Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 04:04 AM JST

PDB ID	:	4UB8 / pdb_00004ub8
Title	:	Native structure of photosystem II (dataset-2) by a femtosecond X-ray laser
Authors	:	Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R.
Deposited on	:	2014-08-12
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

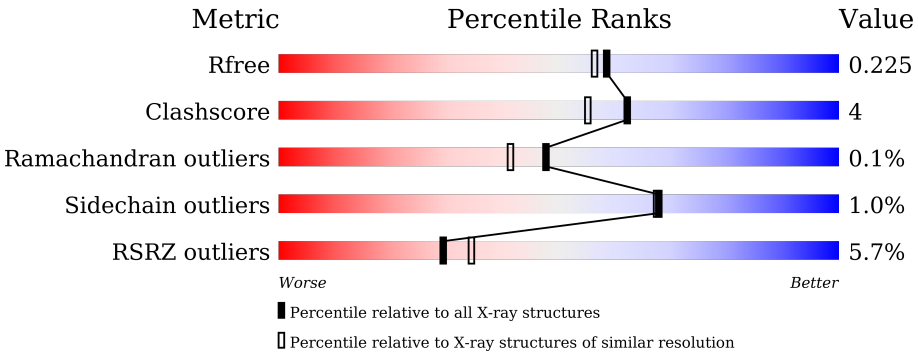
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 Å.

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



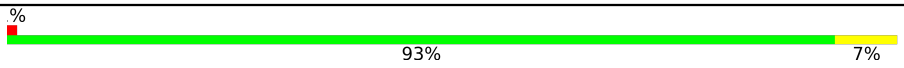
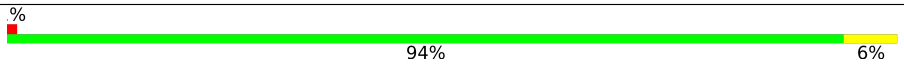
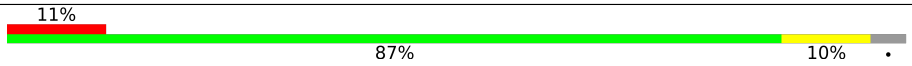
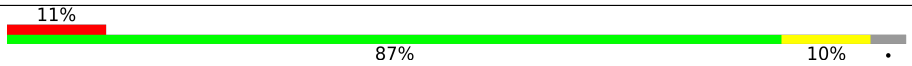
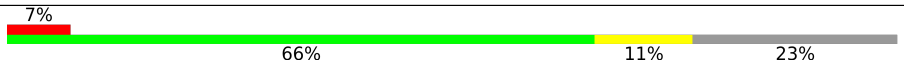
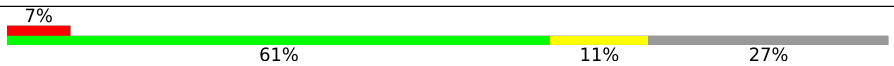
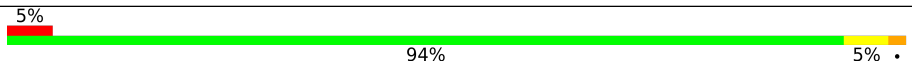
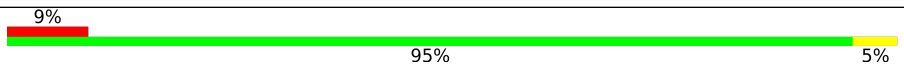
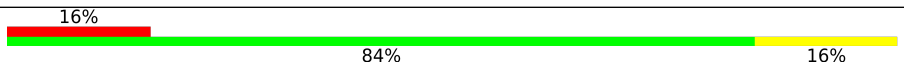
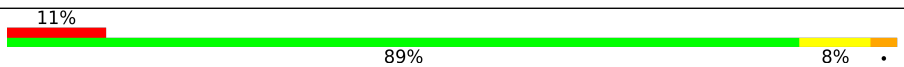
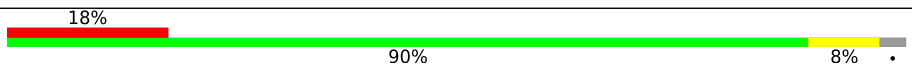
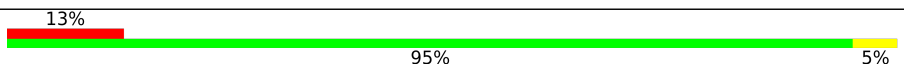
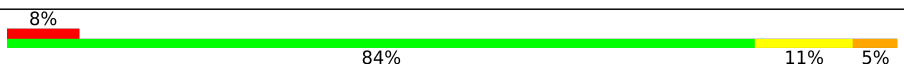
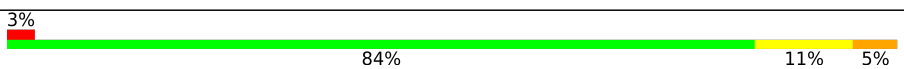
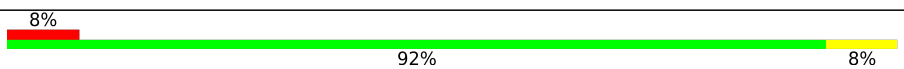
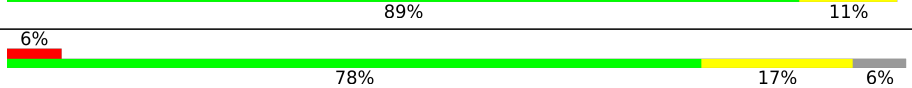
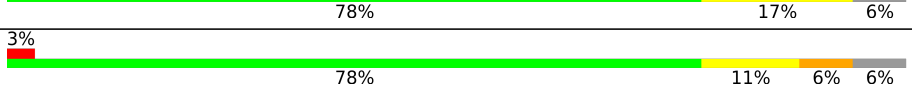
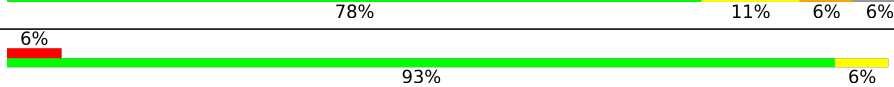
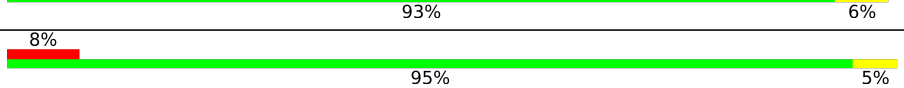
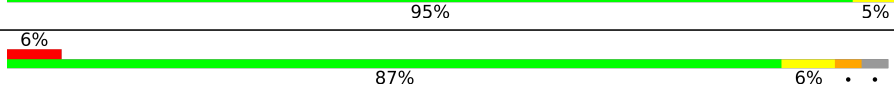
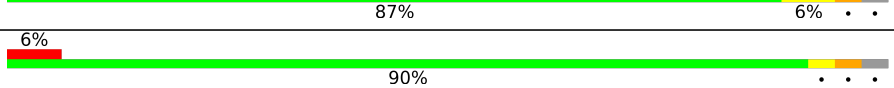
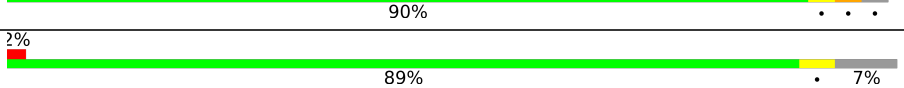
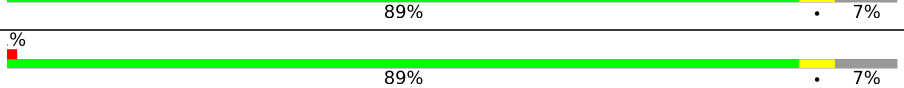
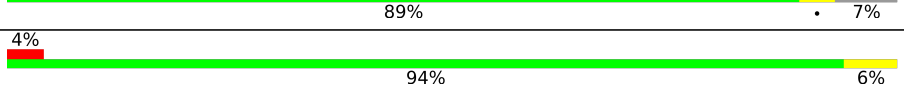
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	344	92% 5%
1	a	344	2% 90% 7%
2	B	505	3% 93% 7%
2	b	505	5% 94% 6%
3	C	455	2% 93% 6%
3	c	455	2% 93% 7%

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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	31	
14	t	31	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	4% 95% 5%
17	Y	30	33% 80% 17%
17	y	30	30% 77% 20%
18	X	40	22% 92% 5%
18	x	40	15% 90% 8%
19	Z	62	32% 94% 6%
19	z	62	34% 90% 10%
20	R	34	88% 79% 18%

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	CL	u	201	-	-	X	-
40	HEC	V	203	X	-	-	-
40	HEC	v	202	X	-	-	-

2 Entry composition (i)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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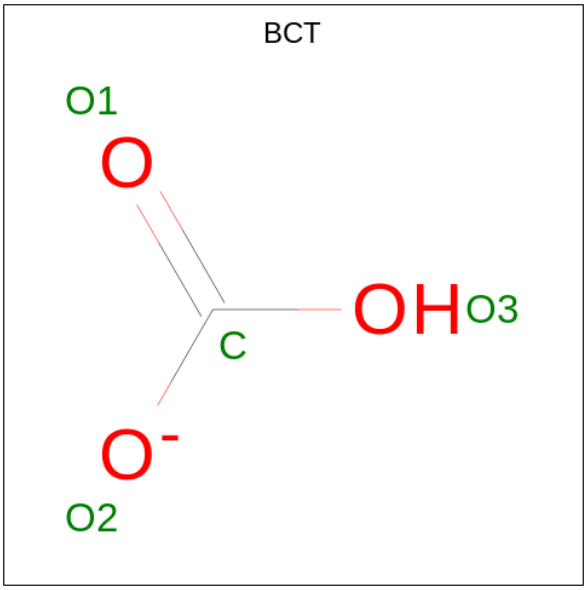
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	a	1	Total Fe 1 1	0	0

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

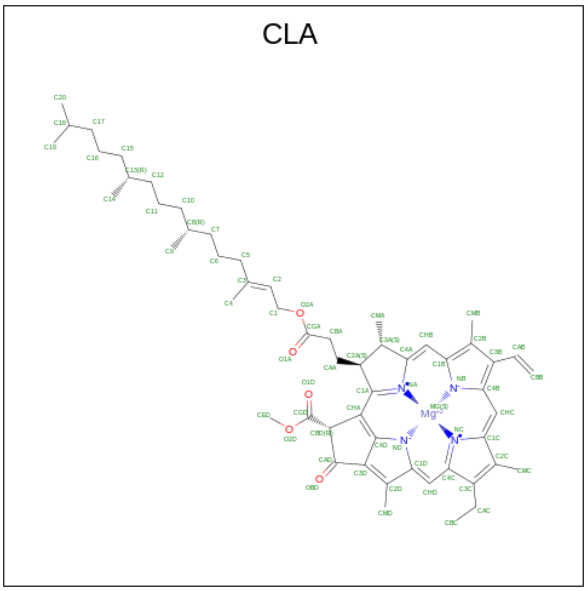
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	2	Total Cl 2 2	0	0
22	V	1	Total Cl 1 1	0	0
22	a	2	Total Cl 2 2	0	0
22	u	1	Total Cl 1 1	0	0

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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



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

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

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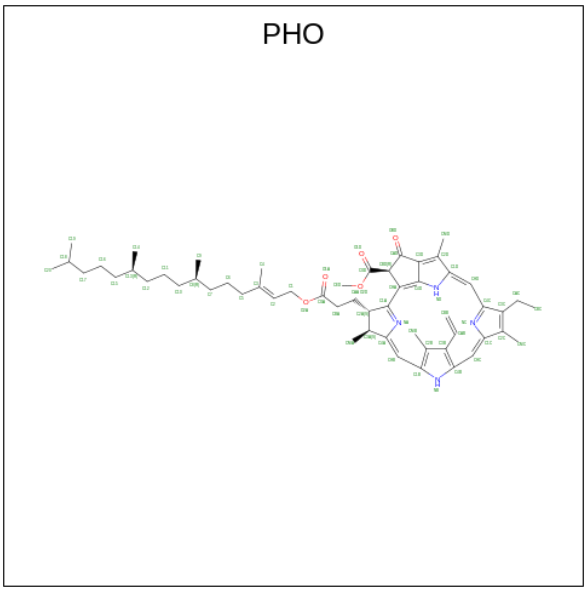
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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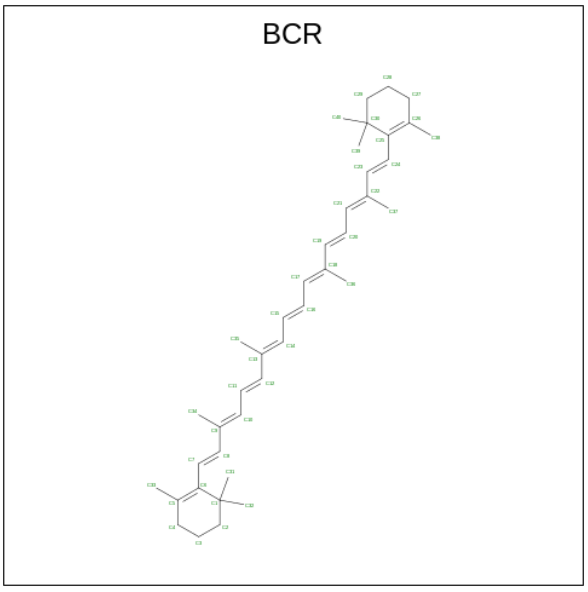
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



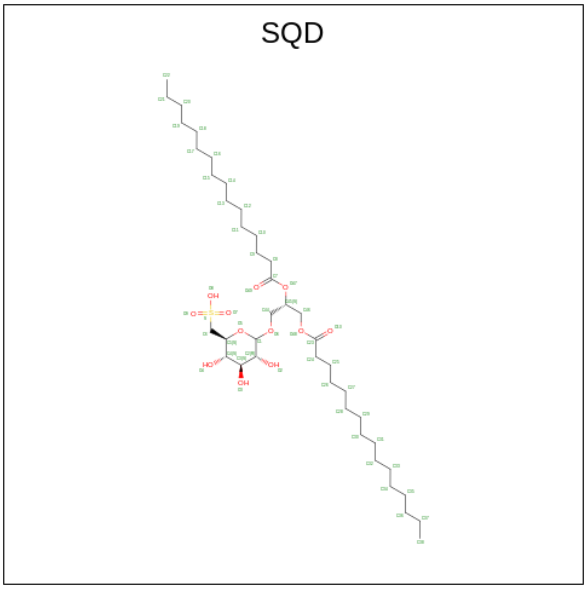
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



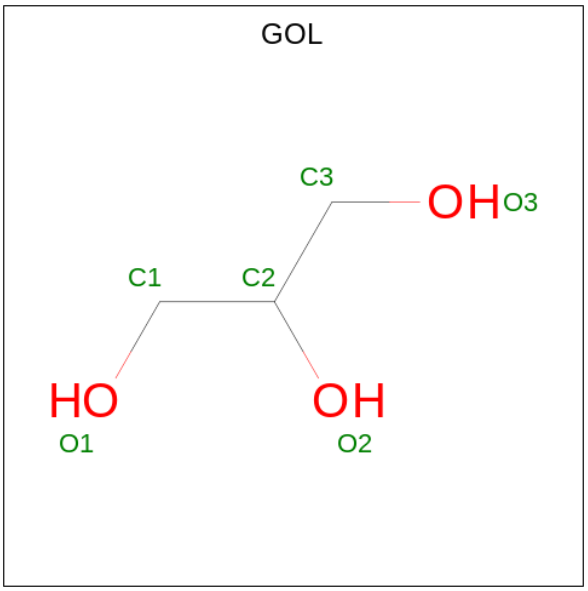
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		
27	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

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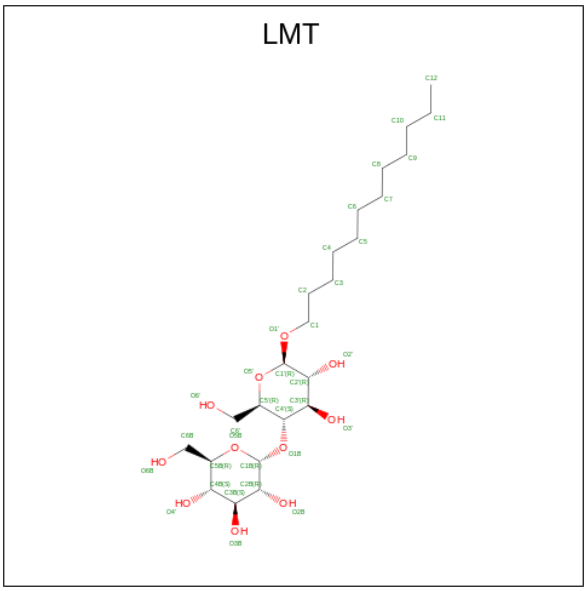
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	v	1	Total C O 6 3 3	0	0
28	v	1	Total C O 6 3 3	0	0

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

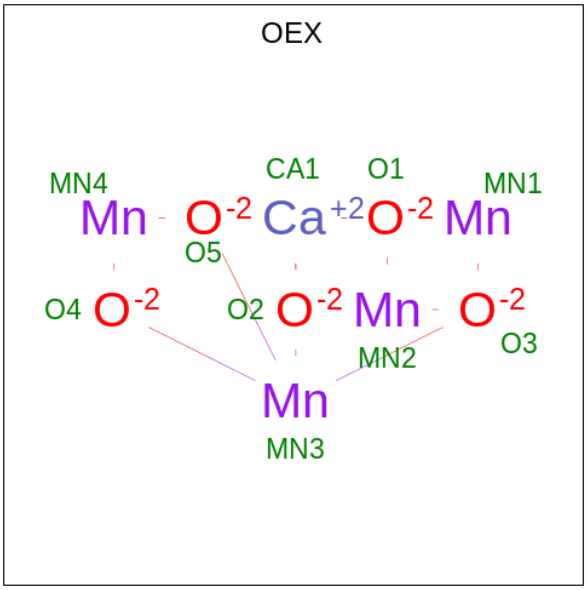
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 28 23 5	0	0
29	B	1	Total C O 33 28 5	0	0
29	C	1	Total C O 34 29 5	0	0
29	D	2	Total C O 57 51 6	0	0
29	I	1	Total C O 40 35 5	0	0
29	J	1	Total C 10 10	0	0
29	M	1	Total C 10 10	0	0
29	X	1	Total C 10 10	0	0
29	a	1	Total C O 30 25 5	0	0
29	b	1	Total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

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



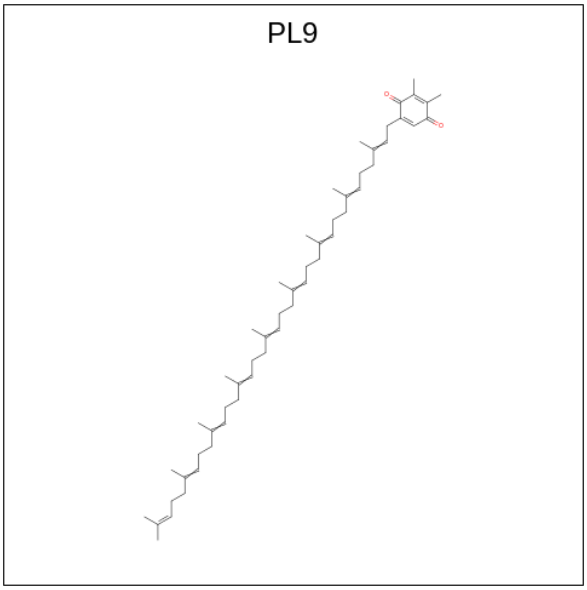
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			33	22	11		
30	B	1	Total	C	O	0	0
			25	19	6		
30	D	1	Total	C	O	0	0
			35	24	11		
30	E	1	Total	C	O	0	0
			35	24	11		
30	I	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C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

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).

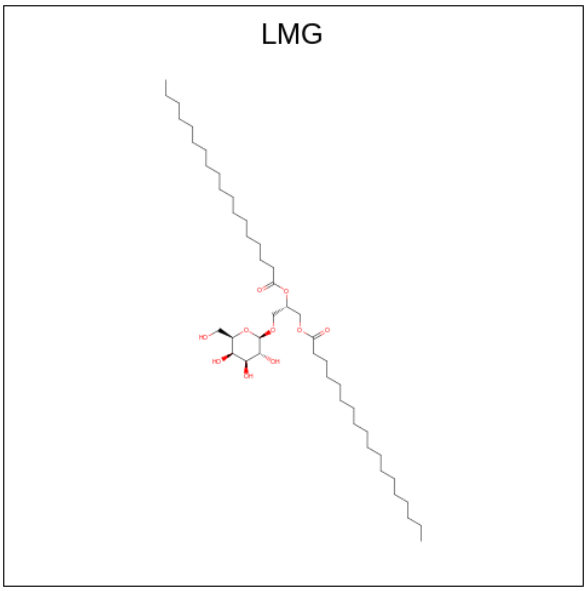


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 55 53 2	0	0
32	D	1	Total C O 55 53 2	0	0
32	a	1	Total C O 55 53 2	0	0
32	d	1	Total C O 55 53 2	0	0

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

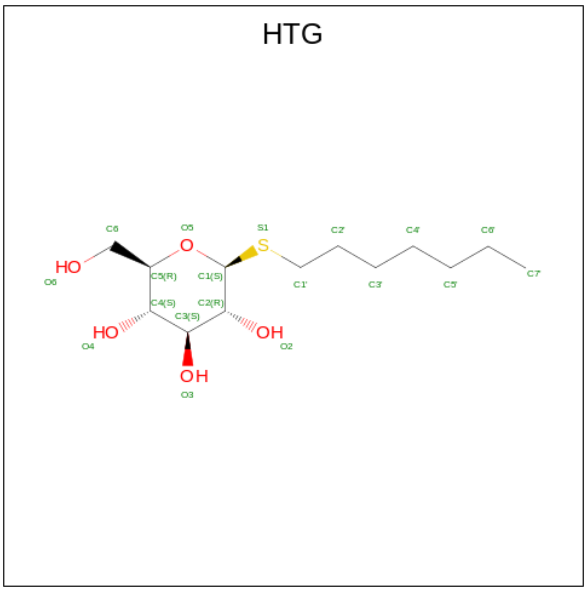
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	f	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0

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



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

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



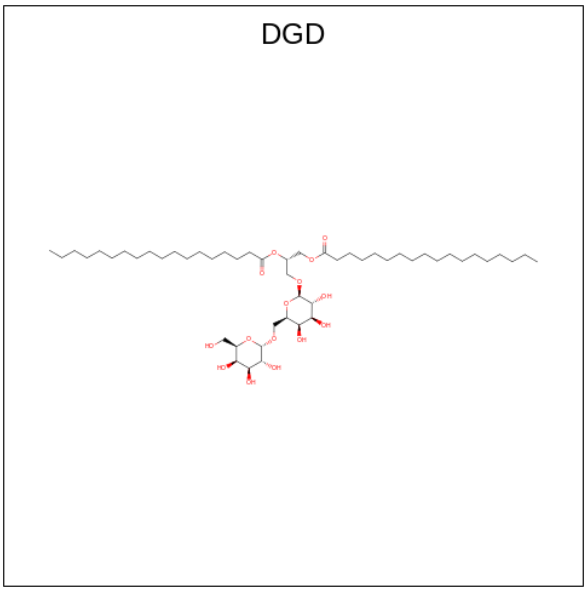
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19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

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

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



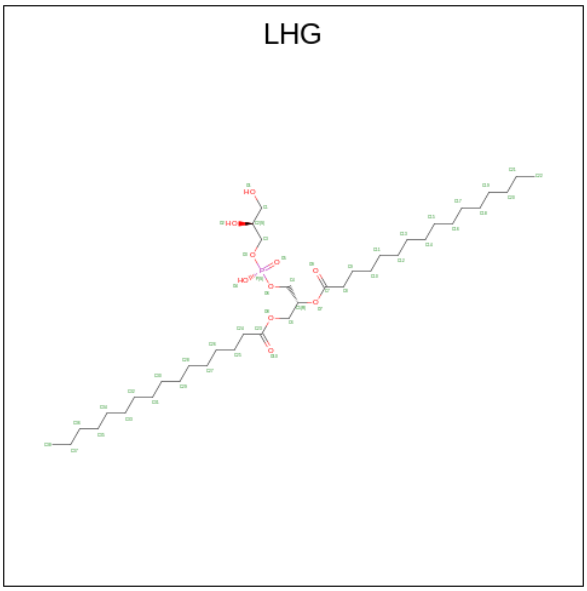
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	D	1	Total C O 62 47 15	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0

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

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



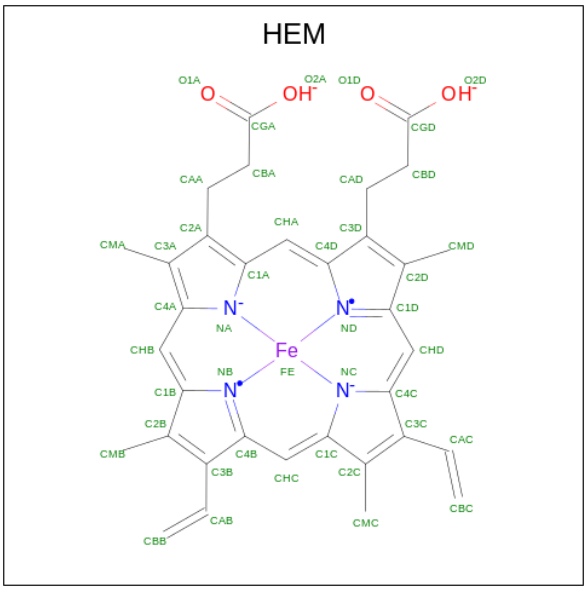
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	E	1	Total C O P 42 31 10 1	0	0
37	L	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49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

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

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

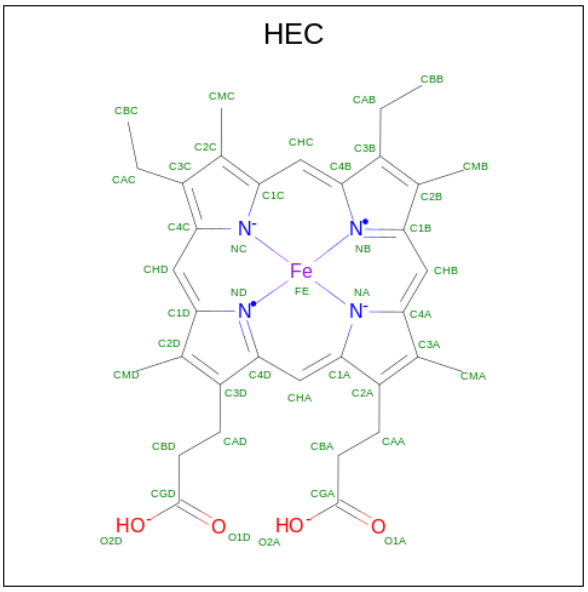


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 41 is water.

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

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

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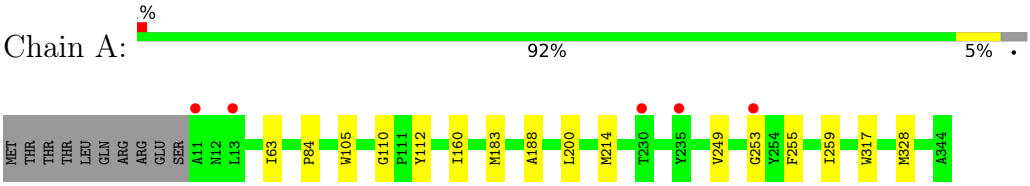
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	t	10	Total O 10 10	0	0
41	u	89	Total O 89 89	0	0
41	v	80	Total O 80 80	0	0
41	y	4	Total O 4 4	0	0
41	x	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

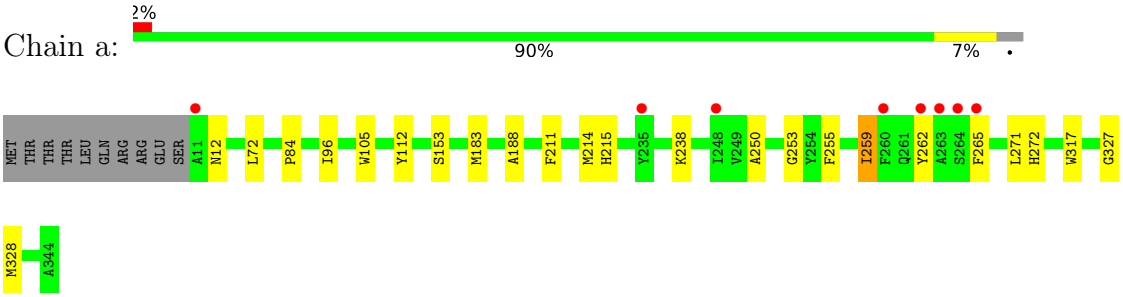
• Molecule 1: Photosystem Q(B) protein

Chain A:



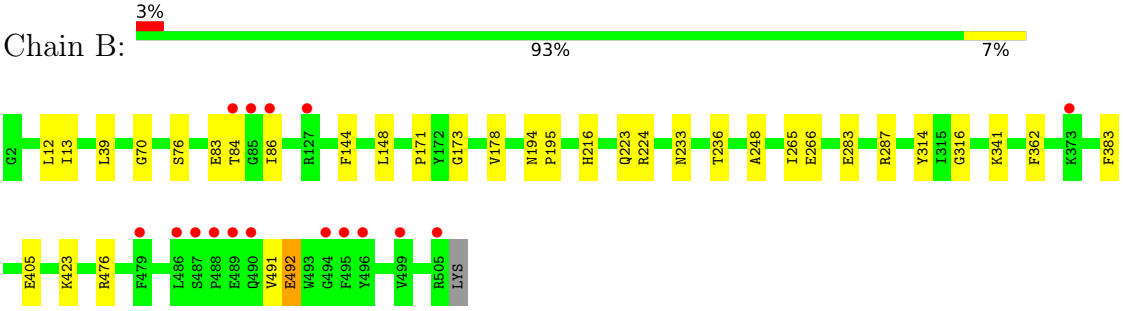
• Molecule 1: Photosystem Q(B) protein

Chain a:



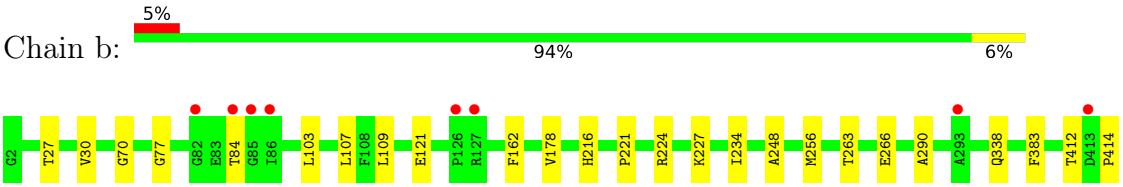
• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

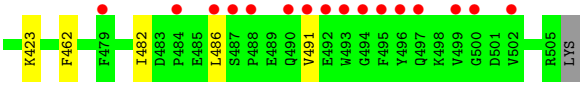
Chain B:



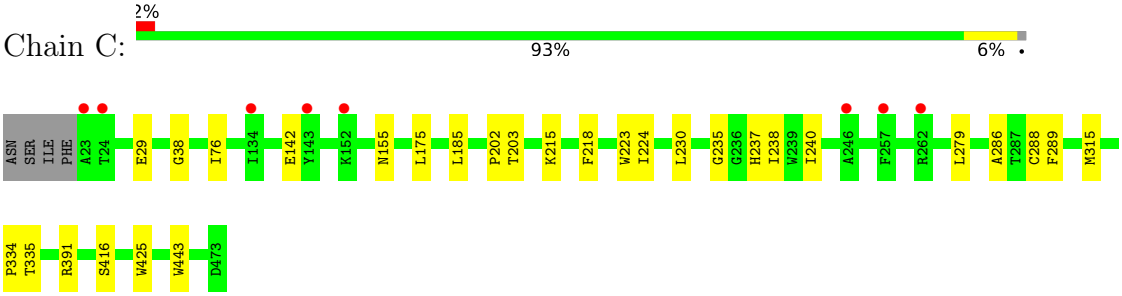
• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

Chain b:

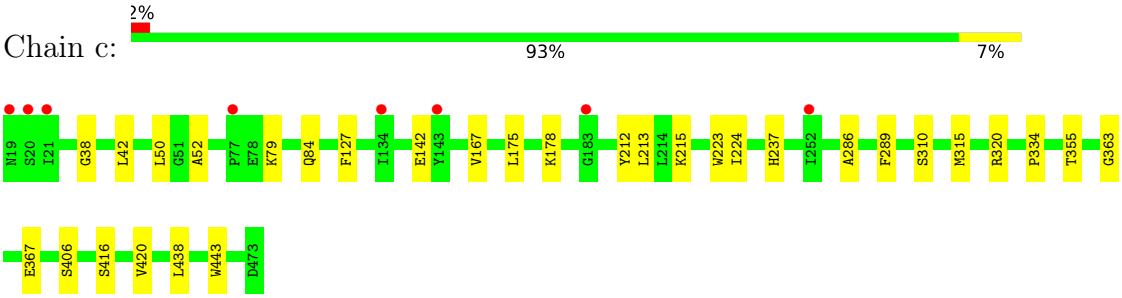




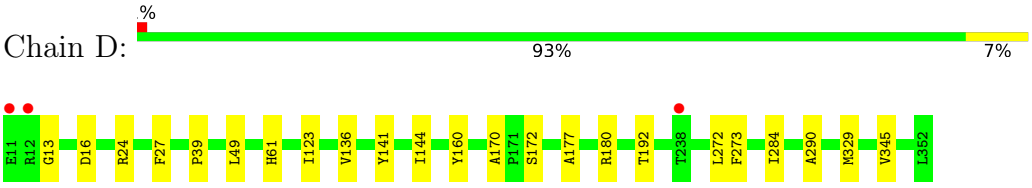
• Molecule 3: Photosystem II 44 kDa reaction center protein



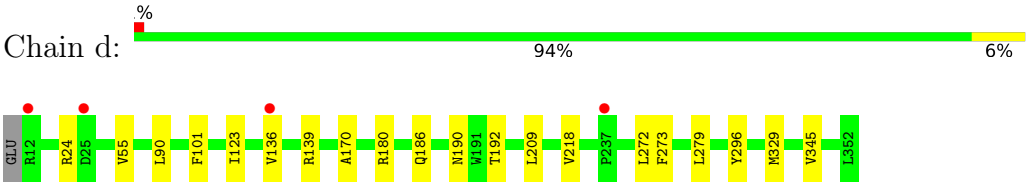
• Molecule 3: Photosystem II 44 kDa reaction center protein



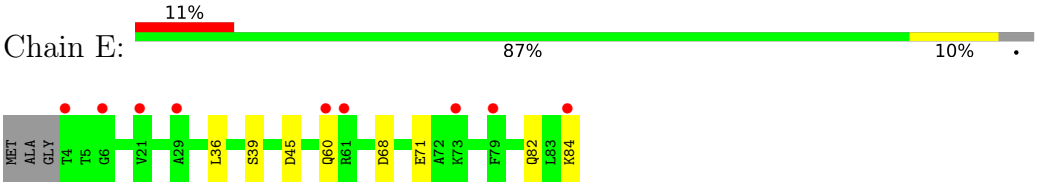
• Molecule 4: Photosystem II D2 protein



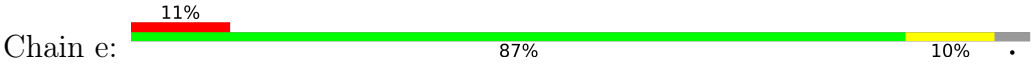
• Molecule 4: Photosystem II D2 protein

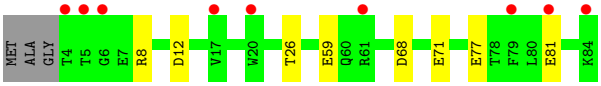


• Molecule 5: Cytochrome b559 subunit alpha



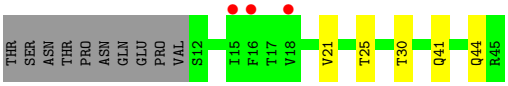
• Molecule 5: Cytochrome b559 subunit alpha





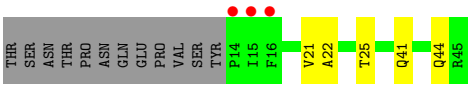
• Molecule 6: Cytochrome b559 subunit beta



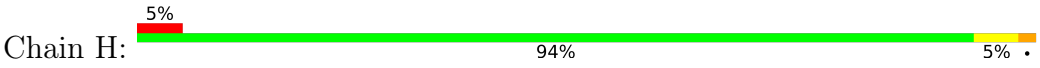


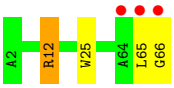
• Molecule 6: Cytochrome b559 subunit beta





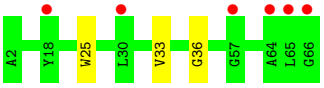
• Molecule 7: Photosystem II reaction center protein H



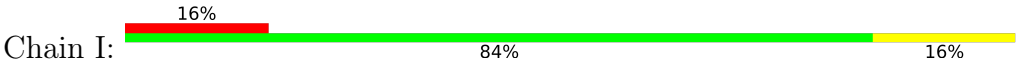


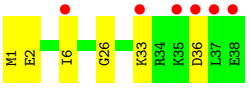
• Molecule 7: Photosystem II reaction center protein H



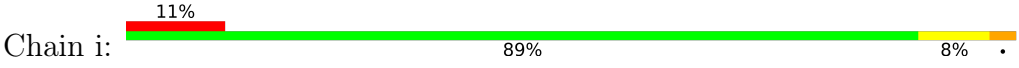


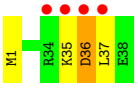
• Molecule 8: Photosystem II reaction center protein I





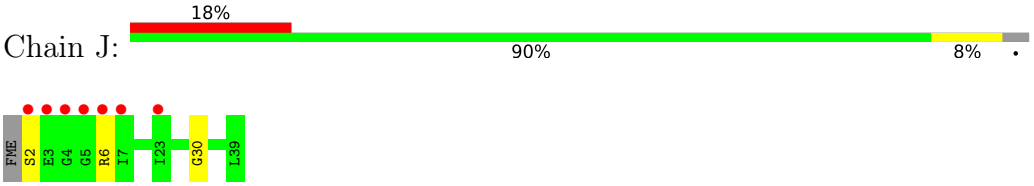
• Molecule 8: Photosystem II reaction center protein I





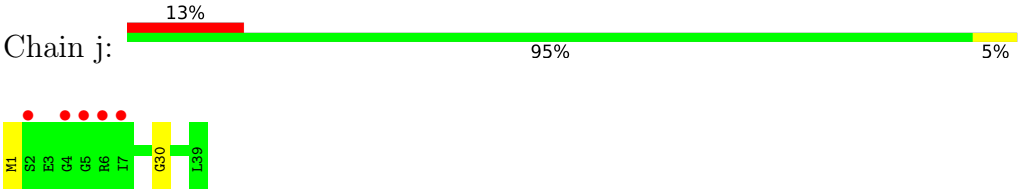
• Molecule 9: Photosystem II reaction center protein J

Chain J:



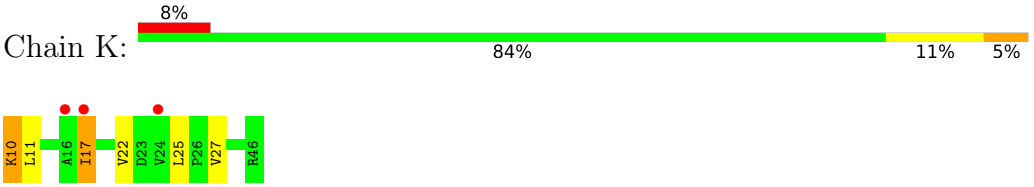
• Molecule 9: Photosystem II reaction center protein J

Chain j:



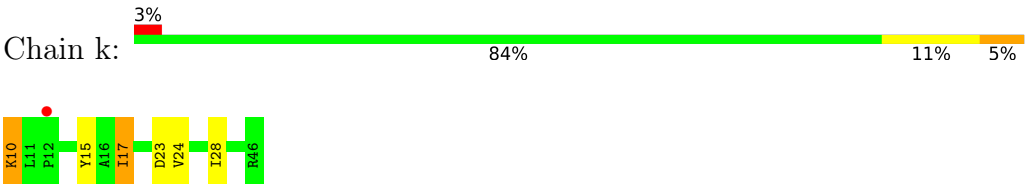
• Molecule 10: Photosystem II reaction center protein K

Chain K:



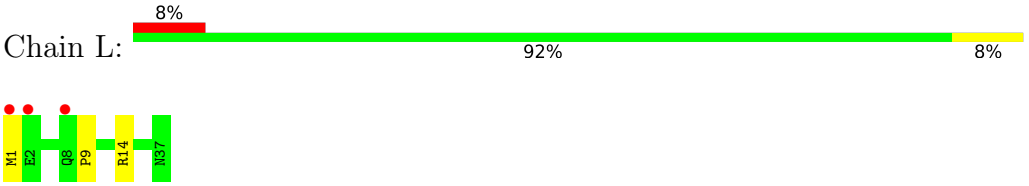
• Molecule 10: Photosystem II reaction center protein K

Chain k:



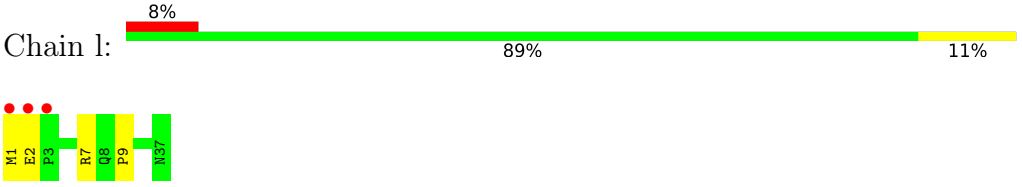
• Molecule 11: Photosystem II reaction center protein L

Chain L:



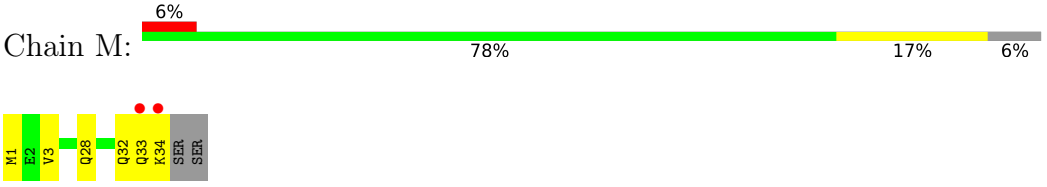
• Molecule 11: Photosystem II reaction center protein L

Chain l:



• Molecule 12: Photosystem II reaction center protein M

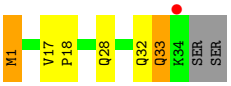
Chain M:



• Molecule 12: Photosystem II reaction center protein M

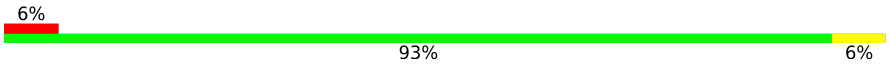
Chain m:

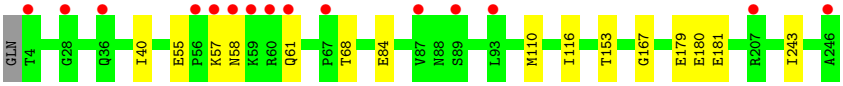




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

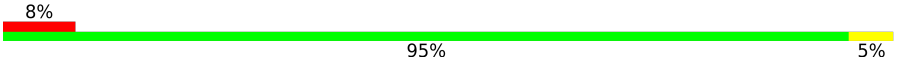
Chain O:

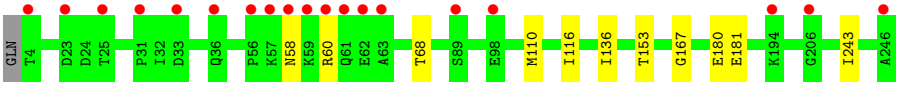




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

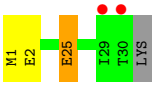




• Molecule 14: Photosystem II reaction center protein T

Chain T:

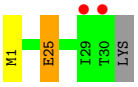




• Molecule 14: Photosystem II reaction center protein T

Chain t:

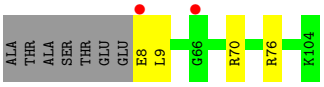




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:





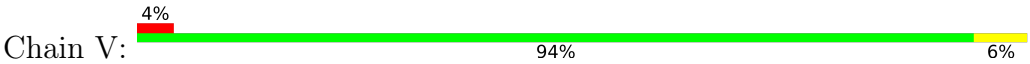
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



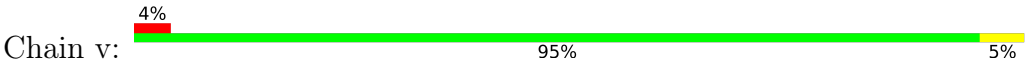


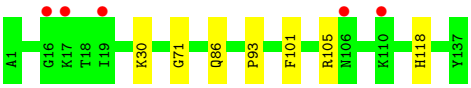
• Molecule 16: Cytochrome c-550



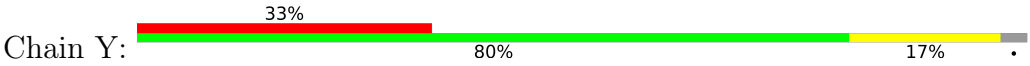


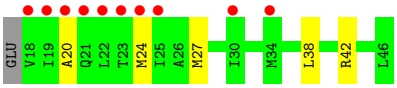
• Molecule 16: Cytochrome c-550



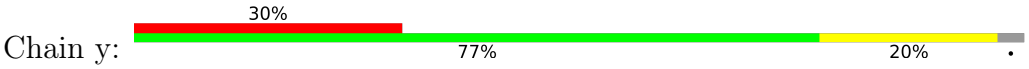


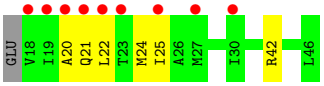
• Molecule 17: Photosystem II reaction center protein Ycf12



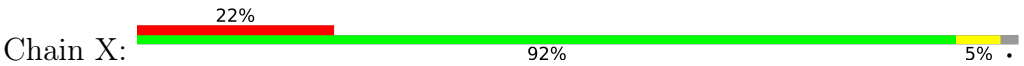


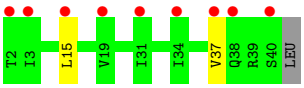
• Molecule 17: Photosystem II reaction center protein Ycf12



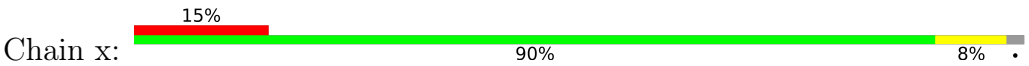


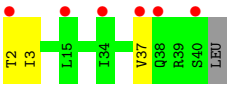
• Molecule 18: Photosystem II reaction center protein X





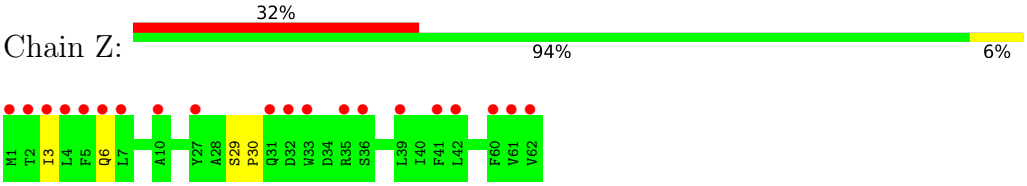
• Molecule 18: Photosystem II reaction center protein X





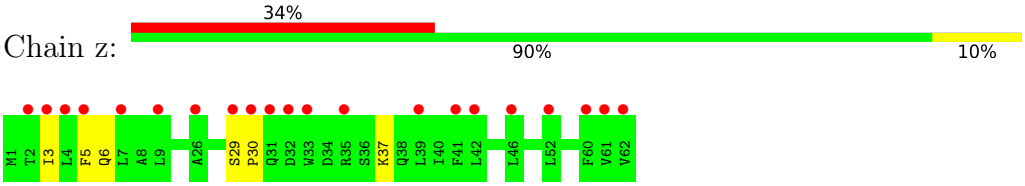
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



