	2	1	1	0	0
			Total	C	O	S		
29	U	1	4	2	1	1	0	0
			Total	C	O	S		
29	V	1	4	2	1	1	0	0
			Total	C	O	S		
29	V	1	4	2	1	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	V	1	4	2	1	1	0	0
			Total	C	O	S		
29	V	1	4	2	1	1	0	0
			Total	C	O	S		
29	V	1	4	2	1	1	0	0
			Total	C	O	S		
29	V	1	4	2	1	1	0	0
			Total	C	O	S		
29	a	1	4	2	1	1	0	0
			Total	C	O	S		
29	a	1	4	2	1	1	0	0
			Total	C	O	S		
29	a	1	4	2	1	1	0	0
			Total	C	O	S		
29	a	1	4	2	1	1	0	0
			Total	C	O	S		
29	a	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	b	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	c	1	4	2	1	1	0	0
			Total	C	O	S		
29	d	1	4	2	1	1	0	0
			Total	C	O	S		
29	d	1	4	2	1	1	0	0
			Total	C	O	S		
29	e	1	4	2	1	1	0	0
			Total	C	O	S		
29	h	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
			Total	C	O	S		
29	o	1	4	2	1	1	0	0

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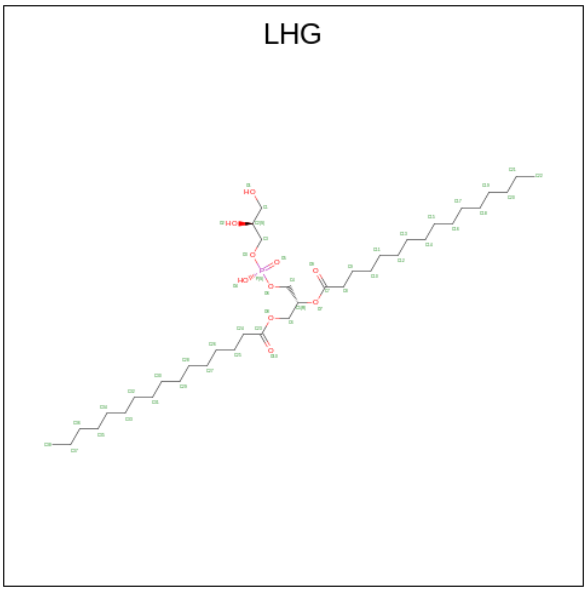
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
29	o	1	4	2	1	1	0	0
29	u	1	4	2	1	1	0	0
29	u	1	4	2	1	1	0	0
29	u	1	4	2	1	1	0	0
29	v	1	4	2	1	1	0	0
29	v	1	4	2	1	1	0	0
29	v	1	4	2	1	1	0	0
29	v	1	4	2	1	1	0	0
29	v	1	4	2	1	1	0	0

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
30	B	1	1	1	0	0
30	O	1	1	1	0	0
30	V	1	1	1	0	0
30	b	1	1	1	0	0
30	c	1	1	1	0	0
30	o	1	1	1	0	0
30	v	1	1	1	0	0

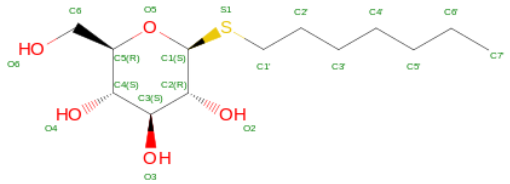
- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
31	B	1	49	38	10	1	0	0
31	D	1	49	38	10	1	0	0
31	D	1	49	38	10	1	0	0
31	D	1	44	33	10	1	0	0
31	E	1	49	38	10	1	0	0
31	F	1	38	27	10	1	0	0
31	b	1	49	38	10	1	0	0
31	d	1	49	38	10	1	0	0
31	d	1	49	38	10	1	0	0
31	d	1	44	33	10	1	0	0
31	e	1	38	29	8	1	0	0
31	f	1	46	35	10	1	0	0

- Molecule 32 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
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 18 12 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C S 9 8 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	D	1	Total C O S 16 10 5 1	0	0
32	O	1	Total C O S 19 13 5 1	0	0
32	U	1	Total C O S 14 8 5 1	0	0
32	V	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0

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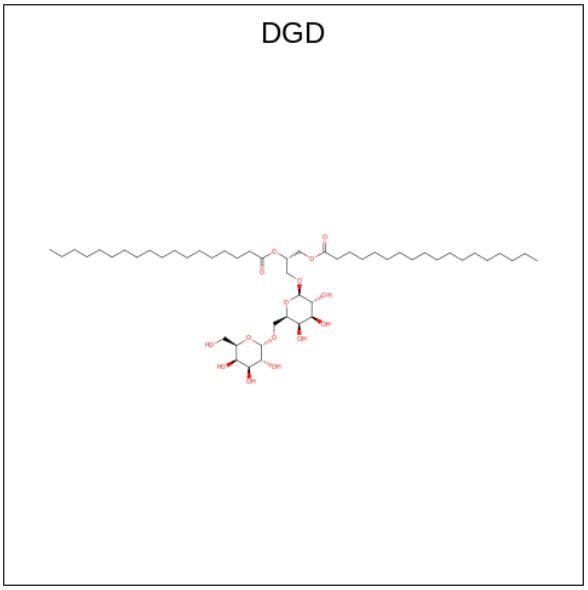
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 17 11 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C S 9 8 1	0	0
32	c	1	Total C O S 15 9 5 1	0	0
32	d	1	Total C O S 16 10 5 1	0	0
32	o	1	Total C O S 19 13 5 1	0	0
32	v	1	Total C O S 16 10 5 1	0	0

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0

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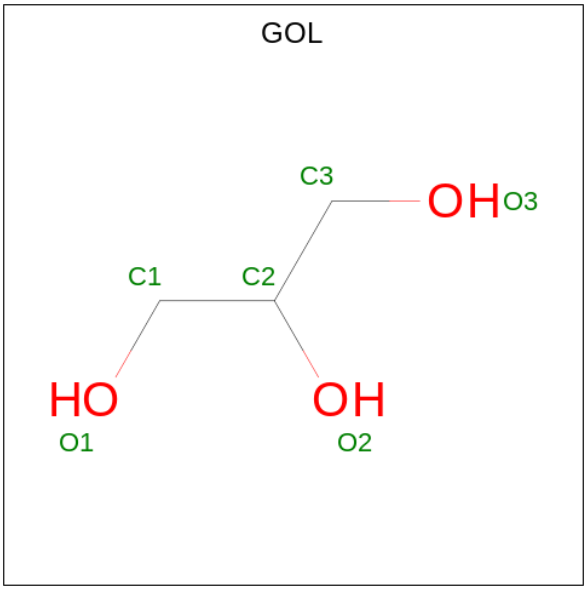
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	D	1	Total C O 45 36 9	0	0
33	H	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 56 41 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	d	1	Total C O 48 39 9	0	0
33	h	1	Total C O 62 47 15	0	0

- Molecule 34 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	C	1	Total C O 6 3 3	0	0
34	D	1	Total C O 6 3 3	0	0
34	b	1	Total C O 6 3 3	0	0
34	c	1	Total C O 6 3 3	0	0

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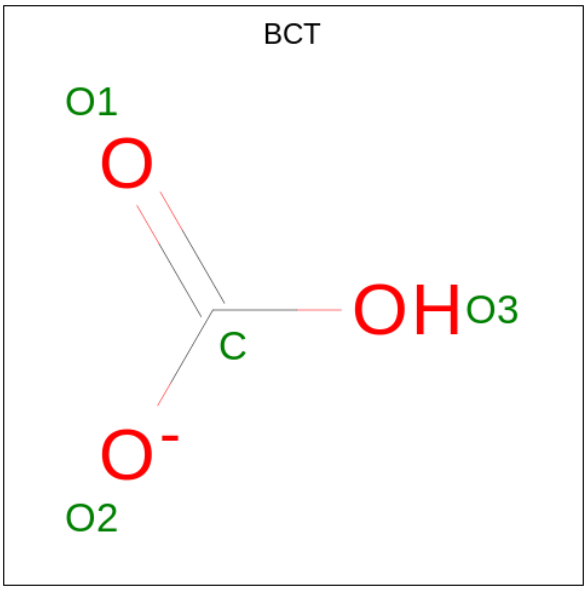
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	e	1	6	3	3	0	0

- Molecule 35 is FE (II) ION (three-letter code: FE2) (formula: Fe).

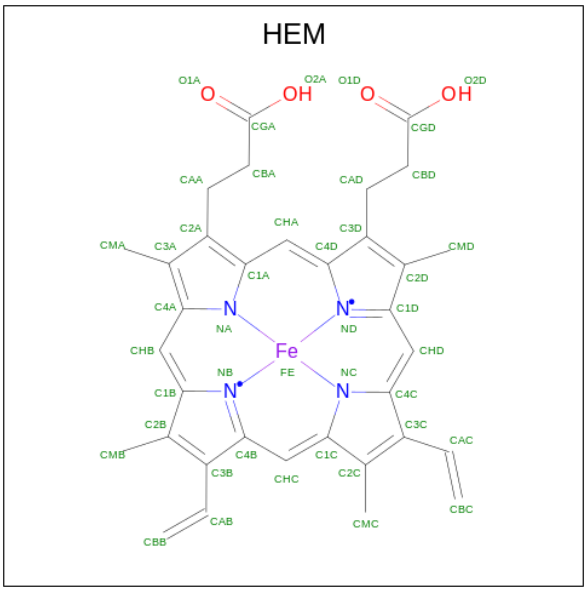
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
35	D	1	1	1	0	0
35	a	1	Total	Fe	0	0
			1	1		

- Molecule 36 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



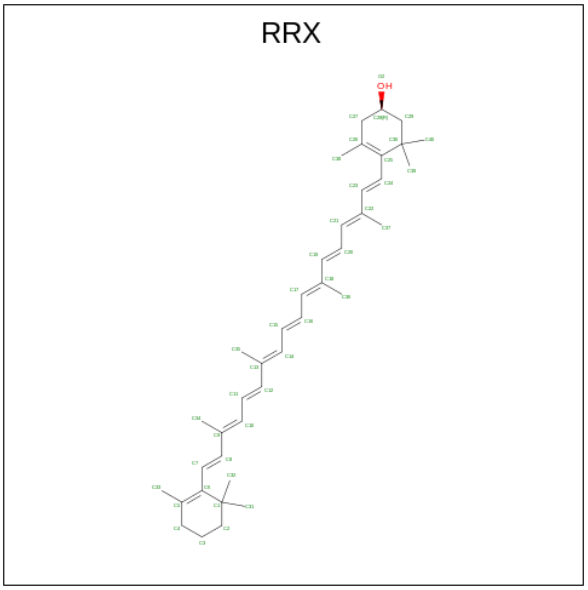
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
36	D	1	8	2	6	0	1
36	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 37 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		
37	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
37	f	1	43	34	1	4	4	0	0

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).

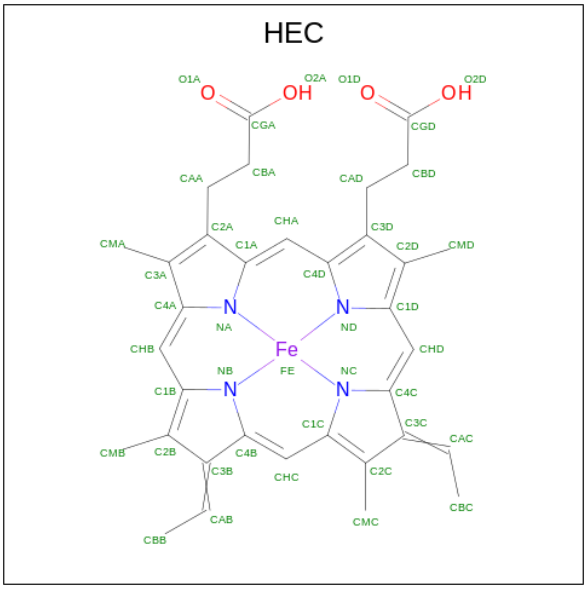


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
38	H	1	41	40	1	0	0
			Total	C	O		
38	h	1	41	40	1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	J	1	Total Mg 1 1	0	0
39	K	1	Total Mg 1 1	0	0
39	j	1	Total Mg 1 1	0	0
39	k	1	Total Mg 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
40	V	1	Total C Fe N O 43 34 1 4 4	0	0
40	v	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	139	Total O 141 141	0	2
41	B	260	Total O 263 263	0	3
41	C	216	Total O 216 216	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	D	126	130	130	0	4
			Total	O		
41	E	20	21	21	0	1
			Total	O		
41	F	6	6	6	0	0
			Total	O		
41	H	43	44	44	0	1
			Total	O		
41	I	6	6	6	0	0
			Total	O		
41	J	11	11	11	0	0
			Total	O		
41	K	8	8	8	0	0
			Total	O		
41	L	11	11	11	0	0
			Total	O		
41	M	10	11	11	0	1
			Total	O		
41	O	148	152	152	0	4
			Total	O		
41	T	13	13	13	0	0
			Total	O		
41	U	71	71	71	0	0
			Total	O		
41	V	102	103	103	0	1
			Total	O		
41	Y	4	5	5	0	1
			Total	O		
41	X	12	12	12	0	0
			Total	O		
41	Z	3	3	3	0	0
			Total	O		
41	a	125	126	126	0	1
			Total	O		
41	b	255	260	260	0	5
			Total	O		
41	c	201	203	203	0	2
			Total	O		
41	d	133	135	135	0	2
			Total	O		
41	e	19	20	20	0	1

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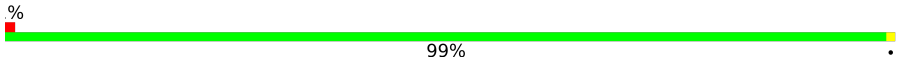
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	f	11	Total O 11 11	0	0
41	h	34	Total O 35 35	0	1
41	i	6	Total O 6 6	0	0
41	j	12	Total O 12 12	0	0
41	k	5	Total O 5 5	0	0
41	l	9	Total O 9 9	0	0
41	m	8	Total O 8 8	0	0
41	o	126	Total O 129 129	0	3
41	t	9	Total O 10 10	0	1
41	u	72	Total O 72 72	0	0
41	v	75	Total O 75 75	0	0
41	y	4	Total O 4 4	0	0
41	x	7	Total O 7 7	0	0
41	z	2	Total O 2 2	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.

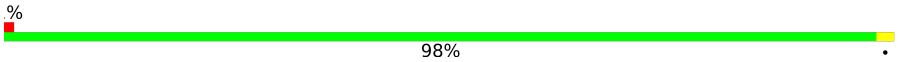
• Molecule 1: Photosystem II protein D1 1

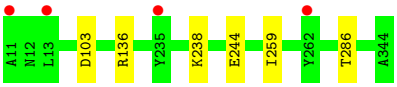
Chain A:



• Molecule 1: Photosystem II protein D1 1

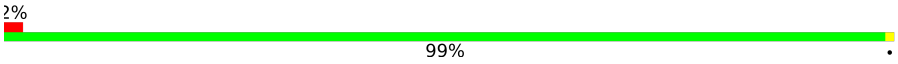
Chain a:

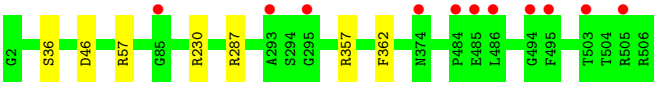




• Molecule 2: Photosystem II CP47 reaction center protein

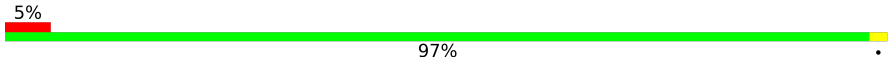
Chain B:

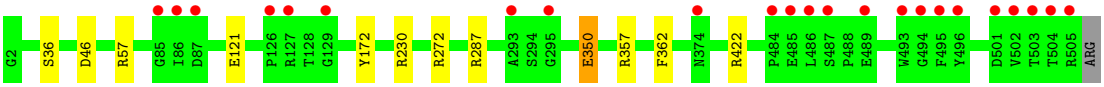




• Molecule 2: Photosystem II CP47 reaction center protein

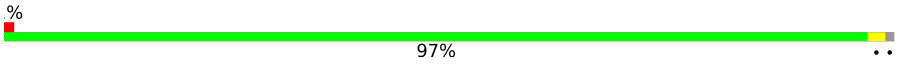
Chain b:

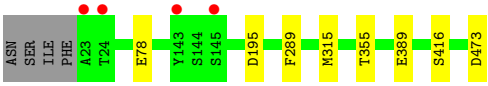




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:





• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 2% 97%

N19 S20 I21 Y143 S144 S145 D195 T200 F257 F289 M315 T355 E389 R390 R391 S416 V417 N418 R461 E462 D473

• Molecule 4: Photosystem II D2 protein

Chain D: % 98%

E11 R12 R26 R139 R180 R233 P237 T238 Q239 A240 M329 HSK336 P347 L352

• Molecule 4: Photosystem II D2 protein

Chain d: 2% 99%

E11 R26 R180 R233 A234 F235 N236 P237 T238 Q239 A240 R294 M329 HSK336 L352

• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 9% 95%

T4 R8 R61 E71 Q74 E77 E81 Q82 L83 LYS

• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 11% 98%

T4 T5 R8 I25 E59 Q60 R61 E77 T78 E81 Q82 L83 K84

• Molecule 6: Cytochrome b559 subunit beta

Chain F: 12% 94% 6%

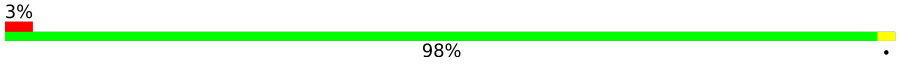
S12 Y13 P14 I15 F16 Q44 R45

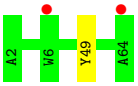
• Molecule 6: Cytochrome b559 subunit beta

Chain f: 3% 94% 6%

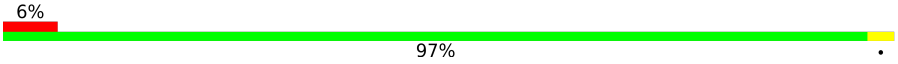
SER TYR P14 R45

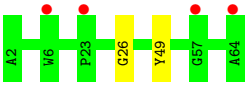
• Molecule 7: Photosystem II reaction center protein H

Chain H: 

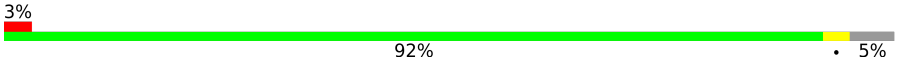


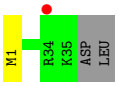
• Molecule 7: Photosystem II reaction center protein H

Chain h: 

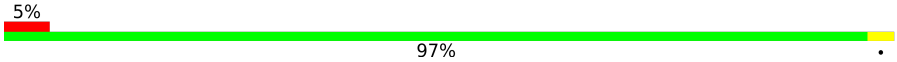


• Molecule 8: Photosystem II reaction center protein I

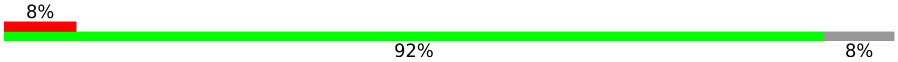
Chain I: 

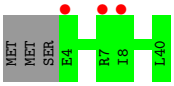


• Molecule 8: Photosystem II reaction center protein I

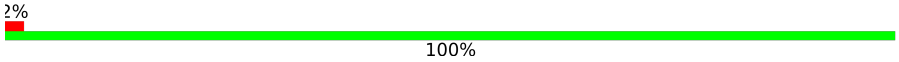
Chain i: 

• Molecule 9: Photosystem II reaction center protein J

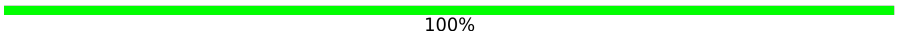
Chain J: 



• Molecule 9: Photosystem II reaction center protein J

Chain j: 

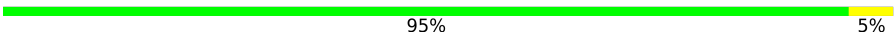
• Molecule 10: Photosystem II reaction center protein K

Chain K: 

There are no outlier residues recorded for this chain.

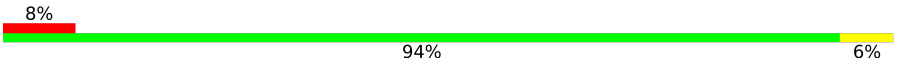
• Molecule 10: Photosystem II reaction center protein K

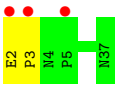
Chain k:



• Molecule 11: Photosystem II reaction center protein L

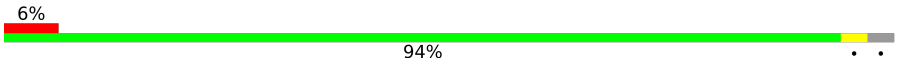
Chain L:

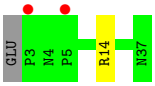




• Molecule 11: Photosystem II reaction center protein L

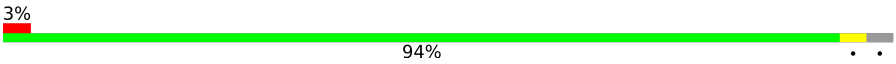
Chain l:





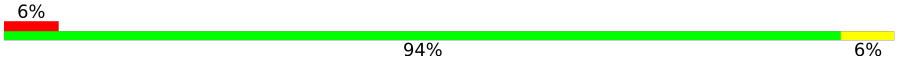
• Molecule 12: Photosystem II reaction center protein M

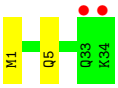
Chain M:



• Molecule 12: Photosystem II reaction center protein M

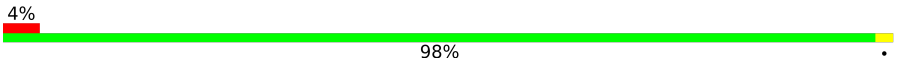
Chain m:

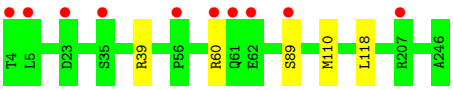




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

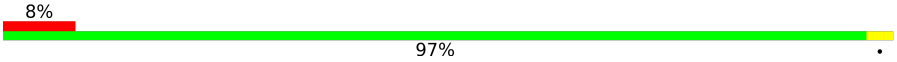
Chain O:

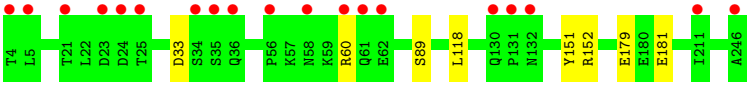




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

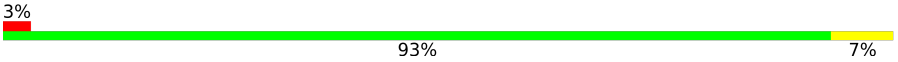




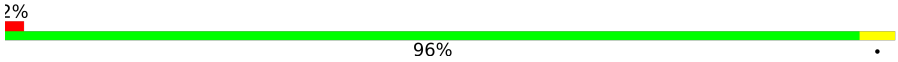
• Molecule 14: Photosystem II reaction center protein T

Chain T:

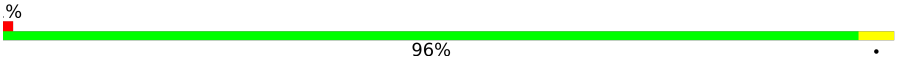
• Molecule 14: Photosystem II reaction center protein T

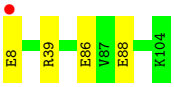
Chain t: 

• Molecule 15: Photosystem II 12 kDa extrinsic protein

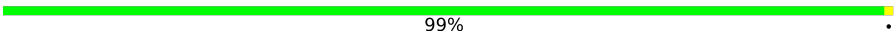
Chain U: 

• Molecule 15: Photosystem II 12 kDa extrinsic protein

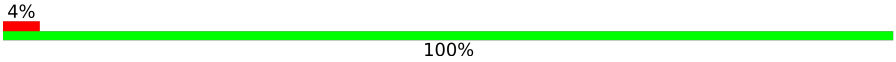
Chain u: 

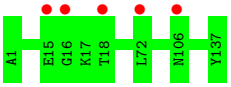


• Molecule 16: Cytochrome c-550

Chain V: 

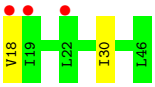
• Molecule 16: Cytochrome c-550

Chain v: 



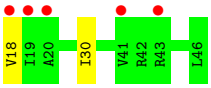
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 10% 93% 7%



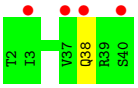
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 17% 93% 7%



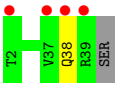
• Molecule 18: Photosystem II reaction center X protein

Chain X: 10% 97%



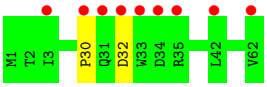
• Molecule 18: Photosystem II reaction center X protein

Chain x: 10% 95%



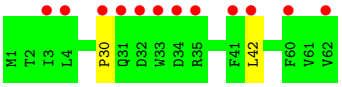
• Molecule 19: Photosystem II reaction center protein Z

Chain Z: 15% 97%



• Molecule 19: Photosystem II reaction center protein Z

Chain z: 19% 97%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.25Å 228.43Å 287.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.10 19.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.99-2.10) 99.5 (19.93-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.154 , 0.197 0.164 , 0.202	Depositor DCC
R_{free} test set	23043 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.9	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	0.97	EDS
Total number of atoms	53800	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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: FME, LHG, PL9, HTG, CA, PHO, CLA, OEX, HEM, BCR, CL, LMT, HEC, LMG, DMS, RRX, DGD, MG, HSK, BCT, FE2, UNL, GOL

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	1.01	0/2711	0.84	2/3699 (0.1%)
1	a	0.97	0/2714	0.83	2/3702 (0.1%)
2	B	0.95	1/4149 (0.0%)	0.84	9/5655 (0.2%)
2	b	0.97	3/4128 (0.1%)	0.86	7/5628 (0.1%)
3	C	0.94	2/3639 (0.1%)	0.82	2/4953 (0.0%)
3	c	0.91	1/3645 (0.0%)	0.81	7/4962 (0.1%)
4	D	0.98	0/2821	0.84	2/3843 (0.1%)
4	d	0.95	0/2813	0.84	1/3831 (0.0%)
5	E	0.87	0/684	0.87	2/935 (0.2%)
5	e	0.86	0/668	0.89	1/913 (0.1%)
6	F	0.94	0/283	0.75	0/386
6	f	0.86	0/265	0.67	0/360
7	H	0.87	0/522	0.77	0/712
7	h	0.90	0/519	0.80	0/708
8	I	0.84	0/281	0.82	0/381
8	i	0.83	0/291	0.79	0/394
9	J	0.87	0/268	0.79	0/363
9	j	0.90	0/285	0.86	0/386
10	K	0.75	0/306	0.77	0/422
10	k	0.72	0/295	0.73	0/407
11	L	1.06	0/298	0.90	1/406 (0.2%)
11	l	1.01	0/303	0.86	1/413 (0.2%)
12	M	0.93	0/257	0.75	0/352
12	m	0.95	0/262	0.86	0/359
13	O	0.89	0/1907	0.91	1/2589 (0.0%)
13	o	0.86	1/1907 (0.1%)	0.88	2/2591 (0.1%)
14	T	1.03	0/258	0.94	1/349 (0.3%)
14	t	0.96	0/258	0.89	0/349
15	U	1.04	1/796 (0.1%)	1.00	2/1078 (0.2%)
15	u	1.05	1/794 (0.1%)	0.93	2/1076 (0.2%)
16	V	0.99	0/1104	0.92	1/1498 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.91	0/1084	0.84	0/1475
17	Y	0.69	0/218	0.81	0/292
17	y	0.63	0/210	0.80	0/281
18	X	0.80	0/295	0.73	0/399
18	x	0.77	0/292	0.74	0/395
19	Z	0.75	0/476	0.71	0/652
19	z	0.65	0/470	0.69	1/645 (0.2%)
All	All	0.94	10/42476 (0.0%)	0.84	47/57839 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	U	88	GLU	CD-OE2	7.36	1.33	1.25
2	B	36	SER	CB-OG	-6.90	1.33	1.42
3	c	389	GLU	CD-OE2	6.24	1.32	1.25
3	C	389[A]	GLU	CD-OE2	6.18	1.32	1.25
3	C	389[B]	GLU	CD-OE2	6.18	1.32	1.25
15	u	88	GLU	CD-OE2	6.17	1.32	1.25
2	b	36	SER	CB-OG	-5.81	1.34	1.42
13	o	151	TYR	CE1-CZ	5.76	1.46	1.38
2	b	350	GLU	CD-OE1	5.74	1.31	1.25
2	b	172	TYR	CE1-CZ	5.01	1.45	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	57	ARG	NE-CZ-NH1	7.50	124.05	120.30
13	O	39	ARG	NE-CZ-NH1	7.26	123.93	120.30
3	c	391[A]	ARG	NE-CZ-NH2	-6.47	117.07	120.30
3	c	391[B]	ARG	NE-CZ-NH2	-6.47	117.07	120.30
2	B	57	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	b	287	ARG	NE-CZ-NH2	-6.43	117.08	120.30
2	B	287[A]	ARG	NE-CZ-NH2	-6.37	117.11	120.30
2	B	287[B]	ARG	NE-CZ-NH2	-6.37	117.11	120.30
3	C	473	ASP	CB-CG-OD1	6.31	123.98	118.30
15	U	39	ARG	NE-CZ-NH2	-6.29	117.15	120.30
2	B	46	ASP	CB-CG-OD2	-6.22	112.70	118.30
4	d	294	ARG	NE-CZ-NH2	-6.14	117.23	120.30
3	c	473	ASP	CB-CG-OD1	6.07	123.77	118.30
16	V	96	ARG	NE-CZ-NH2	-5.82	117.39	120.30
11	l	14	ARG	NE-CZ-NH2	-5.82	117.39	120.30
4	D	233	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	8	ARG	NE-CZ-NH2	-5.75	117.42	120.30
5	E	8	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	b	230	ARG	NE-CZ-NH2	5.68	123.14	120.30
2	b	357	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	B	46	ASP	CB-CG-OD1	5.55	123.30	118.30
2	b	422	ARG	NE-CZ-NH1	5.55	123.07	120.30
19	z	42	LEU	CA-CB-CG	5.54	128.04	115.30
15	U	39	ARG	NE-CZ-NH1	5.48	123.04	120.30
5	E	8	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	206	PHE	CB-CG-CD1	5.40	124.58	120.80
15	u	39	ARG	NE-CZ-NH2	-5.37	117.61	120.30
15	u	39	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	B	287[A]	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	B	287[B]	ARG	NE-CZ-NH1	5.32	122.96	120.30
13	o	33	ASP	CB-CG-OD1	5.29	123.06	118.30
14	T	28	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	B	357	ARG	NE-CZ-NH1	5.23	122.92	120.30
3	C	195	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	a	136	ARG	NE-CZ-NH2	5.17	122.89	120.30
13	o	152	ARG	NE-CZ-NH1	-5.17	117.71	120.30
3	c	195	ASP	CB-CG-OD2	-5.16	113.66	118.30
2	b	46	ASP	CB-CG-OD1	5.15	122.94	118.30
4	D	139	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	c	389	GLU	OE1-CD-OE2	5.13	129.46	123.30
2	B	230	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	a	103	ASP	CB-CG-OD1	5.11	122.90	118.30
11	L	2	GLU	C-N-CA	5.08	143.34	122.00
2	b	272	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	206	PHE	CB-CG-CD2	-5.07	117.25	120.80
3	c	195	ASP	CB-CG-OD1	5.03	122.82	118.30
3	c	461	ARG	NE-CZ-NH2	5.01	122.81	120.30

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	334/334 (100%)	328 (98%)	5 (2%)	1 (0%)	41	41
1	a	334/334 (100%)	327 (98%)	6 (2%)	1 (0%)	41	41
2	B	508/505 (101%)	501 (99%)	7 (1%)	0	100	100
2	b	506/505 (100%)	498 (98%)	8 (2%)	0	100	100
3	C	454/455 (100%)	444 (98%)	9 (2%)	1 (0%)	47	49
3	c	455/455 (100%)	446 (98%)	8 (2%)	1 (0%)	47	49
4	D	341/342 (100%)	336 (98%)	5 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	80/81 (99%)	78 (98%)	2 (2%)	0	100	100
5	e	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	62/63 (98%)	56 (90%)	6 (10%)	0	100	100
7	h	62/63 (98%)	57 (92%)	4 (6%)	1 (2%)	9	5
8	I	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
8	i	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
9	J	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	35/36 (97%)	34 (97%)	0	1 (3%)	4	1
11	l	35/36 (97%)	35 (100%)	0	0	100	100
12	M	32/34 (94%)	32 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	239 (98%)	5 (2%)	1 (0%)	34	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	247/243 (102%)	240 (97%)	6 (2%)	1 (0%)	34	32
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	96/97 (99%)	94 (98%)	2 (2%)	0	100	100
15	u	96/97 (99%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	133 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
17	Y	28/29 (97%)	27 (96%)	1 (4%)	0	100	100
17	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
All	All	5227/5270 (99%)	5106 (98%)	111 (2%)	10 (0%)	47	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	L	3	PRO
3	C	416	SER
3	c	416	SER
13	O	60	ARG
19	Z	30	PRO
13	o	60	ARG
19	z	30	PRO
1	A	259	ILE
1	a	259	ILE
7	h	26	GLY

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	269/270 (100%)	266 (99%)	3 (1%)	73	79
1	a	270/270 (100%)	267 (99%)	3 (1%)	73	79
2	B	404/403 (100%)	403 (100%)	1 (0%)	93	96
2	b	402/403 (100%)	399 (99%)	3 (1%)	84	88
3	C	356/356 (100%)	351 (99%)	5 (1%)	67	73
3	c	356/356 (100%)	349 (98%)	7 (2%)	55	60
4	D	277/276 (100%)	273 (99%)	4 (1%)	67	73
4	d	276/276 (100%)	273 (99%)	3 (1%)	73	79
5	E	72/72 (100%)	69 (96%)	3 (4%)	30	30
5	e	68/72 (94%)	67 (98%)	1 (2%)	65	71
6	F	27/28 (96%)	25 (93%)	2 (7%)	13	10
6	f	26/28 (93%)	26 (100%)	0	100	100
7	H	54/53 (102%)	53 (98%)	1 (2%)	57	63
7	h	54/53 (102%)	53 (98%)	1 (2%)	57	63
8	I	30/33 (91%)	30 (100%)	0	100	100
8	i	31/33 (94%)	31 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	30 (100%)	0	100	100
10	k	28/30 (93%)	26 (93%)	2 (7%)	14	11
11	L	32/34 (94%)	32 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	29/30 (97%)	29 (100%)	0	100	100
12	m	29/30 (97%)	28 (97%)	1 (3%)	37	39
13	O	205/206 (100%)	202 (98%)	3 (2%)	65	71
13	o	203/206 (98%)	199 (98%)	4 (2%)	55	60
14	T	26/26 (100%)	25 (96%)	1 (4%)	33	34
14	t	26/26 (100%)	25 (96%)	1 (4%)	33	34
15	U	85/84 (101%)	82 (96%)	3 (4%)	36	38
15	u	85/84 (101%)	83 (98%)	2 (2%)	49	53
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	115/117 (98%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	Y	22/22 (100%)	20 (91%)	2 (9%)	9 6
17	y	20/22 (91%)	18 (90%)	2 (10%)	7 5
18	X	31/32 (97%)	30 (97%)	1 (3%)	39 41
18	x	32/32 (100%)	31 (97%)	1 (3%)	40 43
19	Z	49/52 (94%)	48 (98%)	1 (2%)	55 60
19	z	47/52 (90%)	47 (100%)	0	100 100
All	All	4268/4304 (99%)	4207 (99%)	61 (1%)	67 73

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	244	GLU
1	A	286	THR
2	B	362	PHE
3	C	78	GLU
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	355	THR
4	D	26	ARG
4	D	180	ARG
4	D	329	MET
4	D	347	PRO
5	E	4	THR
5	E	77[A]	GLU
5	E	77[B]	GLU
6	F	16	PHE
6	F	44	GLN
7	H	49	TYR
13	O	89	SER
13	O	110	MET
13	O	118	LEU
14	T	29	ILE
15	U	51	LYS
15	U	70[A]	ARG
15	U	70[B]	ARG
17	Y	18	VAL
17	Y	30	ILE
18	X	38	GLN

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Mol	Chain	Res	Type
19	Z	32	ASP
1	a	238	LYS
1	a	244	GLU
1	a	286	THR
2	b	121	GLU
2	b	350	GLU
2	b	362	PHE
3	c	19	ASN
3	c	21	ILE
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET
3	c	355	THR
3	c	418	ASN
4	d	26	ARG
4	d	180	ARG
4	d	329	MET
5	e	77	GLU
7	h	49	TYR
10	k	19	ASP
10	k	27	VAL
12	m	5	GLN
13	o	89	SER
13	o	118	LEU
13	o	179	GLU
13	o	181	GLU
14	t	25	GLU
15	u	8	GLU
15	u	86	GLU
17	y	18	VAL
17	y	30	ILE
18	x	38	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	216	HIS
2	B	331	ASN
3	C	28	GLN
3	C	228	ASN
3	C	311	GLN

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Mol	Chain	Res	Type
2	b	53	ASN
2	b	179	GLN
2	b	289	GLN
2	b	331	ASN
3	c	28	GLN
3	c	228	ASN
13	o	82	GLN
13	o	104	GLN
16	v	34	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)

10 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	$\#\|Z\| > 2$
12	FME	M	1	12	8,9,10	1.32	1 (12%)	7,9,11	1.19	0
8	FME	i	1	8	8,9,10	0.35	0	7,9,11	1.72	2 (28%)
14	FME	T	1	14	8,9,10	0.75	0	7,9,11	1.63	2 (28%)
8	FME	I	1	8	8,9,10	0.72	0	7,9,11	1.81	3 (42%)
12	FME	m	1	12	8,9,10	1.09	1 (12%)	7,9,11	1.01	0
4	HSK	d	336[B]	-	7,11,12	1.34	1 (14%)	3,14,16	1.22	0
4	HSK	D	336[B]	-	7,11,12	2.26	1 (14%)	3,14,16	1.56	1 (33%)
4	HSK	d	336[A]	-	7,10,12	1.30	1 (14%)	3,12,16	1.35	0
4	HSK	D	336[A]	-	7,10,12	1.36	1 (14%)	3,12,16	1.89	1 (33%)
14	FME	t	1	14	8,9,10	0.83	0	7,9,11	1.38	1 (14%)

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
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
14	FME	t	1	14	-	3/7/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[B]	HSK	CE1-ND1	-5.83	1.29	1.36
4	D	336[A]	HSK	CE1-ND1	-3.39	1.32	1.36
4	d	336[B]	HSK	CE1-ND1	-3.15	1.32	1.36
4	d	336[A]	HSK	CE1-ND1	-2.72	1.33	1.36
12	M	1	FME	CA-N	2.32	1.49	1.46
12	m	1	FME	CA-N	2.23	1.49	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	C-CA-N	3.30	115.69	109.73
8	I	1	FME	C-CA-N	3.12	115.36	109.73
4	D	336[A]	HSK	CD2-NE2-CE1	2.67	109.94	105.78
4	D	336[B]	HSK	CD2-NE2-CE1	2.39	109.50	105.78
8	I	1	FME	O-C-CA	-2.30	118.74	124.78
8	i	1	FME	O-C-CA	-2.27	118.84	124.78
8	I	1	FME	CA-N-CN	-2.25	119.36	122.82
14	t	1	FME	CE-SD-CG	2.17	107.85	100.40
14	T	1	FME	CE-SD-CG	2.11	107.64	100.40
14	T	1	FME	CA-N-CN	2.04	125.96	122.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

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 353 ligands modelled in this entry, 18 are monoatomic and 52 are unknown - leaving 283 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	$\#\|Z\| > 2$
23	PHO	D	404	-	51,69,69	1.84	9 (17%)	47,99,99	1.25	6 (12%)
29	DMS	B	633	-	3,3,3	2.55	1 (33%)	3,3,3	0.98	0
22	CLA	b	611	41	65,73,73	1.81	15 (23%)	76,113,113	2.29	24 (31%)
22	CLA	b	614	41	65,73,73	1.76	17 (26%)	76,113,113	2.10	24 (31%)
32	HTG	B	629	-	19,19,19	0.97	2 (10%)	23,24,24	1.46	3 (13%)
26	LMG	b	625	-	49,49,55	1.23	3 (6%)	57,57,63	1.18	6 (10%)
37	HEM	F	101	5,6	41,50,50	1.74	7 (17%)	45,82,82	1.92	12 (26%)
36	BCT	d	401[A]	35	2,3,3	0.58	0	2,3,3	1.26	0
22	CLA	c	508	41	65,73,73	2.08	20 (30%)	76,113,113	2.41	22 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	b	608	-	65,73,73	2.05	17 (26%)	76,113,113	2.50	27 (35%)
22	CLA	C	505	-	65,73,73	2.00	19 (29%)	76,113,113	2.20	19 (25%)
25	PL9	d	407	-	55,55,55	1.17	9 (16%)	68,69,69	1.47	9 (13%)
22	CLA	c	505	41	65,73,73	2.23	19 (29%)	76,113,113	2.32	27 (35%)
29	DMS	D	420	-	3,3,3	2.61	1 (33%)	3,3,3	0.95	0
29	DMS	b	638	-	3,3,3	3.10	1 (33%)	3,3,3	1.05	0
29	DMS	o	303	-	3,3,3	1.94	1 (33%)	3,3,3	0.78	0
22	CLA	B	613	-	65,73,73	1.89	11 (16%)	76,113,113	2.30	24 (31%)
28	LMT	B	623	-	36,36,36	0.80	1 (2%)	47,47,47	1.68	10 (21%)
32	HTG	c	541	-	15,15,19	1.17	1 (6%)	18,20,24	3.42	6 (33%)
29	DMS	c	530	-	3,3,3	2.72	1 (33%)	3,3,3	0.75	0
29	DMS	c	532	-	3,3,3	2.72	1 (33%)	3,3,3	0.89	0
22	CLA	B	610	-	65,73,73	1.88	14 (21%)	76,113,113	2.16	21 (27%)
29	DMS	C	530	-	3,3,3	2.06	1 (33%)	3,3,3	0.70	0
22	CLA	B	603	-	65,73,73	2.22	16 (24%)	76,113,113	2.23	24 (31%)
22	CLA	b	606	-	65,73,73	1.99	15 (23%)	76,113,113	2.31	30 (39%)
24	BCR	b	621	-	41,41,41	0.87	1 (2%)	56,56,56	1.47	9 (16%)
24	BCR	B	619	-	41,41,41	1.30	5 (12%)	56,56,56	1.43	7 (12%)
29	DMS	c	540	-	3,3,3	2.84	1 (33%)	3,3,3	0.97	0
29	DMS	u	204	-	3,3,3	2.75	1 (33%)	3,3,3	1.02	0
22	CLA	b	619	-	65,73,73	2.15	17 (26%)	76,113,113	2.45	29 (38%)
32	HTG	D	413	-	16,16,19	1.08	2 (12%)	20,21,24	2.53	6 (30%)
22	CLA	A	408	-	65,73,73	2.07	17 (26%)	76,113,113	2.28	22 (28%)
28	LMT	b	626	-	25,25,36	0.96	1 (4%)	30,30,47	1.57	3 (10%)
29	DMS	c	538	-	3,3,3	3.04	1 (33%)	3,3,3	1.05	0
26	LMG	d	412	39	47,47,55	0.99	3 (6%)	55,55,63	1.30	5 (9%)
32	HTG	O	302	-	19,19,19	1.64	4 (21%)	23,24,24	1.26	3 (13%)
22	CLA	d	405	-	65,73,73	2.12	18 (27%)	76,113,113	2.20	26 (34%)
22	CLA	b	617	-	65,73,73	1.89	14 (21%)	76,113,113	2.00	23 (30%)
29	DMS	o	305	-	3,3,3	2.67	1 (33%)	3,3,3	0.74	0
29	DMS	B	635	-	3,3,3	2.80	1 (33%)	3,3,3	0.64	0
29	DMS	O	304	-	3,3,3	2.65	1 (33%)	3,3,3	0.68	0
34	GOL	c	533	-	5,5,5	0.52	0	5,5,5	0.97	0
24	BCR	y	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.71	14 (25%)
23	PHO	d	404	-	51,69,69	1.73	7 (13%)	47,99,99	1.66	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
28	LMT	M	101	-	36,36,36	0.66	0	47,47,47	1.37	6 (12%)
29	DMS	D	416	-	3,3,3	2.65	1 (33%)	3,3,3	0.10	0
29	DMS	d	415	-	3,3,3	2.34	1 (33%)	3,3,3	0.81	0
29	DMS	O	307	-	3,3,3	2.72	1 (33%)	3,3,3	0.40	0
29	DMS	o	311	-	3,3,3	2.66	1 (33%)	3,3,3	0.88	0
22	CLA	C	506	-	65,73,73	2.03	14 (21%)	76,113,113	2.44	20 (26%)
31	LHG	E	101	-	48,48,48	1.04	2 (4%)	51,54,54	0.94	2 (3%)
26	LMG	C	518	-	49,49,55	1.07	2 (4%)	57,57,63	1.25	7 (12%)
29	DMS	b	631	-	3,3,3	2.63	1 (33%)	3,3,3	0.57	0
29	DMS	B	631	-	3,3,3	2.87	1 (33%)	3,3,3	0.91	0
29	DMS	a	416	-	3,3,3	2.85	1 (33%)	3,3,3	1.15	0
29	DMS	c	534	-	3,3,3	2.69	1 (33%)	3,3,3	0.44	0
22	CLA	c	503	-	65,73,73	2.00	15 (23%)	76,113,113	2.19	26 (34%)
29	DMS	u	202	-	3,3,3	2.76	1 (33%)	3,3,3	1.44	0
29	DMS	o	310	-	3,3,3	2.89	1 (33%)	3,3,3	1.04	0
29	DMS	O	312	-	3,3,3	2.72	1 (33%)	3,3,3	0.68	0
24	BCR	b	623	-	41,41,41	1.17	4 (9%)	56,56,56	1.40	9 (16%)
29	DMS	O	311	-	3,3,3	2.64	1 (33%)	3,3,3	1.71	1 (33%)
29	DMS	A	418	-	3,3,3	2.66	1 (33%)	3,3,3	1.18	0
26	LMG	c	520	-	38,38,55	1.29	2 (5%)	46,46,63	1.33	5 (10%)
32	HTG	U	203	-	14,14,19	0.99	1 (7%)	18,19,24	2.78	8 (44%)
22	CLA	c	513	-	65,73,73	2.20	18 (27%)	76,113,113	2.18	24 (31%)
29	DMS	b	634	-	3,3,3	2.71	1 (33%)	3,3,3	0.67	0
22	CLA	C	510	-	65,73,73	2.04	20 (30%)	76,113,113	2.19	18 (23%)
29	DMS	O	305	-	3,3,3	2.90	1 (33%)	3,3,3	1.17	0
20	OEX	A	401	1,3,41	0,15,15	-	-	-		
22	CLA	B	617	-	65,73,73	1.98	17 (26%)	76,113,113	2.39	28 (36%)
29	DMS	B	641	-	3,3,3	2.83	1 (33%)	3,3,3	1.00	0
28	LMT	j	102	-	23,23,36	0.89	0	27,27,47	1.94	6 (22%)
36	BCT	D	402[A]	35	2,3,3	0.45	0	2,3,3	0.63	0
32	HTG	c	524	-	8,8,19	0.55	0	7,7,24	1.33	1 (14%)
29	DMS	O	310	-	3,3,3	2.71	1 (33%)	3,3,3	0.89	0
29	DMS	O	303	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
22	CLA	c	512	3	65,73,73	2.60	18 (27%)	76,113,113	2.20	21 (27%)
29	DMS	v	204	-	3,3,3	2.69	1 (33%)	3,3,3	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	C	511	3	65,73,73	2.42	16 (24%)	76,113,113	2.49	23 (30%)
29	DMS	A	417	-	3,3,3	2.02	1 (33%)	3,3,3	0.55	0
28	LMT	F	102	-	24,24,36	1.31	3 (12%)	29,29,47	1.44	6 (20%)
29	DMS	C	531	-	3,3,3	2.72	1 (33%)	3,3,3	0.72	0
29	DMS	O	309	-	3,3,3	2.76	1 (33%)	3,3,3	0.91	0
29	DMS	c	535	-	3,3,3	2.61	1 (33%)	3,3,3	0.30	0
29	DMS	c	539	-	3,3,3	2.59	1 (33%)	3,3,3	0.48	0
29	DMS	o	306	-	3,3,3	2.55	1 (33%)	3,3,3	1.00	0
29	DMS	o	308	-	3,3,3	2.81	1 (33%)	3,3,3	0.41	0
32	HTG	o	301	-	19,19,19	1.94	3 (15%)	23,24,24	1.78	7 (30%)
26	LMG	C	519	-	48,48,55	1.29	3 (6%)	56,56,63	1.79	12 (21%)
29	DMS	C	526	-	3,3,3	2.76	1 (33%)	3,3,3	1.19	0
29	DMS	B	640	-	3,3,3	3.00	1 (33%)	3,3,3	1.33	1 (33%)
32	HTG	b	627	-	19,19,19	0.98	1 (5%)	23,24,24	2.00	4 (17%)
22	CLA	c	510	-	65,73,73	2.13	16 (24%)	76,113,113	2.42	26 (34%)
29	DMS	c	536	-	3,3,3	2.69	1 (33%)	3,3,3	1.07	0
22	CLA	C	513	-	65,73,73	2.74	17 (26%)	76,113,113	2.11	23 (30%)
31	LHG	d	410	-	48,48,48	0.63	1 (2%)	51,54,54	1.23	5 (9%)
22	CLA	B	614	-	65,73,73	2.06	16 (24%)	76,113,113	2.12	20 (26%)
32	HTG	B	642	-	18,18,19	1.11	2 (11%)	22,23,24	2.72	10 (45%)
22	CLA	b	618	-	65,73,73	2.01	19 (29%)	76,113,113	2.50	29 (38%)
26	LMG	c	521	-	51,51,55	1.15	3 (5%)	59,59,63	1.12	7 (11%)
29	DMS	I	105	-	3,3,3	2.69	1 (33%)	3,3,3	1.03	0
29	DMS	B	639	-	3,3,3	2.59	1 (33%)	3,3,3	0.95	0
31	LHG	b	624	-	48,48,48	0.75	2 (4%)	51,54,54	1.10	5 (9%)
29	DMS	h	104	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
22	CLA	c	507	-	65,73,73	1.90	14 (21%)	76,113,113	2.37	24 (31%)
34	GOL	b	636	-	5,5,5	0.09	0	5,5,5	0.40	0
29	DMS	C	528	-	3,3,3	2.55	1 (33%)	3,3,3	0.52	0
24	BCR	B	620	-	41,41,41	1.24	3 (7%)	56,56,56	1.34	9 (16%)
31	LHG	D	411	-	43,43,48	1.12	3 (6%)	46,49,54	1.08	4 (8%)
22	CLA	b	607	-	65,73,73	1.88	15 (23%)	76,113,113	2.25	22 (28%)
22	CLA	C	507	41	65,73,73	2.30	22 (33%)	76,113,113	2.18	16 (21%)
23	PHO	a	408	-	51,69,69	1.73	9 (17%)	47,99,99	1.10	4 (8%)
24	BCR	t	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.90	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	HTG	C	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.98	2 (8%)
29	DMS	B	632	-	3,3,3	2.43	1 (33%)	3,3,3	1.58	1 (33%)
29	DMS	a	418	-	3,3,3	2.79	1 (33%)	3,3,3	0.71	0
33	DGD	d	408	-	48,48,67	1.37	5 (10%)	56,56,81	1.58	8 (14%)
28	LMT	A	415	-	36,36,36	1.33	4 (11%)	47,47,47	1.97	15 (31%)
22	CLA	B	605	-	65,73,73	1.90	16 (24%)	76,113,113	2.36	30 (39%)
22	CLA	B	607	-	65,73,73	2.19	18 (27%)	76,113,113	2.14	22 (28%)
32	HTG	V	202	-	19,19,19	1.02	2 (10%)	23,24,24	3.35	7 (30%)
28	LMT	a	401	-	36,36,36	1.26	3 (8%)	47,47,47	2.27	16 (34%)
22	CLA	b	613	-	65,73,73	2.17	19 (29%)	76,113,113	2.05	20 (26%)
22	CLA	c	511	-	65,73,73	1.84	15 (23%)	76,113,113	2.50	27 (35%)
29	DMS	e	105	-	3,3,3	2.74	1 (33%)	3,3,3	1.02	0
29	DMS	o	304	-	3,3,3	2.57	1 (33%)	3,3,3	1.49	0
22	CLA	c	509	-	65,73,73	2.33	17 (26%)	76,113,113	2.14	19 (25%)
29	DMS	b	635	-	3,3,3	2.89	1 (33%)	3,3,3	0.94	0
22	CLA	D	403	-	65,73,73	1.94	18 (27%)	76,113,113	2.24	21 (27%)
29	DMS	C	525	-	3,3,3	2.47	1 (33%)	3,3,3	1.10	0
29	DMS	A	419	-	3,3,3	2.96	1 (33%)	3,3,3	0.81	0
24	BCR	K	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.36	10 (17%)
33	DGD	D	408	-	45,45,67	1.49	4 (8%)	53,53,81	1.70	10 (18%)
29	DMS	v	203	-	3,3,3	2.51	1 (33%)	3,3,3	0.76	0
40	HEC	V	201	16	32,50,50	2.02	6 (18%)	24,82,82	1.70	6 (25%)
24	BCR	K	102	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	3 (5%)
32	HTG	C	536	-	19,19,19	1.22	2 (10%)	23,24,24	1.82	1 (4%)
33	DGD	h	101	-	63,63,67	1.20	4 (6%)	77,77,81	1.43	15 (19%)
34	GOL	e	104	-	5,5,5	0.82	0	5,5,5	1.63	1 (20%)
26	LMG	D	412	39	47,47,55	1.05	3 (6%)	55,55,63	1.14	3 (5%)
29	DMS	o	307	-	3,3,3	2.70	1 (33%)	3,3,3	1.24	0
24	BCR	C	514	-	41,41,41	1.16	4 (9%)	56,56,56	1.31	4 (7%)
24	BCR	c	516	-	41,41,41	1.11	3 (7%)	56,56,56	1.37	8 (14%)
29	DMS	D	415	-	3,3,3	2.59	1 (33%)	3,3,3	1.23	0
24	BCR	A	409	-	41,41,41	1.44	8 (19%)	56,56,56	1.55	7 (12%)
24	BCR	T	101	-	41,41,41	0.95	0	56,56,56	1.79	14 (25%)
29	DMS	a	420	-	3,3,3	2.81	1 (33%)	3,3,3	1.07	0
29	DMS	b	637	-	3,3,3	2.56	1 (33%)	3,3,3	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	DMS	B	638	-	3,3,3	2.31	1 (33%)	3,3,3	1.19	0
29	DMS	b	632	-	3,3,3	2.62	1 (33%)	3,3,3	0.90	0
22	CLA	d	402	-	65,73,73	1.82	15 (23%)	76,113,113	2.03	25 (32%)
28	LMT	z	101	-	33,33,36	8.08	2 (6%)	44,44,47	2.76	11 (25%)
29	DMS	c	529	-	3,3,3	2.92	1 (33%)	3,3,3	0.89	0
29	DMS	U	202	-	3,3,3	2.61	1 (33%)	3,3,3	1.60	1 (33%)
29	DMS	v	206	-	3,3,3	2.65	1 (33%)	3,3,3	1.12	0
29	DMS	C	529	-	3,3,3	2.64	1 (33%)	3,3,3	0.81	0
38	RRX	h	102	-	42,42,42	0.98	2 (4%)	57,58,58	1.61	11 (19%)
22	CLA	b	616	-	65,73,73	2.01	16 (24%)	76,113,113	2.60	24 (31%)
34	GOL	D	417	-	5,5,5	0.48	0	5,5,5	0.47	0
29	DMS	D	419	-	3,3,3	2.73	1 (33%)	3,3,3	0.68	0
28	LMT	m	102	-	24,24,36	0.84	1 (4%)	29,29,47	1.03	3 (10%)
28	LMT	c	522	-	36,36,36	0.98	1 (2%)	47,47,47	1.92	10 (21%)
22	CLA	A	406	41	65,73,73	1.65	17 (26%)	76,113,113	2.13	21 (27%)
29	DMS	b	630	-	3,3,3	1.99	1 (33%)	3,3,3	0.40	0
32	HTG	C	535	-	8,8,19	0.55	0	7,7,24	1.05	1 (14%)
29	DMS	B	637	-	3,3,3	2.59	1 (33%)	3,3,3	1.10	0
25	PL9	D	407	-	55,55,55	1.11	6 (10%)	68,69,69	1.47	7 (10%)
31	LHG	d	411	-	43,43,48	1.03	3 (6%)	46,49,54	0.99	5 (10%)
32	HTG	B	628	-	19,19,19	0.49	0	23,24,24	1.76	2 (8%)
22	CLA	B	604	-	65,73,73	1.69	12 (18%)	76,113,113	2.64	28 (36%)
22	CLA	B	608	41	65,73,73	1.77	14 (21%)	76,113,113	2.06	21 (27%)
29	DMS	d	416	-	3,3,3	2.74	1 (33%)	3,3,3	0.95	0
28	LMT	Z	101	-	36,36,36	0.84	2 (5%)	47,47,47	1.46	7 (14%)
22	CLA	a	409	-	65,73,73	1.70	14 (21%)	76,113,113	2.28	20 (26%)
28	LMT	t	102	-	24,24,36	1.12	2 (8%)	29,29,47	1.45	5 (17%)
22	CLA	C	502	-	65,73,73	2.08	15 (23%)	76,113,113	2.40	23 (30%)
29	DMS	O	308	-	3,3,3	2.72	1 (33%)	3,3,3	1.60	1 (33%)
22	CLA	A	404	-	65,73,73	1.83	15 (23%)	76,113,113	2.27	23 (30%)
29	DMS	C	527	-	3,3,3	2.64	1 (33%)	3,3,3	1.11	0
31	LHG	D	410	-	48,48,48	0.79	3 (6%)	51,54,54	1.07	2 (3%)
20	OEX	a	402	1,3,41	0,15,15	-	-	-		
32	HTG	B	624	-	19,19,19	1.01	1 (5%)	23,24,24	2.08	2 (8%)
32	HTG	c	523	-	19,19,19	0.70	0	23,24,24	1.49	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	PL9	A	410	-	55,55,55	1.15	4 (7%)	68,69,69	2.12	17 (25%)
29	DMS	b	633	-	3,3,3	2.76	1 (33%)	3,3,3	1.10	0
28	LMT	J	102	-	24,24,36	0.80	1 (4%)	29,29,47	1.23	3 (10%)
33	DGD	C	517	-	63,63,67	0.95	4 (6%)	77,77,81	1.17	9 (11%)
29	DMS	V	207	-	3,3,3	2.81	1 (33%)	3,3,3	0.56	0
22	CLA	B	609	-	65,73,73	1.92	15 (23%)	76,113,113	2.38	22 (28%)
22	CLA	c	506	-	65,73,73	1.98	20 (30%)	76,113,113	2.15	25 (32%)
22	CLA	B	612	-	65,73,73	1.94	14 (21%)	76,113,113	2.44	24 (31%)
22	CLA	b	605	41	65,73,73	2.20	16 (24%)	76,113,113	2.48	28 (36%)
22	CLA	c	514	-	65,73,73	2.09	17 (26%)	76,113,113	2.22	26 (34%)
22	CLA	A	405	41	65,73,73	1.99	16 (24%)	76,113,113	2.65	25 (32%)
29	DMS	b	639	-	3,3,3	2.57	1 (33%)	3,3,3	1.52	0
29	DMS	v	207	-	3,3,3	2.99	1 (33%)	3,3,3	1.23	1 (33%)
22	CLA	C	503	-	65,73,73	1.98	16 (24%)	76,113,113	2.09	24 (31%)
22	CLA	b	615	-	65,73,73	1.82	13 (20%)	76,113,113	1.96	22 (28%)
24	BCR	k	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	6 (10%)
29	DMS	C	534	-	3,3,3	2.78	1 (33%)	3,3,3	1.01	0
29	DMS	V	208	-	3,3,3	2.49	1 (33%)	3,3,3	1.17	1 (33%)
29	DMS	V	205	-	3,3,3	2.70	1 (33%)	3,3,3	0.96	0
29	DMS	c	531	-	3,3,3	2.64	1 (33%)	3,3,3	0.66	0
29	DMS	v	205	-	3,3,3	2.46	1 (33%)	3,3,3	0.84	0
32	HTG	d	413	-	16,16,19	0.98	1 (6%)	20,21,24	3.85	6 (30%)
33	DGD	c	519	-	63,63,67	1.04	4 (6%)	77,77,81	1.38	11 (14%)
33	DGD	c	518	-	57,57,67	0.95	4 (7%)	71,71,81	1.09	7 (9%)
29	DMS	E	104	-	3,3,3	2.75	1 (33%)	3,3,3	1.00	0
33	DGD	c	517	-	63,63,67	1.05	3 (4%)	77,77,81	1.06	5 (6%)
23	PHO	A	407	-	51,69,69	1.51	8 (15%)	47,99,99	1.35	9 (19%)
28	LMT	T	102	-	24,24,36	0.57	0	29,29,47	1.55	7 (24%)
36	BCT	D	402[B]	35	2,3,3	0.63	0	2,3,3	0.78	0
24	BCR	a	410	-	41,41,41	1.05	4 (9%)	56,56,56	1.10	5 (8%)
24	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.37	11 (19%)
22	CLA	c	502	-	65,73,73	2.56	18 (27%)	76,113,113	2.71	23 (30%)
31	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.62	4 (7%)
32	HTG	v	208	-	16,16,19	0.92	1 (6%)	20,21,24	3.35	6 (30%)
28	LMT	m	103	-	23,23,36	0.88	0	27,27,47	1.70	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	DGD	C	515	-	63,63,67	1.01	4 (6%)	77,77,81	1.23	7 (9%)
22	CLA	B	616	-	65,73,73	2.44	19 (29%)	76,113,113	2.31	21 (27%)
29	DMS	D	418	-	3,3,3	2.59	1 (33%)	3,3,3	1.66	0
22	CLA	B	615	-	65,73,73	2.01	13 (20%)	76,113,113	2.54	27 (35%)
28	LMT	M	102	-	24,24,36	0.82	0	29,29,47	1.27	3 (10%)
34	GOL	C	533	-	5,5,5	0.54	0	5,5,5	1.67	1 (20%)
36	BCT	d	401[B]	35	2,3,3	0.78	0	2,3,3	0.66	0
22	CLA	c	504	-	65,73,73	2.55	19 (29%)	76,113,113	2.28	17 (22%)
24	BCR	d	406	-	41,41,41	1.10	2 (4%)	56,56,56	1.61	10 (17%)
22	CLA	B	602	41	65,73,73	2.45	19 (29%)	76,113,113	2.25	28 (36%)
22	CLA	C	512	-	65,73,73	2.26	17 (26%)	76,113,113	2.31	26 (34%)
29	DMS	c	537	-	3,3,3	2.64	1 (33%)	3,3,3	1.13	0
22	CLA	C	508	-	65,73,73	2.14	17 (26%)	76,113,113	2.11	20 (26%)
22	CLA	C	504	41	65,73,73	2.24	16 (24%)	76,113,113	2.21	17 (22%)
24	BCR	c	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.37	8 (14%)
28	LMT	l	101	-	24,24,36	0.83	1 (4%)	29,29,47	0.97	1 (3%)
29	DMS	A	416	-	3,3,3	2.74	1 (33%)	3,3,3	1.01	0
29	DMS	O	306	-	3,3,3	2.80	1 (33%)	3,3,3	1.14	0
32	HTG	b	601	-	19,19,19	1.08	2 (10%)	23,24,24	1.44	4 (17%)
40	HEC	v	202	16	32,50,50	2.15	9 (28%)	24,82,82	1.84	7 (29%)
22	CLA	B	606	-	65,73,73	2.16	16 (24%)	76,113,113	2.46	21 (27%)
22	CLA	b	610	-	65,73,73	2.35	15 (23%)	76,113,113	2.44	23 (30%)
33	DGD	H	101	-	63,63,67	1.22	4 (6%)	77,77,81	1.63	13 (16%)
29	DMS	C	532	-	3,3,3	3.06	1 (33%)	3,3,3	0.95	0
29	DMS	o	309	-	3,3,3	2.65	1 (33%)	3,3,3	1.45	0
22	CLA	b	612	-	65,73,73	1.93	15 (23%)	76,113,113	2.25	25 (32%)
29	DMS	V	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
33	DGD	C	516	-	63,63,67	1.06	5 (7%)	77,77,81	1.00	4 (5%)
22	CLA	b	620	-	65,73,73	2.25	17 (26%)	76,113,113	2.28	26 (34%)
22	CLA	d	403	41	65,73,73	1.94	15 (23%)	76,113,113	2.26	24 (31%)
29	DMS	a	417	-	3,3,3	2.82	1 (33%)	3,3,3	1.16	0
37	HEM	f	101	5,6	41,50,50	2.00	8 (19%)	45,82,82	1.58	9 (20%)
22	CLA	a	407	41	65,73,73	1.93	19 (29%)	76,113,113	2.54	23 (30%)
22	CLA	C	501	-	65,73,73	1.91	15 (23%)	76,113,113	2.79	26 (34%)
26	LMG	B	622	-	51,51,55	1.01	3 (5%)	59,59,63	1.26	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	DMS	B	634	-	3,3,3	2.62	1 (33%)	3,3,3	0.54	0
22	CLA	a	406	-	65,73,73	1.72	16 (24%)	76,113,113	2.40	23 (30%)
24	BCR	b	622	-	41,41,41	1.27	4 (9%)	56,56,56	1.15	4 (7%)
29	DMS	c	528	-	3,3,3	2.31	1 (33%)	3,3,3	1.49	1 (33%)
31	LHG	e	101	-	37,37,48	1.12	2 (5%)	40,42,54	0.95	2 (5%)
26	LMG	a	412	-	51,51,55	1.09	3 (5%)	59,59,63	1.05	3 (5%)
24	BCR	B	618	-	41,41,41	0.91	0	56,56,56	1.34	9 (16%)
28	LMT	C	520	-	36,36,36	0.92	1 (2%)	47,47,47	2.14	10 (21%)
29	DMS	V	204	-	3,3,3	2.63	1 (33%)	3,3,3	1.40	1 (33%)
31	LHG	f	102	-	45,45,48	1.08	2 (4%)	48,51,54	1.07	5 (10%)
32	HTG	C	521	-	19,19,19	0.80	0	23,24,24	1.74	4 (17%)
32	HTG	b	602	-	19,19,19	1.11	2 (10%)	23,24,24	1.64	3 (13%)
25	PL9	a	411	-	55,55,55	0.97	3 (5%)	68,69,69	2.26	20 (29%)
31	LHG	D	409	-	48,48,48	0.90	3 (6%)	51,54,54	1.61	6 (11%)
22	CLA	D	405	-	65,73,73	1.93	17 (26%)	76,113,113	1.93	20 (26%)
22	CLA	C	509	-	65,73,73	1.70	16 (24%)	76,113,113	2.67	30 (39%)
38	RRX	H	102	-	42,42,42	1.09	2 (4%)	57,58,58	1.51	9 (15%)
22	CLA	b	609	-	65,73,73	1.65	10 (15%)	76,113,113	2.47	22 (28%)
31	LHG	B	621	-	48,48,48	0.83	2 (4%)	51,54,54	1.31	6 (11%)
24	BCR	D	406	-	41,41,41	1.40	7 (17%)	56,56,56	1.92	15 (26%)
22	CLA	B	611	41	65,73,73	2.23	18 (27%)	76,113,113	2.15	21 (27%)
29	DMS	V	206	-	3,3,3	2.65	1 (33%)	3,3,3	0.79	0
29	DMS	u	203	-	3,3,3	2.54	1 (33%)	3,3,3	1.25	0
29	DMS	a	419	-	3,3,3	2.75	1 (33%)	3,3,3	0.73	0
29	DMS	B	636	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
32	HTG	b	640	-	17,17,19	2.71	5 (29%)	21,22,24	3.94	12 (57%)
26	LMG	A	411	-	51,51,55	1.04	2 (3%)	59,59,63	1.24	7 (11%)
28	LMT	m	101	-	36,36,36	0.74	0	47,47,47	1.53	10 (21%)
31	LHG	F	103	-	37,37,48	1.21	2 (5%)	40,43,54	1.58	4 (10%)

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
23	PHO	D	404	-	-	2/37/103/103	0/5/6/6
22	CLA	b	611	41	1/1/15/20	5/37/115/115	-
22	CLA	b	614	41	1/1/15/20	3/37/115/115	-
32	HTG	B	629	-	-	1/10/30/30	0/1/1/1
26	LMG	b	625	-	-	14/44/64/70	0/1/1/1
37	HEM	F	101	5,6	-	3/12/54/54	-
22	CLA	c	508	41	1/1/15/20	6/37/115/115	-
22	CLA	b	608	-	1/1/15/20	4/37/115/115	-
22	CLA	C	505	-	1/1/15/20	3/37/115/115	-
25	PL9	d	407	-	-	3/53/73/73	0/1/1/1
22	CLA	c	505	41	-	5/37/115/115	-
32	HTG	c	541	-	-	3/6/26/30	0/1/1/1
22	CLA	B	613	-	1/1/15/20	3/37/115/115	-
28	LMT	B	623	-	-	7/21/61/61	0/2/2/2
22	CLA	B	610	-	1/1/15/20	1/37/115/115	-
22	CLA	B	603	-	1/1/15/20	6/37/115/115	-
22	CLA	b	606	-	1/1/15/20	6/37/115/115	-
24	BCR	b	621	-	-	2/29/63/63	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
22	CLA	b	619	-	1/1/15/20	5/37/115/115	-
32	HTG	D	413	-	-	2/7/27/30	0/1/1/1
22	CLA	A	408	-	-	15/37/115/115	-
28	LMT	b	626	-	-	11/17/37/61	0/1/1/2
32	HTG	O	302	-	-	4/10/30/30	0/1/1/1
26	LMG	d	412	39	-	9/42/62/70	0/1/1/1
22	CLA	d	405	-	-	12/37/115/115	-
22	CLA	b	617	-	1/1/15/20	1/37/115/115	-
34	GOL	c	533	-	-	4/4/4/4	-
24	BCR	y	101	-	-	2/29/63/63	0/2/2/2
23	PHO	d	404	-	-	1/37/103/103	0/5/6/6
28	LMT	M	101	-	-	4/21/61/61	0/2/2/2
22	CLA	C	506	-	1/1/15/20	10/37/115/115	-
31	LHG	E	101	-	-	29/53/53/53	-
26	LMG	C	518	-	-	14/44/64/70	0/1/1/1
22	CLA	c	503	-	1/1/15/20	7/37/115/115	-
24	BCR	b	623	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	c	520	-	-	9/33/53/70	0/1/1/1
32	HTG	U	203	-	-	2/5/25/30	0/1/1/1
22	CLA	c	513	-	1/1/15/20	10/37/115/115	-
22	CLA	C	510	-	1/1/15/20	9/37/115/115	-
22	CLA	B	617	-	1/1/15/20	10/37/115/115	-
28	LMT	j	102	-	-	8/15/31/61	0/1/1/2
32	HTG	c	524	-	-	3/6/6/30	-
22	CLA	c	512	3	1/1/15/20	1/37/115/115	-
22	CLA	C	511	3	1/1/15/20	1/37/115/115	-
28	LMT	F	102	-	-	9/15/35/61	0/1/1/2
32	HTG	o	301	-	-	4/10/30/30	0/1/1/1
26	LMG	C	519	-	-	13/43/63/70	0/1/1/1
32	HTG	b	627	-	-	6/10/30/30	0/1/1/1
22	CLA	c	510	-	1/1/15/20	11/37/115/115	-
32	HTG	B	642	-	-	5/9/29/30	0/1/1/1
22	CLA	C	513	-	-	12/37/115/115	-
31	LHG	d	410	-	-	7/53/53/53	-
22	CLA	B	614	-	1/1/15/20	8/37/115/115	-
22	CLA	b	618	-	1/1/15/20	13/37/115/115	-
26	LMG	c	521	-	-	20/46/66/70	0/1/1/1
31	LHG	b	624	-	-	21/53/53/53	-
34	GOL	b	636	-	-	2/4/4/4	-
22	CLA	c	507	-	1/1/15/20	7/37/115/115	-
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
31	LHG	D	411	-	-	14/48/48/53	-
22	CLA	b	607	-	1/1/15/20	2/37/115/115	-
22	CLA	C	507	41	1/1/15/20	8/37/115/115	-
23	PHO	a	408	-	-	5/37/103/103	0/5/6/6
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
32	HTG	C	522	-	-	4/10/30/30	0/1/1/1
33	DGD	d	408	-	-	12/42/62/95	0/1/1/2
28	LMT	A	415	-	-	12/21/61/61	0/2/2/2
22	CLA	B	607	-	1/1/15/20	8/37/115/115	-
22	CLA	B	605	-	-	9/37/115/115	-
32	HTG	V	202	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMT	a	401	-	-	9/21/61/61	0/2/2/2
22	CLA	b	613	-	-	2/37/115/115	-
22	CLA	c	511	-	1/1/15/20	9/37/115/115	-
22	CLA	c	509	-	-	4/37/115/115	-
22	CLA	D	403	-	1/1/15/20	1/37/115/115	-
24	BCR	K	101	-	-	0/29/63/63	0/2/2/2
33	DGD	D	408	-	-	20/39/59/95	0/1/1/2
40	HEC	V	201	16	-	2/10/54/54	-
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
32	HTG	C	536	-	-	3/10/30/30	0/1/1/1
33	DGD	h	101	-	-	15/51/91/95	0/2/2/2
34	GOL	e	104	-	-	1/4/4/4	-
26	LMG	D	412	39	-	12/42/62/70	0/1/1/1
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
24	BCR	c	516	-	-	0/29/63/63	0/2/2/2
24	BCR	A	409	-	-	1/29/63/63	0/2/2/2
24	BCR	T	101	-	-	4/29/63/63	0/2/2/2
28	LMT	z	101	-	1/1/10/10	6/18/58/61	0/2/2/2
22	CLA	d	402	-	-	4/37/115/115	-
38	RRX	h	102	-	-	0/29/65/65	0/2/2/2
22	CLA	b	616	-	1/1/15/20	4/37/115/115	-
34	GOL	D	417	-	-	3/4/4/4	-
32	HTG	C	535	-	-	3/6/6/30	-
28	LMT	m	102	-	-	8/15/35/61	0/1/1/2
28	LMT	c	522	-	-	6/21/61/61	0/2/2/2
22	CLA	A	406	41	-	4/37/115/115	-
25	PL9	D	407	-	-	1/53/73/73	0/1/1/1
31	LHG	d	411	-	-	11/48/48/53	-
32	HTG	B	628	-	-	3/10/30/30	0/1/1/1
22	CLA	B	604	-	1/1/15/20	4/37/115/115	-
22	CLA	B	608	41	1/1/15/20	6/37/115/115	-
28	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
22	CLA	a	409	-	1/1/15/20	12/37/115/115	-
28	LMT	t	102	-	-	9/15/35/61	0/1/1/2
22	CLA	C	502	-	-	6/37/115/115	-
22	CLA	A	404	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	B	624	-	-	3/10/30/30	0/1/1/1
31	LHG	D	410	-	-	6/53/53/53	-
32	HTG	c	523	-	-	5/10/30/30	0/1/1/1
25	PL9	A	410	-	-	10/53/73/73	0/1/1/1
28	LMT	J	102	-	-	8/15/35/61	0/1/1/2
33	DGD	C	517	-	-	13/51/91/95	0/2/2/2
22	CLA	c	506	-	1/1/15/20	3/37/115/115	-
22	CLA	B	609	-	-	2/37/115/115	-
22	CLA	B	612	-	-	3/37/115/115	-
22	CLA	b	605	41	1/1/15/20	17/37/115/115	-
22	CLA	c	514	-	-	13/37/115/115	-
22	CLA	A	405	41	-	6/37/115/115	-
22	CLA	C	503	-	-	3/37/115/115	-
22	CLA	b	615	-	-	5/37/115/115	-
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
33	DGD	c	519	-	-	11/51/91/95	0/2/2/2
32	HTG	d	413	-	-	2/7/27/30	0/1/1/1
33	DGD	c	518	-	-	15/45/85/95	0/2/2/2
33	DGD	c	517	-	-	14/51/91/95	0/2/2/2
23	PHO	A	407	-	-	2/37/103/103	0/5/6/6
28	LMT	T	102	-	-	6/15/35/61	0/1/1/2
24	BCR	a	410	-	-	0/29/63/63	0/2/2/2
24	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
22	CLA	c	502	-	1/1/15/20	6/37/115/115	-
31	LHG	d	409	-	-	11/53/53/53	-
32	HTG	v	208	-	-	3/7/27/30	0/1/1/1
28	LMT	m	103	-	-	6/15/31/61	0/1/1/2
33	DGD	C	515	-	-	16/51/91/95	0/2/2/2
22	CLA	B	616	-	1/1/15/20	9/37/115/115	-
22	CLA	B	615	-	1/1/15/20	11/37/115/115	-
28	LMT	M	102	-	-	6/15/35/61	0/1/1/2
34	GOL	C	533	-	-	2/4/4/4	-
22	CLA	c	504	-	-	2/37/115/115	-
24	BCR	d	406	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	602	41	1/1/15/20	14/37/115/115	-
22	CLA	C	512	-	1/1/15/20	7/37/115/115	-
22	CLA	C	508	-	1/1/15/20	4/37/115/115	-
22	CLA	C	504	41	1/1/15/20	9/37/115/115	-
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
28	LMT	l	101	-	-	6/15/35/61	0/1/1/2
32	HTG	b	601	-	-	4/10/30/30	0/1/1/1
40	HEC	v	202	16	-	2/10/54/54	-
22	CLA	B	606	-	1/1/15/20	7/37/115/115	-
22	CLA	b	610	-	1/1/15/20	9/37/115/115	-
33	DGD	H	101	-	-	12/51/91/95	0/2/2/2
22	CLA	b	612	-	-	2/37/115/115	-
33	DGD	C	516	-	-	20/51/91/95	0/2/2/2
22	CLA	b	620	-	1/1/15/20	15/37/115/115	-
22	CLA	d	403	41	-	5/37/115/115	-
37	HEM	f	101	5,6	-	4/12/54/54	-
22	CLA	a	407	41	-	11/37/115/115	-
22	CLA	C	501	-	1/1/15/20	4/37/115/115	-
26	LMG	B	622	-	-	12/46/66/70	0/1/1/1
22	CLA	a	406	-	1/1/15/20	4/37/115/115	-
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
31	LHG	e	101	-	-	18/41/41/53	-
26	LMG	a	412	-	-	14/46/66/70	0/1/1/1
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
28	LMT	C	520	-	1/1/10/10	13/21/61/61	0/2/2/2
31	LHG	f	102	-	-	16/50/50/53	-
32	HTG	C	521	-	-	3/10/30/30	0/1/1/1
32	HTG	b	602	-	-	1/10/30/30	0/1/1/1
25	PL9	a	411	-	-	10/53/73/73	0/1/1/1
31	LHG	D	409	-	-	10/53/53/53	-
22	CLA	D	405	-	1/1/15/20	7/37/115/115	-
22	CLA	C	509	-	1/1/15/20	8/37/115/115	-
38	RRX	H	102	-	-	0/29/65/65	0/2/2/2
22	CLA	b	609	-	1/1/15/20	2/37/115/115	-
31	LHG	B	621	-	-	14/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	D	406	-	-	2/29/63/63	0/2/2/2
22	CLA	B	611	41	1/1/15/20	3/37/115/115	-
32	HTG	b	640	-	-	4/8/28/30	0/1/1/1
26	LMG	A	411	-	-	23/46/66/70	0/1/1/1
28	LMT	m	101	-	-	6/21/61/61	0/2/2/2
31	LHG	F	103	-	-	15/42/42/53	-

All (1535) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	z	101	LMT	C2-C1	46.12	3.47	1.51
22	C	513	CLA	MG-NA	14.53	2.40	2.06
22	c	512	CLA	MG-NA	13.25	2.37	2.06
22	c	504	CLA	MG-NA	12.94	2.37	2.06
22	C	511	CLA	MG-NA	12.29	2.35	2.06
22	c	502	CLA	MG-NA	12.10	2.35	2.06
22	b	610	CLA	MG-NA	11.77	2.34	2.06
22	B	602	CLA	MG-NA	10.85	2.32	2.06
22	B	607	CLA	MG-NA	9.93	2.29	2.06
22	B	606	CLA	MG-NA	9.56	2.29	2.06
22	C	504	CLA	MG-NA	9.49	2.28	2.06
22	b	620	CLA	MG-NA	9.39	2.28	2.06
22	c	505	CLA	MG-NA	9.29	2.28	2.06
22	C	502	CLA	MG-NA	9.06	2.27	2.06
22	B	612	CLA	MG-NA	9.04	2.27	2.06
22	c	502	CLA	MG-ND	-8.49	1.89	2.05
22	C	512	CLA	MG-NA	8.47	2.26	2.06
22	c	508	CLA	MG-NA	8.33	2.26	2.06
22	B	616	CLA	MG-NA	8.28	2.25	2.06
22	B	617	CLA	MG-NA	8.24	2.25	2.06
22	c	509	CLA	MG-NA	8.07	2.25	2.06
22	B	603	CLA	MG-NA	7.92	2.25	2.06
22	B	611	CLA	MG-NA	7.75	2.24	2.06
22	c	514	CLA	MG-NA	7.49	2.24	2.06
22	b	605	CLA	MG-NA	7.43	2.23	2.06
37	f	101	HEM	C3D-C2D	7.20	1.52	1.36
22	c	510	CLA	MG-ND	-7.15	1.91	2.05
22	C	506	CLA	MG-NA	7.09	2.23	2.06
22	B	611	CLA	MG-NC	7.07	2.23	2.06
22	A	405	CLA	OBD-CAD	7.02	1.34	1.22
22	B	615	CLA	MG-NA	6.98	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	616	CLA	C1B-NB	-6.86	1.29	1.35
22	b	606	CLA	C1D-ND	-6.86	1.29	1.37
22	C	507	CLA	MG-NA	6.85	2.22	2.06
32	o	301	HTG	C1'-S1	-6.80	1.72	1.81
32	b	640	HTG	C1-S1	6.78	1.91	1.80
22	c	513	CLA	MG-NA	6.76	2.22	2.06
22	c	513	CLA	C3B-C2B	6.73	1.49	1.40
22	B	609	CLA	MG-NA	6.68	2.22	2.06
22	B	608	CLA	MG-NA	6.66	2.22	2.06
22	B	614	CLA	MG-NA	6.59	2.21	2.06
40	V	201	HEC	C3C-C2C	-6.57	1.33	1.40
22	A	404	CLA	OBD-CAD	6.54	1.33	1.22
22	b	608	CLA	CHC-C1C	6.52	1.51	1.35
22	C	508	CLA	MG-NC	6.52	2.21	2.06
22	b	619	CLA	MG-NA	6.47	2.21	2.06
22	B	616	CLA	MG-ND	6.46	2.18	2.05
22	C	501	CLA	MG-NA	6.43	2.21	2.06
22	b	615	CLA	MG-NA	6.43	2.21	2.06
37	F	101	HEM	C3D-C2D	6.42	1.50	1.36
23	D	404	PHO	C3B-C2B	6.37	1.49	1.40
22	b	618	CLA	MG-NA	6.33	2.21	2.06
22	C	507	CLA	CHD-C1D	6.31	1.50	1.38
22	C	507	CLA	MG-NC	6.27	2.21	2.06
22	c	503	CLA	MG-NA	6.26	2.21	2.06
22	C	505	CLA	C3C-C2C	6.23	1.50	1.36
22	B	605	CLA	CHD-C4C	6.22	1.53	1.39
22	C	508	CLA	MG-NA	6.22	2.21	2.06
22	b	619	CLA	C3B-C2B	6.20	1.49	1.40
26	b	625	LMG	O8-C28	6.18	1.51	1.33
22	C	506	CLA	CHC-C1C	6.17	1.50	1.35
22	B	613	CLA	C1D-ND	-6.04	1.30	1.37
32	b	640	HTG	O5-C1	6.04	1.51	1.42
22	C	513	CLA	C3B-C2B	6.03	1.48	1.40
22	b	612	CLA	C4B-NB	-6.00	1.29	1.35
22	c	505	CLA	MG-NC	5.98	2.20	2.06
22	B	606	CLA	C3B-C2B	5.94	1.48	1.40
22	c	507	CLA	C3B-C2B	5.94	1.48	1.40
22	b	616	CLA	C3B-C2B	5.89	1.48	1.40
22	C	502	CLA	C3C-C2C	5.87	1.49	1.36
22	B	610	CLA	C1D-ND	-5.87	1.30	1.37
22	c	510	CLA	OBD-CAD	5.86	1.32	1.22
22	c	509	CLA	MG-NC	5.84	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	609	CLA	C1D-ND	-5.84	1.30	1.37
22	B	613	CLA	C3B-C2B	5.81	1.48	1.40
22	a	407	CLA	C4B-NB	-5.80	1.30	1.35
22	C	513	CLA	CHD-C1D	5.80	1.49	1.38
22	d	403	CLA	MG-NA	5.76	2.20	2.06
22	d	405	CLA	MG-NA	5.76	2.19	2.06
22	c	503	CLA	O2D-CGD	5.76	1.47	1.33
22	b	619	CLA	MG-ND	5.75	2.17	2.05
22	b	608	CLA	MG-ND	-5.73	1.94	2.05
22	C	508	CLA	C3B-C2B	5.72	1.48	1.40
22	B	614	CLA	MG-ND	5.71	2.17	2.05
22	C	512	CLA	C3B-C2B	5.71	1.48	1.40
22	b	605	CLA	O2D-CGD	5.68	1.47	1.33
40	v	202	HEC	C2B-C3B	-5.67	1.34	1.40
22	b	607	CLA	MG-NA	5.63	2.19	2.06
22	D	403	CLA	C3B-C2B	5.61	1.48	1.40
22	b	613	CLA	O2D-CGD	5.60	1.46	1.33
22	c	509	CLA	C3B-C2B	5.58	1.48	1.40
22	C	510	CLA	MG-NA	5.58	2.19	2.06
22	b	611	CLA	C3C-C2C	5.56	1.48	1.36
22	c	511	CLA	C3C-C2C	5.55	1.48	1.36
22	c	504	CLA	CHC-C1C	5.54	1.49	1.35
22	B	615	CLA	C1C-NC	-5.51	1.29	1.37
22	B	603	CLA	CHD-C1D	5.47	1.49	1.38
22	d	402	CLA	CHC-C1C	5.46	1.49	1.35
22	C	511	CLA	O2D-CGD	5.45	1.46	1.33
22	A	404	CLA	O2D-CGD	5.42	1.46	1.33
22	b	613	CLA	CHC-C1C	5.41	1.48	1.35
22	b	618	CLA	C3C-C2C	5.40	1.48	1.36
22	B	614	CLA	CHC-C1C	5.39	1.48	1.35
22	B	616	CLA	CHD-C4C	5.38	1.51	1.39
33	d	408	DGD	O2G-C1B	5.37	1.49	1.34
22	b	617	CLA	CHC-C1C	5.35	1.48	1.35
22	B	603	CLA	C3B-C2B	5.34	1.47	1.40
33	D	408	DGD	O1G-C1A	5.34	1.48	1.33
22	B	615	CLA	CHC-C1C	5.34	1.48	1.35
23	a	408	PHO	CBD-CGD	-5.33	1.45	1.52
22	c	512	CLA	CHD-C1D	5.33	1.48	1.38
22	B	613	CLA	CHC-C1C	5.32	1.48	1.35
22	c	508	CLA	C3C-C2C	5.31	1.48	1.36
22	b	608	CLA	MG-NA	5.30	2.18	2.06
22	C	508	CLA	CHC-C1C	5.30	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	405	CLA	C3C-C2C	5.29	1.48	1.36
22	C	504	CLA	C3B-C2B	5.29	1.47	1.40
33	D	408	DGD	O2G-C1B	5.27	1.49	1.34
25	A	410	PL9	C7-C3	5.27	1.56	1.51
22	b	616	CLA	CHC-C1C	5.27	1.48	1.35
22	B	602	CLA	O2A-CGA	5.27	1.48	1.33
33	H	101	DGD	O5D-C1E	5.27	1.49	1.40
22	b	610	CLA	CHC-C1C	5.26	1.48	1.35
22	c	507	CLA	O2D-CGD	5.25	1.46	1.33
22	b	620	CLA	CHC-C1C	5.25	1.48	1.35
26	C	519	LMG	O8-C28	5.21	1.48	1.33
22	B	604	CLA	C3C-C2C	5.21	1.47	1.36
22	B	609	CLA	CHD-C1D	5.21	1.48	1.38
22	d	405	CLA	MG-NC	5.20	2.18	2.06
22	A	405	CLA	C4B-NB	-5.19	1.30	1.35
22	B	607	CLA	CHC-C1C	5.18	1.48	1.35
22	D	405	CLA	MG-NC	5.17	2.18	2.06
22	c	513	CLA	O2D-CGD	5.14	1.45	1.33
29	b	638	DMS	O-S	5.14	1.85	1.50
22	b	605	CLA	O2A-CGA	5.13	1.48	1.33
23	A	407	PHO	C3B-C2B	5.13	1.47	1.40
22	C	503	CLA	MG-NA	5.13	2.18	2.06
22	b	614	CLA	O2D-CGD	5.12	1.45	1.33
22	c	504	CLA	C1D-ND	-5.12	1.31	1.37
22	C	513	CLA	C3C-C2C	5.11	1.47	1.36
22	b	608	CLA	C3C-C2C	5.11	1.47	1.36
22	b	606	CLA	C3C-C2C	5.11	1.47	1.36
22	B	611	CLA	C3C-C2C	5.09	1.47	1.36
29	v	207	DMS	O-S	5.08	1.84	1.50
22	C	506	CLA	C3B-C2B	5.08	1.47	1.40
29	c	538	DMS	O-S	5.07	1.84	1.50
22	C	503	CLA	CHC-C1C	5.07	1.48	1.35
22	A	408	CLA	C3B-C2B	5.07	1.47	1.40
40	V	201	HEC	C2B-C3B	-5.07	1.35	1.40
22	c	513	CLA	CHC-C1C	5.07	1.48	1.35
22	c	504	CLA	C3B-C2B	5.06	1.47	1.40
22	c	509	CLA	CHD-C4C	5.06	1.50	1.39
29	C	532	DMS	O-S	5.06	1.84	1.50
23	d	404	PHO	O2D-CGD	5.06	1.45	1.33
23	d	404	PHO	OBD-CAD	5.06	1.29	1.22
22	c	506	CLA	MG-NA	5.05	2.18	2.06
22	b	611	CLA	MG-NA	5.04	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	613	CLA	MG-ND	5.04	2.15	2.05
22	C	512	CLA	CHD-C1D	5.04	1.48	1.38
22	D	403	CLA	C4B-NB	-5.02	1.30	1.35
22	B	610	CLA	CHC-C1C	5.02	1.47	1.35
22	c	512	CLA	CHC-C1C	5.01	1.47	1.35
22	B	602	CLA	C3C-C2C	5.01	1.47	1.36
22	C	504	CLA	CHC-C1C	5.00	1.47	1.35
22	A	408	CLA	CHC-C1C	5.00	1.47	1.35
26	c	520	LMG	O7-C10	5.00	1.48	1.34
26	C	518	LMG	O8-C28	5.00	1.47	1.33
22	B	615	CLA	C1D-ND	-4.99	1.31	1.37
22	b	612	CLA	OBD-CAD	4.98	1.31	1.22
22	C	512	CLA	C3C-C2C	4.98	1.47	1.36
22	a	407	CLA	CHC-C1C	4.95	1.47	1.35
29	A	419	DMS	O-S	4.95	1.83	1.50
22	B	610	CLA	CHD-C1D	4.95	1.48	1.38
22	d	403	CLA	C1D-ND	-4.95	1.31	1.37
22	B	606	CLA	MG-ND	-4.94	1.96	2.05
22	c	506	CLA	C3C-C2C	4.94	1.47	1.36
22	b	613	CLA	CHD-C1D	4.94	1.48	1.38
22	b	616	CLA	MG-NA	4.94	2.18	2.06
22	a	409	CLA	C3C-C2C	4.94	1.47	1.36
29	c	529	DMS	O-S	4.92	1.83	1.50
22	B	613	CLA	O2D-CGD	4.92	1.45	1.33
22	A	405	CLA	C1B-NB	-4.92	1.30	1.35
22	B	611	CLA	CHC-C1C	4.91	1.47	1.35
29	B	640	DMS	O-S	4.90	1.83	1.50
22	c	514	CLA	CHC-C1C	4.90	1.47	1.35
29	B	631	DMS	O-S	4.89	1.83	1.50
22	C	509	CLA	C3C-C2C	4.89	1.47	1.36
33	d	408	DGD	O1G-C1A	4.88	1.47	1.33
22	d	405	CLA	C3C-C2C	4.88	1.47	1.36
22	B	603	CLA	C1D-ND	-4.87	1.31	1.37
22	d	405	CLA	C3B-C2B	4.86	1.47	1.40
26	c	521	LMG	O7-C10	4.86	1.48	1.34
22	C	512	CLA	CHC-C1C	4.85	1.47	1.35
22	b	620	CLA	C1B-NB	-4.85	1.30	1.35
29	O	305	DMS	O-S	4.82	1.82	1.50
23	a	408	PHO	OBD-CAD	4.82	1.29	1.22
29	B	641	DMS	O-S	4.81	1.82	1.50
22	b	607	CLA	O2D-CGD	4.81	1.44	1.33
29	o	310	DMS	O-S	4.81	1.82	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	f	101	HEM	C3C-C2C	-4.81	1.33	1.40
22	A	408	CLA	CHD-C1D	4.80	1.47	1.38
28	A	415	LMT	O3B-C3B	4.80	1.54	1.43
22	d	402	CLA	C3B-C2B	4.78	1.47	1.40
22	C	513	CLA	CHC-C1C	4.78	1.47	1.35
22	B	616	CLA	CHC-C1C	4.77	1.47	1.35
29	a	416	DMS	O-S	4.77	1.82	1.50
23	D	404	PHO	OBD-CAD	4.77	1.29	1.22
22	d	403	CLA	CHC-C1C	4.77	1.47	1.35
26	c	521	LMG	O8-C28	4.76	1.47	1.33
29	c	540	DMS	O-S	4.76	1.82	1.50
22	a	406	CLA	CHC-C1C	4.76	1.47	1.35
22	a	407	CLA	OBD-CAD	4.76	1.30	1.22
22	b	617	CLA	MG-NA	4.75	2.17	2.06
22	c	514	CLA	C3B-C2B	4.74	1.47	1.40
22	C	505	CLA	CHC-C1C	4.74	1.47	1.35
22	A	408	CLA	C3C-C2C	4.74	1.46	1.36
22	C	507	CLA	C3C-C2C	4.74	1.46	1.36
22	a	409	CLA	CHC-C1C	4.74	1.47	1.35
22	b	605	CLA	OBD-CAD	4.73	1.30	1.22
22	C	505	CLA	CHD-C4C	4.73	1.50	1.39
22	C	503	CLA	C3B-C2B	4.73	1.46	1.40
22	b	607	CLA	C1D-ND	-4.73	1.32	1.37
22	A	408	CLA	C1B-NB	4.73	1.39	1.35
22	c	505	CLA	O2D-CGD	4.72	1.44	1.33
29	B	635	DMS	O-S	4.72	1.82	1.50
22	D	405	CLA	CHC-C1C	4.72	1.47	1.35
29	C	526	DMS	O-S	4.72	1.82	1.50
22	C	503	CLA	C3C-C2C	4.72	1.46	1.36
22	b	620	CLA	C3C-C2C	4.72	1.46	1.36
29	V	207	DMS	O-S	4.71	1.82	1.50
40	v	202	HEC	C3C-C2C	-4.71	1.35	1.40
22	d	405	CLA	O2A-CGA	4.70	1.47	1.33
22	B	616	CLA	O2D-CGD	4.70	1.44	1.33
22	b	610	CLA	O2D-CGD	4.70	1.44	1.33
22	C	501	CLA	CHC-C1C	4.70	1.47	1.35
22	b	619	CLA	CHC-C1C	4.70	1.47	1.35
32	O	302	HTG	C1'-S1	-4.70	1.75	1.81
29	a	417	DMS	O-S	4.70	1.82	1.50
22	d	403	CLA	OBD-CAD	4.69	1.30	1.22
22	b	606	CLA	C1B-NB	-4.69	1.31	1.35
22	b	605	CLA	CHD-C1D	4.69	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	o	308	DMS	O-S	4.69	1.81	1.50
22	c	510	CLA	CHC-C1C	4.68	1.47	1.35
22	C	502	CLA	CHC-C1C	4.68	1.47	1.35
29	A	416	DMS	O-S	4.67	1.81	1.50
22	b	613	CLA	C3C-C2C	4.67	1.46	1.36
29	a	418	DMS	O-S	4.67	1.81	1.50
22	A	408	CLA	MG-ND	-4.67	1.96	2.05
29	b	635	DMS	O-S	4.66	1.81	1.50
29	b	634	DMS	O-S	4.66	1.81	1.50
22	b	619	CLA	CHD-C4C	4.65	1.49	1.39
26	a	412	LMG	O7-C10	4.64	1.47	1.34
31	F	103	LHG	O7-C7	4.64	1.47	1.34
29	a	420	DMS	O-S	4.64	1.81	1.50
22	B	603	CLA	MG-NC	4.63	2.17	2.06
22	b	606	CLA	CHC-C1C	4.63	1.46	1.35
22	d	405	CLA	CHD-C1D	4.63	1.47	1.38
29	O	306	DMS	O-S	4.63	1.81	1.50
22	B	606	CLA	C1D-ND	-4.63	1.32	1.37
22	c	512	CLA	MG-ND	-4.63	1.96	2.05
29	u	204	DMS	O-S	4.63	1.81	1.50
22	B	610	CLA	C3B-C2B	4.63	1.46	1.40
22	C	510	CLA	OBD-CAD	4.63	1.30	1.22
22	c	507	CLA	C3C-C2C	4.62	1.46	1.36
22	B	611	CLA	MG-ND	-4.62	1.96	2.05
22	C	504	CLA	O2D-CGD	4.62	1.44	1.33
22	c	509	CLA	C1C-NC	-4.62	1.30	1.37
22	B	607	CLA	C3B-C2B	4.61	1.46	1.40
22	c	510	CLA	CHD-C1D	4.61	1.47	1.38
22	c	505	CLA	C1C-NC	-4.61	1.30	1.37
29	b	633	DMS	O-S	4.61	1.81	1.50
22	C	513	CLA	O2D-CGD	4.60	1.44	1.33
22	c	507	CLA	MG-ND	-4.60	1.96	2.05
22	A	404	CLA	C3C-C2C	4.59	1.46	1.36
22	a	407	CLA	MG-NA	4.58	2.17	2.06
29	c	534	DMS	O-S	4.58	1.81	1.50
22	C	507	CLA	C3B-C2B	4.58	1.46	1.40
22	C	506	CLA	O2D-CGD	4.57	1.44	1.33
29	h	104	DMS	O-S	4.57	1.81	1.50
29	E	104	DMS	O-S	4.56	1.81	1.50
29	a	419	DMS	O-S	4.56	1.81	1.50
22	b	611	CLA	O2D-CGD	4.55	1.44	1.33
22	b	610	CLA	C3B-C2B	4.55	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	O	309	DMS	O-S	4.55	1.81	1.50
29	O	307	DMS	O-S	4.55	1.81	1.50
22	C	511	CLA	CHD-C1D	4.55	1.47	1.38
29	C	534	DMS	O-S	4.55	1.81	1.50
22	c	509	CLA	CHC-C1C	4.55	1.46	1.35
29	C	531	DMS	O-S	4.54	1.80	1.50
29	d	416	DMS	O-S	4.54	1.80	1.50
29	c	532	DMS	O-S	4.54	1.80	1.50
29	c	530	DMS	O-S	4.54	1.80	1.50
29	D	416	DMS	O-S	4.53	1.80	1.50
22	B	608	CLA	CHC-C1C	4.53	1.46	1.35
22	B	602	CLA	C3B-C2B	4.53	1.46	1.40
29	D	419	DMS	O-S	4.52	1.80	1.50
29	O	312	DMS	O-S	4.52	1.80	1.50
22	c	513	CLA	O2A-CGA	4.52	1.46	1.33
22	a	406	CLA	C1D-ND	-4.51	1.32	1.37
29	u	202	DMS	O-S	4.51	1.80	1.50
22	c	512	CLA	C3C-C2C	4.50	1.46	1.36
22	b	606	CLA	CHD-C4C	4.50	1.49	1.39
22	c	503	CLA	C3B-C2B	4.50	1.46	1.40
22	c	509	CLA	CHD-C1D	4.50	1.47	1.38
22	B	614	CLA	MG-NC	-4.49	1.95	2.06
22	B	611	CLA	CHD-C1D	4.49	1.47	1.38
29	e	105	DMS	O-S	4.49	1.80	1.50
31	E	101	LHG	O7-C7	4.49	1.47	1.34
22	b	615	CLA	CHC-C1C	4.49	1.46	1.35
29	I	105	DMS	O-S	4.48	1.80	1.50
22	c	505	CLA	CHD-C1D	4.48	1.47	1.38
31	F	103	LHG	O8-C23	4.48	1.46	1.33
22	C	508	CLA	CHD-C1D	4.48	1.47	1.38
22	C	504	CLA	C1D-ND	-4.48	1.32	1.37
29	B	636	DMS	O-S	4.48	1.80	1.50
29	O	310	DMS	O-S	4.47	1.80	1.50
29	o	311	DMS	O-S	4.47	1.80	1.50
29	b	632	DMS	O-S	4.47	1.80	1.50
29	V	205	DMS	O-S	4.47	1.80	1.50
22	B	616	CLA	CHD-C1D	4.46	1.47	1.38
26	C	519	LMG	O7-C10	4.46	1.46	1.34
26	A	411	LMG	O7-C10	4.46	1.46	1.34
29	c	536	DMS	O-S	4.46	1.80	1.50
31	e	101	LHG	O8-C23	4.45	1.46	1.33
22	A	408	CLA	OBD-CAD	4.45	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	MG-NC	-4.44	1.95	2.06
29	v	204	DMS	O-S	4.44	1.80	1.50
22	b	612	CLA	C3C-C2C	4.44	1.46	1.36
29	O	308	DMS	O-S	4.44	1.80	1.50
22	c	512	CLA	O2D-CGD	4.44	1.44	1.33
22	c	514	CLA	O2D-CGD	4.44	1.44	1.33
29	c	531	DMS	O-S	4.44	1.80	1.50
22	B	602	CLA	CHC-C1C	4.43	1.46	1.35
22	b	618	CLA	CHC-C1C	4.43	1.46	1.35
29	b	631	DMS	O-S	4.43	1.80	1.50
22	b	620	CLA	C1D-ND	-4.42	1.32	1.37
26	A	411	LMG	O8-C28	4.42	1.46	1.33
26	B	622	LMG	O8-C28	4.42	1.46	1.33
29	O	304	DMS	O-S	4.42	1.80	1.50
29	o	307	DMS	O-S	4.42	1.80	1.50
22	a	409	CLA	O2A-CGA	4.42	1.46	1.33
22	C	509	CLA	MG-NC	-4.41	1.95	2.06
22	b	607	CLA	CHC-C1C	4.41	1.46	1.35
29	A	418	DMS	O-S	4.41	1.80	1.50
22	C	501	CLA	CHD-C1D	4.41	1.47	1.38
29	O	311	DMS	O-S	4.41	1.80	1.50
29	o	305	DMS	O-S	4.41	1.80	1.50
22	c	511	CLA	MG-NA	4.41	2.16	2.06
29	V	204	DMS	O-S	4.40	1.80	1.50
29	B	634	DMS	O-S	4.40	1.80	1.50
22	b	616	CLA	MG-ND	-4.40	1.97	2.05
22	c	503	CLA	CHC-C1C	4.40	1.46	1.35
22	c	511	CLA	CHC-C1C	4.40	1.46	1.35
29	V	203	DMS	O-S	4.40	1.80	1.50
40	v	202	HEC	C3D-C2D	4.40	1.50	1.37
29	o	309	DMS	O-S	4.40	1.79	1.50
22	c	510	CLA	C3C-C2C	4.39	1.46	1.36
22	d	402	CLA	CHD-C1D	4.39	1.46	1.38
29	c	535	DMS	O-S	4.39	1.79	1.50
22	B	604	CLA	CHD-C4C	4.39	1.49	1.39
29	O	303	DMS	O-S	4.38	1.79	1.50
22	c	509	CLA	O2D-CGD	4.38	1.43	1.33
29	v	206	DMS	O-S	4.38	1.79	1.50
29	D	418	DMS	O-S	4.38	1.79	1.50
29	V	206	DMS	O-S	4.38	1.79	1.50
22	C	504	CLA	CHD-C4C	4.37	1.49	1.39
22	C	505	CLA	C1B-NB	-4.37	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	407	PHO	CBD-CGD	-4.37	1.46	1.52
22	C	510	CLA	CHC-C1C	4.37	1.46	1.35
29	B	637	DMS	O-S	4.36	1.79	1.50
22	C	506	CLA	C3C-C2C	4.36	1.46	1.36
29	c	539	DMS	O-S	4.36	1.79	1.50
29	D	420	DMS	O-S	4.36	1.79	1.50
29	D	415	DMS	O-S	4.35	1.79	1.50
29	C	529	DMS	O-S	4.35	1.79	1.50
22	a	407	CLA	C1D-ND	-4.35	1.32	1.37
29	b	639	DMS	O-S	4.35	1.79	1.50
31	E	101	LHG	O8-C23	4.35	1.46	1.33
22	b	612	CLA	CHD-C1D	4.35	1.46	1.38
22	c	503	CLA	CHD-C1D	4.34	1.46	1.38
22	B	605	CLA	C3C-C2C	4.34	1.45	1.36
22	c	514	CLA	O2A-CGA	4.33	1.46	1.33
29	c	537	DMS	O-S	4.33	1.79	1.50
22	B	609	CLA	C3C-C2C	4.33	1.45	1.36
22	b	615	CLA	C3B-C2B	4.33	1.46	1.40
23	a	408	PHO	C3D-C2D	4.33	1.47	1.39
31	D	411	LHG	O8-C23	4.33	1.46	1.33
22	C	510	CLA	O2D-CGD	4.32	1.43	1.33
22	B	603	CLA	C3C-C2C	4.32	1.45	1.36
22	b	609	CLA	C3C-C2C	4.32	1.45	1.36
22	B	614	CLA	CHD-C1D	4.32	1.46	1.38
29	o	304	DMS	O-S	4.32	1.79	1.50
22	c	513	CLA	CHD-C1D	4.32	1.46	1.38
22	d	403	CLA	C3C-C2C	4.32	1.45	1.36
22	C	510	CLA	MG-ND	-4.31	1.97	2.05
22	B	604	CLA	MG-NA	4.31	2.16	2.06
22	c	504	CLA	CHD-C1D	4.31	1.46	1.38
22	c	503	CLA	OBD-CAD	4.31	1.29	1.22
29	C	527	DMS	O-S	4.31	1.79	1.50
33	h	101	DGD	O5D-C1E	4.31	1.47	1.40
22	c	514	CLA	C3C-C2C	4.31	1.45	1.36
22	C	507	CLA	MG-ND	4.31	2.14	2.05
22	c	502	CLA	C3C-C2C	4.30	1.45	1.36
22	b	607	CLA	C3C-C2C	4.30	1.45	1.36
22	D	405	CLA	MG-NA	4.30	2.16	2.06
22	B	607	CLA	C1B-NB	-4.30	1.31	1.35
29	B	633	DMS	O-S	4.29	1.79	1.50
22	c	513	CLA	C3C-C2C	4.29	1.45	1.36
26	a	412	LMG	O8-C28	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	O2D-CGD	4.29	1.43	1.33
22	b	611	CLA	MG-NC	4.28	2.16	2.06
29	C	528	DMS	O-S	4.28	1.79	1.50
22	c	502	CLA	O2D-CGD	4.27	1.43	1.33
22	A	405	CLA	C1D-ND	-4.26	1.32	1.37
29	b	637	DMS	O-S	4.26	1.79	1.50
31	f	102	LHG	O8-C23	4.26	1.45	1.33
22	C	512	CLA	O2D-CGD	4.26	1.43	1.33
22	c	507	CLA	CHC-C1C	4.26	1.45	1.35
22	b	620	CLA	CHD-C1D	4.26	1.46	1.38
22	c	506	CLA	CHC-C1C	4.26	1.45	1.35
26	c	520	LMG	O8-C28	4.25	1.45	1.33
23	D	404	PHO	C3D-C2D	4.25	1.47	1.39
22	C	505	CLA	CHD-C1D	4.25	1.46	1.38
22	d	402	CLA	MG-NA	4.24	2.16	2.06
29	o	306	DMS	O-S	4.23	1.78	1.50
22	b	605	CLA	CHC-C1C	4.23	1.45	1.35
22	C	507	CLA	CHC-C1C	4.23	1.45	1.35
22	c	502	CLA	CHC-C1C	4.22	1.45	1.35
22	d	403	CLA	MG-NC	-4.22	1.96	2.06
22	D	403	CLA	C3C-C2C	4.22	1.45	1.36
22	c	505	CLA	CHC-C1C	4.22	1.45	1.35
22	B	603	CLA	CHC-C1C	4.22	1.45	1.35
22	C	510	CLA	C3C-C2C	4.22	1.45	1.36
33	C	516	DGD	O5D-C1E	4.21	1.47	1.40
29	C	525	DMS	O-S	4.21	1.78	1.50
23	a	408	PHO	C3B-C2B	4.21	1.46	1.40
29	B	639	DMS	O-S	4.20	1.78	1.50
23	d	404	PHO	C3D-C2D	4.19	1.46	1.39
22	B	614	CLA	C3C-C2C	4.19	1.45	1.36
22	b	616	CLA	O2D-CGD	4.19	1.43	1.33
22	B	615	CLA	C4B-NB	-4.19	1.31	1.35
22	c	508	CLA	CHC-C1C	4.18	1.45	1.35
29	v	205	DMS	O-S	4.18	1.78	1.50
22	C	513	CLA	CHD-C4C	4.18	1.48	1.39
22	B	602	CLA	O2D-CGD	4.17	1.43	1.33
29	v	203	DMS	O-S	4.17	1.78	1.50
22	b	609	CLA	CHC-C1C	4.17	1.45	1.35
22	b	608	CLA	O2D-CGD	4.17	1.43	1.33
22	b	611	CLA	CHC-C1C	4.17	1.45	1.35
22	B	608	CLA	CHD-C1D	4.17	1.46	1.38
40	v	202	HEC	CBC-CAC	-4.16	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	C3C-C2C	4.16	1.45	1.36
22	a	409	CLA	O2D-CGD	4.15	1.43	1.33
29	V	208	DMS	O-S	4.15	1.78	1.50
22	c	510	CLA	O2D-CGD	4.15	1.43	1.33
22	b	606	CLA	MG-NA	4.15	2.16	2.06
22	b	617	CLA	C1C-NC	-4.13	1.31	1.37
29	U	202	DMS	O-S	4.13	1.78	1.50
26	D	412	LMG	O7-C10	4.13	1.45	1.34
22	b	608	CLA	C1B-NB	-4.13	1.31	1.35
22	b	610	CLA	C3C-C2C	4.12	1.45	1.36
22	c	514	CLA	CHD-C1D	4.12	1.46	1.38
22	B	612	CLA	MG-ND	-4.12	1.97	2.05
22	c	507	CLA	O2A-CGA	4.11	1.45	1.33
22	C	512	CLA	MG-ND	4.11	2.13	2.05
22	d	402	CLA	O2A-CGA	4.11	1.45	1.33
23	D	404	PHO	CBD-CGD	-4.10	1.46	1.52
22	b	617	CLA	C1D-ND	-4.10	1.32	1.37
22	b	614	CLA	CHD-C1D	4.10	1.46	1.38
22	C	511	CLA	CHC-C1C	4.09	1.45	1.35
29	B	632	DMS	O-S	4.09	1.77	1.50
29	u	203	DMS	O-S	4.08	1.77	1.50
22	b	618	CLA	CHD-C1D	4.08	1.46	1.38
22	B	617	CLA	C3C-C2C	4.07	1.45	1.36
22	B	610	CLA	MG-NC	4.07	2.15	2.06
22	B	615	CLA	O2A-CGA	4.07	1.45	1.33
22	B	602	CLA	C4B-NB	4.07	1.38	1.35
22	B	606	CLA	CHD-C1D	4.07	1.46	1.38
22	A	406	CLA	CHD-C1D	4.07	1.46	1.38
22	B	617	CLA	O2D-CGD	4.06	1.43	1.33
22	b	613	CLA	C1C-NC	-4.05	1.31	1.37
22	b	615	CLA	CHD-C1D	4.05	1.46	1.38
22	a	406	CLA	C3B-C2B	4.05	1.46	1.40
33	h	101	DGD	O3G-C1D	4.05	1.47	1.40
22	C	512	CLA	CHD-C4C	4.04	1.48	1.39
22	B	602	CLA	CHD-C1D	4.04	1.46	1.38
22	C	502	CLA	C3B-C2B	4.04	1.46	1.40
31	e	101	LHG	O7-C7	4.03	1.45	1.34
22	b	619	CLA	MG-NC	4.02	2.15	2.06
28	a	401	LMT	O1'-C1'	4.01	1.47	1.40
22	D	403	CLA	O2D-CGD	4.01	1.43	1.33
22	b	616	CLA	OBD-CAD	4.00	1.29	1.22
22	c	506	CLA	MG-NC	4.00	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	C3B-C2B	4.00	1.45	1.40
22	B	607	CLA	O2D-CGD	3.99	1.42	1.33
22	c	511	CLA	O2D-CGD	3.99	1.42	1.33
22	c	510	CLA	O2A-CGA	3.99	1.45	1.33
28	F	102	LMT	O1'-C1'	3.99	1.47	1.40
22	B	616	CLA	C3C-C2C	3.98	1.45	1.36
22	C	506	CLA	O2A-CGA	3.97	1.45	1.33
23	D	404	PHO	O2A-CGA	3.97	1.44	1.33
22	B	602	CLA	C1D-ND	-3.97	1.32	1.37
22	b	616	CLA	MG-NC	-3.96	1.96	2.06
22	B	605	CLA	CHC-C1C	3.96	1.45	1.35
22	C	508	CLA	CHD-C4C	3.96	1.48	1.39
22	C	505	CLA	C3B-C2B	3.96	1.45	1.40
29	c	528	DMS	O-S	3.96	1.77	1.50
24	C	514	BCR	C30-C25	-3.95	1.48	1.53
22	c	509	CLA	C3C-C2C	3.95	1.45	1.36
22	C	511	CLA	C1C-NC	-3.95	1.31	1.37
22	C	503	CLA	O2D-CGD	3.95	1.42	1.33
22	A	405	CLA	C3D-C2D	3.95	1.49	1.39
22	C	509	CLA	C3B-C2B	3.94	1.45	1.40
22	b	615	CLA	O2D-CGD	3.94	1.42	1.33
22	b	617	CLA	O2A-CGA	3.93	1.44	1.33
23	d	404	PHO	C3B-C2B	3.93	1.45	1.40
32	b	640	HTG	O6-C6	3.93	1.59	1.42
22	B	603	CLA	C1B-NB	-3.92	1.31	1.35
32	b	601	HTG	C1'-S1	-3.92	1.76	1.81
22	C	511	CLA	C3C-C2C	3.91	1.45	1.36
22	c	506	CLA	C3B-C2B	3.91	1.45	1.40
22	C	511	CLA	C3B-C2B	3.90	1.45	1.40
22	b	614	CLA	CHC-C1C	3.90	1.45	1.35
33	C	516	DGD	O1G-C1A	3.90	1.44	1.33
29	d	415	DMS	O-S	3.90	1.76	1.50
22	C	504	CLA	CHD-C1D	3.90	1.46	1.38
22	C	501	CLA	CHD-C4C	3.90	1.48	1.39
22	B	609	CLA	C1B-NB	-3.89	1.31	1.35
22	b	609	CLA	C1B-NB	-3.87	1.31	1.35
22	b	614	CLA	C3C-C2C	3.87	1.45	1.36
22	C	511	CLA	OBD-CAD	3.87	1.29	1.22
22	c	502	CLA	C3B-C2B	3.86	1.45	1.40
33	c	519	DGD	O1G-C1A	3.86	1.44	1.33
22	c	513	CLA	CHD-C4C	3.86	1.48	1.39
22	D	405	CLA	CHD-C1D	3.86	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	h	101	DGD	O2G-C1B	3.85	1.45	1.34
22	B	617	CLA	O2A-CGA	3.85	1.44	1.33
22	A	406	CLA	C1B-NB	-3.85	1.31	1.35
22	b	620	CLA	O2D-CGD	3.85	1.42	1.33
22	d	405	CLA	C4C-C3C	3.85	1.51	1.45
22	C	507	CLA	O2D-CGD	3.84	1.42	1.33
22	C	513	CLA	O2A-CGA	3.84	1.44	1.33
22	c	504	CLA	C3C-C2C	3.84	1.44	1.36
22	b	620	CLA	C3B-C2B	3.83	1.45	1.40
22	C	503	CLA	O2A-CGA	3.83	1.44	1.33
22	B	617	CLA	CHC-C1C	3.81	1.44	1.35
22	D	403	CLA	C1D-ND	-3.81	1.33	1.37
22	C	505	CLA	MG-NA	3.81	2.15	2.06
22	b	605	CLA	C3C-C2C	3.81	1.44	1.36
22	D	403	CLA	C4D-ND	-3.79	1.32	1.37
22	a	406	CLA	C3C-C2C	3.79	1.44	1.36
22	B	603	CLA	CHD-C4C	3.78	1.47	1.39
22	B	607	CLA	C3C-C2C	3.78	1.44	1.36
22	c	503	CLA	CHD-C4C	3.78	1.47	1.39
22	d	403	CLA	CHD-C4C	3.76	1.47	1.39
22	C	509	CLA	O2A-CGA	3.76	1.44	1.33
22	C	507	CLA	CHD-C4C	3.76	1.47	1.39
22	B	613	CLA	MG-NA	3.76	2.15	2.06
28	z	101	LMT	O1'-C1'	3.76	1.46	1.40
22	B	616	CLA	C4B-NB	-3.76	1.31	1.35
33	c	517	DGD	O5D-C1E	3.76	1.46	1.40
26	C	518	LMG	O7-C10	3.76	1.44	1.34
22	b	620	CLA	C1C-NC	-3.76	1.32	1.37
22	C	504	CLA	C1C-NC	-3.75	1.32	1.37
22	C	512	CLA	OBD-CAD	3.75	1.28	1.22
22	c	513	CLA	MG-NC	3.75	2.15	2.06
23	d	404	PHO	O2A-CGA	3.74	1.44	1.33
22	d	405	CLA	CHC-C1C	3.74	1.44	1.35
22	B	610	CLA	C3C-C2C	3.74	1.44	1.36
22	c	507	CLA	CHD-C1D	3.73	1.45	1.38
22	c	512	CLA	C1C-NC	-3.73	1.32	1.37
22	c	512	CLA	CHD-C4C	3.73	1.47	1.39
22	C	501	CLA	C3C-C2C	3.73	1.44	1.36
22	C	509	CLA	CHC-C1C	3.73	1.44	1.35
22	b	605	CLA	C4D-ND	3.73	1.42	1.37
22	b	606	CLA	OBD-CAD	3.73	1.28	1.22
22	b	616	CLA	CHD-C1D	3.72	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	C3D-C2D	3.72	1.49	1.39
22	c	511	CLA	CHD-C1D	3.72	1.45	1.38
26	b	625	LMG	O7-C10	3.72	1.44	1.34
22	b	607	CLA	CHD-C1D	3.71	1.45	1.38
22	B	609	CLA	O2D-CGD	3.71	1.42	1.33
22	c	512	CLA	C3B-C2B	3.71	1.45	1.40
29	B	638	DMS	O-S	3.71	1.75	1.50
22	A	404	CLA	CHC-C1C	3.71	1.44	1.35
22	b	608	CLA	C1D-ND	-3.70	1.33	1.37
22	B	612	CLA	C3C-C2C	3.70	1.44	1.36
22	B	608	CLA	CHD-C4C	3.70	1.47	1.39
22	b	617	CLA	CHD-C4C	3.69	1.47	1.39
22	B	614	CLA	O2D-CGD	3.69	1.42	1.33
22	c	502	CLA	C4C-C3C	3.69	1.51	1.45
22	B	605	CLA	O2D-CGD	3.69	1.42	1.33
40	V	201	HEC	C3D-C2D	3.68	1.48	1.37
22	C	502	CLA	O2A-CGA	3.67	1.44	1.33
22	A	404	CLA	MG-ND	-3.66	1.98	2.05
24	D	406	BCR	C17-C18	3.66	1.40	1.35
22	c	504	CLA	O2D-CGD	3.66	1.42	1.33
22	A	405	CLA	CHC-C1C	3.66	1.44	1.35
22	c	506	CLA	O2A-CGA	3.66	1.44	1.33
22	c	504	CLA	CHD-C4C	3.66	1.47	1.39
22	b	616	CLA	C1D-ND	-3.65	1.33	1.37
22	b	613	CLA	MG-NA	3.65	2.14	2.06
22	C	503	CLA	MG-NC	3.65	2.14	2.06
22	B	605	CLA	MG-NA	3.63	2.14	2.06
22	c	505	CLA	C3C-C2C	3.62	1.44	1.36
22	a	406	CLA	MG-NA	3.62	2.14	2.06
22	C	511	CLA	CHD-C4C	3.62	1.47	1.39
22	b	618	CLA	O2D-CGD	3.61	1.42	1.33
22	A	406	CLA	C1D-ND	-3.61	1.33	1.37
22	b	619	CLA	C3C-C2C	3.60	1.44	1.36
22	c	506	CLA	CHD-C4C	3.60	1.47	1.39
22	b	611	CLA	C1B-NB	-3.59	1.32	1.35
22	b	613	CLA	CHD-C4C	3.59	1.47	1.39
24	b	623	BCR	C30-C25	-3.59	1.48	1.53
22	c	508	CLA	C1B-CHB	3.59	1.51	1.41
22	C	513	CLA	C1C-NC	-3.58	1.32	1.37
32	O	302	HTG	O5-C1	3.58	1.48	1.42
22	A	406	CLA	MG-NA	3.57	2.14	2.06
22	b	606	CLA	O2A-CGA	3.57	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	502	CLA	C1C-NC	-3.56	1.32	1.37
31	d	411	LHG	O8-C23	3.56	1.43	1.33
22	B	609	CLA	O2A-CGA	3.56	1.43	1.33
22	D	403	CLA	CHD-C4C	3.55	1.47	1.39
22	A	404	CLA	CHD-C4C	3.55	1.47	1.39
22	C	508	CLA	O2D-CGD	3.55	1.41	1.33
22	b	617	CLA	O2D-CGD	3.55	1.41	1.33
22	C	510	CLA	CHD-C1D	3.55	1.45	1.38
22	a	407	CLA	C3D-C2D	3.55	1.48	1.39
22	C	505	CLA	MG-NC	3.54	2.14	2.06
22	c	512	CLA	C3D-C2D	3.54	1.48	1.39
22	C	503	CLA	OBD-CAD	3.54	1.28	1.22
22	D	403	CLA	MG-NA	3.53	2.14	2.06
22	B	615	CLA	CHD-C1D	3.53	1.45	1.38
33	c	517	DGD	O2G-C1B	3.53	1.44	1.34
22	C	504	CLA	C3C-C2C	3.52	1.44	1.36
31	f	102	LHG	O7-C7	3.52	1.44	1.34
22	B	612	CLA	C1D-ND	-3.51	1.33	1.37
22	c	512	CLA	MG-NC	3.51	2.14	2.06
22	B	609	CLA	CHC-C1C	3.51	1.44	1.35
31	D	411	LHG	O7-C7	3.51	1.44	1.34
22	C	510	CLA	C1D-ND	-3.51	1.33	1.37
22	C	503	CLA	CHD-C4C	3.50	1.47	1.39
22	B	605	CLA	MG-NC	3.50	2.14	2.06
28	t	102	LMT	O1'-C1'	3.50	1.46	1.40
22	A	408	CLA	CHD-C4C	3.50	1.47	1.39
22	c	513	CLA	C1D-ND	-3.50	1.33	1.37
22	c	506	CLA	CHD-C1D	3.49	1.45	1.38
22	b	619	CLA	C3D-C2D	3.49	1.48	1.39
22	D	405	CLA	C1B-CHB	3.49	1.50	1.41
22	c	512	CLA	OBD-CAD	3.48	1.28	1.22
22	C	507	CLA	C4D-CHA	3.48	1.50	1.38
22	C	507	CLA	C1C-NC	-3.48	1.32	1.37
22	D	403	CLA	MG-ND	3.48	2.12	2.05
22	A	408	CLA	O2D-CGD	3.48	1.41	1.33
22	b	617	CLA	C3C-C2C	3.47	1.44	1.36
33	C	515	DGD	O5D-C1E	3.47	1.46	1.40
22	B	617	CLA	C1D-ND	-3.47	1.33	1.37
26	D	412	LMG	O8-C28	3.46	1.43	1.33
22	b	619	CLA	O2D-CGD	3.46	1.41	1.33
22	b	613	CLA	C3B-C2B	3.46	1.45	1.40
37	F	101	HEM	C3C-C2C	-3.45	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	406	CLA	CHC-C1C	3.45	1.43	1.35
22	C	501	CLA	O2D-CGD	3.45	1.41	1.33
22	b	609	CLA	O2A-CGA	3.45	1.43	1.33
22	b	613	CLA	O2A-CGA	3.45	1.43	1.33
22	C	508	CLA	C1B-NB	3.45	1.38	1.35
22	b	605	CLA	C3B-C2B	3.45	1.45	1.40
22	C	508	CLA	C3C-C2C	3.45	1.44	1.36
32	C	536	HTG	C1'-S1	-3.44	1.77	1.81
22	B	612	CLA	O2A-CGA	3.44	1.43	1.33
22	C	512	CLA	O2A-CGA	3.43	1.43	1.33
22	b	612	CLA	C4D-ND	-3.43	1.33	1.37
22	c	508	CLA	MG-NC	3.43	2.14	2.06
22	C	511	CLA	C1B-CHB	3.43	1.50	1.41
22	b	618	CLA	O2A-CGA	3.43	1.43	1.33
22	B	613	CLA	C1B-CHB	3.43	1.50	1.41
22	b	619	CLA	CHD-C1D	3.43	1.45	1.38
22	B	614	CLA	CHD-C4C	3.43	1.47	1.39
26	B	622	LMG	O7-C10	3.43	1.44	1.34
22	d	402	CLA	O2D-CGD	3.42	1.41	1.33
22	b	610	CLA	C1B-CHB	3.42	1.50	1.41
22	B	606	CLA	O2D-CGD	3.41	1.41	1.33
22	A	406	CLA	C3D-C2D	3.41	1.48	1.39
22	b	610	CLA	C4D-CHA	3.41	1.50	1.38
22	c	510	CLA	C3B-C2B	3.41	1.45	1.40
22	B	604	CLA	OBD-CAD	3.41	1.28	1.22
22	b	614	CLA	C1D-ND	-3.40	1.33	1.37
22	b	616	CLA	C3C-C2C	3.40	1.43	1.36
22	C	505	CLA	O2D-CGD	3.39	1.41	1.33
22	b	613	CLA	C1D-ND	-3.39	1.33	1.37
22	B	617	CLA	CHD-C4C	3.39	1.47	1.39
22	B	604	CLA	O2D-CGD	3.39	1.41	1.33
26	d	412	LMG	O8-C28	3.39	1.43	1.33
22	B	604	CLA	C3D-C2D	3.39	1.48	1.39
22	B	612	CLA	CHC-C1C	3.39	1.43	1.35
22	B	613	CLA	CHD-C1D	3.38	1.45	1.38
22	c	504	CLA	O2A-CGA	3.38	1.43	1.33
22	c	508	CLA	C4B-CHC	3.38	1.50	1.41
23	a	408	PHO	O2D-CGD	3.38	1.41	1.33
28	c	522	LMT	O1'-C1'	3.38	1.46	1.40
22	b	617	CLA	CHD-C1D	3.37	1.44	1.38
22	C	506	CLA	CHD-C4C	3.37	1.46	1.39
22	a	407	CLA	MG-NC	-3.35	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	BCR	C23-C22	3.35	1.53	1.45
22	b	612	CLA	C1D-ND	-3.35	1.33	1.37
22	B	611	CLA	C4D-CHA	3.35	1.50	1.38
22	c	511	CLA	C3D-C2D	3.35	1.48	1.39
22	C	512	CLA	C1B-NB	-3.34	1.32	1.35
29	A	417	DMS	O-S	3.34	1.72	1.50
22	B	615	CLA	C3C-C2C	3.34	1.43	1.36
22	B	604	CLA	CHC-C1C	3.34	1.43	1.35
22	B	613	CLA	C3C-C2C	3.34	1.43	1.36
22	c	503	CLA	C3C-C2C	3.34	1.43	1.36
22	b	618	CLA	C1D-ND	-3.34	1.33	1.37
22	c	509	CLA	O2A-CGA	3.33	1.43	1.33
22	b	613	CLA	OBD-CAD	3.33	1.28	1.22
22	B	604	CLA	CHD-C1D	3.33	1.44	1.38
22	b	607	CLA	OBD-CAD	3.33	1.28	1.22
22	C	509	CLA	OBD-CAD	3.33	1.28	1.22
22	b	620	CLA	O2A-CGA	3.33	1.43	1.33
22	B	611	CLA	C3D-C2D	3.33	1.48	1.39
22	B	611	CLA	O2D-CGD	3.32	1.41	1.33
33	C	517	DGD	O2G-C1B	3.32	1.43	1.34
33	c	517	DGD	O1G-C1A	3.32	1.43	1.33
37	f	101	HEM	C3C-CAC	3.31	1.54	1.47
22	B	607	CLA	C4D-CHA	3.31	1.50	1.38
22	b	605	CLA	CHD-C4C	3.31	1.46	1.39
22	b	609	CLA	O2D-CGD	3.31	1.41	1.33
22	b	612	CLA	CHC-C1C	3.31	1.43	1.35
22	C	513	CLA	OBD-CAD	3.31	1.28	1.22
22	b	617	CLA	OBD-CAD	3.30	1.28	1.22
22	B	602	CLA	C4C-C3C	3.30	1.50	1.45
22	B	614	CLA	C3B-C2B	3.30	1.44	1.40
22	b	614	CLA	MG-NC	3.29	2.14	2.06
33	C	517	DGD	O1G-C1A	3.29	1.43	1.33
23	D	404	PHO	CHA-CBD	-3.29	1.48	1.52
22	C	509	CLA	MG-NA	3.29	2.14	2.06
22	c	508	CLA	C4D-CHA	3.28	1.50	1.38
22	b	610	CLA	CHD-C1D	3.28	1.44	1.38
22	c	509	CLA	OBD-CAD	3.28	1.28	1.22
22	c	508	CLA	CHD-C4C	3.27	1.46	1.39
22	B	617	CLA	MG-NC	-3.27	1.98	2.06
22	B	602	CLA	CHD-C4C	3.27	1.46	1.39
22	B	610	CLA	O2A-CGA	3.26	1.42	1.33
22	c	502	CLA	C1B-CHB	3.26	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	C1C-NC	-3.26	1.32	1.37
22	c	510	CLA	C3D-C2D	3.26	1.48	1.39
22	b	605	CLA	C3D-C2D	3.26	1.48	1.39
22	c	502	CLA	O2A-CGA	3.26	1.42	1.33
22	C	501	CLA	C1D-ND	-3.25	1.33	1.37
33	H	101	DGD	O2G-C1B	3.25	1.43	1.34
22	C	506	CLA	CHD-C1D	3.25	1.44	1.38
22	B	616	CLA	C1D-ND	-3.24	1.33	1.37
22	A	405	CLA	C3C-C2C	3.24	1.43	1.36
22	c	514	CLA	OBD-CAD	3.24	1.28	1.22
22	b	618	CLA	MG-ND	-3.24	1.99	2.05
22	c	504	CLA	C4D-CHA	3.24	1.49	1.38
22	D	403	CLA	CMB-C2B	-3.23	1.44	1.51
37	f	101	HEM	CMA-C3A	3.23	1.58	1.51
22	d	403	CLA	CHD-C1D	3.23	1.44	1.38
26	d	412	LMG	O7-C10	3.23	1.43	1.34
23	D	404	PHO	O2D-CGD	3.22	1.41	1.33
33	h	101	DGD	O1G-C1A	3.22	1.42	1.33
22	c	502	CLA	C1D-ND	-3.22	1.33	1.37
22	c	514	CLA	CHD-C4C	3.21	1.46	1.39
22	c	513	CLA	MG-ND	-3.21	1.99	2.05
22	b	615	CLA	C4B-NB	3.21	1.38	1.35
22	b	605	CLA	C1C-NC	-3.21	1.33	1.37
22	B	614	CLA	C1B-NB	-3.21	1.32	1.35
22	D	405	CLA	O2D-CGD	3.21	1.41	1.33
23	A	407	PHO	C3C-C2C	3.20	1.47	1.37
29	o	303	DMS	O-S	3.20	1.71	1.50
22	b	608	CLA	CHD-C1D	3.20	1.44	1.38
22	b	606	CLA	C3B-C2B	3.20	1.44	1.40
22	d	402	CLA	C3D-C2D	3.20	1.47	1.39
22	b	618	CLA	OBD-CAD	3.19	1.28	1.22
22	b	618	CLA	C4B-CHC	3.19	1.49	1.41
22	c	512	CLA	O2A-CGA	3.19	1.42	1.33
23	A	407	PHO	CAC-C3C	-3.19	1.46	1.52
22	C	501	CLA	C3B-C2B	3.18	1.44	1.40
22	c	505	CLA	OBD-CAD	3.18	1.28	1.22
22	C	509	CLA	C4B-NB	-3.18	1.32	1.35
22	b	614	CLA	C4C-C3C	3.18	1.50	1.45
22	b	613	CLA	C4B-NB	-3.18	1.32	1.35
22	a	409	CLA	C1C-NC	-3.17	1.33	1.37
22	B	606	CLA	CHC-C1C	3.17	1.43	1.35
22	B	611	CLA	C4C-C3C	3.17	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	C3D-C4D	3.17	1.51	1.44
25	a	411	PL9	C7-C3	3.17	1.54	1.51
22	d	405	CLA	OBD-CAD	3.16	1.27	1.22
31	d	409	LHG	O8-C23	3.16	1.42	1.33
22	A	405	CLA	C1D-C2D	3.15	1.51	1.45
22	C	503	CLA	CHD-C1D	3.15	1.44	1.38
22	c	508	CLA	OBD-CAD	3.15	1.27	1.22
22	C	503	CLA	C1D-ND	-3.15	1.33	1.37
22	c	507	CLA	CHD-C4C	3.14	1.46	1.39
22	C	508	CLA	C1C-NC	-3.14	1.33	1.37
22	B	604	CLA	C1C-NC	-3.14	1.33	1.37
22	b	612	CLA	C1B-NB	-3.14	1.32	1.35
29	b	630	DMS	O-S	3.13	1.71	1.50
22	b	610	CLA	CHD-C4C	3.13	1.46	1.39
22	B	605	CLA	C1D-ND	-3.13	1.33	1.37
22	c	510	CLA	MG-NC	3.13	2.13	2.06
22	C	513	CLA	C4D-CHA	3.13	1.49	1.38
22	b	618	CLA	C1C-C2C	3.13	1.50	1.44
33	c	518	DGD	O1G-C1A	3.13	1.42	1.33
22	D	405	CLA	CHD-C4C	3.13	1.46	1.39
22	B	611	CLA	C1C-NC	-3.13	1.33	1.37
22	c	511	CLA	OBD-CAD	3.12	1.27	1.22
22	B	606	CLA	C3C-C2C	3.12	1.43	1.36
22	C	502	CLA	OBD-CAD	3.12	1.27	1.22
22	d	405	CLA	O2D-CGD	3.12	1.40	1.33
22	c	506	CLA	C3D-C2D	3.12	1.47	1.39
22	D	403	CLA	CHD-C1D	3.12	1.44	1.38
22	a	409	CLA	C4D-ND	3.12	1.41	1.37
22	c	509	CLA	C3D-C2D	3.12	1.47	1.39
22	B	612	CLA	C3B-C2B	3.11	1.44	1.40
22	B	605	CLA	C1C-NC	-3.11	1.33	1.37
22	B	616	CLA	OBD-CAD	3.11	1.27	1.22
22	c	503	CLA	C1D-ND	-3.11	1.34	1.37
22	b	610	CLA	O2A-CGA	3.10	1.42	1.33
31	D	409	LHG	O8-C23	3.10	1.42	1.33
22	b	612	CLA	CHD-C4C	3.10	1.46	1.39
22	c	506	CLA	C1B-CHB	3.10	1.49	1.41
24	B	619	BCR	C19-C18	3.09	1.52	1.45
22	c	504	CLA	C1B-CHB	3.08	1.49	1.41
22	D	403	CLA	CHC-C1C	3.08	1.42	1.35
22	c	506	CLA	C4B-CHC	3.08	1.49	1.41
22	c	511	CLA	C1B-NB	-3.08	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	405	CLA	C3D-C2D	3.08	1.47	1.39
22	C	510	CLA	C4C-C3C	3.07	1.50	1.45
22	D	405	CLA	MG-ND	-3.07	1.99	2.05
29	C	530	DMS	O-S	3.07	1.71	1.50
22	c	510	CLA	MG-NA	3.07	2.13	2.06
22	C	512	CLA	MG-NC	3.07	2.13	2.06
32	o	301	HTG	O5-C1	3.07	1.47	1.42
22	A	406	CLA	OBD-CAD	3.07	1.27	1.22
22	A	405	CLA	CHD-C4C	3.06	1.46	1.39
22	c	502	CLA	CHD-C4C	3.06	1.46	1.39
22	C	502	CLA	C3D-C2D	3.05	1.47	1.39
22	C	511	CLA	MG-ND	-3.05	1.99	2.05
22	B	611	CLA	C3B-C2B	3.05	1.44	1.40
22	B	615	CLA	C4D-CHA	3.05	1.49	1.38
22	C	504	CLA	C3D-C2D	3.05	1.47	1.39
22	C	504	CLA	C4D-CHA	3.04	1.49	1.38
22	B	607	CLA	C1D-ND	-3.04	1.34	1.37
22	b	605	CLA	C4B-CHC	3.04	1.49	1.41
33	c	518	DGD	O2G-C2G	-3.04	1.39	1.46
22	C	502	CLA	CHD-C1D	3.03	1.44	1.38
32	b	640	HTG	O5-C5	3.03	1.51	1.44
22	b	608	CLA	C3B-C2B	3.03	1.44	1.40
22	d	405	CLA	C4B-NB	-3.03	1.32	1.35
22	C	510	CLA	C1B-CHB	3.02	1.49	1.41
22	C	509	CLA	C1D-ND	-3.02	1.34	1.37
22	C	513	CLA	C1B-CHB	3.02	1.49	1.41
28	A	415	LMT	C4B-C3B	3.02	1.60	1.52
22	b	615	CLA	CHD-C4C	3.02	1.46	1.39
40	V	201	HEC	CBC-CAC	-3.02	1.38	1.49
22	c	502	CLA	C4D-ND	3.02	1.41	1.37
22	C	513	CLA	MG-ND	3.02	2.11	2.05
22	b	608	CLA	C1C-NC	-3.02	1.33	1.37
22	D	405	CLA	C3D-C2D	3.02	1.47	1.39
22	b	616	CLA	C1B-CHB	3.01	1.49	1.41
22	c	510	CLA	CHD-C4C	3.01	1.46	1.39
22	c	502	CLA	C4D-CHA	3.01	1.49	1.38
22	c	509	CLA	C1D-C2D	3.01	1.51	1.45
22	C	510	CLA	O2A-CGA	3.01	1.42	1.33
22	b	610	CLA	C4B-CHC	3.01	1.49	1.41
22	c	506	CLA	C1C-NC	-3.00	1.33	1.37
22	d	402	CLA	CMB-C2B	-3.00	1.45	1.51
24	k	101	BCR	C12-C13	3.00	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	CLA	C4D-CHA	2.99	1.49	1.38
22	A	408	CLA	O2A-CGA	2.99	1.42	1.33
22	C	511	CLA	O2A-CGA	2.99	1.42	1.33
22	d	405	CLA	CHD-C4C	2.99	1.46	1.39
22	B	608	CLA	O2A-CGA	2.99	1.42	1.33
32	B	642	HTG	C1-S1	2.98	1.85	1.80
22	c	514	CLA	C1D-ND	-2.98	1.34	1.37
33	C	515	DGD	O1G-C1A	2.98	1.42	1.33
22	c	505	CLA	CHD-C4C	2.98	1.46	1.39
22	B	610	CLA	C1B-CHB	2.98	1.49	1.41
22	B	617	CLA	C4D-CHA	2.98	1.49	1.38
22	c	508	CLA	C4B-NB	-2.97	1.32	1.35
25	d	407	PL9	C7-C3	2.97	1.54	1.51
22	b	620	CLA	C4D-CHA	2.97	1.48	1.38
22	A	408	CLA	MG-NC	2.97	2.13	2.06
22	b	609	CLA	CHD-C4C	2.97	1.46	1.39
22	d	405	CLA	C1C-NC	-2.97	1.33	1.37
22	C	510	CLA	CHD-C4C	2.97	1.46	1.39
23	a	408	PHO	C3A-C2A	-2.96	1.52	1.54
22	C	508	CLA	O2A-CGA	2.96	1.42	1.33
22	B	605	CLA	CAA-C2A	-2.96	1.48	1.54
23	A	407	PHO	O2A-CGA	2.96	1.42	1.33
22	a	409	CLA	CHD-C1D	2.96	1.44	1.38
22	B	606	CLA	CHD-C4C	2.95	1.46	1.39
22	d	403	CLA	O2D-CGD	2.95	1.40	1.33
22	B	616	CLA	C1C-NC	-2.95	1.33	1.37
22	c	506	CLA	C4B-NB	-2.95	1.32	1.35
40	V	201	HEC	CBB-CAB	-2.95	1.38	1.49
22	B	612	CLA	OBD-CAD	2.95	1.27	1.22
22	C	513	CLA	C3D-C2D	2.95	1.47	1.39
22	B	605	CLA	O2A-CGA	2.95	1.41	1.33
22	c	514	CLA	C3D-C2D	2.94	1.47	1.39
22	b	614	CLA	C3D-C2D	2.94	1.47	1.39
24	A	409	BCR	C15-C14	2.94	1.52	1.43
22	C	506	CLA	C4D-CHA	2.94	1.48	1.38
22	a	406	CLA	O2D-CGD	2.94	1.40	1.33
22	a	406	CLA	C4B-NB	-2.93	1.32	1.35
22	b	611	CLA	C1D-ND	-2.93	1.34	1.37
22	D	405	CLA	OBD-CAD	2.93	1.27	1.22
22	a	406	CLA	OBD-CAD	2.93	1.27	1.22
22	c	511	CLA	C3B-C2B	2.93	1.44	1.40
22	b	618	CLA	C4C-C3C	2.92	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	622	BCR	C5-C6	2.92	1.39	1.34
22	A	408	CLA	C4B-NB	2.92	1.37	1.35
22	c	505	CLA	C3D-C4D	-2.92	1.37	1.44
24	K	102	BCR	C17-C18	2.92	1.39	1.35
22	C	513	CLA	C1D-ND	-2.92	1.34	1.37
22	B	612	CLA	O2D-CGD	2.92	1.40	1.33
22	B	617	CLA	C3B-C2B	2.92	1.44	1.40
22	C	512	CLA	C1B-CHB	2.91	1.49	1.41
22	B	603	CLA	O2D-CGD	2.91	1.40	1.33
22	a	406	CLA	CHD-C4C	2.91	1.45	1.39
22	B	602	CLA	C4D-CHA	2.91	1.48	1.38
22	c	503	CLA	C3D-C2D	2.90	1.47	1.39
22	b	610	CLA	MG-NC	2.90	2.13	2.06
22	b	608	CLA	O2A-CGA	2.90	1.41	1.33
22	c	512	CLA	C1B-CHB	2.90	1.49	1.41
28	l	101	LMT	O1'-C1'	2.90	1.45	1.40
22	B	613	CLA	C1C-NC	-2.90	1.33	1.37
22	A	404	CLA	C1B-NB	-2.90	1.32	1.35
23	A	407	PHO	CHA-CBD	-2.90	1.48	1.52
22	B	607	CLA	C4C-C3C	2.89	1.50	1.45
22	c	510	CLA	C4D-ND	2.89	1.41	1.37
22	B	605	CLA	OBD-CAD	2.89	1.27	1.22
22	D	405	CLA	C4C-C3C	2.89	1.50	1.45
22	d	403	CLA	C4C-C3C	2.89	1.50	1.45
22	b	619	CLA	C4D-CHA	2.89	1.48	1.38
33	D	408	DGD	O3G-C1D	2.89	1.45	1.40
33	C	517	DGD	O2G-C2G	-2.89	1.39	1.46
22	C	510	CLA	C1B-NB	-2.89	1.32	1.35
22	b	613	CLA	C1B-NB	-2.88	1.32	1.35
22	B	608	CLA	C1B-CHB	2.88	1.49	1.41
22	C	510	CLA	C3B-C2B	2.88	1.44	1.40
22	B	608	CLA	O2D-CGD	2.88	1.40	1.33
22	C	512	CLA	C3D-C2D	2.88	1.47	1.39
22	B	602	CLA	OBD-CAD	2.87	1.27	1.22
22	c	508	CLA	O2D-CGD	2.87	1.40	1.33
22	b	619	CLA	C1B-CHB	2.87	1.49	1.41
22	d	402	CLA	C1B-CHB	2.87	1.49	1.41
22	c	511	CLA	O2A-CGA	2.87	1.41	1.33
22	C	507	CLA	C1D-ND	-2.87	1.34	1.37
22	c	508	CLA	C1C-NC	-2.86	1.33	1.37
24	d	406	BCR	C30-C25	-2.86	1.49	1.53
22	b	615	CLA	O2A-CGA	2.86	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	407	CLA	O2A-CGA	2.86	1.41	1.33
22	d	403	CLA	C3B-C2B	2.86	1.44	1.40
23	D	404	PHO	C3C-C2C	2.86	1.46	1.37
22	D	405	CLA	C3B-C2B	2.86	1.44	1.40
22	B	602	CLA	C1C-NC	-2.85	1.33	1.37
28	Z	101	LMT	O1'-C1'	2.84	1.45	1.40
22	C	501	CLA	O2A-CGA	2.84	1.41	1.33
22	B	603	CLA	C1B-CHB	2.84	1.48	1.41
24	d	406	BCR	C12-C13	2.84	1.52	1.45
22	b	617	CLA	C4D-CHA	2.84	1.48	1.38
22	A	408	CLA	C4C-C3C	2.83	1.49	1.45
24	c	516	BCR	C14-C13	2.83	1.39	1.35
22	c	511	CLA	CHD-C4C	2.82	1.45	1.39
22	b	617	CLA	C3D-C2D	2.82	1.46	1.39
22	c	503	CLA	C4D-CHA	2.82	1.48	1.38
22	B	608	CLA	C3C-C2C	2.82	1.42	1.36
22	B	616	CLA	C3B-C2B	2.82	1.44	1.40
22	C	507	CLA	C3D-C2D	2.82	1.46	1.39
22	B	610	CLA	C4D-ND	-2.82	1.33	1.37
40	v	202	HEC	CBB-CAB	-2.81	1.39	1.49
22	B	616	CLA	C4C-C3C	2.81	1.49	1.45
22	C	501	CLA	OBD-CAD	2.81	1.27	1.22
22	c	507	CLA	C1D-ND	-2.81	1.34	1.37
22	B	616	CLA	C3D-C2D	2.81	1.46	1.39
31	d	409	LHG	O7-C7	2.81	1.42	1.34
32	b	602	HTG	C1'-S1	-2.81	1.77	1.81
22	c	506	CLA	C4D-CHA	2.81	1.48	1.38
22	B	608	CLA	C1C-NC	-2.81	1.33	1.37
22	B	609	CLA	C1D-ND	-2.81	1.34	1.37
22	c	503	CLA	MG-ND	-2.81	2.00	2.05
22	c	514	CLA	C1B-CHB	2.80	1.48	1.41
22	B	612	CLA	CHD-C4C	2.80	1.45	1.39
22	c	510	CLA	C1D-ND	-2.80	1.34	1.37
22	c	505	CLA	C4B-CHC	2.80	1.48	1.41
22	a	407	CLA	C3C-C2C	2.80	1.42	1.36
22	b	619	CLA	C1D-ND	-2.80	1.34	1.37
22	b	610	CLA	C1C-NC	-2.80	1.33	1.37
22	B	614	CLA	C3D-C2D	2.80	1.46	1.39
26	C	519	LMG	O1-C1	2.80	1.45	1.40
22	b	618	CLA	C3D-C4D	-2.79	1.37	1.44
22	b	620	CLA	OBD-CAD	2.79	1.27	1.22
22	D	403	CLA	O2A-CGA	2.79	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	101	BCR	C8-C9	2.79	1.51	1.45
22	b	607	CLA	C1B-NB	-2.79	1.32	1.35
22	B	605	CLA	C1B-CHB	2.78	1.48	1.41
37	F	101	HEM	C3C-CAC	2.78	1.53	1.47
23	d	404	PHO	C3C-C2C	2.78	1.45	1.37
22	c	508	CLA	C3B-C2B	2.77	1.44	1.40
32	B	629	HTG	C1'-S1	-2.77	1.77	1.81
22	c	508	CLA	O2A-CGA	2.77	1.41	1.33
22	d	405	CLA	C4D-CHA	2.77	1.48	1.38
22	C	503	CLA	C1B-NB	-2.77	1.32	1.35
25	A	410	PL9	C6-C1	2.77	1.53	1.48
22	c	508	CLA	C3D-C2D	2.76	1.46	1.39
22	b	611	CLA	O2A-CGA	2.76	1.41	1.33
22	D	403	CLA	C4D-CHA	2.76	1.48	1.38
22	c	511	CLA	C4D-ND	2.76	1.41	1.37
22	C	507	CLA	C4C-C3C	2.76	1.49	1.45
22	B	613	CLA	C1B-NB	-2.75	1.32	1.35
23	a	408	PHO	C3C-C2C	2.75	1.45	1.37
22	B	614	CLA	OBD-CAD	2.75	1.27	1.22
22	b	606	CLA	O2D-CGD	2.75	1.39	1.33
22	B	617	CLA	CHD-C1D	2.74	1.43	1.38
22	c	503	CLA	C1B-CHB	2.74	1.48	1.41
22	b	619	CLA	OBD-CAD	2.74	1.27	1.22
22	C	505	CLA	C4B-CHC	2.73	1.48	1.41
22	C	504	CLA	MG-NC	2.73	2.12	2.06
22	C	501	CLA	C1B-CHB	2.73	1.48	1.41
22	C	505	CLA	C1D-ND	-2.73	1.34	1.37
33	c	519	DGD	O2G-C2G	-2.73	1.39	1.46
22	d	402	CLA	C4D-CHA	2.73	1.48	1.38
22	b	613	CLA	C4B-CHC	2.73	1.48	1.41
22	c	504	CLA	MG-NC	2.73	2.12	2.06
22	B	610	CLA	O2D-CGD	2.72	1.39	1.33
22	B	613	CLA	CHD-C4C	2.72	1.45	1.39
31	d	411	LHG	O7-C7	2.72	1.42	1.34
22	A	404	CLA	CHD-C1D	2.72	1.43	1.38
22	C	505	CLA	C4C-C3C	2.72	1.49	1.45
22	B	617	CLA	C3D-C2D	2.72	1.46	1.39
22	c	505	CLA	C3D-C2D	2.71	1.46	1.39
22	c	504	CLA	C1C-NC	-2.71	1.33	1.37
22	C	508	CLA	OBD-CAD	2.71	1.27	1.22
32	V	202	HTG	O5-C1	2.71	1.46	1.42
22	A	406	CLA	O2D-CGD	2.71	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	C3D-C2D	2.71	1.46	1.39
22	b	613	CLA	C1B-CHB	2.70	1.48	1.41
22	D	403	CLA	C1B-NB	-2.70	1.32	1.35
22	b	605	CLA	C4D-CHA	2.70	1.48	1.38
32	v	208	HTG	C1'-S1	-2.70	1.78	1.81
22	C	501	CLA	C3D-C2D	2.70	1.46	1.39
22	c	511	CLA	MG-ND	-2.70	2.00	2.05
26	B	622	LMG	O1-C1	2.69	1.44	1.40
22	C	503	CLA	C4B-CHC	2.69	1.48	1.41
22	C	508	CLA	MG-ND	-2.69	2.00	2.05
22	b	618	CLA	C1B-NB	-2.69	1.32	1.35
22	A	406	CLA	CHD-C4C	2.69	1.45	1.39
22	D	405	CLA	C4B-CHC	2.69	1.48	1.41
22	A	406	CLA	C4D-CHA	2.69	1.48	1.38
25	d	407	PL9	C7-C8	-2.69	1.46	1.50
22	B	602	CLA	MG-ND	2.68	2.11	2.05
22	B	606	CLA	C4B-CHC	2.68	1.48	1.41
22	B	607	CLA	O2A-CGA	2.68	1.41	1.33
22	c	512	CLA	C4D-CHA	2.67	1.47	1.38
22	B	612	CLA	C4D-CHA	2.67	1.47	1.38
31	D	410	LHG	O8-C23	2.67	1.41	1.33
22	B	615	CLA	CBA-CGA	2.67	1.58	1.50
31	D	409	LHG	C24-C23	2.67	1.58	1.50
22	d	403	CLA	O2A-CGA	2.67	1.41	1.33
37	f	101	HEM	FE-NB	2.67	2.10	1.96
22	C	501	CLA	C4B-CHC	2.67	1.48	1.41
22	B	606	CLA	C1B-CHB	2.66	1.48	1.41
22	c	508	CLA	CHD-C1D	2.66	1.43	1.38
22	b	607	CLA	C3D-C2D	2.66	1.46	1.39
22	b	605	CLA	C1C-C2C	2.66	1.49	1.44
22	B	609	CLA	C3B-C2B	2.66	1.44	1.40
22	b	612	CLA	O2A-CGA	2.65	1.41	1.33
33	c	518	DGD	O3G-C1D	2.65	1.44	1.40
22	A	405	CLA	O2A-CGA	2.64	1.41	1.33
22	B	610	CLA	CHD-C4C	2.64	1.45	1.39
22	b	612	CLA	O2D-CGD	2.64	1.39	1.33
22	C	509	CLA	CHD-C1D	2.64	1.43	1.38
22	c	511	CLA	C4D-CHA	2.64	1.47	1.38
22	C	510	CLA	MG-NC	2.64	2.12	2.06
22	A	406	CLA	C1C-NC	-2.63	1.33	1.37
22	A	408	CLA	MG-NA	2.63	2.12	2.06
22	B	606	CLA	C1C-C2C	2.63	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	410	LHG	O7-C7	2.63	1.41	1.34
22	b	608	CLA	O2A-C1	-2.62	1.38	1.46
37	F	101	HEM	CMB-C2B	2.62	1.56	1.50
22	A	406	CLA	C3D-C4D	-2.62	1.38	1.44
38	H	102	RRX	C26-C25	2.62	1.39	1.34
22	a	409	CLA	C4D-CHA	2.62	1.47	1.38
22	b	618	CLA	C1B-CHB	2.62	1.48	1.41
25	a	411	PL9	C2-C3	2.62	1.41	1.34
22	B	609	CLA	C4C-C3C	2.62	1.49	1.45
22	d	405	CLA	C4B-CHC	2.62	1.48	1.41
22	C	509	CLA	C4D-CHA	2.62	1.47	1.38
33	C	515	DGD	O2G-C1B	2.62	1.41	1.34
32	o	301	HTG	C1-C2	2.62	1.57	1.53
31	B	621	LHG	O8-C23	2.61	1.41	1.33
22	C	508	CLA	C3D-C2D	2.61	1.46	1.39
22	C	503	CLA	C3D-C2D	2.61	1.46	1.39
28	a	401	LMT	O3B-C3B	2.61	1.49	1.43
24	b	622	BCR	C12-C13	2.61	1.51	1.45
22	c	506	CLA	C1D-ND	-2.61	1.34	1.37
22	b	617	CLA	C3B-C2B	2.61	1.44	1.40
22	b	615	CLA	C1C-NC	-2.60	1.33	1.37
22	C	506	CLA	C1B-CHB	2.60	1.48	1.41
22	c	504	CLA	C4B-CHC	2.60	1.48	1.41
22	C	507	CLA	C4B-NB	-2.60	1.32	1.35
40	v	202	HEC	C4D-ND	2.60	1.41	1.36
22	C	502	CLA	C4D-CHA	2.60	1.47	1.38
37	f	101	HEM	CAB-C3B	2.59	1.54	1.47
22	b	610	CLA	C3D-C2D	2.59	1.46	1.39
23	d	404	PHO	CMD-C2D	-2.59	1.45	1.51
22	B	611	CLA	OBD-CAD	2.59	1.26	1.22
22	d	402	CLA	C4C-C3C	2.59	1.49	1.45
22	b	612	CLA	MG-NA	2.59	2.12	2.06
22	b	611	CLA	C4D-CHA	2.58	1.47	1.38
22	C	502	CLA	C4B-NB	-2.58	1.32	1.35
32	b	640	HTG	C1-C2	2.58	1.57	1.53
22	c	513	CLA	C4D-CHA	2.58	1.47	1.38
22	C	506	CLA	C1D-ND	-2.58	1.34	1.37
22	B	607	CLA	CHD-C1D	2.58	1.43	1.38
22	c	510	CLA	C1B-CHB	2.58	1.48	1.41
22	C	511	CLA	C4D-CHA	2.58	1.47	1.38
22	b	613	CLA	C3D-C2D	2.57	1.46	1.39
22	C	511	CLA	C1D-ND	-2.57	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	OBD-CAD	2.57	1.26	1.22
24	A	409	BCR	C27-C26	2.57	1.56	1.51
25	d	407	PL9	C41-C39	2.56	1.56	1.51
28	C	520	LMT	O1'-C1'	2.56	1.44	1.40
22	b	614	CLA	CBD-CGD	-2.56	1.44	1.52
22	C	509	CLA	C4C-C3C	2.56	1.49	1.45
22	c	514	CLA	C1C-NC	-2.56	1.34	1.37
37	F	101	HEM	CAB-C3B	2.56	1.54	1.47
22	C	508	CLA	C4D-CHA	2.56	1.47	1.38
22	C	507	CLA	OBD-CAD	2.56	1.26	1.22
28	t	102	LMT	O5'-C1'	2.56	1.48	1.41
22	A	405	CLA	C4D-ND	-2.56	1.34	1.37
22	c	505	CLA	C1D-ND	-2.55	1.34	1.37
22	B	616	CLA	C1B-CHB	2.55	1.48	1.41
22	c	504	CLA	OBD-CAD	2.55	1.26	1.22
22	b	614	CLA	C1C-NC	-2.54	1.34	1.37
22	b	618	CLA	CHD-C4C	2.54	1.45	1.39
22	c	507	CLA	C4B-CHC	2.54	1.48	1.41
22	C	512	CLA	C4D-CHA	2.54	1.47	1.38
22	c	502	CLA	C4B-CHC	2.54	1.48	1.41
25	D	407	PL9	C6-C5	2.54	1.48	1.35
22	a	409	CLA	C1D-ND	-2.54	1.34	1.37
22	C	510	CLA	C4D-CHA	2.53	1.47	1.38
28	a	401	LMT	O5B-C1B	2.53	1.48	1.41
22	C	505	CLA	O2A-CGA	2.53	1.40	1.33
22	c	504	CLA	C3D-C2D	2.53	1.46	1.39
22	c	505	CLA	C3B-C2B	2.53	1.43	1.40
22	B	616	CLA	O2A-CGA	2.52	1.40	1.33
22	A	404	CLA	C1D-C2D	2.52	1.50	1.45
22	B	607	CLA	CMA-C3A	-2.52	1.47	1.53
28	b	626	LMT	O1'-C1'	2.52	1.44	1.40
22	b	606	CLA	C1B-CHB	2.52	1.48	1.41
32	b	627	HTG	C1'-S1	-2.52	1.78	1.81
28	F	102	LMT	O5'-C1'	2.51	1.48	1.41
22	c	514	CLA	C4D-CHA	2.51	1.47	1.38
22	B	609	CLA	C3D-C2D	2.51	1.46	1.39
22	c	512	CLA	C1D-ND	-2.51	1.34	1.37
24	A	409	BCR	C30-C25	-2.51	1.50	1.53
33	c	518	DGD	O2G-C1B	2.51	1.41	1.34
22	b	615	CLA	C4D-CHA	2.51	1.47	1.38
22	a	409	CLA	MG-NA	2.50	2.12	2.06
25	d	407	PL9	C2-C1	-2.50	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	519	DGD	O2D-C2D	2.50	1.48	1.43
22	d	402	CLA	CAA-C2A	-2.49	1.49	1.54
22	d	402	CLA	C3C-C2C	2.49	1.42	1.36
22	B	609	CLA	MG-ND	2.49	2.10	2.05
24	B	620	BCR	C12-C13	2.49	1.51	1.45
22	b	614	CLA	C4D-CHA	2.49	1.47	1.38
22	B	612	CLA	C2A-C1A	-2.49	1.46	1.52
28	m	102	LMT	O1'-C1'	2.49	1.44	1.40
22	b	613	CLA	C4D-CHA	2.48	1.47	1.38
22	B	604	CLA	CMA-C3A	2.48	1.58	1.53
22	b	611	CLA	CHD-C1D	2.48	1.43	1.38
22	C	504	CLA	C1B-NB	-2.48	1.33	1.35
22	C	509	CLA	O2D-CGD	2.48	1.39	1.33
22	c	505	CLA	C4C-C3C	2.48	1.49	1.45
22	A	405	CLA	CBD-CGD	-2.48	1.44	1.52
22	b	614	CLA	CHD-C4C	2.48	1.44	1.39
22	B	615	CLA	C1D-C2D	2.48	1.50	1.45
22	c	506	CLA	C4C-C3C	2.48	1.49	1.45
22	a	406	CLA	C1B-CHB	2.47	1.47	1.41
38	H	102	RRX	C23-C22	2.47	1.51	1.45
22	c	506	CLA	MG-ND	2.47	2.10	2.05
22	d	402	CLA	C4D-ND	2.47	1.41	1.37
22	b	616	CLA	O2A-CGA	2.47	1.40	1.33
22	B	603	CLA	O2A-CGA	2.46	1.40	1.33
22	b	620	CLA	C1B-CHB	2.46	1.47	1.41
22	c	502	CLA	CHD-C1D	2.46	1.43	1.38
22	B	617	CLA	C1C-NC	-2.46	1.34	1.37
24	B	619	BCR	C37-C22	2.46	1.56	1.50
24	A	409	BCR	C16-C17	2.46	1.51	1.43
22	b	618	CLA	C1C-NC	-2.45	1.34	1.37
22	b	608	CLA	C4D-CHA	2.45	1.47	1.38
22	B	602	CLA	C2-C3	2.45	1.38	1.33
22	b	614	CLA	MG-NA	2.45	2.12	2.06
22	c	508	CLA	O2A-C1	-2.45	1.39	1.46
22	b	605	CLA	MG-NC	2.44	2.12	2.06
25	d	407	PL9	C23-C24	2.44	1.38	1.33
22	C	503	CLA	C1C-C2C	2.44	1.49	1.44
32	O	302	HTG	C1-C2	2.44	1.57	1.53
22	a	406	CLA	C4D-CHA	2.44	1.47	1.38
22	c	508	CLA	C1B-NB	-2.43	1.33	1.35
22	b	618	CLA	C3D-C2D	2.43	1.45	1.39
22	c	504	CLA	C1C-C2C	2.43	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	CHD-C4C	2.43	1.44	1.39
22	C	508	CLA	C1B-CHB	2.43	1.47	1.41
22	a	407	CLA	C1B-CHB	2.43	1.47	1.41
32	c	541	HTG	O5-C1	2.43	1.46	1.42
32	C	536	HTG	O5-C1	2.43	1.46	1.42
33	C	517	DGD	O3G-C3G	2.43	1.48	1.43
22	B	617	CLA	C2-C3	2.43	1.38	1.33
26	c	521	LMG	O1-C1	2.43	1.44	1.40
24	D	406	BCR	C30-C25	-2.43	1.50	1.53
22	c	511	CLA	CMB-C2B	-2.43	1.46	1.51
22	A	408	CLA	C1B-CHB	2.43	1.47	1.41
22	b	616	CLA	C3D-C2D	2.43	1.45	1.39
22	b	606	CLA	C3B-CAB	2.43	1.52	1.47
22	B	604	CLA	O2A-CGA	2.42	1.40	1.33
22	b	614	CLA	C1B-NB	-2.42	1.33	1.35
25	A	410	PL9	C2-C3	2.42	1.41	1.34
22	A	405	CLA	C3B-C2B	2.42	1.43	1.40
22	B	608	CLA	MG-ND	2.42	2.10	2.05
22	b	611	CLA	C1B-CHB	2.42	1.47	1.41
22	a	409	CLA	C3D-C2D	2.42	1.45	1.39
22	B	611	CLA	O2A-CGA	2.42	1.40	1.33
22	C	505	CLA	C3D-C2D	2.42	1.45	1.39
22	B	607	CLA	C3D-C2D	2.41	1.45	1.39
22	c	512	CLA	C4C-C3C	2.40	1.49	1.45
22	c	506	CLA	O2D-CGD	2.40	1.39	1.33
24	b	621	BCR	C15-C14	2.40	1.50	1.43
22	B	605	CLA	C4B-NB	-2.39	1.33	1.35
22	a	409	CLA	C1B-CHB	2.39	1.47	1.41
22	c	513	CLA	C1B-CHB	2.39	1.47	1.41
25	a	411	PL9	C6-C5	2.39	1.47	1.35
23	A	407	PHO	C3D-C2D	2.39	1.43	1.39
26	a	412	LMG	O1-C1	2.39	1.44	1.40
22	b	620	CLA	C3D-C4D	-2.39	1.38	1.44
22	C	502	CLA	CHD-C4C	2.39	1.44	1.39
24	B	619	BCR	C23-C22	2.39	1.51	1.45
22	B	608	CLA	C3B-C2B	2.39	1.43	1.40
33	H	101	DGD	O3G-C1D	2.39	1.44	1.40
22	c	510	CLA	C4D-CHA	2.38	1.46	1.38
22	B	611	CLA	CHD-C4C	2.38	1.44	1.39
22	c	504	CLA	C1B-NB	-2.38	1.33	1.35
22	D	405	CLA	C1D-ND	-2.38	1.34	1.37
22	c	503	CLA	O2A-CGA	2.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	407	PL9	C3-C4	-2.37	1.45	1.49
24	t	101	BCR	C23-C22	2.37	1.51	1.45
22	C	511	CLA	C3D-C2D	2.37	1.45	1.39
22	b	614	CLA	C3B-C2B	2.37	1.43	1.40
22	b	609	CLA	C1C-NC	-2.37	1.34	1.37
25	D	407	PL9	O1-C4	2.37	1.28	1.23
22	b	608	CLA	C1B-CHB	2.37	1.47	1.41
32	C	522	HTG	C1'-S1	-2.36	1.78	1.81
37	F	101	HEM	O1D-CGD	2.36	1.30	1.22
26	d	412	LMG	O1-C1	2.36	1.44	1.40
22	C	507	CLA	O2A-CGA	2.36	1.40	1.33
22	b	620	CLA	C4B-CHC	2.36	1.47	1.41
22	A	406	CLA	C3C-C2C	2.36	1.41	1.36
22	b	612	CLA	C1B-CHB	2.36	1.47	1.41
22	b	619	CLA	O2A-CGA	2.35	1.40	1.33
22	B	603	CLA	C4B-CHC	2.35	1.47	1.41
22	c	502	CLA	C3D-C2D	2.35	1.45	1.39
22	c	505	CLA	O2A-CGA	2.35	1.40	1.33
22	b	612	CLA	C3D-C2D	2.35	1.45	1.39
24	b	622	BCR	C8-C9	2.35	1.51	1.45
31	D	411	LHG	O1-C1	-2.34	1.32	1.42
32	V	202	HTG	C1'-S1	-2.34	1.78	1.81
22	c	507	CLA	C1B-CHB	2.34	1.47	1.41
22	b	607	CLA	O2A-CGA	2.34	1.40	1.33
22	B	608	CLA	CAA-C2A	2.33	1.58	1.54
22	B	607	CLA	C1B-CHB	2.33	1.47	1.41
22	B	607	CLA	C4B-CHC	2.33	1.47	1.41
22	B	616	CLA	MG-NC	2.33	2.11	2.06
24	a	410	BCR	C8-C9	2.33	1.50	1.45
22	B	612	CLA	C3D-C4D	-2.33	1.38	1.44
22	b	608	CLA	C1D-C2D	2.33	1.49	1.45
24	B	619	BCR	C4-C5	2.33	1.55	1.51
22	B	602	CLA	C1C-C2C	2.32	1.49	1.44
22	c	513	CLA	C4B-CHC	2.32	1.47	1.41
22	b	616	CLA	CHD-C4C	2.32	1.44	1.39
32	D	413	HTG	C1-C2	2.32	1.57	1.53
37	f	101	HEM	C2C-C1C	2.32	1.47	1.42
22	c	504	CLA	C4C-C3C	2.32	1.49	1.45
22	A	406	CLA	C4B-NB	-2.32	1.33	1.35
22	c	507	CLA	C4D-CHA	2.31	1.46	1.38
22	C	501	CLA	C1C-NC	-2.31	1.34	1.37
24	K	102	BCR	C1-C6	-2.31	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	101	BCR	C16-C17	2.31	1.50	1.43
31	B	621	LHG	O7-C7	2.30	1.40	1.34
22	B	611	CLA	C1C-C2C	2.30	1.49	1.44
25	D	407	PL9	C38-C39	-2.30	1.27	1.33
22	b	607	CLA	C4D-CHA	2.30	1.46	1.38
22	b	607	CLA	CMB-C2B	-2.30	1.46	1.51
22	c	505	CLA	C1B-CHB	2.30	1.47	1.41
22	C	506	CLA	C3D-C2D	2.30	1.45	1.39
24	b	623	BCR	C24-C25	2.30	1.53	1.45
22	b	607	CLA	C3B-C2B	2.29	1.43	1.40
22	b	611	CLA	CHD-C4C	2.29	1.44	1.39
22	B	606	CLA	O2A-CGA	2.29	1.40	1.33
22	B	605	CLA	C4D-CHA	2.29	1.46	1.38
31	D	409	LHG	P-O4	-2.28	1.44	1.55
22	b	607	CLA	C3D-C4D	-2.28	1.39	1.44
22	a	407	CLA	CMB-C2B	-2.28	1.46	1.51
22	b	616	CLA	C4B-CHC	2.28	1.47	1.41
22	a	407	CLA	C4D-ND	-2.28	1.34	1.37
22	A	404	CLA	C3D-C2D	2.28	1.45	1.39
22	C	512	CLA	C1D-ND	-2.28	1.35	1.37
33	H	101	DGD	O1G-C1A	2.27	1.40	1.33
24	B	620	BCR	C15-C14	2.27	1.50	1.43
22	B	614	CLA	C4C-C3C	2.27	1.49	1.45
31	b	624	LHG	O7-C5	-2.27	1.40	1.46
22	c	509	CLA	C1B-CHB	2.27	1.47	1.41
22	B	616	CLA	C4D-CHA	2.27	1.46	1.38
22	A	406	CLA	C3A-C2A	-2.27	1.48	1.54
24	b	623	BCR	C27-C26	2.27	1.55	1.51
22	b	611	CLA	C4B-CHC	2.26	1.47	1.41
22	c	512	CLA	C1B-NB	-2.26	1.33	1.35
22	A	405	CLA	C4B-CHC	2.26	1.47	1.41
22	c	505	CLA	C1C-C2C	2.26	1.48	1.44
37	f	101	HEM	O1D-CGD	2.26	1.29	1.22
22	b	614	CLA	OBD-CAD	2.25	1.26	1.22
22	C	513	CLA	C4B-CHC	2.25	1.47	1.41
22	B	614	CLA	C4B-NB	2.25	1.37	1.35
22	b	615	CLA	C1B-CHB	2.25	1.47	1.41
22	B	614	CLA	CMB-C2B	-2.25	1.47	1.51
22	C	507	CLA	C4B-CHC	2.25	1.47	1.41
22	C	505	CLA	C2A-C1A	-2.25	1.47	1.52
22	A	404	CLA	C1B-CHB	2.25	1.47	1.41
28	J	102	LMT	O1'-C1'	2.25	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	408	DGD	O3G-C1D	2.25	1.44	1.40
33	c	519	DGD	O2G-C1B	2.25	1.40	1.34
22	B	602	CLA	C4D-ND	2.25	1.40	1.37
24	D	406	BCR	C12-C13	2.24	1.50	1.45
22	c	513	CLA	C3D-C2D	2.24	1.45	1.39
24	A	409	BCR	C39-C30	-2.24	1.49	1.53
22	C	505	CLA	C4D-ND	-2.24	1.34	1.37
22	B	604	CLA	C5-C3	2.24	1.55	1.51
33	C	515	DGD	C4D-C3D	2.24	1.58	1.52
23	a	408	PHO	C4B-NB	-2.24	1.31	1.38
22	c	506	CLA	OBD-CAD	2.24	1.26	1.22
22	A	408	CLA	C3D-C2D	2.24	1.45	1.39
22	B	617	CLA	C3D-C4D	-2.24	1.39	1.44
22	C	504	CLA	O2A-CGA	2.24	1.39	1.33
22	a	409	CLA	C3B-CAB	2.24	1.52	1.47
40	v	202	HEC	O1D-CGD	2.23	1.29	1.22
22	a	406	CLA	MG-ND	-2.23	2.01	2.05
22	c	509	CLA	C4B-CHC	2.23	1.47	1.41
22	c	508	CLA	C1D-ND	-2.23	1.35	1.37
22	B	606	CLA	C4D-CHA	2.23	1.46	1.38
22	B	609	CLA	C4D-CHA	2.22	1.46	1.38
22	c	513	CLA	C4C-C3C	2.22	1.48	1.45
22	c	514	CLA	C4D-ND	2.22	1.40	1.37
22	B	603	CLA	C3D-C2D	2.22	1.45	1.39
22	b	606	CLA	C3D-C4D	-2.22	1.39	1.44
33	d	408	DGD	C4D-C3D	2.22	1.58	1.52
22	b	614	CLA	O2A-CGA	2.22	1.39	1.33
22	B	611	CLA	C1-C2	2.22	1.55	1.49
22	d	403	CLA	C3D-C2D	2.22	1.45	1.39
24	K	101	BCR	C17-C18	2.22	1.38	1.35
22	b	611	CLA	C3B-C2B	2.22	1.43	1.40
24	K	101	BCR	C38-C26	2.22	1.54	1.50
22	B	603	CLA	C3B-CAB	2.21	1.52	1.47
22	a	407	CLA	O2D-CGD	2.21	1.38	1.33
22	c	507	CLA	C3D-C2D	2.21	1.45	1.39
22	d	405	CLA	C1B-CHB	2.21	1.47	1.41
22	C	507	CLA	C1B-CHB	2.21	1.47	1.41
22	A	404	CLA	C1D-ND	-2.21	1.35	1.37
28	A	415	LMT	O5'-C1'	2.21	1.47	1.41
25	d	407	PL9	C18-C19	2.20	1.38	1.33
22	C	502	CLA	C1B-CHB	2.20	1.47	1.41
22	b	609	CLA	O2A-C1	-2.20	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	406	BCR	C19-C18	2.20	1.50	1.45
22	C	506	CLA	OBD-CAD	2.20	1.26	1.22
22	C	502	CLA	C4B-CHC	2.20	1.47	1.41
31	D	410	LHG	O7-C5	-2.20	1.41	1.46
32	B	624	HTG	C1'-S1	-2.19	1.78	1.81
33	C	516	DGD	C1D-C2D	2.19	1.58	1.52
22	d	405	CLA	C1C-C2C	2.19	1.48	1.44
22	D	405	CLA	C4D-CHA	2.19	1.46	1.38
22	c	505	CLA	C4D-CHA	2.19	1.46	1.38
22	b	607	CLA	C4B-CHC	2.18	1.47	1.41
24	A	409	BCR	C19-C18	2.18	1.50	1.45
32	U	203	HTG	O5-C1	2.18	1.45	1.42
31	d	410	LHG	O7-C7	2.18	1.40	1.34
24	c	516	BCR	C15-C14	2.18	1.50	1.43
24	K	102	BCR	C19-C18	2.18	1.50	1.45
22	B	607	CLA	CAA-C2A	-2.18	1.50	1.54
22	b	606	CLA	C4D-CHA	2.18	1.46	1.38
22	B	607	CLA	C3A-C2A	-2.18	1.48	1.54
22	B	611	CLA	C1B-CHB	2.18	1.47	1.41
24	c	516	BCR	C16-C17	2.18	1.50	1.43
22	a	406	CLA	C3B-CAB	2.18	1.52	1.47
22	B	609	CLA	C1C-NC	-2.17	1.34	1.37
22	d	403	CLA	C4D-CHA	2.17	1.46	1.38
22	a	407	CLA	C4D-CHA	2.17	1.46	1.38
40	v	202	HEC	CMC-C2C	2.17	1.56	1.51
22	D	405	CLA	O2A-CGA	2.17	1.39	1.33
31	d	411	LHG	C4-C5	2.17	1.57	1.50
22	b	619	CLA	CAC-C3C	-2.17	1.45	1.51
22	c	506	CLA	C1C-C2C	2.17	1.48	1.44
25	D	407	PL9	C41-C39	2.16	1.55	1.51
22	C	504	CLA	MG-ND	2.16	2.10	2.05
22	c	503	CLA	C4D-ND	2.16	1.40	1.37
28	A	415	LMT	C3B-C2B	2.16	1.57	1.52
24	t	101	BCR	C35-C13	2.16	1.55	1.50
31	b	624	LHG	O8-C23	2.16	1.39	1.33
40	V	201	HEC	O2A-CGA	-2.16	1.23	1.30
22	b	619	CLA	C1C-NC	-2.16	1.34	1.37
22	D	403	CLA	C1B-CHB	2.16	1.47	1.41
22	b	616	CLA	C4D-CHA	2.15	1.46	1.38
22	c	509	CLA	CBD-CGD	-2.15	1.45	1.52
33	C	516	DGD	O2G-C1B	2.15	1.40	1.34
22	B	609	CLA	C2A-C1A	-2.15	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	BCR	C12-C13	2.15	1.50	1.45
24	D	406	BCR	C10-C9	-2.15	1.32	1.35
25	D	407	PL9	C2-C1	-2.15	1.38	1.44
22	a	406	CLA	C1D-C2D	2.15	1.49	1.45
22	a	406	CLA	C1C-NC	-2.15	1.34	1.37
26	D	412	LMG	O8-C9	-2.14	1.40	1.45
22	a	406	CLA	MG-NC	-2.14	2.01	2.06
25	d	407	PL9	C36-C37	-2.14	1.46	1.53
33	D	408	DGD	C4D-C5D	2.14	1.57	1.52
22	C	513	CLA	C4C-C3C	2.14	1.48	1.45
22	B	617	CLA	C4B-CHC	2.14	1.46	1.41
22	b	613	CLA	MG-NC	2.14	2.11	2.06
32	B	629	HTG	O5-C1	2.13	1.45	1.42
22	B	610	CLA	C4B-CHC	2.13	1.46	1.41
22	C	505	CLA	C1B-CHB	2.13	1.46	1.41
22	c	513	CLA	C3D-C4D	-2.13	1.39	1.44
22	b	615	CLA	C3D-C2D	2.13	1.44	1.39
22	a	407	CLA	CHD-C1D	2.13	1.42	1.38
22	C	511	CLA	C3D-C4D	-2.12	1.39	1.44
22	a	407	CLA	C1B-NB	-2.12	1.33	1.35
22	B	610	CLA	C2-C3	2.12	1.38	1.33
32	d	413	HTG	O5-C1	2.12	1.45	1.42
24	D	406	BCR	C24-C25	2.12	1.52	1.45
32	b	602	HTG	O5-C1	2.11	1.45	1.42
22	A	408	CLA	C5-C3	2.11	1.55	1.51
25	A	410	PL9	C6-C5	2.11	1.46	1.35
32	C	522	HTG	O5-C1	2.11	1.45	1.42
22	d	402	CLA	C1D-ND	-2.11	1.35	1.37
22	b	610	CLA	C1C-C2C	2.10	1.48	1.44
22	a	407	CLA	MG-ND	2.10	2.10	2.05
22	C	510	CLA	C4B-CHC	2.10	1.46	1.41
24	a	410	BCR	C19-C18	2.10	1.50	1.45
24	a	410	BCR	C10-C9	2.10	1.38	1.35
24	b	622	BCR	C1-C6	2.10	1.56	1.53
22	C	507	CLA	C4D-ND	2.10	1.40	1.37
22	b	609	CLA	C3D-C2D	2.10	1.44	1.39
24	K	101	BCR	C12-C13	2.10	1.50	1.45
22	C	504	CLA	C1B-CHB	2.09	1.46	1.41
22	C	509	CLA	C1B-CHB	2.09	1.46	1.41
22	b	617	CLA	CMB-C2B	-2.09	1.47	1.51
24	c	515	BCR	C21-C22	-2.09	1.33	1.35
22	b	611	CLA	CMB-C2B	-2.09	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	BCR	C8-C9	2.09	1.50	1.45
22	C	508	CLA	C1D-ND	-2.09	1.35	1.37
22	B	603	CLA	C3D-C4D	-2.09	1.39	1.44
22	B	610	CLA	OBD-CAD	2.08	1.26	1.22
24	a	410	BCR	C12-C13	2.08	1.50	1.45
22	A	404	CLA	C1C-NC	2.08	1.40	1.37
22	C	505	CLA	CMA-C3A	-2.08	1.48	1.53
22	C	505	CLA	C4D-CHA	2.08	1.45	1.38
23	a	408	PHO	C4A-C3A	-2.08	1.47	1.51
28	B	623	LMT	C4B-C5B	2.08	1.57	1.53
32	O	302	HTG	C1-S1	2.07	1.84	1.80
22	A	405	CLA	CHD-C1D	2.07	1.42	1.38
22	c	502	CLA	OBD-CAD	2.07	1.26	1.22
25	D	407	PL9	C2-C3	2.07	1.40	1.34
22	A	404	CLA	O2A-CGA	2.07	1.39	1.33
22	b	606	CLA	CHD-C1D	2.07	1.42	1.38
22	c	514	CLA	C1C-C2C	2.06	1.48	1.44
22	c	514	CLA	C3D-C4D	-2.06	1.39	1.44
22	C	509	CLA	CHD-C4C	2.06	1.43	1.39
25	d	407	PL9	C6-C5	2.06	1.46	1.35
22	C	510	CLA	C1C-NC	-2.06	1.34	1.37
22	C	510	CLA	C1A-CHA	2.05	1.51	1.43
24	y	101	BCR	C5-C6	2.05	1.38	1.34
22	C	512	CLA	C4C-C3C	2.05	1.48	1.45
32	D	413	HTG	C1'-S1	-2.05	1.78	1.81
32	B	642	HTG	C1-C2	2.05	1.56	1.53
22	a	409	CLA	C3B-C2B	2.05	1.43	1.40
22	C	503	CLA	C5-C3	2.05	1.55	1.51
22	a	407	CLA	C1C-NC	-2.04	1.34	1.37
26	b	625	LMG	O7-C8	-2.04	1.41	1.46
28	F	102	LMT	C4'-C5'	2.04	1.57	1.53
22	A	406	CLA	O2A-CGA	2.04	1.39	1.33
22	b	620	CLA	C3D-C2D	2.04	1.44	1.39
23	A	407	PHO	O2D-CGD	2.04	1.38	1.33
22	B	602	CLA	C1B-CHB	2.04	1.46	1.41
22	D	403	CLA	OBD-CAD	2.04	1.26	1.22
37	F	101	HEM	CAA-C2A	2.04	1.55	1.52
22	B	614	CLA	O1D-CGD	2.03	1.26	1.21
24	B	619	BCR	C24-C25	2.03	1.52	1.45
22	B	615	CLA	O2D-CGD	2.03	1.38	1.33
22	B	608	CLA	C4D-CHA	2.03	1.45	1.38
22	B	608	CLA	C1D-C2D	2.03	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Z	101	LMT	O1B-C1B	2.03	1.47	1.41
22	D	403	CLA	C1-C2	2.03	1.55	1.49
22	c	509	CLA	C4D-CHA	2.03	1.45	1.38
24	B	620	BCR	C24-C25	2.03	1.52	1.45
22	a	407	CLA	C4C-C3C	2.03	1.48	1.45
22	d	403	CLA	CMA-C3A	2.02	1.57	1.53
22	A	404	CLA	C4B-CHC	2.02	1.46	1.41
38	h	102	RRX	C30-C25	2.02	1.56	1.53
24	b	623	BCR	C5-C6	2.02	1.37	1.34
24	C	514	BCR	C17-C18	2.02	1.38	1.35
22	b	618	CLA	C4D-CHA	2.02	1.45	1.38
22	C	507	CLA	C1C-C2C	2.02	1.48	1.44
32	b	601	HTG	C1-S1	-2.02	1.77	1.80
33	C	516	DGD	O2G-C2G	-2.02	1.41	1.46
22	C	502	CLA	CMA-C3A	2.02	1.57	1.53
22	B	612	CLA	CHD-C1D	2.02	1.42	1.38
22	C	506	CLA	C1C-NC	-2.02	1.34	1.37
40	v	202	HEC	C2A-C1A	2.02	1.47	1.42
22	b	608	CLA	CHD-C4C	2.02	1.43	1.39
22	B	615	CLA	CHD-C4C	2.01	1.43	1.39
22	b	608	CLA	MG-NC	2.01	2.11	2.06
22	B	605	CLA	C4B-CHC	2.01	1.46	1.41
24	A	409	BCR	C8-C9	2.01	1.50	1.45
22	C	507	CLA	CBD-CGD	-2.01	1.46	1.52
23	D	404	PHO	C3A-C2A	-2.01	1.52	1.54
38	h	102	RRX	C23-C22	2.01	1.50	1.45
22	b	620	CLA	C1C-C2C	2.01	1.48	1.44
22	c	508	CLA	C4C-C3C	2.00	1.48	1.45
22	B	606	CLA	C4B-NB	-2.00	1.33	1.35
24	D	406	BCR	C16-C17	2.00	1.49	1.43
22	B	617	CLA	C1B-CHB	2.00	1.46	1.41
22	A	406	CLA	C3B-C2B	2.00	1.43	1.40
22	c	507	CLA	C1C-NC	-2.00	1.34	1.37
33	d	408	DGD	C4D-C5D	2.00	1.57	1.52

All (2403) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	413	HTG	C1'-S1-C1	13.68	125.67	100.09
32	c	541	HTG	C1'-S1-C1	12.83	124.08	100.09
22	c	504	CLA	C4A-NA-C1A	11.98	112.09	106.71
22	B	616	CLA	C4A-NA-C1A	11.74	111.99	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	V	202	HTG	O5-C1-C2	-11.63	95.69	110.31
22	c	512	CLA	C4A-NA-C1A	11.23	111.75	106.71
28	z	101	LMT	O1'-C1-C2	10.82	147.50	109.56
22	c	502	CLA	C4A-NA-C1A	10.12	111.25	106.71
22	b	610	CLA	C4A-NA-C1A	10.10	111.25	106.71
28	z	101	LMT	C3-C2-C1	10.04	157.97	113.49
22	C	501	CLA	O2D-CGD-O1D	-10.00	104.29	123.84
22	C	508	CLA	C4A-NA-C1A	9.65	111.04	106.71
32	U	203	HTG	C1'-S1-C1	9.54	118.42	100.16
22	C	502	CLA	C2D-C1D-ND	9.47	117.09	110.10
22	A	405	CLA	C2C-C1C-NC	9.46	118.83	109.97
32	v	208	HTG	O5-C1-C2	-9.36	98.54	110.31
32	v	208	HTG	C1'-S1-C1	9.35	117.57	100.09
32	b	640	HTG	C1-O5-C5	9.32	129.78	112.58
22	C	507	CLA	C4A-NA-C1A	9.26	110.87	106.71
22	B	615	CLA	C4A-NA-C1A	9.22	110.85	106.71
22	a	407	CLA	C2D-C1D-ND	8.91	116.67	110.10
22	C	501	CLA	C4A-NA-C1A	8.90	110.71	106.71
22	C	513	CLA	C4A-NA-C1A	8.81	110.67	106.71
22	C	509	CLA	C2D-C1D-ND	8.72	116.53	110.10
32	D	413	HTG	C1'-S1-C1	8.63	116.24	100.09
22	B	612	CLA	C2D-C1D-ND	8.63	116.46	110.10
22	B	604	CLA	C2D-C1D-ND	8.61	116.45	110.10
22	C	504	CLA	C4A-NA-C1A	8.54	110.55	106.71
22	c	511	CLA	C4D-CHA-C1A	-8.43	110.99	121.25
22	c	502	CLA	C2D-C1D-ND	8.42	116.31	110.10
22	a	406	CLA	CAC-C3C-C4C	8.41	135.72	124.81
22	C	501	CLA	O2D-CGD-CBD	8.29	126.01	111.27
22	c	510	CLA	C4A-NA-C1A	8.28	110.43	106.71
22	C	511	CLA	C4A-NA-C1A	8.28	110.43	106.71
32	B	624	HTG	C1'-S1-C1	8.23	115.48	100.09
22	C	510	CLA	C4A-NA-C1A	8.18	110.38	106.71
22	c	511	CLA	C2D-C1D-ND	8.15	116.11	110.10
22	c	513	CLA	C4A-NA-C1A	8.12	110.36	106.71
22	D	403	CLA	C2C-C1C-NC	8.09	117.55	109.97
22	C	511	CLA	C2D-C1D-ND	8.05	116.04	110.10
22	a	406	CLA	C2D-C1D-ND	8.05	116.04	110.10
22	B	606	CLA	C2D-C1D-ND	8.00	116.00	110.10
22	b	608	CLA	C4A-NA-C1A	8.00	110.30	106.71
22	c	509	CLA	C4A-NA-C1A	7.98	110.29	106.71
22	B	604	CLA	C2C-C1C-NC	7.91	117.39	109.97
22	c	505	CLA	C4A-NA-C1A	7.90	110.26	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	505	CLA	C4A-NA-C1A	7.89	110.25	106.71
32	b	627	HTG	C1'-S1-C1	7.89	114.85	100.09
32	C	536	HTG	C1'-S1-C1	7.89	114.84	100.09
32	C	522	HTG	C1'-S1-C1	7.86	114.79	100.09
22	c	508	CLA	O2D-CGD-CBD	7.86	125.23	111.27
22	c	507	CLA	C2D-C1D-ND	7.85	115.89	110.10
22	C	506	CLA	C2D-C1D-ND	7.77	115.83	110.10
22	b	608	CLA	CAC-C3C-C4C	7.71	134.81	124.81
22	C	509	CLA	C2C-C1C-NC	7.71	117.19	109.97
22	b	610	CLA	C2D-C1D-ND	7.68	115.76	110.10
22	d	403	CLA	C2D-C1D-ND	7.64	115.73	110.10
22	b	616	CLA	C2D-C1D-ND	7.62	115.72	110.10
22	C	506	CLA	C4A-NA-C1A	7.60	110.12	106.71
23	d	404	PHO	O2D-CGD-CBD	7.52	120.53	111.00
22	b	616	CLA	CAC-C3C-C4C	7.52	134.56	124.81
22	B	611	CLA	C4A-NA-C1A	7.48	110.07	106.71
22	A	404	CLA	C2D-C1D-ND	7.41	115.56	110.10
22	b	612	CLA	CAC-C3C-C4C	7.37	134.37	124.81
32	b	640	HTG	C6-C5-C4	-7.34	95.80	113.00
22	B	605	CLA	C2D-C1D-ND	7.32	115.50	110.10
25	a	411	PL9	O1-C4-C3	-7.31	112.66	120.72
22	a	407	CLA	C2C-C1C-NC	7.29	116.80	109.97
22	b	618	CLA	C4A-NA-C1A	7.24	109.96	106.71
22	B	603	CLA	C4A-NA-C1A	7.24	109.96	106.71
22	b	607	CLA	C2C-C1C-NC	7.19	116.71	109.97
22	B	606	CLA	C2C-C1C-NC	7.18	116.70	109.97
22	b	611	CLA	C2D-C1D-ND	7.14	115.37	110.10
22	A	405	CLA	C1C-C2C-C3C	-7.13	99.46	106.96
32	d	413	HTG	O5-C1-C2	-7.13	101.34	110.31
22	b	616	CLA	CHD-C4C-C3C	-7.13	114.36	124.84
22	B	613	CLA	CAC-C3C-C4C	7.12	134.05	124.81
22	B	615	CLA	O2D-CGD-O1D	-7.10	109.95	123.84
22	B	612	CLA	C2C-C1C-NC	7.10	116.62	109.97
22	A	408	CLA	C2D-C1D-ND	7.09	115.33	110.10
22	b	609	CLA	CHD-C1D-ND	-7.09	117.94	124.45
31	D	409	LHG	O8-C23-O10	-7.08	105.72	123.59
22	C	512	CLA	C2D-C1D-ND	7.08	115.32	110.10
31	F	103	LHG	O7-C7-C8	7.06	126.73	111.50
22	B	609	CLA	C2D-C1D-ND	7.04	115.29	110.10
22	c	507	CLA	CHD-C1D-ND	-7.04	117.99	124.45
22	c	505	CLA	C4D-CHA-C1A	-7.00	112.73	121.25
22	B	613	CLA	C4A-NA-C1A	6.97	109.84	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	640	HTG	O5-C5-C6	6.91	123.62	106.44
22	A	406	CLA	C2C-C1C-NC	6.91	116.45	109.97
33	d	408	DGD	O2G-C1B-C2B	6.91	126.39	111.50
22	a	409	CLA	C2D-C1D-ND	6.88	115.18	110.10
22	b	612	CLA	C2C-C1C-NC	6.87	116.41	109.97
22	a	409	CLA	CAC-C3C-C4C	6.85	133.70	124.81
22	d	405	CLA	C2C-C1C-NC	6.85	116.39	109.97
22	b	605	CLA	O2D-CGD-CBD	6.84	123.42	111.27
22	b	614	CLA	C2C-C1C-NC	6.83	116.38	109.97
32	B	642	HTG	O6-C6-C5	-6.82	87.88	111.29
22	b	609	CLA	CHD-C4C-C3C	-6.82	114.82	124.84
22	C	511	CLA	C4D-CHA-C1A	-6.80	112.98	121.25
22	C	501	CLA	C2D-C1D-ND	6.74	115.07	110.10
25	A	410	PL9	O1-C4-C3	-6.72	113.32	120.72
22	b	619	CLA	C1C-C2C-C3C	-6.71	99.91	106.96
22	C	507	CLA	C2C-C1C-NC	6.67	116.22	109.97
22	B	609	CLA	O2D-CGD-O1D	-6.66	110.82	123.84
22	b	620	CLA	C2D-C1D-ND	6.62	114.98	110.10
22	c	510	CLA	C2D-C1D-ND	6.55	114.93	110.10
22	b	606	CLA	C2D-C1D-ND	6.55	114.93	110.10
22	c	514	CLA	C2D-C1D-ND	6.54	114.92	110.10
22	B	606	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	B	608	CLA	C2C-C1C-NC	6.54	116.09	109.97
22	C	504	CLA	C1C-C2C-C3C	-6.50	100.12	106.96
25	A	410	PL9	C3-C4-C5	6.50	127.06	118.60
22	b	618	CLA	C4D-CHA-C1A	-6.50	113.34	121.25
22	B	615	CLA	C2C-C1C-NC	6.47	116.03	109.97
32	V	202	HTG	C1'-S1-C1	6.47	112.19	100.09
22	b	608	CLA	C2D-C1D-ND	6.44	114.85	110.10
22	b	619	CLA	C2C-C1C-NC	6.44	116.00	109.97
22	B	609	CLA	C4D-CHA-C1A	-6.42	113.44	121.25
22	b	609	CLA	C2C-C1C-NC	6.40	115.97	109.97
22	B	617	CLA	C2D-C1D-ND	6.39	114.82	110.10
28	C	520	LMT	O5B-C1B-C2B	6.39	123.87	110.35
22	B	609	CLA	CAC-C3C-C4C	6.36	133.06	124.81
22	B	610	CLA	C2C-C1C-NC	6.35	115.92	109.97
22	c	509	CLA	C2D-C1D-ND	6.33	114.77	110.10
22	b	610	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
22	A	404	CLA	C2C-C1C-NC	6.30	115.88	109.97
33	D	408	DGD	O2G-C1B-C2B	6.30	125.08	111.50
22	b	609	CLA	C2D-C1D-ND	6.29	114.74	110.10
22	A	408	CLA	C1D-ND-C4D	-6.29	101.87	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	510	CLA	C2C-C1C-NC	6.29	115.86	109.97
22	c	511	CLA	C1D-ND-C4D	-6.27	101.88	106.33
22	A	405	CLA	CMB-C2B-C3B	6.26	136.39	124.68
22	C	506	CLA	CHD-C4C-C3C	-6.24	115.66	124.84
22	C	505	CLA	C2D-C1D-ND	6.23	114.69	110.10
22	c	506	CLA	C4A-NA-C1A	6.22	109.50	106.71
22	B	617	CLA	C2C-C1C-NC	6.20	115.78	109.97
22	C	505	CLA	C2C-C1C-NC	6.20	115.78	109.97
22	B	607	CLA	C2D-C1D-ND	6.20	114.67	110.10
32	B	628	HTG	C1'-S1-C1	6.20	111.68	100.09
32	C	521	HTG	C1'-S1-C1	6.14	111.58	100.09
22	B	604	CLA	O2D-CGD-O1D	-6.13	111.85	123.84
22	A	408	CLA	C2C-C1C-NC	6.13	115.72	109.97
28	C	520	LMT	C1B-O1B-C4'	6.12	133.12	117.96
22	B	614	CLA	C2D-C1D-ND	6.10	114.60	110.10
22	B	609	CLA	C2C-C1C-NC	6.10	115.69	109.97
22	a	407	CLA	CAC-C3C-C4C	6.09	132.71	124.81
22	B	613	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
22	B	610	CLA	C2D-C1D-ND	6.09	114.59	110.10
22	B	604	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
22	c	508	CLA	C2D-C1D-ND	6.08	114.58	110.10
22	c	503	CLA	C2D-C1D-ND	6.07	114.58	110.10
24	T	101	BCR	C12-C13-C14	-6.06	109.64	118.94
22	d	402	CLA	C2C-C1C-NC	6.06	115.65	109.97
22	B	612	CLA	C1D-ND-C4D	-6.06	102.03	106.33
22	c	507	CLA	CHD-C4C-C3C	-6.06	115.94	124.84
22	c	508	CLA	C4A-NA-C1A	6.05	109.43	106.71
22	c	502	CLA	C2C-C1C-NC	6.04	115.63	109.97
22	a	407	CLA	C3C-C4C-NC	6.02	117.32	110.57
22	C	504	CLA	C2D-C1D-ND	6.01	114.53	110.10
22	B	614	CLA	C4D-CHA-C1A	-6.01	113.94	121.25
22	c	502	CLA	C1D-ND-C4D	-5.97	102.09	106.33
22	C	507	CLA	C1C-C2C-C3C	-5.96	100.69	106.96
22	C	512	CLA	C4A-NA-C1A	5.94	109.38	106.71
22	C	508	CLA	C2D-C1D-ND	5.93	114.47	110.10
22	b	611	CLA	C2C-C1C-NC	5.92	115.52	109.97
22	B	603	CLA	C2C-C1C-NC	5.91	115.51	109.97
22	a	406	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
22	B	614	CLA	C4A-NA-C1A	5.91	109.36	106.71
22	c	506	CLA	C2D-C1D-ND	5.89	114.44	110.10
22	C	501	CLA	C2C-C1C-NC	5.88	115.48	109.97
22	d	403	CLA	C2C-C1C-NC	5.87	115.47	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	614	CLA	C2D-C1D-ND	5.86	114.42	110.10
22	b	618	CLA	C2D-C1D-ND	5.86	114.42	110.10
22	C	501	CLA	CHD-C1D-ND	-5.85	119.08	124.45
22	B	611	CLA	O2D-CGD-O1D	-5.85	112.40	123.84
22	b	616	CLA	CMC-C2C-C1C	5.84	133.94	125.04
22	C	509	CLA	C4D-CHA-C1A	-5.83	114.16	121.25
22	a	409	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
31	d	409	LHG	O8-C23-O10	-5.80	108.96	123.59
22	b	605	CLA	C2D-C1D-ND	5.79	114.37	110.10
32	c	523	HTG	C1'-S1-C1	5.77	110.88	100.09
22	B	611	CLA	C2D-C1D-ND	5.76	114.35	110.10
22	C	506	CLA	CAC-C3C-C4C	5.75	132.27	124.81
22	D	405	CLA	C2D-C1D-ND	5.74	114.33	110.10
22	c	502	CLA	C4D-CHA-C1A	-5.73	114.28	121.25
22	a	406	CLA	CHD-C1D-ND	-5.70	119.21	124.45
22	b	618	CLA	CAC-C3C-C4C	5.69	132.19	124.81
22	A	404	CLA	C1C-C2C-C3C	-5.69	100.98	106.96
22	B	602	CLA	C2C-C1C-NC	5.68	115.30	109.97
22	b	616	CLA	C4D-CHA-C1A	-5.68	114.33	121.25
22	B	616	CLA	C2C-C1C-NC	5.68	115.29	109.97
22	c	508	CLA	C2C-C1C-NC	5.66	115.28	109.97
22	A	406	CLA	CMC-C2C-C1C	5.66	133.66	125.04
22	B	608	CLA	C4D-CHA-C1A	-5.66	114.36	121.25
22	D	403	CLA	C1C-C2C-C3C	-5.65	101.02	106.96
25	a	411	PL9	C7-C3-C2	5.65	130.72	123.30
22	C	503	CLA	C4A-NA-C1A	5.63	109.24	106.71
22	B	602	CLA	CHD-C1D-ND	-5.63	119.28	124.45
22	b	605	CLA	C4A-NA-C1A	5.62	109.23	106.71
22	B	606	CLA	CAC-C3C-C4C	5.62	132.10	124.81
22	B	605	CLA	C4A-NA-C1A	5.61	109.23	106.71
22	b	618	CLA	O2D-CGD-CBD	5.60	121.21	111.27
22	B	610	CLA	C4A-NA-C1A	5.59	109.22	106.71
22	d	405	CLA	C4D-CHA-C1A	-5.57	114.47	121.25
22	B	605	CLA	C4D-CHA-C1A	-5.56	114.48	121.25
22	c	508	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
22	B	605	CLA	C2C-C1C-NC	5.55	115.17	109.97
22	A	406	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
22	b	616	CLA	C2C-C1C-NC	5.54	115.17	109.97
28	C	520	LMT	O1B-C4'-C3'	5.54	122.00	107.28
22	b	607	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
22	B	613	CLA	CHD-C1D-ND	-5.52	119.38	124.45
22	c	514	CLA	C4D-CHA-C1A	-5.52	114.53	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	502	CLA	CHD-C1D-ND	-5.52	119.38	124.45
22	C	504	CLA	C2C-C1C-NC	5.52	115.14	109.97
22	C	506	CLA	CHD-C1D-ND	-5.51	119.39	124.45
22	b	611	CLA	CHD-C4C-C3C	-5.51	116.75	124.84
22	b	611	CLA	C4A-NA-C1A	5.51	109.18	106.71
22	A	405	CLA	C1D-ND-C4D	5.50	110.24	106.33
25	A	410	PL9	C53-C6-C1	5.49	126.22	114.99
28	C	520	LMT	O1B-C1B-O5B	5.49	126.01	110.67
22	A	408	CLA	C4-C3-C5	5.49	124.50	115.27
22	b	612	CLA	C2D-C1D-ND	5.49	114.15	110.10
22	b	605	CLA	C2C-C1C-NC	5.49	115.11	109.97
22	b	619	CLA	C2D-C1D-ND	5.48	114.14	110.10
22	c	505	CLA	C2D-C1D-ND	5.47	114.14	110.10
22	b	619	CLA	C4A-NA-C1A	5.46	109.16	106.71
25	a	411	PL9	C3-C4-C5	5.46	125.70	118.60
22	B	613	CLA	C2D-C1D-ND	5.46	114.13	110.10
22	b	605	CLA	C4D-CHA-C1A	-5.46	114.61	121.25
22	C	510	CLA	C2C-C1C-NC	5.46	115.08	109.97
22	B	604	CLA	C1D-ND-C4D	-5.45	102.46	106.33
22	C	510	CLA	O2D-CGD-O1D	-5.45	113.18	123.84
22	A	405	CLA	C4A-NA-C1A	-5.45	104.26	106.71
22	C	502	CLA	CAC-C3C-C4C	5.44	131.87	124.81
24	A	409	BCR	C38-C26-C25	-5.44	118.42	124.53
24	D	406	BCR	C7-C8-C9	-5.41	118.06	126.23
33	H	101	DGD	O1G-C1A-O1A	-5.41	109.94	123.59
22	B	617	CLA	O2D-CGD-CBD	5.40	120.86	111.27
32	V	202	HTG	O2-C2-C1	5.40	120.18	110.27
22	B	615	CLA	C4D-CHA-C1A	-5.39	114.69	121.25
22	b	620	CLA	O2D-CGD-CBD	5.38	120.83	111.27
31	d	409	LHG	O7-C7-C8	5.35	123.04	111.50
22	b	617	CLA	C2C-C1C-NC	5.34	114.98	109.97
22	B	607	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
22	b	613	CLA	C2D-C1D-ND	5.34	114.04	110.10
22	B	612	CLA	O2D-CGD-CBD	5.34	120.75	111.27
22	C	512	CLA	C2C-C1C-NC	5.34	114.97	109.97
22	c	510	CLA	C4D-CHA-C1A	-5.33	114.77	121.25
28	c	522	LMT	O1B-C1B-O5B	5.33	125.55	110.67
22	d	405	CLA	C1C-C2C-C3C	-5.32	101.37	106.96
22	d	403	CLA	CHD-C1D-ND	-5.32	119.57	124.45
25	D	407	PL9	C40-C39-C41	5.31	124.20	115.27
22	c	503	CLA	C2C-C1C-NC	5.31	114.94	109.97
22	c	503	CLA	C1D-CHD-C4C	-5.30	114.62	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	506	CLA	C2C-C1C-NC	5.28	114.92	109.97
25	a	411	PL9	C7-C3-C4	-5.28	112.58	116.88
22	A	405	CLA	CMB-C2B-C1B	-5.25	120.40	128.46
22	b	613	CLA	CHD-C1D-ND	-5.24	119.64	124.45
22	D	403	CLA	C2A-C1A-CHA	-5.24	114.70	123.86
32	b	640	HTG	C3-C4-C5	5.23	119.58	110.24
38	H	102	RRX	C7-C8-C9	-5.23	118.34	126.23
22	B	616	CLA	C2D-C1D-ND	5.22	113.95	110.10
22	b	611	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
28	z	101	LMT	O5B-C1B-C2B	5.20	121.36	110.35
22	B	615	CLA	C2D-C1D-ND	5.20	113.93	110.10
22	c	514	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
28	t	102	LMT	C1'-O5'-C5'	5.18	123.85	113.69
22	D	405	CLA	C4A-NA-C1A	5.17	109.03	106.71
22	b	607	CLA	C1C-C2C-C3C	-5.17	101.53	106.96
22	b	618	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
22	B	617	CLA	O2A-CGA-CBA	5.15	128.08	111.91
22	b	616	CLA	C3C-C4C-NC	5.15	116.35	110.57
22	B	602	CLA	O2D-CGD-CBD	5.15	120.41	111.27
22	a	407	CLA	CHD-C1D-ND	-5.13	119.74	124.45
22	c	503	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
22	b	613	CLA	C2C-C1C-NC	5.12	114.77	109.97
22	C	503	CLA	C2D-C1D-ND	5.12	113.88	110.10
22	b	613	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
22	c	509	CLA	C1C-C2C-C3C	-5.12	101.58	106.96
22	c	504	CLA	C2D-C1D-ND	5.11	113.87	110.10
28	m	103	LMT	C3'-C4'-C5'	5.11	115.06	109.97
22	A	408	CLA	C4D-CHA-C1A	-5.11	115.03	121.25
28	m	103	LMT	C2'-C3'-C4'	5.10	118.10	110.69
22	c	502	CLA	O2D-CGD-O1D	-5.10	113.87	123.84
33	H	101	DGD	C3G-O3G-C1D	-5.10	103.78	113.74
24	d	406	BCR	C24-C23-C22	-5.10	118.54	126.23
22	d	403	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
22	C	509	CLA	C1C-C2C-C3C	-5.08	101.61	106.96
22	c	511	CLA	CHB-C4A-NA	5.08	131.54	124.51
22	B	610	CLA	C1C-C2C-C3C	-5.07	101.62	106.96
28	a	401	LMT	C4B-C3B-C2B	-5.07	101.97	110.82
22	C	509	CLA	O2D-CGD-O1D	-5.07	113.93	123.84
22	c	510	CLA	CED-O2D-CGD	5.07	127.39	115.94
22	C	510	CLA	CAC-C3C-C4C	5.06	131.38	124.81
22	C	505	CLA	C1C-C2C-C3C	-5.05	101.65	106.96
22	b	610	CLA	C3D-C2D-C1D	-5.05	98.95	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	407	PL9	C7-C3-C4	5.04	120.98	116.88
22	b	607	CLA	C4A-NA-C1A	5.04	108.97	106.71
26	d	412	LMG	O7-C10-C11	5.03	122.35	111.50
22	c	511	CLA	C2C-C1C-NC	5.03	114.69	109.97
22	C	512	CLA	C1C-C2C-C3C	-5.03	101.67	106.96
22	a	407	CLA	C1C-C2C-C3C	-5.03	101.67	106.96
22	B	604	CLA	C4D-CHA-C1A	-5.02	115.14	121.25
22	C	510	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
22	B	606	CLA	C3C-C4C-NC	5.00	116.18	110.57
28	a	401	LMT	C1-O1'-C1'	5.00	122.13	113.84
22	b	620	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
38	h	102	RRX	C7-C8-C9	-4.99	118.70	126.23
22	b	609	CLA	CAC-C3C-C4C	4.99	131.28	124.81
22	A	405	CLA	C2D-C1D-ND	4.98	113.77	110.10
22	C	503	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
22	B	603	CLA	C1C-C2C-C3C	-4.98	101.72	106.96
22	C	509	CLA	C3B-C4B-NB	4.97	115.64	109.21
22	a	406	CLA	CMC-C2C-C1C	4.96	132.59	125.04
31	D	409	LHG	O8-C23-C24	4.95	127.44	111.91
22	B	602	CLA	C2D-C1D-ND	4.94	113.75	110.10
22	c	513	CLA	O2D-CGD-CBD	4.94	120.04	111.27
22	A	406	CLA	CAC-C3C-C4C	4.93	131.21	124.81
22	C	504	CLA	C4D-CHA-C1A	-4.93	115.25	121.25
28	c	522	LMT	O5B-C5B-C4B	4.93	118.65	109.69
28	B	623	LMT	O1B-C1B-O5B	4.93	124.44	110.67
22	C	509	CLA	CAC-C3C-C4C	4.93	131.20	124.81
22	C	511	CLA	CAC-C3C-C4C	4.93	131.20	124.81
22	C	511	CLA	O2D-CGD-O1D	-4.92	114.22	123.84
22	b	613	CLA	CAC-C3C-C4C	4.91	131.19	124.81
22	C	506	CLA	CMC-C2C-C1C	4.91	132.51	125.04
31	d	409	LHG	O8-C23-C24	4.89	127.26	111.91
22	b	619	CLA	CHA-C4D-ND	4.89	142.73	132.50
28	A	415	LMT	C3B-C4B-C5B	4.89	118.96	110.24
22	B	602	CLA	C1C-C2C-C3C	-4.88	101.82	106.96
22	B	614	CLA	CHB-C4A-NA	4.88	131.26	124.51
22	C	507	CLA	O2D-CGD-CBD	4.88	119.94	111.27
22	b	607	CLA	O2D-CGD-CBD	4.88	119.93	111.27
22	d	402	CLA	C4-C3-C5	4.87	123.47	115.27
22	B	609	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	t	101	BCR	C12-C13-C14	-4.87	111.47	118.94
22	B	617	CLA	O2A-CGA-O1A	-4.87	111.30	123.59
22	B	606	CLA	CHD-C4C-C3C	-4.87	117.69	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	502	CLA	C4A-NA-C1A	4.86	108.89	106.71
22	C	509	CLA	CHD-C1D-ND	-4.85	119.99	124.45
22	b	606	CLA	CHD-C1D-ND	-4.85	119.99	124.45
26	C	519	LMG	O6-C5-C6	4.85	118.50	106.44
32	b	602	HTG	C1'-S1-C1	4.84	109.15	100.09
22	c	504	CLA	CHD-C4C-C3C	-4.84	117.72	124.84
28	a	401	LMT	O5'-C5'-C4'	4.84	119.96	109.75
22	B	611	CLA	C2C-C1C-NC	4.84	114.51	109.97
22	c	507	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
28	b	626	LMT	O5'-C5'-C4'	4.83	119.94	109.75
22	a	407	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
26	C	519	LMG	O1-C1-C2	4.83	115.84	108.30
22	B	608	CLA	C2D-C1D-ND	4.82	113.66	110.10
22	c	514	CLA	CHD-C1D-ND	-4.82	120.03	124.45
22	c	508	CLA	C4-C3-C5	4.81	123.37	115.27
22	a	409	CLA	C3B-C4B-NB	4.81	115.43	109.21
22	B	608	CLA	C1C-C2C-C3C	-4.81	101.90	106.96
22	B	607	CLA	C4A-NA-C1A	4.80	108.86	106.71
40	V	201	HEC	CBD-CAD-C3D	-4.80	104.43	112.62
22	C	507	CLA	C4D-CHA-C1A	-4.79	115.41	121.25
22	c	509	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
32	b	640	HTG	O5-C1-S1	4.78	121.26	109.82
22	C	505	CLA	CHD-C4C-C3C	-4.78	117.81	124.84
22	C	504	CLA	CHD-C1D-ND	-4.78	120.06	124.45
22	d	405	CLA	C4A-NA-C1A	4.78	108.85	106.71
22	B	614	CLA	C2C-C1C-NC	4.78	114.45	109.97
22	c	508	CLA	O2D-CGD-O1D	-4.77	114.51	123.84
22	c	506	CLA	C4D-CHA-C1A	-4.77	115.45	121.25
22	d	405	CLA	C2D-C1D-ND	4.76	113.61	110.10
22	b	608	CLA	C4D-CHA-C1A	-4.76	115.46	121.25
22	c	509	CLA	C4D-CHA-C1A	-4.75	115.46	121.25
22	B	617	CLA	CHD-C4C-C3C	-4.75	117.85	124.84
22	b	607	CLA	C2D-C1D-ND	4.75	113.61	110.10
22	c	502	CLA	C1C-C2C-C3C	-4.75	101.96	106.96
22	a	409	CLA	C2C-C1C-NC	4.75	114.42	109.97
22	b	611	CLA	CHD-C1D-ND	-4.74	120.09	124.45
32	o	301	HTG	C1'-S1-C1	4.74	108.95	100.09
28	z	101	LMT	O1B-C1B-C2B	4.73	120.36	108.10
22	c	507	CLA	CMD-C2D-C1D	4.72	133.03	124.71
22	d	403	CLA	C1C-C2C-C3C	-4.72	101.99	106.96
22	b	609	CLA	O2D-CGD-CBD	4.72	119.65	111.27
22	a	406	CLA	C2C-C1C-NC	4.72	114.39	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	620	CLA	C2C-C1C-NC	4.71	114.38	109.97
22	b	615	CLA	C2D-C1D-ND	4.71	113.57	110.10
22	b	606	CLA	CAC-C3C-C4C	4.70	130.91	124.81
22	C	509	CLA	CHD-C4C-C3C	-4.69	117.94	124.84
22	b	616	CLA	C1D-ND-C4D	-4.68	103.01	106.33
32	B	642	HTG	C1-C2-C3	4.68	119.83	110.59
22	b	614	CLA	CHD-C4C-C3C	-4.67	117.98	124.84
22	C	502	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
22	A	405	CLA	CMC-C2C-C1C	4.66	132.14	125.04
22	B	606	CLA	CMB-C2B-C3B	4.66	133.40	124.68
25	a	411	PL9	C20-C19-C21	4.66	123.11	115.27
22	C	506	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
22	B	616	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
22	a	409	CLA	C4D-CHA-C1A	-4.65	115.59	121.25
32	B	629	HTG	C1'-S1-C1	4.65	108.78	100.09
22	b	612	CLA	CMC-C2C-C1C	4.65	132.12	125.04
22	C	513	CLA	C4D-CHA-C1A	-4.64	115.60	121.25
22	C	511	CLA	C1C-C2C-C3C	-4.64	102.08	106.96
22	b	606	CLA	C2C-C1C-NC	4.63	114.31	109.97
32	v	208	HTG	O5-C1-S1	4.63	120.88	109.82
28	j	102	LMT	C3'-C4'-C5'	-4.62	105.36	109.97
22	B	603	CLA	CMC-C2C-C1C	4.62	132.07	125.04
22	B	607	CLA	C2C-C1C-NC	4.62	114.30	109.97
22	c	511	CLA	CHD-C4C-C3C	-4.62	118.05	124.84
22	B	604	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
22	c	502	CLA	CAC-C3C-C4C	4.62	130.80	124.81
28	a	401	LMT	O3B-C3B-C2B	4.61	121.01	110.35
22	b	615	CLA	CHD-C4C-C3C	-4.60	118.07	124.84
22	b	605	CLA	CHD-C4C-C3C	-4.60	118.08	124.84
22	c	506	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
22	B	610	CLA	CAC-C3C-C4C	4.59	130.76	124.81
22	b	618	CLA	O2D-CGD-O1D	-4.58	114.88	123.84
22	D	403	CLA	C4D-CHA-C1A	-4.58	115.68	121.25
22	c	510	CLA	CAC-C3C-C4C	4.57	130.74	124.81
22	D	403	CLA	CMB-C2B-C3B	4.57	133.23	124.68
24	c	516	BCR	C32-C1-C6	-4.57	102.89	110.30
38	H	102	RRX	C24-C23-C22	-4.57	119.33	126.23
22	b	620	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
28	A	415	LMT	C1'-O5'-C5'	4.56	122.64	113.69
22	C	508	CLA	C1C-C2C-C3C	-4.56	102.16	106.96
22	c	509	CLA	C2C-C1C-NC	4.56	114.25	109.97
22	b	609	CLA	CMC-C2C-C1C	4.56	131.98	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Z	101	LMT	O1B-C1B-C2B	4.56	119.91	108.10
22	c	508	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
24	A	409	BCR	C33-C5-C6	-4.55	119.42	124.53
22	c	513	CLA	C2D-C1D-ND	4.55	113.46	110.10
22	A	408	CLA	C1C-C2C-C3C	-4.54	102.18	106.96
22	B	612	CLA	C1C-C2C-C3C	-4.54	102.18	106.96
22	B	610	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
22	b	615	CLA	C4D-CHA-C1A	-4.54	115.73	121.25
22	D	405	CLA	C4D-CHA-C1A	-4.53	115.74	121.25
22	c	510	CLA	C1C-C2C-C3C	-4.53	102.20	106.96
22	c	503	CLA	C4D-CHA-C1A	-4.53	115.74	121.25
22	b	606	CLA	CMB-C2B-C3B	4.52	133.13	124.68
22	b	605	CLA	C1D-CHD-C4C	-4.51	116.32	126.06
22	b	612	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
22	b	613	CLA	O2D-CGD-O1D	-4.51	115.02	123.84
22	c	503	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
22	c	505	CLA	C2C-C1C-NC	4.50	114.19	109.97
32	d	413	HTG	O5-C1-S1	4.50	120.58	109.82
22	a	407	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
22	C	502	CLA	C1C-C2C-C3C	-4.50	102.23	106.96
22	b	617	CLA	CAC-C3C-C4C	4.50	130.64	124.81
22	B	603	CLA	O2D-CGD-O1D	-4.49	115.06	123.84
22	c	502	CLA	O2D-CGD-CBD	4.49	119.25	111.27
22	b	608	CLA	O2D-CGD-CBD	4.48	119.23	111.27
22	b	607	CLA	CAC-C3C-C4C	4.48	130.62	124.81
24	D	406	BCR	C29-C30-C25	4.48	117.37	110.48
22	b	606	CLA	O2D-CGD-CBD	4.47	119.22	111.27
22	c	507	CLA	C4D-CHA-C1A	-4.47	115.80	121.25
22	A	406	CLA	C2D-C1D-ND	4.47	113.40	110.10
22	C	509	CLA	C1D-ND-C4D	-4.47	103.16	106.33
22	C	513	CLA	CHD-C1D-ND	-4.47	120.35	124.45
22	A	404	CLA	C2A-C1A-CHA	-4.47	116.04	123.86
28	A	415	LMT	O3B-C3B-C2B	4.47	120.68	110.35
22	B	612	CLA	CHD-C4C-C3C	-4.47	118.27	124.84
22	b	607	CLA	CMC-C2C-C1C	4.46	131.83	125.04
28	b	626	LMT	C1'-O5'-C5'	4.46	122.44	113.69
22	d	403	CLA	CHD-C4C-NC	4.46	131.22	124.20
22	b	606	CLA	CHD-C4C-C3C	-4.45	118.29	124.84
22	C	511	CLA	C1D-ND-C4D	-4.44	103.18	106.33
22	c	510	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
22	c	511	CLA	C3B-C4B-NB	4.43	114.94	109.21
22	c	514	CLA	C2C-C1C-NC	4.43	114.12	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	410	PL9	C7-C3-C2	4.42	129.11	123.30
22	d	403	CLA	C4A-NA-C1A	4.42	108.69	106.71
22	B	613	CLA	CMC-C2C-C1C	4.42	131.77	125.04
22	b	619	CLA	CMC-C2C-C1C	4.42	131.77	125.04
26	C	519	LMG	O8-C28-C29	4.42	125.77	111.91
24	K	102	BCR	C11-C10-C9	-4.42	121.01	127.31
22	b	617	CLA	CHD-C1D-ND	-4.41	120.40	124.45
23	d	404	PHO	O2D-CGD-O1D	-4.41	115.22	123.84
26	c	520	LMG	O7-C10-C11	4.40	123.06	110.80
22	c	502	CLA	CHD-C4C-C3C	-4.40	118.38	124.84
22	B	614	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
22	c	505	CLA	C1D-ND-C4D	-4.39	103.22	106.33
22	C	502	CLA	C2C-C1C-NC	4.38	114.08	109.97
22	A	404	CLA	CHD-C1D-ND	-4.38	120.43	124.45
22	b	615	CLA	C2C-C1C-NC	4.37	114.07	109.97
22	B	605	CLA	CHD-C4C-C3C	-4.37	118.41	124.84
22	d	405	CLA	O2D-CGD-CBD	4.37	119.03	111.27
22	C	512	CLA	C1-O2A-CGA	4.36	127.89	116.44
22	C	512	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
22	B	607	CLA	O2D-CGD-O1D	-4.36	115.32	123.84
22	a	407	CLA	CMB-C2B-C3B	4.34	132.81	124.68
22	B	605	CLA	C1D-ND-C4D	-4.34	103.25	106.33
28	a	401	LMT	O5B-C5B-C6B	4.34	117.23	106.44
22	A	405	CLA	CHD-C4C-C3C	-4.34	118.47	124.84
22	c	502	CLA	CMD-C2D-C1D	4.34	132.35	124.71
22	B	615	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
22	b	612	CLA	C4D-CHA-C1A	-4.32	115.99	121.25
22	A	404	CLA	CMC-C2C-C1C	4.32	131.62	125.04
22	b	608	CLA	CMC-C2C-C1C	4.31	131.61	125.04
22	c	506	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
22	C	505	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
22	C	508	CLA	CHD-C4C-C3C	-4.30	118.52	124.84
26	C	518	LMG	O8-C28-C29	4.30	125.39	111.91
22	B	606	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
22	b	617	CLA	C2D-C1D-ND	4.29	113.27	110.10
33	d	408	DGD	C3D-C4D-C5D	4.29	116.45	109.77
22	c	513	CLA	CHD-C1D-ND	-4.29	120.51	124.45
22	A	406	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
22	c	507	CLA	C2A-C1A-CHA	-4.29	116.36	123.86
22	C	501	CLA	CAC-C3C-C4C	4.29	130.37	124.81
28	a	401	LMT	O3'-C3'-C2'	-4.28	100.45	110.35
24	t	101	BCR	C23-C22-C21	-4.28	112.37	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	509	CLA	O2D-CGD-CBD	4.28	118.88	111.27
22	B	611	CLA	CHD-C4C-C3C	-4.28	118.55	124.84
26	C	519	LMG	C7-O1-C1	4.27	122.08	113.74
22	b	605	CLA	CHA-C4D-ND	4.26	141.42	132.50
22	c	504	CLA	C2C-C1C-NC	4.26	113.97	109.97
22	B	617	CLA	CHD-C1D-ND	-4.26	120.54	124.45
22	c	512	CLA	C2C-C1C-NC	4.26	113.96	109.97
22	b	609	CLA	CHD-C4C-NC	4.26	130.91	124.20
31	D	411	LHG	O1-C1-C2	-4.26	89.79	110.20
22	b	611	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
22	d	403	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
22	C	510	CLA	C2D-C1D-ND	4.25	113.23	110.10
22	c	512	CLA	O2D-CGD-CBD	4.25	118.82	111.27
22	b	615	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
22	C	512	CLA	C4D-CHA-C1A	-4.25	116.08	121.25
22	b	619	CLA	OBD-CAD-C3D	-4.24	118.31	128.52
25	a	411	PL9	C53-C6-C1	4.23	123.64	114.99
22	B	604	CLA	C3B-C4B-NB	4.23	114.68	109.21
22	c	512	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
22	B	608	CLA	C4A-NA-C1A	-4.22	104.81	106.71
22	b	620	CLA	C4A-NA-C1A	4.22	108.61	106.71
37	F	101	HEM	CBD-CAD-C3D	-4.22	100.90	112.63
22	B	612	CLA	C4A-NA-C1A	4.22	108.60	106.71
22	c	505	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
22	d	405	CLA	CAC-C3C-C4C	4.22	130.28	124.81
22	c	514	CLA	C1-O2A-CGA	4.21	127.50	116.44
22	C	502	CLA	C3B-C4B-NB	4.21	114.65	109.21
22	D	403	CLA	C1D-ND-C4D	4.21	109.33	106.33
22	b	606	CLA	C1-C2-C3	-4.20	118.78	126.04
22	B	606	CLA	C4D-CHA-C1A	-4.20	116.14	121.25
22	a	409	CLA	C1D-ND-C4D	-4.20	103.35	106.33
22	B	609	CLA	CHD-C4C-C3C	-4.19	118.68	124.84
22	c	513	CLA	C2C-C1C-NC	4.19	113.90	109.97
22	c	507	CLA	C2C-C1C-NC	4.19	113.90	109.97
40	v	202	HEC	CBD-CAD-C3D	-4.19	105.48	112.62
22	C	501	CLA	C4D-CHA-C1A	-4.18	116.16	121.25
22	C	502	CLA	CHD-C4C-C3C	-4.18	118.70	124.84
22	b	620	CLA	C3C-C4C-NC	4.17	115.25	110.57
22	b	610	CLA	CHD-C4C-NC	4.17	130.77	124.20
22	C	501	CLA	O1D-CGD-CBD	-4.17	115.96	124.48
22	B	602	CLA	C2A-C1A-CHA	-4.17	116.57	123.86
22	D	403	CLA	C3D-C2D-C1D	-4.16	100.16	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	408	DGD	C3D-C4D-C5D	4.15	116.23	109.77
22	b	615	CLA	CAC-C3C-C4C	4.15	130.19	124.81
22	B	612	CLA	C4D-CHA-C1A	-4.15	116.20	121.25
22	C	511	CLA	C2C-C1C-NC	4.14	113.85	109.97
22	d	402	CLA	C3B-C4B-NB	4.14	114.57	109.21
22	a	406	CLA	CHD-C4C-NC	4.14	130.73	124.20
22	b	608	CLA	CHD-C4C-C3C	-4.14	118.75	124.84
22	b	614	CLA	CAC-C3C-C4C	4.13	130.17	124.81
22	b	619	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
28	c	522	LMT	C1B-O5B-C5B	4.12	121.78	113.69
22	c	510	CLA	C1D-ND-C4D	-4.12	103.41	106.33
22	B	607	CLA	C4D-CHA-C1A	-4.12	116.24	121.25
22	c	513	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
22	D	403	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
22	a	409	CLA	CHD-C1D-ND	-4.10	120.69	124.45
22	a	409	CLA	C3C-C4C-NC	4.10	115.17	110.57
22	B	616	CLA	CHD-C1D-ND	-4.10	120.69	124.45
22	c	507	CLA	CAC-C3C-C4C	4.09	130.12	124.81
28	j	102	LMT	C2'-C3'-C4'	-4.09	104.74	110.69
22	B	602	CLA	C4A-NA-C1A	4.09	108.55	106.71
28	B	623	LMT	O1B-C1B-C2B	4.09	118.70	108.10
22	A	405	CLA	CHD-C1D-ND	-4.09	120.69	124.45
22	b	614	CLA	C3D-C2D-C1D	-4.09	100.26	105.83
22	B	604	CLA	C3C-C4C-NC	4.08	115.15	110.57
22	C	510	CLA	CMC-C2C-C1C	4.08	131.25	125.04
22	b	605	CLA	C3C-C4C-NC	4.08	115.14	110.57
22	B	617	CLA	C3D-C2D-C1D	-4.08	100.27	105.83
22	c	504	CLA	C3D-C2D-C1D	-4.08	100.27	105.83
22	D	405	CLA	C1C-C2C-C3C	-4.07	102.67	106.96
22	b	612	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
22	a	406	CLA	CAC-C3C-C2C	-4.06	120.58	127.53
22	A	405	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
22	c	507	CLA	CHD-C4C-NC	4.05	130.59	124.20
22	C	512	CLA	O2D-CGD-CBD	4.05	118.47	111.27
22	B	603	CLA	C2D-C1D-ND	4.05	113.09	110.10
32	V	202	HTG	O5-C1-S1	4.05	119.50	109.82
22	b	605	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
22	b	609	CLA	C4D-CHA-C1A	-4.04	116.33	121.25
22	d	402	CLA	CAC-C3C-C4C	4.04	130.05	124.81
22	b	618	CLA	C1D-ND-C4D	-4.04	103.47	106.33
22	C	501	CLA	CHD-C4C-C3C	-4.04	118.90	124.84
22	c	508	CLA	CHD-C4C-NC	4.04	130.56	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	502	CLA	O2D-CGD-O1D	-4.04	115.95	123.84
33	C	516	DGD	O2G-C1B-O1B	-4.03	113.95	123.70
22	C	507	CLA	CHB-C4A-NA	4.03	130.09	124.51
22	c	503	CLA	O2D-CGD-CBD	4.03	118.43	111.27
28	A	415	LMT	C1-O1'-C1'	4.03	120.52	113.84
22	B	612	CLA	O2D-CGD-O1D	-4.03	115.97	123.84
22	c	508	CLA	CHD-C1D-ND	-4.02	120.76	124.45
22	b	611	CLA	C4D-CHA-C1A	-4.02	116.35	121.25
22	b	619	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
22	C	511	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
22	C	513	CLA	C2D-C1D-ND	4.02	113.07	110.10
22	b	607	CLA	C3C-C4C-NC	4.02	115.07	110.57
32	d	413	HTG	O5-C5-C4	4.01	116.98	109.69
22	C	502	CLA	C4D-CHA-C1A	-4.01	116.36	121.25
25	a	411	PL9	C30-C29-C31	4.01	122.02	115.27
25	A	410	PL9	O2-C1-C2	-4.01	112.60	121.78
22	B	616	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
31	d	410	LHG	O8-C23-O10	-4.00	113.48	123.59
26	D	412	LMG	O7-C10-C11	4.00	120.12	111.50
22	b	614	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
22	b	617	CLA	CHD-C4C-C3C	-4.00	118.97	124.84
22	b	612	CLA	CAC-C3C-C2C	-3.99	120.70	127.53
22	B	604	CLA	C3D-C2D-C1D	-3.99	100.38	105.83
22	B	617	CLA	C4A-NA-C1A	3.99	108.50	106.71
22	A	408	CLA	C1B-CHB-C4A	-3.99	122.22	130.12
24	t	101	BCR	C28-C27-C26	-3.98	106.97	114.08
22	B	615	CLA	CHD-C1D-ND	-3.98	120.79	124.45
26	A	411	LMG	O1-C1-C2	3.98	114.52	108.30
22	B	617	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
25	d	407	PL9	C40-C39-C41	3.98	121.96	115.27
22	A	405	CLA	CHA-C4D-ND	3.97	140.81	132.50
22	A	405	CLA	CAC-C3C-C4C	3.97	129.96	124.81
22	a	407	CLA	C2A-C1A-CHA	-3.97	116.92	123.86
22	A	408	CLA	C3B-C4B-NB	3.96	114.33	109.21
22	B	605	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
24	y	101	BCR	C39-C30-C25	-3.96	103.88	110.30
22	d	402	CLA	C4D-CHA-C1A	-3.96	116.43	121.25
22	c	503	CLA	CHA-C4D-ND	3.96	140.78	132.50
22	B	606	CLA	CMC-C2C-C1C	3.96	131.06	125.04
22	B	605	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
22	C	506	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
22	B	610	CLA	CHD-C1D-ND	-3.95	120.82	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	403	CLA	CHD-C4C-C3C	-3.95	119.03	124.84
24	d	406	BCR	C35-C13-C14	-3.95	117.39	122.92
22	B	617	CLA	CAC-C3C-C4C	3.95	129.93	124.81
28	c	522	LMT	O1'-C1'-C2'	3.95	114.46	108.30
22	D	403	CLA	CHA-C4D-ND	3.94	140.75	132.50
22	b	610	CLA	CHD-C1D-ND	-3.94	120.84	124.45
33	H	101	DGD	O1G-C1A-C2A	3.93	124.25	111.91
22	B	607	CLA	CMD-C2D-C1D	3.93	131.64	124.71
22	B	605	CLA	C6-C5-C3	-3.93	103.15	113.45
22	C	513	CLA	CHD-C4C-C3C	-3.93	119.06	124.84
22	B	607	CLA	O2D-CGD-CBD	3.93	118.25	111.27
22	b	619	CLA	C4D-CHA-C1A	-3.93	116.47	121.25
22	b	618	CLA	CMD-C2D-C1D	3.92	131.63	124.71
28	c	522	LMT	C1'-O5'-C5'	3.92	121.39	113.69
22	B	615	CLA	CMD-C2D-C1D	3.92	131.62	124.71
37	F	101	HEM	C4D-ND-C1D	3.92	109.12	105.07
22	b	608	CLA	C3C-C4C-NC	3.92	114.97	110.57
22	c	504	CLA	CMC-C2C-C1C	3.92	131.00	125.04
22	C	511	CLA	C3B-C4B-NB	3.91	114.27	109.21
25	a	411	PL9	C16-C14-C13	-3.91	113.20	121.12
28	B	623	LMT	C3B-C4B-C5B	3.91	117.21	110.24
22	A	406	CLA	C4D-CHA-C1A	-3.91	116.49	121.25
22	C	510	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
22	b	605	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
22	C	501	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
22	C	513	CLA	O2D-CGD-CBD	3.90	118.21	111.27
22	C	512	CLA	CHA-C4D-ND	3.90	140.66	132.50
22	b	618	CLA	C2C-C1C-NC	3.90	113.62	109.97
32	D	413	HTG	O5-C1-C2	-3.90	105.41	110.31
24	D	406	BCR	C36-C18-C19	-3.89	111.94	118.08
22	B	617	CLA	O2A-C1-C2	3.89	118.86	108.64
22	c	504	CLA	CAC-C3C-C4C	3.89	129.85	124.81
22	b	620	CLA	CHD-C1D-ND	-3.88	120.89	124.45
22	b	619	CLA	C1-O2A-CGA	3.88	126.62	116.44
22	B	612	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
28	j	102	LMT	O5'-C1'-O1'	3.87	117.84	109.40
22	B	610	CLA	C2A-C1A-CHA	-3.87	117.10	123.86
22	C	503	CLA	C2C-C1C-NC	3.87	113.59	109.97
22	b	607	CLA	CHD-C1D-ND	-3.87	120.90	124.45
22	c	513	CLA	CMD-C2D-C1D	3.87	131.53	124.71
22	B	615	CLA	CHD-C4C-C3C	-3.86	119.16	124.84
22	b	614	CLA	CHD-C1D-ND	-3.86	120.90	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	622	LMG	O8-C28-C29	3.86	124.03	111.91
32	B	642	HTG	C3-C4-C5	-3.86	103.35	110.24
33	H	101	DGD	O6D-C1D-O3G	3.85	119.10	109.97
33	H	101	DGD	O3G-C1D-C2D	-3.85	102.29	108.30
31	B	621	LHG	O4-P-O5	3.85	131.28	112.24
37	f	101	HEM	C4D-ND-C1D	3.85	109.05	105.07
26	C	519	LMG	O7-C10-C11	3.84	119.78	111.50
22	B	612	CLA	C3C-C4C-NC	3.84	114.88	110.57
33	D	408	DGD	O2G-C1B-O1B	-3.83	114.45	123.70
22	c	504	CLA	CHD-C1D-ND	-3.83	120.94	124.45
22	b	617	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
22	B	603	CLA	CHD-C4C-C3C	-3.82	119.22	124.84
22	c	505	CLA	O2D-CGD-CBD	3.82	118.05	111.27
22	B	607	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
22	b	619	CLA	O2D-CGD-CBD	3.81	118.04	111.27
22	b	612	CLA	CHD-C4C-C3C	-3.81	119.23	124.84
22	c	509	CLA	CHD-C1D-ND	-3.81	120.95	124.45
24	b	621	BCR	C34-C9-C8	3.81	124.08	118.08
22	b	605	CLA	CED-O2D-CGD	3.81	124.55	115.94
22	D	405	CLA	C2C-C1C-NC	3.81	113.54	109.97
32	b	602	HTG	O5-C1-C2	3.80	115.09	110.31
22	C	503	CLA	C4D-CHA-C1A	-3.80	116.62	121.25
22	C	508	CLA	C2C-C1C-NC	3.80	113.53	109.97
22	B	604	CLA	CHD-C1D-ND	-3.80	120.96	124.45
22	c	510	CLA	C3B-C4B-NB	3.80	114.12	109.21
22	A	404	CLA	C4D-CHA-C1A	-3.80	116.63	121.25
24	K	101	BCR	C32-C1-C6	-3.80	104.14	110.30
22	A	408	CLA	O2D-CGD-CBD	3.80	118.01	111.27
22	b	618	CLA	C3D-C2D-C1D	-3.80	100.65	105.83
22	B	602	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
22	c	506	CLA	CBC-CAC-C3C	-3.79	101.97	112.43
22	a	409	CLA	C4C-C3C-C2C	-3.79	101.37	106.90
22	B	611	CLA	CAC-C3C-C4C	3.79	129.72	124.81
22	C	506	CLA	CHA-C4D-ND	3.79	140.42	132.50
22	A	408	CLA	C2A-C1A-CHA	-3.79	117.24	123.86
22	C	504	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
22	b	611	CLA	CAC-C3C-C4C	3.78	129.72	124.81
32	b	640	HTG	O6-C6-C5	3.78	124.27	111.29
24	t	101	BCR	C35-C13-C14	-3.78	117.63	122.92
22	B	614	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
26	b	625	LMG	O7-C10-C11	3.78	119.65	111.50
22	b	617	CLA	O2D-CGD-CBD	3.78	117.98	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	h	101	DGD	O1G-C1A-O1A	-3.78	114.06	123.59
32	C	522	HTG	C1-O5-C5	3.77	119.53	112.58
25	a	411	PL9	C31-C29-C28	-3.76	113.50	121.12
22	A	404	CLA	C7-C6-C5	-3.76	103.15	113.36
22	B	611	CLA	C4D-CHA-C1A	-3.76	116.67	121.25
22	b	609	CLA	C3D-C2D-C1D	-3.75	100.71	105.83
22	c	514	CLA	C2A-C1A-CHA	-3.75	117.30	123.86
22	b	620	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
22	c	505	CLA	C3B-C4B-NB	3.75	114.05	109.21
22	B	602	CLA	O2A-CGA-CBA	3.74	123.65	111.91
22	B	615	CLA	CAC-C3C-C4C	3.74	129.66	124.81
22	D	403	CLA	C3C-C4C-NC	3.73	114.75	110.57
22	d	403	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
24	t	101	BCR	C32-C1-C6	3.72	116.33	110.30
22	B	606	CLA	C1D-ND-C4D	-3.71	103.70	106.33
24	B	619	BCR	C34-C9-C10	3.71	128.12	122.92
22	c	512	CLA	O2A-CGA-O1A	-3.71	114.23	123.59
25	D	407	PL9	C40-C39-C38	-3.71	114.17	123.68
33	c	519	DGD	O3G-C1D-C2D	-3.71	102.52	108.30
22	b	613	CLA	C4D-CHA-C1A	-3.70	116.74	121.25
32	b	640	HTG	O4-C4-C5	-3.70	100.10	109.30
22	b	614	CLA	CMC-C2C-C1C	3.70	130.67	125.04
32	B	642	HTG	O5-C1-C2	-3.70	105.66	110.31
22	C	511	CLA	CHA-C4D-ND	3.70	140.23	132.50
22	c	503	CLA	CMC-C2C-C1C	3.69	130.66	125.04
22	b	616	CLA	C3D-C2D-C1D	-3.69	100.79	105.83
22	b	609	CLA	CMD-C2D-C1D	3.69	131.22	124.71
22	b	608	CLA	C2C-C1C-NC	3.69	113.43	109.97
22	B	610	CLA	CMC-C2C-C1C	3.69	130.66	125.04
22	b	619	CLA	C6-C5-C3	-3.68	103.80	113.45
40	v	202	HEC	CMC-C2C-C1C	-3.68	122.81	128.46
22	b	610	CLA	C2C-C1C-NC	3.68	113.42	109.97
22	b	610	CLA	O2D-CGD-CBD	3.68	117.80	111.27
22	C	503	CLA	C5-C3-C2	-3.68	113.68	121.12
22	B	617	CLA	O2D-CGD-O1D	-3.67	116.65	123.84
24	C	514	BCR	C7-C8-C9	-3.67	120.68	126.23
22	C	509	CLA	C3D-C2D-C1D	-3.67	100.82	105.83
22	B	609	CLA	C4-C3-C5	3.67	121.45	115.27
22	B	614	CLA	CAC-C3C-C4C	3.67	129.57	124.81
32	c	541	HTG	O4-C4-C5	3.67	118.40	109.30
22	a	407	CLA	CMC-C2C-C1C	3.67	130.62	125.04
28	c	522	LMT	O1B-C1B-C2B	3.66	117.59	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	520	LMT	O3'-C3'-C4'	3.66	119.64	109.94
22	B	613	CLA	C2C-C1C-NC	3.66	113.40	109.97
22	B	607	CLA	CHD-C1D-ND	-3.66	121.09	124.45
22	C	503	CLA	CAC-C3C-C4C	3.66	129.56	124.81
22	c	504	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
24	y	101	BCR	C35-C13-C12	3.66	123.84	118.08
22	A	404	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
37	F	101	HEM	CBA-CAA-C2A	-3.65	106.39	112.62
22	B	608	CLA	O1D-CGD-CBD	-3.65	117.01	124.48
22	b	605	CLA	C1-O2A-CGA	3.65	126.02	116.44
22	C	503	CLA	CHA-C4D-ND	3.65	140.13	132.50
22	B	605	CLA	CAC-C3C-C4C	3.65	129.54	124.81
25	A	410	PL9	C32-C33-C34	-3.64	118.89	127.66
22	B	615	CLA	CHB-C4A-NA	3.64	129.55	124.51
26	a	412	LMG	O1-C1-C2	3.64	113.99	108.30
24	D	406	BCR	C32-C1-C6	3.64	116.20	110.30
28	T	102	LMT	C3'-C4'-C5'	-3.64	103.75	110.24
22	b	616	CLA	C4C-C3C-C2C	-3.64	101.60	106.90
22	c	511	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
32	b	602	HTG	C1-O5-C5	3.63	119.27	112.58
22	B	615	CLA	O2A-CGA-O1A	-3.63	114.43	123.59
22	a	407	CLA	C4D-CHA-C1A	-3.63	116.84	121.25
33	d	408	DGD	O2G-C1B-O1B	-3.62	114.94	123.70
22	c	514	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
33	c	519	DGD	C1E-O6E-C5E	-3.62	106.58	113.69
22	B	602	CLA	CHA-C4D-ND	3.62	140.08	132.50
22	b	616	CLA	C2A-C1A-CHA	-3.62	117.53	123.86
22	C	512	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
24	T	101	BCR	C23-C22-C21	-3.61	113.39	118.94
22	B	603	CLA	CMB-C2B-C3B	3.61	131.44	124.68
22	C	506	CLA	C3C-C4C-NC	3.61	114.62	110.57
22	A	406	CLA	C3B-C4B-NB	3.61	113.88	109.21
22	c	510	CLA	CHB-C4A-NA	3.61	129.50	124.51
24	D	406	BCR	C40-C30-C25	-3.61	104.45	110.30
22	C	502	CLA	CMC-C2C-C1C	3.60	130.53	125.04
22	C	503	CLA	CMC-C2C-C1C	3.60	130.53	125.04
25	D	407	PL9	C53-C6-C1	3.60	122.36	114.99
28	a	401	LMT	O2'-C2'-C1'	3.60	118.80	110.05
33	c	519	DGD	O5D-C1E-C2E	-3.60	102.68	108.30
40	V	201	HEC	CMB-C2B-C1B	-3.60	122.94	128.46
22	c	511	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
22	b	614	CLA	C4A-NA-C1A	3.59	108.32	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	513	CLA	CBC-CAC-C3C	-3.59	102.54	112.43
22	B	605	CLA	C2A-C1A-CHA	-3.59	117.58	123.86
22	c	513	CLA	C3D-C2D-C1D	-3.59	100.94	105.83
25	a	411	PL9	C16-C17-C18	-3.59	100.10	111.88
22	c	514	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
22	b	609	CLA	CED-O2D-CGD	3.58	124.05	115.94
22	c	507	CLA	C1D-ND-C4D	-3.58	103.79	106.33
22	c	514	CLA	C3D-C2D-C1D	-3.58	100.94	105.83
22	b	613	CLA	O2D-CGD-CBD	3.58	117.63	111.27
22	C	513	CLA	C2C-C1C-NC	3.58	113.32	109.97
22	B	613	CLA	O2D-CGD-CBD	3.58	117.62	111.27
33	C	517	DGD	C6D-O5D-C1E	3.57	120.71	113.74
22	B	609	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
22	A	406	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
22	B	608	CLA	C3D-C2D-C1D	-3.56	100.97	105.83
22	c	506	CLA	CHD-C1D-ND	-3.56	121.18	124.45
22	b	613	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
22	b	616	CLA	C3B-C4B-NB	3.55	113.80	109.21
22	C	503	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
22	A	404	CLA	C1B-CHB-C4A	-3.55	123.09	130.12
22	B	604	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
22	b	611	CLA	CMD-C2D-C1D	3.55	130.97	124.71
32	V	202	HTG	C1-C2-C3	-3.55	103.58	110.59
22	b	617	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
22	b	608	CLA	C3D-C2D-C1D	-3.55	100.99	105.83
24	b	623	BCR	C7-C8-C9	-3.54	120.88	126.23
22	C	513	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
22	b	620	CLA	CAC-C3C-C4C	3.54	129.41	124.81
22	B	608	CLA	CBC-CAC-C3C	-3.54	102.67	112.43
24	k	101	BCR	C35-C13-C14	-3.54	117.97	122.92
22	b	608	CLA	C6-C5-C3	-3.54	104.18	113.45
22	B	607	CLA	C3D-C2D-C1D	-3.54	101.00	105.83
22	A	405	CLA	C3C-C4C-NC	3.53	114.53	110.57
22	D	405	CLA	CAC-C3C-C4C	3.53	129.39	124.81
22	b	608	CLA	C3B-C4B-NB	3.53	113.77	109.21
22	a	406	CLA	C3D-C2D-C1D	-3.53	101.02	105.83
22	c	513	CLA	CHD-C4C-C3C	-3.52	119.66	124.84
22	B	611	CLA	CHA-C4D-ND	3.52	139.86	132.50
22	b	605	CLA	CMB-C2B-C1B	3.51	133.87	128.46
22	b	620	CLA	CHA-C4D-ND	3.51	139.84	132.50
25	D	407	PL9	C2-C3-C4	3.51	123.64	118.80
22	b	606	CLA	C1C-C2C-C3C	-3.51	103.27	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	616	CLA	C4A-NA-C1A	3.50	108.28	106.71
37	F	101	HEM	CAD-C3D-C4D	3.50	130.78	124.66
24	T	101	BCR	C34-C9-C8	3.50	123.59	118.08
37	f	101	HEM	CBA-CAA-C2A	-3.50	106.65	112.62
22	C	506	CLA	CHD-C4C-NC	3.50	129.72	124.20
22	B	616	CLA	CHA-C4D-ND	3.50	139.81	132.50
22	a	409	CLA	CHB-C4A-NA	3.50	129.35	124.51
22	B	615	CLA	C1-O2A-CGA	3.49	125.61	116.44
22	c	505	CLA	CHB-C4A-NA	3.49	129.34	124.51
22	B	603	CLA	CHA-C4D-ND	3.49	139.81	132.50
22	b	609	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
22	B	613	CLA	CHD-C4C-NC	3.49	129.70	124.20
22	a	409	CLA	CMC-C2C-C1C	3.49	130.35	125.04
22	d	402	CLA	C2A-C1A-CHA	-3.49	117.77	123.86
22	b	606	CLA	C1D-CHD-C4C	-3.48	118.54	126.06
22	b	619	CLA	CMB-C2B-C3B	3.48	131.20	124.68
22	C	510	CLA	CHD-C4C-NC	3.48	129.69	124.20
22	b	618	CLA	C4C-C3C-C2C	-3.48	101.83	106.90
22	b	609	CLA	C2A-C1A-CHA	-3.48	117.78	123.86
22	A	404	CLA	C1D-ND-C4D	-3.48	103.86	106.33
22	d	402	CLA	CHD-C1D-ND	-3.47	121.26	124.45
22	b	617	CLA	C7-C6-C5	-3.47	103.94	113.36
28	M	102	LMT	C4'-C3'-C2'	3.47	116.88	110.82
22	B	604	CLA	C2A-C1A-CHA	-3.47	117.80	123.86
24	b	621	BCR	C7-C8-C9	-3.47	121.00	126.23
22	b	608	CLA	CHA-C4D-ND	3.46	139.75	132.50
33	D	408	DGD	O6D-C5D-C4D	3.46	115.73	109.52
22	C	506	CLA	C2C-C1C-NC	3.46	113.21	109.97
24	d	406	BCR	C34-C9-C10	-3.46	118.08	122.92
22	D	403	CLA	C2D-C1D-ND	3.46	112.65	110.10
22	c	512	CLA	CHA-C4D-ND	3.46	139.73	132.50
24	A	409	BCR	C27-C26-C25	3.46	127.75	122.73
22	B	616	CLA	CHD-C4C-C3C	-3.45	119.76	124.84
22	C	512	CLA	CHD-C1D-ND	-3.45	121.28	124.45
22	c	511	CLA	CHA-C4D-ND	3.45	139.72	132.50
22	b	620	CLA	CMB-C2B-C3B	3.45	131.13	124.68
22	C	509	CLA	C2A-C1A-CHA	-3.45	117.83	123.86
22	B	608	CLA	C3B-C4B-NB	3.45	113.67	109.21
22	A	408	CLA	CHD-C4C-C3C	-3.45	119.77	124.84
22	B	614	CLA	CHD-C1D-ND	-3.44	121.29	124.45
22	C	502	CLA	CMD-C2D-C1D	3.44	130.78	124.71
25	a	411	PL9	C22-C23-C24	-3.44	119.37	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	512	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
24	k	101	BCR	C35-C13-C12	3.44	123.50	118.08
22	b	614	CLA	CMD-C2D-C1D	3.44	130.77	124.71
28	j	102	LMT	O5'-C1'-C2'	-3.43	105.69	110.87
22	B	606	CLA	C3D-C2D-C1D	-3.43	101.14	105.83
22	C	501	CLA	C2A-C1A-CHA	-3.43	117.86	123.86
22	b	605	CLA	C4D-C3D-CAD	3.43	112.14	108.10
22	B	605	CLA	CHD-C1D-ND	-3.43	121.30	124.45
37	F	101	HEM	CMC-C2C-C3C	3.43	131.09	124.68
22	a	409	CLA	C4-C3-C5	3.42	121.03	115.27
25	A	410	PL9	C30-C29-C31	3.42	121.03	115.27
22	B	613	CLA	C3C-C4C-NC	3.42	114.41	110.57
22	C	505	CLA	CHD-C4C-NC	3.42	129.59	124.20
22	b	606	CLA	CHA-C4D-ND	3.42	139.66	132.50
22	c	506	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
22	c	511	CLA	C4A-NA-C1A	3.42	108.24	106.71
22	B	614	CLA	C2A-C1A-CHA	-3.42	117.88	123.86
38	h	102	RRX	C29-C28-C27	3.42	114.99	110.30
24	B	618	BCR	C34-C9-C8	3.42	123.47	118.08
32	c	524	HTG	C1-S1-C1'	3.42	112.14	100.40
22	B	607	CLA	CHD-C4C-NC	3.41	129.58	124.20
32	O	302	HTG	O2-C2-C3	-3.41	102.47	110.35
32	b	640	HTG	C4-C3-C2	3.41	116.78	110.82
22	C	502	CLA	C1D-ND-C4D	-3.41	103.91	106.33
22	B	602	CLA	C4D-CHA-C1A	-3.41	117.10	121.25
28	a	401	LMT	O5'-C1'-C2'	-3.41	103.14	110.35
22	C	509	CLA	CHC-C1C-C2C	-3.40	117.31	126.72
22	B	616	CLA	C3D-C2D-C1D	-3.40	101.20	105.83
37	F	101	HEM	CMD-C2D-C1D	3.39	130.21	125.04
22	A	404	CLA	C3D-C2D-C1D	-3.39	101.20	105.83
22	c	514	CLA	C1D-ND-C4D	-3.39	103.92	106.33
22	b	608	CLA	CHB-C4A-NA	3.39	129.20	124.51
22	C	508	CLA	CHD-C4C-NC	3.39	129.54	124.20
28	j	102	LMT	O3'-C3'-C4'	3.39	116.92	110.14
22	c	502	CLA	C3D-C2D-C1D	-3.39	101.21	105.83
22	b	618	CLA	C3C-C4C-NC	3.38	114.37	110.57
22	b	607	CLA	C4D-CHA-C1A	-3.38	117.13	121.25
22	c	513	CLA	CHA-C4D-ND	3.38	139.56	132.50
22	c	514	CLA	CHA-C4D-ND	3.38	139.56	132.50
22	B	611	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
24	y	101	BCR	C34-C9-C8	3.37	123.39	118.08
22	C	505	CLA	C4D-CHA-C1A	-3.37	117.15	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	515	BCR	C33-C5-C6	-3.37	120.75	124.53
22	b	620	CLA	CBC-CAC-C3C	-3.37	103.15	112.43
24	D	406	BCR	C29-C28-C27	-3.37	103.86	111.38
22	c	509	CLA	C3B-C4B-NB	3.36	113.56	109.21
22	c	508	CLA	C4D-CHA-C1A	-3.36	117.16	121.25
22	B	610	CLA	CBC-CAC-C3C	-3.36	103.18	112.43
22	B	616	CLA	C2A-C1A-CHA	-3.36	117.99	123.86
22	b	605	CLA	CAC-C3C-C4C	3.35	129.16	124.81
33	c	519	DGD	O6D-C1D-C2D	3.34	117.42	110.35
31	B	621	LHG	O8-C23-O10	-3.34	115.16	123.59
22	d	405	CLA	CED-O2D-CGD	3.34	123.49	115.94
32	B	642	HTG	O3-C3-C4	-3.34	102.63	110.35
22	b	614	CLA	C4D-CHA-C1A	-3.34	117.18	121.25
22	C	502	CLA	CHD-C1D-ND	-3.34	121.39	124.45
22	d	402	CLA	CHD-C4C-C3C	-3.33	119.94	124.84
22	C	503	CLA	C2A-C1A-CHA	-3.33	118.03	123.86
22	b	618	CLA	CED-O2D-CGD	3.33	123.47	115.94
22	B	613	CLA	C4D-CHA-C1A	-3.33	117.19	121.25
28	B	623	LMT	O1'-C1'-C2'	-3.33	103.10	108.30
22	B	605	CLA	CMB-C2B-C3B	3.33	130.91	124.68
22	b	620	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
24	K	102	BCR	C29-C30-C25	3.33	115.60	110.48
22	b	608	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
22	C	503	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
25	D	407	PL9	C36-C37-C38	-3.32	100.97	111.88
22	c	506	CLA	CMB-C2B-C3B	3.32	130.89	124.68
22	c	504	CLA	CHD-C4C-NC	3.32	129.43	124.20
22	B	616	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
24	D	406	BCR	C24-C23-C22	-3.32	121.22	126.23
33	H	101	DGD	O4E-C4E-C3E	-3.32	102.68	110.35
31	B	621	LHG	O8-C23-C24	3.31	122.31	111.91
22	b	609	CLA	CMB-C2B-C3B	3.31	130.88	124.68
22	b	608	CLA	CMB-C2B-C3B	3.31	130.87	124.68
22	C	506	CLA	CMD-C2D-C1D	3.31	130.54	124.71
22	C	513	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
22	A	408	CLA	CHD-C1D-ND	-3.30	121.42	124.45
28	c	522	LMT	C3B-C4B-C5B	3.30	116.13	110.24
28	F	102	LMT	O5'-C5'-C6'	3.30	114.65	106.44
22	b	615	CLA	CMD-C2D-C1D	3.30	130.53	124.71
22	A	406	CLA	CHD-C4C-NC	3.30	129.41	124.20
22	b	619	CLA	CAC-C3C-C4C	3.30	129.09	124.81
33	h	101	DGD	O6D-C5D-C6D	3.30	113.33	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	506	CLA	C3D-C2D-C1D	-3.30	101.33	105.83
24	B	619	BCR	C30-C25-C26	-3.30	117.97	122.61
28	l	101	LMT	O1'-C1'-C2'	3.29	113.45	108.30
22	b	614	CLA	CHA-C4D-ND	3.29	139.39	132.50
22	b	611	CLA	CHD-C4C-NC	3.29	129.39	124.20
33	C	517	DGD	O1G-C1A-C2A	3.29	122.24	111.91
22	B	611	CLA	O2A-CGA-O1A	-3.29	115.29	123.59
28	M	101	LMT	O1'-C1'-C2'	3.29	113.44	108.30
22	C	509	CLA	O2A-C1-C2	3.29	117.27	108.64
22	A	405	CLA	C2A-C1A-CHA	-3.28	118.11	123.86
22	b	619	CLA	CHD-C4C-C3C	-3.28	120.01	124.84
22	C	511	CLA	CMD-C2D-C1D	3.28	130.50	124.71
22	A	405	CLA	CHC-C1C-C2C	-3.28	117.64	126.72
31	d	409	LHG	O7-C7-O9	-3.28	115.77	123.70
22	B	606	CLA	C2A-C1A-CHA	-3.28	118.13	123.86
22	c	503	CLA	C4A-NA-C1A	3.28	108.18	106.71
22	b	618	CLA	CHB-C4A-NA	3.27	129.04	124.51
22	c	514	CLA	C3C-C4C-NC	3.27	114.24	110.57
31	e	101	LHG	O8-C23-C24	3.27	122.18	111.91
32	B	642	HTG	O2-C2-C3	-3.27	102.79	110.35
22	d	405	CLA	CHD-C4C-C3C	-3.27	120.03	124.84
22	b	620	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
22	B	612	CLA	C1D-CHD-C4C	-3.27	119.01	126.06
22	A	404	CLA	C3C-C4C-NC	3.27	114.24	110.57
22	b	610	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
22	c	502	CLA	CMC-C2C-C1C	3.26	130.01	125.04
22	d	402	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
37	F	101	HEM	CHC-C4B-NB	3.26	127.97	124.43
32	b	601	HTG	O5-C5-C4	3.26	115.61	109.69
22	b	606	CLA	C4D-CHA-C1A	-3.26	117.28	121.25
22	C	505	CLA	O2A-CGA-O1A	-3.26	115.37	123.59
28	A	415	LMT	C1'-C2'-C3'	-3.26	103.21	110.00
22	b	606	CLA	O2A-CGA-CBA	3.25	122.12	111.91
28	C	520	LMT	C2'-C3'-C4'	-3.25	102.25	109.68
22	C	507	CLA	CHA-C4D-ND	3.25	139.30	132.50
32	b	640	HTG	C1-C2-C3	3.25	117.01	110.59
22	b	608	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
22	C	501	CLA	C3B-C4B-NB	3.25	113.41	109.21
24	D	406	BCR	C30-C25-C26	-3.25	118.04	122.61
26	d	412	LMG	O2-C2-C1	-3.25	102.16	110.05
22	C	501	CLA	C1D-ND-C4D	-3.25	104.03	106.33
33	D	408	DGD	C3G-O3G-C1D	3.24	120.08	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	608	CLA	CAC-C3C-C4C	3.24	129.02	124.81
24	B	619	BCR	C29-C28-C27	-3.24	104.13	111.38
24	d	406	BCR	C30-C25-C26	-3.24	118.05	122.61
22	b	617	CLA	O2A-CGA-CBA	3.24	122.08	111.91
22	d	402	CLA	C3C-C4C-NC	3.24	114.20	110.57
22	C	513	CLA	C4-C3-C5	3.24	120.72	115.27
22	C	506	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
22	C	509	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
22	b	606	CLA	C3D-C2D-C1D	-3.24	101.41	105.83
22	b	606	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
22	B	602	CLA	C3B-C4B-NB	3.24	113.39	109.21
22	b	615	CLA	C3D-C2D-C1D	-3.24	101.41	105.83
22	B	612	CLA	CAC-C3C-C4C	3.23	129.01	124.81
22	B	609	CLA	C3C-C4C-NC	3.23	114.20	110.57
22	d	402	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
22	b	616	CLA	CHD-C4C-NC	3.23	129.29	124.20
22	b	605	CLA	C2A-C1A-CHA	-3.23	118.21	123.86
22	b	610	CLA	C4D-CHA-C1A	-3.23	117.32	121.25
22	B	615	CLA	C3D-C2D-C1D	-3.22	101.43	105.83
22	B	609	CLA	CHA-C4D-ND	3.22	139.24	132.50
22	C	512	CLA	CHD-C4C-C3C	-3.22	120.11	124.84
22	C	505	CLA	CHD-C1D-ND	-3.22	121.49	124.45
22	b	609	CLA	C3C-C4C-NC	3.22	114.18	110.57
22	d	403	CLA	CMB-C2B-C3B	3.21	130.69	124.68
23	A	407	PHO	CMB-C2B-C3B	3.21	130.69	124.68
38	h	102	RRX	C2-C1-C6	3.21	115.42	110.48
22	B	603	CLA	CHB-C4A-NA	3.21	128.95	124.51
22	B	605	CLA	CHA-C4D-ND	3.21	139.21	132.50
22	b	605	CLA	CMC-C2C-C1C	3.21	129.92	125.04
22	b	616	CLA	CHD-C1D-ND	-3.21	121.51	124.45
22	C	503	CLA	CMB-C2B-C3B	3.21	130.68	124.68
22	c	503	CLA	C2A-C1A-CHA	-3.20	118.26	123.86
22	c	510	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
28	A	415	LMT	O1B-C4'-C3'	3.20	115.79	107.28
22	c	510	CLA	C3C-C4C-NC	3.20	114.16	110.57
22	C	503	CLA	CHB-C4A-NA	3.20	128.93	124.51
31	E	101	LHG	O7-C7-C8	3.19	118.39	111.50
22	A	406	CLA	CHD-C1D-ND	-3.19	121.52	124.45
22	C	510	CLA	CHD-C1D-ND	-3.19	121.52	124.45
22	C	507	CLA	CBC-CAC-C3C	-3.19	103.63	112.43
22	B	603	CLA	C1D-CHD-C4C	-3.19	119.17	126.06
32	b	640	HTG	O2-C2-C1	3.19	116.13	110.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	603	CLA	O2D-CGD-CBD	3.19	116.94	111.27
22	c	513	CLA	C1-O2A-CGA	3.19	124.81	116.44
23	D	404	PHO	CMA-C3A-C4A	-3.19	107.40	114.38
22	C	503	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
33	c	517	DGD	C2G-O2G-C1B	-3.18	109.96	117.79
31	f	102	LHG	O8-C23-O10	-3.18	115.57	123.59
33	C	515	DGD	O3G-C3G-C2G	-3.18	103.23	110.90
37	F	101	HEM	CMA-C3A-C4A	-3.18	123.58	128.46
22	B	602	CLA	C1-O2A-CGA	3.18	124.78	116.44
22	b	610	CLA	C3B-C4B-NB	3.18	113.32	109.21
22	C	513	CLA	CHD-C4C-NC	3.18	129.21	124.20
24	D	406	BCR	C34-C9-C8	3.17	123.08	118.08
22	c	508	CLA	C3D-C2D-C1D	-3.17	101.50	105.83
22	b	610	CLA	CAC-C3C-C4C	3.17	128.93	124.81
22	D	405	CLA	C2A-C1A-CHA	-3.17	118.31	123.86
22	C	502	CLA	CHA-C4D-ND	3.17	139.13	132.50
33	h	101	DGD	O1G-C1A-C2A	3.17	121.84	111.91
22	C	508	CLA	CHD-C1D-ND	-3.17	121.55	124.45
28	c	522	LMT	C1B-O1B-C4'	3.16	125.80	117.96
22	b	609	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
22	B	610	CLA	C3D-C2D-C1D	-3.15	101.53	105.83
22	b	620	CLA	C4D-CHA-C1A	-3.15	117.42	121.25
22	c	505	CLA	CHD-C4C-C3C	-3.15	120.21	124.84
22	c	514	CLA	C1D-CHD-C4C	-3.15	119.27	126.06
22	c	511	CLA	C3D-C2D-C1D	-3.15	101.53	105.83
32	D	413	HTG	O2-C2-C3	-3.14	103.08	110.35
22	c	505	CLA	CMD-C2D-C1D	3.14	130.25	124.71
22	b	615	CLA	CHD-C1D-ND	-3.14	121.57	124.45
22	A	404	CLA	CHA-C4D-ND	3.14	139.07	132.50
22	b	608	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
22	A	405	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
22	B	611	CLA	C3D-C2D-C1D	-3.13	101.56	105.83
28	J	102	LMT	C4'-C3'-C2'	3.13	116.29	110.82
22	c	508	CLA	CHB-C4A-NA	3.13	128.84	124.51
22	C	506	CLA	O2D-CGD-CBD	3.13	116.83	111.27
28	a	401	LMT	C1'-O5'-C5'	3.13	119.83	113.69
26	c	520	LMG	O8-C28-C29	3.13	121.73	111.91
22	C	505	CLA	CHB-C4A-NA	3.13	128.84	124.51
22	b	609	CLA	CHB-C4A-NA	3.13	128.84	124.51
22	C	506	CLA	CHB-C4A-NA	3.13	128.84	124.51
22	C	504	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
24	b	622	BCR	C29-C30-C25	3.12	115.29	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	403	CLA	C3B-C4B-NB	3.12	113.25	109.21
22	c	503	CLA	C3C-C4C-NC	3.12	114.07	110.57
22	c	511	CLA	CAC-C3C-C4C	3.12	128.86	124.81
22	A	408	CLA	C1D-CHD-C4C	-3.12	119.33	126.06
22	c	511	CLA	C3D-C4D-CHA	-3.12	105.59	112.72
22	c	514	CLA	CMB-C2B-C3B	3.11	130.50	124.68
22	B	609	CLA	CHB-C4A-NA	3.11	128.82	124.51
22	B	602	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
22	B	610	CLA	CMB-C2B-C3B	3.11	130.50	124.68
22	c	512	CLA	C4D-CHA-C1A	-3.11	117.46	121.25
22	C	505	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	C	501	CLA	C3D-C2D-C1D	-3.11	101.58	105.83
22	C	507	CLA	CHD-C4C-C3C	-3.11	120.27	124.84
24	C	514	BCR	C38-C26-C25	-3.11	121.04	124.53
22	A	404	CLA	CHD-C4C-C3C	-3.11	120.27	124.84
22	B	604	CLA	CAC-C3C-C4C	3.11	128.84	124.81
22	b	611	CLA	CHA-C4D-ND	3.11	139.00	132.50
22	B	609	CLA	CMC-C2C-C1C	3.10	129.76	125.04
22	B	606	CLA	CHC-C1C-NC	-3.10	119.50	124.20
22	B	612	CLA	CHA-C4D-ND	3.10	138.98	132.50
22	B	617	CLA	CHA-C4D-ND	3.10	138.98	132.50
26	d	412	LMG	O7-C10-O9	-3.10	116.22	123.70
22	a	409	CLA	C1D-CHD-C4C	-3.10	119.38	126.06
22	B	603	CLA	CAC-C3C-C4C	3.10	128.83	124.81
33	C	517	DGD	O6E-C5E-C6E	3.10	114.13	106.44
22	C	503	CLA	O2D-CGD-CBD	3.10	116.77	111.27
26	c	521	LMG	O7-C10-C11	3.10	118.17	111.50
22	D	403	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
33	H	101	DGD	O4E-C4E-C5E	3.09	116.98	109.30
22	D	405	CLA	CHB-C4A-NA	3.09	128.78	124.51
33	C	516	DGD	O2G-C1B-C2B	3.09	118.15	111.50
31	F	103	LHG	O8-C23-C24	3.08	121.57	111.91
22	C	510	CLA	O2A-CGA-O1A	-3.08	115.82	123.59
22	C	513	CLA	C3D-C2D-C1D	-3.08	101.63	105.83
28	m	101	LMT	C1'-O5'-C5'	-3.08	107.65	113.69
22	B	608	CLA	CGD-CBD-CAD	-3.08	100.76	110.73
22	B	611	CLA	C3C-C4C-NC	3.08	114.02	110.57
33	c	519	DGD	C1D-O6D-C5D	-3.08	107.65	113.69
22	B	611	CLA	C1D-CHD-C4C	-3.07	119.43	126.06
32	B	628	HTG	O5-C1-C2	-3.07	106.45	110.31
22	C	502	CLA	CHD-C4C-NC	3.07	129.04	124.20
24	B	619	BCR	C8-C9-C10	-3.07	114.23	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	406	CLA	C4D-CHA-C1A	-3.07	117.51	121.25
22	a	407	CLA	C1D-ND-C4D	-3.07	104.15	106.33
38	h	102	RRX	C16-C15-C14	-3.07	117.18	123.47
22	b	611	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
33	c	519	DGD	O1G-C1A-C2A	3.06	121.52	111.91
22	B	617	CLA	C1-O2A-CGA	3.06	124.48	116.44
22	b	606	CLA	C2A-C1A-CHA	-3.06	118.50	123.86
22	B	603	CLA	C3C-C4C-NC	3.06	114.00	110.57
22	b	610	CLA	CMD-C2D-C1D	3.06	130.10	124.71
22	C	512	CLA	CMB-C2B-C3B	3.06	130.39	124.68
34	C	533	GOL	O2-C2-C3	3.05	122.57	109.12
22	b	615	CLA	C2A-C1A-CHA	-3.05	118.52	123.86
22	C	503	CLA	C4-C3-C5	3.05	120.40	115.27
22	b	620	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
22	B	605	CLA	O2D-CGD-CBD	3.05	116.68	111.27
22	b	617	CLA	C4A-NA-C1A	3.05	108.08	106.71
22	b	620	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
26	c	520	LMG	O8-C28-O10	-3.05	115.90	123.59
32	b	601	HTG	C1'-S1-C1	3.05	105.79	100.09
24	y	101	BCR	C35-C13-C14	-3.05	118.66	122.92
22	b	619	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
22	C	506	CLA	C4D-CHA-C1A	-3.05	117.54	121.25
22	c	512	CLA	C2D-C1D-ND	3.04	112.35	110.10
22	A	404	CLA	C4D-C3D-CAD	3.04	111.68	108.10
22	b	615	CLA	C1-C2-C3	-3.04	120.79	126.04
26	d	412	LMG	O8-C28-O10	-3.04	115.92	123.59
22	b	617	CLA	CMD-C2D-C1D	3.04	130.07	124.71
22	C	513	CLA	CHA-C4D-ND	3.04	138.85	132.50
22	B	604	CLA	CMC-C2C-C1C	3.04	129.66	125.04
22	b	616	CLA	C1D-CHD-C4C	-3.03	119.51	126.06
22	B	602	CLA	CAC-C3C-C4C	3.03	128.75	124.81
22	b	619	CLA	CHD-C1D-ND	-3.03	121.67	124.45
28	F	102	LMT	O1'-C1'-C2'	3.03	113.03	108.30
22	D	405	CLA	C1D-ND-C4D	-3.03	104.19	106.33
22	b	613	CLA	CHD-C4C-NC	3.03	128.97	124.20
22	d	402	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	b	616	CLA	CED-O2D-CGD	3.02	122.77	115.94
33	C	517	DGD	O5D-C6D-C5D	3.02	114.63	109.05
22	C	505	CLA	O2D-CGD-CBD	3.02	116.63	111.27
28	m	101	LMT	C1-O1'-C1'	3.02	118.84	113.84
22	c	512	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
22	a	407	CLA	C3A-C2A-C1A	-3.01	96.83	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	519	LMG	O1-C7-C8	3.01	118.17	110.90
22	c	512	CLA	C1-O2A-CGA	3.01	124.35	116.44
22	B	604	CLA	CHD-C4C-NC	3.01	128.95	124.20
22	B	617	CLA	CBC-CAC-C3C	-3.01	104.13	112.43
22	d	405	CLA	CHB-C4A-NA	3.01	128.67	124.51
24	B	619	BCR	C29-C30-C25	3.01	115.11	110.48
22	b	613	CLA	C3D-C2D-C1D	-3.01	101.73	105.83
22	c	510	CLA	C1-C2-C3	-3.01	120.84	126.04
22	D	403	CLA	C1D-CHD-C4C	-3.00	119.58	126.06
22	c	513	CLA	C2A-C1A-CHA	-3.00	118.61	123.86
26	A	411	LMG	C4-C3-C2	3.00	116.07	110.82
22	D	403	CLA	CMC-C2C-C1C	3.00	129.61	125.04
28	M	101	LMT	C1'-O5'-C5'	-3.00	107.80	113.69
22	B	612	CLA	CBC-CAC-C3C	-3.00	104.16	112.43
37	f	101	HEM	CAD-CBD-CGD	3.00	120.06	113.60
22	b	617	CLA	C4D-CHA-C1A	-3.00	117.60	121.25
25	A	410	PL9	C2-C3-C4	-3.00	114.66	118.80
22	B	603	CLA	C4D-CHA-C1A	-3.00	117.60	121.25
22	C	503	CLA	CHD-C4C-NC	2.99	128.92	124.20
22	B	603	CLA	C11-C12-C13	-2.99	106.25	115.92
22	B	615	CLA	CED-O2D-CGD	2.99	122.70	115.94
22	B	611	CLA	C1C-C2C-C3C	-2.99	103.82	106.96
24	Y	101	BCR	C34-C9-C8	2.99	122.78	118.08
22	c	512	CLA	CAC-C3C-C4C	2.99	128.69	124.81
22	c	514	CLA	CMD-C2D-C1D	2.98	129.97	124.71
22	b	606	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
22	b	611	CLA	CMC-C2C-C1C	2.98	129.58	125.04
22	d	403	CLA	CMC-C2C-C1C	2.98	129.58	125.04
22	B	614	CLA	C3B-C4B-NB	2.98	113.06	109.21
40	v	202	HEC	CMB-C2B-C1B	-2.98	123.88	128.46
32	o	301	HTG	C1-O5-C5	2.98	118.08	112.58
22	c	505	CLA	O2A-C1-C2	-2.98	100.80	108.64
22	B	614	CLA	CMD-C2D-C1D	2.98	129.96	124.71
22	B	604	CLA	O2D-CGD-CBD	2.98	116.56	111.27
22	A	406	CLA	C3C-C4C-NC	2.98	113.91	110.57
22	c	505	CLA	C2A-C1A-CHA	-2.97	118.66	123.86
22	A	406	CLA	C4A-NA-C1A	-2.97	105.37	106.71
28	m	101	LMT	O1'-C1'-C2'	2.97	112.94	108.30
22	B	613	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
22	C	508	CLA	C3D-C2D-C1D	-2.97	101.78	105.83
22	c	507	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
22	B	616	CLA	CHD-C4C-NC	2.96	128.87	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	T	101	BCR	C35-C13-C14	-2.96	118.77	122.92
22	b	617	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	c	506	CLA	CAC-C3C-C4C	2.96	128.65	124.81
32	c	541	HTG	C6-C5-C4	2.96	119.93	113.00
22	C	508	CLA	CAC-C3C-C4C	2.96	128.65	124.81
22	c	502	CLA	CBC-CAC-C3C	-2.96	104.28	112.43
22	A	404	CLA	CAC-C3C-C4C	2.96	128.65	124.81
28	z	101	LMT	C3B-C4B-C5B	2.95	115.51	110.24
22	b	618	CLA	CHD-C1D-ND	-2.95	121.74	124.45
22	D	403	CLA	CHC-C1C-NC	-2.95	119.72	124.20
22	A	405	CLA	CMD-C2D-C3D	2.95	134.40	127.61
28	m	101	LMT	C1B-C2B-C3B	2.95	116.14	110.00
22	a	407	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
22	d	405	CLA	CMD-C2D-C1D	2.95	129.91	124.71
22	a	406	CLA	C7-C6-C5	-2.95	105.36	113.36
22	b	617	CLA	CHA-C4D-ND	2.94	138.65	132.50
22	c	505	CLA	C3D-C2D-C1D	-2.94	101.82	105.83
31	b	624	LHG	O7-C7-O9	-2.94	116.60	123.70
31	D	411	LHG	O4-P-O5	2.94	126.75	112.24
22	c	509	CLA	CHD-C4C-C3C	-2.93	120.53	124.84
22	C	502	CLA	O2D-CGD-CBD	2.93	116.48	111.27
22	c	511	CLA	C2A-C1A-CHA	-2.93	118.73	123.86
22	B	604	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
22	b	615	CLA	O2D-CGD-CBD	2.93	116.47	111.27
24	d	406	BCR	C34-C9-C8	2.93	122.69	118.08
22	b	606	CLA	C3C-C4C-NC	2.93	113.86	110.57
22	c	506	CLA	CHA-C4D-ND	2.93	138.62	132.50
22	b	620	CLA	O2A-CGA-CBA	2.92	121.08	111.91
28	m	101	LMT	O2B-C2B-C3B	-2.92	103.59	110.35
28	A	415	LMT	O4'-C4B-C5B	-2.92	102.04	109.30
22	B	602	CLA	C1D-CHD-C4C	-2.92	119.76	126.06
22	c	503	CLA	C1-C2-C3	-2.92	120.99	126.04
22	c	513	CLA	C1D-CHD-C4C	-2.92	119.76	126.06
22	c	512	CLA	CMC-C2C-C1C	2.92	129.48	125.04
22	b	612	CLA	CGD-CBD-CAD	-2.92	101.28	110.73
22	C	509	CLA	C4-C3-C5	2.92	120.18	115.27
32	C	521	HTG	C6-C5-C4	-2.92	106.17	113.00
28	M	101	LMT	C3'-C4'-C5'	-2.92	104.24	110.93
28	Z	101	LMT	O1'-C1'-C2'	2.92	112.86	108.30
22	b	615	CLA	CMC-C2C-C1C	2.92	129.48	125.04
31	F	103	LHG	O7-C7-O9	-2.92	116.66	123.70
32	B	624	HTG	C1-C2-C3	2.91	116.34	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	508	CLA	CMD-C2D-C1D	2.91	129.85	124.71
23	d	404	PHO	CMC-C2C-C3C	2.91	130.43	124.94
33	h	101	DGD	C3E-C4E-C5E	-2.91	105.05	110.24
31	b	624	LHG	O7-C7-C8	2.91	117.76	111.50
22	b	617	CLA	CMC-C2C-C1C	2.90	129.46	125.04
28	C	520	LMT	C6B-C5B-C4B	2.90	119.80	113.00
22	b	612	CLA	CMB-C2B-C3B	2.90	130.11	124.68
22	b	619	CLA	C3B-C4B-NB	2.90	112.96	109.21
22	C	511	CLA	CHD-C4C-C3C	-2.90	120.58	124.84
33	D	408	DGD	O1G-C1A-C2A	2.90	121.01	111.91
22	b	615	CLA	CHD-C4C-NC	2.90	128.77	124.20
38	h	102	RRX	C33-C5-C6	-2.90	121.27	124.53
25	A	410	PL9	C7-C8-C9	-2.90	121.97	126.79
22	c	512	CLA	CHD-C4C-C3C	-2.89	120.58	124.84
22	c	505	CLA	C3D-C4D-ND	2.89	114.92	110.24
22	b	606	CLA	C3B-C4B-NB	2.89	112.95	109.21
22	C	512	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	b	610	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	b	613	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
33	C	517	DGD	O6D-C1D-O3G	-2.89	103.14	109.97
22	b	620	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
28	a	401	LMT	O1B-C1B-C2B	2.89	115.58	108.10
33	h	101	DGD	C3G-O3G-C1D	-2.88	108.11	113.74
22	c	507	CLA	O2D-CGD-CBD	2.88	116.39	111.27
24	K	101	BCR	C24-C23-C22	-2.88	121.88	126.23
22	a	407	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
24	c	515	BCR	C11-C10-C9	-2.88	123.20	127.31
22	c	511	CLA	C3C-C4C-NC	2.87	113.79	110.57
22	B	602	CLA	CMD-C2D-C1D	2.87	129.78	124.71
22	d	403	CLA	CHA-C4D-ND	2.87	138.51	132.50
33	H	101	DGD	C2G-O2G-C1B	-2.87	110.72	117.79
24	T	101	BCR	C7-C8-C9	-2.87	121.90	126.23
22	C	504	CLA	C2A-C1A-CHA	-2.87	118.84	123.86
24	k	101	BCR	C7-C8-C9	-2.87	121.90	126.23
24	y	101	BCR	C32-C1-C6	2.87	114.95	110.30
22	b	618	CLA	C4D-C3D-CAD	2.87	111.48	108.10
22	C	508	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
25	a	411	PL9	C21-C19-C18	-2.87	115.31	121.12
38	h	102	RRX	C37-C22-C21	-2.87	118.91	122.92
23	A	407	PHO	C4C-NC-C1C	-2.87	101.21	107.09
22	D	405	CLA	CHD-C4C-C3C	-2.87	120.63	124.84
22	B	606	CLA	C4C-C3C-C2C	-2.87	102.72	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	411	PL9	C37-C38-C39	-2.86	120.76	127.66
22	b	612	CLA	C1D-CHD-C4C	-2.86	119.88	126.06
25	d	407	PL9	O1-C4-C3	-2.86	117.57	120.72
28	m	102	LMT	O2'-C2'-C3'	2.86	116.96	110.35
22	b	610	CLA	O1D-CGD-CBD	-2.86	118.63	124.48
22	d	403	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
22	B	615	CLA	C2A-C1A-CHA	-2.86	118.86	123.86
22	A	405	CLA	C1D-CHD-C4C	-2.86	119.90	126.06
22	b	615	CLA	CHA-C4D-ND	2.85	138.47	132.50
22	a	406	CLA	CMD-C2D-C1D	2.85	129.74	124.71
22	c	509	CLA	CHD-C4C-NC	2.85	128.69	124.20
22	D	405	CLA	CED-O2D-CGD	2.85	122.38	115.94
24	c	515	BCR	C24-C23-C22	-2.85	121.93	126.23
22	b	619	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
31	e	101	LHG	O8-C23-O10	-2.85	116.41	123.59
28	a	401	LMT	O2'-C2'-C3'	-2.85	103.77	110.35
31	B	621	LHG	O6-P-O5	-2.84	97.95	109.07
24	b	621	BCR	C23-C22-C21	-2.84	114.58	118.94
25	A	410	PL9	C31-C32-C33	2.84	121.22	111.88
22	b	608	CLA	C16-C15-C13	-2.84	106.74	115.92
24	b	621	BCR	C33-C5-C6	-2.84	121.34	124.53
22	C	508	CLA	CMD-C2D-C1D	2.84	129.71	124.71
40	V	201	HEC	CMC-C2C-C1C	-2.84	124.10	128.46
22	b	611	CLA	C3C-C4C-NC	2.84	113.75	110.57
22	a	409	CLA	C3D-C2D-C1D	-2.83	101.97	105.83
22	b	614	CLA	O2A-CGA-O1A	-2.83	116.45	123.59
22	d	405	CLA	C3B-C4B-NB	2.83	112.87	109.21
22	c	503	CLA	CAC-C3C-C4C	2.83	128.48	124.81
33	c	518	DGD	C3A-C2A-C1A	-2.83	103.34	113.62
22	B	609	CLA	C5-C3-C2	-2.83	115.40	121.12
22	d	403	CLA	O2D-CGD-CBD	2.83	116.29	111.27
24	y	101	BCR	C34-C9-C10	-2.82	118.97	122.92
25	d	407	PL9	C22-C23-C24	-2.82	120.86	127.66
32	d	413	HTG	C6-C5-C4	-2.82	106.40	113.00
22	c	502	CLA	C3B-C4B-NB	2.82	112.86	109.21
32	b	601	HTG	C2'-C1'-S1	-2.82	103.29	112.40
22	b	619	CLA	CHD-C4C-NC	2.82	128.65	124.20
22	b	619	CLA	C11-C10-C8	-2.82	106.81	115.92
24	D	406	BCR	C39-C30-C25	-2.82	105.73	110.30
22	B	607	CLA	C14-C13-C15	2.82	121.49	111.29
22	B	617	CLA	C4D-CHA-C1A	-2.82	117.82	121.25
37	f	101	HEM	CAD-C3D-C4D	2.81	129.57	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	507	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	b	619	CLA	CMD-C2D-C3D	2.81	134.07	127.61
23	A	407	PHO	CMC-C2C-C3C	2.81	130.24	124.94
26	d	412	LMG	O8-C28-C29	2.80	120.70	111.91
22	B	604	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	C	513	CLA	C2A-C1A-CHA	-2.80	118.97	123.86
24	C	514	BCR	C37-C22-C23	2.79	122.47	118.08
22	B	605	CLA	C3C-C4C-NC	2.79	113.70	110.57
22	C	510	CLA	CMD-C2D-C3D	2.79	134.03	127.61
22	c	507	CLA	CMC-C2C-C1C	2.79	129.28	125.04
22	c	507	CLA	C3B-C4B-NB	2.79	112.81	109.21
24	t	101	BCR	C37-C22-C23	2.78	122.46	118.08
22	c	510	CLA	C4-C3-C5	2.78	119.95	115.27
22	B	617	CLA	C3C-C4C-NC	2.78	113.69	110.57
22	C	511	CLA	CMC-C2C-C1C	2.78	129.28	125.04
24	c	516	BCR	C3-C4-C5	-2.78	109.11	114.08
32	V	202	HTG	C1-O5-C5	-2.78	107.45	112.58
22	c	502	CLA	CHA-C4D-ND	2.78	138.31	132.50
32	D	413	HTG	O2-C2-C1	2.78	115.37	110.27
26	c	520	LMG	O7-C10-O9	-2.78	116.99	123.70
26	C	519	LMG	C9-O8-C28	2.78	127.40	117.12
24	B	620	BCR	C29-C30-C25	2.78	114.75	110.48
24	c	516	BCR	C7-C8-C9	-2.78	122.04	126.23
22	B	614	CLA	CHD-C4C-NC	2.78	128.58	124.20
22	b	612	CLA	CHA-C4D-ND	2.78	138.31	132.50
22	B	608	CLA	C2A-C1A-CHA	-2.78	119.01	123.86
33	C	515	DGD	O6D-C5D-C6D	2.77	112.26	106.67
22	b	610	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
28	T	102	LMT	O5'-C5'-C6'	2.77	113.32	106.44
22	a	407	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
28	Z	101	LMT	C4B-C3B-C2B	2.77	115.65	110.82
32	b	627	HTG	C3-C4-C5	2.77	115.17	110.24
33	h	101	DGD	O2G-C1B-C2B	2.77	117.46	111.50
25	a	411	PL9	O2-C1-C2	-2.76	115.45	121.78
22	B	602	CLA	CHD-C4C-C3C	-2.76	120.78	124.84
31	F	103	LHG	O8-C23-O10	-2.76	116.62	123.59
22	d	402	CLA	CHA-C4D-ND	2.76	138.27	132.50
22	C	512	CLA	C1-C2-C3	-2.76	121.27	126.04
22	d	405	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	C	510	CLA	CHB-C4A-NA	2.76	128.32	124.51
22	c	507	CLA	C4A-NA-C1A	2.76	107.94	106.71
22	B	602	CLA	C3D-C2D-C1D	-2.75	102.07	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	626	LMT	O3'-C3'-C2'	-2.75	103.98	110.35
22	b	615	CLA	C3B-C4B-NB	2.75	112.77	109.21
22	c	506	CLA	CHD-C4C-NC	2.75	128.54	124.20
22	C	501	CLA	CMD-C2D-C1D	2.75	129.56	124.71
22	d	405	CLA	C2A-C1A-CHA	-2.75	119.06	123.86
22	B	603	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
22	C	512	CLA	C2A-C1A-CHA	-2.75	119.06	123.86
33	C	517	DGD	O1G-C1A-O1A	-2.74	116.67	123.59
22	C	509	CLA	CMD-C2D-C1D	2.74	129.54	124.71
25	d	407	PL9	C40-C39-C38	-2.74	116.64	123.68
24	t	101	BCR	C3-C4-C5	-2.74	109.18	114.08
22	c	505	CLA	C7-C6-C5	-2.74	105.92	113.36
22	c	511	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
22	B	603	CLA	O2A-CGA-CBA	2.74	120.50	111.91
22	b	606	CLA	O2A-CGA-O1A	-2.74	116.69	123.59
22	a	406	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
37	f	101	HEM	CBD-CAD-C3D	-2.74	105.03	112.63
22	a	409	CLA	CHD-C4C-NC	2.74	128.51	124.20
22	b	613	CLA	CBC-CAC-C3C	-2.74	104.89	112.43
28	A	415	LMT	O2'-C2'-C3'	2.73	116.67	110.35
22	b	615	CLA	C4A-NA-C1A	2.73	107.93	106.71
22	C	508	CLA	C4-C3-C5	2.73	119.86	115.27
22	C	509	CLA	CHA-C4D-ND	2.73	138.21	132.50
25	d	407	PL9	C10-C9-C11	2.73	119.86	115.27
33	c	518	DGD	O1G-C1A-O1A	-2.73	116.71	123.59
22	B	602	CLA	CMC-C2C-C1C	2.72	129.19	125.04
22	B	613	CLA	C3D-C2D-C1D	-2.72	102.11	105.83
22	b	616	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	c	515	BCR	C15-C14-C13	-2.72	123.43	127.31
22	C	509	CLA	C3C-C4C-NC	2.72	113.62	110.57
22	b	618	CLA	C3D-C4D-ND	2.72	114.63	110.24
32	D	413	HTG	C4-C3-C2	2.72	115.56	110.82
24	T	101	BCR	C8-C9-C10	-2.72	114.77	118.94
22	c	507	CLA	CHB-C4A-NA	2.72	128.27	124.51
24	B	619	BCR	C7-C8-C9	-2.72	122.13	126.23
22	c	506	CLA	C2A-C1A-CHA	-2.71	119.11	123.86
26	a	412	LMG	O7-C10-C11	2.71	117.35	111.50
28	t	102	LMT	O3'-C3'-C4'	2.71	116.62	110.35
22	b	612	CLA	C3B-C4B-NB	2.71	112.72	109.21
22	b	605	CLA	C3D-C4D-CHA	-2.71	106.52	112.72
22	b	610	CLA	CHA-C4D-ND	2.71	138.17	132.50
22	C	502	CLA	CAC-C3C-C2C	-2.71	122.89	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	504	CLA	CMB-C2B-C3B	2.71	129.75	124.68
22	c	509	CLA	C1D-ND-C4D	-2.71	104.41	106.33
33	D	408	DGD	C4D-C3D-C2D	2.71	115.55	110.82
22	B	615	CLA	O2D-CGD-CBD	2.71	116.08	111.27
24	D	406	BCR	C34-C9-C10	-2.71	119.13	122.92
22	c	511	CLA	C3D-C4D-ND	2.71	114.61	110.24
26	D	412	LMG	O8-C28-O10	-2.70	116.77	123.59
22	B	607	CLA	CHA-C4D-ND	2.70	138.16	132.50
22	B	611	CLA	O2D-CGD-CBD	2.70	116.07	111.27
22	b	609	CLA	CHA-C4D-ND	2.70	138.15	132.50
22	c	502	CLA	CHD-C4C-NC	2.70	128.46	124.20
22	c	510	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
22	b	608	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
22	B	617	CLA	C1D-CHD-C4C	-2.70	120.23	126.06
26	C	519	LMG	O8-C28-O10	-2.70	116.78	123.59
22	B	604	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
28	z	101	LMT	O5'-C1'-C2'	-2.70	104.63	110.35
32	B	629	HTG	C4-C3-C2	-2.70	106.11	110.82
22	A	404	CLA	CMD-C2D-C3D	2.70	133.82	127.61
22	C	509	CLA	CMC-C2C-C1C	2.70	129.15	125.04
22	C	511	CLA	C4D-C3D-CAD	2.70	111.28	108.10
26	B	622	LMG	C8-O7-C10	2.70	124.43	117.79
22	D	405	CLA	C4-C3-C5	2.70	119.81	115.27
22	B	612	CLA	CHD-C1D-ND	-2.70	121.98	124.45
22	b	613	CLA	C3C-C4C-NC	2.69	113.59	110.57
22	a	406	CLA	C1D-ND-C4D	-2.69	104.42	106.33
22	c	510	CLA	CHA-C4D-ND	2.69	138.13	132.50
22	d	402	CLA	CMC-C2C-C1C	2.69	129.14	125.04
22	b	613	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
28	m	102	LMT	C1'-O5'-C5'	2.69	118.97	113.69
25	A	410	PL9	C20-C19-C21	2.69	119.80	115.27
22	c	504	CLA	CED-O2D-CGD	2.69	122.02	115.94
24	t	101	BCR	C38-C26-C25	-2.69	121.51	124.53
22	C	509	CLA	CHD-C4C-NC	2.69	128.44	124.20
22	b	605	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
22	b	608	CLA	CAC-C3C-C2C	-2.69	122.93	127.53
33	h	101	DGD	O2D-C2D-C1D	-2.69	103.52	110.05
24	b	621	BCR	C15-C14-C13	-2.69	123.48	127.31
22	b	613	CLA	C3B-C4B-NB	2.69	112.68	109.21
24	K	101	BCR	C11-C10-C9	-2.68	123.48	127.31
32	c	541	HTG	O2-C2-C3	-2.68	104.15	110.35
22	c	513	CLA	CMB-C2B-C3B	2.68	129.70	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	623	LMT	C3'-C4'-C5'	2.68	117.07	110.93
33	c	518	DGD	O1G-C1A-C2A	2.68	120.32	111.91
28	B	623	LMT	O1B-C4'-C5'	-2.68	102.10	109.45
22	c	514	CLA	CHD-C4C-NC	2.68	128.43	124.20
26	C	518	LMG	O7-C10-C11	2.68	117.28	111.50
22	d	403	CLA	CMD-C2D-C3D	2.68	133.78	127.61
22	B	615	CLA	CHA-C4D-ND	2.68	138.10	132.50
22	c	504	CLA	C7-C6-C5	-2.68	106.08	113.36
24	k	101	BCR	C31-C1-C6	2.68	114.64	110.30
22	C	504	CLA	CHA-C4D-ND	2.68	138.10	132.50
22	b	614	CLA	CHD-C4C-NC	2.68	128.42	124.20
22	c	513	CLA	CMC-C2C-C1C	2.68	129.11	125.04
28	A	415	LMT	O3B-C3B-C4B	2.67	116.53	110.35
32	U	203	HTG	C1-O5-C5	2.67	117.51	112.58
22	b	616	CLA	C3D-C4D-ND	2.67	114.56	110.24
29	O	308	DMS	O-S-C2	2.67	120.18	106.54
22	B	613	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
26	c	521	LMG	O4-C4-C5	2.67	115.93	109.30
22	B	610	CLA	CMD-C2D-C3D	2.67	133.75	127.61
22	b	612	CLA	CMD-C2D-C3D	2.67	133.75	127.61
31	d	411	LHG	O7-C7-O9	-2.67	117.25	123.70
22	b	611	CLA	C3B-C4B-NB	2.67	112.66	109.21
22	c	503	CLA	CHD-C4C-NC	2.67	128.41	124.20
22	B	611	CLA	CMD-C2D-C1D	2.67	129.41	124.71
31	f	102	LHG	O7-C7-C8	2.66	117.24	111.50
24	c	516	BCR	C35-C13-C14	-2.66	119.19	122.92
22	c	508	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
22	b	605	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
22	B	613	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
22	b	620	CLA	C3B-C4B-NB	2.66	112.65	109.21
24	K	101	BCR	C29-C28-C27	-2.66	105.44	111.38
33	C	517	DGD	O3G-C3G-C2G	-2.66	104.49	110.90
23	A	407	PHO	OBD-CAD-CBD	-2.65	121.93	125.82
33	H	101	DGD	O2D-C2D-C1D	-2.65	103.61	110.05
24	B	620	BCR	C23-C24-C25	-2.65	119.76	127.20
22	A	406	CLA	CHA-C4D-ND	2.65	138.04	132.50
31	D	409	LHG	O4-P-O5	2.65	125.33	112.24
40	v	202	HEC	CMC-C2C-C3C	2.65	128.93	125.82
26	B	622	LMG	O7-C10-C11	2.65	117.21	111.50
22	A	406	CLA	C3D-C2D-C1D	-2.65	102.22	105.83
22	B	617	CLA	CHD-C4C-NC	2.65	128.37	124.20
22	b	616	CLA	O2D-CGD-CBD	2.64	115.97	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	620	CLA	CMD-C2D-C1D	2.64	129.37	124.71
22	D	405	CLA	O2A-C1-C2	-2.64	101.69	108.64
22	b	605	CLA	O2A-CGA-CBA	2.64	120.19	111.91
22	A	405	CLA	C3B-C4B-NB	2.64	112.62	109.21
22	B	615	CLA	CHC-C1C-NC	-2.64	120.20	124.20
26	C	518	LMG	O8-C9-C8	2.64	116.10	108.43
24	K	101	BCR	C34-C9-C8	2.63	122.23	118.08
22	c	512	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
22	b	607	CLA	CHA-C4D-ND	2.63	138.01	132.50
23	A	407	PHO	C1A-C2A-C3A	-2.63	100.33	102.84
22	b	613	CLA	C4A-NA-C1A	2.63	107.89	106.71
22	d	405	CLA	C1D-ND-C4D	-2.63	104.47	106.33
24	b	622	BCR	C3-C4-C5	-2.63	109.38	114.08
22	b	618	CLA	CHA-C4D-ND	2.63	138.00	132.50
22	B	604	CLA	C4A-NA-C1A	2.63	107.89	106.71
22	C	502	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
22	B	607	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	c	508	CLA	CHA-C4D-ND	2.62	137.98	132.50
22	b	618	CLA	CHD-C4C-NC	2.62	128.33	124.20
22	b	605	CLA	C1D-ND-C4D	-2.62	104.47	106.33
22	B	610	CLA	C4D-CHA-C1A	-2.62	118.06	121.25
29	B	632	DMS	O-S-C1	-2.62	93.19	106.54
22	b	609	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
22	b	606	CLA	C4D-C3D-CAD	2.62	111.18	108.10
22	c	507	CLA	CHA-C4D-ND	2.61	137.97	132.50
22	d	402	CLA	C3A-C2A-C1A	-2.61	97.42	101.34
28	T	102	LMT	C1'-O5'-C5'	-2.61	108.56	113.69
22	c	503	CLA	C1-O2A-CGA	2.61	123.30	116.44
22	b	606	CLA	CMC-C2C-C1C	2.61	129.02	125.04
22	b	617	CLA	CHD-C4C-NC	2.61	128.32	124.20
22	B	608	CLA	CHA-C4D-ND	2.61	137.96	132.50
22	d	403	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
22	A	408	CLA	CHD-C4C-NC	2.61	128.31	124.20
22	B	606	CLA	CHB-C4A-NA	2.61	128.12	124.51
33	H	101	DGD	O2E-C2E-C3E	-2.61	104.32	110.35
22	B	615	CLA	O2A-CGA-CBA	2.61	120.09	111.91
28	j	102	LMT	O5'-C5'-C6'	2.61	112.92	106.44
23	D	404	PHO	C4C-NC-C1C	-2.61	101.74	107.09
24	a	410	BCR	C11-C10-C9	-2.61	123.59	127.31
22	B	607	CLA	CAC-C3C-C4C	2.60	128.19	124.81
22	B	609	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
31	D	409	LHG	C6-O8-C23	2.60	126.75	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	618	CLA	C1-O2A-CGA	2.60	123.27	116.44
22	C	508	CLA	C4D-CHA-C1A	-2.60	118.08	121.25
24	t	101	BCR	C7-C8-C9	-2.60	122.31	126.23
24	B	618	BCR	C24-C23-C22	-2.60	122.31	126.23
22	B	611	CLA	C3B-C4B-NB	2.60	112.57	109.21
22	b	610	CLA	C3C-C4C-NC	2.60	113.48	110.57
22	b	620	CLA	C1-O2A-CGA	2.60	123.25	116.44
22	b	617	CLA	C1-C2-C3	-2.59	121.56	126.04
22	b	612	CLA	C5-C3-C2	-2.59	115.87	121.12
22	C	501	CLA	CHA-C4D-ND	2.59	137.92	132.50
22	C	510	CLA	C4D-CHA-C1A	-2.59	118.09	121.25
22	B	612	CLA	CMC-C2C-C1C	2.59	128.99	125.04
31	E	101	LHG	O8-C23-C24	2.59	120.04	111.91
22	B	615	CLA	C3B-C4B-NB	2.59	112.56	109.21
33	C	517	DGD	O2D-C2D-C3D	2.59	116.34	110.35
24	t	101	BCR	C7-C6-C5	-2.59	115.19	121.46
28	Z	101	LMT	C1'-O5'-C5'	2.59	118.77	113.69
32	o	301	HTG	O2-C2-C1	2.59	115.02	110.27
22	C	501	CLA	C1-O2A-CGA	2.59	123.23	116.44
22	c	507	CLA	C3C-C4C-NC	2.59	113.47	110.57
28	c	522	LMT	O5'-C5'-C4'	2.58	115.20	109.75
23	a	408	PHO	CMB-C2B-C3B	2.58	129.51	124.68
22	B	610	CLA	C3C-C4C-NC	2.58	113.47	110.57
28	m	101	LMT	C1B-O1B-C4'	2.58	124.36	117.96
22	B	610	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	b	612	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
28	M	101	LMT	C1B-O5B-C5B	2.58	118.75	113.69
33	H	101	DGD	C6D-C5D-C4D	2.58	117.48	112.09
22	b	605	CLA	C4-C3-C2	-2.58	117.06	123.68
22	C	507	CLA	CMC-C2C-C3C	2.58	133.12	126.12
22	b	605	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
22	B	605	CLA	CMC-C2C-C1C	2.58	128.96	125.04
22	B	607	CLA	C3B-C4B-NB	2.57	112.54	109.21
22	d	405	CLA	CHA-C4D-ND	2.57	137.88	132.50
22	c	509	CLA	CMD-C2D-C1D	2.57	129.24	124.71
28	Z	101	LMT	C2'-C3'-C4'	2.57	115.55	109.68
24	d	406	BCR	C10-C11-C12	-2.57	115.20	123.22
22	d	405	CLA	O2A-C1-C2	-2.57	101.88	108.64
22	B	602	CLA	O2A-C1-C2	2.57	115.39	108.64
40	v	202	HEC	C1D-C2D-C3D	-2.57	105.21	107.00
28	T	102	LMT	C1-O1'-C1'	2.57	118.09	113.84
22	B	606	CLA	O2A-CGA-O1A	-2.56	117.12	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	T	101	BCR	C15-C14-C13	-2.56	123.65	127.31
26	C	518	LMG	O1-C7-C8	-2.56	104.72	110.90
22	c	503	CLA	C3B-C4B-NB	2.56	112.52	109.21
28	J	102	LMT	O1'-C1'-C2'	2.56	112.30	108.30
28	Z	101	LMT	O1B-C4'-C5'	2.56	116.46	109.45
28	m	101	LMT	C3'-C4'-C5'	-2.56	105.06	110.93
32	b	640	HTG	C1'-S1-C1	2.56	104.88	100.09
22	b	614	CLA	C3C-C4C-NC	2.56	113.44	110.57
22	c	505	CLA	CED-O2D-CGD	2.56	121.72	115.94
22	a	407	CLA	C3D-C4D-ND	2.56	114.37	110.24
32	D	413	HTG	O5-C5-C6	2.55	112.79	106.44
33	c	519	DGD	O1G-C1A-O1A	-2.55	117.15	123.59
22	b	611	CLA	C1D-ND-C4D	-2.55	104.52	106.33
28	C	520	LMT	O1'-C1'-C2'	2.55	112.28	108.30
22	c	505	CLA	CBC-CAC-C3C	-2.55	105.40	112.43
22	B	610	CLA	C3D-C4D-ND	2.55	114.36	110.24
22	c	505	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
22	C	501	CLA	CMB-C2B-C3B	2.55	129.45	124.68
22	C	504	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	C	504	CLA	CHD-C4C-C3C	-2.55	121.10	124.84
24	t	101	BCR	C19-C18-C17	-2.55	115.03	118.94
28	a	401	LMT	O1'-C1'-C2'	2.55	112.28	108.30
24	d	406	BCR	C35-C13-C12	2.54	122.09	118.08
22	C	502	CLA	C1D-CHD-C4C	-2.54	120.57	126.06
28	Z	101	LMT	O5B-C1B-C2B	-2.54	104.96	110.35
22	b	607	CLA	CHD-C4C-NC	2.54	128.21	124.20
33	H	101	DGD	O5E-C6E-C5E	-2.54	102.57	111.29
24	c	515	BCR	C35-C13-C12	2.54	122.08	118.08
22	b	617	CLA	C3B-C4B-NB	2.54	112.50	109.21
22	B	608	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
22	a	406	CLA	C3B-C4B-NB	2.54	112.49	109.21
28	A	415	LMT	O5B-C1B-C2B	2.54	115.72	110.35
24	T	101	BCR	C19-C18-C17	-2.54	115.05	118.94
22	b	607	CLA	C1D-CHD-C4C	-2.54	120.58	126.06
28	C	520	LMT	C1B-C2B-C3B	2.54	115.28	110.00
22	C	503	CLA	C3D-C2D-C1D	-2.53	102.37	105.83
22	c	509	CLA	CHB-C4A-NA	2.53	128.02	124.51
32	U	203	HTG	O5-C5-C6	2.53	112.74	106.44
22	a	406	CLA	C1D-CHD-C4C	-2.53	120.59	126.06
22	d	403	CLA	C4D-CHA-C1A	-2.53	118.17	121.25
22	c	513	CLA	CHD-C4C-NC	2.53	128.19	124.20
31	f	102	LHG	O4-P-O5	2.53	124.76	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	502	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
22	c	514	CLA	C3B-C4B-NB	2.53	112.48	109.21
22	C	502	CLA	C16-C17-C18	-2.53	104.06	115.98
23	d	404	PHO	CMB-C2B-C3B	2.53	129.41	124.68
22	b	610	CLA	C4C-C3C-C2C	-2.53	103.22	106.90
22	B	604	CLA	CHC-C1C-NC	-2.53	120.37	124.20
22	b	615	CLA	CGD-CBD-CAD	-2.53	102.55	110.73
22	d	402	CLA	C4A-NA-C1A	2.52	107.84	106.71
22	b	606	CLA	C1D-ND-C4D	-2.52	104.54	106.33
22	B	610	CLA	CHD-C4C-NC	2.52	128.18	124.20
28	A	415	LMT	O5'-C5'-C6'	2.52	112.70	106.44
22	B	616	CLA	C3B-C4B-NB	2.52	112.47	109.21
25	D	407	PL9	C36-C34-C33	-2.52	116.02	121.12
22	B	604	CLA	CHA-C4D-ND	2.52	137.77	132.50
22	c	503	CLA	CMD-C2D-C3D	2.52	133.41	127.61
33	D	408	DGD	O1G-C1G-C2G	2.52	115.77	108.43
22	b	610	CLA	C1D-CHD-C4C	-2.52	120.62	126.06
23	A	407	PHO	C3D-CAD-CBD	2.52	110.92	107.61
22	b	619	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
22	C	511	CLA	C1D-CHD-C4C	-2.52	120.63	126.06
29	c	528	DMS	O-S-C2	-2.52	93.70	106.54
38	H	102	RRX	C34-C9-C8	2.52	122.04	118.08
22	c	508	CLA	C1-O2A-CGA	2.52	123.04	116.44
33	h	101	DGD	O6D-C1D-O3G	2.52	115.93	109.97
22	C	513	CLA	C5-C3-C2	-2.51	116.03	121.12
24	t	101	BCR	C1-C6-C7	2.51	122.88	115.78
32	b	627	HTG	O2-C2-C3	-2.51	104.54	110.35
22	A	405	CLA	O2D-CGD-CBD	2.51	115.72	111.27
24	y	101	BCR	C15-C14-C13	-2.51	123.73	127.31
28	T	102	LMT	O5'-C5'-C4'	-2.50	105.14	109.69
28	t	102	LMT	O5'-C1'-C2'	2.50	115.65	110.35
22	B	604	CLA	C4-C3-C5	2.50	119.48	115.27
28	z	101	LMT	O1'-C1'-C2'	2.50	112.21	108.30
26	C	519	LMG	O8-C9-C8	2.50	115.72	108.43
32	o	301	HTG	O4-C4-C5	2.50	115.51	109.30
22	b	608	CLA	C1D-ND-C4D	-2.50	104.56	106.33
24	Y	101	BCR	C8-C9-C10	-2.50	115.10	118.94
22	C	501	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
37	f	101	HEM	C4D-C3D-C2D	-2.50	103.25	106.90
24	B	620	BCR	C2-C3-C4	-2.50	105.80	111.38
24	K	101	BCR	C8-C7-C6	-2.50	120.19	127.20
22	c	514	CLA	C4C-C3C-C2C	-2.50	103.26	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	613	CLA	CAC-C3C-C2C	-2.49	123.26	127.53
22	b	616	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
22	b	607	CLA	C3D-C2D-C1D	-2.49	102.44	105.83
22	b	618	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
24	A	409	BCR	C33-C5-C4	2.49	118.39	113.62
22	a	406	CLA	CHA-C4D-ND	2.49	137.70	132.50
22	D	405	CLA	CHD-C1D-ND	-2.48	122.17	124.45
22	d	405	CLA	C3D-C2D-C1D	-2.48	102.45	105.83
22	b	615	CLA	C1D-CHD-C4C	-2.48	120.71	126.06
22	c	511	CLA	CAA-CBA-CGA	-2.48	106.01	113.25
22	c	511	CLA	CHD-C4C-NC	2.48	128.11	124.20
22	A	406	CLA	C6-C5-C3	-2.48	106.96	113.45
22	B	614	CLA	CAA-CBA-CGA	-2.48	106.02	113.25
22	d	402	CLA	C1-C2-C3	-2.48	121.76	126.04
37	f	101	HEM	CMA-C3A-C4A	-2.48	124.66	128.46
22	C	503	CLA	CHD-C1D-ND	-2.48	122.18	124.45
22	c	503	CLA	CMB-C2B-C3B	2.47	129.31	124.68
22	d	402	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
22	c	513	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	y	101	BCR	C15-C16-C17	-2.47	118.41	123.47
33	C	515	DGD	C6D-C5D-C4D	2.47	117.25	112.09
22	b	606	CLA	CMD-C2D-C3D	2.47	133.30	127.61
22	a	409	CLA	CHA-C4D-ND	2.47	137.67	132.50
32	B	642	HTG	O5-C5-C6	2.47	112.58	106.44
22	C	507	CLA	CMB-C2B-C3B	2.47	129.30	124.68
24	y	101	BCR	C10-C11-C12	-2.47	115.51	123.22
22	c	503	CLA	C3D-C4D-CHA	-2.47	107.08	112.72
22	B	605	CLA	O2A-C1-C2	2.47	115.12	108.64
22	a	407	CLA	CED-O2D-CGD	2.47	121.52	115.94
22	c	504	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
23	D	404	PHO	CMD-C2D-C3D	2.47	129.29	124.68
22	b	613	CLA	CMB-C2B-C3B	2.46	129.29	124.68
22	b	607	CLA	O1D-CGD-CBD	-2.46	119.44	124.48
22	C	507	CLA	C2D-C1D-ND	2.46	111.92	110.10
31	B	621	LHG	C10-C9-C8	-2.46	104.34	113.19
26	b	625	LMG	O8-C9-C8	2.46	115.60	108.43
38	H	102	RRX	C37-C22-C21	-2.46	119.47	122.92
22	B	609	CLA	C7-C6-C5	-2.46	106.67	113.36
25	a	411	PL9	C42-C43-C44	-2.46	121.73	127.66
40	V	201	HEC	O2D-CGD-CBD	2.46	121.94	114.03
25	d	407	PL9	C36-C37-C38	-2.46	103.79	111.88
33	c	518	DGD	O6E-C5E-C6E	2.46	112.55	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	511	CLA	CMD-C2D-C1D	2.46	129.04	124.71
22	b	616	CLA	O2A-CGA-CBA	2.46	119.62	111.91
24	T	101	BCR	C36-C18-C19	2.46	121.95	118.08
22	C	501	CLA	C3C-C4C-NC	2.45	113.32	110.57
25	a	411	PL9	C8-C7-C3	2.45	118.91	111.98
40	V	201	HEC	CMB-C2B-C3B	2.45	128.70	125.82
24	c	516	BCR	C35-C13-C12	2.45	121.94	118.08
38	h	102	RRX	C24-C23-C22	-2.45	122.53	126.23
32	B	642	HTG	C6-C5-C4	-2.45	107.26	113.00
22	d	405	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	B	615	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
24	b	623	BCR	C16-C17-C18	-2.45	123.81	127.31
22	c	511	CLA	CED-O2D-CGD	2.45	121.47	115.94
22	B	605	CLA	CAA-C2A-C3A	-2.45	106.08	112.78
22	A	404	CLA	CMB-C2B-C3B	2.45	129.26	124.68
22	c	506	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
22	b	612	CLA	CHC-C1C-C2C	-2.45	119.96	126.72
22	C	508	CLA	C5-C3-C2	-2.44	116.17	121.12
33	C	515	DGD	O2G-C1B-C2B	2.44	116.77	111.50
22	b	611	CLA	CGD-CBD-CAD	-2.44	102.82	110.73
37	F	101	HEM	C4B-CHC-C1C	2.44	125.78	122.56
22	c	507	CLA	C1D-CHD-C4C	-2.44	120.79	126.06
32	U	203	HTG	C3-C4-C5	-2.44	105.88	110.24
22	B	614	CLA	O2A-CGA-CBA	2.44	119.57	111.91
22	b	612	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
33	d	408	DGD	C1G-O1G-C1A	2.44	126.15	117.12
22	B	613	CLA	C1-O2A-CGA	2.44	122.84	116.44
22	C	512	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
22	C	502	CLA	CHB-C4A-NA	2.44	127.88	124.51
33	c	518	DGD	O2G-C1B-C2B	2.44	116.75	111.50
24	b	622	BCR	C40-C30-C25	-2.43	106.35	110.30
22	b	606	CLA	C4C-C3C-C2C	-2.43	103.35	106.90
28	a	401	LMT	C1B-O1B-C4'	2.43	123.98	117.96
22	d	402	CLA	CMB-C2B-C3B	2.43	129.23	124.68
22	B	605	CLA	CGD-CBD-CAD	-2.43	102.86	110.73
26	c	521	LMG	O1-C7-C8	2.43	116.76	110.90
22	c	506	CLA	O2A-CGA-CBA	2.43	119.53	111.91
24	B	619	BCR	C2-C1-C6	2.43	114.22	110.48
22	C	504	CLA	CED-O2D-CGD	2.43	121.43	115.94
26	C	519	LMG	O3-C3-C4	-2.42	104.74	110.35
22	d	405	CLA	C3C-C4C-NC	2.42	113.29	110.57
22	A	408	CLA	C3D-C4D-ND	2.42	114.16	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	508	CLA	C1D-ND-C4D	-2.42	104.61	106.33
22	d	405	CLA	CMC-C2C-C1C	2.42	128.73	125.04
22	B	604	CLA	C3D-C4D-ND	2.42	114.15	110.24
33	D	408	DGD	C1G-O1G-C1A	2.42	126.07	117.12
24	B	618	BCR	C37-C22-C23	2.42	121.88	118.08
22	B	603	CLA	C16-C15-C13	-2.42	108.11	115.92
22	D	405	CLA	C3D-C2D-C1D	-2.42	102.53	105.83
24	b	623	BCR	C38-C26-C25	-2.41	121.82	124.53
22	a	406	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
38	H	102	RRX	C15-C16-C17	-2.41	118.53	123.47
22	B	605	CLA	C1D-CHD-C4C	-2.41	120.86	126.06
22	B	617	CLA	CHB-C4A-NA	2.41	127.85	124.51
32	v	208	HTG	C1-C2-C3	-2.41	105.83	110.59
22	C	512	CLA	C3D-C4D-CHA	-2.41	107.21	112.72
22	B	605	CLA	C4C-C3C-C2C	-2.41	103.39	106.90
28	M	102	LMT	C6'-C5'-C4'	2.41	118.64	113.00
22	C	506	CLA	OBD-CAD-C3D	-2.41	122.73	128.52
22	c	511	CLA	O2D-CGD-CBD	2.41	115.54	111.27
32	U	203	HTG	O3-C3-C2	-2.41	104.79	110.35
22	c	506	CLA	CAA-C2A-C1A	2.40	119.85	111.97
33	h	101	DGD	C1D-O6D-C5D	2.40	118.41	113.69
22	C	511	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
22	A	406	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
24	B	620	BCR	C8-C7-C6	-2.40	120.46	127.20
22	C	511	CLA	C3D-C4D-CHA	-2.40	107.23	112.72
22	B	617	CLA	CMD-C2D-C1D	2.40	128.94	124.71
22	c	514	CLA	C3D-C4D-CHA	-2.40	107.23	112.72
26	c	521	LMG	O8-C9-C8	2.40	115.42	108.43
22	C	502	CLA	C1-C2-C3	-2.40	121.89	126.04
22	B	614	CLA	C1D-ND-C4D	-2.40	104.63	106.33
22	B	603	CLA	C3D-C2D-C1D	-2.40	102.56	105.83
22	b	612	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	B	615	CLA	C1D-ND-C4D	-2.40	104.63	106.33
22	b	620	CLA	OBD-CAD-C3D	-2.40	122.75	128.52
22	c	506	CLA	C1D-CHD-C4C	-2.40	120.89	126.06
22	c	514	CLA	O2A-CGA-CBA	2.40	119.42	111.91
22	B	605	CLA	C7-C6-C5	-2.39	106.86	113.36
22	b	611	CLA	C1-O2A-CGA	2.39	122.72	116.44
38	H	102	RRX	C40-C30-C25	-2.39	106.42	110.30
22	A	406	CLA	CHC-C1C-C2C	-2.39	120.10	126.72
22	C	503	CLA	C3C-C4C-NC	2.39	113.25	110.57
24	c	515	BCR	C3-C4-C5	-2.39	109.81	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	514	CLA	C4-C3-C5	2.39	119.29	115.27
24	b	623	BCR	C35-C13-C14	-2.39	119.57	122.92
32	O	302	HTG	C1-O5-C5	2.39	116.99	112.58
28	F	102	LMT	O5'-C5'-C4'	-2.39	105.36	109.69
22	A	405	CLA	CAC-C3C-C2C	-2.39	123.44	127.53
22	c	511	CLA	CHD-C1D-C2D	-2.39	120.47	125.48
22	C	513	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
22	a	406	CLA	C4A-NA-C1A	2.39	107.78	106.71
32	C	521	HTG	O5-C5-C6	2.39	112.37	106.44
22	D	403	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
32	C	535	HTG	C1-S1-C1'	2.38	108.59	100.40
26	C	518	LMG	O5-C6-C5	-2.38	103.12	111.29
22	c	512	CLA	O2A-CGA-CBA	2.38	119.38	111.91
22	C	509	CLA	C11-C12-C13	-2.38	108.23	115.92
28	F	102	LMT	O1B-C4'-C5'	2.37	115.19	109.30
22	A	405	CLA	C3A-C2A-C1A	-2.37	97.78	101.34
24	B	618	BCR	C7-C8-C9	-2.37	122.65	126.23
22	b	619	CLA	CED-O2D-CGD	2.37	121.31	115.94
22	C	509	CLA	C4A-NA-C1A	2.37	107.77	106.71
22	C	512	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
22	C	512	CLA	C1D-ND-C4D	-2.37	104.65	106.33
23	a	408	PHO	O2D-CGD-CBD	2.37	114.00	111.00
22	d	403	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
22	a	406	CLA	C4C-C3C-C2C	-2.37	103.45	106.90
24	t	101	BCR	C8-C9-C10	-2.37	115.31	118.94
22	c	506	CLA	C1D-ND-C4D	-2.36	104.66	106.33
24	D	406	BCR	C10-C11-C12	-2.36	115.84	123.22
31	d	410	LHG	C32-C31-C30	-2.36	102.42	114.42
25	A	410	PL9	C37-C38-C39	-2.36	121.97	127.66
22	b	618	CLA	C3D-C4D-CHA	-2.36	107.32	112.72
22	B	611	CLA	C17-C16-C15	2.36	124.09	113.24
22	A	408	CLA	C3D-C2D-C1D	-2.36	102.61	105.83
24	B	620	BCR	C38-C26-C25	-2.36	121.88	124.53
22	b	614	CLA	O2D-CGD-CBD	2.36	115.46	111.27
22	C	504	CLA	CHD-C4C-NC	2.36	127.92	124.20
22	c	503	CLA	C1D-ND-C4D	-2.36	104.66	106.33
22	b	614	CLA	C14-C13-C15	-2.36	102.76	111.29
22	b	614	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
31	f	102	LHG	C6-O8-C23	2.35	125.83	117.12
33	c	519	DGD	O6E-C5E-C6E	2.35	112.28	106.44
24	t	101	BCR	C23-C24-C25	-2.35	120.61	127.20
22	b	618	CLA	O2A-CGA-O1A	-2.35	117.67	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	d	405	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
37	f	101	HEM	CMA-C3A-C2A	2.35	129.37	124.94
22	c	513	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
22	C	505	CLA	CHA-C4D-ND	2.35	137.41	132.50
23	a	408	PHO	C4C-NC-C1C	-2.34	102.28	107.09
22	C	508	CLA	C1D-CHD-C4C	-2.34	121.00	126.06
28	a	401	LMT	C1B-C2B-C3B	2.34	114.88	110.00
22	B	612	CLA	C3D-C4D-CHA	-2.34	107.37	112.72
22	B	614	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
24	y	101	BCR	C3-C4-C5	-2.34	109.90	114.08
28	J	102	LMT	O2'-C2'-C3'	-2.34	104.94	110.35
33	C	516	DGD	O1G-C1A-O1A	-2.34	117.69	123.59
22	c	504	CLA	OBD-CAD-C3D	-2.34	122.89	128.52
28	z	101	LMT	O1B-C1B-O5B	2.34	117.21	110.67
22	C	505	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
33	d	408	DGD	O1G-C1A-C2A	2.34	119.24	111.91
38	h	102	RRX	C34-C9-C8	2.34	121.76	118.08
37	F	101	HEM	C3C-C4C-NC	-2.34	106.53	110.94
22	b	614	CLA	C1D-CHD-C4C	-2.33	121.02	126.06
32	U	203	HTG	O4-C4-C5	2.33	115.09	109.30
22	B	606	CLA	CHA-C4D-ND	2.33	137.38	132.50
33	c	517	DGD	C4D-C3D-C2D	-2.33	106.75	110.82
24	t	101	BCR	C15-C14-C13	-2.33	123.99	127.31
22	C	510	CLA	C3B-C4B-NB	2.33	112.22	109.21
22	C	509	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
22	c	502	CLA	C3D-C4D-ND	2.33	114.00	110.24
22	B	617	CLA	CHC-C1C-C2C	-2.33	120.29	126.72
22	b	607	CLA	CMD-C2D-C1D	2.32	128.81	124.71
28	A	415	LMT	O2'-C2'-C1'	2.32	115.69	110.05
22	B	612	CLA	CMD-C2D-C1D	2.32	128.80	124.71
22	c	504	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
24	c	516	BCR	C39-C30-C25	-2.32	106.53	110.30
24	y	101	BCR	C16-C15-C14	-2.32	118.72	123.47
22	a	406	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
26	C	519	LMG	O3-C3-C2	2.32	115.71	110.35
22	c	512	CLA	C4-C3-C5	2.32	119.17	115.27
22	d	405	CLA	C4-C3-C5	2.32	119.17	115.27
22	A	408	CLA	C5-C3-C2	-2.32	116.43	121.12
22	a	407	CLA	C3B-C4B-NB	2.32	112.20	109.21
22	c	510	CLA	C3D-C4D-ND	2.32	113.98	110.24
22	c	510	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
22	c	502	CLA	CHC-C1C-NC	-2.32	120.69	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	608	CLA	CMA-C3A-C4A	2.32	118.00	111.77
22	d	402	CLA	O2D-CGD-CBD	2.31	115.38	111.27
22	D	405	CLA	CHA-C4D-ND	2.31	137.34	132.50
32	o	301	HTG	C1-C2-C3	2.31	115.16	110.59
24	K	101	BCR	C34-C9-C10	-2.31	119.68	122.92
22	b	618	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
22	c	513	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	B	607	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
22	A	408	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
32	c	541	HTG	O5-C1-S1	2.31	115.34	109.82
32	B	642	HTG	C1'-S1-C1	2.31	104.41	100.09
22	A	404	CLA	C3D-C4D-CHA	-2.31	107.44	112.72
28	F	102	LMT	C6'-C5'-C4'	2.31	118.41	113.00
22	C	512	CLA	OBD-CAD-C3D	-2.31	122.97	128.52
22	b	606	CLA	C3D-C4D-CHA	-2.31	107.45	112.72
33	d	408	DGD	O6D-C5D-C6D	2.31	111.68	106.70
22	A	404	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
22	a	406	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
22	b	618	CLA	CMB-C2B-C1B	2.30	132.00	128.46
33	C	515	DGD	O5D-C1E-C2E	-2.30	104.71	108.30
22	b	617	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
25	A	410	PL9	C50-C49-C48	-2.30	116.00	122.65
22	B	611	CLA	CHD-C1D-ND	-2.30	122.34	124.45
24	b	621	BCR	C8-C9-C10	-2.30	115.41	118.94
33	c	519	DGD	C3G-O3G-C1D	2.30	118.23	113.74
22	b	610	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
24	b	623	BCR	C39-C30-C25	-2.30	106.58	110.30
22	B	611	CLA	O2A-CGA-CBA	2.29	119.11	111.91
22	b	617	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	c	515	BCR	C39-C30-C25	-2.29	106.58	110.30
22	c	508	CLA	C5-C3-C2	-2.29	116.48	121.12
22	c	513	CLA	C1-C2-C3	-2.29	122.08	126.04
25	a	411	PL9	C15-C14-C16	2.29	119.12	115.27
31	d	410	LHG	O7-C7-O9	-2.29	118.17	123.70
22	b	614	CLA	C3B-C4B-NB	2.29	112.17	109.21
26	c	521	LMG	O8-C28-C29	2.29	119.09	111.91
33	c	518	DGD	C1E-O6E-C5E	2.29	118.18	113.69
22	b	607	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
22	B	615	CLA	C3C-C4C-NC	2.29	113.14	110.57
22	D	405	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
40	v	202	HEC	CBA-CAA-C2A	-2.29	108.75	112.60
24	A	409	BCR	C24-C23-C22	-2.29	122.78	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	t	101	BCR	C29-C28-C27	-2.29	106.27	111.38
22	C	506	CLA	C1D-ND-C4D	-2.28	104.71	106.33
28	m	102	LMT	O1B-C4'-C5'	2.28	114.97	109.30
22	B	607	CLA	C4-C3-C5	2.28	119.11	115.27
22	c	505	CLA	C4-C3-C5	2.28	119.11	115.27
22	B	604	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
22	b	615	CLA	C7-C6-C5	-2.28	107.16	113.36
24	D	406	BCR	C28-C27-C26	-2.28	110.00	114.08
22	C	505	CLA	CMC-C2C-C1C	2.28	128.51	125.04
23	D	404	PHO	CBA-CAA-C2A	-2.28	107.16	113.81
24	B	618	BCR	C34-C9-C10	-2.28	119.73	122.92
22	b	608	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
22	C	513	CLA	CHB-C4A-NA	2.27	127.66	124.51
22	C	501	CLA	C1D-CHD-C4C	-2.27	121.15	126.06
31	D	410	LHG	O2-C2-C3	-2.27	101.58	109.56
22	A	406	CLA	C4-C3-C5	2.27	119.09	115.27
28	A	415	LMT	O6'-C6'-C5'	2.27	119.09	111.29
24	t	101	BCR	C24-C23-C22	-2.27	122.80	126.23
25	A	410	PL9	C25-C24-C26	2.27	119.09	115.27
22	b	606	CLA	CHD-C4C-NC	2.27	127.78	124.20
22	d	405	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
24	t	101	BCR	C15-C16-C17	-2.27	118.83	123.47
38	H	102	RRX	C16-C15-C14	-2.27	118.83	123.47
22	b	615	CLA	C3C-C4C-NC	2.27	113.11	110.57
22	b	617	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
22	b	612	CLA	C4-C3-C5	2.27	119.08	115.27
24	Y	101	BCR	C24-C23-C22	-2.26	122.81	126.23
22	a	407	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	a	406	CLA	C3C-C4C-NC	2.26	113.11	110.57
22	b	612	CLA	C3C-C4C-NC	2.26	113.11	110.57
26	D	412	LMG	C1-O6-C5	2.26	118.13	113.69
22	b	606	CLA	C1-O2A-CGA	2.26	122.38	116.44
22	c	507	CLA	C4C-C3C-C2C	-2.26	103.60	106.90
22	B	605	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	Y	101	BCR	C36-C18-C19	2.26	121.64	118.08
28	t	102	LMT	O2'-C2'-C1'	2.26	115.54	110.05
22	c	505	CLA	C4D-C3D-CAD	2.26	110.76	108.10
24	b	622	BCR	C8-C7-C6	-2.26	120.85	127.20
38	h	102	RRX	C16-C17-C18	-2.26	124.08	127.31
33	d	408	DGD	C2G-O2G-C1B	2.26	123.36	117.79
22	b	607	CLA	C1-O2A-CGA	2.26	122.37	116.44
28	m	101	LMT	O5'-C1'-O1'	-2.26	104.62	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	521	LMG	C4-C3-C2	2.26	114.77	110.82
22	c	510	CLA	C4D-C3D-CAD	2.26	110.76	108.10
25	A	410	PL9	C22-C23-C24	-2.26	122.22	127.66
22	B	610	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
22	B	602	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
28	C	520	LMT	O4'-C4B-C5B	2.25	114.89	109.30
22	B	616	CLA	C1-O2A-CGA	2.25	122.36	116.44
22	B	613	CLA	C3A-C2A-C1A	2.25	104.71	101.34
22	B	615	CLA	C4-C3-C5	2.25	119.06	115.27
22	B	609	CLA	C1D-CHD-C4C	-2.25	121.20	126.06
22	B	616	CLA	C11-C10-C8	-2.25	108.64	115.92
22	b	605	CLA	CHD-C1D-ND	-2.25	122.39	124.45
22	c	511	CLA	C1-O2A-CGA	2.25	122.35	116.44
33	h	101	DGD	C3G-C2G-C1G	2.25	117.11	111.79
22	B	616	CLA	CMC-C2C-C1C	2.25	128.47	125.04
22	B	608	CLA	C1D-ND-C4D	-2.25	104.74	106.33
22	B	608	CLA	CHC-C1C-NC	-2.25	120.79	124.20
24	Y	101	BCR	C19-C18-C17	-2.25	115.49	118.94
22	b	611	CLA	C1D-CHD-C4C	-2.25	121.21	126.06
22	C	501	CLA	CHD-C4C-NC	2.24	127.74	124.20
24	Y	101	BCR	C39-C30-C25	-2.24	106.66	110.30
22	B	617	CLA	C3B-C4B-NB	2.24	112.11	109.21
22	D	405	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
26	A	411	LMG	O6-C1-C2	-2.24	105.60	110.35
22	B	602	CLA	C1D-ND-C4D	-2.24	104.74	106.33
22	B	612	CLA	C3B-C4B-NB	2.24	112.10	109.21
23	D	404	PHO	C1-C2-C3	-2.24	122.17	126.04
28	M	101	LMT	C1-O1'-C1'	2.24	117.55	113.84
32	c	523	HTG	O5-C1-C2	-2.24	107.50	110.31
26	C	518	LMG	O8-C28-O10	-2.24	117.95	123.59
24	y	101	BCR	C2-C3-C4	-2.24	106.38	111.38
22	b	610	CLA	O2A-CGA-CBA	2.24	118.92	111.91
31	D	409	LHG	O7-C7-O9	-2.23	118.30	123.70
22	c	502	CLA	C3C-C4C-NC	2.23	113.08	110.57
22	b	611	CLA	CBC-CAC-C3C	-2.23	106.27	112.43
22	C	510	CLA	O2A-CGA-CBA	2.23	118.92	111.91
22	B	602	CLA	C3D-C4D-CHA	-2.23	107.61	112.72
22	B	613	CLA	CMB-C2B-C3B	2.23	128.85	124.68
26	A	411	LMG	O4-C4-C5	2.23	114.84	109.30
28	A	415	LMT	O5B-C5B-C6B	2.23	111.98	106.44
22	C	505	CLA	C1-O2A-CGA	2.23	122.30	116.44
24	b	623	BCR	C20-C21-C22	2.23	130.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	C1-C2-C3	-2.23	122.19	126.04
32	b	640	HTG	O3-C3-C4	-2.23	105.19	110.35
22	B	614	CLA	C4C-C3C-C2C	-2.23	103.65	106.90
22	b	605	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
25	A	410	PL9	C15-C14-C16	2.23	119.02	115.27
31	b	624	LHG	O8-C6-C5	2.23	114.92	108.43
22	C	508	CLA	CHB-C4A-NA	2.23	127.59	124.51
32	d	413	HTG	C3-C4-C5	2.23	114.21	110.24
31	f	102	LHG	O7-C7-O9	-2.23	118.32	123.70
22	c	503	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
22	C	512	CLA	O2A-C1-C2	-2.23	102.78	108.64
22	D	405	CLA	C3B-C4B-NB	2.23	112.09	109.21
38	h	102	RRX	C11-C10-C9	-2.22	124.14	127.31
22	c	511	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
22	b	618	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
22	b	611	CLA	CHC-C1C-C2C	-2.22	120.57	126.72
26	C	518	LMG	O7-C10-O9	-2.22	118.33	123.70
32	U	203	HTG	O3-C3-C4	2.22	115.48	110.35
24	A	409	BCR	C8-C7-C6	-2.22	120.97	127.20
31	d	410	LHG	C34-C33-C32	-2.22	103.16	114.42
22	B	616	CLA	CMD-C2D-C3D	2.22	132.72	127.61
22	c	505	CLA	CHD-C4C-NC	2.22	127.70	124.20
22	C	507	CLA	C4-C3-C5	2.22	119.00	115.27
24	B	618	BCR	C15-C14-C13	-2.22	124.14	127.31
24	y	101	BCR	C29-C30-C25	2.22	113.90	110.48
24	a	410	BCR	C8-C7-C6	-2.22	120.97	127.20
22	c	503	CLA	C16-C17-C18	-2.22	105.53	115.98
22	A	406	CLA	C11-C10-C8	-2.22	108.75	115.92
22	B	606	CLA	C4-C3-C5	2.22	119.00	115.27
26	B	622	LMG	O6-C5-C6	2.22	111.94	106.44
32	b	627	HTG	O5-C5-C6	2.21	111.94	106.44
22	b	619	CLA	C5-C3-C2	-2.21	116.64	121.12
22	A	406	CLA	O2D-CGD-CBD	2.21	115.20	111.27
40	v	202	HEC	CAD-CBD-CGD	-2.21	107.56	113.76
24	k	101	BCR	C32-C1-C6	-2.21	106.71	110.30
28	T	102	LMT	O3'-C3'-C2'	2.21	115.46	110.35
22	B	617	CLA	C1D-ND-C4D	-2.21	104.77	106.33
22	B	615	CLA	CHD-C4C-NC	2.21	127.69	124.20
26	A	411	LMG	O6-C5-C4	2.21	113.71	109.69
22	c	509	CLA	CHC-C1C-NC	-2.21	120.85	124.20
28	z	101	LMT	O5'-C5'-C6'	2.21	111.93	106.44
24	Y	101	BCR	C15-C16-C17	-2.21	118.95	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	410	BCR	C40-C30-C25	-2.21	106.72	110.30
24	Y	101	BCR	C38-C26-C25	-2.21	122.05	124.53
24	b	623	BCR	C8-C9-C10	-2.21	115.56	118.94
22	B	606	CLA	CHD-C1D-C2D	-2.21	120.85	125.48
31	D	411	LHG	O7-C7-C8	2.21	116.25	111.50
22	C	511	CLA	CHD-C1D-C2D	-2.21	120.85	125.48
22	C	507	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
22	A	408	CLA	CHB-C4A-NA	2.20	127.56	124.51
37	F	101	HEM	CMA-C3A-C2A	2.20	129.09	124.94
22	c	514	CLA	C4A-NA-C1A	2.20	107.70	106.71
22	c	502	CLA	C3D-C4D-CHA	-2.20	107.69	112.72
22	B	609	CLA	CGD-CBD-CAD	-2.20	103.61	110.73
22	c	506	CLA	CMD-C2D-C1D	2.20	128.59	124.71
22	c	514	CLA	OBD-CAD-C3D	-2.20	123.23	128.52
22	c	514	CLA	CAC-C3C-C4C	2.20	127.66	124.81
22	C	504	CLA	CMC-C2C-C3C	2.20	132.08	126.12
25	A	410	PL9	C37-C36-C34	-2.20	105.75	112.98
31	b	624	LHG	O4-P-O5	2.20	123.10	112.24
24	B	620	BCR	C3-C4-C5	-2.20	110.15	114.08
22	b	616	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
22	b	614	CLA	O2A-CGA-CBA	2.20	118.80	111.91
24	T	101	BCR	C3-C4-C5	-2.19	110.16	114.08
22	C	509	CLA	CMB-C2B-C3B	2.19	128.78	124.68
28	B	623	LMT	O3'-C3'-C2'	-2.19	105.28	110.35
22	d	403	CLA	C16-C15-C13	-2.19	108.83	115.92
22	B	605	CLA	C3D-C4D-CHA	-2.19	107.71	112.72
28	A	415	LMT	O1B-C1B-C2B	2.19	113.78	108.10
22	c	507	CLA	CMB-C2B-C3B	2.19	128.78	124.68
22	B	605	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
22	B	616	CLA	C4D-CHA-C1A	-2.19	118.58	121.25
22	c	512	CLA	CHD-C4C-NC	2.19	127.65	124.20
22	c	509	CLA	CMB-C2B-C3B	2.19	128.77	124.68
22	B	608	CLA	C1D-CHD-C4C	-2.19	121.34	126.06
22	C	506	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
24	B	620	BCR	C36-C18-C19	2.19	121.52	118.08
32	o	301	HTG	O2-C2-C3	-2.19	105.30	110.35
26	C	519	LMG	O7-C10-O9	-2.19	118.42	123.70
22	B	605	CLA	C3B-C4B-NB	2.19	112.03	109.21
22	c	513	CLA	CAC-C3C-C4C	2.18	127.64	124.81
22	B	608	CLA	CMB-C2B-C3B	2.18	128.76	124.68
23	A	407	PHO	CMD-C2D-C3D	2.18	128.76	124.68
22	B	609	CLA	CMD-C2D-C1D	2.18	128.56	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	503	CLA	CBC-CAC-C3C	-2.18	106.41	112.43
22	B	612	CLA	C2A-C1A-CHA	-2.18	120.04	123.86
22	b	616	CLA	CAC-C3C-C2C	-2.18	123.80	127.53
22	c	513	CLA	CBA-CAA-C2A	-2.18	107.43	113.86
33	h	101	DGD	O6E-C5E-C6E	2.18	111.86	106.44
33	h	101	DGD	O2E-C2E-C1E	2.18	115.34	110.05
22	c	514	CLA	C4D-C3D-CAD	2.18	110.66	108.10
31	D	409	LHG	O2-C2-C3	-2.18	101.92	109.56
22	C	510	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
22	b	614	CLA	C1-O2A-CGA	2.18	122.15	116.44
33	c	517	DGD	C1D-O6D-C5D	-2.18	109.42	113.69
24	Y	101	BCR	C35-C13-C12	2.18	121.50	118.08
24	b	623	BCR	C27-C26-C25	2.17	125.89	122.73
22	b	619	CLA	C4-C3-C5	2.17	118.93	115.27
22	B	602	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
24	k	101	BCR	C3-C4-C5	-2.17	110.20	114.08
22	c	511	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
22	C	510	CLA	C1-O2A-CGA	2.17	122.14	116.44
33	h	101	DGD	O3E-C3E-C4E	2.17	115.36	110.35
38	H	102	RRX	C15-C14-C13	2.17	130.40	127.31
32	C	521	HTG	C1-O5-C5	2.17	116.58	112.58
25	a	411	PL9	C11-C9-C8	-2.17	116.73	121.12
24	K	101	BCR	C33-C5-C6	-2.17	122.09	124.53
22	c	505	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	b	608	CLA	CAA-C2A-C1A	2.17	119.07	111.97
22	c	513	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
28	m	101	LMT	O5B-C5B-C6B	2.16	111.82	106.44
22	B	617	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
24	K	101	BCR	C40-C30-C25	-2.16	106.79	110.30
22	c	504	CLA	CHA-C4D-ND	2.16	137.02	132.50
31	d	410	LHG	O2-C2-C1	-2.16	99.60	109.12
22	B	609	CLA	CAC-C3C-C2C	-2.16	123.83	127.53
37	f	101	HEM	C4B-CHC-C1C	2.16	125.41	122.56
22	d	405	CLA	O2A-CGA-CBA	2.16	118.69	111.91
22	c	512	CLA	C5-C3-C2	-2.16	116.74	121.12
22	D	403	CLA	C4A-NA-C1A	-2.16	105.73	106.71
32	c	523	HTG	O5-C5-C6	2.16	111.81	106.44
22	A	404	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
23	a	408	PHO	C6-C5-C3	2.16	119.12	113.45
22	A	405	CLA	C16-C15-C13	-2.16	108.94	115.92
25	d	407	PL9	C53-C6-C1	2.16	119.40	114.99
31	B	621	LHG	C34-C33-C32	-2.16	103.47	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	603	CLA	C3D-C4D-CHA	-2.16	107.79	112.72
29	B	640	DMS	O-S-C2	2.16	117.54	106.54
23	A	407	PHO	C5-C3-C2	2.16	125.48	121.12
24	b	621	BCR	C23-C24-C25	-2.16	121.15	127.20
22	C	512	CLA	CMC-C2C-C3C	2.15	131.97	126.12
22	D	405	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
22	b	612	CLA	CHD-C4C-NC	2.15	127.60	124.20
22	B	603	CLA	CHC-C1C-NC	-2.15	120.94	124.20
32	v	208	HTG	O3-C3-C2	2.15	115.33	110.35
26	B	622	LMG	O7-C10-O9	-2.15	118.50	123.70
26	A	411	LMG	O8-C28-C29	2.15	118.65	111.91
31	d	411	LHG	O7-C7-C8	2.15	116.13	111.50
23	A	407	PHO	C1-C2-C3	-2.15	122.33	126.04
22	c	512	CLA	CMB-C2B-C3B	2.15	128.69	124.68
24	Y	101	BCR	C12-C13-C14	-2.15	115.65	118.94
28	F	102	LMT	O6'-C6'-C5'	2.15	118.65	111.29
22	c	510	CLA	C3D-C4D-CHA	-2.15	107.81	112.72
29	U	202	DMS	O-S-C1	2.14	117.48	106.54
22	C	509	CLA	C1-C2-C3	-2.14	122.33	126.04
22	B	613	CLA	C1D-ND-C4D	-2.14	104.81	106.33
22	B	613	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
22	B	614	CLA	C7-C6-C5	-2.14	107.54	113.36
22	c	512	CLA	C3B-C4B-NB	2.14	111.98	109.21
24	K	102	BCR	C38-C26-C25	-2.14	122.12	124.53
22	b	619	CLA	CAC-C3C-C2C	-2.14	123.87	127.53
32	U	203	HTG	O4-C4-C3	2.14	115.30	110.35
26	b	625	LMG	C3-C4-C5	2.14	114.06	110.24
22	b	607	CLA	C2A-C3A-C4A	-2.14	98.41	101.87
22	d	403	CLA	C6-C7-C8	-2.14	109.01	115.92
22	C	513	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
29	O	311	DMS	C2-S-C1	2.14	109.44	98.44
33	c	517	DGD	O2E-C2E-C3E	-2.14	105.41	110.35
24	B	618	BCR	C23-C22-C21	-2.13	115.67	118.94
22	C	503	CLA	C4C-C3C-C2C	-2.13	103.79	106.90
22	b	619	CLA	C3D-C4D-CHA	-2.13	107.84	112.72
22	d	402	CLA	C5-C3-C2	-2.13	116.80	121.12
31	d	411	LHG	O8-C23-O10	-2.13	118.21	123.59
28	z	101	LMT	C4B-C3B-C2B	2.13	114.55	110.82
24	d	406	BCR	C36-C18-C17	2.13	125.91	122.92
23	d	404	PHO	CMA-C3A-C4A	-2.13	109.71	114.38
33	C	515	DGD	C1D-O6D-C5D	-2.13	109.51	113.69
22	C	508	CLA	C3B-C4B-NB	2.13	111.96	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	622	LMG	O8-C28-O10	-2.13	118.22	123.59
24	B	620	BCR	C36-C18-C17	-2.13	119.94	122.92
22	b	614	CLA	C6-C5-C3	-2.13	107.88	113.45
22	b	609	CLA	C4A-NA-C1A	2.13	107.66	106.71
32	c	541	HTG	C1-C2-C3	2.13	114.79	110.59
22	D	403	CLA	O2D-CGD-CBD	2.13	115.05	111.27
22	b	610	CLA	C4-C3-C5	2.13	118.85	115.27
22	B	608	CLA	CMD-C2D-C1D	2.12	128.46	124.71
26	B	622	LMG	O4-C4-C3	-2.12	105.44	110.35
22	A	404	CLA	O2A-CGA-CBA	2.12	118.58	111.91
22	c	505	CLA	CHA-C4D-ND	2.12	136.94	132.50
22	d	403	CLA	C1-O2A-CGA	2.12	122.02	116.44
33	c	519	DGD	C3E-C4E-C5E	-2.12	106.45	110.24
22	B	606	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
24	B	618	BCR	C29-C30-C25	2.12	113.74	110.48
22	c	506	CLA	C3C-C4C-NC	2.12	112.94	110.57
22	a	409	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
22	B	603	CLA	C1-C2-C3	-2.11	122.39	126.04
33	d	408	DGD	C4D-C3D-C2D	2.11	114.51	110.82
28	z	101	LMT	O2B-C2B-C1B	2.11	115.17	110.05
28	B	623	LMT	C2'-C3'-C4'	2.11	114.50	109.68
33	C	517	DGD	O6D-C5D-C6D	2.11	110.92	106.67
22	B	612	CLA	C3D-C4D-ND	2.11	113.65	110.24
22	B	616	CLA	CHB-C4A-NA	2.11	127.43	124.51
22	c	507	CLA	CED-O2D-CGD	2.11	120.71	115.94
22	A	405	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
22	C	508	CLA	CMB-C2B-C3B	2.11	128.62	124.68
22	c	508	CLA	C1D-CHD-C4C	-2.11	121.51	126.06
22	c	506	CLA	CHB-C4A-NA	2.11	127.43	124.51
31	d	411	LHG	O6-P-O5	-2.11	100.83	109.07
28	M	102	LMT	O2'-C2'-C3'	2.11	115.22	110.35
22	c	503	CLA	C4D-C3D-CAD	2.11	110.58	108.10
26	c	521	LMG	O7-C10-O9	-2.11	118.61	123.70
22	C	511	CLA	CHD-C4C-NC	2.11	127.52	124.20
24	b	621	BCR	C37-C22-C21	2.11	125.87	122.92
22	c	510	CLA	CHD-C4C-NC	2.11	127.52	124.20
29	V	204	DMS	C2-S-C1	2.10	109.27	98.44
40	V	201	HEC	O1D-CGD-CBD	-2.10	116.33	123.08
22	d	403	CLA	C4D-C3D-CAD	2.10	110.57	108.10
24	K	101	BCR	C19-C18-C17	-2.10	115.72	118.94
22	b	611	CLA	C4-C3-C5	2.10	118.81	115.27
24	c	516	BCR	C38-C26-C25	-2.10	122.17	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D	410	LHG	O8-C23-C24	2.10	118.50	111.91
22	C	509	CLA	C1-O2A-CGA	2.10	121.95	116.44
25	d	407	PL9	C8-C7-C3	2.10	117.91	111.98
22	B	609	CLA	C11-C10-C8	-2.10	109.14	115.92
22	b	620	CLA	CMC-C2C-C1C	2.09	128.23	125.04
23	D	404	PHO	CMB-C2B-C3B	2.09	128.60	124.68
31	b	624	LHG	O6-P-O5	-2.09	100.88	109.07
22	b	618	CLA	C4-C3-C5	2.09	118.79	115.27
22	c	509	CLA	C1-O2A-CGA	2.09	121.93	116.44
22	c	507	CLA	CGD-CBD-CAD	-2.09	103.96	110.73
22	C	505	CLA	CMD-C2D-C3D	2.09	132.43	127.61
24	a	410	BCR	C35-C13-C12	2.09	121.37	118.08
38	h	102	RRX	C31-C1-C6	-2.09	106.91	110.30
22	b	618	CLA	C3B-C4B-NB	2.09	111.91	109.21
22	b	608	CLA	CMD-C2D-C1D	2.09	128.39	124.71
24	D	406	BCR	C19-C18-C17	2.09	122.14	118.94
22	B	602	CLA	C5-C3-C2	2.09	125.34	121.12
22	C	513	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
33	C	515	DGD	C3G-C2G-C1G	-2.09	106.85	111.79
32	b	601	HTG	C3-C4-C5	2.09	113.96	110.24
22	c	509	CLA	CHA-C4D-ND	2.09	136.86	132.50
22	B	607	CLA	CHC-C1C-C2C	-2.08	120.95	126.72
22	B	608	CLA	O2D-CGD-CBD	2.08	114.97	111.27
28	T	102	LMT	O1'-C1'-C2'	2.08	111.56	108.30
24	T	101	BCR	C11-C10-C9	-2.08	124.34	127.31
22	d	402	CLA	C4C-C3C-C2C	-2.08	103.86	106.90
22	d	402	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	Y	101	BCR	C7-C8-C9	-2.08	123.09	126.23
24	d	406	BCR	C32-C1-C6	2.08	113.68	110.30
32	V	202	HTG	O5-C5-C6	2.08	111.61	106.44
22	c	510	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
22	d	403	CLA	CBC-CAC-C3C	-2.08	106.69	112.43
22	c	512	CLA	C1D-CHD-C4C	-2.08	121.57	126.06
22	c	503	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
28	B	623	LMT	O5'-C5'-C6'	2.08	111.60	106.44
22	c	506	CLA	C4C-C3C-C2C	-2.08	103.87	106.90
28	t	102	LMT	C4'-C3'-C2'	-2.08	107.20	110.82
22	B	607	CLA	C3C-C4C-NC	2.07	112.90	110.57
22	B	605	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
22	C	511	CLA	C3A-C2A-C1A	2.07	104.44	101.34
22	B	617	CLA	C4C-C3C-C2C	-2.07	103.88	106.90
22	a	407	CLA	CMD-C2D-C3D	2.07	132.38	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	609	CLA	CHC-C1C-NC	-2.07	121.06	124.20
24	B	618	BCR	C11-C10-C9	-2.07	124.35	127.31
22	d	402	CLA	C1D-CHD-C4C	-2.07	121.59	126.06
22	b	608	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
22	C	503	CLA	C1-C2-C3	2.07	129.62	126.04
22	c	505	CLA	C3D-C4D-CHA	-2.07	107.99	112.72
22	A	408	CLA	CMC-C2C-C3C	2.07	131.73	126.12
22	C	505	CLA	C1D-CHD-C4C	-2.07	121.59	126.06
22	d	402	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
33	h	101	DGD	CDA-CCA-CBA	-2.07	103.93	114.42
22	C	507	CLA	C3B-C4B-NB	2.07	111.88	109.21
22	b	613	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
22	B	613	CLA	C4-C3-C5	2.06	118.74	115.27
22	B	604	CLA	C1-O2A-CGA	2.06	121.86	116.44
22	c	508	CLA	CAC-C3C-C4C	2.06	127.49	124.81
22	d	405	CLA	C1-O2A-CGA	2.06	121.86	116.44
22	D	403	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	c	508	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
22	A	408	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
32	o	301	HTG	O3-C3-C4	-2.06	105.58	110.35
26	b	625	LMG	O7-C10-O9	-2.06	118.72	123.70
38	H	102	RRX	C32-C1-C6	2.06	113.64	110.30
24	d	406	BCR	C7-C8-C9	-2.06	123.12	126.23
24	b	623	BCR	C3-C4-C5	-2.06	110.40	114.08
26	c	520	LMG	C3-C4-C5	2.06	113.91	110.24
22	B	616	CLA	CMB-C2B-C3B	2.06	128.53	124.68
22	B	602	CLA	CED-O2D-CGD	2.06	120.59	115.94
22	c	510	CLA	C4C-C3C-C2C	-2.06	103.90	106.90
22	C	501	CLA	C6-C5-C3	-2.06	108.06	113.45
22	b	606	CLA	OBD-CAD-C3D	-2.06	123.57	128.52
28	a	401	LMT	C3B-C4B-C5B	2.06	113.91	110.24
28	a	401	LMT	O6B-C6B-C5B	2.05	118.34	111.29
33	H	101	DGD	O2G-C1B-C2B	2.05	115.93	111.50
22	c	510	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	b	614	CLA	CHC-C1C-NC	-2.05	121.09	124.20
22	c	508	CLA	C4C-C3C-C2C	-2.05	103.91	106.90
22	B	607	CLA	C16-C15-C13	2.05	122.55	115.92
25	a	411	PL9	C10-C9-C11	2.05	118.72	115.27
22	c	505	CLA	C5-C3-C2	-2.05	116.97	121.12
22	B	602	CLA	C4C-C3C-C2C	-2.05	103.91	106.90
22	B	616	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
24	y	101	BCR	C4-C5-C6	2.05	125.71	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	504	CLA	C6-C5-C3	2.05	118.83	113.45
24	A	409	BCR	C34-C9-C8	2.05	121.31	118.08
22	c	509	CLA	C3D-C4D-ND	2.05	113.55	110.24
22	b	605	CLA	CMD-C2D-C1D	2.05	128.32	124.71
22	D	403	CLA	C3A-C2A-C1A	-2.05	98.27	101.34
31	d	411	LHG	C10-C9-C8	-2.05	105.83	113.19
33	D	408	DGD	C2G-O2G-C1B	2.05	122.83	117.79
29	v	207	DMS	O-S-C2	2.05	116.98	106.54
22	C	513	CLA	O2A-CGA-CBA	2.05	118.33	111.91
22	C	513	CLA	CMD-C2D-C1D	2.05	128.32	124.71
22	b	607	CLA	CHB-C4A-NA	2.05	127.34	124.51
22	b	612	CLA	O2D-CGD-CBD	-2.04	107.64	111.27
22	c	504	CLA	CMD-C2D-C3D	2.04	132.32	127.61
22	b	612	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	B	608	CLA	C1-O2A-CGA	2.04	121.81	116.44
32	O	302	HTG	C1-C2-C3	2.04	114.62	110.59
22	C	501	CLA	CBA-CAA-C2A	2.04	119.89	113.86
33	C	516	DGD	O2D-C2D-C3D	-2.04	105.63	110.35
22	C	512	CLA	CMD-C2D-C1D	2.04	128.31	124.71
37	F	101	HEM	C1B-NB-C4B	2.04	107.18	105.07
24	C	514	BCR	C34-C9-C8	2.04	121.29	118.08
22	B	610	CLA	CHC-C1C-C2C	-2.04	121.08	126.72
24	T	101	BCR	C37-C22-C21	2.04	125.78	122.92
22	B	614	CLA	C3C-C4C-NC	2.04	112.86	110.57
33	h	101	DGD	C2G-O2G-C1B	-2.04	112.78	117.79
25	a	411	PL9	C40-C39-C41	2.04	118.70	115.27
25	D	407	PL9	C22-C23-C24	-2.04	122.76	127.66
22	B	603	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
32	v	208	HTG	O4-C4-C3	-2.04	105.64	110.35
24	B	620	BCR	C11-C10-C9	-2.04	124.41	127.31
22	B	617	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
33	c	518	DGD	C3B-C2B-C1B	-2.03	106.22	113.62
22	C	509	CLA	CAC-C3C-C2C	-2.03	124.05	127.53
26	b	625	LMG	C9-C8-C7	-2.03	106.98	111.79
22	b	615	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
26	A	411	LMG	O3-C3-C4	2.03	115.05	110.35
28	B	623	LMT	O5B-C1B-C2B	2.03	114.65	110.35
22	B	613	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
32	B	642	HTG	C2'-C1'-S1	2.03	118.97	112.40
22	B	604	CLA	C3D-C4D-CHA	-2.03	108.08	112.72
24	T	101	BCR	C30-C25-C26	-2.03	119.75	122.61
22	A	408	CLA	C4A-NA-C1A	2.03	107.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	511	CLA	C4-C3-C5	2.03	118.68	115.27
22	B	611	CLA	CHD-C4C-NC	2.03	127.40	124.20
28	c	522	LMT	O2'-C2'-C1'	2.03	114.97	110.05
22	C	511	CLA	CBC-CAC-C3C	-2.03	106.85	112.43
22	c	503	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
24	T	101	BCR	C7-C6-C5	-2.02	116.56	121.46
24	b	621	BCR	C11-C10-C9	-2.02	124.42	127.31
22	a	409	CLA	C4A-NA-C1A	2.02	107.62	106.71
22	B	605	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
22	C	513	CLA	CAC-C3C-C4C	2.02	127.43	124.81
22	c	505	CLA	CAC-C3C-C4C	2.02	127.43	124.81
32	B	629	HTG	O2-C2-C1	2.02	113.98	110.27
22	B	612	CLA	C7-C6-C5	-2.02	107.87	113.36
24	c	515	BCR	C34-C9-C8	2.02	121.26	118.08
22	b	606	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
24	a	410	BCR	C16-C15-C14	-2.02	119.34	123.47
22	b	611	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
24	c	516	BCR	C15-C14-C13	-2.02	124.43	127.31
22	c	506	CLA	O2D-CGD-CBD	2.02	114.85	111.27
26	b	625	LMG	C1-O6-C5	-2.02	109.73	113.69
22	B	613	CLA	C1C-C2C-C3C	-2.02	104.84	106.96
22	C	509	CLA	C16-C15-C13	-2.02	109.41	115.92
22	C	501	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
22	C	512	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
22	b	607	CLA	CHC-C1C-NC	-2.01	121.15	124.20
34	e	104	GOL	C3-C2-C1	-2.01	103.87	111.70
31	D	411	LHG	O7-C5-C4	2.01	115.69	108.40
22	b	620	CLA	C6-C5-C3	2.01	118.73	113.45
33	c	517	DGD	O1G-C1G-C2G	-2.01	102.58	108.43
22	b	609	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
22	b	617	CLA	C17-C16-C15	-2.01	104.00	113.24
28	m	101	LMT	C2'-C3'-C4'	2.01	114.27	109.68
29	V	208	DMS	C2-S-C1	2.01	108.78	98.44
22	B	615	CLA	C3D-C4D-ND	2.01	113.48	110.24
22	B	610	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	C	513	CLA	CMB-C2B-C3B	2.01	128.43	124.68
33	c	519	DGD	C1D-C2D-C3D	-2.01	105.82	110.00
22	B	612	CLA	CMB-C2B-C3B	2.00	128.43	124.68
22	c	510	CLA	CMC-C2C-C1C	2.00	128.09	125.04
24	D	406	BCR	C36-C18-C17	2.00	125.73	122.92
22	B	605	CLA	CMD-C2D-C3D	2.00	132.22	127.61
22	b	613	CLA	C3D-C4D-ND	2.00	113.48	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	508	CLA	CHA-C4D-ND	2.00	136.69	132.50
22	a	407	CLA	CHC-C1C-C2C	-2.00	121.18	126.72
28	M	101	LMT	O6'-C6'-C5'	-2.00	104.42	111.29
22	a	409	CLA	C1-O2A-CGA	2.00	121.69	116.44
26	a	412	LMG	O4-C4-C3	-2.00	105.72	110.35