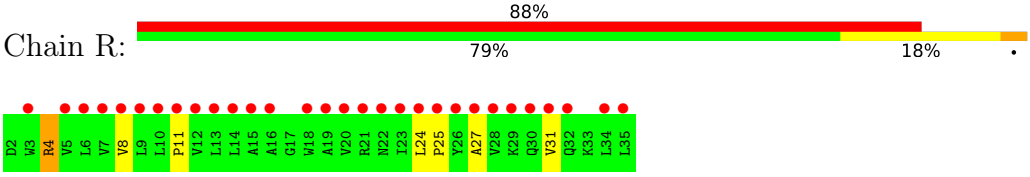
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.81Å 230.00Å 288.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.90 – 1.95 61.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.1 (61.90-1.95) 86.4 (61.90-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.08 (at 1.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.188 , 0.225 0.188 , 0.225	Depositor DCC
R_{free} test set	29342 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	53958	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, LHG, PHO, BCT, HTG, CL, SQD, HEC, OEX, DGD, CA, MG, HEM, FE2, GOL, LMG, FME, LMT, CLA, BCR, PL9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.67	0/2725	0.86	0/3716
1	a	0.67	1/2731 (0.0%)	0.85	0/3724
2	B	0.60	0/4193	0.83	0/5712
2	b	0.59	0/4201	0.83	3/5723 (0.1%)
3	C	0.56	0/3634	0.82	2/4947 (0.0%)
3	c	0.57	1/3676 (0.0%)	0.82	0/5004
4	D	0.64	0/2821	0.80	2/3844 (0.1%)
4	d	0.64	0/2818	0.82	3/3840 (0.1%)
5	E	0.48	0/693	0.84	0/944
5	e	0.43	0/681	0.82	0/928
6	F	0.57	0/284	0.79	0/387
6	f	0.49	0/265	0.83	0/360
7	H	0.50	0/535	0.78	0/728
7	h	0.43	0/524	0.76	0/713
8	I	0.46	0/311	0.82	0/419
8	i	0.49	0/311	0.74	0/419
9	J	0.47	0/278	0.77	0/376
9	j	0.50	0/278	0.76	0/376
10	K	0.49	0/303	0.75	0/416
10	k	0.59	1/303 (0.3%)	0.83	0/416
11	L	0.55	0/319	0.70	0/433
11	l	0.59	0/319	0.71	0/433
12	M	0.64	0/270	0.88	0/368
12	m	0.72	1/262 (0.4%)	0.92	0/357
13	O	0.52	0/1926	0.82	2/2611 (0.1%)
13	o	0.48	0/1919	0.79	0/2601
14	T	0.65	0/266	0.77	0/362
14	t	0.69	0/266	0.80	0/362
15	U	0.52	0/785	0.78	0/1064
15	u	0.53	0/785	0.73	0/1064
16	V	0.57	0/1096	0.78	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.55	0/1085	0.81	1/1473 (0.1%)
17	Y	0.41	0/216	0.76	0/289
17	y	0.42	0/216	0.78	0/289
18	X	0.41	0/298	0.74	0/403
18	x	0.40	0/290	0.73	0/392
19	Z	0.40	0/490	0.82	0/669
19	z	0.43	0/490	0.81	0/669
20	R	0.36	0/279	0.71	0/383
All	All	0.58	4/43142 (0.0%)	0.81	13/58701 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	17	VAL	CA-CB	7.01	1.58	1.54
10	k	28	ILE	CA-CB	5.54	1.56	1.54
3	c	310	SER	C-O	5.35	1.30	1.24
1	a	327	GLY	C-O	5.09	1.29	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	v	105	ARG	N-CA-C	6.08	118.70	111.71
4	d	170	ALA	CA-C-N	-5.61	114.15	119.76
4	d	170	ALA	C-N-CA	-5.61	114.15	119.76
2	b	414	PRO	N-CA-C	5.54	117.45	110.70
2	b	221	PRO	O-C-N	5.42	123.80	121.31
13	O	55	GLU	CA-C-N	5.34	125.64	119.92
13	O	55	GLU	C-N-CA	5.34	125.64	119.92
4	d	55	VAL	N-CA-C	5.21	115.47	108.17
3	C	76	ILE	CA-C-N	5.06	124.84	119.28
3	C	76	ILE	C-N-CA	5.06	124.84	119.28
4	D	170	ALA	CA-C-N	-5.06	114.70	119.76
4	D	170	ALA	C-N-CA	-5.06	114.70	119.76
2	b	77	GLY	N-CA-C	5.04	120.72	114.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2631	0	2538	12	0
1	a	2634	0	2543	20	0
2	B	4023	0	3904	29	0
2	b	4028	0	3910	25	0
3	C	3506	0	3439	20	0
3	c	3544	0	3480	21	0
4	D	2726	0	2627	20	0
4	d	2720	0	2626	15	0
5	E	668	0	658	7	0
5	e	662	0	648	5	0
6	F	275	0	282	3	0
6	f	257	0	269	3	0
7	H	519	0	545	5	0
7	h	511	0	532	6	0
8	I	314	0	328	4	0
8	i	314	0	328	2	0
9	J	272	0	279	3	0
9	j	282	0	290	1	0
10	K	293	0	305	5	0
10	k	293	0	305	5	0
11	L	309	0	327	2	0
11	l	309	0	327	3	0
12	M	274	0	299	6	0
12	m	269	0	288	5	0
13	O	1883	0	1865	10	0
13	o	1879	0	1858	7	0
14	T	264	0	267	3	0
14	t	264	0	267	1	0
15	U	774	0	773	2	0
15	u	774	0	773	4	0
16	V	1072	0	1086	7	0
16	v	1064	0	1073	3	0
17	Y	215	0	246	3	0
17	y	215	0	246	4	0
18	X	292	0	328	2	0
18	x	287	0	317	2	0
19	Z	479	0	516	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	479	0	516	4	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	V	1	0	0	1	0
22	a	2	0	0	0	0
22	u	1	0	0	2	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	195	0	216	6	0
24	B	1040	0	1152	24	0
24	C	845	0	936	20	0
24	D	195	0	216	7	0
24	a	195	0	216	5	0
24	b	1040	0	1152	23	0
24	c	845	0	936	27	0
24	d	195	0	216	5	0
25	A	128	0	148	1	0
25	a	64	0	74	1	0
25	d	64	0	74	1	0
26	A	40	0	56	3	0
26	B	120	0	168	8	0
26	C	80	0	112	3	0
26	D	40	0	56	1	0
26	H	40	0	56	4	0
26	K	40	0	56	1	0
26	T	40	0	56	7	0
26	Y	40	0	56	2	0
26	a	40	0	56	0	0
26	b	120	0	168	8	0
26	c	80	0	112	9	0
26	d	40	0	56	3	0
26	h	40	0	56	4	0
26	k	40	0	56	1	0
26	t	40	0	56	4	0
26	y	40	0	56	1	0
27	A	108	0	156	4	0
27	F	43	0	53	3	0
27	a	108	0	155	4	0
27	b	54	0	78	2	0
27	f	43	0	53	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	l	54	0	78	2	0
28	A	18	0	24	2	0
28	B	42	0	56	3	0
28	C	12	0	16	1	0
28	F	6	0	8	0	0
28	O	6	0	8	0	0
28	T	12	0	16	2	0
28	V	30	0	40	4	0
28	a	12	0	16	2	0
28	b	30	0	40	3	0
28	c	18	0	24	2	0
28	f	6	0	7	0	0
28	t	6	0	8	1	0
28	v	24	0	32	1	0
29	A	28	0	0	0	0
29	B	33	0	0	0	0
29	C	34	0	0	0	0
29	D	57	0	0	0	0
29	I	40	0	0	0	0
29	J	10	0	0	0	0
29	M	10	0	0	0	0
29	X	10	0	0	0	0
29	a	30	0	0	0	0
29	b	33	0	0	0	0
29	d	53	0	0	0	0
29	i	40	0	0	0	0
29	j	10	0	0	0	0
29	k	42	0	0	0	0
29	m	10	0	0	0	0
29	x	10	0	0	0	0
30	A	33	0	39	0	0
30	B	25	0	35	1	0
30	D	35	0	46	1	0
30	E	35	0	46	0	0
30	I	35	0	46	2	0
30	M	70	0	92	3	0
30	a	70	0	92	4	0
30	b	50	0	70	1	0
30	f	35	0	46	0	0
30	m	70	0	92	2	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	A	55	0	80	4	0
32	D	55	0	80	0	0
32	a	55	0	80	10	0
32	d	55	0	80	0	0
33	B	1	0	0	0	0
33	F	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	f	1	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	2	0
34	C	153	0	216	7	0
34	J	51	0	72	2	0
34	Z	37	0	44	1	0
34	b	51	0	72	1	0
34	c	153	0	216	3	0
34	j	51	0	72	1	0
34	z	39	0	48	4	0
35	B	95	0	130	4	0
35	C	38	0	52	3	0
35	D	16	0	17	2	0
35	O	19	0	26	0	0
35	V	19	0	26	1	0
35	b	76	0	104	1	0
35	c	38	0	52	0	0
35	d	16	0	17	2	0
36	C	186	0	246	7	0
36	D	62	0	82	1	0
36	H	62	0	82	2	0
36	c	186	0	246	3	0
36	d	62	0	82	5	0
36	h	62	0	82	0	0
37	D	147	0	222	10	0
37	E	42	0	57	2	0
37	L	49	0	74	1	0
37	d	147	0	222	4	0
37	e	42	0	57	4	0
37	l	49	0	74	4	0
38	E	43	0	30	0	0
38	e	43	0	30	2	0
39	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	149	0	0	1	0
41	B	280	0	0	4	0
41	C	209	0	0	3	0
41	D	161	0	0	1	0
41	E	28	0	0	1	0
41	F	7	0	0	0	0
41	H	40	0	0	0	0
41	I	8	0	0	0	0
41	J	12	0	0	1	0
41	K	6	0	0	1	0
41	L	12	0	0	0	0
41	M	15	0	0	0	0
41	O	165	0	0	2	0
41	T	13	0	0	0	0
41	U	76	0	0	2	0
41	V	111	0	0	1	0
41	X	8	0	0	0	0
41	Y	1	0	0	0	0
41	a	151	0	0	1	0
41	b	249	0	0	2	0
41	c	189	0	0	3	0
41	d	139	0	0	1	0
41	e	15	0	0	0	0
41	f	7	0	0	0	0
41	h	36	0	0	0	0
41	i	5	0	0	0	0
41	j	7	0	0	0	0
41	k	3	0	0	0	0
41	l	10	0	0	1	0
41	m	12	0	0	0	0
41	o	137	0	0	0	0
41	t	10	0	0	0	0
41	u	89	0	0	3	0
41	v	80	0	0	1	0
41	x	5	0	0	0	0
41	y	4	0	0	0	0
All	All	53958	0	52755	427	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (427) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:HG2	32:A:419:PL9:H102	1.51	0.93
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.49	0.92
1:a:214:MET:HG2	32:a:416:PL9:H102	1.54	0.87
24:B:616:CLA:H71	24:B:617:CLA:H192	1.64	0.78
22:u:201:CL:CL	41:u:337:HOH:O	2.40	0.75
4:d:192:THR:HG23	24:d:402:CLA:HBC2	1.68	0.75
24:C:503:CLA:H193	35:C:522:HTG:H3'1	1.67	0.74
24:c:504:CLA:H61	24:c:514:CLA:H42	1.68	0.74
8:I:26:GLY:HA3	30:I:102:LMT:H6'1	1.70	0.73
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.71	0.73
24:c:503:CLA:H202	24:c:509:CLA:HBB1	1.72	0.72
2:B:39:LEU:HD22	30:a:401:LMT:H62	1.73	0.71
26:B:620:BCR:H331	26:B:620:BCR:HC8	1.73	0.71
32:A:419:PL9:H471	27:F:101:SQD:H302	1.71	0.71
36:D:407:DGD:HD4	5:E:45:ASP:HB3	1.73	0.70
22:u:201:CL:CL	41:v:301:HOH:O	2.47	0.69
13:O:58:ASN:HD21	13:O:61:GLN:HB2	1.60	0.66
27:A:411:SQD:H251	37:D:410:LHG:H131	1.78	0.66
4:d:101:PHE:HB3	36:d:407:DGD:HG2	1.78	0.66
18:x:2:THR:HG22	18:x:3:ILE:HG12	1.77	0.65
24:B:615:CLA:H18	34:B:621:LMG:H421	1.78	0.64
2:b:234:ILE:HB	28:b:632:GOL:H31	1.79	0.63
24:C:511:CLA:H192	24:C:511:CLA:HBC3	1.80	0.62
3:c:213[B]:LEU:HD11	26:c:516:BCR:H373	1.82	0.62
16:v:71:GLY:HA2	28:v:203:GOL:H32	1.81	0.62
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.82	0.62
2:B:248:ALA:HA	24:B:604:CLA:H42	1.81	0.62
24:b:620:CLA:H2	24:b:621:CLA:HBB2	1.82	0.62
1:a:238:LYS:NZ	41:a:628:HOH:O	2.32	0.61
2:B:266:GLU:HB3	28:B:628:GOL:H11	1.82	0.61
2:B:171:PRO:HD3	7:H:66:GLY:HA2	1.81	0.61
24:a:406:CLA:HBB1	24:a:406:CLA:HMB3	1.81	0.61
24:B:606:CLA:HHC	24:B:606:CLA:HBB1	1.81	0.60
13:O:68:THR:HG22	13:O:110[B]:MET:HG2	1.82	0.60
3:c:213[A]:LEU:HG	24:c:508:CLA:H202	1.83	0.60
32:A:419:PL9:H502	4:D:39:PRO:HG3	1.83	0.60
27:A:416:SQD:H271	2:b:109:LEU:HD13	1.84	0.59
24:b:616:CLA:H142	37:l:102:LHG:H371	1.85	0.59
3:c:167:VAL:HG13	24:c:514:CLA:H71	1.85	0.59
2:b:227:LYS:NZ	30:b:626:LMT:O6'	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:407:DGD:HAW1	27:f:101:SQD:H383	1.85	0.58
2:b:266:GLU:HB3	28:b:633:GOL:H11	1.86	0.57
3:c:286:ALA:HB2	24:c:504:CLA:HMD1	1.86	0.57
41:B:953:HOH:O	7:H:12[A]:ARG:NH2	2.38	0.57
1:a:211:PHE:CE2	32:a:416:PL9:H13	2.39	0.57
5:E:45:ASP:OD2	20:R:4:ARG:NH2	2.38	0.57
24:c:505:CLA:HHC	24:c:505:CLA:HBB1	1.86	0.57
35:B:622:HTG:H4'2	30:a:401:LMT:H61	1.87	0.57
24:B:602:CLA:H91	26:H:101:BCR:H21C	1.86	0.56
24:C:510:CLA:HMB1	24:C:510:CLA:HBB1	1.87	0.56
24:C:513:CLA:H101	24:C:514:CLA:H141	1.87	0.56
24:c:503:CLA:C4D	24:c:505:CLA:H2	2.34	0.56
1:a:262:TYR:HB3	37:e:101:LHG:HC62	1.88	0.56
3:c:438:LEU:HD11	24:c:507:CLA:HBB1	1.86	0.55
6:F:30:THR:HG21	34:J:101:LMG:H412	1.88	0.55
28:A:413:GOL:H11	12:M:1:FME:HG2	1.88	0.55
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.19	0.55
34:B:621:LMG:H242	4:D:284:ILE:HD13	1.86	0.55
26:Y:101:BCR:H321	26:Y:101:BCR:HC8	1.88	0.55
24:b:620:CLA:H2	24:b:621:CLA:CBB	2.36	0.55
24:c:508:CLA:HMC2	24:c:509:CLA:H102	1.89	0.55
35:d:411:HTG:H1	7:h:25:TRP:CG	2.42	0.55
24:C:514:CLA:HAB	26:C:515:BCR:H24C	1.88	0.55
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.88	0.55
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.41	0.55
37:D:410:LHG:H112	37:D:410:LHG:H382	1.88	0.55
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.39	0.55
32:a:416:PL9:HC2	32:a:416:PL9:H103	1.89	0.54
28:a:412:GOL:H11	12:m:1:FME:HG2	1.88	0.54
24:A:406:CLA:H91	34:J:101:LMG:H221	1.88	0.54
30:B:634:LMT:H2'	28:B:635:GOL:H2	1.88	0.54
4:d:24:ARG:HD3	18:x:37:VAL:HG22	1.89	0.54
4:D:13:GLY:HA3	35:D:411:HTG:H62	1.89	0.54
2:b:216:HIS:HE1	24:b:614:CLA:C1A	2.21	0.54
2:b:482:ILE:HD12	2:b:486:LEU:HD13	1.90	0.54
3:c:215:LYS:HG3	3:c:223:TRP:HA	1.90	0.54
26:y:101:BCR:H321	26:y:101:BCR:HC8	1.89	0.53
24:d:404:CLA:H162	7:h:33:VAL:HG13	1.91	0.53
26:d:405:BCR:H313	36:d:407:DGD:HA91	1.89	0.53
6:F:21:VAL:O	6:F:25:THR:HG23	2.08	0.53
26:T:102:BCR:H19C	26:b:623:BCR:H363	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:627:HTG:H7'1	13:o:180:GLU:HG3	1.91	0.53
34:c:501:LMG:H242	24:c:507:CLA:H92	1.90	0.53
10:K:17:ILE:H	10:K:17:ILE:HD13	1.73	0.53
24:c:515:CLA:H171	26:c:526:BCR:H373	1.91	0.53
11:l:2:GLU:O	41:l:207:HOH:O	2.18	0.53
12:m:28:GLN:O	12:m:32:GLN:HG3	2.09	0.53
28:b:631:GOL:H11	15:u:22:GLY:HA2	1.91	0.53
16:V:70:GLU:HB2	28:V:205:GOL:H12	1.90	0.52
32:A:419:PL9:H101	32:A:419:PL9:H13	1.90	0.52
37:D:410:LHG:H132	37:D:410:LHG:H372	1.91	0.52
27:b:601:SQD:H1	27:b:601:SQD:H462	1.90	0.52
36:d:407:DGD:O1B	36:d:407:DGD:O2D	2.28	0.52
26:B:620:BCR:H331	26:B:620:BCR:C8	2.35	0.52
3:C:215:LYS:NZ	41:C:769:HOH:O	2.42	0.52
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.92	0.52
12:M:28:GLN:O	12:M:32:GLN:HG3	2.10	0.52
2:B:86[B]:ILE:HD12	2:B:86[B]:ILE:H	1.74	0.52
12:M:33:GLN:HB2	12:m:33:GLN:HB2	1.92	0.52
24:c:515:CLA:HAB	26:c:526:BCR:H24C	1.91	0.52
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.91	0.51
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.46	0.51
26:t:101:BCR:H321	26:t:101:BCR:HC8	1.93	0.51
13:o:68:THR:HG22	13:o:110[B]:MET:HG2	1.91	0.51
4:D:61:HIS:HD2	41:D:599:HOH:O	1.92	0.51
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.91	0.51
4:D:192:THR:HG23	24:D:403:CLA:HBC2	1.91	0.51
8:I:36:ASP:OD1	8:I:36:ASP:N	2.43	0.51
3:C:391:ARG:NH2	41:C:776:HOH:O	2.44	0.51
1:a:271:LEU:HD11	32:a:416:PL9:HC8	1.93	0.51
3:C:443:TRP:CZ2	24:C:509:CLA:HMD1	2.47	0.50
24:c:508:CLA:H71	26:c:516:BCR:H10C	1.93	0.50
28:c:525:GOL:H2	41:c:708:HOH:O	2.10	0.50
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.10	0.50
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.92	0.50
3:C:155:ASN:OD1	41:C:757:HOH:O	2.19	0.50
41:U:230[A]:HOH:O	22:V:202:CL:CL	2.56	0.50
1:a:72:LEU:HD11	30:a:401:LMT:H52	1.93	0.50
26:H:101:BCR:H331	26:H:101:BCR:C8	2.42	0.50
2:B:83:GLU:C	2:B:86[B]:ILE:HD11	2.37	0.50
3:c:212:TYR:O	3:c:215:LYS:HG2	2.11	0.50
28:T:103:GOL:H12	30:m:103:LMT:H12	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:183:MET:HA	24:a:406:CLA:HMD1	1.93	0.49
2:b:412:THR:O	41:b:758:HOH:O	2.19	0.49
5:e:77:GLU:O	5:e:81:GLU:HG2	2.11	0.49
24:C:509:CLA:HBC3	24:C:511:CLA:H71	1.92	0.49
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.47	0.49
19:z:37:LYS:NZ	34:z:101:LMG:HC5	2.27	0.49
11:L:14:ARG:HB3	14:T:25[A]:GLU:HG2	1.93	0.49
27:a:411:SQD:H302	24:c:510:CLA:H71	1.94	0.49
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.94	0.49
2:b:103:LEU:HB2	24:b:611:CLA:H62	1.94	0.49
3:C:185:LEU:HB2	3:C:230:LEU:HD13	1.92	0.49
34:C:501:LMG:H152	36:C:517:DGD:HA82	1.94	0.49
5:e:26:THR:HB	38:e:102:HEM:HAB	1.95	0.49
10:k:15:TYR:CZ	19:z:5:PHE:HZ	2.30	0.49
1:a:153:SER:HB2	24:a:406:CLA:H43	1.93	0.49
3:c:223:TRP:CG	3:c:224:ILE:H	2.30	0.49
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.48	0.49
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.95	0.49
3:C:223:TRP:CG	3:C:224:ILE:H	2.31	0.49
4:D:24:ARG:NH2	27:F:101:SQD:O4	2.46	0.49
10:k:24:VAL:HG13	17:y:25:ILE:HD13	1.95	0.48
3:c:320:ARG:HB2	28:c:525:GOL:H32	1.94	0.48
24:b:610:CLA:HHC	24:b:610:CLA:HBB1	1.96	0.48
2:B:76[A]:SER:OG	35:B:622:HTG:O6	2.30	0.48
8:I:2:GLU:O	8:I:6:ILE:HG12	2.14	0.48
27:a:411:SQD:H142	37:d:410:LHG:H152	1.95	0.48
24:A:405:CLA:CBD	24:D:401:CLA:HAC2	2.43	0.48
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.96	0.48
3:C:286:ALA:HB2	24:C:503:CLA:HMD2	1.96	0.48
3:c:79:LYS:HB3	3:c:84:GLN:NE2	2.28	0.48
4:d:272:LEU:C	4:d:272:LEU:HD23	2.39	0.48
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.49	0.48
26:H:101:BCR:H331	26:H:101:BCR:HC8	1.95	0.48
26:T:102:BCR:HC8	26:T:102:BCR:H311	1.95	0.48
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.49	0.48
3:c:363:GLY:O	3:c:367:GLU:HG2	2.14	0.48
24:d:404:CLA:H142	7:h:36:GLY:HA3	1.95	0.48
26:b:623:BCR:H331	26:b:623:BCR:C8	2.43	0.48
24:b:611:CLA:H72	26:b:624:BCR:H311	1.96	0.47
37:l:102:LHG:H331	12:m:18:PRO:HB3	1.96	0.47
24:C:514:CLA:HBC1	34:Z:101:LMG:H171	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:102:BCR:H331	26:T:102:BCR:HC7	1.56	0.47
3:C:203:THR:O	3:C:235:GLY:HA3	2.14	0.47
37:E:101:LHG:HC61	37:E:101:LHG:H241	1.70	0.47
32:a:416:PL9:H512	27:f:101:SQD:H311	1.95	0.47
24:c:508:CLA:C3D	24:c:509:CLA:H193	2.45	0.47
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.96	0.47
1:a:265:PHE:HE2	32:a:416:PL9:H122	1.80	0.47
6:f:21:VAL:O	6:f:25:THR:HG23	2.14	0.47
10:k:17:ILE:HD13	10:k:17:ILE:H	1.80	0.47
16:v:30:LYS:HD3	16:v:118:HIS:NE2	2.29	0.47
34:C:501:LMG:H211	36:C:517:DGD:HA61	1.96	0.47
14:T:25[A]:GLU:HG3	28:T:101:GOL:H2	1.96	0.47
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.49	0.47
28:B:635:GOL:H31	30:M:101:LMT:H6D	1.96	0.47
16:V:14:SER:HA	28:V:208:GOL:H12	1.97	0.47
9:J:2:SER:N	41:J:208:HOH:O	2.48	0.47
13:O:84:GLU:OE2	41:O:543:HOH:O	2.20	0.47
4:D:272:LEU:C	4:D:272:LEU:HD23	2.40	0.47
13:O:110[B]:MET:HE2	13:O:116:ILE:HD11	1.97	0.47
24:b:606:CLA:H91	26:h:101:BCR:H21C	1.97	0.47
24:c:511:CLA:HBB1	24:c:511:CLA:HMB1	1.96	0.47
27:a:411:SQD:H251	37:d:410:LHG:H121	1.96	0.46
2:b:248:ALA:HA	24:b:608:CLA:H42	1.96	0.46
34:j:101:LMG:H192	34:j:101:LMG:H221	1.62	0.46
1:A:84:PRO:HA	1:A:112:TYR:CG	2.50	0.46
16:V:24:LYS:HD3	28:V:207:GOL:H2	1.98	0.46
24:b:609:CLA:H43	24:b:610:CLA:H2	1.97	0.46
10:k:10:LYS:HD2	10:k:10:LYS:N	2.31	0.46
4:D:49:LEU:HD13	26:D:405:BCR:C15	2.45	0.46
1:A:160:ILE:HD11	36:C:517:DGD:HBT2	1.98	0.46
24:C:502:CLA:H192	24:C:507:CLA:C1B	2.45	0.46
2:B:476:ARG:NH1	41:B:951:HOH:O	2.46	0.46
24:B:612:CLA:H161	24:B:612:CLA:H192	1.81	0.46
13:o:58:ASN:C	13:o:60:ARG:H	2.24	0.46
26:t:101:BCR:H331	26:t:101:BCR:HC7	1.60	0.46
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.50	0.46
3:C:38:GLY:HA3	24:C:512:CLA:HMD2	1.98	0.46
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.15	0.46
35:d:411:HTG:H1	7:h:25:TRP:CD1	2.50	0.46
24:C:509:CLA:H122	24:C:509:CLA:H162	1.75	0.46
26:c:516:BCR:H15C	26:c:516:BCR:H351	1.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:502:CLA:C4D	24:C:504:CLA:H2	2.46	0.46
36:C:518:DGD:HAE2	36:C:518:DGD:HA81	1.68	0.46
24:C:507:CLA:HMC1	24:C:508:CLA:H102	1.98	0.45
4:D:141:TYR:OH	37:D:408:LHG:O4	2.29	0.45
37:D:410:LHG:H331	37:D:410:LHG:H302	1.57	0.45
4:D:123:ILE:HD11	36:H:102:DGD:HAE1	1.97	0.45
2:b:162:PHE:O	24:b:611:CLA:HHD	2.16	0.45
37:D:410:LHG:H141	37:D:410:LHG:H322	1.99	0.45
26:K:101:BCR:H24C	26:K:101:BCR:H371	1.73	0.45
25:a:408:PHO:NC	25:a:408:PHO:ND	2.62	0.45
2:b:462:PHE:CE1	24:b:618:CLA:HMB2	2.52	0.45
8:i:36:ASP:OD1	8:i:36:ASP:N	2.49	0.45
36:C:519:DGD:HBF1	37:D:410:LHG:H211	1.98	0.45
4:D:123:ILE:HD11	36:H:102:DGD:HAH2	1.97	0.45
2:B:223:GLN:NE2	41:B:937:HOH:O	2.30	0.45
24:D:404:CLA:H171	18:X:15[A]:LEU:HD13	1.99	0.45
3:c:50:LEU:HD11	24:c:515:CLA:HBB1	1.98	0.45
4:d:186:GLN:HB2	24:d:402:CLA:HBC1	1.99	0.45
24:d:404:CLA:H3A	24:d:404:CLA:HBA1	1.76	0.45
4:D:141:TYR:HA	4:D:144:ILE:HD12	1.99	0.45
20:R:8:VAL:O	20:R:11:PRO:HD2	2.17	0.45
3:C:218:PHE:HE2	34:C:501:LMG:H111	1.80	0.45
32:a:416:PL9:H221	32:a:416:PL9:H201	1.71	0.45
34:z:101:LMG:H111	34:z:101:LMG:H142	1.68	0.45
26:T:102:BCR:H11C	26:b:623:BCR:H382	1.98	0.44
2:b:256:MET:HA	2:b:263:THR:HG21	1.98	0.44
3:c:178:LYS:NZ	41:c:714:HOH:O	2.49	0.44
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.99	0.44
24:C:504:CLA:HAB	34:C:521:LMG:H241	1.99	0.44
3:C:288:CYS:SG	36:C:517:DGD:HB32	2.58	0.44
13:O:57:LYS:HE3	2:b:338:GLN:HA	1.99	0.44
28:a:412:GOL:C1	12:m:1:FME:HG2	2.47	0.44
26:c:526:BCR:H11C	26:c:526:BCR:H341	1.89	0.44
1:A:200:LEU:HG	36:C:519:DGD:HAT2	1.98	0.44
26:A:410:BCR:H24C	26:A:410:BCR:H371	1.76	0.44
4:D:16:ASP:OD2	30:D:402:LMT:O6'	2.34	0.44
26:T:102:BCR:HC8	26:T:102:BCR:H321	1.99	0.44
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.52	0.44
41:A:615[B]:HOH:O	16:V:30:LYS:HE2	2.17	0.44
2:B:233:ASN:O	2:B:236:THR:HG22	2.18	0.44
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:618:BCR:H383	27:l:101:SQD:H101	2.00	0.44
36:c:519:DGD:HAE2	36:c:519:DGD:HA81	1.80	0.44
26:h:101:BCR:H24C	26:h:101:BCR:H371	1.74	0.44
26:B:619:BCR:H24C	26:B:619:BCR:H371	1.81	0.44
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.53	0.44
24:b:619:CLA:H62	24:b:619:CLA:H41	1.45	0.44
30:M:102:LMT:H6D	11:l:9:PRO:HA	2.00	0.44
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.53	0.44
14:t:25[A]:GLU:HG3	28:t:102:GOL:H2	2.00	0.44
28:A:413:GOL:C1	12:M:1:FME:HG2	2.48	0.44
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.53	0.44
5:E:60:GLN:NE2	41:E:228:HOH:O	2.51	0.44
34:c:520:LMG:H301	34:c:520:LMG:H182	2.00	0.44
8:i:35:LYS:O	8:i:37:LEU:N	2.51	0.44
2:B:491:VAL:HG12	4:D:136:VAL:HG13	2.00	0.44
5:E:68:ASP:OD1	5:E:71:GLU:N	2.42	0.44
16:V:55[B]:ARG:NH1	41:V:388:HOH:O	2.51	0.44
1:a:215:HIS:ND1	32:a:416:PL9:O1	2.50	0.44
26:c:526:BCR:H15C	26:c:526:BCR:H351	1.87	0.44
27:F:101:SQD:H342	27:F:101:SQD:H311	1.65	0.43
26:b:624:BCR:C8	26:b:624:BCR:H331	2.48	0.43
15:u:81:HIS:HD2	41:u:326:HOH:O	1.99	0.43
26:Y:101:BCR:H15C	26:Y:101:BCR:H351	1.89	0.43
27:b:601:SQD:O8	11:l:7:ARG:HD2	2.18	0.43
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	1.99	0.43
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.99	0.43
35:V:204:HTG:H4'1	35:V:204:HTG:H1'1	1.78	0.43
1:a:84:PRO:HA	1:a:112:TYR:CG	2.53	0.43
2:b:290:ALA:O	41:b:730:HOH:O	2.21	0.43
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.75	0.43
26:k:103:BCR:H24C	26:k:103:BCR:H371	1.59	0.43
13:o:136:ILE:HD12	13:o:243:ILE:HD13	2.00	0.43
24:B:607:CLA:H61	24:B:607:CLA:H102	1.72	0.43
4:D:273:PHE:CE2	37:L:101:LHG:H112	2.52	0.43
3:c:443:TRP:CZ2	24:c:510:CLA:HMD1	2.53	0.43
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.53	0.43
17:y:20:ALA:O	17:y:24:MET:HG2	2.18	0.43
2:B:13:ILE:HG12	24:B:613:CLA:HAC2	2.01	0.43
24:B:615:CLA:H112	24:B:615:CLA:H71	1.62	0.43
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.53	0.43
1:A:63:ILE:HB	3:C:335:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:614:CLA:H43	37:D:408:LHG:H372	2.01	0.43
26:B:619:BCR:H363	26:t:101:BCR:H19C	2.00	0.43
3:C:279:LEU:HD22	24:C:510:CLA:HED2	2.00	0.43
35:D:411:HTG:H1	7:H:25:TRP:CD1	2.53	0.43
27:a:411:SQD:H361	27:a:411:SQD:H332	1.86	0.43
5:e:8:ARG:HH21	5:e:12:ASP:HB3	1.83	0.43
24:B:615:CLA:H41	24:B:615:CLA:H62	1.88	0.43
2:b:30:VAL:HG12	24:b:610:CLA:HHD	2.00	0.43
3:c:38:GLY:HA3	24:c:513:CLA:HMD2	2.01	0.43
27:A:411:SQD:H131	37:D:410:LHG:H142	1.99	0.43
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.53	0.43
2:B:216:HIS:CE1	24:B:610:CLA:NA	2.86	0.43
24:D:401:CLA:H203	24:D:401:CLA:H162	1.80	0.43
26:T:102:BCR:H24C	26:T:102:BCR:H371	1.84	0.43
17:Y:20:ALA:O	17:Y:24:MET:HG2	2.18	0.43
24:b:620:CLA:H112	24:b:620:CLA:H91	1.79	0.43
3:c:52:ALA:HB2	24:c:513:CLA:HMA2	2.01	0.43
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.34	0.43
12:M:34:LYS:HG2	30:M:102:LMT:O3B	2.18	0.43
24:b:618:CLA:H18	37:d:408:LHG:H202	2.01	0.43
3:c:406:SER:HA	3:c:420:VAL:HG23	2.00	0.43
24:c:505:CLA:HBB1	34:c:521:LMG:H231	2.01	0.43
24:c:511:CLA:H191	24:c:514:CLA:HAC1	2.00	0.43
25:A:408:PHO:NC	25:A:408:PHO:ND	2.67	0.43
24:B:604:CLA:H3A	24:B:604:CLA:CGA	2.48	0.43
34:C:520:LMG:H211	34:C:520:LMG:H242	1.81	0.43
9:J:6:ARG:H	9:J:6:ARG:HG2	1.69	0.43
10:K:10:LYS:HD2	10:K:10:LYS:N	2.34	0.43
3:c:175:LEU:HD23	3:c:237:HIS:CG	2.54	0.43
24:c:510:CLA:H203	36:c:518:DGD:HA92	2.01	0.43
4:d:139:ARG:NH2	41:d:635:HOH:O	2.51	0.43
2:B:283:GLU:OE2	2:B:287[B]:ARG:NE	2.51	0.42
24:D:401:CLA:HBB1	24:D:401:CLA:HMB3	2.01	0.42
13:O:180:GLU:CD	13:O:180:GLU:H	2.27	0.42
15:U:76:ARG:NH2	41:U:201:HOH:O	2.51	0.42
24:c:507:CLA:HAA1	24:c:507:CLA:HBD	2.01	0.42
27:l:101:SQD:H462	27:l:101:SQD:H1	2.01	0.42
3:C:202:PRO:HD2	35:C:523:HTG:H62	2.01	0.42
24:C:514:CLA:HAB	26:C:515:BCR:H371	2.00	0.42
11:L:9:PRO:HA	30:m:102:LMT:H6D	2.01	0.42
24:b:606:CLA:H143	24:b:606:CLA:C1B	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:622:BCR:H24C	26:b:622:BCR:H371	1.76	0.42
5:e:26:THR:HB	38:e:102:HEM:CAB	2.48	0.42
37:e:101:LHG:H152	6:f:22:ALA:HB1	2.01	0.42
2:B:492:GLU:HG3	41:B:915:HOH:O	2.19	0.42
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.77	0.42
34:C:520:LMG:H192	10:K:27:VAL:HG11	2.02	0.42
4:D:24:ARG:HD3	18:X:37:VAL:HG22	2.00	0.42
5:E:84:LYS:HD3	5:E:84:LYS:HA	1.91	0.42
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.85	0.42
24:b:611:CLA:H111	24:b:611:CLA:H152	1.80	0.42
4:d:209:LEU:HD23	4:d:209:LEU:C	2.43	0.42
4:d:273:PHE:CE2	37:l:102:LHG:H112	2.54	0.42
19:z:29:SER:HA	19:z:30:PRO:HD3	1.85	0.42
35:B:622:HTG:H5'2	30:a:401:LMT:H82	2.01	0.42
24:B:607:CLA:H111	24:B:607:CLA:H142	1.83	0.42
36:c:518:DGD:HB32	36:c:518:DGD:HB61	1.33	0.42
12:M:3:VAL:HG11	14:T:2:GLU:HG2	2.01	0.42
32:a:416:PL9:H171	32:a:416:PL9:H151	1.67	0.42
3:c:127:PHE:CE1	34:z:101:LMG:H152	2.55	0.42
26:c:526:BCR:H24C	26:c:526:BCR:H371	1.81	0.42
24:B:615:CLA:HAA1	24:B:615:CLA:HBD	2.00	0.42
3:C:425:TRP:CD1	24:C:505:CLA:HMA2	2.55	0.42
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.92	0.42
13:O:179:GLU:HG2	41:O:499:HOH:O	2.19	0.42
1:a:259:ILE:HA	37:e:101:LHG:H202	2.01	0.42
26:c:516:BCR:H24C	26:c:516:BCR:H371	1.83	0.42
3:C:218:PHE:CE2	34:C:501:LMG:H111	2.54	0.42
1:A:249:VAL:HG12	2:B:491:VAL:HG21	2.02	0.42
26:B:618:BCR:H11C	26:B:618:BCR:H341	1.86	0.42
17:Y:38:LEU:O	17:Y:42:ARG:HD3	2.20	0.42
24:A:405:CLA:HBD	24:D:401:CLA:HAC2	2.00	0.41
24:A:409:CLA:H61	24:A:409:CLA:H102	1.76	0.41
32:a:416:PL9:H401	32:a:416:PL9:H421	1.91	0.41
2:b:27:THR:HG22	2:b:107:LEU:HD13	2.01	0.41
15:u:81:HIS:HE1	41:u:309:HOH:O	2.02	0.41
19:z:37:LYS:HZ3	34:z:101:LMG:HC5	1.84	0.41
24:B:617:CLA:H62	24:B:617:CLA:H41	1.52	0.41
15:U:8:GLU:HG2	15:U:9:LEU:H	1.84	0.41
16:V:68:ASN:OD1	28:V:205:GOL:H2	2.19	0.41
17:Y:27:MET:HE2	17:Y:27:MET:HB3	1.97	0.41
24:a:409:CLA:H61	24:a:409:CLA:H102	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:622:BCR:H12C	34:b:625:LMG:C43	2.50	0.41
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.01	0.41
1:A:253:GLY:HA3	2:B:491:VAL:HB	2.02	0.41
35:B:623:HTG:H1	35:B:623:HTG:H2'2	1.86	0.41
5:E:36:LEU:HA	5:E:39:SER:OG	2.20	0.41
2:b:491:VAL:HG13	4:d:136:VAL:HG13	2.02	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.84	0.41
26:b:624:BCR:H15C	26:b:624:BCR:H351	1.94	0.41
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.41
24:c:503:CLA:C3D	24:c:505:CLA:H2	2.51	0.41
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	2.01	0.41
26:B:620:BCR:H371	26:B:620:BCR:H24C	1.82	0.41
26:T:102:BCR:H11C	26:T:102:BCR:H341	1.97	0.41
20:R:24:LEU:N	20:R:25:PRO:HD2	2.36	0.41
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.90	0.41
24:C:507:CLA:H52	30:I:102:LMT:H71	2.02	0.41
28:C:524:GOL:O1	16:V:49:ASN:ND2	2.48	0.41
5:E:82:GLN:C	5:E:84:LYS:H	2.29	0.41
27:f:101:SQD:H81	27:f:101:SQD:H45	1.80	0.41
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.03	0.41
24:B:617:CLA:H93	24:B:617:CLA:H61	1.95	0.41
3:C:334:PRO:HA	13:O:153:THR:OG1	2.20	0.41
3:c:42:LEU:HD21	24:c:513:CLA:H2A	2.03	0.41
24:A:406:CLA:HBB1	24:A:406:CLA:HMB1	2.03	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.02	0.41
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.76	0.41
2:b:216:HIS:CE1	24:b:614:CLA:NA	2.89	0.41
4:d:273:PHE:CZ	37:l:102:LHG:H112	2.56	0.41
26:d:405:BCR:HC22	36:d:407:DGD:HA72	2.03	0.41
26:h:101:BCR:C8	26:h:101:BCR:H331	2.51	0.41
13:o:110[B]:MET:HE2	13:o:116:ILE:HD11	2.03	0.41
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.55	0.41
24:D:401:CLA:O1A	24:D:401:CLA:H43	2.20	0.41
10:K:25:LEU:HB2	41:K:201:HOH:O	2.21	0.41
20:R:27:ALA:O	20:R:31:VAL:HG23	2.21	0.41
24:b:606:CLA:H72	24:b:606:CLA:H2	2.02	0.41
24:b:620:CLA:H112	24:b:620:CLA:H152	1.85	0.41
24:c:514:CLA:O1A	41:c:782:HOH:O	2.22	0.41
4:d:279:LEU:HD22	25:d:403:PHO:HBC3	2.03	0.41
5:e:68:ASP:OD1	5:e:71:GLU:N	2.48	0.41
26:A:410:BCR:H11C	26:A:410:BCR:H341	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:416:SQD:H301	27:A:416:SQD:H272	1.85	0.40
2:B:423:LYS:HD3	2:B:423:LYS:HA	1.79	0.40
24:C:508:CLA:H61	24:C:508:CLA:H92	1.75	0.40
26:d:405:BCR:H351	26:d:405:BCR:H15C	1.81	0.40
37:d:410:LHG:H331	37:d:410:LHG:H302	1.50	0.40
8:I:33:LYS:HA	8:I:33:LYS:HD3	1.89	0.40
37:D:410:LHG:H242	37:D:410:LHG:H272	1.95	0.40
26:t:101:BCR:H382	26:t:101:BCR:H23C	2.03	0.40
24:B:604:CLA:HAB	24:B:606:CLA:H171	2.03	0.40
24:B:617:CLA:H111	24:B:617:CLA:H152	1.93	0.40
4:D:27:PHE:CD1	37:E:101:LHG:HC12	2.57	0.40
1:a:153:SER:CB	24:a:406:CLA:H43	2.51	0.40
24:b:610:CLA:H41	24:b:610:CLA:H62	1.77	0.40
24:b:613:CLA:HAB	4:d:123:ILE:HG12	2.04	0.40
26:h:101:BCR:H312	26:h:101:BCR:HC32	1.90	0.40
26:A:410:BCR:H351	26:A:410:BCR:H15C	1.84	0.40
3:C:238:ILE:HD13	35:C:523:HTG:H2'1	2.03	0.40
37:e:101:LHG:H251	37:e:101:LHG:H282	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	36	28
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	36	28
2	B	512/505 (101%)	507 (99%)	5 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	454/455 (100%)	445 (98%)	7 (2%)	2 (0%)	30	21
3	c	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	30	21

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100 100
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
All	All	5279/5382 (98%)	5168 (98%)	104 (2%)	7 (0%)	48 41

All (7) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	272/279 (98%)	272 (100%)	0	100 100
1	a	273/279 (98%)	272 (100%)	1 (0%)	84 85
2	B	412/403 (102%)	409 (99%)	3 (1%)	76 76
2	b	413/403 (102%)	411 (100%)	2 (0%)	81 82
3	C	357/356 (100%)	353 (99%)	4 (1%)	65 64
3	c	362/356 (102%)	358 (99%)	4 (1%)	65 64
4	D	277/277 (100%)	275 (99%)	2 (1%)	76 76
4	d	277/277 (100%)	274 (99%)	3 (1%)	65 64
5	E	74/73 (101%)	74 (100%)	0	100 100
5	e	72/73 (99%)	71 (99%)	1 (1%)	59 56
6	F	28/38 (74%)	27 (96%)	1 (4%)	31 21
6	f	26/38 (68%)	25 (96%)	1 (4%)	29 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	H	55/54 (102%)	52 (94%)	3 (6%)	19 8
7	h	54/54 (100%)	54 (100%)	0	100 100
8	I	34/34 (100%)	34 (100%)	0	100 100
8	i	34/34 (100%)	34 (100%)	0	100 100
9	J	26/26 (100%)	26 (100%)	0	100 100
9	j	26/26 (100%)	26 (100%)	0	100 100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15 5
10	k	30/30 (100%)	28 (93%)	2 (7%)	15 5
11	L	36/35 (103%)	35 (97%)	1 (3%)	38 30
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 30
12	M	31/32 (97%)	31 (100%)	0	100 100
12	m	30/32 (94%)	29 (97%)	1 (3%)	33 24
13	O	210/207 (101%)	209 (100%)	1 (0%)	81 82
13	o	209/207 (101%)	208 (100%)	1 (0%)	81 82
14	T	27/27 (100%)	25 (93%)	2 (7%)	13 4
14	t	27/27 (100%)	25 (93%)	2 (7%)	13 4
15	U	84/89 (94%)	83 (99%)	1 (1%)	63 61
15	u	84/89 (94%)	84 (100%)	0	100 100
16	V	118/117 (101%)	117 (99%)	1 (1%)	73 74
16	v	117/117 (100%)	116 (99%)	1 (1%)	70 70
17	Y	22/23 (96%)	22 (100%)	0	100 100
17	y	22/23 (96%)	21 (96%)	1 (4%)	24 14
18	X	33/33 (100%)	33 (100%)	0	100 100
18	x	32/33 (97%)	32 (100%)	0	100 100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29 19
19	z	52/52 (100%)	50 (96%)	2 (4%)	29 19
20	R	29/29 (100%)	28 (97%)	1 (3%)	32 23
All	All	4383/4399 (100%)	4336 (99%)	47 (1%)	68 64

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	84	THR

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Mol	Chain	Res	Type
2	B	362	PHE
2	B	492	GLU
3	C	29	GLU
3	C	142	GLU
3	C	289	PHE
3	C	315	MET
4	D	329	MET
4	D	345	VAL
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	65	LEU
10	K	10	LYS
10	K	17	ILE
11	L	1	MET
13	O	181	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	70	ARG
16	V	86	GLN
19	Z	3	ILE
19	Z	6	GLN
20	R	4	ARG
1	a	12	ASN
2	b	84	THR
2	b	121	GLU
3	c	142	GLU
3	c	289	PHE
3	c	315	MET
3	c	355	THR
4	d	90	LEU
4	d	329	MET
4	d	345	VAL
5	e	59	GLU
6	f	44	GLN
10	k	10	LYS
10	k	17	ILE
11	l	1	MET
12	m	33	GLN
13	o	181	GLU
14	t	25[A]	GLU
14	t	25[B]	GLU

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Mol	Chain	Res	Type
16	v	86	GLN
17	y	42	ARG
19	z	3	ILE
19	z	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
2	B	331	ASN
2	B	490	GLN
3	C	44	ASN
3	C	201	ASN
3	C	322	GLN
4	D	61	HIS
4	D	186	GLN
4	D	255	GLN
5	E	74	GLN
19	Z	31	GLN
1	a	165	GLN
2	b	289	GLN
2	b	331	ASN
2	b	490	GLN
2	b	497	GLN
3	c	28	GLN
3	c	44	ASN
3	c	415	ASN
4	d	186	GLN
4	d	301	GLN
4	d	350	ASN
10	k	40	GLN
12	m	28	GLN
12	m	32	GLN
13	o	155	ASN
15	u	78	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	i	1	8	8,9,10	0.62	0	7,9,11	1.17	1 (14%)
9	FME	j	1	9	8,9,10	0.63	0	7,9,11	1.32	1 (14%)
14	FME	t	1	14	8,9,10	0.85	0	7,9,11	2.28	4 (57%)
12	FME	M	1	12	8,9,10	0.63	0	7,9,11	1.32	0
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.32	2 (28%)
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	1.73	3 (42%)
12	FME	m	1	12	8,9,10	0.69	0	7,9,11	1.05	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
8	FME	i	1	8	-	0/7/9/11	-
9	FME	j	1	9	-	2/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	C-CA-N	3.68	116.36	109.73
14	t	1	FME	O-C-CA	-3.00	116.92	124.78
14	T	1	FME	O-C-CA	-2.78	117.48	124.78

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

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	2	0
12	m	1	FME	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 252 ligands modelled in this entry, 17 are monoatomic and 19 are unknown - leaving 216 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	LMG	c	501	-	51,51,55	0.88	2 (3%)	59,59,63	1.25	6 (10%)
37	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.09	3 (6%)
25	PHO	A	407	-	58,69,69	2.76	11 (18%)	56,99,99	2.78	14 (25%)
37	LHG	e	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.04	3 (6%)
37	LHG	d	408	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	5 (9%)
24	CLA	B	614	2	69,73,73	2.02	18 (26%)	83,113,113	2.76	33 (39%)
24	CLA	b	611	2	69,73,73	2.01	20 (28%)	83,113,113	2.88	32 (38%)
24	CLA	c	513	3	69,73,73	2.02	19 (27%)	83,113,113	2.75	29 (34%)
24	CLA	b	613	2	69,73,73	2.08	20 (28%)	83,113,113	2.81	32 (38%)
24	CLA	b	606	41	69,73,73	2.09	20 (28%)	83,113,113	2.79	26 (31%)
26	BCR	c	516	-	41,41,41	1.08	1 (2%)	56,56,56	1.41	9 (16%)
31	OEX	A	418	41,3,1	0,14,14	-	-	-		
40	HEC	V	203	16	50,50,50	1.71	9 (18%)	68,82,82	1.82	15 (22%)
24	CLA	b	610	2	69,73,73	2.00	19 (27%)	83,113,113	2.98	31 (37%)
36	DGD	c	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.09	6 (7%)
28	GOL	c	524	-	5,5,5	0.32	0	5,5,5	0.37	0
37	LHG	d	410	-	48,48,48	0.94	2 (4%)	51,54,54	0.97	3 (5%)
24	CLA	C	514	3	69,73,73	2.00	20 (28%)	83,113,113	2.81	31 (37%)
34	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	4 (6%)
28	GOL	c	525	-	5,5,5	0.36	0	5,5,5	0.58	0
38	HEM	e	102	5,6	50,50,50	1.56	7 (14%)	66,82,82	1.76	17 (25%)
36	DGD	c	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	3 (3%)
28	GOL	B	633	-	5,5,5	0.30	0	5,5,5	0.66	0
26	BCR	b	623	-	41,41,41	1.08	1 (2%)	56,56,56	1.13	5 (8%)
24	CLA	B	609	2	69,73,73	2.06	20 (28%)	83,113,113	2.77	29 (34%)
24	CLA	c	504	3	69,73,73	2.01	19 (27%)	83,113,113	2.74	29 (34%)
24	CLA	B	611	41	69,73,73	2.05	20 (28%)	83,113,113	2.79	31 (37%)
26	BCR	A	410	-	41,41,41	1.02	1 (2%)	56,56,56	1.33	7 (12%)
26	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.33	8 (14%)
28	GOL	V	205	-	5,5,5	0.37	0	5,5,5	0.30	0
28	GOL	b	633	-	5,5,5	0.37	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	607	2	69,73,73	2.07	20 (28%)	83,113,113	2.89	33 (39%)
36	DGD	H	102	-	63,63,67	0.93	3 (4%)	77,77,81	0.90	3 (3%)
24	CLA	C	503	3	69,73,73	2.05	20 (28%)	83,113,113	2.72	30 (36%)
36	DGD	c	519	-	63,63,67	0.89	2 (3%)	77,77,81	0.97	3 (3%)
30	LMT	a	401	-	36,36,36	0.45	0	47,47,47	0.97	3 (6%)
27	SQD	b	601	-	53,54,54	1.02	3 (5%)	62,65,65	1.63	10 (16%)
28	GOL	A	413	-	5,5,5	0.43	0	5,5,5	0.62	0
24	CLA	b	620	2	69,73,73	2.04	20 (28%)	83,113,113	2.83	28 (33%)
30	LMT	A	417	-	34,34,36	0.38	0	45,45,47	1.06	3 (6%)
30	LMT	m	103	-	36,36,36	0.56	1 (2%)	47,47,47	1.05	4 (8%)
28	GOL	C	524	-	5,5,5	0.34	0	5,5,5	0.89	0
34	LMG	c	521	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	5 (8%)
35	HTG	O	303	-	19,19,19	1.07	1 (5%)	23,24,24	0.93	1 (4%)
36	DGD	D	407	-	63,63,67	0.96	4 (6%)	77,77,81	1.30	9 (11%)
37	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.09	5 (9%)
32	PL9	d	406	-	55,55,55	0.71	1 (1%)	68,69,69	1.55	14 (20%)
30	LMT	m	102	-	36,36,36	0.49	0	47,47,47	0.99	2 (4%)
26	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.39	8 (14%)
28	GOL	T	101	-	5,5,5	0.45	0	5,5,5	0.31	0
30	LMT	B	634	-	25,25,36	0.49	0	30,30,47	0.71	0
24	CLA	c	508	3	69,73,73	2.02	20 (28%)	83,113,113	2.70	31 (37%)
24	CLA	B	607	2	69,73,73	2.03	19 (27%)	83,113,113	2.88	31 (37%)
28	GOL	b	630	-	5,5,5	0.34	0	5,5,5	0.16	0
35	HTG	B	630	-	19,19,19	0.97	2 (10%)	23,24,24	1.31	1 (4%)
37	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.16	5 (9%)
24	CLA	b	612	41	69,73,73	1.96	19 (27%)	83,113,113	2.75	31 (37%)
30	LMT	b	602	-	25,25,36	0.46	0	30,30,47	1.26	3 (10%)
35	HTG	B	623	-	19,19,19	0.88	1 (5%)	23,24,24	1.25	3 (13%)
28	GOL	V	206	-	5,5,5	0.37	0	5,5,5	0.46	0
35	HTG	c	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.50	2 (8%)
34	LMG	c	520	-	51,51,55	0.95	2 (3%)	59,59,63	0.92	2 (3%)
34	LMG	z	101	-	39,39,55	1.11	2 (5%)	47,47,63	1.17	4 (8%)
24	CLA	D	401	41	69,73,73	2.04	20 (28%)	83,113,113	2.82	34 (40%)
26	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	5 (8%)
24	CLA	D	404	4	69,73,73	2.02	19 (27%)	83,113,113	2.88	32 (38%)
36	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.02	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	619	2	69,73,73	1.99	20 (28%)	83,113,113	2.90	33 (39%)
24	CLA	c	514	3	69,73,73	2.02	20 (28%)	83,113,113	2.91	32 (38%)
28	GOL	V	207	-	5,5,5	0.37	0	5,5,5	0.46	0
24	CLA	C	510	3	69,73,73	2.12	20 (28%)	83,113,113	2.78	31 (37%)
24	CLA	c	510	3	69,73,73	2.07	20 (28%)	83,113,113	2.83	30 (36%)
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	10 (17%)
25	PHO	d	403	-	58,69,69	2.82	11 (18%)	56,99,99	2.88	16 (28%)
26	BCR	B	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.24	5 (8%)
28	GOL	v	204	-	5,5,5	0.32	0	5,5,5	0.37	0
24	CLA	b	608	2	69,73,73	2.06	20 (28%)	83,113,113	2.89	31 (37%)
37	LHG	D	410	-	48,48,48	0.94	2 (4%)	51,54,54	0.94	3 (5%)
26	BCR	B	620	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	13 (23%)
24	CLA	B	613	2	69,73,73	2.03	21 (30%)	83,113,113	2.72	27 (32%)
28	GOL	B	625	-	5,5,5	0.31	0	5,5,5	0.56	0
35	HTG	b	603	-	19,19,19	1.07	2 (10%)	23,24,24	1.28	1 (4%)
24	CLA	B	616	2	69,73,73	2.05	20 (28%)	83,113,113	2.78	31 (37%)
24	CLA	B	605	2	69,73,73	1.95	22 (31%)	83,113,113	2.91	30 (36%)
24	CLA	b	614	2	69,73,73	2.07	19 (27%)	83,113,113	2.78	31 (37%)
24	CLA	d	404	4	69,73,73	2.05	20 (28%)	83,113,113	2.91	29 (34%)
25	PHO	A	408	-	58,69,69	2.80	13 (22%)	56,99,99	3.01	17 (30%)
24	CLA	c	505	3	69,73,73	2.03	19 (27%)	83,113,113	2.84	29 (34%)
24	CLA	d	401	41	69,73,73	2.01	17 (24%)	83,113,113	2.79	31 (37%)
26	BCR	T	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	11 (19%)
28	GOL	A	412	-	5,5,5	0.26	0	5,5,5	0.68	0
31	OEX	a	415	41,3,1	0,14,14	-	-	-		
27	SQD	l	101	-	53,54,54	1.00	3 (5%)	62,65,65	1.40	9 (14%)
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	7 (9%)
24	CLA	B	610	2	69,73,73	2.00	17 (24%)	83,113,113	2.86	30 (36%)
24	CLA	C	507	3	69,73,73	2.04	20 (28%)	83,113,113	2.71	31 (37%)
35	HTG	b	628	-	19,19,19	1.10	2 (10%)	23,24,24	1.83	3 (13%)
26	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.25	5 (8%)
24	CLA	B	603	2	69,73,73	2.02	21 (30%)	83,113,113	2.91	30 (36%)
24	CLA	B	617	2	69,73,73	1.98	21 (30%)	83,113,113	2.77	29 (34%)
26	BCR	k	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.33	5 (8%)
24	CLA	a	407	41	69,73,73	2.05	20 (28%)	83,113,113	2.86	33 (39%)
28	GOL	B	628	-	5,5,5	0.40	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	LHG	D	409	-	48,48,48	0.85	2 (4%)	51,54,54	1.08	5 (9%)
24	CLA	D	403	4	69,73,73	2.04	20 (28%)	83,113,113	2.82	30 (36%)
24	CLA	A	409	1	69,73,73	2.03	20 (28%)	83,113,113	2.85	31 (37%)
24	CLA	B	608	41	69,73,73	2.01	20 (28%)	83,113,113	2.72	33 (39%)
24	CLA	C	512	3	69,73,73	2.01	19 (27%)	83,113,113	2.83	28 (33%)
24	CLA	B	615	2	69,73,73	1.98	20 (28%)	83,113,113	3.03	31 (37%)
28	GOL	T	103	-	5,5,5	0.41	0	5,5,5	0.24	0
35	HTG	C	523	-	19,19,19	1.02	2 (10%)	23,24,24	1.77	5 (21%)
34	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.14	5 (8%)
27	SQD	a	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.60	11 (17%)
26	BCR	b	622	-	41,41,41	1.14	2 (4%)	56,56,56	1.36	4 (7%)
35	HTG	d	411	-	16,16,19	1.21	2 (12%)	20,21,24	1.55	1 (5%)
34	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.44	7 (15%)
24	CLA	B	606	2	69,73,73	1.99	19 (27%)	83,113,113	2.93	30 (36%)
28	GOL	C	525	-	5,5,5	0.33	0	5,5,5	0.72	0
34	LMG	C	501	-	51,51,55	0.97	2 (3%)	59,59,63	1.10	3 (5%)
24	CLA	A	405	1	69,73,73	2.03	21 (30%)	83,113,113	2.77	31 (37%)
35	HTG	B	624	-	19,19,19	1.06	2 (10%)	23,24,24	1.89	4 (17%)
26	BCR	a	410	-	41,41,41	1.14	1 (2%)	56,56,56	1.35	8 (14%)
26	BCR	D	405	-	41,41,41	1.05	1 (2%)	56,56,56	1.70	12 (21%)
30	LMT	M	101	-	36,36,36	0.57	1 (2%)	47,47,47	0.84	0
24	CLA	C	502	3	69,73,73	1.98	20 (28%)	83,113,113	2.72	29 (34%)
30	LMT	D	402	-	36,36,36	0.48	0	47,47,47	1.01	3 (6%)
30	LMT	E	102	-	36,36,36	0.46	0	47,47,47	0.75	0
30	LMT	f	102	-	36,36,36	0.47	0	47,47,47	0.77	0
35	HTG	b	604	-	19,19,19	1.02	2 (10%)	23,24,24	1.10	2 (8%)
28	GOL	b	629	-	5,5,5	0.38	0	5,5,5	0.29	0
34	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.11	5 (8%)
24	CLA	a	409	1	69,73,73	2.04	19 (27%)	83,113,113	2.83	32 (38%)
28	GOL	v	201	-	5,5,5	0.35	0	5,5,5	0.39	0
23	BCT	a	418	21	2,3,3	0.60	0	2,3,3	0.82	0
32	PL9	a	416	-	55,55,55	0.63	2 (3%)	68,69,69	1.85	18 (26%)
27	SQD	A	416	-	53,54,54	1.05	3 (5%)	62,65,65	1.15	7 (11%)
24	CLA	b	618	2	69,73,73	2.00	20 (28%)	83,113,113	2.83	29 (34%)
35	HTG	V	204	-	19,19,19	1.00	2 (10%)	23,24,24	1.33	3 (13%)
24	CLA	B	604	2	69,73,73	2.05	20 (28%)	83,113,113	2.82	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	PL9	A	419	-	55,55,55	0.63	1 (1%)	68,69,69	1.85	19 (27%)
24	CLA	a	406	1	69,73,73	2.03	20 (28%)	83,113,113	2.75	29 (34%)
26	BCR	t	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.32	8 (14%)
40	HEC	v	202	16	50,50,50	1.69	8 (16%)	68,82,82	1.77	17 (25%)
24	CLA	C	509	3	69,73,73	2.07	20 (28%)	83,113,113	2.80	28 (33%)
26	BCR	b	624	-	41,41,41	0.99	1 (2%)	56,56,56	1.25	8 (14%)
28	GOL	f	104	33	5,5,5	0.35	0	5,5,5	0.24	0
28	GOL	t	102	-	5,5,5	0.34	0	5,5,5	0.30	0
27	SQD	f	101	-	42,43,54	1.18	3 (7%)	51,54,65	1.44	7 (13%)
24	CLA	c	506	41	69,73,73	2.02	20 (28%)	83,113,113	2.82	30 (36%)
24	CLA	c	511	3	69,73,73	2.13	20 (28%)	83,113,113	2.79	29 (34%)
28	GOL	B	629	-	5,5,5	0.32	0	5,5,5	0.39	0
24	CLA	B	612	2	69,73,73	2.03	20 (28%)	83,113,113	2.89	29 (34%)
24	CLA	c	515	3	69,73,73	2.06	21 (30%)	83,113,113	2.83	32 (38%)
30	LMT	a	417	-	36,36,36	0.44	0	47,47,47	0.84	2 (4%)
34	LMG	J	101	39	51,51,55	0.84	2 (3%)	59,59,63	1.01	4 (6%)
34	LMG	b	625	-	51,51,55	0.90	2 (3%)	59,59,63	1.03	4 (6%)
28	GOL	V	201	-	5,5,5	0.38	0	5,5,5	0.43	0
35	HTG	c	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	2 (8%)
27	SQD	A	411	-	53,54,54	0.97	3 (5%)	62,65,65	1.58	11 (17%)
24	CLA	b	621	2	69,73,73	2.07	21 (30%)	83,113,113	2.77	30 (36%)
24	CLA	C	505	41	69,73,73	2.05	20 (28%)	83,113,113	2.76	29 (34%)
28	GOL	b	631	-	5,5,5	0.34	0	5,5,5	0.45	0
35	HTG	B	631	-	19,19,19	1.03	2 (10%)	23,24,24	1.44	2 (8%)
24	CLA	B	602	41	69,73,73	2.06	20 (28%)	83,113,113	2.85	30 (36%)
28	GOL	v	203	-	5,5,5	0.27	0	5,5,5	0.49	0
34	LMG	j	101	39	51,51,55	0.93	3 (5%)	59,59,63	0.98	3 (5%)
28	GOL	c	527	-	5,5,5	0.41	0	5,5,5	0.31	0
24	CLA	C	513	3	69,73,73	2.02	20 (28%)	83,113,113	2.81	33 (39%)
30	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.86	0
35	HTG	C	522	-	19,19,19	1.01	2 (10%)	23,24,24	1.28	2 (8%)
28	GOL	a	413	-	5,5,5	0.43	0	5,5,5	0.27	0
23	BCT	A	404	21	2,3,3	0.65	0	2,3,3	0.87	0
36	DGD	d	407	-	63,63,67	0.94	3 (4%)	77,77,81	1.04	6 (7%)
30	LMT	b	626	-	25,25,36	0.50	0	30,30,47	0.64	0
28	GOL	B	627	-	5,5,5	0.34	0	5,5,5	0.71	0
28	GOL	B	635	-	5,5,5	0.40	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	PHO	a	408	-	58,69,69	2.78	13 (22%)	56,99,99	2.85	14 (25%)
35	HTG	B	622	-	19,19,19	1.20	1 (5%)	23,24,24	1.43	3 (13%)
24	CLA	C	504	3	69,73,73	2.04	20 (28%)	83,113,113	2.82	28 (33%)
28	GOL	F	103	33	5,5,5	0.36	0	5,5,5	0.37	0
28	GOL	a	412	-	5,5,5	0.34	0	5,5,5	0.57	0
36	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.06	4 (5%)
24	CLA	c	509	41	69,73,73	1.99	19 (27%)	83,113,113	2.79	28 (33%)
24	CLA	c	503	3	69,73,73	2.02	20 (28%)	83,113,113	2.82	31 (37%)
28	GOL	v	205	-	5,5,5	0.35	0	5,5,5	0.46	0
32	PL9	D	406	-	55,55,55	0.77	2 (3%)	68,69,69	1.50	16 (23%)
24	CLA	b	617	2	69,73,73	2.00	21 (30%)	83,113,113	2.67	30 (36%)
24	CLA	b	616	2	69,73,73	2.04	20 (28%)	83,113,113	2.85	30 (36%)
28	GOL	b	632	-	5,5,5	0.44	0	5,5,5	0.52	0
38	HEM	E	103	5,6	50,50,50	1.52	6 (12%)	66,82,82	1.80	16 (24%)
35	HTG	b	627	-	19,19,19	0.86	1 (5%)	23,24,24	1.35	4 (17%)
24	CLA	C	506	3	69,73,73	2.04	20 (28%)	83,113,113	2.65	27 (32%)
24	CLA	b	615	41	69,73,73	2.05	20 (28%)	83,113,113	2.73	29 (34%)
28	GOL	V	208	-	5,5,5	0.37	0	5,5,5	0.27	0
37	LHG	D	408	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
28	GOL	A	414	-	5,5,5	0.41	0	5,5,5	0.20	0
24	CLA	C	511	3	69,73,73	2.06	20 (28%)	83,113,113	2.76	30 (36%)
26	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	11 (19%)
37	LHG	l	102	-	48,48,48	0.95	2 (4%)	51,54,54	1.02	3 (5%)
24	CLA	d	402	4	69,73,73	2.03	20 (28%)	83,113,113	2.81	28 (33%)
26	BCR	d	405	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	13 (23%)
36	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	0.89	3 (3%)
24	CLA	c	507	3	69,73,73	2.02	19 (27%)	83,113,113	2.66	24 (28%)
26	BCR	Y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	8 (14%)
24	CLA	C	508	41	69,73,73	2.05	20 (28%)	83,113,113	2.80	30 (36%)
24	CLA	b	609	2	69,73,73	2.07	22 (31%)	83,113,113	2.82	29 (34%)
30	LMT	I	102	-	36,36,36	0.45	0	47,47,47	1.18	4 (8%)
28	GOL	B	626	-	5,5,5	0.29	0	5,5,5	0.48	0
26	BCR	c	526	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	10 (17%)
28	GOL	O	302	-	5,5,5	0.36	0	5,5,5	0.35	0
26	BCR	B	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.00	3 (5%)
35	HTG	D	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.03	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	c	512	3	69,73,73	2.04	19 (27%)	83,113,113	2.74	31 (37%)
27	SQD	a	402	-	53,54,54	1.03	3 (5%)	62,65,65	1.19	6 (9%)
27	SQD	F	101	-	42,43,54	1.12	3 (7%)	51,54,65	1.55	9 (17%)
24	CLA	A	406	41	69,73,73	2.09	20 (28%)	83,113,113	2.80	32 (38%)

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
34	LMG	c	501	-	-	14/46/66/70	0/1/1/1
37	LHG	E	101	-	-	20/46/46/53	-
25	PHO	A	407	-	-	3/37/103/103	0/5/6/6
37	LHG	e	101	-	-	18/46/46/53	-
37	LHG	d	408	-	-	9/53/53/53	-
24	CLA	B	614	2	-	9/39/115/115	-
24	CLA	b	611	2	-	10/39/115/115	-
24	CLA	c	513	3	-	5/39/115/115	-
24	CLA	b	613	2	-	2/39/115/115	-
24	CLA	b	606	41	-	16/39/115/115	-
26	BCR	c	516	-	-	4/29/63/63	0/2/2/2
40	HEC	V	203	16	1/1/3/7	6/14/54/54	-
24	CLA	b	610	2	-	5/39/115/115	-
36	DGD	c	517	-	-	12/51/91/95	0/2/2/2
28	GOL	c	524	-	-	0/4/4/4	-
37	LHG	d	410	-	-	13/53/53/53	-
24	CLA	C	514	3	-	5/39/115/115	-
34	LMG	B	621	-	-	7/46/66/70	0/1/1/1
28	GOL	c	525	-	-	1/4/4/4	-
38	HEM	e	102	5,6	-	4/14/54/54	-
36	DGD	c	518	-	-	15/51/91/95	0/2/2/2
28	GOL	B	633	-	-	0/4/4/4	-
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
24	CLA	B	609	2	-	1/39/115/115	-
24	CLA	c	504	3	-	5/39/115/115	-
24	CLA	B	611	41	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
28	GOL	V	205	-	-	4/4/4/4	-
28	GOL	b	633	-	-	2/4/4/4	-
24	CLA	b	607	2	-	3/39/115/115	-
36	DGD	H	102	-	-	11/51/91/95	0/2/2/2
24	CLA	C	503	3	-	10/39/115/115	-
36	DGD	c	519	-	-	12/51/91/95	0/2/2/2
30	LMT	a	401	-	-	9/21/61/61	0/2/2/2
27	SQD	b	601	-	-	20/49/69/69	0/1/1/1
28	GOL	A	413	-	-	2/4/4/4	-
24	CLA	b	620	2	-	5/39/115/115	-
30	LMT	A	417	-	-	3/19/59/61	0/2/2/2
30	LMT	m	103	-	-	6/21/61/61	0/2/2/2
28	GOL	C	524	-	-	2/4/4/4	-
34	LMG	c	521	-	-	6/46/66/70	0/1/1/1
35	HTG	O	303	-	-	2/10/30/30	0/1/1/1
36	DGD	D	407	-	-	17/51/91/95	0/2/2/2
37	LHG	d	409	-	-	11/53/53/53	-
32	PL9	d	406	-	-	3/53/73/73	0/1/1/1
30	LMT	m	102	-	-	3/21/61/61	0/2/2/2
26	BCR	C	516	-	-	3/29/63/63	0/2/2/2
28	GOL	T	101	-	-	2/4/4/4	-
30	LMT	B	634	-	-	5/17/37/61	0/1/1/2
24	CLA	c	508	3	-	8/39/115/115	-
24	CLA	B	607	2	-	4/39/115/115	-
28	GOL	b	630	-	-	0/4/4/4	-
35	HTG	B	630	-	-	1/10/30/30	0/1/1/1
37	LHG	L	101	-	-	12/53/53/53	-
24	CLA	b	612	41	-	5/39/115/115	-
30	LMT	b	602	-	-	7/17/37/61	0/1/1/2
35	HTG	B	623	-	-	5/10/30/30	0/1/1/1
28	GOL	V	206	-	-	2/4/4/4	-
35	HTG	c	522	-	-	1/10/30/30	0/1/1/1
34	LMG	c	520	-	-	5/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	z	101	-	-	13/34/54/70	0/1/1/1
24	CLA	D	401	41	-	5/39/115/115	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	D	404	4	-	7/39/115/115	-
36	DGD	C	518	-	-	19/51/91/95	0/2/2/2
24	CLA	b	619	2	-	14/39/115/115	-
24	CLA	c	514	3	-	14/39/115/115	-
28	GOL	V	207	-	-	0/4/4/4	-
24	CLA	C	510	3	-	4/39/115/115	-
24	CLA	c	510	3	-	2/39/115/115	-
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
25	PHO	d	403	-	-	3/37/103/103	0/5/6/6
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
28	GOL	v	204	-	-	2/4/4/4	-
24	CLA	b	608	2	-	7/39/115/115	-
37	LHG	D	410	-	-	14/53/53/53	-
26	BCR	B	620	-	-	5/29/63/63	0/2/2/2
24	CLA	B	613	2	-	2/39/115/115	-
28	GOL	B	625	-	-	2/4/4/4	-
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
24	CLA	B	616	2	-	10/39/115/115	-
24	CLA	B	605	2	-	4/39/115/115	-
24	CLA	b	614	2	-	4/39/115/115	-
24	CLA	d	404	4	-	6/39/115/115	-
25	PHO	A	408	-	-	1/37/103/103	0/5/6/6
24	CLA	c	505	3	-	4/39/115/115	-
24	CLA	d	401	41	-	7/39/115/115	-
26	BCR	T	102	-	-	0/29/63/63	0/2/2/2
28	GOL	A	412	-	-	2/4/4/4	-
27	SQD	l	101	-	-	20/49/69/69	0/1/1/1
36	DGD	h	102	-	-	9/51/91/95	0/2/2/2
24	CLA	B	610	2	-	3/39/115/115	-
24	CLA	C	507	3	-	8/39/115/115	-
35	HTG	b	628	-	-	2/10/30/30	0/1/1/1
26	BCR	H	101	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	603	2	-	7/39/115/115	-
24	CLA	B	617	2	-	9/39/115/115	-
26	BCR	k	103	-	-	1/29/63/63	0/2/2/2
24	CLA	a	407	41	-	5/39/115/115	-
28	GOL	B	628	-	-	2/4/4/4	-
37	LHG	D	409	-	-	9/53/53/53	-
24	CLA	D	403	4	-	4/39/115/115	-
24	CLA	A	409	1	-	12/39/115/115	-
24	CLA	B	608	41	-	6/39/115/115	-
24	CLA	C	512	3	-	1/39/115/115	-
24	CLA	B	615	2	-	14/39/115/115	-
28	GOL	T	103	-	-	3/4/4/4	-
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
34	LMG	C	521	-	-	14/46/66/70	0/1/1/1
27	SQD	a	411	-	-	9/49/69/69	0/1/1/1
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
35	HTG	d	411	-	-	2/7/27/30	0/1/1/1
34	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
24	CLA	B	606	2	-	3/39/115/115	-
28	GOL	C	525	-	-	0/4/4/4	-
34	LMG	C	501	-	-	16/46/66/70	0/1/1/1
24	CLA	A	405	1	-	1/39/115/115	-
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
26	BCR	D	405	-	-	6/29/63/63	0/2/2/2
30	LMT	M	101	-	-	8/21/61/61	0/2/2/2
24	CLA	C	502	3	-	11/39/115/115	-
30	LMT	D	402	-	-	9/21/61/61	0/2/2/2
30	LMT	E	102	-	-	9/21/61/61	0/2/2/2
30	LMT	f	102	-	-	7/21/61/61	0/2/2/2
35	HTG	b	604	-	-	1/10/30/30	0/1/1/1
28	GOL	b	629	-	-	2/4/4/4	-
34	LMG	C	520	-	-	13/46/66/70	0/1/1/1
24	CLA	a	409	1	-	11/39/115/115	-
28	GOL	v	201	-	-	0/4/4/4	-
32	PL9	a	416	-	-	17/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	416	-	-	17/49/69/69	0/1/1/1
24	CLA	b	618	2	-	6/39/115/115	-
35	HTG	V	204	-	-	3/10/30/30	0/1/1/1
24	CLA	B	604	2	-	3/39/115/115	-
32	PL9	A	419	-	-	8/53/73/73	0/1/1/1
24	CLA	a	406	1	-	3/39/115/115	-
40	HEC	v	202	16	1/1/3/7	6/14/54/54	-
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2
24	CLA	C	509	3	-	3/39/115/115	-
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
28	GOL	f	104	33	-	3/4/4/4	-
28	GOL	t	102	-	-	0/4/4/4	-
27	SQD	f	101	-	-	16/38/58/69	0/1/1/1
24	CLA	c	506	41	-	8/39/115/115	-
24	CLA	c	511	3	-	9/39/115/115	-
28	GOL	B	629	-	-	0/4/4/4	-
24	CLA	B	612	2	-	3/39/115/115	-
24	CLA	c	515	3	-	6/39/115/115	-
30	LMT	a	417	-	-	2/21/61/61	0/2/2/2
34	LMG	J	101	39	-	9/46/66/70	0/1/1/1
34	LMG	b	625	-	-	18/46/66/70	0/1/1/1
28	GOL	V	201	-	-	0/4/4/4	-
35	HTG	c	523	-	-	1/10/30/30	0/1/1/1
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
24	CLA	b	621	2	-	10/39/115/115	-
24	CLA	C	505	41	-	6/39/115/115	-
28	GOL	b	631	-	-	2/4/4/4	-
35	HTG	B	631	-	-	1/10/30/30	0/1/1/1
24	CLA	B	602	41	-	15/39/115/115	-
28	GOL	v	203	-	-	4/4/4/4	-
34	LMG	j	101	39	-	12/46/66/70	0/1/1/1
28	GOL	c	527	-	-	2/4/4/4	-
24	CLA	C	513	3	-	10/39/115/115	-
30	LMT	M	102	-	-	5/21/61/61	0/2/2/2
35	HTG	C	522	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	a	413	-	-	4/4/4/4	-
36	DGD	d	407	-	-	20/51/91/95	0/2/2/2
30	LMT	b	626	-	-	6/17/37/61	0/1/1/2
28	GOL	B	627	-	-	2/4/4/4	-
28	GOL	B	635	-	-	2/4/4/4	-
25	PHO	a	408	-	-	2/37/103/103	0/5/6/6
35	HTG	B	622	-	-	1/10/30/30	0/1/1/1
24	CLA	C	504	3	-	4/39/115/115	-
28	GOL	F	103	33	-	2/4/4/4	-
28	GOL	a	412	-	-	2/4/4/4	-
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
24	CLA	c	509	41	-	3/39/115/115	-
24	CLA	c	503	3	-	5/39/115/115	-
28	GOL	v	205	-	-	2/4/4/4	-
32	PL9	D	406	-	-	1/53/73/73	0/1/1/1
24	CLA	b	617	2	-	3/39/115/115	-
24	CLA	b	616	2	-	4/39/115/115	-
28	GOL	b	632	-	-	2/4/4/4	-
38	HEM	E	103	5,6	-	4/14/54/54	-
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
24	CLA	C	506	3	-	7/39/115/115	-
24	CLA	b	615	41	-	6/39/115/115	-
28	GOL	V	208	-	-	2/4/4/4	-
37	LHG	D	408	-	-	9/53/53/53	-
28	GOL	A	414	-	-	2/4/4/4	-
24	CLA	C	511	3	-	8/39/115/115	-
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
37	LHG	l	102	-	-	18/53/53/53	-
24	CLA	d	402	4	-	3/39/115/115	-
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
36	DGD	C	519	-	-	5/51/91/95	0/2/2/2
24	CLA	c	507	3	-	5/39/115/115	-
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
24	CLA	C	508	41	-	12/39/115/115	-
24	CLA	b	609	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	I	102	-	-	10/21/61/61	0/2/2/2
28	GOL	B	626	-	-	2/4/4/4	-
26	BCR	c	526	-	-	1/29/63/63	0/2/2/2
28	GOL	O	302	-	-	2/4/4/4	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	HTG	D	411	-	-	1/7/27/30	0/1/1/1
24	CLA	c	512	3	-	7/39/115/115	-
27	SQD	a	402	-	-	17/49/69/69	0/1/1/1
27	SQD	F	101	-	-	12/38/58/69	0/1/1/1
24	CLA	A	406	41	-	5/39/115/115	-

All (1622) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C1B-C2B	9.08	1.49	1.39
25	d	403	PHO	C1B-C2B	9.05	1.49	1.39
25	d	403	PHO	C1D-C2D	9.03	1.49	1.39
25	a	408	PHO	C1D-C2D	8.84	1.49	1.39
25	A	407	PHO	C1D-C2D	8.67	1.49	1.39
25	A	408	PHO	C1D-C2D	8.40	1.48	1.39
25	A	407	PHO	C1B-C2B	8.33	1.48	1.39
25	a	408	PHO	C1B-C2B	8.28	1.48	1.39
25	a	408	PHO	C3B-C4B	8.26	1.51	1.41
25	A	408	PHO	C3B-C4B	7.81	1.50	1.41
25	A	407	PHO	C3B-C4B	7.33	1.49	1.41
25	d	403	PHO	C3B-C4B	7.22	1.49	1.41
25	d	403	PHO	C3B-C2B	6.65	1.49	1.40
25	d	403	PHO	C4D-CHA	6.61	1.50	1.39
25	A	408	PHO	C3B-C2B	6.51	1.49	1.40
25	a	408	PHO	C3B-C2B	6.44	1.49	1.40
25	A	407	PHO	C3B-C2B	6.39	1.49	1.40
25	A	407	PHO	C4D-CHA	6.26	1.49	1.39
25	a	408	PHO	C4D-CHA	6.17	1.49	1.39
25	A	408	PHO	C4D-CHA	6.08	1.49	1.39
24	b	609	CLA	C1D-ND	6.00	1.45	1.37
25	A	407	PHO	C3C-C2C	5.94	1.49	1.36
25	a	408	PHO	C3C-C2C	5.92	1.49	1.36
24	A	406	CLA	C1D-ND	5.75	1.44	1.37
24	c	511	CLA	C1D-ND	5.72	1.44	1.37
24	b	614	CLA	C1D-ND	5.68	1.44	1.37
24	b	606	CLA	C3C-C2C	5.67	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C3D-C2D	5.63	1.49	1.39
24	B	609	CLA	C3C-C2C	5.61	1.48	1.36
24	A	409	CLA	C3C-C2C	5.60	1.48	1.36
24	a	406	CLA	C1D-ND	5.58	1.44	1.37
25	A	408	PHO	C3C-C2C	5.58	1.48	1.36
25	d	403	PHO	C3D-C2D	5.58	1.49	1.39
25	d	403	PHO	C3C-C2C	5.56	1.48	1.36
38	e	102	HEM	FE-NB	5.54	2.12	1.94
24	B	605	CLA	C1D-ND	5.54	1.44	1.37
24	B	612	CLA	C3C-C2C	5.51	1.48	1.36
24	B	602	CLA	C3C-C2C	5.50	1.48	1.36
24	C	504	CLA	C1D-ND	5.47	1.44	1.37
24	B	611	CLA	C3C-C2C	5.45	1.48	1.36
24	C	509	CLA	C3C-C2C	5.45	1.48	1.36
40	V	203	HEC	FE-NB	5.44	2.11	1.94
24	B	609	CLA	C1D-ND	5.43	1.44	1.37
24	C	506	CLA	C3C-C2C	5.42	1.48	1.36
24	c	506	CLA	C3C-C2C	5.42	1.48	1.36
24	C	503	CLA	C3C-C2C	5.40	1.48	1.36
24	c	511	CLA	C3C-C2C	5.39	1.48	1.36
24	C	504	CLA	C3C-C2C	5.38	1.48	1.36
24	b	620	CLA	C3C-C2C	5.38	1.48	1.36
24	c	503	CLA	C3C-C2C	5.37	1.48	1.36
24	a	406	CLA	C3C-C2C	5.35	1.48	1.36
24	b	617	CLA	C3C-C2C	5.35	1.48	1.36
25	A	407	PHO	C3D-C2D	5.35	1.49	1.39
24	D	404	CLA	C3C-C2C	5.35	1.48	1.36
24	b	618	CLA	C3C-C2C	5.35	1.48	1.36
24	c	514	CLA	C3C-C2C	5.35	1.48	1.36
24	B	616	CLA	C1D-ND	5.34	1.44	1.37
24	a	407	CLA	C1D-ND	5.34	1.44	1.37
24	b	610	CLA	C1D-ND	5.34	1.44	1.37
24	c	512	CLA	C3C-C2C	5.34	1.48	1.36
24	b	614	CLA	O2D-CGD	5.34	1.46	1.33
24	b	606	CLA	C1D-ND	5.33	1.44	1.37
24	c	508	CLA	C1D-ND	5.33	1.44	1.37
24	b	613	CLA	C3C-C2C	5.33	1.48	1.36
24	d	402	CLA	C3C-C2C	5.32	1.48	1.36
24	c	504	CLA	C3C-C2C	5.32	1.48	1.36
24	b	621	CLA	C1D-ND	5.32	1.44	1.37
24	a	409	CLA	C3C-C2C	5.32	1.48	1.36
24	b	620	CLA	C1D-ND	5.31	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C3C-C2C	5.30	1.48	1.36
24	c	509	CLA	C3C-C2C	5.30	1.48	1.36
24	C	513	CLA	C3C-C2C	5.28	1.48	1.36
24	b	607	CLA	C3C-C2C	5.27	1.47	1.36
24	B	607	CLA	C1D-ND	5.27	1.44	1.37
24	c	510	CLA	C3C-C2C	5.26	1.47	1.36
24	C	510	CLA	O2D-CGD	5.26	1.46	1.33
24	B	604	CLA	C3C-C2C	5.26	1.47	1.36
24	C	511	CLA	C3C-C2C	5.25	1.47	1.36
24	B	606	CLA	O2D-CGD	5.25	1.46	1.33
24	b	614	CLA	C3C-C2C	5.25	1.47	1.36
24	b	606	CLA	O2D-CGD	5.25	1.46	1.33
24	C	505	CLA	C3C-C2C	5.23	1.47	1.36
24	C	507	CLA	C3C-C2C	5.22	1.47	1.36
24	c	505	CLA	C1D-ND	5.22	1.44	1.37
25	A	407	PHO	OBD-CAD	5.21	1.29	1.22
24	b	608	CLA	C1D-ND	5.21	1.44	1.37
24	b	615	CLA	C3C-C2C	5.21	1.47	1.36
24	B	602	CLA	O2D-CGD	5.20	1.45	1.33
24	B	610	CLA	C3C-C2C	5.19	1.47	1.36
24	b	608	CLA	C3C-C2C	5.19	1.47	1.36
24	c	505	CLA	C3C-C2C	5.19	1.47	1.36
24	D	401	CLA	C3C-C2C	5.18	1.47	1.36
24	c	515	CLA	C3C-C2C	5.18	1.47	1.36
24	c	511	CLA	O2D-CGD	5.18	1.45	1.33
24	C	508	CLA	C1D-ND	5.17	1.44	1.37
24	A	406	CLA	C3C-C2C	5.17	1.47	1.36
24	C	503	CLA	C1D-ND	5.17	1.44	1.37
24	C	511	CLA	C1D-ND	5.17	1.44	1.37
24	c	506	CLA	O2D-CGD	5.17	1.45	1.33
24	B	603	CLA	C3C-C2C	5.17	1.47	1.36
24	b	612	CLA	C3C-C2C	5.16	1.47	1.36
24	c	507	CLA	C3C-C2C	5.16	1.47	1.36
24	c	513	CLA	C3C-C2C	5.16	1.47	1.36
24	B	617	CLA	O2D-CGD	5.15	1.45	1.33
24	a	407	CLA	C3C-C2C	5.15	1.47	1.36
24	B	613	CLA	C3C-C2C	5.14	1.47	1.36
24	b	618	CLA	O2D-CGD	5.14	1.45	1.33
24	C	510	CLA	C1D-ND	5.14	1.44	1.37
24	b	621	CLA	O2D-CGD	5.14	1.45	1.33
24	C	507	CLA	C1D-ND	5.14	1.44	1.37
24	d	401	CLA	C3C-C2C	5.13	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C3C-C2C	5.13	1.47	1.36
24	b	616	CLA	C1D-ND	5.13	1.44	1.37
24	c	508	CLA	C3C-C2C	5.12	1.47	1.36
24	c	515	CLA	O2D-CGD	5.12	1.45	1.33
24	b	618	CLA	C1D-ND	5.11	1.44	1.37
24	b	616	CLA	C3C-C2C	5.11	1.47	1.36
24	B	614	CLA	C3C-C2C	5.10	1.47	1.36
24	B	607	CLA	C3C-C2C	5.10	1.47	1.36
40	v	202	HEC	FE-NB	5.09	2.10	1.94
24	b	613	CLA	O2D-CGD	5.09	1.45	1.33
24	b	611	CLA	C1D-ND	5.08	1.44	1.37
24	B	607	CLA	O2D-CGD	5.08	1.45	1.33
24	a	406	CLA	O2D-CGD	5.08	1.45	1.33
24	B	617	CLA	C3C-C2C	5.07	1.47	1.36
24	b	621	CLA	C3C-C2C	5.07	1.47	1.36
24	B	610	CLA	C1D-ND	5.07	1.44	1.37
24	C	507	CLA	O2D-CGD	5.06	1.45	1.33
25	a	408	PHO	O2D-CGD	5.06	1.45	1.33
24	b	611	CLA	C3C-C2C	5.06	1.47	1.36
24	B	615	CLA	C3C-C2C	5.06	1.47	1.36
24	B	616	CLA	O2D-CGD	5.06	1.45	1.33
24	c	512	CLA	O2D-CGD	5.05	1.45	1.33
24	c	510	CLA	C1D-ND	5.05	1.44	1.37
26	c	526	BCR	C23-C22	-5.04	1.35	1.45
24	b	609	CLA	O2D-CGD	5.04	1.45	1.33
24	c	515	CLA	C1D-ND	5.04	1.44	1.37
24	b	607	CLA	O2D-CGD	5.04	1.45	1.33
24	B	606	CLA	C3C-C2C	5.03	1.47	1.36
24	B	610	CLA	CHC-C1C	5.02	1.48	1.38
24	b	610	CLA	C3C-C2C	5.02	1.47	1.36
24	c	514	CLA	O2D-CGD	5.02	1.45	1.33
24	C	508	CLA	C3C-C2C	5.02	1.47	1.36
24	c	513	CLA	O2D-CGD	5.01	1.45	1.33
24	a	409	CLA	C1D-ND	5.00	1.43	1.37
24	B	612	CLA	C1D-ND	5.00	1.43	1.37
24	b	613	CLA	C1D-ND	4.98	1.43	1.37
24	C	512	CLA	O2D-CGD	4.98	1.45	1.33
24	C	509	CLA	O2D-CGD	4.98	1.45	1.33
24	b	616	CLA	O2D-CGD	4.98	1.45	1.33
25	d	403	PHO	O2D-CGD	4.98	1.45	1.33
24	C	502	CLA	C3C-C2C	4.98	1.47	1.36
24	C	514	CLA	C1D-ND	4.97	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	C3C-C2C	4.97	1.47	1.36
24	b	617	CLA	O2D-CGD	4.97	1.45	1.33
24	B	602	CLA	C1D-ND	4.97	1.43	1.37
24	A	406	CLA	O2D-CGD	4.97	1.45	1.33
24	B	615	CLA	O2D-CGD	4.97	1.45	1.33
24	c	503	CLA	O2D-CGD	4.96	1.45	1.33
24	B	613	CLA	CHC-C1C	4.96	1.48	1.38
24	b	620	CLA	O2D-CGD	4.95	1.45	1.33
24	B	604	CLA	O2D-CGD	4.94	1.45	1.33
24	a	409	CLA	O2D-CGD	4.94	1.45	1.33
24	d	404	CLA	C3C-C2C	4.94	1.47	1.36
24	B	606	CLA	C1D-ND	4.92	1.43	1.37
24	B	608	CLA	C3C-C2C	4.92	1.47	1.36
24	A	409	CLA	O2D-CGD	4.92	1.45	1.33
24	d	404	CLA	O2D-CGD	4.92	1.45	1.33
24	b	617	CLA	CHC-C1C	4.92	1.48	1.38
25	a	408	PHO	C3D-C2D	4.92	1.48	1.39
24	C	506	CLA	O2D-CGD	4.90	1.45	1.33
24	B	604	CLA	C1D-ND	4.90	1.43	1.37
38	E	103	HEM	FE-NB	4.90	2.10	1.94
24	C	514	CLA	C3C-C2C	4.89	1.47	1.36
24	B	614	CLA	O2D-CGD	4.89	1.45	1.33
24	b	607	CLA	C1D-ND	4.89	1.43	1.37
24	C	505	CLA	C1D-ND	4.89	1.43	1.37
24	B	609	CLA	O2D-CGD	4.88	1.45	1.33
24	C	513	CLA	O2D-CGD	4.88	1.45	1.33
24	b	619	CLA	O2D-CGD	4.88	1.45	1.33
24	d	401	CLA	C1D-ND	4.88	1.43	1.37
24	b	611	CLA	O2D-CGD	4.88	1.45	1.33
24	c	513	CLA	C1D-ND	4.87	1.43	1.37
24	B	614	CLA	C1D-ND	4.87	1.43	1.37
24	c	509	CLA	O2D-CGD	4.87	1.45	1.33
24	d	404	CLA	C1D-ND	4.86	1.43	1.37
24	B	611	CLA	C1D-ND	4.86	1.43	1.37
24	b	619	CLA	C3C-C2C	4.86	1.47	1.36
24	B	603	CLA	O2D-CGD	4.86	1.45	1.33
24	b	611	CLA	CHC-C1C	4.86	1.48	1.38
24	D	401	CLA	O2D-CGD	4.85	1.45	1.33
24	B	613	CLA	O2D-CGD	4.85	1.45	1.33
24	c	503	CLA	C1D-ND	4.84	1.43	1.37
24	c	515	CLA	CHC-C1C	4.84	1.48	1.38
26	C	515	BCR	C23-C22	-4.84	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	505	CLA	CHC-C1C	4.84	1.48	1.38
24	b	608	CLA	O2D-CGD	4.83	1.45	1.33
24	b	616	CLA	CHC-C1C	4.83	1.48	1.38
24	C	514	CLA	O2D-CGD	4.83	1.45	1.33
24	b	612	CLA	O2D-CGD	4.83	1.45	1.33
24	D	403	CLA	C3C-C2C	4.83	1.47	1.36
24	b	607	CLA	CHC-C1C	4.83	1.48	1.38
24	C	508	CLA	O2D-CGD	4.82	1.45	1.33
24	c	505	CLA	O2D-CGD	4.82	1.45	1.33
26	d	405	BCR	C23-C22	-4.82	1.35	1.45
25	A	407	PHO	O2D-CGD	4.82	1.45	1.33
24	d	402	CLA	C1D-ND	4.82	1.43	1.37
26	y	101	BCR	C23-C22	-4.82	1.35	1.45
24	b	608	CLA	CHC-C1C	4.81	1.48	1.38
24	D	401	CLA	C1D-ND	4.81	1.43	1.37
24	a	407	CLA	CHC-C1C	4.81	1.48	1.38
24	c	508	CLA	O2D-CGD	4.80	1.44	1.33
24	D	404	CLA	O2D-CGD	4.80	1.44	1.33
24	B	602	CLA	CHC-C1C	4.80	1.48	1.38
24	B	616	CLA	CHC-C1C	4.80	1.48	1.38
26	C	516	BCR	C23-C22	-4.79	1.35	1.45
24	c	514	CLA	CHC-C1C	4.78	1.48	1.38
24	C	503	CLA	CHC-C1C	4.78	1.48	1.38
24	B	616	CLA	C3C-C2C	4.77	1.46	1.36
24	A	405	CLA	O2D-CGD	4.76	1.44	1.33
24	b	619	CLA	C1D-ND	4.75	1.43	1.37
24	B	615	CLA	CHC-C1C	4.75	1.48	1.38
24	C	510	CLA	CHD-C1D	4.75	1.47	1.38
24	b	615	CLA	CHC-C1C	4.75	1.48	1.38
24	A	409	CLA	CHC-C1C	4.74	1.48	1.38
24	c	510	CLA	CHC-C1C	4.74	1.48	1.38
24	C	503	CLA	O2D-CGD	4.73	1.44	1.33
24	C	502	CLA	O2D-CGD	4.72	1.44	1.33
26	B	620	BCR	C23-C22	-4.72	1.35	1.45
24	c	510	CLA	O2D-CGD	4.72	1.44	1.33
24	A	405	CLA	C1D-ND	4.72	1.43	1.37
24	c	511	CLA	CHD-C1D	4.72	1.47	1.38
24	b	606	CLA	CHC-C1C	4.72	1.48	1.38
24	C	509	CLA	CHD-C1D	4.71	1.47	1.38
25	A	408	PHO	O2D-CGD	4.70	1.44	1.33
24	C	509	CLA	C1D-ND	4.70	1.43	1.37
24	C	506	CLA	C1D-ND	4.70	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	O2D-CGD	4.70	1.44	1.33
24	d	402	CLA	O2A-CGA	4.69	1.47	1.33
24	c	512	CLA	C1D-ND	4.69	1.43	1.37
24	A	405	CLA	CHC-C1C	4.69	1.48	1.38
26	b	624	BCR	C23-C22	-4.68	1.35	1.45
24	d	404	CLA	CHC-C1C	4.68	1.48	1.38
24	B	611	CLA	O2D-CGD	4.68	1.44	1.33
24	C	504	CLA	O2D-CGD	4.68	1.44	1.33
24	c	504	CLA	O2D-CGD	4.67	1.44	1.33
24	B	612	CLA	O2D-CGD	4.67	1.44	1.33
24	D	404	CLA	CHC-C1C	4.66	1.48	1.38
24	c	509	CLA	C1D-ND	4.66	1.43	1.37
24	C	513	CLA	C1D-ND	4.66	1.43	1.37
24	c	514	CLA	C1D-ND	4.66	1.43	1.37
24	A	406	CLA	CHC-C1C	4.66	1.48	1.38
26	k	103	BCR	C23-C22	-4.65	1.35	1.45
26	D	405	BCR	C23-C22	-4.65	1.35	1.45
24	D	403	CLA	C1D-ND	4.65	1.43	1.37
24	b	621	CLA	CHD-C1D	4.65	1.47	1.38
24	C	505	CLA	CHC-C1C	4.65	1.48	1.38
24	c	507	CLA	O2D-CGD	4.64	1.44	1.33
24	C	505	CLA	O2D-CGD	4.64	1.44	1.33
26	a	410	BCR	C23-C22	-4.63	1.36	1.45
24	c	507	CLA	CHC-C1C	4.63	1.47	1.38
24	d	402	CLA	O2D-CGD	4.63	1.44	1.33
24	C	508	CLA	CHC-C1C	4.62	1.47	1.38
24	B	612	CLA	CHC-C1C	4.62	1.47	1.38
24	C	506	CLA	CHC-C1C	4.62	1.47	1.38
26	h	101	BCR	C23-C22	-4.62	1.36	1.45
24	c	512	CLA	CHC-C1C	4.62	1.47	1.38
24	B	605	CLA	CHC-C1C	4.62	1.47	1.38
24	c	504	CLA	C1D-ND	4.61	1.43	1.37
24	c	507	CLA	C1D-ND	4.61	1.43	1.37
24	D	403	CLA	O2A-CGA	4.61	1.46	1.33
35	B	622	HTG	C1'-S1	-4.61	1.75	1.81
24	B	605	CLA	C3C-C2C	4.61	1.46	1.36
24	B	603	CLA	CHC-C1C	4.60	1.47	1.38
24	B	613	CLA	CHD-C1D	4.60	1.47	1.38
24	d	401	CLA	O2D-CGD	4.60	1.44	1.33
24	C	512	CLA	CHC-C1C	4.59	1.47	1.38
24	B	615	CLA	C1D-ND	4.59	1.43	1.37
24	C	512	CLA	C1D-ND	4.59	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	CHC-C1C	4.59	1.47	1.38
24	b	610	CLA	CHC-C1C	4.58	1.47	1.38
26	T	102	BCR	C23-C22	-4.57	1.36	1.45
24	a	407	CLA	CHD-C1D	4.57	1.47	1.38
25	A	408	PHO	OBD-CAD	4.57	1.28	1.22
24	b	614	CLA	CHD-C1D	4.57	1.47	1.38
24	b	609	CLA	C3C-C2C	4.56	1.46	1.36
24	C	514	CLA	CHC-C1C	4.56	1.47	1.38
24	B	609	CLA	CHC-C1C	4.54	1.47	1.38
24	B	610	CLA	O2D-CGD	4.54	1.44	1.33
34	z	101	LMG	O8-C28	4.54	1.46	1.33
24	c	511	CLA	CHC-C1C	4.54	1.47	1.38
24	C	504	CLA	CHC-C1C	4.53	1.47	1.38
24	b	613	CLA	O2A-CGA	4.53	1.46	1.33
24	D	404	CLA	C1D-ND	4.53	1.43	1.37
24	B	604	CLA	CHC-C1C	4.53	1.47	1.38
24	C	513	CLA	CHC-C1C	4.53	1.47	1.38
24	c	504	CLA	CHC-C1C	4.52	1.47	1.38
24	B	616	CLA	O2A-CGA	4.52	1.46	1.33
26	c	516	BCR	C23-C22	-4.52	1.36	1.45
24	c	506	CLA	CHC-C1C	4.51	1.47	1.38
24	c	513	CLA	CHC-C1C	4.51	1.47	1.38
26	b	623	BCR	C23-C22	-4.50	1.36	1.45
24	b	613	CLA	CHD-C1D	4.50	1.47	1.38
26	t	101	BCR	C23-C22	-4.49	1.36	1.45
24	b	615	CLA	O2D-CGD	4.49	1.44	1.33
26	H	101	BCR	C23-C22	-4.49	1.36	1.45
24	A	406	CLA	OBD-CAD	4.48	1.30	1.22
24	C	509	CLA	CHC-C1C	4.48	1.47	1.38
26	Y	101	BCR	C23-C22	-4.48	1.36	1.45
24	B	608	CLA	CHC-C1C	4.47	1.47	1.38
36	D	407	DGD	O1G-C1A	4.47	1.46	1.33
24	C	510	CLA	O2A-CGA	4.47	1.46	1.33
24	b	615	CLA	C1D-ND	4.46	1.43	1.37
24	b	613	CLA	CHC-C1C	4.46	1.47	1.38
24	c	509	CLA	CHC-C1C	4.46	1.47	1.38
24	B	608	CLA	O2D-CGD	4.46	1.44	1.33
27	A	416	SQD	O48-C23	4.46	1.46	1.33
24	B	602	CLA	O2A-CGA	4.44	1.46	1.33
24	b	617	CLA	C1D-ND	4.43	1.43	1.37
24	c	505	CLA	CHD-C1D	4.43	1.47	1.38
24	b	619	CLA	CHC-C1C	4.43	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	407	DGD	O2G-C1B	4.43	1.46	1.34
24	B	609	CLA	CHD-C1D	4.42	1.47	1.38
24	B	611	CLA	CHC-C1C	4.42	1.47	1.38
24	c	510	CLA	O2A-CGA	4.42	1.46	1.33
26	b	622	BCR	C23-C22	-4.42	1.36	1.45
24	D	403	CLA	CHD-C1D	4.42	1.47	1.38
24	B	607	CLA	CHD-C1D	4.42	1.47	1.38
24	b	615	CLA	CHD-C1D	4.41	1.47	1.38
24	b	620	CLA	CHC-C1C	4.41	1.47	1.38
25	a	408	PHO	OBD-CAD	4.41	1.28	1.22
34	C	501	LMG	O7-C10	4.41	1.46	1.34
27	f	101	SQD	O47-C7	4.41	1.46	1.34
34	C	520	LMG	O8-C28	4.40	1.46	1.33
24	D	401	CLA	CHC-C1C	4.40	1.47	1.38
27	a	402	SQD	O48-C23	4.40	1.46	1.33
24	c	506	CLA	C1D-ND	4.40	1.43	1.37
24	D	403	CLA	O2D-CGD	4.40	1.43	1.33
24	c	515	CLA	CHD-C1D	4.40	1.46	1.38
24	A	409	CLA	C1D-ND	4.40	1.43	1.37
24	b	621	CLA	CHC-C1C	4.40	1.47	1.38
24	a	407	CLA	O2D-CGD	4.39	1.43	1.33
36	D	407	DGD	O2G-C1B	4.39	1.46	1.34
24	a	407	CLA	O2A-CGA	4.39	1.46	1.33
24	C	502	CLA	CHC-C1C	4.39	1.47	1.38
24	a	409	CLA	O2A-CGA	4.39	1.46	1.33
26	B	618	BCR	C23-C22	-4.39	1.36	1.45
24	c	509	CLA	O2A-CGA	4.38	1.46	1.33
37	e	101	LHG	O8-C23	4.38	1.46	1.33
24	A	406	CLA	CHD-C1D	4.38	1.46	1.38
24	B	602	CLA	CHD-C1D	4.37	1.46	1.38
24	c	507	CLA	CHD-C1D	4.37	1.46	1.38
24	c	508	CLA	CHC-C1C	4.37	1.47	1.38
24	b	612	CLA	CHC-C1C	4.37	1.47	1.38
27	F	101	SQD	O47-C7	4.37	1.46	1.34
26	K	101	BCR	C23-C22	-4.36	1.36	1.45
24	b	606	CLA	CHD-C1D	4.36	1.46	1.38
24	C	511	CLA	CHC-C1C	4.36	1.47	1.38
34	C	521	LMG	O7-C10	4.35	1.46	1.34
26	A	410	BCR	C23-C22	-4.35	1.36	1.45
24	c	503	CLA	CHC-C1C	4.35	1.47	1.38
24	c	508	CLA	CHD-C1D	4.34	1.46	1.38
24	C	510	CLA	CHC-C1C	4.34	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	CHC-C1C	4.34	1.47	1.38
24	d	402	CLA	CHD-C1D	4.34	1.46	1.38
24	B	608	CLA	C1D-ND	4.33	1.43	1.37
24	c	512	CLA	CHD-C1D	4.33	1.46	1.38
26	B	619	BCR	C23-C22	-4.33	1.36	1.45
24	D	403	CLA	CHC-C1C	4.32	1.47	1.38
34	c	521	LMG	O7-C10	4.32	1.46	1.34
24	B	603	CLA	CHD-C1D	4.32	1.46	1.38
24	c	513	CLA	CHD-C1D	4.32	1.46	1.38
24	b	610	CLA	O2D-CGD	4.32	1.43	1.33
24	B	606	CLA	O2A-CGA	4.32	1.46	1.33
24	C	507	CLA	CHD-C1D	4.32	1.46	1.38
24	C	507	CLA	CHC-C1C	4.31	1.47	1.38
24	c	510	CLA	CHD-C1D	4.31	1.46	1.38
24	c	512	CLA	CHB-C1B	4.31	1.49	1.39
24	C	513	CLA	O2A-CGA	4.31	1.45	1.33
24	B	603	CLA	C1D-ND	4.31	1.43	1.37
36	d	407	DGD	O1G-C1A	4.31	1.45	1.33
24	C	506	CLA	CHD-C1D	4.30	1.46	1.38
24	B	604	CLA	O2A-CGA	4.30	1.45	1.33
24	b	618	CLA	CHC-C1C	4.30	1.47	1.38
24	B	617	CLA	CHC-C1C	4.29	1.47	1.38
24	C	502	CLA	C1D-ND	4.29	1.43	1.37
24	a	409	CLA	CHC-C1C	4.29	1.47	1.38
24	B	614	CLA	CHC-C1C	4.29	1.47	1.38
24	C	508	CLA	O2A-CGA	4.29	1.45	1.33
24	C	511	CLA	CHD-C1D	4.29	1.46	1.38
24	b	606	CLA	O2A-CGA	4.29	1.45	1.33
37	E	101	LHG	O8-C23	4.29	1.45	1.33
27	b	601	SQD	O47-C7	4.29	1.46	1.34
24	b	614	CLA	CHC-C1C	4.28	1.47	1.38
24	C	503	CLA	CHD-C1D	4.28	1.46	1.38
24	D	401	CLA	OBD-CAD	4.28	1.29	1.22
24	C	505	CLA	CHD-C1D	4.28	1.46	1.38
24	c	515	CLA	O2A-CGA	4.28	1.45	1.33
24	b	617	CLA	O2A-CGA	4.28	1.45	1.33
36	c	519	DGD	O1G-C1A	4.27	1.45	1.33
24	B	617	CLA	C1D-ND	4.27	1.43	1.37
24	c	514	CLA	O2A-CGA	4.26	1.45	1.33
24	d	401	CLA	O2A-CGA	4.26	1.45	1.33
34	C	501	LMG	O8-C28	4.26	1.45	1.33
24	c	503	CLA	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	CHD-C1D	4.26	1.46	1.38
34	c	520	LMG	O8-C28	4.26	1.45	1.33
36	C	518	DGD	O1G-C1A	4.25	1.45	1.33
24	b	617	CLA	CHD-C1D	4.25	1.46	1.38
24	C	502	CLA	O2A-CGA	4.25	1.45	1.33
24	C	505	CLA	CHB-C1B	4.25	1.48	1.39
24	D	404	CLA	CHD-C1D	4.25	1.46	1.38
24	A	406	CLA	CHD-C4C	4.25	1.48	1.39
24	c	508	CLA	O2A-CGA	4.25	1.45	1.33
24	B	612	CLA	CHD-C1D	4.24	1.46	1.38
24	b	614	CLA	OBD-CAD	4.24	1.29	1.22
24	a	406	CLA	CHC-C1C	4.24	1.47	1.38
24	b	607	CLA	CHD-C1D	4.24	1.46	1.38
24	B	608	CLA	O2A-CGA	4.23	1.45	1.33
40	V	203	HEC	FE-NC	4.23	2.09	1.95
24	b	607	CLA	C3D-C2D	4.23	1.50	1.39
24	b	616	CLA	CHD-C1D	4.23	1.46	1.38
24	b	619	CLA	CHD-C1D	4.23	1.46	1.38
24	B	605	CLA	O2D-CGD	4.23	1.43	1.33
24	a	409	CLA	CHD-C1D	4.23	1.46	1.38
24	B	609	CLA	O2A-CGA	4.22	1.45	1.33
24	c	503	CLA	CHD-C1D	4.22	1.46	1.38
24	b	612	CLA	CHD-C1D	4.22	1.46	1.38
25	d	403	PHO	OBD-CAD	4.22	1.28	1.22
24	B	608	CLA	OBD-CAD	4.22	1.29	1.22
24	d	402	CLA	CHC-C1C	4.21	1.47	1.38
24	B	614	CLA	CHD-C1D	4.21	1.46	1.38
34	Z	101	LMG	O7-C10	4.21	1.46	1.34
24	b	619	CLA	CHD-C4C	4.21	1.48	1.39
27	A	416	SQD	O47-C7	4.21	1.46	1.34
34	C	521	LMG	O8-C28	4.21	1.45	1.33
24	d	404	CLA	CHD-C1D	4.20	1.46	1.38
24	D	403	CLA	CHB-C1B	4.20	1.48	1.39
34	c	521	LMG	O8-C28	4.20	1.45	1.33
24	C	507	CLA	O2A-CGA	4.20	1.45	1.33
24	C	509	CLA	O2A-CGA	4.20	1.45	1.33
24	c	504	CLA	O2A-CGA	4.19	1.45	1.33
24	C	506	CLA	O2A-CGA	4.19	1.45	1.33
24	b	616	CLA	O2A-CGA	4.19	1.45	1.33
24	B	611	CLA	CHC-C4B	4.18	1.48	1.39
27	f	101	SQD	O48-C23	4.18	1.45	1.33
37	e	101	LHG	O7-C7	4.18	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	O2A-CGA	4.18	1.45	1.33
24	B	610	CLA	O2A-CGA	4.18	1.45	1.33
34	b	625	LMG	O8-C28	4.17	1.45	1.33
27	F	101	SQD	O48-C23	4.17	1.45	1.33
24	a	406	CLA	CHD-C1D	4.17	1.46	1.38
38	e	102	HEM	FE-NC	4.17	2.09	1.95
40	v	202	HEC	FE-NC	4.16	2.09	1.95
24	d	401	CLA	CHD-C1D	4.16	1.46	1.38
24	c	511	CLA	O2A-CGA	4.16	1.45	1.33
34	z	101	LMG	O7-C10	4.16	1.46	1.34
24	C	504	CLA	O2A-CGA	4.16	1.45	1.33
24	c	512	CLA	O2A-CGA	4.16	1.45	1.33
24	B	617	CLA	CHD-C1D	4.16	1.46	1.38
24	b	608	CLA	CHD-C1D	4.16	1.46	1.38
24	b	620	CLA	CHD-C1D	4.16	1.46	1.38
36	c	518	DGD	O1G-C1A	4.16	1.45	1.33
24	C	502	CLA	CHD-C1D	4.16	1.46	1.38
37	l	102	LHG	O8-C23	4.16	1.45	1.33
24	B	609	CLA	C3D-C2D	4.15	1.50	1.39
37	D	410	LHG	O7-C7	4.15	1.46	1.34
24	B	608	CLA	CHB-C1B	4.15	1.48	1.39
24	d	404	CLA	O2A-CGA	4.15	1.45	1.33
24	b	610	CLA	O2A-CGA	4.15	1.45	1.33
24	b	614	CLA	O2A-CGA	4.14	1.45	1.33
27	l	101	SQD	O47-C7	4.14	1.46	1.34
24	C	503	CLA	C3D-C2D	4.14	1.50	1.39
24	c	511	CLA	CHD-C4C	4.14	1.48	1.39
24	b	619	CLA	O2A-CGA	4.14	1.45	1.33
24	B	605	CLA	CHD-C1D	4.14	1.46	1.38
24	B	617	CLA	O2A-CGA	4.13	1.45	1.33
24	c	503	CLA	CHB-C1B	4.13	1.48	1.39
24	b	621	CLA	O2A-CGA	4.13	1.45	1.33
24	c	513	CLA	CHD-C4C	4.12	1.48	1.39
24	b	609	CLA	O2A-CGA	4.12	1.45	1.33
24	A	409	CLA	CHC-C4B	4.12	1.48	1.39
37	d	409	LHG	O8-C23	4.12	1.45	1.33
24	C	505	CLA	CHD-C4C	4.12	1.48	1.39
24	c	515	CLA	CHD-C4C	4.12	1.48	1.39
24	C	512	CLA	O2A-CGA	4.11	1.45	1.33
24	d	401	CLA	OBD-CAD	4.11	1.29	1.22
24	b	608	CLA	O2A-CGA	4.11	1.45	1.33
24	b	609	CLA	CHC-C4B	4.11	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E	101	LHG	O7-C7	4.11	1.45	1.34
24	a	407	CLA	CHD-C4C	4.11	1.48	1.39
37	d	410	LHG	O8-C23	4.11	1.45	1.33
24	B	611	CLA	CHD-C1D	4.10	1.46	1.38
24	b	610	CLA	CHD-C1D	4.10	1.46	1.38
24	C	505	CLA	O2A-CGA	4.10	1.45	1.33
36	H	102	DGD	O2G-C1B	4.10	1.45	1.34
24	c	514	CLA	CHD-C1D	4.09	1.46	1.38
24	C	508	CLA	CHD-C1D	4.09	1.46	1.38
24	b	616	CLA	C3D-C2D	4.09	1.50	1.39
24	C	513	CLA	CHD-C1D	4.09	1.46	1.38
24	C	503	CLA	O2A-CGA	4.09	1.45	1.33
24	b	612	CLA	C1D-ND	4.08	1.42	1.37
24	C	514	CLA	OBD-CAD	4.08	1.29	1.22
24	c	508	CLA	CHD-C4C	4.08	1.48	1.39
25	d	403	PHO	O2A-CGA	4.08	1.45	1.33
24	a	406	CLA	CHB-C1B	4.08	1.48	1.39
24	d	402	CLA	CHD-C4C	4.08	1.48	1.39
24	B	606	CLA	CHC-C1C	4.08	1.46	1.38
24	C	507	CLA	C3D-C2D	4.08	1.50	1.39
24	d	401	CLA	C3D-C2D	4.07	1.50	1.39
24	b	618	CLA	O2A-CGA	4.07	1.45	1.33
24	C	510	CLA	CHB-C1B	4.07	1.48	1.39
36	h	102	DGD	O1G-C1A	4.07	1.45	1.33
24	B	607	CLA	O2A-CGA	4.07	1.45	1.33
37	l	102	LHG	O7-C7	4.07	1.45	1.34
34	c	501	LMG	O8-C28	4.07	1.45	1.33
24	B	616	CLA	C3D-C2D	4.07	1.50	1.39
27	b	601	SQD	O48-C23	4.07	1.45	1.33
34	B	621	LMG	O8-C28	4.07	1.45	1.33
24	C	514	CLA	CHD-C1D	4.07	1.46	1.38
24	b	621	CLA	CHD-C4C	4.07	1.48	1.39
27	a	402	SQD	O47-C7	4.06	1.45	1.34
34	C	520	LMG	O7-C10	4.06	1.45	1.34
24	D	401	CLA	O2A-CGA	4.06	1.45	1.33
34	c	520	LMG	O7-C10	4.06	1.45	1.34
24	B	610	CLA	CHB-C1B	4.06	1.48	1.39
24	c	507	CLA	CHD-C4C	4.06	1.48	1.39
24	C	512	CLA	CHD-C4C	4.06	1.48	1.39
24	C	511	CLA	O2A-CGA	4.06	1.45	1.33
24	b	615	CLA	CHB-C1B	4.05	1.48	1.39
36	C	517	DGD	O2G-C1B	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	O2A-CGA	4.05	1.45	1.33
24	A	409	CLA	C3D-C2D	4.05	1.50	1.39
34	B	621	LMG	O7-C10	4.05	1.45	1.34
35	d	411	HTG	C1'-S1	-4.05	1.76	1.81
24	B	608	CLA	CHC-C4B	4.05	1.48	1.39
24	C	509	CLA	C3D-C2D	4.05	1.50	1.39
25	a	408	PHO	O2A-CGA	4.05	1.45	1.33
24	b	611	CLA	CHD-C1D	4.05	1.46	1.38
24	B	616	CLA	CHD-C1D	4.04	1.46	1.38
24	B	611	CLA	O2A-CGA	4.04	1.45	1.33
24	b	620	CLA	OBD-CAD	4.04	1.29	1.22
27	l	101	SQD	O48-C23	4.03	1.45	1.33
24	b	611	CLA	O2A-CGA	4.03	1.45	1.33
24	b	618	CLA	CHB-C1B	4.03	1.48	1.39
24	b	609	CLA	CHB-C1B	4.03	1.48	1.39
24	D	401	CLA	CHD-C1D	4.03	1.46	1.38
24	B	617	CLA	OBD-CAD	4.03	1.29	1.22
24	D	401	CLA	C3D-C2D	4.03	1.50	1.39
24	c	506	CLA	O2A-CGA	4.03	1.45	1.33
24	b	606	CLA	CHD-C4C	4.03	1.48	1.39
24	c	511	CLA	OBD-CAD	4.03	1.29	1.22
24	c	510	CLA	C3D-C2D	4.03	1.50	1.39
35	b	603	HTG	C1'-S1	-4.03	1.76	1.81
24	C	507	CLA	CHB-C1B	4.02	1.48	1.39
24	b	620	CLA	C3D-C2D	4.02	1.50	1.39
24	C	503	CLA	CHB-C1B	4.01	1.48	1.39
24	B	610	CLA	OBD-CAD	4.01	1.29	1.22
24	A	406	CLA	CHB-C1B	4.01	1.48	1.39
24	b	617	CLA	CHB-C1B	4.00	1.48	1.39
24	c	514	CLA	CHD-C4C	4.00	1.48	1.39
24	B	606	CLA	CHD-C1D	4.00	1.46	1.38
24	B	612	CLA	C3D-C2D	4.00	1.50	1.39
24	b	620	CLA	O2A-CGA	3.99	1.45	1.33
24	b	608	CLA	CHD-C4C	3.98	1.48	1.39
24	B	605	CLA	CHB-C1B	3.98	1.48	1.39
24	d	402	CLA	C1B-NB	-3.98	1.32	1.37
24	c	504	CLA	C3D-C2D	3.98	1.50	1.39
24	c	507	CLA	OBD-CAD	3.98	1.29	1.22
24	A	405	CLA	CHB-C1B	3.98	1.48	1.39
24	c	513	CLA	CHB-C1B	3.98	1.48	1.39
24	c	513	CLA	O2A-CGA	3.98	1.45	1.33
24	B	617	CLA	CHB-C1B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	202	HEC	CBC-CAC	-3.97	1.33	1.51
24	B	604	CLA	CHD-C1D	3.97	1.46	1.38
24	A	405	CLA	C3D-C2D	3.97	1.50	1.39
24	B	610	CLA	CHD-C1D	3.97	1.46	1.38
24	c	505	CLA	O2A-CGA	3.97	1.44	1.33
24	B	612	CLA	O2A-CGA	3.97	1.44	1.33
24	C	502	CLA	C3D-C2D	3.96	1.49	1.39
36	c	517	DGD	O2G-C1B	3.96	1.45	1.34
36	c	519	DGD	O2G-C1B	3.96	1.45	1.34
34	j	101	LMG	O8-C28	3.95	1.44	1.33
24	C	503	CLA	CHD-C4C	3.95	1.48	1.39
24	C	509	CLA	CHD-C4C	3.95	1.48	1.39
24	B	614	CLA	O2A-CGA	3.95	1.44	1.33
36	H	102	DGD	O1G-C1A	3.95	1.44	1.33
24	C	510	CLA	OBD-CAD	3.95	1.29	1.22
37	d	410	LHG	O7-C7	3.95	1.45	1.34
24	C	504	CLA	CHD-C1D	3.95	1.46	1.38
27	a	411	SQD	O48-C23	3.95	1.44	1.33
24	d	401	CLA	CHC-C1C	3.95	1.46	1.38
24	d	404	CLA	C1B-NB	-3.95	1.32	1.37
24	b	621	CLA	CHB-C1B	3.94	1.48	1.39
24	c	506	CLA	CHD-C1D	3.94	1.46	1.38
24	c	504	CLA	CHD-C4C	3.94	1.48	1.39
37	D	410	LHG	O8-C23	3.94	1.44	1.33
24	C	511	CLA	CHD-C4C	3.93	1.48	1.39
24	c	510	CLA	CHC-C4B	3.93	1.48	1.39
24	C	510	CLA	CHD-C4C	3.93	1.48	1.39
35	O	303	HTG	C1'-S1	-3.93	1.76	1.81
24	C	508	CLA	CHC-C4B	3.93	1.48	1.39
24	b	614	CLA	CHB-C1B	3.93	1.48	1.39
24	a	406	CLA	CHD-C4C	3.93	1.48	1.39
24	b	619	CLA	C3D-C2D	3.93	1.49	1.39
24	c	509	CLA	CHB-C1B	3.93	1.48	1.39
24	C	511	CLA	CHB-C1B	3.93	1.48	1.39
24	b	616	CLA	CHB-C1B	3.93	1.48	1.39
24	C	511	CLA	C3D-C2D	3.92	1.49	1.39
24	d	401	CLA	CHB-C1B	3.92	1.48	1.39
40	V	203	HEC	CBC-CAC	-3.92	1.34	1.51
24	d	404	CLA	CHD-C4C	3.92	1.48	1.39
24	b	615	CLA	CHC-C4B	3.92	1.48	1.39
24	C	514	CLA	CHB-C1B	3.92	1.48	1.39
24	b	615	CLA	C3D-C2D	3.92	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	518	DGD	O2G-C1B	3.92	1.45	1.34
24	A	409	CLA	CHD-C1D	3.92	1.46	1.38
24	C	512	CLA	CHD-C1D	3.91	1.46	1.38
24	B	605	CLA	O2A-CGA	3.91	1.44	1.33
24	b	606	CLA	C3D-C2D	3.91	1.49	1.39
24	d	404	CLA	CHC-C4B	3.91	1.48	1.39
24	C	506	CLA	CHB-C1B	3.91	1.48	1.39
24	C	509	CLA	CHB-C1B	3.91	1.48	1.39
27	a	411	SQD	O47-C7	3.91	1.45	1.34
24	C	510	CLA	C3D-C2D	3.90	1.49	1.39
34	j	101	LMG	O7-C10	3.90	1.45	1.34
24	c	505	CLA	CHC-C4B	3.89	1.48	1.39
24	b	614	CLA	CHD-C4C	3.89	1.48	1.39
24	B	613	CLA	C1D-ND	3.89	1.42	1.37
27	A	411	SQD	O47-C7	3.89	1.45	1.34
24	b	613	CLA	CHC-C4B	3.89	1.48	1.39
37	d	408	LHG	O8-C23	3.89	1.44	1.33
24	a	409	CLA	CHD-C4C	3.89	1.48	1.39
24	D	404	CLA	O2A-CGA	3.88	1.44	1.33
38	E	103	HEM	FE-NC	3.88	2.08	1.95
24	c	506	CLA	C3D-C2D	3.88	1.49	1.39
24	b	615	CLA	CHD-C4C	3.88	1.48	1.39
25	A	407	PHO	O2A-CGA	3.88	1.44	1.33
24	b	615	CLA	O2A-CGA	3.88	1.44	1.33
24	C	513	CLA	C3D-C2D	3.88	1.49	1.39
24	B	613	CLA	CHB-C1B	3.88	1.48	1.39
24	B	611	CLA	CHD-C4C	3.88	1.48	1.39
24	C	512	CLA	CHB-C1B	3.87	1.48	1.39
24	b	607	CLA	O2A-CGA	3.87	1.44	1.33
24	c	512	CLA	CHD-C4C	3.87	1.48	1.39
37	L	101	LHG	O8-C23	3.87	1.44	1.33
24	c	504	CLA	CHB-C1B	3.87	1.48	1.39
24	B	608	CLA	CHD-C1D	3.87	1.45	1.38
24	B	612	CLA	CHC-C4B	3.87	1.48	1.39
24	C	505	CLA	C3D-C2D	3.86	1.49	1.39
24	c	506	CLA	OBD-CAD	3.86	1.29	1.22
24	A	409	CLA	O2A-CGA	3.86	1.44	1.33
24	B	607	CLA	C3D-C2D	3.86	1.49	1.39
24	b	611	CLA	CHC-C4B	3.86	1.48	1.39
24	D	403	CLA	CHD-C4C	3.85	1.48	1.39
24	C	504	CLA	OBD-CAD	3.85	1.29	1.22
27	A	411	SQD	O48-C23	3.85	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	C3D-C2D	3.85	1.49	1.39
36	C	519	DGD	O1G-C1A	3.85	1.44	1.33
24	b	616	CLA	CHC-C4B	3.85	1.48	1.39
24	b	612	CLA	C3D-C2D	3.85	1.49	1.39
35	b	628	HTG	C1'-S1	-3.85	1.76	1.81
24	b	610	CLA	CHC-C4B	3.84	1.48	1.39
24	b	617	CLA	CHC-C4B	3.83	1.48	1.39
24	A	406	CLA	C3D-C2D	3.83	1.49	1.39
24	b	616	CLA	CHD-C4C	3.83	1.48	1.39
24	C	508	CLA	CHD-C4C	3.83	1.48	1.39
24	B	611	CLA	C3D-C2D	3.83	1.49	1.39
24	b	610	CLA	CHD-C4C	3.83	1.48	1.39
24	A	406	CLA	O2A-CGA	3.83	1.44	1.33
24	B	603	CLA	OBD-CAD	3.82	1.29	1.22
24	B	604	CLA	C3D-C2D	3.82	1.49	1.39
24	c	514	CLA	CHC-C4B	3.82	1.48	1.39
24	B	615	CLA	O2A-CGA	3.82	1.44	1.33
24	b	608	CLA	CHC-C4B	3.82	1.48	1.39
36	h	102	DGD	O2G-C1B	3.81	1.45	1.34
24	B	602	CLA	C3D-C2D	3.81	1.49	1.39
24	b	615	CLA	OBD-CAD	3.81	1.29	1.22
24	b	613	CLA	CHD-C4C	3.81	1.47	1.39
24	b	621	CLA	C3D-C2D	3.81	1.49	1.39
24	b	607	CLA	OBD-CAD	3.80	1.29	1.22
24	C	504	CLA	C3D-C2D	3.80	1.49	1.39
24	b	610	CLA	OBD-CAD	3.80	1.29	1.22
24	B	614	CLA	CHD-C4C	3.80	1.47	1.39
24	C	508	CLA	OBD-CAD	3.80	1.29	1.22
36	c	517	DGD	O1G-C1A	3.80	1.44	1.33
24	c	515	CLA	C3D-C2D	3.80	1.49	1.39
24	C	507	CLA	CHD-C4C	3.80	1.47	1.39
24	C	506	CLA	CHD-C4C	3.80	1.47	1.39
24	B	614	CLA	CHB-C1B	3.80	1.47	1.39
24	d	402	CLA	C3D-C2D	3.80	1.49	1.39
24	B	604	CLA	CHB-C1B	3.79	1.47	1.39
24	c	510	CLA	OBD-CAD	3.79	1.29	1.22
24	c	515	CLA	OBD-CAD	3.79	1.29	1.22
24	c	509	CLA	C3D-C2D	3.79	1.49	1.39
24	b	614	CLA	C3D-C2D	3.79	1.49	1.39
24	a	407	CLA	CHC-C4B	3.79	1.47	1.39
24	A	409	CLA	OBD-CAD	3.79	1.29	1.22
24	B	602	CLA	CHC-C4B	3.79	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	CHD-C4C	3.78	1.47	1.39
36	C	517	DGD	O1G-C1A	3.78	1.44	1.33
24	B	612	CLA	CHD-C4C	3.78	1.47	1.39
40	v	202	HEC	CBB-CAB	-3.78	1.34	1.51
24	B	611	CLA	CHB-C1B	3.78	1.47	1.39
24	b	606	CLA	CHC-C4B	3.78	1.47	1.39
24	C	503	CLA	CHC-C4B	3.78	1.47	1.39
24	d	402	CLA	CHB-C1B	3.78	1.47	1.39
24	C	511	CLA	CHC-C4B	3.77	1.47	1.39
24	c	511	CLA	CHB-C1B	3.77	1.47	1.39
24	c	511	CLA	C3D-C2D	3.77	1.49	1.39
24	c	505	CLA	C3D-C2D	3.77	1.49	1.39
24	b	620	CLA	CHD-C4C	3.77	1.47	1.39
24	B	615	CLA	CHD-C4C	3.77	1.47	1.39
24	B	602	CLA	CHD-C4C	3.76	1.47	1.39
24	a	409	CLA	C3D-C2D	3.76	1.49	1.39
24	b	611	CLA	C3D-C2D	3.75	1.49	1.39
24	B	609	CLA	CHD-C4C	3.75	1.47	1.39
24	b	607	CLA	CHC-C4B	3.75	1.47	1.39
24	C	514	CLA	CHD-C4C	3.75	1.47	1.39
34	c	501	LMG	O7-C10	3.75	1.44	1.34
24	B	606	CLA	CHB-C1B	3.75	1.47	1.39
24	b	613	CLA	C3D-C2D	3.75	1.49	1.39
24	B	606	CLA	CHC-C4B	3.75	1.47	1.39
24	C	510	CLA	CHC-C4B	3.75	1.47	1.39
24	b	609	CLA	CHD-C1D	3.75	1.45	1.38
24	c	505	CLA	CHB-C1B	3.75	1.47	1.39
24	b	611	CLA	CHD-C4C	3.75	1.47	1.39
24	D	401	CLA	CHD-C4C	3.75	1.47	1.39
24	a	407	CLA	C3D-C2D	3.74	1.49	1.39
24	c	508	CLA	C3D-C2D	3.74	1.49	1.39
24	B	610	CLA	C3D-C2D	3.74	1.49	1.39
24	C	505	CLA	OBD-CAD	3.74	1.28	1.22
24	C	514	CLA	C3D-C2D	3.74	1.49	1.39
24	d	404	CLA	C3D-C2D	3.73	1.49	1.39
24	b	609	CLA	OBD-CAD	3.73	1.28	1.22
24	D	404	CLA	C3D-C2D	3.73	1.49	1.39
24	B	603	CLA	C3D-C2D	3.73	1.49	1.39
34	J	101	LMG	O7-C10	3.73	1.44	1.34
24	B	615	CLA	OBD-CAD	3.73	1.28	1.22
24	b	606	CLA	CHB-C1B	3.72	1.47	1.39
24	C	513	CLA	CHD-C4C	3.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	O2A-CGA	3.72	1.44	1.33
24	a	406	CLA	C3D-C2D	3.72	1.49	1.39
24	b	608	CLA	CHB-C1B	3.72	1.47	1.39
24	b	618	CLA	C3D-C2D	3.72	1.49	1.39
24	C	504	CLA	CHD-C4C	3.72	1.47	1.39
36	c	518	DGD	O2G-C1B	3.72	1.44	1.34
37	L	101	LHG	O7-C7	3.72	1.44	1.34
24	B	606	CLA	CHD-C4C	3.71	1.47	1.39
34	J	101	LMG	O8-C28	3.71	1.44	1.33
24	b	607	CLA	CHB-C1B	3.71	1.47	1.39
24	c	513	CLA	OBD-CAD	3.71	1.28	1.22
35	B	624	HTG	C1'-S1	-3.71	1.76	1.81
38	e	102	HEM	C4D-ND	-3.70	1.33	1.40
24	B	608	CLA	C3D-C2D	3.70	1.49	1.39
24	b	607	CLA	CHD-C4C	3.70	1.47	1.39
24	c	510	CLA	CHD-C4C	3.70	1.47	1.39
24	b	612	CLA	O2A-CGA	3.70	1.44	1.33
24	c	512	CLA	CHC-C4B	3.70	1.47	1.39
24	A	405	CLA	O2A-CGA	3.69	1.44	1.33
34	b	625	LMG	O7-C10	3.69	1.44	1.34
24	D	404	CLA	OBD-CAD	3.69	1.28	1.22
24	B	610	CLA	CHD-C4C	3.69	1.47	1.39
24	c	511	CLA	CHC-C4B	3.69	1.47	1.39
24	c	507	CLA	CHB-C1B	3.69	1.47	1.39
24	D	403	CLA	C3D-C2D	3.69	1.49	1.39
24	B	614	CLA	C3D-C2D	3.69	1.49	1.39
24	C	511	CLA	OBD-CAD	3.69	1.28	1.22
24	B	608	CLA	CHD-C4C	3.69	1.47	1.39
24	c	505	CLA	CHD-C4C	3.69	1.47	1.39
24	B	616	CLA	CHB-C1B	3.69	1.47	1.39
25	A	408	PHO	O2A-CGA	3.68	1.44	1.33
24	B	616	CLA	CHD-C4C	3.68	1.47	1.39
24	D	403	CLA	OBD-CAD	3.68	1.28	1.22
24	c	507	CLA	CHC-C4B	3.68	1.47	1.39
24	B	603	CLA	O2A-CGA	3.68	1.44	1.33
24	C	504	CLA	CHC-C4B	3.67	1.47	1.39
24	b	609	CLA	C3D-C2D	3.67	1.49	1.39
24	D	404	CLA	CHC-C4B	3.67	1.47	1.39
24	A	409	CLA	CHB-C1B	3.67	1.47	1.39
24	c	515	CLA	CHC-C4B	3.67	1.47	1.39
24	B	603	CLA	CHD-C4C	3.67	1.47	1.39
24	D	403	CLA	CHC-C4B	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CHC-C4B	3.66	1.47	1.39
35	c	523	HTG	C1'-S1	-3.66	1.76	1.81
24	c	508	CLA	C1B-NB	-3.66	1.33	1.37
24	c	510	CLA	CHB-C1B	3.66	1.47	1.39
37	D	408	LHG	O8-C23	3.66	1.44	1.33
24	C	512	CLA	C3D-C2D	3.66	1.49	1.39
24	B	607	CLA	CHC-C4B	3.65	1.47	1.39
24	c	509	CLA	CHD-C1D	3.65	1.45	1.38
24	a	407	CLA	OBD-CAD	3.65	1.28	1.22
24	B	604	CLA	CHD-C4C	3.65	1.47	1.39
24	C	506	CLA	OBD-CAD	3.65	1.28	1.22
24	c	503	CLA	CHD-C4C	3.64	1.47	1.39
24	B	607	CLA	CHB-C1B	3.64	1.47	1.39
24	B	615	CLA	C1B-NB	-3.64	1.33	1.37
24	B	616	CLA	OBD-CAD	3.64	1.28	1.22
24	c	503	CLA	OBD-CAD	3.64	1.28	1.22
24	c	509	CLA	CHD-C4C	3.64	1.47	1.39
24	B	614	CLA	CHC-C4B	3.64	1.47	1.39
24	B	610	CLA	CHC-C4B	3.63	1.47	1.39
24	C	506	CLA	CHC-C4B	3.63	1.47	1.39
24	B	617	CLA	CHD-C4C	3.63	1.47	1.39
24	B	604	CLA	CHC-C4B	3.62	1.47	1.39
38	E	103	HEM	C4D-ND	-3.62	1.34	1.40
24	C	504	CLA	CHB-C1B	3.62	1.47	1.39
24	B	613	CLA	C3D-C2D	3.62	1.49	1.39
24	C	512	CLA	OBD-CAD	3.62	1.28	1.22
24	B	607	CLA	CHD-C4C	3.62	1.47	1.39
24	b	612	CLA	CHC-C4B	3.61	1.47	1.39
24	C	506	CLA	C3D-C2D	3.61	1.49	1.39
24	A	405	CLA	OBD-CAD	3.61	1.28	1.22
37	d	409	LHG	O7-C7	3.61	1.44	1.34
24	c	513	CLA	C3D-C2D	3.60	1.49	1.39
24	b	618	CLA	CHD-C4C	3.60	1.47	1.39
24	b	613	CLA	CHB-C1B	3.60	1.47	1.39
24	C	502	CLA	CHB-C1B	3.60	1.47	1.39
24	B	614	CLA	OBD-CAD	3.59	1.28	1.22
36	C	519	DGD	O2G-C1B	3.59	1.44	1.34
35	B	631	HTG	C1'-S1	-3.59	1.76	1.81
24	B	606	CLA	C3D-C2D	3.59	1.48	1.39
24	B	612	CLA	OBD-CAD	3.59	1.28	1.22
24	B	613	CLA	CHD-C4C	3.58	1.47	1.39
35	D	411	HTG	C1'-S1	-3.58	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	CHD-C1D	3.58	1.45	1.38
24	d	404	CLA	CHB-C1B	3.58	1.47	1.39
24	c	512	CLA	C3D-C2D	3.58	1.48	1.39
24	B	615	CLA	CHB-C1B	3.57	1.47	1.39
24	b	610	CLA	C3D-C2D	3.57	1.48	1.39
24	C	502	CLA	OBD-CAD	3.57	1.28	1.22
24	b	613	CLA	OBD-CAD	3.57	1.28	1.22
24	B	607	CLA	C1B-NB	-3.57	1.33	1.37
24	b	618	CLA	CHD-C1D	3.57	1.45	1.38
24	b	612	CLA	CHB-C1B	3.56	1.47	1.39
24	B	603	CLA	C1B-NB	-3.56	1.33	1.37
24	C	508	CLA	CHB-C1B	3.56	1.47	1.39
24	d	401	CLA	CHD-C4C	3.55	1.47	1.39
24	A	405	CLA	CHC-C4B	3.55	1.47	1.39
24	B	617	CLA	C3D-C2D	3.55	1.48	1.39
24	b	611	CLA	CHB-C1B	3.55	1.47	1.39
24	b	608	CLA	OBD-CAD	3.55	1.28	1.22
24	d	402	CLA	CHC-C4B	3.55	1.47	1.39
24	b	620	CLA	CHC-C4B	3.53	1.47	1.39
24	a	406	CLA	O2A-CGA	3.53	1.43	1.33
24	A	405	CLA	CHD-C4C	3.53	1.47	1.39
24	c	509	CLA	CHC-C4B	3.53	1.47	1.39
24	C	508	CLA	C3D-C2D	3.53	1.48	1.39
24	B	616	CLA	CHC-C4B	3.53	1.47	1.39
24	B	615	CLA	C3D-C2D	3.53	1.48	1.39
24	B	603	CLA	CHB-C1B	3.53	1.47	1.39
24	b	619	CLA	OBD-CAD	3.53	1.28	1.22
24	a	407	CLA	CHB-C1B	3.52	1.47	1.39
24	c	508	CLA	CHB-C1B	3.52	1.47	1.39
35	C	523	HTG	C1'-S1	-3.52	1.76	1.81
24	b	621	CLA	OBD-CAD	3.52	1.28	1.22
24	D	404	CLA	CHD-C4C	3.52	1.47	1.39
24	c	506	CLA	CHD-C4C	3.52	1.47	1.39
24	c	503	CLA	C3D-C2D	3.52	1.48	1.39
24	b	611	CLA	OBD-CAD	3.52	1.28	1.22
24	C	509	CLA	CHC-C4B	3.52	1.47	1.39
24	B	615	CLA	CHD-C1D	3.52	1.45	1.38
37	D	409	LHG	O8-C23	3.52	1.43	1.33
24	b	608	CLA	C3D-C2D	3.52	1.48	1.39
24	b	613	CLA	C1B-NB	-3.52	1.33	1.37
24	C	513	CLA	CHB-C1B	3.52	1.47	1.39
24	b	610	CLA	CHB-C1B	3.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	b	604	HTG	C1'-S1	-3.51	1.76	1.81
24	B	604	CLA	OBD-CAD	3.51	1.28	1.22
24	b	617	CLA	C3D-C2D	3.51	1.48	1.39
24	c	514	CLA	CHB-C1B	3.50	1.47	1.39
35	B	630	HTG	C1'-S1	-3.50	1.77	1.81
24	a	409	CLA	CHB-C1B	3.50	1.47	1.39
24	B	613	CLA	CHC-C4B	3.50	1.47	1.39
40	V	203	HEC	CBB-CAB	-3.50	1.35	1.51
24	c	514	CLA	OBD-CAD	3.50	1.28	1.22
24	C	513	CLA	CHC-C4B	3.49	1.47	1.39
24	C	514	CLA	CHC-C4B	3.49	1.47	1.39
24	C	502	CLA	CHD-C4C	3.49	1.47	1.39
24	b	616	CLA	OBD-CAD	3.49	1.28	1.22
24	D	404	CLA	CHB-C1B	3.49	1.47	1.39
24	a	406	CLA	OBD-CAD	3.49	1.28	1.22
24	b	620	CLA	CHB-C1B	3.48	1.47	1.39
24	B	603	CLA	CHC-C4B	3.48	1.47	1.39
24	a	409	CLA	OBD-CAD	3.48	1.28	1.22
24	b	609	CLA	C1C-C2C	3.48	1.51	1.44
24	C	502	CLA	CHC-C4B	3.48	1.47	1.39
24	b	617	CLA	OBD-CAD	3.48	1.28	1.22
40	v	202	HEC	C4B-NB	-3.47	1.34	1.40
24	c	506	CLA	CHB-C1B	3.47	1.47	1.39
37	D	409	LHG	O7-C7	3.47	1.44	1.34
24	b	614	CLA	CHC-C4B	3.47	1.47	1.39
38	E	103	HEM	C1B-NB	-3.47	1.34	1.40
24	B	602	CLA	CHB-C1B	3.47	1.47	1.39
24	C	510	CLA	C1B-NB	-3.47	1.33	1.37
24	d	404	CLA	OBD-CAD	3.46	1.28	1.22
24	B	611	CLA	OBD-CAD	3.46	1.28	1.22
24	c	504	CLA	C4B-NB	-3.45	1.33	1.37
24	b	618	CLA	CHC-C4B	3.44	1.47	1.39
24	B	605	CLA	CHD-C4C	3.44	1.47	1.39
24	C	513	CLA	C1B-NB	-3.44	1.33	1.37
37	D	408	LHG	O7-C7	3.44	1.44	1.34
24	b	619	CLA	CHB-C1B	3.43	1.47	1.39
24	B	609	CLA	CHB-C1B	3.43	1.47	1.39
24	B	612	CLA	CHB-C1B	3.42	1.47	1.39
24	c	506	CLA	CHC-C4B	3.42	1.47	1.39
35	C	522	HTG	C1'-S1	-3.41	1.77	1.81
24	c	504	CLA	OBD-CAD	3.40	1.28	1.22
24	c	507	CLA	C3D-C2D	3.40	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	OBD-CAD	3.40	1.28	1.22
24	C	507	CLA	C1B-NB	-3.40	1.33	1.37
24	D	401	CLA	CHB-C1B	3.40	1.47	1.39
24	B	615	CLA	C4B-NB	-3.40	1.33	1.37
24	B	607	CLA	OBD-CAD	3.40	1.28	1.22
24	b	618	CLA	OBD-CAD	3.40	1.28	1.22
24	D	401	CLA	CHC-C4B	3.39	1.47	1.39
24	C	505	CLA	CHC-C4B	3.39	1.47	1.39
24	b	609	CLA	CHD-C4C	3.38	1.47	1.39
37	d	408	LHG	O7-C7	3.38	1.43	1.34
35	V	204	HTG	C1'-S1	-3.37	1.77	1.81
24	c	509	CLA	OBD-CAD	3.37	1.28	1.22
24	d	401	CLA	C1B-NB	-3.37	1.33	1.37
40	V	203	HEC	C1D-ND	-3.36	1.34	1.40
24	C	507	CLA	C4B-NB	-3.36	1.33	1.37
24	C	513	CLA	OBD-CAD	3.35	1.28	1.22
24	B	615	CLA	CHC-C4B	3.35	1.46	1.39
35	c	522	HTG	C1'-S1	-3.34	1.77	1.81
24	b	612	CLA	OBD-CAD	3.34	1.28	1.22
24	B	614	CLA	C1B-NB	-3.34	1.33	1.37
24	c	515	CLA	CHB-C1B	3.33	1.46	1.39
24	c	503	CLA	CHC-C4B	3.33	1.46	1.39
24	c	505	CLA	OBD-CAD	3.33	1.28	1.22
24	a	409	CLA	C4B-NB	-3.33	1.33	1.37
24	c	513	CLA	CHC-C4B	3.32	1.46	1.39
24	b	617	CLA	CHD-C4C	3.32	1.46	1.39
24	b	619	CLA	CHC-C4B	3.32	1.46	1.39
35	B	623	HTG	C1'-S1	-3.32	1.77	1.81
24	c	508	CLA	OBD-CAD	3.32	1.28	1.22
24	A	405	CLA	C4B-NB	-3.31	1.33	1.37
24	b	612	CLA	CHD-C4C	3.31	1.46	1.39
24	c	504	CLA	CHC-C4B	3.31	1.46	1.39
24	c	512	CLA	C1B-NB	-3.31	1.33	1.37
24	C	503	CLA	OBD-CAD	3.31	1.28	1.22
38	e	102	HEM	C1B-NB	-3.30	1.34	1.40
24	A	406	CLA	C1B-NB	-3.30	1.33	1.37
24	c	506	CLA	C1B-NB	-3.29	1.33	1.37
24	c	508	CLA	CHC-C4B	3.29	1.46	1.39
24	b	614	CLA	C1B-NB	-3.29	1.33	1.37
24	B	609	CLA	OBD-CAD	3.28	1.28	1.22
24	a	406	CLA	CHC-C4B	3.28	1.46	1.39
40	v	202	HEC	C1D-ND	-3.28	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	OBD-CAD	3.28	1.28	1.22
24	b	608	CLA	C3B-C4B	3.27	1.50	1.42
24	b	621	CLA	C4B-NB	-3.27	1.33	1.37
24	b	606	CLA	OBD-CAD	3.27	1.28	1.22
24	C	510	CLA	C4B-NB	-3.26	1.33	1.37
24	B	611	CLA	C1B-NB	-3.26	1.33	1.37
24	B	609	CLA	C1B-NB	-3.26	1.33	1.37
24	D	404	CLA	C3B-C4B	3.26	1.50	1.42
24	C	512	CLA	CHC-C4B	3.26	1.46	1.39
24	B	602	CLA	C1B-NB	-3.25	1.33	1.37
24	b	621	CLA	CHC-C4B	3.24	1.46	1.39
24	C	507	CLA	OBD-CAD	3.23	1.28	1.22
24	C	511	CLA	C4B-NB	-3.22	1.33	1.37
24	D	401	CLA	C4B-NB	-3.22	1.33	1.37
24	B	609	CLA	CHC-C4B	3.22	1.46	1.39
24	B	613	CLA	OBD-CAD	3.22	1.28	1.22
24	C	502	CLA	C1B-NB	-3.22	1.33	1.37
24	B	603	CLA	C4B-NB	-3.22	1.33	1.37
24	C	507	CLA	CHC-C4B	3.21	1.46	1.39
24	a	409	CLA	CHC-C4B	3.21	1.46	1.39
24	c	505	CLA	C1B-NB	-3.21	1.33	1.37
24	C	511	CLA	C1B-NB	-3.21	1.33	1.37
24	c	510	CLA	C1C-C2C	3.21	1.50	1.44
35	b	627	HTG	C1'-S1	-3.20	1.77	1.81
24	C	513	CLA	C4B-NB	-3.20	1.33	1.37
24	c	511	CLA	C1B-C2B	3.19	1.50	1.43
24	c	511	CLA	C1B-NB	-3.19	1.33	1.37
24	b	619	CLA	C1B-NB	-3.18	1.33	1.37
24	b	612	CLA	C1B-NB	-3.18	1.33	1.37
24	D	403	CLA	C1B-C2B	3.17	1.50	1.43
24	B	602	CLA	OBD-CAD	3.17	1.27	1.22
24	c	509	CLA	C4B-NB	-3.17	1.33	1.37
24	a	407	CLA	C3B-C4B	3.17	1.50	1.42
24	a	409	CLA	C1B-NB	-3.16	1.33	1.37
24	c	513	CLA	C1B-C2B	3.15	1.50	1.43
24	b	611	CLA	C3B-C4B	3.14	1.50	1.42
24	d	401	CLA	C4B-NB	-3.14	1.33	1.37
24	a	409	CLA	C1B-C2B	3.14	1.50	1.43
24	d	401	CLA	CHC-C4B	3.13	1.46	1.39
24	C	508	CLA	C1B-NB	-3.13	1.33	1.37
24	D	403	CLA	C1B-NB	-3.13	1.33	1.37
24	B	605	CLA	C1B-C2B	3.13	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C3B-C4B	3.12	1.50	1.42
24	B	605	CLA	C3D-C2D	3.12	1.47	1.39
24	A	405	CLA	C4C-C3C	3.10	1.50	1.45
24	b	621	CLA	C1B-C2B	3.10	1.50	1.43
24	A	409	CLA	C1B-NB	-3.10	1.34	1.37
24	d	401	CLA	C1B-C2B	3.10	1.50	1.43
24	B	616	CLA	C1B-NB	-3.09	1.34	1.37
24	C	509	CLA	C4B-NB	-3.09	1.34	1.37
24	b	606	CLA	C1B-NB	-3.08	1.34	1.37
24	A	406	CLA	CHC-C4B	3.08	1.46	1.39
24	C	508	CLA	C4B-NB	-3.08	1.34	1.37
24	C	509	CLA	OBD-CAD	3.08	1.27	1.22
24	B	617	CLA	C1B-C2B	3.07	1.50	1.43
24	b	620	CLA	C3B-C4B	3.07	1.49	1.42
24	C	506	CLA	C1B-NB	-3.07	1.34	1.37
24	c	503	CLA	C1B-NB	-3.07	1.34	1.37
24	c	507	CLA	C4C-C3C	3.07	1.50	1.45
24	B	613	CLA	C4C-C3C	3.07	1.50	1.45
24	B	613	CLA	C1B-NB	-3.06	1.34	1.37
24	b	613	CLA	C4B-NB	-3.06	1.34	1.37
24	B	608	CLA	C3B-C4B	3.06	1.49	1.42
24	c	507	CLA	C1B-C2B	3.06	1.50	1.43
24	B	606	CLA	C3B-C4B	3.06	1.49	1.42
24	C	514	CLA	C1B-C2B	3.06	1.50	1.43
24	b	612	CLA	C1B-C2B	3.05	1.50	1.43
24	b	615	CLA	C1C-C2C	3.05	1.50	1.44
24	B	604	CLA	C1B-C2B	3.05	1.50	1.43
24	C	512	CLA	C1B-C2B	3.04	1.50	1.43
24	c	510	CLA	C1B-NB	-3.04	1.34	1.37
40	V	203	HEC	C4B-NB	-3.04	1.35	1.40
24	b	610	CLA	C3B-C4B	3.04	1.49	1.42
24	B	617	CLA	CHC-C4B	3.04	1.46	1.39
24	B	614	CLA	C4C-C3C	3.03	1.50	1.45
24	b	616	CLA	C1B-C2B	3.02	1.50	1.43
24	B	607	CLA	C1C-C2C	3.02	1.50	1.44
24	D	404	CLA	C1B-C2B	3.02	1.50	1.43
24	c	513	CLA	C1B-NB	-3.02	1.34	1.37
24	D	404	CLA	C1B-NB	-3.00	1.34	1.37
24	c	513	CLA	C4B-NB	-3.00	1.34	1.37
24	c	505	CLA	C3B-C4B	3.00	1.49	1.42
24	c	514	CLA	C3B-C4B	3.00	1.49	1.42
24	b	607	CLA	C4B-NB	-2.99	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	C4B-NB	-2.99	1.34	1.37
24	d	402	CLA	OBD-CAD	2.99	1.27	1.22
24	B	604	CLA	C1C-C2C	2.99	1.50	1.44
24	B	614	CLA	C4B-NB	-2.98	1.34	1.37
24	B	617	CLA	C1B-NB	-2.98	1.34	1.37
24	C	509	CLA	C4C-C3C	2.98	1.50	1.45
24	C	510	CLA	C4C-C3C	2.98	1.50	1.45
24	B	604	CLA	C4B-NB	-2.98	1.34	1.37
24	C	505	CLA	C1B-NB	-2.97	1.34	1.37
24	A	409	CLA	C4B-NB	-2.97	1.34	1.37
24	b	607	CLA	C1B-NB	-2.97	1.34	1.37
24	b	618	CLA	C1B-C2B	2.97	1.50	1.43
24	B	616	CLA	C1B-C2B	2.97	1.50	1.43
24	C	506	CLA	C4C-C3C	2.96	1.50	1.45
24	c	509	CLA	C4D-CHA	2.96	1.48	1.38
24	b	615	CLA	C3B-C4B	2.95	1.49	1.42
24	D	403	CLA	C1C-C2C	2.95	1.50	1.44
24	a	406	CLA	C4C-C3C	2.95	1.50	1.45
24	c	515	CLA	C1B-NB	-2.95	1.34	1.37
24	b	621	CLA	C4C-C3C	2.95	1.50	1.45
24	D	401	CLA	C4D-CHA	2.94	1.48	1.38
24	B	608	CLA	C1B-NB	-2.94	1.34	1.37
24	B	602	CLA	C3B-C4B	2.94	1.49	1.42
24	b	606	CLA	C3B-C4B	2.94	1.49	1.42
24	c	506	CLA	C1C-C2C	2.94	1.50	1.44
24	A	406	CLA	C4B-NB	-2.94	1.34	1.37
24	B	608	CLA	C1B-C2B	2.94	1.50	1.43
24	B	610	CLA	C1B-NB	-2.93	1.34	1.37
24	b	608	CLA	C1C-C2C	2.93	1.50	1.44
24	C	512	CLA	C3B-C4B	2.93	1.49	1.42
27	A	416	SQD	C6-S	-2.93	1.66	1.77
27	a	402	SQD	C6-S	-2.91	1.66	1.77
27	A	411	SQD	C6-S	-2.91	1.66	1.77
24	b	608	CLA	C1B-NB	-2.90	1.34	1.37
24	b	607	CLA	C3B-C4B	2.90	1.49	1.42
27	f	101	SQD	C6-S	-2.90	1.66	1.77
25	A	408	PHO	CHA-CBD	-2.89	1.48	1.51
24	D	403	CLA	C4C-C3C	2.89	1.50	1.45
24	b	620	CLA	C1B-NB	-2.89	1.34	1.37
24	c	506	CLA	C4B-NB	-2.89	1.34	1.37
24	b	615	CLA	C4C-C3C	2.88	1.50	1.45
24	C	505	CLA	C1B-C2B	2.88	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	C4B-NB	-2.88	1.34	1.37
24	B	613	CLA	C4B-NB	-2.87	1.34	1.37
24	C	502	CLA	C4B-NB	-2.87	1.34	1.37
24	c	505	CLA	C1C-C2C	2.86	1.50	1.44
24	a	406	CLA	C1B-C2B	2.86	1.50	1.43
24	D	404	CLA	C1C-C2C	2.86	1.50	1.44
24	C	509	CLA	C1B-NB	-2.86	1.34	1.37
24	b	611	CLA	C4B-NB	-2.85	1.34	1.37
24	C	512	CLA	C1B-NB	-2.85	1.34	1.37
24	b	618	CLA	C1C-C2C	2.85	1.50	1.44
24	b	607	CLA	C1B-C2B	2.85	1.50	1.43
24	C	514	CLA	C4B-NB	-2.85	1.34	1.37
24	C	506	CLA	C1B-C2B	2.84	1.50	1.43
24	d	404	CLA	C1C-C2C	2.84	1.50	1.44
24	D	401	CLA	C4C-C3C	2.84	1.49	1.45
24	C	508	CLA	C1B-C2B	2.84	1.49	1.43
24	b	610	CLA	C1B-NB	-2.84	1.34	1.37
24	C	512	CLA	C4D-CHA	2.84	1.48	1.38
24	c	509	CLA	C1B-NB	-2.84	1.34	1.37
24	b	620	CLA	C1B-C2B	2.83	1.49	1.43
24	b	616	CLA	C3B-C4B	2.83	1.49	1.42
24	b	615	CLA	C1B-C2B	2.83	1.49	1.43
24	C	511	CLA	C3B-C4B	2.83	1.49	1.42
24	b	611	CLA	C1C-C2C	2.83	1.50	1.44
24	C	502	CLA	C1B-C2B	2.83	1.49	1.43
24	C	503	CLA	C4C-C3C	2.83	1.49	1.45
24	b	609	CLA	C4C-C3C	2.82	1.49	1.45
24	C	512	CLA	C4B-NB	-2.82	1.34	1.37
24	B	615	CLA	C1B-C2B	2.82	1.49	1.43
24	c	510	CLA	C3B-C4B	2.82	1.49	1.42
24	A	405	CLA	C1C-C2C	2.82	1.50	1.44
24	c	507	CLA	C1B-NB	-2.82	1.34	1.37
24	c	512	CLA	C1B-C2B	2.81	1.49	1.43
24	B	610	CLA	C3B-C4B	2.81	1.49	1.42
24	b	619	CLA	C1B-C2B	2.81	1.49	1.43
24	b	618	CLA	C1B-NB	-2.81	1.34	1.37
24	b	609	CLA	C1B-C2B	2.81	1.49	1.43
24	c	506	CLA	C4D-CHA	2.80	1.48	1.38
24	B	605	CLA	OBD-CAD	2.80	1.27	1.22
24	C	508	CLA	C1C-C2C	2.80	1.50	1.44
24	c	504	CLA	C1B-C2B	2.80	1.49	1.43
24	C	505	CLA	C4B-NB	-2.80	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	C3B-C4B	2.79	1.49	1.42
24	c	515	CLA	C3B-C4B	2.79	1.49	1.42
24	C	510	CLA	C1B-C2B	2.79	1.49	1.43
24	b	620	CLA	C4D-CHA	2.78	1.48	1.38
24	C	505	CLA	C4C-C3C	2.78	1.49	1.45
24	B	614	CLA	C4D-CHA	2.78	1.48	1.38
24	C	503	CLA	C1C-C2C	2.78	1.49	1.44
24	B	612	CLA	C3B-C4B	2.78	1.49	1.42
24	d	404	CLA	C3B-C4B	2.78	1.49	1.42
24	b	606	CLA	C4B-NB	-2.78	1.34	1.37
24	B	606	CLA	C1B-NB	-2.78	1.34	1.37
24	c	504	CLA	C1B-NB	-2.77	1.34	1.37
24	c	512	CLA	C4B-NB	-2.77	1.34	1.37
24	B	612	CLA	C1B-C2B	2.77	1.49	1.43
24	b	615	CLA	C1B-NB	-2.77	1.34	1.37
24	b	608	CLA	C4B-NB	-2.76	1.34	1.37
24	b	608	CLA	C1B-C2B	2.76	1.49	1.43
24	b	619	CLA	C4C-C3C	2.76	1.49	1.45
24	B	606	CLA	C1B-C2B	2.76	1.49	1.43
24	d	404	CLA	C4B-NB	-2.76	1.34	1.37
24	C	513	CLA	C1C-C2C	2.76	1.49	1.44
24	c	509	CLA	C1B-C2B	2.76	1.49	1.43
24	B	604	CLA	C3B-C4B	2.75	1.49	1.42
24	c	512	CLA	C1C-C2C	2.75	1.49	1.44
24	B	612	CLA	C1C-C2C	2.75	1.49	1.44
24	c	507	CLA	C3B-C4B	2.74	1.49	1.42
24	b	609	CLA	C4D-CHA	2.74	1.48	1.38
24	a	407	CLA	C4D-CHA	2.74	1.48	1.38
24	B	607	CLA	C4D-CHA	2.74	1.48	1.38
24	C	504	CLA	C4B-NB	-2.74	1.34	1.37
24	B	617	CLA	C4B-NB	-2.74	1.34	1.37
24	C	514	CLA	C3B-C4B	2.74	1.49	1.42
24	a	406	CLA	C4D-CHA	2.74	1.48	1.38
24	B	611	CLA	C1B-C2B	2.73	1.49	1.43
24	c	507	CLA	C1C-C2C	2.73	1.49	1.44
24	b	610	CLA	C1B-C2B	2.73	1.49	1.43
24	b	617	CLA	C1B-C2B	2.73	1.49	1.43
24	C	506	CLA	C4B-NB	-2.73	1.34	1.37
24	B	610	CLA	C1B-C2B	2.72	1.49	1.43
27	a	411	SQD	C6-S	-2.72	1.67	1.77
24	c	511	CLA	C4B-NB	-2.72	1.34	1.37
24	A	405	CLA	C4D-CHA	2.72	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	621	CLA	C4D-CHA	2.72	1.48	1.38
24	c	513	CLA	C4D-CHA	2.71	1.48	1.38
24	C	502	CLA	C1C-C2C	2.71	1.49	1.44
24	b	610	CLA	C4D-CHA	2.71	1.48	1.38
24	D	401	CLA	C1B-NB	-2.71	1.34	1.37
24	C	503	CLA	C4D-CHA	2.71	1.48	1.38
24	B	605	CLA	C1B-NB	-2.70	1.34	1.37
24	c	503	CLA	C4C-C3C	2.70	1.49	1.45
24	c	514	CLA	C1B-NB	-2.70	1.34	1.37
24	B	604	CLA	C1B-NB	-2.70	1.34	1.37
24	C	513	CLA	C3B-C4B	2.70	1.49	1.42
24	d	404	CLA	C1B-C2B	2.69	1.49	1.43
24	B	603	CLA	C4C-C3C	2.69	1.49	1.45
24	c	511	CLA	C4D-CHA	2.69	1.48	1.38
24	B	616	CLA	C4D-CHA	2.69	1.48	1.38
24	b	621	CLA	C1B-NB	-2.69	1.34	1.37
24	c	504	CLA	C3B-C4B	2.69	1.49	1.42
24	B	609	CLA	C4D-CHA	2.68	1.47	1.38
24	C	503	CLA	C4B-NB	-2.68	1.34	1.37
24	C	508	CLA	C4D-CHA	2.68	1.47	1.38
24	B	616	CLA	C3B-C4B	2.68	1.49	1.42
24	c	515	CLA	C4C-C3C	2.68	1.49	1.45
24	c	508	CLA	C4B-NB	-2.68	1.34	1.37
24	b	611	CLA	C4D-CHA	2.68	1.47	1.38
24	c	515	CLA	C4B-NB	-2.67	1.34	1.37
24	C	510	CLA	C1C-C2C	2.67	1.49	1.44
24	A	406	CLA	C1B-C2B	2.67	1.49	1.43
24	c	510	CLA	C4D-CHA	2.67	1.47	1.38
24	B	611	CLA	C4C-C3C	2.67	1.49	1.45
24	b	613	CLA	C4D-CHA	2.67	1.47	1.38
24	c	510	CLA	C4C-C3C	2.66	1.49	1.45
24	b	619	CLA	C3B-C4B	2.66	1.49	1.42
24	B	609	CLA	C3B-C4B	2.66	1.49	1.42
24	C	509	CLA	C1B-C2B	2.66	1.49	1.43
24	c	503	CLA	C4D-CHA	2.66	1.47	1.38
24	A	406	CLA	C3B-C4B	2.66	1.49	1.42
24	b	619	CLA	C4D-CHA	2.66	1.47	1.38
24	b	610	CLA	C1C-C2C	2.65	1.49	1.44
24	A	409	CLA	C1B-C2B	2.65	1.49	1.43
24	B	608	CLA	C4D-CHA	2.65	1.47	1.38
24	C	509	CLA	C3B-C4B	2.65	1.49	1.42
24	b	614	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C1B-NB	-2.65	1.34	1.37
24	a	406	CLA	C3B-C4B	2.65	1.49	1.42
24	b	615	CLA	C4D-CHA	2.65	1.47	1.38
24	b	617	CLA	C1C-C2C	2.65	1.49	1.44
24	B	613	CLA	C3B-C4B	2.65	1.49	1.42
24	D	403	CLA	C3B-C4B	2.65	1.49	1.42
24	A	409	CLA	C1C-C2C	2.65	1.49	1.44
24	B	611	CLA	C4B-NB	-2.65	1.34	1.37
24	d	402	CLA	C1C-C2C	2.65	1.49	1.44
24	C	507	CLA	C4D-CHA	2.64	1.47	1.38
24	B	614	CLA	C1C-C2C	2.64	1.49	1.44
24	B	602	CLA	C4D-CHA	2.64	1.47	1.38
24	d	402	CLA	C4D-CHA	2.64	1.47	1.38
24	b	616	CLA	C4D-CHA	2.64	1.47	1.38
24	B	609	CLA	C4B-NB	-2.64	1.34	1.37
24	C	513	CLA	C4D-CHA	2.64	1.47	1.38
24	B	612	CLA	C4D-CHA	2.63	1.47	1.38
24	B	606	CLA	C1C-C2C	2.63	1.49	1.44
24	c	512	CLA	C4D-CHA	2.63	1.47	1.38
32	a	416	PL9	C6-C5	2.63	1.49	1.35
24	B	603	CLA	C3B-C4B	2.63	1.48	1.42
24	C	510	CLA	C4D-CHA	2.63	1.47	1.38
34	Z	101	LMG	O8-C28	2.63	1.46	1.33
24	a	409	CLA	C4D-CHA	2.63	1.47	1.38
24	C	504	CLA	C4C-C3C	2.63	1.49	1.45
24	C	505	CLA	C4D-CHA	2.63	1.47	1.38
24	c	512	CLA	C3B-C4B	2.62	1.48	1.42
24	C	511	CLA	C4D-CHA	2.62	1.47	1.38
24	B	603	CLA	C1C-C2C	2.62	1.49	1.44
24	C	504	CLA	C3B-C4B	2.62	1.48	1.42
24	B	613	CLA	C1B-C2B	2.62	1.49	1.43
24	C	504	CLA	C1C-C2C	2.62	1.49	1.44
24	c	507	CLA	C4D-CHA	2.62	1.47	1.38
24	B	613	CLA	C4D-CHA	2.61	1.47	1.38
24	c	509	CLA	C1C-C2C	2.61	1.49	1.44
24	c	514	CLA	C4C-C3C	2.61	1.49	1.45
24	C	509	CLA	C4D-CHA	2.60	1.47	1.38
24	C	503	CLA	C1B-C2B	2.60	1.49	1.43
24	c	511	CLA	C1C-C2C	2.60	1.49	1.44
24	C	502	CLA	C4D-CHA	2.60	1.47	1.38
24	B	611	CLA	C4D-CHA	2.60	1.47	1.38
24	D	401	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	601	SQD	C6-S	-2.60	1.67	1.77
24	C	511	CLA	C1C-C2C	2.60	1.49	1.44
24	C	502	CLA	C4C-C3C	2.60	1.49	1.45
24	b	614	CLA	C3B-C4B	2.60	1.48	1.42
24	B	605	CLA	C3B-C4B	2.60	1.48	1.42
24	c	514	CLA	C1C-C2C	2.59	1.49	1.44
24	c	504	CLA	C4D-CHA	2.59	1.47	1.38
24	c	515	CLA	C1B-C2B	2.59	1.49	1.43
35	D	411	HTG	C1-S1	-2.59	1.76	1.80
24	b	611	CLA	C1B-C2B	2.59	1.49	1.43
24	b	614	CLA	C4C-C3C	2.58	1.49	1.45
24	B	608	CLA	C4C-C3C	2.58	1.49	1.45
24	B	613	CLA	C1C-C2C	2.58	1.49	1.44
24	C	509	CLA	C1C-C2C	2.58	1.49	1.44
24	b	618	CLA	C4C-C3C	2.58	1.49	1.45
24	b	608	CLA	C4D-CHA	2.58	1.47	1.38
24	B	605	CLA	C4D-CHA	2.58	1.47	1.38
24	b	618	CLA	C4D-CHA	2.58	1.47	1.38
24	b	607	CLA	C1C-C2C	2.58	1.49	1.44
24	c	508	CLA	C4D-CHA	2.58	1.47	1.38
24	d	404	CLA	C4D-CHA	2.58	1.47	1.38
24	a	409	CLA	C4C-C3C	2.57	1.49	1.45
24	a	407	CLA	C1C-C2C	2.57	1.49	1.44
32	A	419	PL9	C6-C5	2.57	1.48	1.35
24	b	621	CLA	C3B-C4B	2.57	1.48	1.42
24	c	506	CLA	C4C-C3C	2.57	1.49	1.45
24	b	606	CLA	C4D-CHA	2.56	1.47	1.38
24	c	503	CLA	C1B-C2B	2.56	1.49	1.43
24	b	617	CLA	C4D-CHA	2.56	1.47	1.38
24	A	409	CLA	C3B-C4B	2.56	1.48	1.42
32	d	406	PL9	C6-C5	2.55	1.48	1.35
24	D	404	CLA	C4B-NB	-2.55	1.34	1.37
24	C	511	CLA	C1B-C2B	2.55	1.49	1.43
24	A	405	CLA	C1B-C2B	2.55	1.49	1.43
24	C	505	CLA	C3B-C4B	2.55	1.48	1.42
24	C	503	CLA	C3B-C4B	2.55	1.48	1.42
24	B	617	CLA	C4D-CHA	2.55	1.47	1.38
24	c	505	CLA	C1B-C2B	2.54	1.49	1.43
24	B	607	CLA	C1B-C2B	2.54	1.49	1.43
24	c	511	CLA	C4C-C3C	2.54	1.49	1.45
24	C	507	CLA	C1B-C2B	2.54	1.49	1.43
24	C	513	CLA	C4C-C3C	2.54	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	CLA	C3B-C4B	2.54	1.48	1.42
24	b	617	CLA	C3B-C4B	2.54	1.48	1.42
24	B	612	CLA	C1B-NB	-2.54	1.34	1.37
24	c	515	CLA	C4D-CHA	2.54	1.47	1.38
24	D	403	CLA	C3D-C4D	-2.54	1.38	1.44
24	D	404	CLA	C4D-CHA	2.54	1.47	1.38
24	B	612	CLA	C4C-C3C	2.54	1.49	1.45
24	c	514	CLA	C1B-C2B	2.54	1.49	1.43
24	b	613	CLA	C3B-C4B	2.53	1.48	1.42
24	B	609	CLA	C1C-C2C	2.53	1.49	1.44
24	C	502	CLA	C3B-C4B	2.53	1.48	1.42
24	B	603	CLA	C4D-CHA	2.53	1.47	1.38
24	b	607	CLA	C4C-C3C	2.53	1.49	1.45
24	B	602	CLA	C1C-C2C	2.53	1.49	1.44
24	B	616	CLA	C4C-C3C	2.53	1.49	1.45
24	B	616	CLA	C4B-NB	-2.53	1.34	1.37
24	c	514	CLA	C4B-NB	-2.53	1.34	1.37
24	c	510	CLA	C1B-C2B	2.53	1.49	1.43
24	c	511	CLA	C3B-C4B	2.52	1.48	1.42
24	B	615	CLA	C4D-CHA	2.52	1.47	1.38
24	C	504	CLA	C1B-C2B	2.52	1.49	1.43
24	B	603	CLA	C1B-C2B	2.52	1.49	1.43
24	C	506	CLA	C4D-CHA	2.52	1.47	1.38
24	C	504	CLA	C4D-CHA	2.52	1.47	1.38
24	a	407	CLA	C1B-NB	-2.52	1.34	1.37
24	b	613	CLA	C1C-C2C	2.52	1.49	1.44
24	B	605	CLA	C1C-C2C	2.51	1.49	1.44
32	D	406	PL9	C6-C5	2.51	1.48	1.35
24	c	506	CLA	C1B-C2B	2.51	1.49	1.43
24	b	613	CLA	C4C-C3C	2.51	1.49	1.45
24	c	506	CLA	C3B-C4B	2.51	1.48	1.42
24	D	401	CLA	C1C-C2C	2.51	1.49	1.44
24	B	613	CLA	C3D-C4D	-2.51	1.38	1.44
24	b	613	CLA	C1B-C2B	2.50	1.49	1.43
24	B	604	CLA	C4D-CHA	2.50	1.47	1.38
36	H	102	DGD	O5D-C1E	2.50	1.44	1.40
24	C	506	CLA	C1C-C2C	2.50	1.49	1.44
24	b	606	CLA	C1C-C2C	2.50	1.49	1.44
24	c	508	CLA	C3B-C4B	2.50	1.48	1.42
24	b	612	CLA	C3B-C4B	2.50	1.48	1.42
24	C	513	CLA	C1B-C2B	2.49	1.49	1.43
25	d	403	PHO	C4B-NB	-2.49	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C4D-CHA	2.49	1.47	1.38
24	d	402	CLA	C4C-C3C	2.49	1.49	1.45
24	b	612	CLA	C4D-CHA	2.49	1.47	1.38
24	B	606	CLA	C4D-CHA	2.49	1.47	1.38
24	a	407	CLA	C4B-NB	-2.49	1.34	1.37
24	C	514	CLA	C1B-NB	-2.48	1.34	1.37
24	B	609	CLA	C1B-C2B	2.48	1.49	1.43
24	B	609	CLA	C4C-C3C	2.48	1.49	1.45
24	B	608	CLA	C1C-C2C	2.48	1.49	1.44
24	b	612	CLA	C1C-C2C	2.48	1.49	1.44
38	E	103	HEM	C1C-C2C	-2.48	1.40	1.45
24	b	615	CLA	C4B-NB	-2.48	1.34	1.37
24	a	409	CLA	C3B-C4B	2.48	1.48	1.42
27	l	101	SQD	C6-S	-2.47	1.68	1.77
24	C	505	CLA	C1C-C2C	2.47	1.49	1.44
24	c	513	CLA	C4C-C3C	2.47	1.49	1.45
24	c	509	CLA	C4C-C3C	2.47	1.49	1.45
24	c	515	CLA	C1C-C2C	2.47	1.49	1.44
24	c	511	CLA	C3B-C2B	2.47	1.49	1.41
35	C	522	HTG	C1-S1	-2.47	1.76	1.80
24	b	609	CLA	C4B-NB	-2.47	1.34	1.37
24	B	617	CLA	C3B-C2B	2.47	1.49	1.41
25	a	408	PHO	CHA-CBD	-2.47	1.48	1.51
24	c	514	CLA	C4D-CHA	2.46	1.47	1.38
24	c	505	CLA	C4D-CHA	2.46	1.47	1.38
36	h	102	DGD	O5D-C1E	2.46	1.44	1.40
24	c	507	CLA	C3D-C4D	-2.46	1.38	1.44
24	d	404	CLA	C4C-C3C	2.46	1.49	1.45
24	C	507	CLA	C4C-C3C	2.45	1.49	1.45
24	a	407	CLA	C4C-C3C	2.45	1.49	1.45
24	b	620	CLA	C4C-C3C	2.45	1.49	1.45
35	c	522	HTG	C1-S1	-2.45	1.77	1.80
24	A	409	CLA	C4D-CHA	2.45	1.47	1.38
24	B	607	CLA	C4B-NB	-2.44	1.34	1.37
24	c	511	CLA	C3D-C4D	-2.44	1.38	1.44
24	C	511	CLA	C3B-C2B	2.44	1.49	1.41
24	B	614	CLA	C1B-C2B	2.44	1.49	1.43
24	c	508	CLA	C3D-C4D	-2.43	1.38	1.44
24	C	512	CLA	C4C-C3C	2.43	1.49	1.45
24	a	407	CLA	C3D-C4D	-2.43	1.38	1.44
24	b	606	CLA	C1B-C2B	2.43	1.49	1.43
24	c	508	CLA	C1B-C2B	2.43	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C1C-C2C	2.43	1.49	1.44
24	a	409	CLA	C1C-NC	-2.43	1.34	1.37
24	d	401	CLA	C4D-CHA	2.43	1.47	1.38
24	B	610	CLA	C4D-CHA	2.43	1.47	1.38
24	b	609	CLA	C1B-NB	-2.43	1.34	1.37
24	b	610	CLA	C4C-C3C	2.43	1.49	1.45
24	b	614	CLA	C4D-CHA	2.42	1.47	1.38
24	B	615	CLA	C3D-C4D	-2.42	1.38	1.44
24	B	607	CLA	C3B-C4B	2.42	1.48	1.42
24	c	508	CLA	C4C-C3C	2.42	1.49	1.45
24	b	610	CLA	C4B-NB	-2.42	1.34	1.37
24	b	619	CLA	C4B-NB	-2.42	1.34	1.37
24	a	407	CLA	C1B-C2B	2.42	1.48	1.43
24	b	617	CLA	C1B-NB	-2.41	1.34	1.37
24	C	503	CLA	C3D-C4D	-2.41	1.38	1.44
24	B	602	CLA	C3D-C4D	-2.41	1.38	1.44
24	C	514	CLA	C4D-CHA	2.41	1.47	1.38
24	B	615	CLA	C3B-C4B	2.41	1.48	1.42
25	A	408	PHO	C4B-NB	-2.40	1.34	1.38
24	A	405	CLA	C3B-C2B	2.40	1.49	1.41
40	v	202	HEC	C4B-C3B	2.40	1.49	1.45
35	b	628	HTG	C1-S1	-2.40	1.77	1.80
24	C	507	CLA	C3B-C4B	2.40	1.48	1.42
24	C	510	CLA	C3B-C4B	2.40	1.48	1.42
24	A	405	CLA	C3B-C4B	2.39	1.48	1.42
24	d	402	CLA	C1B-C2B	2.39	1.48	1.43
27	F	101	SQD	C6-S	-2.39	1.68	1.77
30	M	101	LMT	O1'-C1'	2.39	1.44	1.40
24	C	507	CLA	C1C-C2C	2.38	1.49	1.44
24	B	609	CLA	C3B-C2B	2.38	1.49	1.41
24	a	409	CLA	C1C-C2C	2.38	1.49	1.44
24	c	510	CLA	C3B-C2B	2.37	1.49	1.41
24	b	613	CLA	C3D-C4D	-2.37	1.38	1.44
24	c	503	CLA	C1C-C2C	2.37	1.49	1.44
24	B	605	CLA	C4C-C3C	2.37	1.49	1.45
24	b	608	CLA	C4C-C3C	2.37	1.49	1.45
24	b	618	CLA	C3B-C2B	2.36	1.49	1.41
38	e	102	HEM	C1C-C2C	-2.36	1.40	1.45
24	B	605	CLA	C3D-C4D	-2.36	1.38	1.44
24	d	402	CLA	C4B-NB	-2.36	1.34	1.37
24	c	505	CLA	C4C-C3C	2.36	1.49	1.45
35	c	523	HTG	C1-S1	-2.36	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C3B-C2B	2.36	1.49	1.41
24	C	504	CLA	C3D-C4D	-2.35	1.38	1.44
24	c	514	CLA	C3D-C4D	-2.35	1.38	1.44
24	B	617	CLA	C4C-C3C	2.35	1.49	1.45
24	c	505	CLA	C4B-NB	-2.35	1.34	1.37
24	b	607	CLA	C4D-CHA	2.35	1.46	1.38
24	d	401	CLA	C4C-C3C	2.35	1.49	1.45
24	C	506	CLA	C3D-C4D	-2.35	1.38	1.44
24	C	510	CLA	C3D-C4D	-2.35	1.38	1.44
24	B	611	CLA	C1C-C2C	2.35	1.49	1.44
24	B	612	CLA	C3D-C4D	-2.35	1.38	1.44
24	C	512	CLA	C1C-C2C	2.35	1.49	1.44
35	B	631	HTG	C1-S1	-2.35	1.77	1.80
24	A	409	CLA	C4C-C3C	2.35	1.49	1.45
24	C	511	CLA	C4C-C3C	2.34	1.49	1.45
24	b	609	CLA	C3B-C4B	2.34	1.48	1.42
24	D	401	CLA	C3D-C4D	-2.34	1.38	1.44
24	b	621	CLA	C3B-C2B	2.34	1.49	1.41
24	b	616	CLA	C3D-C4D	-2.34	1.38	1.44
24	A	406	CLA	C4D-CHA	2.34	1.46	1.38
35	d	411	HTG	C1-S1	-2.34	1.77	1.80
24	B	613	CLA	C3B-C2B	2.33	1.49	1.41
24	A	405	CLA	C1B-NB	-2.33	1.34	1.37
24	B	614	CLA	C3B-C2B	2.33	1.49	1.41
24	b	618	CLA	C3B-C4B	2.33	1.48	1.42
24	a	406	CLA	C1C-C2C	2.33	1.49	1.44
24	B	602	CLA	C4C-C3C	2.33	1.49	1.45
35	V	204	HTG	C1-S1	-2.32	1.77	1.80
24	B	603	CLA	C3B-C2B	2.32	1.49	1.41
24	c	504	CLA	C4C-C3C	2.32	1.49	1.45
24	c	507	CLA	C4B-NB	-2.32	1.34	1.37
24	C	508	CLA	C4C-C3C	2.32	1.49	1.45
24	b	617	CLA	C3D-C4D	-2.32	1.38	1.44
24	C	508	CLA	C3B-C4B	2.31	1.48	1.42
24	B	616	CLA	C1C-C2C	2.31	1.49	1.44
24	b	614	CLA	C1C-C2C	2.31	1.49	1.44
24	c	506	CLA	C3D-C4D	-2.31	1.39	1.44
24	B	612	CLA	C3B-C2B	2.31	1.49	1.41
24	C	508	CLA	C3B-C2B	2.30	1.49	1.41
24	B	606	CLA	C4B-NB	-2.30	1.35	1.37
24	b	608	CLA	C3B-C2B	2.30	1.49	1.41
24	B	604	CLA	C3B-C2B	2.30	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	V	203	HEC	C4B-C3B	2.30	1.49	1.45
24	c	503	CLA	C3B-C2B	2.30	1.49	1.41
24	b	616	CLA	C1C-C2C	2.30	1.49	1.44
24	c	504	CLA	C1C-C2C	2.30	1.49	1.44
24	B	607	CLA	C4C-C3C	2.29	1.49	1.45
30	m	103	LMT	O1'-C1'	2.29	1.44	1.40
24	b	612	CLA	C4B-NB	-2.29	1.35	1.37
24	B	602	CLA	C3B-C2B	2.29	1.48	1.41
24	C	509	CLA	C3D-C4D	-2.29	1.39	1.44
24	b	610	CLA	C3D-C4D	-2.29	1.39	1.44
24	C	506	CLA	C3B-C2B	2.29	1.48	1.41
24	B	608	CLA	C3D-C4D	-2.28	1.39	1.44
24	B	611	CLA	C3D-C4D	-2.28	1.39	1.44
24	C	513	CLA	C3B-C2B	2.28	1.48	1.41
24	B	604	CLA	C3D-C4D	-2.28	1.39	1.44
24	B	610	CLA	C3D-C4D	-2.28	1.39	1.44
24	A	406	CLA	C4C-C3C	2.28	1.49	1.45
24	B	605	CLA	C3B-C2B	2.28	1.48	1.41
24	b	618	CLA	C4B-NB	-2.28	1.35	1.37
24	b	608	CLA	C3D-C4D	-2.28	1.39	1.44
24	C	504	CLA	C1B-NB	-2.28	1.35	1.37
24	b	616	CLA	C4C-C3C	2.28	1.49	1.45
24	c	513	CLA	C3B-C4B	2.28	1.48	1.42
24	A	405	CLA	MG-ND	-2.27	2.01	2.05
24	d	404	CLA	C3D-C4D	-2.27	1.39	1.44
24	B	606	CLA	C4C-C3C	2.27	1.49	1.45
24	b	615	CLA	C3B-C2B	2.27	1.48	1.41
24	b	619	CLA	C3B-C2B	2.27	1.48	1.41
24	D	404	CLA	C4C-C3C	2.26	1.48	1.45
25	a	408	PHO	C1D-ND	-2.26	1.34	1.38
24	b	617	CLA	C4C-C3C	2.26	1.48	1.45
24	C	507	CLA	C3D-C4D	-2.26	1.39	1.44
24	b	611	CLA	C1B-NB	-2.26	1.35	1.37
24	c	513	CLA	C3D-C4D	-2.25	1.39	1.44
24	B	609	CLA	C3D-C4D	-2.25	1.39	1.44
24	D	401	CLA	C3B-C2B	2.25	1.48	1.41
24	C	511	CLA	C3D-C4D	-2.25	1.39	1.44
24	b	621	CLA	C1C-C2C	2.24	1.48	1.44
24	c	504	CLA	C3D-C4D	-2.24	1.39	1.44
25	a	408	PHO	C4B-NB	-2.24	1.34	1.38
24	C	514	CLA	C1C-C2C	2.24	1.48	1.44
24	B	604	CLA	C4C-C3C	2.24	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	CLA	C3B-C2B	2.24	1.48	1.41
24	d	402	CLA	C3B-C2B	2.24	1.48	1.41
24	d	402	CLA	C3D-C4D	-2.24	1.39	1.44
36	D	407	DGD	O3G-C1D	2.24	1.44	1.40
24	C	514	CLA	C4C-C3C	2.24	1.48	1.45
24	C	508	CLA	C3D-C4D	-2.23	1.39	1.44
24	C	509	CLA	C3B-C2B	2.23	1.48	1.41
32	a	416	PL9	C2-C3	2.23	1.40	1.34
24	C	514	CLA	C3B-C2B	2.23	1.48	1.41
24	b	607	CLA	C3B-C2B	2.23	1.48	1.41
24	B	617	CLA	C3B-C4B	2.23	1.48	1.42
24	b	606	CLA	C3D-C4D	-2.23	1.39	1.44
24	C	502	CLA	C3D-C4D	-2.22	1.39	1.44
24	B	616	CLA	C3D-C4D	-2.22	1.39	1.44
24	b	606	CLA	C3B-C2B	2.22	1.48	1.41
38	e	102	HEM	C3B-C4B	2.21	1.49	1.44
24	a	406	CLA	C1B-NB	-2.21	1.35	1.37
24	b	611	CLA	C4C-C3C	2.21	1.48	1.45
24	a	406	CLA	C3D-C4D	-2.21	1.39	1.44
24	B	608	CLA	C3B-C2B	2.21	1.48	1.41
24	b	620	CLA	C3B-C2B	2.21	1.48	1.41
24	c	515	CLA	C3D-C4D	-2.21	1.39	1.44
24	C	502	CLA	C3B-C2B	2.20	1.48	1.41
24	d	404	CLA	C1D-C2D	2.20	1.49	1.45
24	b	611	CLA	C3B-C2B	2.20	1.48	1.41
24	C	505	CLA	C3D-C4D	-2.20	1.39	1.44
24	b	609	CLA	C3B-C2B	2.20	1.48	1.41
35	b	604	HTG	C1-S1	-2.20	1.77	1.80
24	c	505	CLA	C3D-C4D	-2.20	1.39	1.44
24	B	617	CLA	C3D-C4D	-2.19	1.39	1.44
24	b	614	CLA	C4B-NB	-2.19	1.35	1.37
24	b	612	CLA	C3D-C4D	-2.19	1.39	1.44
24	b	609	CLA	MG-NA	2.19	2.11	2.06
24	B	610	CLA	C1C-C2C	2.19	1.48	1.44
24	C	513	CLA	C3D-C4D	-2.19	1.39	1.44
24	B	611	CLA	C3B-C2B	2.19	1.48	1.41
24	a	406	CLA	C4B-NB	-2.18	1.35	1.37
24	c	513	CLA	C3B-C2B	2.18	1.48	1.41
24	B	607	CLA	C3B-C2B	2.18	1.48	1.41
24	c	515	CLA	C1D-C2D	2.17	1.49	1.45
24	a	406	CLA	C3B-C2B	2.17	1.48	1.41
24	C	510	CLA	C3B-C2B	2.17	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C4B-NB	-2.17	1.35	1.37
24	C	503	CLA	C1B-NB	-2.17	1.35	1.37
32	D	406	PL9	C2-C3	2.17	1.40	1.34
24	C	503	CLA	C3B-C2B	2.17	1.48	1.41
24	c	510	CLA	C4B-NB	-2.17	1.35	1.37
24	A	406	CLA	C3D-C4D	-2.16	1.39	1.44
24	b	617	CLA	C4B-NB	-2.16	1.35	1.37
24	b	617	CLA	C3B-C2B	2.16	1.48	1.41
24	c	510	CLA	C3D-C4D	-2.16	1.39	1.44
24	B	617	CLA	C1C-NC	-2.16	1.34	1.37
24	D	404	CLA	C3B-C2B	2.16	1.48	1.41
24	c	508	CLA	C1C-C2C	2.16	1.48	1.44
24	c	512	CLA	C3B-C2B	2.16	1.48	1.41
38	E	103	HEM	C1D-ND	-2.16	1.34	1.38
24	c	508	CLA	C3B-C2B	2.15	1.48	1.41
40	V	203	HEC	C1B-NB	-2.15	1.34	1.38
24	c	506	CLA	C3B-C2B	2.15	1.48	1.41
24	b	609	CLA	MG-ND	-2.15	2.01	2.05
24	B	602	CLA	C1B-C2B	2.14	1.48	1.43
24	b	613	CLA	C3B-C2B	2.14	1.48	1.41
24	b	620	CLA	C1C-C2C	2.14	1.48	1.44
24	c	512	CLA	C4C-C3C	2.14	1.48	1.45
24	C	512	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	613	CLA	MG-NA	2.14	2.11	2.06
24	c	514	CLA	C3B-C2B	2.14	1.48	1.41
24	c	503	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	616	CLA	C1C-NC	-2.13	1.34	1.37
24	D	403	CLA	C3B-C2B	2.13	1.48	1.41
24	b	619	CLA	C3D-C4D	-2.12	1.39	1.44
24	b	615	CLA	C3D-C4D	-2.11	1.39	1.44
24	c	515	CLA	C3B-C2B	2.11	1.48	1.41
24	a	407	CLA	C3B-C2B	2.11	1.48	1.41
24	C	507	CLA	C3B-C2B	2.11	1.48	1.41
24	A	406	CLA	C3B-C2B	2.11	1.48	1.41
24	c	509	CLA	C3B-C2B	2.11	1.48	1.41
24	B	606	CLA	C3D-C4D	-2.11	1.39	1.44
25	A	407	PHO	CHA-CBD	-2.11	1.49	1.51
24	b	619	CLA	C1C-C2C	2.10	1.48	1.44
24	A	409	CLA	C3B-C2B	2.10	1.48	1.41
24	B	617	CLA	C1C-C2C	2.10	1.48	1.44
35	C	523	HTG	C1-S1	-2.09	1.77	1.80
24	b	612	CLA	C3B-C2B	2.09	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C3D-C4D	-2.09	1.39	1.44
24	B	605	CLA	MG-NA	2.09	2.11	2.06
24	B	615	CLA	C4C-C3C	2.08	1.48	1.45
24	B	603	CLA	C3D-C4D	-2.08	1.39	1.44
24	B	603	CLA	C1C-NC	-2.08	1.34	1.37
35	b	603	HTG	C1-S1	-2.08	1.77	1.80
24	A	405	CLA	MG-NA	2.08	2.11	2.06
24	b	621	CLA	C3D-C4D	-2.08	1.39	1.44
24	B	612	CLA	C4B-NB	-2.08	1.35	1.37
24	b	617	CLA	C1C-NC	-2.08	1.34	1.37
35	B	624	HTG	C1-S1	-2.07	1.77	1.80
24	C	505	CLA	C3B-C2B	2.07	1.48	1.41
25	A	408	PHO	C3A-C2A	-2.06	1.52	1.54
24	b	616	CLA	C3B-C2B	2.06	1.48	1.41
40	V	203	HEC	C1A-C2A	-2.06	1.41	1.45
24	c	503	CLA	C3B-C4B	2.06	1.47	1.42
24	B	605	CLA	C4B-NB	-2.06	1.35	1.37
24	d	402	CLA	C3B-C4B	2.05	1.47	1.42
24	C	514	CLA	C3D-C4D	-2.05	1.39	1.44
24	b	606	CLA	C4C-C3C	2.05	1.48	1.45
24	b	620	CLA	C4B-NB	-2.05	1.35	1.37
36	D	407	DGD	O5D-C1E	2.05	1.43	1.40
24	b	620	CLA	C3D-C4D	-2.05	1.39	1.44
24	B	605	CLA	MG-ND	-2.05	2.01	2.05
24	c	509	CLA	C3B-C4B	2.05	1.47	1.42
35	B	630	HTG	C1-S1	-2.05	1.77	1.80
24	b	618	CLA	C3D-C4D	-2.04	1.39	1.44
26	b	622	BCR	C19-C18	2.04	1.50	1.45
24	b	616	CLA	C4B-NB	-2.04	1.35	1.37
24	b	611	CLA	C3D-C4D	-2.04	1.39	1.44
24	b	609	CLA	C3D-C4D	-2.03	1.39	1.44
38	e	102	HEM	C1D-ND	-2.03	1.34	1.38
36	d	407	DGD	O5D-C1E	2.03	1.43	1.40
24	A	409	CLA	C3D-C4D	-2.02	1.39	1.44
24	A	406	CLA	C1C-C2C	2.02	1.48	1.44
40	v	202	HEC	C1D-C2D	2.02	1.48	1.44
24	b	614	CLA	C3B-C2B	2.01	1.48	1.41
24	D	403	CLA	C1C-NC	-2.01	1.34	1.37
34	j	101	LMG	O1-C1	2.01	1.43	1.40
24	B	615	CLA	C3B-C2B	2.01	1.48	1.41
24	b	621	CLA	C1C-NC	-2.01	1.34	1.37