All (52) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	404	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	B	617	CLA	ND
22	C	501	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	508	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	D	403	CLA	ND
22	D	405	CLA	ND
22	a	406	CLA	ND
22	a	409	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	608	CLA	ND
22	b	609	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	614	CLA	ND
22	b	616	CLA	ND
22	b	617	CLA	ND
22	b	618	CLA	ND
22	b	619	CLA	ND
22	b	620	CLA	ND
22	c	502	CLA	ND
22	c	503	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
28	C	520	LMT	C1B
28	z	101	LMT	C1B

All (1209) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	405	CLA	CHA-CBD-CGD-O1D
22	A	408	CLA	C4-C3-C5-C6
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	602	CLA	C11-C10-C8-C9
22	B	606	CLA	C4-C3-C5-C6
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CHA-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	C2-C3-C5-C6
22	C	507	CLA	C4-C3-C5-C6
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	513	CLA	O2A-C1-C2-C3
22	b	605	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	CHA-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O1D
22	b	606	CLA	CHA-CBD-CGD-O1D
22	b	618	CLA	CHA-CBD-CGD-O1D
22	b	618	CLA	CHA-CBD-CGD-O2D
22	b	618	CLA	CAD-CBD-CGD-O1D
22	b	618	CLA	CAD-CBD-CGD-O2D
22	b	618	CLA	C4-C3-C5-C6
22	c	503	CLA	CHA-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	508	CLA	C2-C3-C5-C6
22	c	508	CLA	C4-C3-C5-C6
22	d	403	CLA	CHA-CBD-CGD-O1D
24	B	618	BCR	C1-C6-C7-C8
24	D	406	BCR	C21-C22-C23-C24
24	T	101	BCR	C11-C12-C13-C35
24	T	101	BCR	C35-C13-C14-C15
24	d	406	BCR	C21-C22-C23-C24
24	t	101	BCR	C11-C12-C13-C35
24	t	101	BCR	C35-C13-C14-C15
25	a	411	PL9	C28-C29-C31-C32
25	a	411	PL9	C30-C29-C31-C32
26	C	519	LMG	O6-C1-O1-C7
26	a	412	LMG	O6-C1-O1-C7
28	A	415	LMT	C2'-C1'-O1'-C1
28	A	415	LMT	O5'-C1'-O1'-C1
28	F	102	LMT	O5'-C1'-O1'-C1
28	J	102	LMT	C2'-C1'-O1'-C1
28	J	102	LMT	O5'-C1'-O1'-C1
28	M	102	LMT	C2'-C1'-O1'-C1
28	b	626	LMT	C2'-C1'-O1'-C1
28	b	626	LMT	O5'-C1'-O1'-C1
28	m	102	LMT	C2'-C1'-O1'-C1
28	m	102	LMT	O5'-C1'-O1'-C1
31	B	621	LHG	C4-O6-P-O4
31	E	101	LHG	O2-C2-C3-O3
31	E	101	LHG	C3-O3-P-O5
31	F	103	LHG	C3-O3-P-O4
31	F	103	LHG	C3-O3-P-O5
31	F	103	LHG	C3-O3-P-O6
31	b	624	LHG	C4-O6-P-O3
31	b	624	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
31	b	624	LHG	C4-O6-P-O5
31	d	410	LHG	O1-C1-C2-C3
31	e	101	LHG	C3-O3-P-O4
31	e	101	LHG	C3-O3-P-O5
31	f	102	LHG	O1-C1-C2-C3
31	f	102	LHG	C3-O3-P-O5
32	B	624	HTG	O5-C1-S1-C1'
32	B	642	HTG	C2'-C1'-S1-C1
32	C	521	HTG	C2'-C1'-S1-C1
32	b	627	HTG	O5-C1-S1-C1'
32	b	627	HTG	C2'-C1'-S1-C1
32	c	523	HTG	C2-C1-S1-C1'
32	c	523	HTG	C2'-C1'-S1-C1
32	c	541	HTG	O5-C1-S1-C1'
33	D	408	DGD	C2B-C1B-O2G-C2G
33	D	408	DGD	O1B-C1B-O2G-C2G
33	d	408	DGD	C2B-C1B-O2G-C2G
33	d	408	DGD	O1B-C1B-O2G-C2G
34	C	533	GOL	C1-C2-C3-O3
34	b	636	GOL	O1-C1-C2-C3
34	c	533	GOL	O1-C1-C2-O2
34	c	533	GOL	O1-C1-C2-C3
34	c	533	GOL	C1-C2-C3-O3
22	B	611	CLA	C15-C16-C17-C18
22	B	616	CLA	C13-C15-C16-C17
28	A	415	LMT	C3'-C4'-O1B-C1B
28	C	520	LMT	C3'-C4'-O1B-C1B
22	C	513	CLA	CBD-CGD-O2D-CED
28	B	623	LMT	O5B-C1B-O1B-C4'
28	C	520	LMT	C4'-C5'-C6'-O6'
28	C	520	LMT	O5B-C1B-O1B-C4'
22	b	605	CLA	C3-C5-C6-C7
22	B	617	CLA	CBA-CGA-O2A-C1
26	A	411	LMG	O10-C28-O8-C9
26	C	519	LMG	O6-C5-C6-O5
32	v	208	HTG	O5-C5-C6-O6
28	F	102	LMT	O5'-C5'-C6'-O6'
28	m	102	LMT	O5'-C5'-C6'-O6'
25	A	410	PL9	C30-C29-C31-C32
22	A	408	CLA	C2-C3-C5-C6
22	B	615	CLA	C3-C5-C6-C7
22	B	617	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	C3-C5-C6-C7
26	A	411	LMG	C29-C28-O8-C9
31	e	101	LHG	C24-C23-O8-C6
32	C	522	HTG	S1-C1'-C2'-C3'
32	v	208	HTG	S1-C1'-C2'-C3'
22	B	611	CLA	O1D-CGD-O2D-CED
28	C	520	LMT	O5'-C5'-C6'-O6'
28	Z	101	LMT	C4'-C5'-C6'-O6'
32	C	536	HTG	C4-C5-C6-O6
31	e	101	LHG	O10-C23-O8-C6
22	C	513	CLA	O1D-CGD-O2D-CED
28	C	520	LMT	O5B-C5B-C6B-O6B
28	C	520	LMT	C4B-C5B-C6B-O6B
22	B	609	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
31	F	103	LHG	O2-C2-C3-O3
28	a	401	LMT	O5B-C1B-O1B-C4'
28	c	522	LMT	C3-C4-C5-C6
31	D	411	LHG	C11-C12-C13-C14
22	B	617	CLA	O1A-CGA-O2A-C1
32	C	536	HTG	O5-C5-C6-O6
32	b	627	HTG	O5-C5-C6-O6
28	A	415	LMT	C4'-C5'-C6'-O6'
22	C	508	CLA	CBD-CGD-O2D-CED
26	B	622	LMG	O6-C5-C6-O5
26	D	412	LMG	C35-C36-C37-C38
28	T	102	LMT	O5'-C5'-C6'-O6'
26	C	519	LMG	C4-C5-C6-O5
28	a	401	LMT	C2B-C1B-O1B-C4'
22	c	514	CLA	C3-C5-C6-C7
32	D	413	HTG	S1-C1'-C2'-C3'
32	c	524	HTG	S1-C1'-C2'-C3'
22	B	608	CLA	O1D-CGD-O2D-CED
32	b	640	HTG	O5-C5-C6-O6
32	b	601	HTG	C4-C5-C6-O6
26	c	521	LMG	O6-C5-C6-O5
28	Z	101	LMT	O5'-C5'-C6'-O6'
28	Z	101	LMT	C4B-C5B-C6B-O6B
22	B	606	CLA	C2-C3-C5-C6
22	b	618	CLA	C2-C3-C5-C6
22	B	605	CLA	CBD-CGD-O2D-CED
28	j	102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
28	z	101	LMT	O5B-C5B-C6B-O6B
28	m	102	LMT	C4'-C5'-C6'-O6'
28	a	401	LMT	O5'-C1'-O1'-C1
25	A	410	PL9	C24-C26-C27-C28
25	a	411	PL9	C19-C21-C22-C23
31	F	103	LHG	C24-C23-O8-C6
22	C	509	CLA	CBD-CGD-O2D-CED
33	C	515	DGD	C5A-C6A-C7A-C8A
31	E	101	LHG	C1-C2-C3-O3
28	b	626	LMT	C4'-C5'-C6'-O6'
22	b	612	CLA	O1D-CGD-O2D-CED
22	b	620	CLA	CBA-CGA-O2A-C1
31	E	101	LHG	C24-C23-O8-C6
28	z	101	LMT	C4B-C5B-C6B-O6B
32	v	208	HTG	C4-C5-C6-O6
28	M	101	LMT	O5'-C5'-C6'-O6'
32	C	522	HTG	C1'-C2'-C3'-C4'
28	F	102	LMT	C4'-C5'-C6'-O6'
28	T	102	LMT	C4'-C5'-C6'-O6'
32	b	627	HTG	C4-C5-C6-O6
28	A	415	LMT	O5'-C5'-C6'-O6'
22	d	405	CLA	C13-C15-C16-C17
22	a	409	CLA	C3-C5-C6-C7
33	D	408	DGD	O2G-C2G-C3G-O3G
31	F	103	LHG	O10-C23-O8-C6
28	j	102	LMT	C4'-C5'-C6'-O6'
22	b	609	CLA	C2-C3-C5-C6
25	A	410	PL9	C28-C29-C31-C32
22	C	513	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C9
22	b	620	CLA	C6-C7-C8-C9
22	c	514	CLA	C11-C10-C8-C9
22	C	506	CLA	CBD-CGD-O2D-CED
24	d	406	BCR	C37-C22-C23-C24
28	J	102	LMT	C4'-C5'-C6'-O6'
22	B	615	CLA	C5-C6-C7-C8
22	B	616	CLA	C10-C11-C12-C13
22	c	508	CLA	C5-C6-C7-C8
26	c	520	LMG	C29-C28-O8-C9
22	D	405	CLA	C8-C10-C11-C12
31	D	409	LHG	C23-C24-C25-C26
31	d	409	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
33	C	516	DGD	C1B-C2B-C3B-C4B
26	c	521	LMG	C4-C5-C6-O5
32	B	642	HTG	C1'-C2'-C3'-C4'
32	b	627	HTG	C1'-C2'-C3'-C4'
28	b	626	LMT	O5'-C5'-C6'-O6'
22	B	602	CLA	C10-C11-C12-C13
22	c	507	CLA	C5-C6-C7-C8
22	C	502	CLA	O1D-CGD-O2D-CED
22	c	502	CLA	O1D-CGD-O2D-CED
22	c	514	CLA	O1D-CGD-O2D-CED
28	Z	101	LMT	O5B-C5B-C6B-O6B
32	b	601	HTG	O5-C5-C6-O6
28	A	415	LMT	O1'-C1-C2-C3
22	B	602	CLA	C15-C16-C17-C18
22	B	614	CLA	C13-C15-C16-C17
28	C	520	LMT	O1'-C1-C2-C3
22	C	509	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C5-C6-C7-C8
22	C	513	CLA	C8-C10-C11-C12
26	C	518	LMG	C28-C29-C30-C31
26	C	519	LMG	C10-C11-C12-C13
22	b	610	CLA	C6-C7-C8-C10
22	c	513	CLA	C12-C13-C15-C16
22	B	602	CLA	C3-C5-C6-C7
22	b	620	CLA	O1A-CGA-O2A-C1
22	B	607	CLA	C2A-CAA-CBA-CGA
22	b	610	CLA	C2A-CAA-CBA-CGA
22	b	610	CLA	C10-C11-C12-C13
22	c	507	CLA	C10-C11-C12-C13
32	B	642	HTG	C4-C5-C6-O6
31	E	101	LHG	O10-C23-O8-C6
22	a	406	CLA	CBD-CGD-O2D-CED
26	B	622	LMG	C4-C5-C6-O5
28	C	520	LMT	O5'-C1'-O1'-C1
28	M	102	LMT	O5'-C1'-O1'-C1
22	b	619	CLA	C5-C6-C7-C8
25	D	407	PL9	C39-C41-C42-C43
28	c	522	LMT	O1'-C1-C2-C3
28	m	103	LMT	O1'-C1-C2-C3
28	m	101	LMT	O5'-C5'-C6'-O6'
22	b	620	CLA	C15-C16-C17-C18
22	d	402	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	H	101	DGD	C6B-C7B-C8B-C9B
26	C	518	LMG	C10-C11-C12-C13
22	C	501	CLA	O1D-CGD-O2D-CED
22	B	616	CLA	C5-C6-C7-C8
22	b	619	CLA	C10-C11-C12-C13
22	b	619	CLA	CBD-CGD-O2D-CED
26	c	520	LMG	O10-C28-O8-C9
22	B	615	CLA	C8-C10-C11-C12
22	b	612	CLA	C13-C15-C16-C17
31	B	621	LHG	C4-O6-P-O3
31	E	101	LHG	C3-O3-P-O6
31	e	101	LHG	C3-O3-P-O6
31	f	102	LHG	C3-O3-P-O6
31	f	102	LHG	C23-C24-C25-C26
22	B	602	CLA	CBA-CGA-O2A-C1
31	F	103	LHG	C23-C24-C25-C26
22	B	616	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	C8-C10-C11-C12
22	c	503	CLA	C16-C17-C18-C19
26	C	519	LMG	C11-C10-O7-C8
26	b	625	LMG	C21-C22-C23-C24
26	c	521	LMG	C21-C22-C23-C24
28	B	623	LMT	C5-C6-C7-C8
28	a	401	LMT	C6-C7-C8-C9
28	m	102	LMT	C5-C6-C7-C8
31	D	411	LHG	C17-C18-C19-C20
31	b	624	LHG	C13-C14-C15-C16
22	c	514	CLA	C16-C17-C18-C19
31	D	409	LHG	C27-C28-C29-C30
31	F	103	LHG	C12-C13-C14-C15
31	d	409	LHG	C11-C10-C9-C8
31	f	102	LHG	C27-C28-C29-C30
33	C	515	DGD	C2A-C3A-C4A-C5A
33	C	516	DGD	C8B-C9B-CAB-CBB
33	D	408	DGD	CAA-CBA-CCA-CDA
33	c	518	DGD	C5A-C6A-C7A-C8A
26	C	519	LMG	O9-C10-O7-C8
22	B	613	CLA	C13-C15-C16-C17
31	D	411	LHG	C14-C15-C16-C17
33	C	517	DGD	C6B-C7B-C8B-C9B
28	Z	101	LMT	C5-C6-C7-C8
31	d	411	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	D	412	LMG	C36-C37-C38-C39
28	M	102	LMT	O1'-C1-C2-C3
31	B	621	LHG	C10-C11-C12-C13
31	d	411	LHG	C13-C14-C15-C16
33	C	516	DGD	CBA-CCA-CDA-CEA
33	D	408	DGD	C6A-C7A-C8A-C9A
22	c	512	CLA	O1D-CGD-O2D-CED
26	C	519	LMG	C2-C1-O1-C7
33	C	516	DGD	C2E-C1E-O5D-C6D
26	B	622	LMG	C39-C40-C41-C42
26	b	625	LMG	C19-C20-C21-C22
28	m	101	LMT	C11-C10-C9-C8
32	C	536	HTG	C2'-C3'-C4'-C5'
33	C	515	DGD	C7B-C8B-C9B-CAB
33	h	101	DGD	C7A-C8A-C9A-CAA
22	B	616	CLA	C16-C17-C18-C20
22	C	502	CLA	C16-C17-C18-C20
22	C	506	CLA	C16-C17-C18-C20
22	b	606	CLA	C16-C17-C18-C19
22	d	405	CLA	C16-C17-C18-C20
33	d	408	DGD	C6A-C7A-C8A-C9A
22	A	408	CLA	C11-C12-C13-C14
22	d	405	CLA	C14-C13-C15-C16
26	c	521	LMG	C28-C29-C30-C31
26	A	411	LMG	C13-C14-C15-C16
28	j	102	LMT	C5-C6-C7-C8
31	E	101	LHG	C25-C26-C27-C28
31	F	103	LHG	C14-C15-C16-C17
31	d	409	LHG	C27-C28-C29-C30
32	C	535	HTG	C2'-C3'-C4'-C5'
33	C	517	DGD	C9B-CAB-CBB-CCB
33	C	515	DGD	CAA-CBA-CCA-CDA
31	D	411	LHG	O1-C1-C2-C3
31	E	101	LHG	O1-C1-C2-C3
34	D	417	GOL	O1-C1-C2-C3
34	D	417	GOL	C1-C2-C3-O3
28	A	415	LMT	O5B-C5B-C6B-O6B
31	D	411	LHG	C10-C11-C12-C13
33	c	517	DGD	C9A-CAA-CBA-CCA
28	t	102	LMT	C4'-C5'-C6'-O6'
26	C	518	LMG	C35-C36-C37-C38
26	b	625	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
26	b	625	LMG	C20-C21-C22-C23
28	c	522	LMT	C7-C8-C9-C10
22	D	405	CLA	C16-C17-C18-C19
22	D	405	CLA	C16-C17-C18-C20
22	A	405	CLA	C2C-C3C-CAC-CBC
26	b	625	LMG	C34-C35-C36-C37
28	t	102	LMT	C7-C8-C9-C10
31	B	621	LHG	C11-C12-C13-C14
31	b	624	LHG	C30-C31-C32-C33
31	d	411	LHG	C10-C11-C12-C13
33	C	517	DGD	CBA-CCA-CDA-CEA
33	C	517	DGD	CBB-CCB-CDB-CEB
26	d	412	LMG	C36-C37-C38-C39
28	F	102	LMT	C7-C8-C9-C10
33	C	516	DGD	C4B-C5B-C6B-C7B
33	D	408	DGD	C2B-C3B-C4B-C5B
33	c	517	DGD	CCA-CDA-CEA-CFA
32	D	413	HTG	C1'-C2'-C3'-C4'
26	c	521	LMG	C10-C11-C12-C13
22	A	408	CLA	C13-C15-C16-C17
22	c	510	CLA	C8-C10-C11-C12
22	B	602	CLA	O1A-CGA-O2A-C1
26	c	520	LMG	C36-C37-C38-C39
31	f	102	LHG	C13-C14-C15-C16
33	C	517	DGD	O6E-C5E-C6E-O5E
26	A	411	LMG	C36-C37-C38-C39
26	b	625	LMG	C35-C36-C37-C38
28	T	102	LMT	C7-C8-C9-C10
28	l	101	LMT	C5-C6-C7-C8
33	c	517	DGD	C4A-C5A-C6A-C7A
33	c	517	DGD	C6A-C7A-C8A-C9A
33	c	517	DGD	C5B-C6B-C7B-C8B
33	c	519	DGD	C2A-C3A-C4A-C5A
22	b	607	CLA	C5-C6-C7-C8
28	F	102	LMT	C2-C1-O1'-C1'
28	T	102	LMT	C2-C1-O1'-C1'
28	m	101	LMT	C2-C1-O1'-C1'
22	B	616	CLA	C16-C17-C18-C19
22	C	506	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C20
32	C	521	HTG	S1-C1'-C2'-C3'
26	A	411	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	a	401	LMT	O1'-C1-C2-C3
33	C	515	DGD	C3B-C4B-C5B-C6B
33	c	518	DGD	C8B-C9B-CAB-CBB
26	D	412	LMG	C12-C13-C14-C15
31	b	624	LHG	C14-C15-C16-C17
33	C	516	DGD	C9A-CAA-CBA-CCA
31	e	101	LHG	C23-C24-C25-C26
33	d	408	DGD	C1A-C2A-C3A-C4A
28	T	102	LMT	O1'-C1-C2-C3
23	a	408	PHO	C4-C3-C5-C6
26	c	521	LMG	C11-C10-O7-C8
26	B	622	LMG	C29-C30-C31-C32
33	C	515	DGD	C8B-C9B-CAB-CBB
31	D	411	LHG	O1-C1-C2-O2
34	C	533	GOL	O2-C2-C3-O3
34	b	636	GOL	O1-C1-C2-O2
34	c	533	GOL	O2-C2-C3-O3
31	D	409	LHG	C31-C32-C33-C34
31	e	101	LHG	C11-C12-C13-C14
31	f	102	LHG	C30-C31-C32-C33
33	C	515	DGD	CAB-CBB-CCB-CDB
22	B	602	CLA	O1D-CGD-O2D-CED
31	E	101	LHG	C26-C27-C28-C29
22	a	406	CLA	C4C-C3C-CAC-CBC
26	a	412	LMG	C36-C37-C38-C39
26	c	521	LMG	O9-C10-O7-C8
22	B	617	CLA	C2-C1-O2A-CGA
22	c	510	CLA	C2-C1-O2A-CGA
26	A	411	LMG	C12-C13-C14-C15
26	C	518	LMG	C11-C12-C13-C14
24	B	618	BCR	C5-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
33	d	408	DGD	C4B-C5B-C6B-C7B
22	b	620	CLA	C5-C6-C7-C8
28	m	102	LMT	C1-C2-C3-C4
28	C	520	LMT	C11-C10-C9-C8
26	B	622	LMG	C10-C11-C12-C13
33	D	408	DGD	C1B-C2B-C3B-C4B
26	a	412	LMG	C37-C38-C39-C40
26	c	521	LMG	C38-C39-C40-C41
33	H	101	DGD	C7A-C8A-C9A-CAA
22	C	506	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	C13-C15-C16-C17
22	C	503	CLA	O1D-CGD-O2D-CED
28	J	102	LMT	C5-C6-C7-C8
31	E	101	LHG	C17-C18-C19-C20
33	D	408	DGD	C9A-CAA-CBA-CCA
22	A	408	CLA	C11-C12-C13-C15
22	B	615	CLA	C12-C13-C15-C16
22	B	617	CLA	C12-C13-C15-C16
22	a	407	CLA	C6-C7-C8-C10
22	d	405	CLA	C11-C10-C8-C7
22	d	405	CLA	C12-C13-C15-C16
28	t	102	LMT	C5-C6-C7-C8
22	b	606	CLA	C16-C17-C18-C20
22	d	405	CLA	C16-C17-C18-C19
31	e	101	LHG	O9-C7-O7-C5
28	A	415	LMT	C5-C6-C7-C8
22	A	408	CLA	C5-C6-C7-C8
22	b	610	CLA	C13-C15-C16-C17
28	F	102	LMT	O1'-C1-C2-C3
28	b	626	LMT	O1'-C1-C2-C3
31	E	101	LHG	C32-C33-C34-C35
31	d	411	LHG	C18-C19-C20-C21
22	C	511	CLA	O1D-CGD-O2D-CED
32	c	524	HTG	C2'-C1'-S1-C1
22	C	509	CLA	O1D-CGD-O2D-CED
26	a	412	LMG	C34-C35-C36-C37
28	m	103	LMT	C5-C6-C7-C8
33	d	408	DGD	C6B-C7B-C8B-C9B
31	B	621	LHG	C12-C13-C14-C15
22	c	507	CLA	C16-C17-C18-C19
22	a	409	CLA	C10-C11-C12-C13
22	b	614	CLA	C15-C16-C17-C18
25	A	410	PL9	C9-C11-C12-C13
25	a	411	PL9	C9-C11-C12-C13
31	D	409	LHG	C15-C16-C17-C18
32	o	301	HTG	C3'-C4'-C5'-C6'
31	e	101	LHG	C7-C8-C9-C10
26	A	411	LMG	C11-C10-O7-C8
31	e	101	LHG	C8-C7-O7-C5
33	C	516	DGD	C7A-C8A-C9A-CAA
33	D	408	DGD	C2A-C3A-C4A-C5A
33	D	408	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
31	E	101	LHG	C12-C13-C14-C15
33	C	516	DGD	C3A-C4A-C5A-C6A
32	B	624	HTG	C1'-C2'-C3'-C4'
26	D	412	LMG	C17-C18-C19-C20
33	c	517	DGD	C4B-C5B-C6B-C7B
32	c	541	HTG	O5-C5-C6-O6
25	a	411	PL9	C4-C3-C7-C8
33	c	518	DGD	C5B-C6B-C7B-C8B
22	B	604	CLA	C6-C7-C8-C9
22	B	615	CLA	C14-C13-C15-C16
22	B	617	CLA	C14-C13-C15-C16
22	C	509	CLA	C6-C7-C8-C9
22	a	407	CLA	C6-C7-C8-C9
22	b	615	CLA	C14-C13-C15-C16
22	c	513	CLA	C14-C13-C15-C16
22	d	405	CLA	C11-C10-C8-C9
31	E	101	LHG	C15-C16-C17-C18
31	F	103	LHG	C10-C11-C12-C13
26	D	412	LMG	C30-C31-C32-C33
26	d	412	LMG	C39-C40-C41-C42
32	d	413	HTG	O5-C5-C6-O6
31	d	409	LHG	C9-C10-C11-C12
33	c	518	DGD	C4B-C5B-C6B-C7B
22	C	502	CLA	C16-C17-C18-C19
22	c	514	CLA	C16-C17-C18-C20
26	A	411	LMG	O9-C10-O7-C8
26	A	411	LMG	C30-C31-C32-C33
31	D	411	LHG	C13-C14-C15-C16
31	F	103	LHG	C27-C28-C29-C30
22	d	403	CLA	C2C-C3C-CAC-CBC
22	a	409	CLA	O1A-CGA-O2A-C1
22	b	605	CLA	C10-C11-C12-C13
22	c	510	CLA	C15-C16-C17-C18
26	a	412	LMG	C21-C22-C23-C24
33	C	516	DGD	C8A-C9A-CAA-CBA
26	d	412	LMG	C29-C30-C31-C32
26	d	412	LMG	C34-C35-C36-C37
31	b	624	LHG	C27-C28-C29-C30
31	d	409	LHG	C30-C31-C32-C33
26	D	412	LMG	O6-C5-C6-O5
33	c	517	DGD	O6E-C5E-C6E-O5E
22	a	406	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	C	518	LMG	C32-C33-C34-C35
26	a	412	LMG	C20-C21-C22-C23
26	B	622	LMG	C31-C32-C33-C34
33	c	517	DGD	C2B-C3B-C4B-C5B
22	c	510	CLA	CBD-CGD-O2D-CED
28	M	101	LMT	C4'-C5'-C6'-O6'
28	M	102	LMT	C11-C10-C9-C8
31	D	410	LHG	C1-C2-C3-O3
31	F	103	LHG	C1-C2-C3-O3
28	l	101	LMT	C11-C10-C9-C8
28	m	103	LMT	C2-C3-C4-C5
31	E	101	LHG	C9-C10-C11-C12
22	c	504	CLA	C8-C10-C11-C12
22	c	510	CLA	C10-C11-C12-C13
22	c	513	CLA	C15-C16-C17-C18
28	m	101	LMT	O1'-C1-C2-C3
26	A	411	LMG	C18-C19-C20-C21
28	t	102	LMT	C9-C10-C11-C12
28	z	101	LMT	C5-C6-C7-C8
32	B	628	HTG	C3'-C4'-C5'-C6'
22	A	408	CLA	C15-C16-C17-C18
26	d	412	LMG	O6-C5-C6-O5
26	a	412	LMG	C7-C8-C9-O8
26	c	521	LMG	O1-C7-C8-C9
28	a	401	LMT	C7-C8-C9-C10
31	e	101	LHG	C4-C5-C6-O8
33	D	408	DGD	C1G-C2G-C3G-O3G
33	c	519	DGD	CAA-CBA-CCA-CDA
26	C	519	LMG	C8-C7-O1-C1
26	c	521	LMG	C8-C7-O1-C1
33	C	516	DGD	C2G-C3G-O3G-C1D
33	C	516	DGD	C5D-C6D-O5D-C1E
33	c	518	DGD	C2G-C3G-O3G-C1D
33	c	518	DGD	C5D-C6D-O5D-C1E
28	c	522	LMT	C5-C6-C7-C8
31	E	101	LHG	C19-C20-C21-C22
22	b	620	CLA	C13-C15-C16-C17
26	a	412	LMG	C32-C33-C34-C35
28	B	623	LMT	C9-C10-C11-C12
33	c	518	DGD	C7A-C8A-C9A-CAA
28	c	522	LMT	O5'-C5'-C6'-O6'
31	E	101	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	f	102	LHG	C17-C18-C19-C20
33	d	408	DGD	CBB-CCB-CDB-CEB
22	B	614	CLA	C15-C16-C17-C18
31	d	410	LHG	O1-C1-C2-O2
31	f	102	LHG	O1-C1-C2-O2
28	l	101	LMT	C7-C8-C9-C10
26	b	625	LMG	C17-C18-C19-C20
28	F	102	LMT	C2-C3-C4-C5
31	E	101	LHG	C33-C34-C35-C36
33	C	517	DGD	CDB-CEB-CFB-CGB
28	a	401	LMT	O5B-C5B-C6B-O6B
26	A	411	LMG	C22-C23-C24-C25
28	C	520	LMT	C4-C5-C6-C7
26	C	519	LMG	C28-C29-C30-C31
22	a	409	CLA	CBA-CGA-O2A-C1
33	C	515	DGD	O6E-C5E-C6E-O5E
26	c	521	LMG	C29-C30-C31-C32
31	D	409	LHG	C29-C30-C31-C32
31	D	411	LHG	C30-C31-C32-C33
31	d	410	LHG	C11-C10-C9-C8
32	B	628	HTG	O5-C5-C6-O6
22	b	608	CLA	C15-C16-C17-C18
22	B	602	CLA	C2-C1-O2A-CGA
28	B	623	LMT	C4-C5-C6-C7
31	b	624	LHG	C29-C30-C31-C32
22	B	605	CLA	O1D-CGD-O2D-CED
32	C	522	HTG	O5-C5-C6-O6
22	a	409	CLA	O1D-CGD-O2D-CED
26	A	411	LMG	C20-C21-C22-C23
31	B	621	LHG	C17-C18-C19-C20
28	F	102	LMT	C3-C4-C5-C6
28	m	103	LMT	C9-C10-C11-C12
28	j	102	LMT	C7-C8-C9-C10
32	C	522	HTG	C2'-C3'-C4'-C5'
33	C	517	DGD	C2A-C3A-C4A-C5A
28	F	102	LMT	C2'-C1'-O1'-C1
26	A	411	LMG	O1-C7-C8-O7
26	A	411	LMG	O7-C8-C9-O8
26	c	521	LMG	O1-C7-C8-O7
28	a	401	LMT	O5'-C5'-C6'-O6'
28	J	102	LMT	O1'-C1-C2-C3
28	A	415	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	C	518	LMG	C29-C30-C31-C32
33	c	519	DGD	C2B-C3B-C4B-C5B
22	B	604	CLA	C6-C7-C8-C10
22	B	614	CLA	C12-C13-C15-C16
22	B	616	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C7
22	b	615	CLA	C12-C13-C15-C16
22	c	510	CLA	C12-C13-C15-C16
22	c	514	CLA	C11-C10-C8-C7
26	D	412	LMG	C39-C40-C41-C42
26	b	625	LMG	C29-C30-C31-C32
31	d	409	LHG	C29-C30-C31-C32
22	a	409	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	c	510	CLA	C14-C13-C15-C16
22	A	408	CLA	CBD-CGD-O2D-CED
28	m	102	LMT	C2-C3-C4-C5
32	O	302	HTG	C3'-C4'-C5'-C6'
28	a	401	LMT	C3-C4-C5-C6
22	A	405	CLA	O1D-CGD-O2D-CED
26	A	411	LMG	C17-C18-C19-C20
26	C	518	LMG	C15-C16-C17-C18
28	J	102	LMT	C11-C10-C9-C8
33	c	517	DGD	O6D-C5D-C6D-O5D
22	b	618	CLA	C5-C6-C7-C8
26	c	520	LMG	C11-C10-O7-C8
33	C	515	DGD	C4B-C5B-C6B-C7B
32	C	535	HTG	C2'-C1'-S1-C1
31	E	101	LHG	C29-C30-C31-C32
22	C	506	CLA	C5-C6-C7-C8
22	b	616	CLA	C13-C15-C16-C17
22	b	620	CLA	C8-C10-C11-C12
26	D	412	LMG	C18-C19-C20-C21
31	f	102	LHG	C29-C30-C31-C32
33	c	519	DGD	CBB-CCB-CDB-CEB
22	c	507	CLA	C16-C17-C18-C20
31	b	624	LHG	O6-C4-C5-C6
31	D	409	LHG	C28-C29-C30-C31
33	C	515	DGD	C6A-C7A-C8A-C9A
33	C	516	DGD	C1A-C2A-C3A-C4A
22	d	405	CLA	C8-C10-C11-C12
28	m	103	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
22	b	609	CLA	C4-C3-C5-C6
26	D	412	LMG	C40-C41-C42-C43
26	b	625	LMG	C36-C37-C38-C39
28	T	102	LMT	C4-C5-C6-C7
22	C	508	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	C16-C17-C18-C19
28	B	623	LMT	C11-C10-C9-C8
32	V	202	HTG	C4'-C5'-C6'-C7'
33	D	408	DGD	C5B-C6B-C7B-C8B
31	D	411	LHG	C2-C3-O3-P
31	d	411	LHG	C2-C3-O3-P
28	t	102	LMT	C4-C5-C6-C7
31	d	411	LHG	C30-C31-C32-C33
28	M	101	LMT	C2-C1-O1'-C1'
28	M	102	LMT	C2-C1-O1'-C1'
28	l	101	LMT	C2-C1-O1'-C1'
26	C	518	LMG	C39-C40-C41-C42
33	h	101	DGD	CDB-CEB-CFB-CGB
22	b	611	CLA	C3-C5-C6-C7
28	J	102	LMT	C3-C4-C5-C6
22	C	513	CLA	CBA-CGA-O2A-C1
31	F	103	LHG	C28-C29-C30-C31
31	d	411	LHG	C16-C17-C18-C19
33	C	516	DGD	C3B-C4B-C5B-C6B
28	J	102	LMT	O5'-C5'-C6'-O6'
33	H	101	DGD	O1G-C1G-C2G-C3G
33	h	101	DGD	O1G-C1G-C2G-C3G
33	C	516	DGD	C5A-C6A-C7A-C8A
26	B	622	LMG	C40-C41-C42-C43
31	d	410	LHG	C32-C33-C34-C35
32	U	203	HTG	C4-C5-C6-O6
33	d	408	DGD	C7A-C8A-C9A-CAA
33	d	408	DGD	C8A-C9A-CAA-CBA
22	C	512	CLA	C10-C11-C12-C13
33	c	517	DGD	CDA-CEA-CFA-CGA
31	D	409	LHG	C30-C31-C32-C33
33	c	518	DGD	C2B-C3B-C4B-C5B
31	e	101	LHG	C26-C27-C28-C29
22	a	409	CLA	C8-C10-C11-C12
26	d	412	LMG	C38-C39-C40-C41
28	c	522	LMT	C4-C5-C6-C7
31	b	624	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	B	621	LHG	C28-C29-C30-C31
33	C	516	DGD	C7B-C8B-C9B-CAB
33	H	101	DGD	CAB-CBB-CCB-CDB
28	t	102	LMT	C11-C10-C9-C8
22	b	616	CLA	C8-C10-C11-C12
31	D	409	LHG	C32-C33-C34-C35
22	b	615	CLA	C2C-C3C-CAC-CBC
26	d	412	LMG	C11-C12-C13-C14
33	H	101	DGD	CCA-CDA-CEA-CFA
26	a	412	LMG	O7-C8-C9-O8
31	e	101	LHG	O7-C5-C6-O8
26	B	622	LMG	C18-C19-C20-C21
31	B	621	LHG	C16-C17-C18-C19
33	h	101	DGD	CCA-CDA-CEA-CFA
22	B	615	CLA	C16-C17-C18-C20
33	h	101	DGD	C7B-C8B-C9B-CAB
22	A	408	CLA	C8-C10-C11-C12
22	c	507	CLA	C15-C16-C17-C18
26	b	625	LMG	C13-C14-C15-C16
26	c	520	LMG	O9-C10-O7-C8
22	D	403	CLA	C2-C1-O2A-CGA
22	c	511	CLA	C6-C7-C8-C9
32	b	640	HTG	C2'-C3'-C4'-C5'
22	B	609	CLA	C13-C15-C16-C17
26	C	518	LMG	C16-C17-C18-C19
26	c	520	LMG	C39-C40-C41-C42
28	C	520	LMT	C6-C7-C8-C9
33	c	518	DGD	C6B-C7B-C8B-C9B
24	b	621	BCR	C1-C6-C7-C8
24	y	101	BCR	C1-C6-C7-C8
33	C	517	DGD	C8A-C9A-CAA-CBA
24	A	409	BCR	C17-C18-C19-C20
33	D	408	DGD	CCA-CDA-CEA-CFA
31	e	101	LHG	C15-C16-C17-C18
33	C	515	DGD	C1B-C2B-C3B-C4B
22	C	510	CLA	O1D-CGD-O2D-CED
33	D	408	DGD	C4A-C5A-C6A-C7A
22	c	510	CLA	C13-C15-C16-C17
26	C	518	LMG	C38-C39-C40-C41
31	B	621	LHG	C9-C10-C11-C12
31	D	409	LHG	C11-C12-C13-C14
31	E	101	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
31	e	101	LHG	C18-C19-C20-C21
22	B	602	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	a	409	CLA	C11-C10-C8-C7
22	b	605	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	b	620	CLA	C11-C12-C13-C15
22	d	405	CLA	C6-C7-C8-C10
24	T	101	BCR	C13-C14-C15-C16
24	t	101	BCR	C13-C14-C15-C16
22	a	407	CLA	C2C-C3C-CAC-CBC
33	c	519	DGD	C8B-C9B-CAB-CBB
26	D	412	LMG	C13-C14-C15-C16
26	b	625	LMG	C32-C33-C34-C35
31	f	102	LHG	C14-C15-C16-C17
31	D	410	LHG	C32-C33-C34-C35
32	b	602	HTG	O5-C1-S1-C1'
32	c	523	HTG	O5-C1-S1-C1'
31	E	101	LHG	C23-C24-C25-C26
33	c	519	DGD	CBA-CCA-CDA-CEA
22	d	403	CLA	C13-C15-C16-C17
31	f	102	LHG	C28-C29-C30-C31
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	617	CLA	CAD-CBD-CGD-O2D
22	D	405	CLA	CAD-CBD-CGD-O2D
22	a	406	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O2D
23	a	408	PHO	CAD-CBD-CGD-O2D
26	C	519	LMG	C30-C31-C32-C33
28	t	102	LMT	O1'-C1-C2-C3
22	c	514	CLA	C13-C15-C16-C17
33	H	101	DGD	O2G-C1B-C2B-C3B
33	c	519	DGD	C9B-CAB-CBB-CCB
26	A	411	LMG	O6-C1-O1-C7
33	C	516	DGD	O6E-C1E-O5D-C6D
25	d	407	PL9	C39-C41-C42-C43
26	A	411	LMG	O1-C7-C8-C9
32	V	202	HTG	C4-C5-C6-O6
22	A	404	CLA	C2C-C3C-CAC-CBC
31	b	624	LHG	O6-C4-C5-O7
22	C	503	CLA	C8-C10-C11-C12
32	C	535	HTG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
33	H	101	DGD	C5B-C6B-C7B-C8B
22	B	602	CLA	CHA-CBD-CGD-O1D
22	B	603	CLA	CHA-CBD-CGD-O2D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	C	506	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	b	610	CLA	CHA-CBD-CGD-O1D
22	b	611	CLA	CHA-CBD-CGD-O1D
22	c	503	CLA	CHA-CBD-CGD-O2D
22	c	505	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	511	CLA	CHA-CBD-CGD-O1D
22	A	405	CLA	C4C-C3C-CAC-CBC
24	T	101	BCR	C12-C13-C14-C15
24	t	101	BCR	C12-C13-C14-C15
33	c	518	DGD	C2E-C1E-O5D-C6D
22	C	504	CLA	C13-C15-C16-C17
22	C	513	CLA	O1A-CGA-O2A-C1
34	e	104	GOL	O1-C1-C2-O2
26	c	521	LMG	C11-C12-C13-C14
33	D	408	DGD	C5A-C6A-C7A-C8A
25	A	410	PL9	C4-C3-C7-C8
22	B	614	CLA	C11-C12-C13-C14
22	B	614	CLA	C14-C13-C15-C16
22	d	405	CLA	C6-C7-C8-C9
28	l	101	LMT	C3-C4-C5-C6
31	d	409	LHG	C18-C19-C20-C21
33	C	517	DGD	C8B-C9B-CAB-CBB
26	d	412	LMG	C40-C41-C42-C43
33	H	101	DGD	C5A-C6A-C7A-C8A
28	C	520	LMT	C3-C4-C5-C6
32	B	642	HTG	C3'-C4'-C5'-C6'
32	b	640	HTG	S1-C1'-C2'-C3'
22	b	618	CLA	C3-C5-C6-C7
28	j	102	LMT	C11-C10-C9-C8
22	C	505	CLA	C16-C17-C18-C19
22	a	407	CLA	C16-C17-C18-C20
31	d	410	LHG	C3-O3-P-O6
33	C	515	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
32	o	301	HTG	C4-C5-C6-O6
25	d	407	PL9	C43-C44-C46-C47
33	H	101	DGD	CCB-CDB-CEB-CFB
31	B	621	LHG	C4-O6-P-O5
31	E	101	LHG	C3-O3-P-O4
31	f	102	LHG	C3-O3-P-O4
22	B	605	CLA	C2C-C3C-CAC-CBC
22	B	611	CLA	C8-C10-C11-C12
22	C	509	CLA	C10-C11-C12-C13
26	a	412	LMG	C35-C36-C37-C38
33	h	101	DGD	C8A-C9A-CAA-CBA
22	b	613	CLA	O1D-CGD-O2D-CED
33	h	101	DGD	O2G-C1B-C2B-C3B
22	B	602	CLA	CAD-CBD-CGD-O1D
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	608	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CAD-CBD-CGD-O1D
22	b	611	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
22	c	507	CLA	CAD-CBD-CGD-O1D
22	c	511	CLA	CAD-CBD-CGD-O1D
33	c	517	DGD	C4D-C5D-C6D-O5D
26	B	622	LMG	O8-C28-C29-C30
22	b	610	CLA	C8-C10-C11-C12
22	b	615	CLA	C15-C16-C17-C18
26	c	521	LMG	C31-C32-C33-C34
22	d	402	CLA	C2C-C3C-CAC-CBC
33	C	515	DGD	C3A-C4A-C5A-C6A
31	E	101	LHG	C7-C8-C9-C10
22	b	605	CLA	CBA-CGA-O2A-C1
22	c	511	CLA	O1D-CGD-O2D-CED
31	d	409	LHG	C1-C2-C3-O3
31	b	624	LHG	C16-C17-C18-C19
22	a	409	CLA	C16-C17-C18-C19
25	d	407	PL9	C45-C44-C46-C47
22	B	606	CLA	O1D-CGD-O2D-CED
22	A	406	CLA	C11-C10-C8-C7
22	A	408	CLA	C12-C13-C15-C16
22	C	504	CLA	C12-C13-C15-C16
22	D	405	CLA	C6-C7-C8-C10
22	a	407	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	a	407	CLA	C12-C13-C15-C16
22	b	620	CLA	C6-C7-C8-C10
32	B	624	HTG	C2-C1-S1-C1'
32	c	541	HTG	C2-C1-S1-C1'
32	c	523	HTG	C2'-C3'-C4'-C5'
33	C	517	DGD	O6D-C5D-C6D-O5D
28	B	623	LMT	C2-C1-O1'-C1'
33	H	101	DGD	C7B-C8B-C9B-CAB
31	F	103	LHG	C11-C10-C9-C8
32	B	628	HTG	C4'-C5'-C6'-C7'
31	d	409	LHG	C16-C17-C18-C19
26	A	411	LMG	C7-C8-C9-O8
28	Z	101	LMT	O1'-C1-C2-C3
33	H	101	DGD	O1G-C1G-C2G-O2G
31	b	624	LHG	C12-C13-C14-C15
32	b	640	HTG	C4-C5-C6-O6
22	b	611	CLA	O1D-CGD-O2D-CED
31	B	621	LHG	C34-C35-C36-C37
33	h	101	DGD	CDA-CEA-CFA-CGA
22	c	514	CLA	O1A-CGA-O2A-C1
33	c	519	DGD	C2A-C1A-O1G-C1G
33	C	517	DGD	C3B-C4B-C5B-C6B
22	B	602	CLA	CAA-CBA-CGA-O2A
22	B	607	CLA	C11-C10-C8-C9
22	B	616	CLA	C14-C13-C15-C16
22	a	407	CLA	C11-C12-C13-C14
22	a	407	CLA	C14-C13-C15-C16
22	a	409	CLA	C11-C12-C13-C14
22	b	605	CLA	C6-C7-C8-C9
31	d	410	LHG	C26-C27-C28-C29
28	j	102	LMT	O1'-C1-C2-C3
33	c	518	DGD	O6E-C1E-O5D-C6D
26	c	521	LMG	C40-C41-C42-C43
31	D	409	LHG	C24-C25-C26-C27
28	m	102	LMT	C7-C8-C9-C10
32	O	302	HTG	C4'-C5'-C6'-C7'
33	c	518	DGD	C1A-C2A-C3A-C4A
28	M	102	LMT	C5-C6-C7-C8
31	E	101	LHG	C27-C28-C29-C30
22	A	408	CLA	C10-C11-C12-C13
22	C	510	CLA	C8-C10-C11-C12
31	b	624	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
26	C	518	LMG	C19-C20-C21-C22
28	b	626	LMT	C7-C8-C9-C10
26	D	412	LMG	C38-C39-C40-C41
22	b	605	CLA	O1A-CGA-O2A-C1
22	b	605	CLA	C16-C17-C18-C20
22	C	504	CLA	O1D-CGD-O2D-CED
24	b	621	BCR	C5-C6-C7-C8
22	A	404	CLA	C4C-C3C-CAC-CBC
26	C	518	LMG	C18-C19-C20-C21
22	c	514	CLA	CBA-CGA-O2A-C1
22	B	603	CLA	C13-C15-C16-C17
22	c	511	CLA	C8-C10-C11-C12
22	B	607	CLA	O1D-CGD-O2D-CED
32	B	642	HTG	O5-C5-C6-O6
28	b	626	LMT	C2-C3-C4-C5
31	D	410	LHG	C3-O3-P-O6
26	B	622	LMG	C38-C39-C40-C41
26	a	412	LMG	C19-C20-C21-C22
33	C	515	DGD	O6D-C5D-C6D-O5D
28	z	101	LMT	O1'-C1-C2-C3
23	D	404	PHO	CHA-CBD-CGD-O2D
33	c	519	DGD	C3B-C4B-C5B-C6B
31	e	101	LHG	C13-C14-C15-C16
22	b	610	CLA	O1D-CGD-O2D-CED
25	A	410	PL9	C20-C19-C21-C22
26	c	521	LMG	C15-C16-C17-C18
32	c	524	HTG	C1'-C2'-C3'-C4'
28	m	103	LMT	C4'-C5'-C6'-O6'
22	C	506	CLA	C6-C7-C8-C10
22	a	409	CLA	C11-C12-C13-C15
22	c	511	CLA	C6-C7-C8-C10
22	c	514	CLA	C11-C12-C13-C15
22	c	510	CLA	C3-C5-C6-C7
22	b	620	CLA	C11-C12-C13-C14
22	c	505	CLA	C8-C10-C11-C12
33	c	518	DGD	C7B-C8B-C9B-CAB
22	C	509	CLA	C8-C10-C11-C12
22	c	502	CLA	C16-C17-C18-C20
31	d	411	LHG	O1-C1-C2-C3
32	o	301	HTG	C1'-C2'-C3'-C4'
33	h	101	DGD	CBA-CCA-CDA-CEA
28	b	626	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	D	411	LHG	C18-C19-C20-C21
33	C	517	DGD	CAA-CBA-CCA-CDA
22	C	510	CLA	C2-C3-C5-C6
28	t	102	LMT	C2-C3-C4-C5
22	b	615	CLA	C10-C11-C12-C13
37	f	101	HEM	CAA-CBA-CGA-O1A
28	b	626	LMT	C11-C10-C9-C8
28	j	102	LMT	C3-C4-C5-C6
33	H	101	DGD	C8A-C9A-CAA-CBA
22	C	507	CLA	C15-C16-C17-C18
22	c	502	CLA	C13-C15-C16-C17
31	d	409	LHG	C17-C18-C19-C20
28	z	101	LMT	C2B-C1B-O1B-C4'
26	A	411	LMG	C40-C41-C42-C43
31	D	411	LHG	C9-C10-C11-C12
26	A	411	LMG	C21-C22-C23-C24
26	c	520	LMG	C31-C32-C33-C34
26	d	412	LMG	C13-C14-C15-C16
32	U	203	HTG	C2'-C1'-S1-C1
33	d	408	DGD	C5B-C6B-C7B-C8B
22	A	406	CLA	C13-C15-C16-C17
33	h	101	DGD	C4D-C5D-C6D-O5D
23	a	408	PHO	C2-C3-C5-C6
26	b	625	LMG	O8-C28-C29-C30
22	b	618	CLA	C2-C1-O2A-CGA
31	F	103	LHG	C9-C10-C11-C12
22	B	605	CLA	C16-C17-C18-C20
31	E	101	LHG	O7-C5-C6-O8
26	c	521	LMG	C20-C21-C22-C23
37	F	101	HEM	CAD-CBD-CGD-O1D
22	B	604	CLA	CBD-CGD-O2D-CED
31	B	621	LHG	C29-C30-C31-C32
22	D	405	CLA	C6-C7-C8-C9
23	a	408	PHO	C14-C13-C15-C16
31	D	411	LHG	C1-C2-C3-O3
22	B	612	CLA	C15-C16-C17-C18
31	d	411	LHG	C27-C28-C29-C30
31	b	624	LHG	C5-C6-O8-C23
22	A	405	CLA	C15-C16-C17-C18
22	C	510	CLA	C4-C3-C5-C6
22	b	620	CLA	C4-C3-C5-C6
22	B	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	408	CLA	C6-C7-C8-C10
22	B	607	CLA	C6-C7-C8-C10
22	B	608	CLA	C12-C13-C15-C16
22	C	503	CLA	C6-C7-C8-C10
22	c	503	CLA	C11-C12-C13-C15
26	c	520	LMG	O7-C10-C11-C12
31	D	410	LHG	C4-O6-P-O3
33	h	101	DGD	C9B-CAB-CBB-CCB
26	A	411	LMG	C31-C32-C33-C34
22	b	606	CLA	C2A-CAA-CBA-CGA
31	b	624	LHG	C25-C26-C27-C28
22	B	615	CLA	C10-C11-C12-C13
37	F	101	HEM	CAD-CBD-CGD-O2D
26	B	622	LMG	C34-C35-C36-C37
31	E	101	LHG	C14-C15-C16-C17
22	b	605	CLA	C4-C3-C5-C6
25	a	411	PL9	C25-C24-C26-C27
28	A	415	LMT	C7-C8-C9-C10
28	Z	101	LMT	C4-C5-C6-C7
22	C	504	CLA	C5-C6-C7-C8
25	A	410	PL9	C18-C19-C21-C22
26	C	518	LMG	C20-C21-C22-C23
26	D	412	LMG	C32-C33-C34-C35
22	c	513	CLA	O1A-CGA-O2A-C1
37	f	101	HEM	CAA-CBA-CGA-O2A
26	C	519	LMG	O7-C8-C9-O8
22	b	620	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	C16-C17-C18-C19
28	m	101	LMT	C7-C8-C9-C10
22	C	506	CLA	C2-C1-O2A-CGA
22	d	402	CLA	C2-C1-O2A-CGA
22	b	618	CLA	C14-C13-C15-C16
22	c	509	CLA	C11-C10-C8-C9
31	d	411	LHG	C12-C13-C14-C15
32	b	601	HTG	C4'-C5'-C6'-C7'
33	c	519	DGD	O1A-C1A-O1G-C1G
33	C	516	DGD	C9B-CAB-CBB-CCB
26	a	412	LMG	O8-C28-C29-C30
26	c	521	LMG	C8-C9-O8-C28
28	C	520	LMT	C7-C8-C9-C10
24	Y	101	BCR	C1-C6-C7-C8
22	b	618	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	f	102	LHG	C12-C13-C14-C15
22	B	617	CLA	C13-C15-C16-C17
22	d	403	CLA	C15-C16-C17-C18
22	A	408	CLA	O1A-CGA-O2A-C1
25	a	411	PL9	C15-C14-C16-C17
26	B	622	LMG	C20-C21-C22-C23
22	c	506	CLA	C2-C3-C5-C6
22	b	618	CLA	C16-C17-C18-C19
22	c	502	CLA	C16-C17-C18-C19
26	C	518	LMG	C13-C14-C15-C16
31	D	411	LHG	C29-C30-C31-C32
28	l	101	LMT	C1-C2-C3-C4
40	V	201	HEC	CAD-CBD-CGD-O2D
28	t	102	LMT	O5'-C5'-C6'-O6'
22	b	605	CLA	CAA-CBA-CGA-O2A
22	C	513	CLA	C4-C3-C5-C6
25	A	410	PL9	C15-C14-C16-C17
25	a	411	PL9	C39-C41-C42-C43
22	B	603	CLA	C11-C12-C13-C15
22	B	614	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C10-C8-C7
22	C	510	CLA	C6-C7-C8-C10
22	b	618	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C10-C8-C7
37	f	101	HEM	CAD-CBD-CGD-O1D
22	c	513	CLA	CBA-CGA-O2A-C1
31	E	101	LHG	O1-C1-C2-O2
33	c	517	DGD	C3A-C4A-C5A-C6A
26	A	411	LMG	C2-C1-O1-C7
33	h	101	DGD	CBB-CCB-CDB-CEB
28	m	101	LMT	C4'-C5'-C6'-O6'
28	B	623	LMT	C2B-C1B-O1B-C4'
32	O	302	HTG	C2'-C1'-S1-C1
31	B	621	LHG	C35-C36-C37-C38
22	b	620	CLA	C2-C3-C5-C6
22	A	408	CLA	C16-C17-C18-C20
22	B	607	CLA	C11-C12-C13-C14
22	C	504	CLA	C6-C7-C8-C9
22	C	504	CLA	C14-C13-C15-C16
22	a	407	CLA	C11-C10-C8-C9
22	b	610	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	619	CLA	C14-C13-C15-C16
22	c	513	CLA	C6-C7-C8-C9
22	c	514	CLA	C11-C12-C13-C14
26	a	412	LMG	C39-C40-C41-C42
31	E	101	LHG	C34-C35-C36-C37
22	D	405	CLA	C13-C15-C16-C17
22	A	404	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	b	607	CLA	CAD-CBD-CGD-O2D
22	b	608	CLA	CAD-CBD-CGD-O2D
22	b	611	CLA	CAD-CBD-CGD-O2D
22	b	620	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O2D
22	c	505	CLA	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
22	c	511	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	CAD-CBD-CGD-O2D
22	c	514	CLA	CAD-CBD-CGD-O2D
22	d	405	CLA	CAD-CBD-CGD-O2D
23	A	407	PHO	CAD-CBD-CGD-O2D
22	d	405	CLA	C10-C11-C12-C13
40	v	202	HEC	CAD-CBD-CGD-O2D
31	b	624	LHG	C10-C11-C12-C13
33	D	408	DGD	C8A-C9A-CAA-CBA
22	c	513	CLA	CAA-CBA-CGA-O2A
40	v	202	HEC	CAD-CBD-CGD-O1D
33	D	408	DGD	C3A-C4A-C5A-C6A
22	b	605	CLA	C2-C3-C5-C6
25	a	411	PL9	C13-C14-C16-C17
23	d	404	PHO	C2C-C3C-CAC-CBC
31	e	101	LHG	O6-C4-C5-O7
40	V	201	HEC	CAD-CBD-CGD-O1D
33	D	408	DGD	C8B-C9B-CAB-CBB
22	B	605	CLA	O2A-C1-C2-C3
22	B	614	CLA	O2A-C1-C2-C3
22	C	512	CLA	O2A-C1-C2-C3
22	b	617	CLA	O2A-C1-C2-C3
22	d	402	CLA	O2A-C1-C2-C3
23	A	407	PHO	O2A-C1-C2-C3
28	M	101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	d	408	DGD	C3B-C4B-C5B-C6B
22	B	605	CLA	C16-C17-C18-C19
33	C	515	DGD	C8A-C9A-CAA-CBA
22	A	405	CLA	CHA-CBD-CGD-O2D
22	A	406	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	CHA-CBD-CGD-O1D
22	B	604	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O2D
22	B	608	CLA	CHA-CBD-CGD-O2D
22	B	617	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O1D
22	a	407	CLA	CHA-CBD-CGD-O1D
22	a	407	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	b	610	CLA	CHA-CBD-CGD-O2D
22	b	613	CLA	CHA-CBD-CGD-O2D
22	b	616	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	511	CLA	CHA-CBD-CGD-O2D
22	d	403	CLA	CHA-CBD-CGD-O2D
28	A	415	LMT	C11-C10-C9-C8
25	A	410	PL9	C13-C14-C16-C17
28	j	102	LMT	O5'-C1'-O1'-C1
32	d	413	HTG	C1'-C2'-C3'-C4'
32	o	301	HTG	O5-C5-C6-O6
22	C	512	CLA	CAA-CBA-CGA-O2A
22	c	506	CLA	CAA-CBA-CGA-O2A
26	C	519	LMG	O1-C7-C8-O7
31	d	409	LHG	O7-C7-C8-C9
33	D	408	DGD	O2G-C1B-C2B-C3B
22	B	616	CLA	C8-C10-C11-C12
33	C	517	DGD	O1G-C1A-C2A-C3A
22	C	504	CLA	C6-C7-C8-C10
22	C	513	CLA	C2-C3-C5-C6
22	b	608	CLA	C12-C13-C15-C16
31	f	102	LHG	C11-C12-C13-C14
22	A	406	CLA	C11-C10-C8-C9
22	B	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	C14-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C9
22	C	510	CLA	C6-C7-C8-C9
22	c	503	CLA	C11-C12-C13-C14
31	b	624	LHG	O2-C2-C3-O3
31	b	624	LHG	C7-C8-C9-C10
31	d	411	LHG	C24-C25-C26-C27
26	A	411	LMG	O8-C28-C29-C30
22	C	512	CLA	C3-C5-C6-C7
25	a	411	PL9	C21-C22-C23-C24
31	b	624	LHG	C17-C18-C19-C20
32	b	601	HTG	C3'-C4'-C5'-C6'
33	c	519	DGD	C7A-C8A-C9A-CAA
23	D	404	PHO	C8-C10-C11-C12
23	a	408	PHO	C8-C10-C11-C12
26	c	521	LMG	C39-C40-C41-C42
22	c	508	CLA	C10-C11-C12-C13
26	b	625	LMG	C12-C13-C14-C15
26	c	521	LMG	C22-C23-C24-C25
33	h	101	DGD	C3B-C4B-C5B-C6B
22	b	608	CLA	C1A-C2A-CAA-CBA
32	c	523	HTG	C3'-C4'-C5'-C6'
22	B	617	CLA	C16-C17-C18-C19
37	f	101	HEM	CAD-CBD-CGD-O2D
25	A	410	PL9	C21-C22-C23-C24
32	C	521	HTG	O5-C5-C6-O6
26	a	412	LMG	C15-C16-C17-C18
22	C	501	CLA	C2A-CAA-CBA-CGA
28	A	415	LMT	C4-C5-C6-C7
33	d	408	DGD	C9A-CAA-CBA-CCA
26	C	519	LMG	C11-C12-C13-C14
33	c	518	DGD	CBB-CCB-CDB-CEB
33	c	517	DGD	C2A-C3A-C4A-C5A
22	c	506	CLA	CAA-CBA-CGA-O1A
31	B	621	LHG	C33-C34-C35-C36
33	C	516	DGD	CBB-CCB-CDB-CEB
31	D	410	LHG	C4-O6-P-O5
31	E	101	LHG	C4-O6-P-O5
31	d	410	LHG	C3-O3-P-O4
22	C	512	CLA	CAA-CBA-CGA-O1A
22	C	510	CLA	CAA-CBA-CGA-O2A
24	y	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	D	410	LHG	C25-C26-C27-C28
33	c	518	DGD	CAB-CBB-CCB-CDB
33	h	101	DGD	C2B-C3B-C4B-C5B
31	e	101	LHG	C11-C10-C9-C8
22	c	513	CLA	CAA-CBA-CGA-O1A
33	h	101	DGD	C5B-C6B-C7B-C8B
22	B	603	CLA	CAD-CBD-CGD-O1D
22	B	610	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O1D
22	b	616	CLA	CAD-CBD-CGD-O1D
31	E	101	LHG	C31-C32-C33-C34
22	B	605	CLA	C11-C10-C8-C9
22	B	606	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C12-C13-C14
22	C	506	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	C	513	CLA	C6-C7-C8-C9
22	b	614	CLA	C11-C12-C13-C14
34	D	417	GOL	O2-C2-C3-O3
33	C	515	DGD	C7A-C8A-C9A-CAA
22	A	404	CLA	C15-C16-C17-C18
33	D	408	DGD	O1B-C1B-C2B-C3B
22	C	505	CLA	CAA-CBA-CGA-O2A
31	b	624	LHG	O7-C7-C8-C9
33	C	516	DGD	O2G-C1B-C2B-C3B
32	V	202	HTG	C2'-C3'-C4'-C5'
32	B	629	HTG	C3'-C4'-C5'-C6'
24	D	406	BCR	C37-C22-C23-C24
22	A	404	CLA	C11-C10-C8-C7
22	B	612	CLA	C11-C12-C13-C15
22	C	513	CLA	C12-C13-C15-C16
22	a	409	CLA	C12-C13-C15-C16
22	b	619	CLA	C12-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C10
22	c	513	CLA	C11-C10-C8-C7
32	b	627	HTG	C2-C1-S1-C1'
32	O	302	HTG	C2'-C3'-C4'-C5'
22	b	606	CLA	CAA-CBA-CGA-O2A
31	f	102	LHG	C31-C32-C33-C34
28	b	626	LMT	C5'-C4'-O1B-C1B
22	A	408	CLA	C16-C17-C18-C19
28	b	626	LMT	C2-C1-O1'-C1'

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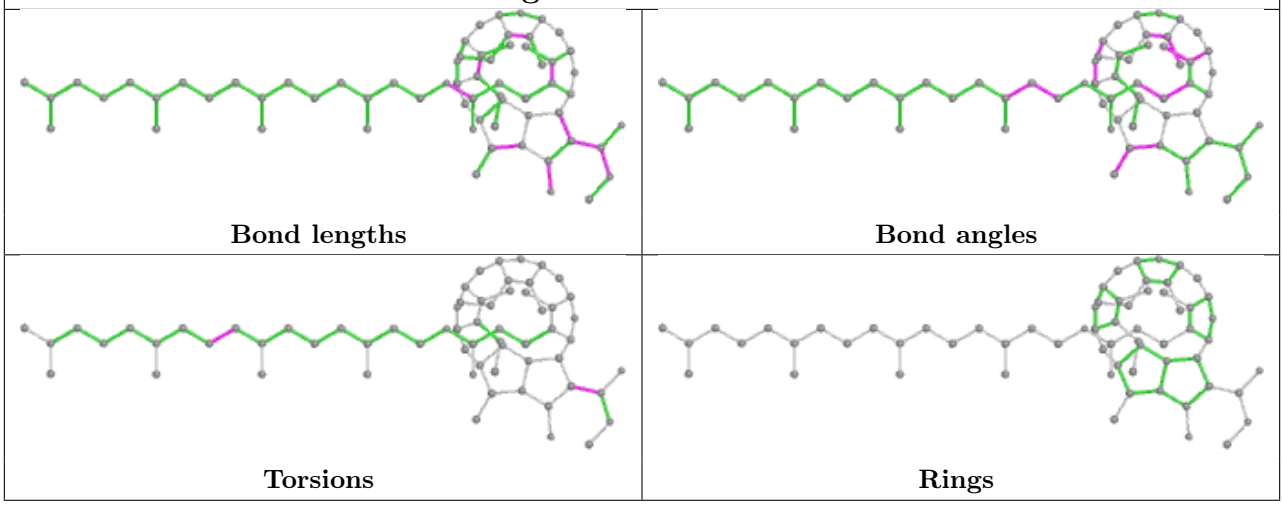
Mol	Chain	Res	Type	Atoms
28	z	101	LMT	C2-C1-O1'-C1'
22	c	511	CLA	CAA-CBA-CGA-O2A
26	b	625	LMG	O9-C10-O7-C8
22	C	501	CLA	CAA-CBA-CGA-O1A
33	C	516	DGD	O1B-C1B-C2B-C3B
26	c	520	LMG	C4-C5-C6-O5
22	b	620	CLA	C10-C11-C12-C13
31	D	411	LHG	O2-C2-C3-O3
22	C	501	CLA	CAA-CBA-CGA-O2A
22	c	502	CLA	CAA-CBA-CGA-O2A
33	c	517	DGD	O1G-C1A-C2A-C3A
22	c	514	CLA	C5-C6-C7-C8
22	C	510	CLA	CAA-CBA-CGA-O1A
37	F	101	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

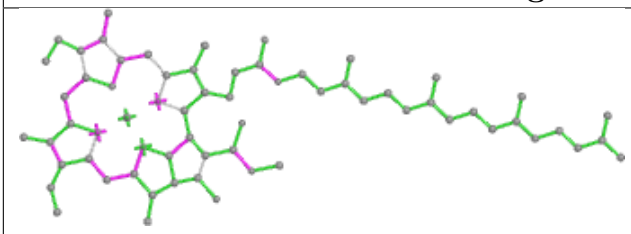
No monomer is involved in short contacts.

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.

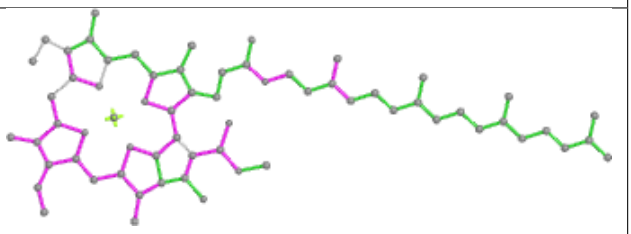
Ligand PHO D 404



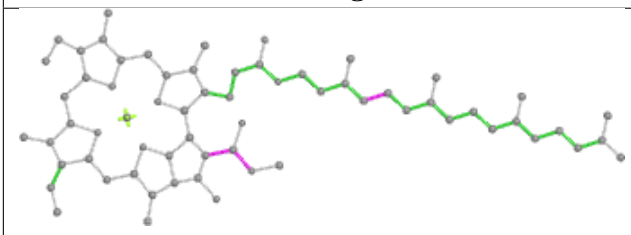
Ligand CLA b 611



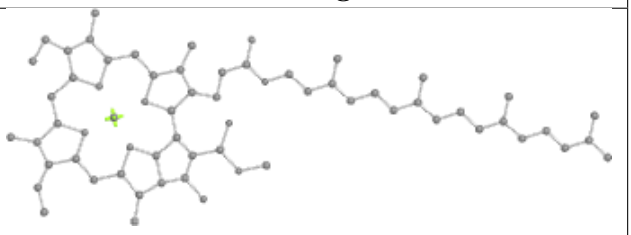
Bond lengths



Bond angles

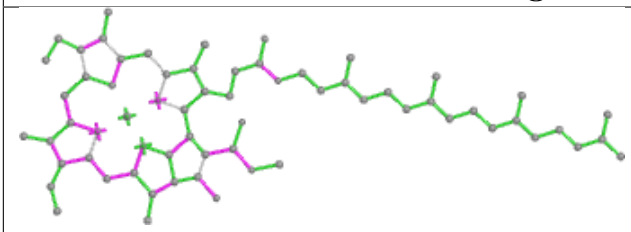


Torsions



Rings

Ligand CLA b 614



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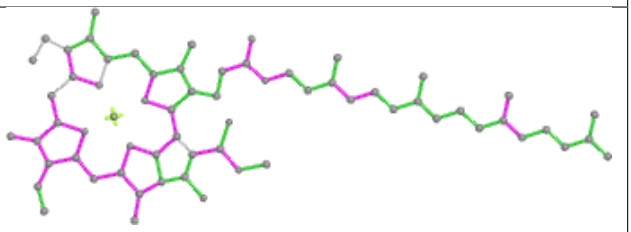

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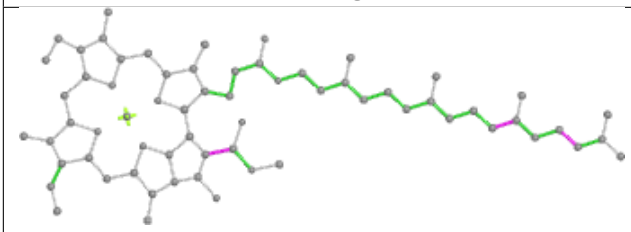
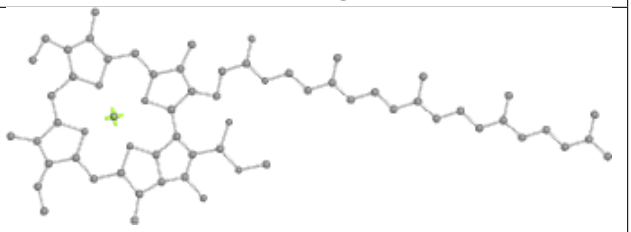
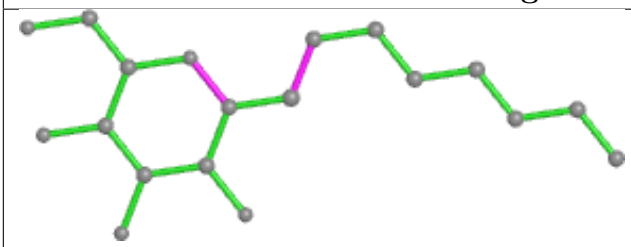


Torsions

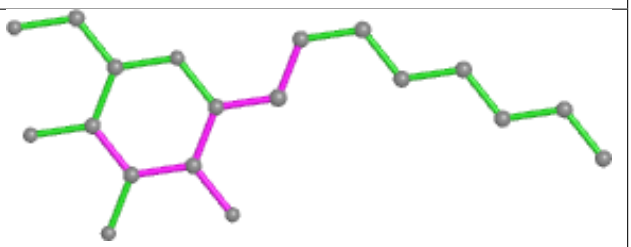


Rings

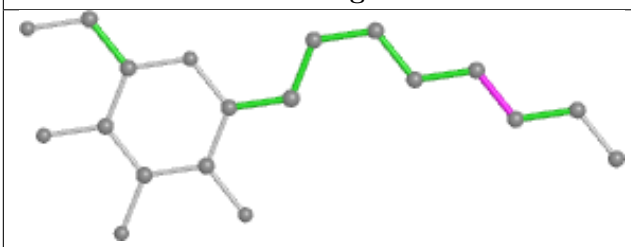
Ligand HTG B 629



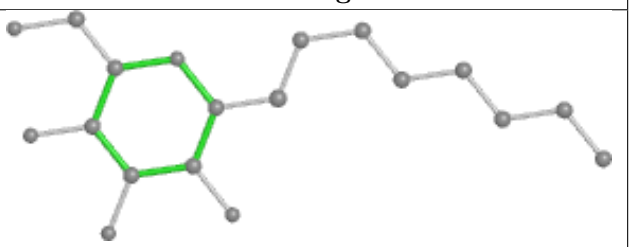
Bond lengths



Bond angles

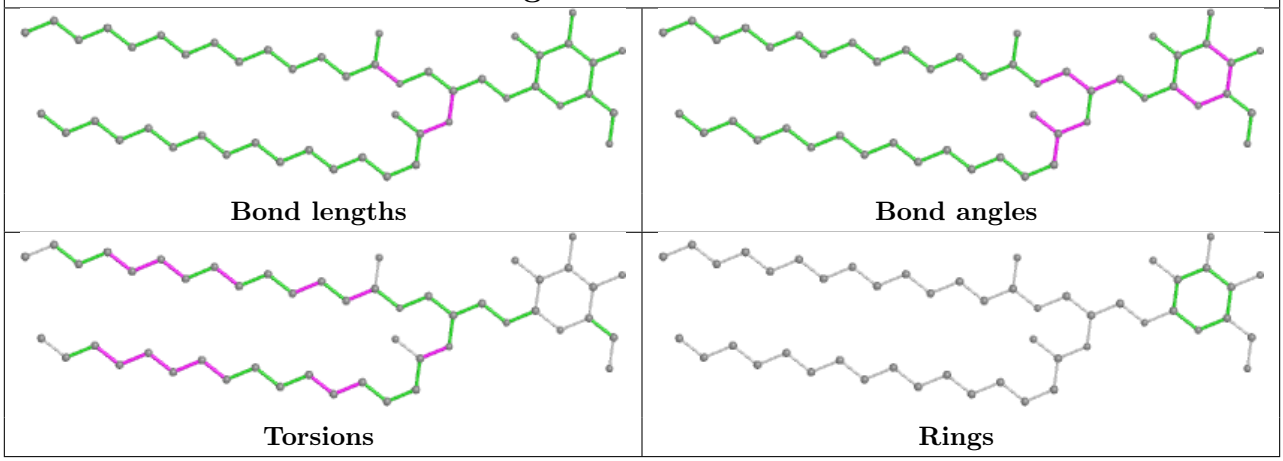


Torsions

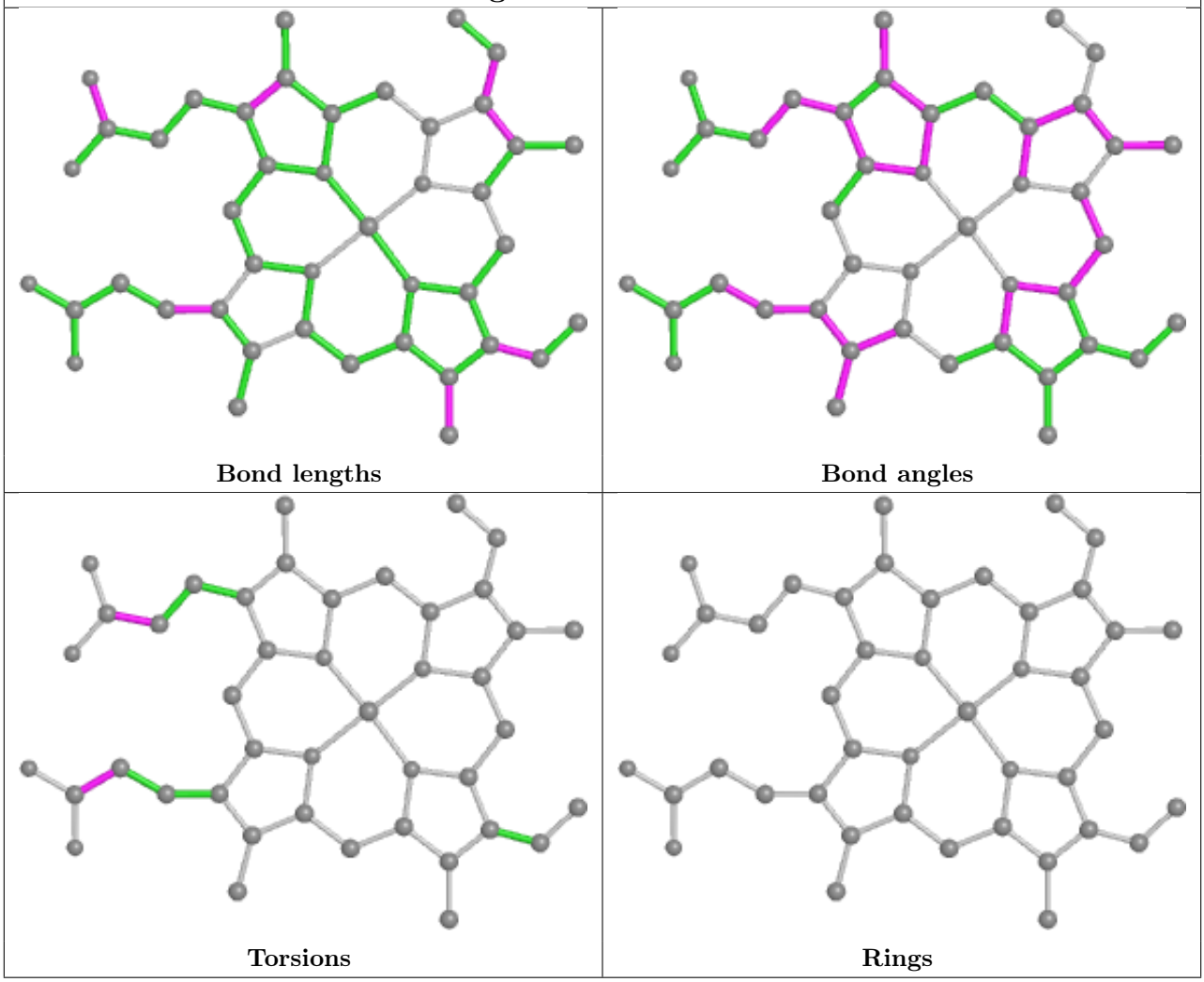


Rings

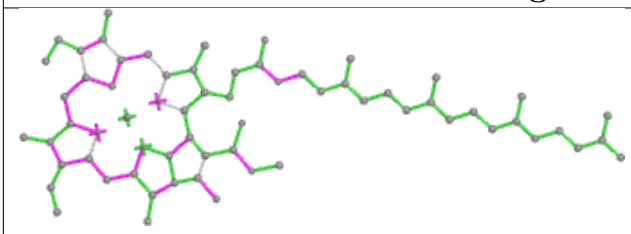
Ligand LMG b 625



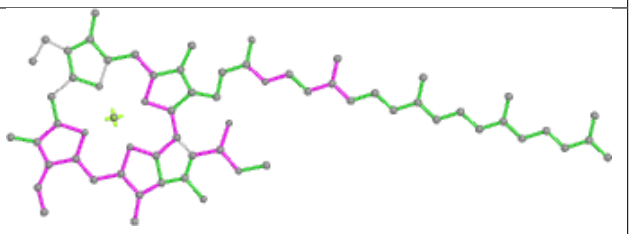
Ligand HEM F 101



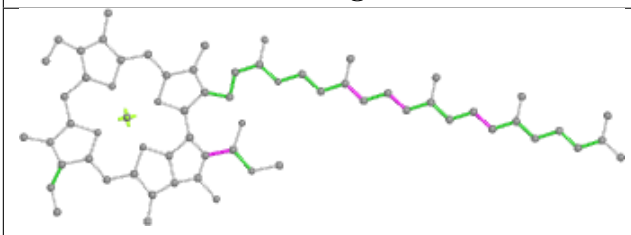
Ligand CLA c 508



Bond lengths



Bond angles



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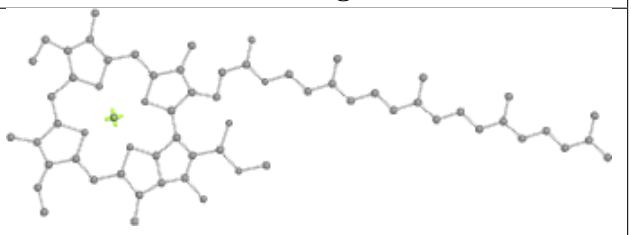

Rings

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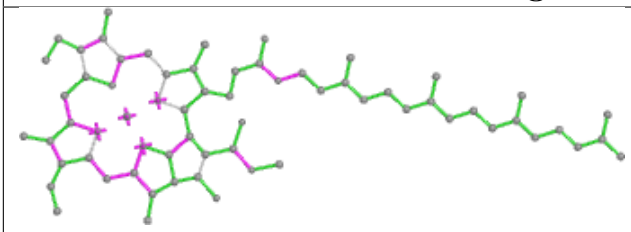

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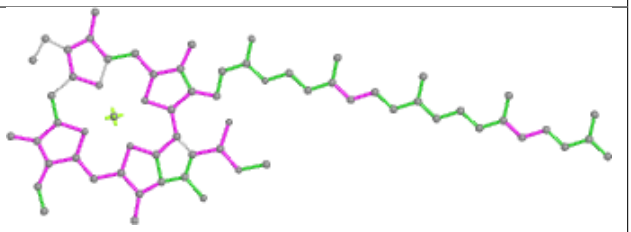

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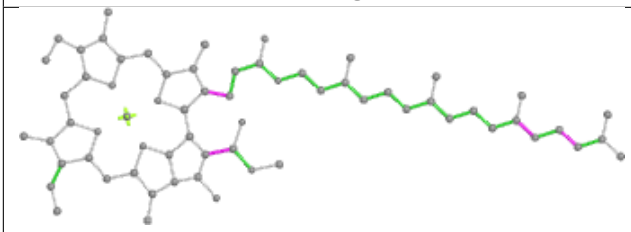

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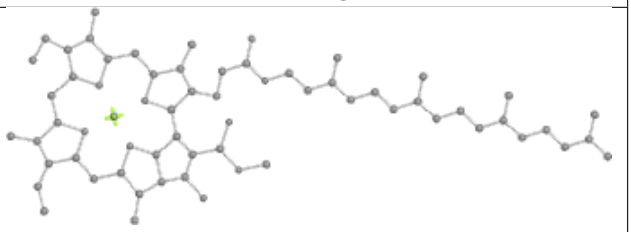

Rings

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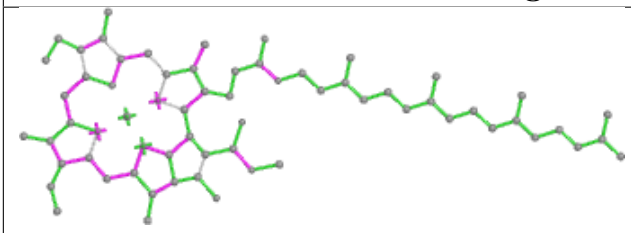

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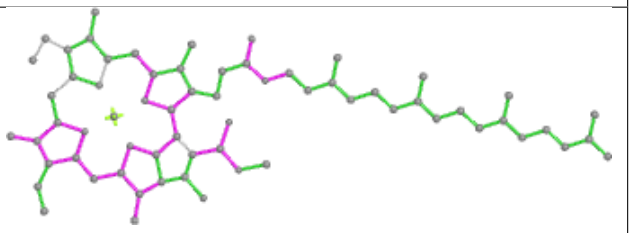

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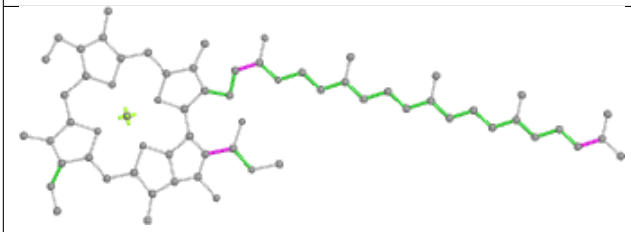

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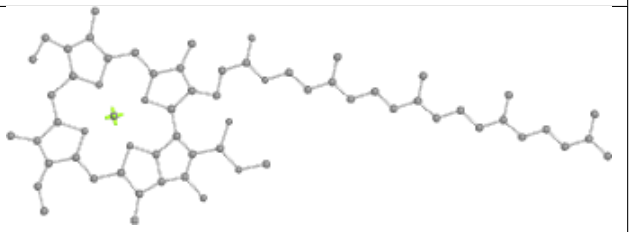

Rings

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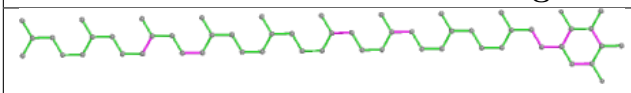
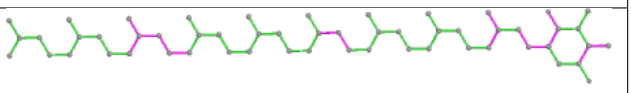
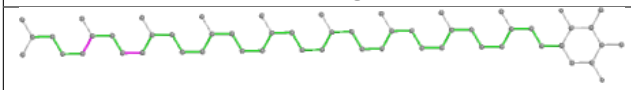
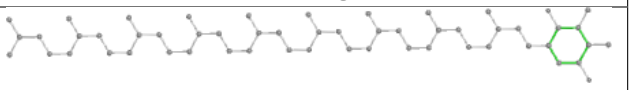
 Bond lengths	 Bond angles
 Torsions	 Rings

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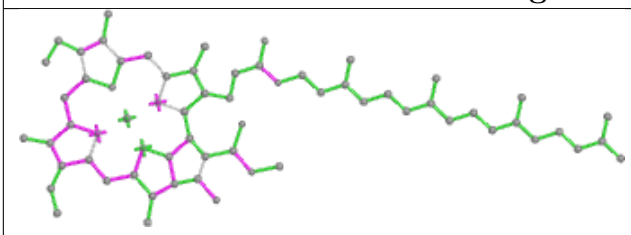
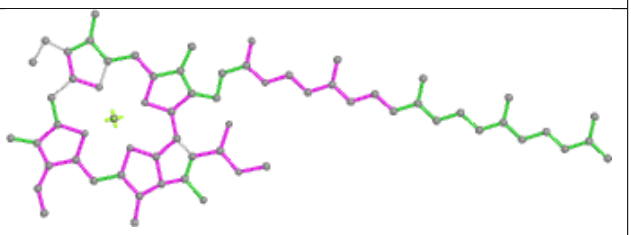
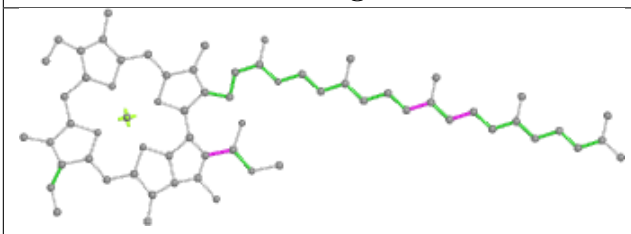
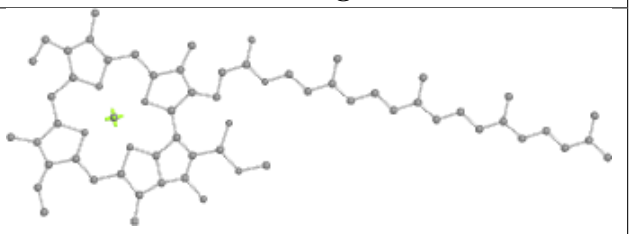
 Bond lengths	 Bond angles
 Torsions	 Rings

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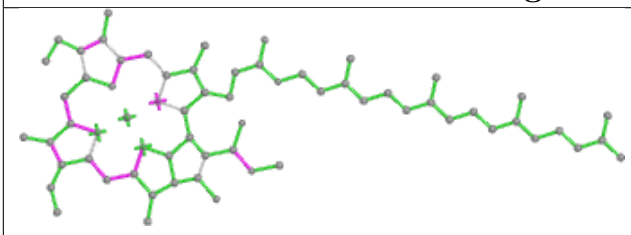
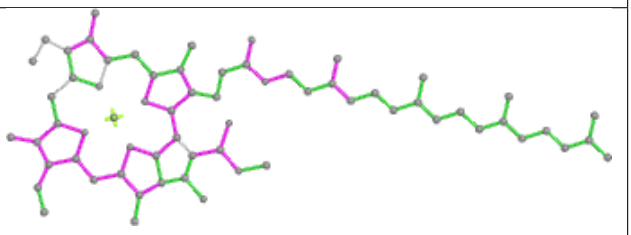
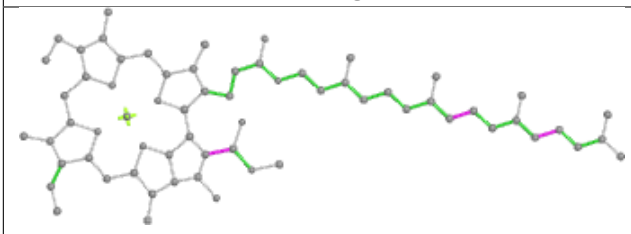
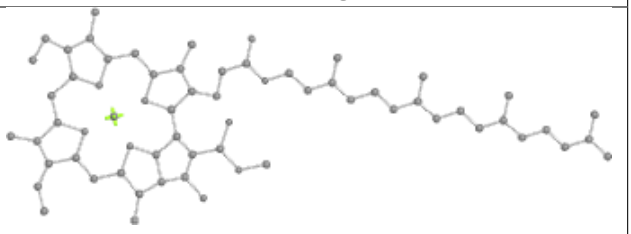
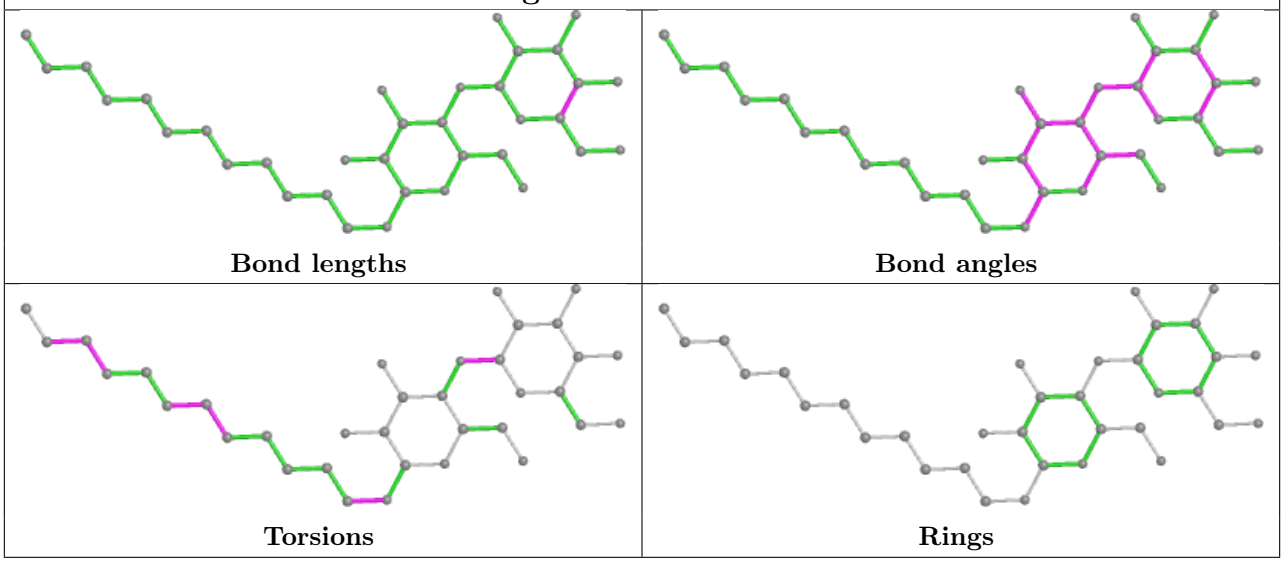
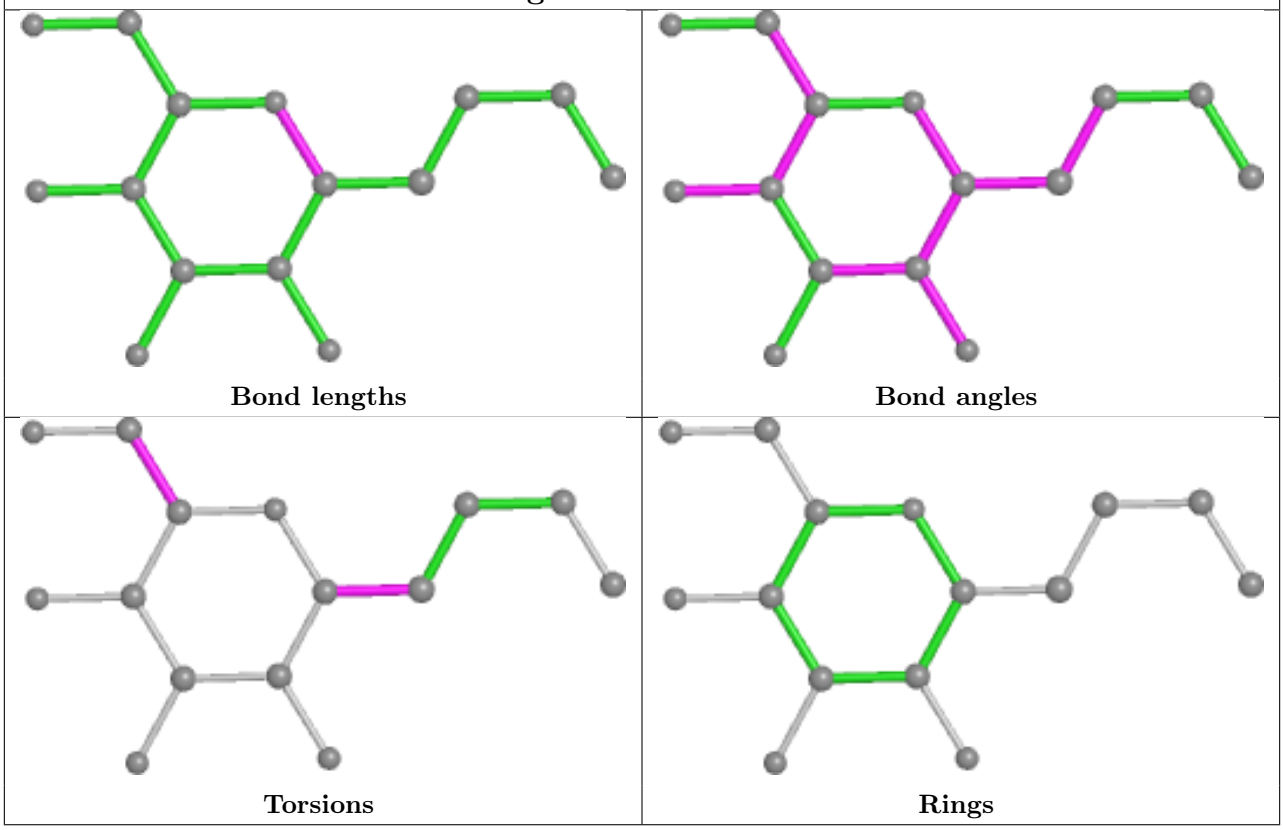
 Bond lengths	 Bond angles
 Torsions	 Rings