All (2758) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	PHO	C2D-C1D-ND	12.92	118.45	109.53
25	a	408	PHO	C2D-C1D-ND	12.33	118.04	109.53
25	A	407	PHO	C2D-C1D-ND	11.58	117.52	109.53
25	d	403	PHO	C2D-C1D-ND	11.27	117.31	109.53
24	B	615	CLA	C1D-ND-C4D	-10.22	99.08	106.33
24	b	610	CLA	C1D-ND-C4D	-10.12	99.15	106.33
24	B	610	CLA	C1D-ND-C4D	-10.04	99.20	106.33
24	A	409	CLA	C1D-ND-C4D	-9.95	99.27	106.33
24	B	606	CLA	C1D-ND-C4D	-9.75	99.41	106.33
24	C	514	CLA	C1D-ND-C4D	-9.61	99.51	106.33
24	c	514	CLA	C1D-ND-C4D	-9.57	99.53	106.33
24	C	504	CLA	C1D-ND-C4D	-9.54	99.56	106.33
24	A	406	CLA	C1D-ND-C4D	-9.53	99.57	106.33
24	C	512	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	B	604	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	c	512	CLA	C1D-ND-C4D	-9.51	99.58	106.33
24	B	612	CLA	C1D-ND-C4D	-9.43	99.63	106.33
24	D	404	CLA	C1D-ND-C4D	-9.40	99.66	106.33
24	c	513	CLA	C1D-ND-C4D	-9.40	99.66	106.33
24	c	505	CLA	C1D-ND-C4D	-9.36	99.69	106.33
24	b	611	CLA	C1D-ND-C4D	-9.32	99.72	106.33
24	a	409	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	c	515	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	B	605	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	c	503	CLA	C1D-ND-C4D	-9.28	99.74	106.33
24	d	404	CLA	C1D-ND-C4D	-9.28	99.75	106.33
24	b	607	CLA	C1D-ND-C4D	-9.26	99.75	106.33
24	b	616	CLA	C1D-ND-C4D	-9.25	99.76	106.33
24	c	510	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	b	614	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	B	603	CLA	C1D-ND-C4D	-9.15	99.83	106.33
24	b	606	CLA	C1D-ND-C4D	-9.13	99.85	106.33
24	B	615	CLA	C2D-C1D-ND	9.11	116.82	110.10
24	a	407	CLA	C1D-ND-C4D	-9.07	99.89	106.33
24	c	509	CLA	C1D-ND-C4D	-9.05	99.90	106.33
24	C	509	CLA	C1D-ND-C4D	-9.05	99.90	106.33
24	b	618	CLA	C1D-ND-C4D	-9.05	99.91	106.33
24	b	620	CLA	C1D-ND-C4D	-9.04	99.92	106.33
24	b	619	CLA	C1D-ND-C4D	-9.02	99.93	106.33
24	B	602	CLA	C1D-ND-C4D	-9.01	99.93	106.33
24	b	610	CLA	C2D-C1D-ND	9.00	116.74	110.10
24	B	609	CLA	C1D-ND-C4D	-8.99	99.95	106.33
24	B	617	CLA	C1D-ND-C4D	-8.97	99.96	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	409	CLA	C2D-C1D-ND	8.95	116.70	110.10
24	C	505	CLA	C1D-ND-C4D	-8.92	100.00	106.33
24	b	617	CLA	C1D-ND-C4D	-8.92	100.00	106.33
24	c	506	CLA	C1D-ND-C4D	-8.88	100.03	106.33
24	c	509	CLA	C2D-C1D-ND	8.87	116.64	110.10
24	b	615	CLA	C1D-ND-C4D	-8.84	100.06	106.33
24	b	608	CLA	C1D-ND-C4D	-8.83	100.06	106.33
24	b	613	CLA	C1D-ND-C4D	-8.82	100.07	106.33
24	B	607	CLA	C1D-ND-C4D	-8.80	100.09	106.33
24	C	510	CLA	C1D-ND-C4D	-8.77	100.11	106.33
24	C	512	CLA	C2D-C1D-ND	8.75	116.55	110.10
24	c	510	CLA	C2D-C1D-ND	8.71	116.52	110.10
24	c	511	CLA	C1D-ND-C4D	-8.71	100.15	106.33
24	B	610	CLA	C2D-C1D-ND	8.67	116.50	110.10
24	C	513	CLA	C1D-ND-C4D	-8.65	100.19	106.33
24	a	406	CLA	C1D-ND-C4D	-8.65	100.19	106.33
24	C	508	CLA	C1D-ND-C4D	-8.64	100.20	106.33
24	c	503	CLA	C2D-C1D-ND	8.62	116.45	110.10
24	C	511	CLA	C1D-ND-C4D	-8.61	100.22	106.33
24	B	611	CLA	C1D-ND-C4D	-8.59	100.23	106.33
24	b	618	CLA	C2D-C1D-ND	8.59	116.44	110.10
24	b	621	CLA	C1D-ND-C4D	-8.58	100.24	106.33
24	d	401	CLA	C1D-ND-C4D	-8.57	100.24	106.33
24	c	506	CLA	C2D-C1D-ND	8.57	116.42	110.10
24	b	616	CLA	C2D-C1D-ND	8.57	116.42	110.10
24	c	514	CLA	C2D-C1D-ND	8.56	116.41	110.10
24	B	605	CLA	C2D-C1D-ND	8.51	116.37	110.10
24	B	607	CLA	C2D-C1D-ND	8.50	116.37	110.10
24	b	619	CLA	C2D-C1D-ND	8.49	116.36	110.10
24	C	507	CLA	C1D-ND-C4D	-8.48	100.31	106.33
24	c	505	CLA	C2D-C1D-ND	8.47	116.35	110.10
24	B	614	CLA	C1D-ND-C4D	-8.43	100.35	106.33
24	d	404	CLA	C2B-C1B-NB	8.42	115.87	110.23
24	C	503	CLA	C1D-ND-C4D	-8.41	100.36	106.33
24	b	611	CLA	C2D-C1D-ND	8.40	116.29	110.10
24	B	608	CLA	C1D-ND-C4D	-8.40	100.37	106.33
24	D	401	CLA	C1D-ND-C4D	-8.38	100.38	106.33
24	c	508	CLA	C1D-ND-C4D	-8.37	100.39	106.33
24	C	508	CLA	C2D-C1D-ND	8.36	116.27	110.10
24	B	606	CLA	C2D-C1D-ND	8.36	116.26	110.10
24	b	615	CLA	C2D-C1D-ND	8.36	116.26	110.10
24	b	612	CLA	C1D-ND-C4D	-8.33	100.42	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	502	CLA	C1D-ND-C4D	-8.33	100.42	106.33
24	B	612	CLA	C2D-C1D-ND	8.32	116.23	110.10
24	D	404	CLA	C2D-C1D-ND	8.32	116.23	110.10
24	B	616	CLA	C2D-C1D-ND	8.31	116.23	110.10
24	B	602	CLA	C2B-C1B-NB	8.31	115.80	110.23
24	c	504	CLA	C1D-ND-C4D	-8.29	100.44	106.33
24	D	404	CLA	C2B-C1B-NB	8.27	115.77	110.23
24	B	614	CLA	C2D-C1D-ND	8.26	116.19	110.10
24	d	402	CLA	C4A-NA-C1A	-8.26	102.99	106.71
24	B	616	CLA	C1D-ND-C4D	-8.25	100.47	106.33
24	b	612	CLA	C2D-C1D-ND	8.24	116.18	110.10
24	D	403	CLA	C1D-ND-C4D	-8.24	100.48	106.33
24	b	609	CLA	C2D-C1D-ND	8.24	116.17	110.10
24	C	514	CLA	C2D-C1D-ND	8.23	116.17	110.10
24	c	515	CLA	C2B-C1B-NB	8.23	115.75	110.23
24	C	506	CLA	C1D-ND-C4D	-8.21	100.50	106.33
24	B	604	CLA	C2D-C1D-ND	8.17	116.12	110.10
24	B	608	CLA	C2D-C1D-ND	8.16	116.12	110.10
24	b	607	CLA	C2D-C1D-ND	8.16	116.12	110.10
25	a	408	PHO	O2D-CGD-CBD	8.16	121.33	111.00
24	c	514	CLA	C2B-C1B-NB	8.15	115.69	110.23
24	b	609	CLA	C1D-ND-C4D	-8.14	100.55	106.33
24	B	609	CLA	C2D-C1D-ND	8.12	116.09	110.10
24	B	613	CLA	C2B-C1B-NB	8.11	115.67	110.23
24	C	513	CLA	C2D-C1D-ND	8.09	116.06	110.10
24	A	405	CLA	C4A-NA-C1A	-8.07	103.08	106.71
24	b	614	CLA	C2D-C1D-ND	8.05	116.04	110.10
24	B	603	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	B	617	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	d	404	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	b	620	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	a	407	CLA	C2D-C1D-ND	8.03	116.02	110.10
24	c	507	CLA	C1D-ND-C4D	-8.03	100.63	106.33
24	c	510	CLA	C2B-C1B-NB	8.01	115.60	110.23
24	B	611	CLA	C2D-C1D-ND	8.00	116.00	110.10
24	c	512	CLA	C2D-C1D-ND	7.99	115.99	110.10
24	d	401	CLA	C2D-C1D-ND	7.97	115.98	110.10
24	C	504	CLA	C2D-C1D-ND	7.97	115.98	110.10
24	d	402	CLA	C1D-ND-C4D	-7.95	100.69	106.33
24	a	409	CLA	C2D-C1D-ND	7.93	115.95	110.10
24	B	603	CLA	C2B-C1B-NB	7.93	115.55	110.23
24	b	611	CLA	C2B-C1B-NB	7.92	115.54	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	502	CLA	C2D-C1D-ND	7.91	115.93	110.10
24	C	505	CLA	C2D-C1D-ND	7.90	115.92	110.10
24	a	407	CLA	C2B-C1B-NB	7.88	115.52	110.23
24	C	509	CLA	C2D-C1D-ND	7.88	115.91	110.10
24	B	602	CLA	C2D-C1D-ND	7.87	115.91	110.10
24	C	507	CLA	C2D-C1D-ND	7.87	115.90	110.10
24	C	513	CLA	C2B-C1B-NB	7.85	115.50	110.23
24	C	511	CLA	C2D-C1D-ND	7.79	115.84	110.10
24	D	401	CLA	C2D-C1D-ND	7.79	115.84	110.10
24	B	613	CLA	C1D-ND-C4D	-7.76	100.83	106.33
24	b	617	CLA	C2D-C1D-ND	7.72	115.79	110.10
24	c	513	CLA	C2D-C1D-ND	7.69	115.77	110.10
24	a	406	CLA	C2D-C1D-ND	7.68	115.76	110.10
24	c	515	CLA	C2D-C1D-ND	7.67	115.76	110.10
24	D	401	CLA	C2B-C1B-NB	7.67	115.37	110.23
24	A	405	CLA	C1D-ND-C4D	-7.65	100.90	106.33
25	d	403	PHO	O2D-CGD-CBD	7.65	120.69	111.00
24	A	405	CLA	C2D-C1D-ND	7.64	115.73	110.10
24	c	504	CLA	C2D-C1D-ND	7.63	115.73	110.10
24	b	606	CLA	C2D-C1D-ND	7.60	115.71	110.10
24	b	621	CLA	C2D-C1D-ND	7.59	115.70	110.10
24	D	403	CLA	C2D-C1D-ND	7.56	115.68	110.10
25	A	408	PHO	C4D-ND-C1D	-7.52	101.18	108.83
24	B	615	CLA	C2B-C1B-NB	7.50	115.26	110.23
24	C	504	CLA	C2B-C1B-NB	7.46	115.23	110.23
24	a	409	CLA	C2B-C1B-NB	7.45	115.23	110.23
24	B	612	CLA	C2B-C1B-NB	7.45	115.22	110.23
24	b	613	CLA	C2B-C1B-NB	7.45	115.22	110.23
24	b	620	CLA	C2B-C1B-NB	7.44	115.22	110.23
24	C	503	CLA	C2D-C1D-ND	7.42	115.57	110.10
24	b	608	CLA	C2B-C1B-NB	7.41	115.20	110.23
24	b	610	CLA	C2B-C1B-NB	7.41	115.20	110.23
25	A	408	PHO	C2B-C1B-NB	7.40	114.63	109.53
24	b	608	CLA	C2D-C1D-ND	7.38	115.54	110.10
24	C	512	CLA	C2B-C1B-NB	7.37	115.17	110.23
24	B	609	CLA	C2B-C1B-NB	7.36	115.16	110.23
24	b	607	CLA	C2B-C1B-NB	7.35	115.16	110.23
24	b	619	CLA	C2B-C1B-NB	7.33	115.15	110.23
24	B	606	CLA	C2B-C1B-NB	7.28	115.11	110.23
24	A	406	CLA	C2D-C1D-ND	7.27	115.47	110.10
24	c	508	CLA	C2D-C1D-ND	7.27	115.46	110.10
24	c	504	CLA	C2B-C1B-NB	7.26	115.10	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	C2B-C1B-NB	7.26	115.10	110.23
24	c	506	CLA	C2B-C1B-NB	7.23	115.08	110.23
24	A	406	CLA	C2B-C1B-NB	7.22	115.07	110.23
24	b	613	CLA	C2D-C1D-ND	7.21	115.42	110.10
24	B	605	CLA	CMD-C2D-C1D	7.21	137.42	124.71
24	b	615	CLA	C2B-C1B-NB	7.20	115.06	110.23
24	C	510	CLA	C2D-C1D-ND	7.20	115.41	110.10
24	B	612	CLA	C4A-NA-C1A	-7.20	103.47	106.71
24	B	616	CLA	C4A-NA-C1A	-7.19	103.47	106.71
24	A	409	CLA	C2B-C1B-NB	7.18	115.05	110.23
24	b	606	CLA	C2B-C1B-NB	7.16	115.03	110.23
24	b	609	CLA	CMD-C2D-C1D	7.14	137.29	124.71
24	B	607	CLA	C4A-NA-C1A	-7.09	103.52	106.71
24	D	403	CLA	C4A-NA-C1A	-7.07	103.53	106.71
25	A	407	PHO	C4D-ND-C1D	-7.07	101.64	108.83
24	c	511	CLA	C2D-C1D-ND	7.03	115.28	110.10
24	b	620	CLA	C4A-NA-C1A	-7.01	103.55	106.71
25	d	403	PHO	C2B-C1B-NB	6.98	114.34	109.53
24	B	616	CLA	C2B-C1B-NB	6.95	114.89	110.23
25	a	408	PHO	C4D-ND-C1D	-6.94	101.77	108.83
24	c	511	CLA	C2B-C1B-NB	6.93	114.88	110.23
24	C	508	CLA	CMD-C2D-C1D	6.93	136.93	124.71
24	C	509	CLA	C2B-C1B-NB	6.92	114.87	110.23
24	B	611	CLA	C2B-C1B-NB	6.92	114.87	110.23
24	B	613	CLA	C2D-C1D-ND	6.90	115.19	110.10
24	c	505	CLA	C4A-NA-C1A	-6.90	103.61	106.71
24	C	510	CLA	C2B-C1B-NB	6.89	114.85	110.23
24	b	621	CLA	C2B-C1B-NB	6.87	114.84	110.23
24	d	404	CLA	CMD-C2D-C1D	6.86	136.81	124.71
24	D	403	CLA	CMD-C2D-C1D	6.85	136.79	124.71
24	B	615	CLA	CMD-C2D-C1D	6.85	136.79	124.71
24	C	514	CLA	C2B-C1B-NB	6.84	114.82	110.23
24	C	506	CLA	C2B-C1B-NB	6.84	114.81	110.23
24	b	610	CLA	CMD-C2D-C1D	6.81	136.72	124.71
25	a	408	PHO	C2B-C1B-NB	6.80	114.22	109.53
24	c	513	CLA	C2B-C1B-NB	6.80	114.79	110.23
24	c	505	CLA	C2B-C1B-NB	6.79	114.78	110.23
24	c	508	CLA	C2B-C1B-NB	6.77	114.77	110.23
24	c	507	CLA	C4A-NA-C1A	-6.75	103.67	106.71
24	C	504	CLA	C4A-NA-C1A	-6.71	103.69	106.71
24	b	616	CLA	C2B-C1B-NB	6.71	114.73	110.23
24	B	607	CLA	C2B-C1B-NB	6.70	114.72	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	407	PHO	C1C-C2C-C3C	-6.70	103.04	108.61
24	d	402	CLA	C2B-C1B-NB	6.69	114.72	110.23
24	A	405	CLA	C2C-C1C-NC	6.67	116.22	109.97
24	A	405	CLA	C2B-C1B-NB	6.65	114.69	110.23
24	b	616	CLA	CHD-C4C-C3C	-6.64	115.08	124.84
24	b	607	CLA	C4A-NA-C1A	-6.64	103.72	106.71
24	B	610	CLA	CHD-C4C-C3C	-6.63	115.09	124.84
24	a	406	CLA	C2C-C1C-NC	6.62	116.17	109.97
24	b	618	CLA	CHD-C4C-C3C	-6.60	115.14	124.84
25	A	407	PHO	O2D-CGD-CBD	6.60	119.36	111.00
24	d	402	CLA	C2D-C1D-ND	6.59	114.96	110.10
25	d	403	PHO	C4D-ND-C1D	-6.59	102.13	108.83
24	d	404	CLA	C4A-NA-C1A	-6.58	103.75	106.71
24	b	606	CLA	CMD-C2D-C1D	6.58	136.31	124.71
24	C	506	CLA	C2D-C1D-ND	6.57	114.95	110.10
24	B	603	CLA	C4A-NA-C1A	-6.57	103.75	106.71
24	c	515	CLA	CHD-C1D-ND	-6.56	118.42	124.45
24	d	404	CLA	CHD-C1D-ND	-6.53	118.45	124.45
24	C	509	CLA	C4A-NA-C1A	-6.53	103.77	106.71
25	A	408	PHO	O2D-CGD-CBD	6.52	119.25	111.00
24	B	614	CLA	C2B-C1B-NB	6.50	114.59	110.23
24	c	507	CLA	C2B-C1B-NB	6.48	114.58	110.23
24	b	612	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
24	c	512	CLA	C2B-C1B-NB	6.48	114.57	110.23
24	c	515	CLA	CMD-C2D-C1D	6.47	136.12	124.71
35	b	628	HTG	C1'-S1-C1	6.47	112.19	100.09
24	c	511	CLA	CMD-C2D-C1D	6.47	136.11	124.71
24	b	608	CLA	C4A-NA-C1A	-6.46	103.80	106.71
24	d	401	CLA	C2B-C1B-NB	6.45	114.56	110.23
24	B	614	CLA	C2C-C1C-NC	6.45	116.02	109.97
24	C	508	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
24	B	607	CLA	CHD-C4C-C3C	-6.44	115.37	124.84
24	B	610	CLA	CMD-C2D-C1D	6.44	136.07	124.71
24	D	401	CLA	CMD-C2D-C1D	6.43	136.05	124.71
24	B	602	CLA	CMD-C2D-C1D	6.43	136.05	124.71
24	a	406	CLA	C2B-C1B-NB	6.43	114.54	110.23
24	b	613	CLA	CMD-C2D-C1D	6.43	136.04	124.71
24	b	610	CLA	CHD-C4C-C3C	-6.42	115.40	124.84
24	c	508	CLA	CMD-C2D-C1D	6.42	136.02	124.71
24	a	407	CLA	CMD-C2D-C1D	6.40	135.99	124.71
24	B	602	CLA	C4A-NA-C1A	-6.39	103.83	106.71
24	C	502	CLA	C2B-C1B-NB	6.38	114.51	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	512	CLA	CMD-C2D-C1D	6.38	135.96	124.71
24	B	617	CLA	C2B-C1B-NB	6.38	114.51	110.23
24	B	606	CLA	C4A-NA-C1A	-6.37	103.84	106.71
24	B	613	CLA	C4A-NA-C1A	-6.37	103.84	106.71
24	a	406	CLA	CMD-C2D-C1D	6.37	135.94	124.71
24	A	409	CLA	CHD-C4C-C3C	-6.36	115.49	124.84
24	A	406	CLA	CMD-C2D-C1D	6.36	135.92	124.71
24	C	504	CLA	CMD-C2D-C1D	6.35	135.91	124.71
24	B	604	CLA	C2B-C1B-NB	6.35	114.49	110.23
24	D	401	CLA	C2C-C1C-NC	6.35	115.92	109.97
24	d	401	CLA	C2C-C1C-NC	6.35	115.92	109.97
24	B	605	CLA	C2C-C1C-NC	6.34	115.91	109.97
25	d	403	PHO	C1C-C2C-C3C	-6.33	103.35	108.61
24	B	605	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
24	c	503	CLA	C2B-C1B-NB	6.31	114.46	110.23
24	b	606	CLA	CHD-C4C-C3C	-6.30	115.57	124.84
24	c	505	CLA	CMD-C2D-C1D	6.29	135.79	124.71
24	B	606	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
24	c	510	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
24	B	615	CLA	CHD-C1D-ND	-6.28	118.69	124.45
24	C	505	CLA	CHD-C1D-ND	-6.28	118.69	124.45
24	b	608	CLA	CMD-C2D-C1D	6.26	135.75	124.71
24	b	610	CLA	CHD-C1D-ND	-6.26	118.70	124.45
24	B	604	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
24	c	506	CLA	CHD-C1D-ND	-6.25	118.71	124.45
24	B	617	CLA	O2D-CGD-CBD	6.24	122.35	111.27
24	C	510	CLA	O2D-CGD-CBD	6.23	122.34	111.27
24	b	606	CLA	CHD-C1D-ND	-6.23	118.73	124.45
24	C	510	CLA	CMD-C2D-C1D	6.22	135.68	124.71
24	b	609	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	b	618	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	D	403	CLA	C2C-C1C-NC	6.19	115.77	109.97
24	D	403	CLA	CHD-C1D-ND	-6.19	118.77	124.45
24	B	609	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
24	b	611	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
24	C	503	CLA	C2B-C1B-NB	6.18	114.37	110.23
24	d	402	CLA	C2C-C1C-NC	6.17	115.75	109.97
24	b	619	CLA	C2C-C1C-NC	6.17	115.75	109.97
24	C	505	CLA	CMD-C2D-C1D	6.15	135.56	124.71
24	B	606	CLA	C2C-C1C-NC	6.15	115.73	109.97
24	d	402	CLA	CMD-C2D-C1D	6.14	135.54	124.71
24	C	508	CLA	C2B-C1B-NB	6.13	114.34	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	505	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
24	c	509	CLA	CHD-C4C-C3C	-6.11	115.85	124.84
24	b	618	CLA	CMD-C2D-C1D	6.11	135.48	124.71
24	B	612	CLA	CHD-C4C-C3C	-6.10	115.88	124.84
24	B	608	CLA	C2B-C1B-NB	6.09	114.31	110.23
24	b	609	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
24	c	514	CLA	CHD-C1D-ND	-6.09	118.86	124.45
35	d	411	HTG	C1'-S1-C1	6.08	111.46	100.09
24	b	614	CLA	C2C-C1C-NC	6.07	115.66	109.97
24	C	504	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
24	d	401	CLA	CHD-C1D-ND	-6.06	118.89	124.45
24	b	611	CLA	CMD-C2D-C1D	6.06	135.39	124.71
24	C	506	CLA	CMD-C2D-C1D	6.05	135.37	124.71
24	b	614	CLA	C4A-NA-C1A	-6.05	103.99	106.71
24	C	512	CLA	CHD-C1D-ND	-6.04	118.90	124.45
25	A	407	PHO	C2B-C1B-NB	6.04	113.70	109.53
24	b	608	CLA	O2D-CGD-CBD	6.03	121.99	111.27
24	b	617	CLA	C2B-C1B-NB	6.03	114.27	110.23
24	A	409	CLA	CHD-C1D-ND	-6.02	118.92	124.45
24	c	512	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
24	b	621	CLA	C2C-C1C-NC	6.02	115.61	109.97
24	b	617	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
24	C	506	CLA	C2C-C1C-NC	6.02	115.61	109.97
24	c	507	CLA	CMD-C2D-C1D	6.01	135.31	124.71
24	C	507	CLA	C2C-C1C-NC	6.01	115.60	109.97
24	B	614	CLA	CMD-C2D-C1D	6.00	135.30	124.71
24	d	404	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
24	c	509	CLA	O2D-CGD-CBD	6.00	121.94	111.27
24	D	404	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
24	B	603	CLA	CMD-C2D-C1D	5.99	135.28	124.71
24	b	607	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
24	c	507	CLA	C2D-C1D-ND	5.98	114.51	110.10
24	c	509	CLA	C2C-C1C-NC	5.97	115.57	109.97
24	c	503	CLA	C2C-C1C-NC	5.97	115.56	109.97
24	B	602	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
24	B	609	CLA	C2C-C1C-NC	5.97	115.56	109.97
24	c	503	CLA	CMD-C2D-C1D	5.96	135.21	124.71
24	b	615	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
24	C	511	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
24	c	513	CLA	CMD-C2D-C1D	5.95	135.20	124.71
24	C	509	CLA	C2C-C1C-NC	5.94	115.54	109.97
24	b	613	CLA	C4A-NA-C1A	-5.93	104.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	CLA	CMD-C2D-C1D	5.93	135.16	124.71
24	B	608	CLA	C2C-C1C-NC	5.92	115.52	109.97
35	B	624	HTG	C1'-S1-C1	5.92	111.17	100.09
25	A	408	PHO	C1C-C2C-C3C	-5.92	103.69	108.61
24	D	401	CLA	CHD-C1D-ND	-5.91	119.03	124.45
24	c	507	CLA	O2D-CGD-CBD	5.90	121.76	111.27
24	A	406	CLA	CHD-C1D-ND	-5.90	119.03	124.45
24	b	618	CLA	C2B-C1B-NB	5.90	114.19	110.23
24	b	612	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	B	602	CLA	CHD-C1D-ND	-5.90	119.04	124.45
24	D	404	CLA	CMD-C2D-C1D	5.89	135.10	124.71
24	b	609	CLA	C4A-NA-C1A	-5.89	104.06	106.71
24	c	506	CLA	CMD-C2D-C1D	5.89	135.09	124.71
24	b	621	CLA	CMD-C2D-C1D	5.89	135.09	124.71
24	B	611	CLA	CMD-C2D-C1D	5.89	135.09	124.71
24	C	505	CLA	C2C-C1C-NC	5.88	115.48	109.97
24	B	603	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
24	a	409	CLA	C2C-C1C-NC	5.86	115.46	109.97
24	c	507	CLA	C2C-C1C-NC	5.85	115.46	109.97
24	b	614	CLA	C2B-C1B-NB	5.85	114.15	110.23
24	B	615	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	a	407	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
24	a	407	CLA	C4A-NA-C1A	-5.84	104.08	106.71
24	B	613	CLA	CMD-C2D-C1D	5.83	134.99	124.71
24	B	617	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
24	b	620	CLA	CHD-C1D-ND	-5.83	119.10	124.45
24	b	609	CLA	C2B-C1B-NB	5.83	114.14	110.23
24	C	503	CLA	CHD-C4C-C3C	-5.83	116.28	124.84
24	B	616	CLA	CHD-C4C-C3C	-5.83	116.28	124.84
24	B	605	CLA	C2B-C1B-NB	5.82	114.14	110.23
24	C	511	CLA	CMD-C2D-C1D	5.82	134.98	124.71
35	c	522	HTG	C1'-S1-C1	5.82	110.97	100.09
24	b	612	CLA	C2B-C1B-NB	5.81	114.13	110.23
24	C	512	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	C	513	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	b	611	CLA	C4A-NA-C1A	-5.81	104.09	106.71
24	b	614	CLA	CMD-C2D-C1D	5.80	134.94	124.71
24	d	401	CLA	CMD-C2D-C1D	5.80	134.94	124.71
24	C	504	CLA	C2C-C1C-NC	5.78	115.39	109.97
24	C	507	CLA	CMD-C2D-C1D	5.78	134.90	124.71
24	C	505	CLA	C2B-C1B-NB	5.78	114.11	110.23
24	B	615	CLA	C4A-NA-C1A	-5.78	104.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	C2B-C1B-NB	5.78	114.10	110.23
24	b	609	CLA	O2D-CGD-CBD	5.77	121.52	111.27
24	A	405	CLA	CMD-C2D-C1D	5.76	134.87	124.71
24	C	513	CLA	C4A-NA-C1A	-5.76	104.11	106.71
24	c	511	CLA	O2D-CGD-CBD	5.75	121.49	111.27
24	B	616	CLA	CMD-C2D-C1D	5.75	134.85	124.71
24	c	508	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	c	512	CLA	CMD-C2D-C1D	5.74	134.84	124.71
24	B	607	CLA	O2D-CGD-CBD	5.74	121.47	111.27
24	B	611	CLA	C4A-NA-C1A	-5.74	104.13	106.71
24	C	510	CLA	C2C-C1C-NC	5.73	115.34	109.97
24	c	514	CLA	O2D-CGD-CBD	5.73	121.45	111.27
24	c	509	CLA	C2B-C1B-NB	5.73	114.07	110.23
24	b	607	CLA	O2D-CGD-CBD	5.73	121.45	111.27
24	B	605	CLA	CHD-C1D-ND	-5.73	119.19	124.45
24	D	403	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
24	c	513	CLA	C2C-C1C-NC	5.72	115.33	109.97
24	B	605	CLA	C4A-NA-C1A	-5.72	104.13	106.71
24	b	620	CLA	CMD-C2D-C1D	5.72	134.79	124.71
24	B	614	CLA	CHD-C1D-ND	-5.71	119.21	124.45
24	B	608	CLA	C4A-NA-C1A	-5.71	104.14	106.71
24	C	503	CLA	C4A-NA-C1A	-5.71	104.14	106.71
24	b	613	CLA	CHD-C1D-ND	-5.70	119.22	124.45
24	a	407	CLA	CHD-C1D-ND	-5.70	119.22	124.45
24	D	404	CLA	CHD-C1D-ND	-5.69	119.22	124.45
24	B	610	CLA	C2B-C1B-NB	5.69	114.05	110.23
24	b	611	CLA	CHD-C1D-ND	-5.69	119.22	124.45
24	C	506	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
24	b	614	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
24	C	505	CLA	O2D-CGD-CBD	5.67	121.34	111.27
24	b	610	CLA	C2C-C1C-NC	5.67	115.28	109.97
24	B	611	CLA	C2C-C1C-NC	5.67	115.28	109.97
24	B	614	CLA	C4A-NA-C1A	-5.67	104.16	106.71
24	c	511	CLA	C2C-C1C-NC	5.66	115.28	109.97
24	D	403	CLA	C2B-C1B-NB	5.66	114.03	110.23
24	B	603	CLA	CHD-C1D-ND	-5.66	119.25	124.45
24	B	604	CLA	C2C-C1C-NC	5.65	115.27	109.97
24	c	503	CLA	O2D-CGD-CBD	5.65	121.31	111.27
24	c	504	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
24	C	502	CLA	CMD-C2D-C1D	5.65	134.66	124.71
24	c	506	CLA	C2C-C1C-NC	5.65	115.26	109.97
24	b	620	CLA	C2C-C1C-NC	5.64	115.25	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	O2D-CGD-CBD	5.64	121.29	111.27
24	C	503	CLA	C2C-C1C-NC	5.64	115.25	109.97
24	B	606	CLA	CHD-C1D-ND	-5.64	119.28	124.45
24	b	616	CLA	CMD-C2D-C1D	5.64	134.65	124.71
24	c	513	CLA	CHD-C1D-ND	-5.63	119.28	124.45
24	c	512	CLA	CHD-C1D-ND	-5.63	119.28	124.45
24	B	611	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
24	B	616	CLA	C2C-C1C-NC	5.62	115.24	109.97
24	b	609	CLA	CHD-C1D-ND	-5.62	119.29	124.45
24	B	611	CLA	CHD-C1D-ND	-5.62	119.29	124.45
24	b	612	CLA	CMD-C2D-C1D	5.60	134.59	124.71
24	b	613	CLA	C2C-C1C-NC	5.60	115.22	109.97
24	b	616	CLA	C2C-C1C-NC	5.59	115.21	109.97
24	C	513	CLA	C2C-C1C-NC	5.59	115.21	109.97
24	B	608	CLA	CMD-C2D-C1D	5.59	134.56	124.71
24	B	607	CLA	CMD-C2D-C1D	5.59	134.56	124.71
24	C	508	CLA	CHD-C1D-ND	-5.58	119.32	124.45
24	C	502	CLA	C2C-C1C-NC	5.58	115.20	109.97
24	B	606	CLA	CMD-C2D-C1D	5.58	134.55	124.71
24	C	507	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
24	C	514	CLA	CMD-C2D-C1D	5.57	134.54	124.71
24	C	504	CLA	CHD-C1D-ND	-5.56	119.34	124.45
24	C	506	CLA	O2D-CGD-CBD	5.55	121.14	111.27
24	B	608	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
24	a	409	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
27	A	411	SQD	O6-C1-C2	5.55	116.97	108.30
24	B	613	CLA	C2C-C1C-NC	5.55	115.17	109.97
24	b	608	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
24	c	513	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
24	c	504	CLA	C2C-C1C-NC	5.53	115.16	109.97
24	B	617	CLA	C2C-C1C-NC	5.53	115.15	109.97
24	B	610	CLA	CHD-C1D-ND	-5.52	119.38	124.45
24	c	509	CLA	CMD-C2D-C1D	5.52	134.44	124.71
24	c	514	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
24	b	615	CLA	C2C-C1C-NC	5.52	115.14	109.97
24	C	510	CLA	CHD-C1D-ND	-5.52	119.38	124.45
24	c	503	CLA	CHD-C4C-C3C	-5.51	116.73	124.84
24	d	402	CLA	CHD-C1D-ND	-5.51	119.39	124.45
24	c	506	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
24	B	617	CLA	CMD-C2D-C1D	5.51	134.43	124.71
24	b	620	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
24	C	512	CLA	C2C-C1C-NC	5.50	115.13	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	619	CLA	C1-C2-C3	-5.50	116.53	126.04
24	c	511	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
24	B	612	CLA	CHD-C1D-ND	-5.49	119.41	124.45
24	c	503	CLA	CHD-C1D-ND	-5.49	119.41	124.45
24	C	514	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
24	c	508	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
24	b	619	CLA	CHD-C1D-ND	-5.48	119.41	124.45
24	C	514	CLA	CHD-C1D-ND	-5.48	119.42	124.45
24	C	509	CLA	CHD-C1D-ND	-5.48	119.42	124.45
24	C	507	CLA	CHD-C1D-ND	-5.47	119.42	124.45
24	C	511	CLA	C2C-C1C-NC	5.47	115.10	109.97
24	c	515	CLA	C2C-C1C-NC	5.46	115.09	109.97
24	B	612	CLA	CMD-C2D-C1D	5.46	134.34	124.71
24	C	510	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
24	C	502	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
24	c	515	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
24	B	607	CLA	C2C-C1C-NC	5.46	115.09	109.97
24	b	619	CLA	O2D-CGD-CBD	5.46	120.96	111.27
24	a	406	CLA	C4A-NA-C1A	-5.46	104.25	106.71
24	c	508	CLA	CHD-C1D-ND	-5.45	119.45	124.45
24	B	603	CLA	C2C-C1C-NC	5.45	115.07	109.97
38	E	103	HEM	CAD-CBD-CGD	5.41	125.25	113.60
24	b	612	CLA	C3C-C4C-NC	5.41	116.64	110.57
24	b	621	CLA	C4A-NA-C1A	-5.40	104.28	106.71
24	C	508	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	C	513	CLA	O2D-CGD-CBD	5.40	120.86	111.27
24	A	406	CLA	C2C-C1C-NC	5.39	115.03	109.97
24	B	609	CLA	C4A-NA-C1A	-5.39	104.28	106.71
24	C	503	CLA	CMD-C2D-C1D	5.39	134.21	124.71
24	c	504	CLA	CHD-C1D-ND	-5.39	119.50	124.45
24	b	613	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
24	c	504	CLA	O2D-CGD-CBD	5.38	120.83	111.27
24	B	615	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	c	505	CLA	CHD-C1D-ND	-5.37	119.52	124.45
24	C	502	CLA	O2D-CGD-CBD	5.37	120.81	111.27
24	b	606	CLA	C4A-NA-C1A	-5.36	104.30	106.71
24	C	514	CLA	C2C-C1C-NC	5.36	115.00	109.97
24	c	510	CLA	C2C-C1C-NC	5.36	114.99	109.97
24	c	504	CLA	CMD-C2D-C1D	5.35	134.15	124.71
24	B	612	CLA	C2C-C1C-NC	5.34	114.98	109.97
27	b	601	SQD	O6-C1-C2	5.34	116.64	108.30
24	c	510	CLA	O2D-CGD-CBD	5.34	120.75	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	619	CLA	CMD-C2D-C1D	5.34	134.12	124.71
24	C	509	CLA	O2D-CGD-CBD	5.33	120.73	111.27
24	a	406	CLA	CHD-C1D-ND	-5.32	119.56	124.45
24	c	509	CLA	CHD-C1D-ND	-5.32	119.56	124.45
25	A	408	PHO	C3D-C4D-ND	5.32	114.97	107.72
24	b	614	CLA	CHD-C1D-ND	-5.32	119.56	124.45
24	b	611	CLA	O2D-CGD-CBD	5.31	120.71	111.27
24	C	508	CLA	C4A-NA-C1A	-5.31	104.32	106.71
24	a	409	CLA	CMD-C2D-C1D	5.31	134.06	124.71
24	B	615	CLA	O2D-CGD-CBD	5.30	120.69	111.27
24	b	608	CLA	CHD-C1D-ND	-5.30	119.58	124.45
24	C	508	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
24	c	514	CLA	C4A-NA-C1A	-5.29	104.33	106.71
24	b	609	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
24	D	404	CLA	O2D-CGD-CBD	5.28	120.65	111.27
24	B	604	CLA	CMD-C2D-C1D	5.28	134.01	124.71
24	C	513	CLA	CMD-C2D-C1D	5.27	134.01	124.71
24	B	610	CLA	C4A-NA-C1A	-5.27	104.33	106.71
24	C	502	CLA	CHD-C1D-ND	-5.27	119.61	124.45
25	A	407	PHO	C3D-C4D-ND	5.27	114.90	107.72
24	b	621	CLA	CHD-C1D-ND	-5.26	119.62	124.45
35	B	631	HTG	C1'-S1-C1	5.26	109.93	100.09
24	c	510	CLA	C4A-NA-C1A	-5.26	104.34	106.71
24	B	608	CLA	CHD-C1D-ND	-5.25	119.63	124.45
24	B	602	CLA	C2C-C1C-NC	5.24	114.88	109.97
24	c	512	CLA	C2C-C1C-NC	5.24	114.88	109.97
24	b	606	CLA	O2D-CGD-CBD	5.24	120.58	111.27
24	B	602	CLA	O2D-CGD-CBD	5.24	120.58	111.27
24	C	509	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
24	c	511	CLA	C4A-NA-C1A	-5.24	104.35	106.71
24	d	402	CLA	O2D-CGD-CBD	5.24	120.57	111.27
24	b	607	CLA	CHD-C1D-ND	-5.24	119.64	124.45
24	d	402	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
25	a	408	PHO	C1C-C2C-C3C	-5.23	104.26	108.61
24	C	511	CLA	C4A-NA-C1A	-5.22	104.36	106.71
24	c	507	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
24	b	618	CLA	C1-C2-C3	-5.20	117.04	126.04
24	C	508	CLA	C3B-C2B-C1B	-5.20	100.88	107.16
24	B	605	CLA	O2D-CGD-CBD	5.20	120.50	111.27
24	b	608	CLA	C2C-C1C-NC	5.20	114.84	109.97
24	b	616	CLA	O2D-CGD-CBD	5.19	120.50	111.27
24	B	604	CLA	CHD-C1D-ND	-5.19	119.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	621	CLA	C3B-C4B-NB	5.19	115.33	110.52
24	b	610	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
24	c	505	CLA	C2C-C1C-NC	5.18	114.83	109.97
24	B	615	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
24	b	609	CLA	C3C-C4C-NC	5.18	116.38	110.57
24	B	614	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
24	B	616	CLA	CHD-C1D-ND	-5.17	119.70	124.45
24	C	511	CLA	O2D-CGD-CBD	5.17	120.45	111.27
24	B	615	CLA	C3B-C2B-C1B	-5.16	100.93	107.16
24	A	405	CLA	C3C-C4C-NC	5.16	116.36	110.57
24	b	621	CLA	O2D-CGD-CBD	5.16	120.43	111.27
24	B	607	CLA	CHD-C1D-ND	-5.15	119.72	124.45
24	A	409	CLA	C2C-C1C-NC	5.14	114.79	109.97
24	b	615	CLA	CMD-C2D-C1D	5.14	133.78	124.71
24	D	403	CLA	C3C-C4C-NC	5.14	116.34	110.57
24	B	616	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
24	B	604	CLA	O2D-CGD-CBD	5.13	120.39	111.27
24	B	610	CLA	C2C-C1C-NC	5.13	114.78	109.97
24	A	406	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
24	d	404	CLA	C2C-C1C-NC	5.13	114.78	109.97
24	b	617	CLA	C3C-C4C-NC	5.12	116.32	110.57
35	c	523	HTG	C1'-S1-C1	5.12	109.67	100.09
24	C	511	CLA	CHD-C1D-ND	-5.11	119.75	124.45
24	c	514	CLA	C2C-C1C-NC	5.11	114.76	109.97
24	b	619	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
24	b	618	CLA	C3C-C4C-NC	5.10	116.29	110.57
24	b	607	CLA	C2C-C1C-NC	5.09	114.74	109.97
24	d	401	CLA	C3B-C4B-NB	5.09	115.24	110.52
24	a	407	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
24	D	404	CLA	C4A-NA-C1A	-5.07	104.42	106.71
24	d	401	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
24	b	613	CLA	O2D-CGD-CBD	5.07	120.28	111.27
24	a	409	CLA	CHD-C1D-ND	-5.07	119.80	124.45
24	b	616	CLA	CHD-C1D-ND	-5.07	119.80	124.45
24	a	407	CLA	C2C-C1C-NC	5.06	114.71	109.97
24	B	605	CLA	C3C-C4C-NC	5.05	116.24	110.57
24	A	409	CLA	C3B-C2B-C1B	-5.05	101.07	107.16
24	B	604	CLA	C3C-C4C-NC	5.05	116.23	110.57
24	B	603	CLA	C3B-C2B-C1B	-5.04	101.07	107.16
24	b	606	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	b	611	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
24	b	616	CLA	C4A-NA-C1A	-5.04	104.44	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	621	CLA	CHD-C4C-C3C	-5.04	117.44	124.84
25	d	403	PHO	C1-C2-C3	-5.03	117.34	126.04
24	B	617	CLA	CHD-C1D-ND	-5.03	119.83	124.45
24	B	611	CLA	O2D-CGD-CBD	5.02	120.19	111.27
24	c	506	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	c	514	CLA	C3B-C2B-C1B	-5.01	101.11	107.16
24	C	503	CLA	O2D-CGD-CBD	5.01	120.17	111.27
24	A	405	CLA	C3B-C2B-C1B	-5.01	101.12	107.16
24	c	504	CLA	C3B-C2B-C1B	-5.01	101.12	107.16
24	B	613	CLA	O2D-CGD-CBD	5.01	120.16	111.27
24	c	509	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	D	404	CLA	C2C-C1C-NC	4.99	114.65	109.97
24	b	612	CLA	CHD-C1D-ND	-4.99	119.87	124.45
24	B	613	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
24	A	405	CLA	CHD-C4C-C3C	-4.98	117.51	124.84
24	B	611	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
24	D	404	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
24	c	509	CLA	C3C-C4C-NC	4.98	116.16	110.57
24	C	513	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
24	c	515	CLA	C3B-C2B-C1B	-4.97	101.16	107.16
24	C	513	CLA	CHD-C1D-ND	-4.97	119.88	124.45
26	D	405	BCR	C24-C23-C22	-4.97	118.73	126.23
24	c	513	CLA	C3B-C2B-C1B	-4.97	101.17	107.16
24	d	404	CLA	C3B-C2B-C1B	-4.97	101.17	107.16
24	c	503	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
24	B	605	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	a	409	CLA	C3B-C2B-C1B	-4.96	101.17	107.16
24	b	611	CLA	C2C-C1C-NC	4.96	114.62	109.97
24	b	617	CLA	C4A-NA-C1A	-4.96	104.48	106.71
24	b	617	CLA	O2D-CGD-CBD	4.96	120.08	111.27
24	b	618	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
24	c	506	CLA	C4A-NA-C1A	-4.96	104.48	106.71
24	c	511	CLA	CHD-C1D-ND	-4.96	119.90	124.45
24	c	508	CLA	C4A-NA-C1A	-4.95	104.48	106.71
24	b	616	CLA	C3C-C4C-NC	4.93	116.10	110.57
24	b	618	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	b	601	SQD	O47-C7-C8	4.93	122.13	111.50
24	C	512	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
24	C	503	CLA	CHD-C1D-ND	-4.93	119.92	124.45
24	c	515	CLA	C4A-NA-C1A	-4.93	104.49	106.71
24	c	505	CLA	O2D-CGD-CBD	4.93	120.03	111.27
24	b	613	CLA	C3B-C2B-C1B	-4.93	101.21	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	b	603	HTG	C1'-S1-C1	4.93	109.30	100.09
24	b	617	CLA	CMD-C2D-C1D	4.92	133.39	124.71
24	c	512	CLA	O2D-CGD-CBD	4.92	120.01	111.27
24	C	509	CLA	CMD-C2D-C1D	4.92	133.38	124.71
24	B	607	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
24	C	514	CLA	C3B-C2B-C1B	-4.92	101.23	107.16
24	B	609	CLA	CHD-C1D-ND	-4.91	119.94	124.45
24	b	607	CLA	CMD-C2D-C1D	4.91	133.36	124.71
24	A	409	CLA	CMD-C2D-C1D	4.91	133.36	124.71
24	C	506	CLA	C4A-NA-C1A	-4.90	104.50	106.71
24	c	510	CLA	C3C-C4C-NC	4.90	116.06	110.57
24	D	401	CLA	CHD-C4C-C3C	-4.89	117.65	124.84
24	b	614	CLA	O2D-CGD-CBD	4.89	119.96	111.27
27	f	101	SQD	O47-C7-C8	4.89	122.03	111.50
24	d	404	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
24	B	609	CLA	CMD-C2D-C1D	4.88	133.32	124.71
24	B	613	CLA	C3C-C4C-NC	4.88	116.05	110.57
24	c	510	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
24	b	607	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
36	D	407	DGD	O2G-C1B-C2B	4.87	122.00	111.50
25	a	408	PHO	C3D-C4D-ND	4.87	114.36	107.72
24	a	406	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
24	D	401	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
24	D	401	CLA	C1C-C2C-C3C	-4.86	101.84	106.96
24	c	503	CLA	C4A-NA-C1A	-4.86	104.52	106.71
35	B	630	HTG	C1'-S1-C1	4.85	109.17	100.09
24	b	619	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
24	c	505	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
24	B	608	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
35	C	522	HTG	C1'-S1-C1	4.84	109.15	100.09
24	c	510	CLA	C3B-C2B-C1B	-4.84	101.31	107.16
40	v	202	HEC	C4B-NB-C1B	4.84	110.08	105.07
24	B	602	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
24	C	504	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
24	b	616	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
35	C	523	HTG	C1-O5-C5	4.83	121.49	112.58
24	B	613	CLA	C3B-C2B-C1B	-4.82	101.35	107.16
40	V	203	HEC	C4B-NB-C1B	4.81	110.05	105.07
25	d	403	PHO	C3D-C4D-ND	4.81	114.28	107.72
27	a	411	SQD	O47-C7-C8	4.81	121.87	111.50
24	b	615	CLA	C4A-NA-C1A	-4.80	104.55	106.71
24	B	610	CLA	C3D-C2D-C1D	-4.80	99.28	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	505	CLA	CHD-C4C-C3C	-4.80	117.79	124.84
24	D	401	CLA	C3B-C2B-C1B	-4.80	101.37	107.16
24	b	615	CLA	CHD-C1D-ND	-4.79	120.05	124.45
24	B	606	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	A	409	CLA	C3D-C4D-ND	4.79	117.98	110.24
24	C	507	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
24	B	614	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
24	B	607	CLA	C3C-C4C-NC	4.78	115.93	110.57
24	C	502	CLA	C4A-NA-C1A	-4.78	104.56	106.71
24	B	603	CLA	O2D-CGD-CBD	4.77	119.75	111.27
24	C	510	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
24	a	409	CLA	O2D-CGD-CBD	4.76	119.73	111.27
24	A	406	CLA	C3D-C4D-ND	4.76	117.94	110.24
24	c	511	CLA	C3B-C2B-C1B	-4.76	101.41	107.16
27	a	411	SQD	O6-C1-C2	4.76	115.73	108.30
24	a	406	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
40	V	203	HEC	CBC-CAC-C3C	4.75	125.52	112.43
24	b	617	CLA	C2C-C1C-NC	4.74	114.42	109.97
24	c	509	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
24	B	617	CLA	C3B-C4B-NB	4.74	114.91	110.52
24	C	505	CLA	C4A-NA-C1A	-4.73	104.58	106.71
24	a	407	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
24	d	401	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	B	612	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
24	c	514	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	C	508	CLA	O2D-CGD-CBD	4.71	119.63	111.27
24	c	506	CLA	O2D-CGD-CBD	4.69	119.61	111.27
24	B	602	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
24	C	505	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
34	c	521	LMG	O7-C10-C11	4.69	121.60	111.50
24	c	503	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
24	C	504	CLA	C3C-C4C-NC	4.68	115.82	110.57
24	b	611	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
38	E	103	HEM	CHC-C4B-NB	4.68	129.50	124.42
24	c	505	CLA	C3C-C4C-NC	4.68	115.82	110.57
35	C	523	HTG	C1'-S1-C1	4.68	108.84	100.09
24	c	508	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
24	b	620	CLA	O2D-CGD-CBD	4.67	119.57	111.27
24	b	615	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
38	e	102	HEM	CAD-CBD-CGD	4.67	123.65	113.60
24	C	502	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
34	C	521	LMG	O7-C10-C11	4.67	121.56	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	611	CLA	C3C-C4C-NC	4.67	115.80	110.57
24	B	611	CLA	C3C-C4C-NC	4.66	115.80	110.57
24	B	609	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
24	C	513	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	613	CLA	CHD-C1D-ND	-4.65	120.18	124.45
24	c	504	CLA	C4A-NA-C1A	-4.65	104.62	106.71
24	d	401	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
24	b	621	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
35	B	624	HTG	O5-C1-C2	4.64	116.15	110.31
24	B	606	CLA	C3C-C4C-NC	4.64	115.77	110.57
24	B	612	CLA	C3D-C2D-C1D	-4.64	99.51	105.83
24	b	610	CLA	C4A-NA-C1A	-4.63	104.62	106.71
24	b	612	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	b	615	CLA	C3C-C4C-NC	4.63	115.77	110.57
24	C	512	CLA	C3B-C2B-C1B	-4.63	101.58	107.16
24	C	508	CLA	C3C-C4C-NC	4.63	115.76	110.57
24	c	510	CLA	CMD-C2D-C1D	4.62	132.86	124.71
24	c	510	CLA	CHD-C1D-ND	-4.62	120.21	124.45
24	B	616	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
24	D	403	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
24	C	506	CLA	C3B-C2B-C1B	-4.60	101.60	107.16
24	b	614	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	c	507	CLA	C3C-C4C-NC	4.60	115.73	110.57
24	B	606	CLA	C3D-C4D-ND	4.59	117.67	110.24
34	C	501	LMG	O7-C10-C11	4.59	121.39	111.50
24	c	512	CLA	C3D-C4D-ND	4.59	117.66	110.24
24	C	503	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
24	B	610	CLA	O2D-CGD-CBD	4.58	119.42	111.27
24	c	506	CLA	C3B-C2B-C1B	-4.58	101.64	107.16
24	B	615	CLA	C3D-C4D-ND	4.58	117.64	110.24
24	A	409	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
24	B	604	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
26	D	405	BCR	C7-C8-C9	-4.57	119.33	126.23
24	d	402	CLA	C3C-C4C-NC	4.57	115.69	110.57
24	b	606	CLA	C3B-C2B-C1B	-4.56	101.65	107.16
26	y	101	BCR	C33-C5-C6	-4.56	119.40	124.53
24	b	620	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	b	607	CLA	C3C-C4C-NC	4.55	115.68	110.57
27	F	101	SQD	O6-C1-C2	4.55	115.41	108.30
24	B	611	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
24	b	609	CLA	C3B-C2B-C1B	-4.54	101.68	107.16
24	b	619	CLA	C3B-C2B-C1B	-4.53	101.70	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	617	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	C	511	CLA	C3B-C2B-C1B	-4.53	101.70	107.16
24	C	503	CLA	C3C-C4C-NC	4.53	115.65	110.57
24	a	407	CLA	O2D-CGD-CBD	4.52	119.31	111.27
24	b	607	CLA	C3D-C4D-ND	4.52	117.55	110.24
24	C	506	CLA	C3C-C4C-NC	4.52	115.64	110.57
24	C	506	CLA	CHD-C1D-ND	-4.52	120.30	124.45
24	C	514	CLA	C3D-C4D-ND	4.52	117.55	110.24
24	B	612	CLA	O2D-CGD-CBD	4.52	119.30	111.27
24	B	609	CLA	C3C-C4C-NC	4.51	115.63	110.57
24	C	507	CLA	O2D-CGD-CBD	4.51	119.28	111.27
24	B	617	CLA	C4A-NA-C1A	-4.51	104.68	106.71
24	b	615	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
24	D	404	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
24	C	502	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
24	C	504	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	c	507	CLA	CHD-C1D-ND	-4.50	120.32	124.45
24	B	610	CLA	C3D-C4D-ND	4.50	117.51	110.24
24	C	514	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	B	616	CLA	C3C-C4C-NC	4.49	115.61	110.57
24	B	614	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
30	b	602	LMT	C1'-O5'-C5'	4.49	122.50	113.69
24	b	610	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
24	C	511	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
24	C	509	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
24	b	612	CLA	O2D-CGD-CBD	4.47	119.22	111.27
24	b	617	CLA	CHD-C1D-ND	-4.47	120.34	124.45
24	A	405	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	B	609	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
24	b	616	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
24	b	612	CLA	C4A-NA-C1A	-4.47	104.70	106.71
24	B	606	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
24	b	608	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
24	B	604	CLA	C3D-C4D-ND	4.46	117.46	110.24
24	D	401	CLA	O2D-CGD-CBD	4.46	119.20	111.27
24	b	609	CLA	C1C-C2C-C3C	-4.46	102.26	106.96
27	l	101	SQD	O47-C7-C8	4.45	121.10	111.50
24	A	406	CLA	C3B-C2B-C1B	-4.45	101.78	107.16
24	c	515	CLA	C3D-C4D-ND	4.45	117.44	110.24
24	A	405	CLA	CHD-C1D-ND	-4.45	120.36	124.45
24	D	404	CLA	C3C-C4C-NC	4.45	115.56	110.57
24	D	404	CLA	C3D-C4D-ND	4.45	117.43	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	615	CLA	O2D-CGD-CBD	4.44	119.16	111.27
24	b	606	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	c	515	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	B	612	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	A	406	CLA	C4A-NA-C1A	-4.44	104.71	106.71
24	B	613	CLA	CAC-C3C-C4C	4.44	130.57	124.81
24	C	503	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
35	B	622	HTG	C1'-S1-C1	4.43	108.38	100.09
24	C	514	CLA	CAC-C3C-C4C	4.43	130.55	124.81
24	c	507	CLA	C3B-C2B-C1B	-4.43	101.82	107.16
24	C	509	CLA	C3D-C4D-ND	4.42	117.39	110.24
24	A	406	CLA	O2D-CGD-CBD	4.41	119.11	111.27
24	C	504	CLA	C3D-C4D-ND	4.41	117.38	110.24
24	b	621	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
24	B	603	CLA	C3C-C4C-NC	4.41	115.52	110.57
24	B	617	CLA	C3C-C4C-NC	4.41	115.51	110.57
24	B	604	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
24	d	404	CLA	C3C-C4C-NC	4.40	115.51	110.57
24	B	607	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
24	B	610	CLA	C3C-C4C-NC	4.40	115.51	110.57
36	d	407	DGD	O2G-C1B-C2B	4.39	120.97	111.50
24	B	604	CLA	C4A-NA-C1A	-4.39	104.73	106.71
24	a	409	CLA	C3D-C4D-ND	4.39	117.34	110.24
24	C	512	CLA	C4A-NA-C1A	-4.39	104.73	106.71
24	d	404	CLA	C3D-C4D-ND	4.39	117.34	110.24
24	C	502	CLA	C3C-C4C-NC	4.39	115.49	110.57
27	A	411	SQD	O47-C7-C8	4.38	120.95	111.50
24	c	511	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
24	A	405	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
24	B	617	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
24	b	610	CLA	O2D-CGD-CBD	4.37	119.04	111.27
24	b	607	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	C	514	CLA	C4A-NA-C1A	-4.36	104.75	106.71
24	a	409	CLA	C3B-C4B-NB	4.35	114.55	110.52
24	c	505	CLA	C1D-CHD-C4C	-4.35	116.68	126.06
24	B	608	CLA	C3C-C4C-NC	4.34	115.44	110.57
24	c	514	CLA	C3D-C4D-ND	4.34	117.25	110.24
24	B	603	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
25	A	408	PHO	C1-C2-C3	-4.33	118.55	126.04
24	A	409	CLA	C3C-C4C-NC	4.33	115.43	110.57
24	B	614	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
24	C	509	CLA	C3D-C2D-C1D	-4.33	99.92	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	603	CLA	C3D-C4D-ND	4.33	117.24	110.24
24	b	613	CLA	C3D-C4D-ND	4.33	117.23	110.24
24	c	504	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
24	b	606	CLA	C3D-C4D-ND	4.32	117.23	110.24
38	e	102	HEM	CHC-C4B-NB	4.32	129.11	124.42
26	Y	101	BCR	C33-C5-C6	-4.32	119.68	124.53
24	b	610	CLA	C3D-C4D-ND	4.32	117.22	110.24
36	C	517	DGD	O2G-C1B-C2B	4.32	120.81	111.50
24	c	513	CLA	C3D-C4D-ND	4.31	117.21	110.24
24	b	618	CLA	C4A-NA-C1A	-4.31	104.77	106.71
26	k	103	BCR	C24-C23-C22	-4.30	119.73	126.23
24	B	607	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
24	B	605	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
24	c	507	CLA	CAC-C3C-C4C	4.29	130.38	124.81
24	d	401	CLA	C3D-C4D-ND	4.29	117.18	110.24
24	b	608	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
24	B	602	CLA	C3C-C4C-NC	4.28	115.37	110.57
24	A	409	CLA	C4A-NA-C1A	-4.28	104.78	106.71
24	C	505	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
24	b	613	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
24	b	620	CLA	C3B-C2B-C1B	-4.28	102.00	107.16
24	b	610	CLA	C3C-C4C-NC	4.28	115.37	110.57
24	B	610	CLA	CMB-C2B-C1B	4.27	131.88	125.37
24	B	612	CLA	C3D-C4D-ND	4.27	117.14	110.24
24	b	610	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
24	C	505	CLA	C3D-C4D-ND	4.26	117.14	110.24
24	B	614	CLA	C3C-C4C-NC	4.26	115.35	110.57
32	A	419	PL9	C32-C33-C34	-4.25	117.42	127.66
24	b	608	CLA	C1D-CHD-C4C	-4.25	116.89	126.06
24	C	510	CLA	C3C-C4C-NC	4.25	115.34	110.57
24	C	514	CLA	C3C-C4C-NC	4.25	115.34	110.57
24	C	513	CLA	C3C-C4C-NC	4.25	115.33	110.57
24	B	609	CLA	C3D-C4D-ND	4.25	117.11	110.24
24	b	618	CLA	C3B-C4B-NB	4.24	114.45	110.52
26	b	622	BCR	C33-C5-C6	-4.24	119.77	124.53
24	B	608	CLA	O2D-CGD-CBD	4.23	118.79	111.27
24	c	512	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
38	E	103	HEM	C4C-NC-C1C	4.23	109.49	105.35
24	c	506	CLA	C3C-C4C-NC	4.23	115.31	110.57
24	C	510	CLA	C3D-C4D-ND	4.23	117.07	110.24
24	c	510	CLA	C3D-C4D-ND	4.22	117.07	110.24
24	c	504	CLA	C3C-C4C-NC	4.22	115.31	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
24	c	503	CLA	O2D-CGD-O1D	-4.21	115.60	123.84
26	D	405	BCR	C38-C26-C25	-4.21	119.80	124.53
24	C	512	CLA	C3C-C4C-NC	4.21	115.29	110.57
24	a	406	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
24	D	401	CLA	C3B-C4B-NB	4.21	114.42	110.52
24	b	619	CLA	C4A-NA-C1A	-4.21	104.81	106.71
24	c	512	CLA	C3B-C4B-NB	4.20	114.42	110.52
24	b	614	CLA	C3D-C4D-ND	4.20	117.04	110.24
24	a	409	CLA	C3C-C4C-NC	4.20	115.28	110.57
24	C	514	CLA	O2D-CGD-CBD	4.20	118.72	111.27
24	B	602	CLA	C3D-C4D-ND	4.19	117.02	110.24
24	d	401	CLA	O2D-CGD-CBD	4.19	118.72	111.27
24	d	401	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
24	b	610	CLA	CMB-C2B-C1B	4.18	131.74	125.37
24	C	511	CLA	C3C-C4C-NC	4.18	115.26	110.57
24	B	613	CLA	C3B-C4B-NB	4.18	114.39	110.52
24	c	511	CLA	C1D-CHD-C4C	-4.18	117.04	126.06
24	C	504	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
24	a	407	CLA	C3D-C4D-ND	4.18	116.99	110.24
24	C	510	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
24	b	619	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
24	c	513	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
24	C	512	CLA	C3D-C4D-ND	4.16	116.97	110.24
24	B	613	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
24	B	608	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
24	a	406	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
24	c	511	CLA	C3B-C4B-NB	4.15	114.37	110.52
24	c	505	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
24	b	617	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
24	c	512	CLA	C3C-C4C-NC	4.15	115.23	110.57
24	c	513	CLA	C4A-NA-C1A	-4.15	104.84	106.71
24	b	619	CLA	C3D-C4D-ND	4.15	116.95	110.24
24	b	611	CLA	C3D-C4D-ND	4.15	116.95	110.24
26	d	405	BCR	C38-C26-C25	-4.15	119.87	124.53
24	b	620	CLA	C3D-C4D-ND	4.15	116.94	110.24
27	a	402	SQD	O47-C7-C8	4.14	120.43	111.50
24	C	503	CLA	C3D-C4D-ND	4.14	116.94	110.24
24	b	613	CLA	C3C-C4C-NC	4.14	115.21	110.57
24	a	409	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
24	b	606	CLA	C3C-C4C-NC	4.14	115.21	110.57
24	b	617	CLA	C3D-C2D-C1D	-4.13	100.19	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
24	c	503	CLA	C3C-C4C-NC	4.13	115.20	110.57
24	C	507	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
24	C	510	CLA	O2D-CGD-O1D	-4.13	115.77	123.84
24	d	402	CLA	C3B-C2B-C1B	-4.12	102.18	107.16
24	C	509	CLA	C3C-C4C-NC	4.12	115.20	110.57
24	B	617	CLA	C3D-C4D-ND	4.12	116.91	110.24
24	c	505	CLA	C3D-C4D-ND	4.12	116.90	110.24
24	A	406	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
24	C	503	CLA	O2D-CGD-O1D	-4.12	115.79	123.84
24	B	606	CLA	CMB-C2B-C1B	4.11	131.64	125.37
26	y	101	BCR	C15-C14-C13	-4.11	121.44	127.31
24	c	503	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
27	b	601	SQD	O7-S-C6	4.10	111.81	106.94
24	b	620	CLA	C3C-C4C-NC	4.10	115.17	110.57
24	b	615	CLA	C3D-C4D-ND	4.10	116.87	110.24
24	b	614	CLA	C3C-C4C-NC	4.09	115.16	110.57
24	b	617	CLA	C3D-C4D-ND	4.09	116.85	110.24
24	C	507	CLA	C4A-NA-C1A	-4.08	104.87	106.71
24	c	511	CLA	C3D-C4D-ND	4.08	116.84	110.24
24	b	616	CLA	C3D-C4D-ND	4.07	116.83	110.24
26	d	405	BCR	C15-C14-C13	-4.07	121.50	127.31
26	H	101	BCR	C38-C26-C25	-4.07	119.96	124.53
24	B	606	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	b	614	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	b	608	CLA	C3C-C4C-NC	4.06	115.12	110.57
24	b	610	CLA	O2D-CGD-O1D	-4.06	115.91	123.84
24	c	513	CLA	O2D-CGD-CBD	4.05	118.47	111.27
24	B	608	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
24	b	621	CLA	C3D-C4D-ND	4.05	116.79	110.24
24	C	505	CLA	C3B-C4B-NB	4.05	114.27	110.52
26	c	516	BCR	C7-C8-C9	-4.05	120.12	126.23
24	C	513	CLA	C3D-C4D-ND	4.05	116.78	110.24
24	C	507	CLA	C3C-C4C-NC	4.05	115.11	110.57
24	c	512	CLA	C3B-C2B-C1B	-4.04	102.28	107.16
24	A	406	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
24	c	506	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
24	b	616	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
24	b	607	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
24	C	505	CLA	CAC-C3C-C4C	4.03	130.04	124.81
24	d	401	CLA	C3C-C4C-NC	4.03	115.09	110.57
24	d	402	CLA	O2D-CGD-O1D	-4.03	115.95	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	C3D-C4D-ND	4.03	116.76	110.24
24	B	610	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
24	b	618	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
24	b	608	CLA	C3D-C4D-ND	4.02	116.75	110.24
24	c	508	CLA	C3B-C4B-NB	4.02	114.25	110.52
24	d	402	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	C	506	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	c	515	CLA	O2D-CGD-CBD	4.02	118.41	111.27
24	d	402	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
24	c	511	CLA	C3C-C4C-NC	4.01	115.07	110.57
24	C	502	CLA	C3D-C4D-ND	4.01	116.73	110.24
24	a	409	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
24	D	401	CLA	C3D-C4D-ND	4.01	116.72	110.24
24	b	616	CLA	CMB-C2B-C1B	4.00	131.47	125.37
24	c	507	CLA	CMB-C2B-C1B	4.00	131.47	125.37
24	B	615	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
24	b	621	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	C	506	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
24	c	513	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
24	c	506	CLA	C3D-C4D-ND	4.00	116.71	110.24
24	c	515	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	C	507	CLA	C3D-C4D-ND	4.00	116.70	110.24
27	F	101	SQD	O47-C7-C8	3.99	120.11	111.50
24	b	612	CLA	C3B-C2B-C1B	-3.99	102.35	107.16
24	C	511	CLA	C3D-C4D-ND	3.98	116.68	110.24
26	C	516	BCR	C7-C8-C9	-3.97	120.24	126.23
24	c	508	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
24	a	407	CLA	C3C-C4C-NC	3.97	115.02	110.57
24	B	605	CLA	CMC-C2C-C1C	3.97	131.08	125.04
24	B	609	CLA	O2D-CGD-CBD	3.97	118.32	111.27
24	b	618	CLA	C1C-C2C-C3C	-3.97	102.79	106.96
36	c	518	DGD	O2G-C1B-C2B	3.96	120.04	111.50
24	B	609	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
24	a	406	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
24	B	607	CLA	CMC-C2C-C1C	3.96	131.06	125.04
34	c	501	LMG	O7-C10-C11	3.95	120.02	111.50
26	C	515	BCR	C33-C5-C6	-3.95	120.09	124.53
24	c	509	CLA	C3D-C4D-ND	3.95	116.63	110.24
24	C	511	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
24	c	508	CLA	C3D-C4D-ND	3.95	116.62	110.24
24	B	606	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
24	B	615	CLA	C3C-C4C-NC	3.94	114.99	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	C3B-C2B-C1B	-3.94	102.41	107.16
40	v	202	HEC	CHB-C1B-NB	3.93	128.69	124.42
24	c	504	CLA	C3D-C4D-ND	3.93	116.60	110.24
24	c	508	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
24	c	503	CLA	C3D-C4D-ND	3.93	116.59	110.24
24	c	508	CLA	C3C-C4C-NC	3.92	114.97	110.57
24	B	609	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
37	E	101	LHG	O7-C7-C8	3.92	119.95	111.50
26	d	405	BCR	C7-C8-C9	-3.92	120.31	126.23
24	b	618	CLA	C3D-C4D-ND	3.92	116.57	110.24
24	a	406	CLA	C3C-C4C-NC	3.91	114.96	110.57
24	b	617	CLA	C4C-C3C-C2C	-3.91	101.20	106.90
24	C	513	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
24	B	604	CLA	C1D-CHD-C4C	-3.90	117.63	126.06
34	Z	101	LMG	O7-C10-C11	3.90	119.92	111.50
24	c	509	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
24	C	508	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
34	C	520	LMG	O8-C28-C29	3.90	124.15	111.91
24	b	619	CLA	C3C-C4C-NC	3.90	114.95	110.57
24	C	512	CLA	O2D-CGD-CBD	3.90	118.20	111.27
24	C	505	CLA	C3B-C2B-C1B	-3.90	102.45	107.16
24	A	406	CLA	C3B-C4B-NB	3.90	114.13	110.52
36	C	518	DGD	O2G-C1B-C2B	3.89	119.89	111.50
24	d	402	CLA	C3B-C4B-NB	3.89	114.13	110.52
24	C	507	CLA	C3B-C4B-NB	3.89	114.13	110.52
24	d	401	CLA	C4A-NA-C1A	-3.89	104.96	106.71
24	B	611	CLA	C3D-C4D-ND	3.89	116.53	110.24
34	c	501	LMG	C7-O1-C1	-3.89	106.15	113.74
24	b	608	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
24	a	407	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
35	B	623	HTG	C1'-S1-C1	3.87	107.33	100.09
24	b	619	CLA	C3B-C4B-NB	3.87	114.11	110.52
24	a	406	CLA	CAC-C3C-C4C	3.87	129.83	124.81
24	b	612	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
24	C	512	CLA	C3B-C4B-NB	3.86	114.10	110.52
27	l	101	SQD	O6-C1-C2	3.86	114.33	108.30
38	e	102	HEM	C4C-NC-C1C	3.86	109.13	105.35
24	d	402	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
24	c	513	CLA	C3B-C4B-NB	3.85	114.09	110.52
24	A	409	CLA	C1C-C2C-C3C	-3.85	102.90	106.96
24	c	504	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
32	a	416	PL9	C15-C14-C16	3.85	121.75	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	611	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
24	b	612	CLA	C3B-C4B-NB	3.84	114.08	110.52
24	D	403	CLA	O2D-CGD-CBD	3.84	118.09	111.27
24	b	613	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	B	613	CLA	C3D-C4D-ND	3.83	116.44	110.24
24	B	614	CLA	C3B-C4B-NB	3.83	114.06	110.52
37	d	409	LHG	O7-C7-C8	3.82	119.74	111.50
24	C	509	CLA	C3B-C4B-NB	3.82	114.06	110.52
27	b	601	SQD	C3-C4-C5	3.82	117.06	110.24
24	c	504	CLA	CMB-C2B-C1B	3.82	131.19	125.37
24	D	403	CLA	C3B-C4B-NB	3.82	114.06	110.52
24	C	504	CLA	O2D-CGD-CBD	3.82	118.06	111.27
26	c	526	BCR	C33-C5-C6	-3.82	120.24	124.53
35	b	604	HTG	C1'-S1-C1	3.82	107.23	100.09
24	C	509	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
24	a	406	CLA	C3B-C4B-NB	3.81	114.05	110.52
24	b	606	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
26	B	618	BCR	C33-C5-C6	-3.81	120.25	124.53
26	C	515	BCR	C7-C8-C9	-3.81	120.48	126.23
26	d	405	BCR	C33-C5-C6	-3.81	120.25	124.53
24	b	611	CLA	CMC-C2C-C1C	3.80	130.83	125.04
24	B	604	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
37	D	409	LHG	O7-C7-C8	3.80	119.69	111.50
24	a	406	CLA	C3D-C4D-ND	3.80	116.38	110.24
24	c	513	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
24	C	511	CLA	C3B-C4B-NB	3.79	114.03	110.52
24	D	403	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	c	510	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	B	615	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
24	B	612	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
34	Z	101	LMG	C1-C2-C3	3.78	117.87	110.00
36	D	407	DGD	C4D-C3D-C2D	3.78	117.42	110.82
24	c	510	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
24	c	512	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	D	403	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
24	B	607	CLA	C3D-C4D-ND	3.76	116.32	110.24
35	b	627	HTG	C1'-S1-C1	3.76	107.12	100.09
24	D	403	CLA	C3D-C4D-ND	3.76	116.31	110.24
24	b	618	CLA	C1D-CHD-C4C	-3.76	117.96	126.06
24	b	610	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
24	B	617	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
24	b	609	CLA	CMC-C2C-C1C	3.75	130.75	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	101	BCR	C33-C5-C6	-3.74	120.32	124.53
24	C	510	CLA	C4A-NA-C1A	-3.74	105.02	106.71
24	b	620	CLA	C3B-C4B-NB	3.74	113.98	110.52
24	C	505	CLA	CMC-C2C-C1C	3.74	130.73	125.04
24	b	608	CLA	O2A-CGA-O1A	-3.74	114.16	123.59
24	C	514	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
24	b	620	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
24	B	603	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
24	b	608	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
24	C	502	CLA	CAC-C3C-C4C	3.73	129.65	124.81
24	A	406	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
24	C	513	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
24	c	504	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
24	b	614	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
24	b	615	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
24	c	511	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
24	c	512	CLA	C4A-NA-C1A	-3.72	105.03	106.71
24	B	612	CLA	C1-C2-C3	-3.72	119.61	126.04
24	b	612	CLA	C3D-C4D-ND	3.72	116.25	110.24
26	T	102	BCR	C33-C5-C6	-3.72	120.35	124.53
36	c	517	DGD	O2G-C1B-C2B	3.72	119.51	111.50
24	B	608	CLA	C3D-C4D-ND	3.71	116.24	110.24
37	e	101	LHG	O7-C7-C8	3.71	119.50	111.50
38	e	102	HEM	CHD-C1D-ND	3.71	128.45	124.42
26	D	405	BCR	C33-C5-C6	-3.71	120.37	124.53
24	C	512	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
24	c	508	CLA	O2D-CGD-CBD	3.70	117.85	111.27
24	B	602	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
24	D	401	CLA	CAA-C2A-C3A	-3.70	102.65	112.78
34	J	101	LMG	O7-C10-C11	3.70	119.47	111.50
24	B	614	CLA	C3D-C4D-ND	3.70	116.22	110.24
40	v	202	HEC	C4C-NC-C1C	3.69	108.97	105.35
24	C	503	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
24	b	614	CLA	C3B-C2B-C1B	-3.69	102.71	107.16
24	B	605	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
24	b	612	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
35	V	204	HTG	C1'-S1-C1	3.68	106.98	100.09
24	B	613	CLA	C4C-C3C-C2C	-3.68	101.53	106.90
24	c	515	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
24	C	510	CLA	C1-C2-C3	-3.68	119.67	126.04
40	V	203	HEC	C4C-NC-C1C	3.68	108.95	105.35
32	A	419	PL9	C27-C28-C29	-3.68	118.80	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	520	LMG	O7-C10-C11	3.67	119.42	111.50
24	C	507	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
24	B	607	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
24	C	512	CLA	C1-O2A-CGA	3.67	126.07	116.44
24	b	621	CLA	CAC-C3C-C4C	3.67	129.57	124.81
24	C	508	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
24	c	511	CLA	CAC-C3C-C4C	3.66	129.56	124.81
24	c	511	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
32	D	406	PL9	C40-C39-C41	3.66	121.42	115.27
24	B	616	CLA	O2D-CGD-CBD	3.65	117.76	111.27
24	B	610	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	B	611	CLA	CAC-C3C-C4C	3.65	129.55	124.81
27	A	416	SQD	O47-C7-C8	3.65	119.37	111.50
24	b	620	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	c	515	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
24	C	502	CLA	O2D-CGD-O1D	-3.64	116.71	123.84
24	B	614	CLA	C1-C2-C3	-3.64	119.75	126.04
24	b	621	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
24	b	606	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	B	609	CLA	C3B-C4B-NB	3.64	113.89	110.52
24	D	403	CLA	C1-C2-C3	-3.64	119.75	126.04
24	C	511	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	C	510	CLA	C3B-C4B-NB	3.64	113.89	110.52
40	V	203	HEC	CHC-C4B-NB	3.64	128.86	124.37
24	b	619	CLA	CAC-C3C-C4C	3.63	129.53	124.81
24	C	509	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
38	e	102	HEM	CHD-C4C-NC	3.63	128.37	124.44
40	v	202	HEC	CHC-C4B-NB	3.63	128.85	124.37
24	D	404	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
24	c	506	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
32	a	416	PL9	C22-C23-C24	-3.63	118.92	127.66
34	B	621	LMG	O7-C10-C11	3.63	119.32	111.50
24	c	511	CLA	C1-C2-C3	-3.62	119.78	126.04
24	C	510	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	a	409	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	c	507	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
24	A	406	CLA	CBC-CAC-C3C	-3.61	102.47	112.43
24	C	506	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	b	615	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
38	E	103	HEM	C1B-NB-C4B	3.61	108.80	105.07
24	d	402	CLA	O2A-CGA-CBA	3.61	123.22	111.91
26	d	405	BCR	C24-C23-C22	-3.60	120.79	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	615	CLA	C4-C3-C5	3.60	121.33	115.27
24	a	409	CLA	CMB-C2B-C1B	3.60	130.86	125.37
24	C	503	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
27	a	411	SQD	C1-O5-C5	-3.60	106.62	113.69
24	B	610	CLA	C3B-C2B-C1B	-3.60	102.81	107.16
34	c	501	LMG	C8-O7-C10	-3.60	108.93	117.79
24	C	502	CLA	C1C-C2C-C3C	-3.60	103.18	106.96
24	d	401	CLA	CHC-C1C-C2C	-3.58	116.77	126.73
24	C	505	CLA	C3C-C4C-NC	3.58	114.59	110.57
24	c	503	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
24	C	505	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
24	A	409	CLA	O2D-CGD-CBD	3.58	117.62	111.27
24	B	602	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
32	a	416	PL9	C17-C18-C19	-3.57	119.06	127.66
24	C	504	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
34	z	101	LMG	O7-C10-C11	3.57	119.19	111.50
24	c	512	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
40	V	203	HEC	CHA-C4D-ND	3.56	128.29	124.42
24	c	507	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
24	B	604	CLA	C3B-C4B-NB	3.56	113.82	110.52
37	d	410	LHG	O7-C7-C8	3.56	119.17	111.50
24	a	409	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
24	B	617	CLA	CAC-C3C-C4C	3.55	129.42	124.81
24	C	505	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
24	B	605	CLA	CMB-C2B-C1B	3.55	130.78	125.37
35	b	628	HTG	O5-C1-C2	3.55	114.78	110.31
24	c	508	CLA	CAC-C3C-C4C	3.55	129.41	124.81
24	b	619	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
24	a	409	CLA	C4A-NA-C1A	-3.55	105.11	106.71
24	c	508	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
24	B	615	CLA	O2A-CGA-O1A	-3.54	114.67	123.59
24	c	506	CLA	C3B-C4B-NB	3.53	113.79	110.52
24	D	404	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
24	A	409	CLA	C4-C3-C5	3.53	121.21	115.27
32	A	419	PL9	C22-C23-C24	-3.53	119.17	127.66
24	D	403	CLA	CED-O2D-CGD	3.53	123.91	115.94
24	b	620	CLA	C4-C3-C5	3.53	121.20	115.27
24	c	504	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
25	A	407	PHO	C1-C2-C3	-3.52	119.95	126.04
26	h	101	BCR	C38-C26-C25	-3.52	120.57	124.53
24	C	506	CLA	C3D-C2D-C1D	-3.52	101.02	105.83
24	B	616	CLA	C3D-C4D-ND	3.52	115.93	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	514	CLA	CMB-C2B-C1B	3.52	130.73	125.37
24	B	608	CLA	CMC-C2C-C1C	3.52	130.40	125.04
24	C	508	CLA	CMC-C2C-C1C	3.52	130.40	125.04
24	d	404	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
24	C	503	CLA	CMB-C2B-C1B	3.51	130.72	125.37
24	c	506	CLA	C4-C3-C5	3.51	121.17	115.27
24	d	404	CLA	CMC-C2C-C1C	3.51	130.38	125.04
27	l	101	SQD	O7-S-C6	3.51	111.11	106.94
24	b	611	CLA	CAC-C3C-C4C	3.51	129.36	124.81
32	a	416	PL9	C32-C33-C34	-3.51	119.22	127.66
27	f	101	SQD	C1-O5-C5	3.50	120.57	113.69
24	b	608	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
36	D	407	DGD	C1D-C2D-C3D	3.50	117.28	110.00
24	B	615	CLA	CAC-C3C-C4C	3.49	129.34	124.81
24	D	404	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
24	A	405	CLA	C3D-C4D-ND	3.49	115.88	110.24
24	C	508	CLA	C3D-C4D-ND	3.49	115.88	110.24
37	l	102	LHG	O7-C7-C8	3.49	119.02	111.50
24	C	506	CLA	CAC-C3C-C4C	3.49	129.33	124.81
24	a	407	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
25	d	403	PHO	O2D-CGD-O1D	-3.48	117.04	123.84
24	C	512	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
24	B	612	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
38	E	103	HEM	CHD-C4C-NC	3.48	128.20	124.44
24	B	616	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
24	B	617	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
24	c	514	CLA	CBC-CAC-C3C	-3.47	102.86	112.43
24	b	607	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
37	D	410	LHG	O7-C7-C8	3.47	118.98	111.50
24	A	405	CLA	CAC-C3C-C4C	3.47	129.31	124.81
24	c	510	CLA	O2D-CGD-O1D	-3.46	117.06	123.84
24	b	608	CLA	C3B-C4B-NB	3.46	113.73	110.52
40	v	202	HEC	CHA-C4D-ND	3.46	128.18	124.42
40	V	203	HEC	CHB-C1B-NB	3.46	128.17	124.42
37	L	101	LHG	O7-C7-C8	3.46	118.95	111.50
34	c	520	LMG	O7-C10-C11	3.46	118.95	111.50
24	b	614	CLA	C3B-C4B-NB	3.45	113.72	110.52
24	C	506	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
24	b	607	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
24	b	613	CLA	C1-C2-C3	-3.44	120.09	126.04
24	b	619	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
26	B	620	BCR	C38-C26-C25	-3.44	120.66	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	509	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
24	d	404	CLA	C3B-C4B-NB	3.44	113.71	110.52
24	c	514	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
37	D	408	LHG	O7-C7-C8	3.43	118.90	111.50
24	D	403	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
24	B	616	CLA	CMB-C2B-C1B	3.43	130.59	125.37
26	t	101	BCR	C33-C5-C6	-3.43	120.68	124.53
24	c	509	CLA	CMB-C2B-C1B	3.42	130.59	125.37
24	b	620	CLA	C1D-CHD-C4C	-3.42	118.67	126.06
24	B	611	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
24	d	404	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
27	A	411	SQD	O8-S-C6	3.42	111.18	105.74
24	C	510	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
24	b	619	CLA	CHC-C1C-C2C	-3.41	117.25	126.73
25	A	408	PHO	C1A-C2A-C3A	-3.41	99.59	102.84
24	b	608	CLA	C4-C3-C5	3.41	121.01	115.27
24	c	505	CLA	CMC-C2C-C1C	3.41	130.23	125.04
25	d	403	PHO	CMB-C2B-C3B	3.41	131.06	124.68
24	C	504	CLA	C3B-C4B-NB	3.41	113.68	110.52
26	b	622	BCR	C7-C8-C9	-3.41	121.08	126.23
24	b	617	CLA	C4-C3-C5	3.41	121.00	115.27
24	B	606	CLA	CMC-C2C-C1C	3.41	130.23	125.04
24	B	603	CLA	CAA-C2A-C3A	-3.41	103.45	112.78
32	A	419	PL9	C37-C38-C39	-3.40	119.46	127.66
24	B	603	CLA	C4-C3-C5	3.40	121.00	115.27
24	a	406	CLA	CHC-C1C-C2C	-3.40	117.30	126.73
24	B	605	CLA	C3D-C4D-ND	3.40	115.73	110.24
24	b	611	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
24	c	507	CLA	C3D-C2D-C1D	-3.39	101.20	105.83
24	d	404	CLA	O2D-CGD-CBD	3.39	117.30	111.27
24	b	621	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
36	h	102	DGD	O2G-C1B-C2B	3.39	118.81	111.50
24	b	617	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
24	B	603	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
24	B	612	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
26	C	515	BCR	C38-C26-C25	-3.38	120.73	124.53
24	c	514	CLA	C3C-C4C-NC	3.38	114.36	110.57
24	D	404	CLA	C3B-C4B-NB	3.38	113.65	110.52
26	Y	101	BCR	C38-C26-C25	-3.38	120.74	124.53
24	B	603	CLA	C3B-C4B-NB	3.37	113.65	110.52
25	A	408	PHO	C4-C3-C5	3.37	120.94	115.27
24	C	502	CLA	C1D-CHD-C4C	-3.37	118.79	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	505	CLA	C4-C3-C5	3.37	120.94	115.27
24	C	514	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
24	b	616	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
24	c	505	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
24	D	401	CLA	CHC-C1C-C2C	-3.37	117.38	126.73
24	B	615	CLA	C3B-C4B-NB	3.37	113.64	110.52
24	c	514	CLA	CMB-C2B-C1B	3.36	130.49	125.37
24	b	620	CLA	CAC-C3C-C4C	3.36	129.17	124.81
30	I	102	LMT	O1B-C4'-C3'	3.36	116.21	107.28
24	c	513	CLA	C3C-C4C-NC	3.36	114.33	110.57
27	f	101	SQD	O7-S-C6	3.35	110.92	106.94
24	c	515	CLA	C3B-C4B-NB	3.35	113.62	110.52
24	B	605	CLA	C3B-C4B-NB	3.35	113.62	110.52
32	a	416	PL9	C37-C38-C39	-3.35	119.60	127.66
40	v	202	HEC	CBC-CAC-C3C	3.35	121.66	112.43
24	B	616	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
24	B	616	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
24	D	401	CLA	CAC-C3C-C4C	3.34	129.15	124.81
24	D	401	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
24	a	406	CLA	O2A-CGA-O1A	-3.34	115.17	123.59
24	B	615	CLA	CMC-C2C-C1C	3.34	130.12	125.04
24	B	615	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
24	b	618	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
24	d	401	CLA	CHB-C1B-NB	-3.33	120.73	124.26
24	B	611	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
24	c	504	CLA	C1-C2-C3	-3.33	120.28	126.04
32	a	416	PL9	C7-C8-C9	-3.33	121.25	126.79
24	b	621	CLA	O2A-CGA-CBA	3.33	122.36	111.91
26	c	516	BCR	C38-C26-C25	-3.33	120.79	124.53
24	c	505	CLA	CAC-C3C-C4C	3.32	129.12	124.81
24	C	509	CLA	O2A-CGA-O1A	-3.32	115.21	123.59
24	C	514	CLA	CMC-C2C-C1C	3.32	130.10	125.04
24	b	607	CLA	CAA-C2A-C3A	-3.32	103.69	112.78
24	B	603	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
24	d	402	CLA	C1-C2-C3	-3.32	120.31	126.04
24	A	405	CLA	CAA-C2A-C3A	-3.32	103.70	112.78
24	B	604	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
24	c	507	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
24	c	513	CLA	C4-C3-C5	3.31	120.84	115.27
24	C	502	CLA	C3B-C4B-NB	3.31	113.58	110.52
24	b	612	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
24	b	614	CLA	CMB-C2B-C1B	3.31	130.41	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	409	CLA	C1-C2-C3	-3.31	120.32	126.04
38	e	102	HEM	C1B-NB-C4B	3.30	108.49	105.07
24	a	409	CLA	C4C-C3C-C2C	-3.30	102.08	106.90
24	b	616	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
25	a	408	PHO	O1D-CGD-CBD	-3.29	119.25	124.74
24	d	401	CLA	CMA-C3A-C2A	-3.29	100.55	113.83
36	D	407	DGD	C1E-O6E-C5E	3.29	120.15	113.69
24	A	405	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
24	B	610	CLA	CHD-C4C-NC	3.29	129.38	124.20
24	b	621	CLA	CHC-C1C-C2C	-3.29	117.60	126.73
24	c	513	CLA	CAC-C3C-C4C	3.29	129.07	124.81
24	c	507	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
24	C	506	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
24	C	513	CLA	C3B-C4B-NB	3.28	113.56	110.52
24	B	611	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
24	D	403	CLA	CMB-C2B-C1B	3.28	130.36	125.37
36	D	407	DGD	C3D-C4D-C5D	3.28	116.09	110.24
32	A	419	PL9	C10-C9-C11	3.28	120.78	115.27
24	C	502	CLA	CMB-C2B-C1B	3.27	130.36	125.37
24	a	407	CLA	CMB-C2B-C1B	3.27	130.35	125.37
32	A	419	PL9	C15-C14-C16	3.27	120.77	115.27
24	c	503	CLA	CMB-C2B-C1B	3.27	130.35	125.37
37	D	408	LHG	O8-C23-O10	-3.27	115.34	123.59
24	b	610	CLA	CMC-C2C-C1C	3.26	130.00	125.04
25	d	403	PHO	C4-C3-C5	3.26	120.76	115.27
24	b	618	CLA	O2D-CGD-CBD	3.26	117.06	111.27
24	B	604	CLA	CAA-C2A-C3A	-3.26	103.86	112.78
24	B	604	CLA	CMC-C2C-C1C	3.26	130.00	125.04
27	a	411	SQD	O8-S-C6	3.26	110.93	105.74
27	a	402	SQD	O48-C23-C24	3.26	122.13	111.91
24	B	612	CLA	CAC-C3C-C4C	3.25	129.03	124.81
24	B	617	CLA	CHC-C1C-C2C	-3.25	117.69	126.73
27	a	411	SQD	C1-C2-C3	-3.25	103.23	110.00
36	C	519	DGD	O3G-C3G-C2G	-3.25	103.07	110.90
32	D	406	PL9	C42-C43-C44	-3.24	119.85	127.66
24	b	611	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	b	608	CLA	CMC-C2C-C1C	3.24	129.98	125.04
24	c	503	CLA	C3B-C4B-NB	3.24	113.52	110.52
24	C	512	CLA	CAC-C3C-C4C	3.24	129.02	124.81
24	D	401	CLA	C3C-C4C-NC	3.24	114.20	110.57
24	B	606	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	a	409	CLA	CHC-C1C-C2C	-3.24	117.73	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	504	CLA	C3B-C4B-NB	3.24	113.52	110.52
24	c	509	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
24	B	612	CLA	C3B-C4B-NB	3.23	113.52	110.52
24	c	508	CLA	CHC-C1C-C2C	-3.23	117.75	126.73
24	A	409	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
24	C	504	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
24	b	612	CLA	CMC-C2C-C1C	3.23	129.95	125.04
34	j	101	LMG	O7-C10-C11	3.22	118.44	111.50
24	b	613	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
25	A	408	PHO	CMB-C2B-C3B	3.22	130.70	124.68
24	C	503	CLA	O2A-CGA-O1A	-3.22	115.47	123.59
24	C	506	CLA	C3B-C4B-NB	3.22	113.50	110.52
24	b	621	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
24	b	607	CLA	C3B-C4B-NB	3.22	113.50	110.52
26	C	516	BCR	C24-C23-C22	-3.22	121.38	126.23
24	C	514	CLA	C1-C2-C3	-3.21	120.48	126.04
27	F	101	SQD	O7-S-C6	3.21	110.76	106.94
24	c	513	CLA	CHC-C1C-C2C	-3.21	117.80	126.73
38	E	103	HEM	CHB-C1B-NB	3.21	128.34	124.37
24	C	509	CLA	CHC-C1C-C2C	-3.21	117.81	126.73
32	a	416	PL9	C20-C19-C21	3.21	120.67	115.27
24	a	406	CLA	O2A-CGA-CBA	3.21	121.98	111.91
24	b	610	CLA	O2A-CGA-O1A	-3.21	115.49	123.59
40	V	203	HEC	CHA-C1A-NA	3.21	127.91	124.44
24	C	509	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
24	b	614	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
25	A	407	PHO	C1A-C2A-C3A	-3.20	99.79	102.84
24	C	506	CLA	CMB-C2B-C1B	3.20	130.25	125.37
24	b	615	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
24	C	514	CLA	C3B-C4B-NB	3.20	113.48	110.52
24	d	402	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
24	c	506	CLA	CAC-C3C-C4C	3.20	128.96	124.81
24	b	608	CLA	O2A-CGA-CBA	3.20	121.94	111.91
24	b	610	CLA	CHD-C4C-NC	3.19	129.24	124.20
24	C	511	CLA	C1-C2-C3	-3.19	120.52	126.04
24	A	405	CLA	O2D-CGD-CBD	3.19	116.93	111.27
24	b	615	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
24	c	515	CLA	CAC-C3C-C4C	3.19	128.94	124.81
24	b	617	CLA	C1-C2-C3	-3.19	120.53	126.04
32	a	416	PL9	C30-C29-C31	3.19	120.63	115.27
24	b	609	CLA	C3D-C4D-ND	3.18	115.39	110.24
24	C	507	CLA	CAC-C3C-C4C	3.18	128.94	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	C3B-C4B-NB	3.18	113.47	110.52
24	b	606	CLA	CHD-C4C-NC	3.18	129.22	124.20
24	D	404	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
24	B	613	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	B	614	CLA	CHC-C1C-C2C	-3.18	117.90	126.73
24	B	614	CLA	CED-O2D-CGD	3.18	123.13	115.94
32	A	419	PL9	C7-C8-C9	-3.18	121.50	126.79
32	a	416	PL9	C10-C9-C11	3.18	120.61	115.27
24	b	617	CLA	C3B-C4B-NB	3.18	113.46	110.52
24	b	607	CLA	CAC-C3C-C4C	3.18	128.93	124.81
24	c	509	CLA	CAC-C3C-C4C	3.17	128.93	124.81
24	D	401	CLA	CBC-CAC-C3C	-3.17	103.68	112.43
24	B	608	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
24	C	512	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
32	a	416	PL9	C27-C28-C29	-3.16	120.05	127.66
24	c	512	CLA	CMC-C2C-C1C	3.16	129.85	125.04
24	b	619	CLA	CMB-C2B-C1B	3.16	130.18	125.37
26	d	405	BCR	C3-C4-C5	-3.16	108.44	114.08
24	A	406	CLA	CAA-C2A-C3A	-3.16	104.14	112.78
24	C	509	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	C	502	CLA	CMC-C2C-C1C	3.15	129.84	125.04
24	B	614	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	B	605	CLA	C1-C2-C3	-3.15	120.59	126.04
24	B	603	CLA	CHC-C1C-C2C	-3.15	117.98	126.73
24	D	401	CLA	C4A-NA-C1A	-3.15	105.29	106.71
24	A	405	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
27	a	411	SQD	C45-O47-C7	-3.15	110.04	117.79
27	A	416	SQD	O48-C23-C24	3.15	121.78	111.91
24	b	617	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
32	a	416	PL9	C42-C43-C44	-3.14	120.11	127.66
24	B	611	CLA	C1D-CHD-C4C	-3.13	119.30	126.06
24	B	612	CLA	CMB-C2B-C1B	3.13	130.14	125.37
24	a	407	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
24	B	612	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
24	C	512	CLA	C4-C3-C5	3.13	120.53	115.27
24	c	509	CLA	C4A-NA-C1A	-3.13	105.30	106.71
24	b	613	CLA	O2A-CGA-CBA	3.13	121.72	111.91
24	B	611	CLA	C1-C2-C3	-3.13	120.64	126.04
26	k	103	BCR	C33-C5-C6	-3.13	121.02	124.53
27	b	601	SQD	O48-C23-C24	3.12	121.71	111.91
24	a	407	CLA	CAA-C2A-C3A	-3.12	104.23	112.78
24	b	609	CLA	CAC-C3C-C4C	3.12	128.86	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
32	A	419	PL9	C20-C19-C21	3.12	120.51	115.27
24	C	507	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
36	H	102	DGD	O2G-C1B-C2B	3.11	118.21	111.50
24	B	607	CLA	C3B-C4B-NB	3.11	113.40	110.52
24	a	406	CLA	CAA-C2A-C3A	-3.11	104.26	112.78
24	B	603	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
24	C	512	CLA	CMB-C2B-C1B	3.11	130.10	125.37
38	e	102	HEM	CBA-CAA-C2A	-3.11	103.99	112.63
24	c	505	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
30	I	102	LMT	C1B-O5B-C5B	3.11	119.79	113.69
24	d	404	CLA	CAC-C3C-C4C	3.11	128.84	124.81
26	H	101	BCR	C7-C8-C9	-3.10	121.55	126.23
37	e	101	LHG	O8-C23-C24	3.10	121.64	111.91
24	C	503	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	c	506	CLA	CMC-C2C-C1C	3.10	129.76	125.04
24	C	510	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	B	617	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	b	610	CLA	C4-C3-C5	3.10	120.48	115.27
34	Z	101	LMG	C7-O1-C1	-3.10	107.69	113.74
24	c	511	CLA	CHB-C1B-NB	-3.10	120.98	124.26
24	B	605	CLA	O2A-CGA-O1A	-3.10	115.78	123.59
24	A	409	CLA	CHD-C4C-NC	3.10	129.08	124.20
24	B	602	CLA	C4C-C3C-C2C	-3.10	102.39	106.90
24	a	409	CLA	CAC-C3C-C4C	3.09	128.82	124.81
24	d	401	CLA	C1D-CHD-C4C	-3.09	119.39	126.06
24	B	609	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
24	b	615	CLA	C3B-C4B-NB	3.09	113.38	110.52
24	C	514	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
24	D	404	CLA	CMB-C2B-C1B	3.08	130.07	125.37
24	D	403	CLA	O2A-CGA-CBA	3.08	121.58	111.91
24	c	508	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
24	a	409	CLA	C4-C3-C5	3.08	120.45	115.27
27	A	411	SQD	C1-C2-C3	-3.08	103.58	110.00
32	a	416	PL9	C7-C3-C4	3.08	119.38	116.88
24	B	609	CLA	CMA-C3A-C4A	-3.07	103.51	111.77
24	B	617	CLA	C1C-C2C-C3C	-3.07	103.72	106.96
24	b	616	CLA	C3B-C4B-NB	3.07	113.36	110.52
24	b	612	CLA	CAA-C2A-C3A	-3.07	104.37	112.78
24	a	407	CLA	CAC-C3C-C4C	3.07	128.79	124.81
35	C	523	HTG	O5-C5-C4	3.07	115.26	109.69
24	B	613	CLA	O2D-CGD-O1D	-3.07	117.84	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	CMC-C2C-C1C	3.06	129.71	125.04
37	d	408	LHG	O7-C7-C8	3.06	118.11	111.50
24	C	502	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
24	b	618	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
24	c	504	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
24	c	504	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
24	b	610	CLA	C3B-C4B-NB	3.05	113.35	110.52
24	c	510	CLA	C4C-C3C-C2C	-3.05	102.44	106.90
24	B	616	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
24	c	513	CLA	C1-C2-C3	-3.05	120.77	126.04
24	b	620	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
24	b	620	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
24	b	616	CLA	CAC-C3C-C4C	3.05	128.76	124.81
24	A	409	CLA	CMC-C2C-C1C	3.05	129.68	125.04
24	A	406	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
24	B	615	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
24	D	403	CLA	CMC-C2C-C1C	3.04	129.68	125.04
26	K	101	BCR	C20-C21-C22	-3.04	122.97	127.31
24	b	611	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
24	C	508	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
26	k	103	BCR	C38-C26-C25	-3.04	121.11	124.53
24	B	613	CLA	C1D-CHD-C4C	-3.04	119.50	126.06
24	B	615	CLA	O2A-CGA-CBA	3.04	121.44	111.91
35	O	303	HTG	C1'-S1-C1	3.04	105.77	100.09
24	c	512	CLA	C4-C3-C5	3.04	120.38	115.27
35	B	624	HTG	C1-C2-C3	3.04	116.58	110.59
27	A	411	SQD	C45-O47-C7	-3.04	110.32	117.79
24	C	509	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
26	c	526	BCR	C15-C14-C13	-3.03	122.98	127.31
24	B	610	CLA	C3B-C4B-NB	3.03	113.33	110.52
24	B	608	CLA	C3B-C4B-NB	3.03	113.32	110.52
24	c	507	CLA	C3B-C4B-NB	3.03	113.32	110.52
24	C	506	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
24	c	513	CLA	CHD-C4C-NC	3.03	128.97	124.20
26	A	410	BCR	C33-C5-C6	-3.03	121.13	124.53
24	A	406	CLA	CAC-C3C-C4C	3.03	128.74	124.81
24	B	607	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
24	b	616	CLA	C1-C2-C3	-3.02	120.82	126.04
32	A	419	PL9	C42-C43-C44	-3.02	120.39	127.66
34	Z	101	LMG	O6-C1-C2	3.02	116.74	110.35
24	b	608	CLA	CAC-C3C-C4C	3.02	128.73	124.81
24	c	510	CLA	C3B-C4B-NB	3.02	113.31	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	403	CLA	CAC-C3C-C4C	3.02	128.72	124.81
24	c	514	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
24	C	514	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	D	404	CLA	CAC-C3C-C4C	3.01	128.72	124.81
24	B	611	CLA	CAA-C2A-C3A	-3.01	104.53	112.78
24	b	607	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
24	A	406	CLA	C3C-C4C-NC	3.01	113.94	110.57
24	C	507	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
24	B	616	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
24	b	606	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
24	c	513	CLA	CMC-C2C-C1C	3.00	129.62	125.04
30	I	102	LMT	C1'-O5'-C5'	3.00	119.59	113.69
32	d	406	PL9	C10-C9-C11	3.00	120.32	115.27
24	b	617	CLA	C2A-C1A-CHA	-3.00	118.61	123.86
24	B	608	CLA	C4-C3-C5	3.00	120.32	115.27
24	b	609	CLA	CMB-C2B-C1B	3.00	129.94	125.37
24	b	613	CLA	CAC-C3C-C4C	3.00	128.70	124.81
24	C	512	CLA	CHC-C1C-C2C	-2.99	118.41	126.73
24	B	610	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
24	C	510	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
40	V	203	HEC	CHD-C1D-ND	2.99	128.06	124.37
24	d	402	CLA	O2A-CGA-O1A	-2.99	116.05	123.59
24	c	508	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	b	607	CLA	C4-C3-C5	2.99	120.30	115.27
24	b	609	CLA	C1D-CHD-C4C	-2.99	119.61	126.06
24	D	401	CLA	O2A-CGA-O1A	-2.99	116.06	123.59
24	b	616	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
24	B	606	CLA	C3B-C4B-NB	2.98	113.28	110.52
24	c	514	CLA	CHD-C4C-NC	2.98	128.91	124.20
32	d	406	PL9	C40-C39-C41	2.98	120.29	115.27
26	c	516	BCR	C31-C1-C6	-2.98	105.46	110.30
24	c	503	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
34	b	625	LMG	O8-C28-C29	2.98	121.26	111.91
24	c	509	CLA	CMC-C2C-C1C	2.98	129.57	125.04
24	b	614	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
32	A	419	PL9	C25-C24-C26	2.98	120.28	115.27
24	d	402	CLA	C4-C3-C5	2.97	120.28	115.27
40	v	202	HEC	CBB-CAB-C3B	2.97	120.63	112.43
24	B	611	CLA	O2A-CGA-CBA	2.97	121.24	111.91
26	A	410	BCR	C15-C14-C13	-2.97	123.07	127.31
24	B	610	CLA	C1-C2-C3	-2.97	120.90	126.04
37	D	408	LHG	O8-C23-C24	2.97	121.23	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	503	CLA	C1-C2-C3	-2.97	120.91	126.04
24	d	402	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	b	612	CLA	CHC-C1C-C2C	-2.97	118.48	126.73
24	d	404	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	A	405	CLA	CAA-C2A-C1A	-2.97	102.25	111.97
24	C	508	CLA	CHD-C4C-NC	2.96	128.87	124.20
24	b	612	CLA	CMB-C2B-C1B	2.96	129.88	125.37
27	f	101	SQD	O5-C5-C4	2.96	115.07	109.69
27	b	601	SQD	C44-O6-C1	-2.96	107.96	113.74
24	B	609	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
24	c	515	CLA	CMC-C2C-C1C	2.96	129.54	125.04
24	C	507	CLA	C4-C3-C5	2.95	120.24	115.27
24	A	406	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
26	D	405	BCR	C28-C27-C26	-2.95	108.81	114.08
24	c	511	CLA	CHC-C1C-C2C	-2.95	118.54	126.73
24	d	404	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
37	D	409	LHG	O8-C23-O10	-2.95	116.16	123.59
24	b	613	CLA	C3B-C4B-NB	2.95	113.25	110.52
24	c	509	CLA	C3B-C4B-NB	2.94	113.25	110.52
24	d	402	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
24	c	503	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
38	e	102	HEM	C4A-NA-C1A	2.94	108.23	105.35
24	C	511	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
32	D	406	PL9	C53-C6-C1	2.94	121.00	114.99
24	A	405	CLA	C3B-C4B-NB	2.94	113.24	110.52
26	B	620	BCR	C24-C23-C22	-2.94	121.80	126.23
40	v	202	HEC	C1D-ND-C4D	2.93	108.10	105.07
24	a	407	CLA	CBC-CAC-C3C	-2.93	104.34	112.43
24	d	401	CLA	C2A-C1A-CHA	-2.93	118.73	123.86
24	B	610	CLA	CHC-C1C-C2C	-2.93	118.59	126.73
24	a	409	CLA	CHB-C1B-NB	-2.93	121.16	124.26
24	b	606	CLA	C4-C3-C5	2.93	120.20	115.27
24	B	607	CLA	C1-O2A-CGA	2.93	124.13	116.44
24	B	605	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
36	c	519	DGD	O2G-C1B-C2B	2.93	117.81	111.50
24	b	615	CLA	CAC-C3C-C4C	2.93	128.61	124.81
24	b	613	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	d	404	CLA	C4-C3-C5	2.93	120.19	115.27
24	A	409	CLA	C2A-C1A-CHA	-2.93	118.74	123.86
24	c	511	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	b	614	CLA	CMC-C2C-C1C	2.92	129.49	125.04
36	c	519	DGD	O1G-C1A-C2A	2.92	121.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	CAA-C2A-C3A	-2.92	104.77	112.78
26	Y	101	BCR	C15-C14-C13	-2.92	123.14	127.31
24	b	616	CLA	CHD-C4C-NC	2.92	128.81	124.20
27	A	411	SQD	C44-O6-C1	-2.92	108.03	113.74
25	A	407	PHO	CMA-C3A-C4A	-2.92	107.98	114.38
24	A	405	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
24	B	604	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
24	B	612	CLA	CMC-C2C-C1C	2.92	129.49	125.04
24	B	606	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	B	602	CLA	C3B-C4B-NB	2.92	113.22	110.52
24	b	618	CLA	CMB-C2B-C1B	2.92	129.81	125.37
24	d	402	CLA	CHC-C1C-C2C	-2.92	118.63	126.73
24	B	614	CLA	C4-C3-C5	2.92	120.18	115.27
24	C	502	CLA	CBC-CAC-C3C	-2.91	104.39	112.43
27	l	101	SQD	O8-S-C6	2.91	110.39	105.74
24	c	515	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	C	514	CLA	C4-C3-C5	2.91	120.17	115.27
26	Y	101	BCR	C16-C17-C18	-2.91	123.15	127.31
24	c	509	CLA	O2A-CGA-CBA	2.91	121.05	111.91
26	B	619	BCR	C29-C30-C25	2.91	114.96	110.48
24	B	607	CLA	C4-C3-C5	2.91	120.17	115.27
24	C	504	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
24	A	405	CLA	CMC-C2C-C1C	2.91	129.47	125.04
24	c	512	CLA	CHD-C4C-NC	2.91	128.79	124.20
24	b	616	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
32	d	406	PL9	C7-C8-C9	-2.91	121.95	126.79
24	c	509	CLA	CHC-C1C-C2C	-2.91	118.66	126.73
24	A	409	CLA	CMB-C2B-C1B	2.91	129.80	125.37
24	A	409	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	c	503	CLA	CAC-C3C-C4C	2.91	128.58	124.81
24	B	611	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
24	C	510	CLA	CHB-C1B-NB	-2.90	121.18	124.26
32	A	419	PL9	C53-C6-C1	2.90	120.93	114.99
24	C	513	CLA	C1-C2-C3	-2.90	121.02	126.04
24	c	505	CLA	CMB-C2B-C1B	2.90	129.79	125.37
24	c	506	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
24	B	608	CLA	C1-O2A-CGA	2.89	124.03	116.44
27	A	411	SQD	C1-O5-C5	-2.89	108.01	113.69
24	C	508	CLA	C4-C3-C5	2.89	120.14	115.27
24	d	401	CLA	CAC-C3C-C4C	2.89	128.56	124.81
24	C	511	CLA	C4-C3-C5	2.89	120.13	115.27
24	A	406	CLA	CHD-C4C-NC	2.89	128.76	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	C4-C3-C5	2.89	120.13	115.27
24	B	607	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
26	C	515	BCR	C16-C17-C18	-2.88	123.19	127.31
24	c	507	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
26	b	624	BCR	C38-C26-C25	-2.88	121.29	124.53
24	B	608	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
24	b	608	CLA	CMA-C3A-C2A	-2.88	102.21	113.83
24	B	615	CLA	CHD-C4C-NC	2.88	128.74	124.20
24	b	615	CLA	O2A-CGA-CBA	2.88	120.94	111.91
24	b	609	CLA	C1-C2-C3	-2.87	121.07	126.04
24	a	407	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
26	K	101	BCR	C37-C22-C21	-2.87	118.90	122.92
24	B	612	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
24	C	513	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
24	b	619	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	b	610	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
24	c	515	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
24	A	406	CLA	C1-C2-C3	-2.87	121.08	126.04
24	C	511	CLA	CAC-C3C-C4C	2.87	128.53	124.81
24	b	617	CLA	O2A-CGA-CBA	2.87	120.91	111.91
24	b	607	CLA	C1-C2-C3	-2.87	121.08	126.04
24	a	407	CLA	CHD-C4C-NC	2.87	128.72	124.20
32	d	406	PL9	C7-C3-C4	-2.86	114.55	116.88
24	C	508	CLA	CAC-C3C-C4C	2.86	128.53	124.81
24	c	515	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
24	b	621	CLA	CHB-C1B-NB	-2.86	121.23	124.26
24	A	406	CLA	C4-C3-C5	2.86	120.08	115.27
36	c	518	DGD	C2G-O2G-C1B	-2.86	110.75	117.79
24	c	514	CLA	O2A-CGA-CBA	2.86	120.88	111.91
26	y	101	BCR	C28-C27-C26	-2.86	108.97	114.08
32	d	406	PL9	C53-C6-C1	2.86	120.83	114.99
24	d	401	CLA	C4C-C3C-C2C	-2.86	102.74	106.90
24	c	512	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
26	b	622	BCR	C15-C14-C13	-2.85	123.24	127.31
24	B	607	CLA	CHD-C4C-NC	2.85	128.70	124.20
24	b	606	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	b	609	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
24	b	608	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
40	v	202	HEC	CHA-C1A-NA	2.85	127.52	124.44
24	d	401	CLA	CAA-C2A-C3A	-2.85	104.99	112.78
24	B	610	CLA	CMA-C3A-C4A	-2.84	104.14	111.77
26	h	101	BCR	C16-C17-C18	-2.84	123.25	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	CAC-C3C-C4C	2.84	128.49	124.81
24	B	605	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
24	B	613	CLA	CMC-C2C-C1C	2.84	129.36	125.04
27	a	411	SQD	C44-O6-C1	-2.84	108.20	113.74
32	a	416	PL9	C53-C6-C1	2.83	120.78	114.99
24	D	404	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
24	C	507	CLA	CBC-CAC-C3C	-2.83	104.63	112.43
25	d	403	PHO	C1A-C2A-C3A	-2.83	100.15	102.84
30	A	417	LMT	O5'-C5'-C4'	2.83	115.72	109.75
24	b	609	CLA	O1D-CGD-CBD	-2.83	118.70	124.48
24	B	614	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
24	C	507	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
26	b	624	BCR	C37-C22-C23	2.82	122.53	118.08
37	L	101	LHG	O8-C23-C24	2.82	120.77	111.91
24	B	607	CLA	CAC-C3C-C4C	2.82	128.47	124.81
26	T	102	BCR	C29-C28-C27	-2.82	105.07	111.38
38	E	103	HEM	CBD-CAD-C3D	-2.82	104.79	112.63
24	a	407	CLA	O2A-CGA-CBA	2.82	120.76	111.91
24	C	511	CLA	CHD-C4C-NC	2.82	128.65	124.20
37	d	410	LHG	O8-C23-C24	2.82	120.75	111.91
24	c	512	CLA	CBC-CAC-C3C	-2.82	104.66	112.43
27	F	101	SQD	O9-S-C6	2.82	110.29	106.94
34	Z	101	LMG	C4-C3-C2	2.82	115.74	110.82
24	B	616	CLA	CAC-C3C-C4C	2.82	128.46	124.81
24	C	505	CLA	CHC-C1C-C2C	-2.81	118.91	126.73
24	b	613	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	B	605	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
24	b	616	CLA	CMC-C2C-C1C	2.81	129.32	125.04
25	A	407	PHO	O1D-CGD-CBD	-2.81	120.06	124.74
36	c	517	DGD	C2G-O2G-C1B	-2.81	110.88	117.79
24	C	510	CLA	CAC-C3C-C4C	2.81	128.45	124.81
25	A	408	PHO	O2D-CGD-O1D	-2.81	118.35	123.84
24	C	504	CLA	C4-C3-C5	2.80	119.99	115.27
27	b	601	SQD	O47-C7-O49	-2.80	116.93	123.70
40	V	203	HEC	C1D-ND-C4D	2.80	107.97	105.07
24	b	617	CLA	CAC-C3C-C4C	2.80	128.44	124.81
24	b	606	CLA	O2A-CGA-CBA	2.80	120.70	111.91
24	B	606	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
24	c	506	CLA	CMB-C2B-C1B	2.80	129.63	125.37
24	B	615	CLA	CBC-CAC-C3C	-2.80	104.72	112.43
32	A	419	PL9	C8-C7-C3	2.80	119.89	111.98
24	B	606	CLA	CHD-C4C-NC	2.80	128.61	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	503	CLA	O2A-CGA-CBA	2.80	120.69	111.91
24	a	407	CLA	C1-C2-C3	-2.79	121.21	126.04
24	C	509	CLA	O2A-CGA-CBA	2.79	120.68	111.91
24	b	613	CLA	CMC-C2C-C1C	2.79	129.29	125.04
24	b	620	CLA	CMB-C2B-C1B	2.79	129.62	125.37
24	c	503	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
24	C	509	CLA	C1-C2-C3	-2.79	121.22	126.04
24	b	606	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
24	B	605	CLA	C4-C3-C5	2.79	119.97	115.27
24	D	403	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
24	B	609	CLA	CHD-C4C-NC	2.79	128.60	124.20
25	a	408	PHO	CMA-C3A-C4A	-2.79	108.27	114.38
24	d	401	CLA	CMB-C2B-C1B	2.79	129.62	125.37
24	c	514	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
24	C	513	CLA	C4-C3-C5	2.79	119.96	115.27
24	c	509	CLA	C4-C3-C5	2.79	119.96	115.27
38	E	103	HEM	CMD-C2D-C1D	2.78	129.28	125.04
24	C	503	CLA	CAC-C3C-C4C	2.78	128.42	124.81
24	B	608	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
24	b	615	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
24	b	617	CLA	CMB-C2B-C1B	2.78	129.61	125.37
24	a	406	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
24	b	612	CLA	C4-C3-C5	2.78	119.95	115.27
24	C	513	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
24	B	604	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
34	z	101	LMG	O8-C28-C29	2.78	120.63	111.91
24	D	401	CLA	CHB-C1B-NB	-2.78	121.31	124.26
24	b	618	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	c	508	CLA	CBC-CAC-C3C	-2.77	104.78	112.43
26	h	101	BCR	C11-C10-C9	-2.77	123.35	127.31
24	a	406	CLA	CAA-C2A-C1A	-2.77	102.89	111.97
24	B	608	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
24	B	612	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	c	509	CLA	O2A-CGA-O1A	-2.77	116.60	123.59
24	C	513	CLA	CMC-C2C-C1C	2.77	129.26	125.04
24	B	604	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
24	b	617	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
24	a	409	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
37	d	408	LHG	O8-C23-C24	2.77	120.59	111.91
24	a	407	CLA	CMC-C2C-C1C	2.77	129.25	125.04
24	B	602	CLA	CHD-C4C-NC	2.76	128.56	124.20
24	b	619	CLA	O2A-CGA-CBA	2.76	120.58	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	F	101	SQD	C3-C4-C5	2.76	115.17	110.24
24	b	612	CLA	CAC-C3C-C4C	2.76	128.40	124.81
24	B	615	CLA	CHC-C1C-C2C	-2.76	119.05	126.73
24	B	602	CLA	O2A-CGA-CBA	2.76	120.58	111.91
24	c	506	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
24	b	609	CLA	C3B-C4B-NB	2.76	113.08	110.52
26	T	102	BCR	C2-C1-C6	2.76	114.73	110.48
34	j	101	LMG	O8-C28-O10	-2.76	116.63	123.59
24	C	514	CLA	CHC-C1C-C2C	-2.76	119.08	126.73
34	b	625	LMG	O7-C10-C11	2.75	117.44	111.50
24	b	616	CLA	C2A-C1A-CHA	-2.75	119.04	123.86
24	B	608	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
26	c	516	BCR	C15-C14-C13	-2.75	123.38	127.31
24	B	606	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
24	C	502	CLA	CHC-C1C-C2C	-2.75	119.09	126.73
24	b	618	CLA	C4-C3-C5	2.75	119.90	115.27
26	y	101	BCR	C16-C17-C18	-2.75	123.39	127.31
24	C	503	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
24	b	621	CLA	C1-C2-C3	-2.75	121.29	126.04
24	C	502	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