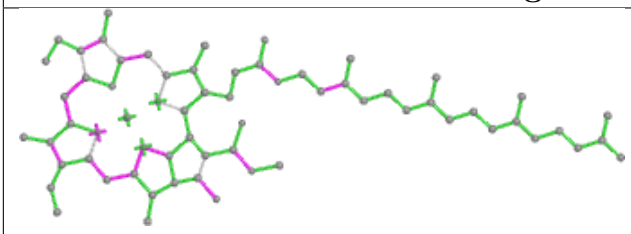
Ligand LMT B 623



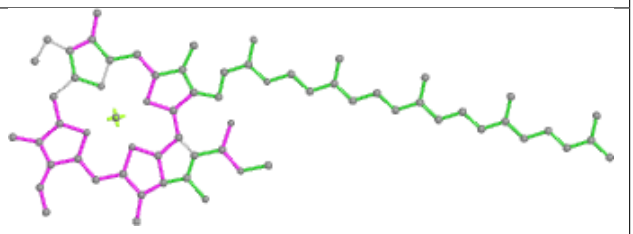
Ligand HTG c 541



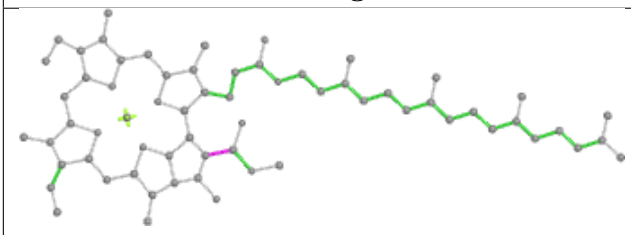
Ligand CLA B 610



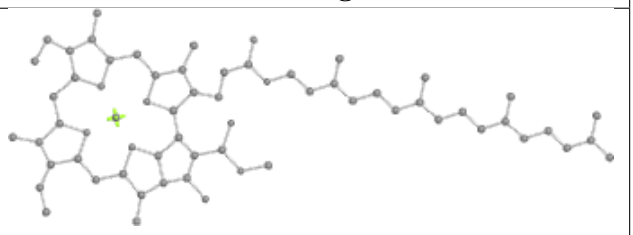
Bond lengths



Bond angles

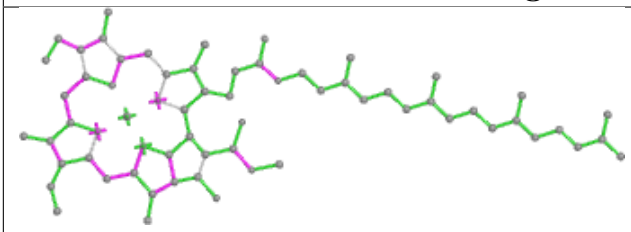


Torsions

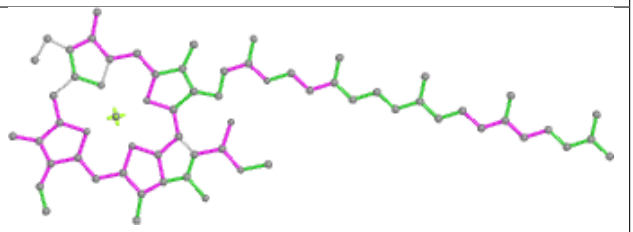


Rings

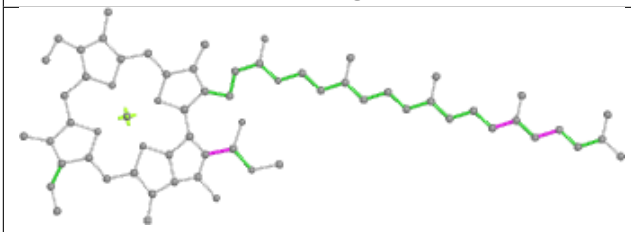
Ligand CLA B 603



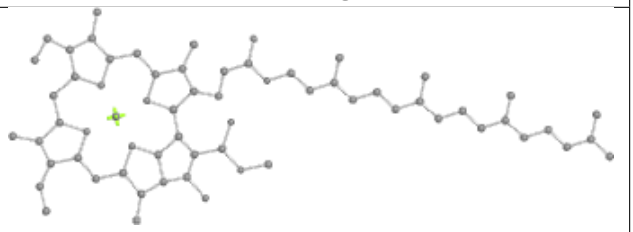
Bond lengths



Bond angles

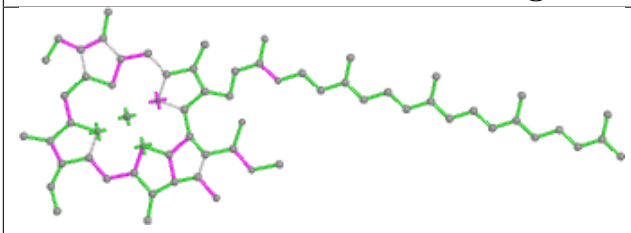


Torsions

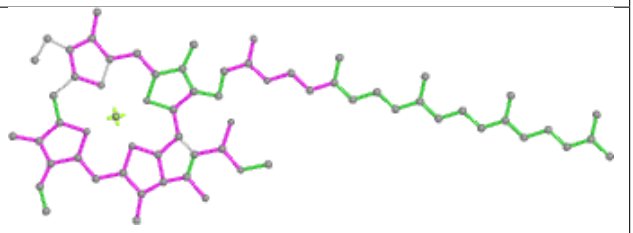


Rings

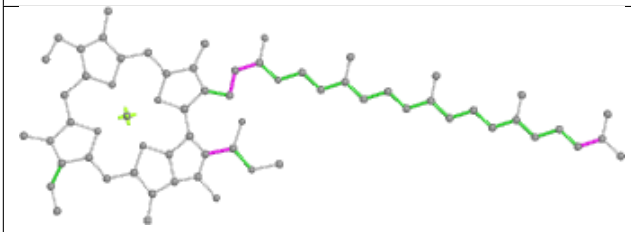
Ligand CLA b 606



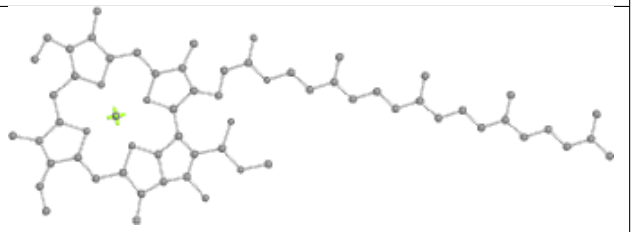
Bond lengths



Bond angles

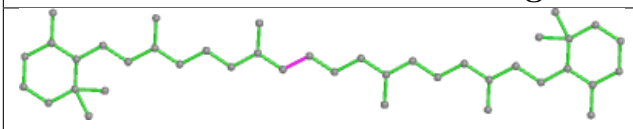


Torsions



Rings

Ligand BCR b 621



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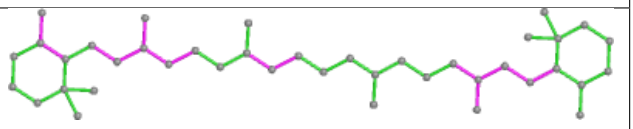
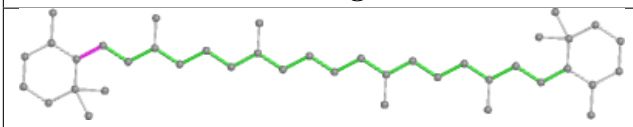
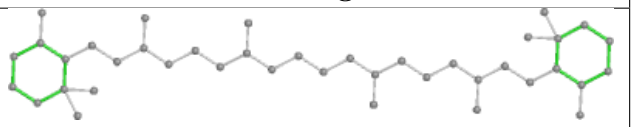


Bond angles

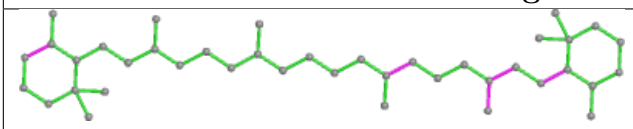


Torsions

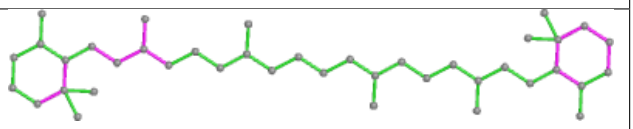


Rings

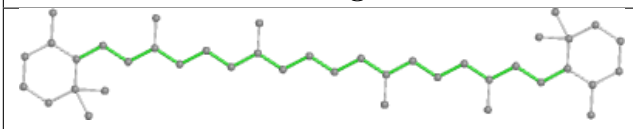
Ligand BCR B 619



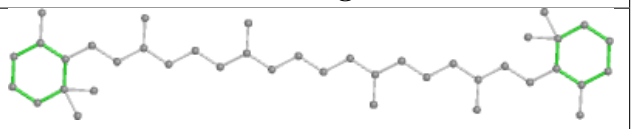
Bond lengths



Bond angles

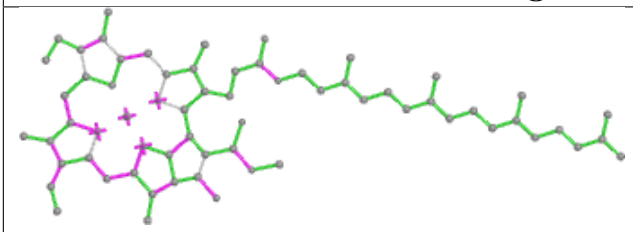


Torsions

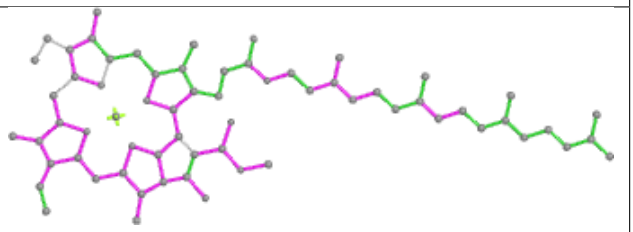


Rings

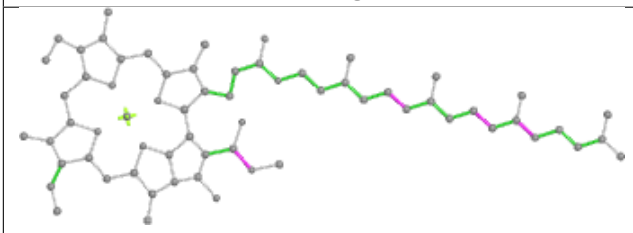
Ligand CLA b 619



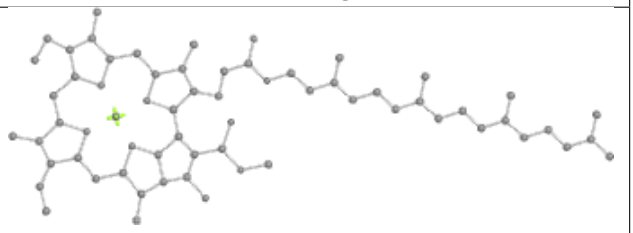
Bond lengths



Bond angles

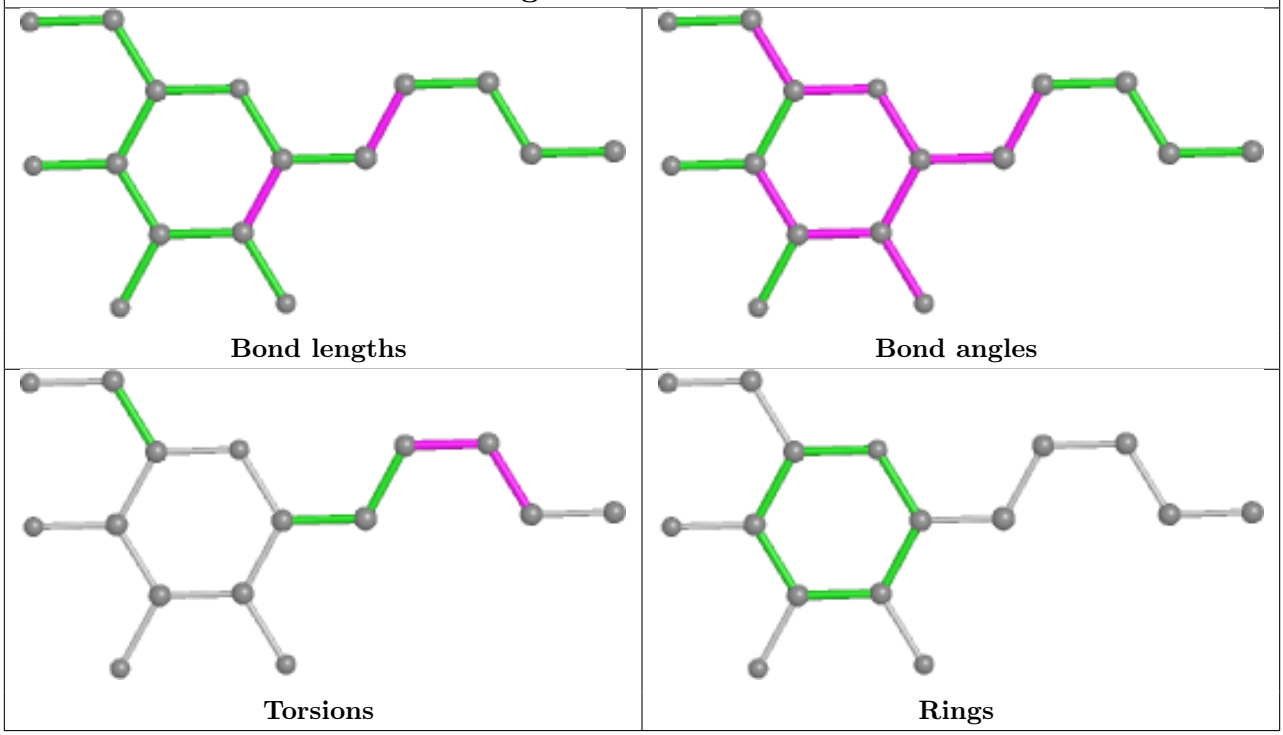


Torsions

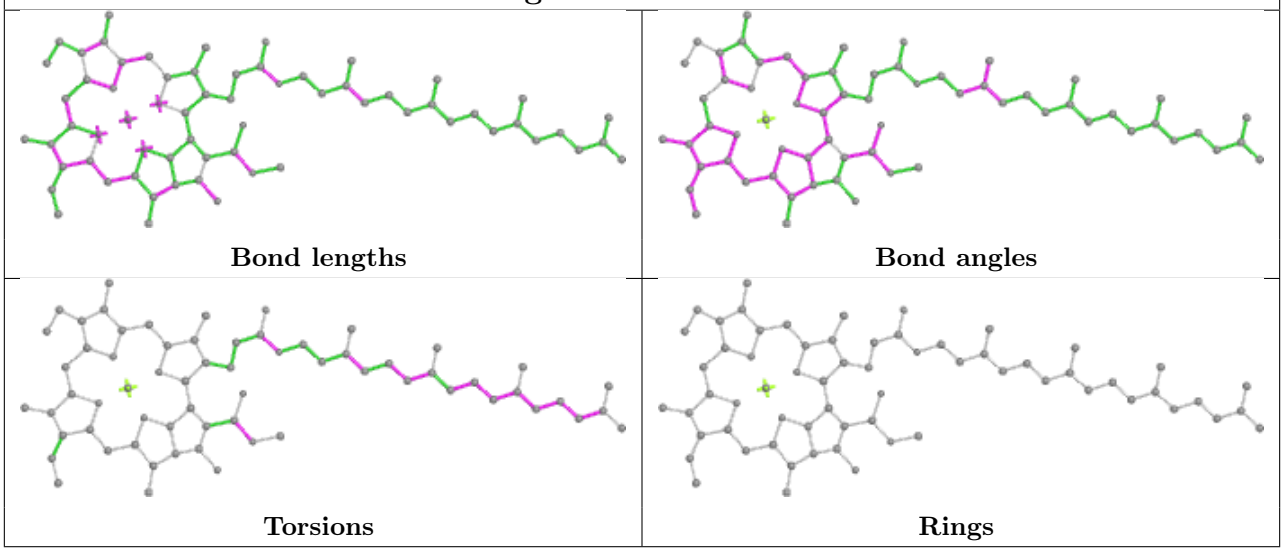


Rings

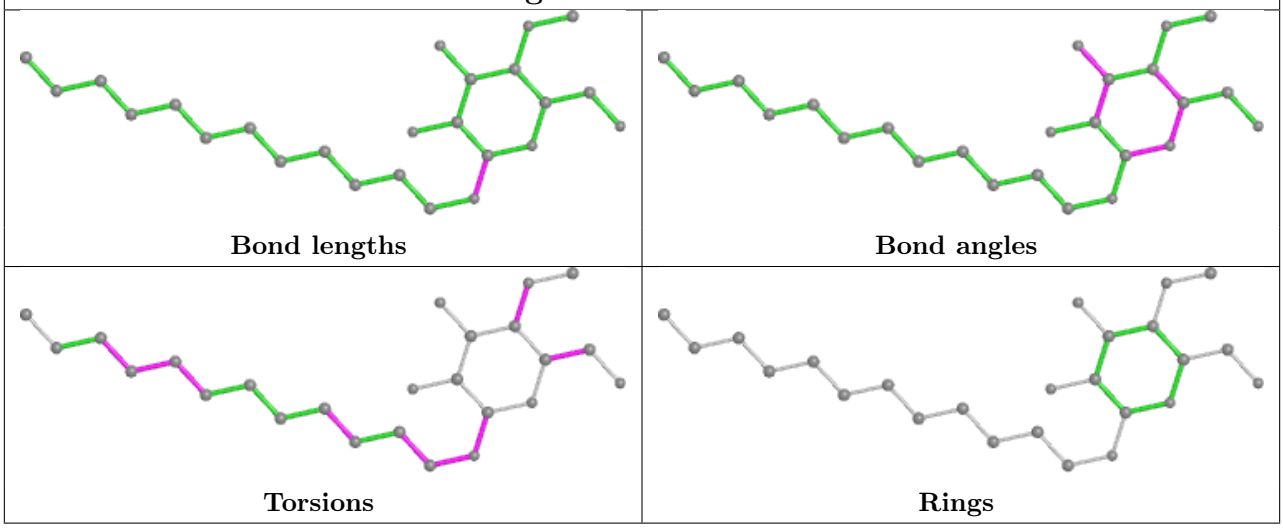
Ligand HTG D 413



Ligand CLA A 408



Ligand LMT b 626



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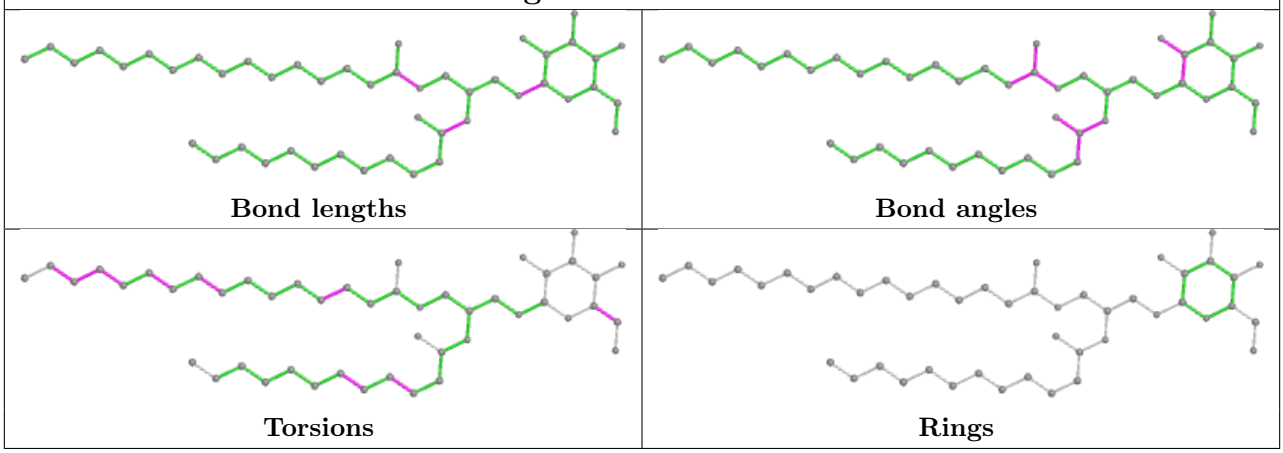
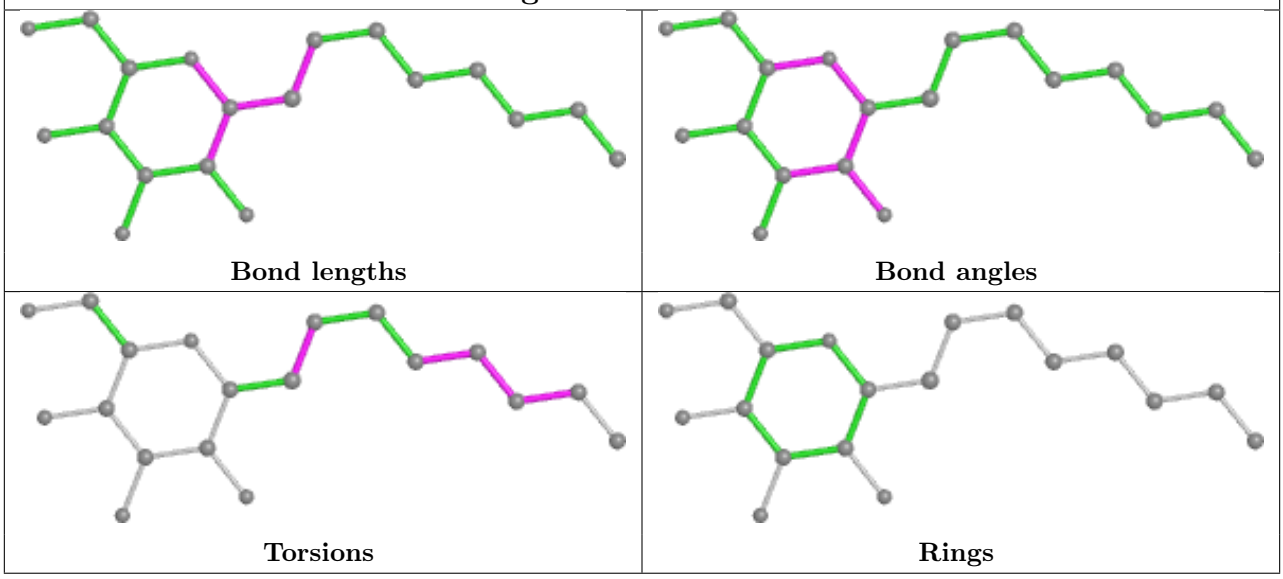
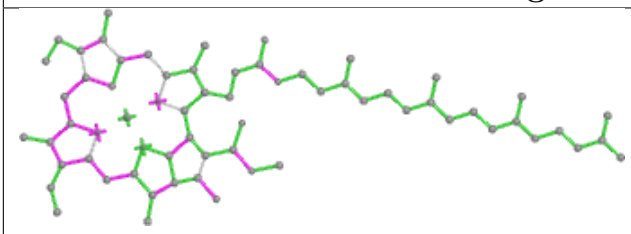


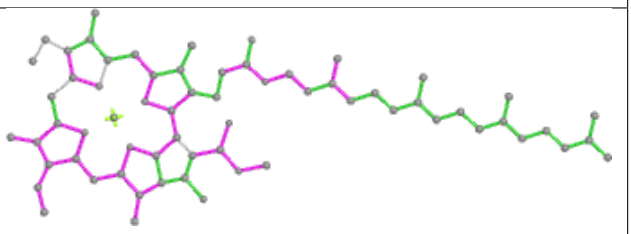
Ligand HTG O 302



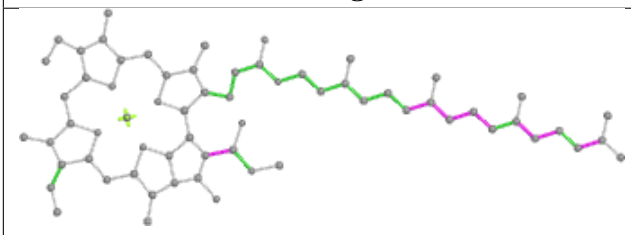
Ligand CLA d 405



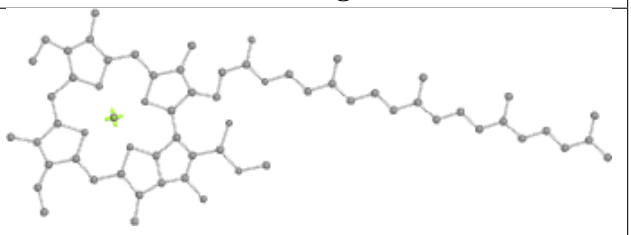
Bond lengths



Bond angles

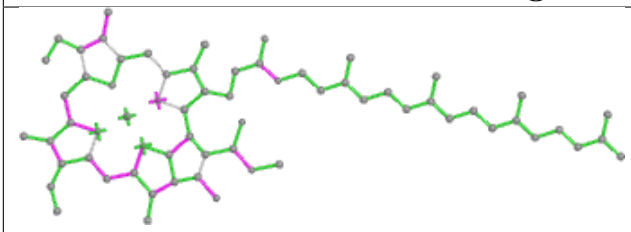


Torsions



Rings

Ligand CLA b 617



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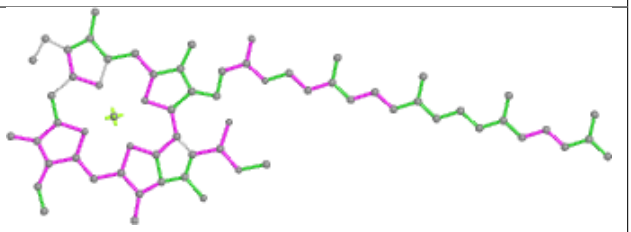
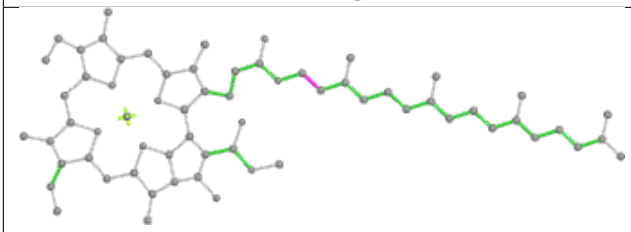
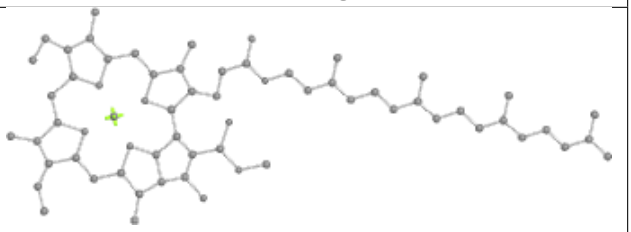


Bond angles

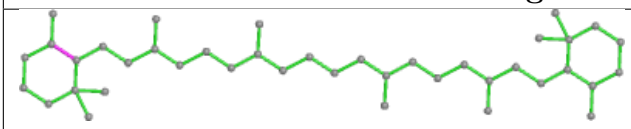


Torsions

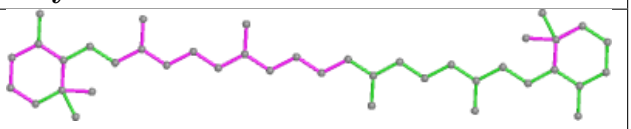


Rings

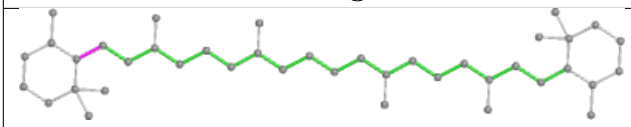
Ligand BCR y 101



Bond lengths



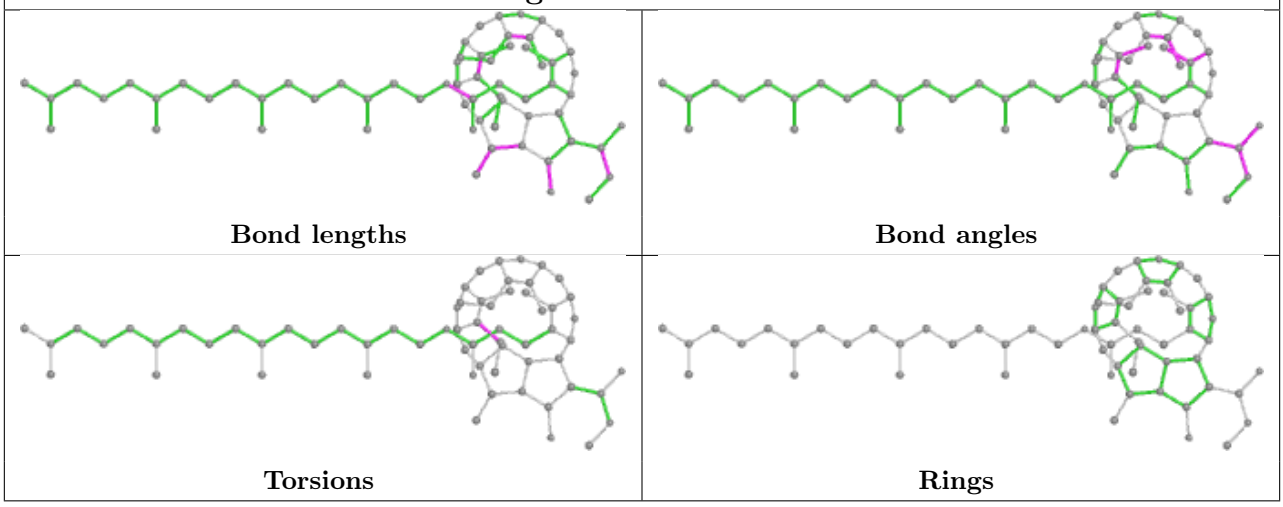
Bond angles



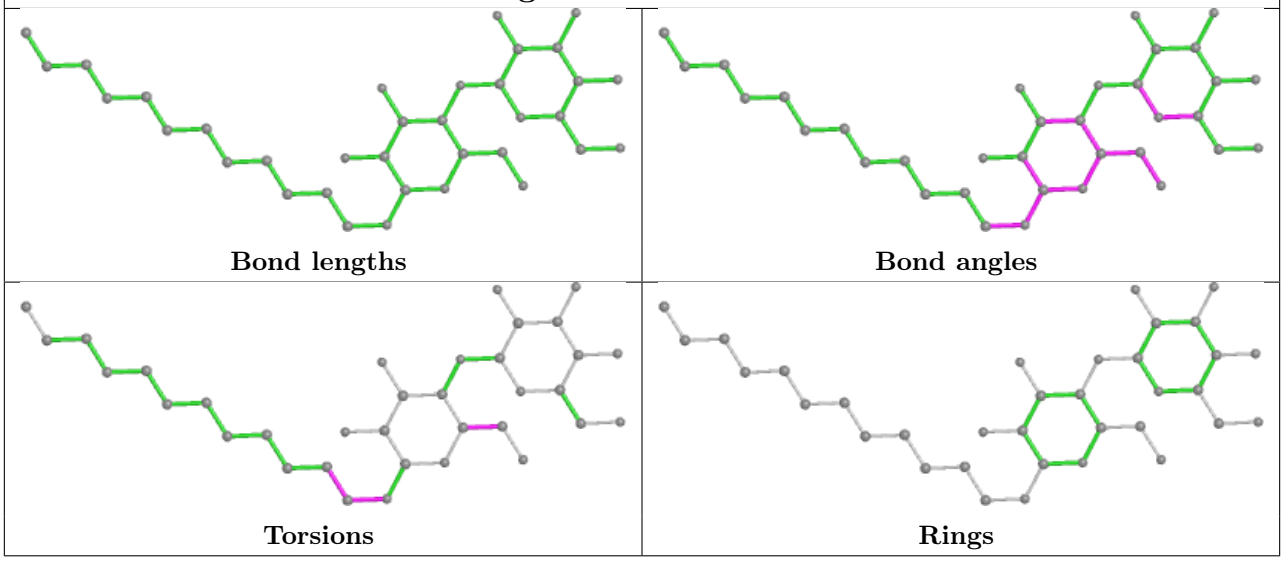
Torsions

Rings

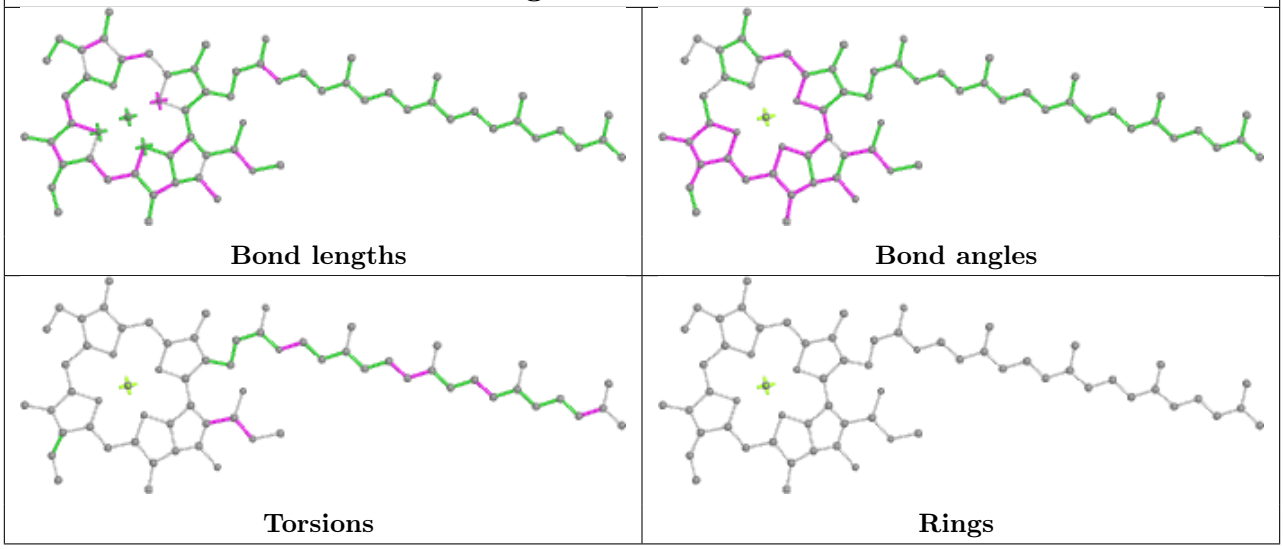
Ligand PHO d 404



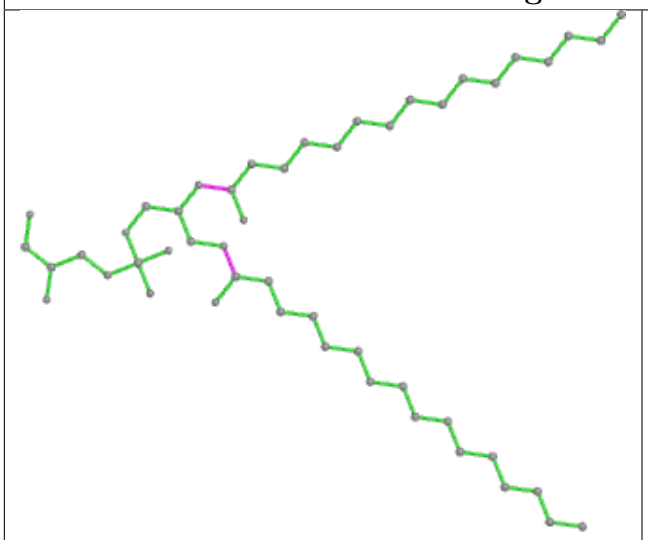
Ligand LMT M 101



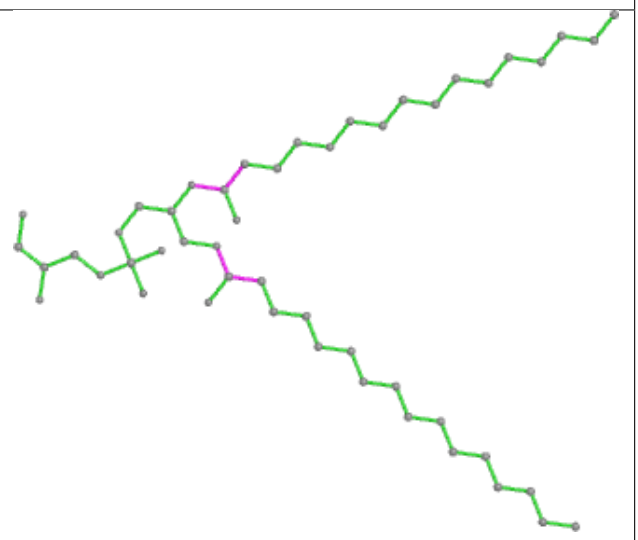
Ligand CLA C 506



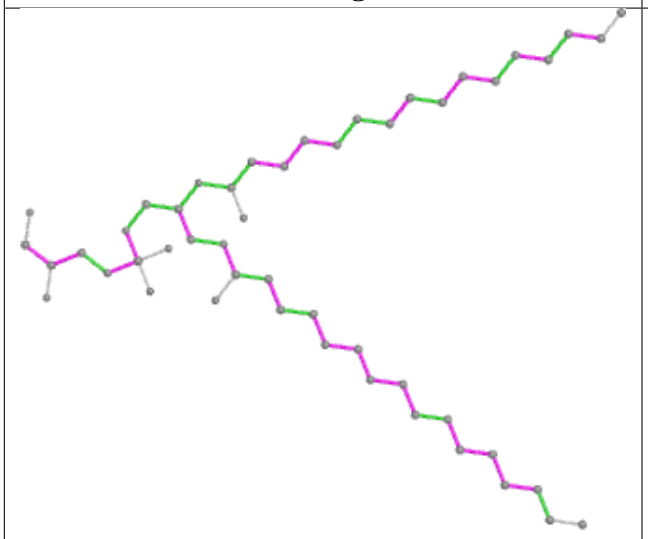
Ligand LHG E 101



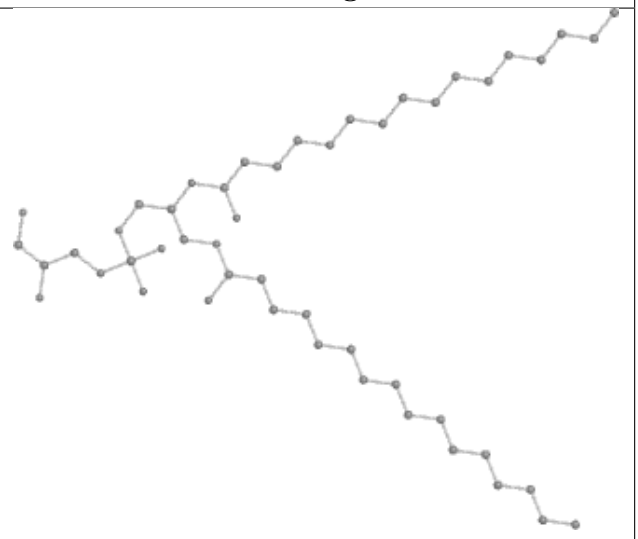
Bond lengths



Bond angles

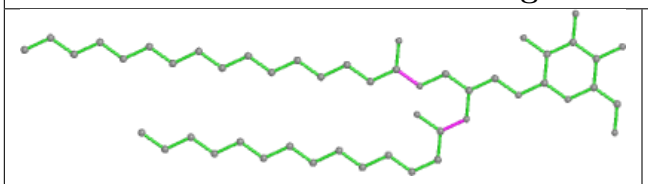


Torsions



Rings

Ligand LMG C 518



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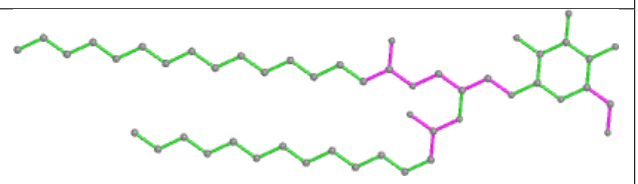
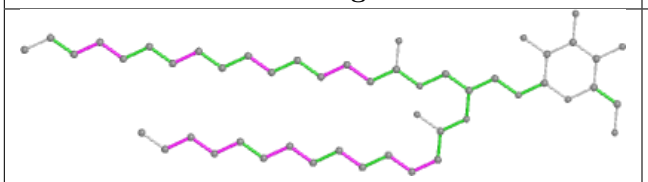


Bond angles



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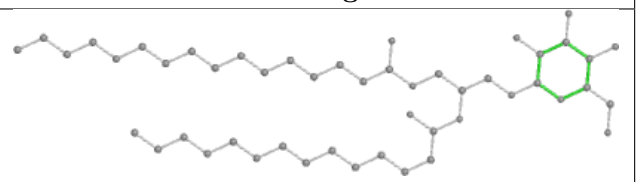
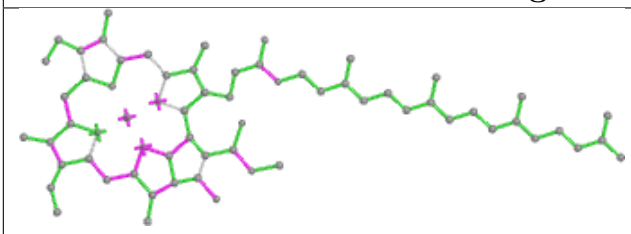
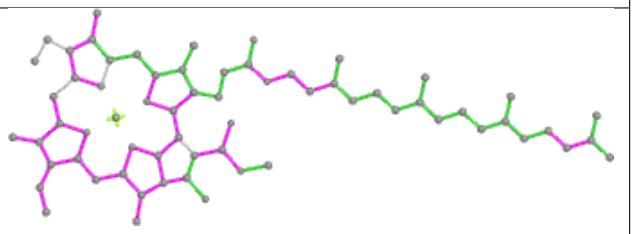


Rings

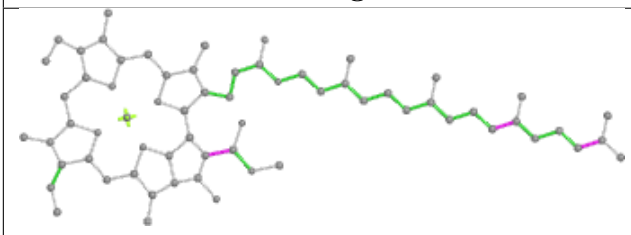
Ligand CLA c 503



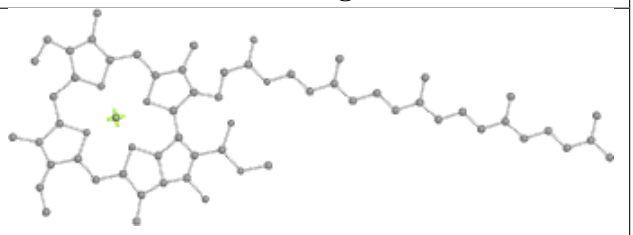
Bond lengths



Bond angles

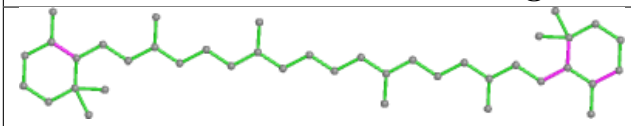


Torsions

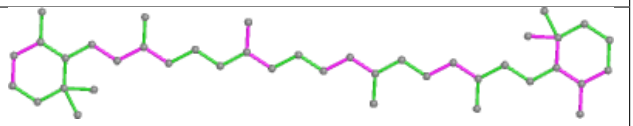


Rings

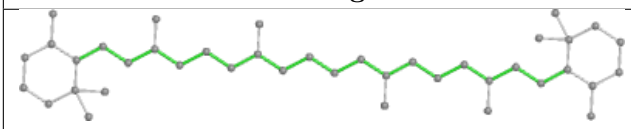
Ligand BCR b 623



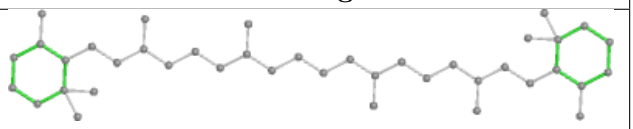
Bond lengths



Bond angles

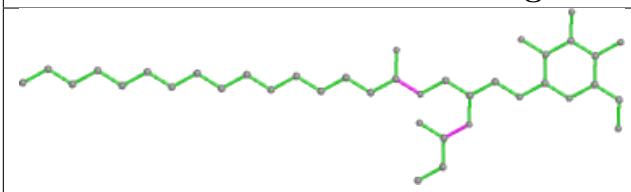


Torsions

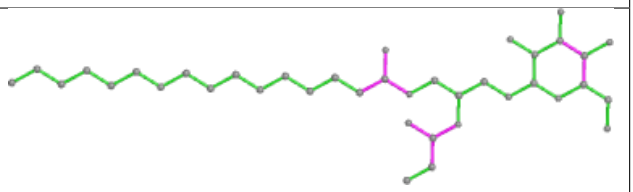


Rings

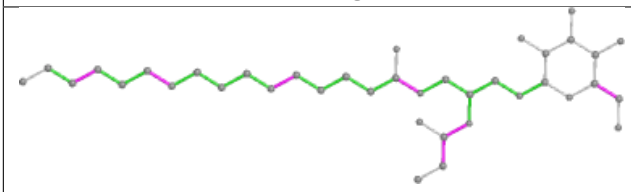
Ligand LMG c 520



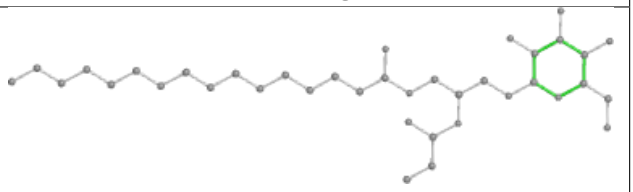
Bond lengths



Bond angles

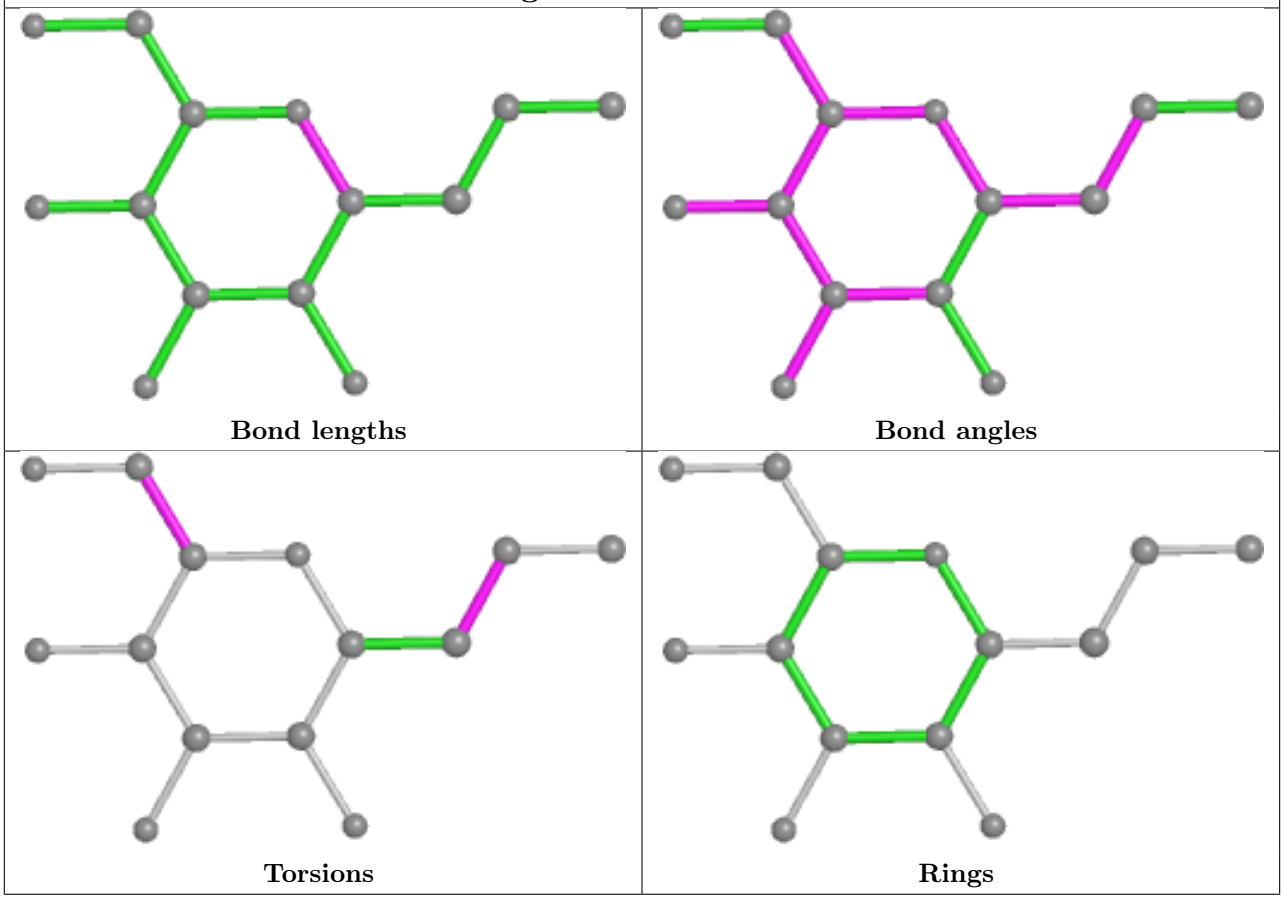


Torsions

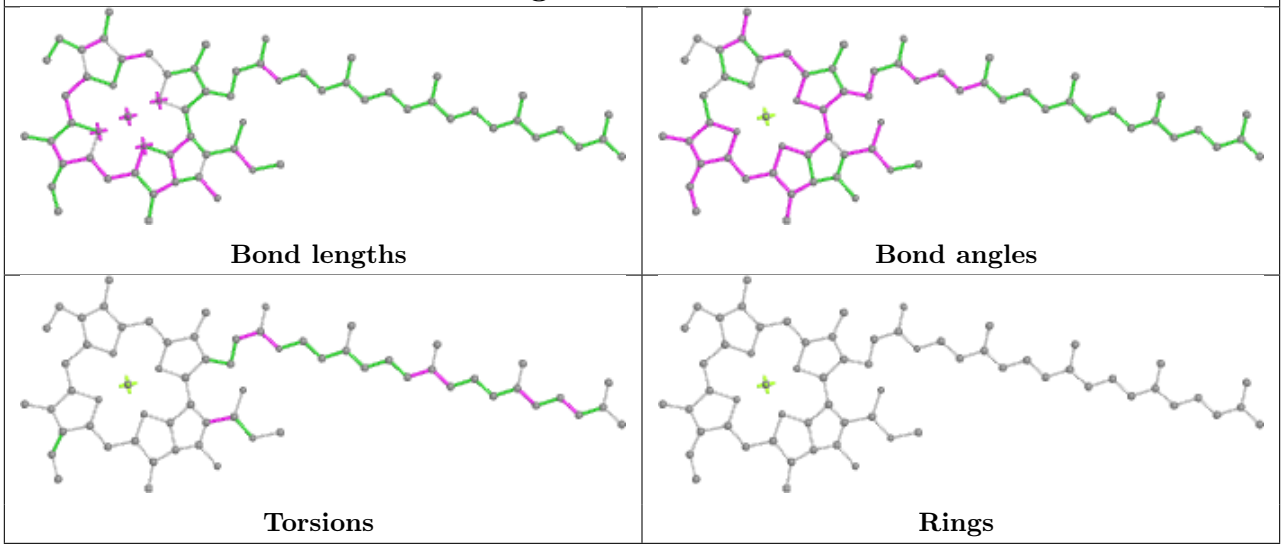


Rings

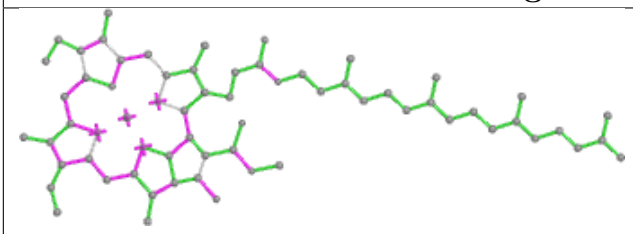
Ligand HTG U 203



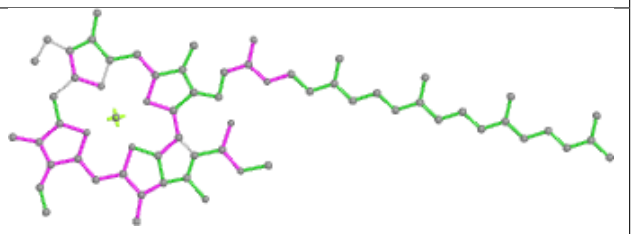
Ligand CLA c 513



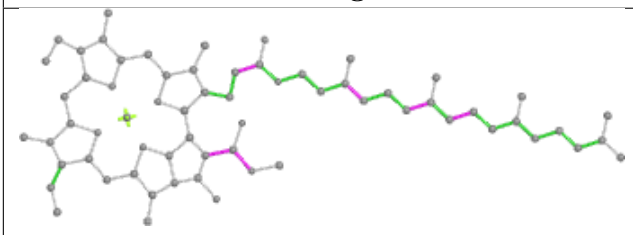
Ligand CLA C 510



Bond lengths



Bond angles



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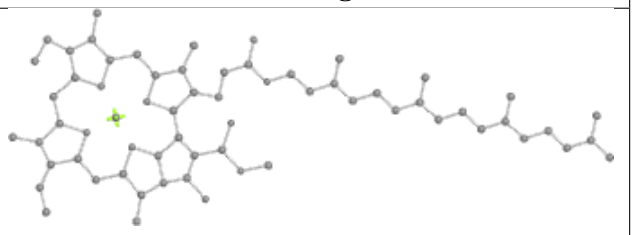
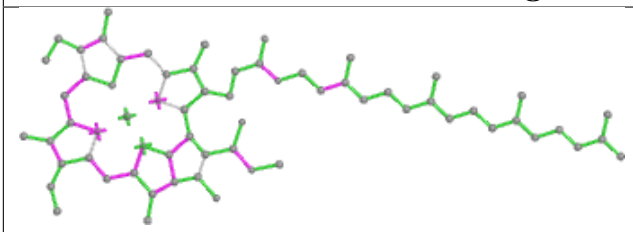


Rings

Ligand CLA B 617



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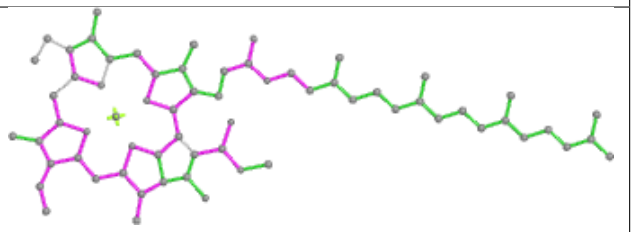
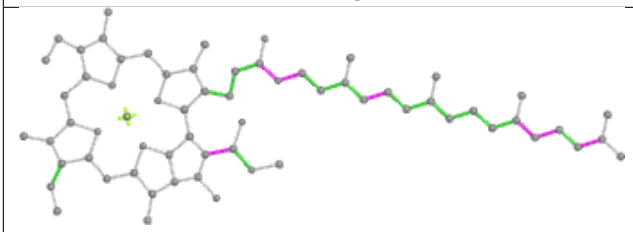


Bond angles



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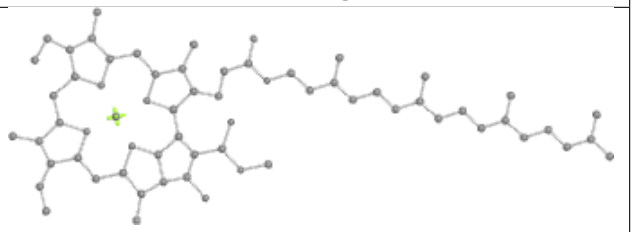
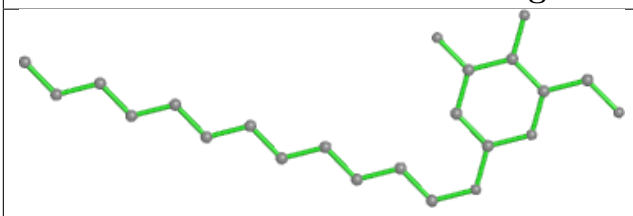


Rings

Ligand LMT j 102



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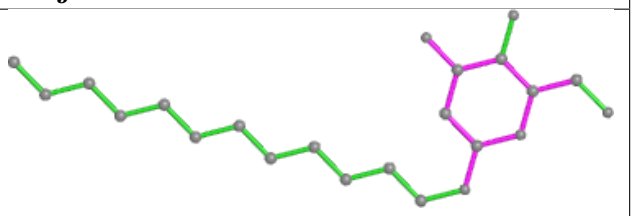
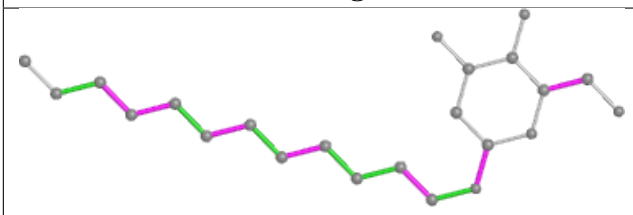


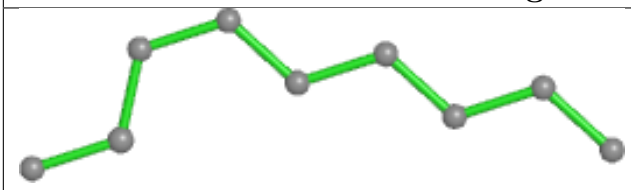
Bond angles



Torsions

Rings

Ligand HTG c 524



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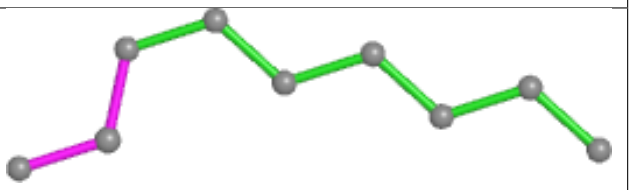
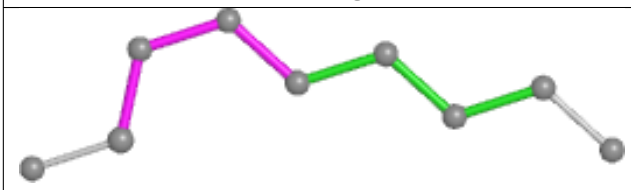


Bond angles



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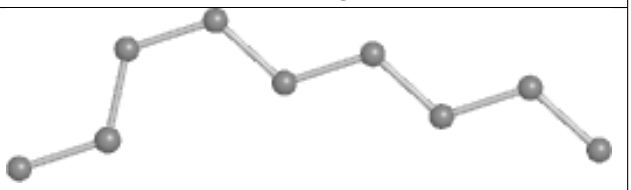
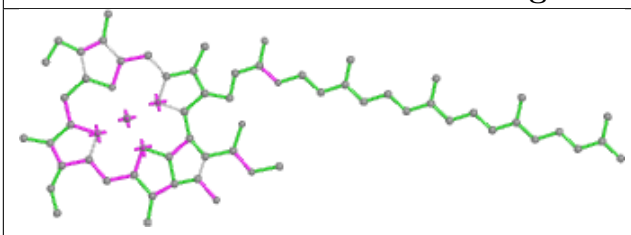


Rings

Ligand CLA c 512



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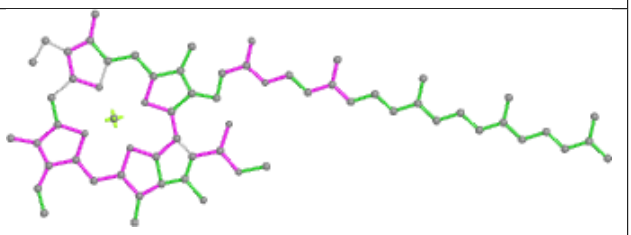
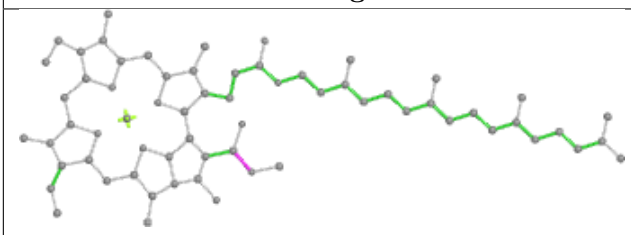


Bond angles



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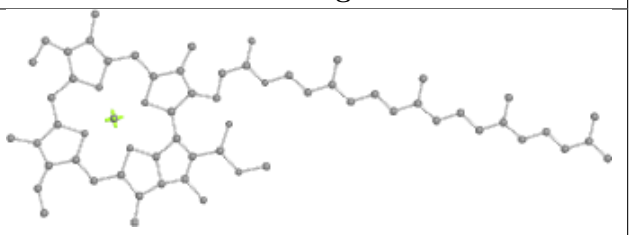
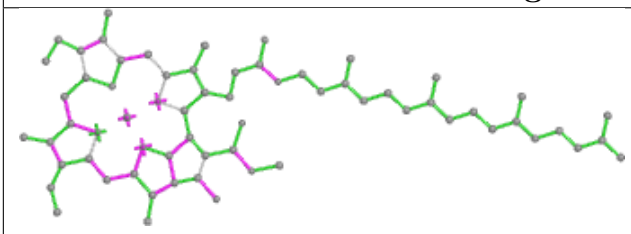


Rings

Ligand CLA C 511



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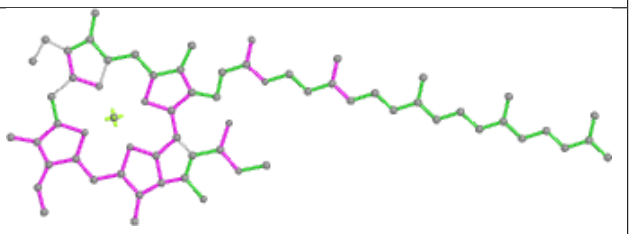
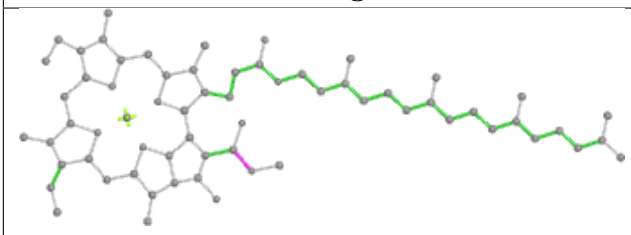


Bond angles



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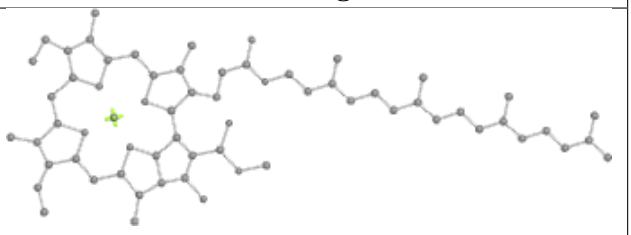
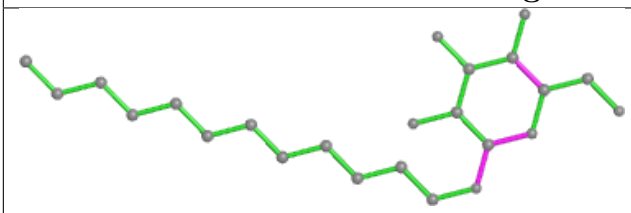


Rings

Ligand LMT F 102



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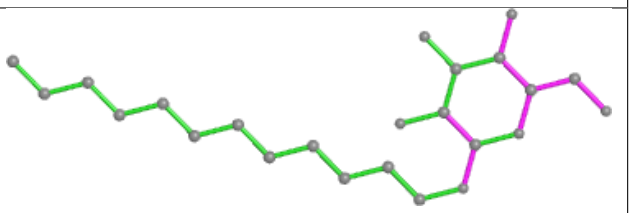
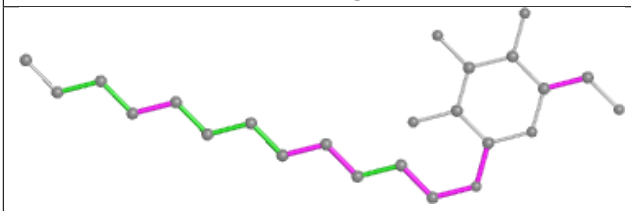


Bond angles



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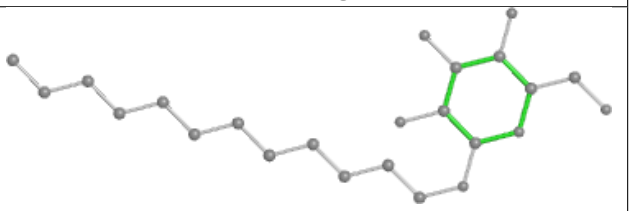
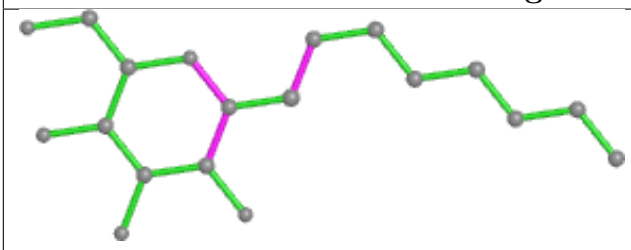


Rings

Ligand HTG o 301



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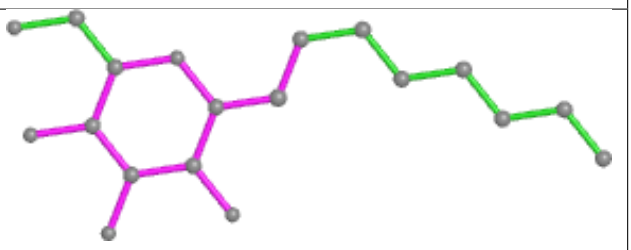
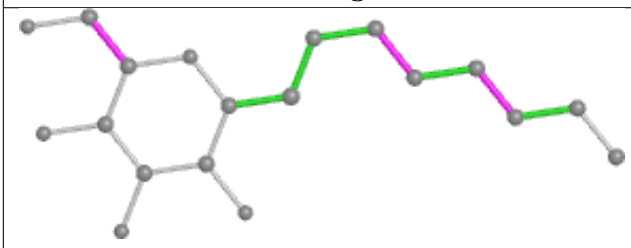
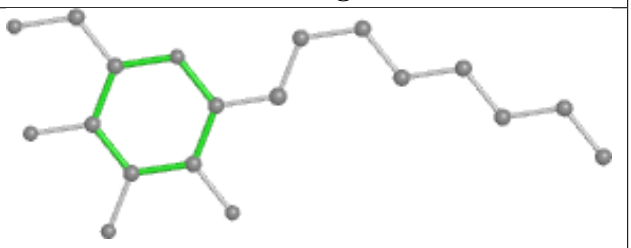


Bond angles

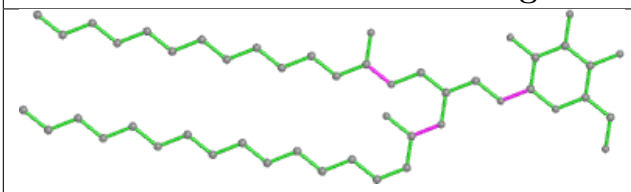


Torsions



Rings

Ligand LMG C 519



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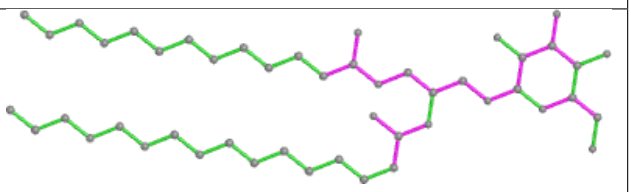
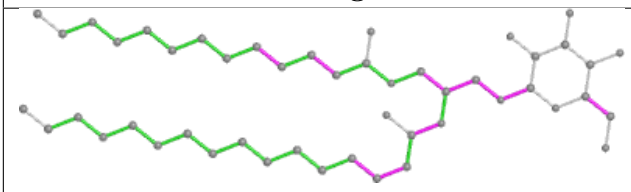


Bond angles



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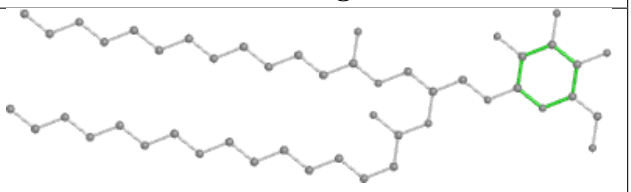
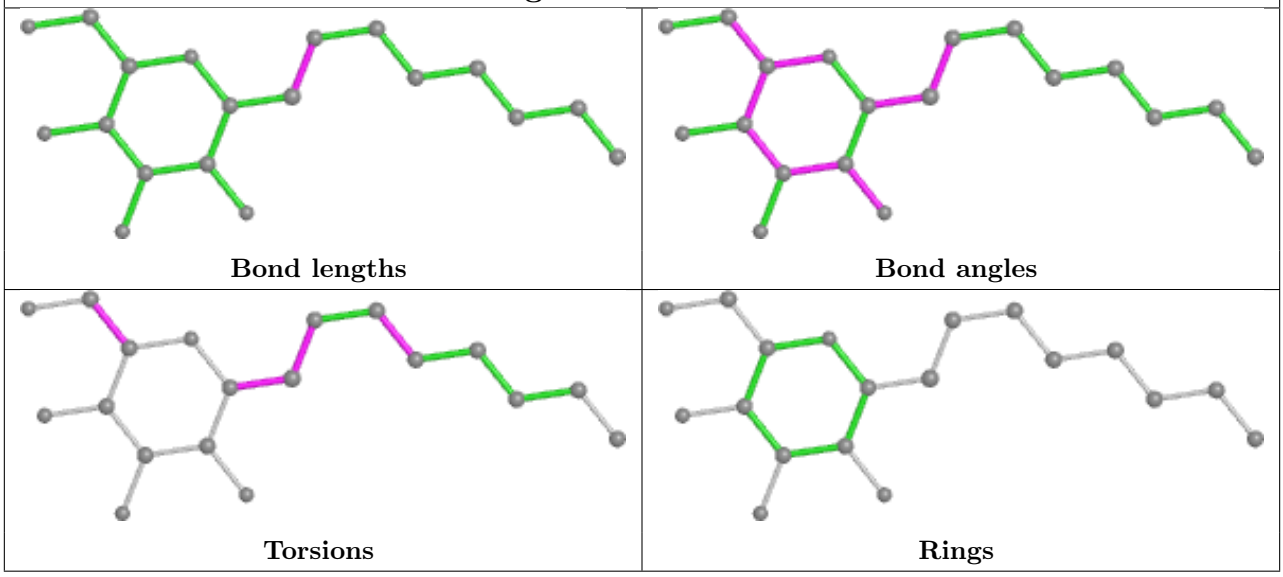
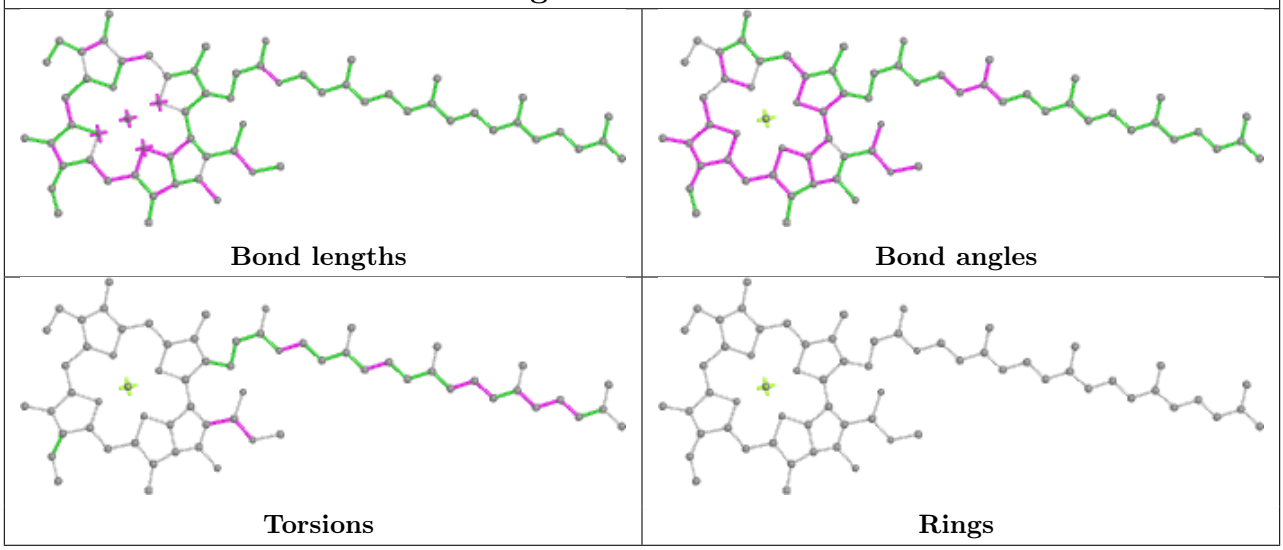


Rings

Ligand HTG b 627



Ligand CLA c 510



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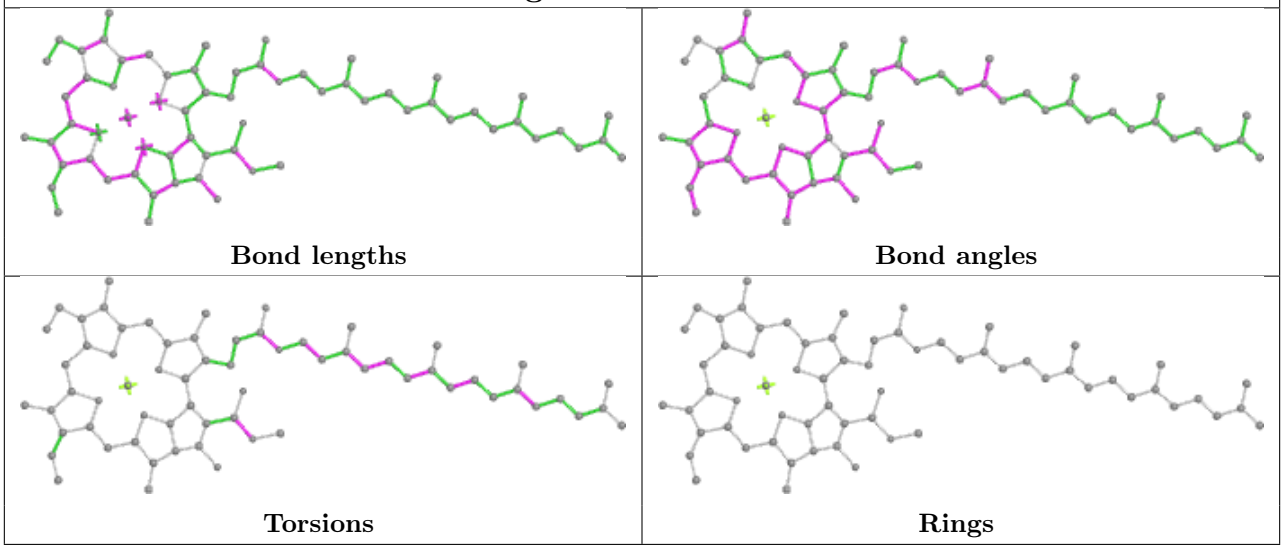
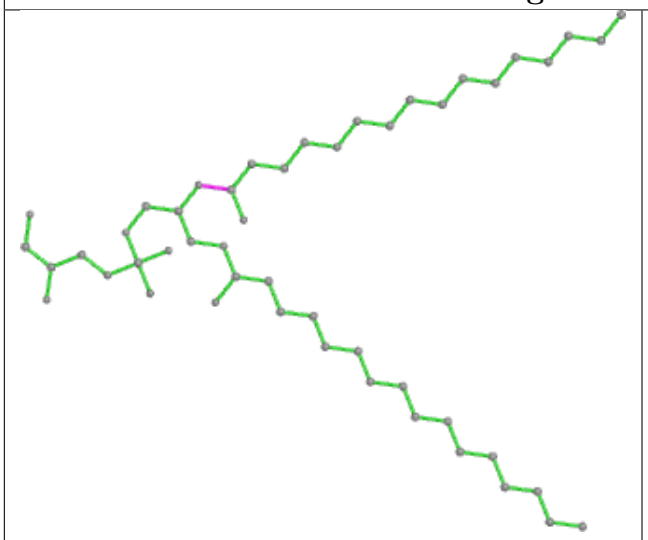
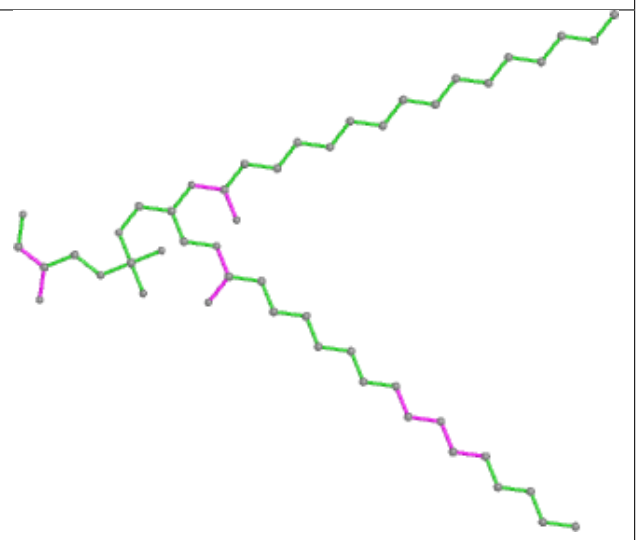


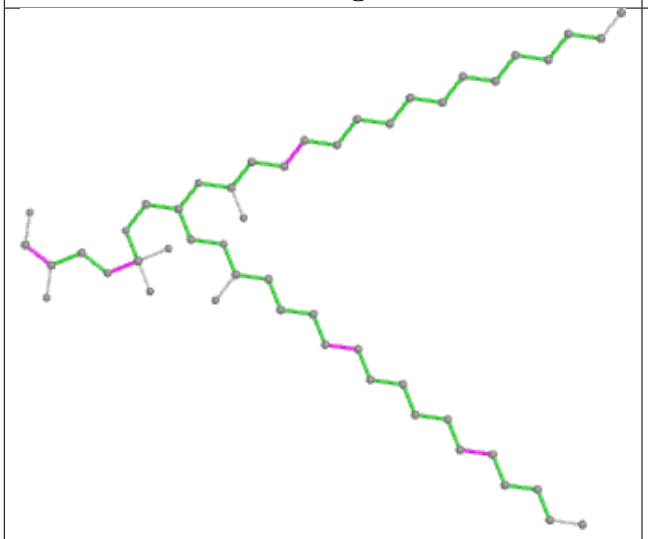
Ligand LHG d 410



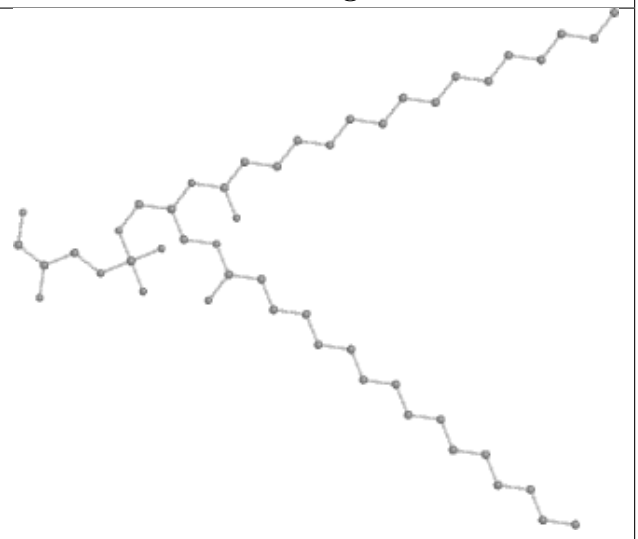
Bond lengths



Bond angles

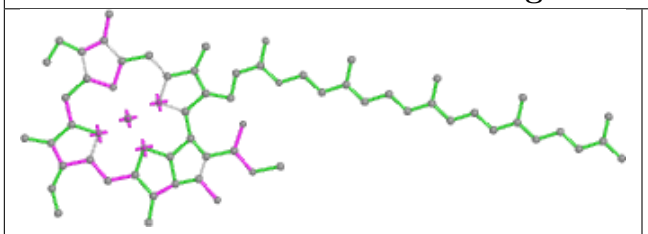


Torsions

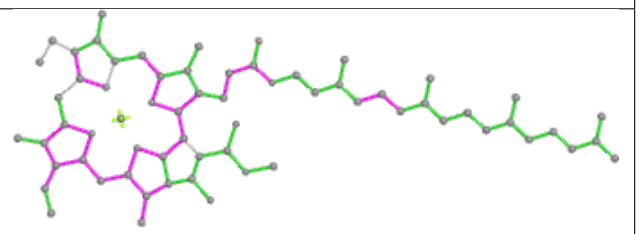


Rings

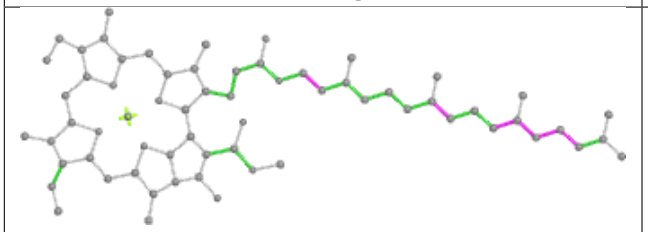
Ligand CLA B 614



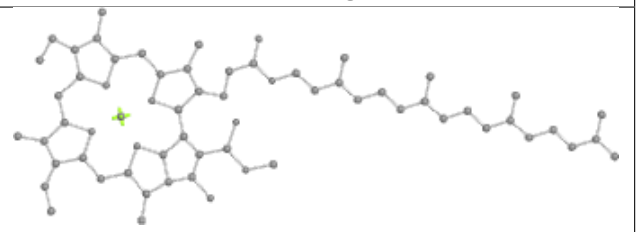
Bond lengths



Bond angles

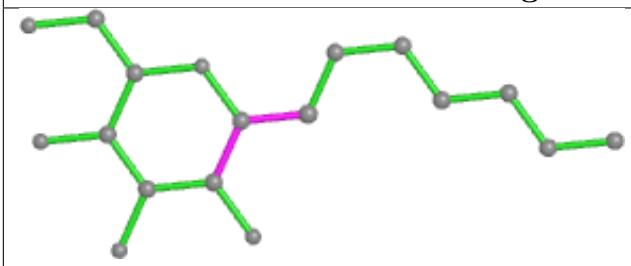


Torsions

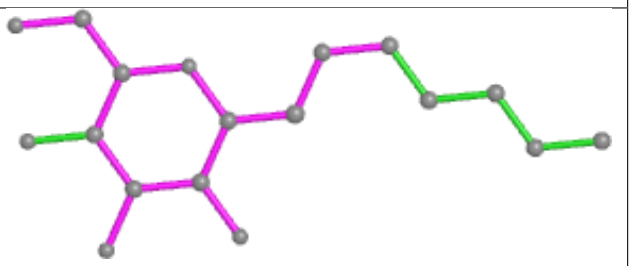


Rings

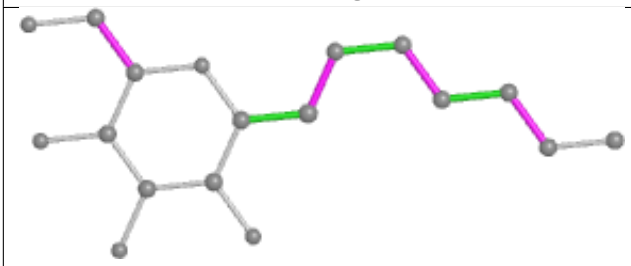
Ligand HTG B 642



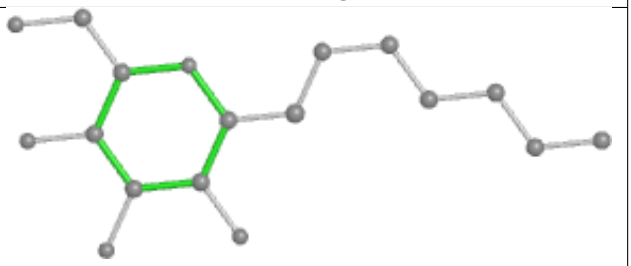
Bond lengths



Bond angles

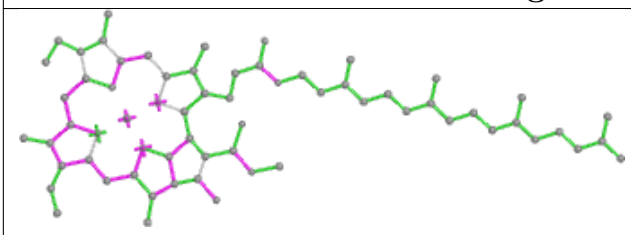


Torsions



Rings

Ligand CLA b 618



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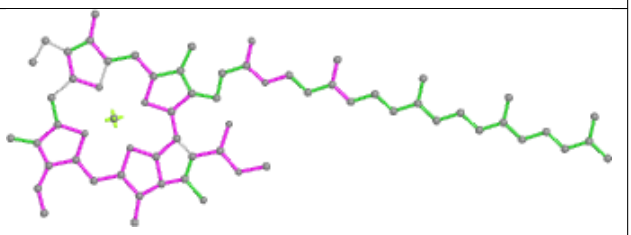
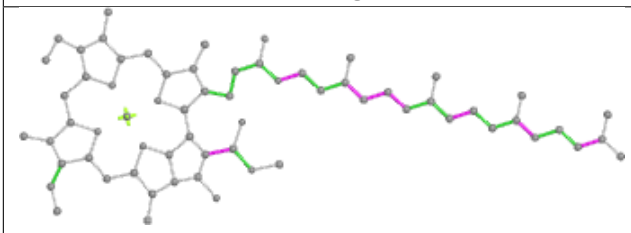


Bond angles



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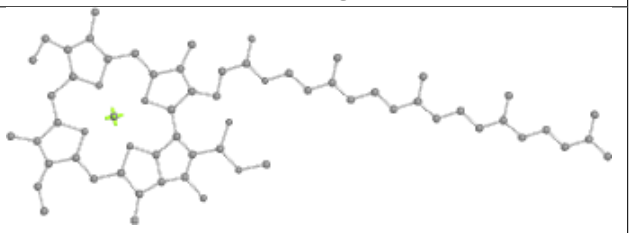
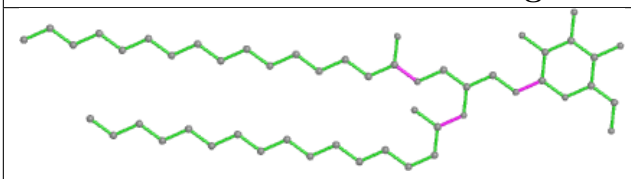


Rings

Ligand LMG c 521



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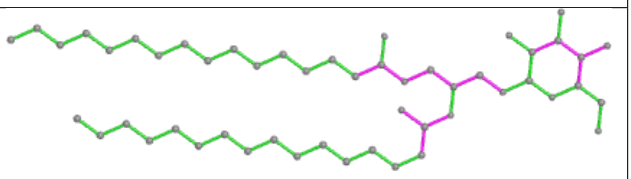
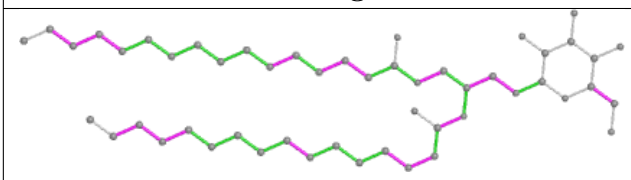
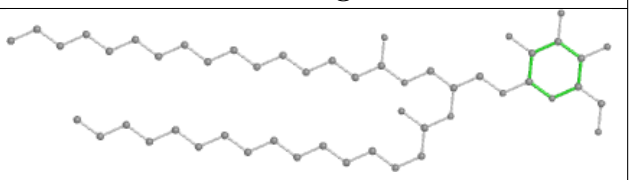


Bond angles

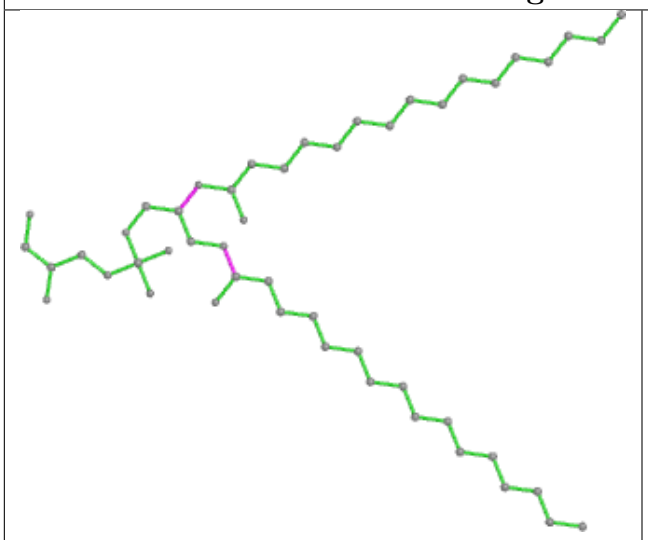


Torsions



Rings

Ligand LHG b 624



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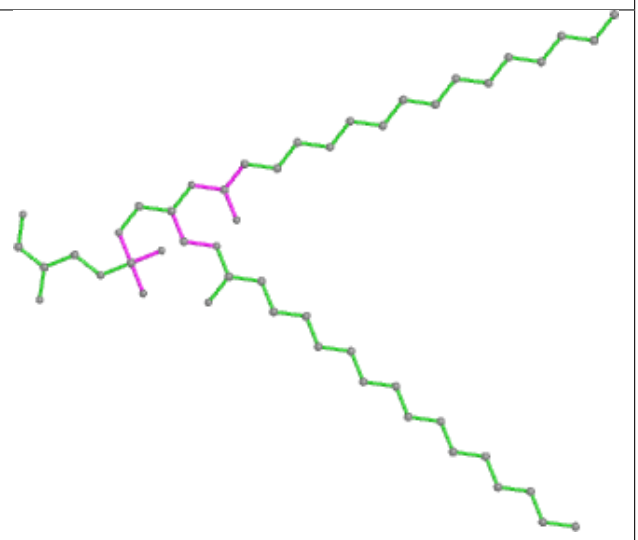
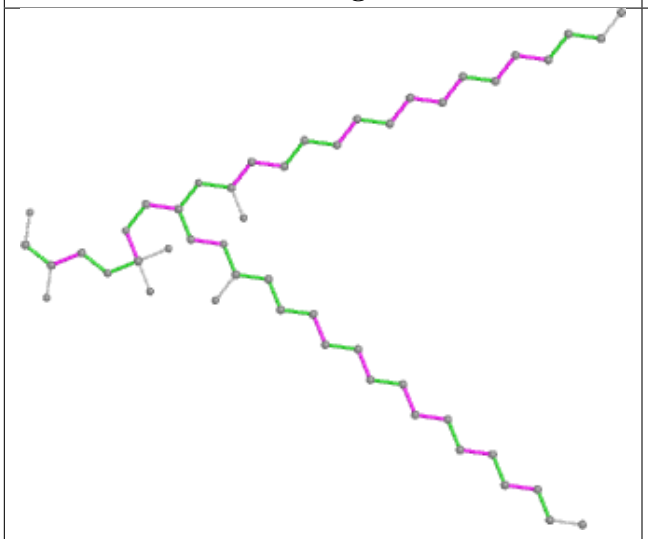


Bond angles



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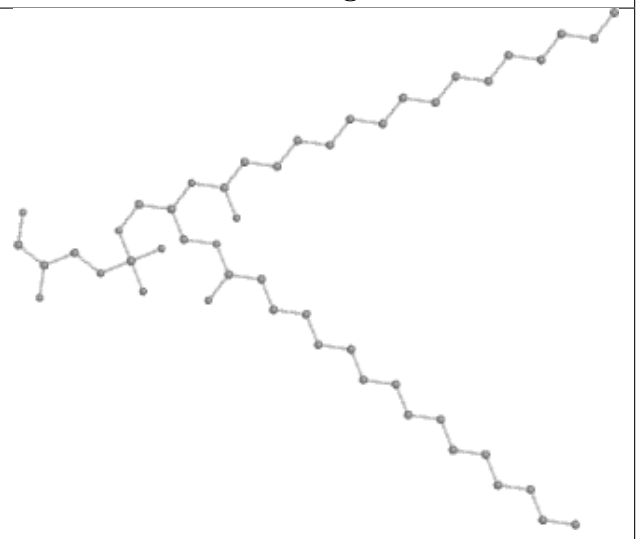
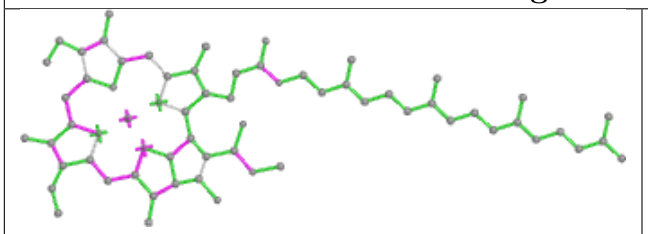


Rings

Ligand CLA c 507



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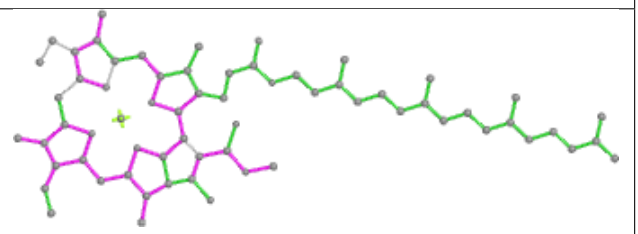
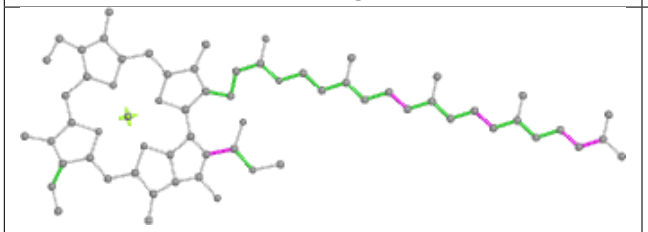


Bond angles



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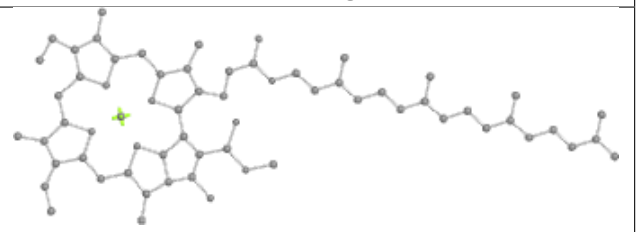
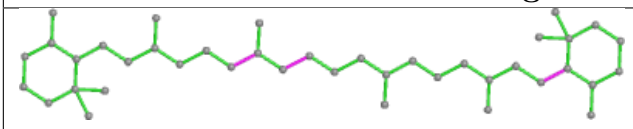


Rings

Ligand BCR B 620



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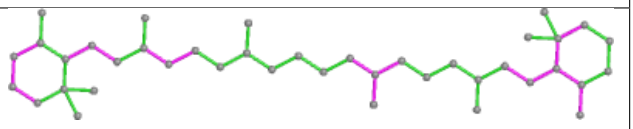
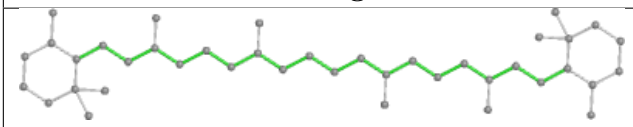


Bond angles



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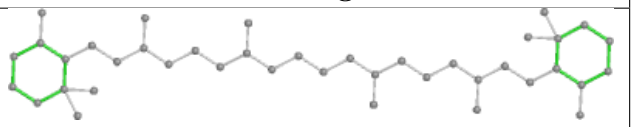
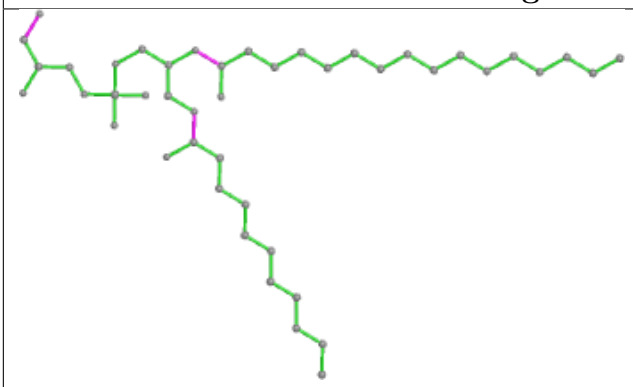


Rings

Ligand LHG D 411



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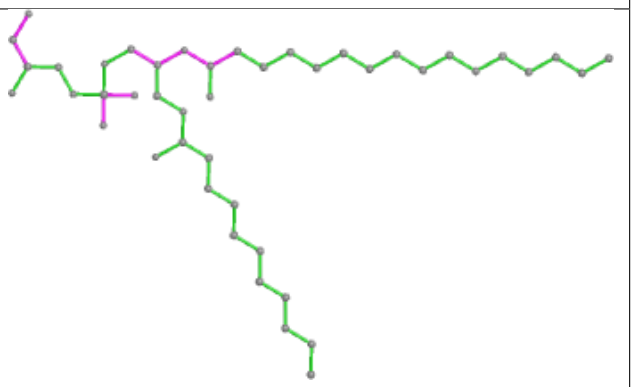

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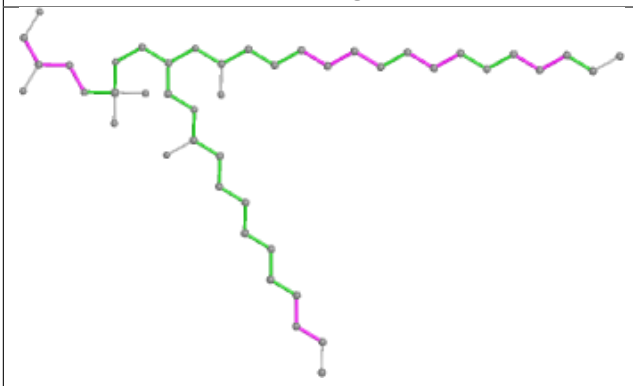

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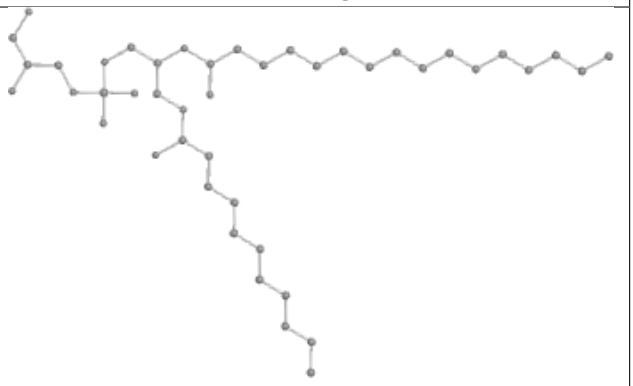
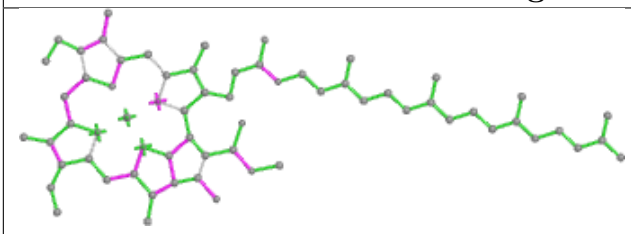


Rings

Ligand CLA b 607



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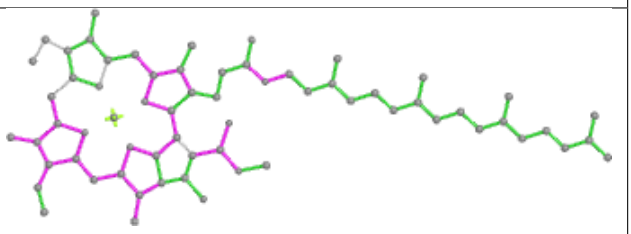

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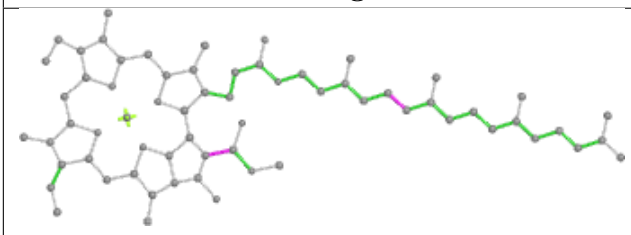

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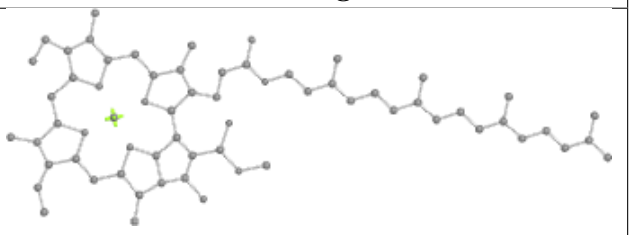
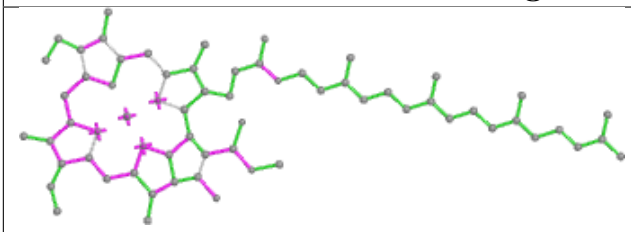


Rings

Ligand CLA C 507



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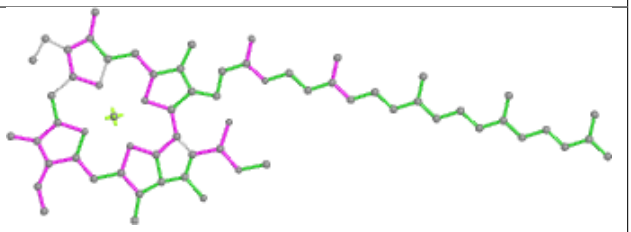
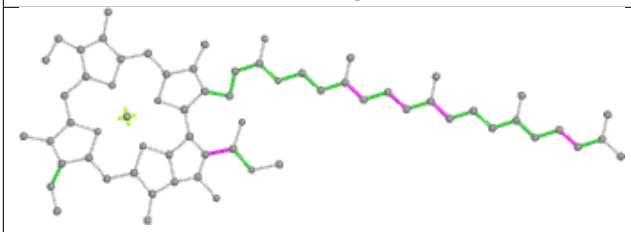
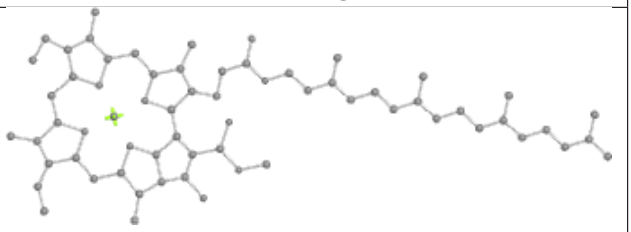


Bond angles

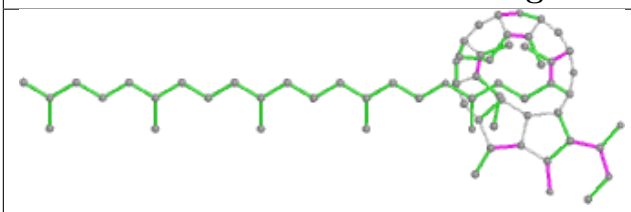


Torsions



Rings

Ligand PHO a 408



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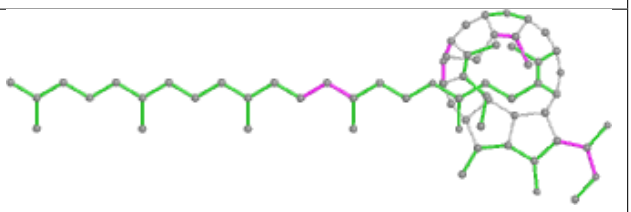

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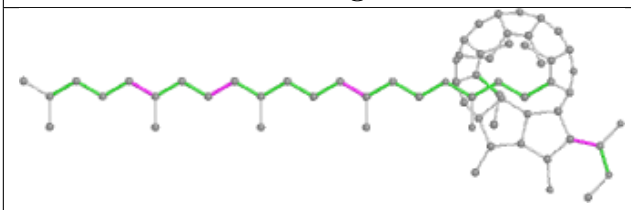

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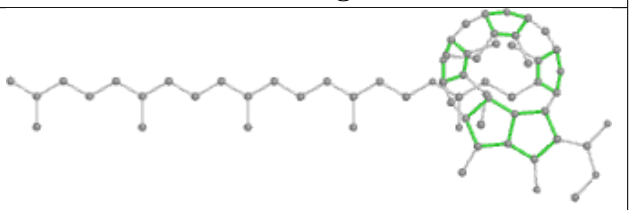
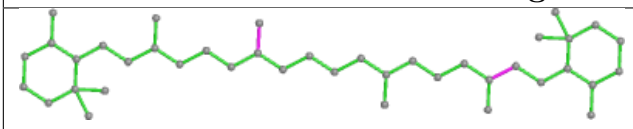


Rings

Ligand BCR t 101



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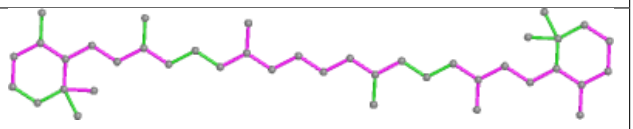
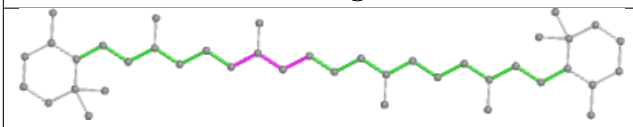


Bond angles



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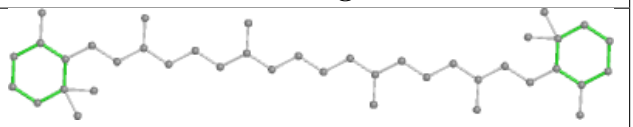
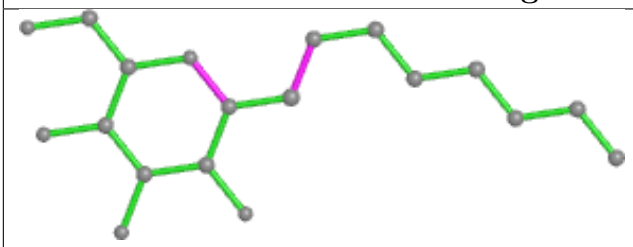


Rings

Ligand HTG C 522



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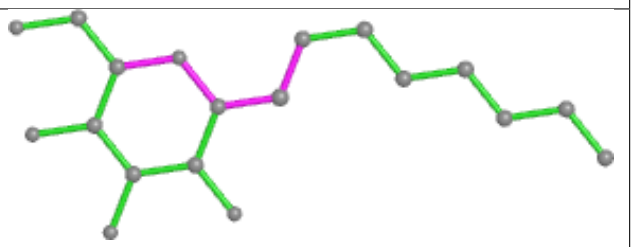
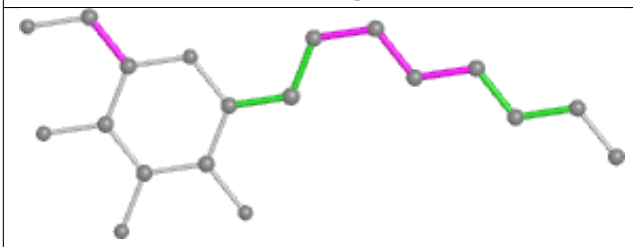


Bond angles



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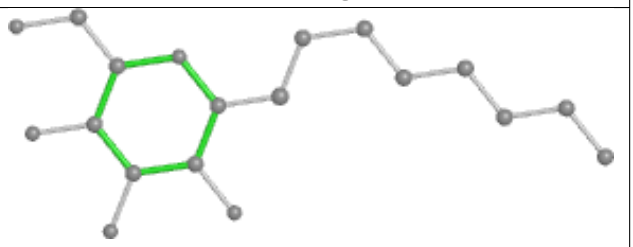
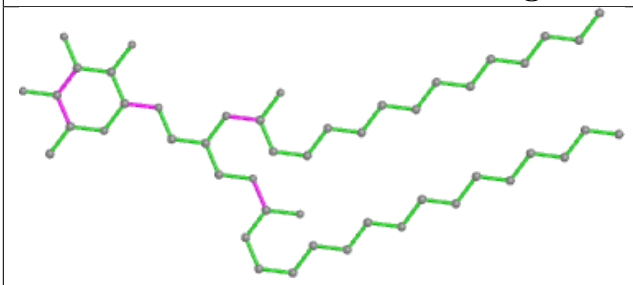


Rings

Ligand DGD d 408



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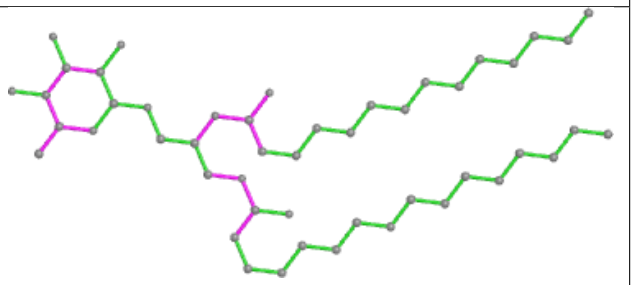
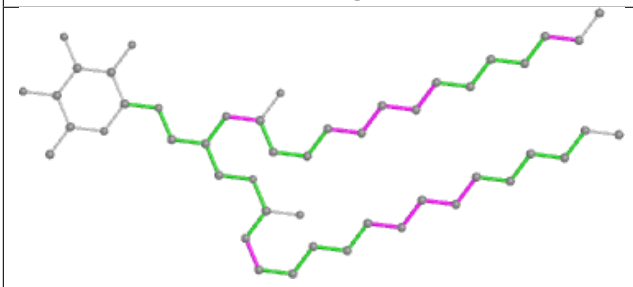


Bond angles



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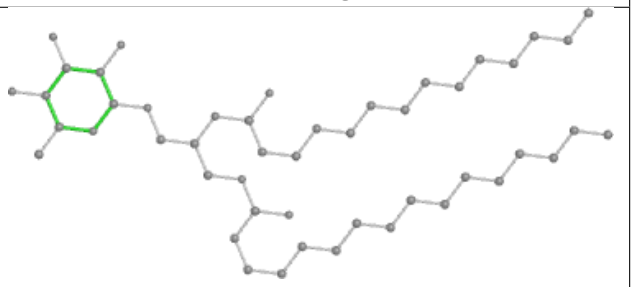
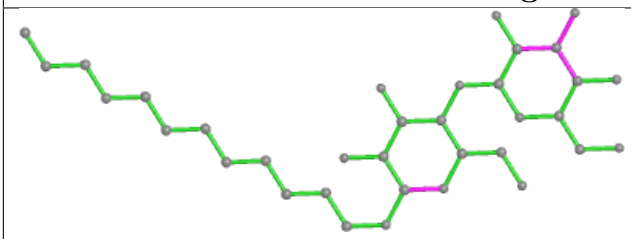


Rings

Ligand LMT A 415



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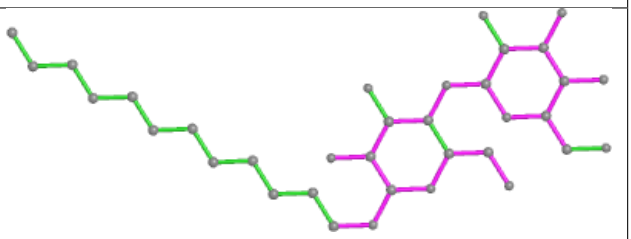
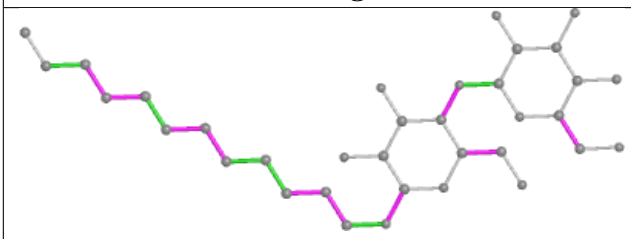
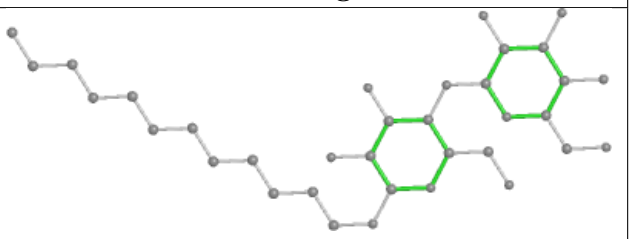


Bond angles

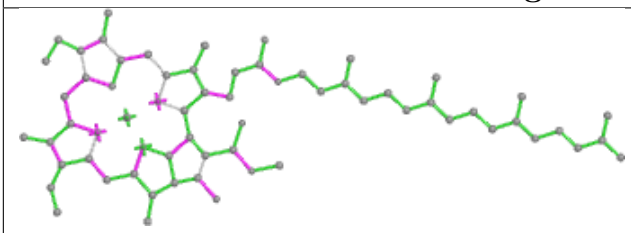


Torsions

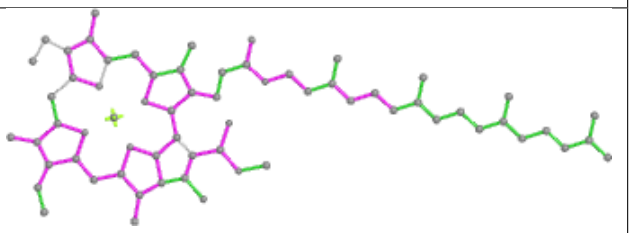


Rings

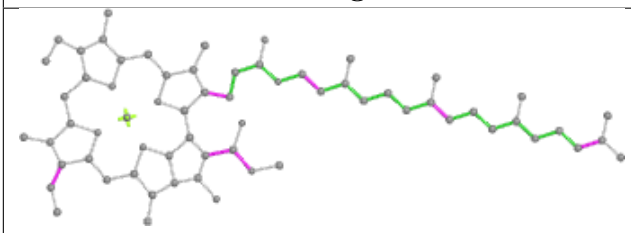
Ligand CLA B 605



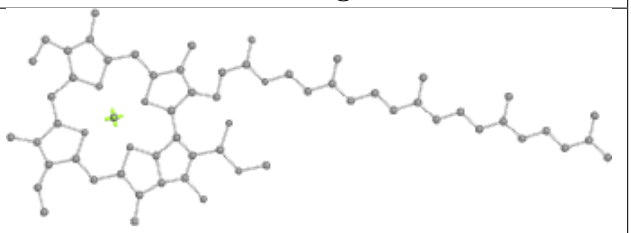
Bond lengths



Bond angles

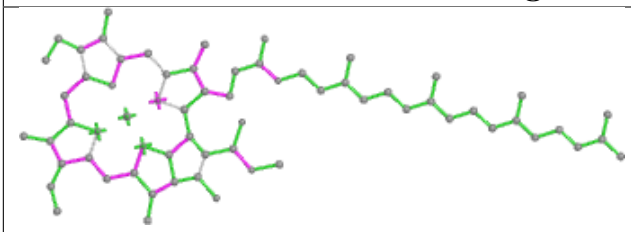


Torsions



Rings

Ligand CLA B 607



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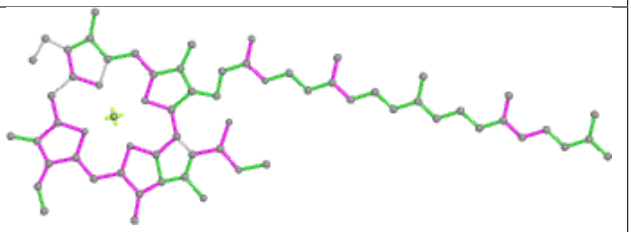
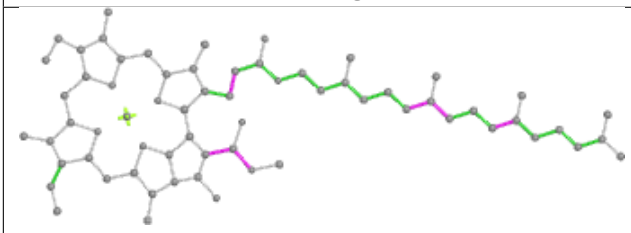
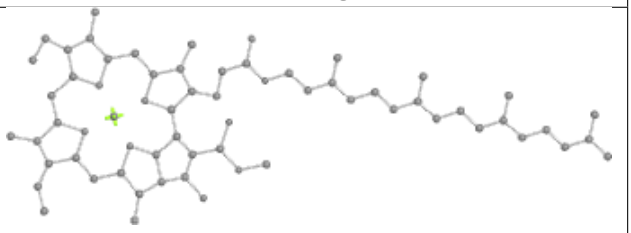


Bond angles

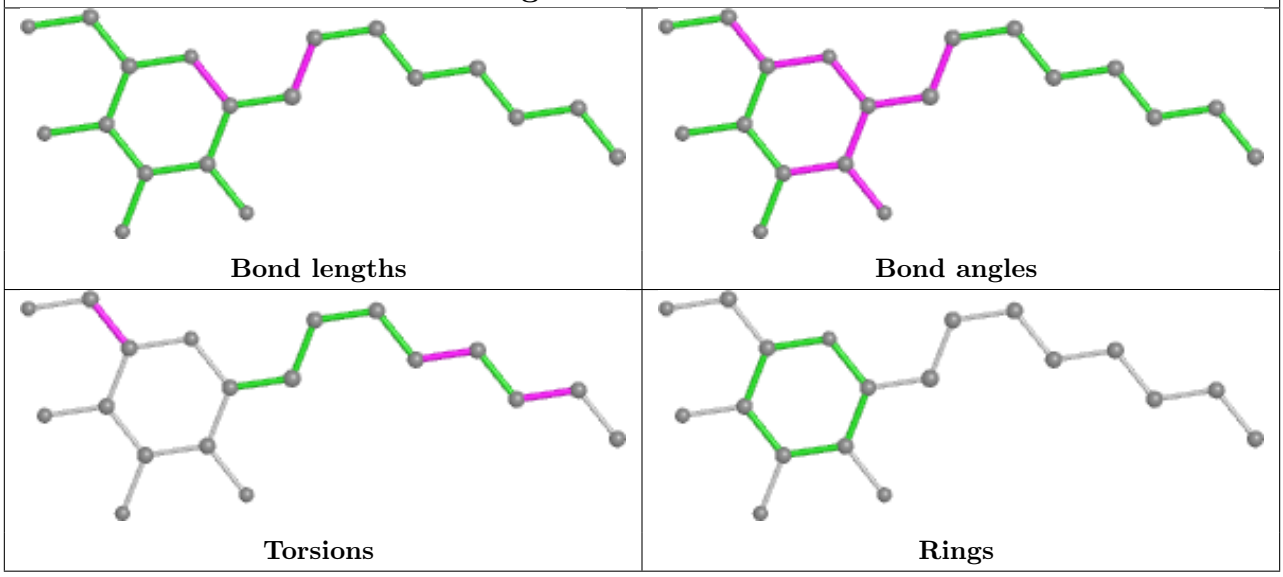


Torsions

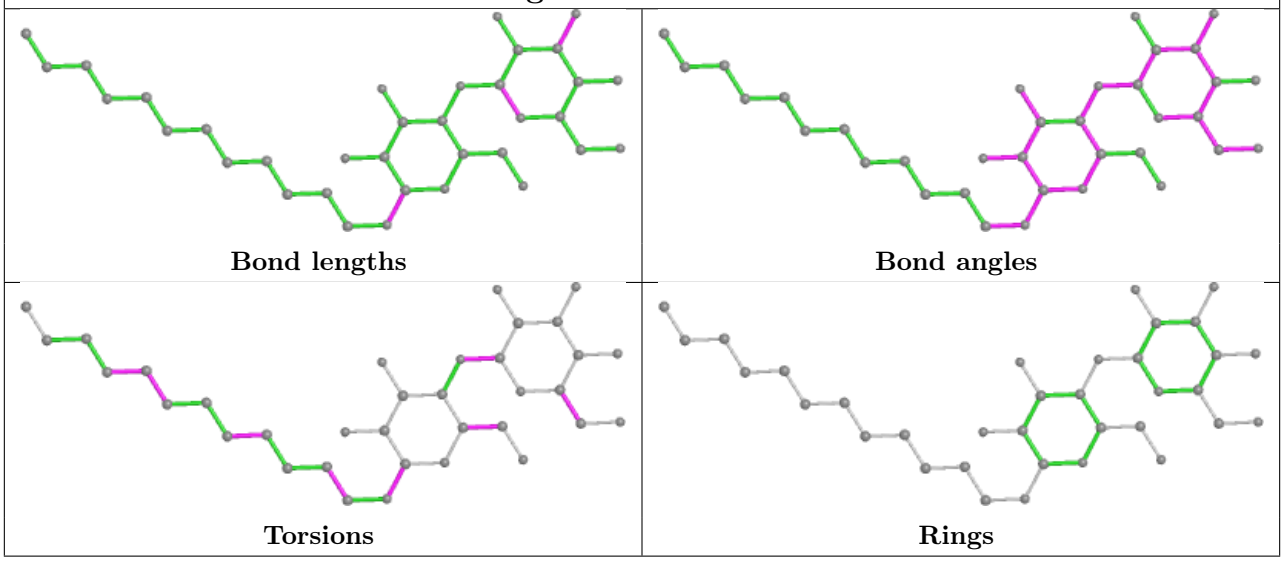


Rings

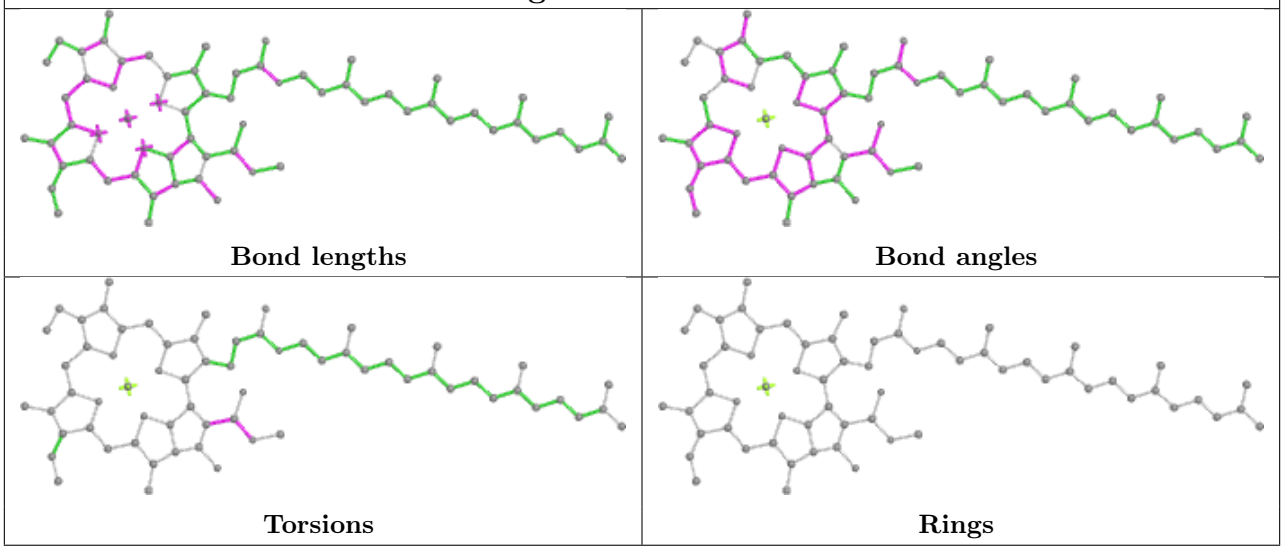
Ligand HTG V 202



Ligand LMT a 401



Ligand CLA b 613



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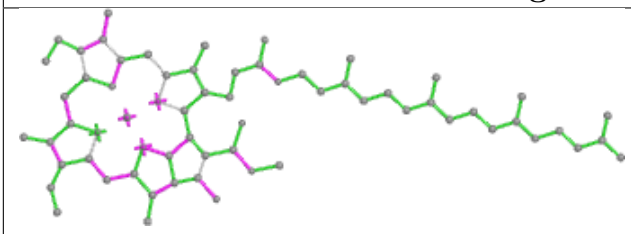
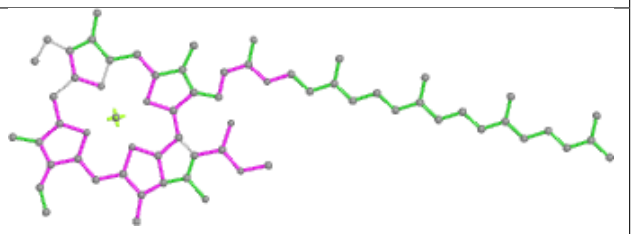
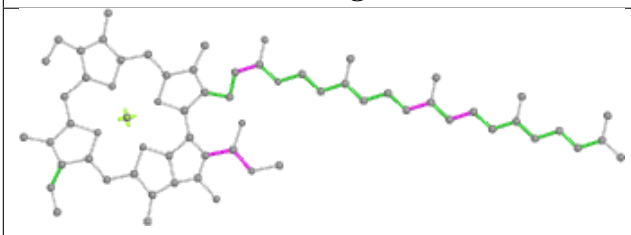


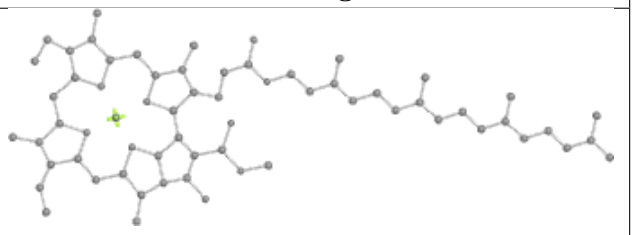
Bond lengths



Bond angles

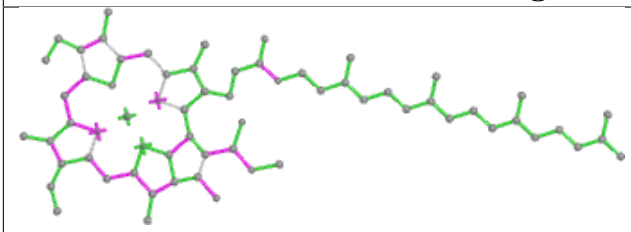


Torsions



Rings

Ligand CLA c 509



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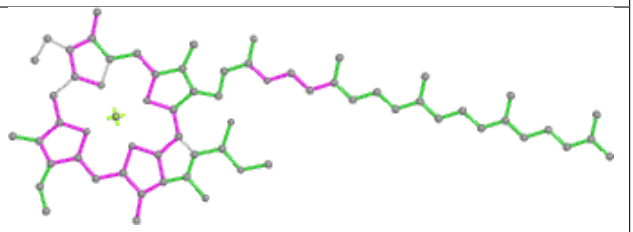
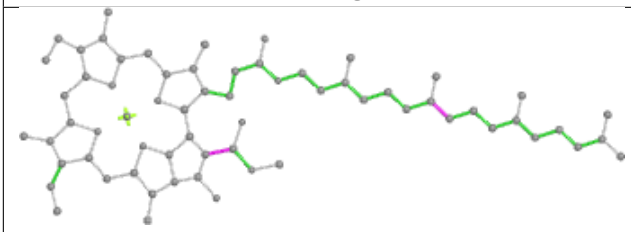
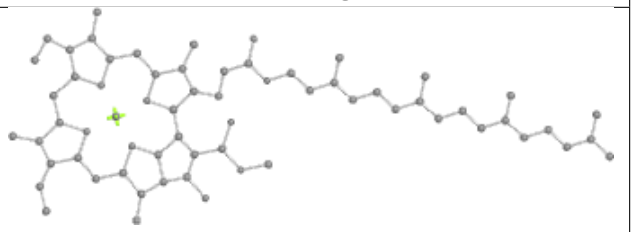


Bond angles

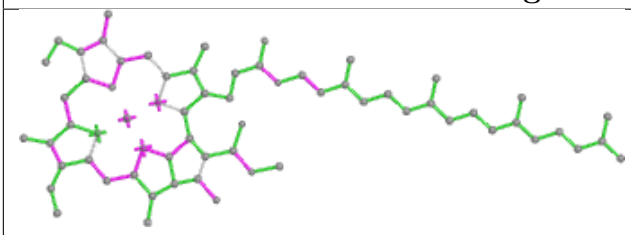


Torsions



Rings

Ligand CLA D 403



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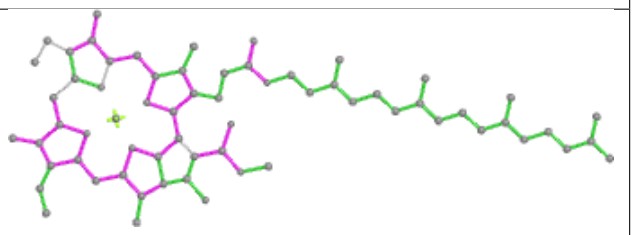
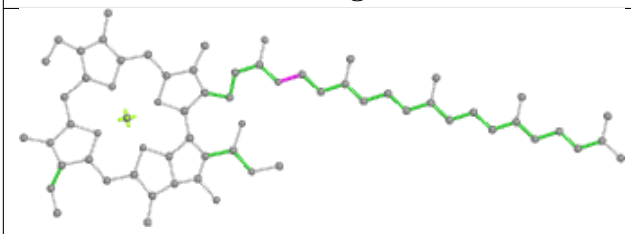


Bond angles



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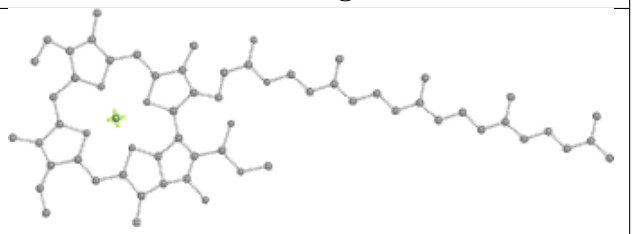
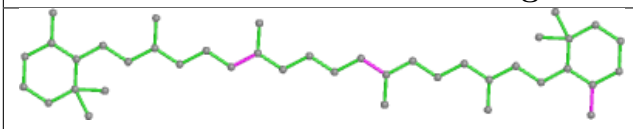


Rings

Ligand BCR K 101



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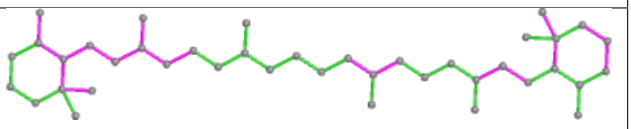
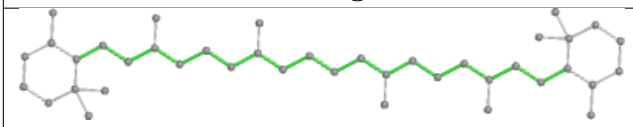


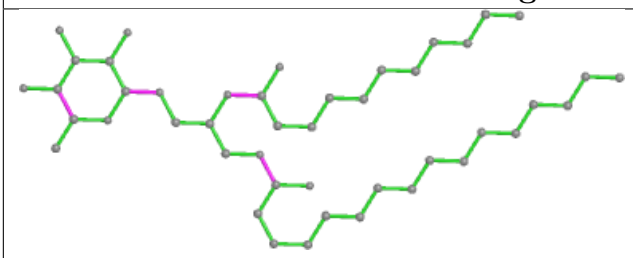
Bond angles



Torsions

Rings

Ligand DGD D 408



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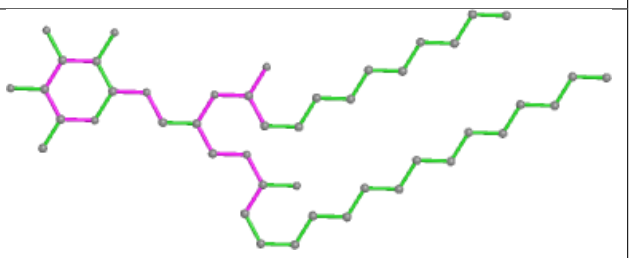
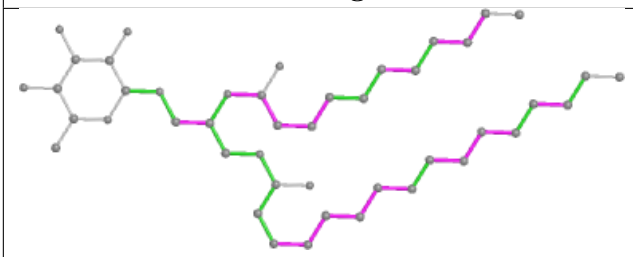
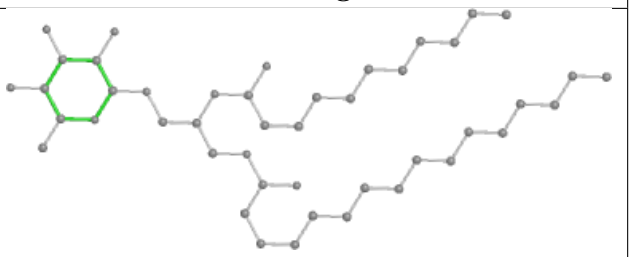


Bond angles

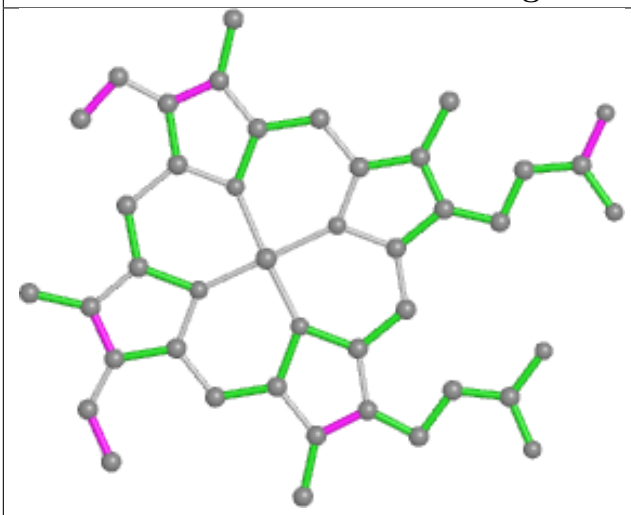


Torsions



Rings

Ligand HEC V 201



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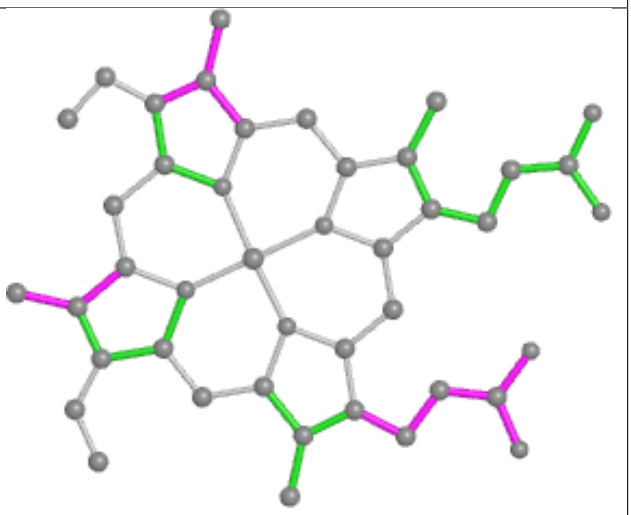
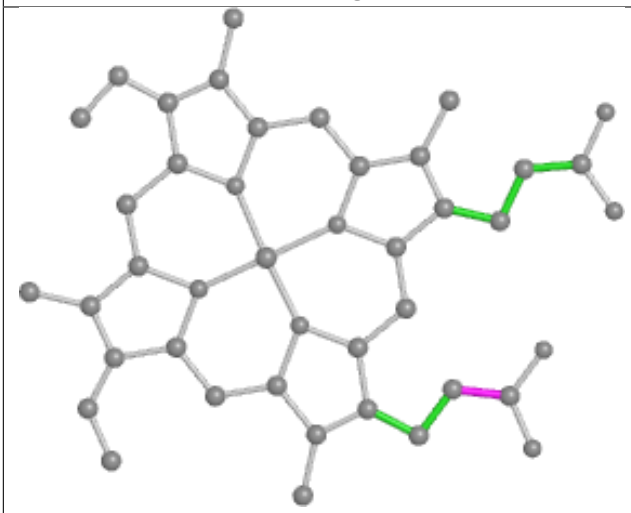
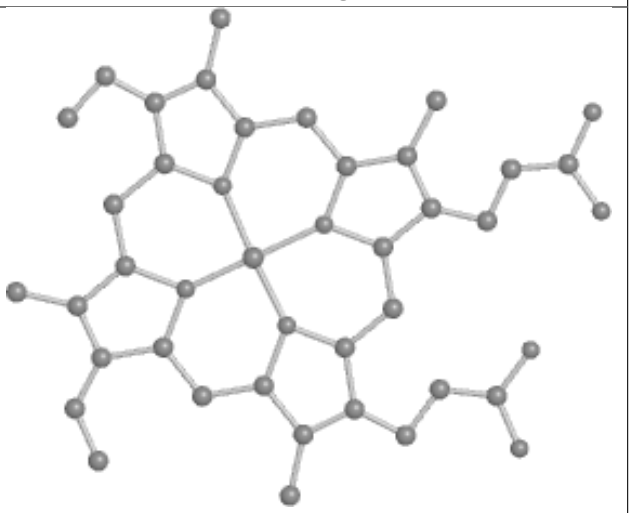


Bond angles

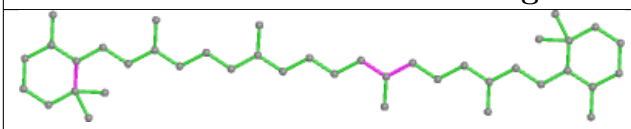


Torsions



Rings

Ligand BCR K 102



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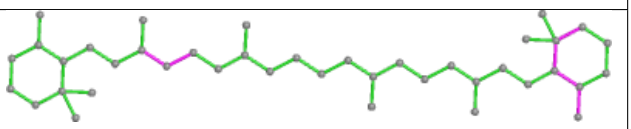
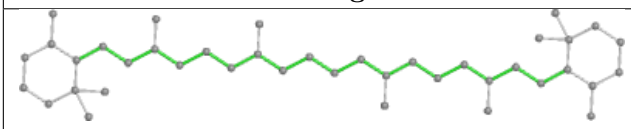
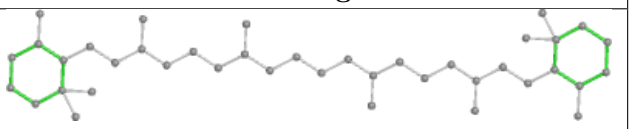


Bond angles

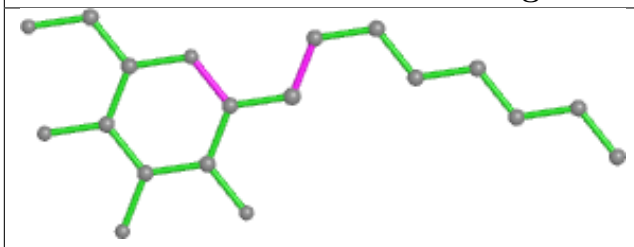


Torsions



Rings

Ligand HTG C 536



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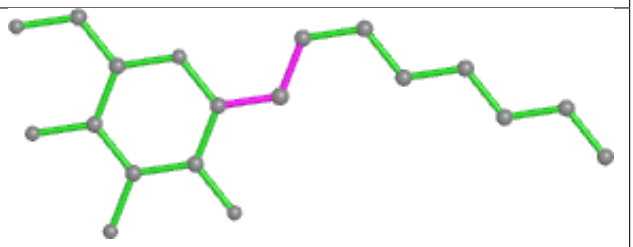
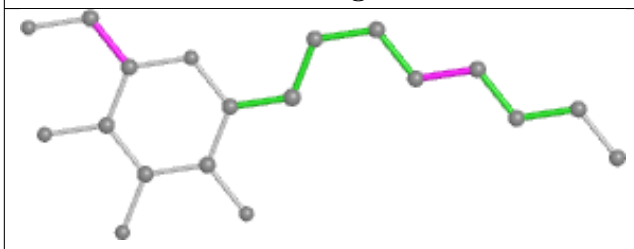
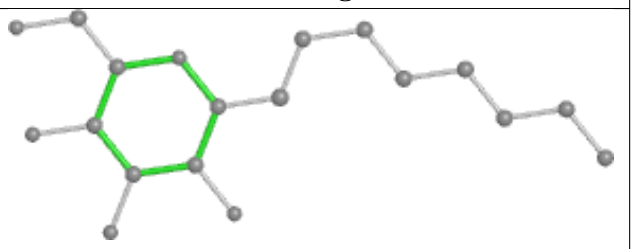


Bond angles

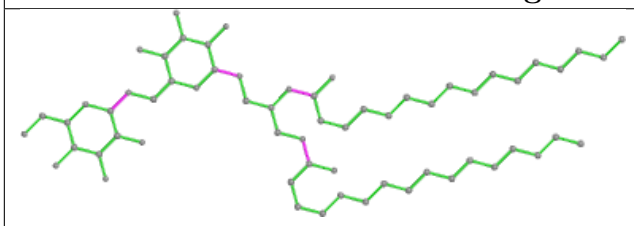


Torsions



Rings

Ligand DGD h 101



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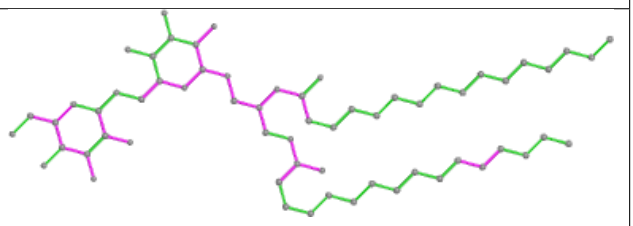
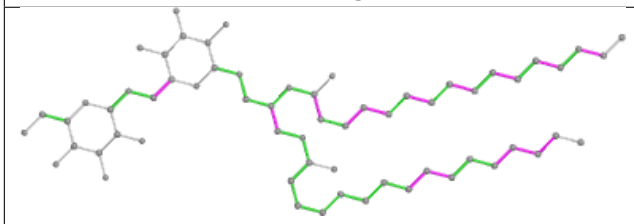
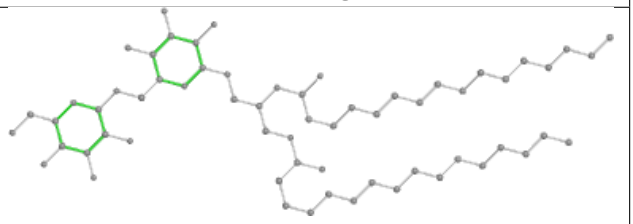


Bond angles

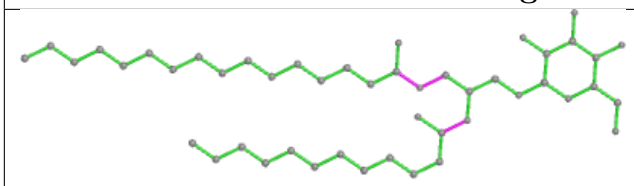


Torsions



Rings

Ligand LMG D 412



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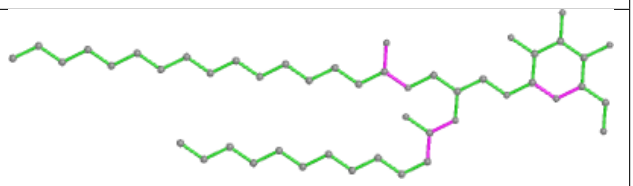
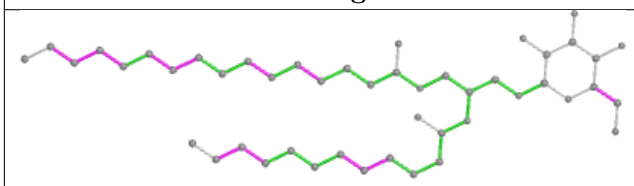
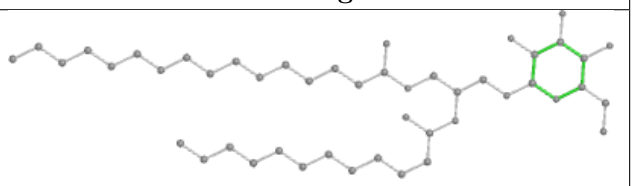


Bond angles

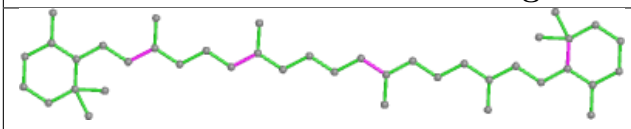


Torsions

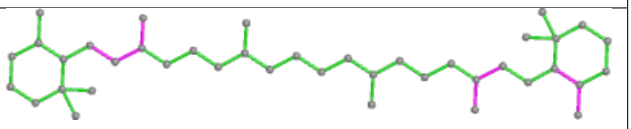


Rings

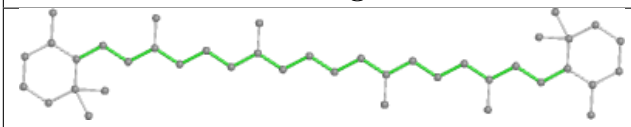
Ligand BCR C 514



Bond lengths



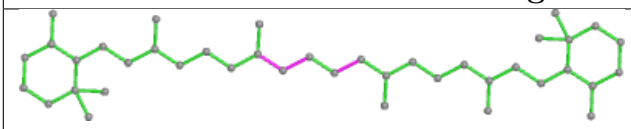
Bond angles



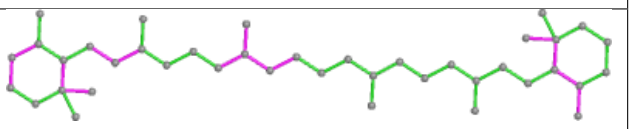
Torsions

Rings

Ligand BCR c 516



Bond lengths



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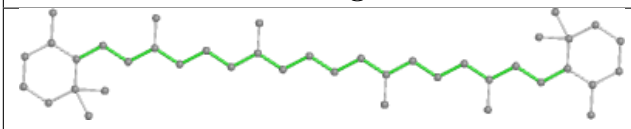
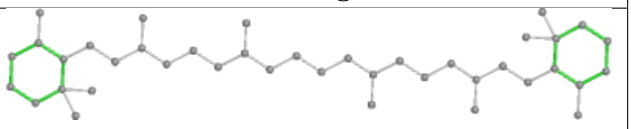
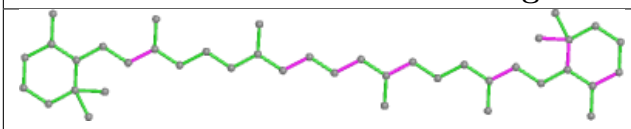


Torsions



Rings

Ligand BCR A 409



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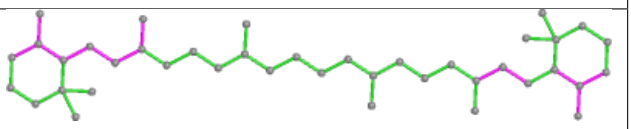
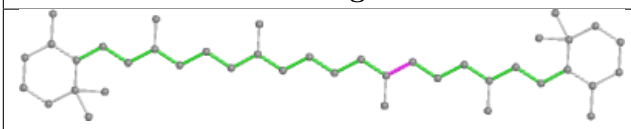


Bond angles



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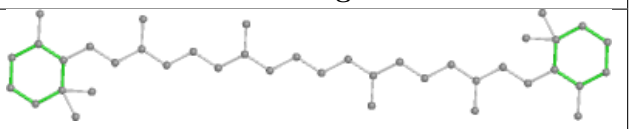
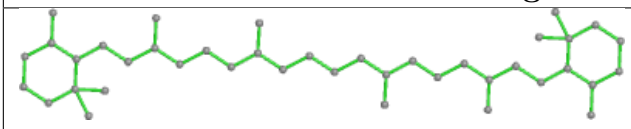


Rings

Ligand BCR T 101



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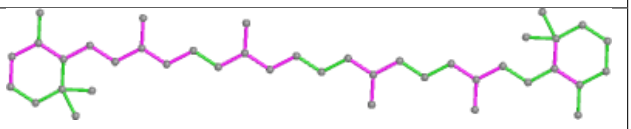

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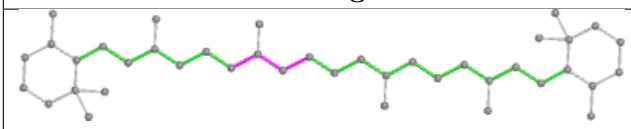

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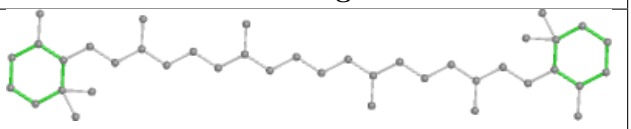
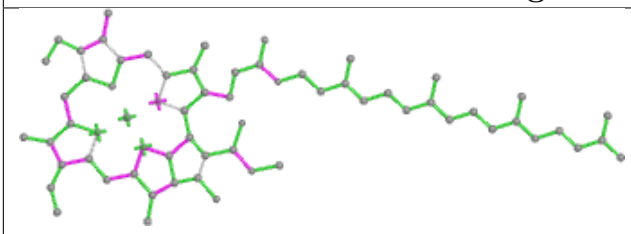


Rings

Ligand CLA d 402



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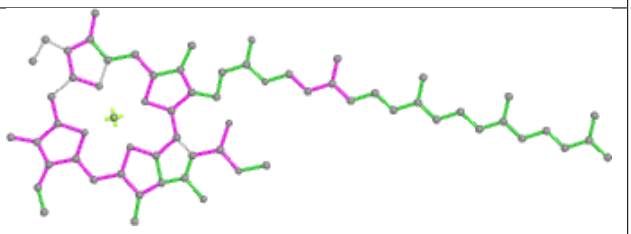
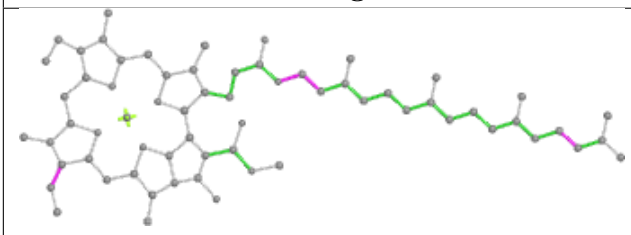


Bond angles



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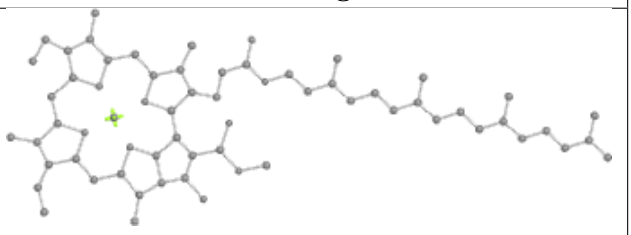
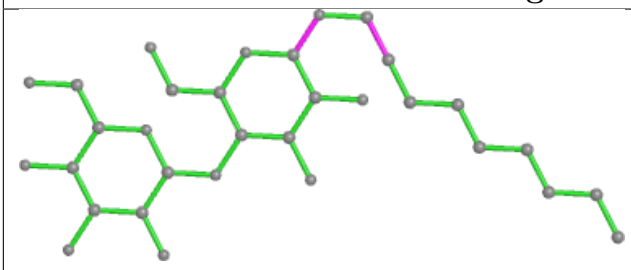


Rings

Ligand LMT z 101



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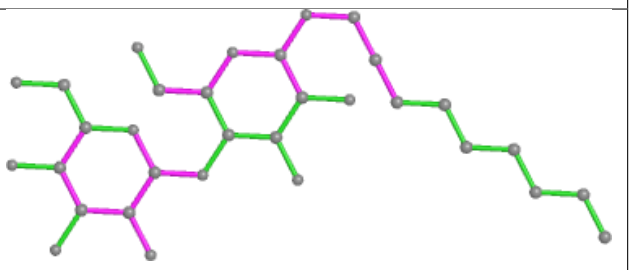
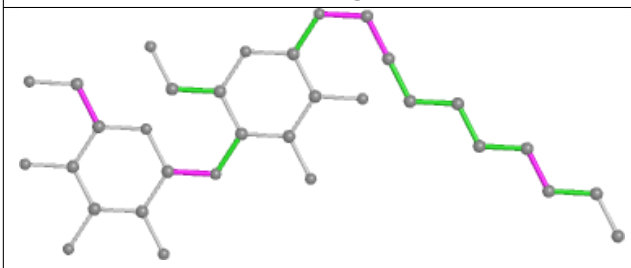


Bond angles



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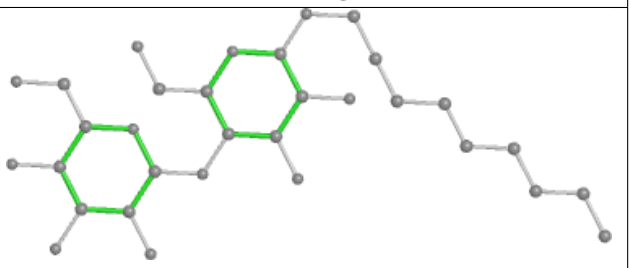
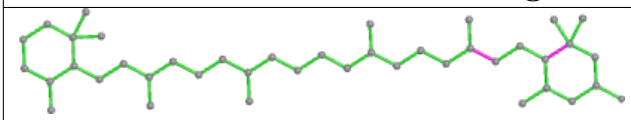


Rings

Ligand RRX h 102



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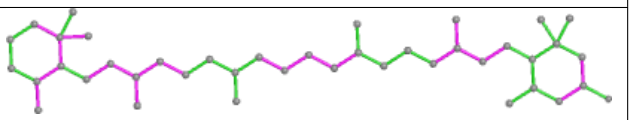

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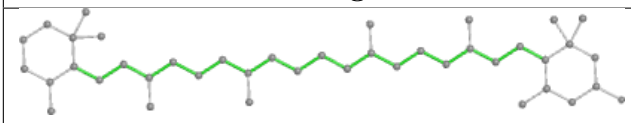

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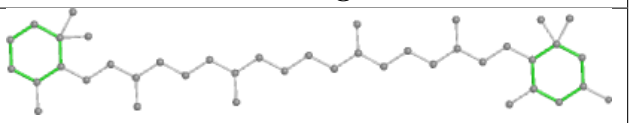
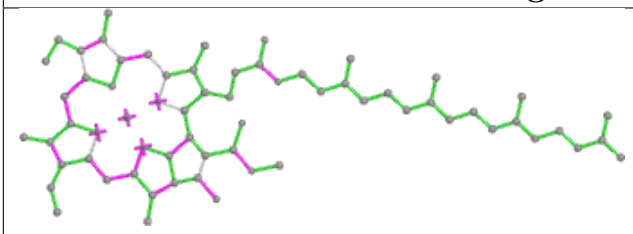


Rings

Ligand CLA b 616



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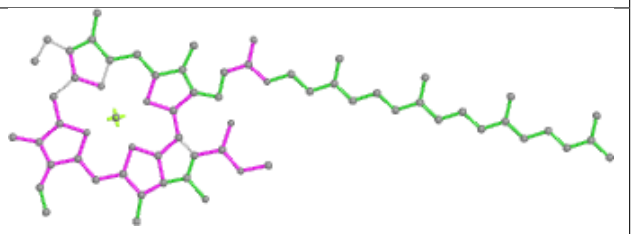

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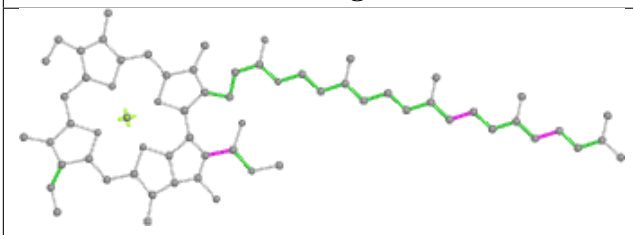

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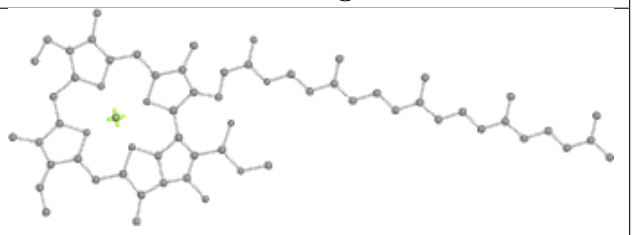
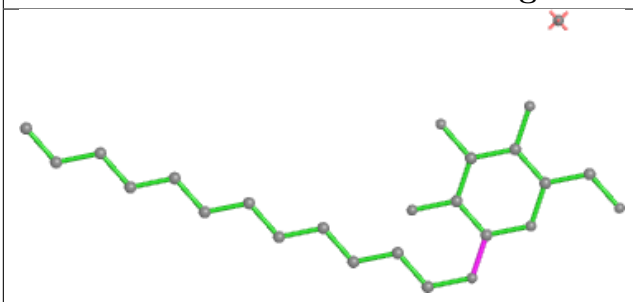


Rings

Ligand LMT m 102



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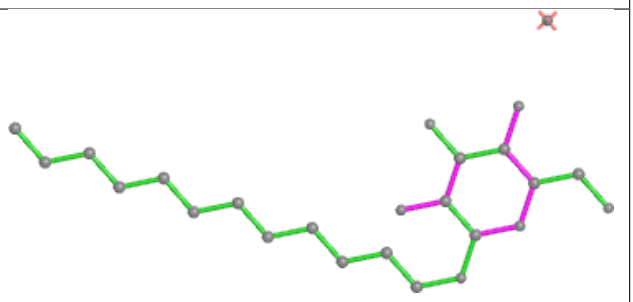
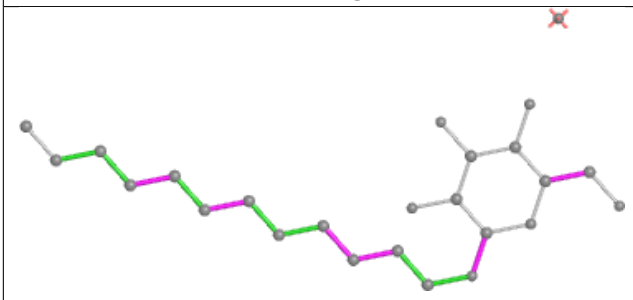


Bond angles



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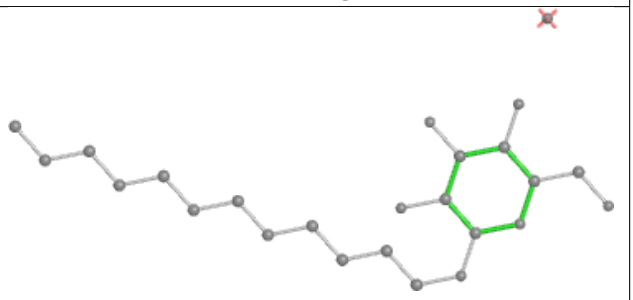
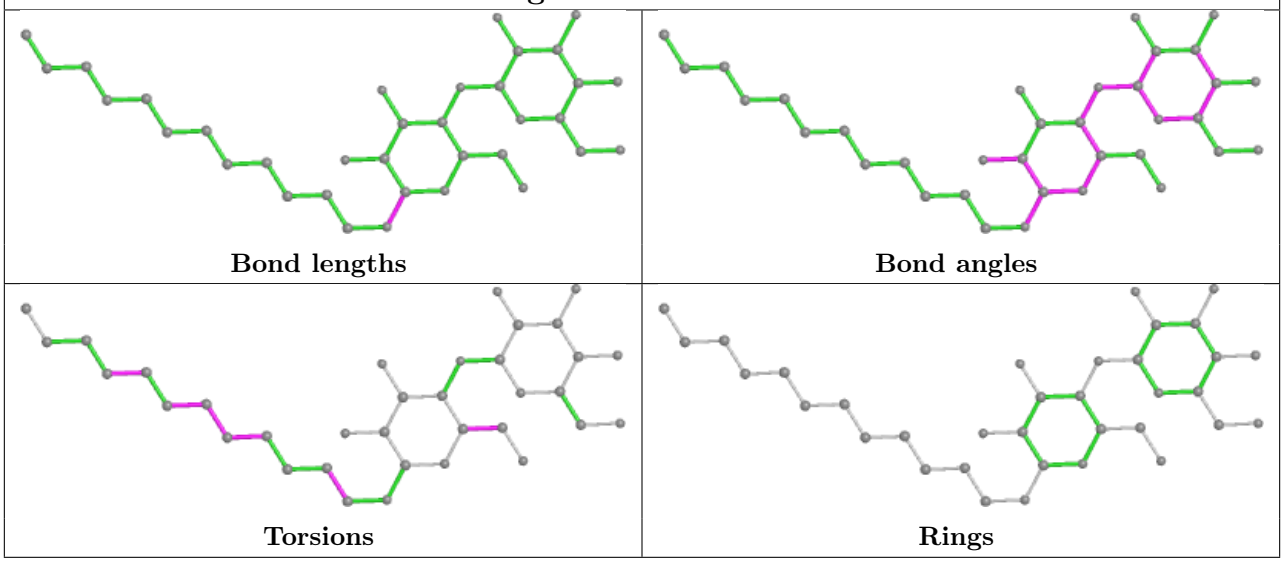
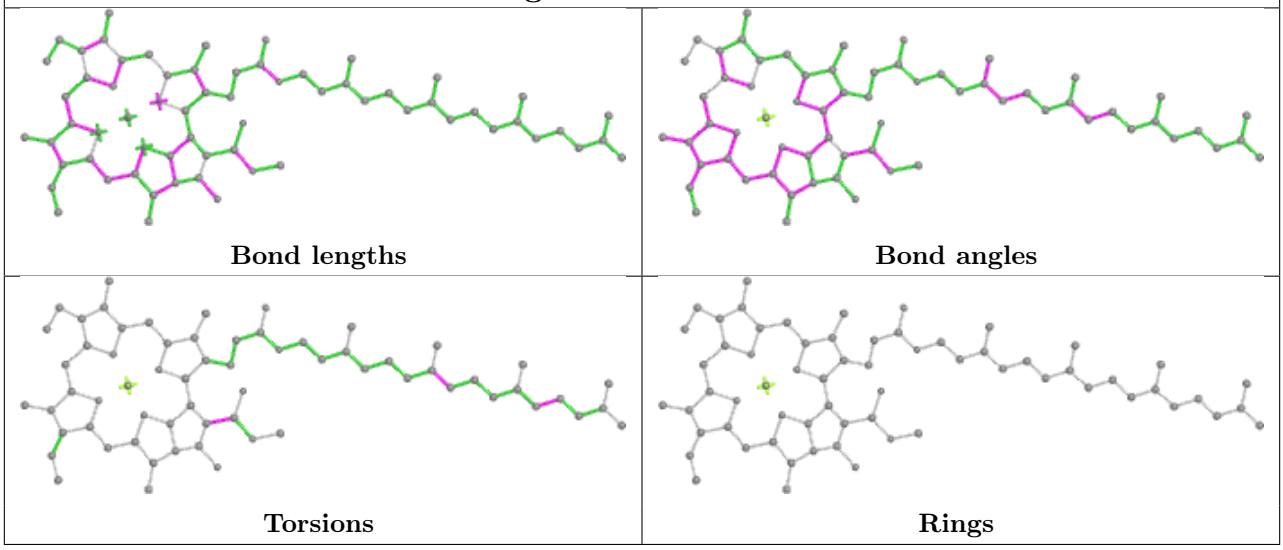


Rings

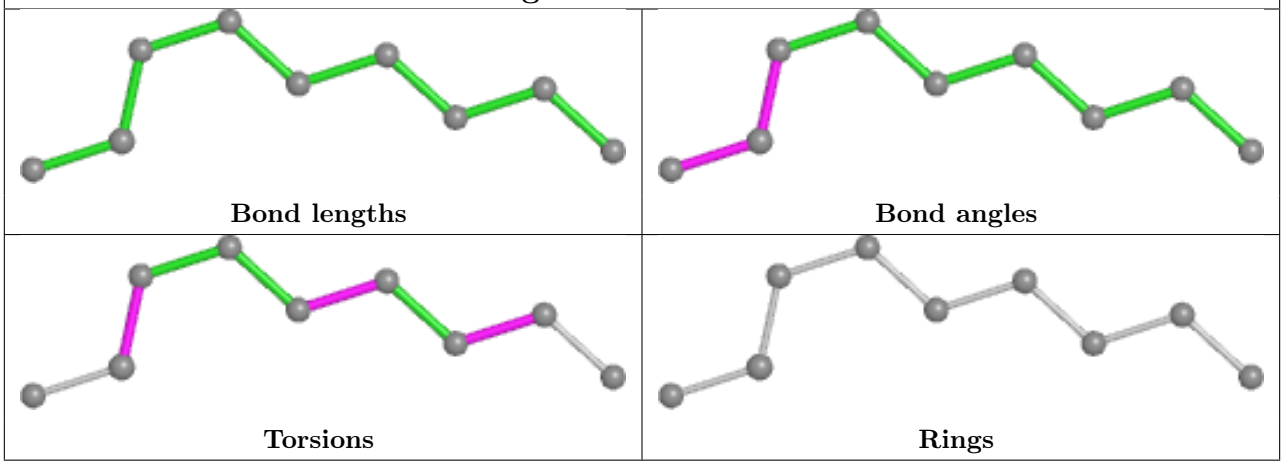
Ligand LMT c 522

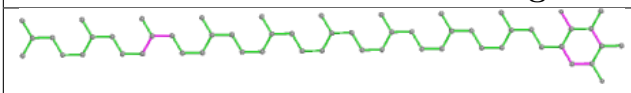
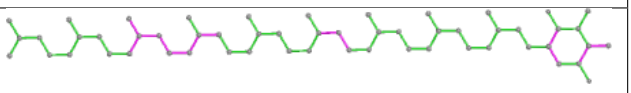
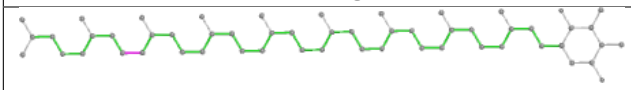
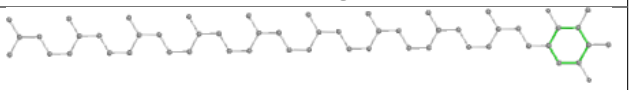


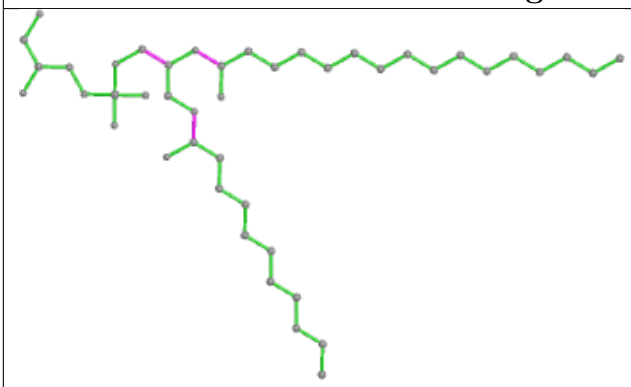
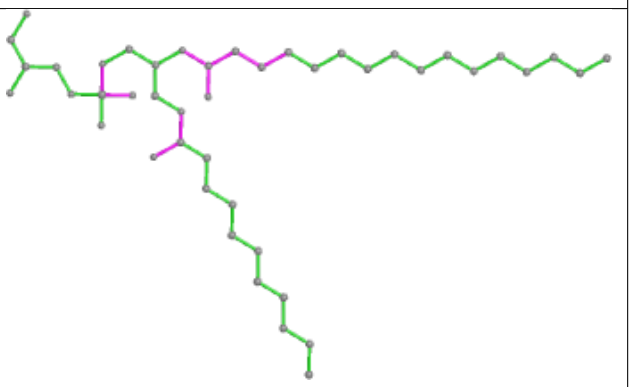
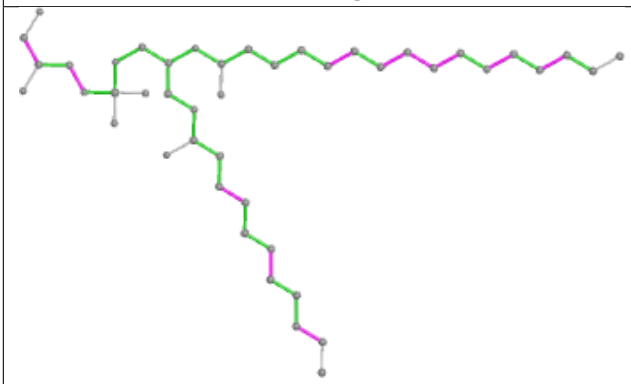
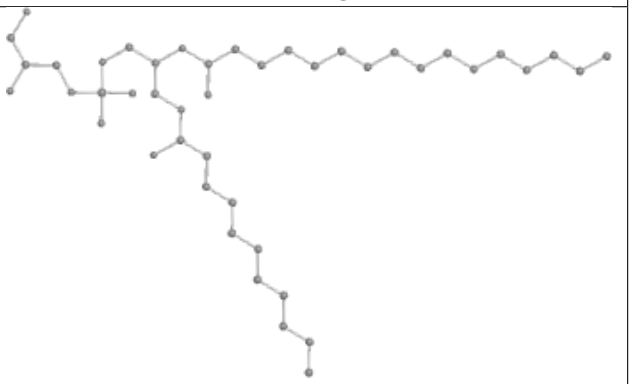
Ligand CLA A 406



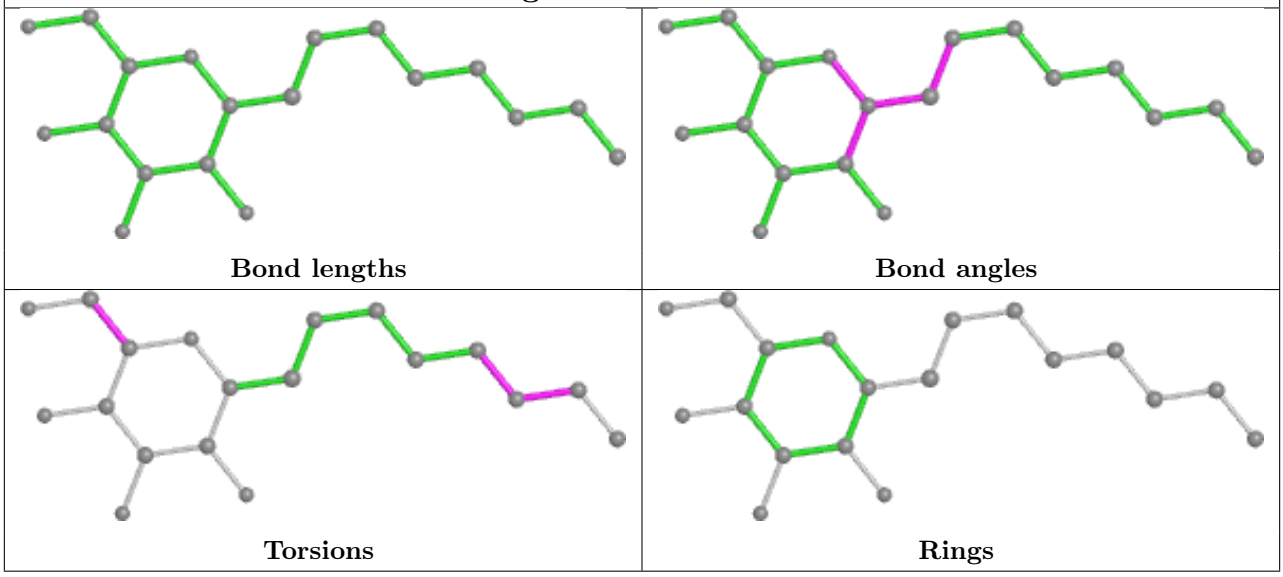
Ligand HTG C 535



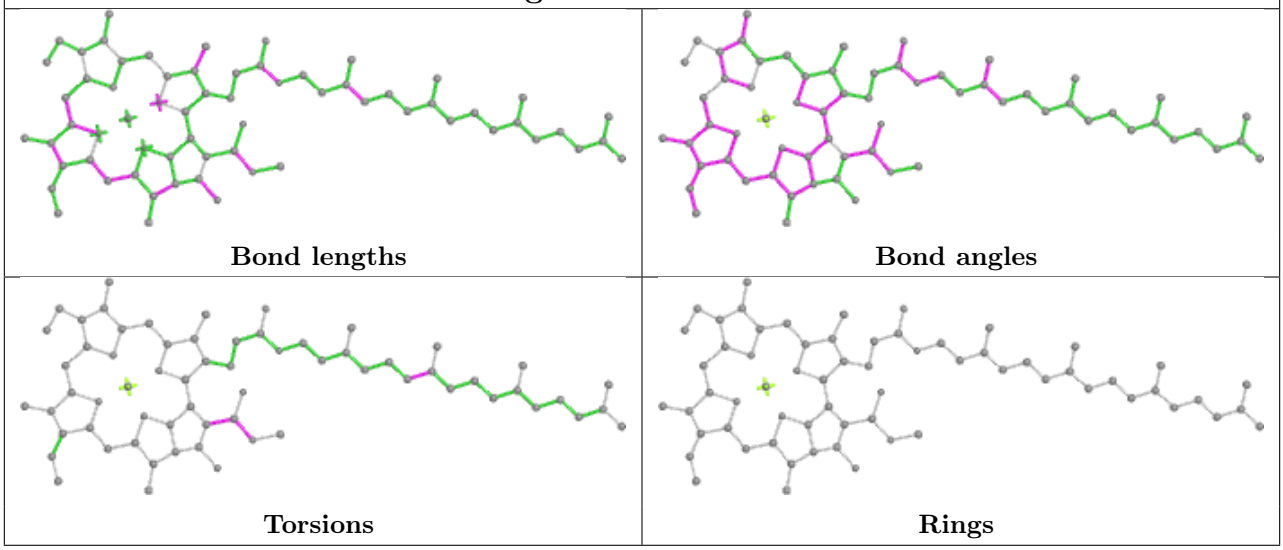
Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG d 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HTG B 628



Ligand CLA B 604



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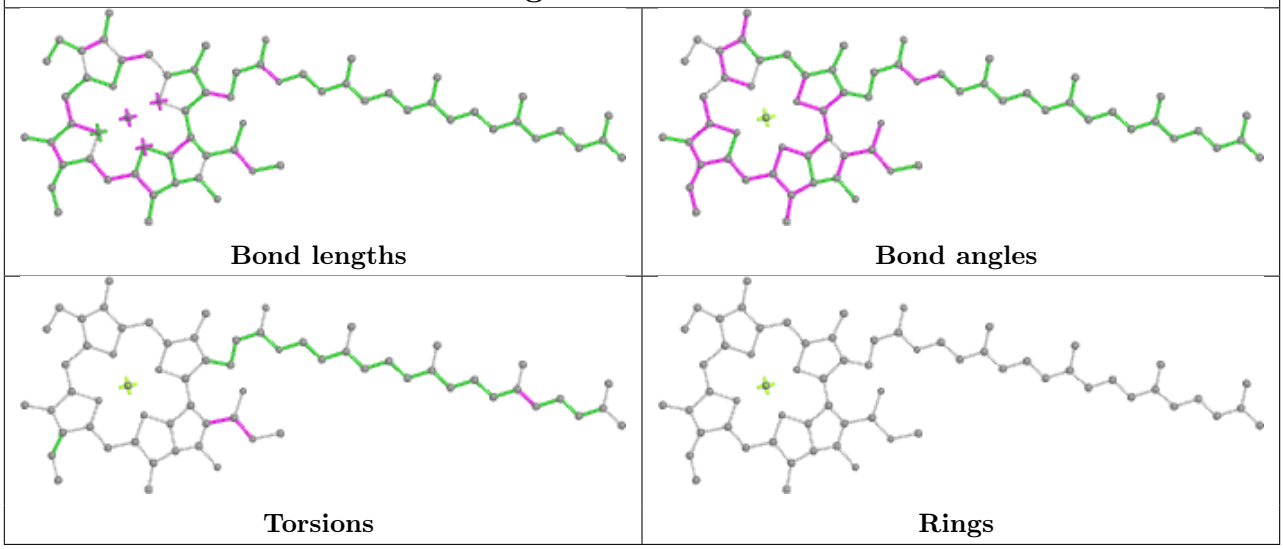
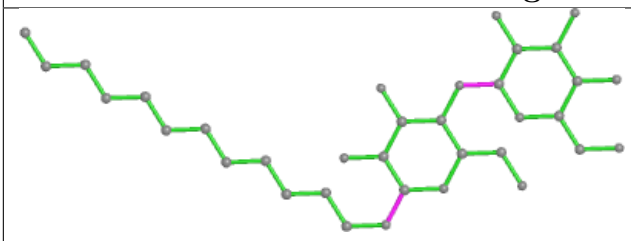
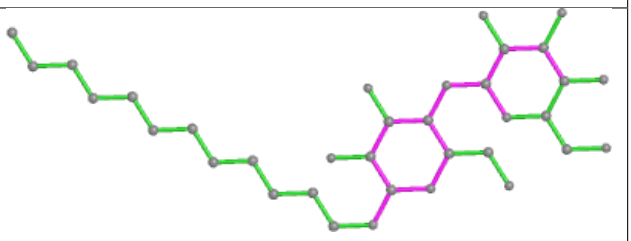


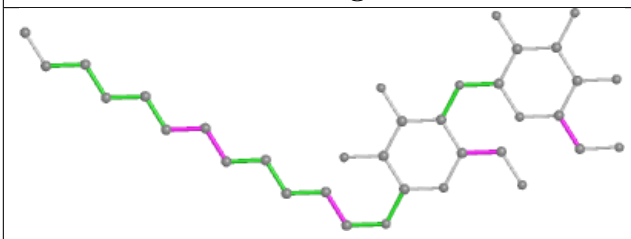
Ligand LMT Z 101



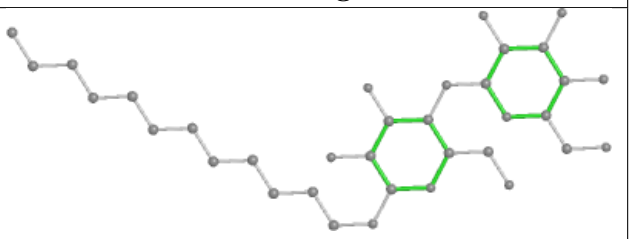
Bond lengths



Bond angles

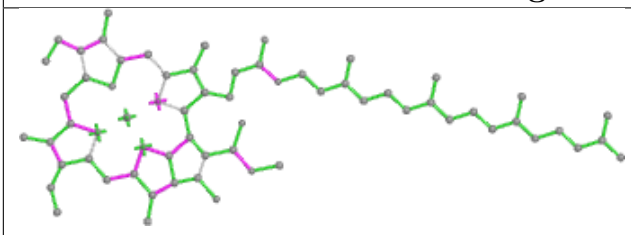


Torsions



Rings

Ligand CLA a 409



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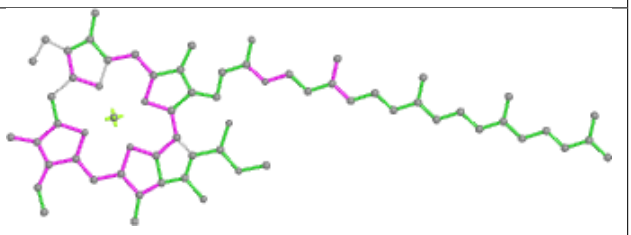
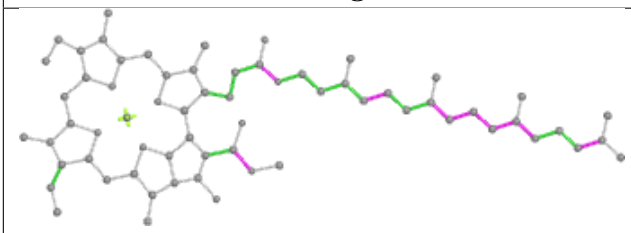
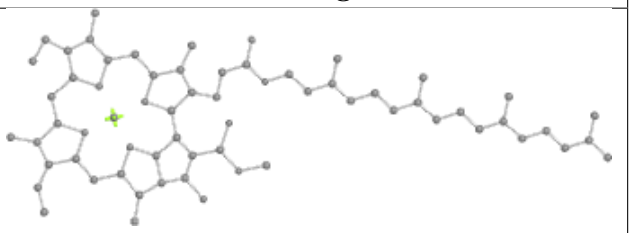


Bond angles

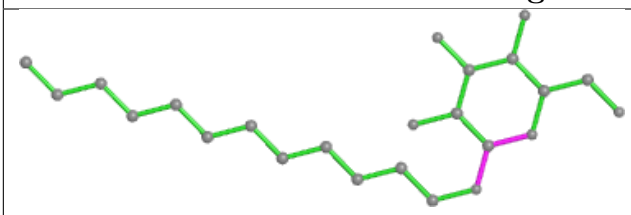


Torsions

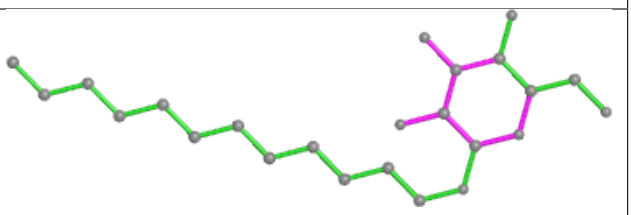


Rings

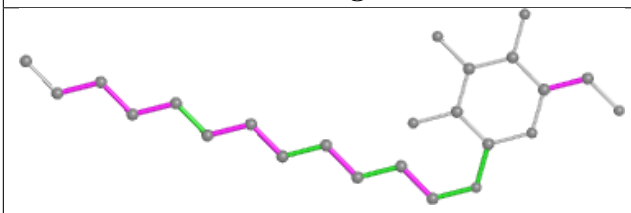
Ligand LMT t 102



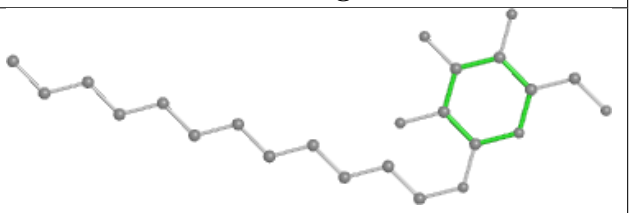
Bond lengths



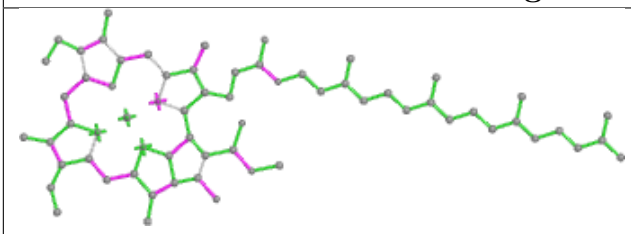
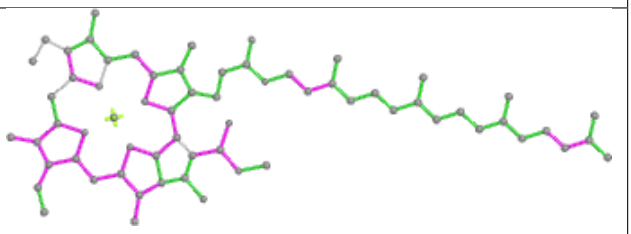
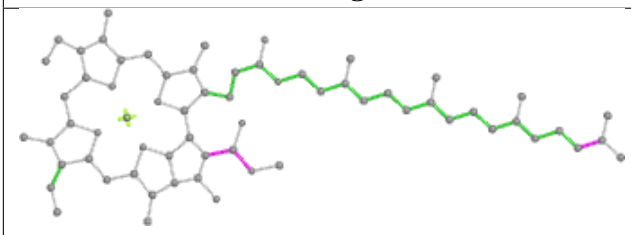
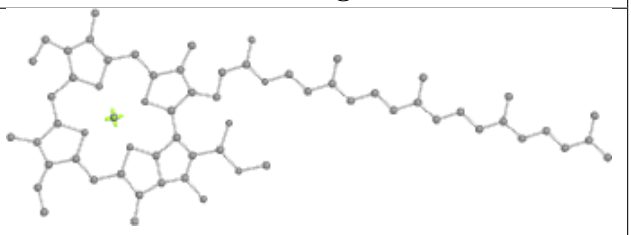
Bond angles

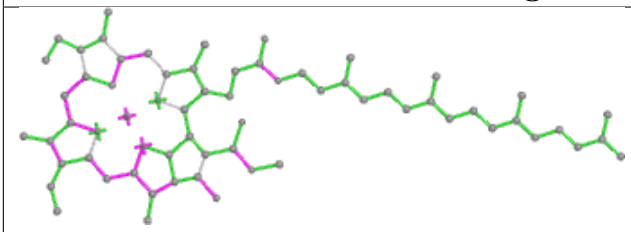
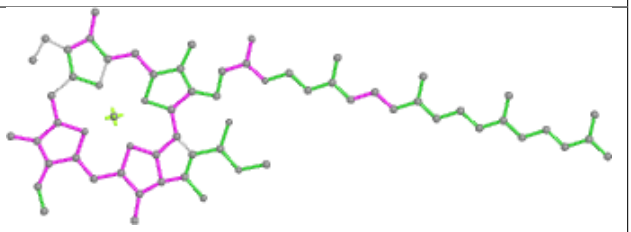
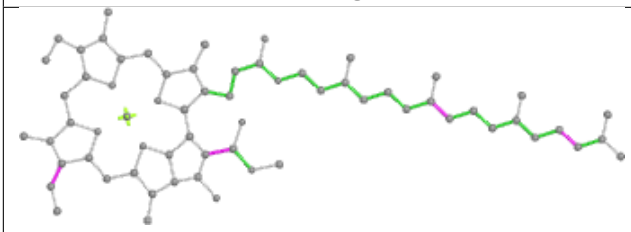
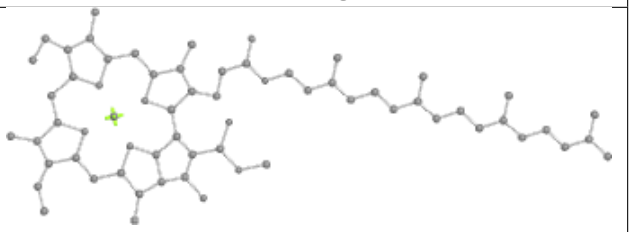


Torsions

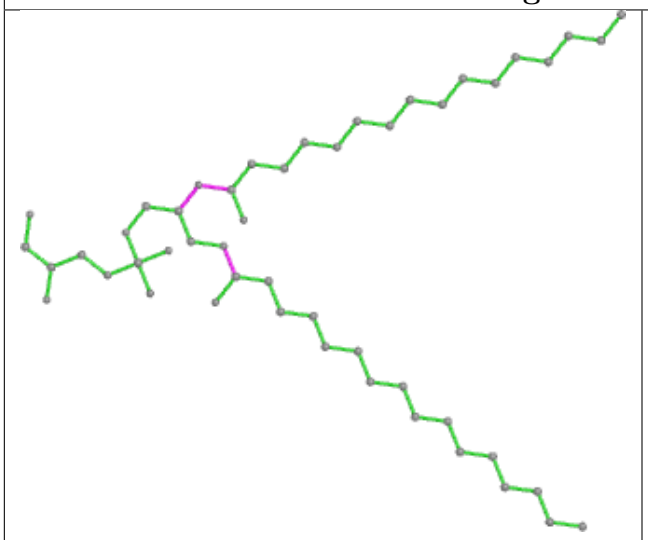


Rings

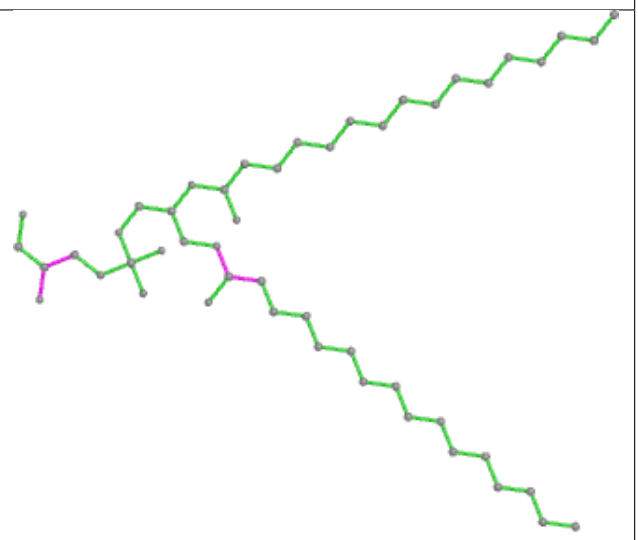
Ligand CLA C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

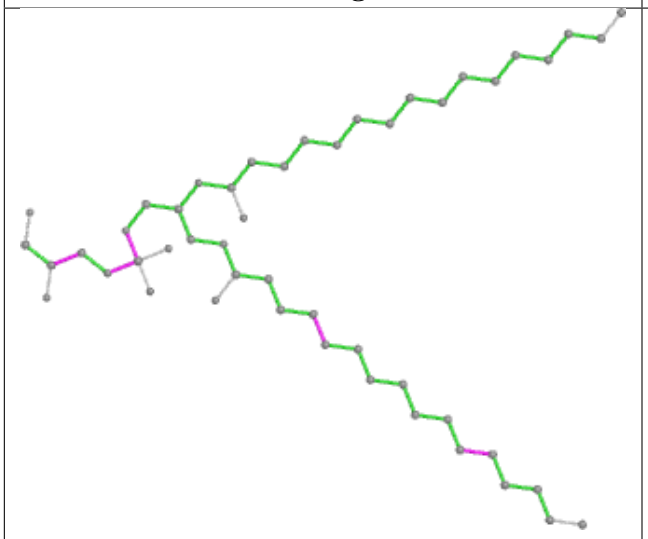
Ligand LHG D 410



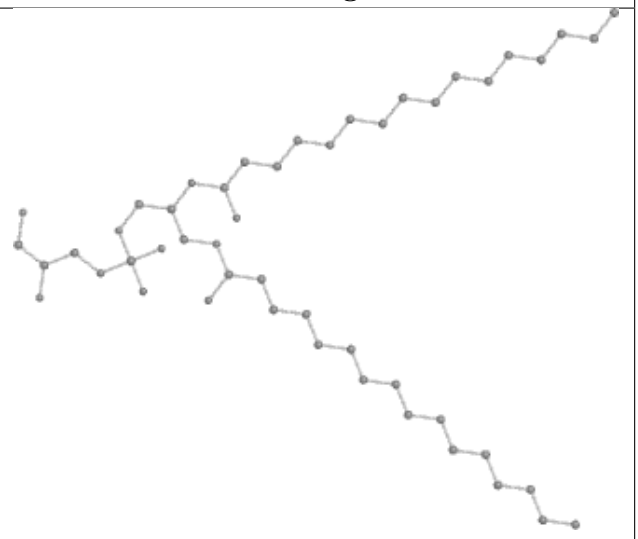
Bond lengths



Bond angles

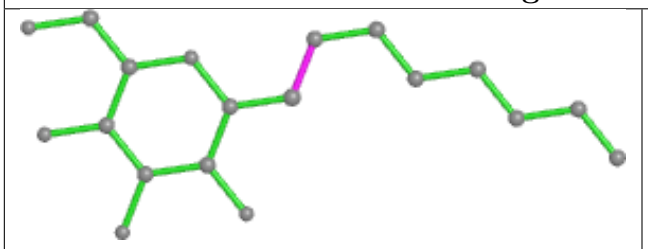


Torsions

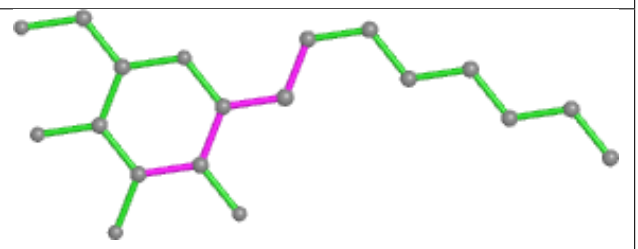


Rings

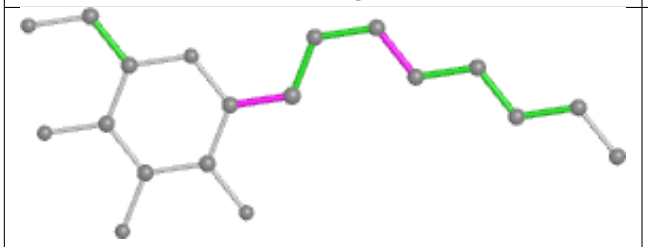
Ligand HTG B 624



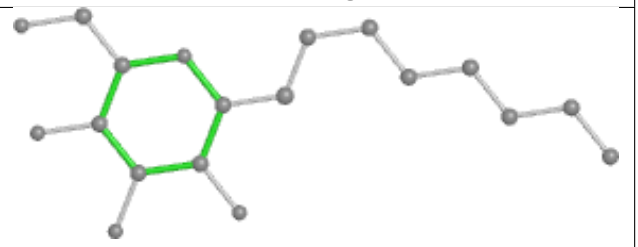
Bond lengths



Bond angles

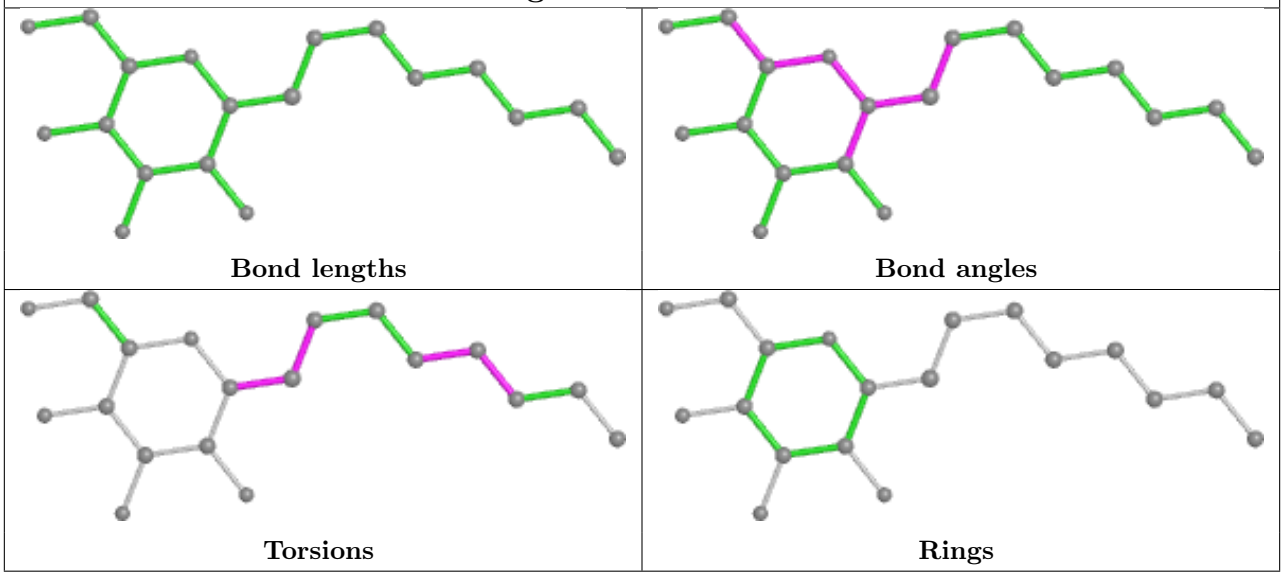


Torsions

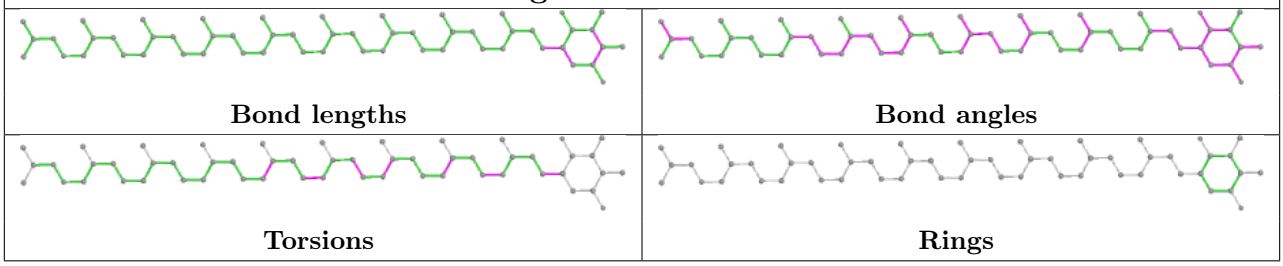


Rings

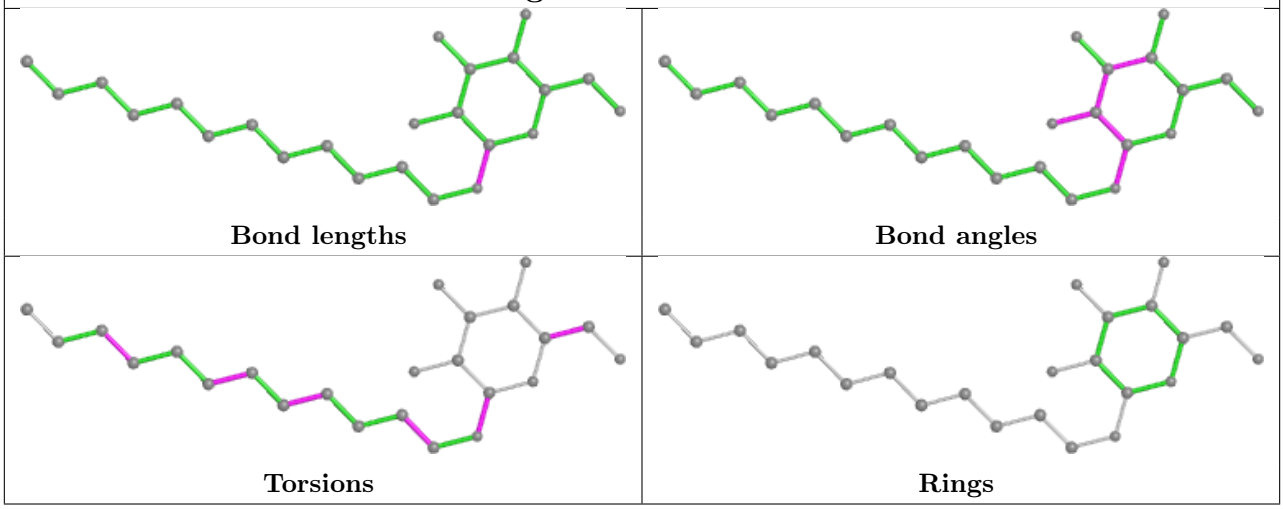
Ligand HTG c 523



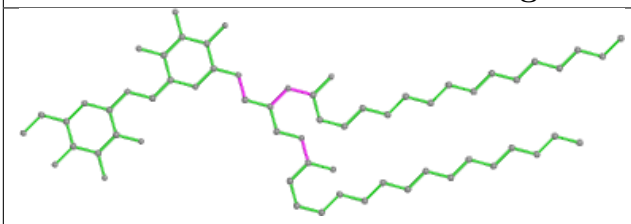
Ligand PL9 A 410



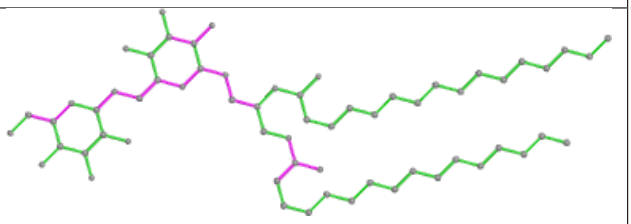
Ligand LMT J 102



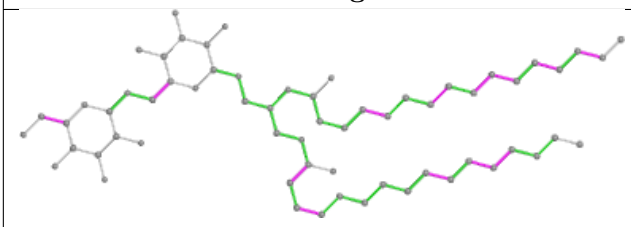
Ligand DGD C 517



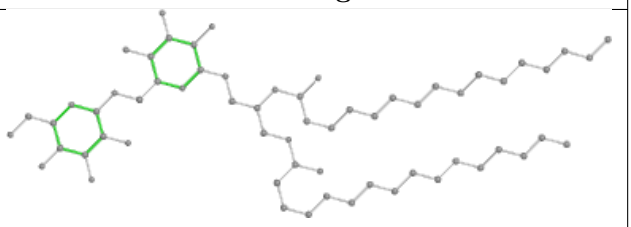
Bond lengths



Bond angles

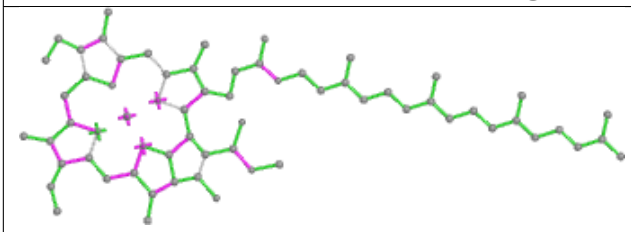


Torsions



Rings

Ligand CLA B 609



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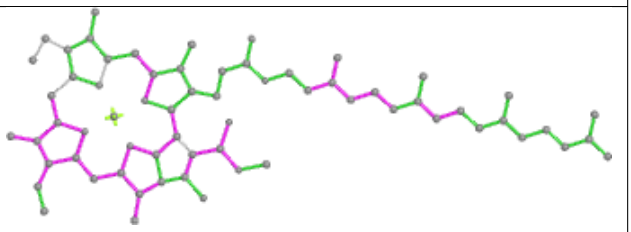
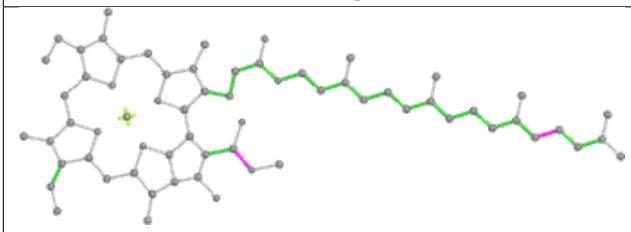
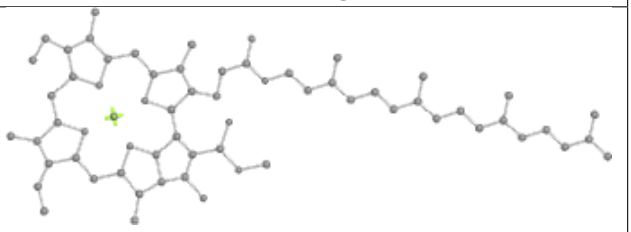


Bond angles

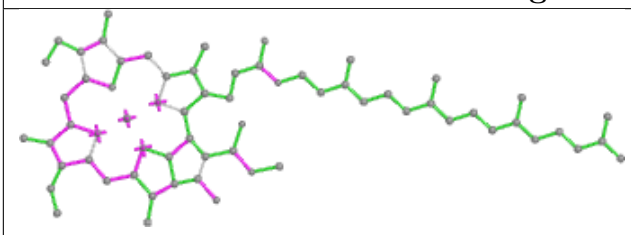


Torsions



Rings

Ligand CLA c 506



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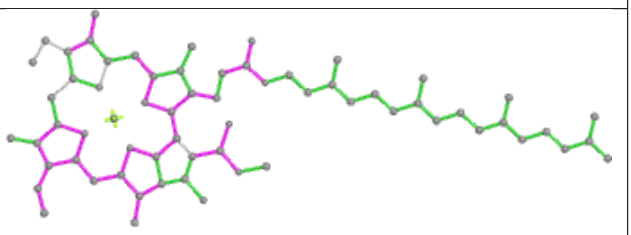
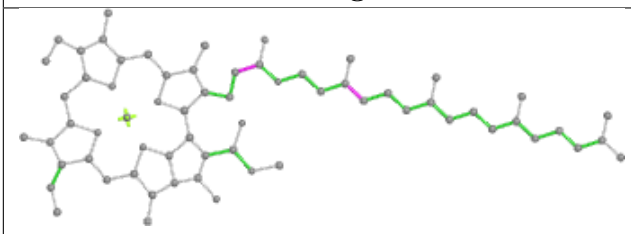
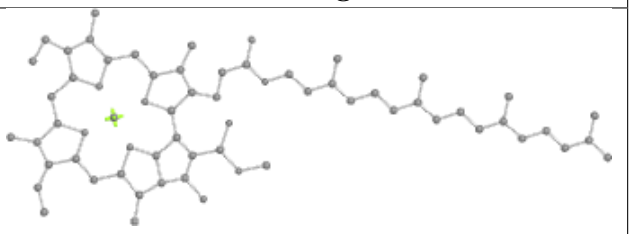


Bond angles

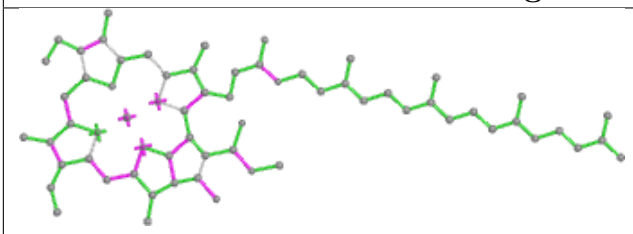


Torsions



Rings

Ligand CLA B 612



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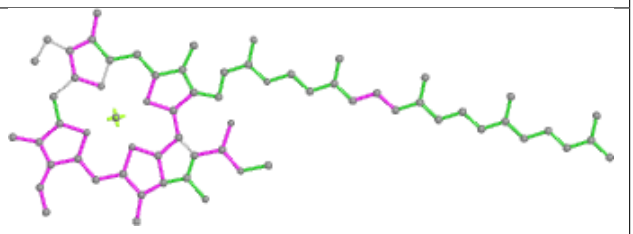
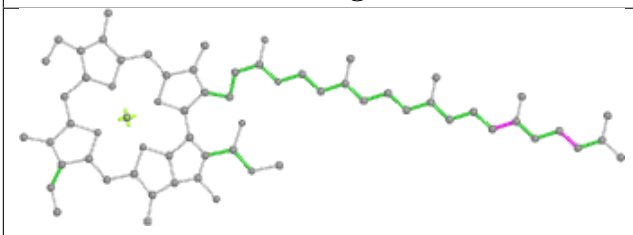


Bond angles



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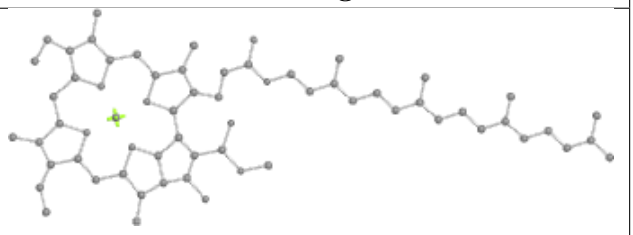
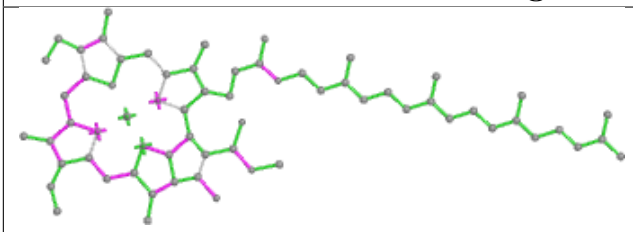


Rings

Ligand CLA b 605



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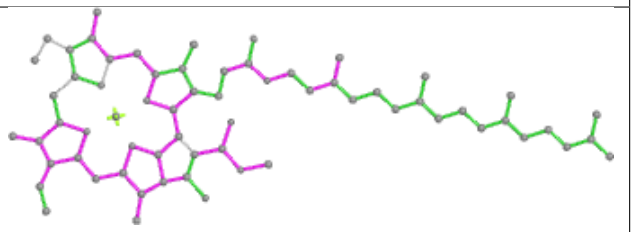
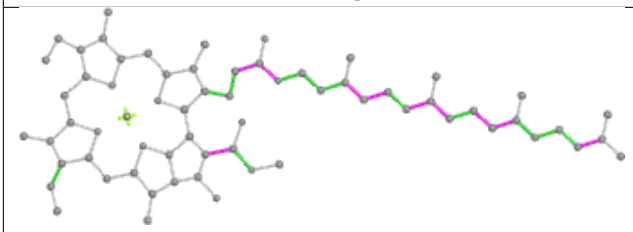


Bond angles



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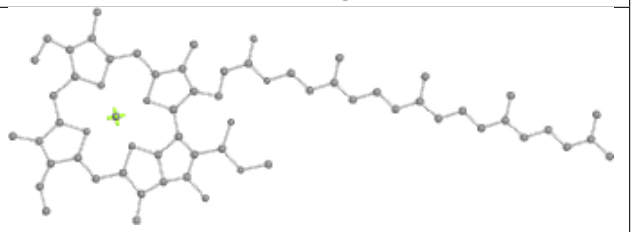
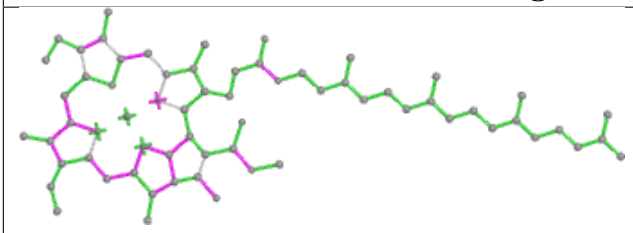
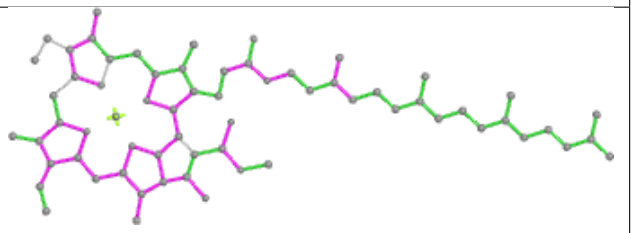


Rings

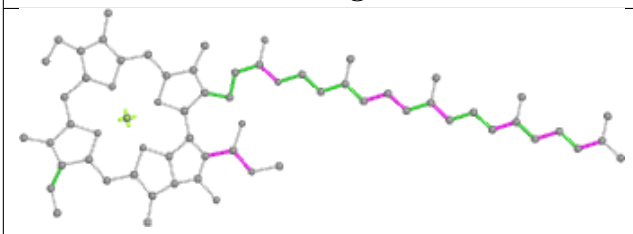
Ligand CLA c 514



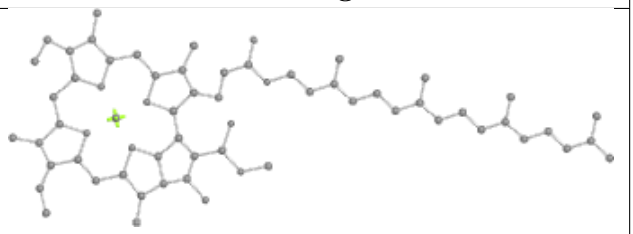
Bond lengths



Bond angles

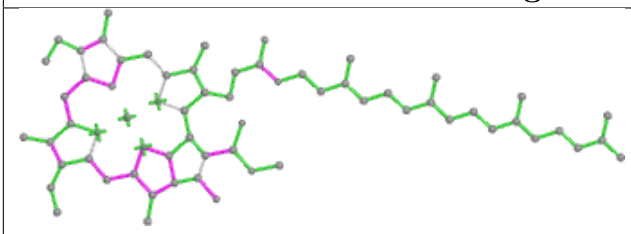


Torsions

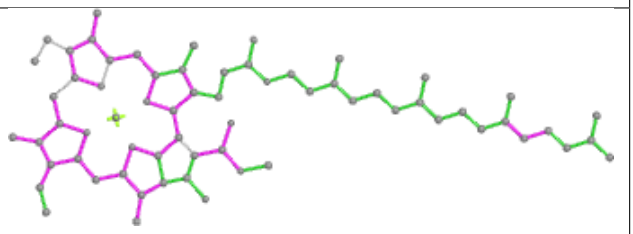


Rings

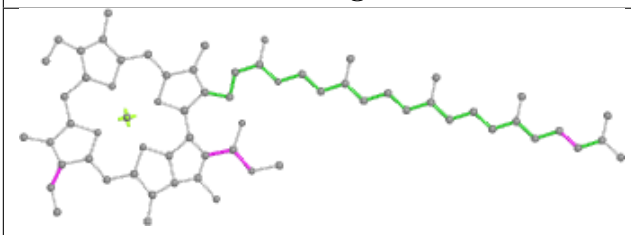
Ligand CLA A 405



Bond lengths



Bond angles



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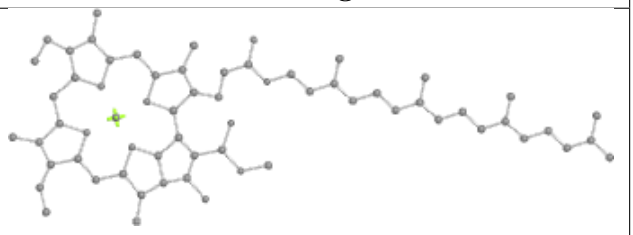
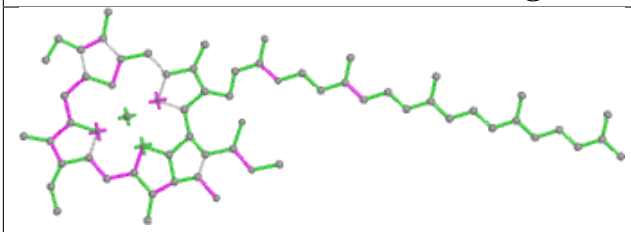
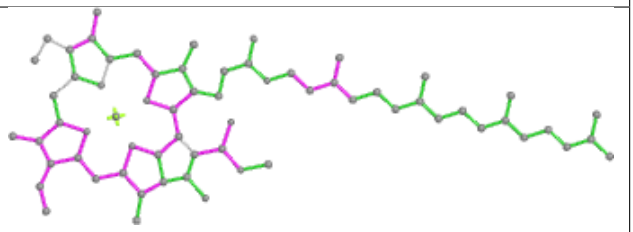


Rings

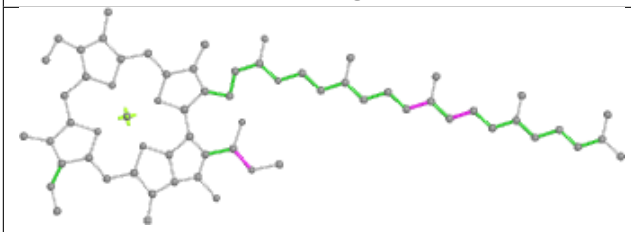
Ligand CLA C 503



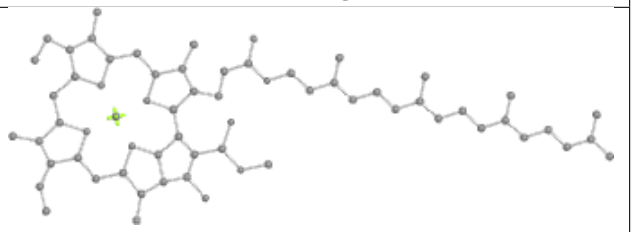
Bond lengths



Bond angles

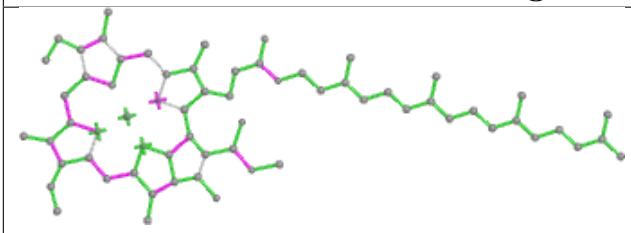


Torsions



Rings

Ligand CLA b 615



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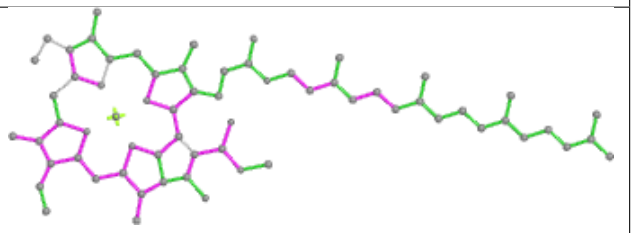

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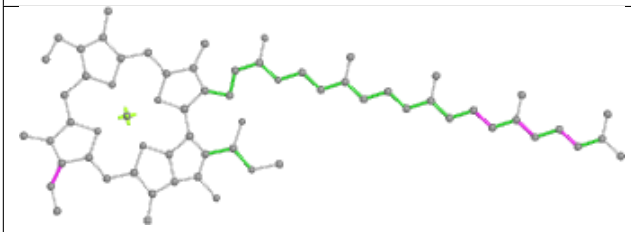

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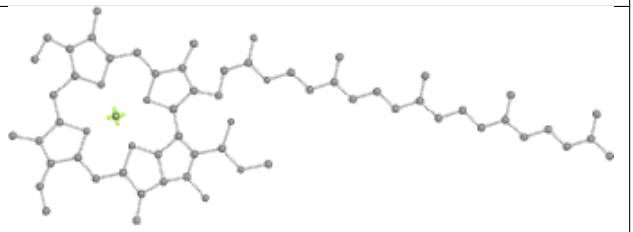
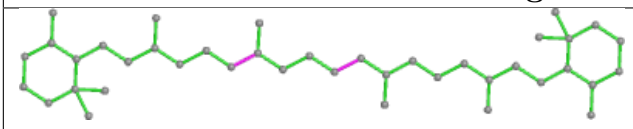


Rings

Ligand BCR k 101



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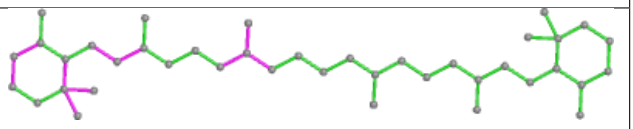

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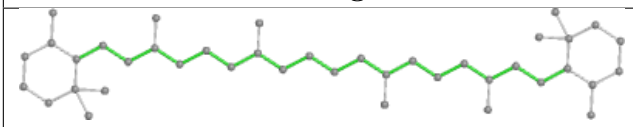

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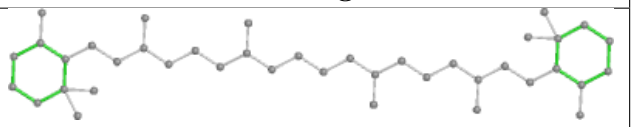
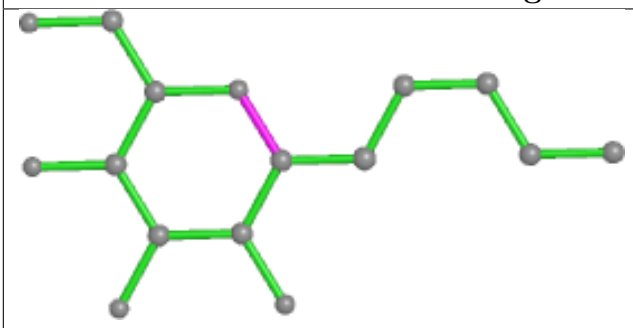


Rings

Ligand HTG d 413



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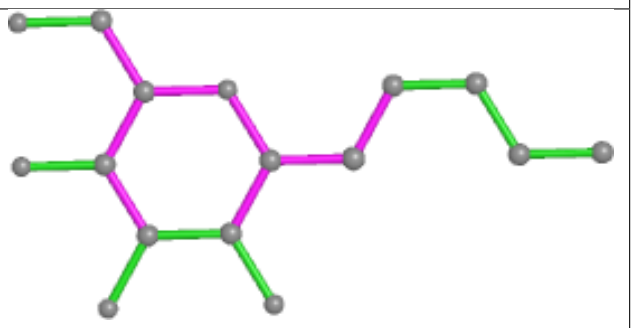
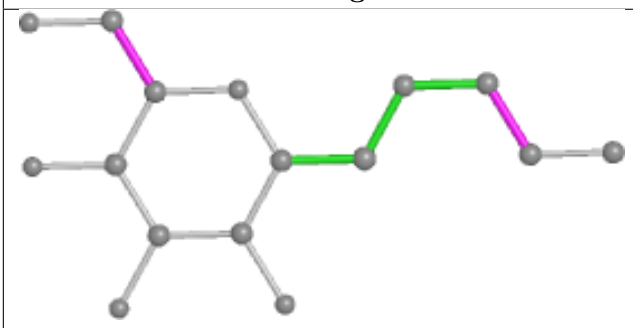


Bond angles



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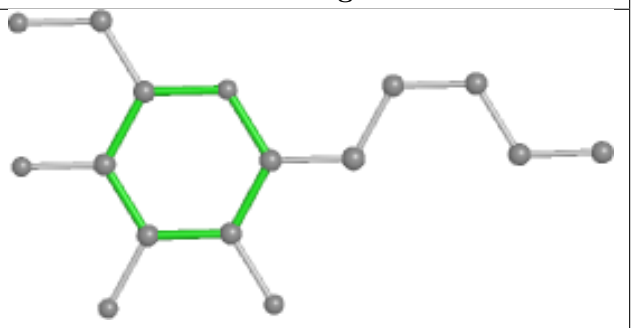
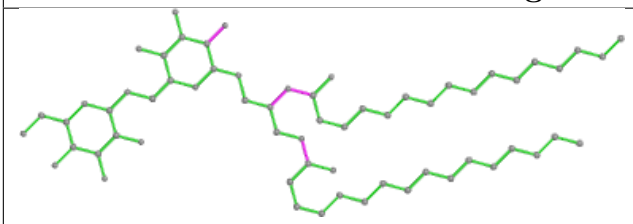


Rings

Ligand DGD c 519



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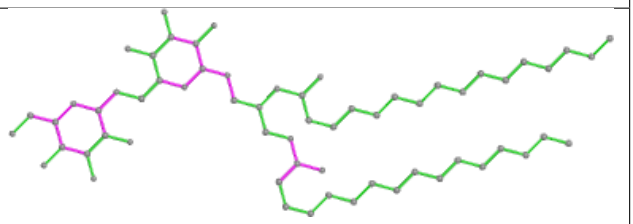
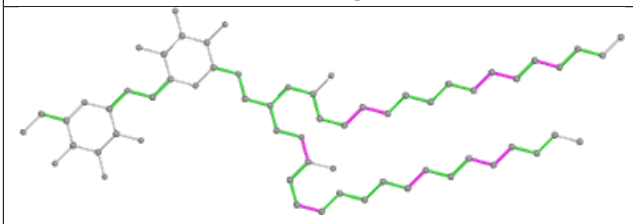


Bond angles



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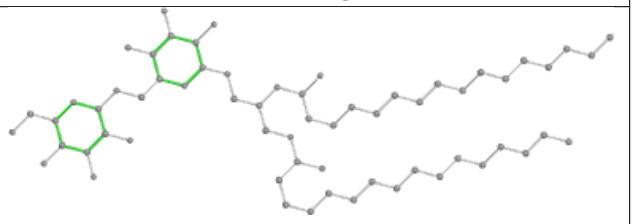

Rings

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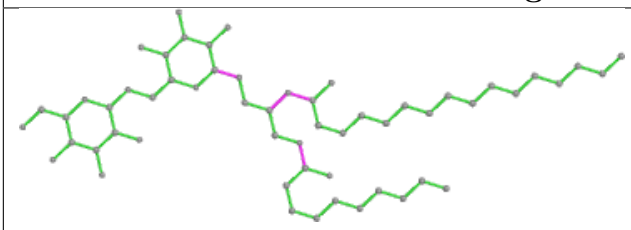

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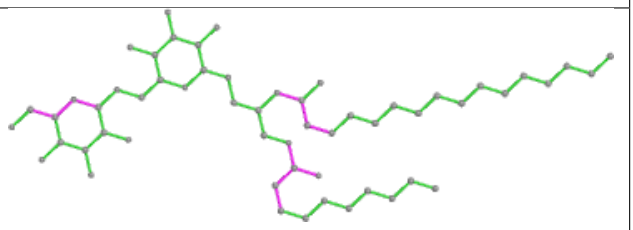
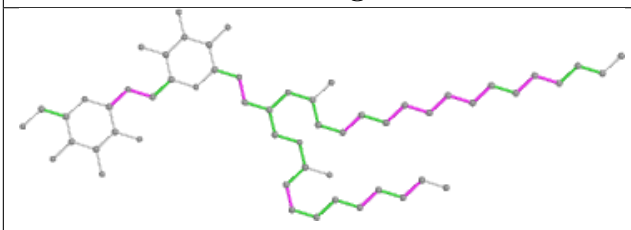


Bond angles



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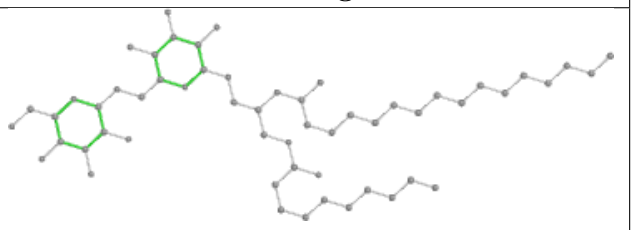

Rings

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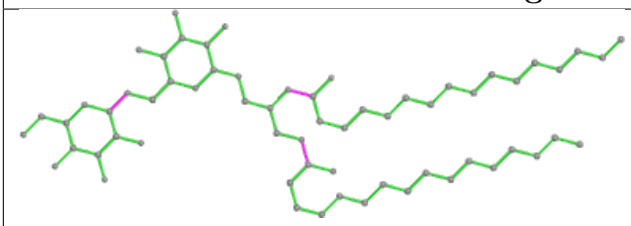

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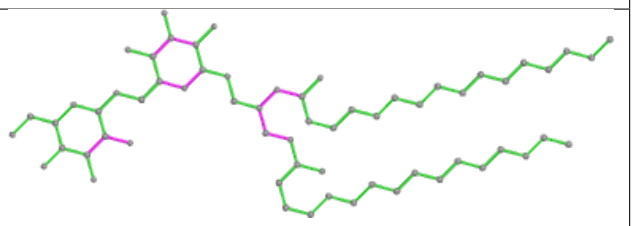

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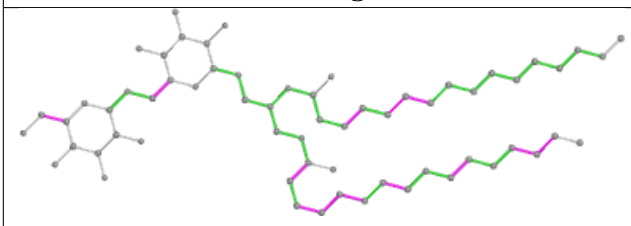

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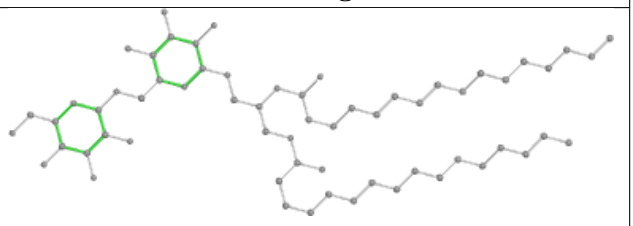
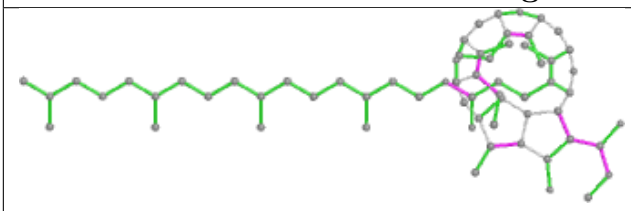


Rings

Ligand PHO A 407



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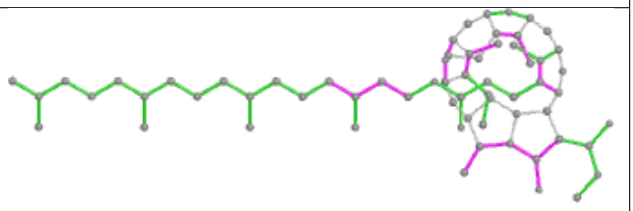

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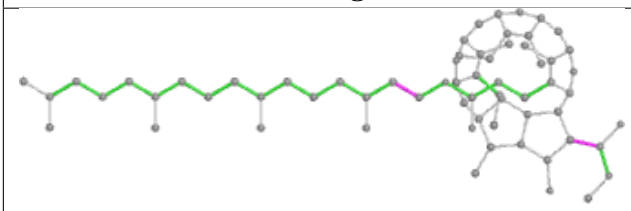

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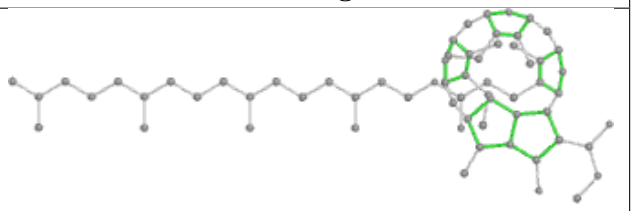
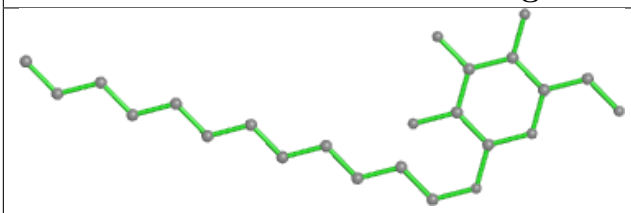


Rings

Ligand LMT T 102



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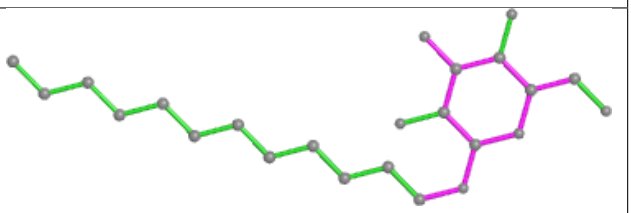

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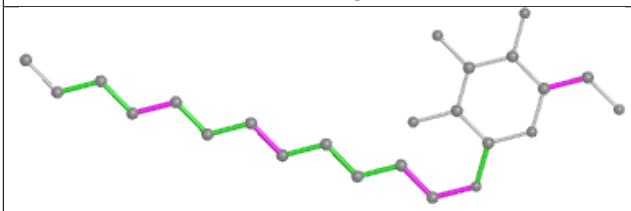

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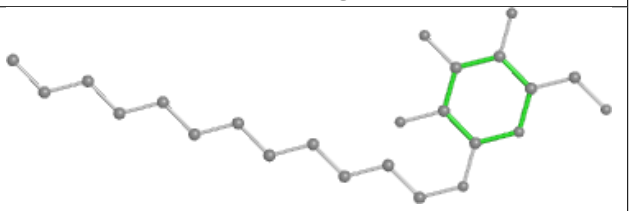
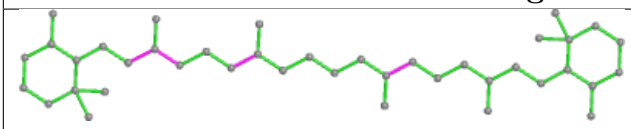


Rings

Ligand BCR a 410



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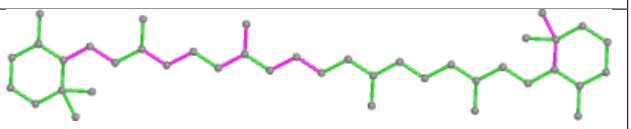

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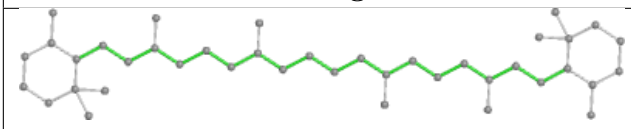
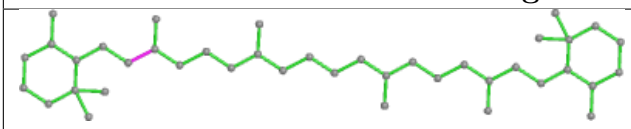


Torsions

Rings

Ligand BCR Y 101



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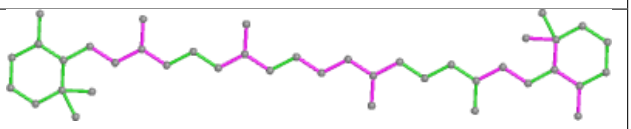
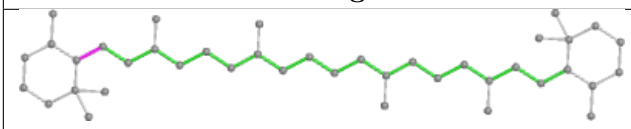


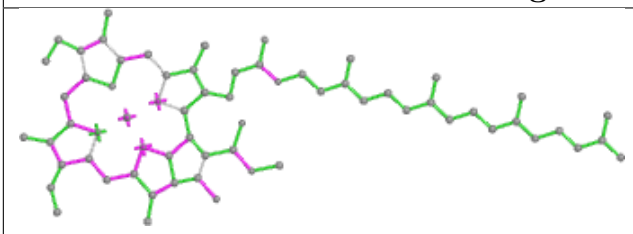
Bond angles



Torsions

Rings

Ligand CLA c 502



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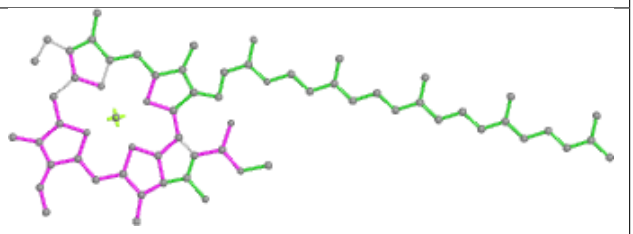
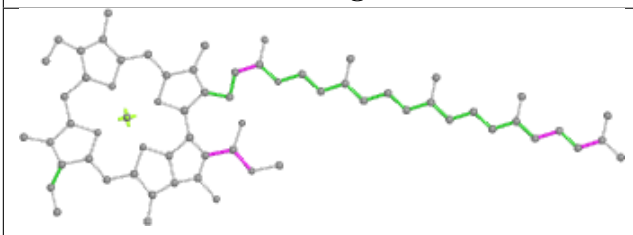
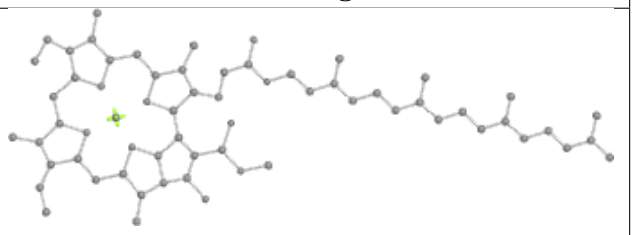


Bond angles

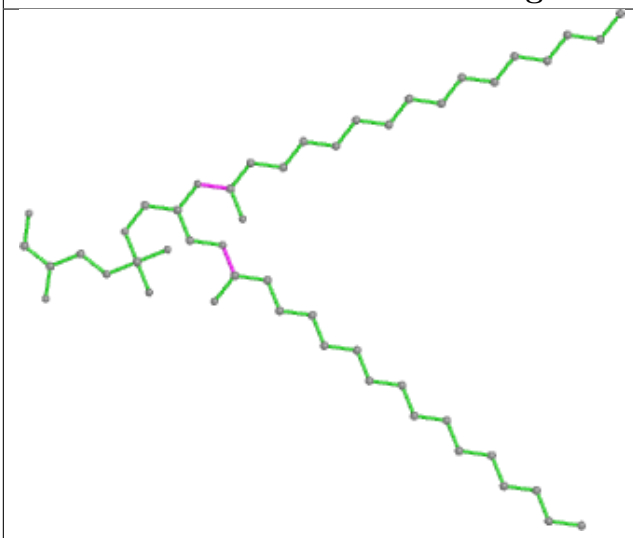


Torsions



Rings

Ligand LHG d 409



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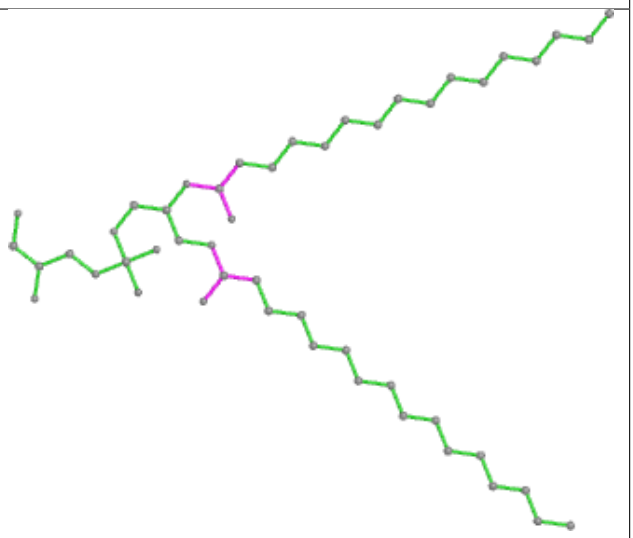
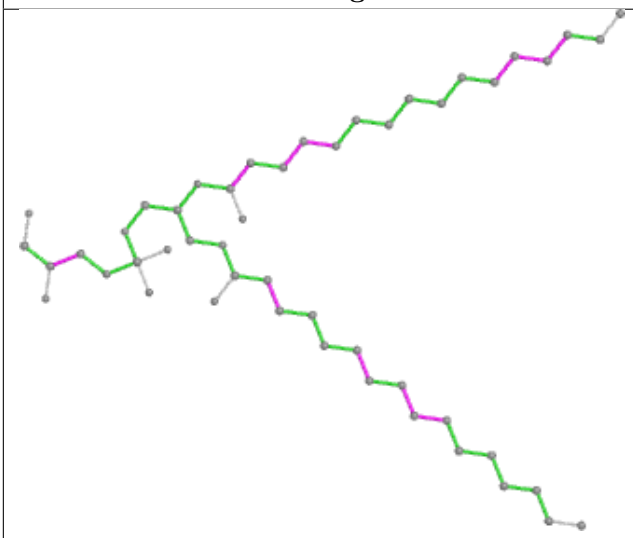
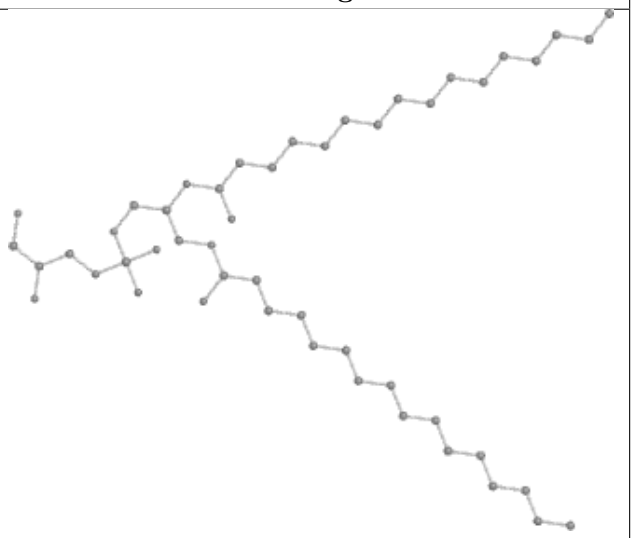


Bond angles

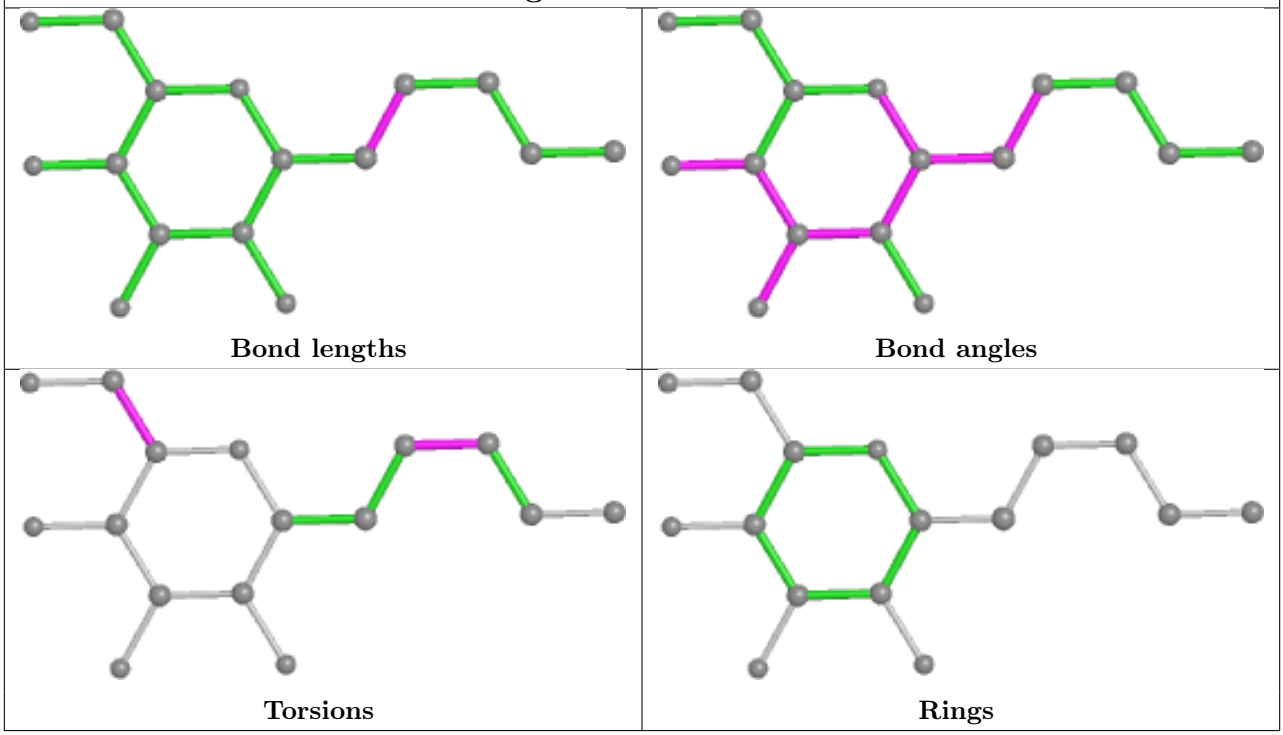


Torsions

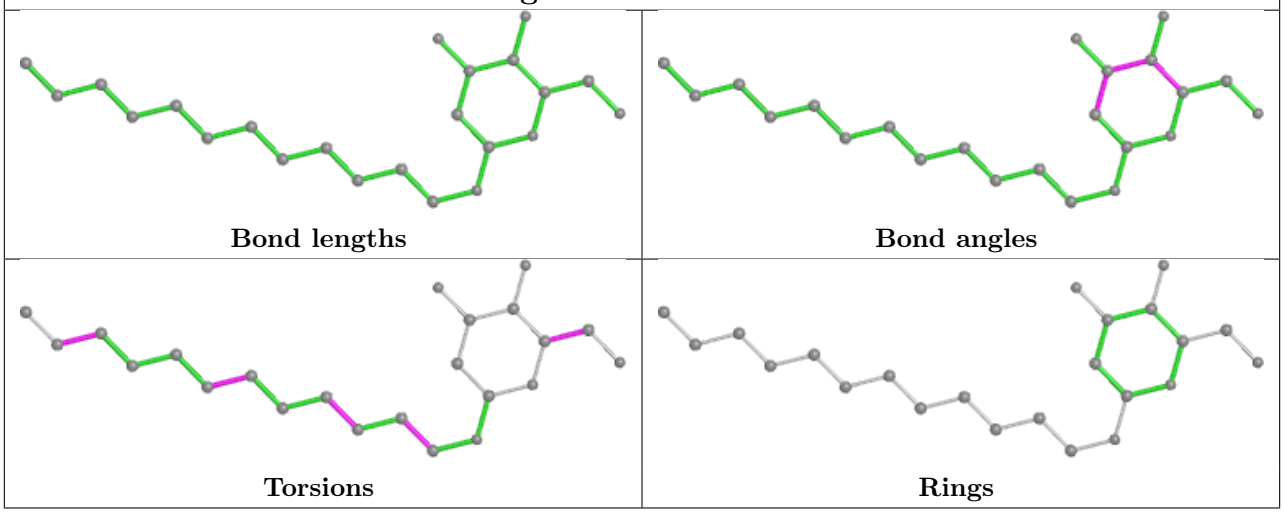


Rings

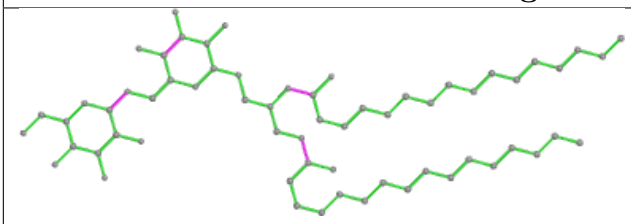
Ligand HTG v 208



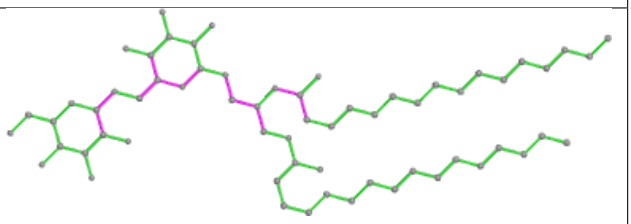
Ligand LMT m 103



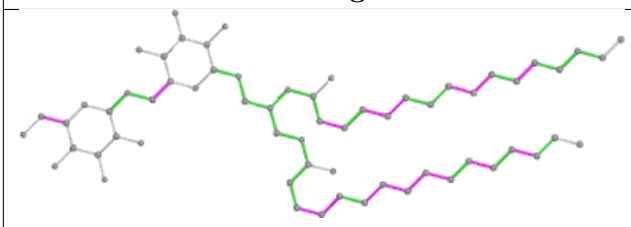
Ligand DGD C 515



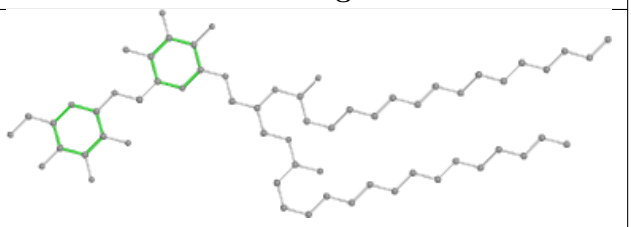
Bond lengths



Bond angles

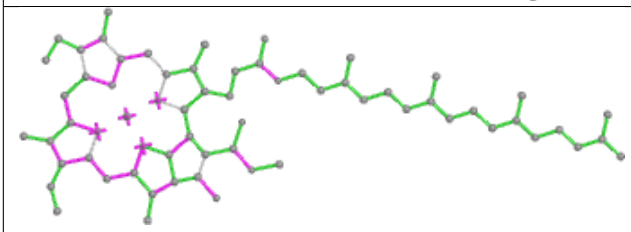


Torsions



Rings

Ligand CLA B 616



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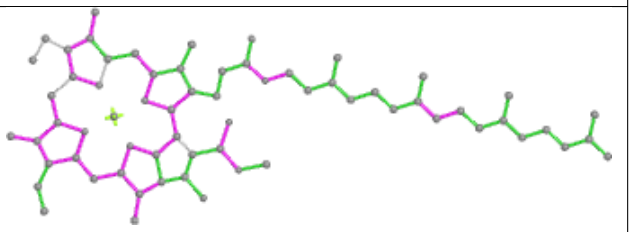
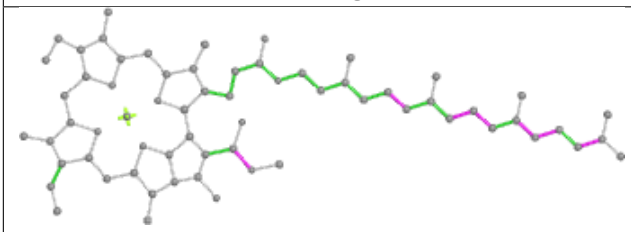


Bond angles



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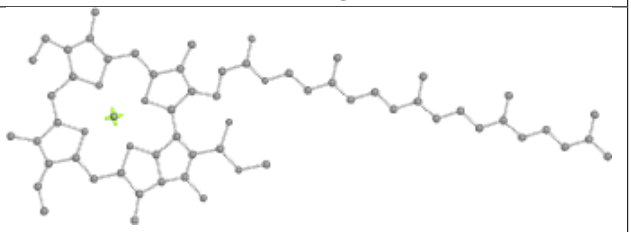
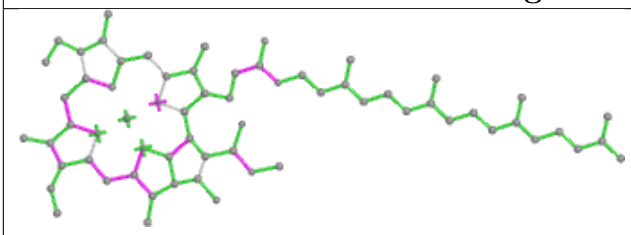


Rings

Ligand CLA B 615



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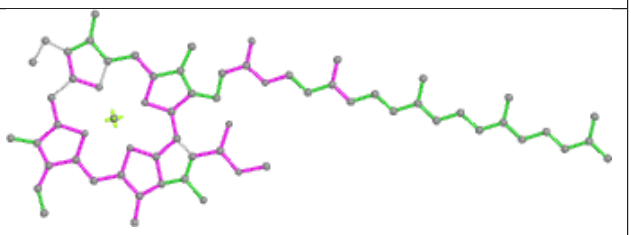
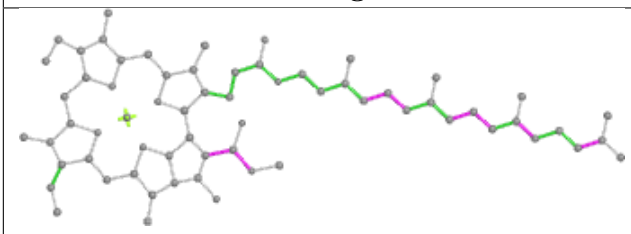
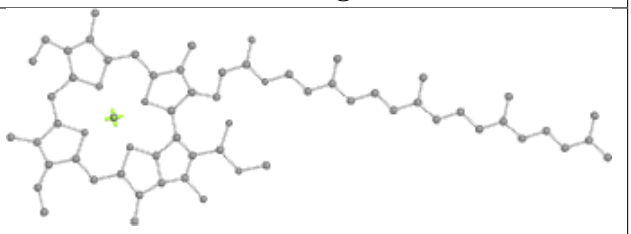


Bond angles

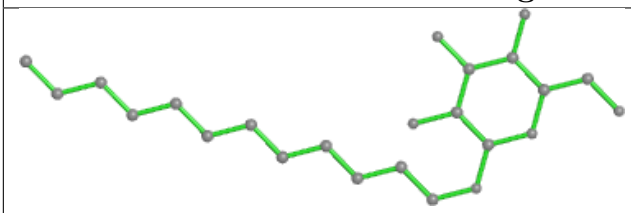


Torsions



Rings

Ligand LMT M 102



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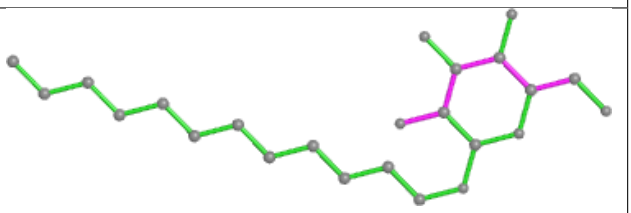
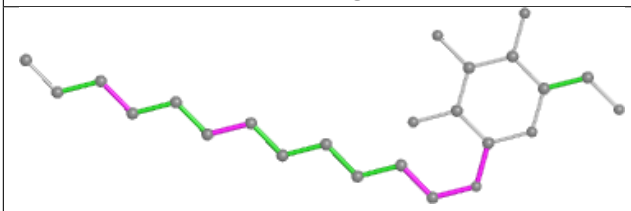


Bond angles



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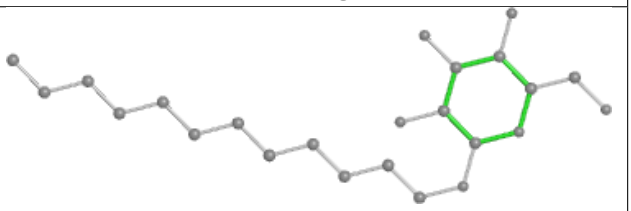
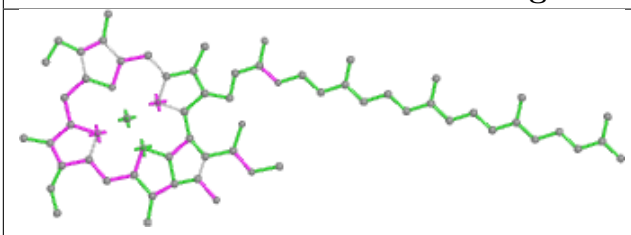


Rings

Ligand CLA c 504



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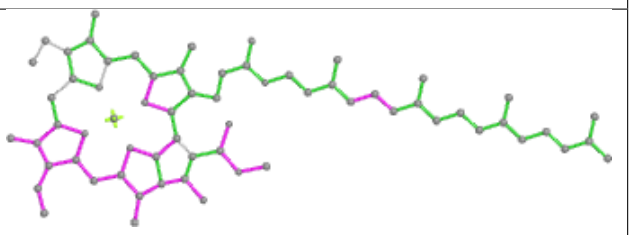
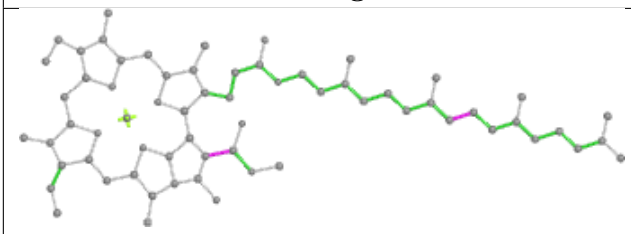


Bond angles



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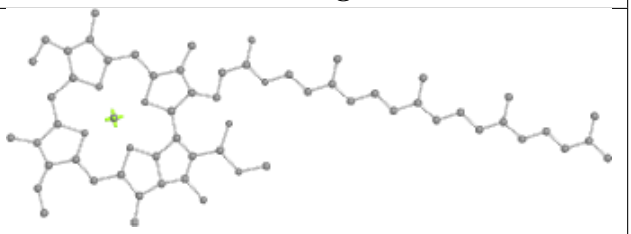
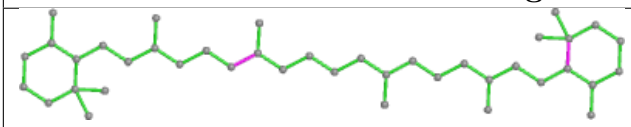


Rings

Ligand BCR d 406



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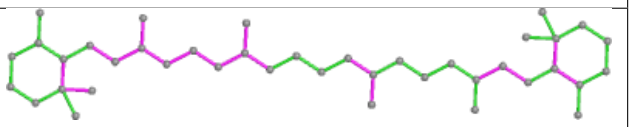
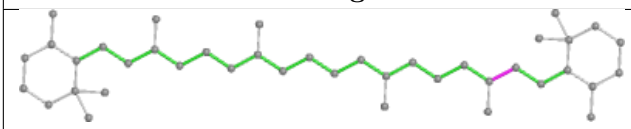


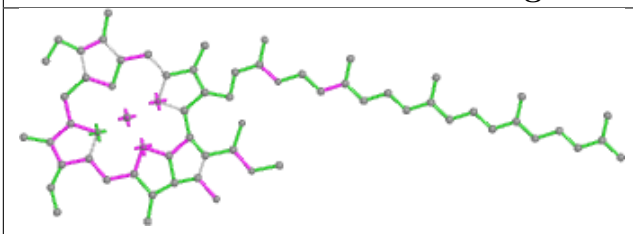
Bond angles



Torsions

Rings

Ligand CLA B 602



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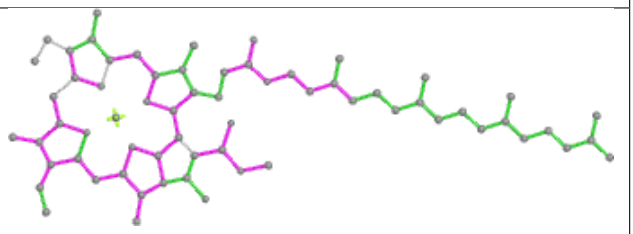
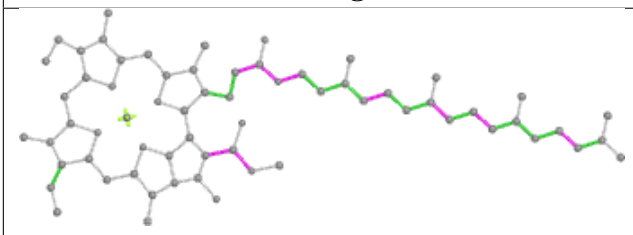
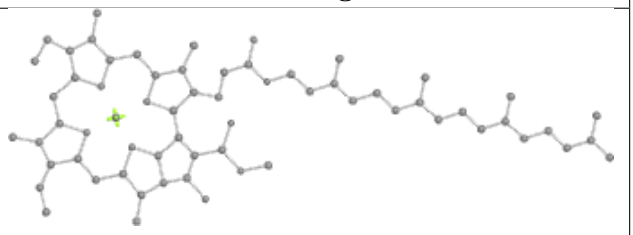


Bond angles

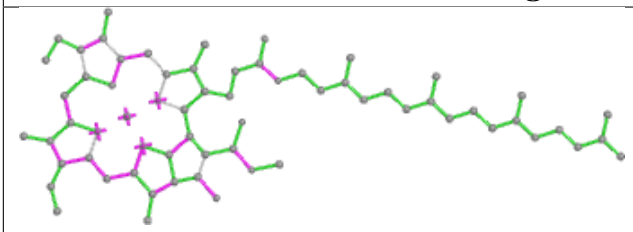


Torsions



Rings

Ligand CLA C 512



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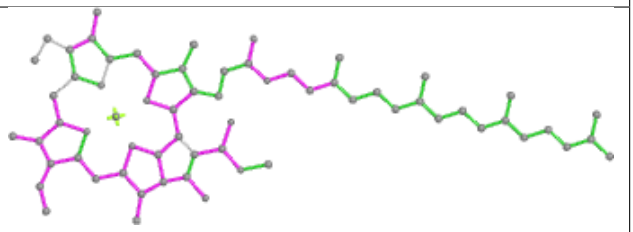
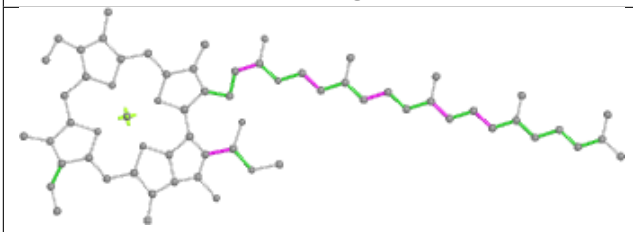


Bond angles



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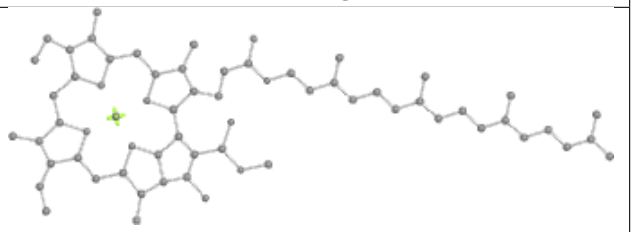
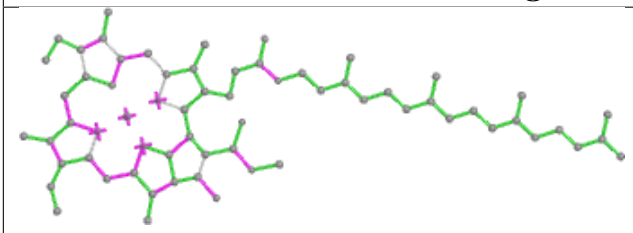


Rings

Ligand CLA C 508



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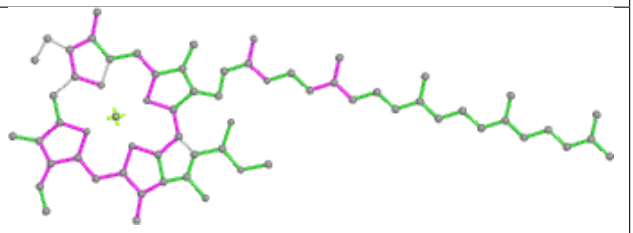
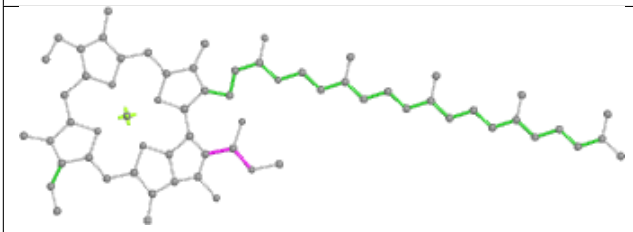
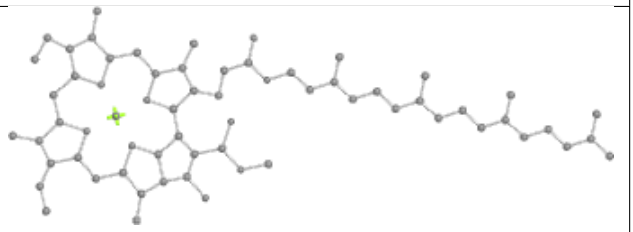


Bond angles

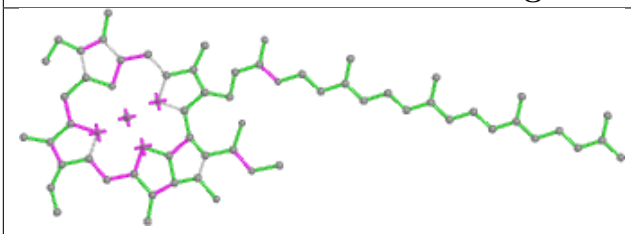


Torsions



Rings

Ligand CLA C 504



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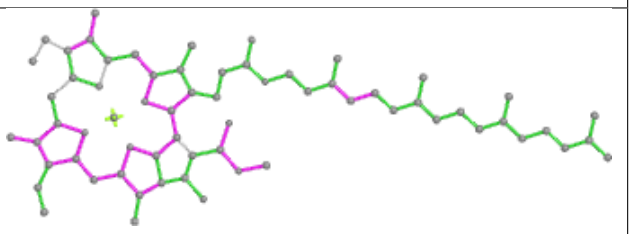

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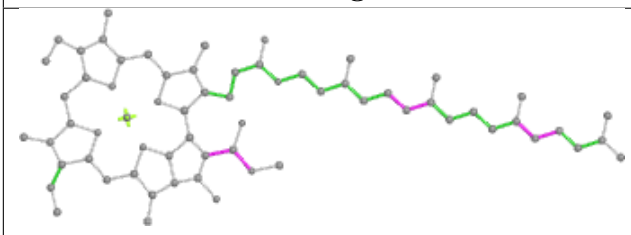

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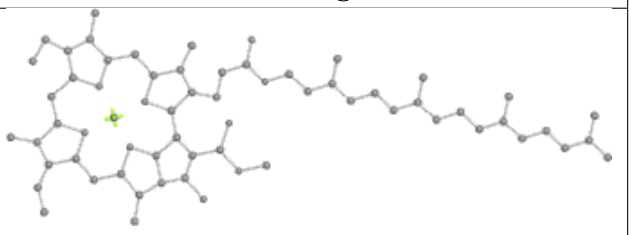
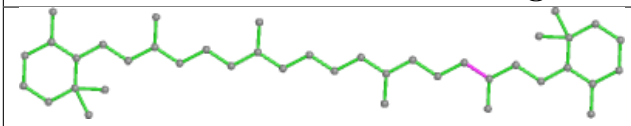


Rings

Ligand BCR c 515



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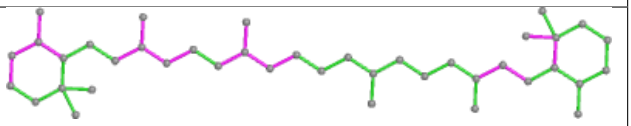
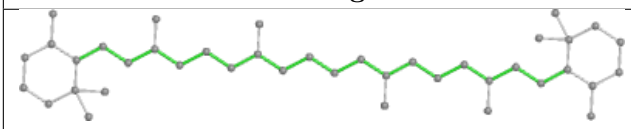


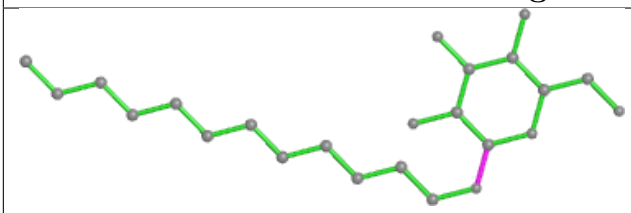
Bond angles



Torsions

Rings

Ligand LMT l 101



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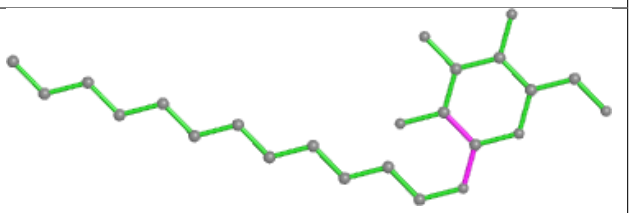
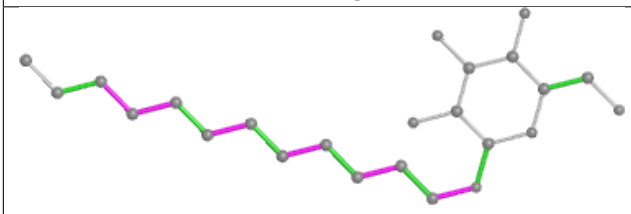


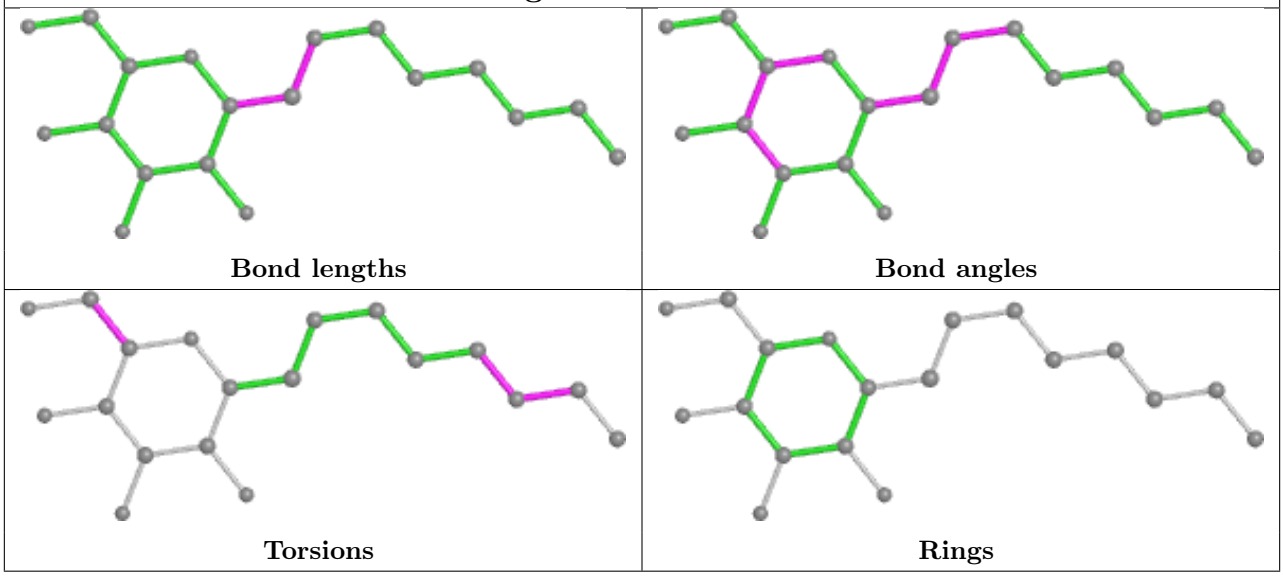
Bond angles



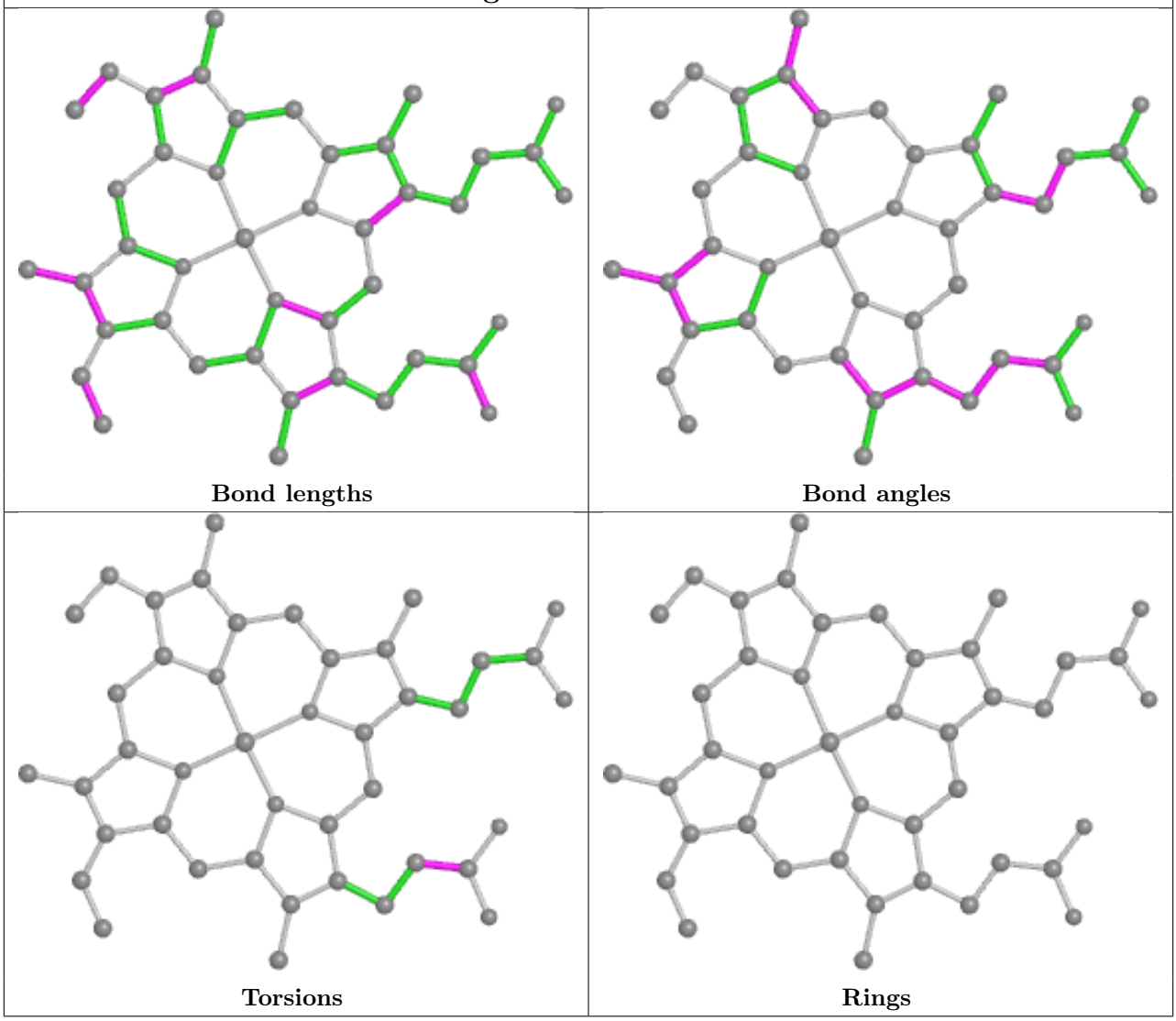
Torsions

Rings

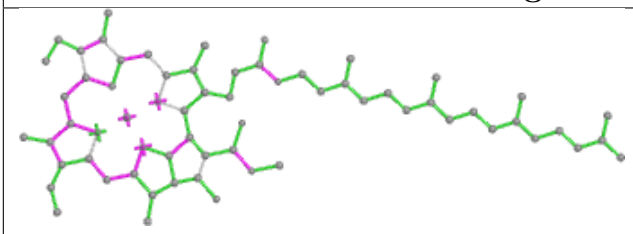
Ligand HTG b 601



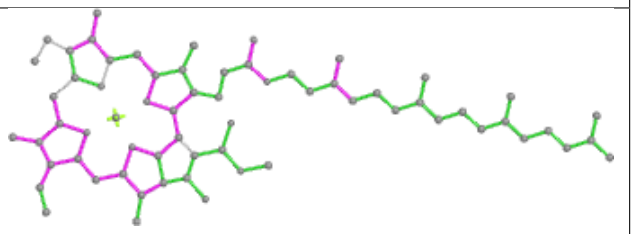
Ligand HEC v 202



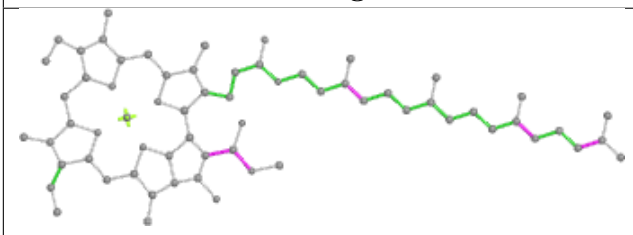
Ligand CLA B 606



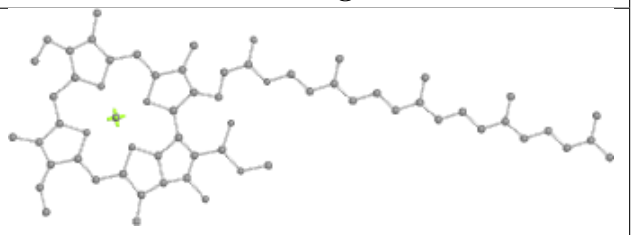
Bond lengths



Bond angles

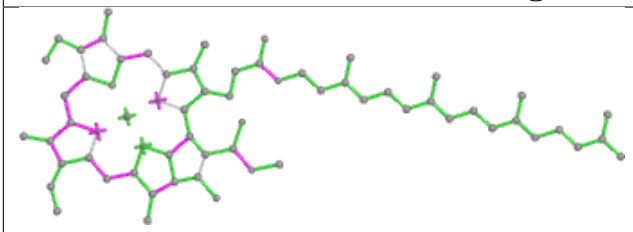


Torsions

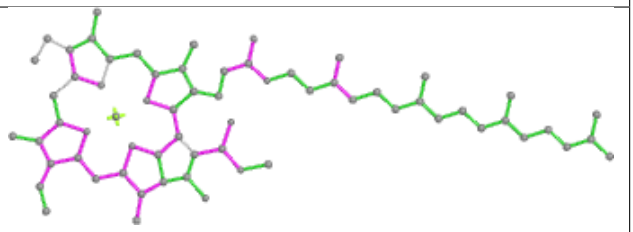


Rings

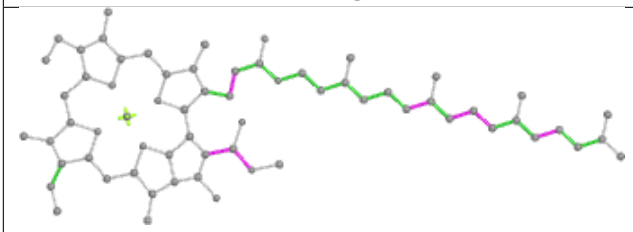
Ligand CLA b 610



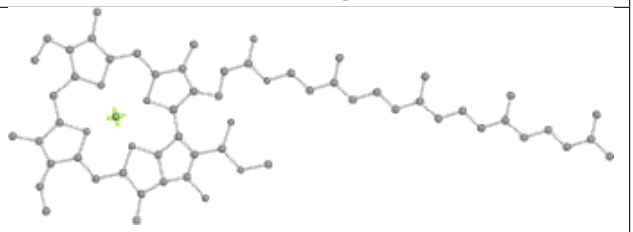
Bond lengths



Bond angles

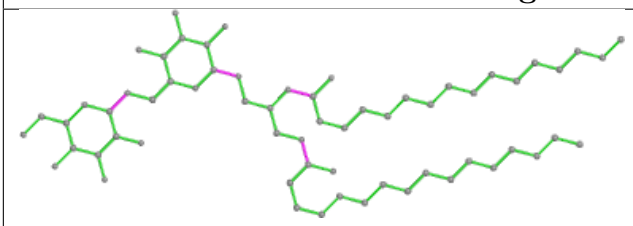


Torsions

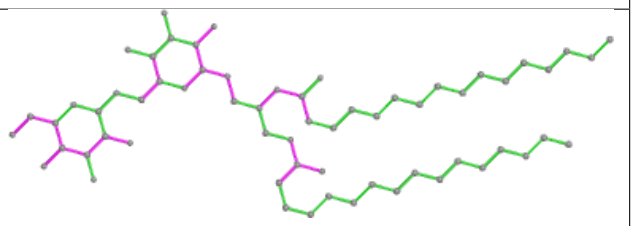


Rings

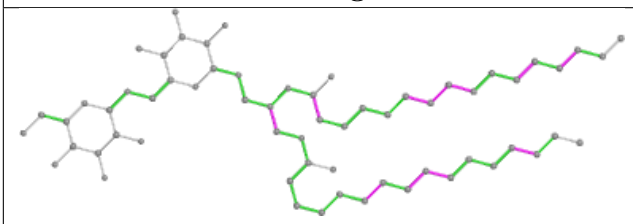
Ligand DGD H 101



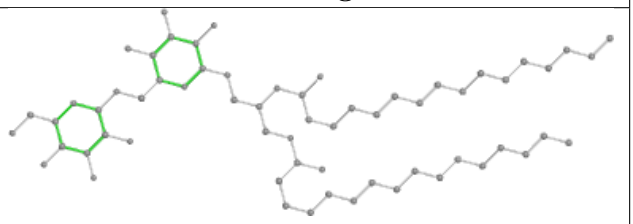
Bond lengths



Bond angles

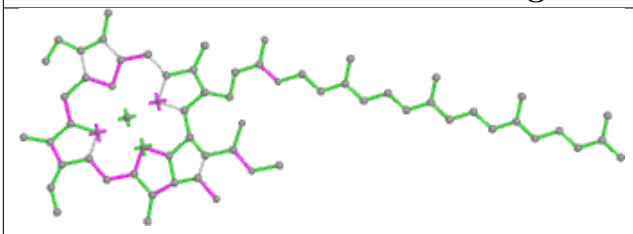


Torsions



Rings

Ligand CLA b 612



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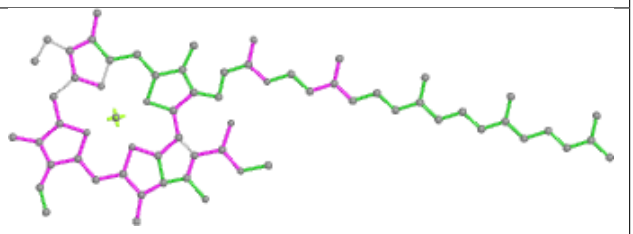
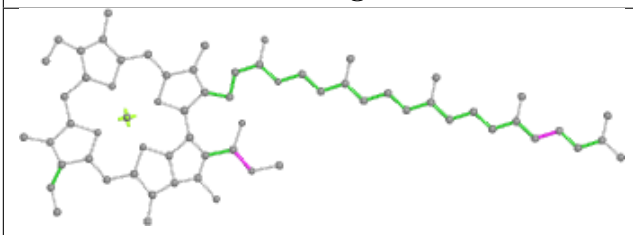


Bond angles



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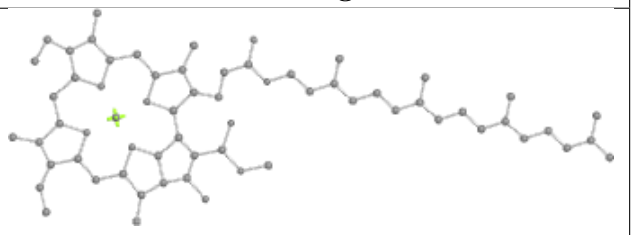
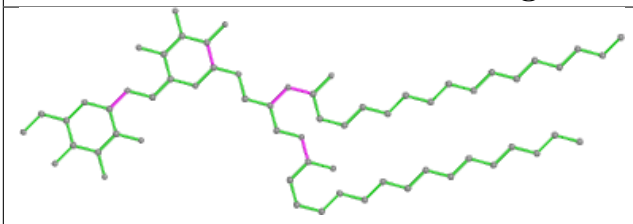


Rings

Ligand DGD C 516



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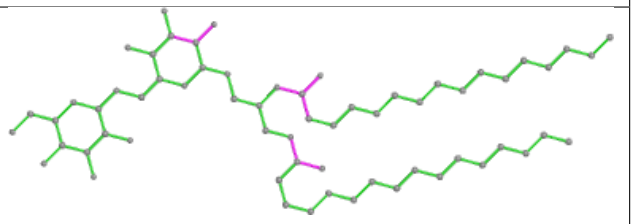
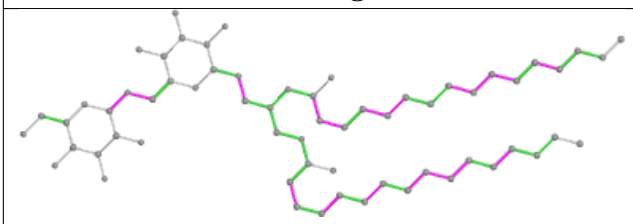


Bond angles



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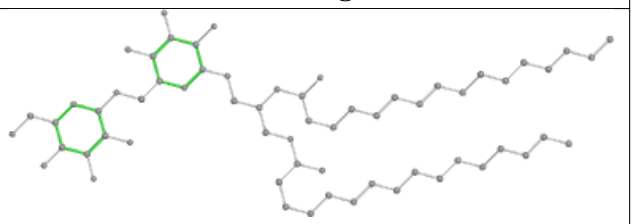
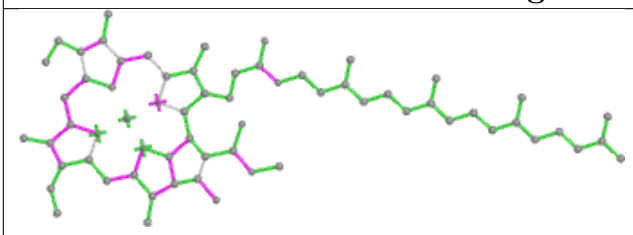


Rings

Ligand CLA b 620



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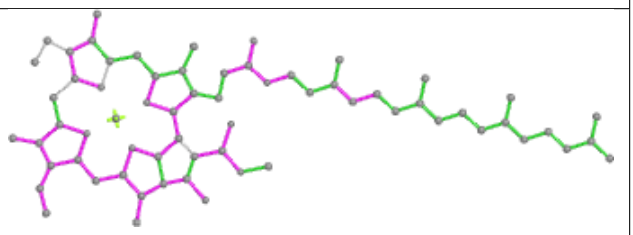

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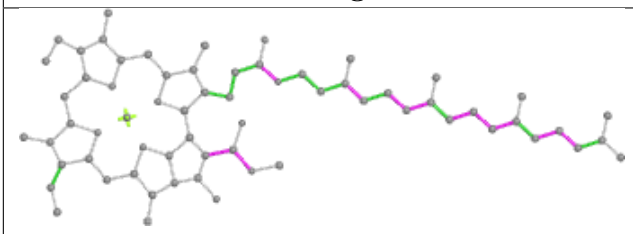

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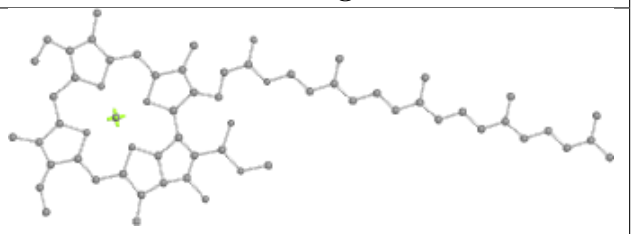
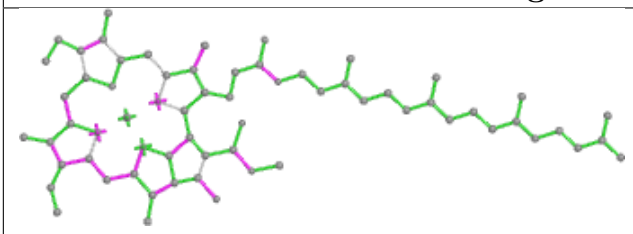


Rings

Ligand CLA d 403



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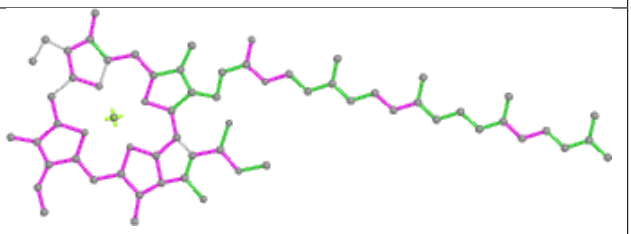
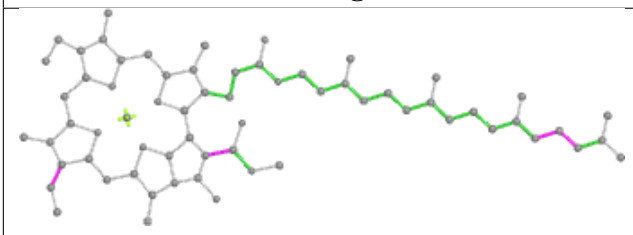


Bond angles



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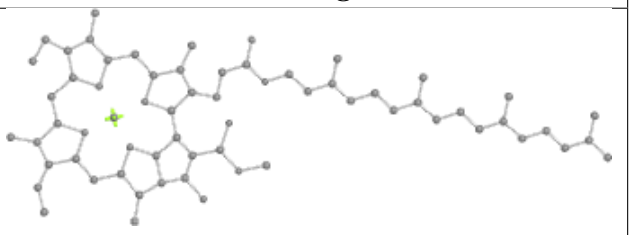
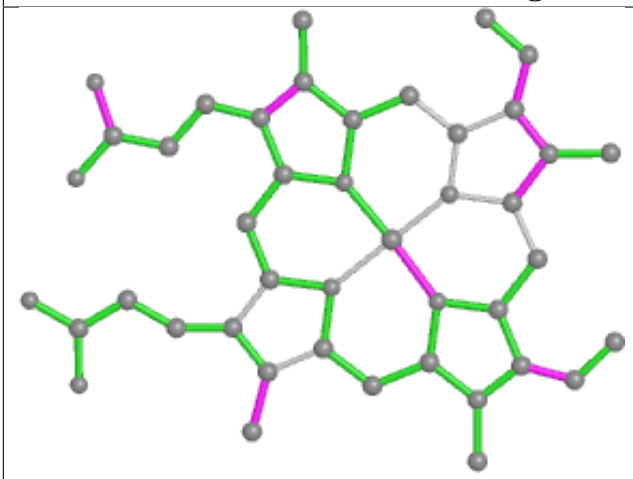


Rings

Ligand HEM f 101



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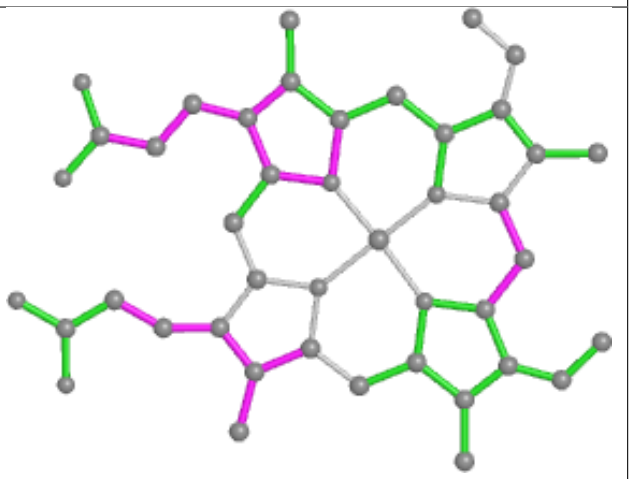
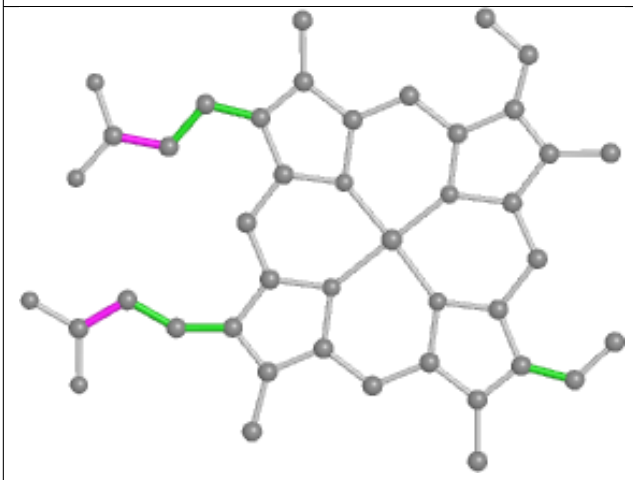


Bond angles



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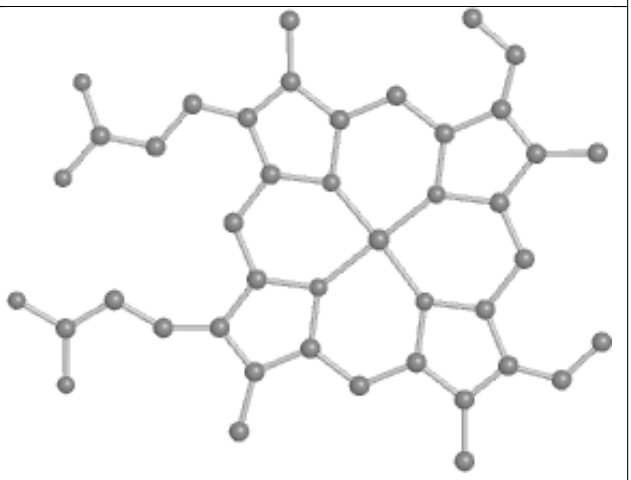
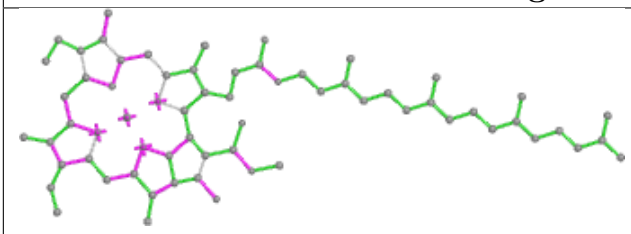


Rings

Ligand CLA a 407



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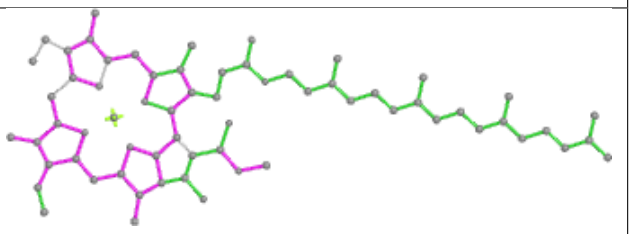
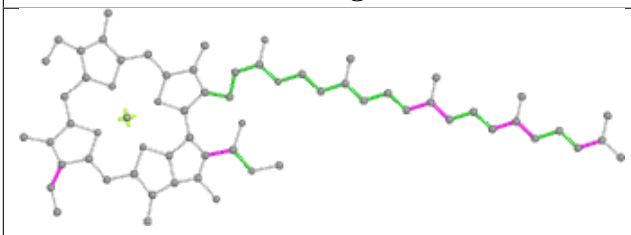


Bond angles



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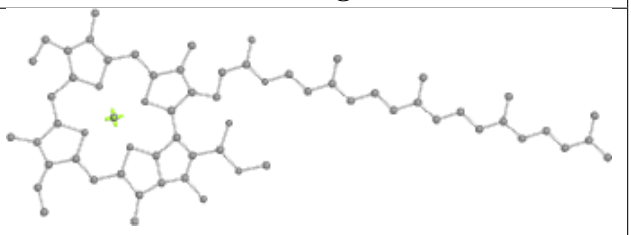
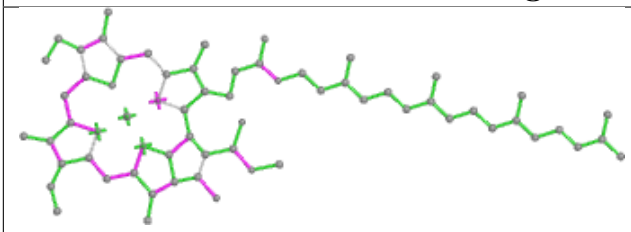


Rings

Ligand CLA C 501



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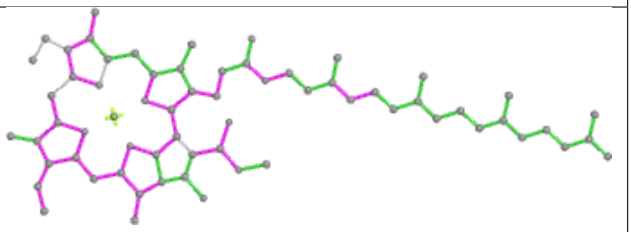
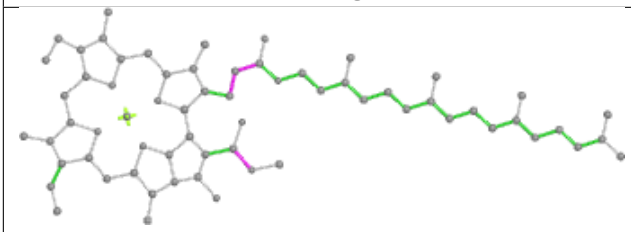


Bond angles



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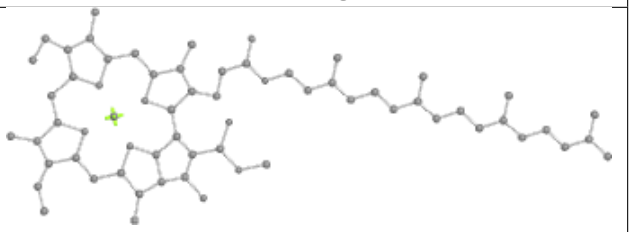
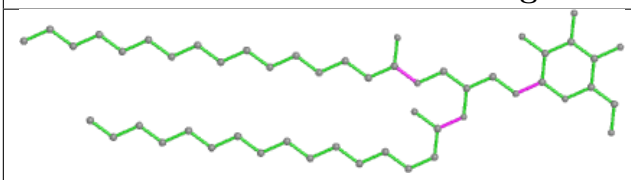


Rings

Ligand LMG B 622



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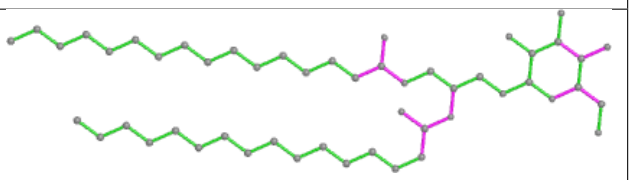

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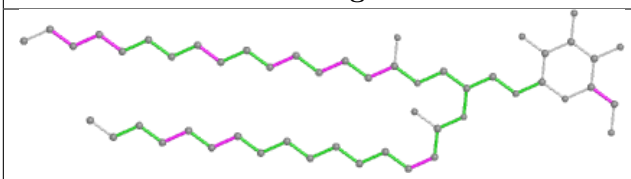

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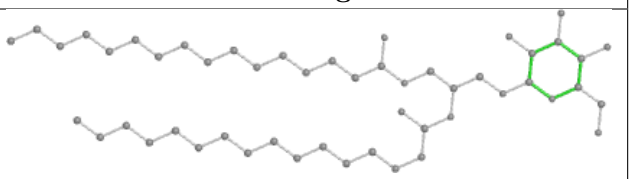
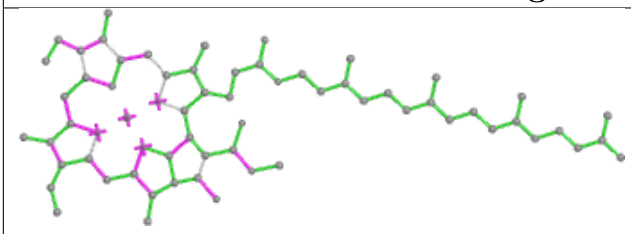


Rings

Ligand CLA a 406



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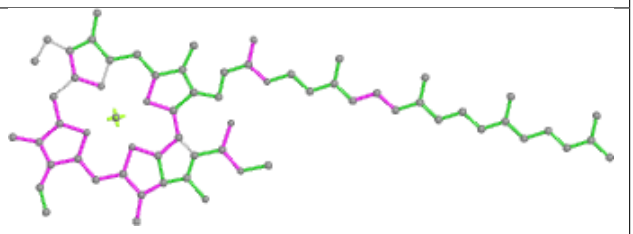
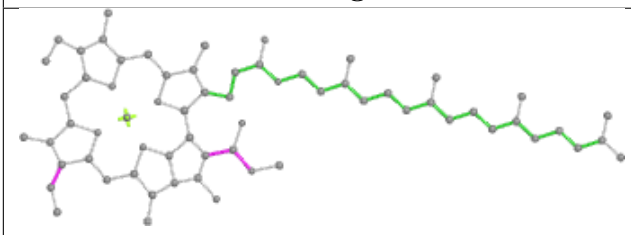


Bond angles



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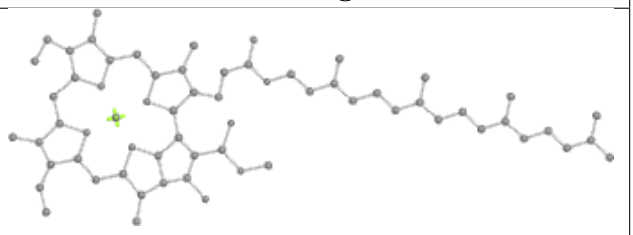
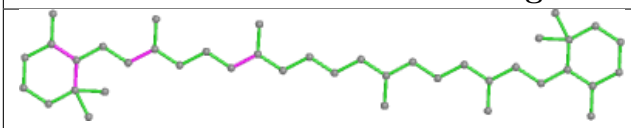


Rings

Ligand BCR b 622



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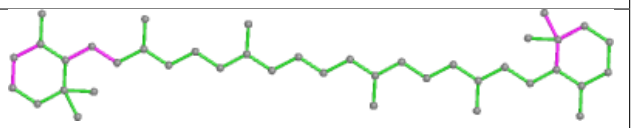
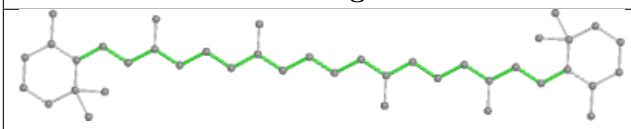


Bond angles



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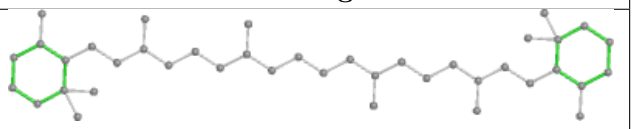
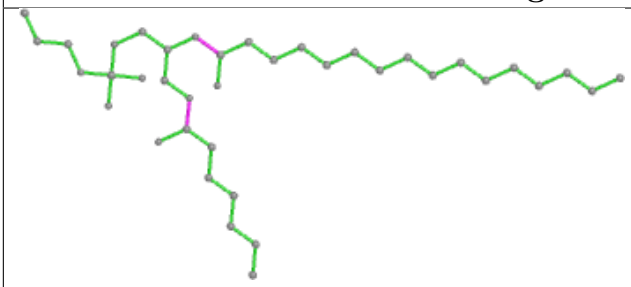


Rings

Ligand LHG e 101



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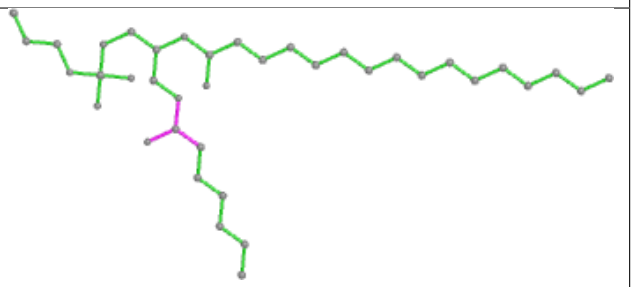
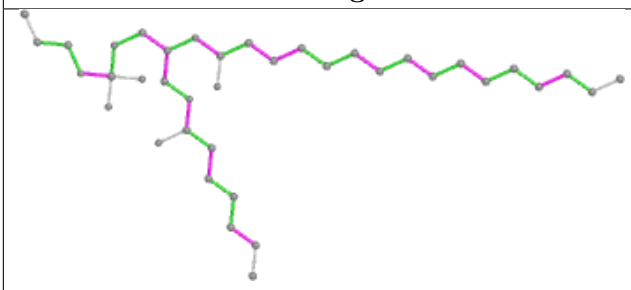
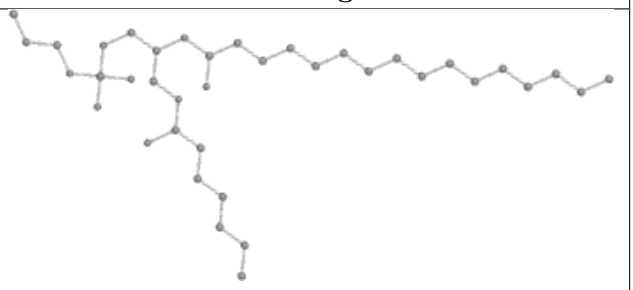


Bond angles

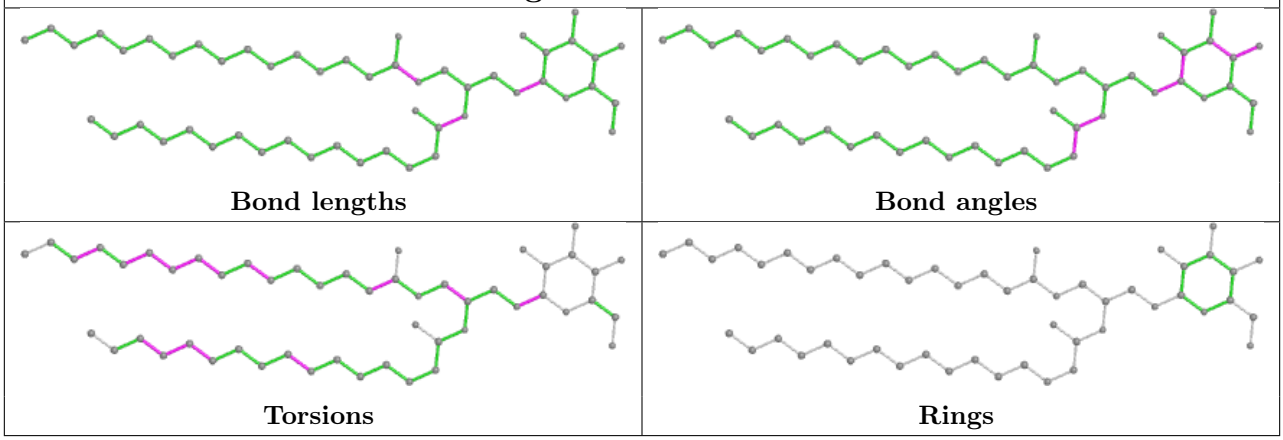


Torsions

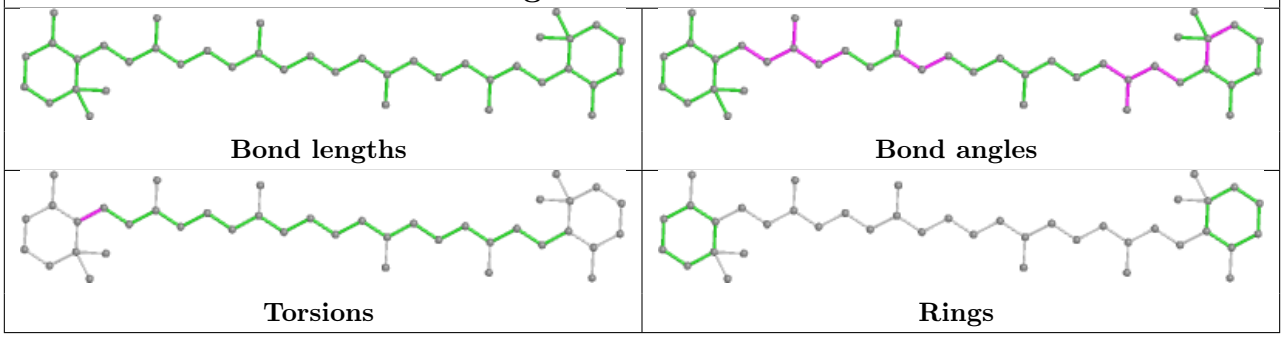


Rings

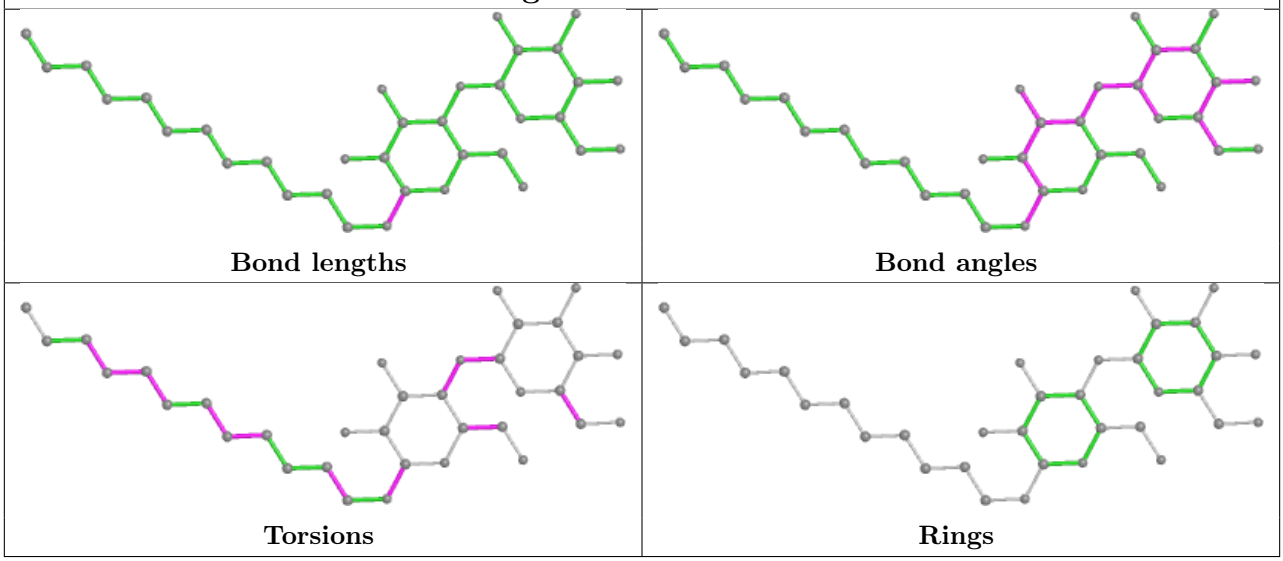
Ligand LMG a 412



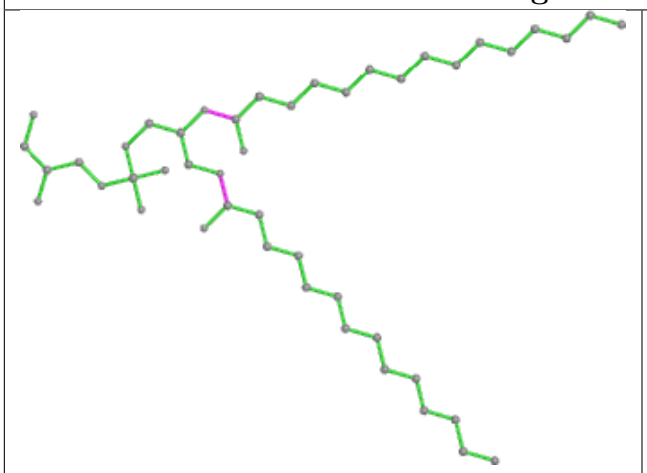
Ligand BCR B 618



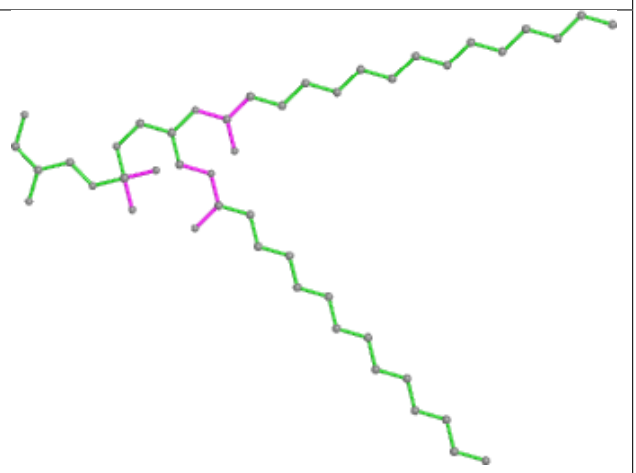
Ligand LMT C 520



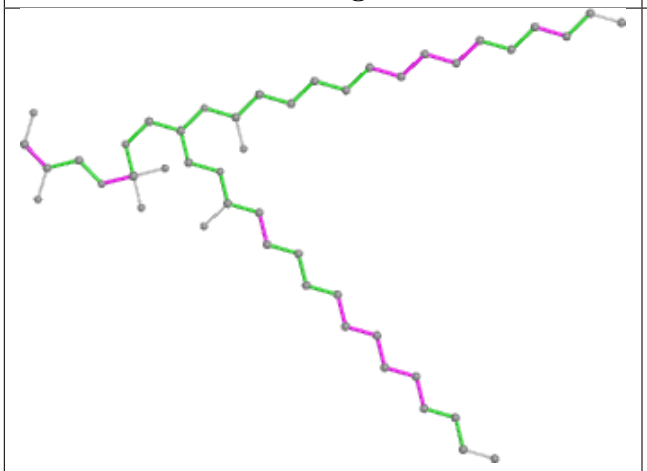
Ligand LHG f 102



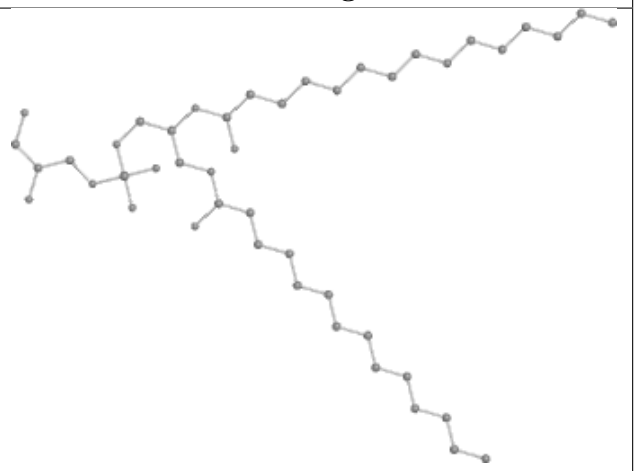
Bond lengths



Bond angles

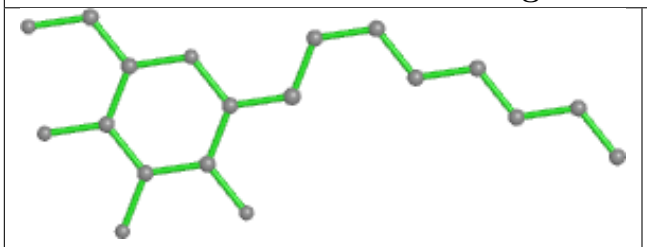


Torsions



Rings

Ligand HTG C 521



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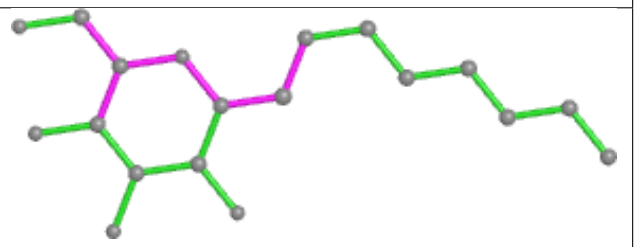
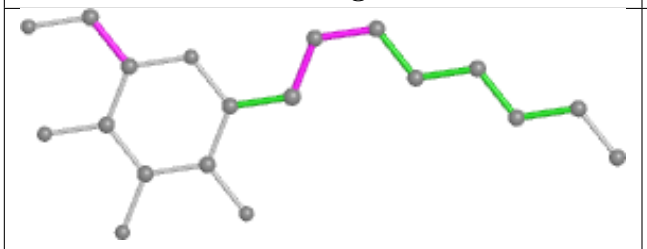
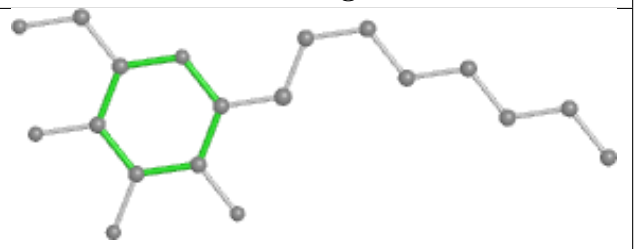