24	C	504	CLA	CAC-C3C-C4C	2.74	128.37	124.81
24	c	514	CLA	CMC-C2C-C1C	2.74	129.22	125.04
24	b	614	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
24	B	602	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
24	C	508	CLA	CMB-C2B-C1B	2.74	129.54	125.37
32	a	416	PL9	C25-C24-C26	2.74	119.88	115.27
37	D	410	LHG	O8-C23-C24	2.74	120.51	111.91
24	b	607	CLA	CMB-C2B-C1B	2.74	129.54	125.37
24	B	611	CLA	C4-C3-C5	2.74	119.88	115.27
24	c	513	CLA	CBC-CAC-C3C	-2.74	104.89	112.43
37	L	101	LHG	C6-C5-C4	-2.74	105.32	111.79
24	A	409	CLA	CAA-C2A-C3A	-2.73	105.29	112.78
24	C	514	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
24	b	610	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
24	c	514	CLA	C3B-C4B-NB	2.73	113.05	110.52
24	C	503	CLA	CMC-C2C-C1C	2.73	129.20	125.04
24	b	611	CLA	C3B-C4B-NB	2.73	113.05	110.52
27	f	101	SQD	O48-C23-C24	2.73	120.47	111.91
24	b	610	CLA	OBD-CAD-C3D	-2.73	121.96	128.52
27	A	416	SQD	C3-C4-C5	2.73	115.10	110.24
26	D	405	BCR	C15-C14-C13	-2.73	123.42	127.31
24	B	609	CLA	O2A-CGA-CBA	2.73	120.46	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	613	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
24	b	610	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
26	Y	101	BCR	C37-C22-C23	2.72	122.36	118.08
24	B	613	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
24	D	404	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
24	B	602	CLA	C1-C2-C3	-2.72	121.34	126.04
24	c	505	CLA	C3B-C4B-NB	2.72	113.04	110.52
36	C	517	DGD	O1G-C1A-O1A	-2.72	116.74	123.59
24	C	511	CLA	CHC-C1C-C2C	-2.72	119.19	126.73
24	b	607	CLA	CHC-C1C-C2C	-2.72	119.19	126.73
24	c	510	CLA	CMC-C2C-C1C	2.71	129.17	125.04
24	c	512	CLA	CHC-C1C-C2C	-2.71	119.19	126.73
24	b	606	CLA	C2A-C1A-CHA	-2.71	119.11	123.86
26	b	623	BCR	C38-C26-C25	-2.71	121.48	124.53
26	K	101	BCR	C24-C23-C22	-2.71	122.14	126.23
32	d	406	PL9	C37-C38-C39	-2.71	121.13	127.66
26	B	620	BCR	C2-C1-C6	2.71	114.65	110.48
36	c	517	DGD	O1G-C1A-O1A	-2.71	116.75	123.59
24	d	404	CLA	CHD-C4C-NC	2.71	128.47	124.20
36	C	518	DGD	O1G-C1A-C2A	2.71	120.41	111.91
37	E	101	LHG	C5-O7-C7	-2.71	111.12	117.79
24	A	405	CLA	CHC-C1C-C2C	-2.71	119.21	126.73
32	A	419	PL9	C45-C44-C46	2.71	119.82	115.27
27	a	411	SQD	O48-C23-C24	2.71	120.40	111.91
24	B	604	CLA	O2A-CGA-CBA	2.71	120.40	111.91
34	z	101	LMG	O6-C5-C4	2.70	114.60	109.69
24	c	515	CLA	C1-C2-C3	-2.70	121.37	126.04
38	e	102	HEM	C4D-ND-C1D	2.70	107.86	105.07
25	a	408	PHO	CMB-C2B-C3B	2.70	129.73	124.68
26	B	620	BCR	C28-C27-C26	-2.70	109.26	114.08
26	T	102	BCR	C28-C27-C26	-2.70	109.26	114.08
24	b	619	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
24	C	503	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
32	d	406	PL9	C15-C14-C16	2.70	119.81	115.27
26	c	526	BCR	C7-C8-C9	-2.70	122.16	126.23
25	a	408	PHO	C1-O2A-CGA	2.70	123.52	116.44
24	C	510	CLA	C4-C3-C5	2.69	119.80	115.27
24	b	611	CLA	CHD-C4C-NC	2.69	128.44	124.20
27	F	101	SQD	C1-C2-C3	-2.69	104.39	110.00
27	A	411	SQD	O48-C23-C24	2.69	120.34	111.91
26	K	101	BCR	C7-C8-C9	-2.69	122.17	126.23
32	A	419	PL9	C35-C34-C36	2.69	119.79	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	V	203	HEC	C3B-C4B-NB	-2.69	107.17	110.17
30	m	102	LMT	C1'-O5'-C5'	-2.69	108.41	113.69
26	d	405	BCR	C28-C27-C26	-2.69	109.28	114.08
24	B	612	CLA	C4-C3-C5	2.69	119.79	115.27
36	h	102	DGD	O1G-C1A-C2A	2.69	120.33	111.91
24	b	612	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
24	c	505	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
24	b	613	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
24	B	615	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	c	509	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	C	507	CLA	C1-C2-C3	-2.68	121.41	126.04
27	A	411	SQD	O9-S-C6	2.68	110.12	106.94
24	B	604	CLA	CAC-C3C-C4C	2.68	128.29	124.81
24	c	510	CLA	C1-C2-C3	-2.68	121.41	126.04
24	D	403	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	B	614	CLA	C1D-CHD-C4C	-2.68	120.28	126.06
24	a	407	CLA	CHC-C1C-C2C	-2.68	119.30	126.73
24	D	404	CLA	CHD-C4C-NC	2.68	128.42	124.20
24	c	505	CLA	O2A-CGA-CBA	2.68	120.31	111.91
24	C	508	CLA	CBC-CAC-C3C	-2.68	105.05	112.43
24	A	405	CLA	CMA-C3A-C2A	-2.67	103.04	113.83
24	c	504	CLA	O2A-CGA-CBA	2.67	120.30	111.91
27	b	601	SQD	C1-C2-C3	-2.67	104.43	110.00
35	b	628	HTG	C1-O5-C5	2.67	117.51	112.58
24	c	510	CLA	C4-C3-C5	2.67	119.77	115.27
32	D	406	PL9	C25-C24-C26	2.67	119.76	115.27
24	b	609	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
24	b	606	CLA	C3B-C4B-NB	2.67	112.99	110.52
24	B	616	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
24	B	614	CLA	O2A-CGA-CBA	2.67	120.28	111.91
24	d	401	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
27	a	411	SQD	O47-C7-O49	-2.67	117.26	123.70
24	B	606	CLA	C4-C3-C5	2.67	119.75	115.27
24	B	608	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
24	b	611	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
24	b	618	CLA	O2A-CGA-CBA	2.66	120.26	111.91
24	C	512	CLA	CHD-C4C-NC	2.66	128.40	124.20
27	A	411	SQD	O48-C23-O10	-2.66	116.87	123.59
24	B	615	CLA	CMB-C2B-C1B	2.66	129.42	125.37
24	C	509	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
24	b	609	CLA	O2A-CGA-CBA	2.66	120.26	111.91
24	B	608	CLA	CAC-C3C-C4C	2.65	128.25	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	618	BCR	C7-C8-C9	-2.65	122.23	126.23
24	b	613	CLA	C2A-C1A-CHA	-2.64	119.23	123.86
32	a	416	PL9	C40-C39-C41	2.64	119.72	115.27
27	l	101	SQD	O48-C23-C24	2.64	120.20	111.91
35	D	411	HTG	C1'-S1-C1	2.64	105.03	100.09
24	C	513	CLA	CHD-C4C-NC	2.64	128.36	124.20
37	d	408	LHG	O8-C23-O10	-2.64	116.94	123.59
24	D	404	CLA	C4-C3-C5	2.63	119.70	115.27
24	D	403	CLA	C1D-CHD-C4C	-2.63	120.38	126.06
24	c	515	CLA	O2A-CGA-CBA	2.63	120.16	111.91
24	c	510	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
24	B	607	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
24	B	605	CLA	CAC-C3C-C4C	2.63	128.22	124.81
30	b	602	LMT	O5'-C5'-C4'	2.63	115.29	109.75
24	b	614	CLA	C1-C2-C3	-2.63	121.50	126.04
24	c	504	CLA	CAC-C3C-C4C	2.63	128.22	124.81
24	c	505	CLA	CHD-C4C-NC	2.63	128.34	124.20
30	m	103	LMT	C1-O1'-C1'	-2.63	109.48	113.84
24	A	409	CLA	C3B-C4B-NB	2.63	112.95	110.52
30	I	102	LMT	C2'-C3'-C4'	-2.63	103.69	109.68
24	D	401	CLA	CMA-C3A-C2A	-2.62	103.24	113.83
24	A	409	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
24	b	615	CLA	CMB-C2B-C1B	2.62	129.36	125.37
24	b	614	CLA	CHD-C4C-NC	2.62	128.34	124.20
24	b	608	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
24	B	605	CLA	O2A-CGA-CBA	2.62	120.12	111.91
24	D	401	CLA	CMA-C3A-C4A	-2.62	104.74	111.77
24	b	611	CLA	CHC-C1C-C2C	-2.62	119.47	126.73
24	c	507	CLA	CMC-C2C-C1C	2.61	129.02	125.04
32	d	406	PL9	C20-C19-C21	2.61	119.67	115.27
24	c	510	CLA	CHD-C4C-NC	2.61	128.32	124.20
34	C	521	LMG	C8-O7-C10	-2.61	111.36	117.79
34	c	521	LMG	O8-C28-C29	2.61	120.10	111.91
24	c	511	CLA	O2A-CGA-CBA	2.61	120.10	111.91
26	c	516	BCR	C3-C4-C5	-2.61	109.42	114.08
24	a	407	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
32	D	406	PL9	C15-C14-C16	2.61	119.66	115.27
24	c	508	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
24	b	619	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
24	C	513	CLA	O2A-CGA-CBA	2.61	120.09	111.91
24	a	407	CLA	C3B-C4B-NB	2.61	112.93	110.52
35	V	204	HTG	C1-C2-C3	-2.61	105.44	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	512	CLA	C1-C2-C3	-2.61	121.53	126.04
24	a	409	CLA	CHB-C4A-NA	2.61	128.12	124.51
34	C	521	LMG	O8-C28-C29	2.61	120.08	111.91
35	b	627	HTG	C1-O5-C5	2.61	117.39	112.58
24	b	618	CLA	CAC-C3C-C4C	2.61	128.19	124.81
24	B	608	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
24	B	609	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
24	c	508	CLA	CED-O2D-CGD	2.60	121.82	115.94
24	b	619	CLA	C4-C3-C5	2.60	119.65	115.27
40	v	202	HEC	C3B-C4B-NB	-2.60	107.27	110.17
24	C	511	CLA	O1D-CGD-CBD	-2.60	119.16	124.48
24	b	614	CLA	CAC-C3C-C4C	2.60	128.18	124.81
36	c	517	DGD	O1G-C1A-C2A	2.60	120.06	111.91
24	C	513	CLA	CAC-C3C-C4C	2.60	128.18	124.81
24	B	608	CLA	O2A-CGA-CBA	2.60	120.06	111.91
24	B	607	CLA	C1-C2-C3	-2.60	121.55	126.04
24	b	610	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
32	A	419	PL9	C30-C29-C31	2.59	119.63	115.27
24	C	507	CLA	O2A-CGA-CBA	2.59	120.04	111.91
27	F	101	SQD	O48-C23-C24	2.59	120.04	111.91
37	D	409	LHG	C5-O7-C7	-2.59	111.41	117.79
24	b	607	CLA	CHD-C4C-NC	2.59	128.28	124.20
24	b	613	CLA	CMB-C2B-C1B	2.59	129.31	125.37
24	d	404	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
36	C	518	DGD	O2G-C1B-O1B	-2.59	117.44	123.70
24	a	406	CLA	O2D-CGD-CBD	2.59	115.87	111.27
24	b	619	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
38	e	102	HEM	CBD-CAD-C3D	-2.59	105.44	112.63
40	v	202	HEC	O2A-CGA-O1A	-2.59	116.85	123.30
24	d	404	CLA	CHC-C1C-C2C	-2.59	119.55	126.73
24	B	617	CLA	C1-O2A-CGA	2.59	123.23	116.44
24	C	504	CLA	C1-C2-C3	-2.58	121.57	126.04
25	A	408	PHO	O2A-CGA-O1A	-2.58	117.07	123.59
37	E	101	LHG	O8-C23-C24	2.58	120.02	111.91
24	C	510	CLA	C1-O2A-CGA	2.58	123.22	116.44
26	a	410	BCR	C15-C14-C13	-2.58	123.62	127.31
26	c	526	BCR	C11-C10-C9	-2.58	123.63	127.31
24	b	608	CLA	CHC-C1C-C2C	-2.58	119.56	126.73
24	C	503	CLA	C3B-C4B-NB	2.58	112.91	110.52
24	B	603	CLA	CHD-C4C-NC	2.58	128.27	124.20
24	c	505	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
24	C	505	CLA	CMB-C2B-C1B	2.58	129.29	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	z	101	LMG	C3-C4-C5	2.58	114.83	110.24
24	B	603	CLA	CBC-CAC-C3C	-2.58	105.33	112.43
24	a	406	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
24	d	402	CLA	CAC-C3C-C4C	2.57	128.15	124.81
24	C	505	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
24	b	617	CLA	CHC-C1C-C2C	-2.57	119.59	126.73
24	C	513	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
24	c	503	CLA	O2A-CGA-CBA	2.57	119.97	111.91
24	A	409	CLA	C1-C2-C3	-2.57	121.60	126.04
24	C	504	CLA	CMB-C2B-C1B	2.57	129.28	125.37
24	b	615	CLA	CMC-C2C-C1C	2.57	128.95	125.04
24	B	612	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
24	C	504	CLA	CHD-C4C-NC	2.57	128.25	124.20
24	c	508	CLA	CHD-C4C-NC	2.57	128.25	124.20
25	a	408	PHO	C1A-C2A-C3A	-2.56	100.40	102.84
24	C	507	CLA	CHD-C4C-NC	2.56	128.24	124.20
24	A	406	CLA	CMC-C2C-C1C	2.56	128.94	125.04
24	c	515	CLA	CMB-C2B-C1B	2.56	129.27	125.37
24	B	610	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
26	h	101	BCR	C10-C11-C12	-2.55	115.24	123.22
26	B	620	BCR	C36-C18-C17	-2.55	119.35	122.92
26	A	410	BCR	C7-C8-C9	-2.55	122.38	126.23
24	B	602	CLA	C4-C3-C5	2.55	119.57	115.27
24	C	505	CLA	C4-C3-C5	2.55	119.56	115.27
24	C	511	CLA	C1-O2A-CGA	2.55	123.14	116.44
24	b	610	CLA	O2A-CGA-CBA	2.55	119.92	111.91
24	d	401	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
24	a	406	CLA	CMB-C2B-C1B	2.55	129.25	125.37
24	D	403	CLA	CMA-C3A-C2A	-2.55	103.54	113.83
24	D	404	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
36	D	407	DGD	O1G-C1A-C2A	2.55	119.90	111.91
24	d	404	CLA	CMB-C2B-C1B	2.55	129.25	125.37
26	B	619	BCR	C28-C27-C26	-2.55	109.53	114.08
24	B	617	CLA	CHD-C4C-NC	2.55	128.22	124.20
24	a	406	CLA	CMA-C3A-C4A	-2.54	104.93	111.77
24	B	607	CLA	CHC-C1C-C2C	-2.54	119.66	126.73
35	V	204	HTG	O5-C1-C2	-2.54	107.11	110.31
32	a	416	PL9	C35-C34-C36	2.54	119.55	115.27
24	b	621	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
26	D	405	BCR	C37-C22-C23	2.54	122.08	118.08
26	c	526	BCR	C20-C21-C22	-2.54	123.69	127.31
24	c	505	CLA	C1-C2-C3	-2.54	121.65	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	CLA	C1-C2-C3	-2.54	121.66	126.04
26	H	101	BCR	C29-C30-C25	2.53	114.38	110.48
24	d	402	CLA	CMC-C2C-C1C	2.53	128.90	125.04
24	b	619	CLA	CBC-CAC-C3C	-2.53	105.44	112.43
24	B	602	CLA	CAC-C3C-C4C	2.53	128.10	124.81
24	B	605	CLA	CHD-C4C-NC	2.53	128.20	124.20
30	a	417	LMT	C1-O1'-C1'	-2.53	109.64	113.84
24	c	514	CLA	CBA-CAA-C2A	-2.53	106.39	113.86
24	B	609	CLA	CMC-C2C-C1C	2.53	128.89	125.04
24	b	608	CLA	CHD-C4C-NC	2.53	128.19	124.20
24	c	507	CLA	C1-O2A-CGA	2.53	123.08	116.44
26	t	101	BCR	C11-C10-C9	-2.53	123.70	127.31
32	d	406	PL9	C8-C7-C3	2.53	119.12	111.98
24	B	611	CLA	C3B-C4B-NB	2.52	112.86	110.52
38	e	102	HEM	CHB-C1B-NB	2.52	127.48	124.37
26	C	516	BCR	C33-C5-C6	-2.52	121.70	124.53
24	A	409	CLA	O2A-CGA-CBA	2.52	119.82	111.91
37	D	409	LHG	O8-C23-C24	2.52	119.81	111.91
24	C	505	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
24	c	513	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
24	c	511	CLA	CHD-C4C-NC	2.52	128.17	124.20
26	c	526	BCR	C38-C26-C25	-2.52	121.70	124.53
30	A	417	LMT	C1'-O5'-C5'	2.51	118.62	113.69
24	c	504	CLA	CHD-C4C-NC	2.51	128.16	124.20
24	c	512	CLA	O2A-CGA-CBA	2.51	119.79	111.91
24	C	509	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
24	B	611	CLA	CMA-C3A-C4A	-2.51	105.03	111.77
30	m	103	LMT	O5B-C5B-C4B	2.51	114.25	109.69
24	c	510	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
24	A	405	CLA	CMA-C3A-C4A	-2.51	105.04	111.77
24	b	611	CLA	C1-C2-C3	-2.51	121.71	126.04
26	c	526	BCR	C24-C23-C22	-2.50	122.45	126.23
38	E	103	HEM	C4A-NA-C1A	2.50	107.80	105.35
38	E	103	HEM	C4B-C3B-C2B	-2.50	105.13	107.11
37	D	409	LHG	O7-C7-O9	-2.50	117.65	123.70
24	d	402	CLA	CMA-C3A-C2A	-2.50	103.73	113.83
24	c	511	CLA	CMC-C2C-C1C	2.50	128.85	125.04
32	d	406	PL9	C42-C43-C44	-2.50	121.63	127.66
24	b	615	CLA	CHD-C4C-NC	2.50	128.15	124.20
24	D	401	CLA	CHD-C4C-NC	2.50	128.15	124.20
24	A	409	CLA	CHC-C1C-C2C	-2.50	119.78	126.73
34	c	501	LMG	O8-C28-C29	2.50	119.75	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	607	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
24	b	614	CLA	C4-C3-C5	2.50	119.47	115.27
24	C	507	CLA	CMC-C2C-C1C	2.50	128.84	125.04
24	b	611	CLA	C4-C3-C5	2.49	119.46	115.27
24	d	401	CLA	CAA-CBA-CGA	2.49	120.53	113.25
24	B	603	CLA	CAA-CBA-CGA	-2.49	105.97	113.25
24	b	619	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
24	A	405	CLA	O2A-CGA-CBA	2.49	119.72	111.91
27	a	402	SQD	O9-S-C6	2.49	109.90	106.94
24	D	401	CLA	CMC-C2C-C1C	2.49	128.83	125.04
26	T	102	BCR	C1-C6-C7	2.49	122.81	115.78
24	B	604	CLA	CHD-C4C-NC	2.49	128.12	124.20
24	c	515	CLA	CHD-C4C-NC	2.49	128.12	124.20
24	D	403	CLA	C2A-C1A-CHA	-2.48	119.51	123.86
24	b	611	CLA	CMB-C2B-C1B	2.48	129.15	125.37
24	B	610	CLA	CBC-CAC-C3C	-2.48	105.58	112.43
24	b	607	CLA	O2A-CGA-CBA	2.48	119.70	111.91
24	c	513	CLA	CHB-C1B-NB	-2.48	121.63	124.26
24	D	404	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
24	C	504	CLA	O2A-CGA-CBA	2.48	119.70	111.91
26	a	410	BCR	C34-C9-C10	-2.48	119.44	122.92
26	B	620	BCR	C3-C4-C5	-2.48	109.64	114.08
24	c	503	CLA	OBD-CAD-C3D	-2.48	122.55	128.52
32	D	406	PL9	C7-C8-C9	-2.48	122.66	126.79
24	b	607	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
34	c	520	LMG	O8-C28-C29	2.48	119.68	111.91
38	E	103	HEM	O2A-CGA-CBA	2.48	121.99	114.03
24	b	612	CLA	CAA-CBA-CGA	2.48	120.49	113.25
24	c	514	CLA	C4-C3-C5	2.48	119.44	115.27
24	B	602	CLA	CMC-C2C-C1C	2.48	128.81	125.04
37	d	409	LHG	O8-C23-C24	2.48	119.68	111.91
24	B	616	CLA	CHD-C4C-NC	2.47	128.10	124.20
32	A	419	PL9	C7-C3-C4	2.47	118.89	116.88
24	c	511	CLA	C4-C3-C5	2.47	119.43	115.27
24	C	508	CLA	CHC-C1C-C2C	-2.47	119.87	126.73
24	C	504	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
24	c	510	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
26	d	405	BCR	C37-C22-C23	2.47	121.97	118.08
24	c	509	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
24	A	406	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
34	c	501	LMG	O7-C10-O9	-2.46	117.75	123.70
27	b	601	SQD	O48-C23-O10	-2.46	117.38	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	505	CLA	CHC-C1C-C2C	-2.46	119.90	126.73
24	c	512	CLA	CAC-C3C-C4C	2.46	128.00	124.81
24	b	620	CLA	CHD-C4C-NC	2.46	128.08	124.20
24	B	616	CLA	C1-O2A-CGA	2.46	122.89	116.44
24	C	503	CLA	CHD-C4C-NC	2.46	128.08	124.20
24	a	407	CLA	C4-C3-C5	2.46	119.41	115.27
24	C	506	CLA	CMC-C2C-C1C	2.46	128.78	125.04
24	A	406	CLA	CMA-C3A-C2A	-2.45	103.93	113.83
24	b	607	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
34	C	501	LMG	O8-C28-C29	2.45	119.61	111.91
24	c	513	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
24	C	514	CLA	O2A-CGA-CBA	2.45	119.61	111.91
24	a	409	CLA	O2A-CGA-CBA	2.45	119.61	111.91
24	c	513	CLA	O2A-CGA-CBA	2.45	119.60	111.91
24	c	503	CLA	CHD-C4C-NC	2.45	128.06	124.20
32	D	406	PL9	C37-C38-C39	-2.45	121.77	127.66
26	B	620	BCR	C15-C14-C13	-2.45	123.82	127.31
24	b	615	CLA	C1-C2-C3	-2.45	121.81	126.04
24	C	512	CLA	CMC-C2C-C1C	2.45	128.76	125.04
24	c	515	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
24	C	508	CLA	O2A-CGA-CBA	2.44	119.56	111.91
24	b	612	CLA	CHD-C4C-NC	2.44	128.05	124.20
26	K	101	BCR	C2-C1-C6	2.44	114.23	110.48
38	e	102	HEM	CHA-C4D-ND	2.44	127.38	124.37
24	b	615	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
24	b	613	CLA	CMA-C3A-C2A	-2.44	104.00	113.83
24	A	409	CLA	CMA-C3A-C2A	-2.44	104.00	113.83
24	c	510	CLA	CAC-C3C-C4C	2.44	127.97	124.81
26	h	101	BCR	C7-C8-C9	-2.44	122.55	126.23
24	B	604	CLA	CHC-C1C-C2C	-2.44	119.96	126.73
25	d	403	PHO	O2A-CGA-CBA	2.43	119.55	111.91
27	l	101	SQD	C1-O5-C5	-2.43	108.91	113.69
24	a	409	CLA	CHD-C4C-NC	2.43	128.04	124.20
24	B	603	CLA	CAC-C3C-C4C	2.43	127.97	124.81
24	D	401	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
36	d	407	DGD	O6E-C5E-C4E	2.43	114.11	109.69
24	d	404	CLA	CGD-CBD-CAD	-2.43	102.86	110.73
26	b	624	BCR	C2-C1-C6	2.43	114.22	110.48
24	c	503	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
26	t	101	BCR	C15-C16-C17	-2.43	118.49	123.47
24	b	612	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
27	l	101	SQD	O9-S-C6	2.43	109.83	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
37	D	410	LHG	O8-C23-O10	-2.43	117.46	123.59
24	c	508	CLA	O2A-CGA-CBA	2.43	119.53	111.91
26	B	618	BCR	C34-C9-C10	-2.43	119.52	122.92
25	A	407	PHO	CMB-C2B-C3B	2.43	129.22	124.68
26	t	101	BCR	C1-C6-C7	2.43	122.64	115.78
24	C	514	CLA	CAA-C2A-C3A	-2.43	106.14	112.78
24	C	506	CLA	C4-C3-C5	2.42	119.35	115.27
36	h	102	DGD	O1G-C1A-O1A	-2.42	117.48	123.59
24	b	611	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
26	t	101	BCR	C2-C1-C6	2.42	114.21	110.48
24	b	612	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
24	b	617	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
24	d	404	CLA	O2A-CGA-CBA	2.42	119.49	111.91
24	B	603	CLA	C1-C2-C3	-2.41	121.87	126.04
26	B	618	BCR	C11-C10-C9	-2.41	123.87	127.31
37	d	408	LHG	O7-C7-O9	-2.41	117.88	123.70
26	A	410	BCR	C37-C22-C21	-2.41	119.55	122.92
24	a	406	CLA	CMA-C3A-C2A	-2.41	104.11	113.83
40	v	202	HEC	CHD-C1D-ND	2.41	127.34	124.37
24	D	401	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	C	502	CLA	O2A-CGA-CBA	2.41	119.46	111.91
24	B	616	CLA	C4-C3-C5	2.41	119.32	115.27
30	a	401	LMT	O5'-C5'-C4'	2.41	114.83	109.75
24	B	613	CLA	C4-C3-C5	2.41	119.32	115.27
25	A	408	PHO	CMD-C2D-C3D	2.41	129.18	124.68
24	b	614	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
24	B	605	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
32	d	406	PL9	O1-C4-C3	-2.40	118.08	120.72
26	B	620	BCR	C7-C8-C9	-2.40	122.61	126.23
24	d	404	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
24	b	607	CLA	CMA-C3A-C4A	-2.40	105.32	111.77
24	c	509	CLA	CHD-C4C-NC	2.40	127.98	124.20
36	c	517	DGD	O3G-C3G-C2G	-2.40	105.11	110.90
24	B	606	CLA	C1-O2A-CGA	2.40	122.73	116.44
30	m	103	LMT	C1B-O5B-C5B	2.40	118.39	113.69
24	B	611	CLA	CMB-C2B-C1B	2.40	129.02	125.37
24	C	513	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
25	A	408	PHO	CMC-C2C-C1C	2.39	129.25	124.73
24	D	404	CLA	O2A-CGA-CBA	2.39	119.41	111.91
26	D	405	BCR	C10-C11-C12	-2.39	115.75	123.22
26	d	405	BCR	C29-C30-C25	2.39	114.16	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	410	BCR	C33-C5-C6	-2.39	121.84	124.53
24	B	603	CLA	CMA-C3A-C4A	-2.39	105.35	111.77
38	E	103	HEM	C4D-ND-C1D	2.39	107.54	105.07
24	c	508	CLA	CGD-CBD-CAD	-2.39	103.00	110.73
24	a	407	CLA	OBD-CAD-C3D	-2.39	122.78	128.52
25	A	407	PHO	CBA-CAA-C2A	-2.39	106.84	113.81
26	H	101	BCR	C37-C22-C21	-2.39	119.58	122.92
34	c	521	LMG	C8-O7-C10	-2.39	111.92	117.79
24	c	512	CLA	O1D-CGD-CBD	-2.39	119.60	124.48
24	b	606	CLA	CMB-C2B-C1B	2.38	129.00	125.37
37	d	410	LHG	O8-C23-O10	-2.38	117.58	123.59
24	C	503	CLA	C4-C3-C5	2.38	119.28	115.27
26	C	516	BCR	C3-C4-C5	-2.38	109.82	114.08
24	b	620	CLA	CMC-C2C-C1C	2.38	128.67	125.04
24	B	612	CLA	O2A-CGA-CBA	2.38	119.38	111.91
35	b	627	HTG	C1-C2-C3	2.38	115.29	110.59
24	C	502	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
24	A	406	CLA	O2A-CGA-CBA	2.38	119.37	111.91
24	C	513	CLA	C1-O2A-CGA	2.38	122.68	116.44
37	l	102	LHG	O8-C23-C24	2.38	119.36	111.91
24	C	502	CLA	CHB-C1B-NB	-2.37	121.74	124.26
36	D	407	DGD	O6E-C5E-C4E	2.37	114.01	109.69
24	C	510	CLA	CMB-C2B-C1B	2.37	128.99	125.37
24	B	602	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	C	512	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	D	404	CLA	CHB-C1B-NB	-2.37	121.75	124.26
24	c	505	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
24	c	515	CLA	C4-C3-C5	2.37	119.26	115.27
24	B	614	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
30	m	103	LMT	O1'-C1'-C2'	2.37	112.01	108.30
36	c	518	DGD	O1G-C1A-C2A	2.37	119.35	111.91
24	B	614	CLA	CMB-C2B-C1B	2.37	128.98	125.37
24	c	503	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	c	514	CLA	C4C-C3C-C2C	-2.37	103.45	106.90
24	b	613	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
24	b	616	CLA	C4-C3-C5	2.37	119.25	115.27
24	C	504	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
36	C	519	DGD	O2G-C1B-C2B	2.37	116.60	111.50
24	b	617	CLA	OBD-CAD-C3D	-2.37	122.83	128.52
24	c	506	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
24	b	615	CLA	CMA-C3A-C4A	-2.36	105.42	111.77
24	b	609	CLA	O2A-CGA-O1A	-2.36	117.63	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	609	CLA	C4-C3-C5	2.36	119.25	115.27
24	c	506	CLA	CHD-C4C-NC	2.36	127.93	124.20
32	D	406	PL9	C12-C13-C14	-2.36	121.97	127.66
24	d	401	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
24	B	614	CLA	O2D-CGD-CBD	2.36	115.46	111.27
24	c	503	CLA	CMC-C2C-C1C	2.36	128.63	125.04
24	A	409	CLA	CMA-C3A-C4A	-2.36	105.44	111.77
24	c	513	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
26	A	410	BCR	C38-C26-C25	-2.35	121.88	124.53
24	B	609	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
24	c	503	CLA	C4-C3-C5	2.35	119.23	115.27
24	b	619	CLA	CHB-C1B-NB	-2.35	121.77	124.26
36	d	407	DGD	O1G-C1A-C2A	2.35	119.28	111.91
30	D	402	LMT	O1B-C4'-C3'	2.35	113.52	107.28
24	C	505	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
36	H	102	DGD	O1G-C1A-O1A	-2.35	117.67	123.59
35	C	522	HTG	O5-C1-C2	2.35	113.26	110.31
26	D	405	BCR	C30-C25-C24	2.35	122.41	115.78
24	c	511	CLA	CMB-C2B-C1B	2.35	128.94	125.37
26	C	516	BCR	C21-C20-C19	-2.35	115.90	123.22
37	D	408	LHG	O7-C7-O9	-2.34	118.03	123.70
40	V	203	HEC	C4A-NA-C1A	2.34	107.64	105.35
27	A	411	SQD	O47-C7-O49	-2.34	118.04	123.70
27	a	402	SQD	O48-C23-O10	-2.34	117.68	123.59
36	C	518	DGD	O1G-C1A-O1A	-2.34	117.68	123.59
24	B	606	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
34	J	101	LMG	O8-C28-O10	-2.34	117.68	123.59
24	B	607	CLA	CMB-C2B-C1B	2.34	128.94	125.37
24	c	505	CLA	C2A-C1A-CHA	-2.34	119.76	123.86
27	a	402	SQD	O8-S-C6	2.34	109.47	105.74
24	C	514	CLA	CHD-C4C-NC	2.34	127.89	124.20
27	f	101	SQD	O47-C7-O49	-2.34	118.05	123.70
26	a	410	BCR	C35-C13-C14	-2.33	119.65	122.92
24	c	514	CLA	CED-O2D-CGD	2.33	121.22	115.94
24	B	608	CLA	CHD-C4C-NC	2.33	127.88	124.20
24	C	507	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
32	d	406	PL9	C22-C23-C24	-2.33	122.04	127.66
24	b	614	CLA	C1-O2A-CGA	2.33	122.56	116.44
24	B	610	CLA	C4-C3-C5	2.33	119.19	115.27
24	B	616	CLA	CED-O2D-CGD	2.33	121.21	115.94
26	B	620	BCR	C16-C17-C18	-2.33	123.99	127.31
26	y	101	BCR	C10-C11-C12	-2.33	115.95	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	522	HTG	C1-O5-C5	2.33	116.87	112.58
24	B	608	CLA	OBD-CAD-C3D	-2.33	122.92	128.52
24	c	514	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
24	c	511	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
24	B	616	CLA	C11-C10-C8	-2.33	108.40	115.92
24	d	401	CLA	O2A-CGA-CBA	2.33	119.21	111.91
24	C	506	CLA	CHD-C4C-NC	2.33	127.87	124.20
24	A	409	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
24	c	506	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
24	c	508	CLA	C4-C3-C5	2.32	119.18	115.27
26	C	516	BCR	C11-C10-C9	-2.32	124.00	127.31
24	B	609	CLA	C1-C2-C3	-2.32	122.03	126.04
24	C	505	CLA	C1-O2A-CGA	2.32	122.53	116.44
36	C	517	DGD	O1G-C1A-C2A	2.32	119.19	111.91
27	A	416	SQD	O5-C5-C4	2.32	113.91	109.69
24	b	613	CLA	CHD-C4C-NC	2.32	127.86	124.20
30	a	401	LMT	C1'-O5'-C5'	2.32	118.24	113.69
24	A	406	CLA	CAA-CBA-CGA	2.32	120.02	113.25
24	c	513	CLA	CMB-C2B-C1B	2.32	128.90	125.37
27	F	101	SQD	C44-O6-C1	-2.31	109.22	113.74
24	C	510	CLA	CHD-C4C-NC	2.31	127.85	124.20
24	b	616	CLA	O2A-CGA-CBA	2.31	119.17	111.91
34	B	621	LMG	O8-C28-C29	2.31	119.16	111.91
24	b	620	CLA	C11-C10-C8	-2.31	108.45	115.92
32	d	406	PL9	C35-C34-C36	2.31	119.16	115.27
24	C	508	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
26	T	102	BCR	C35-C13-C12	2.31	121.72	118.08
26	a	410	BCR	C37-C22-C21	-2.31	119.69	122.92
25	d	403	PHO	CMA-C3A-C4A	-2.31	109.32	114.38
24	b	621	CLA	CMB-C2B-C1B	2.30	128.88	125.37
35	B	622	HTG	C1-O5-C5	2.30	116.83	112.58
24	B	617	CLA	O2A-CGA-CBA	2.30	119.14	111.91
24	b	620	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
26	h	101	BCR	C31-C1-C6	-2.30	106.57	110.30
26	Y	101	BCR	C10-C11-C12	-2.30	116.04	123.22
24	B	614	CLA	CMC-C2C-C1C	2.30	128.54	125.04
24	a	409	CLA	CMA-C3A-C4A	-2.30	105.59	111.77
36	h	102	DGD	O4D-C4D-C3D	-2.30	105.04	110.35
37	d	409	LHG	C5-O7-C7	-2.30	112.13	117.79
24	b	613	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
40	V	203	HEC	O2D-CGD-CBD	2.30	121.41	114.03
24	C	503	CLA	CBC-CAC-C3C	-2.30	106.10	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	510	CLA	O2A-CGA-CBA	2.30	119.11	111.91
24	B	611	CLA	CMC-C2C-C1C	2.29	128.53	125.04
34	C	520	LMG	O8-C28-O10	-2.29	117.81	123.59
24	c	504	CLA	CHB-C1B-NB	-2.29	121.83	124.26
24	C	504	CLA	CMC-C2C-C1C	2.29	128.53	125.04
24	b	613	CLA	C11-C10-C8	-2.29	108.52	115.92
26	b	624	BCR	C16-C17-C18	-2.29	124.04	127.31
24	c	514	CLA	CHB-C4A-NA	2.29	127.68	124.51
35	B	623	HTG	C1-C2-C3	2.29	115.11	110.59
36	h	102	DGD	O2G-C1B-O1B	-2.29	118.17	123.70
27	b	601	SQD	O9-S-C6	2.29	109.66	106.94
24	b	621	CLA	O1D-CGD-CBD	-2.29	119.81	124.48
36	H	102	DGD	O1G-C1A-C2A	2.28	119.08	111.91
24	c	504	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	c	512	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	B	606	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
24	B	615	CLA	CHB-C1B-NB	-2.28	121.84	124.26
27	a	411	SQD	O9-S-C6	2.28	109.65	106.94
24	A	406	CLA	CED-O2D-CGD	2.28	121.09	115.94
24	A	409	CLA	CHB-C4A-NA	2.28	127.66	124.51
26	D	405	BCR	C37-C22-C21	-2.28	119.73	122.92
26	h	101	BCR	C29-C30-C25	2.28	113.98	110.48
24	D	404	CLA	CMC-C2C-C1C	2.28	128.50	125.04
24	a	409	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
40	V	203	HEC	CBB-CAB-C3B	2.27	118.70	112.43
24	b	614	CLA	CGD-CBD-CAD	-2.27	103.37	110.73
25	a	408	PHO	C4D-CHA-CBD	-2.27	107.49	108.52
24	A	406	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
40	v	202	HEC	O2A-CGA-CBA	2.27	121.33	114.03
24	C	508	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
24	B	617	CLA	CHB-C1B-NB	-2.27	121.85	124.26
26	Y	101	BCR	C40-C30-C25	-2.27	106.62	110.30
24	C	510	CLA	O2A-CGA-CBA	2.27	119.03	111.91
34	Z	101	LMG	C9-C8-C7	-2.27	106.42	111.79
24	c	506	CLA	CHB-C1B-NB	-2.27	121.86	124.26
25	a	408	PHO	O2D-CGD-O1D	-2.26	119.41	123.84
26	b	623	BCR	C37-C22-C21	-2.26	119.75	122.92
24	b	607	CLA	C1-O2A-CGA	2.26	122.38	116.44
24	a	406	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
24	B	611	CLA	OBD-CAD-C3D	-2.26	123.08	128.52
24	b	618	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
25	A	408	PHO	O2A-CGA-CBA	2.26	118.99	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	613	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
24	B	617	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
24	C	510	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	D	401	CLA	C1-C2-C3	-2.25	122.15	126.04
26	b	624	BCR	C3-C4-C5	-2.25	110.06	114.08
24	C	505	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
34	B	621	LMG	C9-C8-C7	-2.25	106.47	111.79
27	f	101	SQD	O9-S-C6	2.25	109.61	106.94
27	F	101	SQD	C1-O5-C5	-2.25	109.27	113.69
24	C	506	CLA	O2A-CGA-CBA	2.25	118.97	111.91
38	e	102	HEM	CHA-C1A-NA	2.25	127.98	123.85
24	B	602	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
24	b	619	CLA	C4-C3-C2	-2.25	117.92	123.68
26	T	102	BCR	C29-C30-C25	2.24	113.94	110.48
35	B	631	HTG	C1-O5-C5	2.24	116.72	112.58
24	D	401	CLA	O2A-CGA-CBA	2.24	118.94	111.91
26	c	526	BCR	C2-C1-C6	2.24	113.93	110.48
32	a	416	PL9	C45-C44-C46	2.24	119.04	115.27
24	b	609	CLA	CHD-C4C-NC	2.24	127.73	124.20
24	b	618	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
26	T	102	BCR	C7-C6-C5	-2.24	116.05	121.46
36	D	407	DGD	O6D-C5D-C6D	2.24	111.18	106.67
24	b	618	CLA	CMC-C2C-C1C	2.24	128.44	125.04
24	C	514	CLA	CHB-C1B-NB	-2.23	121.89	124.26
26	b	622	BCR	C29-C30-C25	2.23	113.92	110.48
24	C	509	CLA	CMB-C2B-C1B	2.23	128.77	125.37
26	d	405	BCR	C29-C28-C27	-2.23	106.39	111.38
24	C	502	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
30	A	417	LMT	C1B-O1B-C4'	-2.23	112.44	117.96
32	D	406	PL9	C27-C28-C29	-2.23	122.29	127.66
26	B	620	BCR	C34-C9-C8	2.23	121.59	118.08
24	B	610	CLA	O2A-CGA-CBA	2.23	118.90	111.91
24	B	616	CLA	CHA-C1A-NA	-2.23	121.29	126.40
24	c	511	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
24	B	603	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
24	A	406	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
32	D	406	PL9	C40-C39-C38	-2.23	117.97	123.68
24	b	611	CLA	O2A-CGA-CBA	2.22	118.89	111.91
26	a	410	BCR	C38-C26-C25	-2.22	122.03	124.53
36	d	407	DGD	O5D-C1E-C2E	2.22	111.78	108.30
24	b	612	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
40	V	203	HEC	CHD-C4C-NC	2.22	127.94	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	515	CLA	CHB-C4A-NA	2.22	127.59	124.51
34	B	621	LMG	C30-C29-C28	-2.22	105.54	113.62
24	b	614	CLA	O2A-CGA-CBA	2.22	118.88	111.91
38	E	103	HEM	CHA-C4D-ND	2.22	127.11	124.37
26	k	103	BCR	C11-C10-C9	-2.22	124.14	127.31
24	b	619	CLA	CHD-C4C-NC	2.22	127.70	124.20
40	v	202	HEC	C3C-C4C-NC	-2.22	107.66	110.15
30	b	602	LMT	O5'-C1'-C2'	2.22	115.05	110.35
32	A	419	PL9	C35-C34-C33	-2.22	117.98	123.68
24	b	608	CLA	C7-C6-C5	-2.22	107.33	113.36
24	b	614	CLA	CED-O2D-CGD	2.22	120.95	115.94
24	B	604	CLA	CED-O2D-CGD	2.22	120.95	115.94
38	e	102	HEM	C2A-C1A-NA	-2.22	107.67	110.15
24	D	404	CLA	CMA-C3A-C2A	-2.22	104.89	113.83
26	b	623	BCR	C29-C30-C25	2.22	113.89	110.48
34	j	101	LMG	O8-C28-C29	2.21	118.86	111.91
24	b	616	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
26	d	405	BCR	C16-C17-C18	-2.21	124.15	127.31
26	K	101	BCR	C29-C30-C25	2.21	113.89	110.48
24	c	506	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
24	C	502	CLA	CHD-C4C-NC	2.21	127.69	124.20
24	a	407	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	b	617	CLA	CHD-C4C-NC	2.21	127.69	124.20
24	B	608	CLA	C1-C2-C3	-2.21	122.22	126.04
34	c	501	LMG	O1-C1-C2	2.21	111.75	108.30
24	b	611	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
24	C	513	CLA	CED-O2D-CGD	2.21	120.94	115.94
27	A	416	SQD	O48-C23-O10	-2.21	118.02	123.59
24	C	508	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
24	b	606	CLA	CMC-C2C-C1C	2.20	128.39	125.04
26	K	101	BCR	C11-C10-C9	-2.20	124.17	127.31
24	B	603	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
37	L	101	LHG	O8-C23-O10	-2.20	118.04	123.59
26	D	405	BCR	C29-C28-C27	-2.20	106.46	111.38
25	A	408	PHO	C4A-C3A-C2A	-2.20	100.75	102.84
24	b	614	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
24	C	513	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
34	J	101	LMG	C9-C8-C7	-2.20	106.59	111.79
24	C	509	CLA	CHD-C4C-NC	2.20	127.66	124.20
24	C	511	CLA	O2A-CGA-CBA	2.19	118.79	111.91
24	B	610	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	C	510	CLA	CMC-C2C-C1C	2.19	128.37	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	607	CLA	CMC-C2C-C1C	2.19	128.37	125.04
26	y	101	BCR	C35-C13-C14	-2.19	119.86	122.92
27	a	402	SQD	C45-O47-C7	-2.19	112.41	117.79
24	c	506	CLA	O2A-CGA-CBA	2.19	118.77	111.91
24	B	605	CLA	CHB-C1B-NB	-2.18	121.94	124.26
24	d	404	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
24	D	403	CLA	CBC-CAC-C3C	-2.18	106.41	112.43
40	v	202	HEC	CMD-C2D-C1D	2.18	128.36	125.04
24	b	612	CLA	C1-O2A-CGA	2.18	122.17	116.44
24	D	401	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
26	T	102	BCR	C21-C20-C19	-2.18	116.41	123.22
35	B	622	HTG	O5-C1-C2	2.18	113.06	110.31
24	B	611	CLA	CHD-C4C-NC	2.18	127.64	124.20
37	d	409	LHG	O8-C23-O10	-2.18	118.10	123.59
24	C	506	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
34	c	521	LMG	O7-C10-O9	-2.18	118.44	123.70
26	B	620	BCR	C10-C11-C12	-2.17	116.44	123.22
24	B	612	CLA	CHB-C1B-NB	-2.17	121.96	124.26
26	y	101	BCR	C21-C20-C19	-2.17	116.44	123.22
24	c	503	CLA	C1-O2A-CGA	2.17	122.14	116.44
26	t	101	BCR	C21-C20-C19	-2.17	116.45	123.22
35	c	523	HTG	C1-O5-C5	2.17	116.58	112.58
24	c	508	CLA	CMC-C2C-C1C	2.17	128.34	125.04
24	C	505	CLA	CHD-C4C-NC	2.17	127.62	124.20
26	T	102	BCR	C19-C18-C17	-2.17	115.62	118.94
36	h	102	DGD	C3G-O3G-C1D	-2.16	109.51	113.74
36	d	407	DGD	C1E-O6E-C5E	2.16	117.93	113.69
24	b	606	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
24	b	616	CLA	OBD-CAD-C3D	-2.16	123.32	128.52
26	Y	101	BCR	C21-C20-C19	-2.16	116.48	123.22
24	c	512	CLA	CHB-C1B-NB	-2.16	121.97	124.26
24	B	604	CLA	CAA-CBA-CGA	2.16	119.56	113.25
24	c	504	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
37	L	101	LHG	O7-C7-O9	-2.16	118.48	123.70
38	e	102	HEM	C4C-CHD-C1D	-2.16	121.40	126.06
24	b	607	CLA	CMA-C3A-C2A	-2.16	105.12	113.83
37	d	408	LHG	C5-O7-C7	-2.16	112.48	117.79
24	B	613	CLA	CHB-C1B-NB	-2.16	121.97	124.26
24	C	514	CLA	CHB-C4A-NA	2.16	127.49	124.51
24	c	510	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
26	c	516	BCR	C28-C27-C26	-2.15	110.23	114.08
24	b	621	CLA	CED-O2D-CGD	2.15	120.81	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	CED-O2D-CGD	2.15	120.80	115.94
32	D	406	PL9	C20-C19-C21	2.15	118.89	115.27
24	C	507	CLA	CMB-C2B-C1B	2.15	128.65	125.37
24	B	607	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
24	c	515	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
27	l	101	SQD	O47-C7-O49	-2.15	118.51	123.70
24	D	401	CLA	CMB-C2B-C1B	2.15	128.64	125.37
24	B	613	CLA	C11-C10-C8	-2.15	108.97	115.92
24	C	513	CLA	CBA-CAA-C2A	-2.15	107.52	113.86
26	c	526	BCR	C16-C17-C18	-2.15	124.24	127.31
24	b	610	CLA	CHB-C1B-NB	-2.15	121.98	124.26
26	a	410	BCR	C40-C30-C25	-2.15	106.82	110.30
37	d	409	LHG	O7-C7-O9	-2.15	118.51	123.70
24	B	602	CLA	C2A-C1A-CHA	-2.15	120.11	123.86
24	C	514	CLA	CBC-CAC-C3C	-2.15	106.52	112.43
24	B	610	CLA	CGD-CBD-CAD	-2.15	103.78	110.73
38	E	103	HEM	O2D-CGD-CBD	2.14	120.92	114.03
24	B	615	CLA	CED-O2D-CGD	2.14	120.79	115.94
38	e	102	HEM	C4B-C3B-C2B	-2.14	105.41	107.11
30	D	402	LMT	O5'-C5'-C4'	2.14	114.26	109.75
24	C	508	CLA	C11-C12-C13	-2.14	109.01	115.92
35	b	604	HTG	O5-C1-C2	2.14	113.00	110.31
26	B	619	BCR	C2-C1-C6	2.14	113.77	110.48
24	b	609	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
36	C	518	DGD	O6D-C1D-O3G	-2.14	104.91	109.97
24	b	619	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	a	409	CLA	CED-O2D-CGD	2.14	120.77	115.94
26	c	516	BCR	C35-C13-C14	-2.14	119.93	122.92
26	c	516	BCR	C2-C1-C6	2.14	113.77	110.48
24	C	511	CLA	CMA-C3A-C4A	-2.13	106.03	111.77
32	D	406	PL9	C15-C14-C13	-2.13	118.20	123.68
34	C	520	LMG	O6-C5-C6	2.13	111.74	106.44
32	D	406	PL9	C10-C9-C11	2.13	118.86	115.27
24	B	604	CLA	C1-O2A-CGA	2.13	122.04	116.44
24	B	602	CLA	CHB-C1B-C2B	-2.13	121.22	127.24
24	B	616	CLA	OBD-CAD-C3D	-2.13	123.39	128.52
24	C	506	CLA	CHB-C1B-NB	-2.13	122.00	124.26
24	D	401	CLA	CAA-CBA-CGA	2.13	119.48	113.25
26	y	101	BCR	C24-C23-C22	-2.13	123.02	126.23
26	c	516	BCR	C33-C5-C6	-2.13	122.14	124.53
26	h	101	BCR	C36-C18-C17	-2.13	119.94	122.92
24	B	617	CLA	C2A-C1A-CHA	-2.13	120.14	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	101	BCR	C16-C17-C18	-2.12	124.28	127.31
24	C	509	CLA	C4-C3-C5	2.12	118.84	115.27
26	C	515	BCR	C15-C14-C13	-2.12	124.28	127.31
32	a	416	PL9	C51-C49-C50	2.12	119.29	114.60
24	B	612	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
36	C	517	DGD	O6D-C5D-C6D	2.12	110.94	106.67
24	b	610	CLA	CAC-C3C-C4C	2.12	127.56	124.81
35	C	523	HTG	O5-C1-C2	2.11	112.97	110.31
24	a	407	CLA	CHB-C1B-C2B	-2.11	121.27	127.24
24	b	620	CLA	C1-C2-C3	-2.11	122.39	126.04
32	A	419	PL9	C40-C39-C41	2.11	118.83	115.27
34	C	521	LMG	O7-C10-O9	-2.11	118.60	123.70
24	B	611	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
24	B	616	CLA	O2A-CGA-CBA	2.11	118.53	111.91
24	b	621	CLA	C4-C3-C5	2.11	118.82	115.27
24	c	515	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
34	c	521	LMG	O8-C28-O10	-2.11	118.27	123.59
24	B	608	CLA	CMB-C2B-C1B	2.11	128.58	125.37
24	B	613	CLA	O2A-CGA-CBA	2.11	118.52	111.91
27	A	416	SQD	O9-S-C6	2.11	109.44	106.94
36	c	519	DGD	O1G-C1A-O1A	-2.11	118.28	123.59
24	c	506	CLA	C1-O2A-CGA	2.10	121.97	116.44
35	C	523	HTG	C1-C2-C3	-2.10	106.43	110.59
24	D	403	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
24	c	508	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
24	d	401	CLA	CHD-C4C-NC	2.10	127.52	124.20
26	y	101	BCR	C1-C6-C7	2.10	121.73	115.78
35	D	411	HTG	O5-C1-C2	2.10	112.96	110.31
24	C	507	CLA	CGD-CBD-CAD	-2.10	103.93	110.73
30	m	102	LMT	C3'-C4'-C5'	-2.10	106.11	110.93
24	c	514	CLA	CMA-C3A-C4A	-2.10	106.12	111.77
24	b	611	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
35	B	624	HTG	C1-O5-C5	2.10	116.45	112.58
25	A	407	PHO	C4A-C3A-C2A	-2.10	100.84	102.84
24	C	511	CLA	CMB-C2B-C1B	2.10	128.56	125.37
34	J	101	LMG	C7-O1-C1	-2.10	109.64	113.74
24	B	609	CLA	C1-O2A-CGA	2.09	121.94	116.44
24	b	621	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
26	B	620	BCR	C2-C3-C4	-2.09	106.70	111.38
24	B	611	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
36	D	407	DGD	O2G-C1B-O1B	-2.09	118.64	123.70
27	a	411	SQD	O48-C23-O10	-2.09	118.31	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	617	CLA	CMB-C2B-C1B	2.09	128.56	125.37
24	b	621	CLA	CHD-C4C-NC	2.09	127.50	124.20
24	B	614	CLA	CMA-C3A-C4A	-2.09	106.15	111.77
25	A	408	PHO	CAC-C3C-C4C	2.09	129.57	124.27
27	A	416	SQD	O8-S-C6	2.09	109.07	105.74
24	B	604	CLA	CMB-C2B-C1B	2.09	128.55	125.37
24	B	615	CLA	C1-C2-C3	-2.09	122.43	126.04
26	b	624	BCR	C10-C11-C12	-2.09	116.70	123.22
24	a	409	CLA	CMA-C3A-C2A	-2.09	105.40	113.83
26	D	405	BCR	C29-C30-C25	2.09	113.70	110.48
25	d	403	PHO	C4-C3-C2	-2.09	118.32	123.68
24	c	512	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
24	D	404	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
26	b	624	BCR	C15-C14-C13	-2.09	124.33	127.31
24	B	602	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
24	C	511	CLA	C6-C7-C8	-2.08	109.18	115.92
34	C	520	LMG	C30-C29-C28	-2.08	106.04	113.62
24	b	620	CLA	CHA-C1A-NA	-2.08	121.63	126.40
35	B	623	HTG	C1-O5-C5	2.08	116.42	112.58
34	C	521	LMG	O6-C5-C6	2.08	111.61	106.44
26	H	101	BCR	C24-C23-C22	-2.08	123.09	126.23
24	c	512	CLA	CHB-C4A-NA	2.08	127.39	124.51
34	b	625	LMG	O7-C10-O9	-2.08	118.67	123.70
26	K	101	BCR	C31-C1-C6	-2.08	106.93	110.30
24	c	515	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
24	c	510	CLA	C1-O2A-CGA	2.08	121.89	116.44
24	B	605	CLA	CHA-C1A-NA	-2.08	121.64	126.40
24	b	611	CLA	CHB-C4A-NA	2.08	127.38	124.51
24	A	405	CLA	CAA-CBA-CGA	-2.08	107.19	113.25
24	B	609	CLA	CHB-C4A-NA	2.08	127.38	124.51
24	b	613	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
32	D	406	PL9	C51-C49-C50	2.07	119.19	114.60
24	B	614	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
24	a	406	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
24	B	613	CLA	CMB-C2B-C1B	2.07	128.53	125.37
26	b	623	BCR	C3-C4-C5	-2.07	110.37	114.08
24	C	503	CLA	C16-C15-C13	-2.07	109.22	115.92
24	B	607	CLA	C6-C7-C8	-2.07	109.22	115.92
24	D	403	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
24	c	510	CLA	CHB-C4A-NA	2.07	127.38	124.51
24	b	609	CLA	CHA-C1A-NA	-2.07	121.65	126.40
24	b	618	CLA	CHB-C1B-NB	-2.07	122.06	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	610	CLA	C5-C3-C2	-2.07	116.93	121.12
24	C	504	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
24	C	508	CLA	CHA-C1A-NA	-2.07	121.66	126.40
40	V	203	HEC	C2A-C1A-NA	-2.07	108.31	110.32
37	l	102	LHG	C6-C5-C4	-2.06	106.90	111.79
24	C	512	CLA	CHB-C1B-NB	-2.06	122.07	124.26
24	B	602	CLA	CHB-C4A-NA	2.06	127.36	124.51
24	c	503	CLA	C1-C2-C3	-2.06	122.48	126.04
26	C	516	BCR	C40-C30-C25	-2.06	106.95	110.30
24	B	616	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
26	t	101	BCR	C35-C13-C12	2.06	121.32	118.08
24	B	604	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
34	C	501	LMG	O7-C10-O9	-2.06	118.72	123.70
34	b	625	LMG	O8-C28-O10	-2.06	118.39	123.59
24	C	505	CLA	C1-C2-C3	-2.06	122.48	126.04
24	B	603	CLA	CMA-C3A-C2A	-2.06	105.53	113.83
30	a	401	LMT	O5B-C5B-C4B	2.06	113.43	109.69
24	B	614	CLA	CMA-C3A-C2A	-2.06	105.53	113.83
26	y	101	BCR	C40-C30-C25	-2.06	106.96	110.30
24	c	508	CLA	CHB-C4A-NA	2.06	127.35	124.51
24	C	512	CLA	O2A-C1-C2	-2.05	103.23	108.64
24	C	513	CLA	CHB-C4A-NA	2.05	127.35	124.51
24	D	404	CLA	CGD-CBD-CAD	-2.05	104.08	110.73
24	b	608	CLA	C5-C3-C2	-2.05	116.96	121.12
24	B	609	CLA	CAC-C3C-C4C	2.05	127.47	124.81
26	B	620	BCR	C23-C24-C25	-2.05	121.44	127.20
32	D	406	PL9	C22-C23-C24	-2.05	122.73	127.66
25	A	407	PHO	CBC-CAC-C3C	-2.05	109.88	112.88
24	A	405	CLA	CMB-C2B-C3B	2.05	131.54	126.59
24	C	510	CLA	C16-C15-C13	-2.05	109.31	115.92
24	C	510	CLA	C4-C3-C2	-2.05	118.43	123.68
24	C	507	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
30	a	417	LMT	C1B-O1B-C4'	-2.05	112.90	117.96
26	d	405	BCR	C40-C30-C25	-2.05	106.98	110.30
24	c	509	CLA	CAA-C2A-C1A	2.04	118.68	111.97
36	h	102	DGD	C6D-C5D-C4D	2.04	116.36	112.09
24	d	402	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
24	b	612	CLA	O2A-CGA-CBA	2.04	118.32	111.91
25	d	403	PHO	O2A-CGA-O1A	-2.04	118.43	123.59
24	B	606	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
24	d	401	CLA	CHC-C1C-NC	2.04	127.30	124.20
26	A	410	BCR	C8-C7-C6	-2.04	121.47	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	617	CLA	C4-C3-C5	2.04	118.70	115.27
40	v	202	HEC	CHB-C1B-C2B	-2.04	121.79	124.98
24	C	513	CLA	CMA-C3A-C4A	-2.04	106.29	111.77
24	A	405	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
35	b	627	HTG	O5-C1-C2	2.04	112.88	110.31
24	B	617	CLA	O2A-C1-C2	2.04	113.99	108.64
26	t	101	BCR	C7-C6-C5	-2.04	116.53	121.46
24	c	515	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
27	l	101	SQD	C45-O47-C7	-2.04	112.78	117.79
30	D	402	LMT	C3B-C4B-C5B	2.04	113.87	110.24
24	b	615	CLA	C4-C3-C5	2.04	118.70	115.27
25	d	403	PHO	C4A-C3A-C2A	-2.04	100.90	102.84
24	C	508	CLA	C3B-C4B-NB	2.04	112.40	110.52
24	B	614	CLA	CHA-C1A-NA	-2.03	121.74	126.40
24	B	609	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	A	405	CLA	CHB-C1B-C2B	-2.03	121.49	127.24
24	B	614	CLA	CHD-C4C-NC	2.03	127.41	124.20
26	d	405	BCR	C38-C26-C27	2.03	117.52	113.62
24	C	513	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
26	b	623	BCR	C11-C12-C13	-2.03	120.71	126.42
26	B	618	BCR	C21-C20-C19	-2.03	116.88	123.22
36	c	517	DGD	O2G-C1B-O1B	-2.03	118.80	123.70
24	B	606	CLA	CED-O2D-CGD	2.03	120.53	115.94
26	k	103	BCR	C20-C21-C22	-2.03	124.41	127.31
24	c	504	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	B	607	CLA	CHB-C1B-C2B	-2.03	121.51	127.24
38	E	103	HEM	CHA-C1A-NA	2.03	127.58	123.85
24	a	407	CLA	CAA-CBA-CGA	2.03	119.18	113.25
24	c	506	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
24	b	607	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
24	A	405	CLA	O2A-C1-C2	2.03	113.96	108.64
25	a	408	PHO	CED-O2D-CGD	2.03	120.52	115.94
24	b	608	CLA	CHB-C1B-C2B	-2.03	121.52	127.24
24	B	614	CLA	C2A-C1A-CHA	-2.03	120.32	123.86
24	C	512	CLA	C11-C10-C8	-2.03	109.37	115.92
26	T	102	BCR	C36-C18-C19	2.03	121.27	118.08
24	b	616	CLA	CBC-CAC-C3C	-2.02	106.85	112.43
24	c	512	CLA	C1-O2A-CGA	2.02	121.75	116.44
24	D	401	CLA	OBD-CAD-C3D	-2.02	123.65	128.52
32	A	419	PL9	C25-C24-C23	-2.02	118.49	123.68
24	b	621	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
38	e	102	HEM	O2D-CGD-CBD	2.02	120.52	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	CHA-C1A-NA	-2.02	121.78	126.40
26	C	516	BCR	C15-C16-C17	-2.02	119.34	123.47
32	d	406	PL9	C12-C13-C14	-2.02	122.80	127.66
40	v	202	HEC	O2D-CGD-CBD	2.02	120.51	114.03
26	c	526	BCR	C21-C20-C19	-2.02	116.92	123.22
26	K	101	BCR	C38-C26-C25	-2.02	122.27	124.53
24	C	511	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
24	c	504	CLA	CMC-C2C-C1C	2.01	128.10	125.04
24	b	615	CLA	CHB-C4A-NA	2.01	127.29	124.51
26	A	410	BCR	C36-C18-C17	-2.01	120.11	122.92
36	d	407	DGD	O6D-C5D-C6D	2.01	110.72	106.67
36	C	519	DGD	O1G-C1A-C2A	2.01	118.22	111.91
24	b	611	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
38	E	103	HEM	O2D-CGD-O1D	-2.01	118.29	123.30
26	b	624	BCR	C21-C20-C19	-2.01	116.95	123.22
37	e	101	LHG	O8-C23-O10	-2.01	118.53	123.59
32	D	406	PL9	C31-C32-C33	-2.01	105.29	111.88
26	a	410	BCR	C20-C21-C22	-2.01	124.45	127.31
24	B	608	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
24	B	614	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	c	514	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
24	c	508	CLA	C2A-C1A-CHA	-2.00	120.35	123.86
24	B	610	CLA	CHB-C1B-NB	-2.00	122.14	124.26
24	b	617	CLA	CHB-C4A-NA	2.00	127.28	124.51
35	D	411	HTG	O5-C1-S1	-2.00	105.04	109.82
34	Z	101	LMG	C9-O8-C28	2.00	122.13	117.10
24	b	617	CLA	C4D-CHA-C1A	-2.00	118.81	121.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	203	HEC	NA
40	v	202	HEC	NA

All (1243) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2-C3-C5-C6
24	B	615	CLA	C4-C3-C5-C6
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	508	CLA	C2-C3-C5-C6
24	C	508	CLA	C4-C3-C5-C6
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	C	514	CLA	C2B-C3B-CAB-CBB
24	C	514	CLA	C4B-C3B-CAB-CBB
24	D	401	CLA	CHA-CBD-CGD-O1D
24	D	401	CLA	CHA-CBD-CGD-O2D
24	b	610	CLA	C2-C3-C5-C6
24	b	610	CLA	C4-C3-C5-C6
24	b	611	CLA	C2B-C3B-CAB-CBB
24	b	611	CLA	C4B-C3B-CAB-CBB
24	b	611	CLA	CHA-CBD-CGD-O1D
24	b	611	CLA	CHA-CBD-CGD-O2D
24	b	619	CLA	CHA-CBD-CGD-O1D
24	b	619	CLA	CHA-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O1D
24	b	619	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
24	c	515	CLA	C2B-C3B-CAB-CBB
24	c	515	CLA	C4B-C3B-CAB-CBB
26	B	618	BCR	C1-C6-C7-C8
26	D	405	BCR	C37-C22-C23-C24
26	D	405	BCR	C23-C24-C25-C30
26	Y	101	BCR	C21-C22-C23-C24
26	Y	101	BCR	C37-C22-C23-C24
26	d	405	BCR	C37-C22-C23-C24
26	d	405	BCR	C23-C24-C25-C30
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
27	A	411	SQD	C5-C6-S-O8
27	A	416	SQD	O6-C44-C45-O47
27	F	101	SQD	C8-C7-O47-C45
27	a	402	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
27	b	601	SQD	O5-C1-O6-C44
27	b	601	SQD	O49-C7-O47-C45
27	b	601	SQD	C5-C6-S-O7
27	b	601	SQD	C5-C6-S-O8
27	b	601	SQD	C5-C6-S-O9
27	f	101	SQD	O49-C7-O47-C45
27	f	101	SQD	C8-C7-O47-C45
27	f	101	SQD	C5-C6-S-O7
27	f	101	SQD	C5-C6-S-O8
27	f	101	SQD	C5-C6-S-O9
27	l	101	SQD	O49-C7-O47-C45
28	A	414	GOL	O1-C1-C2-C3
28	B	626	GOL	O1-C1-C2-C3
28	B	627	GOL	O1-C1-C2-C3
28	C	524	GOL	O1-C1-C2-C3
28	F	103	GOL	O1-C1-C2-C3
28	O	302	GOL	O1-C1-C2-C3
28	T	101	GOL	O1-C1-C2-C3
28	T	103	GOL	O1-C1-C2-C3
28	V	205	GOL	O1-C1-C2-C3
28	V	205	GOL	C1-C2-C3-O3
28	V	208	GOL	O1-C1-C2-C3
28	a	412	GOL	C1-C2-C3-O3
28	b	631	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
28	v	203	GOL	C1-C2-C3-O3
28	v	204	GOL	O1-C1-C2-C3
28	v	205	GOL	O1-C1-C2-C3
30	B	634	LMT	C2'-C1'-O1'-C1
30	B	634	LMT	O5'-C1'-O1'-C1
30	E	102	LMT	C2'-C1'-O1'-C1
30	E	102	LMT	O5'-C1'-O1'-C1
30	I	102	LMT	C2'-C1'-O1'-C1
30	I	102	LMT	O5'-C1'-O1'-C1
30	M	101	LMT	O5'-C1'-O1'-C1
30	a	401	LMT	C2'-C1'-O1'-C1
30	a	401	LMT	O5'-C1'-O1'-C1
30	a	417	LMT	C2'-C1'-O1'-C1
30	b	602	LMT	C2'-C1'-O1'-C1
30	b	602	LMT	O5'-C1'-O1'-C1
30	b	626	LMT	C2'-C1'-O1'-C1
30	b	626	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
30	f	102	LMT	C2'-C1'-O1'-C1
30	f	102	LMT	O5'-C1'-O1'-C1
32	a	416	PL9	C18-C19-C21-C22
32	a	416	PL9	C20-C19-C21-C22
32	a	416	PL9	C28-C29-C31-C32
32	a	416	PL9	C30-C29-C31-C32
34	C	501	LMG	O9-C10-O7-C8
34	C	501	LMG	C11-C10-O7-C8
34	Z	101	LMG	C2-C1-O1-C7
34	Z	101	LMG	O6-C1-O1-C7
34	Z	101	LMG	O9-C10-O7-C8
34	z	101	LMG	O9-C10-O7-C8
35	B	623	HTG	C2'-C1'-S1-C1
35	C	522	HTG	C2'-C1'-S1-C1
35	V	204	HTG	C2-C1-S1-C1'
35	V	204	HTG	O5-C1-S1-C1'
36	D	407	DGD	O1B-C1B-O2G-C2G
36	D	407	DGD	C2D-C1D-O3G-C3G
36	D	407	DGD	O6D-C1D-O3G-C3G
36	D	407	DGD	C2E-C1E-O5D-C6D
36	D	407	DGD	O6E-C1E-O5D-C6D
36	d	407	DGD	O1B-C1B-O2G-C2G
36	d	407	DGD	C2E-C1E-O5D-C6D
36	d	407	DGD	O6E-C1E-O5D-C6D
37	D	409	LHG	C3-O3-P-O6
37	D	409	LHG	C4-O6-P-O4
37	E	101	LHG	C4-O6-P-O3
37	E	101	LHG	C4-O6-P-O5
37	E	101	LHG	O10-C23-O8-C6
37	E	101	LHG	C24-C23-O8-C6
37	L	101	LHG	C4-O6-P-O4
37	d	409	LHG	O2-C2-C3-O3
37	d	409	LHG	C3-O3-P-O4
37	d	409	LHG	C4-O6-P-O4
37	e	101	LHG	C4-O6-P-O5
37	e	101	LHG	O7-C5-C6-O8
37	l	102	LHG	C4-O6-P-O3
37	l	102	LHG	C4-O6-P-O4
37	l	102	LHG	C4-O6-P-O5
37	e	101	LHG	O10-C23-O8-C6
27	F	101	SQD	O49-C7-O47-C45
27	F	101	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
27	b	601	SQD	C8-C7-O47-C45
27	l	101	SQD	C8-C7-O47-C45
34	Z	101	LMG	C11-C10-O7-C8
34	z	101	LMG	C11-C10-O7-C8
36	D	407	DGD	C2B-C1B-O2G-C2G
36	d	407	DGD	C2B-C1B-O2G-C2G
32	a	416	PL9	C25-C24-C26-C27
37	e	101	LHG	C24-C23-O8-C6
30	M	101	LMT	O5'-C5'-C6'-O6'
34	Z	101	LMG	C4-C5-C6-O5
30	I	102	LMT	O5B-C5B-C6B-O6B
24	b	619	CLA	C3-C5-C6-C7
24	b	621	CLA	C3-C5-C6-C7
27	F	101	SQD	O10-C23-O48-C46
34	Z	101	LMG	O6-C5-C6-O5
30	M	101	LMT	C4'-C5'-C6'-O6'
27	b	601	SQD	C31-C32-C33-C34
30	I	102	LMT	C3'-C4'-O1B-C1B
34	C	521	LMG	O6-C5-C6-O5
40	V	203	HEC	C2C-C3C-CAC-CBC
35	C	522	HTG	S1-C1'-C2'-C3'
37	d	410	LHG	C30-C31-C32-C33
30	D	402	LMT	O5B-C5B-C6B-O6B
24	B	617	CLA	C4-C3-C5-C6
24	b	619	CLA	C4-C3-C5-C6
32	A	419	PL9	C25-C24-C26-C27
32	a	416	PL9	C15-C14-C16-C17
24	B	617	CLA	C2-C3-C5-C6
24	b	619	CLA	C2-C3-C5-C6
32	A	419	PL9	C23-C24-C26-C27
32	a	416	PL9	C13-C14-C16-C17
32	a	416	PL9	C23-C24-C26-C27
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	611	CLA	C2A-CAA-CBA-CGA
30	a	417	LMT	O5'-C1'-O1'-C1
36	c	518	DGD	C3B-C4B-C5B-C6B
35	C	523	HTG	O5-C5-C6-O6
37	d	409	LHG	C1-C2-C3-O3
24	C	507	CLA	C3-C5-C6-C7
24	c	508	CLA	C15-C16-C17-C18
24	b	608	CLA	CBD-CGD-O2D-CED
36	d	407	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
36	d	407	DGD	C2A-C1A-O1G-C1G
24	B	603	CLA	C14-C13-C15-C16
24	d	401	CLA	CBD-CGD-O2D-CED
26	B	620	BCR	C7-C8-C9-C34
26	d	405	BCR	C7-C8-C9-C34
26	D	405	BCR	C21-C22-C23-C24
26	d	405	BCR	C21-C22-C23-C24
30	D	402	LMT	C4B-C5B-C6B-O6B
24	C	510	CLA	C8-C10-C11-C12
24	c	514	CLA	C10-C11-C12-C13
40	V	203	HEC	C4C-C3C-CAC-CBC
24	B	603	CLA	C15-C16-C17-C18
24	b	609	CLA	C15-C16-C17-C18
24	b	621	CLA	C10-C11-C12-C13
35	b	628	HTG	C1'-C2'-C3'-C4'
24	B	615	CLA	C10-C11-C12-C13
24	b	620	CLA	C10-C11-C12-C13
28	V	206	GOL	O1-C1-C2-O2
28	b	629	GOL	O2-C2-C3-O3
28	b	631	GOL	O1-C1-C2-O2
28	b	633	GOL	O1-C1-C2-O2
27	F	101	SQD	C23-C24-C25-C26
27	l	101	SQD	C7-C8-C9-C10
34	C	521	LMG	C28-C29-C30-C31
24	C	510	CLA	C2-C1-O2A-CGA
24	b	606	CLA	C2-C1-O2A-CGA
24	B	612	CLA	C15-C16-C17-C18
24	b	606	CLA	C10-C11-C12-C13
24	b	618	CLA	C8-C10-C11-C12
36	C	518	DGD	C1B-C2B-C3B-C4B
24	B	614	CLA	C11-C10-C8-C7
24	B	605	CLA	C3-C5-C6-C7
24	b	606	CLA	C8-C10-C11-C12
27	f	101	SQD	C31-C32-C33-C34
36	d	407	DGD	O6D-C1D-O3G-C3G
24	A	409	CLA	C15-C16-C17-C18
24	B	614	CLA	C8-C10-C11-C12
32	D	406	PL9	C39-C41-C42-C43
32	a	416	PL9	C9-C11-C12-C13
32	a	416	PL9	C14-C16-C17-C18
30	E	102	LMT	O1'-C1-C2-C3
30	M	101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
40	v	202	HEC	C2B-C3B-CAB-CBB
36	D	407	DGD	C1A-C2A-C3A-C4A
36	C	519	DGD	C6B-C7B-C8B-C9B
24	B	602	CLA	C3-C5-C6-C7
24	B	617	CLA	C3-C5-C6-C7
24	b	608	CLA	C5-C6-C7-C8
37	d	408	LHG	C24-C23-O8-C6
36	d	407	DGD	O1A-C1A-O1G-C1G
24	c	512	CLA	C8-C10-C11-C12
24	B	614	CLA	C15-C16-C17-C18
24	B	616	CLA	C10-C11-C12-C13
24	c	511	CLA	C13-C15-C16-C17
37	L	101	LHG	C4-O6-P-O3
37	d	409	LHG	C3-O3-P-O6
37	e	101	LHG	C3-O3-P-O6
35	B	623	HTG	C1'-C2'-C3'-C4'
24	A	409	CLA	C8-C10-C11-C12
24	B	614	CLA	C13-C15-C16-C17
24	b	619	CLA	C15-C16-C17-C18
30	a	401	LMT	C4B-C5B-C6B-O6B
37	D	410	LHG	C30-C31-C32-C33
24	a	406	CLA	C2C-C3C-CAC-CBC
40	V	203	HEC	C2B-C3B-CAB-CBB
24	b	611	CLA	C3-C5-C6-C7
30	D	402	LMT	C5'-C4'-O1B-C1B
30	I	102	LMT	C4B-C5B-C6B-O6B
34	J	101	LMG	C35-C36-C37-C38
37	E	101	LHG	C8-C7-O7-C5
27	a	402	SQD	C16-C17-C18-C19
35	B	623	HTG	C2'-C3'-C4'-C5'
36	C	517	DGD	CBA-CCA-CDA-CEA
36	C	517	DGD	C4B-C5B-C6B-C7B
36	C	517	DGD	C5B-C6B-C7B-C8B
36	D	407	DGD	CBA-CCA-CDA-CEA
36	c	517	DGD	C5A-C6A-C7A-C8A
37	d	410	LHG	C9-C10-C11-C12
37	d	410	LHG	C13-C14-C15-C16
24	b	620	CLA	C16-C17-C18-C20
36	h	102	DGD	C6A-C7A-C8A-C9A
37	d	410	LHG	C29-C30-C31-C32
37	E	101	LHG	O9-C7-O7-C5
27	f	101	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	B	621	LMG	C36-C37-C38-C39
34	C	521	LMG	C17-C18-C19-C20
34	b	625	LMG	C16-C17-C18-C19
30	E	102	LMT	C4-C5-C6-C7
34	C	520	LMG	C38-C39-C40-C41
36	H	102	DGD	C7A-C8A-C9A-CAA
27	F	101	SQD	C28-C29-C30-C31
37	D	408	LHG	C30-C31-C32-C33
27	a	411	SQD	C7-C8-C9-C10
34	C	501	LMG	C2-C1-O1-C7
36	c	518	DGD	C2E-C1E-O5D-C6D
27	b	601	SQD	C17-C18-C19-C20
27	f	101	SQD	C25-C26-C27-C28
36	d	407	DGD	C4B-C5B-C6B-C7B
37	d	408	LHG	O10-C23-O8-C6
24	C	502	CLA	C16-C17-C18-C19
32	d	406	PL9	C15-C14-C16-C17
27	b	601	SQD	C11-C10-C9-C8
36	D	407	DGD	C4A-C5A-C6A-C7A
36	d	407	DGD	C8B-C9B-CAB-CBB
37	l	102	LHG	C14-C15-C16-C17
32	d	406	PL9	C13-C14-C16-C17
24	A	406	CLA	C6-C7-C8-C9
24	C	511	CLA	C6-C7-C8-C9
24	c	508	CLA	C14-C13-C15-C16
36	C	517	DGD	O6D-C5D-C6D-O5D
34	C	520	LMG	C10-C11-C12-C13
27	l	101	SQD	C28-C29-C30-C31
30	B	634	LMT	C2-C3-C4-C5
30	b	602	LMT	C3-C4-C5-C6
34	C	521	LMG	C16-C17-C18-C19
36	C	518	DGD	C4B-C5B-C6B-C7B
36	c	518	DGD	C5A-C6A-C7A-C8A
36	c	518	DGD	C2B-C3B-C4B-C5B
37	d	410	LHG	C10-C11-C12-C13
28	A	413	GOL	C1-C2-C3-O3
28	B	625	GOL	C1-C2-C3-O3
28	B	628	GOL	O1-C1-C2-C3
28	B	635	GOL	O1-C1-C2-C3
28	V	206	GOL	O1-C1-C2-C3
28	a	413	GOL	C1-C2-C3-O3
28	b	629	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	b	632	GOL	C1-C2-C3-O3
28	b	633	GOL	O1-C1-C2-C3
28	c	527	GOL	O1-C1-C2-C3
28	f	104	GOL	C1-C2-C3-O3
24	c	514	CLA	C3-C5-C6-C7
24	b	611	CLA	C13-C15-C16-C17
36	C	519	DGD	CBA-CCA-CDA-CEA
27	a	402	SQD	C10-C11-C12-C13
30	B	634	LMT	C3-C4-C5-C6
30	D	402	LMT	C3'-C4'-O1B-C1B
34	b	625	LMG	C30-C31-C32-C33
34	c	501	LMG	C12-C13-C14-C15
36	C	518	DGD	C5A-C6A-C7A-C8A
36	h	102	DGD	C7A-C8A-C9A-CAA
37	D	410	LHG	C31-C32-C33-C34
30	m	103	LMT	O5B-C5B-C6B-O6B
24	C	506	CLA	C4B-C3B-CAB-CBB
24	c	507	CLA	C4B-C3B-CAB-CBB
24	c	514	CLA	C4B-C3B-CAB-CBB
24	b	620	CLA	C16-C17-C18-C19
34	C	501	LMG	O6-C1-O1-C7
32	d	406	PL9	C39-C41-C42-C43
27	a	402	SQD	C17-C18-C19-C20
27	a	402	SQD	C25-C26-C27-C28
27	a	402	SQD	C34-C35-C36-C37
27	l	101	SQD	C29-C30-C31-C32
34	Z	101	LMG	C19-C20-C21-C22
37	E	101	LHG	C9-C10-C11-C12
30	I	102	LMT	C5-C6-C7-C8
34	c	501	LMG	C16-C17-C18-C19
36	h	102	DGD	C5B-C6B-C7B-C8B
27	l	101	SQD	C31-C32-C33-C34
37	d	410	LHG	C15-C16-C17-C18
24	B	617	CLA	C8-C10-C11-C12
30	M	101	LMT	C2-C1-O1'-C1'
34	C	521	LMG	C15-C16-C17-C18
34	J	101	LMG	C19-C20-C21-C22
36	H	102	DGD	CCA-CDA-CEA-CFA
36	c	517	DGD	O6D-C5D-C6D-O5D
30	m	103	LMT	C11-C10-C9-C8
36	H	102	DGD	CBA-CCA-CDA-CEA
24	b	606	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	c	512	CLA	C2-C3-C5-C6
28	A	414	GOL	O1-C1-C2-O2
28	B	625	GOL	O2-C2-C3-O3
28	B	626	GOL	O1-C1-C2-O2
28	B	627	GOL	O1-C1-C2-O2
28	B	635	GOL	O1-C1-C2-O2
28	F	103	GOL	O1-C1-C2-O2
28	T	103	GOL	O1-C1-C2-O2
28	V	205	GOL	O1-C1-C2-O2
28	V	208	GOL	O1-C1-C2-O2
28	a	412	GOL	O2-C2-C3-O3
28	v	205	GOL	O1-C1-C2-O2
24	C	508	CLA	C5-C6-C7-C8
37	l	102	LHG	C31-C32-C33-C34
24	C	506	CLA	C2B-C3B-CAB-CBB
24	D	403	CLA	C2B-C3B-CAB-CBB
24	c	507	CLA	C2B-C3B-CAB-CBB
24	c	514	CLA	C2B-C3B-CAB-CBB
24	d	401	CLA	C2C-C3C-CAC-CBC
34	b	625	LMG	C17-C18-C19-C20
34	z	101	LMG	C12-C13-C14-C15
36	C	518	DGD	CAB-CBB-CCB-CDB
24	B	617	CLA	C2-C1-O2A-CGA
36	d	407	DGD	C4A-C5A-C6A-C7A
36	d	407	DGD	CCB-CDB-CEB-CFB
30	I	102	LMT	C6-C7-C8-C9
37	L	101	LHG	C34-C35-C36-C37
26	B	618	BCR	C5-C6-C7-C8
26	B	620	BCR	C5-C6-C7-C8
26	D	405	BCR	C23-C24-C25-C26
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	b	622	BCR	C1-C6-C7-C8
26	b	622	BCR	C5-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C26
34	c	501	LMG	C30-C31-C32-C33
24	B	602	CLA	C10-C11-C12-C13
34	b	625	LMG	C11-C10-O7-C8
27	l	101	SQD	C26-C27-C28-C29
37	d	410	LHG	C12-C13-C14-C15
36	C	518	DGD	C1A-C2A-C3A-C4A
30	A	417	LMT	O1'-C1-C2-C3