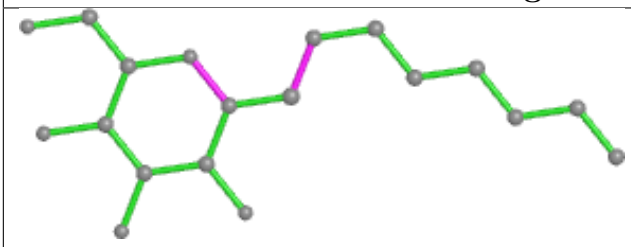
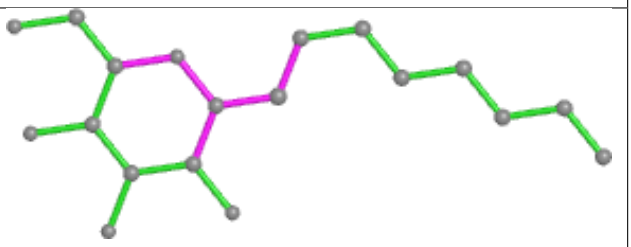
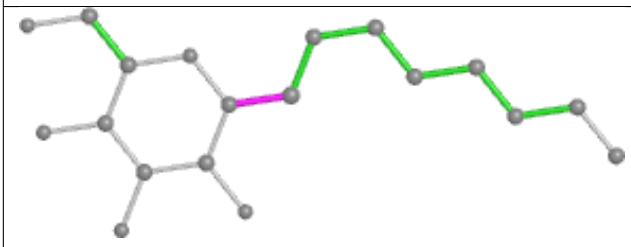
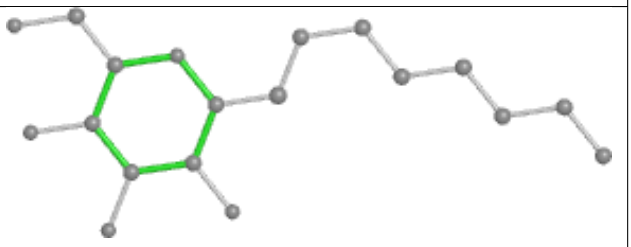
Bond angles

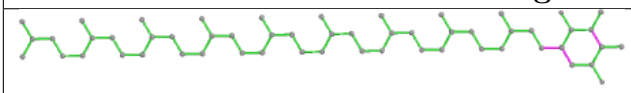
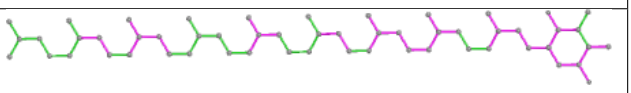
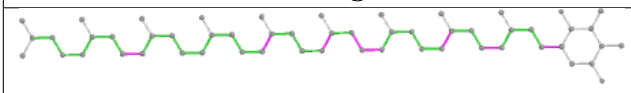
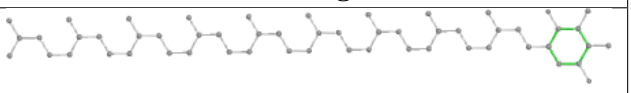


Torsions

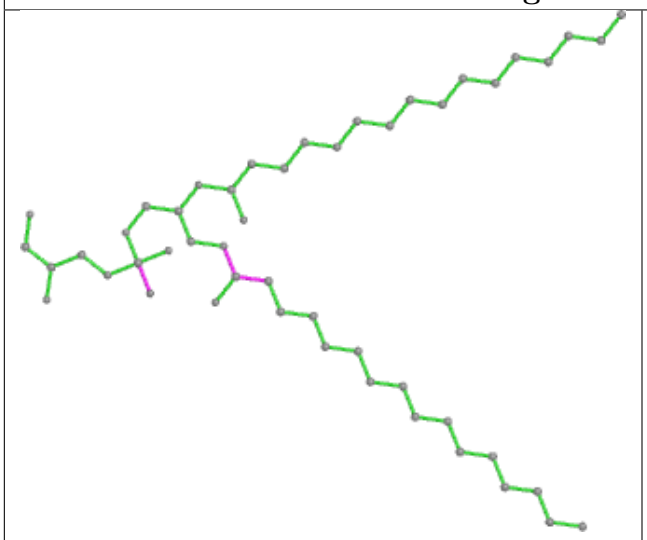


Rings

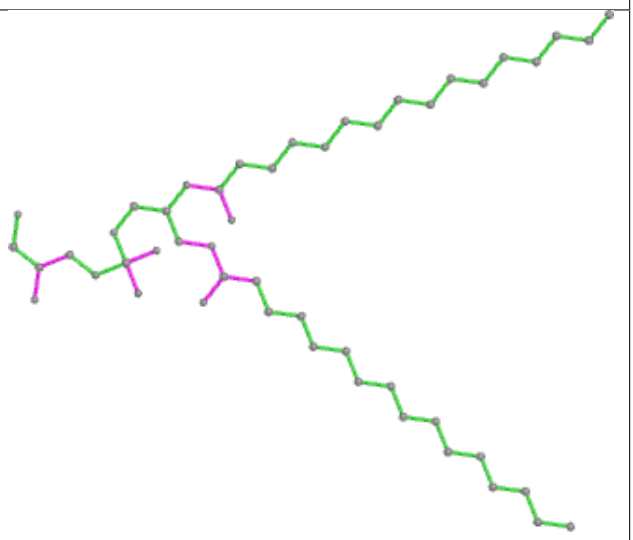
Ligand HTG b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 a 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

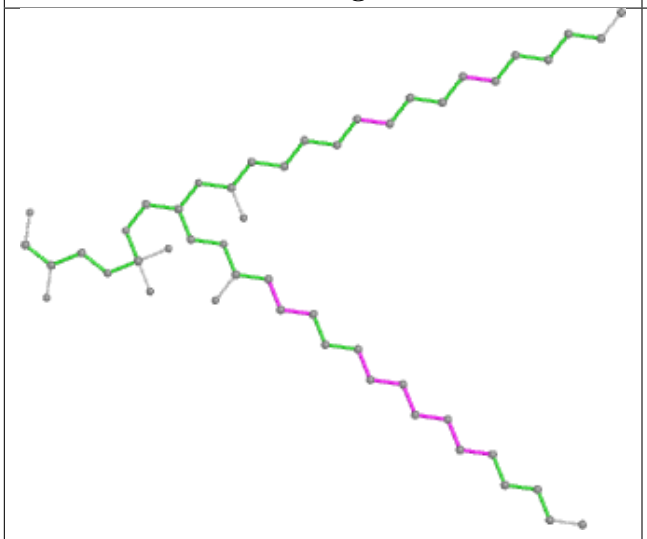
Ligand LHG D 409



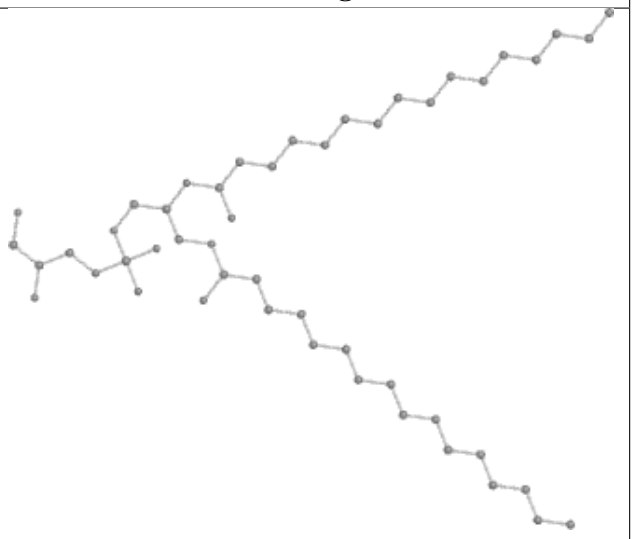
Bond lengths



Bond angles

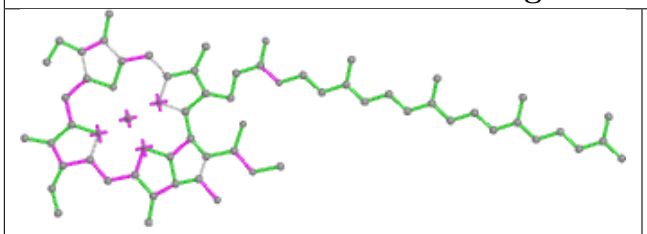


Torsions



Rings

Ligand CLA D 405



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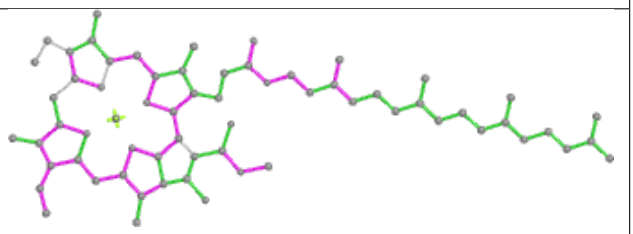
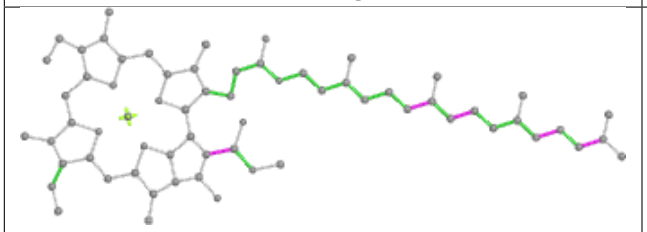
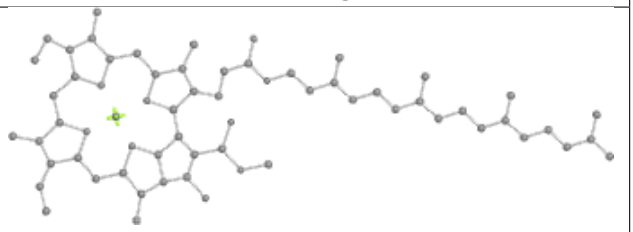


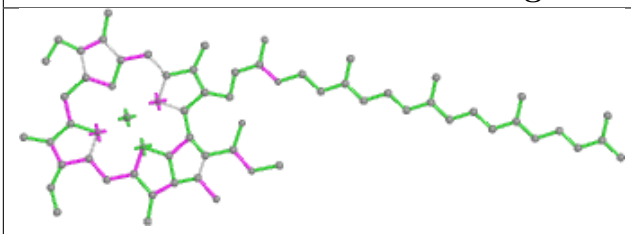
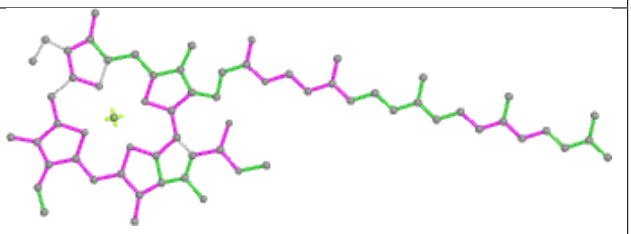
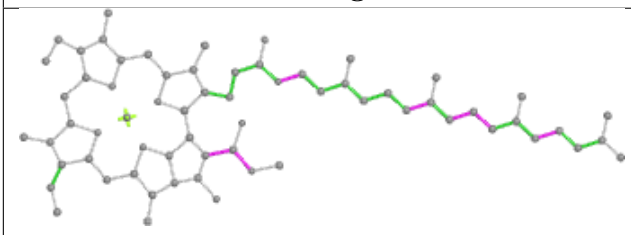
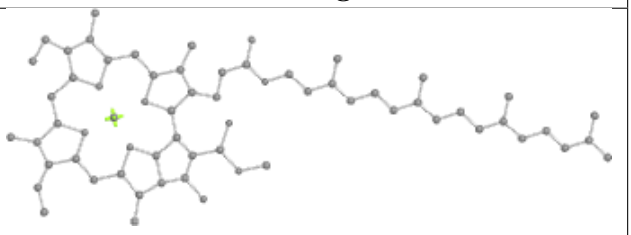
Bond angles

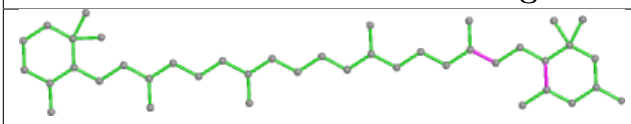
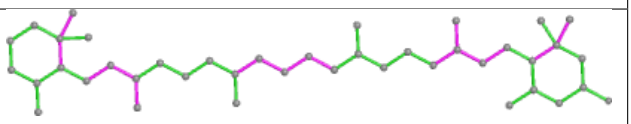
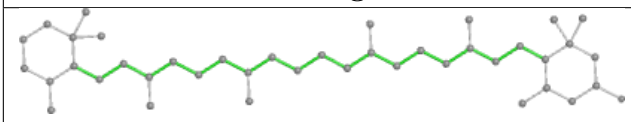
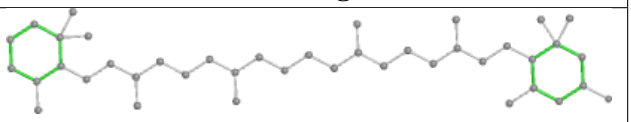


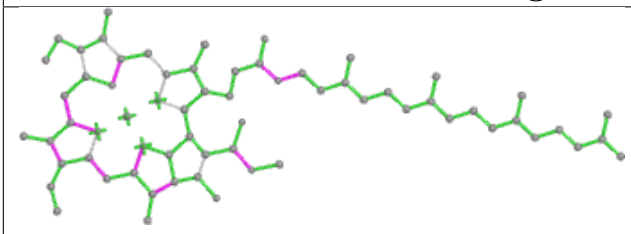
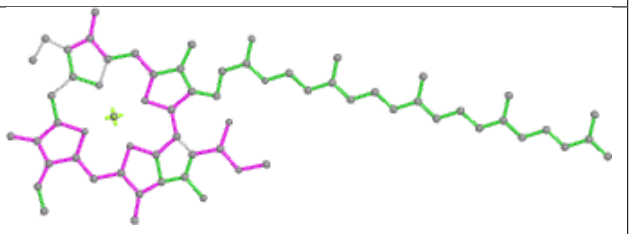
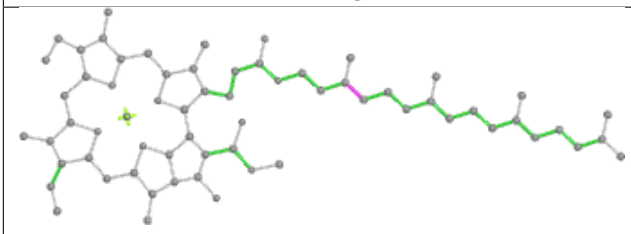
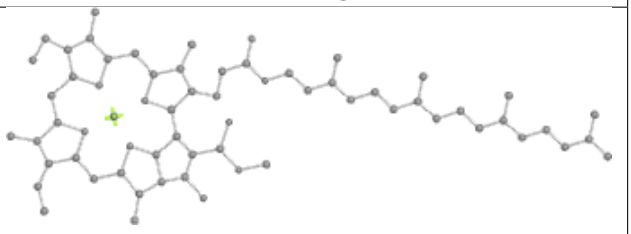
Torsions



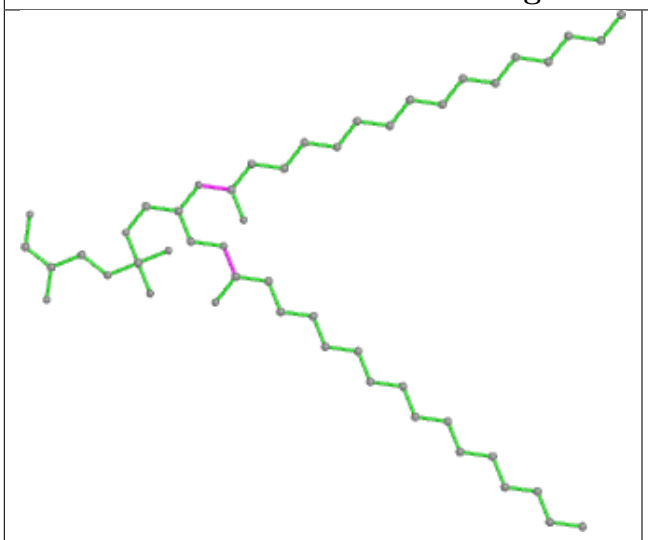
Rings

Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

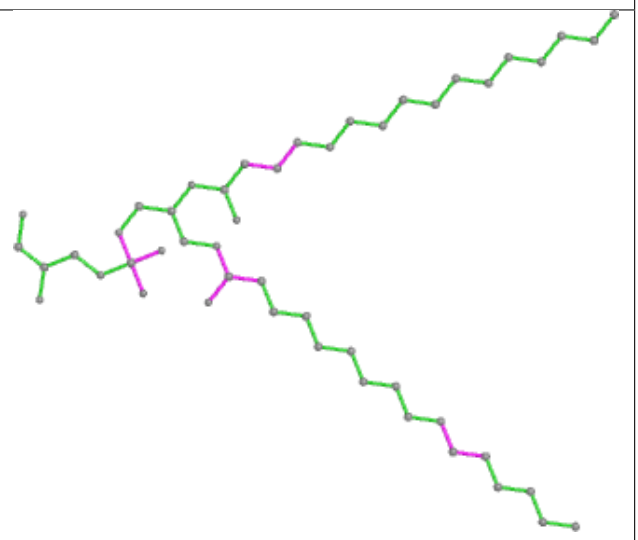
Ligand RRX H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

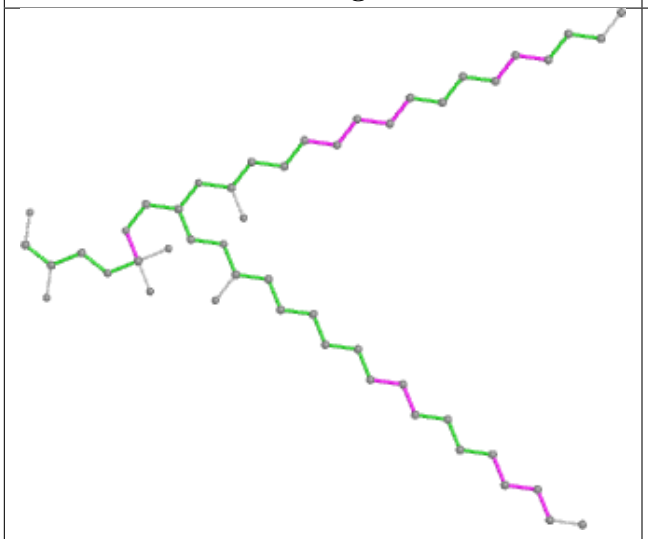
Ligand LHG B 621



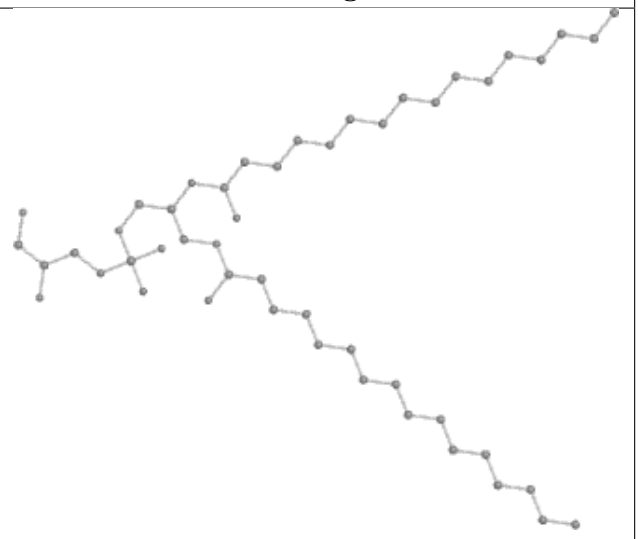
Bond lengths



Bond angles

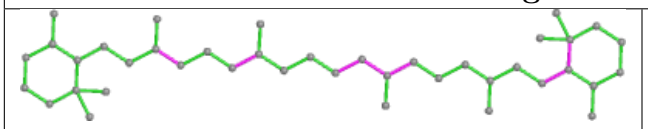


Torsions



Rings

Ligand BCR D 406



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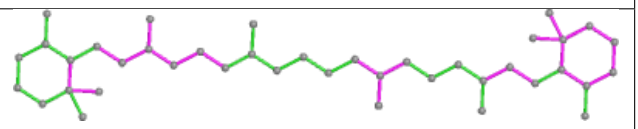
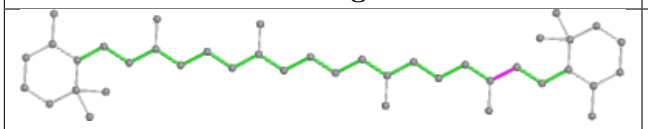
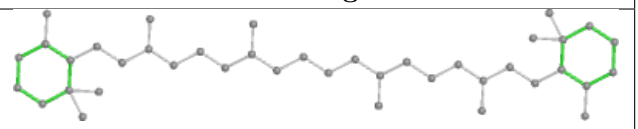


Bond angles

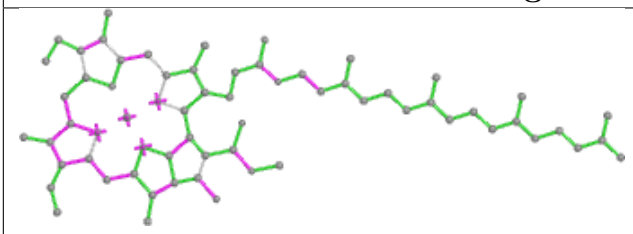


Torsions

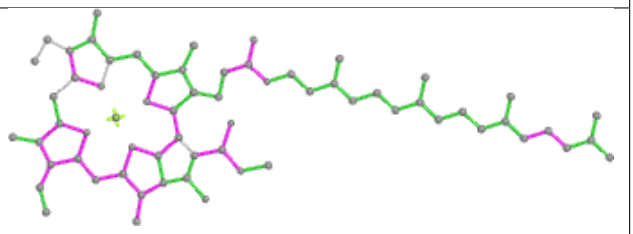


Rings

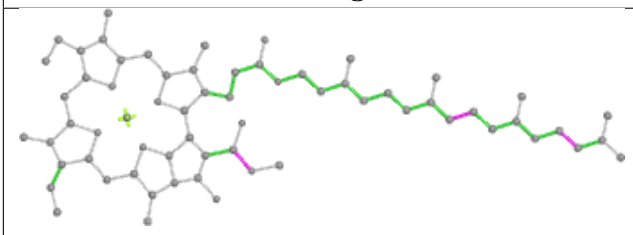
Ligand CLA B 611



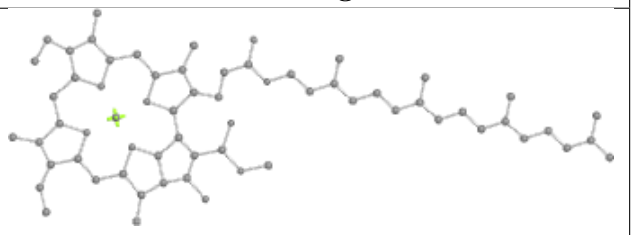
Bond lengths



Bond angles

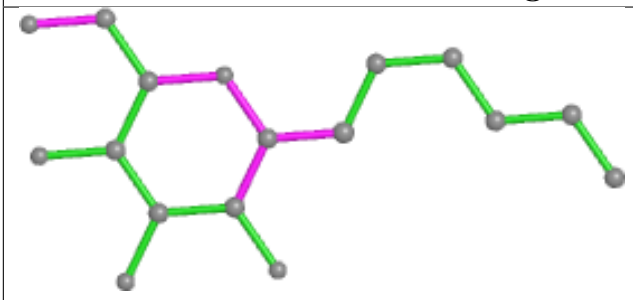


Torsions

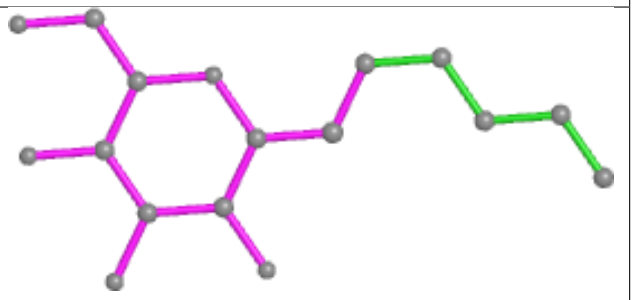


Rings

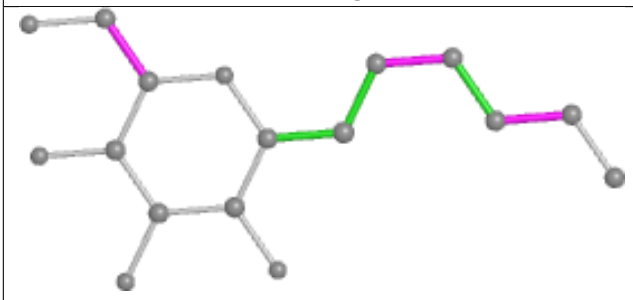
Ligand HTG b 640



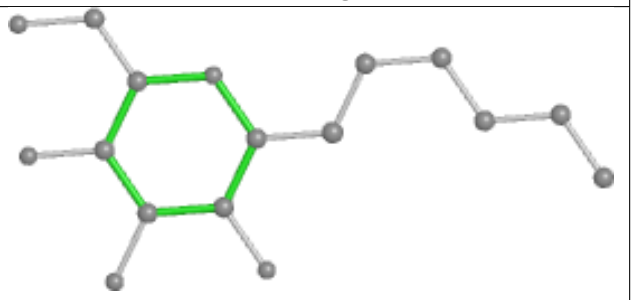
Bond lengths



Bond angles

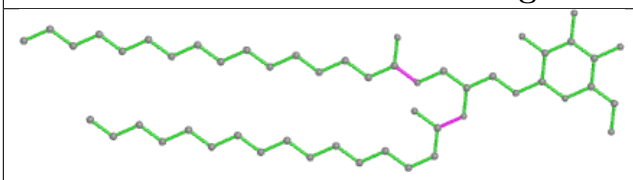


Torsions

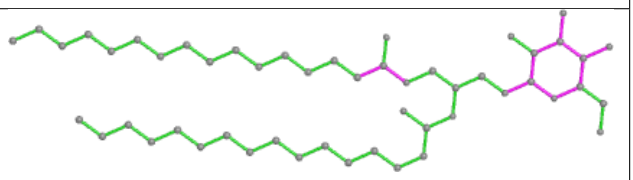


Rings

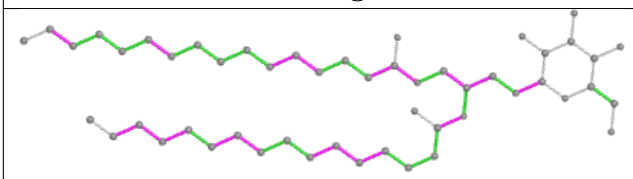
Ligand LMG A 411



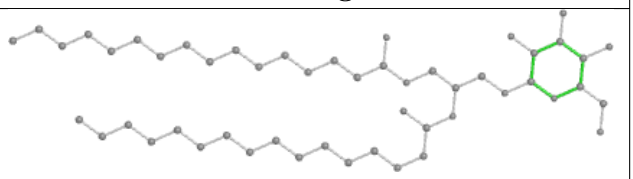
Bond lengths



Bond angles

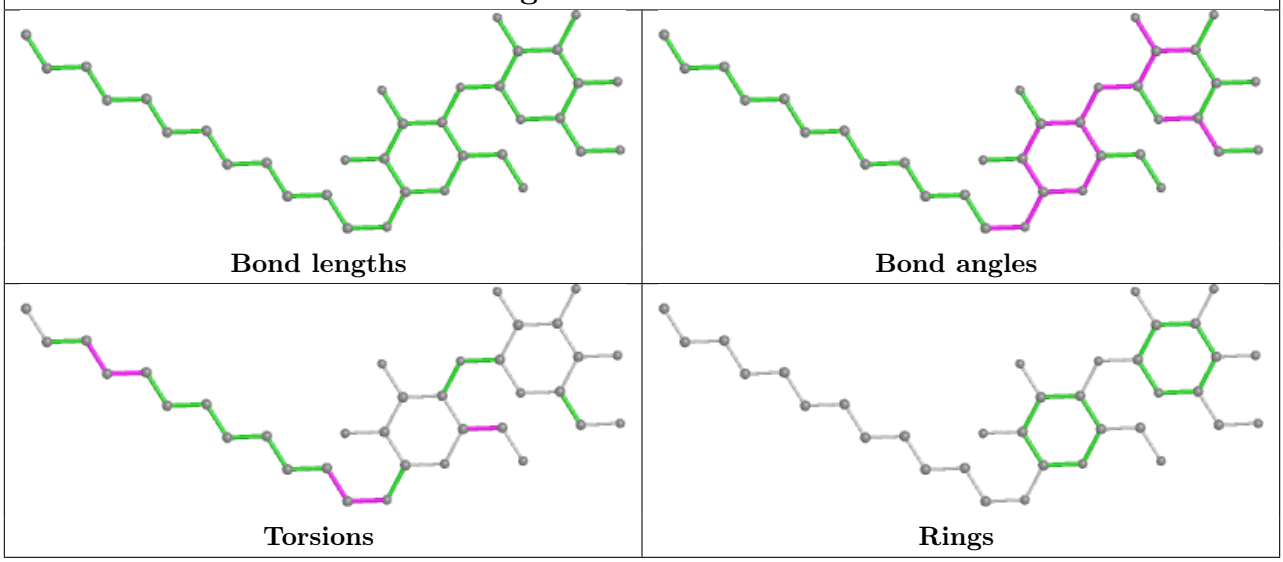


Torsions

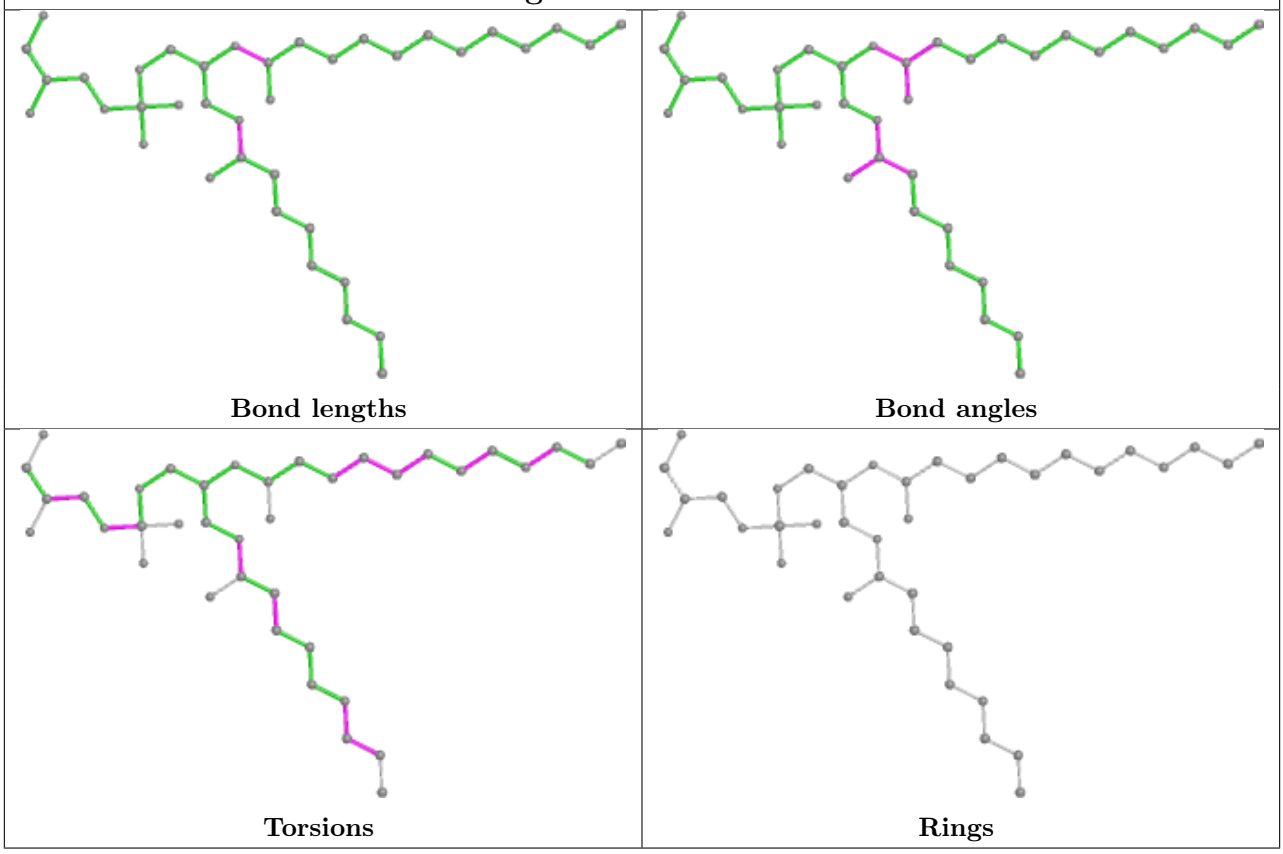


Rings

Ligand LMT m 101



Ligand LHG F 103



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	334/334 (100%)	-0.79	3 (0%)	84	86	24, 33, 56, 90	0
1	a	334/334 (100%)	-0.78	4 (1%)	79	82	27, 35, 59, 92	0
2	B	505/505 (100%)	-0.58	11 (2%)	62	66	23, 38, 68, 90	0
2	b	504/505 (99%)	-0.47	23 (4%)	32	38	29, 39, 71, 131	0
3	C	451/455 (99%)	-0.64	4 (0%)	84	86	28, 41, 60, 115	0
3	c	455/455 (100%)	-0.53	8 (1%)	68	72	32, 45, 62, 110	0
4	D	341/342 (99%)	-0.76	5 (1%)	73	77	25, 34, 52, 118	0
4	d	341/342 (99%)	-0.78	7 (2%)	63	68	27, 35, 56, 98	0
5	E	80/81 (98%)	0.21	7 (8%)	10	12	37, 58, 90, 102	0
5	e	81/81 (100%)	0.27	9 (11%)	5	7	40, 54, 83, 105	0
6	F	34/34 (100%)	0.07	4 (11%)	4	5	36, 46, 86, 115	0
6	f	32/34 (94%)	-0.39	1 (3%)	49	55	38, 46, 70, 77	0
7	H	63/63 (100%)	-0.34	2 (3%)	47	54	34, 46, 59, 106	0
7	h	63/63 (100%)	-0.24	4 (6%)	20	24	35, 49, 66, 85	0
8	I	34/37 (91%)	-0.41	1 (2%)	51	57	36, 47, 67, 90	0
8	i	36/37 (97%)	-0.26	2 (5%)	24	29	38, 49, 90, 96	0
9	J	37/40 (92%)	-0.28	3 (8%)	12	15	32, 50, 104, 120	0
9	j	40/40 (100%)	-0.42	1 (2%)	57	62	39, 52, 67, 90	0
10	K	37/37 (100%)	-0.48	0	100	100	41, 49, 62, 73	0
10	k	37/37 (100%)	-0.44	0	100	100	44, 52, 74, 77	0
11	L	36/36 (100%)	-0.46	3 (8%)	11	14	26, 32, 77, 105	0
11	l	35/36 (97%)	-0.51	2 (5%)	23	29	29, 33, 69, 106	0
12	M	32/34 (94%)	-0.81	1 (3%)	49	55	31, 35, 55, 89	0
12	m	33/34 (97%)	-0.52	2 (6%)	21	26	32, 37, 76, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	243/243 (100%)	-0.24	10 (4%)	37	43	28, 45, 73, 129	0
13	o	243/243 (100%)	-0.13	19 (7%)	13	17	29, 47, 80, 114	0
14	T	29/30 (96%)	-0.58	1 (3%)	45	51	28, 35, 58, 126	0
14	t	29/30 (96%)	-0.65	1 (3%)	45	51	29, 34, 61, 103	0
15	U	97/97 (100%)	-0.45	2 (2%)	63	68	30, 40, 60, 89	0
15	u	97/97 (100%)	-0.43	1 (1%)	82	85	34, 42, 63, 108	0
16	V	137/137 (100%)	-0.66	0	100	100	29, 39, 58, 77	0
16	v	137/137 (100%)	-0.28	5 (3%)	42	49	36, 49, 70, 90	0
17	Y	29/29 (100%)	0.56	3 (10%)	6	8	48, 62, 85, 111	0
17	y	29/29 (100%)	0.57	5 (17%)	1	1	53, 69, 83, 94	0
18	X	39/39 (100%)	0.07	4 (10%)	6	8	41, 51, 80, 108	0
18	x	38/39 (97%)	-0.09	4 (10%)	6	8	42, 52, 97, 107	0
19	Z	62/62 (100%)	0.11	9 (14%)	2	3	46, 59, 102, 129	0
19	z	62/62 (100%)	0.47	12 (19%)	1	1	57, 73, 113, 130	0
All	All	5246/5270 (99%)	-0.49	183 (3%)	44	50	23, 41, 73, 131	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	12	SER	9.3
18	X	40	SER	8.9
14	T	30	THR	7.0
2	b	486	LEU	7.0
7	H	64	ALA	6.9
4	D	11	GLU	6.3
2	b	495	PHE	6.2
17	Y	19	ILE	6.1
13	o	246	ALA	5.8
2	b	485	GLU	5.8
13	O	61	GLN	5.8
13	o	4	THR	5.6
11	L	3	PRO	5.6
2	b	502	VAL	5.1
5	e	5	THR	5.0
14	t	30	THR	4.8
19	Z	32	ASP	4.7
6	f	14	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
3	C	23	ALA	4.6
18	x	2	THR	4.6
13	O	60	ARG	4.5
18	x	38	GLN	4.4
13	O	4	THR	4.4
19	z	3	ILE	4.4
19	Z	34	ASP	4.4
11	l	3	PRO	4.4
5	e	59	GLU	4.3
19	z	32	ASP	4.2
18	X	38	GLN	4.2
3	c	19	ASN	4.2
13	O	89	SER	4.1
2	b	503	THR	4.1
17	y	18	VAL	4.0
2	b	494	GLY	4.0
17	y	19	ILE	4.0
19	Z	31	GLN	3.9
4	D	238	THR	3.9
4	d	236	ASN	3.9
4	D	12	ARG	3.9
19	Z	3	ILE	3.9
13	O	62	GLU	3.9
13	o	36	GLN	3.8
19	Z	30	PRO	3.8
3	c	21	ILE	3.8
3	C	24	THR	3.8
19	z	62	VAL	3.8
2	b	484	PRO	3.7
15	u	8	GLU	3.7
18	x	39	ARG	3.7
5	E	82	GLN	3.7
1	A	11	ALA	3.6
8	I	34	ARG	3.6
19	z	4	LEU	3.6
18	x	37	VAL	3.6
13	o	60	ARG	3.5
1	a	11	ALA	3.5
16	v	16	GLY	3.5
2	b	504	THR	3.5
4	d	238	THR	3.5
6	F	14	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
13	o	23	ASP	3.5
4	D	240	ALA	3.4
2	b	493	TRP	3.4
13	o	25	THR	3.4
13	o	132	ASN	3.4
13	o	24	ASP	3.3
19	z	34	ASP	3.3
3	c	143	TYR	3.3
13	O	35	SER	3.3
13	o	35	SER	3.3
19	z	30	PRO	3.2
7	h	64	ALA	3.2
5	e	81	GLU	3.2
9	J	7	ARG	3.2
13	o	211	ILE	3.2
17	Y	18	VAL	3.2
15	U	8	GLU	3.1
2	B	503	THR	3.1
2	b	85	GLY	3.1
3	c	20	SER	3.1
4	d	233	ARG	3.1
13	o	56	PRO	3.1
11	l	5	PRO	3.1
2	b	129	GLY	3.0
7	h	57	GLY	3.0
19	z	33	TRP	3.0
5	E	83	LEU	3.0
2	B	293	ALA	3.0
1	A	12	ASN	3.0
17	y	20	ALA	2.9
2	B	486	LEU	2.9
5	e	61	ARG	2.9
8	i	36	ASP	2.9
19	z	60	PHE	2.9
19	z	42	LEU	2.9
9	j	1	MET	2.9
12	m	33	GLN	2.9
7	h	6	TRP	2.8
2	b	496	TYR	2.8
3	c	145	SER	2.8
13	o	61	GLN	2.8
4	d	240	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
13	o	62	GLU	2.8
13	o	34	SER	2.8
2	b	126	PRO	2.7
19	Z	42	LEU	2.7
19	Z	35	ARG	2.7
2	b	293	ALA	2.7
2	B	485	GLU	2.7
13	O	56	PRO	2.7
13	o	5	LEU	2.7
13	O	5	LEU	2.7
1	a	262	TYR	2.6
19	Z	33	TRP	2.6
17	y	43	ARG	2.6
12	M	33	GLN	2.6
5	E	74	GLN	2.6
5	e	78	THR	2.6
11	L	2	GLU	2.6
2	B	495	PHE	2.6
11	L	5	PRO	2.6
6	F	13	TYR	2.5
1	a	13	LEU	2.5
12	m	34	LYS	2.5
18	X	3	ILE	2.5
3	C	143	TYR	2.5
2	b	374	ASN	2.5
2	b	87	ASP	2.5
5	e	4	THR	2.5
6	F	16	PHE	2.5
2	b	487	SER	2.4
2	b	86	ILE	2.4
3	C	145	SER	2.4
5	e	84	LYS	2.4
7	H	6	TRP	2.4
4	d	237	PRO	2.4
13	o	131	PRO	2.4
17	Y	22	LEU	2.4
3	c	462	GLU	2.4
2	b	505	ARG	2.4
19	z	35	ARG	2.4
13	o	130[A]	GLN	2.4
2	B	85	GLY	2.4
15	U	27	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	4	THR	2.3
19	z	31	GLN	2.3
2	B	295	GLY	2.3
4	d	234	ALA	2.3
5	E	81	GLU	2.3
13	o	58	ASN	2.3
5	e	25	ILE	2.3
16	v	15	GLU	2.3
5	E	61	ARG	2.3
2	b	127	ARG	2.3
13	O	207	ARG	2.3
4	d	11	GLU	2.2
2	B	494	GLY	2.2
2	b	501	ASP	2.2
16	v	106	ASN	2.2
4	D	237	PRO	2.2
9	J	4	GLU	2.2
19	Z	62	VAL	2.2
2	B	374	ASN	2.2
2	b	489	GLU	2.2
2	B	484	PRO	2.2
2	B	505	ARG	2.2
5	e	83	LEU	2.1
8	i	37	LEU	2.1
3	c	257	PHE	2.1
13	O	23	ASP	2.1
16	v	18	THR	2.1
9	J	8	ILE	2.1
16	v	72	LEU	2.1
17	y	41	VAL	2.1
13	o	21	THR	2.1
1	A	262	TYR	2.1
1	a	235	TYR	2.1
5	E	71	GLU	2.1
19	z	41	PHE	2.1
7	h	23	PRO	2.0
3	c	200	THR	2.0
18	X	37	VAL	2.0
2	b	295	GLY	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
12	FME	M	1	10/11	0.93	0.13	39,42,73,78	0
12	FME	m	1	10/11	0.94	0.13	40,46,74,76	0
8	FME	I	1	10/11	0.95	0.08	36,43,47,48	0
14	FME	t	1	10/11	0.96	0.08	31,41,67,75	0
8	FME	i	1	10/11	0.97	0.08	40,45,49,51	0
14	FME	T	1	10/11	0.98	0.06	35,40,67,76	0
4	HSK	d	336[B]	11/12	0.99	0.06	35,42,52,56	8
4	HSK	D	336[B]	11/12	0.99	0.07	35,37,42,45	8
4	HSK	D	336[A]	10/12	0.99	0.07	32,36,37,37	7
4	HSK	d	336[A]	10/12	0.99	0.06	35,38,42,42	7

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
27	UNL	J	103	16/-	0.42	0.27	74,97,111,112	0
27	UNL	b	603	16/-	0.47	0.26	73,94,114,115	0
27	UNL	I	102	14/-	0.52	0.22	82,96,101,101	0
27	UNL	j	104	16/-	0.52	0.27	77,91,113,115	0
32	HTG	D	413	16/19	0.52	0.33	80,99,115,116	0
28	LMT	m	103	23/35	0.53	0.23	59,80,125,127	0
32	HTG	C	536	19/19	0.53	0.32	79,117,138,138	0
28	LMT	J	102	24/35	0.53	0.26	62,83,124,131	0
27	UNL	B	625	15/-	0.54	0.23	83,93,115,120	0
27	UNL	c	525	5/-	0.56	0.16	72,83,84,84	0
32	HTG	B	624	19/19	0.56	0.40	65,99,109,114	0
32	HTG	b	602	19/19	0.56	0.20	71,113,132,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	DGD	d	408	48/66	0.56	0.30	70,100,122,132	0
27	UNL	C	524	26/-	0.58	0.24	76,97,109,120	0
32	HTG	C	522	19/19	0.58	0.33	61,92,117,117	0
28	LMT	a	401	35/35	0.59	0.33	38,67,86,100	35
28	LMT	A	415	35/35	0.59	0.27	54,88,106,116	0
27	UNL	e	103	11/-	0.60	0.33	67,81,102,104	0
28	LMT	l	101	24/35	0.61	0.23	59,76,130,142	0
27	UNL	i	101	16/-	0.61	0.23	82,85,100,101	0
27	UNL	E	103	16/-	0.62	0.25	78,88,108,109	0
32	HTG	d	413	16/19	0.63	0.32	66,100,118,131	0
33	DGD	D	408	45/66	0.63	0.25	70,93,120,129	0
27	UNL	K	103	10/-	0.63	0.23	78,89,97,98	0
32	HTG	c	541	15/19	0.64	0.37	74,104,117,120	0
32	HTG	U	203	14/19	0.64	0.48	76,107,133,154	0
27	UNL	I	101	16/-	0.65	0.21	78,88,102,110	0
27	UNL	H	104	7/-	0.65	0.18	78,82,85,88	0
28	LMT	j	102	23/35	0.67	0.21	71,81,105,108	0
27	UNL	u	201	13/-	0.68	0.26	57,67,80,84	0
28	LMT	M	101	35/35	0.68	0.21	43,73,83,90	0
28	LMT	m	101	35/35	0.68	0.23	38,70,81,85	0
28	LMT	m	102	25/35	0.68	0.26	45,72,116,124	0
28	LMT	F	102	24/35	0.68	0.25	60,97,113,121	0
27	UNL	a	415	40/-	0.69	0.24	75,97,121,124	0
28	LMT	t	102	24/35	0.69	0.20	67,87,121,126	0
32	HTG	c	524	9/19	0.70	0.19	73,79,97,114	0
32	HTG	B	629	19/19	0.70	0.20	59,118,133,135	0
27	UNL	A	414	28/-	0.70	0.23	76,94,110,114	0
27	UNL	j	103	33/-	0.70	0.24	67,112,139,141	0
32	HTG	b	627	19/19	0.70	0.25	69,91,106,109	0
34	GOL	e	104	6/6	0.70	0.23	72,77,81,84	0
26	LMG	c	521	51/55	0.71	0.23	51,93,114,122	0
29	DMS	c	540	4/4	0.71	0.33	99,101,109,120	0
27	UNL	i	102	14/-	0.71	0.23	91,101,109,109	0
26	LMG	C	519	48/55	0.71	0.23	52,89,111,119	0
29	DMS	O	312	4/4	0.72	0.29	78,88,109,113	0
27	UNL	c	527	16/-	0.72	0.24	73,83,115,120	0
27	UNL	c	526	32/-	0.72	0.24	67,94,116,119	0
28	LMT	b	626	25/35	0.72	0.20	62,76,105,114	0
27	UNL	Z	102	6/-	0.73	0.19	71,83,89,90	0
27	UNL	A	413	7/-	0.74	0.21	84,90,95,96	0
31	LHG	E	101	49/49	0.74	0.25	60,95,130,135	0
27	UNL	E	102	13/-	0.75	0.18	81,91,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	DMS	c	538	4/4	0.75	0.19	70,106,108,128	0
27	UNL	U	201	14/-	0.76	0.23	54,74,82,82	0
28	LMT	T	102	24/35	0.76	0.20	43,78,107,110	0
32	HTG	c	523	19/19	0.76	0.23	86,101,115,118	0
27	UNL	e	102	8/-	0.77	0.18	77,82,84,84	0
28	LMT	z	101	32/35	0.77	0.18	53,88,118,138	0
28	LMT	M	102	24/35	0.77	0.15	51,70,94,108	0
27	UNL	T	103	13/-	0.78	0.28	80,89,96,101	0
27	UNL	a	414	8/-	0.78	0.16	77,81,86,90	0
29	DMS	a	418	4/4	0.78	0.19	97,107,116,118	0
29	DMS	O	309	4/4	0.79	0.33	80,106,109,118	0
27	UNL	B	630	16/-	0.80	0.18	69,81,89,89	0
27	UNL	b	641	40/-	0.80	0.18	60,77,94,97	0
27	UNL	B	643	40/-	0.80	0.20	60,76,101,112	0
27	UNL	A	412	8/-	0.80	0.16	64,74,78,79	0
29	DMS	d	416	4/4	0.81	0.24	99,114,115,118	0
27	UNL	i	104	14/-	0.81	0.18	69,80,99,101	0
31	LHG	e	101	38/49	0.81	0.23	63,94,111,113	0
28	LMT	Z	101	35/35	0.81	0.19	48,88,101,103	0
27	UNL	a	413	8/-	0.81	0.15	76,83,90,95	0
34	GOL	D	417	6/6	0.81	0.21	63,70,73,74	0
27	UNL	A	421	40/-	0.81	0.16	56,78,120,123	0
27	UNL	d	417	36/-	0.82	0.15	49,87,101,107	0
29	DMS	a	419	4/4	0.82	0.27	96,109,116,119	0
29	DMS	D	419	4/4	0.82	0.22	96,114,118,120	0
27	UNL	C	523	9/-	0.82	0.13	75,77,85,87	0
27	UNL	A	420	36/-	0.82	0.15	41,86,102,108	0
29	DMS	v	207	4/4	0.82	0.20	75,78,83,99	0
27	UNL	B	627	16/-	0.83	0.17	53,64,87,88	0
28	LMT	C	520	35/35	0.83	0.23	71,97,104,104	0
29	DMS	B	640	4/4	0.83	0.31	70,86,87,96	0
32	HTG	B	642	18/19	0.83	0.22	25,38,48,49	18
27	UNL	X	101	16/-	0.83	0.16	47,53,78,80	0
34	GOL	b	636	6/6	0.83	0.31	61,76,83,103	0
29	DMS	c	532	4/4	0.83	0.22	64,81,98,107	0
29	DMS	c	534	4/4	0.84	0.26	80,90,95,100	0
29	DMS	A	419	4/4	0.84	0.22	94,96,101,109	0
29	DMS	V	207	4/4	0.84	0.29	85,97,101,104	0
26	LMG	a	412	51/55	0.84	0.14	51,69,85,98	0
32	HTG	b	640	17/19	0.84	0.20	27,44,57,61	17
25	PL9	A	410	55/55	0.84	0.19	51,77,105,110	0
27	UNL	b	628	36/-	0.84	0.17	50,73,110,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	DMS	O	306	4/4	0.85	0.25	76,88,93,106	0
29	DMS	O	308	4/4	0.85	0.24	67,71,84,97	0
27	UNL	B	626	40/-	0.85	0.15	46,68,109,118	0
26	LMG	A	411	51/55	0.85	0.15	54,68,92,105	0
28	LMT	B	623	35/35	0.85	0.16	56,68,85,93	0
27	UNL	H	103	7/-	0.85	0.11	69,72,89,93	0
25	PL9	a	411	55/55	0.85	0.18	54,73,105,110	0
28	LMT	c	522	35/35	0.85	0.26	65,89,117,127	0
27	UNL	h	103	8/-	0.85	0.17	66,79,89,91	0
27	UNL	t	103	16/-	0.85	0.19	71,86,109,110	0
29	DMS	I	105	4/4	0.85	0.41	76,86,99,99	0
32	HTG	b	601	19/19	0.85	0.15	57,66,80,92	0
26	LMG	C	518	49/55	0.86	0.18	42,73,104,111	0
29	DMS	O	310	4/4	0.86	0.29	70,98,98,109	0
29	DMS	c	536	4/4	0.86	0.37	97,97,105,115	0
26	LMG	c	520	38/55	0.86	0.14	43,70,87,91	0
29	DMS	c	539	4/4	0.86	0.16	106,108,113,115	0
32	HTG	v	208	16/19	0.87	0.23	60,80,108,119	0
32	HTG	B	628	19/19	0.87	0.14	47,69,90,102	0
26	LMG	B	622	51/55	0.87	0.13	48,60,79,84	0
27	UNL	a	421	40/-	0.87	0.12	55,75,110,112	0
29	DMS	O	304	4/4	0.87	0.44	85,104,105,105	0
29	DMS	u	203	4/4	0.87	0.31	48,83,83,92	0
32	HTG	C	521	19/19	0.88	0.19	70,88,102,103	0
27	UNL	x	101	16/-	0.88	0.20	56,65,93,94	0
32	HTG	C	535	9/19	0.88	0.15	72,80,85,97	0
27	UNL	I	104	13/-	0.88	0.16	57,66,93,95	0
29	DMS	b	633	4/4	0.89	0.17	77,78,82,98	0
27	UNL	I	103	16/-	0.89	0.22	47,62,98,98	0
29	DMS	o	307	4/4	0.89	0.31	63,84,93,93	0
29	DMS	o	310	4/4	0.89	0.25	73,80,91,101	0
27	UNL	i	103	16/-	0.89	0.21	50,59,84,85	0
33	DGD	h	101	62/66	0.89	0.14	35,47,64,65	0
29	DMS	a	416	4/4	0.89	0.19	75,83,103,104	0
22	CLA	B	602	65/65	0.89	0.13	39,52,116,127	0
27	UNL	b	629	16/-	0.89	0.13	48,62,81,82	0
26	LMG	b	625	49/55	0.90	0.12	47,57,79,86	0
29	DMS	o	306	4/4	0.90	0.35	87,88,103,119	0
31	LHG	f	102	46/49	0.90	0.14	52,78,107,120	0
24	BCR	d	406	40/40	0.90	0.11	30,42,75,76	0
29	DMS	C	529	4/4	0.90	0.33	90,90,93,97	0
29	DMS	V	206	4/4	0.90	0.39	61,85,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	C	513	65/65	0.90	0.11	46,58,99,105	0
38	RRX	h	102	41/41	0.90	0.12	38,46,63,72	0
29	DMS	v	204	4/4	0.91	0.27	89,92,96,99	0
29	DMS	v	206	4/4	0.91	0.20	63,73,80,85	0
22	CLA	b	605	65/65	0.91	0.14	41,60,107,122	0
30	CA	v	209	1/1	0.91	0.19	90,90,90,90	0
22	CLA	b	620	65/65	0.91	0.11	32,44,112,139	0
27	UNL	D	414	16/-	0.91	0.17	44,53,66,73	0
29	DMS	O	307	4/4	0.91	0.25	87,92,93,94	0
24	BCR	D	406	40/40	0.91	0.10	32,40,73,76	0
24	BCR	K	101	40/40	0.91	0.16	36,47,54,58	0
29	DMS	B	639	4/4	0.91	0.27	75,84,91,94	0
24	BCR	K	102	40/40	0.91	0.10	42,53,57,60	0
33	DGD	H	101	62/66	0.91	0.13	34,46,55,59	0
29	DMS	U	202	4/4	0.91	0.15	40,61,69,82	0
29	DMS	C	527	4/4	0.91	0.15	75,76,79,93	0
24	BCR	T	101	40/40	0.91	0.11	40,52,78,83	0
29	DMS	C	534	4/4	0.91	0.30	67,81,87,87	0
24	BCR	c	515	40/40	0.91	0.11	50,62,69,70	0
32	HTG	O	302	19/19	0.91	0.12	41,57,74,75	0
29	DMS	O	311	4/4	0.92	0.15	80,88,88,91	0
29	DMS	h	104	4/4	0.92	0.19	103,104,106,109	0
32	HTG	o	301	19/19	0.92	0.11	49,58,70,73	0
31	LHG	F	103	38/49	0.92	0.15	56,82,111,112	0
33	DGD	C	516	62/66	0.92	0.11	31,45,103,116	0
29	DMS	B	634	4/4	0.92	0.35	83,86,86,94	0
29	DMS	C	532	4/4	0.92	0.25	58,72,80,81	0
22	CLA	B	617	65/65	0.92	0.12	31,43,129,145	0
29	DMS	u	202	4/4	0.92	0.17	48,69,70,82	0
24	BCR	t	101	40/40	0.92	0.10	36,52,72,74	0
29	DMS	D	420	4/4	0.92	0.33	93,98,108,110	0
29	DMS	a	417	4/4	0.92	0.35	69,78,88,92	0
38	RRX	H	102	41/41	0.92	0.11	36,42,56,60	0
27	UNL	d	414	16/-	0.92	0.17	44,56,84,88	0
26	LMG	d	412	47/55	0.93	0.12	37,47,99,103	0
29	DMS	B	633	4/4	0.93	0.15	94,98,98,100	0
29	DMS	E	104	4/4	0.93	0.28	91,95,98,105	0
29	DMS	e	105	4/4	0.93	0.33	80,93,97,97	0
22	CLA	c	507	65/65	0.93	0.10	42,51,109,121	0
29	DMS	B	635	4/4	0.93	0.21	90,94,95,106	0
34	GOL	c	533	6/6	0.93	0.25	58,62,76,81	0
32	HTG	V	202	19/19	0.93	0.27	50,62,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	y	101	40/40	0.93	0.09	40,47,57,59	0
29	DMS	o	309	4/4	0.93	0.26	70,78,79,91	0
29	DMS	B	638	4/4	0.94	0.27	43,55,65,71	0
29	DMS	O	303	4/4	0.94	0.19	72,84,93,96	0
29	DMS	V	208	4/4	0.94	0.11	83,84,90,91	0
22	CLA	C	506	65/65	0.94	0.10	39,55,121,136	0
29	DMS	O	305	4/4	0.94	0.17	77,88,91,93	0
22	CLA	C	512	65/65	0.94	0.09	39,51,96,105	0
22	CLA	c	513	65/65	0.94	0.10	43,56,94,107	0
24	BCR	Y	101	40/40	0.94	0.10	37,43,55,57	0
29	DMS	b	637	4/4	0.94	0.18	71,82,87,95	0
33	DGD	c	518	56/66	0.94	0.09	37,45,80,86	0
29	DMS	u	204	4/4	0.94	0.09	70,83,95,98	0
29	DMS	b	638	4/4	0.94	0.23	80,89,92,92	0
29	DMS	A	418	4/4	0.94	0.23	82,92,94,95	0
24	BCR	b	623	40/40	0.94	0.09	33,44,60,61	0
22	CLA	c	514	65/65	0.94	0.11	44,66,111,118	0
24	BCR	c	516	40/40	0.94	0.09	37,46,57,58	0
22	CLA	b	610	65/65	0.94	0.09	31,42,81,83	0
29	DMS	V	204	4/4	0.94	0.13	68,73,75,90	0
29	DMS	b	634	4/4	0.95	0.20	73,77,82,89	0
29	DMS	b	635	4/4	0.95	0.22	70,71,71,73	0
22	CLA	c	508	65/65	0.95	0.09	34,44,68,76	0
29	DMS	v	203	4/4	0.95	0.18	76,78,80,82	0
29	DMS	D	418	4/4	0.95	0.24	83,92,96,114	0
29	DMS	v	205	4/4	0.95	0.16	61,68,69,70	0
29	DMS	b	639	4/4	0.95	0.27	87,93,94,106	0
26	LMG	D	412	47/55	0.95	0.10	34,44,84,95	0
22	CLA	C	508	65/65	0.95	0.09	33,39,105,122	0
31	LHG	D	409	49/49	0.95	0.10	37,48,64,69	0
31	LHG	D	411	44/49	0.95	0.11	35,44,110,117	0
29	DMS	c	535	4/4	0.95	0.21	84,92,99,112	0
29	DMS	B	636	4/4	0.95	0.25	65,83,88,91	0
31	LHG	d	411	44/49	0.95	0.13	37,47,109,121	0
33	DGD	C	517	62/66	0.95	0.08	27,42,77,83	0
29	DMS	c	537	4/4	0.95	0.31	85,94,103,106	0
29	DMS	V	205	4/4	0.95	0.25	77,79,80,89	0
21	CL	v	201	1/1	0.95	0.26	93,93,93,93	0
33	DGD	c	519	62/66	0.95	0.09	32,45,73,87	0
24	BCR	B	618	40/40	0.95	0.08	31,39,51,54	0
24	BCR	B	619	40/40	0.95	0.08	30,40,55,70	0
34	GOL	C	533	6/6	0.95	0.17	46,53,57,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	DMS	B	641	4/4	0.95	0.25	65,66,71,83	0
29	DMS	A	416	4/4	0.95	0.21	71,73,77,85	0
22	CLA	C	507	65/65	0.95	0.10	37,44,68,75	0
29	DMS	C	531	4/4	0.95	0.12	86,87,90,92	0
29	DMS	a	420	4/4	0.95	0.17	87,90,91,93	0
22	CLA	D	405	65/65	0.95	0.09	31,39,114,126	0
39	MG	K	104	1/1	0.95	0.09	56,56,56,56	0
22	CLA	c	512	65/65	0.96	0.10	40,49,56,65	0
22	CLA	C	503	65/65	0.96	0.08	33,41,47,58	0
22	CLA	B	603	65/65	0.96	0.08	30,38,46,50	0
22	CLA	d	405	65/65	0.96	0.08	31,43,111,120	0
24	BCR	A	409	40/40	0.96	0.08	28,35,42,44	0
22	CLA	a	409	65/65	0.96	0.11	29,37,126,135	0
22	CLA	B	607	65/65	0.96	0.09	32,39,71,87	0
24	BCR	B	620	40/40	0.96	0.08	31,41,57,60	0
24	BCR	C	514	40/40	0.96	0.09	35,46,60,63	0
29	DMS	V	203	4/4	0.96	0.15	74,84,87,92	0
22	CLA	b	606	65/65	0.96	0.09	32,37,48,59	0
29	DMS	B	637	4/4	0.96	0.12	69,73,81,82	0
22	CLA	B	611	65/65	0.96	0.09	30,37,44,57	0
22	CLA	b	611	65/65	0.96	0.07	26,32,50,58	0
22	CLA	b	614	65/65	0.96	0.07	30,40,46,51	0
22	CLA	b	616	65/65	0.96	0.08	29,36,44,50	0
24	BCR	a	410	40/40	0.96	0.07	32,39,45,46	0
29	DMS	C	528	4/4	0.96	0.25	74,81,82,82	0
33	DGD	C	515	62/66	0.96	0.11	30,41,105,109	0
24	BCR	b	621	40/40	0.96	0.07	36,42,55,58	0
24	BCR	b	622	40/40	0.96	0.08	29,44,58,67	0
30	CA	V	209	1/1	0.96	0.15	93,93,93,93	0
30	CA	c	501	1/1	0.96	0.10	62,62,62,62	0
29	DMS	b	631	4/4	0.96	0.08	66,78,80,82	0
29	DMS	b	632	4/4	0.96	0.12	63,72,72,73	0
22	CLA	b	619	65/65	0.96	0.08	32,42,59,67	0
22	CLA	C	509	65/65	0.96	0.10	33,42,68,76	0
22	CLA	c	504	65/65	0.96	0.08	34,47,56,58	0
22	CLA	c	505	65/65	0.96	0.07	35,40,74,82	0
22	CLA	C	510	65/65	0.96	0.08	33,40,52,66	0
22	CLA	A	408	65/65	0.96	0.09	25,34,110,115	0
29	DMS	c	530	4/4	0.96	0.17	70,88,95,104	0
22	CLA	c	509	65/65	0.96	0.08	34,41,100,113	0
22	CLA	c	510	65/65	0.96	0.10	30,42,76,81	0
25	PL9	d	407	55/55	0.96	0.08	27,34,46,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	LHG	b	624	49/49	0.97	0.09	33,42,65,76	0
31	LHG	d	409	49/49	0.97	0.12	40,47,64,70	0
31	LHG	d	410	49/49	0.97	0.11	27,38,58,73	0
29	DMS	C	530	4/4	0.97	0.16	40,54,55,58	0
22	CLA	C	504	65/65	0.97	0.07	32,38,72,74	0
23	PHO	A	407	64/64	0.97	0.07	25,30,33,38	0
23	PHO	D	404	64/64	0.97	0.08	25,34,41,45	0
23	PHO	a	408	64/64	0.97	0.07	27,33,38,42	0
29	DMS	c	531	4/4	0.97	0.27	90,91,96,98	0
22	CLA	b	607	65/65	0.97	0.07	29,36,47,51	0
22	CLA	b	608	65/65	0.97	0.08	29,35,75,79	0
22	CLA	C	505	65/65	0.97	0.07	34,41,54,60	0
22	CLA	B	608	65/65	0.97	0.08	24,31,47,62	0
22	CLA	b	612	65/65	0.97	0.07	26,35,44,49	0
22	CLA	b	613	65/65	0.97	0.10	35,40,50,54	0
22	CLA	B	610	65/65	0.97	0.10	33,41,49,54	0
22	CLA	B	604	65/65	0.97	0.07	26,34,44,55	0
29	DMS	d	415	4/4	0.97	0.18	64,70,75,87	0
22	CLA	b	617	65/65	0.97	0.08	30,35,74,80	0
22	CLA	b	618	65/65	0.97	0.09	29,36,123,128	0
22	CLA	B	614	65/65	0.97	0.07	26,32,69,94	0
29	DMS	o	304	4/4	0.97	0.14	85,86,87,87	0
29	DMS	o	305	4/4	0.97	0.31	88,91,92,102	0
22	CLA	B	615	65/65	0.97	0.07	27,36,115,119	0
22	CLA	c	502	65/65	0.97	0.07	38,43,56,64	0
29	DMS	o	308	4/4	0.97	0.26	71,77,85,85	0
22	CLA	c	503	65/65	0.97	0.07	31,38,55,64	0
22	CLA	C	511	65/65	0.97	0.09	36,44,50,53	0
29	DMS	o	311	4/4	0.97	0.20	80,91,94,116	0
29	DMS	B	632	4/4	0.97	0.09	53,54,55,69	0
22	CLA	B	616	65/65	0.97	0.07	32,39,61,67	0
22	CLA	c	506	65/65	0.97	0.07	34,43,57,71	0
24	BCR	k	101	40/40	0.97	0.12	41,48,56,58	0
33	DGD	c	517	62/66	0.97	0.09	32,46,93,108	0
22	CLA	B	605	65/65	0.97	0.08	26,33,65,73	0
22	CLA	D	403	65/65	0.97	0.08	23,28,49,53	0
22	CLA	C	501	65/65	0.97	0.08	32,41,55,66	0
25	PL9	D	407	55/55	0.97	0.08	26,35,43,54	0
22	CLA	a	406	65/65	0.97	0.10	25,31,40,56	0
22	CLA	c	511	65/65	0.97	0.08	30,40,54,58	0
29	DMS	C	525	4/4	0.97	0.10	42,51,52,58	0
31	LHG	B	621	49/49	0.97	0.10	33,41,61,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	DMS	C	526	4/4	0.97	0.20	60,61,66,69	0
36	BCT	d	401[A]	4/4	0.97	0.12	50,52,55,67	4
36	BCT	d	401[B]	4/4	0.97	0.12	21,31,31,38	4
37	HEM	F	101	43/43	0.97	0.09	43,52,63,69	0
22	CLA	a	407	65/65	0.97	0.08	25,33,104,120	0
22	CLA	C	502	65/65	0.97	0.07	30,36,52,61	0
39	MG	J	101	1/1	0.97	0.04	45,45,45,45	0
22	CLA	A	404	65/65	0.97	0.09	22,28,40,59	0
39	MG	k	102	1/1	0.97	0.13	61,61,61,61	0
30	CA	O	301	1/1	0.98	0.05	57,57,57,57	0
22	CLA	B	613	65/65	0.98	0.07	28,33,40,43	0
30	CA	b	604	1/1	0.98	0.07	63,63,63,63	0
23	PHO	d	404	64/64	0.98	0.09	27,34,41,48	0
30	CA	o	302	1/1	0.98	0.07	58,58,58,58	0
29	DMS	c	528	4/4	0.98	0.10	41,54,55,56	0
29	DMS	c	529	4/4	0.98	0.16	52,56,57,67	0
22	CLA	A	405	65/65	0.98	0.07	22,27,39,48	0
31	LHG	D	410	49/49	0.98	0.12	30,38,53,67	0
22	CLA	b	615	65/65	0.98	0.08	25,33,52,55	0
22	CLA	B	609	65/65	0.98	0.07	28,35,44,47	0
22	CLA	b	609	65/65	0.98	0.09	28,33,47,48	0
22	CLA	d	402	65/65	0.98	0.09	25,30,48,56	0
36	BCT	D	402[A]	4/4	0.98	0.16	24,36,36,40	4
36	BCT	D	402[B]	4/4	0.98	0.16	36,44,46,50	4
29	DMS	D	415	4/4	0.98	0.11	65,68,77,91	0
29	DMS	b	630	4/4	0.98	0.10	37,40,40,42	0
29	DMS	D	416	4/4	0.98	0.17	68,80,85,89	0
37	HEM	f	101	43/43	0.98	0.07	42,50,58,63	0
22	CLA	d	403	65/65	0.98	0.07	26,29,43,53	0
22	CLA	B	606	65/65	0.98	0.09	28,34,51,56	0
22	CLA	A	406	65/65	0.98	0.06	24,33,95,113	0
22	CLA	B	612	65/65	0.98	0.07	25,32,48,55	0
39	MG	j	101	1/1	0.98	0.06	50,50,50,50	0
29	DMS	B	631	4/4	0.98	0.09	31,35,36,42	0
40	HEC	V	201	43/43	0.98	0.10	28,32,39,44	0
40	HEC	v	202	43/43	0.98	0.09	37,44,49,57	0
30	CA	B	601	1/1	0.99	0.10	60,60,60,60	0
21	CL	A	402	1/1	0.99	0.04	31,31,31,31	0
29	DMS	o	303	4/4	0.99	0.05	31,40,41,44	0
21	CL	a	404	1/1	0.99	0.02	35,35,35,35	0
21	CL	a	405	1/1	0.99	0.06	34,34,34,34	0
20	OEX	a	402	10/10	0.99	0.04	28,33,39,41	0

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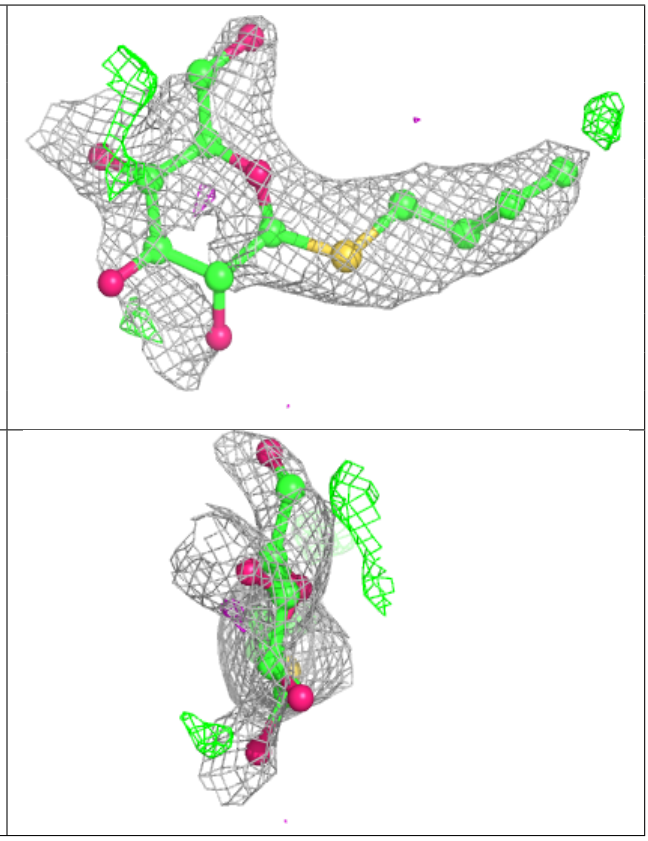
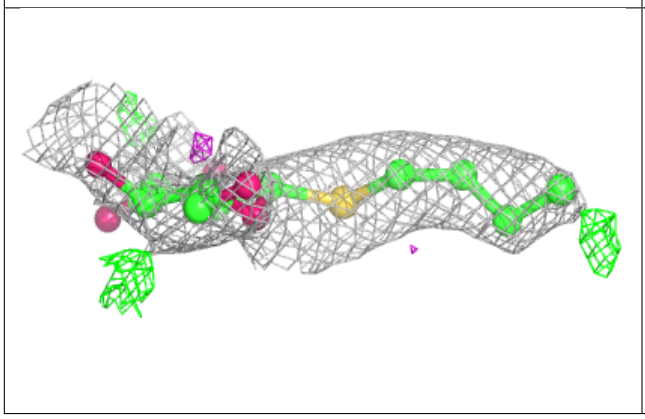
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	DMS	A	417	4/4	0.99	0.07	32,36,37,38	0
35	FE2	D	401	1/1	1.00	0.06	41,41,41,41	0
35	FE2	a	403	1/1	1.00	0.07	40,40,40,40	0
21	CL	A	403	1/1	1.00	0.04	29,29,29,29	0
20	OEX	A	401	10/10	1.00	0.04	28,31,39,40	0

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 HTG D 413:

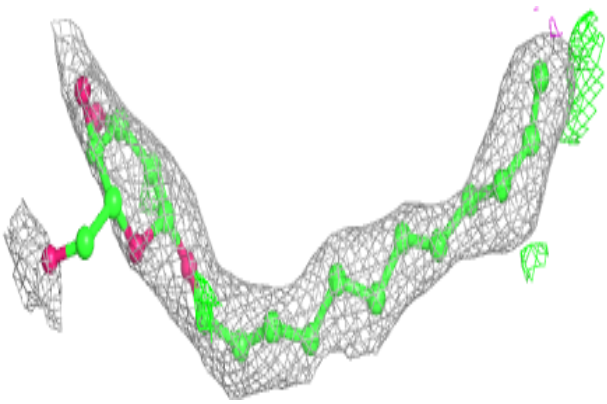
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

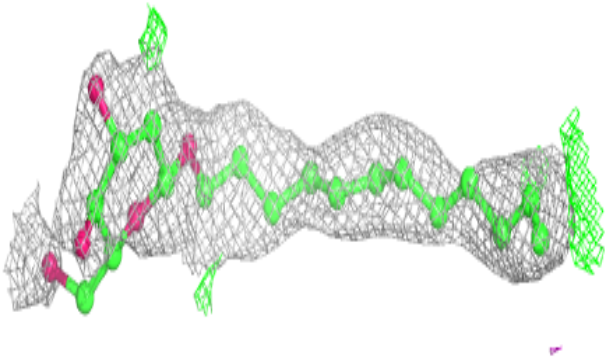


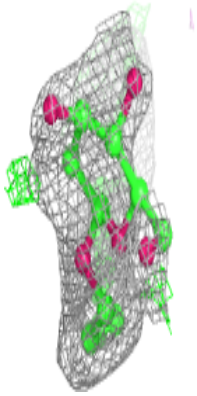


Electron density around LMT m 103:

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

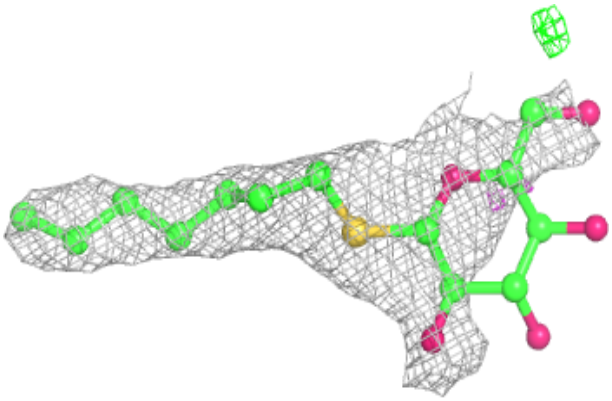


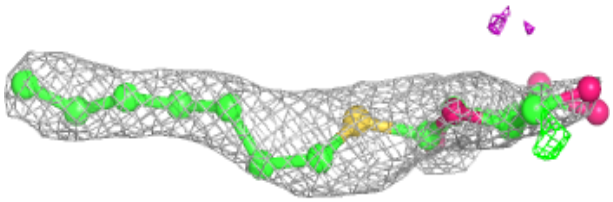


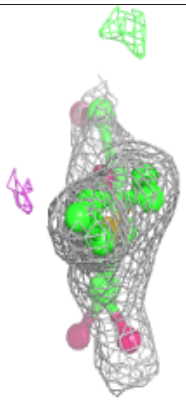


Electron density around HTG C 536:

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

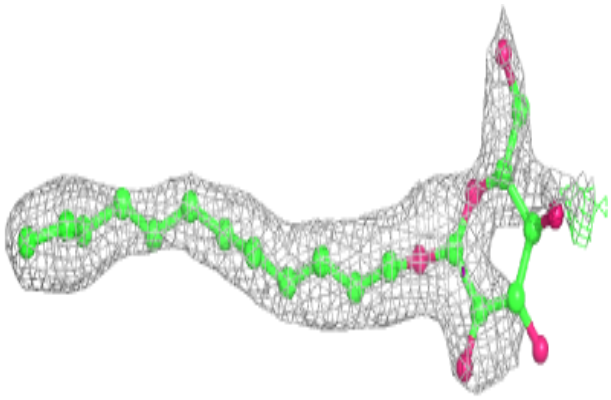


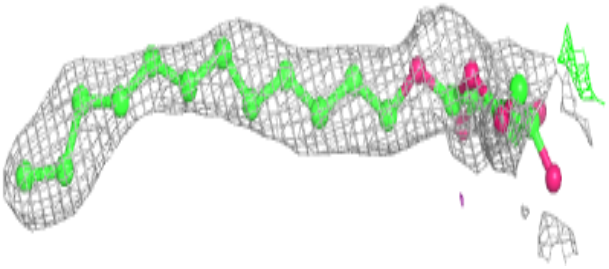




Electron density around LMT J 102:

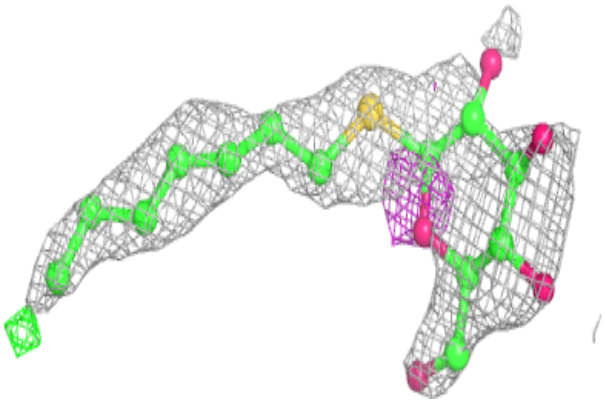
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

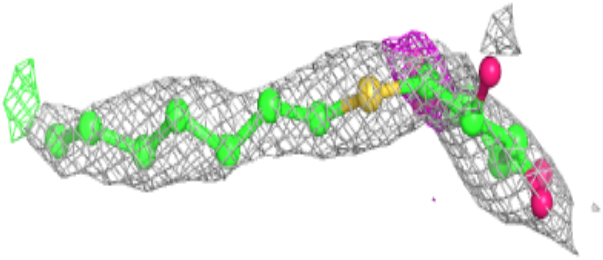


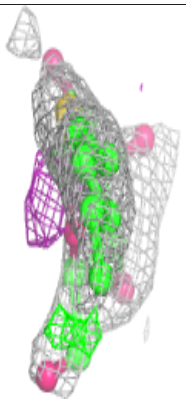


Electron density around HTG B 624:

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

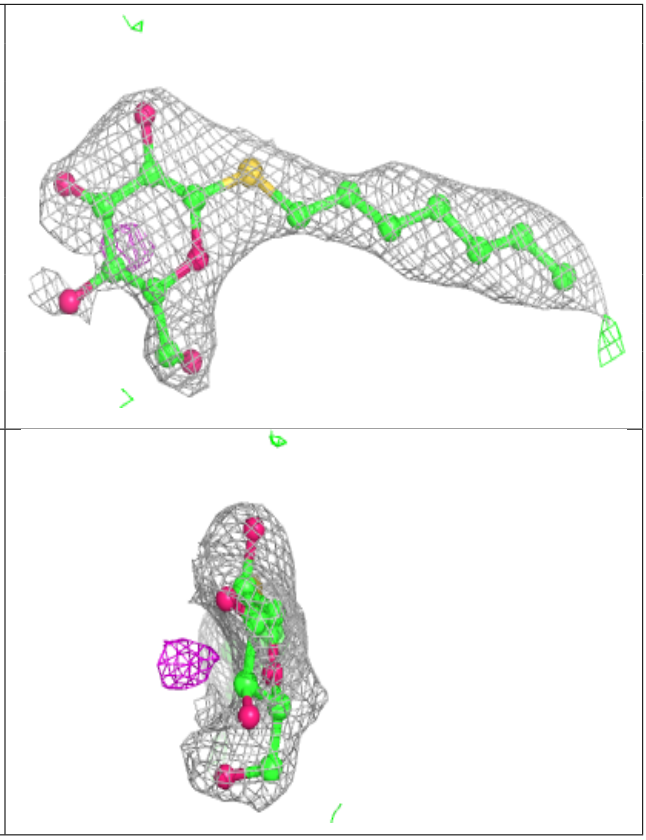






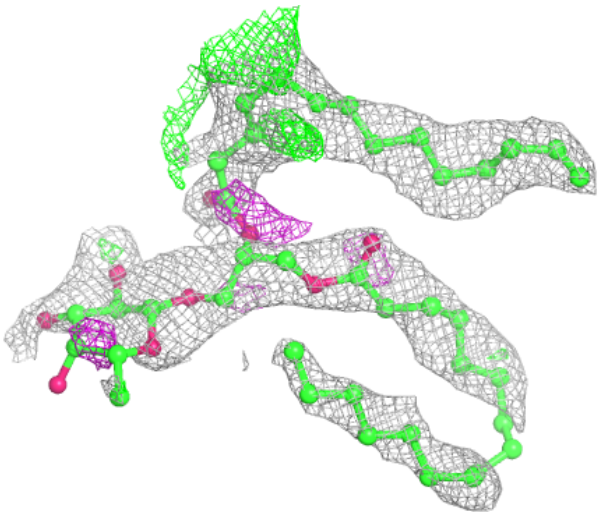
Electron density around HTG b 602:

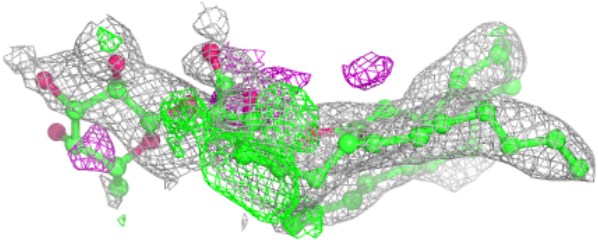
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

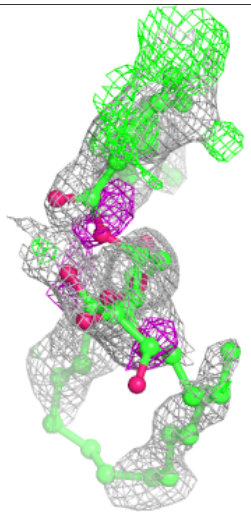


Electron density around DGD d 408:

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

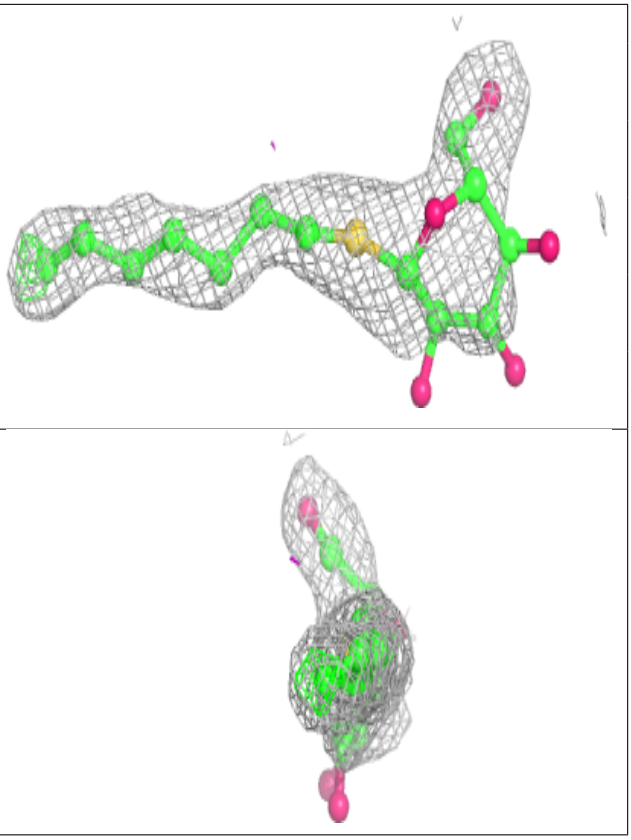


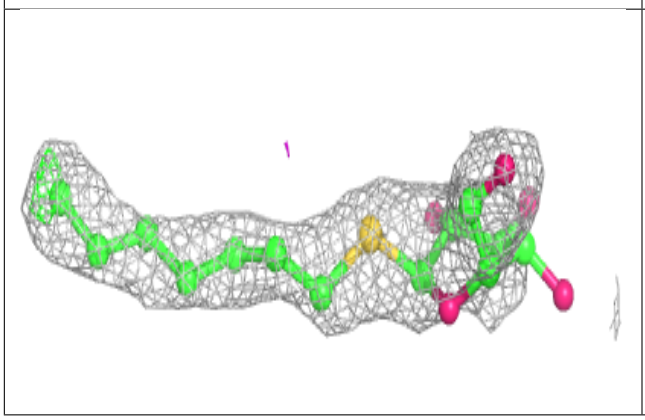




Electron density around HTG C 522:

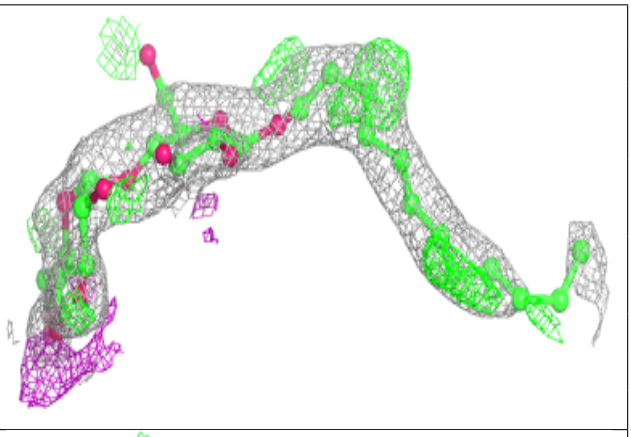
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

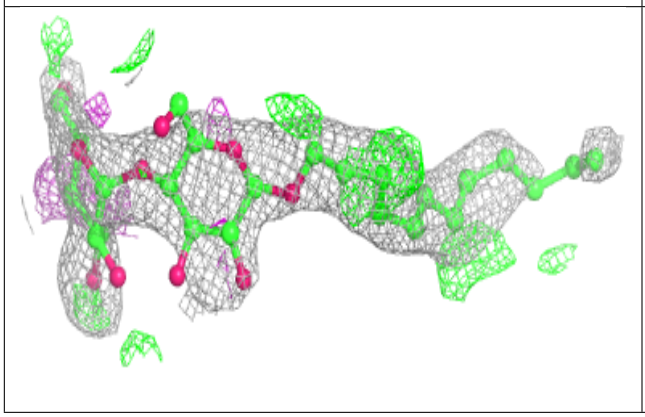


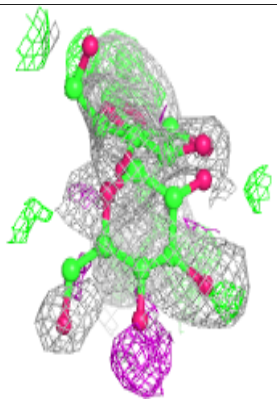


Electron density around LMT a 401:

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

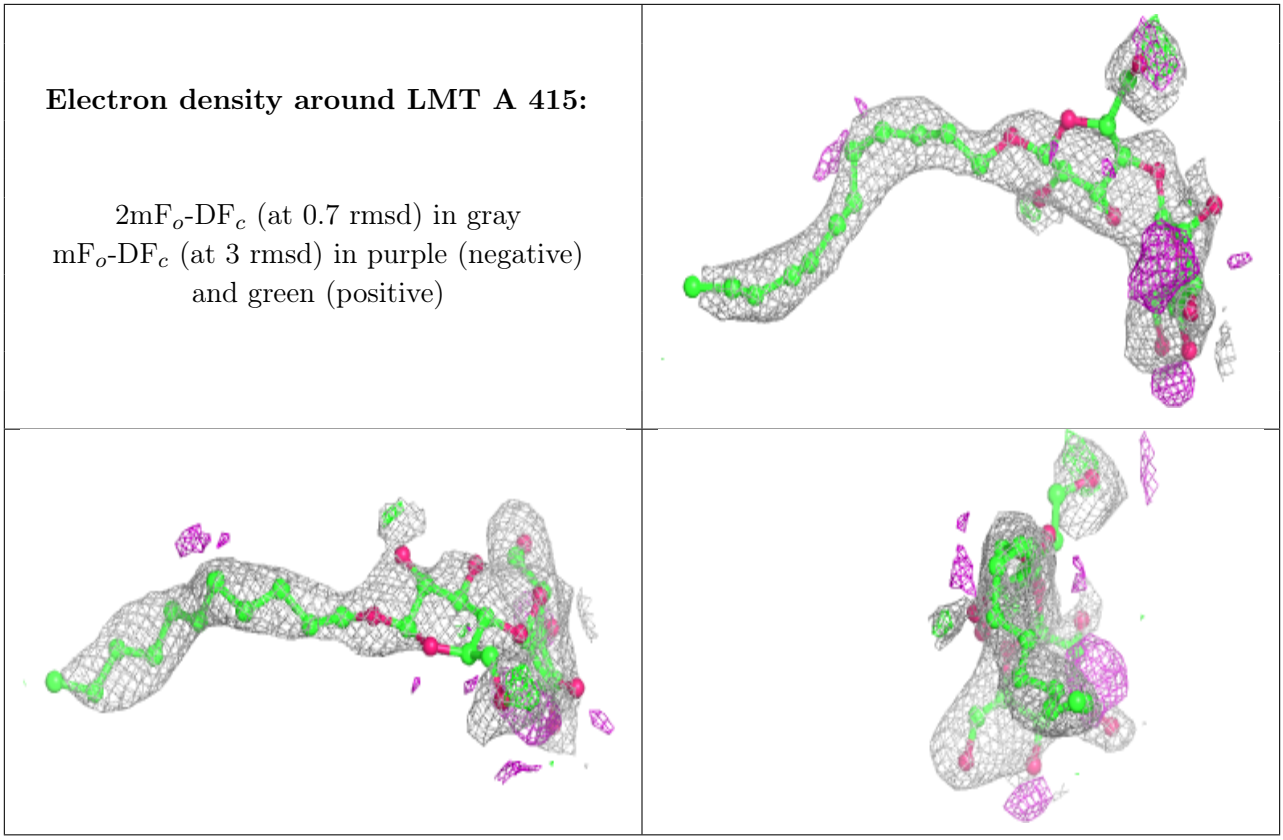






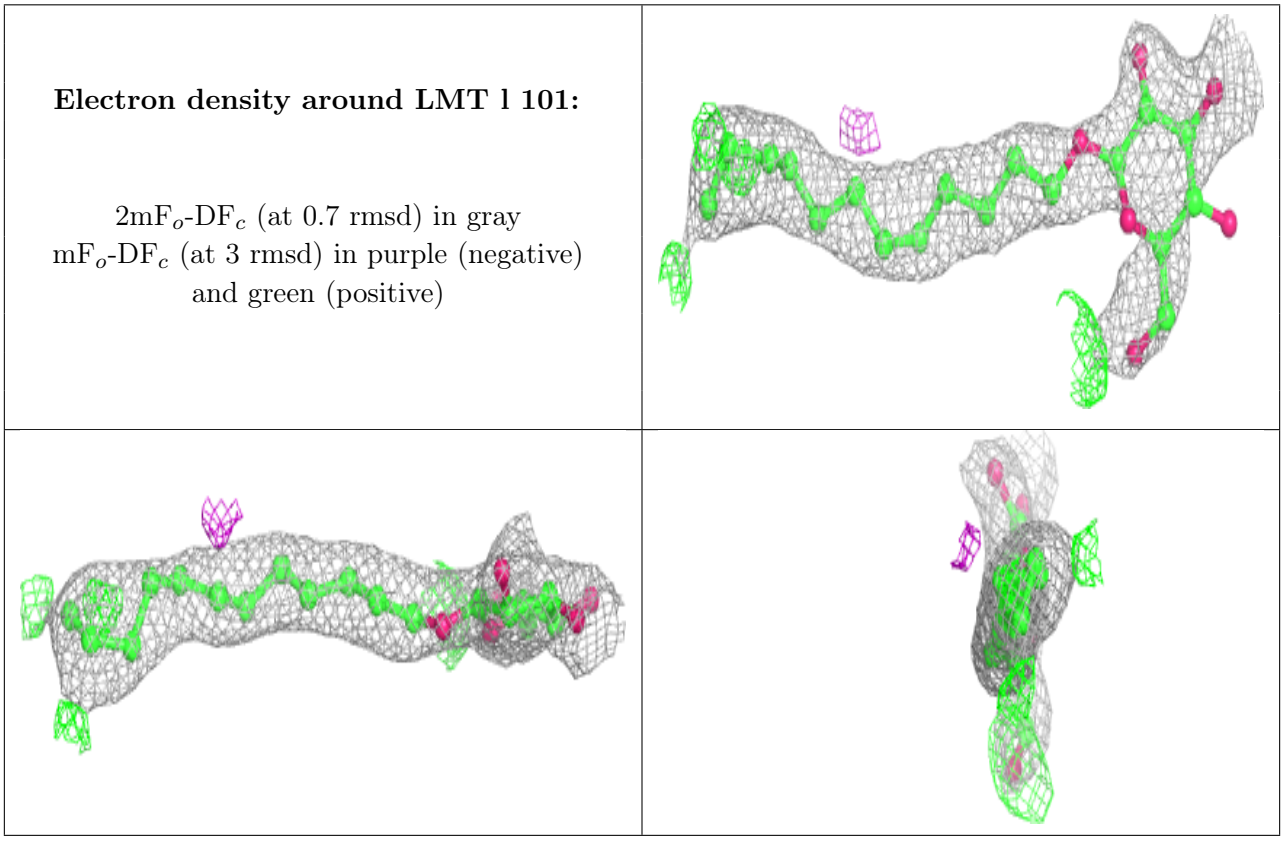
Electron density around LMT A 415:

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



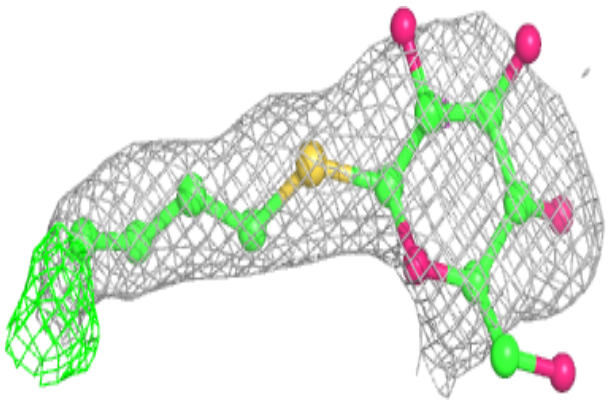
Electron density around LMT l 101:

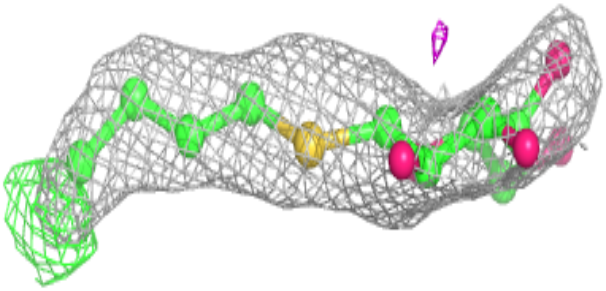
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

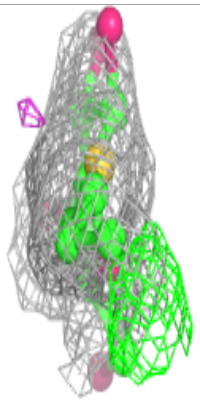


Electron density around HTG d 413:

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

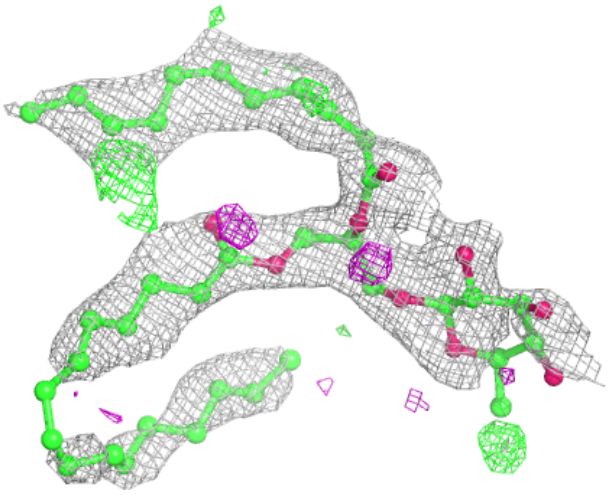


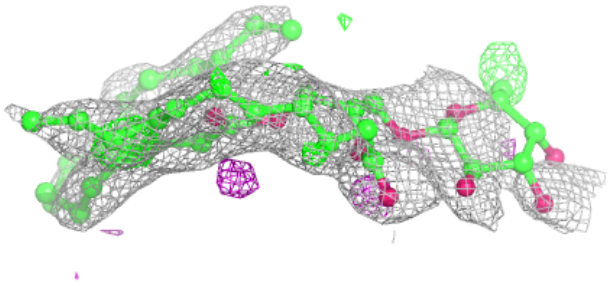


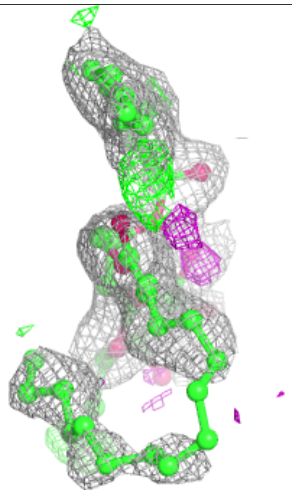


Electron density around DGD D 408:

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

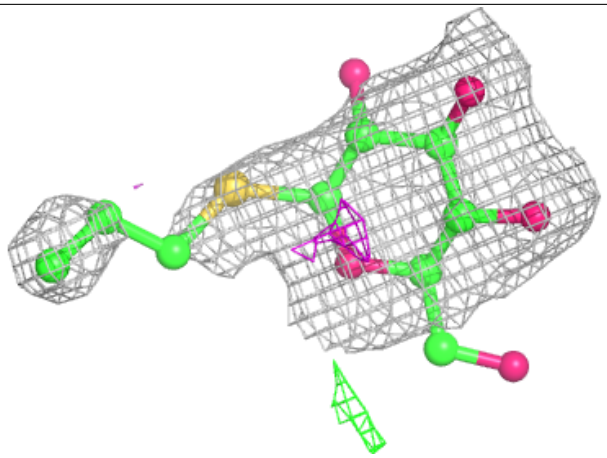


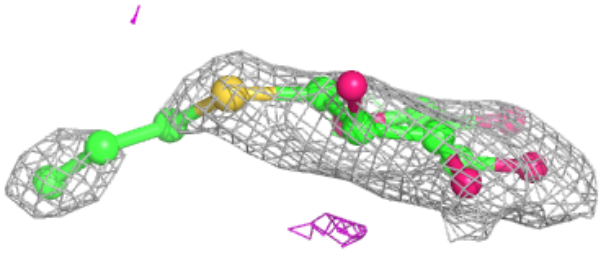


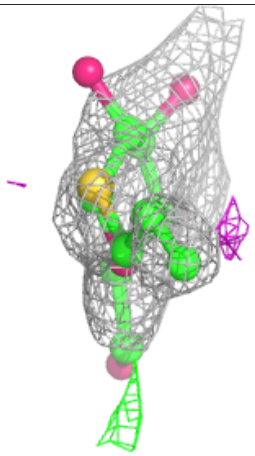


Electron density around HTG c 541:

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

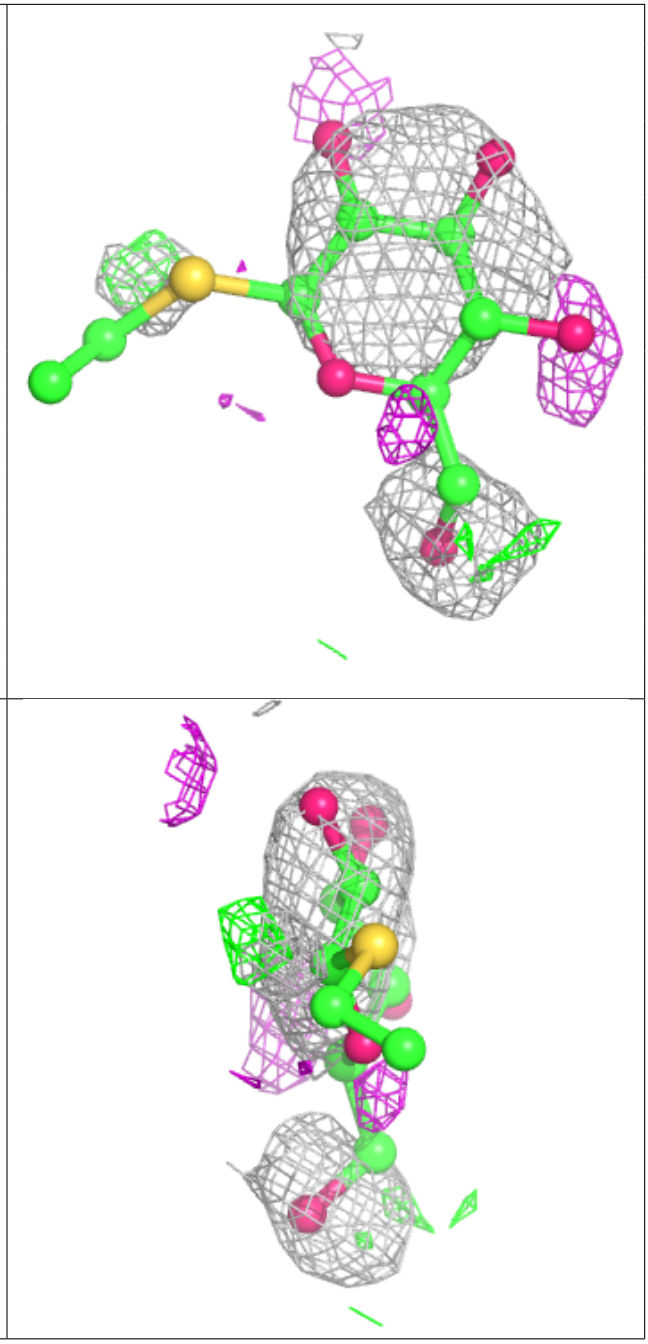






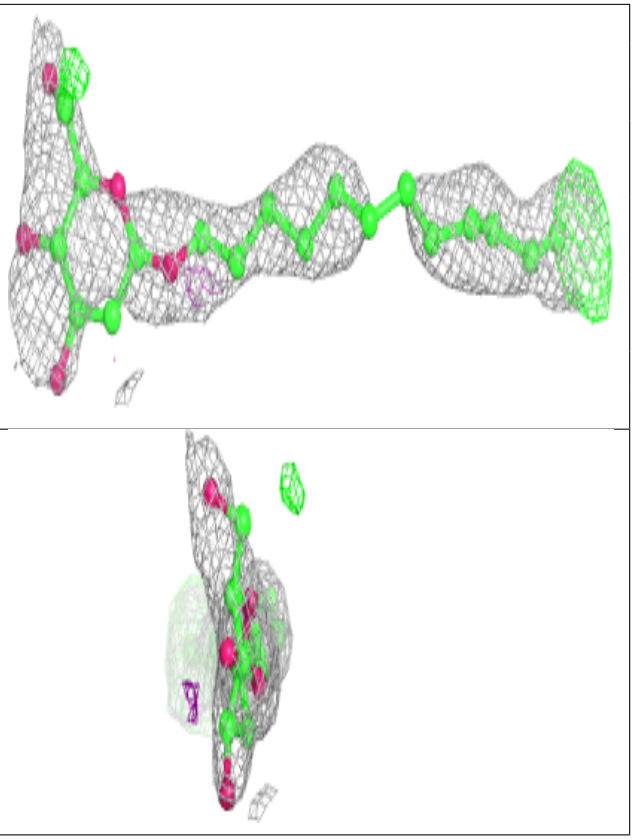
Electron density around HTG U 203:

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



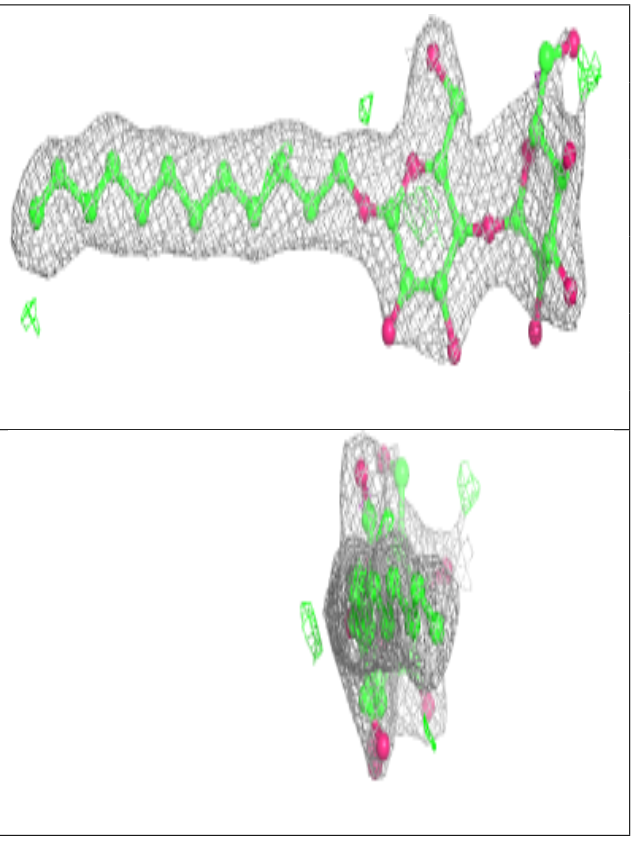
Electron density around LMT j 102:

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



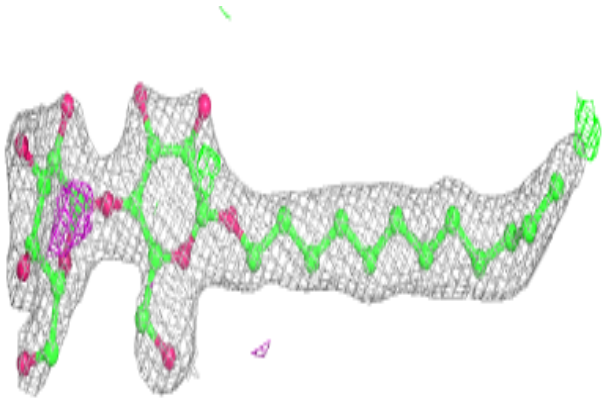
Electron density around LMT M 101:

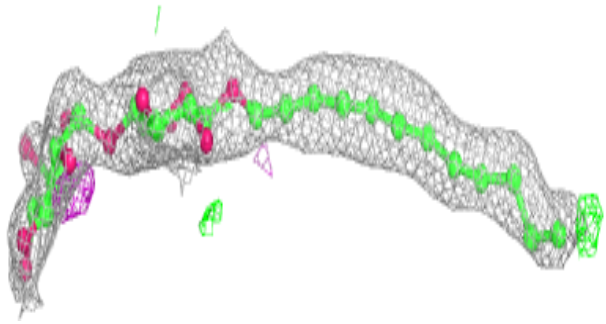
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

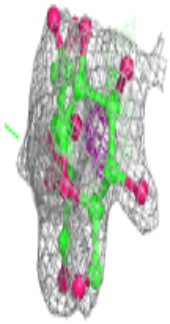


Electron density around LMT m 101:

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

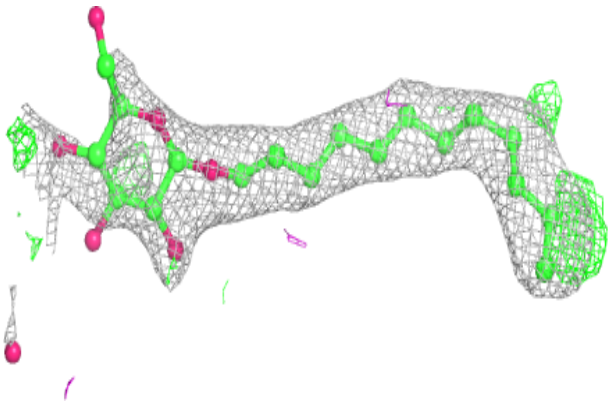


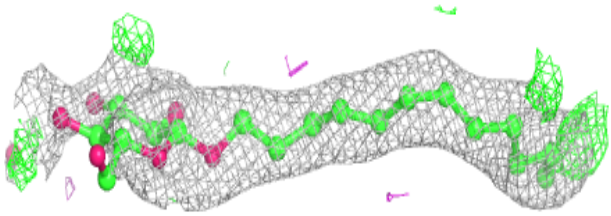


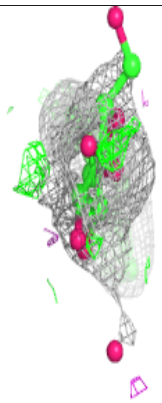


Electron density around LMT m 102:

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

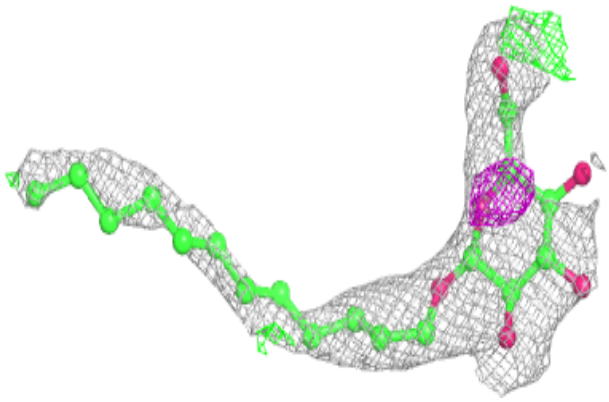


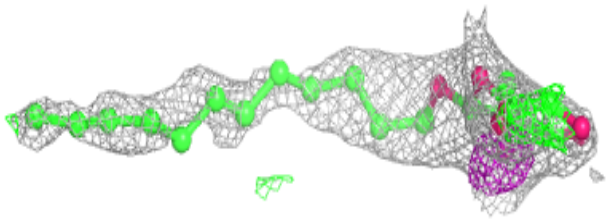


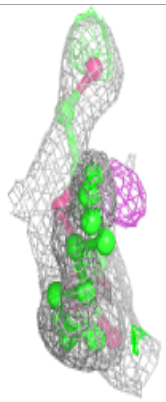


Electron density around LMT F 102:

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

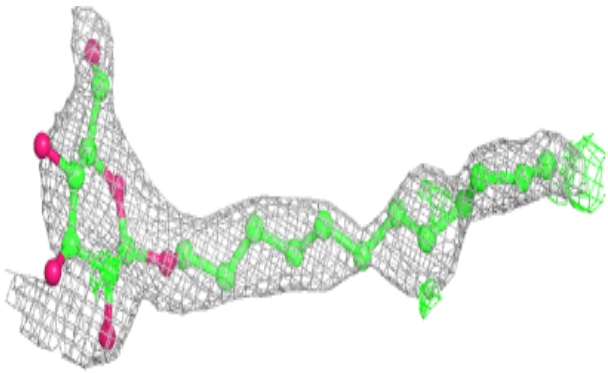


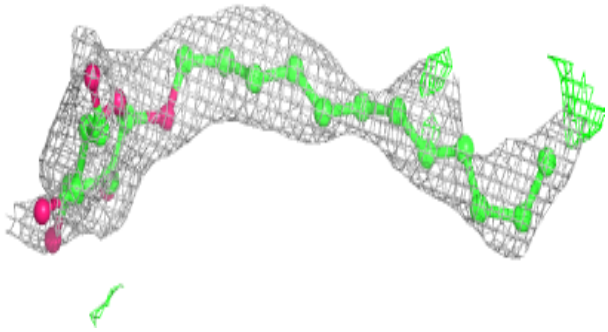


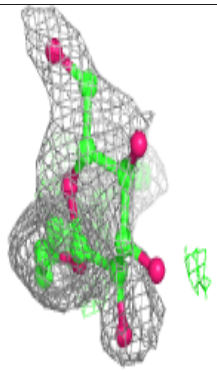


Electron density around LMT t 102:

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

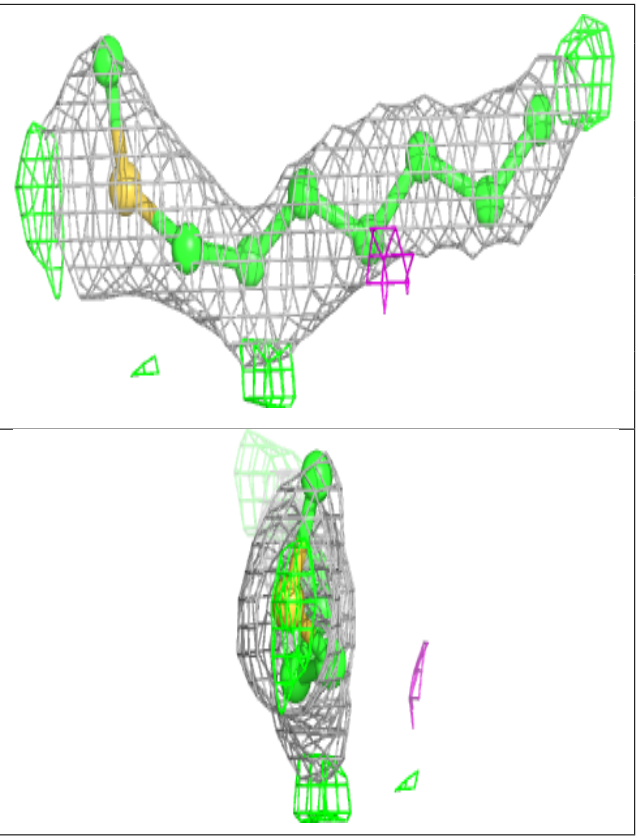






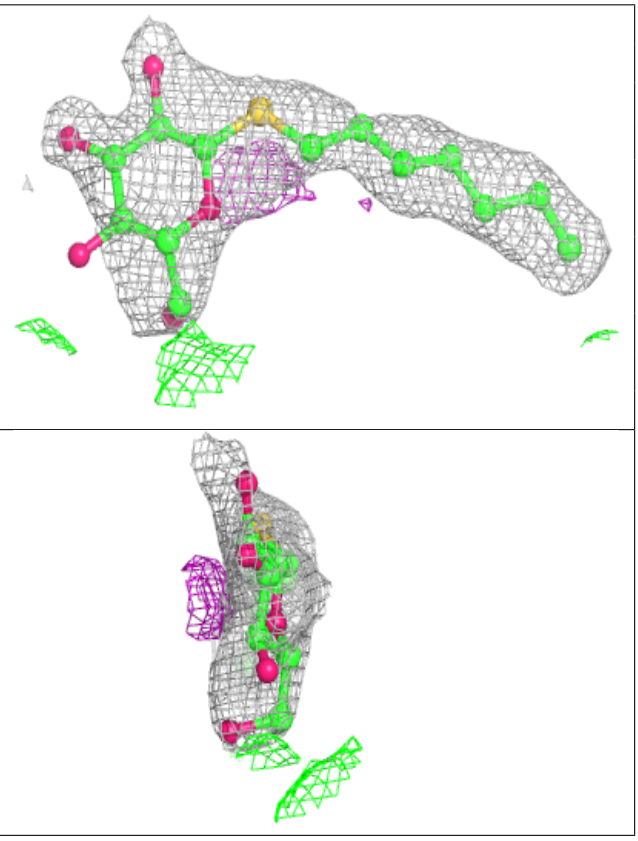
Electron density around HTG c 524:

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



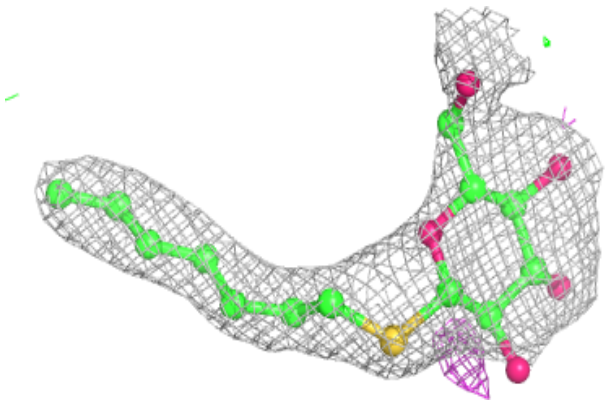
Electron density around HTG B 629:

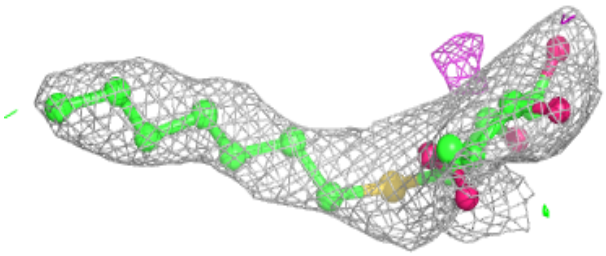
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

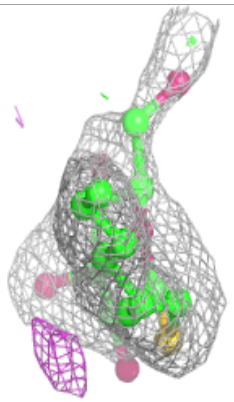


Electron density around HTG b 627:

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

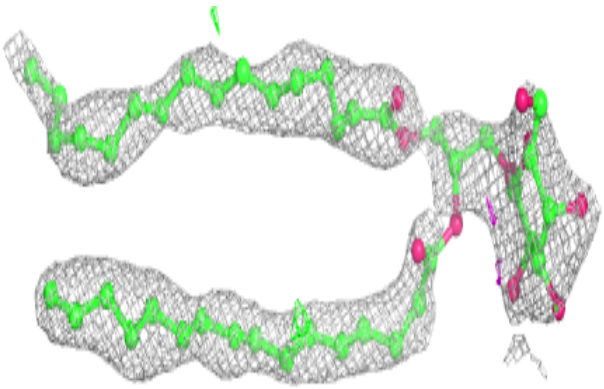


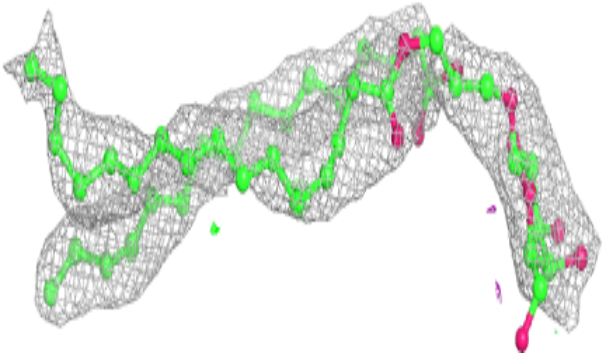


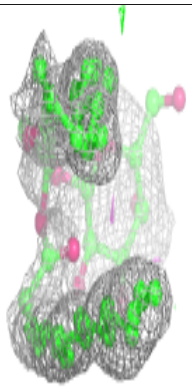


Electron density around LMG c 521:

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

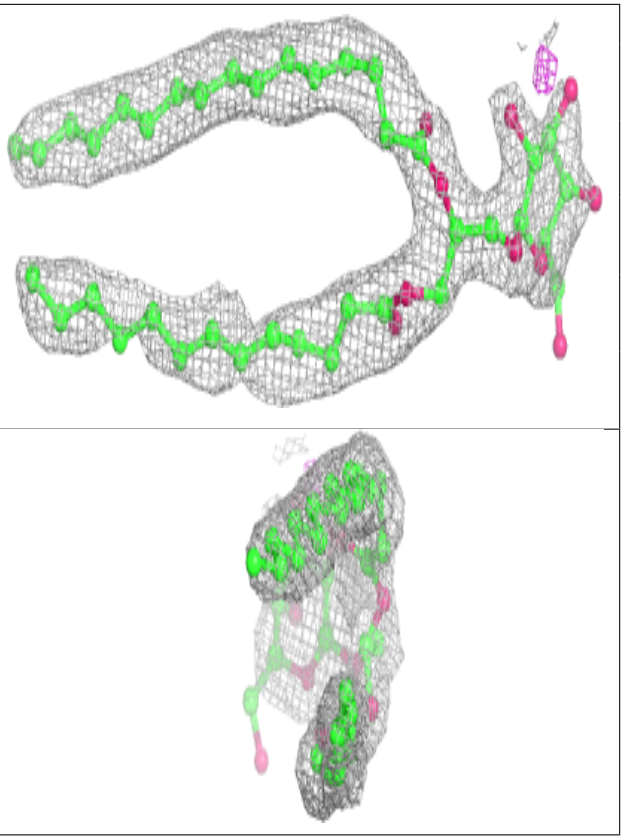






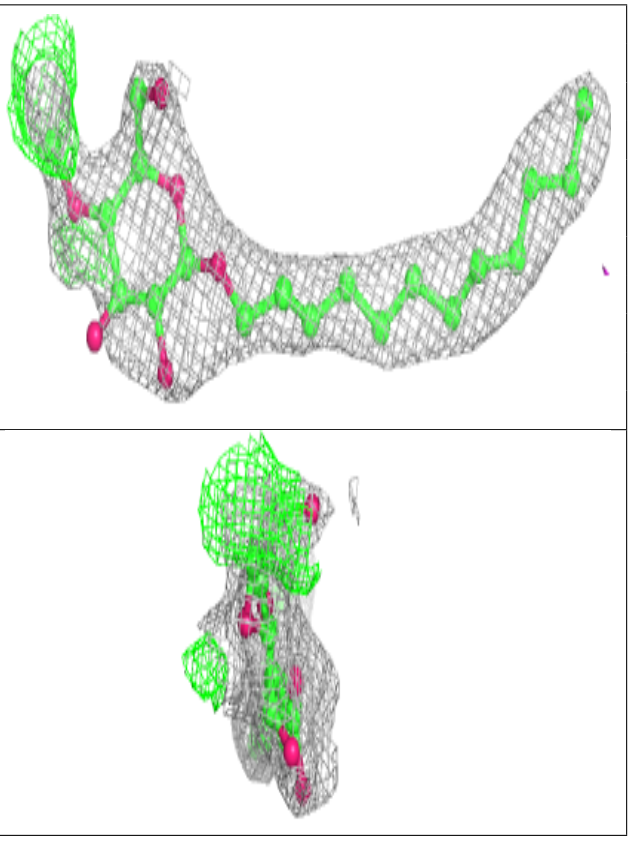
Electron density around LMG C 519:

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



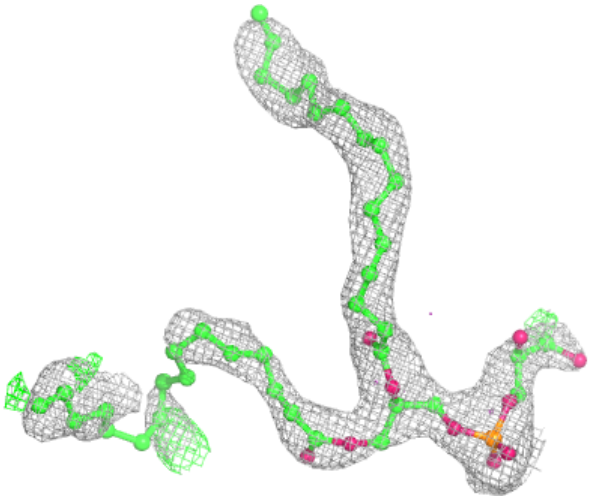
Electron density around LMT b 626:

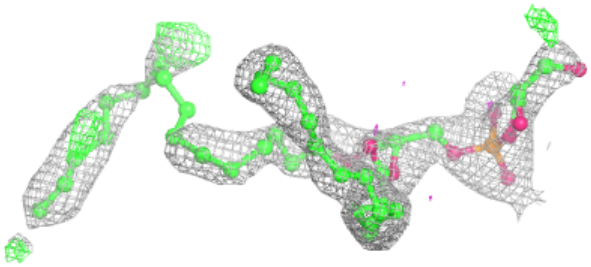
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

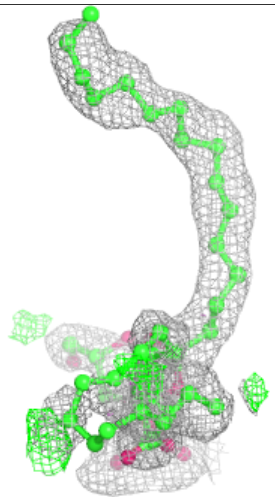


Electron density around LHG E 101:

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

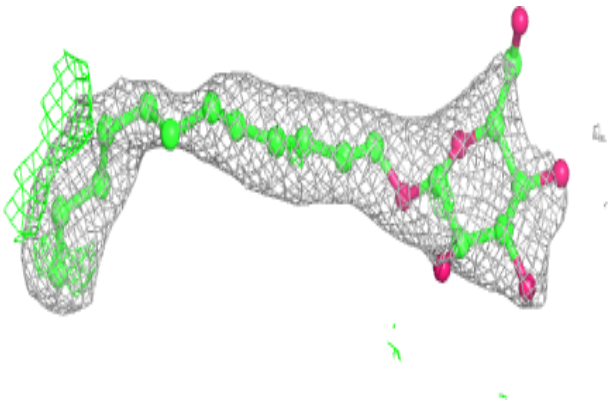


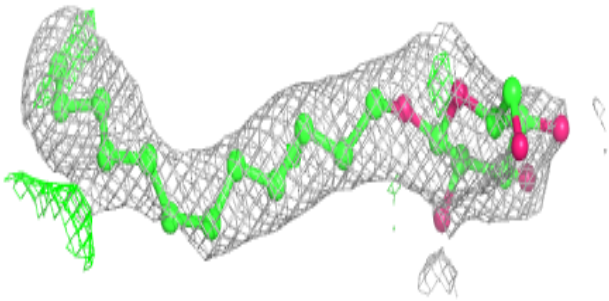


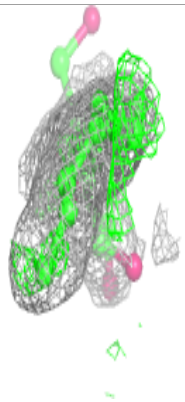


Electron density around LMT T 102:

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

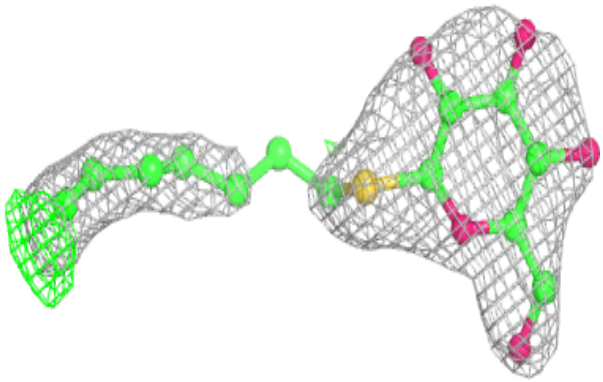


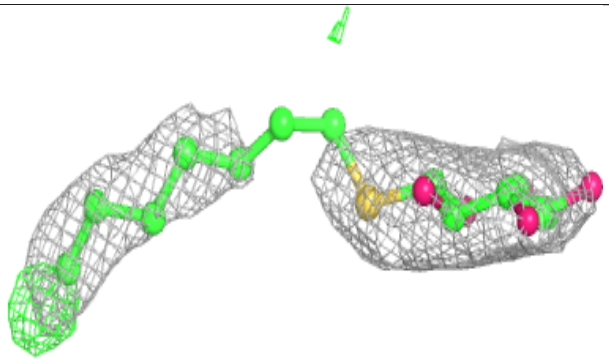


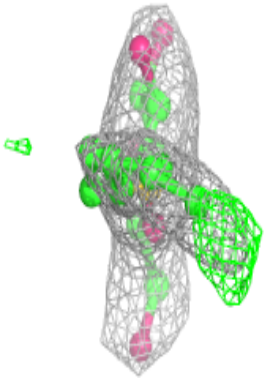


Electron density around HTG c 523:

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

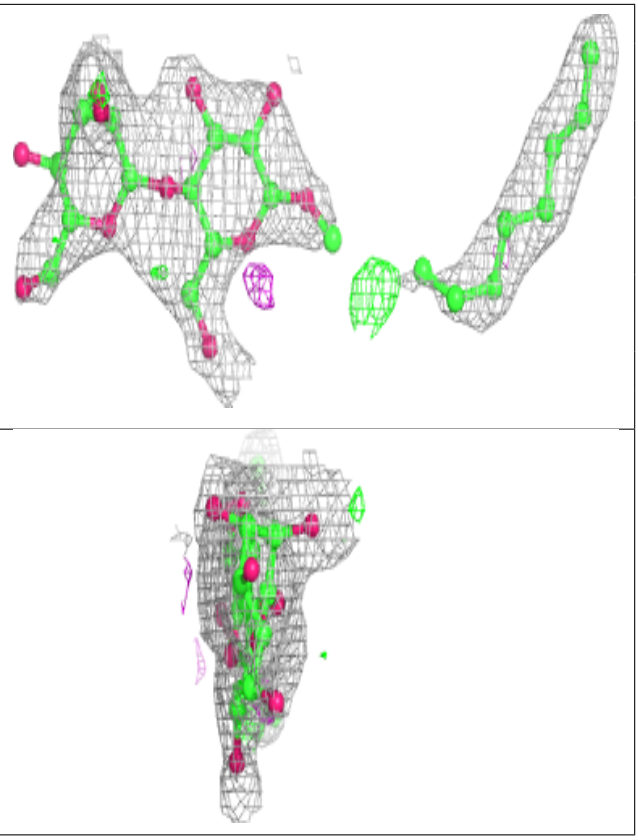






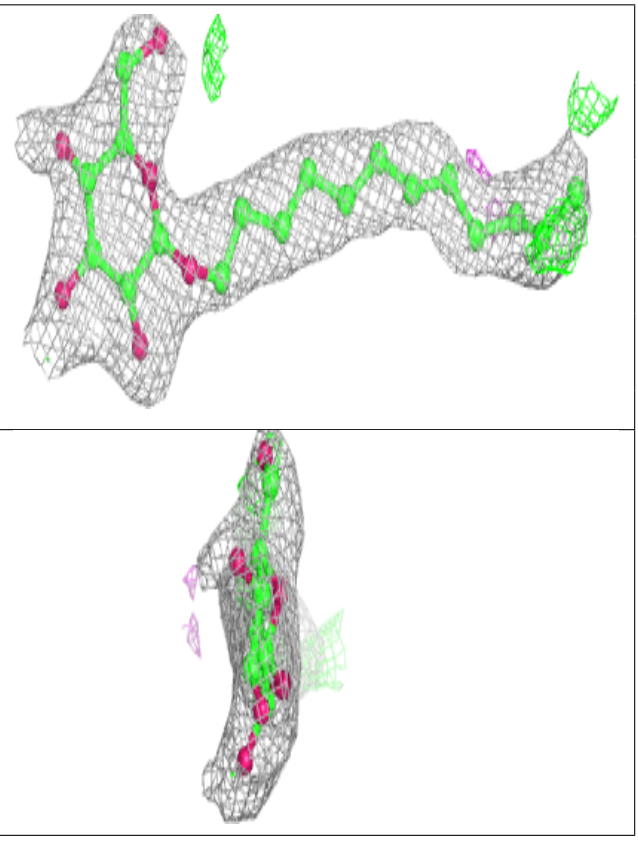
Electron density around LMT z 101:

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



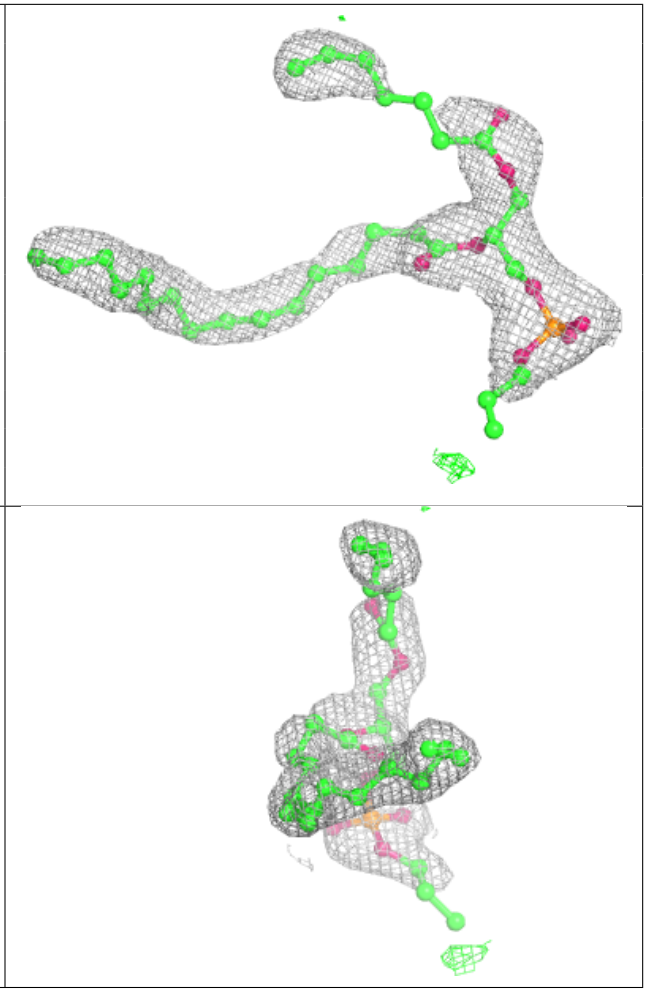
Electron density around LMT M 102:

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



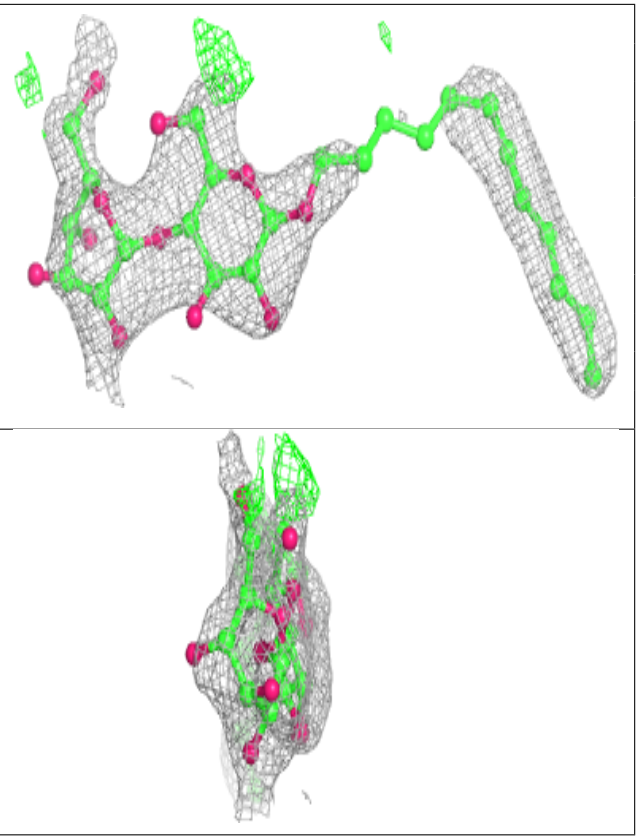
Electron density around LHG e 101:

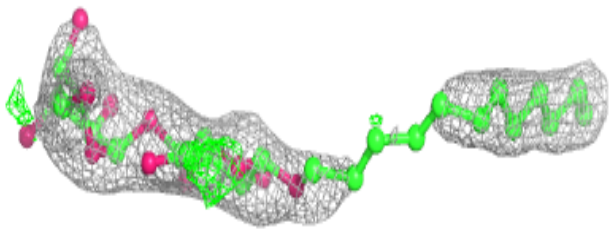
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMT Z 101:

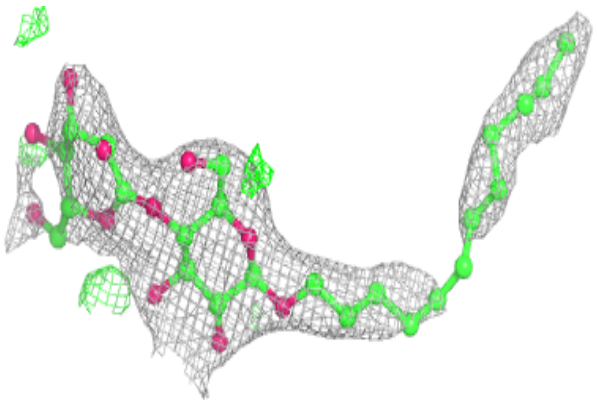
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

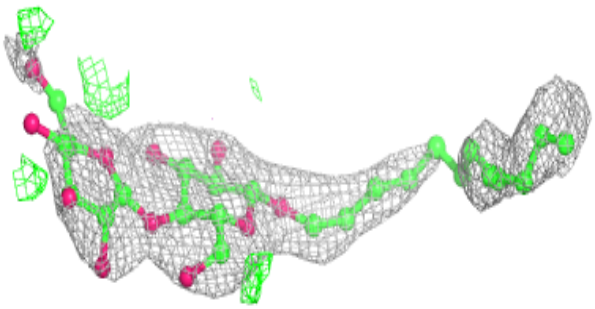


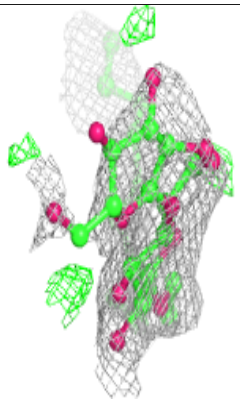


Electron density around LMT C 520:

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

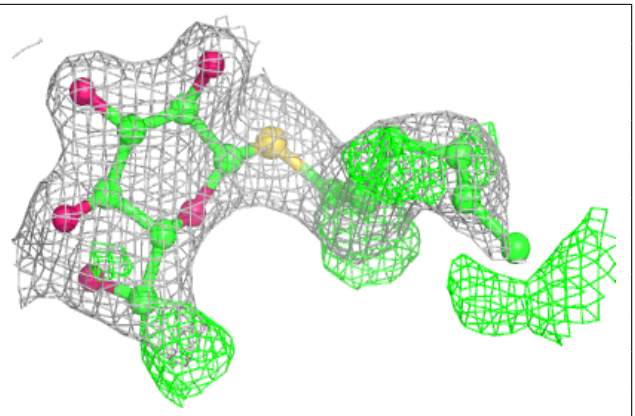


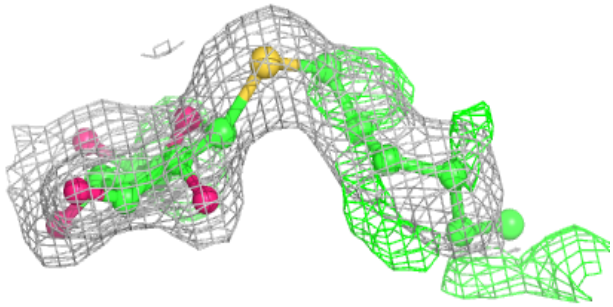


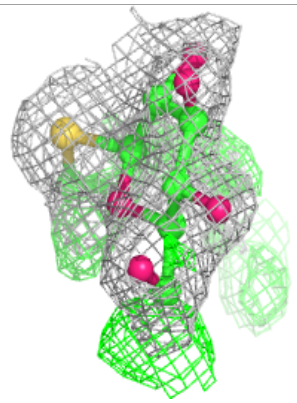


Electron density around HTG B 642:

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

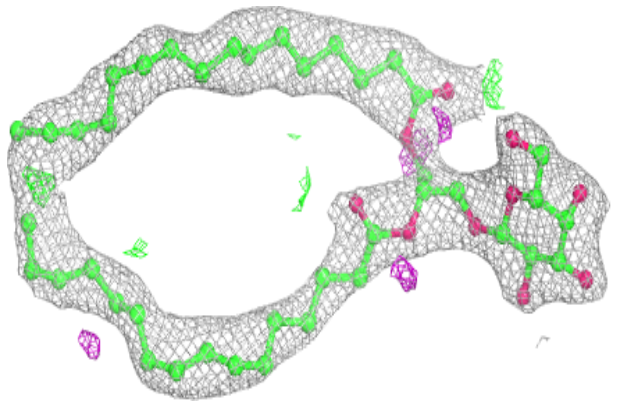


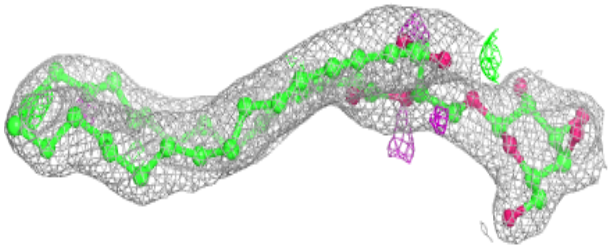


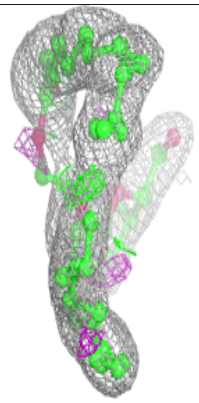


Electron density around LMG a 412:

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

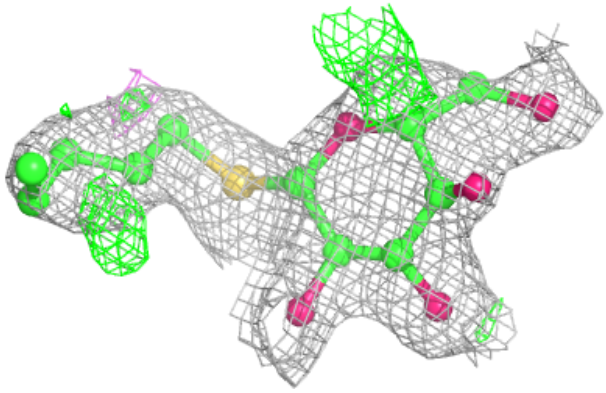


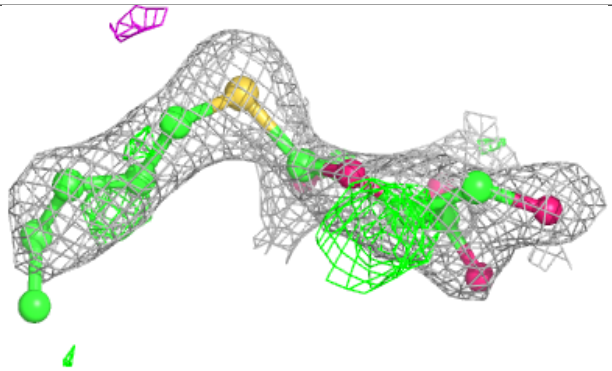


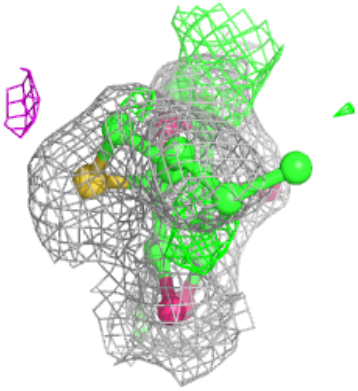


Electron density around HTG b 640:

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

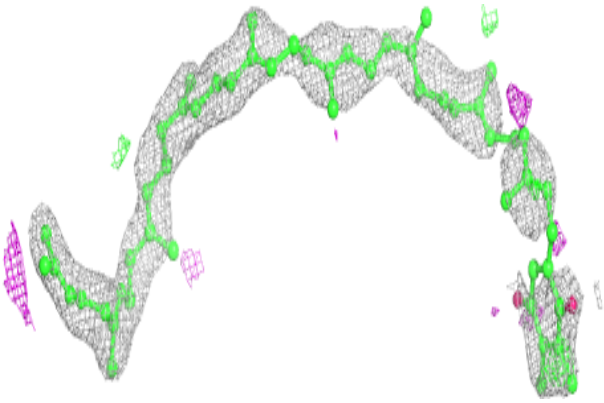


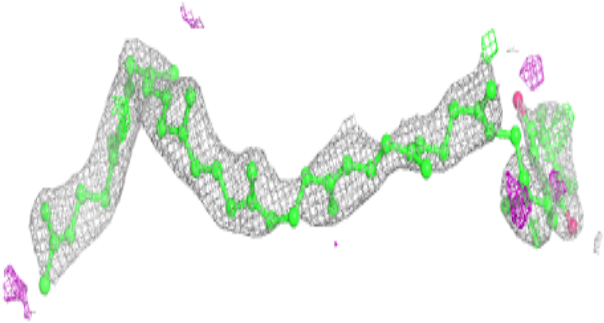


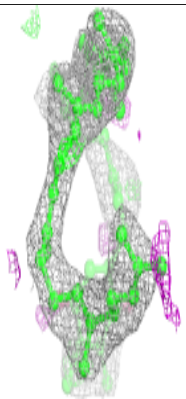


Electron density around PL9 A 410:

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

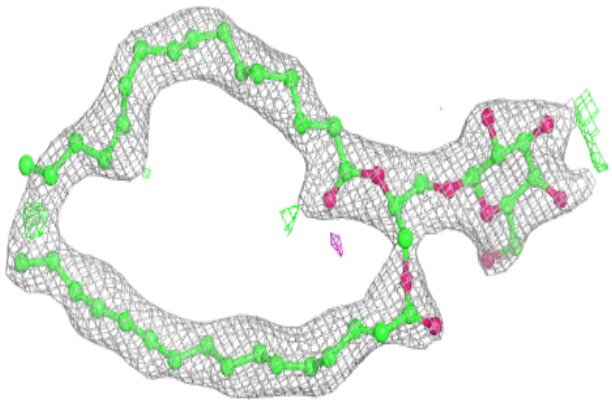


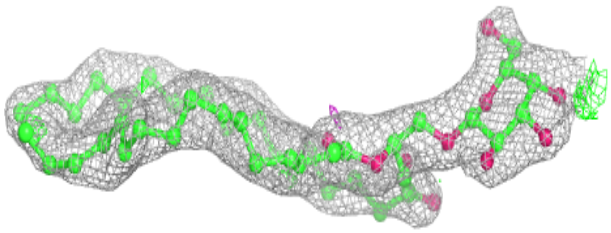


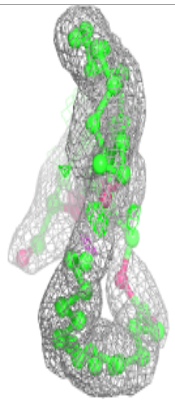


Electron density around LMG A 411:

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

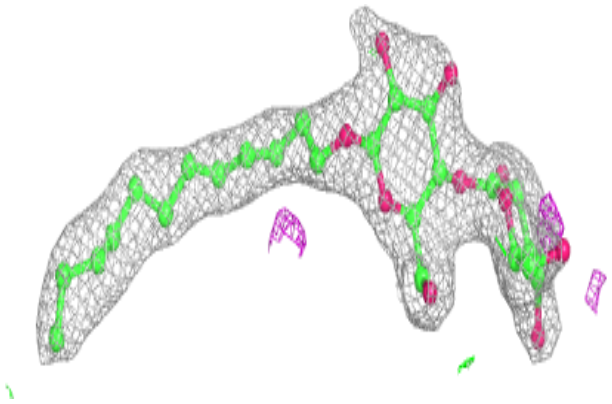


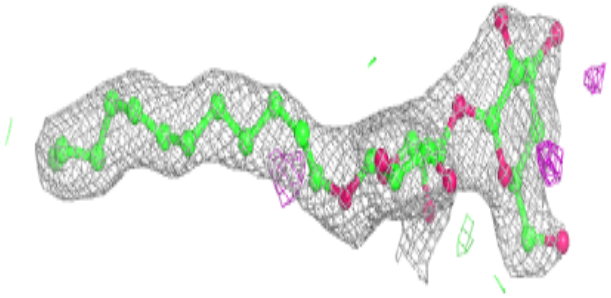


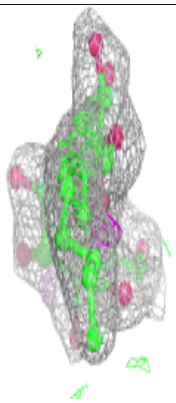


Electron density around LMT B 623:

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

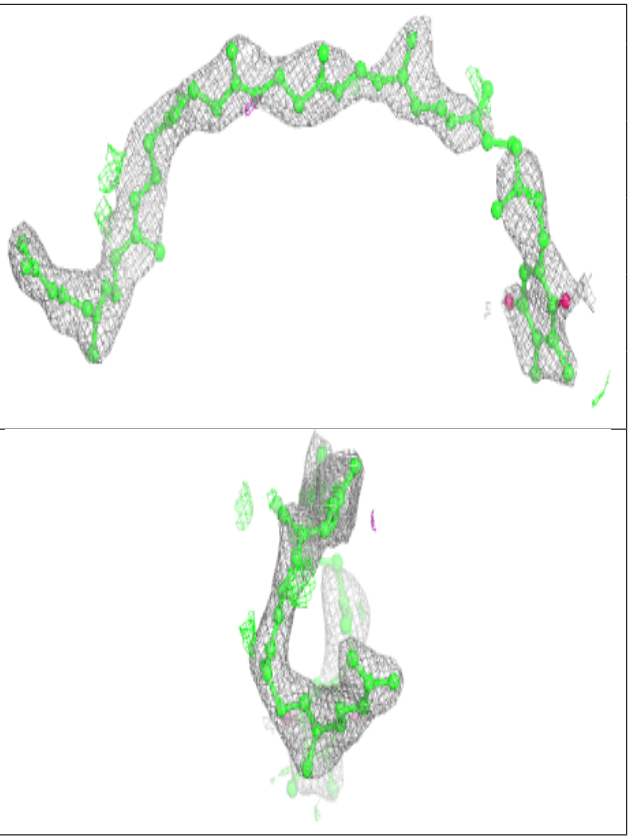






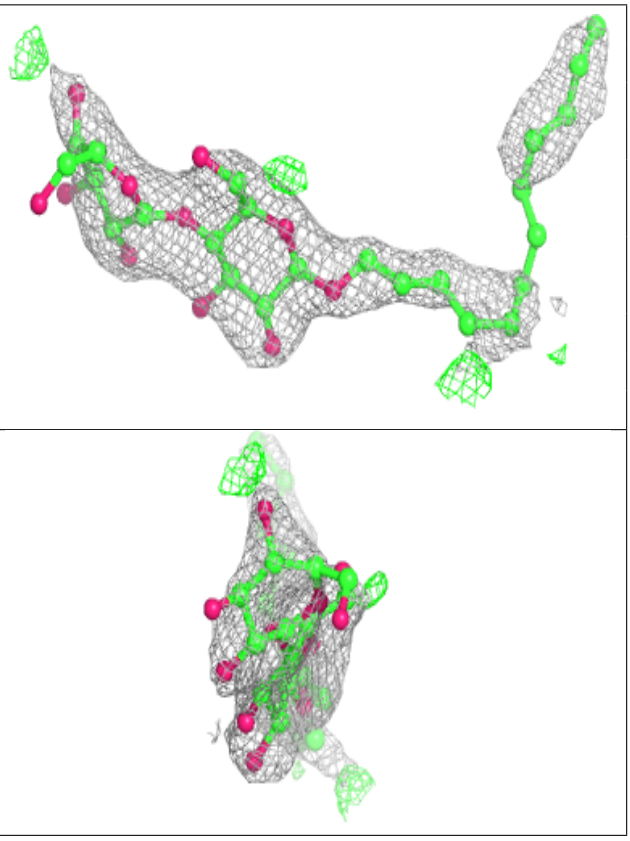
Electron density around PL9 a 411:

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



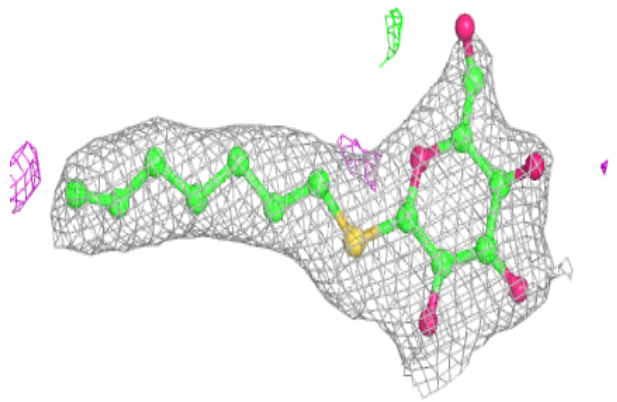
Electron density around LMT c 522:

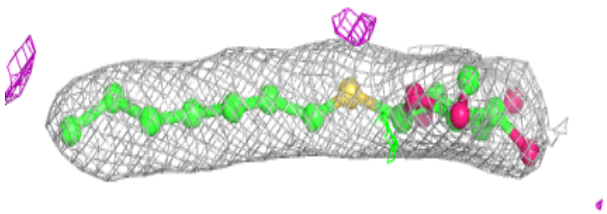
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

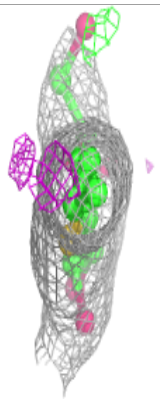


Electron density around HTG b 601:

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

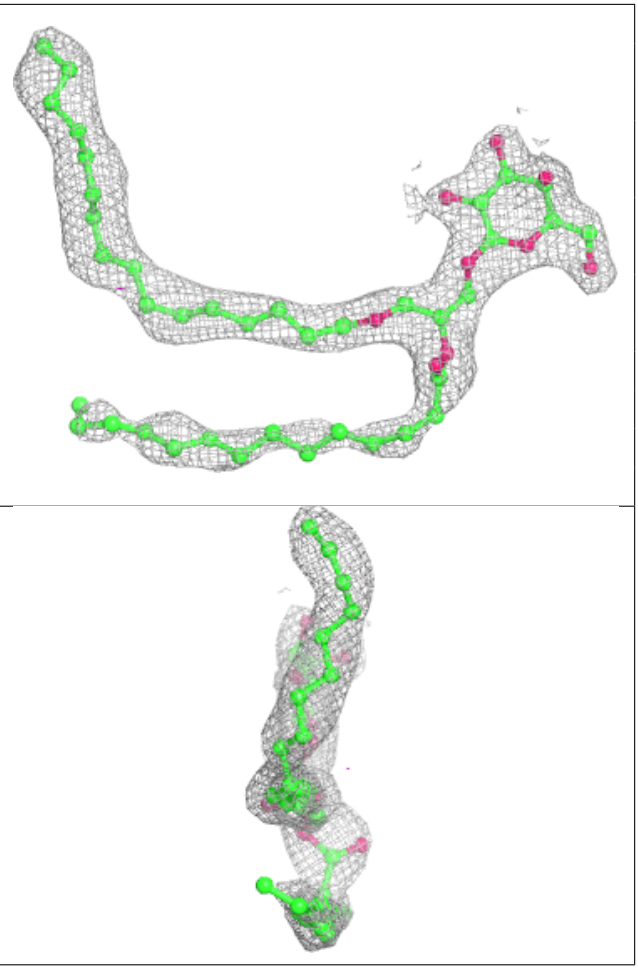


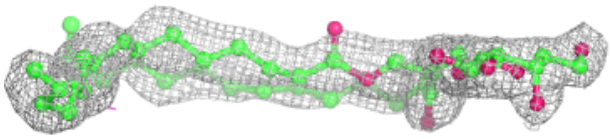




Electron density around LMG C 518:

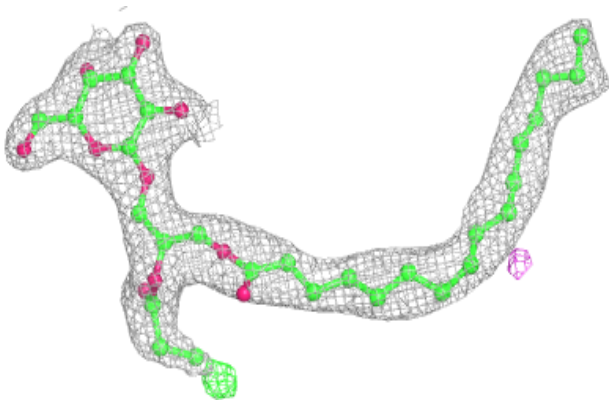
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

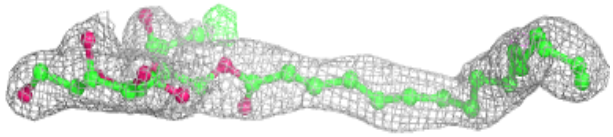


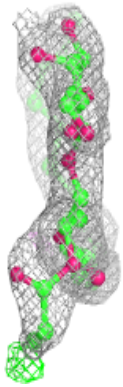


Electron density around LMG c 520:

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

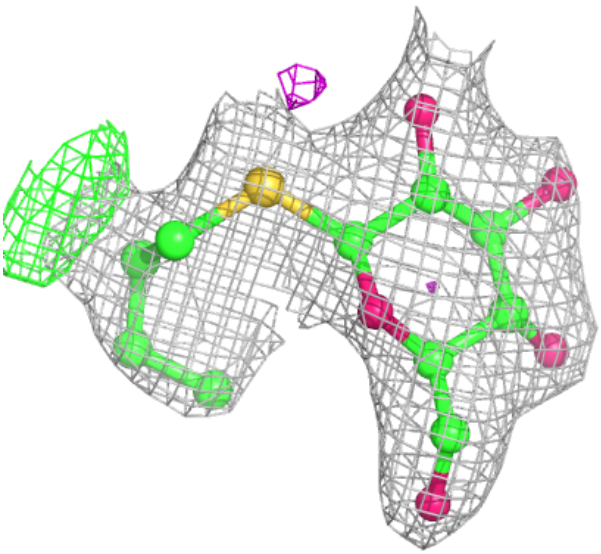


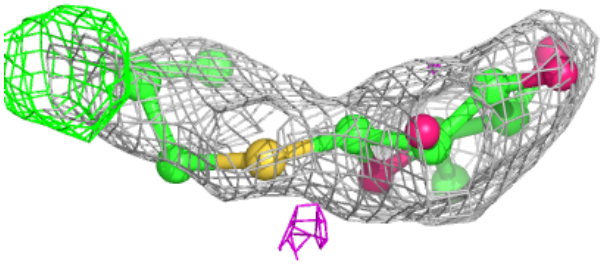


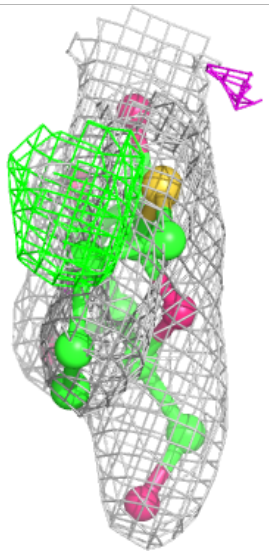


Electron density around HTG v 208:

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

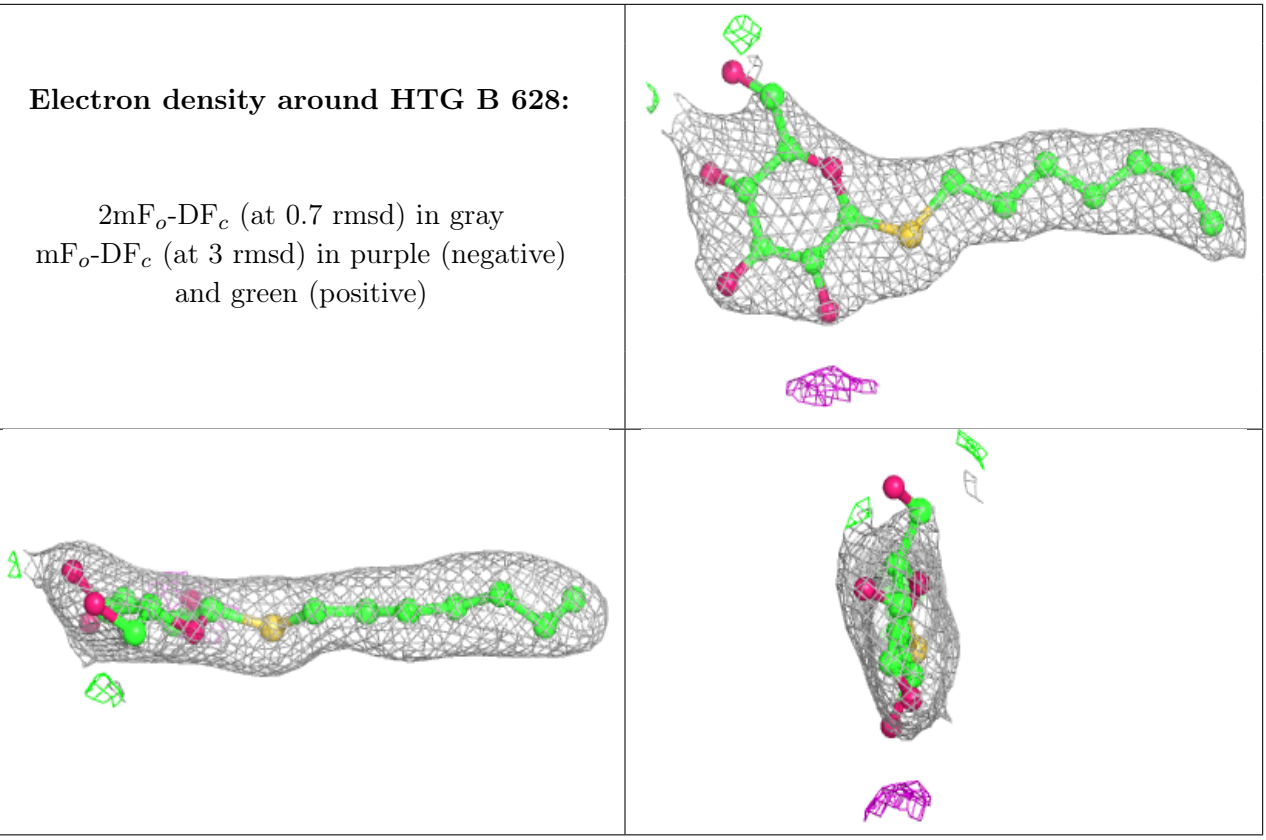






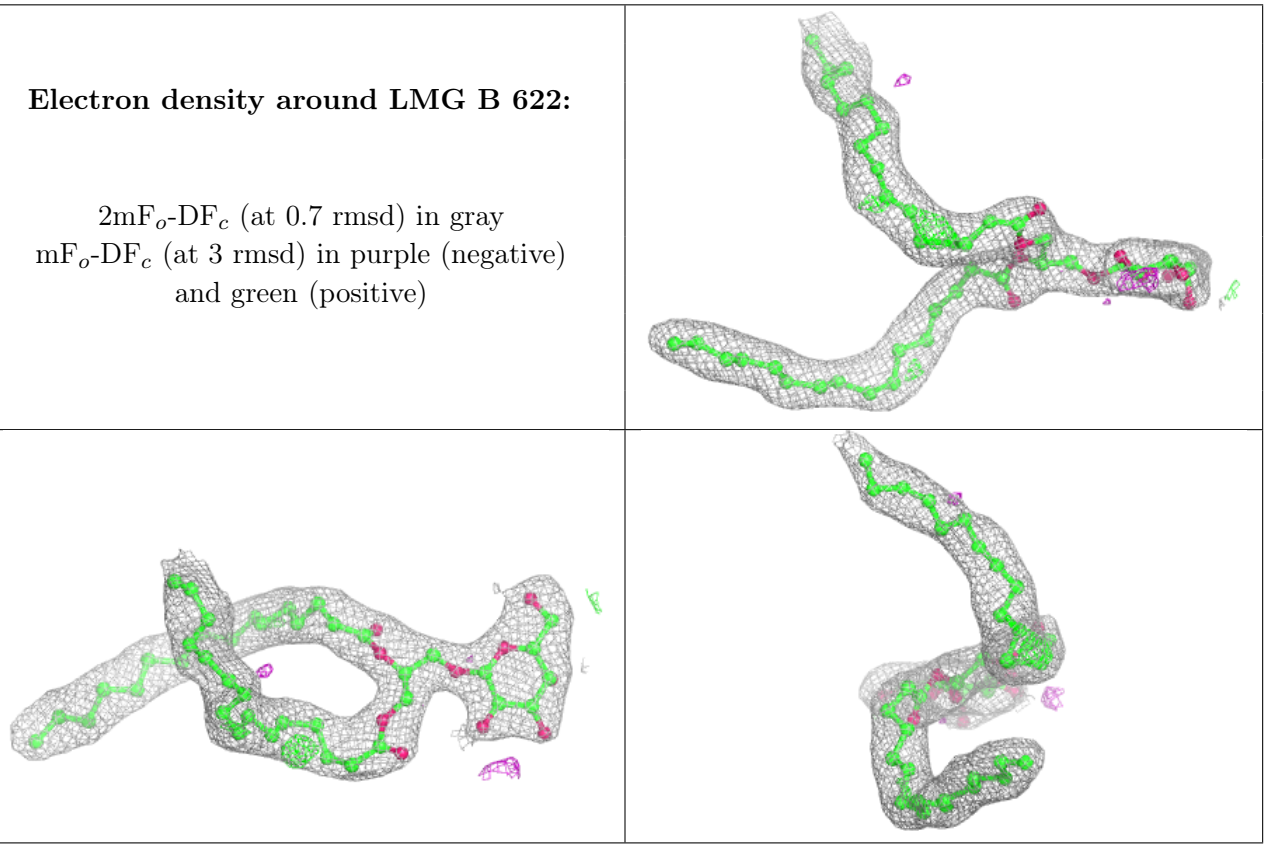
Electron density around HTG B 628:

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



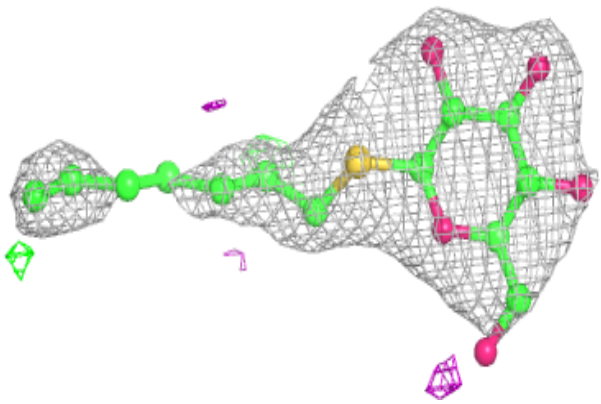
Electron density around LMG B 622:

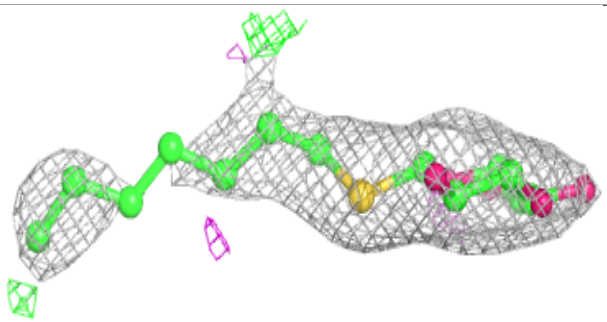
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

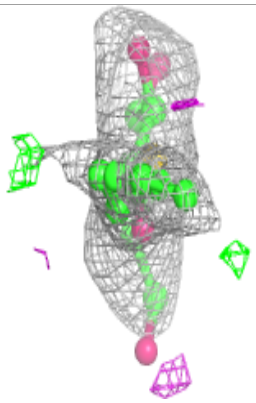


Electron density around HTG C 521:

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

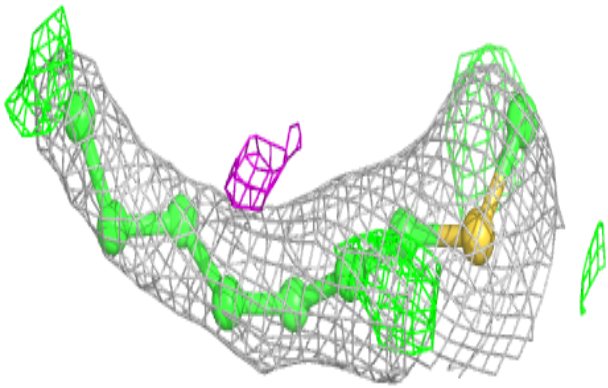


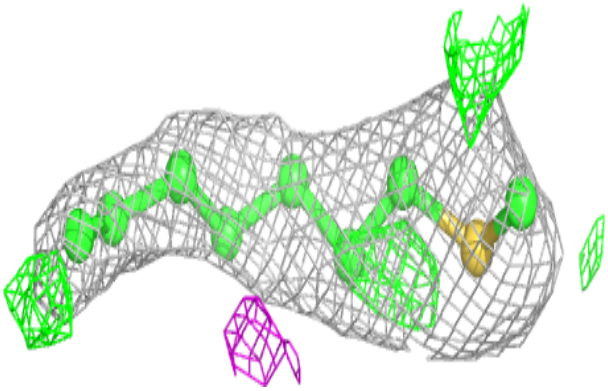


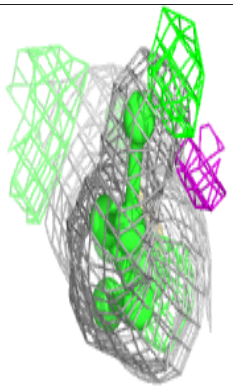


Electron density around HTG C 535:

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

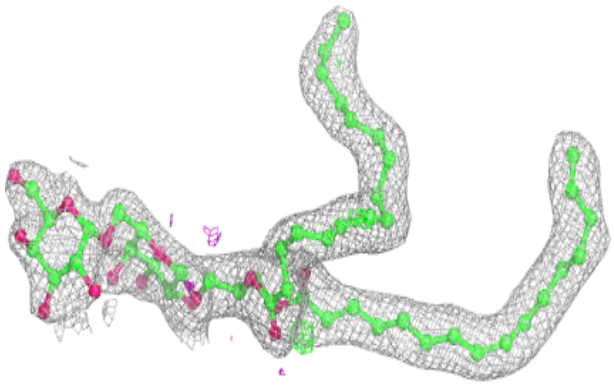


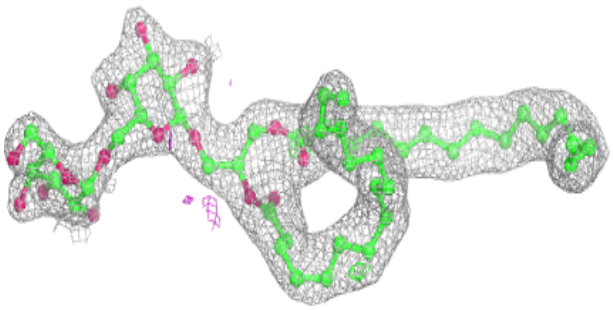


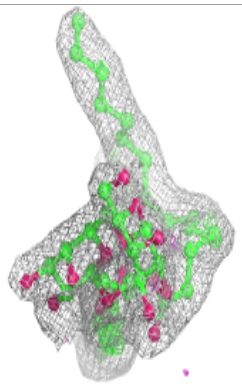


Electron density around DGD h 101:

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

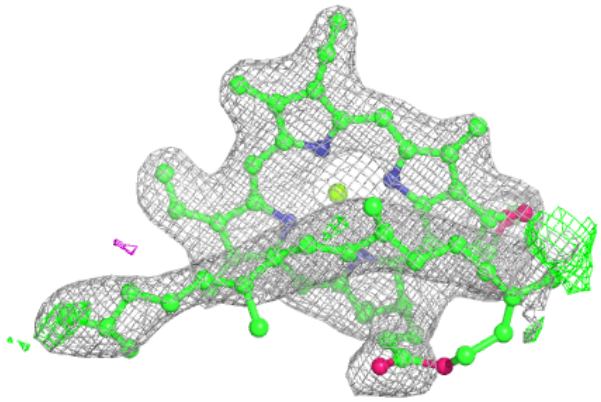


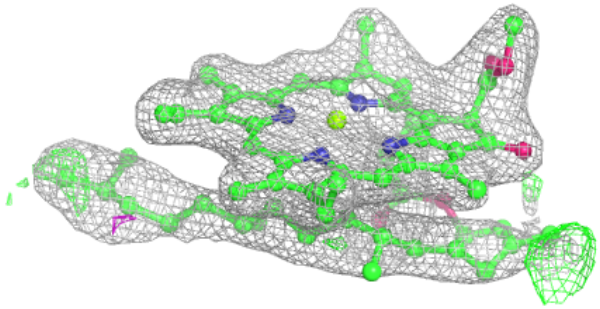


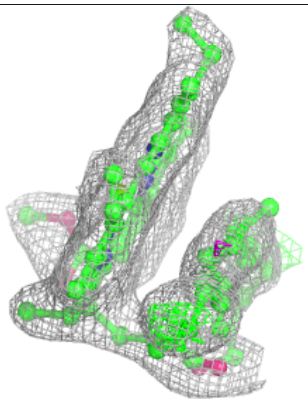


Electron density around CLA B 602:

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

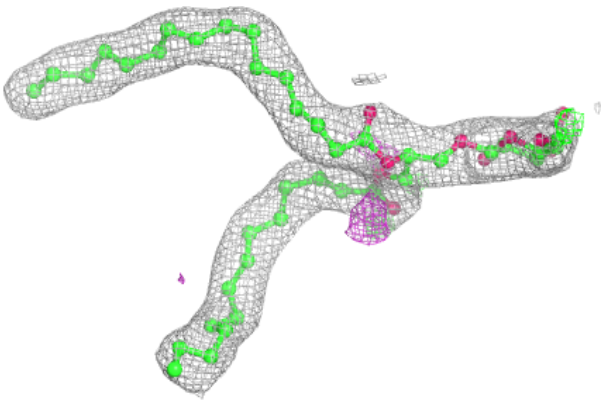


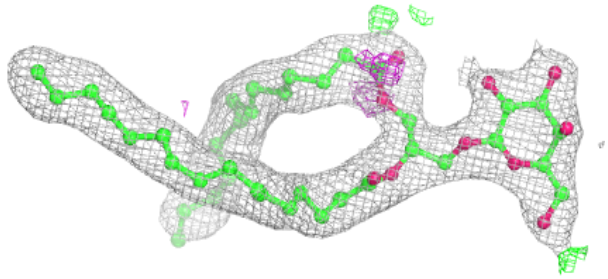


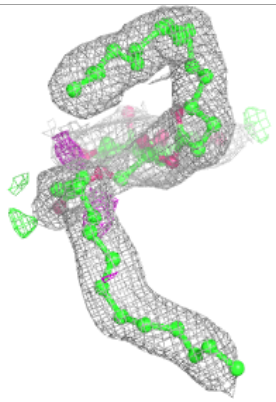


Electron density around LMG b 625:

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

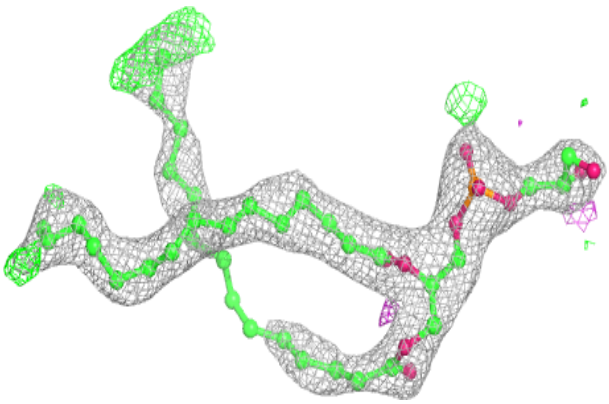


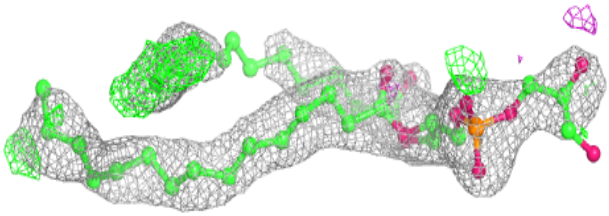


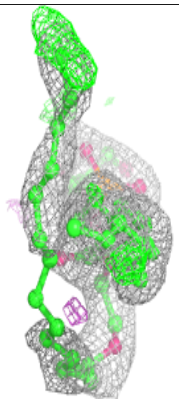


Electron density around LHG f 102:

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

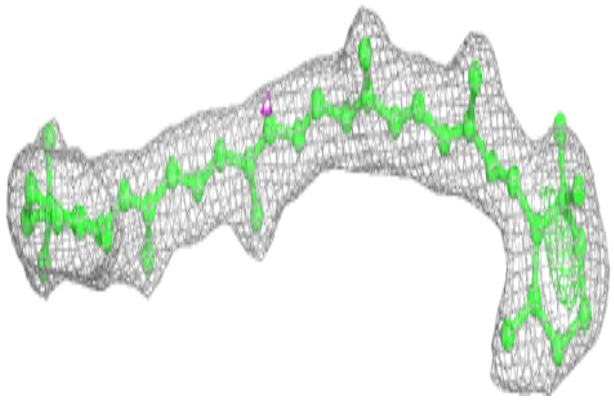


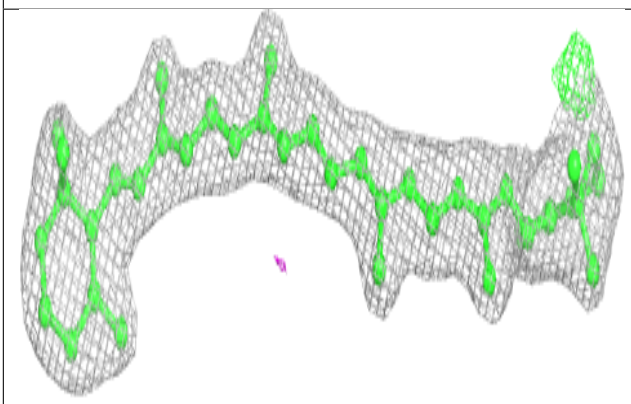


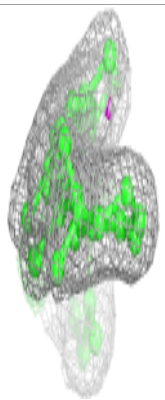


Electron density around BCR d 406:

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

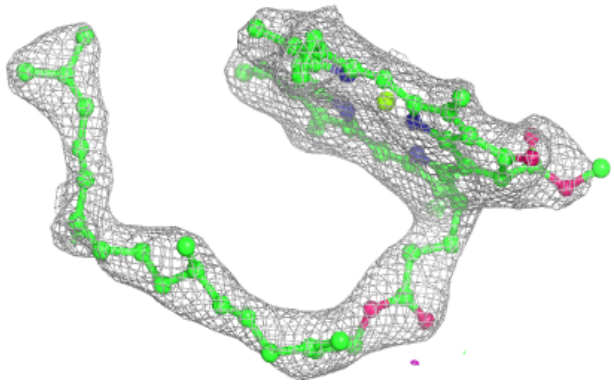


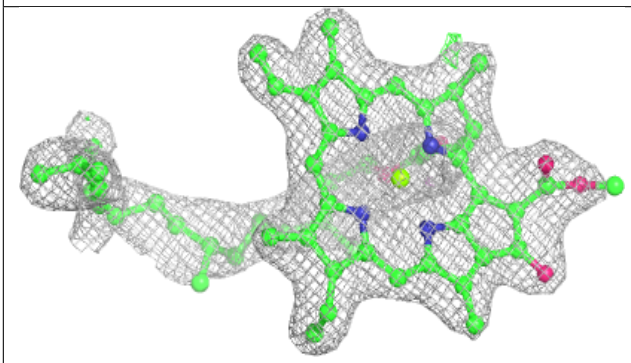


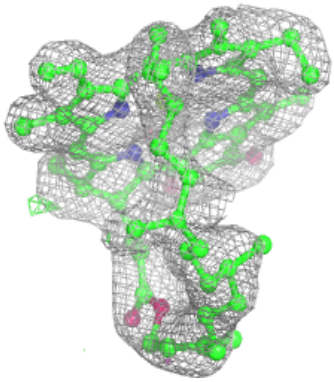


Electron density around CLA C 513:

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

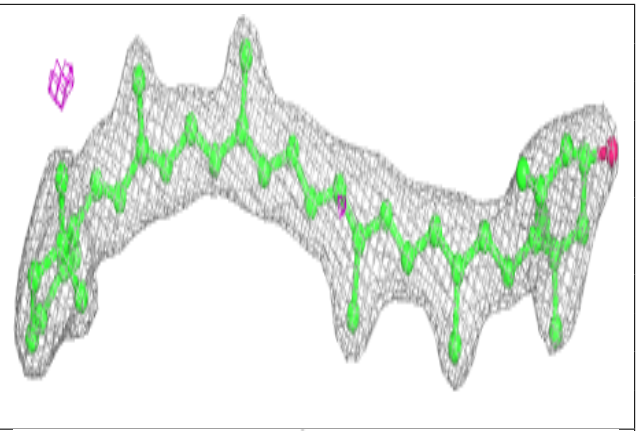


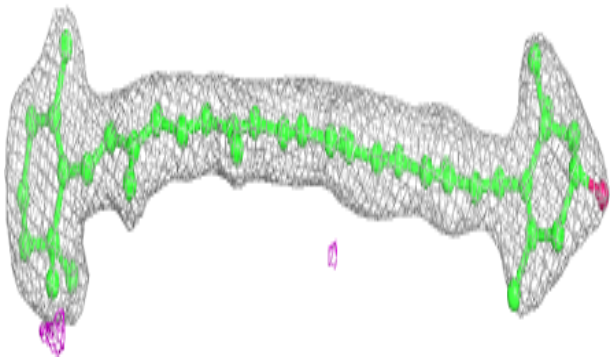




Electron density around RRX h 102:

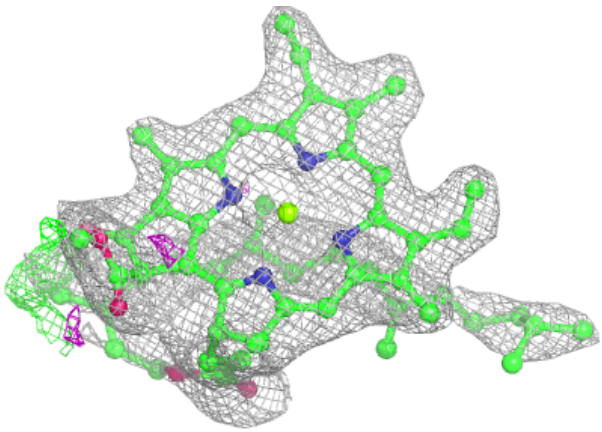
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

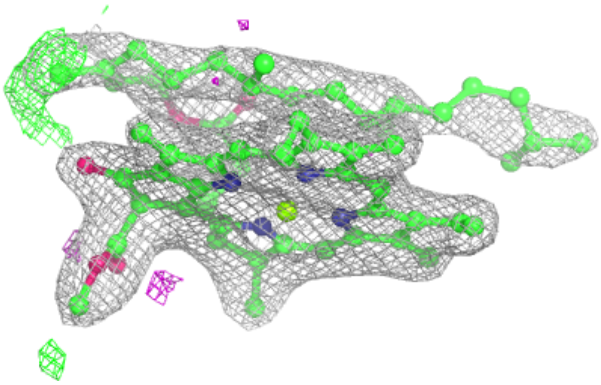


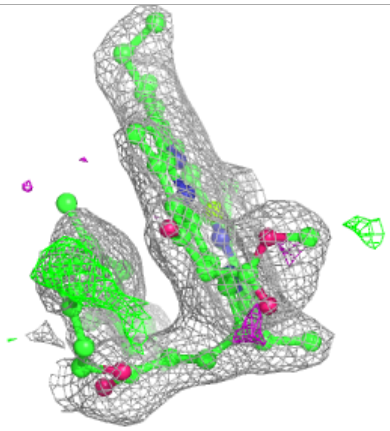


Electron density around CLA b 605:

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

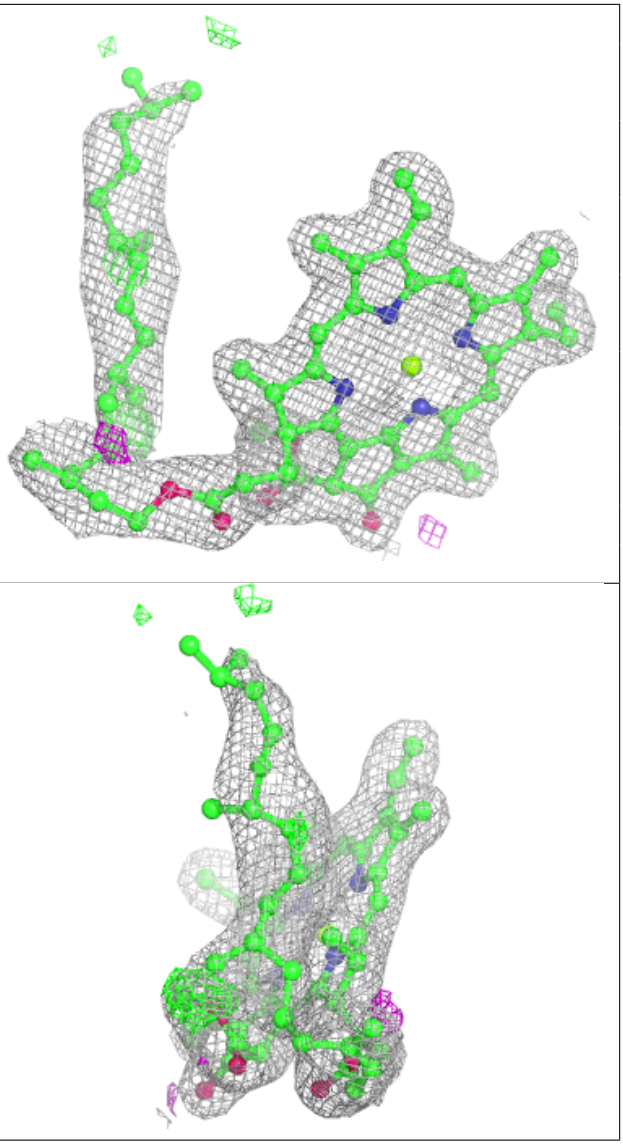






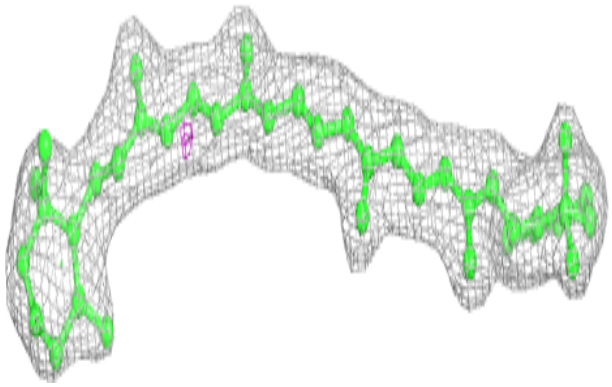
Electron density around CLA b 620:

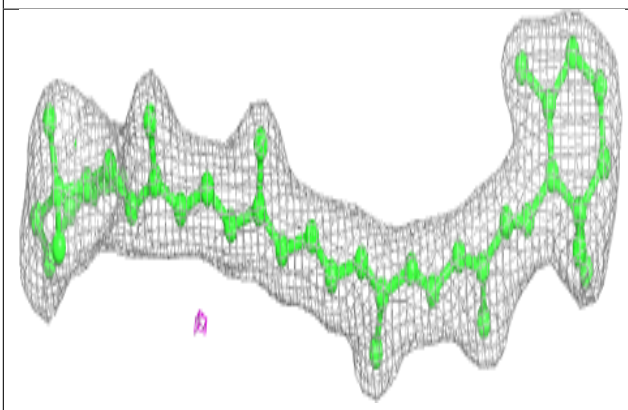
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

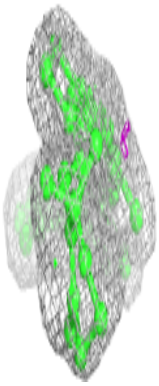


Electron density around BCR D 406:

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

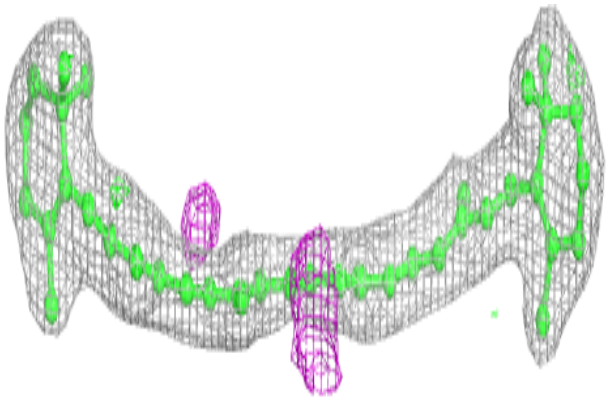


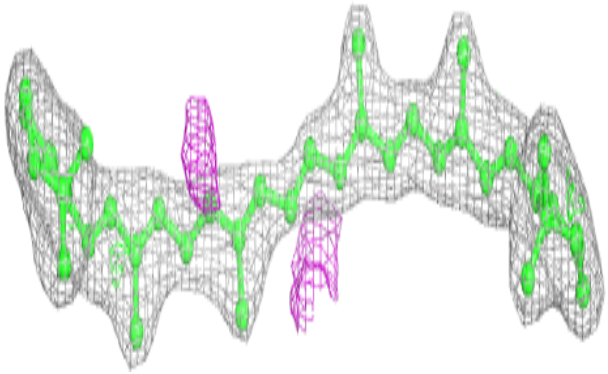


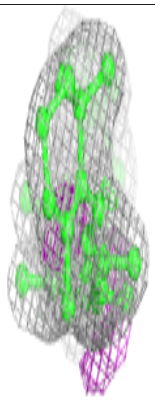


Electron density around BCR K 101:

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

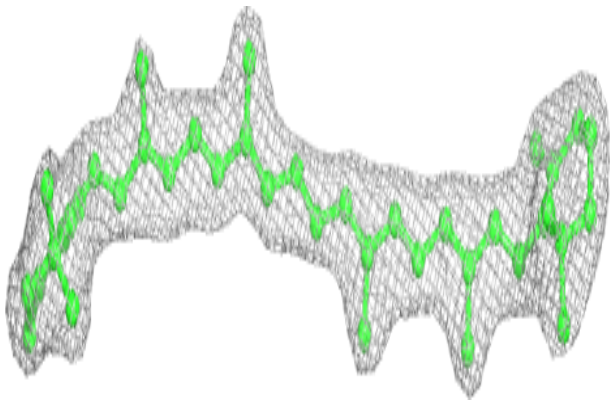


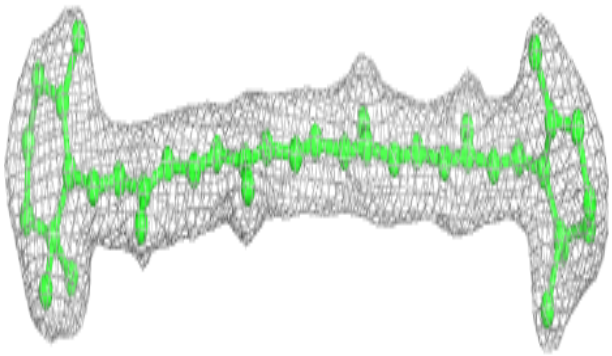


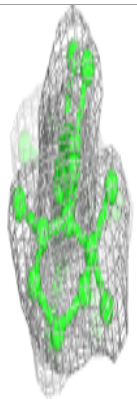


Electron density around BCR K 102:

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

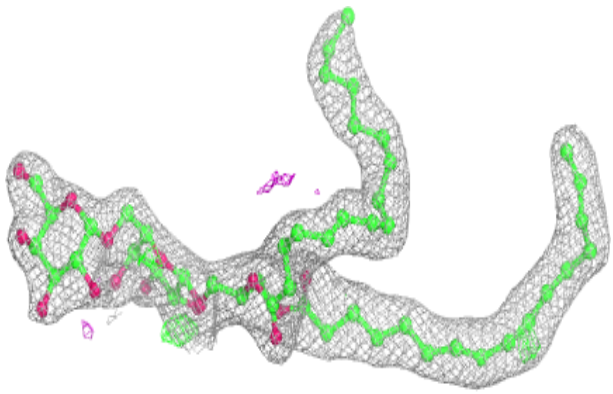


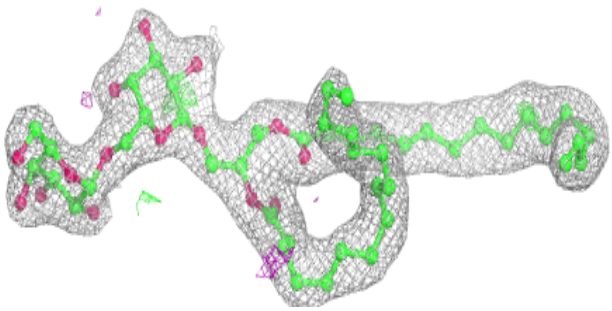




Electron density around DGD H 101:

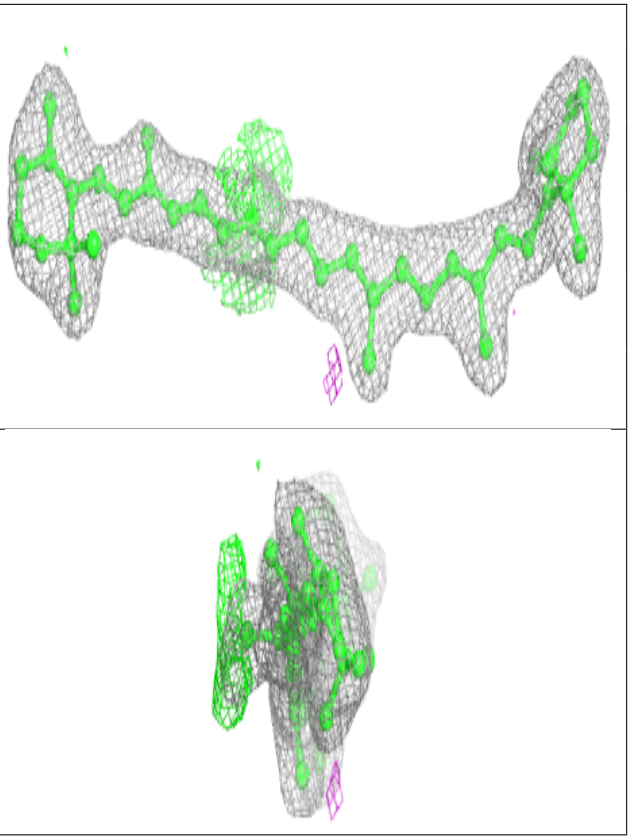
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

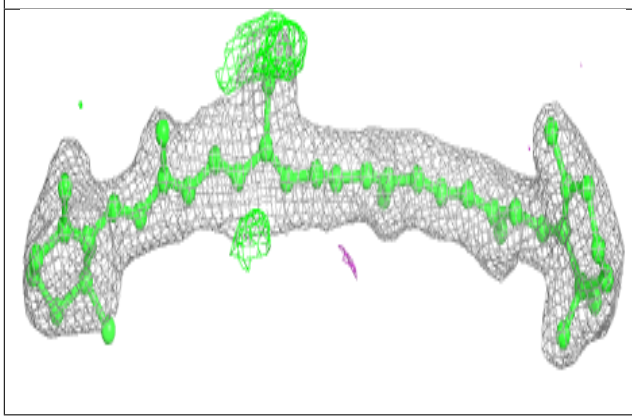




Electron density around BCR T 101:

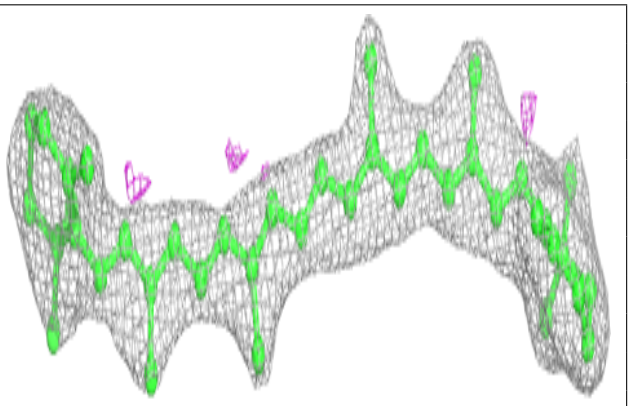
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

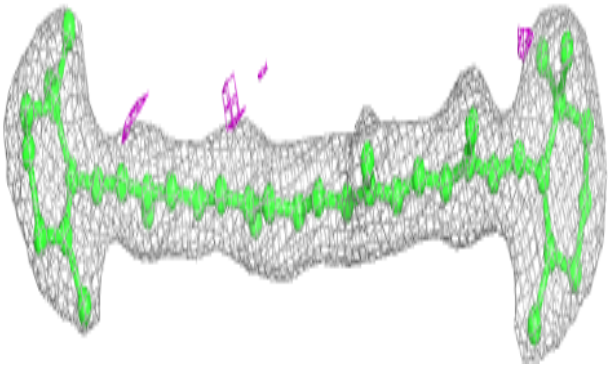


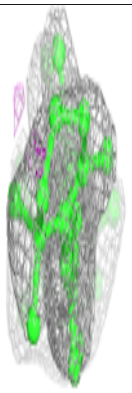


Electron density around BCR c 515:

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

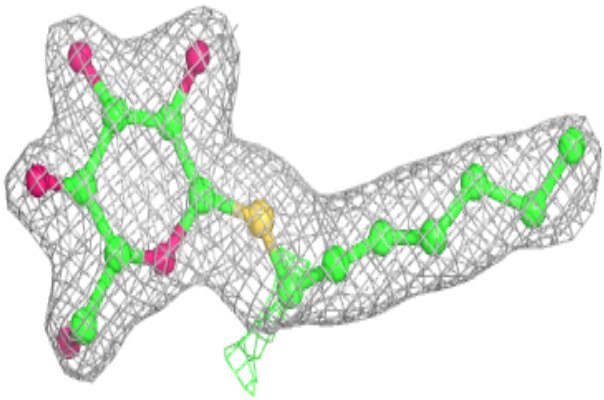


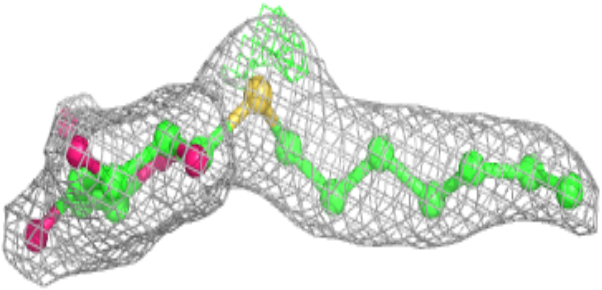


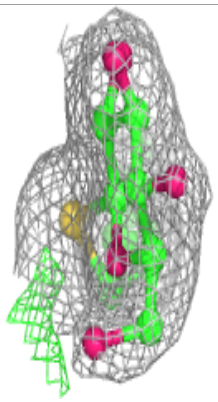


Electron density around HTG O 302:

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

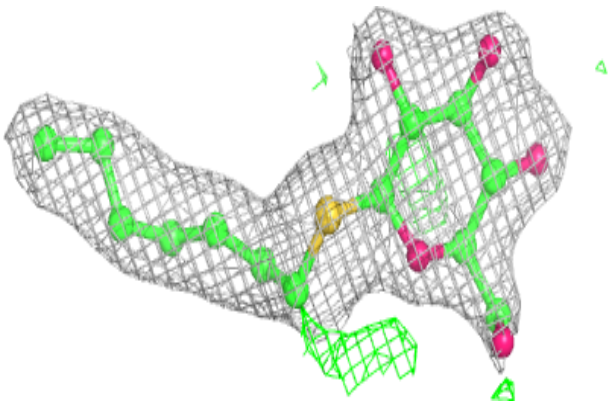


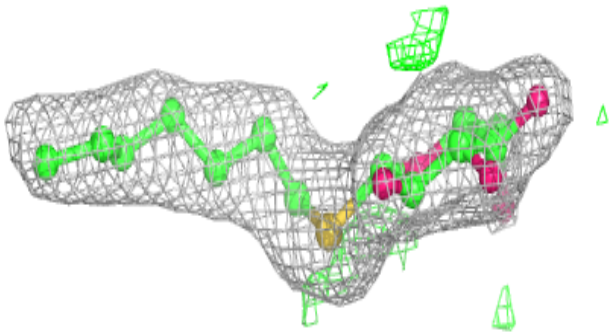


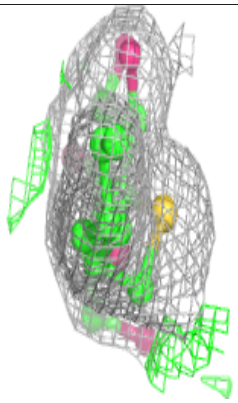


Electron density around HTG o 301:

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

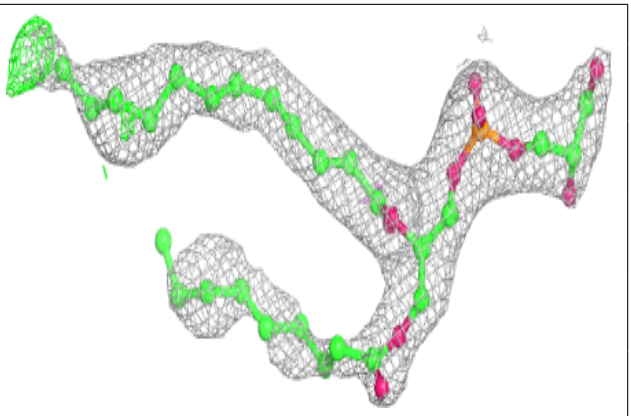


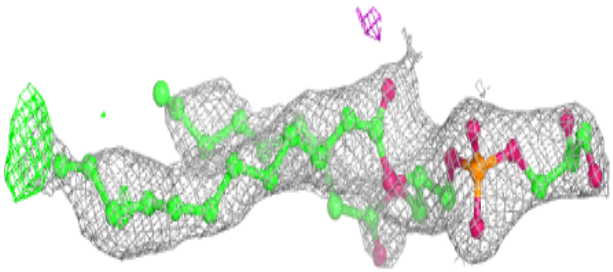


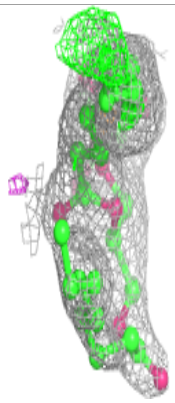


Electron density around LHG F 103:

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

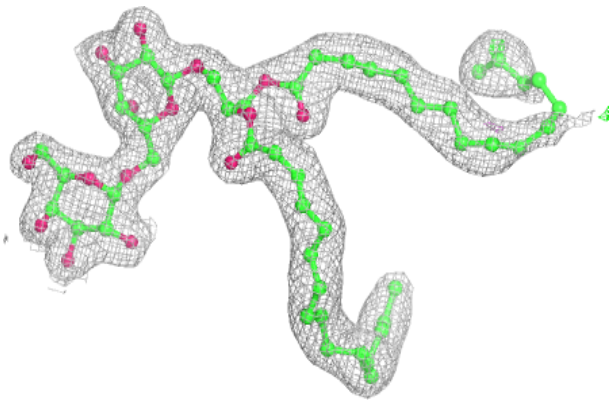


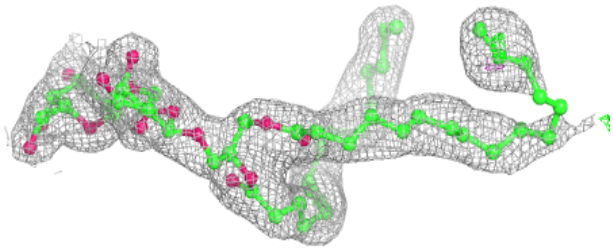


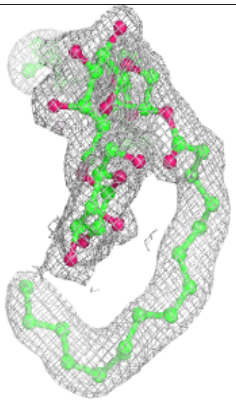


Electron density around DGD C 516:

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

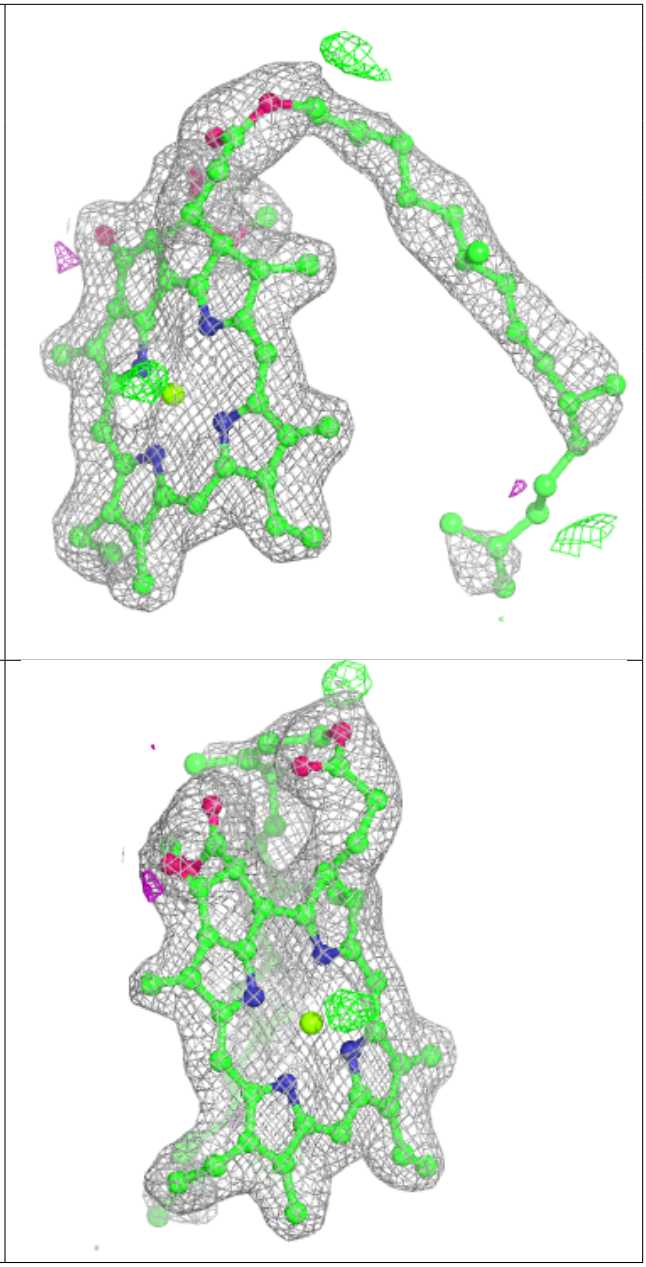






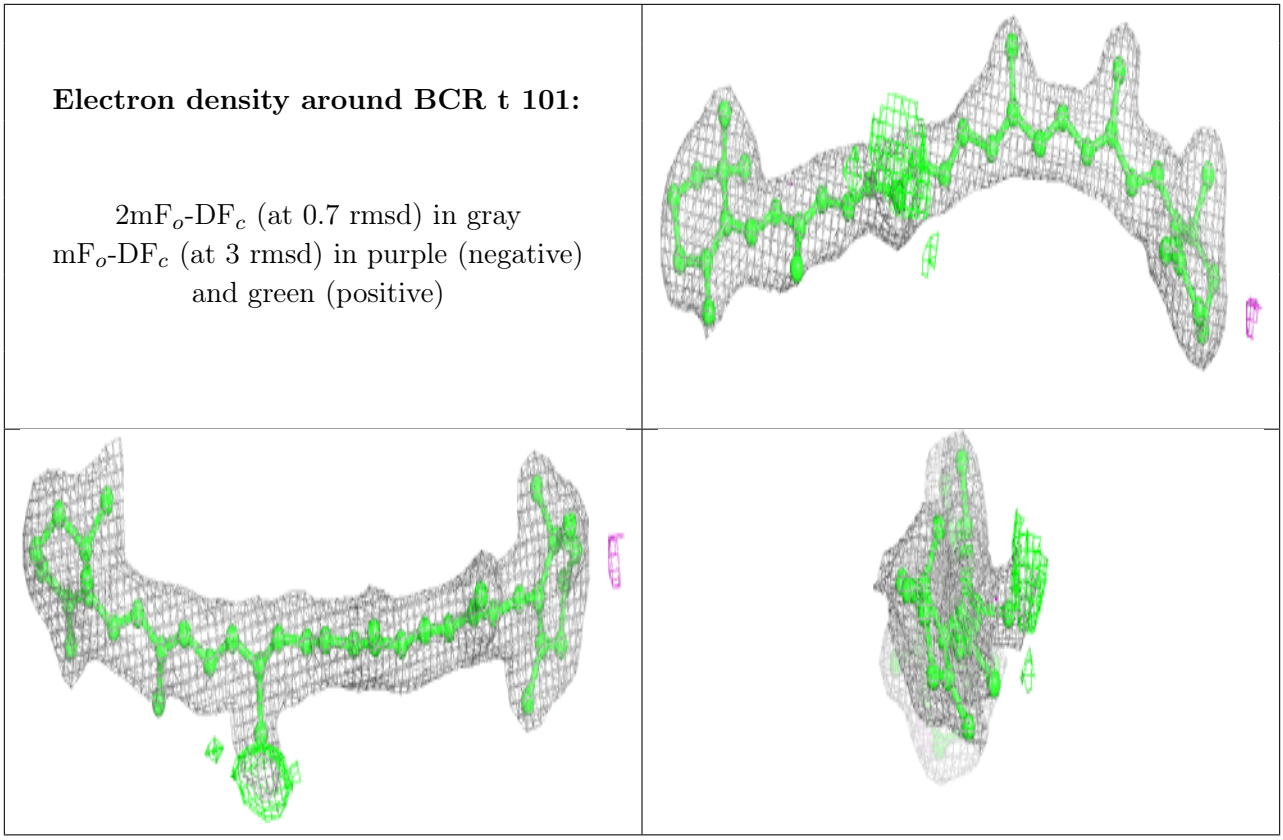
Electron density around CLA B 617:

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



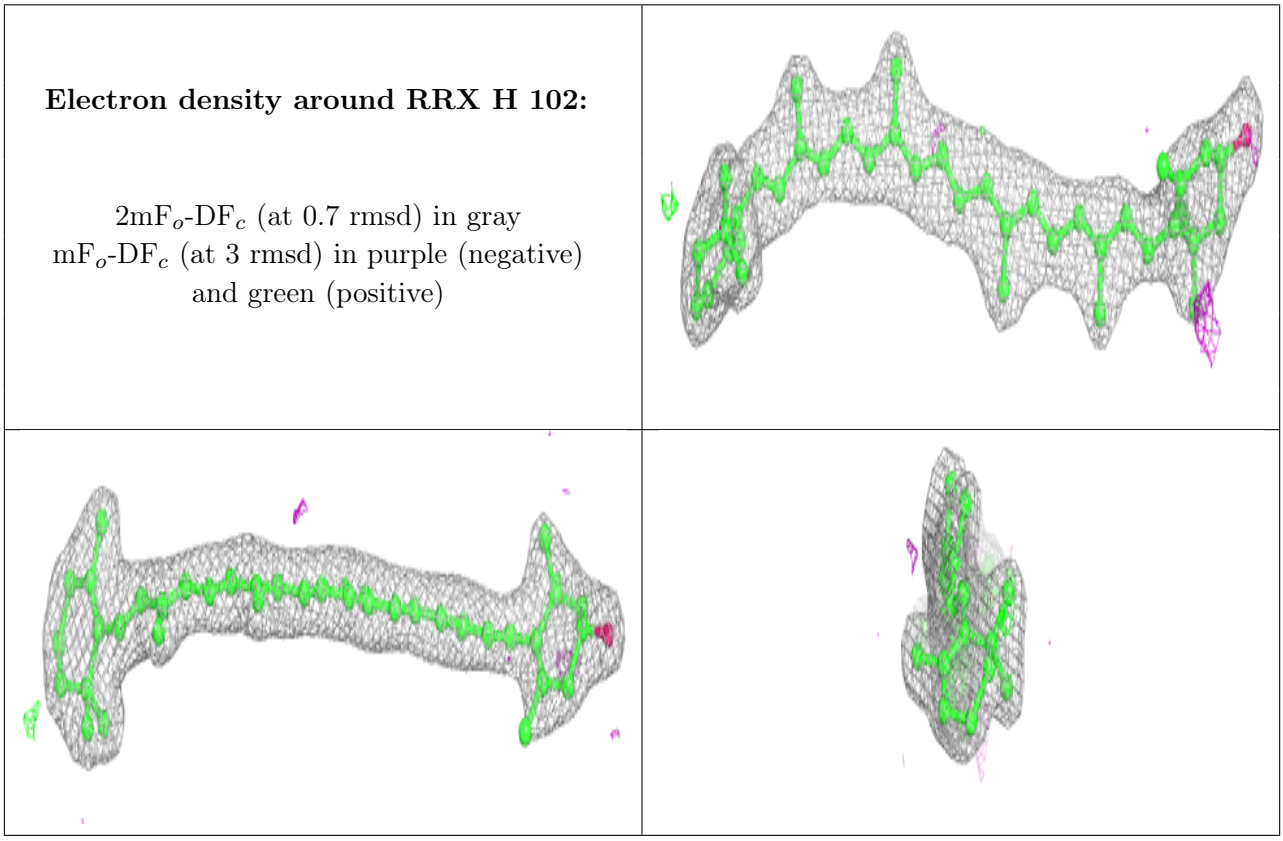
Electron density around BCR t 101:

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



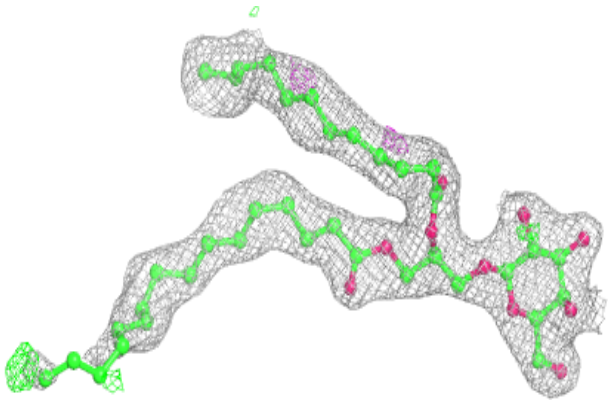
Electron density around RRX H 102:

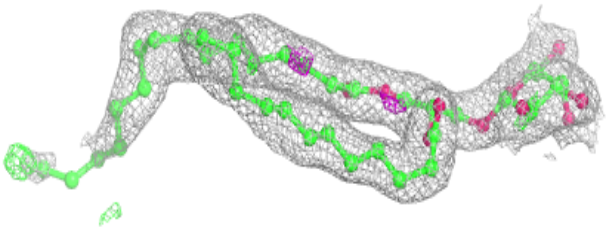
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

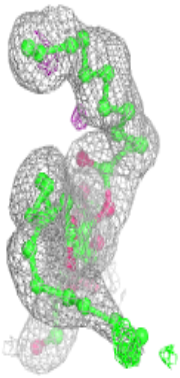


Electron density around LMG d 412:

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

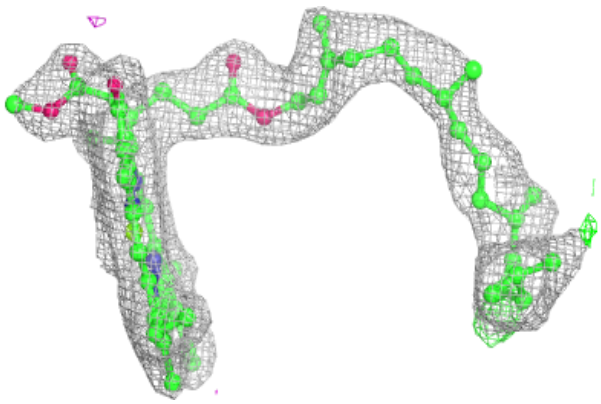


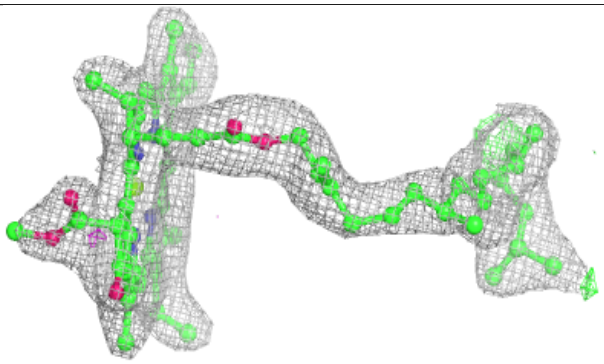


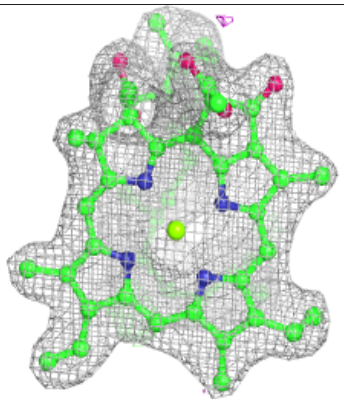


Electron density around CLA c 507:

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

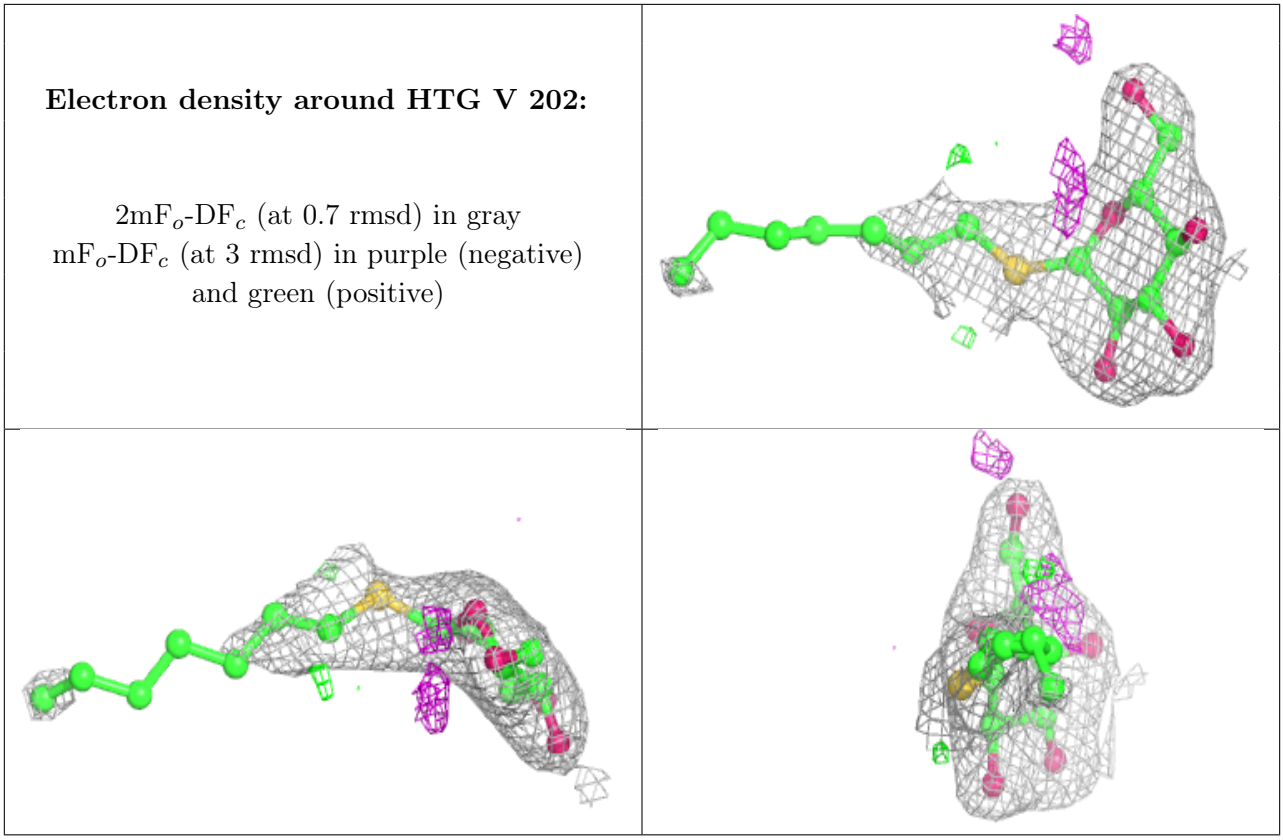






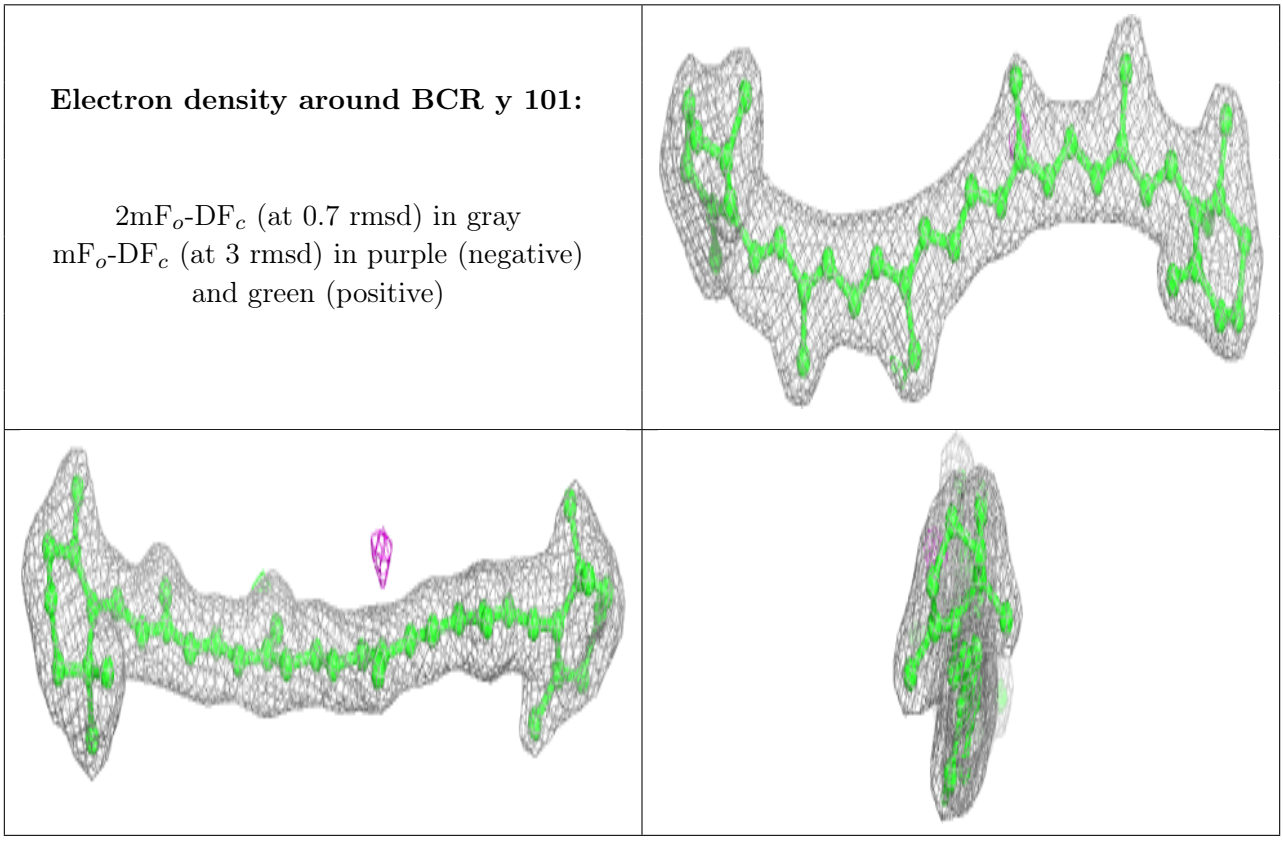
Electron density around HTG V 202:

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



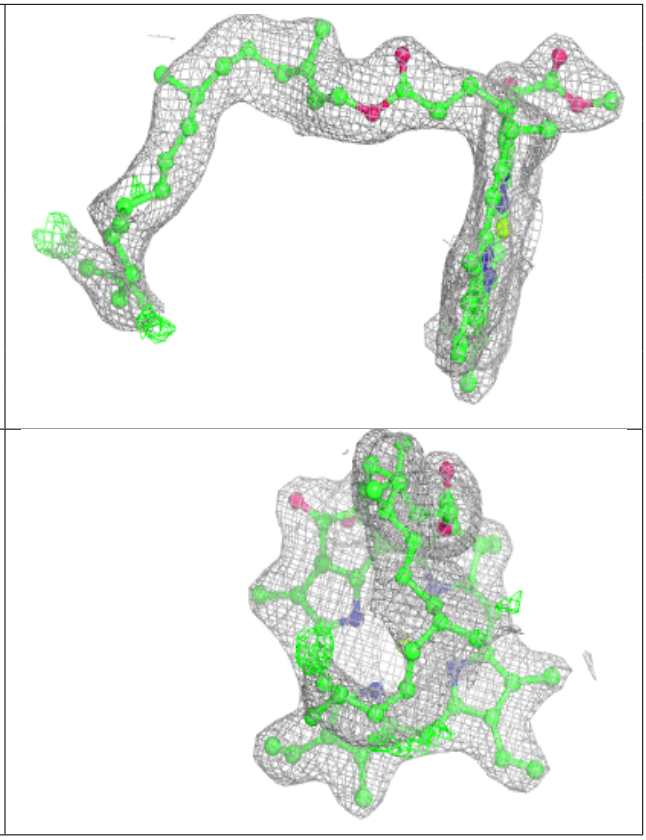
Electron density around BCR y 101:

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



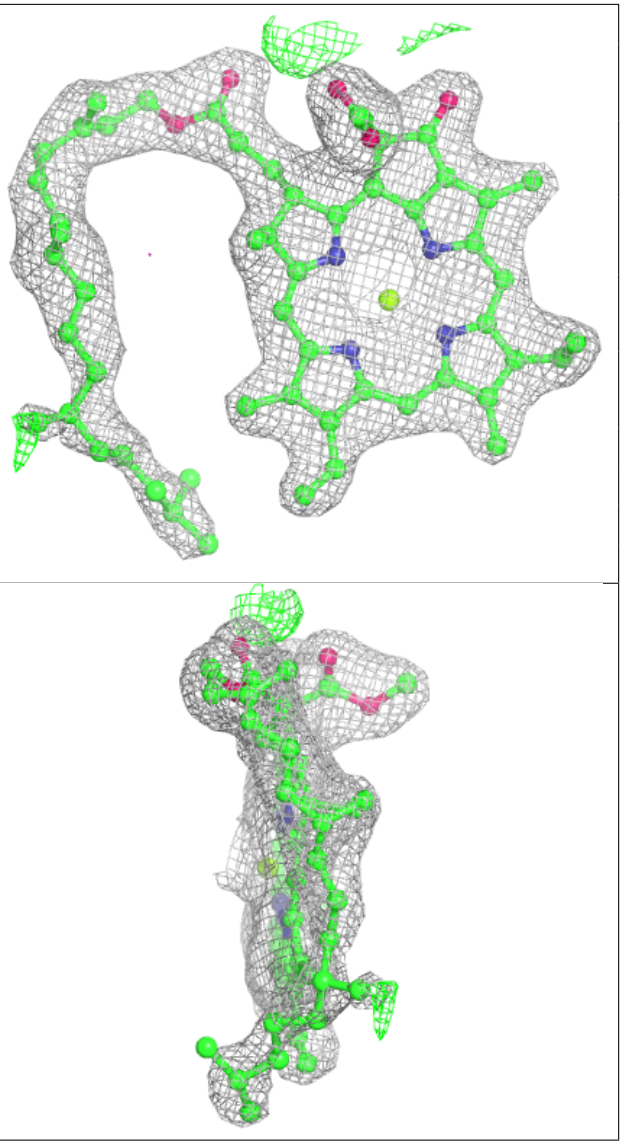
Electron density around CLA C 506:

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



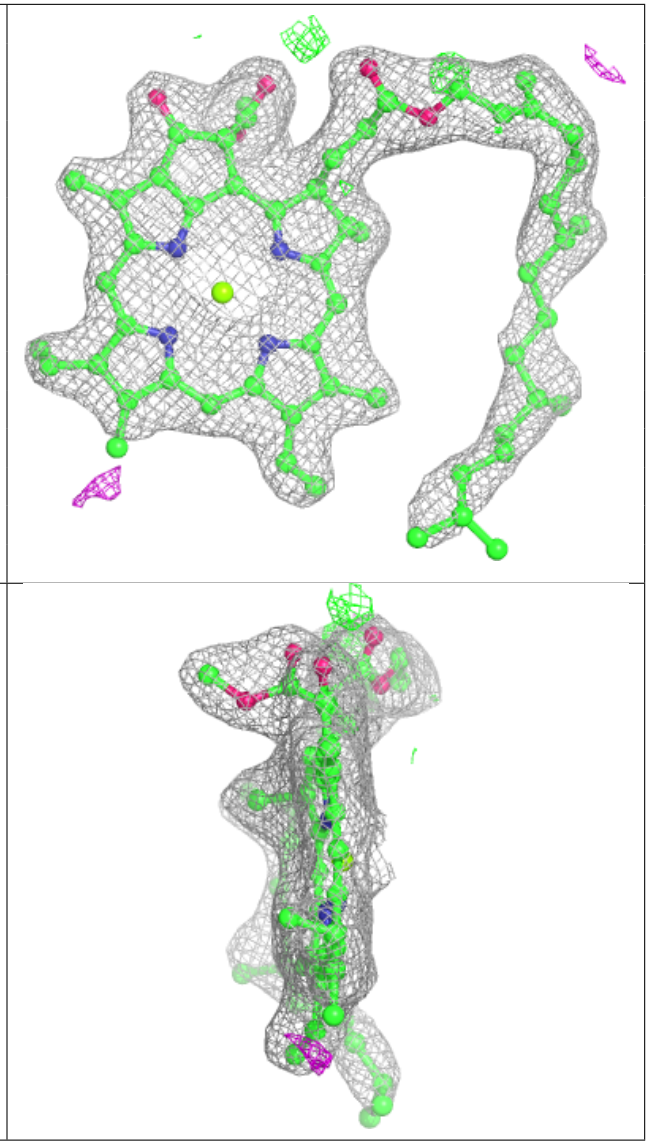
Electron density around CLA C 512:

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



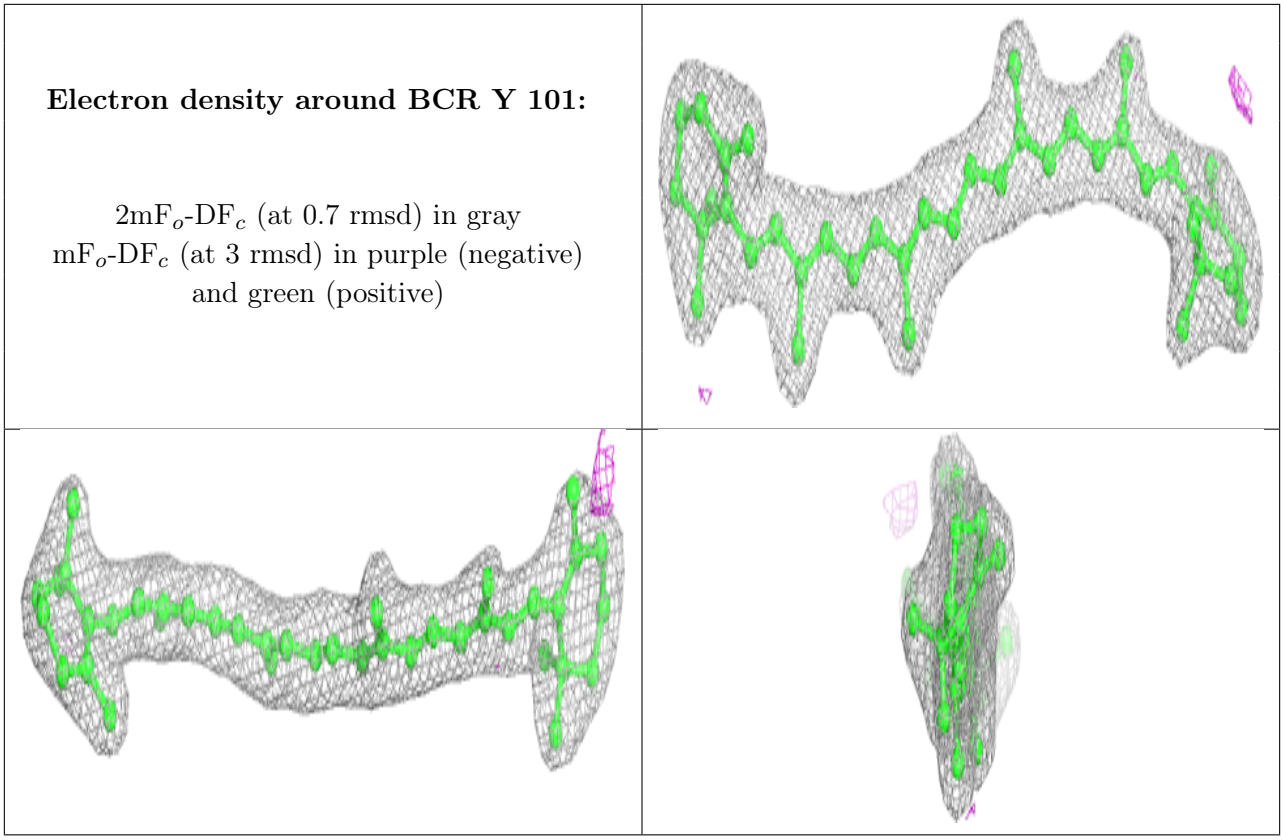
Electron density around CLA c 513:

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



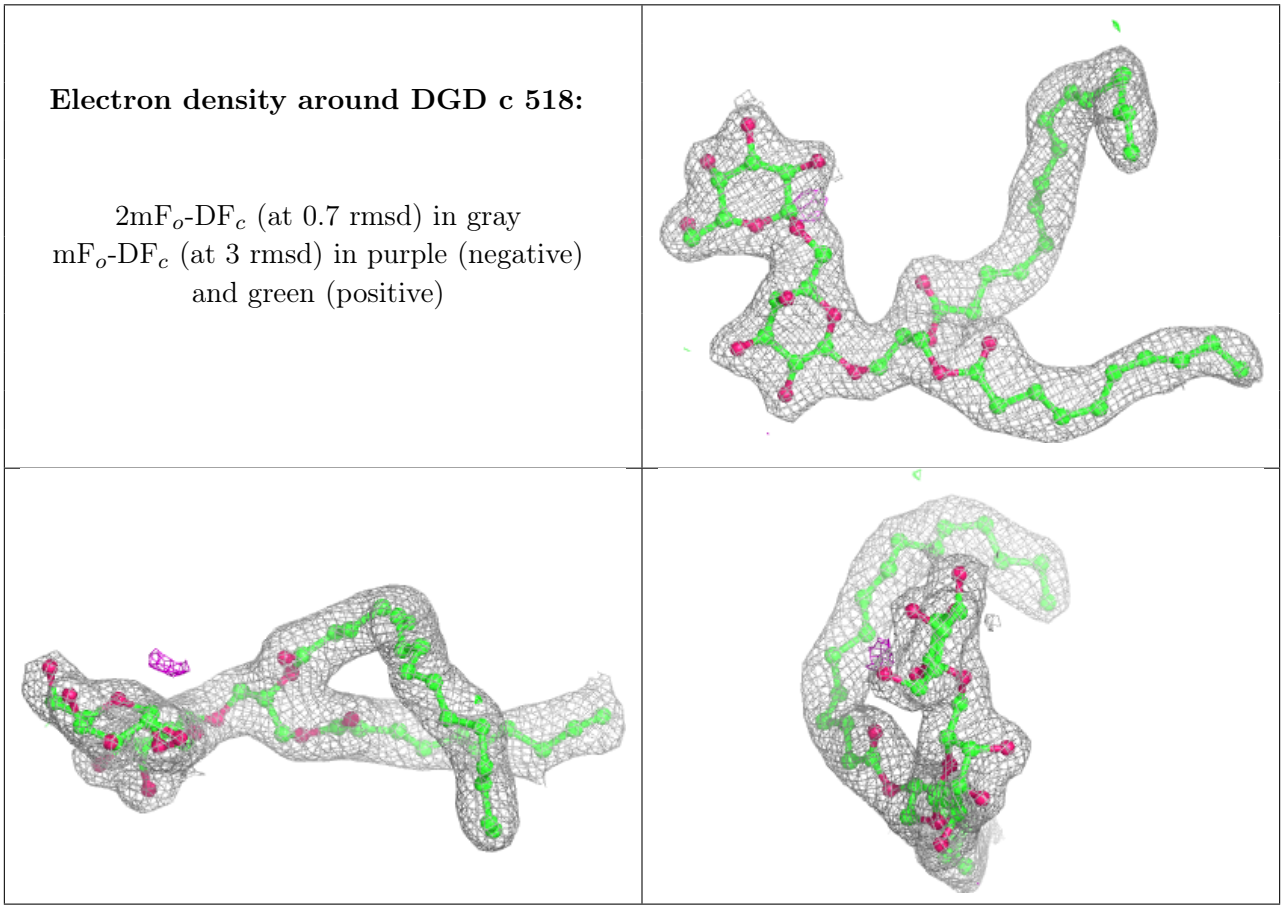
Electron density around BCR Y 101:

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



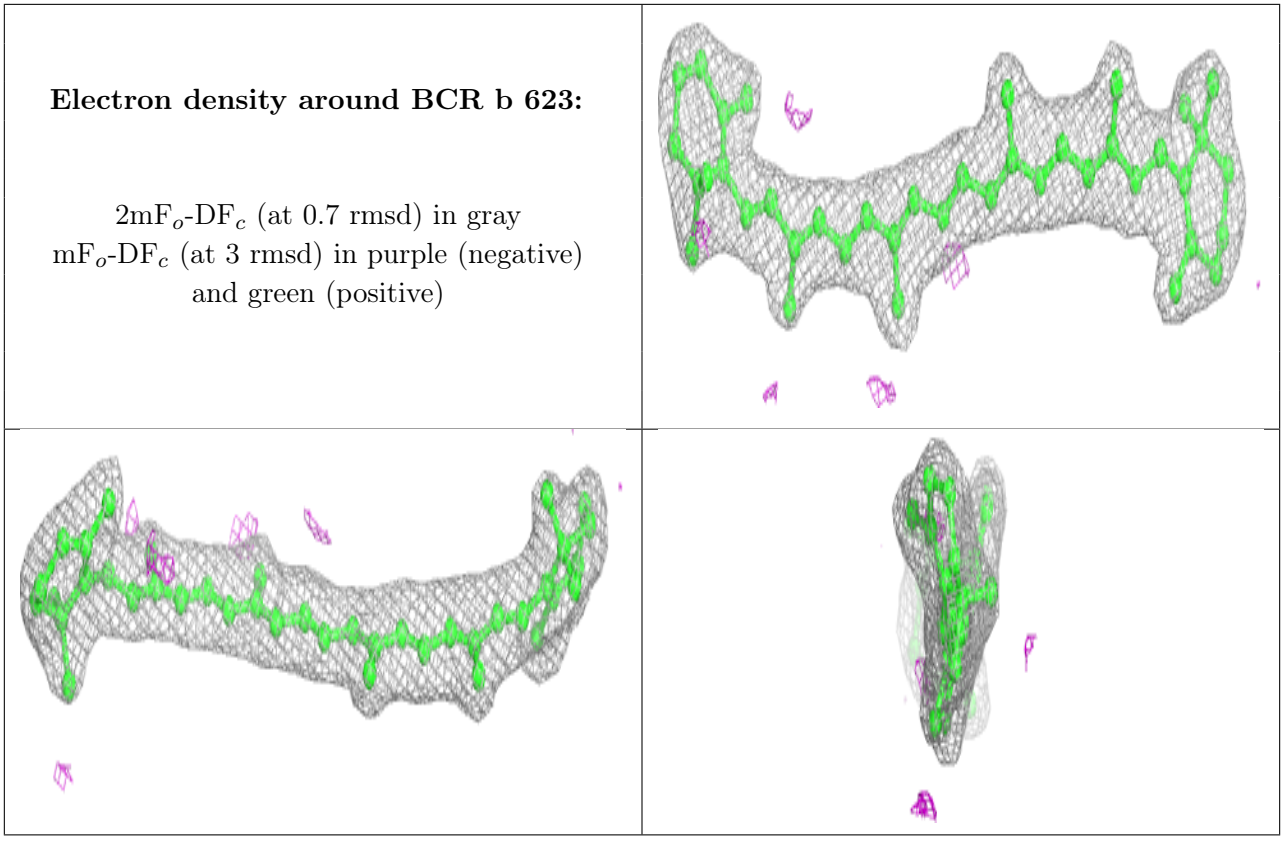
Electron density around DGD c 518:

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



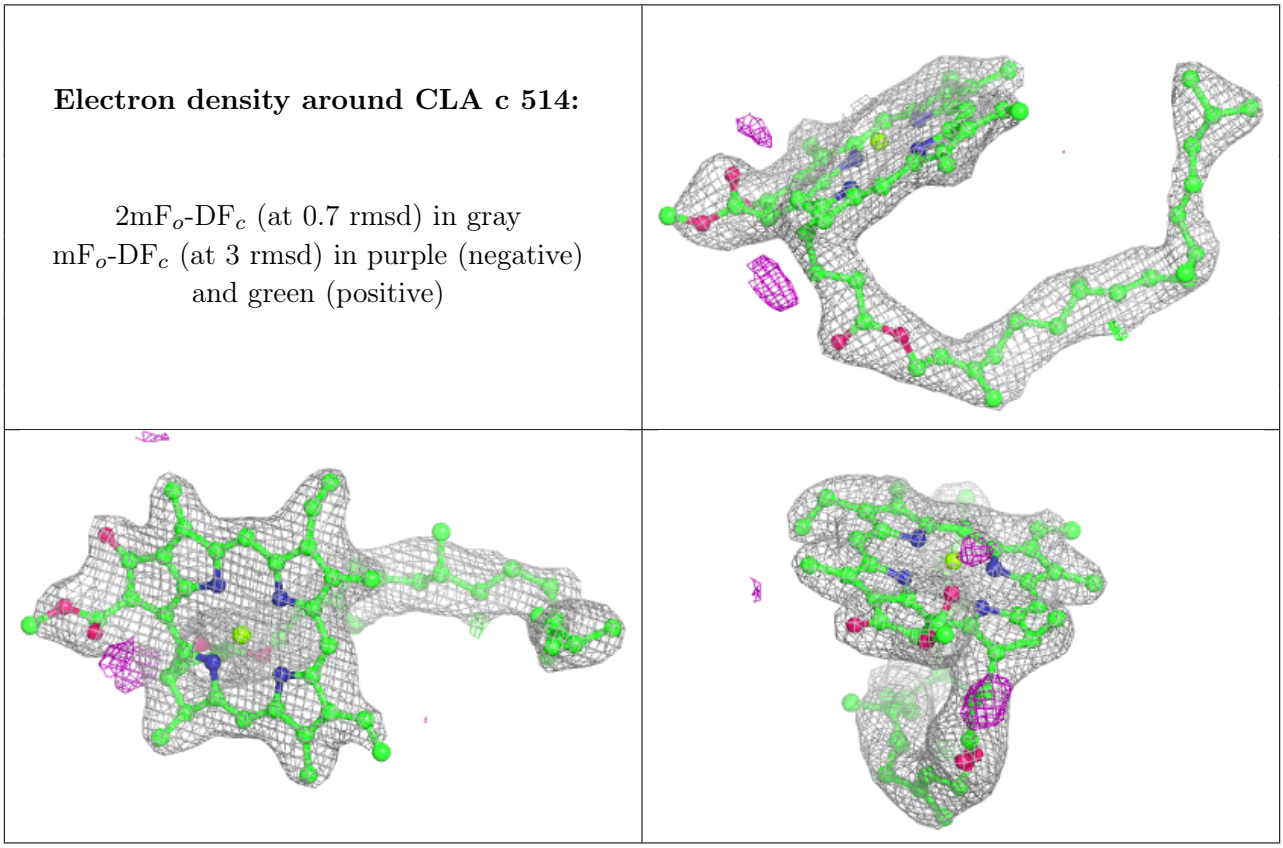
Electron density around BCR b 623:

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



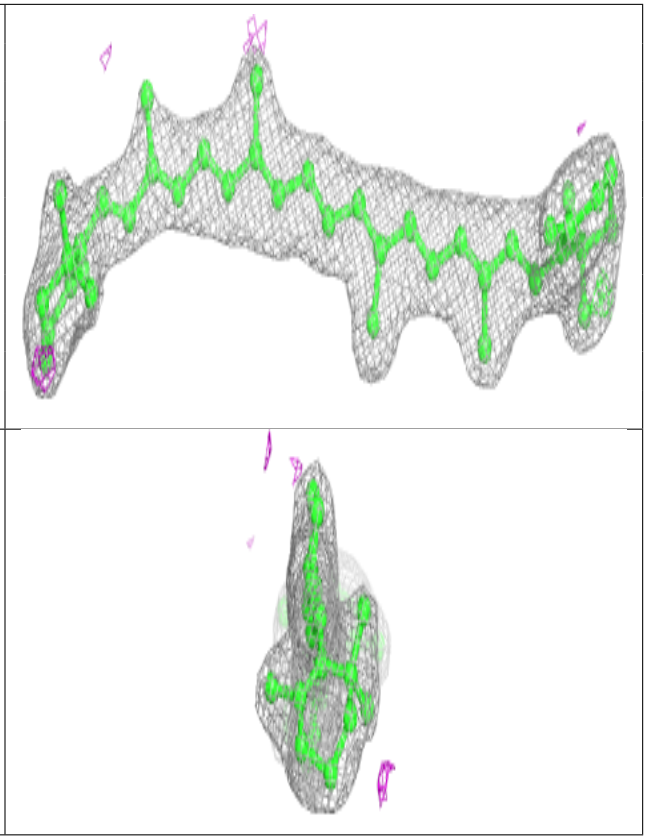
Electron density around CLA c 514:

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



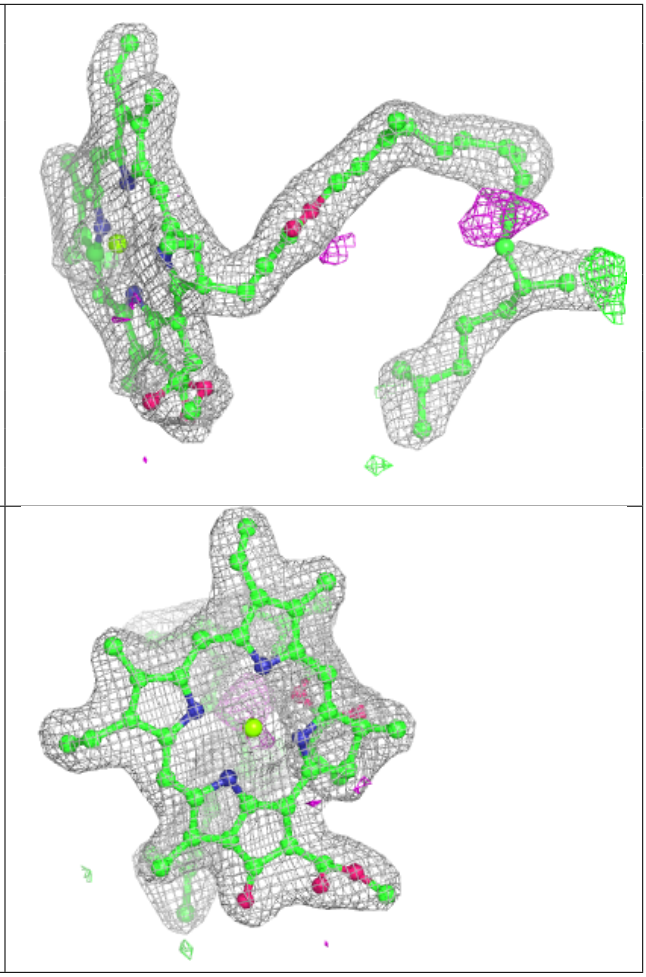
Electron density around BCR c 516:

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



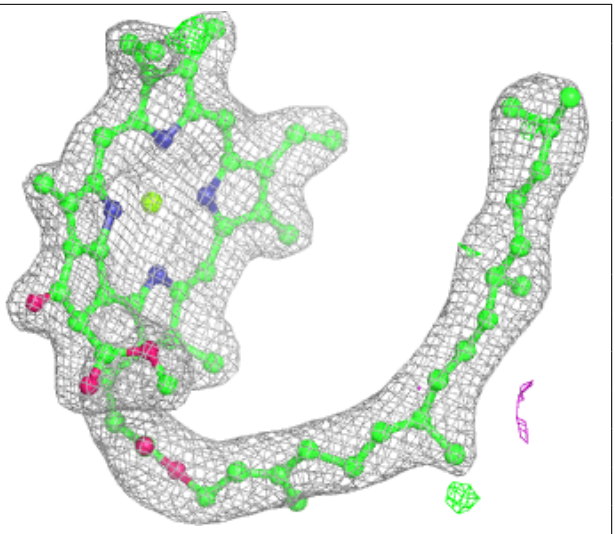
Electron density around CLA b 610:

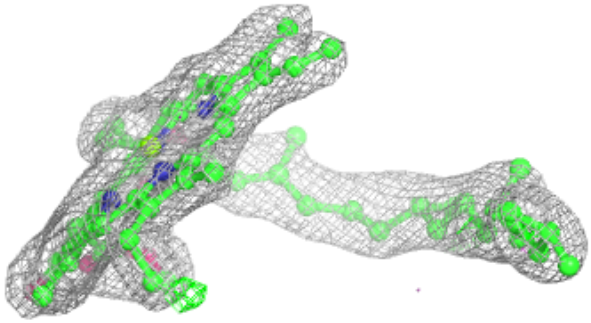
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

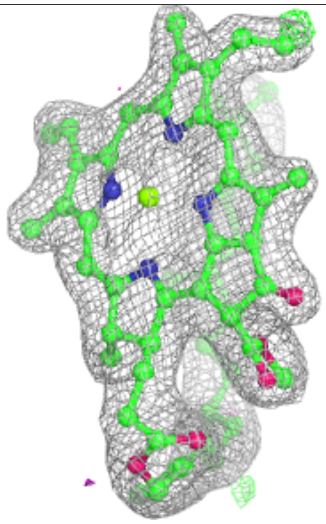


Electron density around CLA c 508:

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

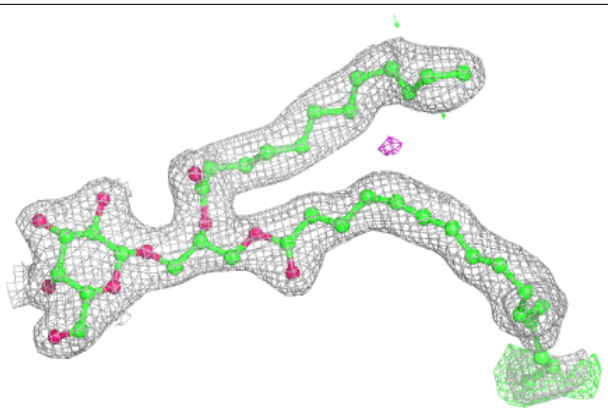


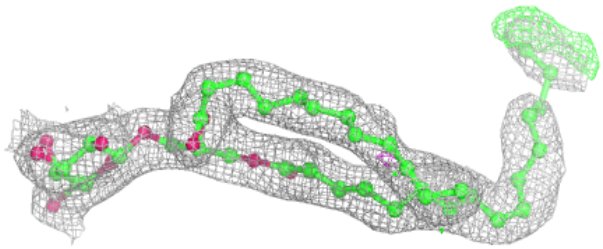


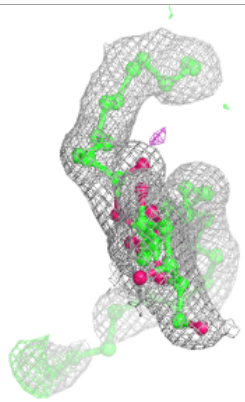


Electron density around LMG D 412:

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

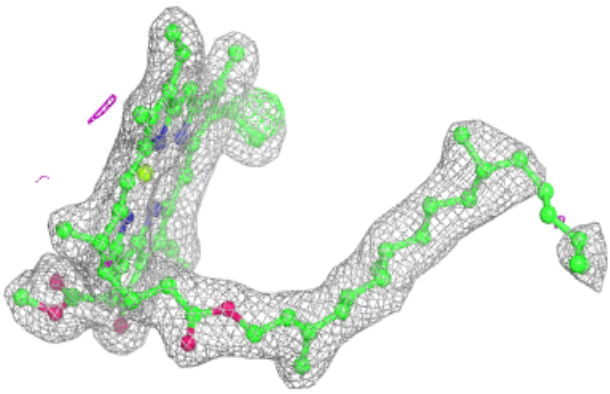


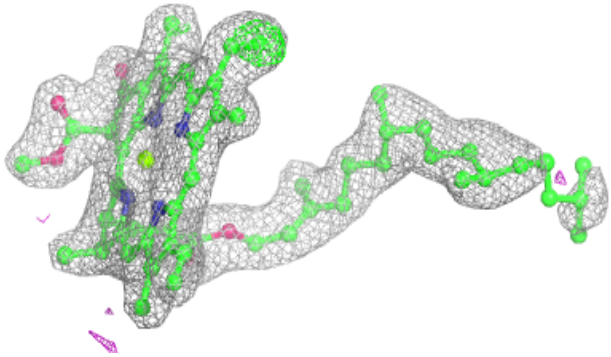


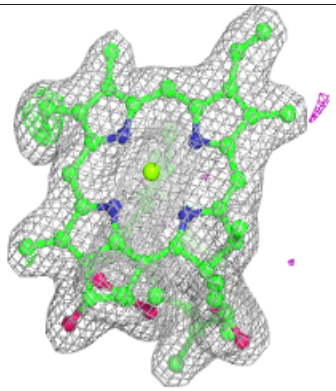


Electron density around CLA C 508:

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

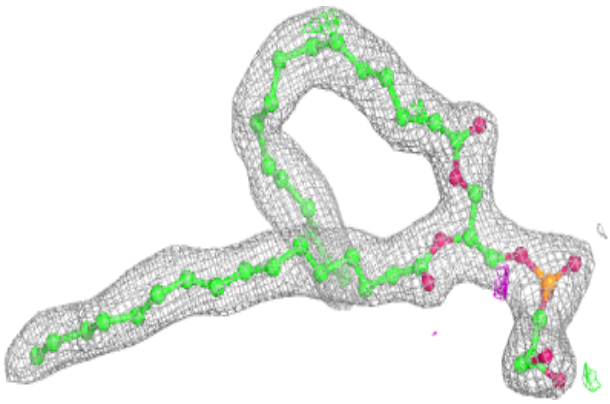


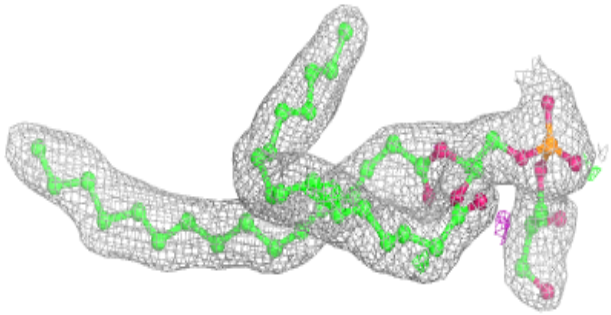


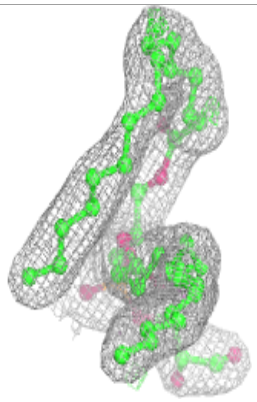


Electron density around LHG D 409:

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

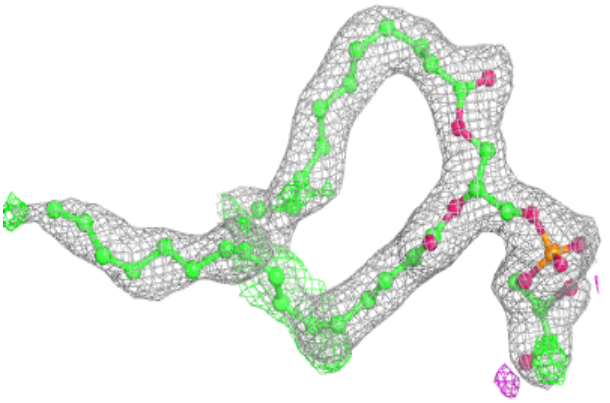


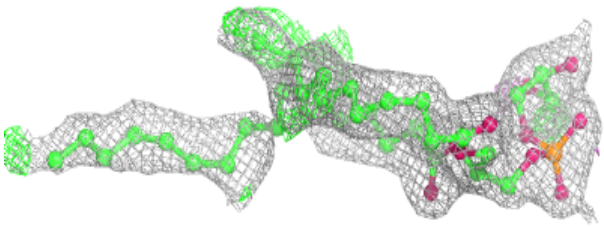


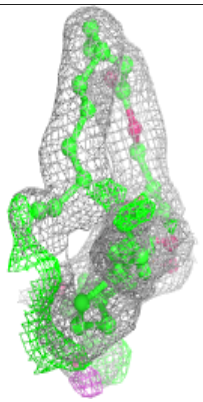


Electron density around LHG D 411:

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

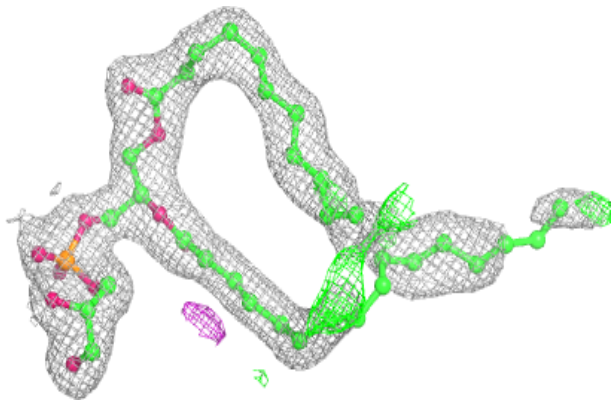


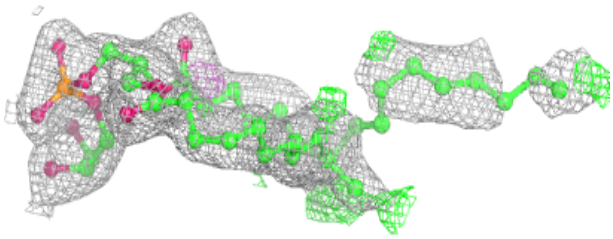


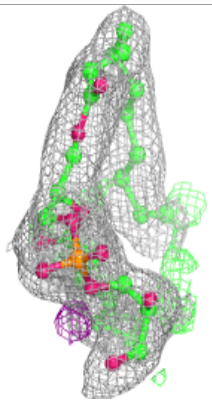


Electron density around LHG d 411:

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

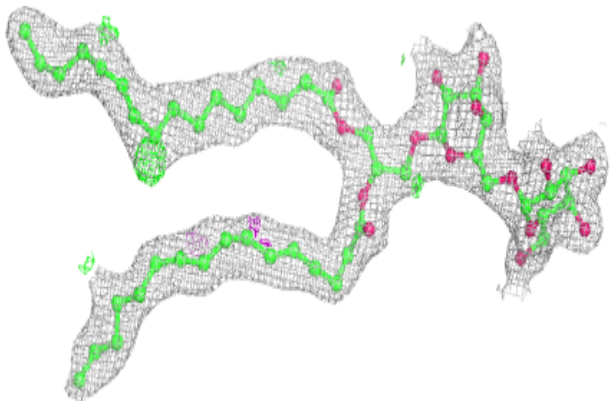


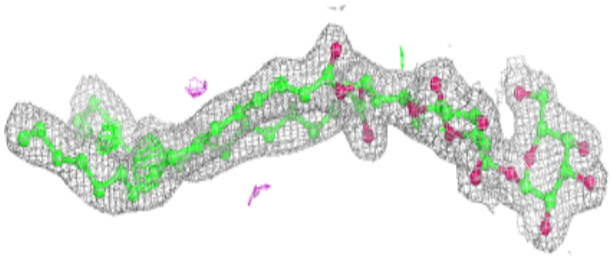


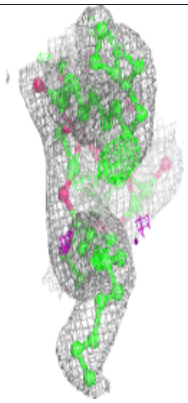


Electron density around DGD C 517:

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

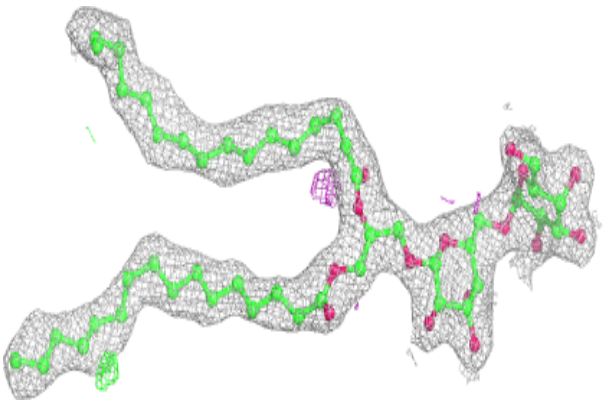


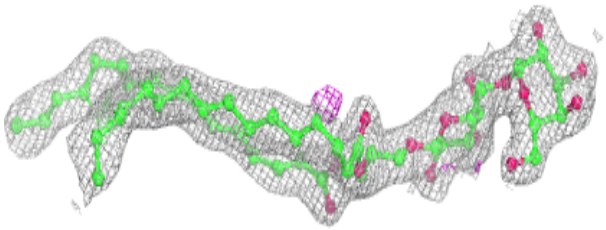


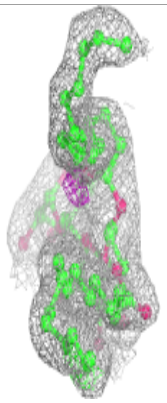


Electron density around DGD c 519:

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

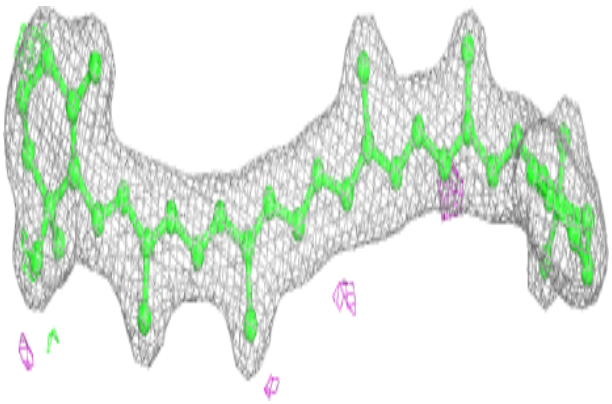


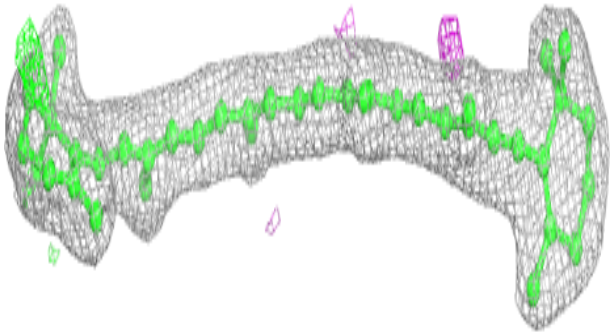


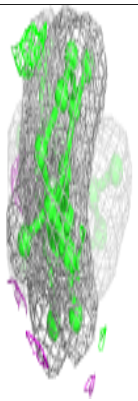


Electron density around BCR B 618:

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

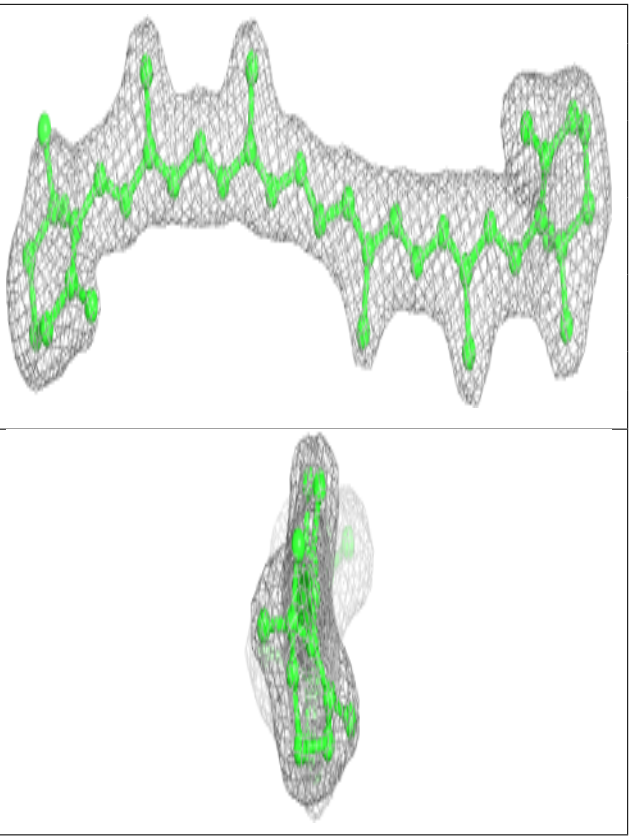






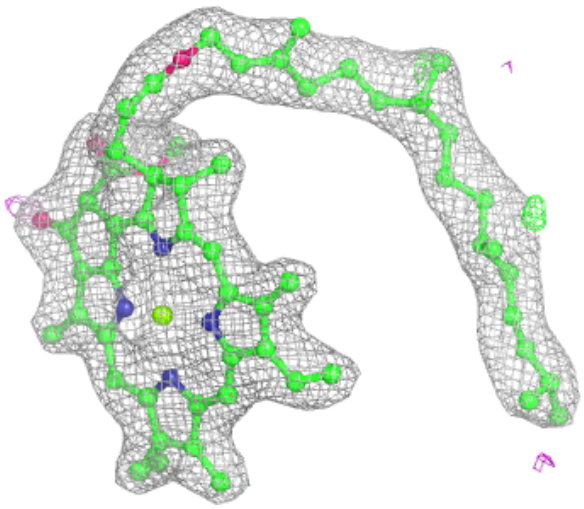
Electron density around BCR B 619:

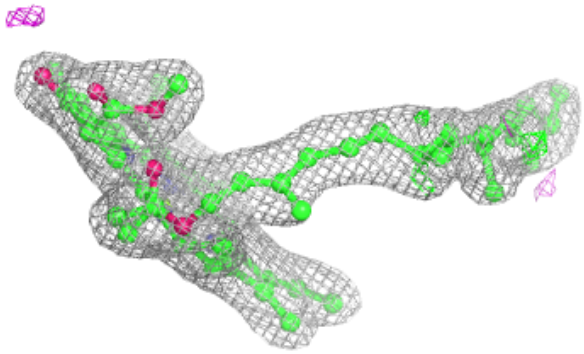
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

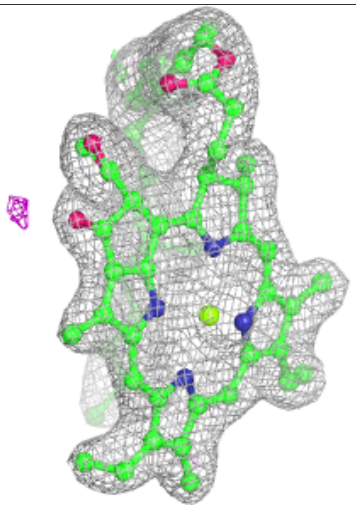


Electron density around CLA C 507:

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

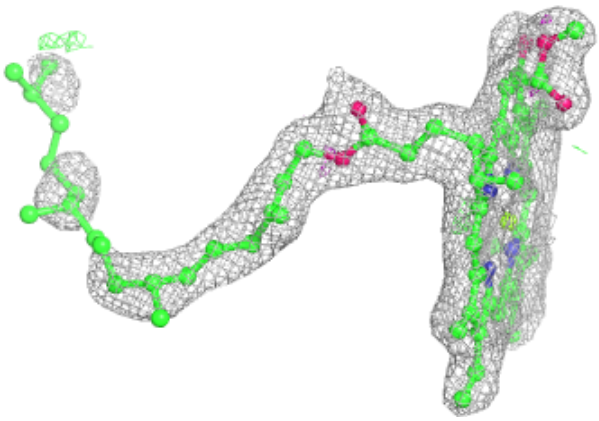


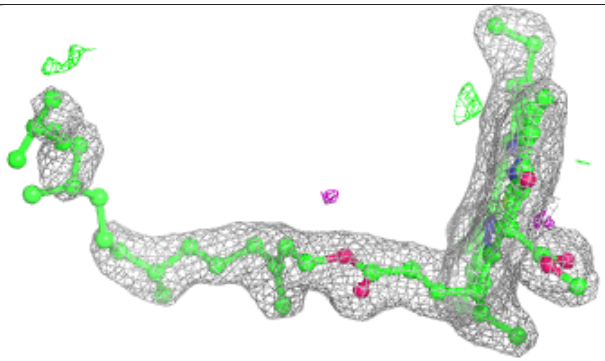


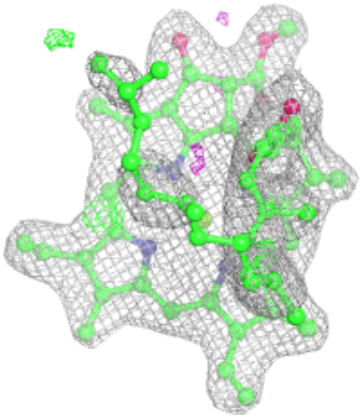


Electron density around CLA D 405:

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

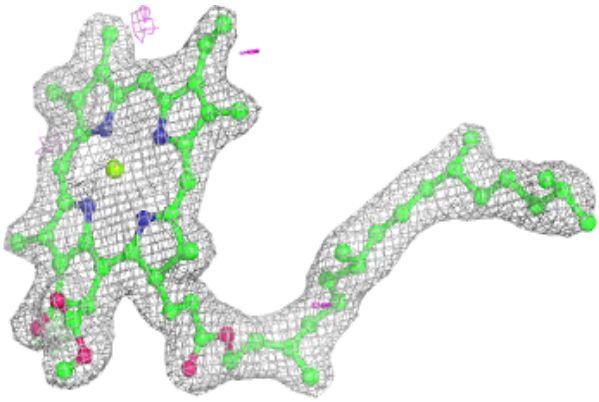


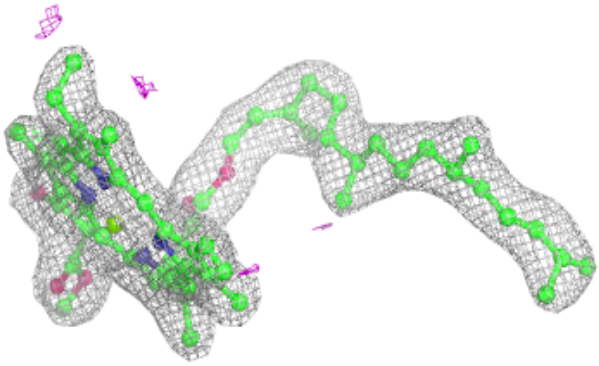


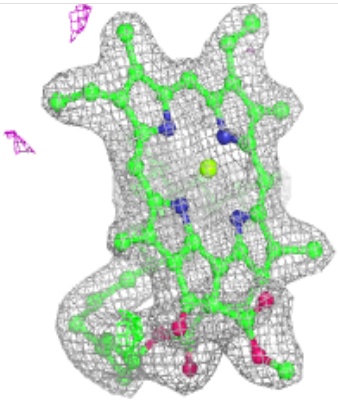


Electron density around CLA c 512:

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

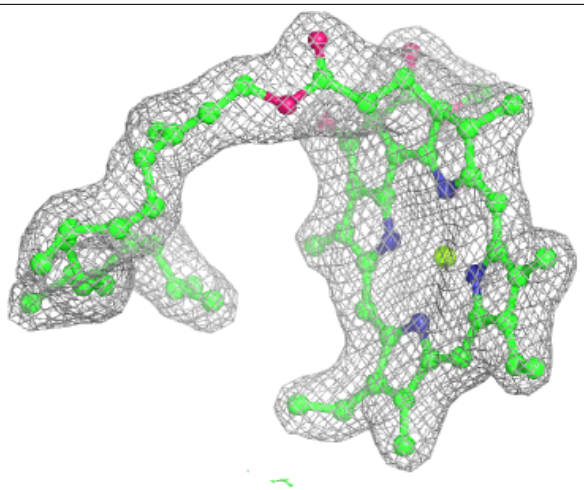


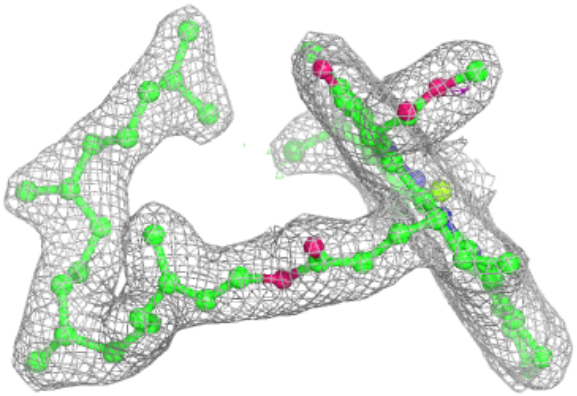


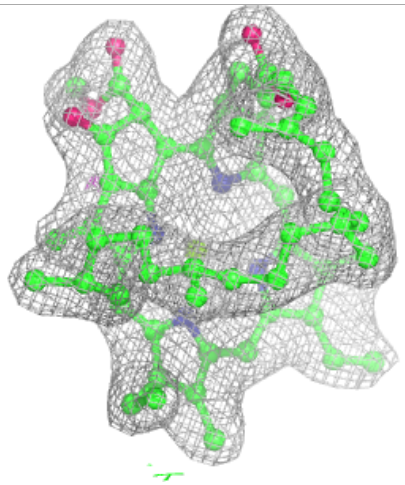


Electron density around CLA C 503:

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

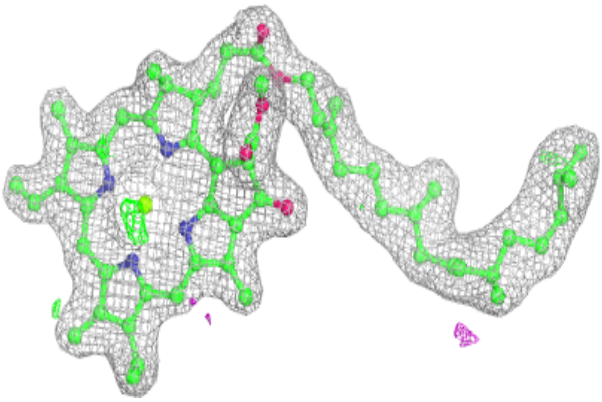


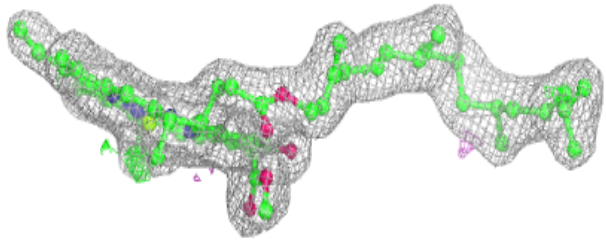


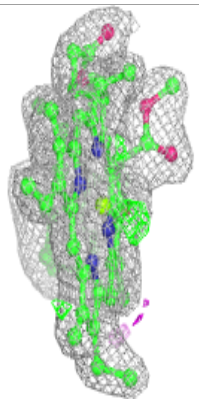


Electron density around CLA B 603:

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

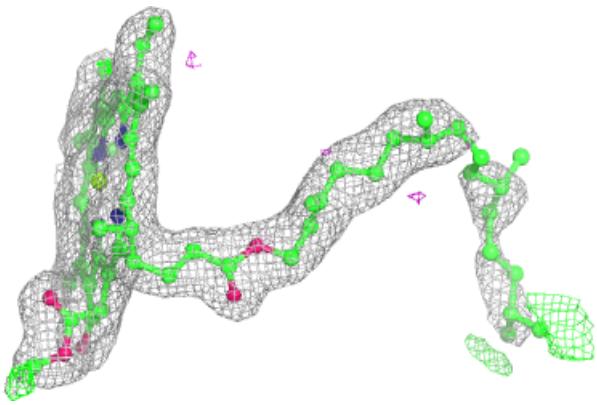


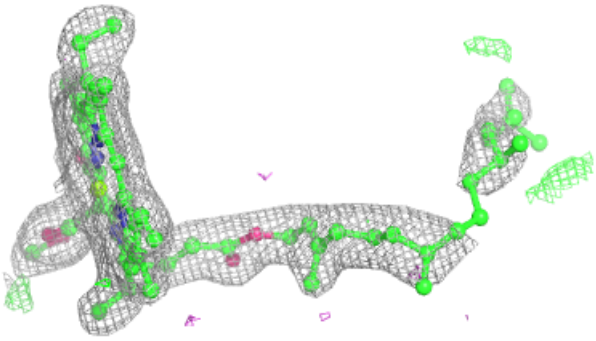


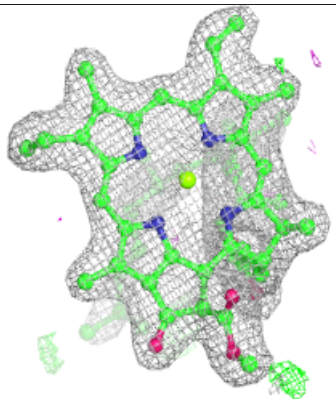


Electron density around CLA d 405:

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

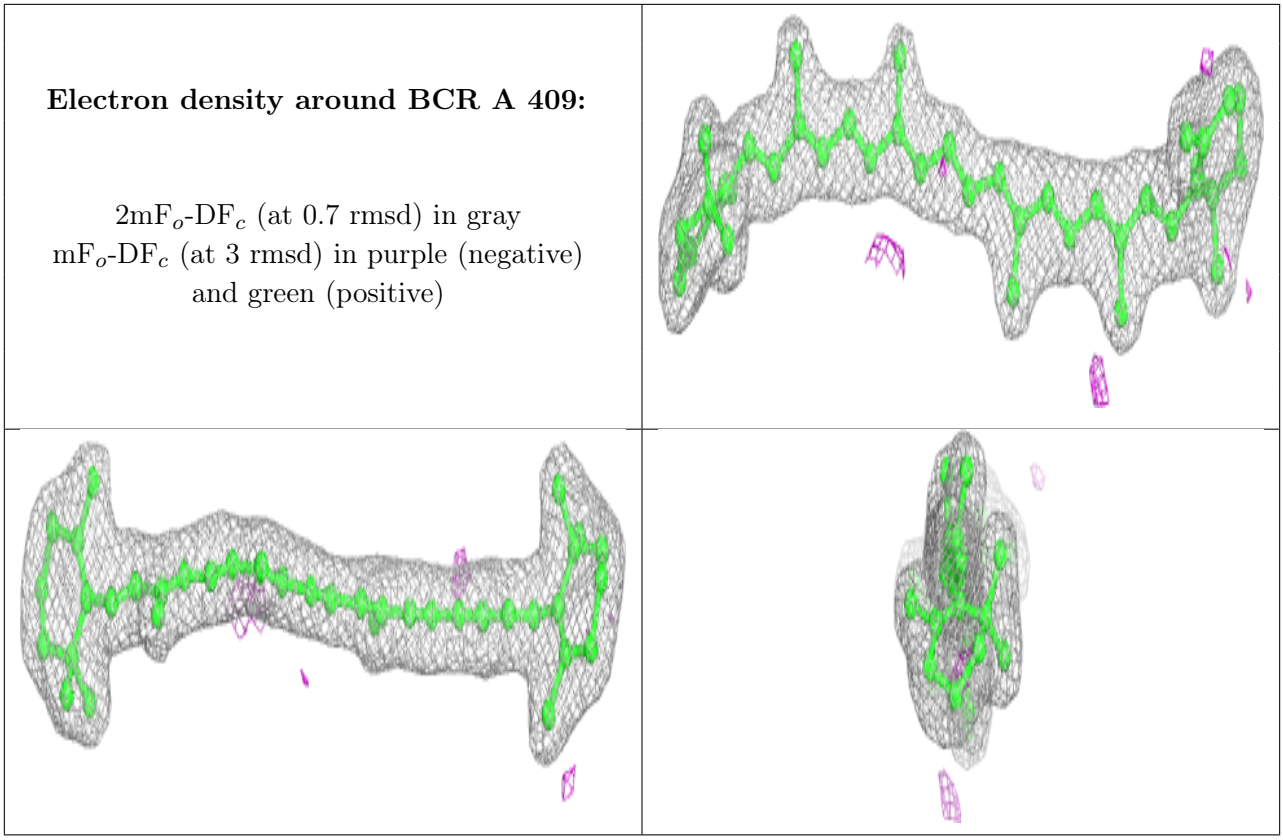






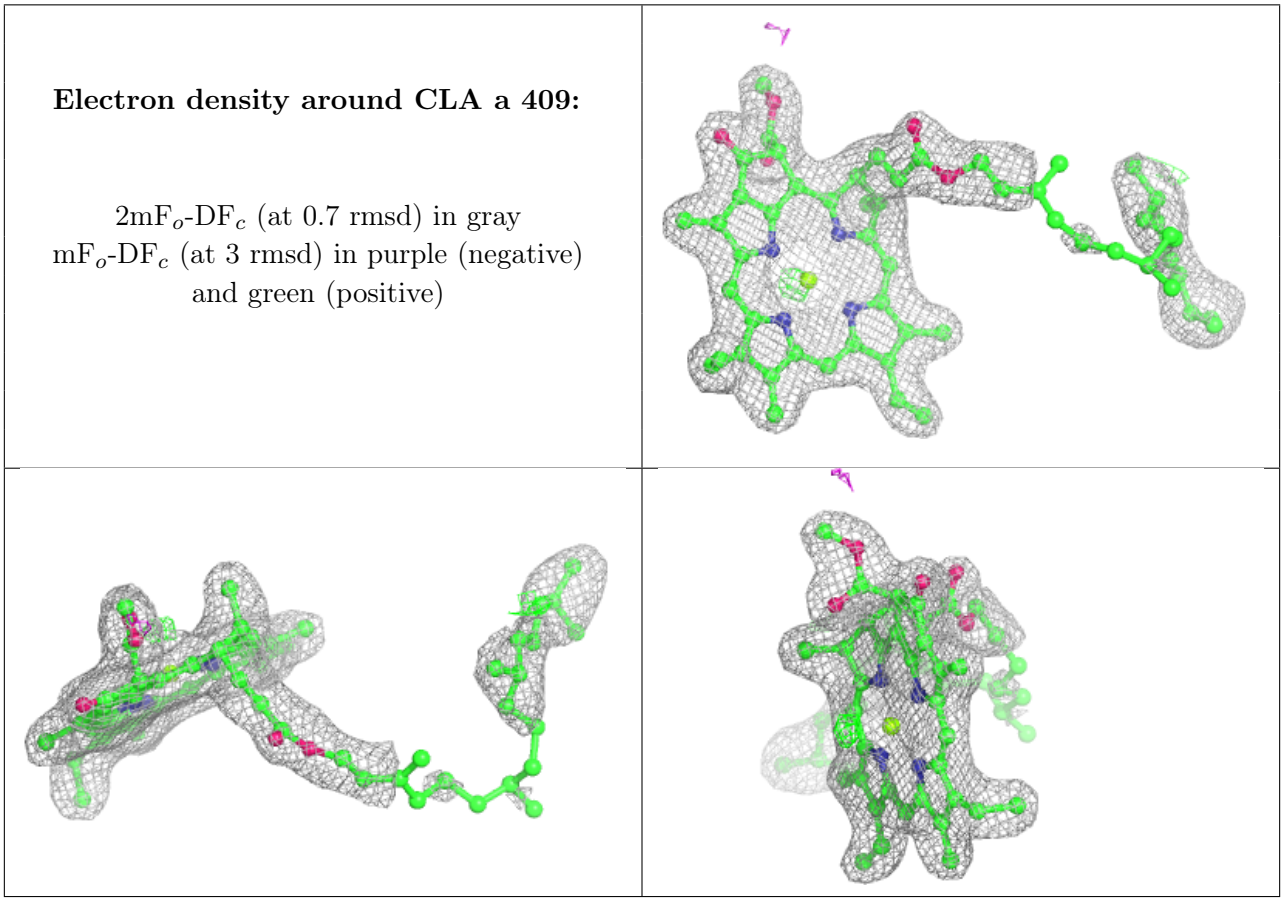
Electron density around BCR A 409:

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



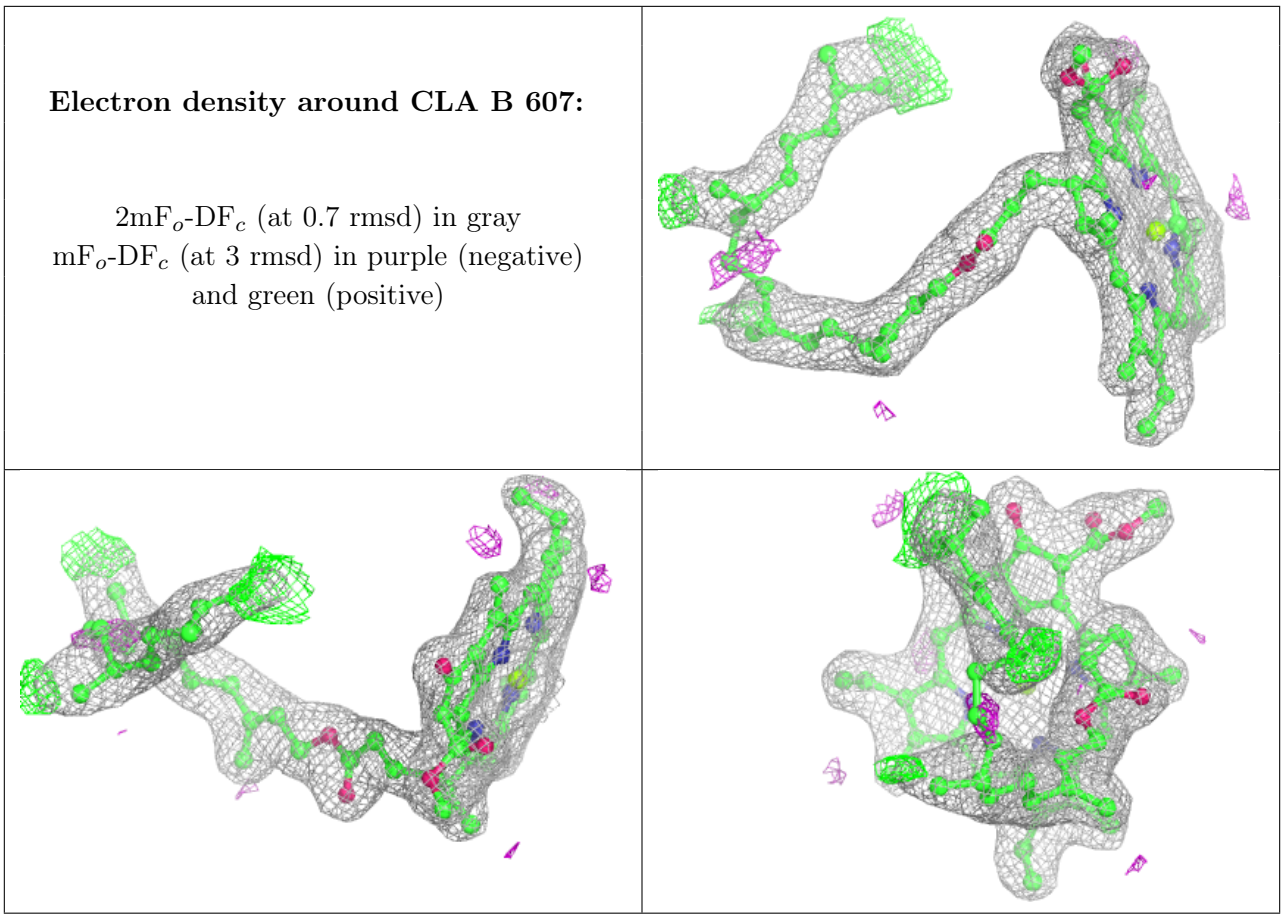
Electron density around CLA a 409:

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



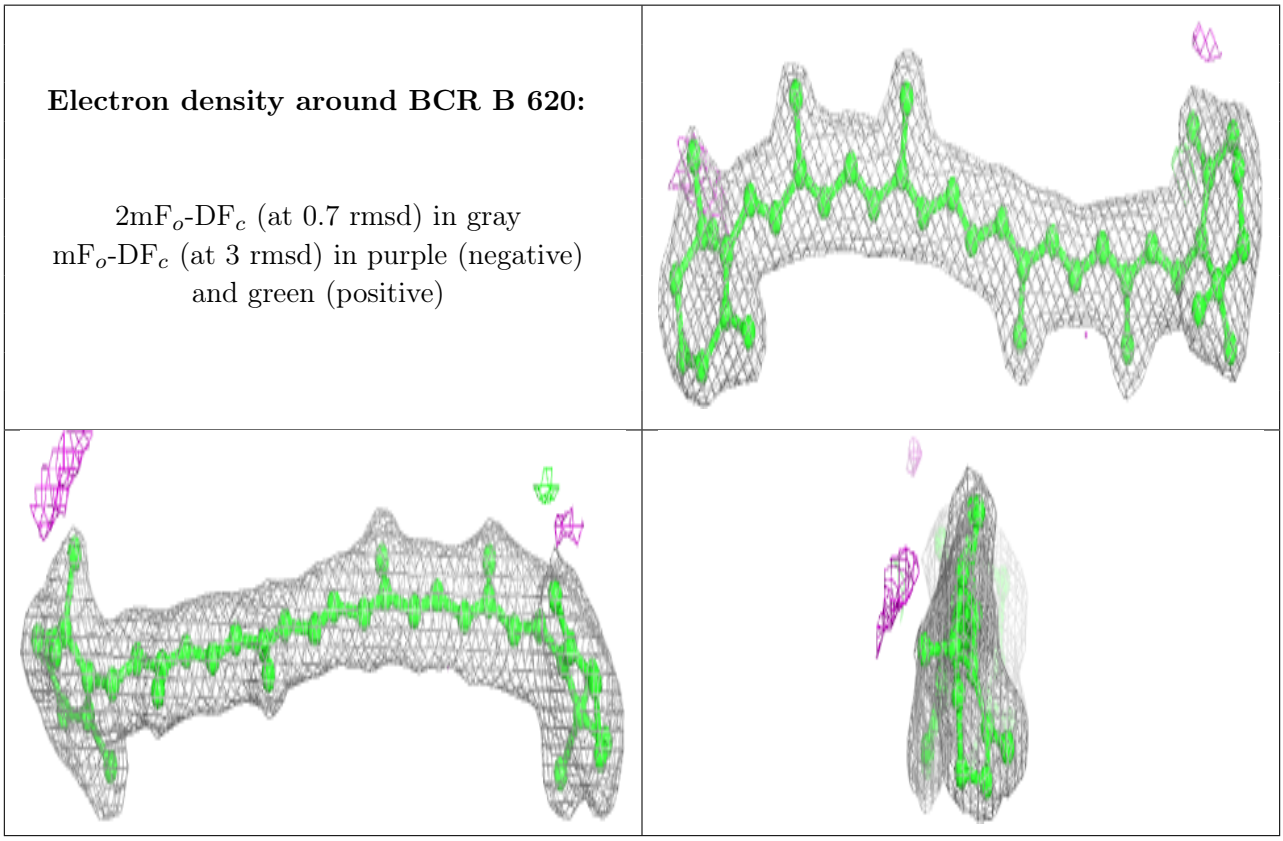
Electron density around CLA B 607:

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



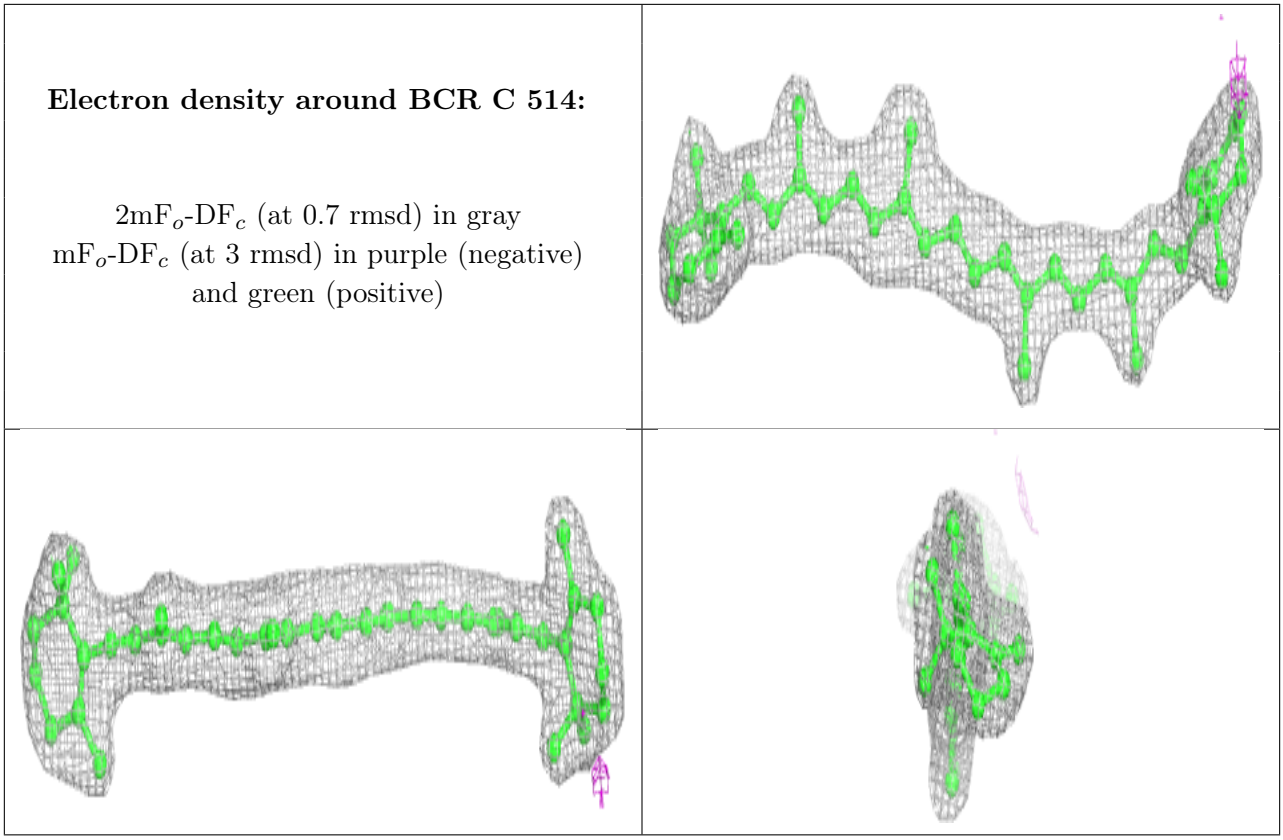
Electron density around BCR B 620:

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



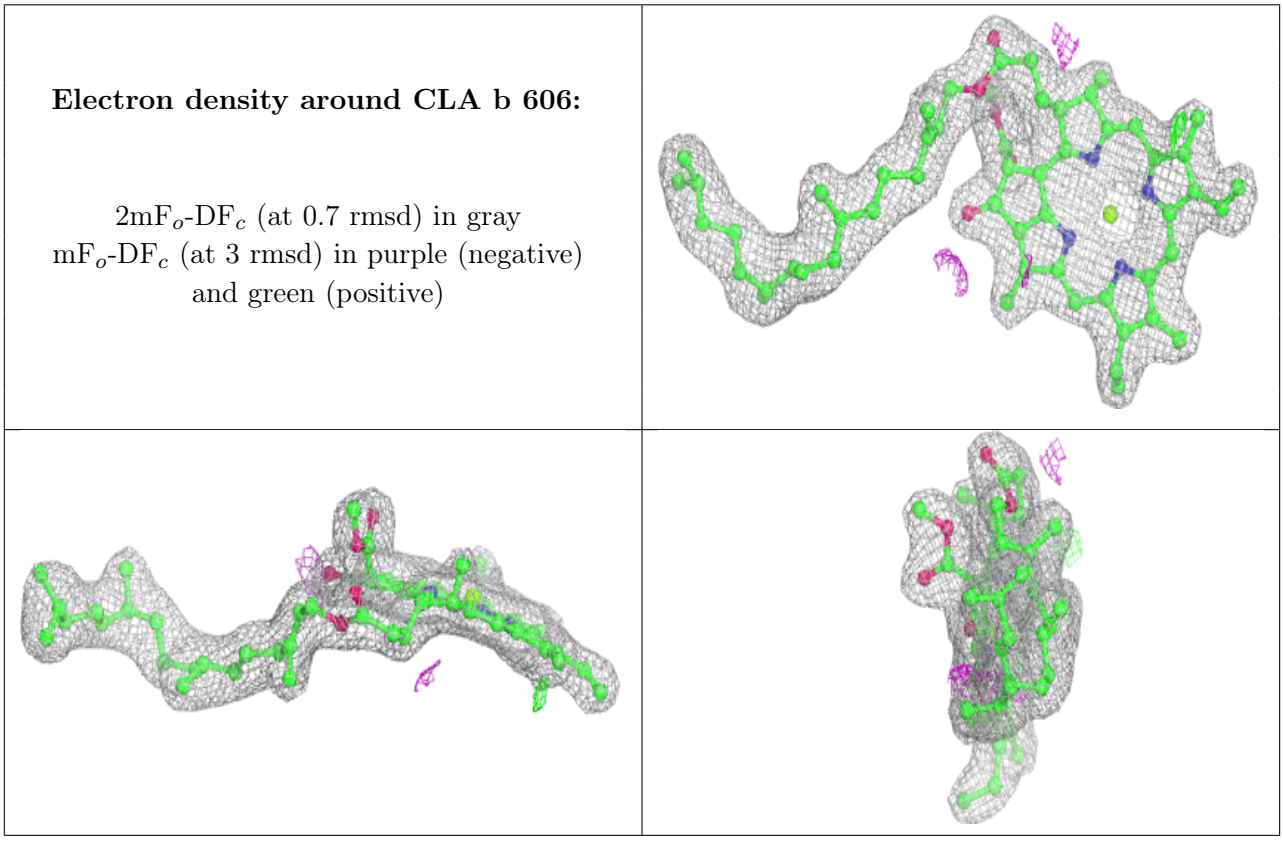
Electron density around BCR C 514:

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



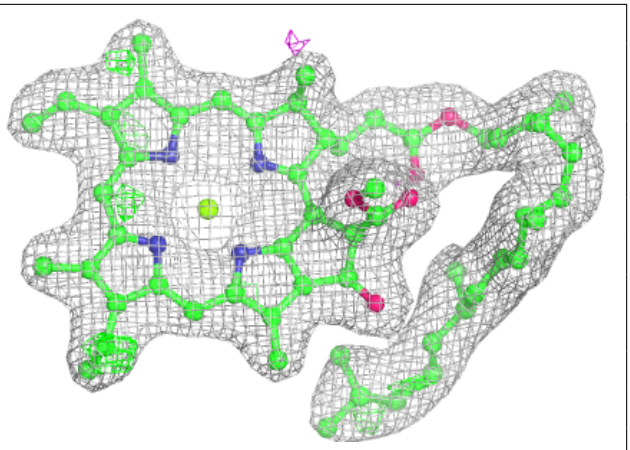
Electron density around CLA b 606:

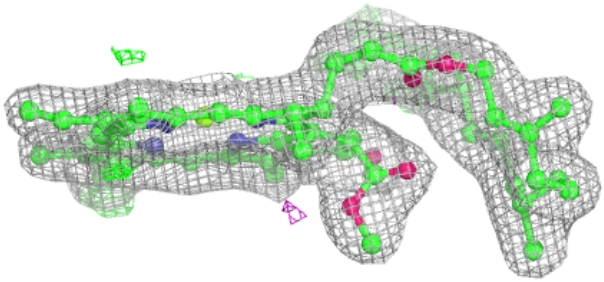
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

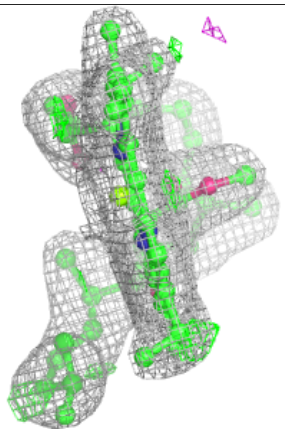


Electron density around CLA B 611:

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

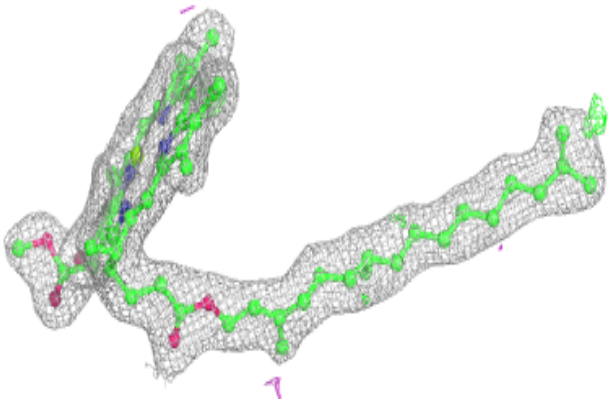


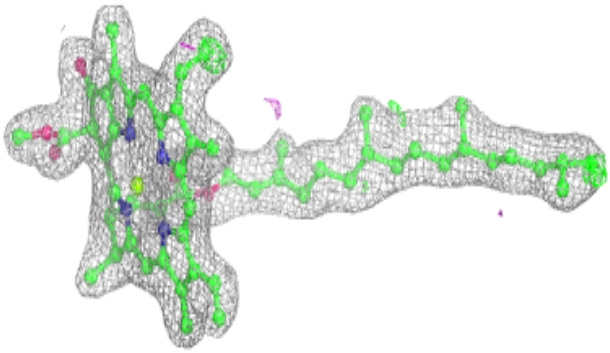


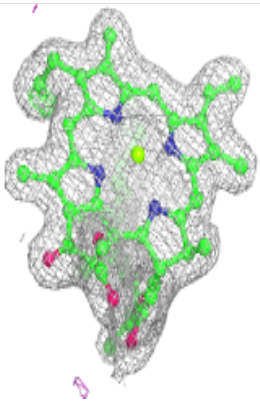


Electron density around CLA b 611:

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

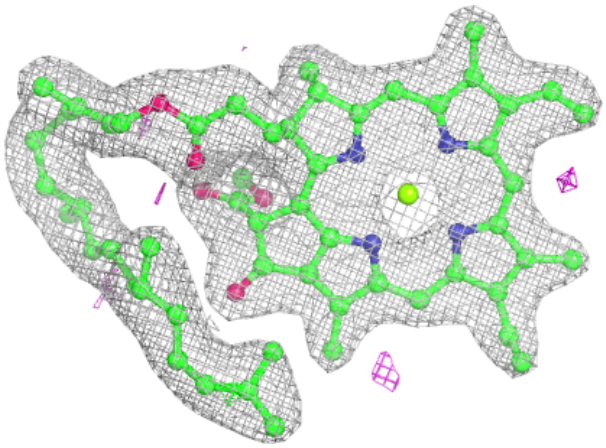


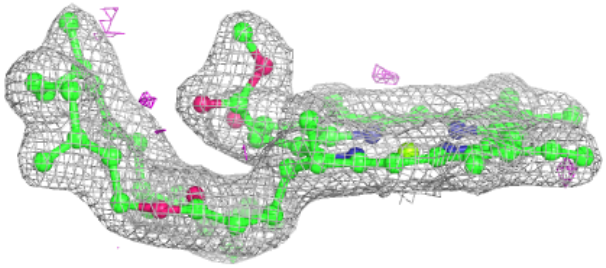


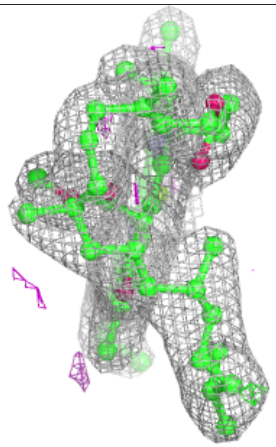


Electron density around CLA b 614:

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

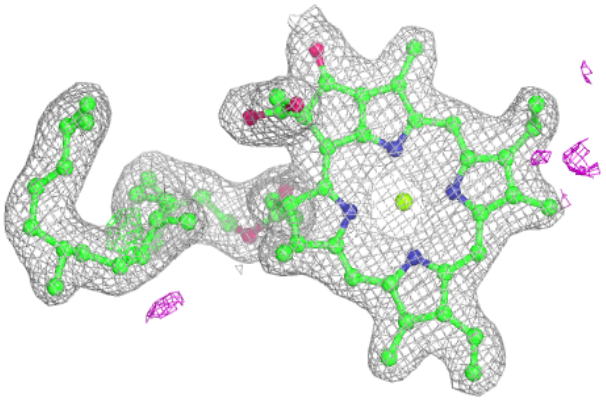


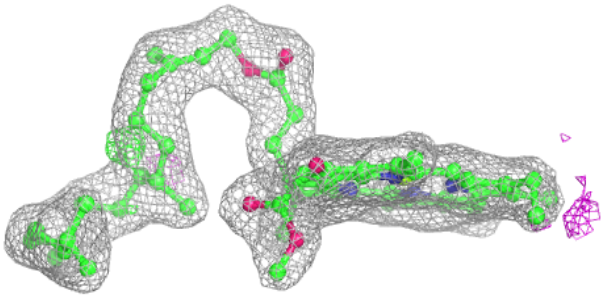


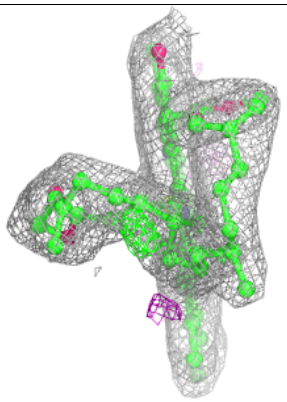


Electron density around CLA b 616:

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

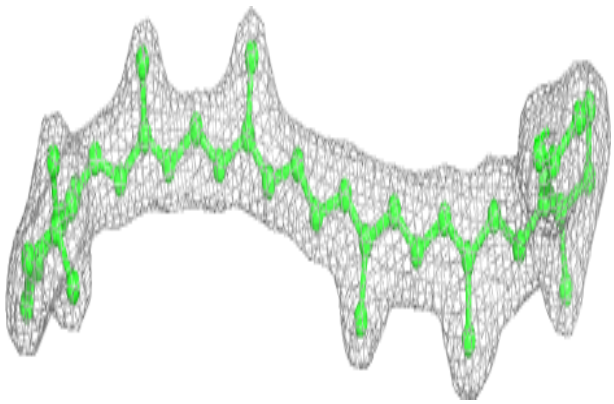


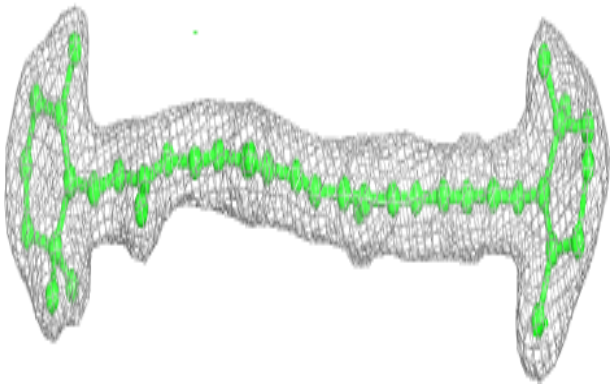


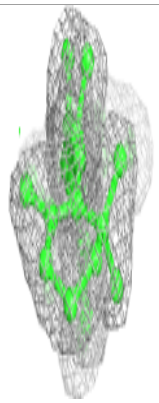


Electron density around BCR a 410:

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

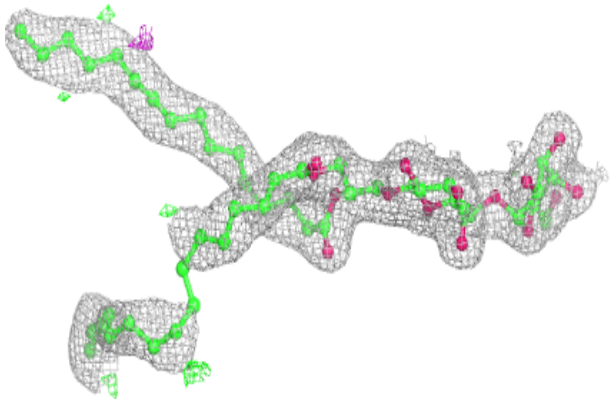


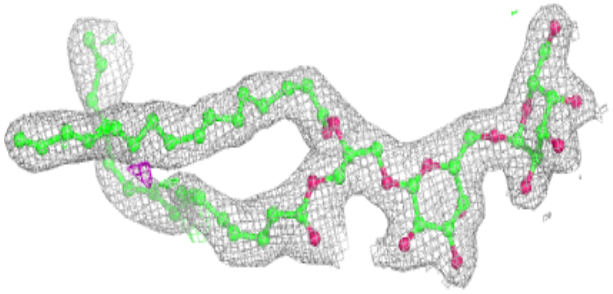


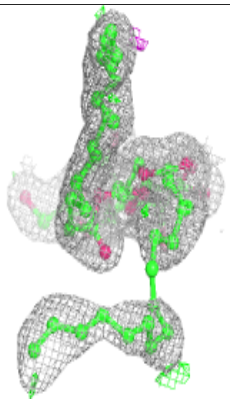


Electron density around DGD C 515:

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

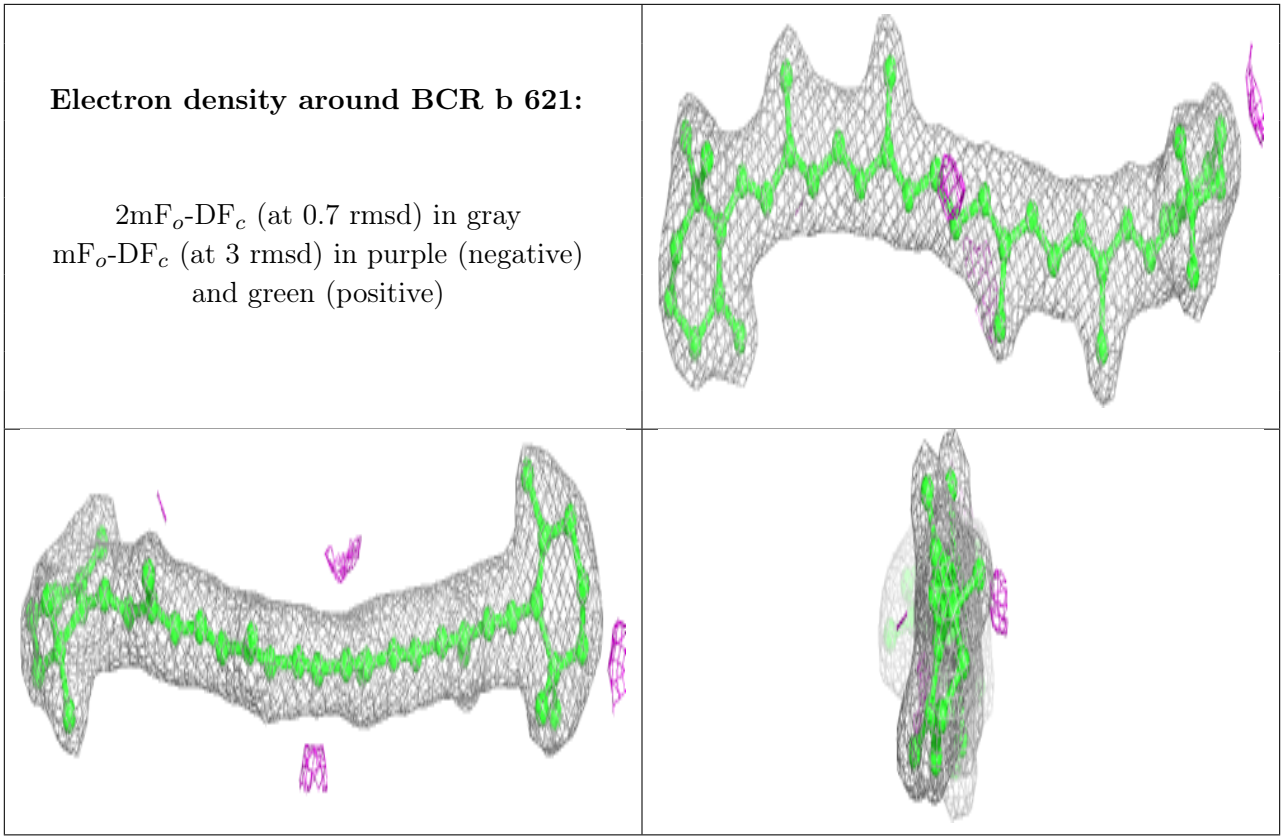






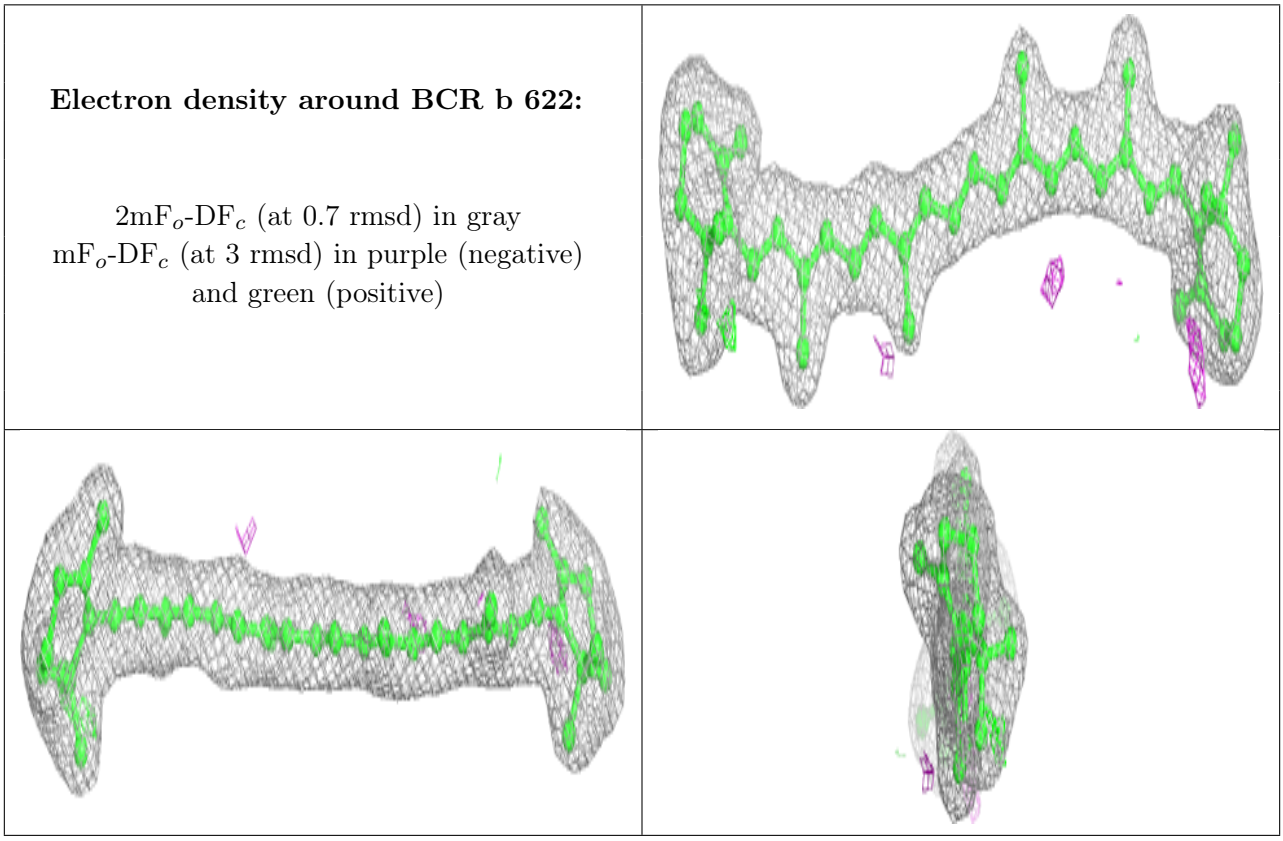
Electron density around BCR b 621:

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



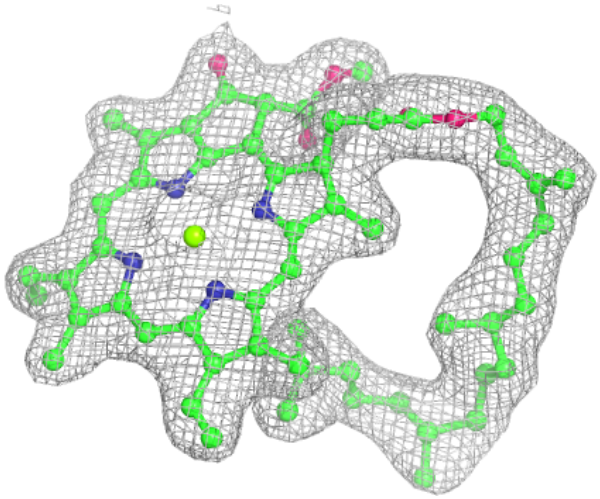
Electron density around BCR b 622:

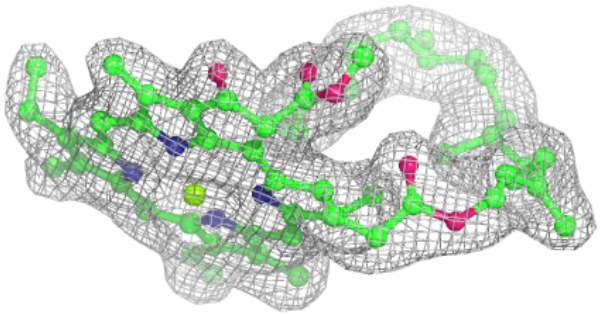
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

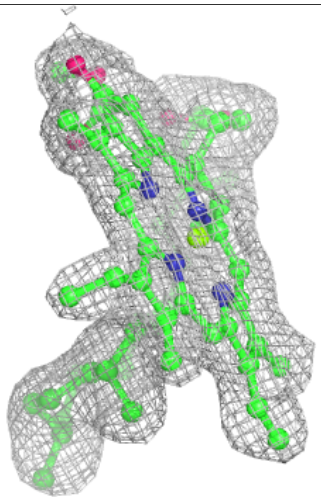


Electron density around CLA b 619:

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

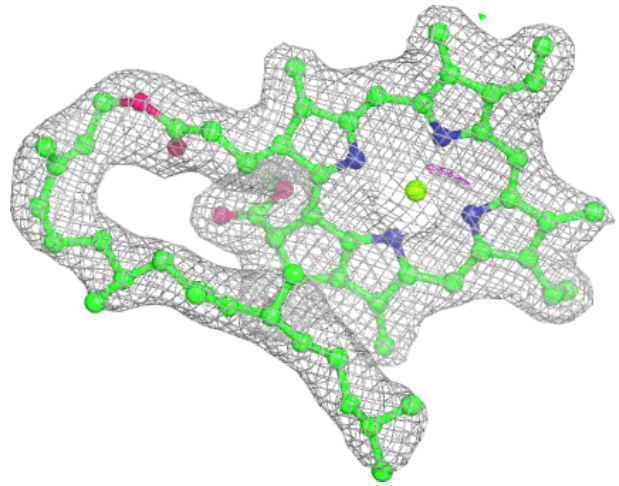


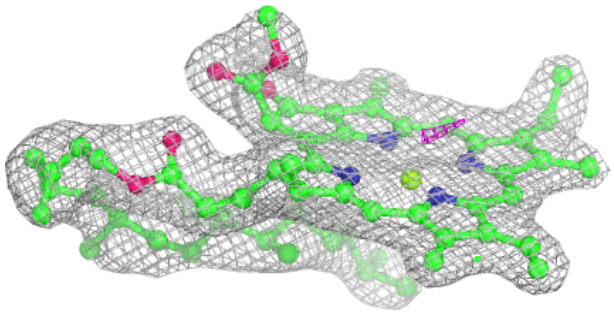


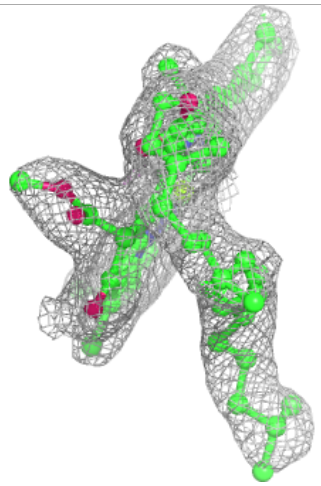


Electron density around CLA C 509:

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

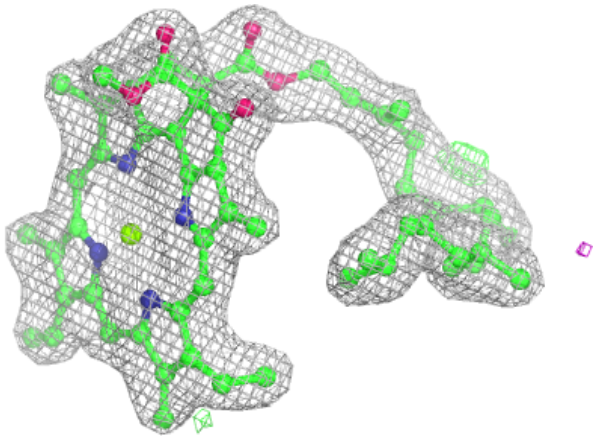


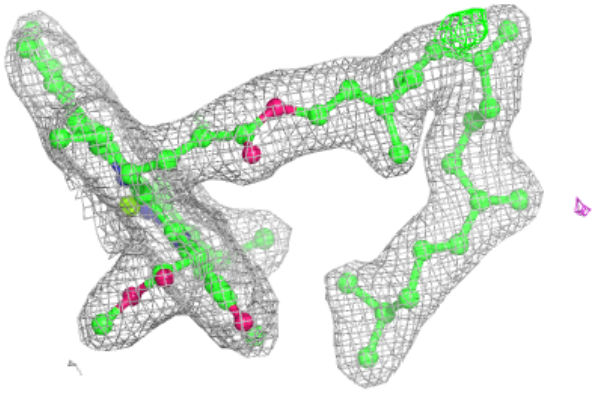


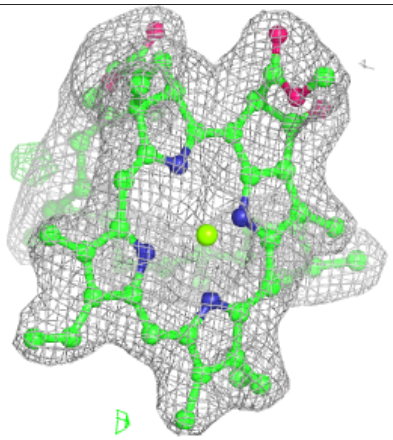


Electron density around CLA c 504:

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

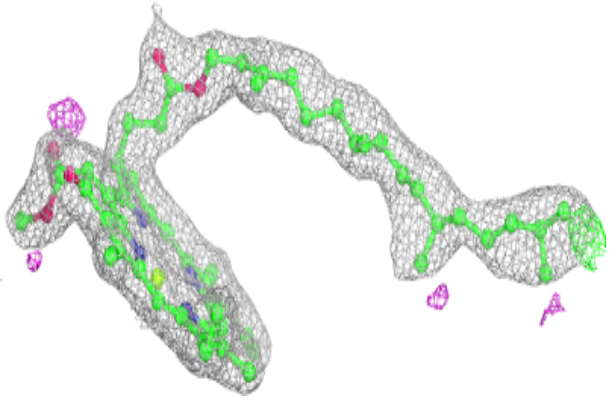


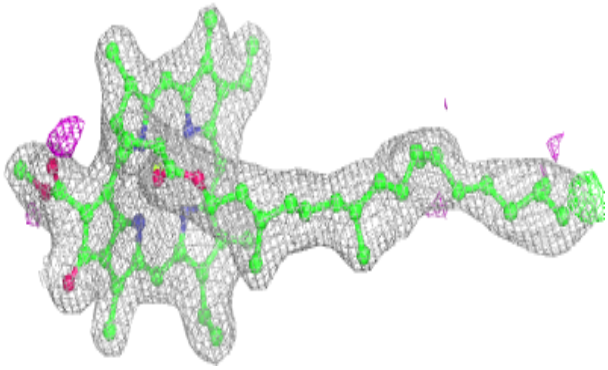


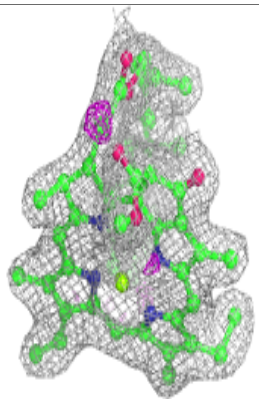


Electron density around CLA c 505:

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

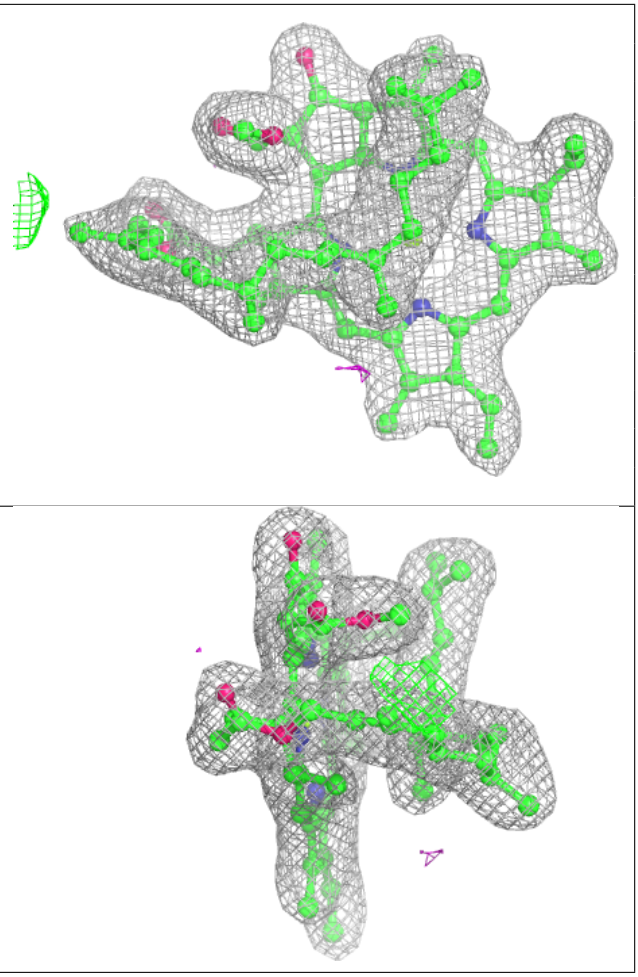






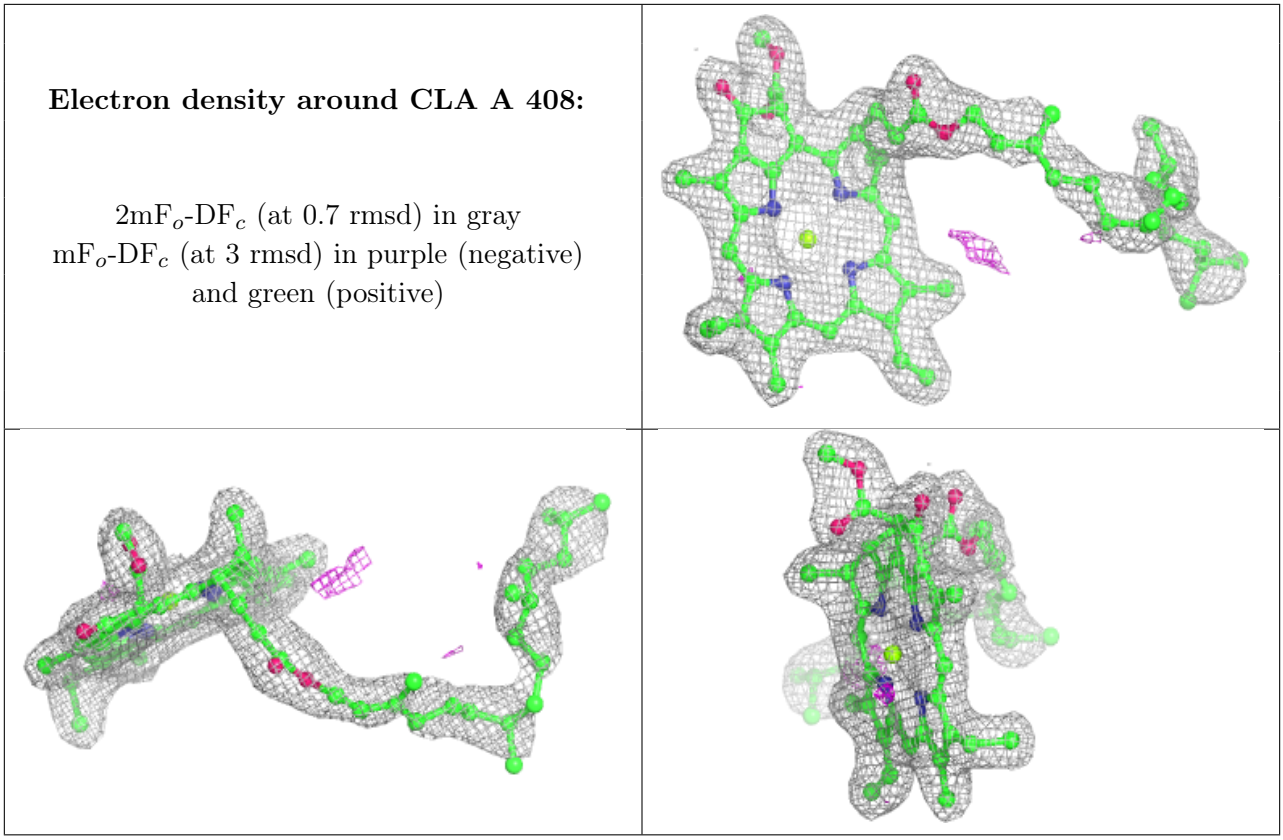
Electron density around CLA C 510:

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



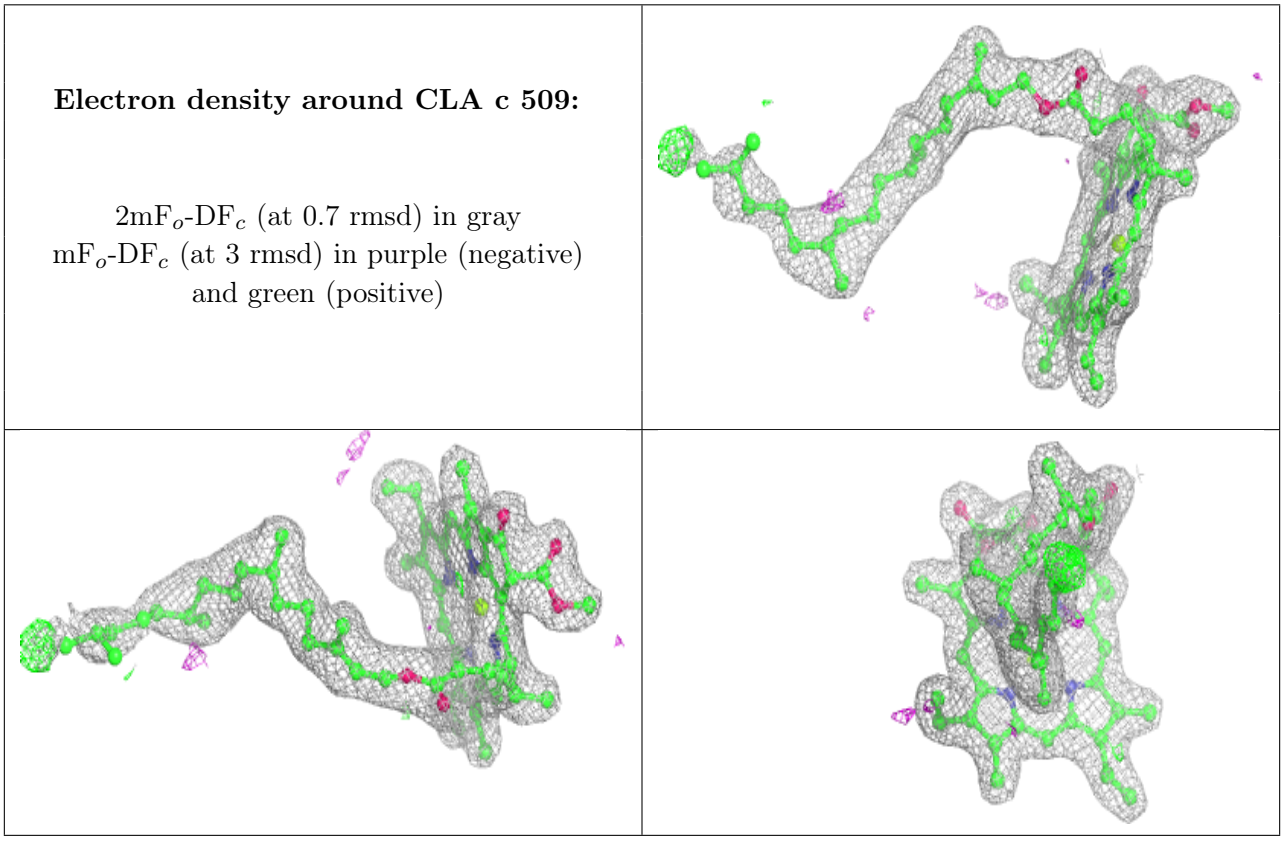
Electron density around CLA A 408:

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



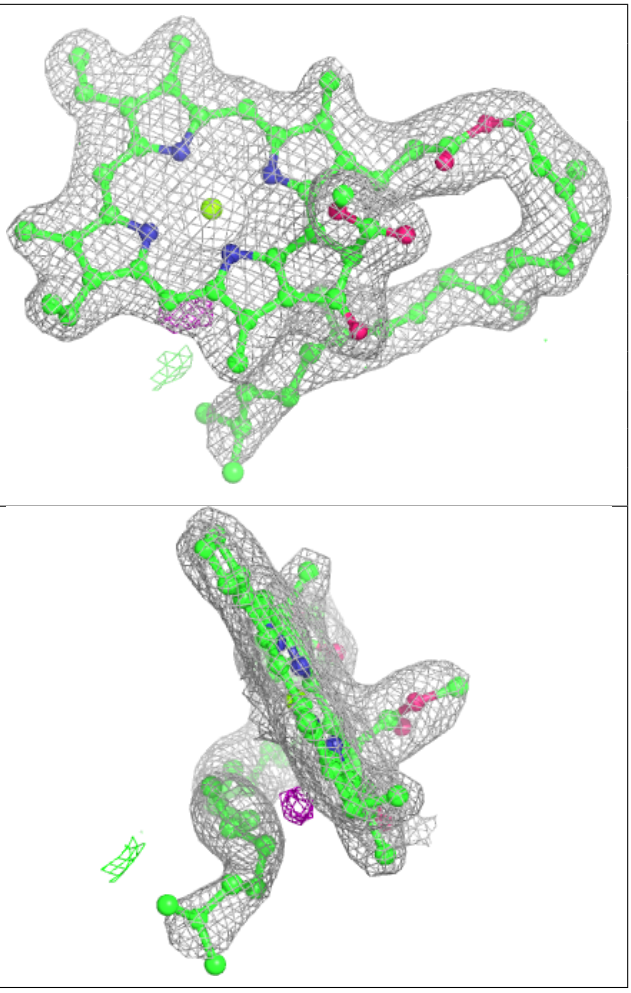
Electron density around CLA c 509:

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



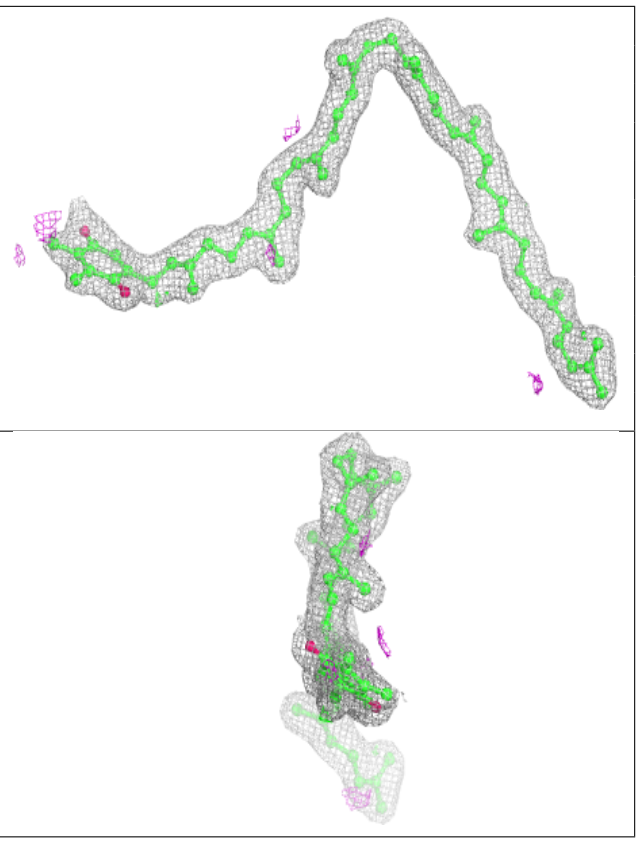
Electron density around CLA c 510:

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



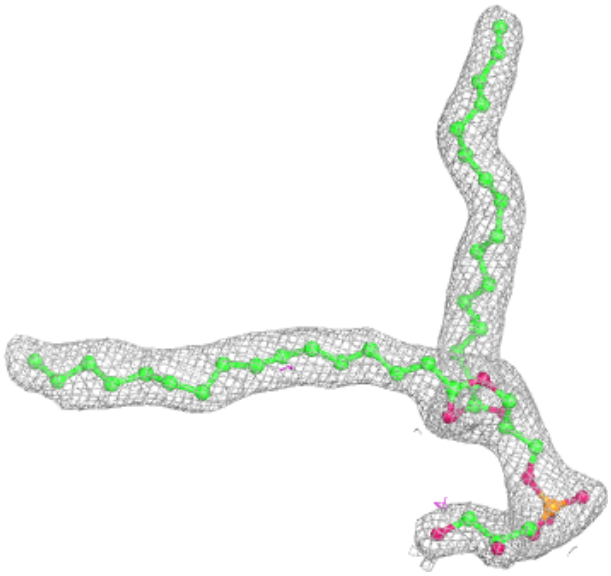
Electron density around PL9 d 407:

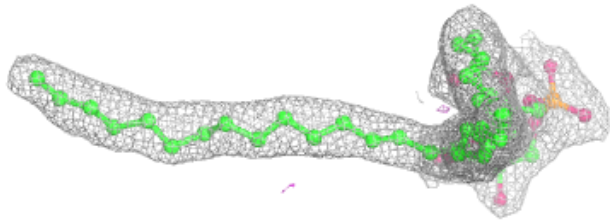
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

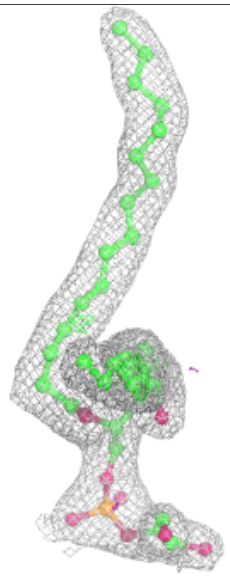


Electron density around LHG b 624:

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

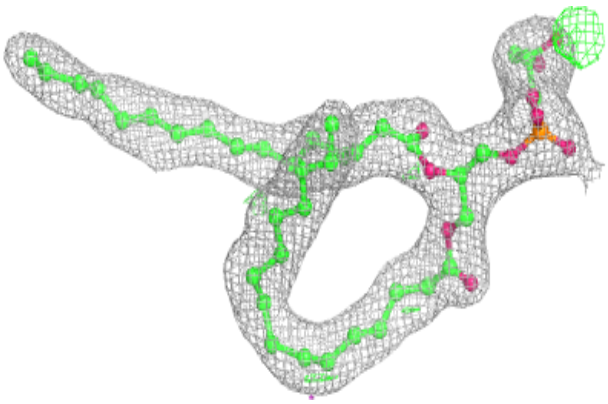


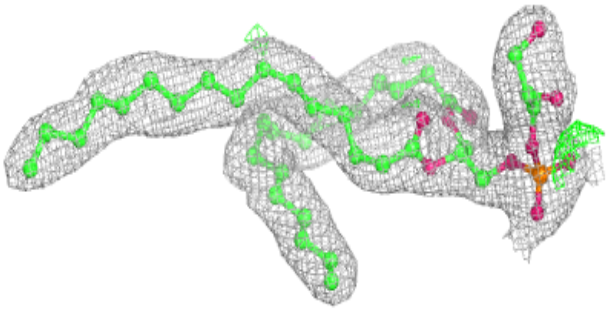


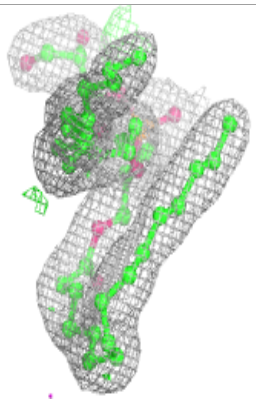


Electron density around LHG d 409:

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

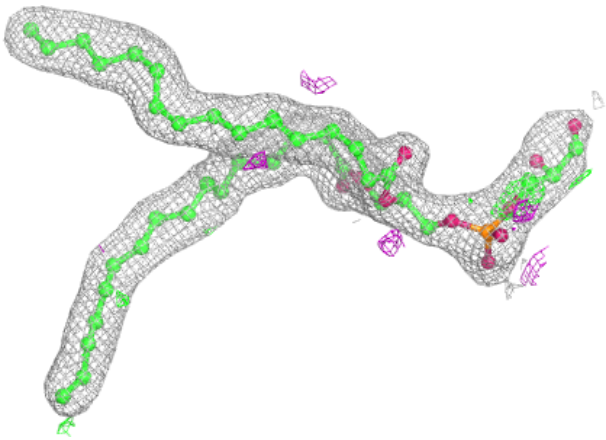


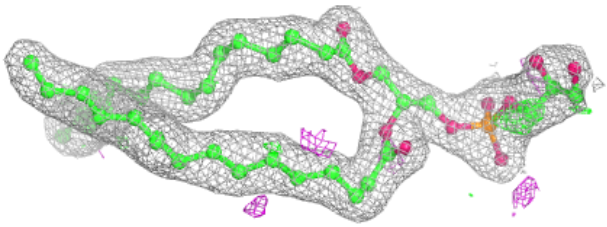


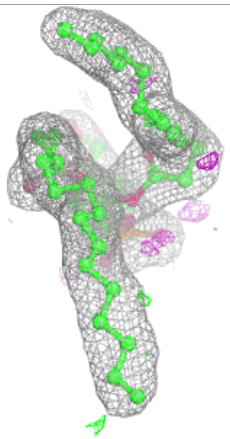


Electron density around LHG d 410:

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

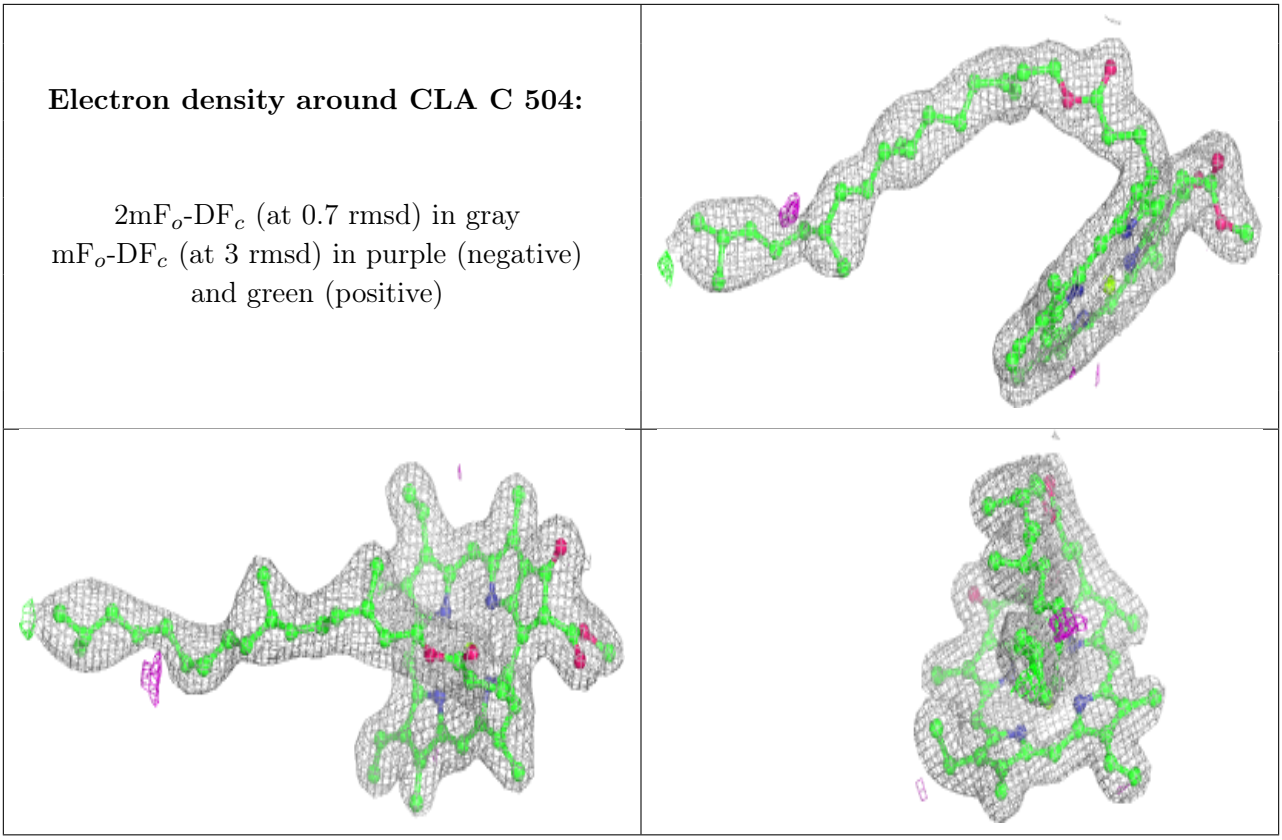






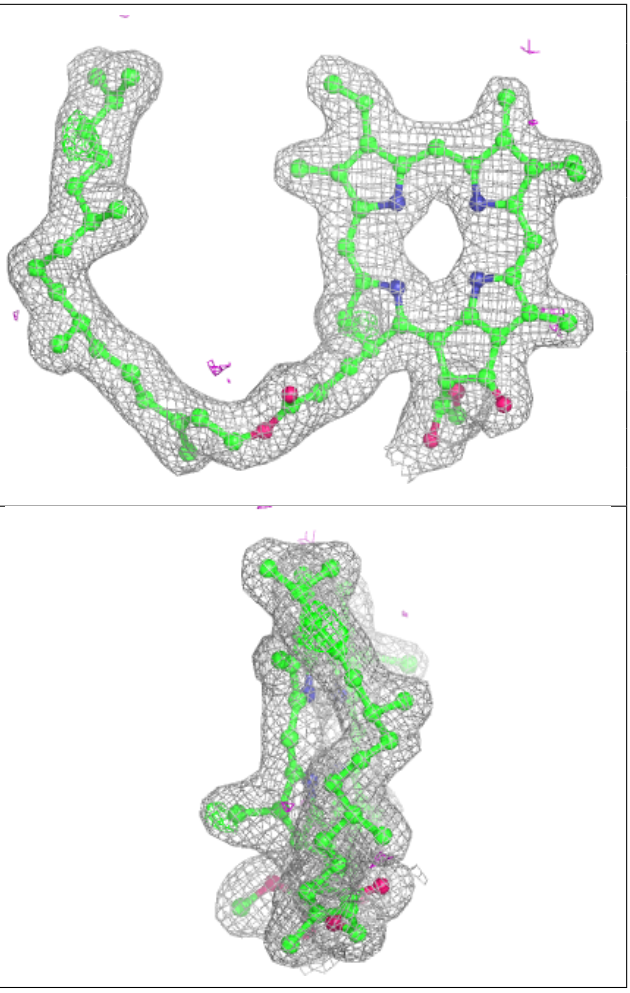
Electron density around CLA C 504:

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



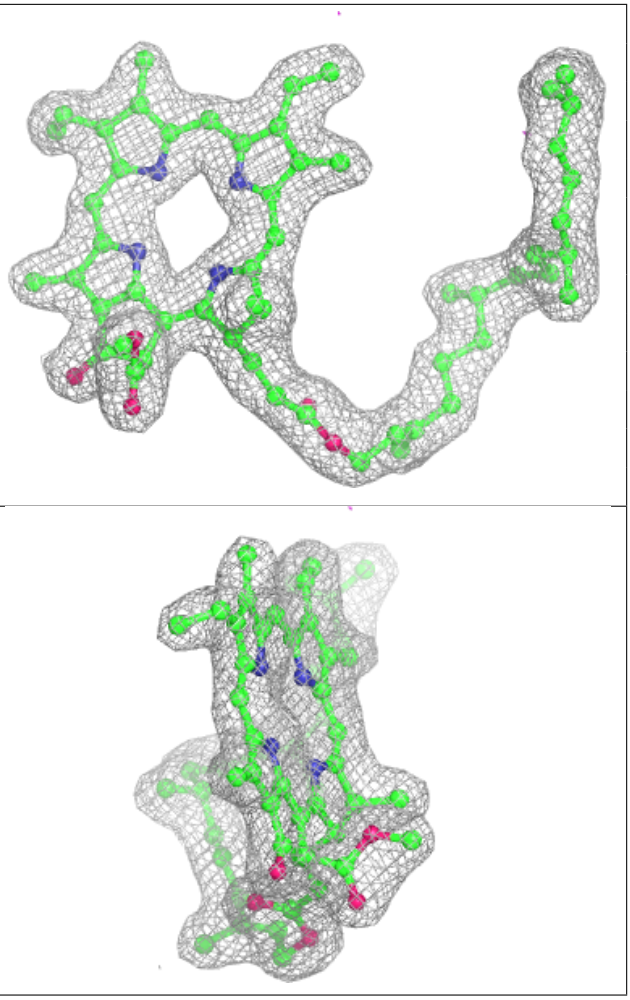
Electron density around PHO A 407:

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



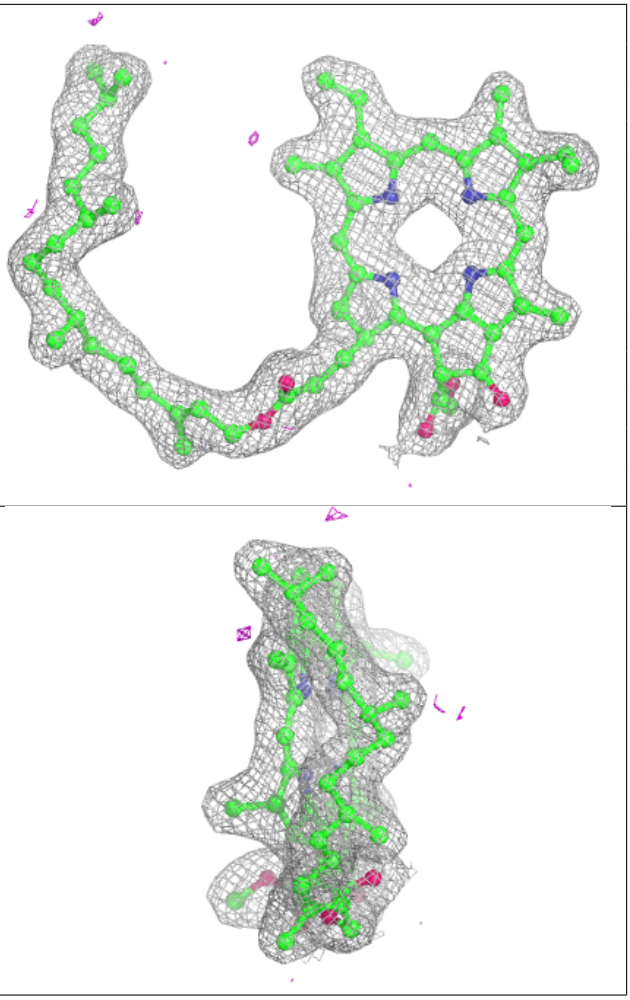
Electron density around PHO D 404:

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



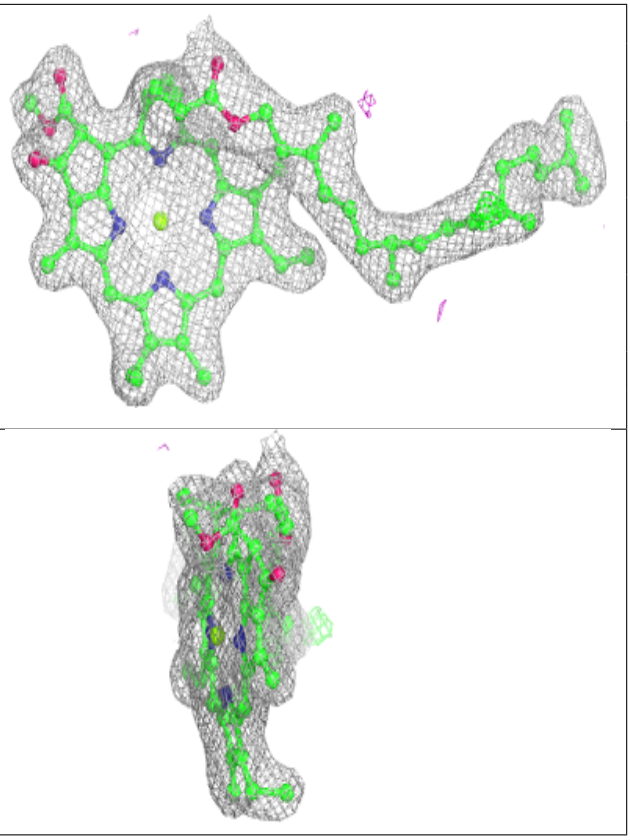
Electron density around PHO a 408:

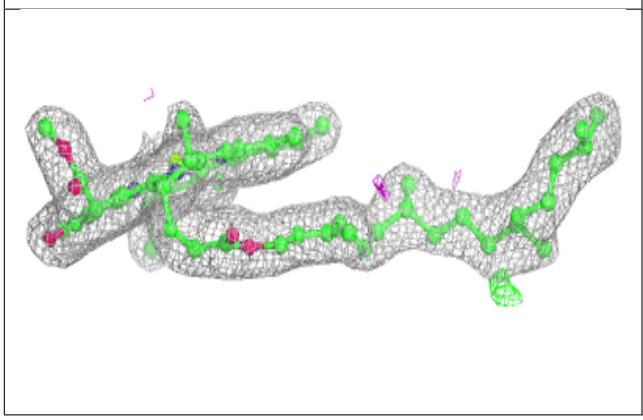
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 607:

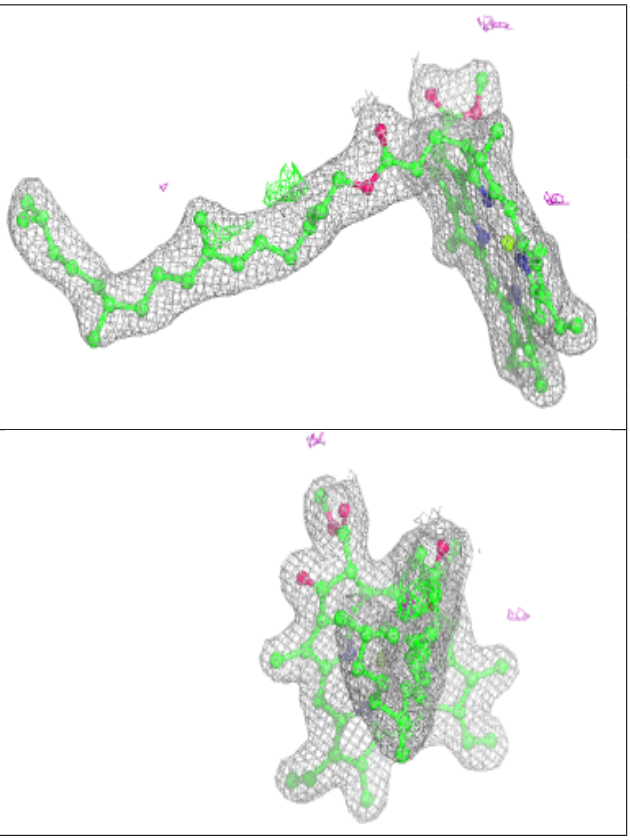
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

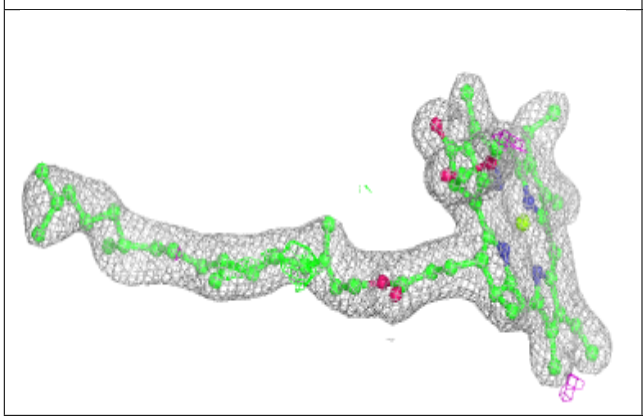




Electron density around CLA b 608:

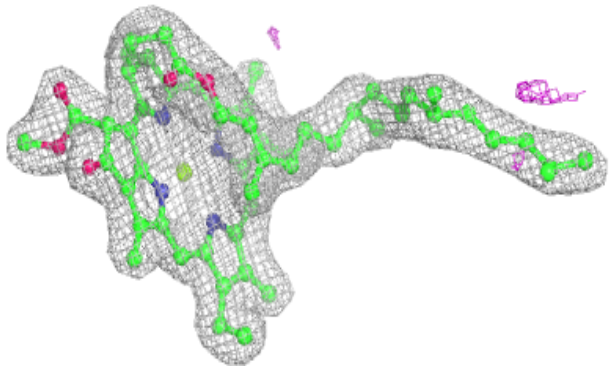
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

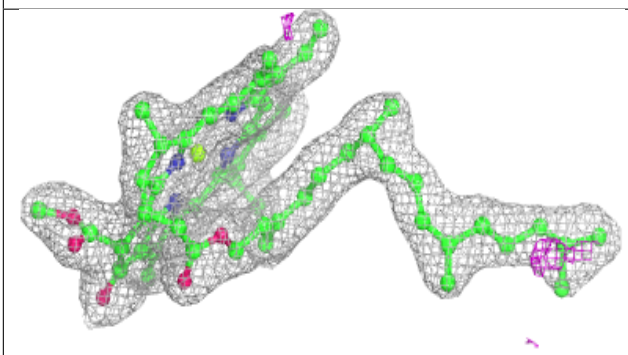


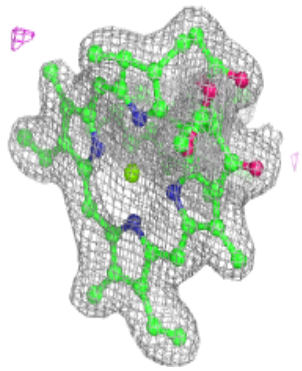


Electron density around CLA C 505:

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

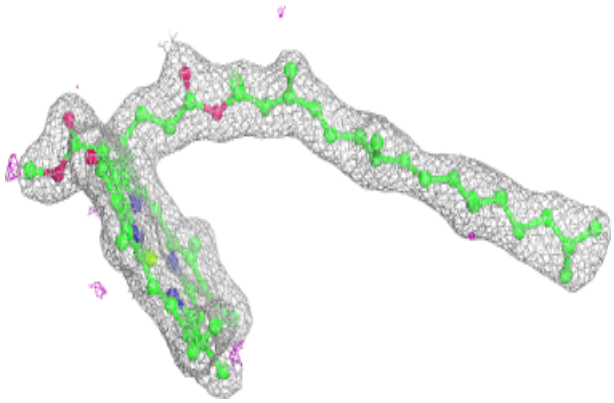


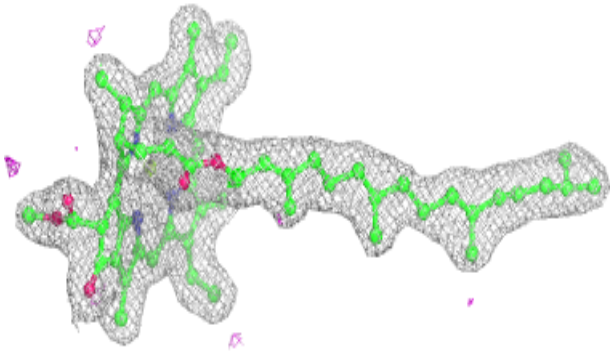


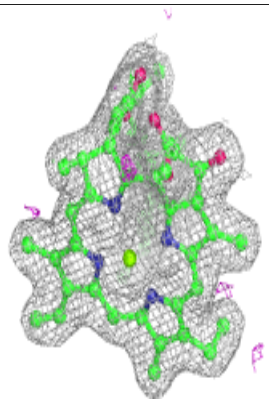


Electron density around CLA B 608:

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

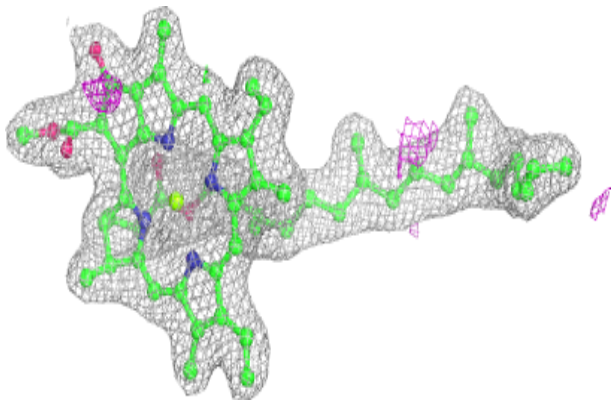


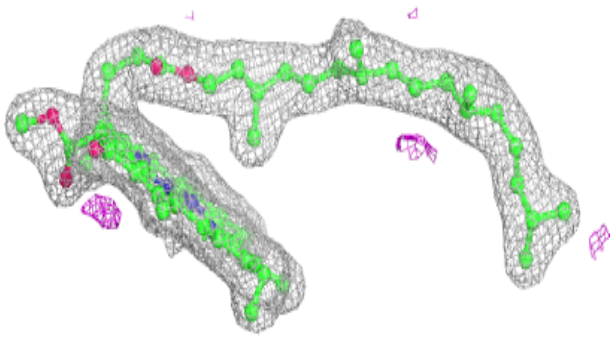


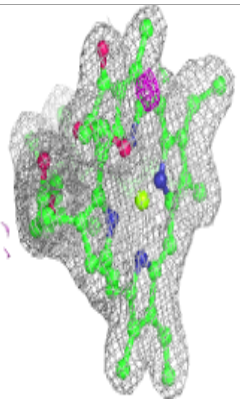


Electron density around CLA b 612:

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

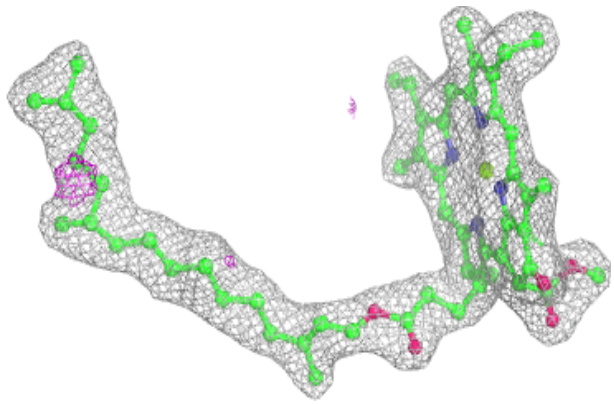


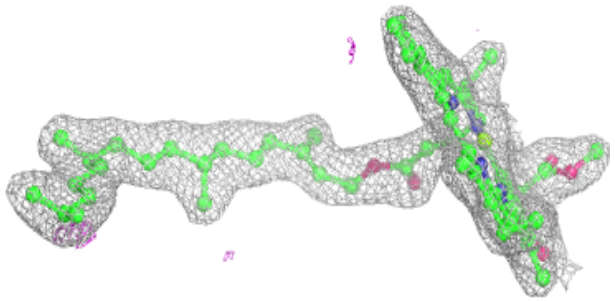


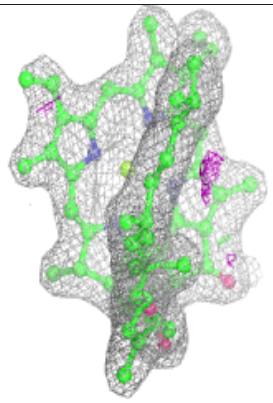


Electron density around CLA b 613:

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

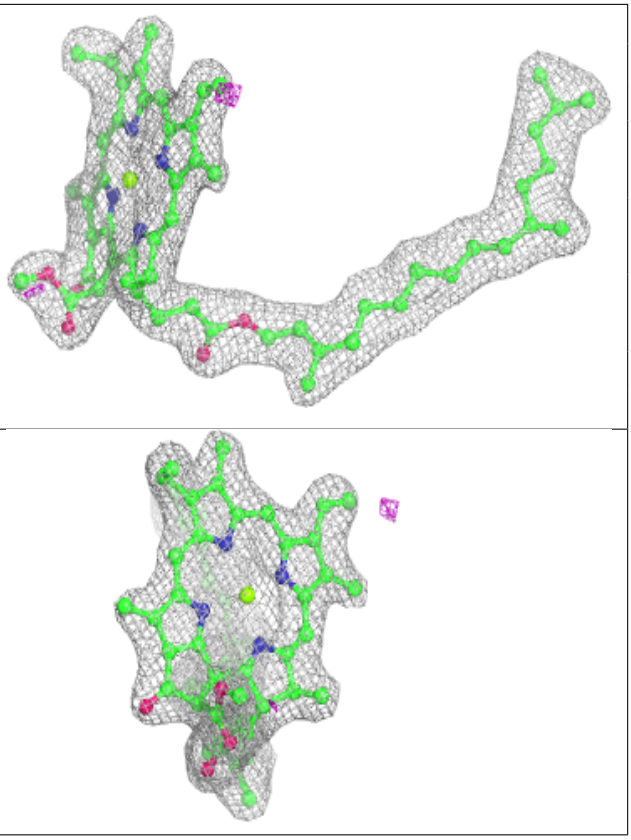


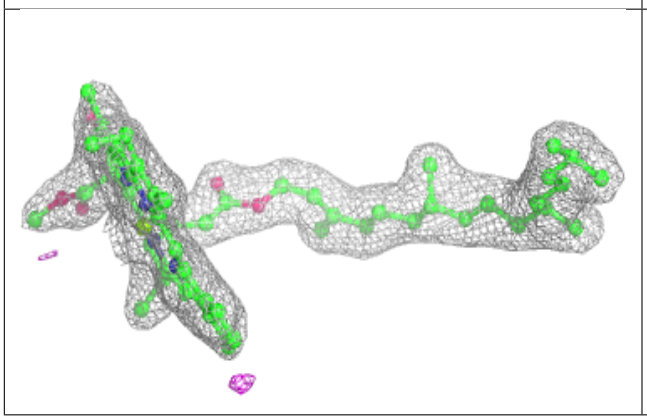




Electron density around CLA B 610:

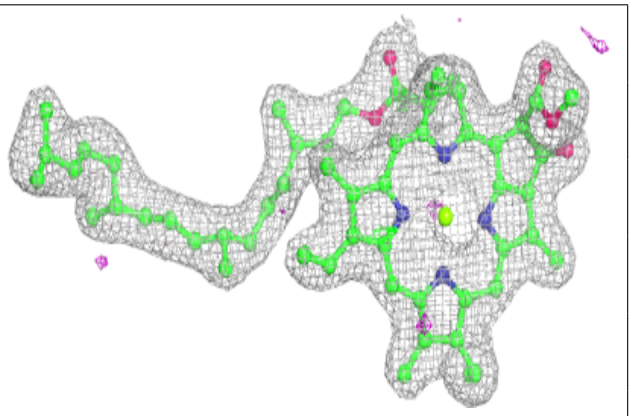
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

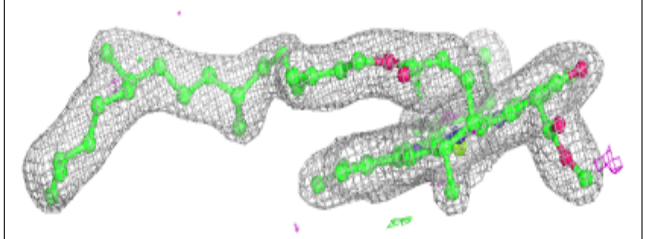


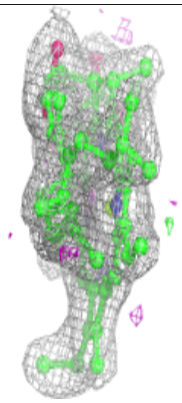


Electron density around CLA B 604:

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

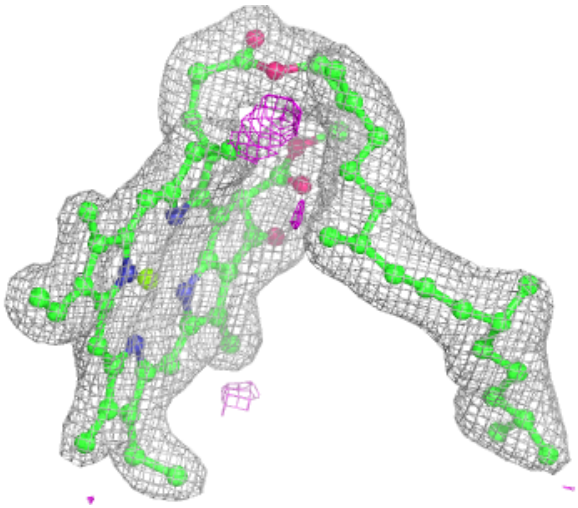


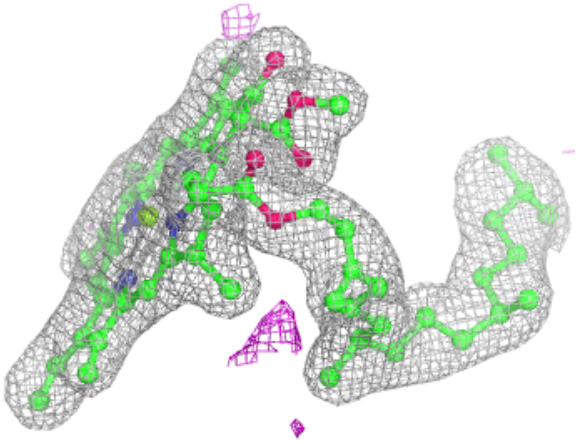


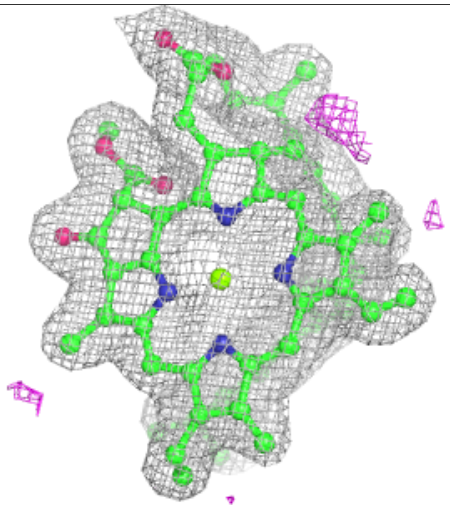


Electron density around CLA b 617:

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

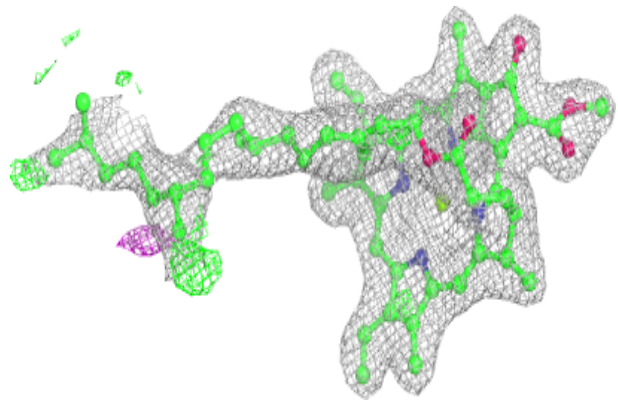


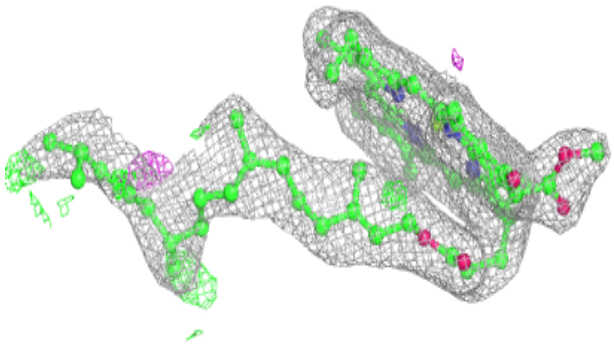


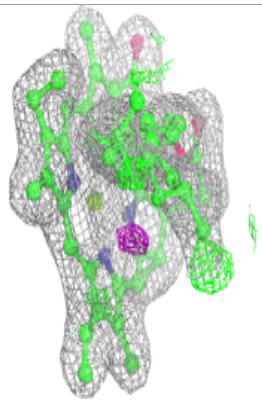


Electron density around CLA b 618:

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

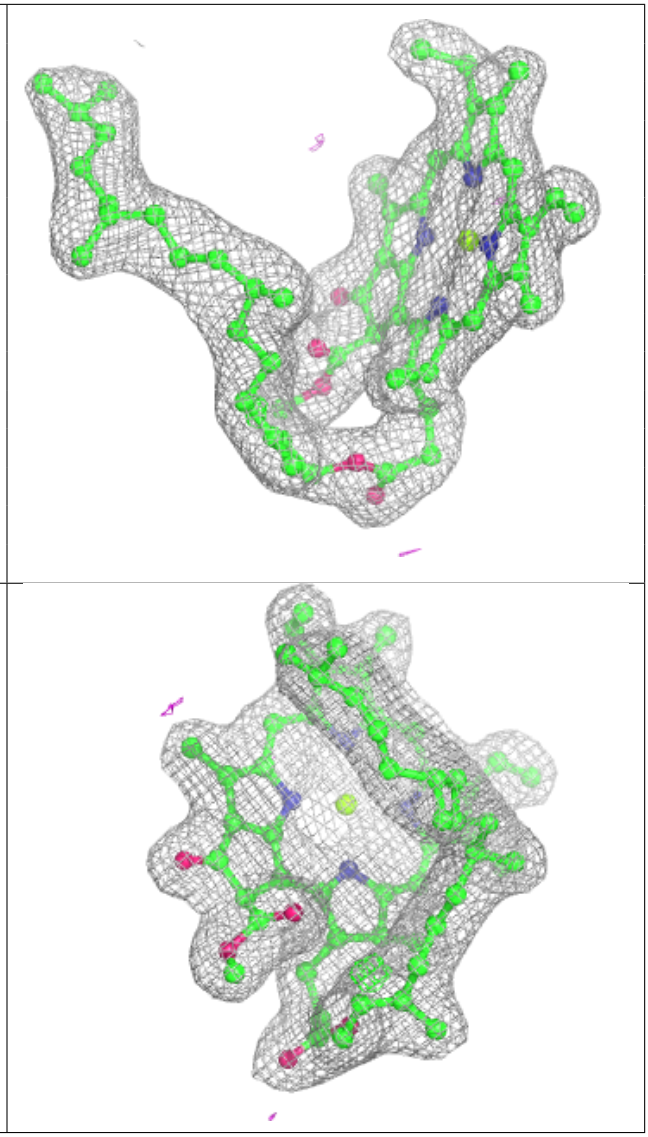






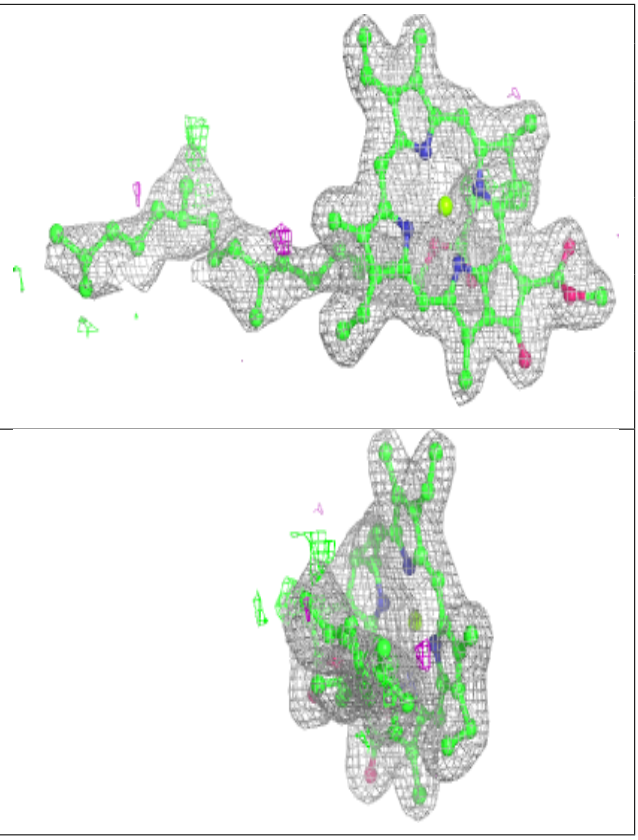
Electron density around CLA B 614:

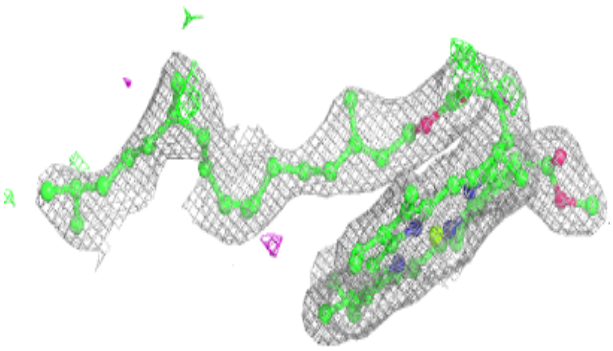
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 615:

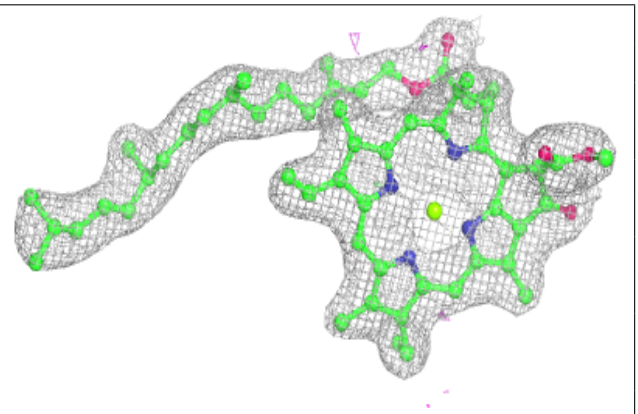
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

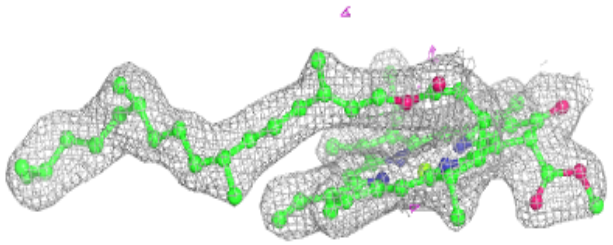


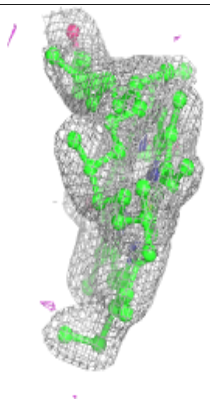


Electron density around CLA c 502:

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

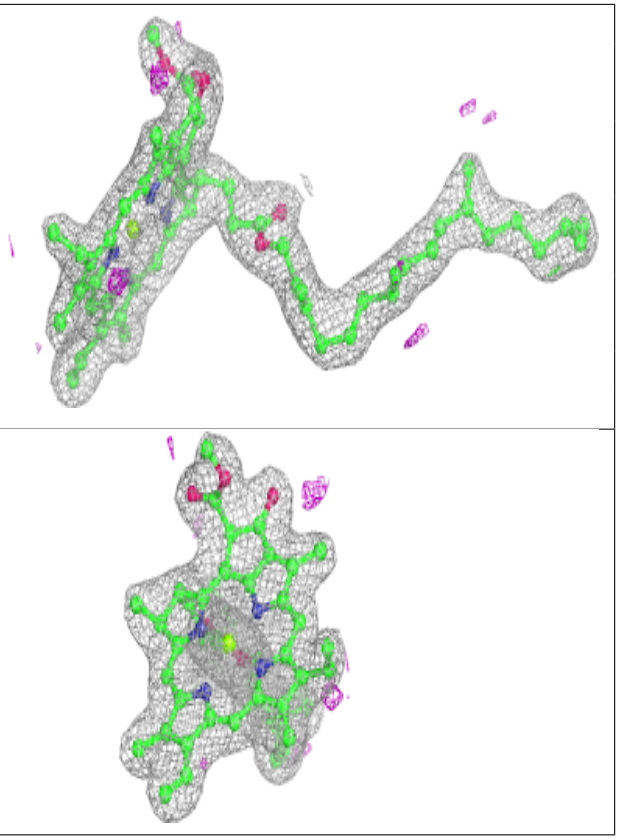


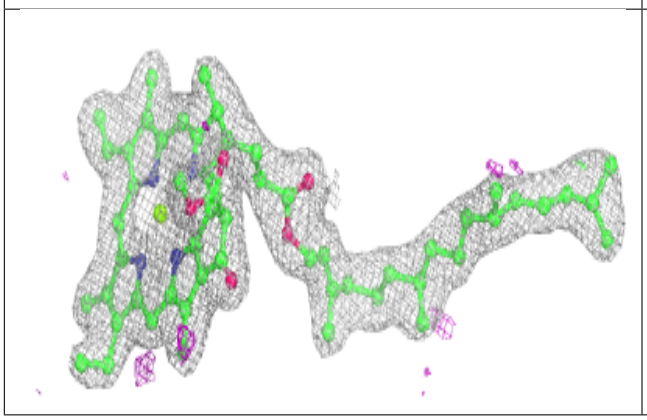




Electron density around CLA c 503:

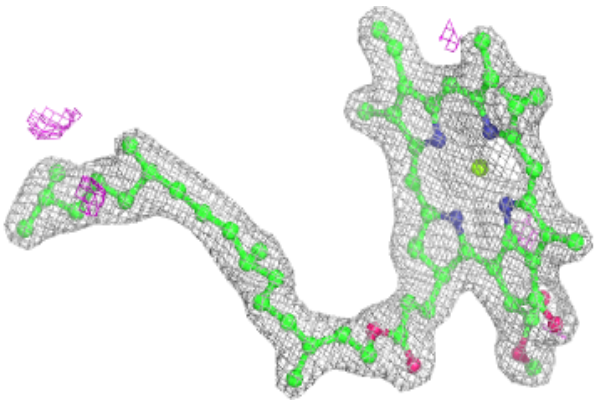
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

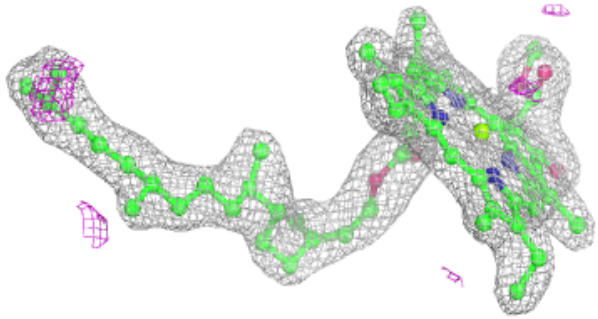


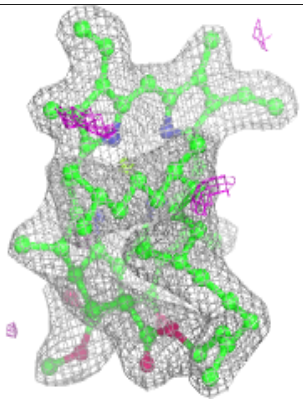


Electron density around CLA C 511:

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

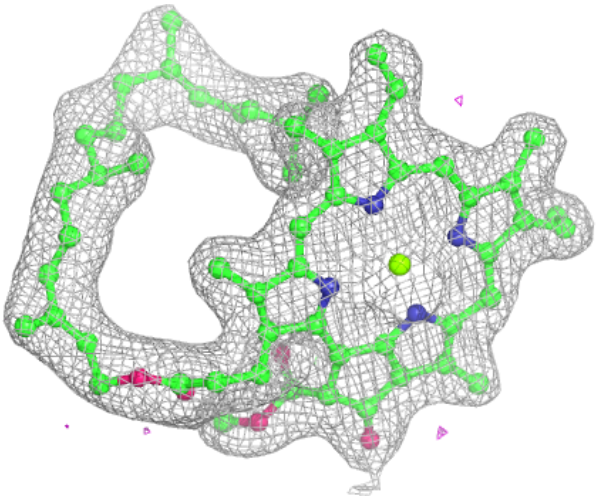


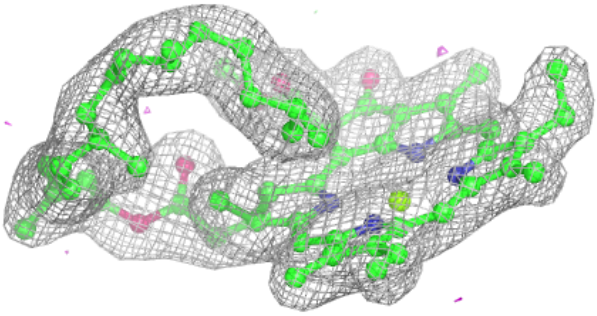


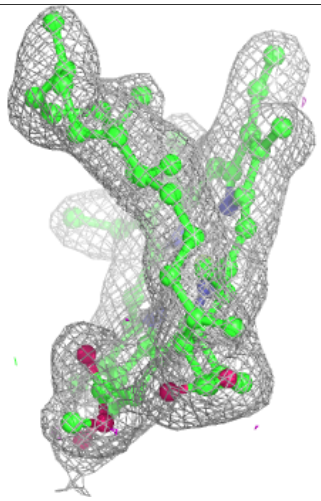


Electron density around CLA B 616:

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

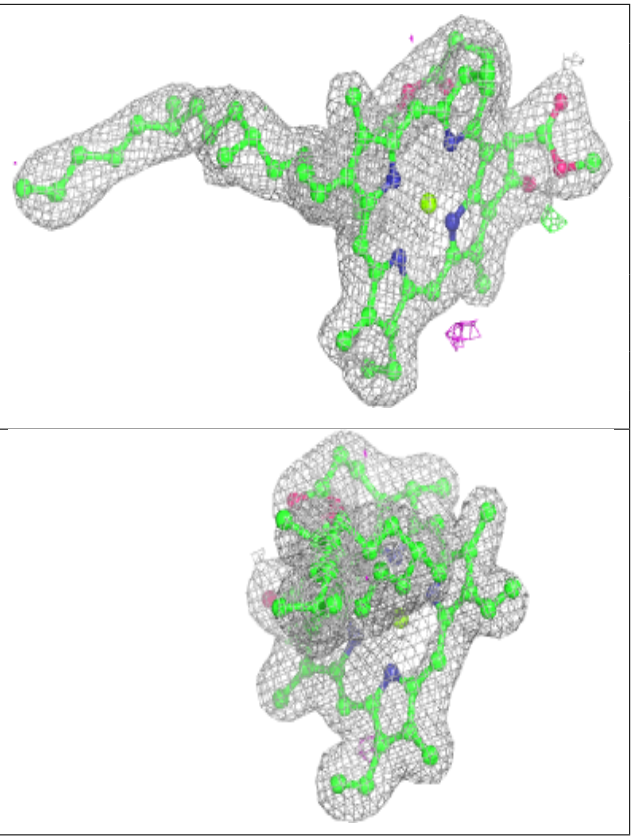


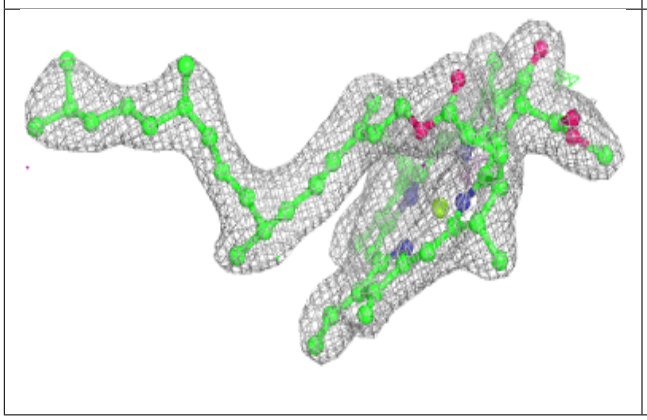




Electron density around CLA c 506:

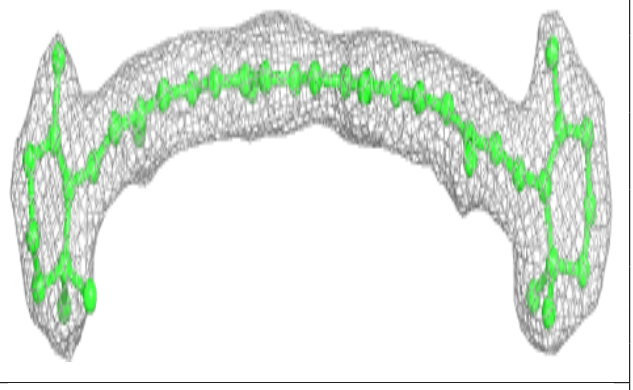
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

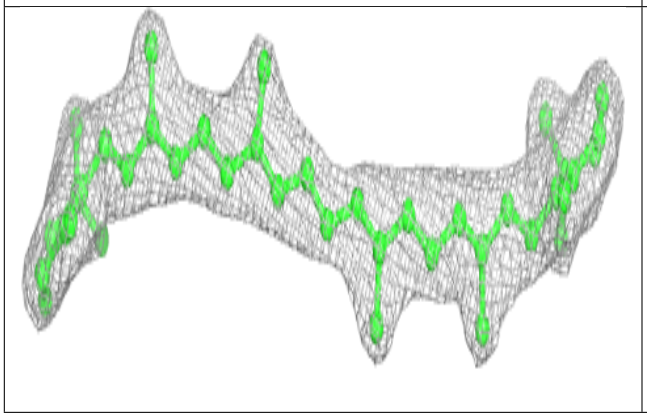


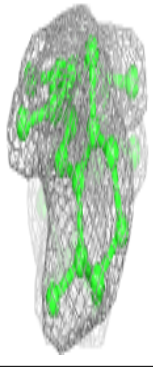


Electron density around BCR k 101:

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

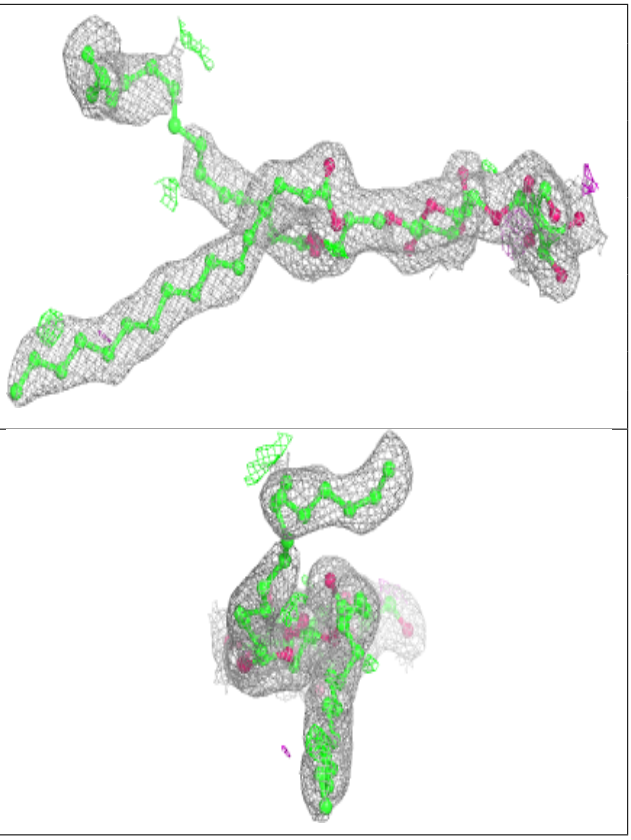






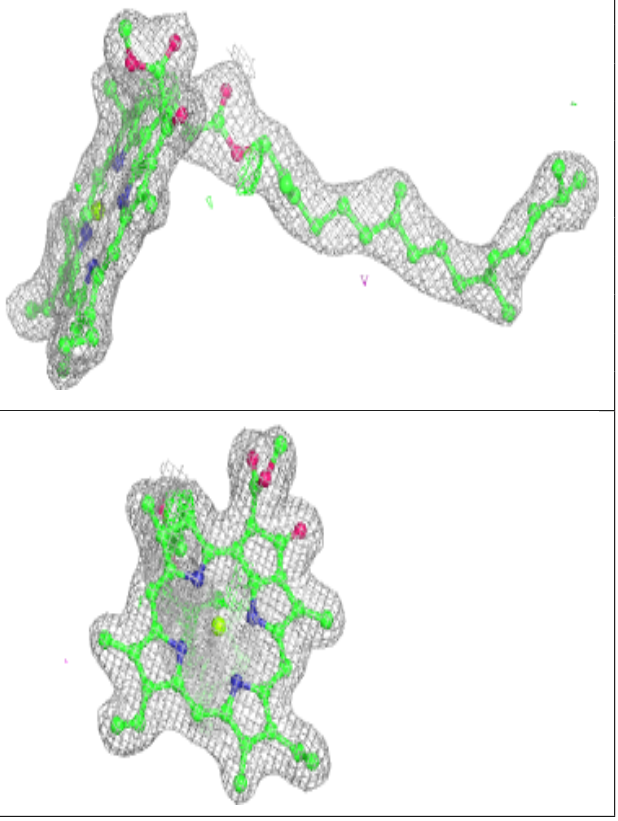
Electron density around DGD c 517:

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



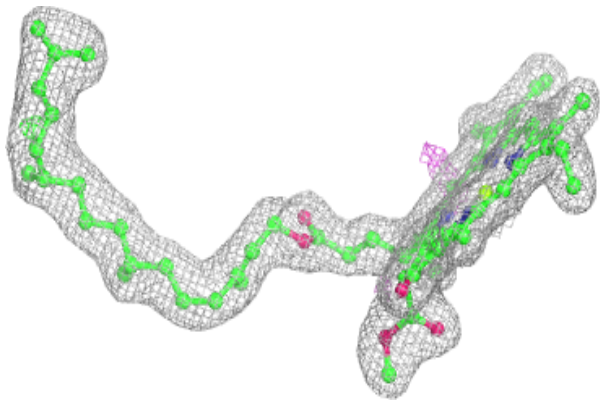
Electron density around CLA B 605:

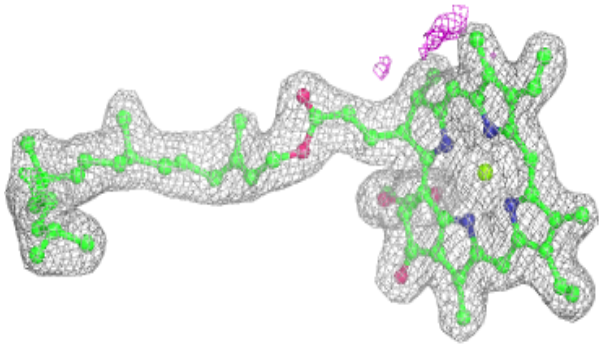
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

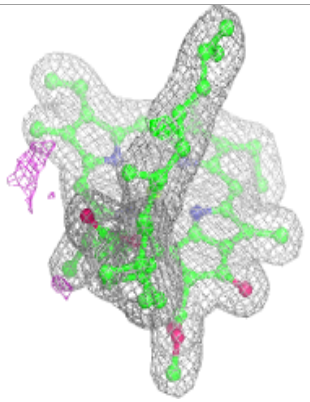


Electron density around CLA D 403:

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

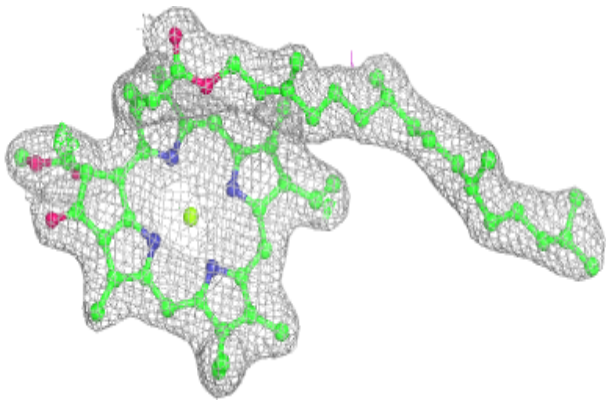


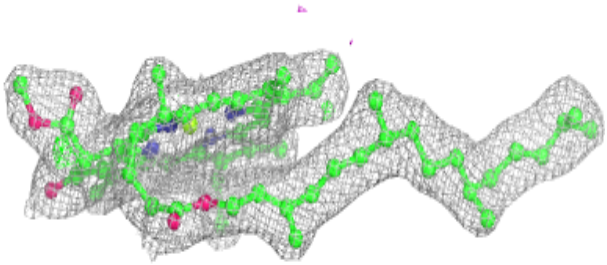


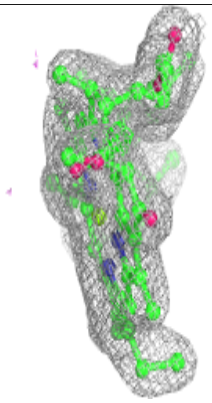


Electron density around CLA C 501:

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

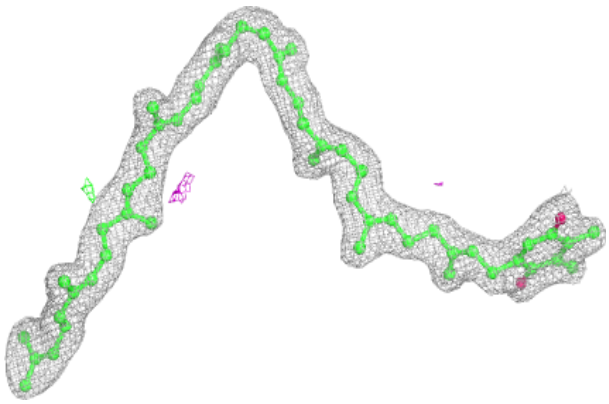


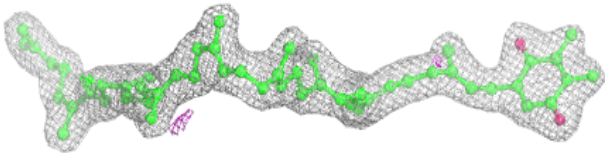


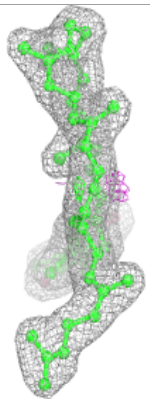


Electron density around PL9 D 407:

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

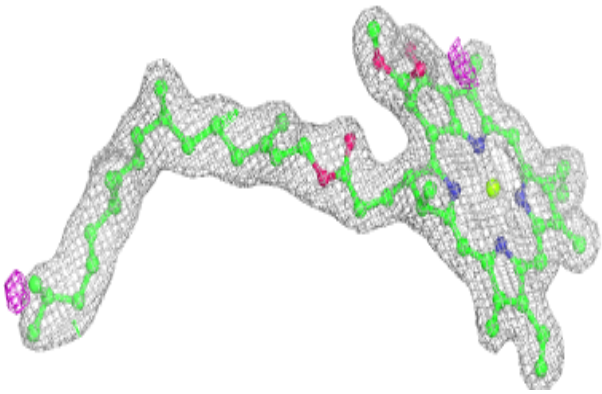


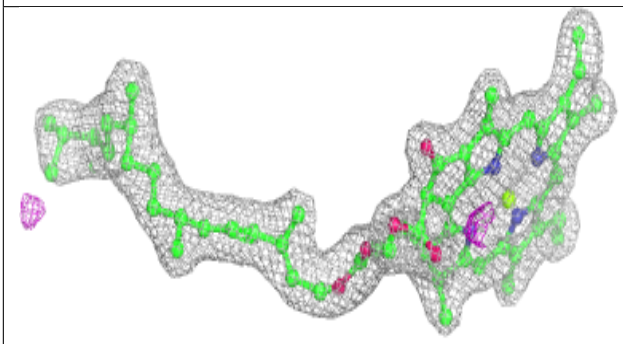


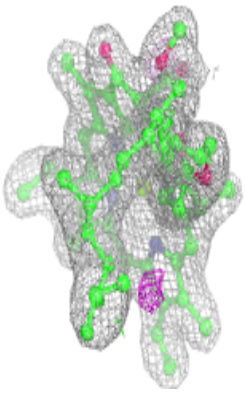


Electron density around CLA a 406:

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

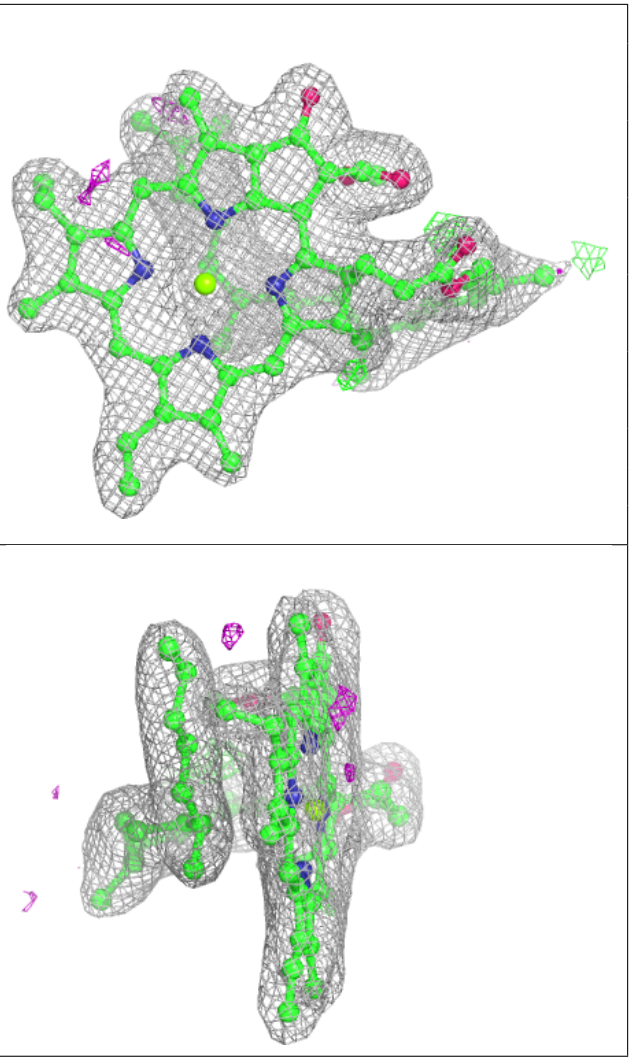






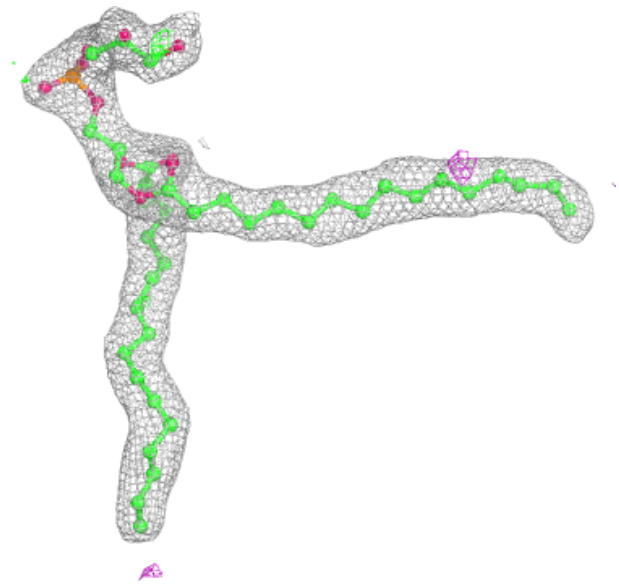
Electron density around CLA c 511:

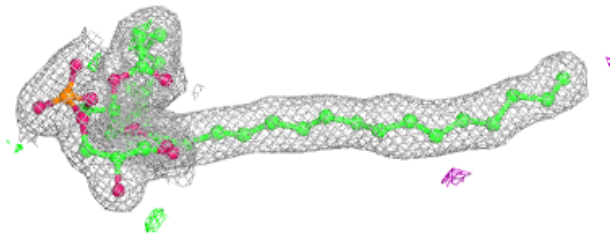
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

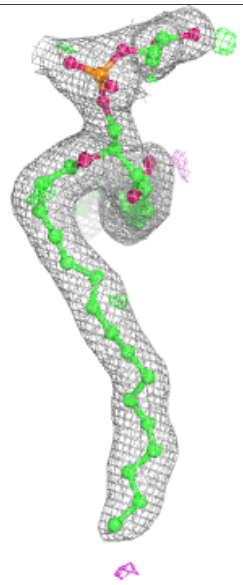


Electron density around LHG B 621:

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

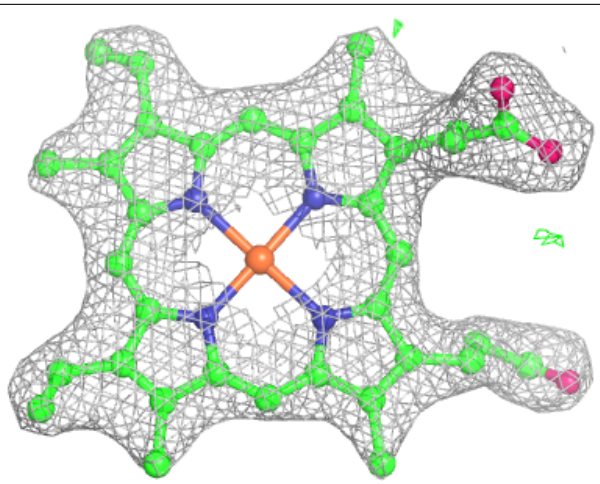


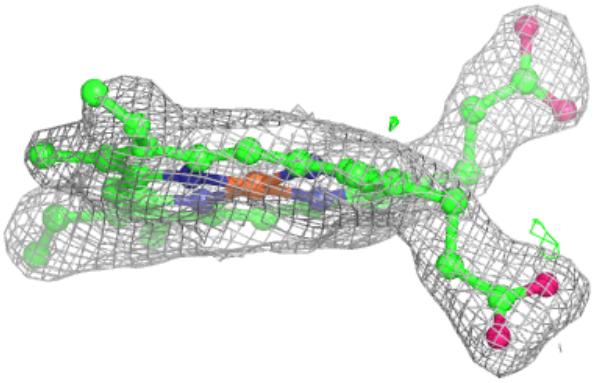


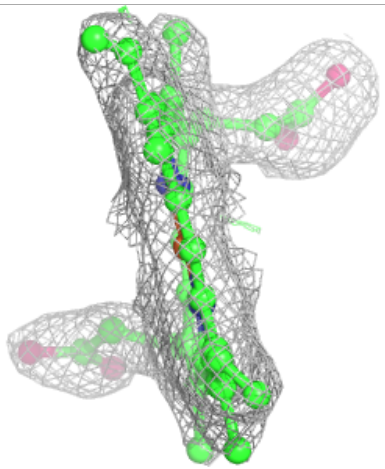


Electron density around HEM F 101:

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

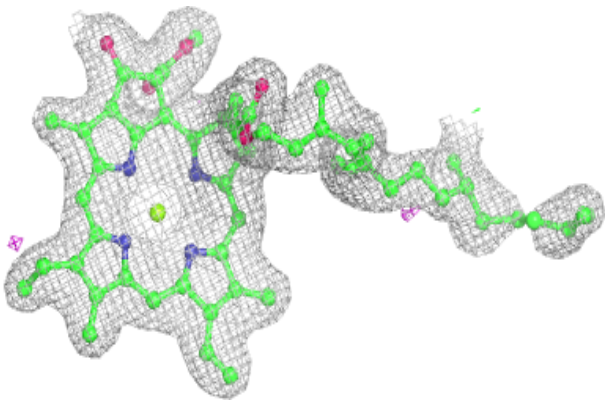


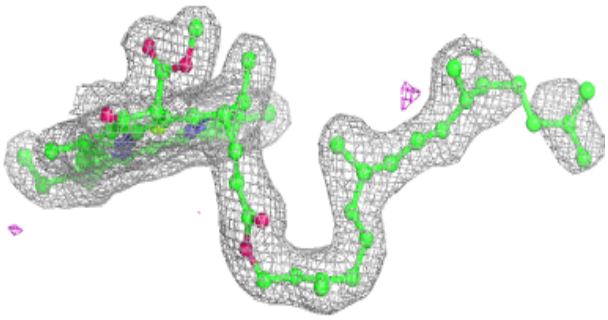


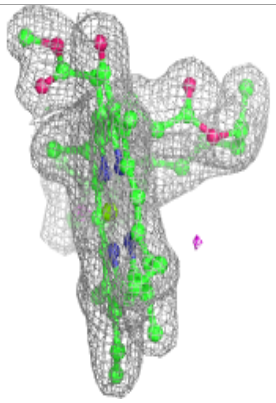


Electron density around CLA a 407:

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

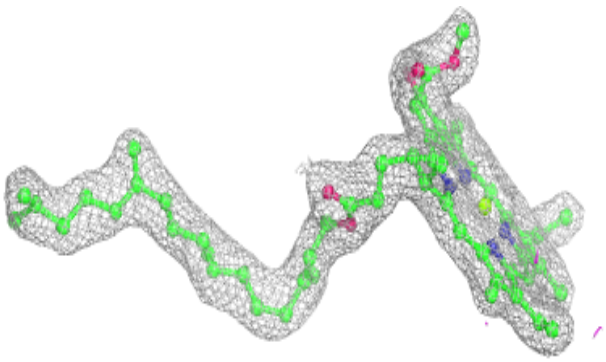


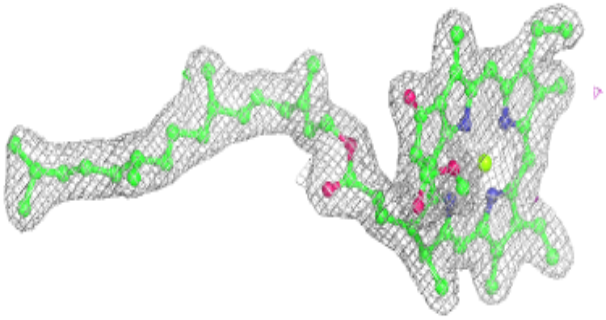


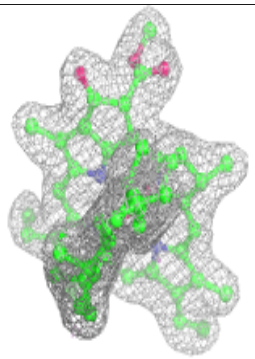


Electron density around CLA C 502:

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

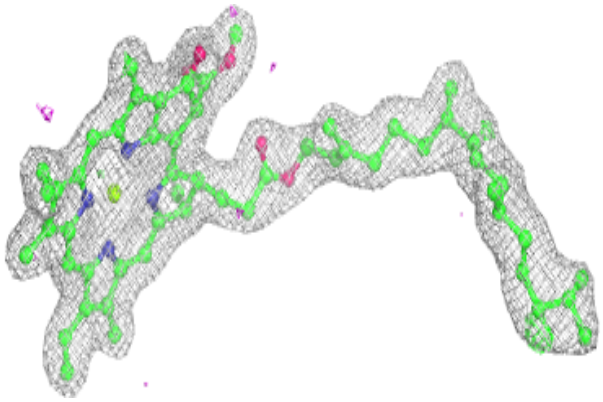


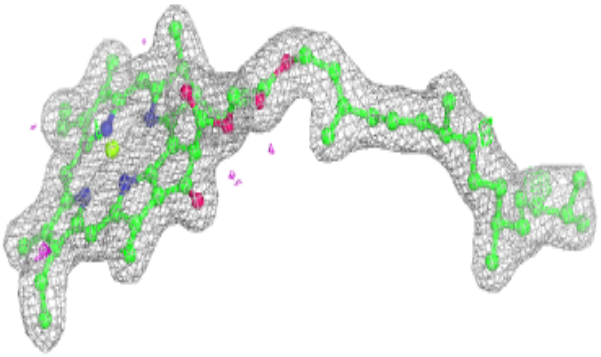


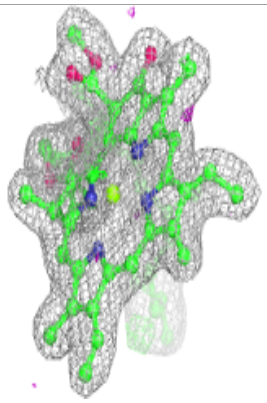


Electron density around CLA A 404:

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

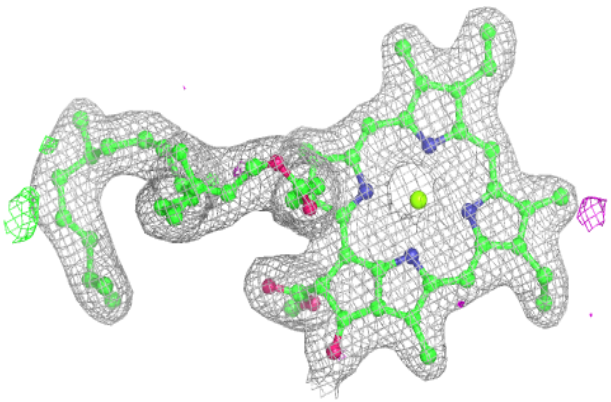


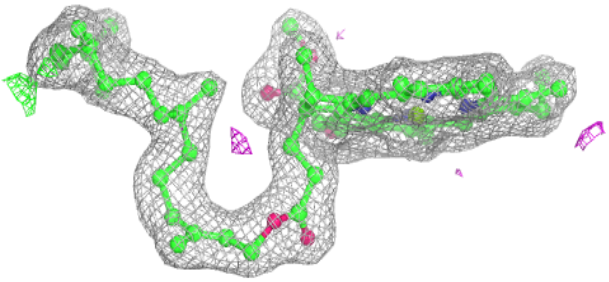


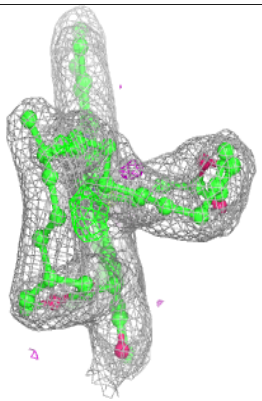


Electron density around CLA B 613:

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

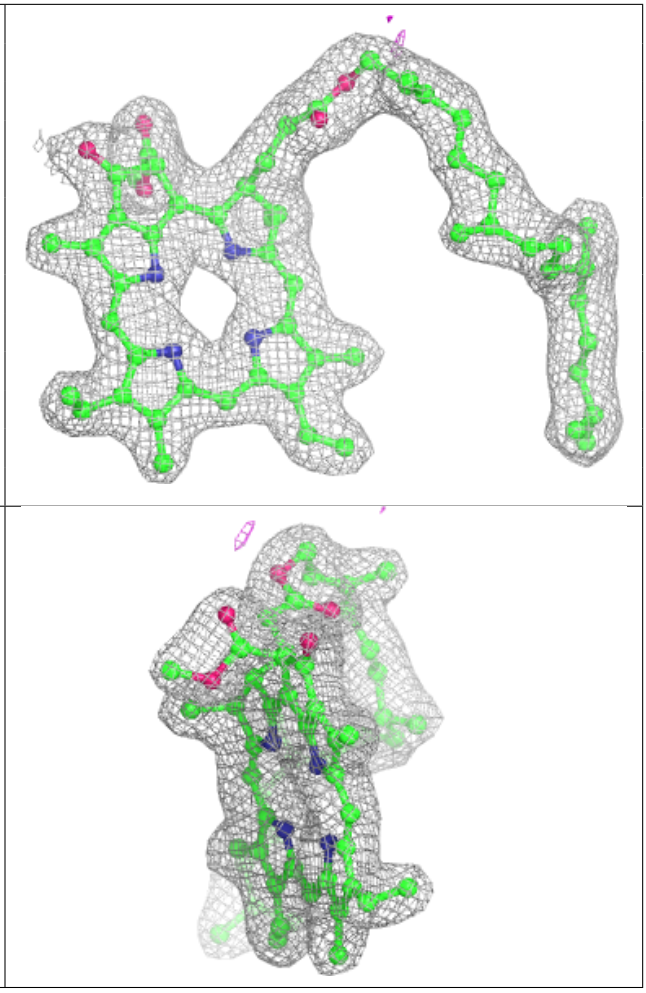






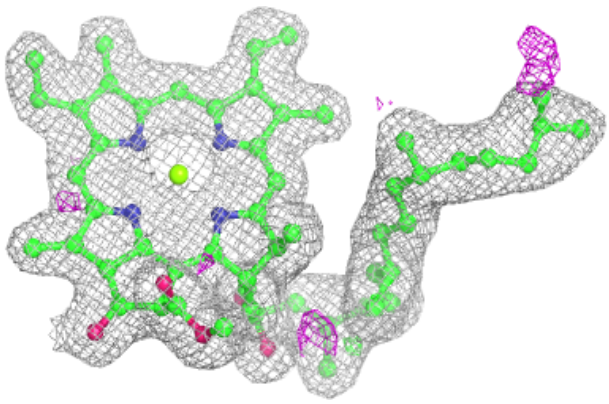
Electron density around PHO d 404:

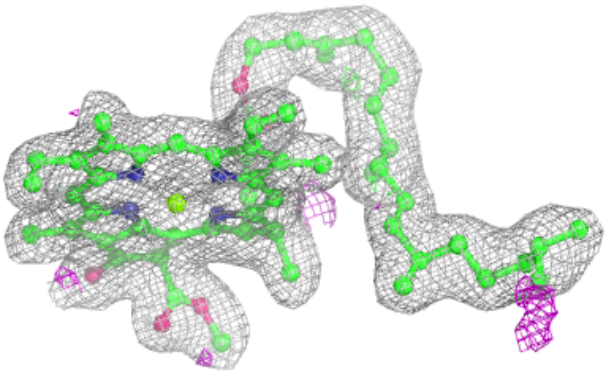
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

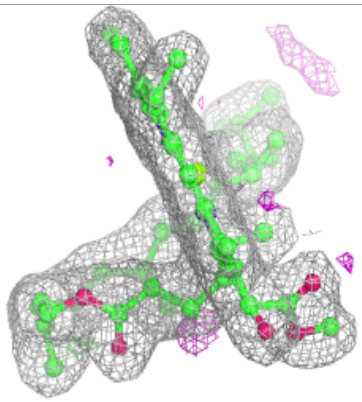


Electron density around CLA A 405:

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

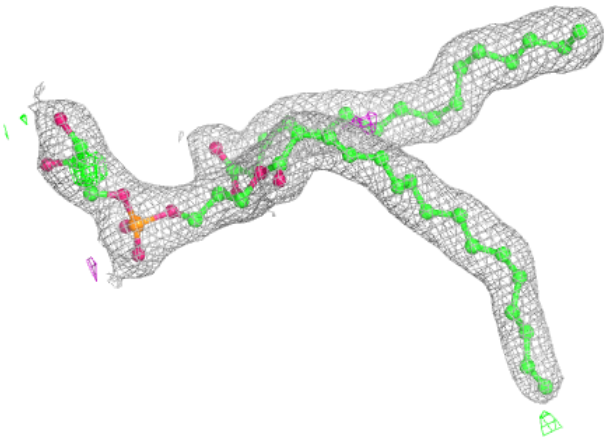


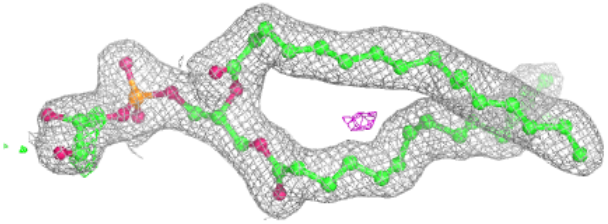


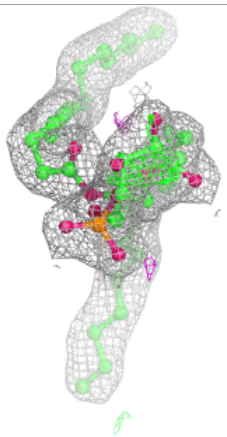


Electron density around LHG D 410:

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

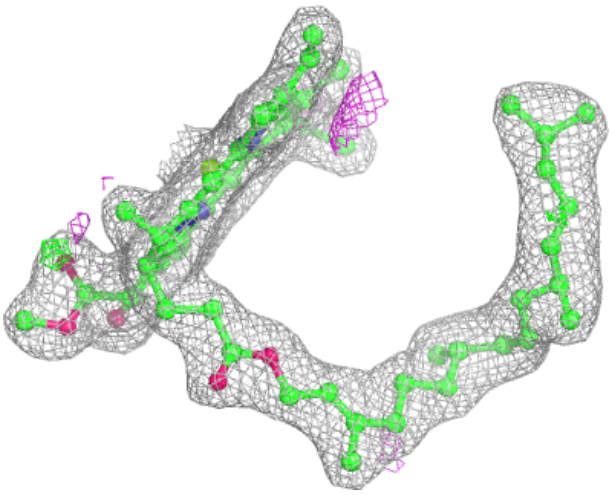


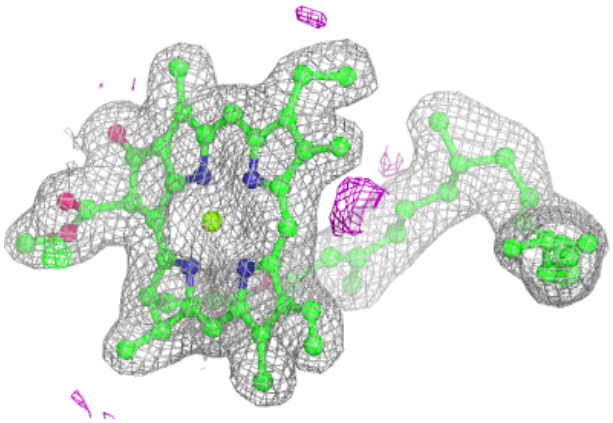


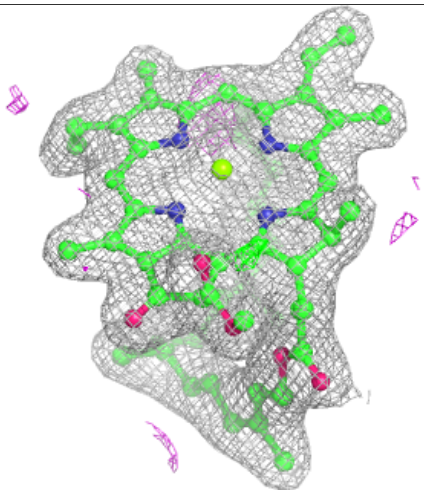


Electron density around CLA b 615:

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

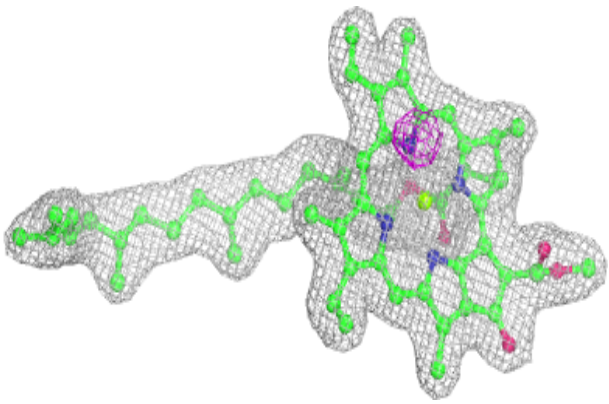


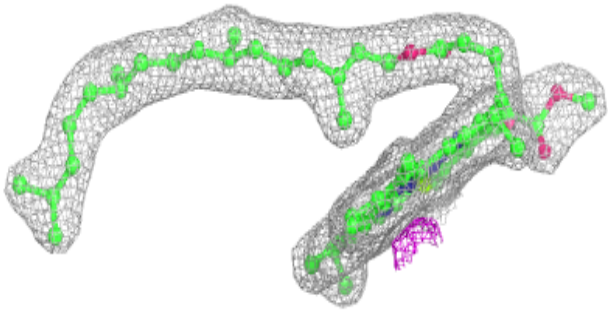


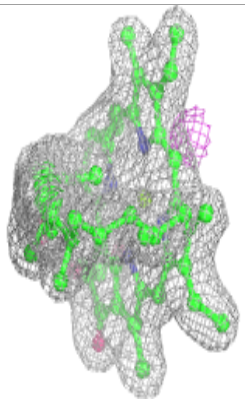


Electron density around CLA B 609:

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

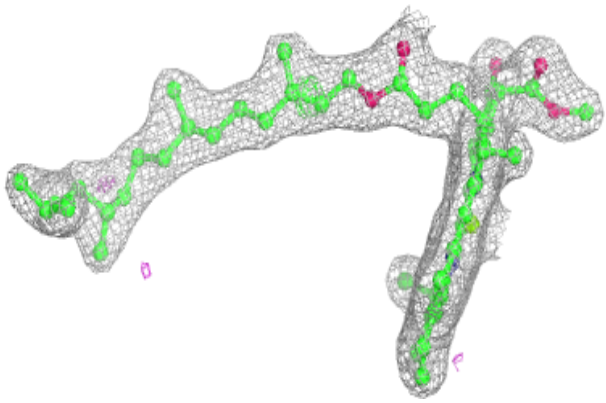


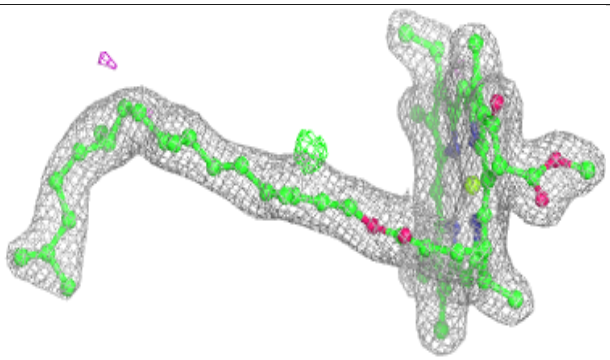


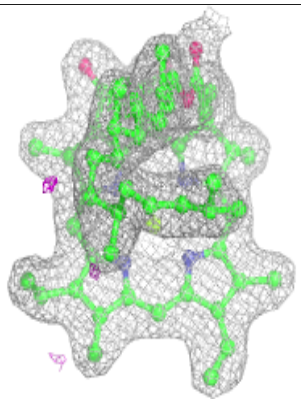


Electron density around CLA b 609:

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

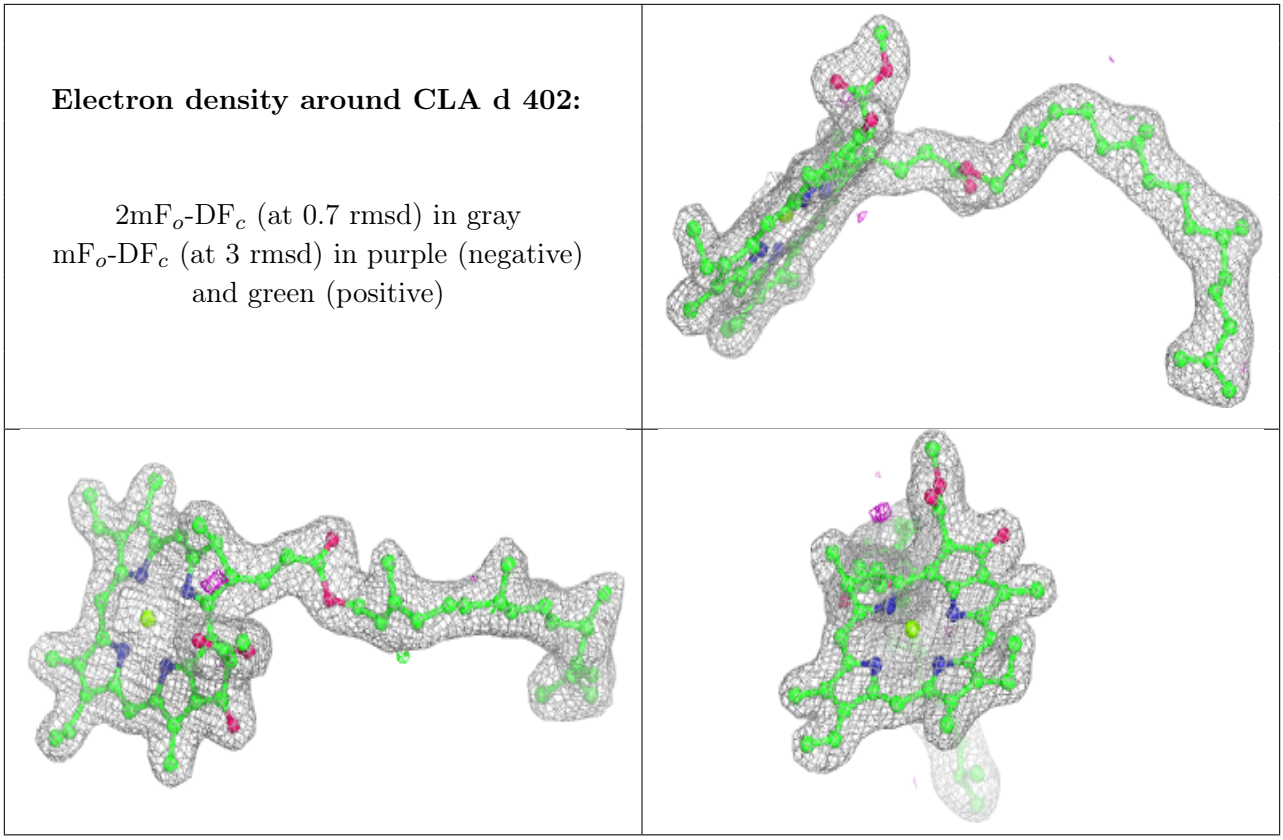






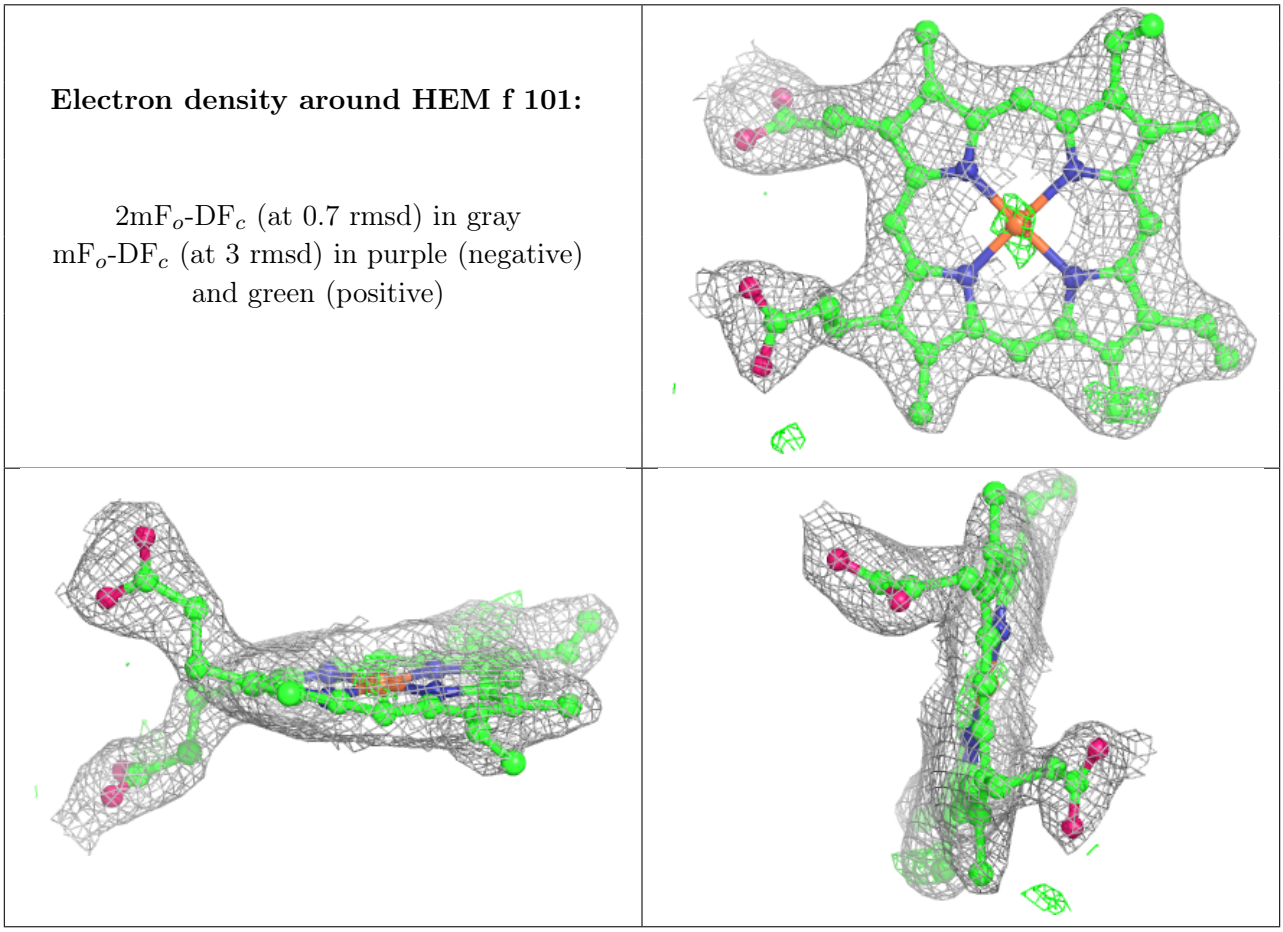
Electron density around CLA d 402:

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



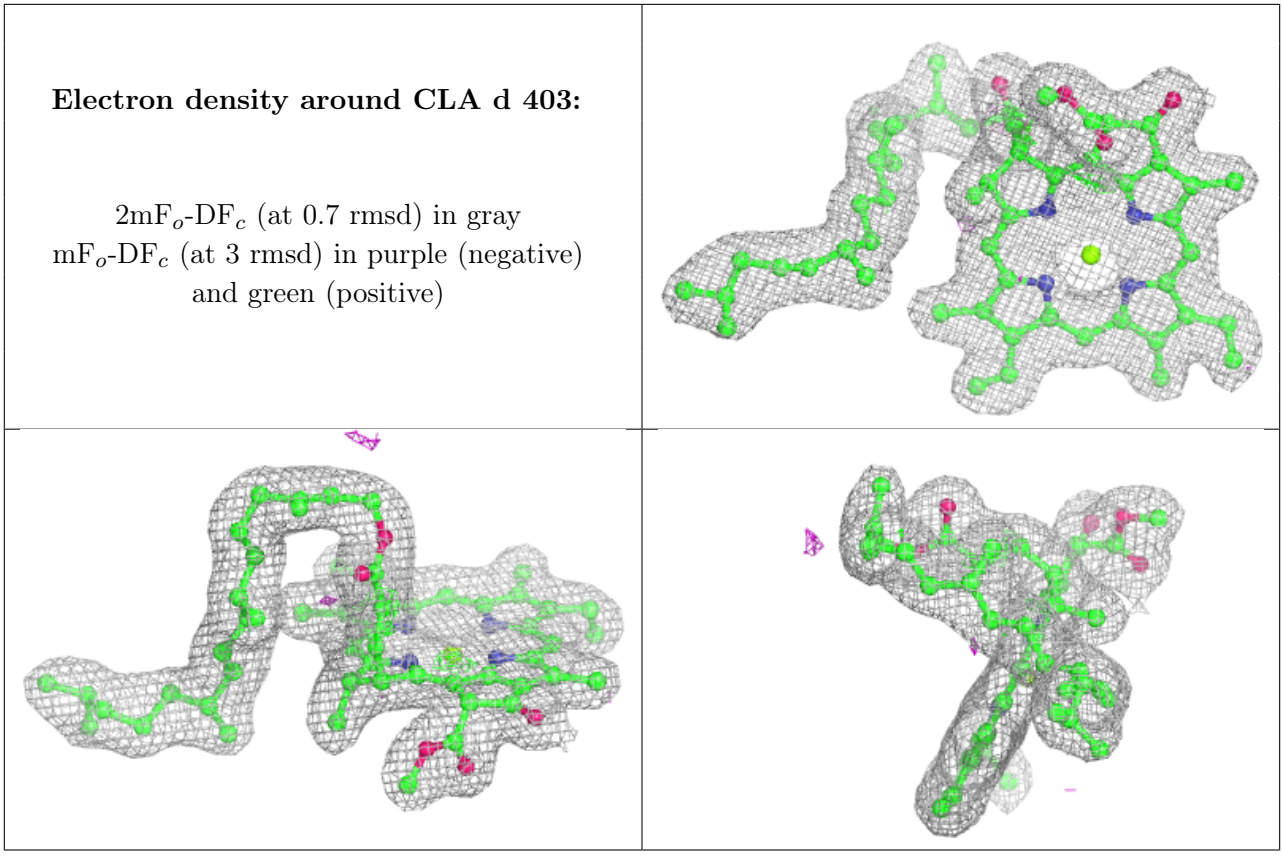
Electron density around HEM f 101:

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



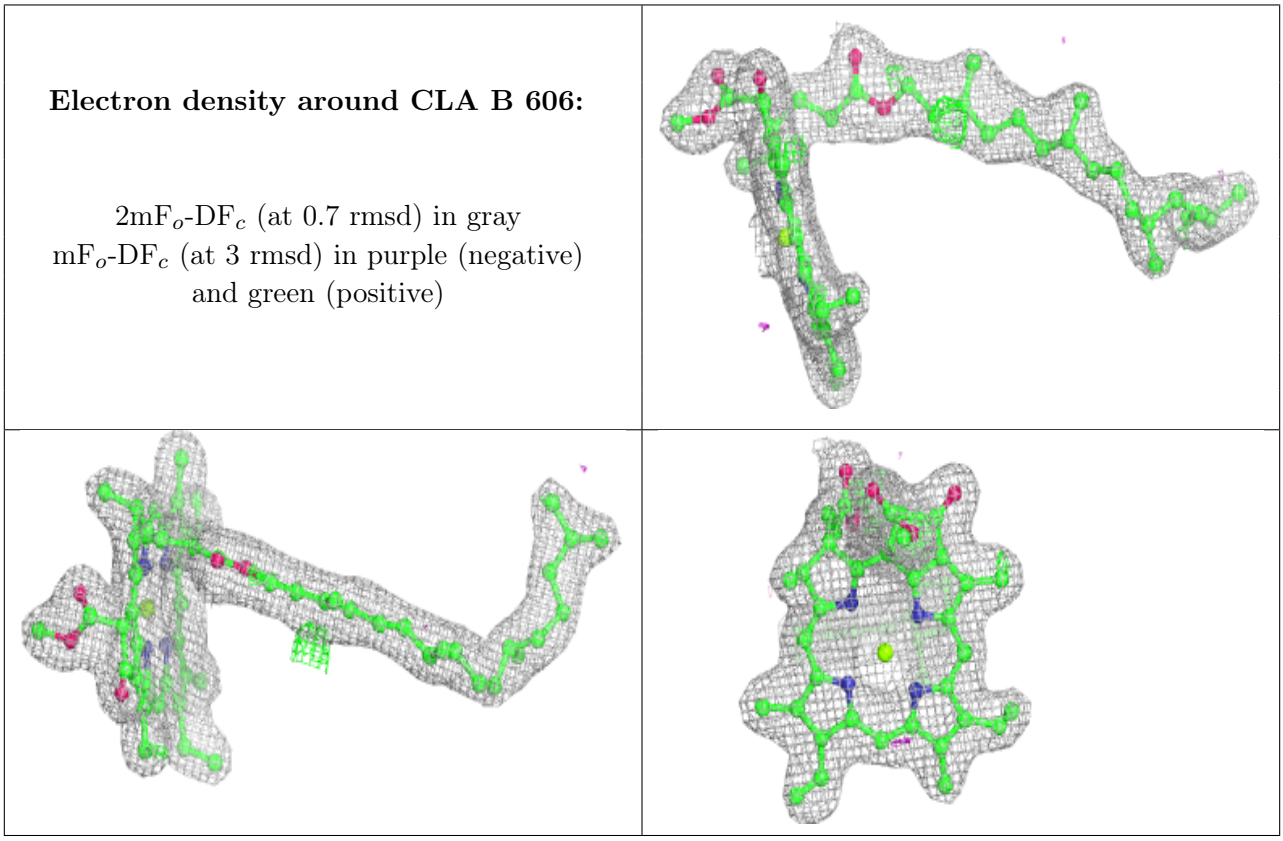
Electron density around CLA d 403:

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



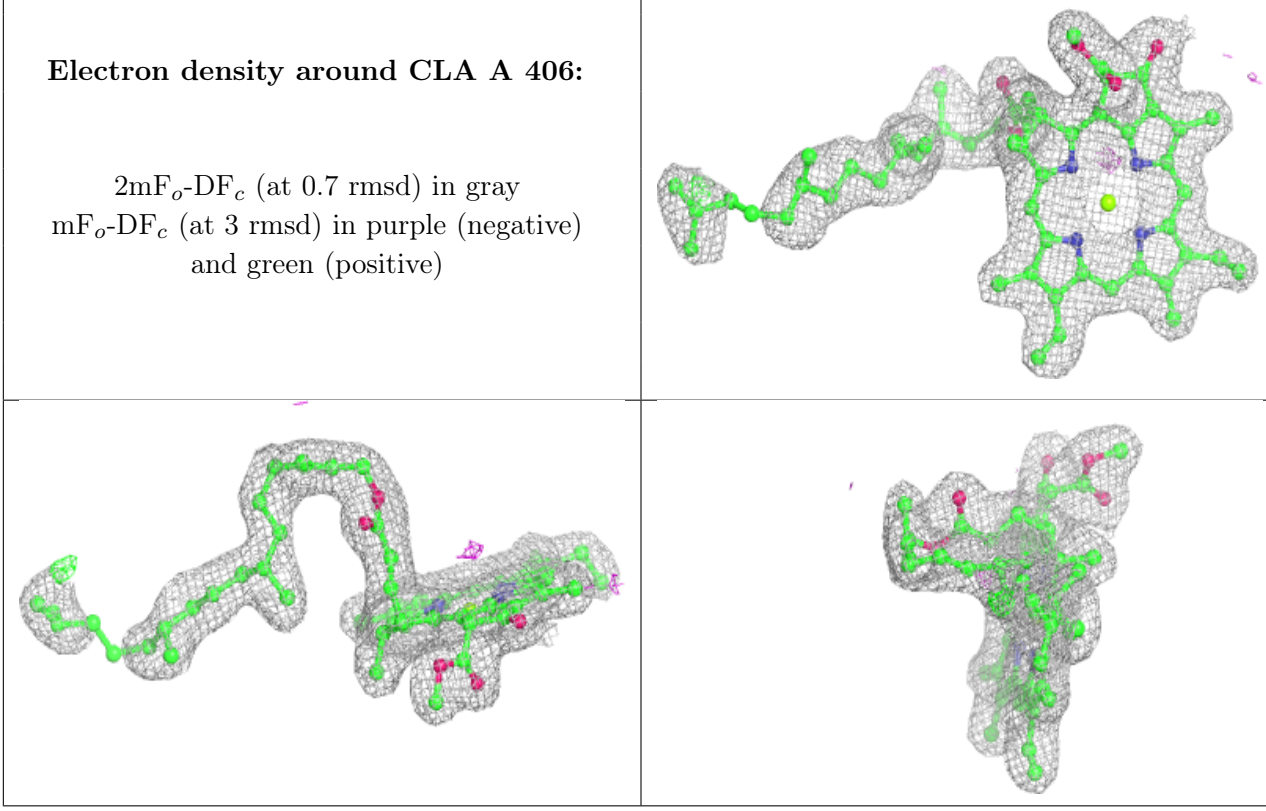
Electron density around CLA B 606:

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



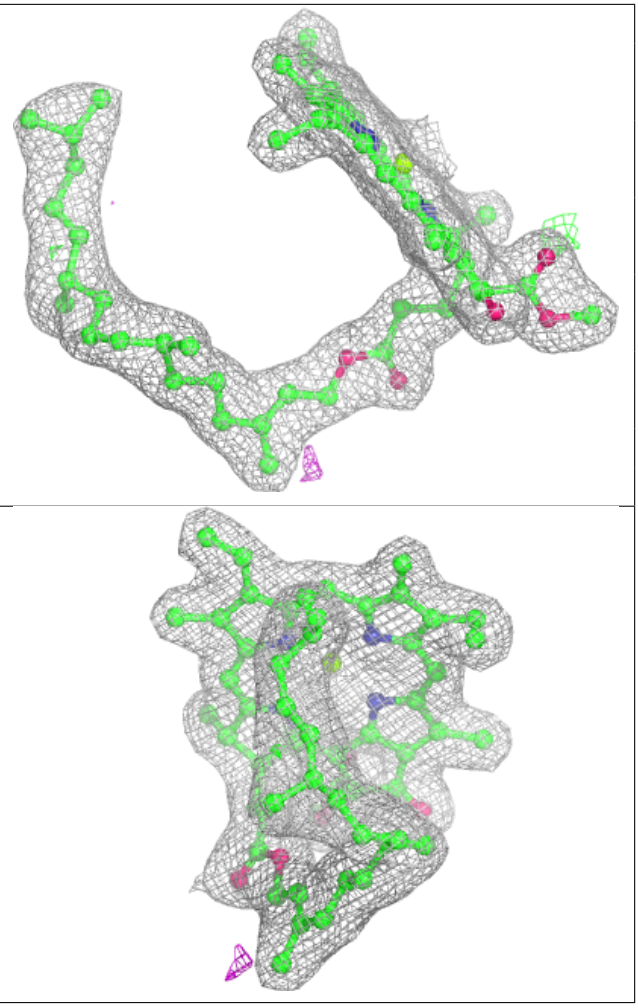
Electron density around CLA A 406:

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



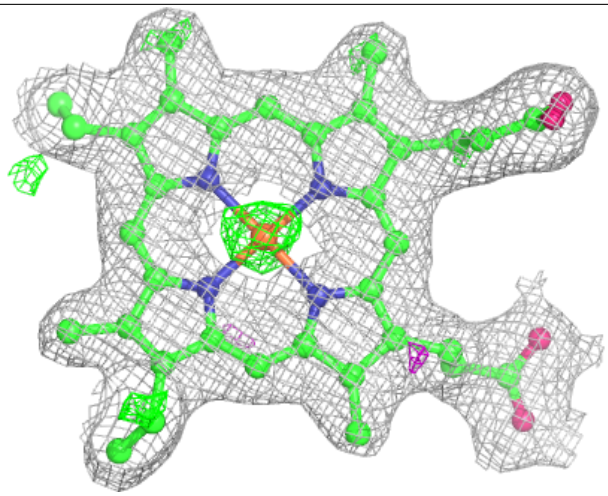
Electron density around CLA B 612:

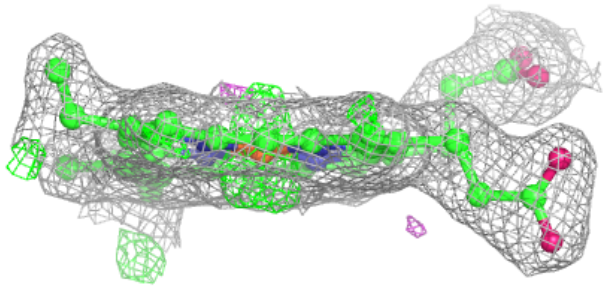
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

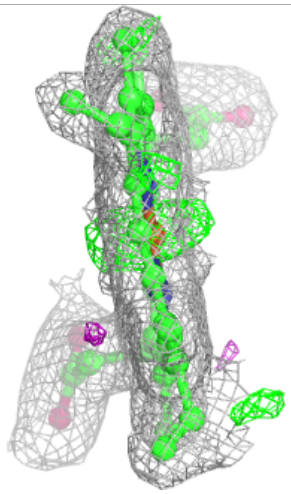


Electron density around HEC V 201:

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

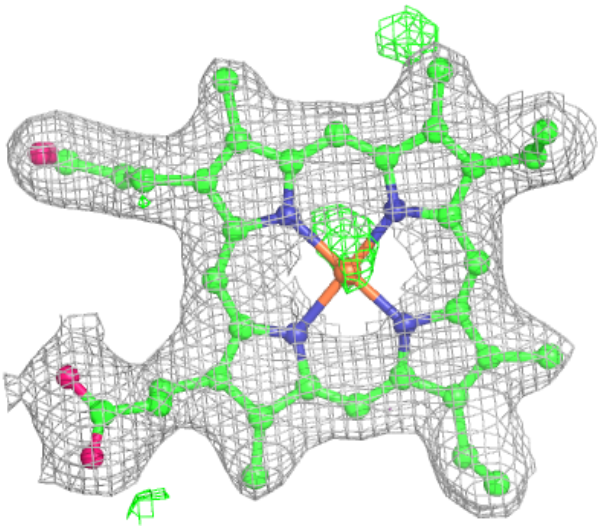


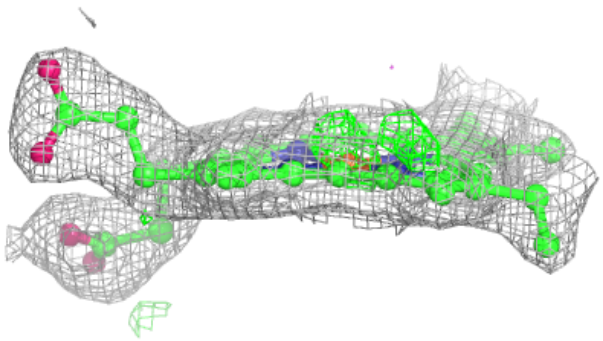


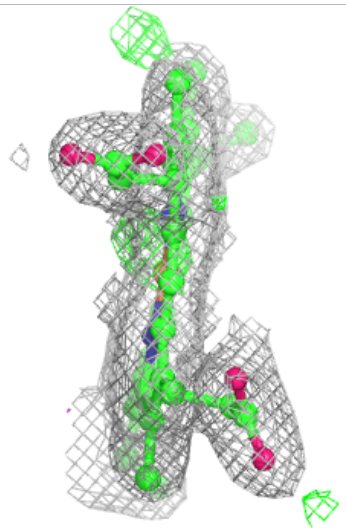


Electron density around HEC v 202:

$2mF_o$-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.