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

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Mol	Chain	Res	Type	Atoms
34	C	520	LMG	O9-C10-O7-C8
37	D	408	LHG	C23-C24-C25-C26
34	C	501	LMG	C14-C15-C16-C17
34	C	501	LMG	C13-C14-C15-C16
37	D	408	LHG	C29-C30-C31-C32
37	e	101	LHG	C14-C15-C16-C17
24	C	502	CLA	C16-C17-C18-C20
27	A	411	SQD	C10-C11-C12-C13
36	C	518	DGD	CAA-CBA-CCA-CDA
36	c	517	DGD	C2A-C3A-C4A-C5A
36	c	517	DGD	O6E-C5E-C6E-O5E
24	D	404	CLA	C4-C3-C5-C6
24	B	606	CLA	C2-C3-C5-C6
25	A	407	PHO	C2-C3-C5-C6
32	A	419	PL9	C4-C3-C7-C8
32	a	416	PL9	C4-C3-C7-C8
36	c	519	DGD	CBA-CCA-CDA-CEA
37	d	410	LHG	C31-C32-C33-C34
37	e	101	LHG	C13-C14-C15-C16
24	B	614	CLA	C11-C10-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	C	513	CLA	C11-C10-C8-C9
30	D	402	LMT	C6-C7-C8-C9
37	D	410	LHG	C32-C33-C34-C35
34	J	101	LMG	O6-C5-C6-O5
35	d	411	HTG	C4-C5-C6-O6
30	a	401	LMT	C7-C8-C9-C10
37	D	410	LHG	C10-C11-C12-C13
24	c	513	CLA	O1A-CGA-O2A-C1
24	c	514	CLA	O1A-CGA-O2A-C1
24	C	512	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
34	b	625	LMG	O9-C10-O7-C8
27	A	416	SQD	C18-C19-C20-C21
30	a	401	LMT	C5-C6-C7-C8
36	D	407	DGD	C9B-CAB-CBB-CCB
24	b	618	CLA	C10-C11-C12-C13
24	a	409	CLA	C13-C15-C16-C17
24	c	511	CLA	C8-C10-C11-C12
37	l	102	LHG	O6-C4-C5-C6
35	b	627	HTG	S1-C1'-C2'-C3'
36	h	102	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CBA-CGA-O2A-C1
34	c	501	LMG	O9-C10-O7-C8
24	d	404	CLA	C4-C3-C5-C6
27	b	601	SQD	C28-C29-C30-C31
36	C	518	DGD	C9A-CAA-CBA-CCA
34	C	501	LMG	C28-C29-C30-C31
37	D	410	LHG	C28-C29-C30-C31
36	C	517	DGD	O6E-C5E-C6E-O5E
24	b	606	CLA	C3-C5-C6-C7
27	A	416	SQD	O6-C44-C45-C46
27	b	601	SQD	C44-C45-C46-O48
27	f	101	SQD	C44-C45-C46-O48
34	C	501	LMG	O1-C7-C8-C9
36	c	518	DGD	C4B-C5B-C6B-C7B
36	d	407	DGD	O1G-C1G-C2G-C3G
37	L	101	LHG	C13-C14-C15-C16
37	d	408	LHG	C29-C30-C31-C32
37	e	101	LHG	C4-C5-C6-O8
37	l	102	LHG	C25-C26-C27-C28
30	a	401	LMT	O5B-C5B-C6B-O6B
34	j	101	LMG	O6-C5-C6-O5
24	c	505	CLA	C8-C10-C11-C12
37	l	102	LHG	C13-C14-C15-C16
36	C	518	DGD	C2G-C3G-O3G-C1D
36	C	518	DGD	C5D-C6D-O5D-C1E
36	c	518	DGD	C2G-C3G-O3G-C1D
36	c	518	DGD	C5D-C6D-O5D-C1E
34	C	520	LMG	C39-C40-C41-C42
30	M	102	LMT	O5'-C5'-C6'-O6'
36	c	517	DGD	C4D-C5D-C6D-O5D
34	C	521	LMG	C18-C19-C20-C21
40	v	202	HEC	C4B-C3B-CAB-CBB
27	a	411	SQD	C10-C11-C12-C13
28	C	524	GOL	O1-C1-C2-O2
28	T	101	GOL	O1-C1-C2-O2
28	a	413	GOL	O2-C2-C3-O3
28	v	203	GOL	O1-C1-C2-O2
28	v	204	GOL	O1-C1-C2-O2
35	V	204	HTG	C2'-C3'-C4'-C5'
24	d	401	CLA	O1D-CGD-O2D-CED
24	a	409	CLA	C10-C11-C12-C13
24	B	610	CLA	C4-C3-C5-C6

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

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C14-C13-C15-C16
24	B	616	CLA	C14-C13-C15-C16
24	D	404	CLA	C11-C10-C8-C9
24	b	606	CLA	C6-C7-C8-C9
24	b	619	CLA	C11-C12-C13-C14
24	c	508	CLA	C11-C10-C8-C9
24	c	511	CLA	C14-C13-C15-C16
24	c	513	CLA	CBD-CGD-O2D-CED
27	l	101	SQD	C11-C10-C9-C8
34	J	101	LMG	C16-C17-C18-C19
36	C	517	DGD	CAA-CBA-CCA-CDA
37	D	409	LHG	C32-C33-C34-C35
24	b	621	CLA	CBA-CGA-O2A-C1
24	C	503	CLA	C16-C17-C18-C20
35	b	627	HTG	C2'-C3'-C4'-C5'
36	h	102	DGD	CDA-CEA-CFA-CGA
27	b	601	SQD	C9-C10-C11-C12
36	c	519	DGD	C3B-C4B-C5B-C6B
24	c	515	CLA	C10-C11-C12-C13
24	A	409	CLA	CBA-CGA-O2A-C1
27	l	101	SQD	C12-C13-C14-C15
24	B	616	CLA	C4B-C3B-CAB-CBB
24	C	503	CLA	C4B-C3B-CAB-CBB
24	D	403	CLA	C4B-C3B-CAB-CBB
24	b	612	CLA	C4B-C3B-CAB-CBB
24	c	503	CLA	C4B-C3B-CAB-CBB
24	c	504	CLA	C4B-C3B-CAB-CBB
24	c	506	CLA	C4B-C3B-CAB-CBB
24	d	402	CLA	C4B-C3B-CAB-CBB
37	e	101	LHG	O6-C4-C5-C6
37	e	101	LHG	C11-C12-C13-C14
40	V	203	HEC	C4B-C3B-CAB-CBB
32	A	419	PL9	C30-C29-C31-C32
24	B	616	CLA	C2-C3-C5-C6
36	c	517	DGD	CBB-CCB-CDB-CEB
27	a	411	SQD	C11-C12-C13-C14
34	c	501	LMG	C29-C30-C31-C32
24	a	406	CLA	C4C-C3C-CAC-CBC
27	a	402	SQD	C26-C27-C28-C29
24	C	513	CLA	CBA-CGA-O2A-C1
24	B	602	CLA	C3A-C2A-CAA-CBA
34	B	621	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
36	H	102	DGD	C5B-C6B-C7B-C8B
36	c	518	DGD	CAA-CBA-CCA-CDA
34	Z	101	LMG	C14-C15-C16-C17
34	j	101	LMG	C13-C14-C15-C16
37	E	101	LHG	C25-C26-C27-C28
24	b	616	CLA	C15-C16-C17-C18
27	l	101	SQD	C44-C45-C46-O48
34	Z	101	LMG	C7-C8-C9-O8
36	D	407	DGD	O1G-C1G-C2G-C3G
37	E	101	LHG	C4-C5-C6-O8
34	c	501	LMG	C19-C20-C21-C22
34	c	521	LMG	C38-C39-C40-C41
34	J	101	LMG	C17-C18-C19-C20
36	c	518	DGD	C8A-C9A-CAA-CBA
34	c	501	LMG	C34-C35-C36-C37
34	c	521	LMG	C30-C31-C32-C33
36	h	102	DGD	C9B-CAB-CBB-CCB
27	A	416	SQD	C23-C24-C25-C26
34	b	625	LMG	C28-C29-C30-C31
24	b	608	CLA	O1D-CGD-O2D-CED
28	A	413	GOL	O2-C2-C3-O3
28	B	628	GOL	O1-C1-C2-O2
28	O	302	GOL	O1-C1-C2-O2
28	V	205	GOL	O2-C2-C3-O3
28	v	203	GOL	O2-C2-C3-O3
37	L	101	LHG	C14-C15-C16-C17
37	l	102	LHG	O6-C4-C5-O7
30	b	626	LMT	C1-C2-C3-C4
30	b	626	LMT	C3'-C4'-O1B-C1B
24	A	409	CLA	O1A-CGA-O2A-C1
34	B	621	LMG	C28-C29-C30-C31
24	B	616	CLA	C2B-C3B-CAB-CBB
24	C	503	CLA	C2B-C3B-CAB-CBB
24	b	612	CLA	C2B-C3B-CAB-CBB
24	c	503	CLA	C2B-C3B-CAB-CBB
24	d	402	CLA	C2B-C3B-CAB-CBB
36	C	517	DGD	CDA-CEA-CFA-CGA
36	c	517	DGD	C4A-C5A-C6A-C7A
24	a	409	CLA	C8-C10-C11-C12
36	d	407	DGD	C9A-CAA-CBA-CCA
37	E	101	LHG	C17-C18-C19-C20
27	l	101	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
34	C	501	LMG	O1-C7-C8-O7
37	E	101	LHG	O7-C5-C6-O8
36	H	102	DGD	CBB-CCB-CDB-CEB
34	z	101	LMG	C11-C12-C13-C14
36	c	518	DGD	C4A-C5A-C6A-C7A
30	E	102	LMT	C5-C6-C7-C8
24	C	510	CLA	C10-C11-C12-C13
24	A	409	CLA	C14-C13-C15-C16
24	C	505	CLA	C14-C13-C15-C16
24	C	507	CLA	C6-C7-C8-C9
24	C	507	CLA	C11-C12-C13-C14
24	b	607	CLA	C14-C13-C15-C16
24	c	507	CLA	C11-C12-C13-C14
24	c	514	CLA	C6-C7-C8-C9
34	C	501	LMG	C11-C12-C13-C14
24	B	617	CLA	C5-C6-C7-C8
24	C	511	CLA	C8-C10-C11-C12
30	m	103	LMT	C1-C2-C3-C4
24	C	514	CLA	C16-C17-C18-C19
30	f	102	LMT	C4'-C5'-C6'-O6'
30	E	102	LMT	C2-C3-C4-C5
26	B	620	BCR	C7-C8-C9-C10
26	d	405	BCR	C7-C8-C9-C10
24	c	506	CLA	C15-C16-C17-C18
24	b	616	CLA	C13-C15-C16-C17
24	B	616	CLA	C8-C10-C11-C12
24	B	603	CLA	C12-C13-C15-C16
24	B	612	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C15
24	B	615	CLA	C12-C13-C15-C16
24	C	505	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C15
24	b	606	CLA	C6-C7-C8-C10
24	b	621	CLA	C11-C12-C13-C15
24	c	511	CLA	C12-C13-C15-C16
32	A	419	PL9	C28-C29-C31-C32
24	b	621	CLA	O1A-CGA-O2A-C1
36	D	407	DGD	C2A-C3A-C4A-C5A
27	f	101	SQD	C32-C33-C34-C35
27	A	411	SQD	C16-C17-C18-C19
30	B	634	LMT	C11-C10-C9-C8
34	B	621	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	d	401	CLA	C4C-C3C-CAC-CBC
24	b	612	CLA	C3-C5-C6-C7
30	I	102	LMT	C5'-C4'-O1B-C1B
24	c	511	CLA	C10-C11-C12-C13
27	a	402	SQD	C30-C31-C32-C33
30	E	102	LMT	C3-C4-C5-C6
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	511	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	b	618	CLA	CAD-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O2D
24	c	514	CLA	CAD-CBD-CGD-O2D
24	c	515	CLA	CAD-CBD-CGD-O2D
24	d	404	CLA	CAD-CBD-CGD-O2D
34	c	501	LMG	C20-C21-C22-C23
24	B	602	CLA	C8-C10-C11-C12
24	C	507	CLA	C5-C6-C7-C8
36	H	102	DGD	CDB-CEB-CFB-CGB
24	c	505	CLA	CBD-CGD-O2D-CED
34	z	101	LMG	O6-C1-O1-C7
36	C	518	DGD	O6E-C1E-O5D-C6D
24	C	509	CLA	C13-C15-C16-C17
27	F	101	SQD	C44-C45-C46-O48
27	a	402	SQD	O6-C44-C45-C46
37	D	410	LHG	C2-C3-O3-P
37	d	410	LHG	C2-C3-O3-P
24	c	514	CLA	CBD-CGD-O2D-CED
37	D	410	LHG	C34-C35-C36-C37
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	512	CLA	O1A-CGA-O2A-C1
30	f	102	LMT	C9-C10-C11-C12
27	F	101	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
34	Z	101	LMG	O7-C8-C9-O8
24	c	511	CLA	C16-C17-C18-C19
28	a	413	GOL	O1-C1-C2-O2
28	c	527	GOL	O1-C1-C2-O2
28	f	104	GOL	O2-C2-C3-O3
34	j	101	LMG	C29-C30-C31-C32
24	b	621	CLA	C4-C3-C5-C6
24	b	621	CLA	C2-C3-C5-C6
27	b	601	SQD	C13-C14-C15-C16
27	A	416	SQD	C5-C6-S-O8
24	B	602	CLA	C2A-CAA-CBA-CGA
24	c	512	CLA	CBA-CGA-O2A-C1
34	j	101	LMG	C10-C11-C12-C13
27	l	101	SQD	C15-C16-C17-C18
36	D	407	DGD	CCA-CDA-CEA-CFA
24	C	507	CLA	C1A-C2A-CAA-CBA
37	D	409	LHG	C4-O6-P-O3
37	d	409	LHG	C4-O6-P-O3
37	l	102	LHG	C10-C11-C12-C13
34	b	625	LMG	C15-C16-C17-C18
24	D	404	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
36	C	518	DGD	C8A-C9A-CAA-CBA
24	D	404	CLA	C4B-C3B-CAB-CBB
24	a	407	CLA	C4B-C3B-CAB-CBB
32	a	416	PL9	C3-C7-C8-C9
37	D	409	LHG	C3-O3-P-O4
37	D	409	LHG	C4-O6-P-O5
37	L	101	LHG	C4-O6-P-O5
37	e	101	LHG	C3-O3-P-O5
27	A	416	SQD	C17-C18-C19-C20
36	H	102	DGD	CDA-CEA-CFA-CGA
34	C	520	LMG	C16-C17-C18-C19
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	b	606	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
27	A	411	SQD	C5-C6-S-O7

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Mol	Chain	Res	Type	Atoms
36	c	519	DGD	C1B-C2B-C3B-C4B
30	M	101	LMT	C2-C3-C4-C5
34	c	501	LMG	C22-C23-C24-C25
34	Z	101	LMG	C12-C13-C14-C15
24	c	513	CLA	O1D-CGD-O2D-CED
27	A	411	SQD	C17-C18-C19-C20
36	d	407	DGD	C5A-C6A-C7A-C8A
24	b	614	CLA	C4-C3-C5-C6
24	A	406	CLA	C12-C13-C15-C16
24	C	502	CLA	C12-C13-C15-C16
24	b	611	CLA	C12-C13-C15-C16
37	e	101	LHG	O6-C4-C5-O7
34	z	101	LMG	C18-C19-C20-C21
34	j	101	LMG	C28-C29-C30-C31
36	c	517	DGD	CAB-CBB-CCB-CDB
36	h	102	DGD	C9A-CAA-CBA-CCA
24	C	514	CLA	C16-C17-C18-C20
34	C	521	LMG	C4-C5-C6-O5
24	B	602	CLA	CAA-CBA-CGA-O2A
24	a	409	CLA	O1A-CGA-O2A-C1
27	b	601	SQD	O47-C45-C46-O48
36	d	407	DGD	O1G-C1G-C2G-O2G
34	C	521	LMG	C8-C7-O1-C1
27	A	416	SQD	C19-C20-C21-C22
40	v	202	HEC	C2C-C3C-CAC-CBC
24	d	404	CLA	C2-C3-C5-C6
37	D	410	LHG	C33-C34-C35-C36
24	B	612	CLA	C14-C13-C15-C16
24	b	621	CLA	C11-C12-C13-C14
27	l	101	SQD	C32-C33-C34-C35
35	b	627	HTG	C3'-C4'-C5'-C6'
30	A	417	LMT	O5'-C1'-O1'-C1
27	b	601	SQD	C18-C19-C20-C21
30	f	102	LMT	C4-C5-C6-C7
36	h	102	DGD	O2G-C1B-C2B-C3B
34	j	101	LMG	C20-C21-C22-C23
34	C	521	LMG	C30-C31-C32-C33
34	c	521	LMG	C29-C30-C31-C32
34	b	625	LMG	C19-C20-C21-C22
34	B	621	LMG	O8-C28-C29-C30
24	B	604	CLA	C5-C6-C7-C8
24	C	502	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	c	504	CLA	C2B-C3B-CAB-CBB
24	c	506	CLA	C2B-C3B-CAB-CBB
24	A	406	CLA	C13-C15-C16-C17
30	E	102	LMT	C1-C2-C3-C4
37	e	101	LHG	O8-C23-C24-C25
37	e	101	LHG	C26-C27-C28-C29
36	C	518	DGD	CBB-CCB-CDB-CEB
24	C	510	CLA	C3-C5-C6-C7
34	j	101	LMG	C40-C41-C42-C43
27	b	601	SQD	C46-C45-O47-C7
27	l	101	SQD	C46-C45-O47-C7
24	B	611	CLA	C2A-CAA-CBA-CGA
24	b	615	CLA	C2A-CAA-CBA-CGA
24	c	514	CLA	C15-C16-C17-C18
24	c	511	CLA	C2-C1-O2A-CGA
24	c	514	CLA	C2-C1-O2A-CGA
24	c	515	CLA	C2-C1-O2A-CGA
30	m	103	LMT	C9-C10-C11-C12
34	b	625	LMG	O10-C28-O8-C9
37	D	410	LHG	O10-C23-O8-C6
24	C	506	CLA	C16-C17-C18-C19
34	c	520	LMG	C28-C29-C30-C31
24	b	606	CLA	C4-C3-C5-C6
34	j	101	LMG	C30-C31-C32-C33
26	C	515	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	c	516	BCR	C23-C24-C25-C30
30	b	602	LMT	O1'-C1-C2-C3
27	b	601	SQD	C24-C25-C26-C27
36	c	519	DGD	C7B-C8B-C9B-CAB
34	b	625	LMG	C29-C28-O8-C9
34	C	521	LMG	C29-C30-C31-C32
30	D	402	LMT	O5'-C1'-O1'-C1
30	M	102	LMT	O5'-C1'-O1'-C1
36	C	517	DGD	O6E-C1E-O5D-C6D
34	J	101	LMG	C10-C11-C12-C13
24	c	508	CLA	C10-C11-C12-C13
27	f	101	SQD	O47-C45-C46-O48
24	B	602	CLA	C15-C16-C17-C18
37	e	101	LHG	C4-O6-P-O3
36	d	407	DGD	C5B-C6B-C7B-C8B
24	C	504	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	c	518	DGD	C9A-CAA-CBA-CCA
24	C	503	CLA	C16-C17-C18-C19
24	a	409	CLA	CBA-CGA-O2A-C1
25	A	408	PHO	C2C-C3C-CAC-CBC
24	a	409	CLA	C4-C3-C5-C6
34	C	520	LMG	C18-C19-C20-C21
35	c	522	HTG	C3'-C4'-C5'-C6'
24	C	507	CLA	C6-C7-C8-C10
24	C	511	CLA	C6-C7-C8-C10
24	b	607	CLA	C12-C13-C15-C16
36	c	519	DGD	C8B-C9B-CAB-CBB
37	E	101	LHG	C26-C27-C28-C29
24	A	409	CLA	C11-C10-C8-C9
24	B	616	CLA	C11-C10-C8-C9
24	b	611	CLA	C14-C13-C15-C16
26	h	101	BCR	C9-C10-C11-C12
37	d	408	LHG	C30-C31-C32-C33
27	F	101	SQD	C26-C27-C28-C29
37	D	408	LHG	C26-C27-C28-C29
37	l	102	LHG	C11-C12-C13-C14
36	c	519	DGD	O1A-C1A-O1G-C1G
34	C	521	LMG	O9-C10-O7-C8
24	D	401	CLA	C15-C16-C17-C18
32	a	416	PL9	C12-C11-C9-C10
37	e	101	LHG	C23-C24-C25-C26
30	m	102	LMT	O5'-C5'-C6'-O6'
34	C	520	LMG	C21-C22-C23-C24
27	l	101	SQD	C24-C23-O48-C46
36	c	519	DGD	C2A-C1A-O1G-C1G
37	D	410	LHG	C24-C23-O8-C6
38	E	103	HEM	C2C-C3C-CAC-CBC
32	A	419	PL9	C2-C3-C7-C8
37	D	410	LHG	C15-C16-C17-C18
40	v	202	HEC	C4C-C3C-CAC-CBC
24	b	606	CLA	CAA-CBA-CGA-O2A
24	c	505	CLA	O1D-CGD-O2D-CED
27	l	101	SQD	C9-C10-C11-C12
24	C	503	CLA	CBD-CGD-O2D-CED
34	B	621	LMG	C10-C11-C12-C13
27	l	101	SQD	C13-C14-C15-C16
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	505	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	b	616	CLA	C4B-C3B-CAB-CBB
27	A	416	SQD	O5-C1-O6-C44
24	B	615	CLA	C5-C6-C7-C8
34	z	101	LMG	C15-C16-C17-C18
37	L	101	LHG	O6-C4-C5-C6
34	C	521	LMG	C39-C40-C41-C42
38	E	103	HEM	CAD-CBD-CGD-O1D
36	D	407	DGD	C3A-C4A-C5A-C6A
24	b	615	CLA	C16-C17-C18-C19
34	C	501	LMG	O8-C28-C29-C30
34	C	501	LMG	C15-C16-C17-C18
36	C	519	DGD	CBB-CCB-CDB-CEB
36	c	519	DGD	C6A-C7A-C8A-C9A
38	e	102	HEM	CAA-CBA-CGA-O1A
24	C	508	CLA	CBD-CGD-O2D-CED
27	F	101	SQD	C30-C31-C32-C33
27	a	402	SQD	C18-C19-C20-C21
34	J	101	LMG	C20-C21-C22-C23
24	B	602	CLA	C2-C1-O2A-CGA
24	b	613	CLA	C2-C1-O2A-CGA
24	d	402	CLA	C2-C1-O2A-CGA
24	b	610	CLA	C10-C11-C12-C13
37	D	410	LHG	C24-C25-C26-C27
36	C	517	DGD	C2E-C1E-O5D-C6D
36	c	517	DGD	C2E-C1E-O5D-C6D
24	C	502	CLA	C2A-CAA-CBA-CGA
27	f	101	SQD	O6-C44-C45-O47
30	b	602	LMT	C7-C8-C9-C10
37	D	408	LHG	C32-C33-C34-C35
24	D	401	CLA	C2C-C3C-CAC-CBC
30	f	102	LMT	C2-C3-C4-C5
36	C	517	DGD	C5A-C6A-C7A-C8A
37	d	408	LHG	C32-C33-C34-C35
24	B	614	CLA	C11-C12-C13-C14
24	C	502	CLA	C11-C12-C13-C14
24	C	513	CLA	C14-C13-C15-C16
24	b	610	CLA	C11-C10-C8-C9
24	b	615	CLA	C11-C12-C13-C14
24	c	506	CLA	C11-C12-C13-C14
24	b	615	CLA	C16-C17-C18-C20
27	A	416	SQD	C34-C35-C36-C37
27	a	411	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
34	C	520	LMG	C11-C12-C13-C14
38	e	102	HEM	CAA-CBA-CGA-O2A
24	a	409	CLA	C15-C16-C17-C18
36	C	518	DGD	C7B-C8B-C9B-CAB
30	m	103	LMT	C4-C5-C6-C7
34	c	520	LMG	C7-C8-C9-O8
34	z	101	LMG	C7-C8-C9-O8
24	c	511	CLA	C16-C17-C18-C20
36	c	517	DGD	O6E-C1E-O5D-C6D
26	D	405	BCR	C7-C8-C9-C34
34	c	520	LMG	C4-C5-C6-O5
24	c	503	CLA	CBD-CGD-O2D-CED
36	H	102	DGD	C6B-C7B-C8B-C9B
40	V	203	HEC	CAD-CBD-CGD-O2D
34	C	501	LMG	C37-C38-C39-C40
37	D	409	LHG	C26-C27-C28-C29
24	A	406	CLA	C6-C7-C8-C10
24	D	403	CLA	C12-C13-C15-C16
24	c	507	CLA	C11-C12-C13-C15
34	b	625	LMG	C37-C38-C39-C40
24	D	404	CLA	C8-C10-C11-C12
34	c	501	LMG	C10-C11-C12-C13
38	E	103	HEM	CAD-CBD-CGD-O2D
36	C	518	DGD	C4A-C5A-C6A-C7A
26	H	101	BCR	C9-C10-C11-C12
27	A	416	SQD	C15-C16-C17-C18
36	C	519	DGD	C2A-C3A-C4A-C5A
30	m	102	LMT	C3-C4-C5-C6
34	Z	101	LMG	C11-C12-C13-C14
40	V	203	HEC	CAD-CBD-CGD-O1D
27	b	601	SQD	C27-C28-C29-C30
35	B	622	HTG	S1-C1'-C2'-C3'
24	A	409	CLA	C3-C5-C6-C7
24	C	508	CLA	C2A-CAA-CBA-CGA
28	f	104	GOL	O1-C1-C2-O2
30	b	602	LMT	C4-C5-C6-C7
24	c	514	CLA	O1D-CGD-O2D-CED
37	D	408	LHG	C11-C12-C13-C14
30	b	626	LMT	C6-C7-C8-C9
24	C	508	CLA	C16-C17-C18-C19
27	a	402	SQD	C28-C29-C30-C31
34	b	625	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
36	d	407	DGD	C1B-C2B-C3B-C4B
24	C	505	CLA	C2B-C3B-CAB-CBB
24	D	404	CLA	C2B-C3B-CAB-CBB
24	a	407	CLA	C2B-C3B-CAB-CBB
24	b	606	CLA	C2B-C3B-CAB-CBB
24	b	616	CLA	C2B-C3B-CAB-CBB
30	M	102	LMT	C5-C6-C7-C8
34	C	501	LMG	C16-C17-C18-C19
27	l	101	SQD	O10-C23-O48-C46
37	d	410	LHG	C33-C34-C35-C36
34	c	521	LMG	C28-C29-C30-C31
27	a	411	SQD	O6-C44-C45-O47
36	D	407	DGD	O2G-C2G-C3G-O3G
37	d	408	LHG	C23-C24-C25-C26
35	d	411	HTG	O5-C5-C6-O6
24	C	503	CLA	O1D-CGD-O2D-CED
36	c	518	DGD	C1A-C2A-C3A-C4A
37	E	101	LHG	C18-C19-C20-C21
27	a	402	SQD	C35-C36-C37-C38
32	a	416	PL9	C45-C44-C46-C47
24	b	618	CLA	C2-C1-O2A-CGA
24	b	619	CLA	C2-C1-O2A-CGA
24	a	409	CLA	C2-C3-C5-C6
24	b	620	CLA	C13-C15-C16-C17
27	A	416	SQD	C11-C12-C13-C14
34	b	625	LMG	C29-C30-C31-C32
32	a	416	PL9	C2-C3-C7-C8
27	a	402	SQD	O10-C23-O48-C46
35	B	631	HTG	S1-C1'-C2'-C3'
35	O	303	HTG	S1-C1'-C2'-C3'
24	c	503	CLA	C2A-CAA-CBA-CGA
36	D	407	DGD	CAA-CBA-CCA-CDA
26	B	620	BCR	C1-C6-C7-C8
26	B	620	BCR	C23-C24-C25-C30
26	C	516	BCR	C1-C6-C7-C8
26	c	516	BCR	C1-C6-C7-C8
26	c	516	BCR	C5-C6-C7-C8
26	c	516	BCR	C23-C24-C25-C26
26	c	526	BCR	C1-C6-C7-C8
26	k	103	BCR	C1-C6-C7-C8
24	C	502	CLA	C15-C16-C17-C18
37	d	409	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
34	c	501	LMG	O8-C28-C29-C30
38	e	102	HEM	CAD-CBD-CGD-O1D
28	T	103	GOL	C1-C2-C3-O3
28	a	413	GOL	O1-C1-C2-C3
24	B	613	CLA	O1A-CGA-O2A-C1
24	B	614	CLA	C10-C11-C12-C13
24	b	606	CLA	C2-C3-C5-C6
25	d	403	PHO	C2C-C3C-CAC-CBC
34	C	520	LMG	C31-C32-C33-C34
30	M	101	LMT	C1-C2-C3-C4
24	B	609	CLA	C16-C17-C18-C19
24	A	409	CLA	C10-C11-C12-C13
24	b	615	CLA	C15-C16-C17-C18
24	b	617	CLA	C8-C10-C11-C12
30	b	626	LMT	C5-C6-C7-C8
37	l	102	LHG	C17-C18-C19-C20
40	v	202	HEC	CAD-CBD-CGD-O2D
34	c	520	LMG	C39-C40-C41-C42
36	C	518	DGD	C4E-C5E-C6E-O5E
30	m	103	LMT	C5-C6-C7-C8
24	C	508	CLA	C4B-C3B-CAB-CBB
24	C	505	CLA	C4-C3-C5-C6
24	A	409	CLA	C11-C12-C13-C15
24	A	409	CLA	C12-C13-C15-C16
24	B	602	CLA	C11-C10-C8-C7
24	C	513	CLA	C12-C13-C15-C16
27	a	402	SQD	C24-C23-O48-C46
27	b	601	SQD	C19-C20-C21-C22
37	e	101	LHG	C15-C16-C17-C18
28	A	412	GOL	O1-C1-C2-O2
28	b	632	GOL	O2-C2-C3-O3
27	A	416	SQD	C2-C1-O6-C44
30	D	402	LMT	C2'-C1'-O1'-C1
37	D	408	LHG	C17-C18-C19-C20
36	c	519	DGD	O1G-C1A-C2A-C3A
24	a	409	CLA	C16-C17-C18-C20
35	D	411	HTG	C2'-C1'-S1-C1
35	b	604	HTG	O5-C1-S1-C1'
34	C	521	LMG	C11-C12-C13-C14
24	c	515	CLA	C4-C3-C5-C6
37	E	101	LHG	C7-C8-C9-C10
24	A	406	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	C	502	CLA	C14-C13-C15-C16
24	C	513	CLA	C6-C7-C8-C9
24	b	617	CLA	C11-C10-C8-C9
24	C	511	CLA	O1A-CGA-O2A-C1
27	f	101	SQD	C24-C25-C26-C27
24	B	608	CLA	C3A-C2A-CAA-CBA
24	b	612	CLA	C3A-C2A-CAA-CBA
24	C	513	CLA	CAA-CBA-CGA-O2A
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	514	CLA	CAD-CBD-CGD-O2D
24	b	609	CLA	CAD-CBD-CGD-O2D
24	b	621	CLA	CAD-CBD-CGD-O2D
24	c	505	CLA	CAD-CBD-CGD-O2D
25	A	407	PHO	CAD-CBD-CGD-O2D
34	z	101	LMG	C17-C18-C19-C20
37	l	102	LHG	C12-C13-C14-C15
24	B	607	CLA	C10-C11-C12-C13
24	B	614	CLA	C2-C1-O2A-CGA
37	d	408	LHG	C11-C10-C9-C8
30	D	402	LMT	C4'-C5'-C6'-O6'
36	C	519	DGD	C8A-C9A-CAA-CBA
24	b	608	CLA	C4-C3-C5-C6
24	c	506	CLA	C4-C3-C5-C6
34	B	621	LMG	C17-C18-C19-C20
36	c	518	DGD	C7A-C8A-C9A-CAA
36	H	102	DGD	O1B-C1B-C2B-C3B
27	l	101	SQD	O5-C1-O6-C44
24	c	514	CLA	CAA-CBA-CGA-O2A
27	f	101	SQD	O47-C7-C8-C9
36	D	407	DGD	C4B-C5B-C6B-C7B
24	D	403	CLA	O2A-C1-C2-C3
25	a	408	PHO	O2A-C1-C2-C3
30	D	402	LMT	C7-C8-C9-C10
34	c	521	LMG	C31-C32-C33-C34
37	L	101	LHG	C27-C28-C29-C30
38	E	103	HEM	C4C-C3C-CAC-CBC
37	l	102	LHG	C27-C28-C29-C30
40	v	202	HEC	CAD-CBD-CGD-O1D
34	j	101	LMG	C19-C20-C21-C22
24	C	504	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	B	608	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	c	506	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O2D
24	c	512	CLA	CHA-CBD-CGD-O2D
24	d	401	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O2D
36	C	517	DGD	C2A-C3A-C4A-C5A
37	D	410	LHG	C29-C30-C31-C32
27	A	411	SQD	C32-C33-C34-C35
36	d	407	DGD	O2G-C2G-C3G-O3G
30	b	602	LMT	C6-C7-C8-C9
24	B	603	CLA	C8-C10-C11-C12
24	B	608	CLA	C3-C5-C6-C7
38	e	102	HEM	CAD-CBD-CGD-O2D
24	D	401	CLA	C4C-C3C-CAC-CBC
37	D	410	LHG	C25-C26-C27-C28
25	d	403	PHO	CHA-CBD-CGD-O2D
28	c	525	GOL	O2-C2-C3-O3
34	b	625	LMG	O8-C28-C29-C30
24	B	617	CLA	C11-C10-C8-C7
24	C	508	CLA	C11-C10-C8-C7
34	b	625	LMG	C36-C37-C38-C39
24	B	604	CLA	C6-C7-C8-C9
24	B	605	CLA	C6-C7-C8-C9
24	a	407	CLA	C6-C7-C8-C9
37	D	409	LHG	C14-C15-C16-C17
24	B	608	CLA	C2B-C3B-CAB-CBB
27	A	416	SQD	C12-C13-C14-C15
27	A	411	SQD	O47-C7-C8-C9
34	z	101	LMG	C13-C14-C15-C16
34	C	521	LMG	C11-C10-O7-C8
37	E	101	LHG	O7-C7-C8-C9
24	B	613	CLA	CBA-CGA-O2A-C1
27	b	601	SQD	C29-C30-C31-C32
28	A	412	GOL	O1-C1-C2-C3
32	a	416	PL9	C43-C44-C46-C47
24	c	514	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
34	c	501	LMG	C11-C12-C13-C14
24	C	511	CLA	CBA-CGA-O2A-C1
30	M	101	LMT	C9-C10-C11-C12
24	c	513	CLA	C1A-C2A-CAA-CBA
24	C	508	CLA	C16-C17-C18-C20
35	B	623	HTG	C4-C5-C6-O6
24	b	621	CLA	C2-C1-O2A-CGA
37	d	409	LHG	C31-C32-C33-C34
36	c	519	DGD	O1A-C1A-C2A-C3A
24	A	405	CLA	C2C-C3C-CAC-CBC
34	C	520	LMG	O7-C10-C11-C12
24	C	504	CLA	C15-C16-C17-C18
24	d	404	CLA	C3-C5-C6-C7
27	a	411	SQD	C32-C33-C34-C35
30	A	417	LMT	C2'-C1'-O1'-C1
30	M	102	LMT	C2'-C1'-O1'-C1
24	A	409	CLA	C4B-C3B-CAB-CBB
24	b	606	CLA	C4B-C3B-CAB-CBB
24	b	614	CLA	C4B-C3B-CAB-CBB
24	b	620	CLA	C4B-C3B-CAB-CBB
37	d	409	LHG	C4-O6-P-O5
30	f	102	LMT	C2B-C1B-O1B-C4'
37	E	101	LHG	O9-C7-C8-C9
26	C	516	BCR	C5-C6-C7-C8
25	a	408	PHO	C8-C10-C11-C12
24	C	513	CLA	CAA-CBA-CGA-O1A
24	B	603	CLA	C2A-CAA-CBA-CGA
27	A	411	SQD	O49-C7-C8-C9
27	f	101	SQD	O49-C7-C8-C9
27	A	416	SQD	C33-C34-C35-C36
32	A	419	PL9	C46-C47-C48-C49
24	B	608	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	a	407	CLA	CAD-CBD-CGD-O1D
24	b	612	CLA	CAD-CBD-CGD-O1D
24	c	508	CLA	CAD-CBD-CGD-O1D
27	A	411	SQD	C5-C6-S-O9
27	A	416	SQD	C5-C6-S-O7
27	A	416	SQD	C5-C6-S-O9
34	b	625	LMG	O10-C28-C29-C30
30	a	401	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	617	CLA	C11-C10-C8-C9
24	C	508	CLA	C11-C10-C8-C9
24	a	409	CLA	C11-C12-C13-C14
24	b	608	CLA	C6-C7-C8-C9
24	b	619	CLA	C14-C13-C15-C16
24	d	404	CLA	C14-C13-C15-C16
27	a	402	SQD	C15-C16-C17-C18
24	C	502	CLA	C13-C15-C16-C17
24	C	506	CLA	CAA-CBA-CGA-O2A
37	L	101	LHG	O7-C7-C8-C9
37	d	408	LHG	O8-C23-C24-C25
37	l	102	LHG	O7-C7-C8-C9
37	l	102	LHG	C29-C30-C31-C32
37	d	409	LHG	C14-C15-C16-C17
34	J	101	LMG	O7-C10-C11-C12
37	D	408	LHG	O8-C23-C24-C25
34	C	520	LMG	O9-C10-C11-C12
32	A	419	PL9	C45-C44-C46-C47
30	M	102	LMT	C4'-C5'-C6'-O6'
24	B	605	CLA	C6-C7-C8-C10
24	a	407	CLA	C6-C7-C8-C10
24	a	409	CLA	C11-C12-C13-C15
24	b	608	CLA	C2-C3-C5-C6
24	b	608	CLA	C6-C7-C8-C10
24	b	611	CLA	C11-C12-C13-C15
24	b	617	CLA	C11-C10-C8-C7
24	c	506	CLA	C2-C3-C5-C6
24	c	509	CLA	C11-C10-C8-C7
24	d	404	CLA	C12-C13-C15-C16
32	a	416	PL9	C12-C11-C9-C8
35	c	523	HTG	C2-C1-S1-C1'
37	l	102	LHG	O9-C7-C8-C9
27	F	101	SQD	C33-C34-C35-C36
27	a	411	SQD	C31-C32-C33-C34
36	h	102	DGD	C6B-C7B-C8B-C9B
37	D	409	LHG	C16-C17-C18-C19
24	b	618	CLA	CAA-CBA-CGA-O2A
24	c	507	CLA	CAA-CBA-CGA-O2A
34	z	101	LMG	O7-C10-C11-C12
36	C	518	DGD	O2G-C1B-C2B-C3B
37	E	101	LHG	O8-C23-C24-C25
26	C	516	BCR	C7-C8-C9-C10

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

There are no ring outliers.

151 monomers are involved in 280 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	c	501	LMG	1	0
37	E	101	LHG	2	0
37	e	101	LHG	4	0
37	d	408	LHG	1	0
24	B	614	CLA	2	0
24	b	611	CLA	4	0
24	c	513	CLA	3	0
24	b	613	CLA	1	0
24	b	606	CLA	3	0
26	c	516	BCR	4	0
24	b	610	CLA	4	0
37	d	410	LHG	3	0
24	C	514	CLA	4	0
34	B	621	LMG	2	0
28	c	525	GOL	2	0
38	e	102	HEM	2	0
36	c	518	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	623	BCR	3	0
24	c	504	CLA	2	0
24	B	611	CLA	1	0
26	A	410	BCR	3	0
26	h	101	BCR	4	0
28	V	205	GOL	2	0
28	b	633	GOL	1	0
36	H	102	DGD	2	0
24	C	503	CLA	2	0
36	c	519	DGD	1	0
30	a	401	LMT	4	0
27	b	601	SQD	2	0
28	A	413	GOL	2	0
24	b	620	CLA	4	0
30	m	103	LMT	1	0
28	C	524	GOL	1	0
34	c	521	LMG	1	0
36	D	407	DGD	1	0
30	m	102	LMT	1	0
28	T	101	GOL	1	0
30	B	634	LMT	1	0
24	c	508	CLA	4	0
24	B	607	CLA	2	0
37	L	101	LHG	1	0
35	B	623	HTG	1	0
34	c	520	LMG	1	0
34	z	101	LMG	4	0
24	D	401	CLA	5	0
26	C	515	BCR	3	0
24	D	404	CLA	1	0
36	C	518	DGD	1	0
24	b	619	CLA	1	0
24	c	514	CLA	4	0
28	V	207	GOL	1	0
24	C	510	CLA	2	0
24	c	510	CLA	3	0
26	y	101	BCR	1	0
25	d	403	PHO	1	0
26	B	618	BCR	3	0
24	b	608	CLA	1	0
37	D	410	LHG	8	0
26	B	620	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	613	CLA	2	0
24	B	616	CLA	1	0
24	b	614	CLA	2	0
24	d	404	CLA	3	0
25	A	408	PHO	1	0
24	c	505	CLA	4	0
26	T	102	BCR	7	0
27	l	101	SQD	2	0
24	B	610	CLA	2	0
24	C	507	CLA	3	0
26	H	101	BCR	4	0
24	B	617	CLA	5	0
26	k	103	BCR	1	0
28	B	628	GOL	1	0
24	D	403	CLA	1	0
24	A	409	CLA	1	0
24	C	512	CLA	1	0
24	B	615	CLA	4	0
28	T	103	GOL	1	0
35	C	523	HTG	2	0
34	C	521	LMG	1	0
27	a	411	SQD	4	0
26	b	622	BCR	2	0
35	d	411	HTG	2	0
34	Z	101	LMG	1	0
24	B	606	CLA	2	0
34	C	501	LMG	4	0
24	A	405	CLA	3	0
26	D	405	BCR	1	0
30	M	101	LMT	1	0
24	C	502	CLA	2	0
30	D	402	LMT	1	0
34	C	520	LMG	2	0
24	a	409	CLA	1	0
32	a	416	PL9	10	0
27	A	416	SQD	2	0
24	b	618	CLA	2	0
35	V	204	HTG	1	0
24	B	604	CLA	3	0
32	A	419	PL9	4	0
24	a	406	CLA	4	0
26	t	101	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	509	CLA	3	0
26	b	624	BCR	3	0
28	t	102	GOL	1	0
27	f	101	SQD	3	0
24	c	511	CLA	2	0
24	B	612	CLA	1	0
24	c	515	CLA	3	0
34	J	101	LMG	2	0
34	b	625	LMG	1	0
27	A	411	SQD	2	0
24	b	621	CLA	2	0
24	C	505	CLA	1	0
28	b	631	GOL	1	0
24	B	602	CLA	1	0
28	v	203	GOL	1	0
34	j	101	LMG	1	0
24	C	513	CLA	1	0
30	M	102	LMT	2	0
35	C	522	HTG	1	0
36	d	407	DGD	5	0
30	b	626	LMT	1	0
28	B	635	GOL	2	0
25	a	408	PHO	1	0
35	B	622	HTG	3	0
24	C	504	CLA	2	0
28	a	412	GOL	2	0
36	C	517	DGD	4	0
24	c	509	CLA	3	0
24	c	503	CLA	3	0
24	b	616	CLA	1	0
28	b	632	GOL	1	0
35	b	627	HTG	1	0
28	V	208	GOL	1	0
37	D	408	LHG	2	0
24	C	511	CLA	2	0
26	K	101	BCR	1	0
37	l	102	LHG	4	0
24	d	402	CLA	2	0
26	d	405	BCR	3	0
36	C	519	DGD	2	0
24	c	507	CLA	3	0
26	Y	101	BCR	2	0

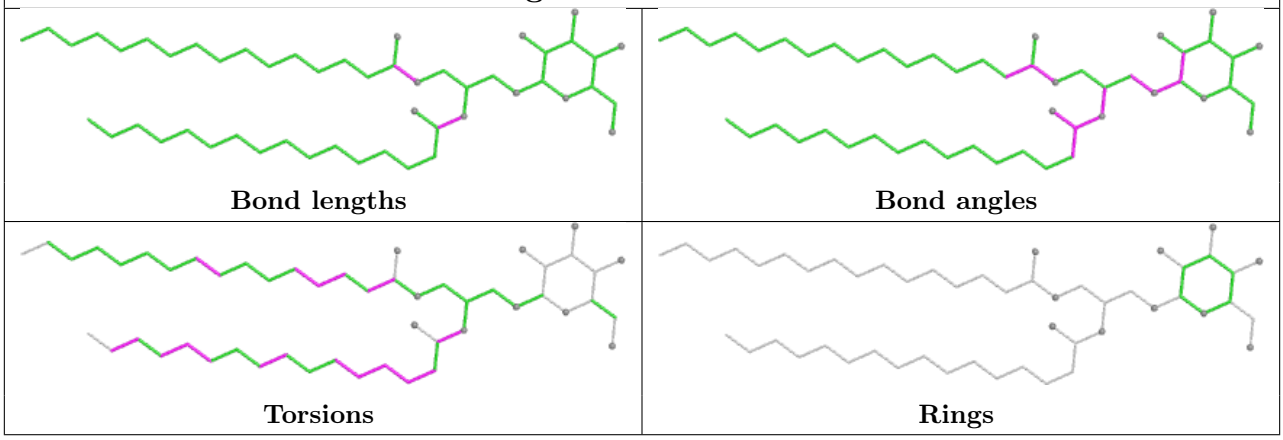
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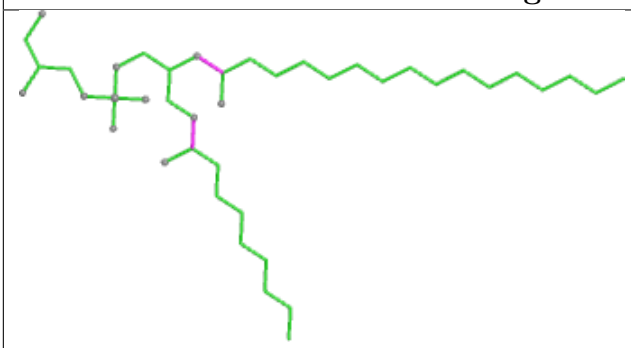
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	508	CLA	2	0
24	b	609	CLA	1	0
30	I	102	LMT	2	0
26	c	526	BCR	5	0
26	B	619	BCR	2	0
35	D	411	HTG	2	0
27	F	101	SQD	3	0
24	A	406	CLA	2	0

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.

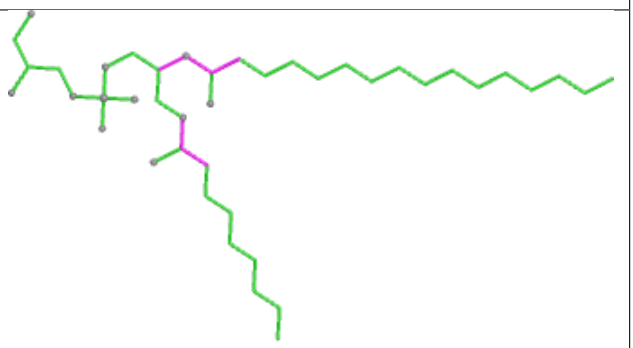
Ligand LMG c 501



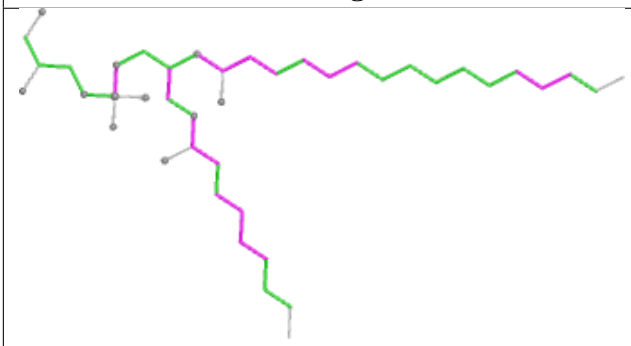
Ligand LHG E 101



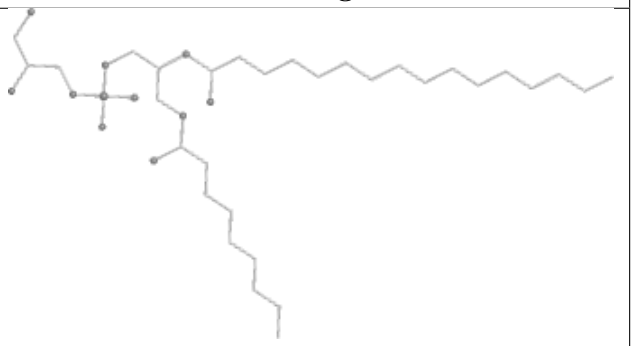
Bond lengths



Bond angles

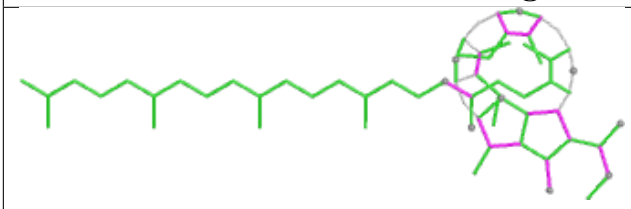


Torsions

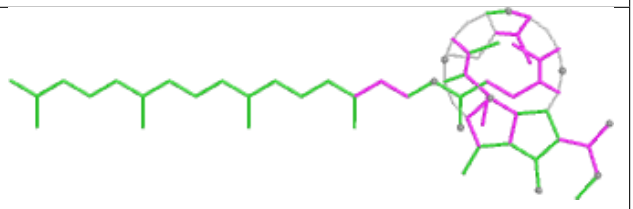


Rings

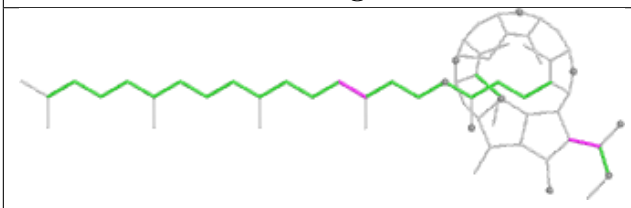
Ligand PHO A 407



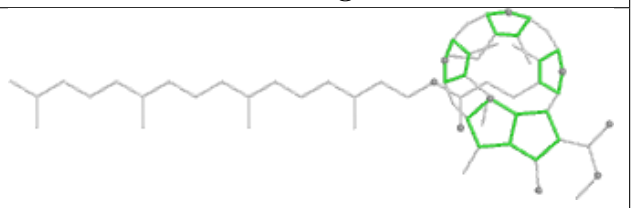
Bond lengths



Bond angles

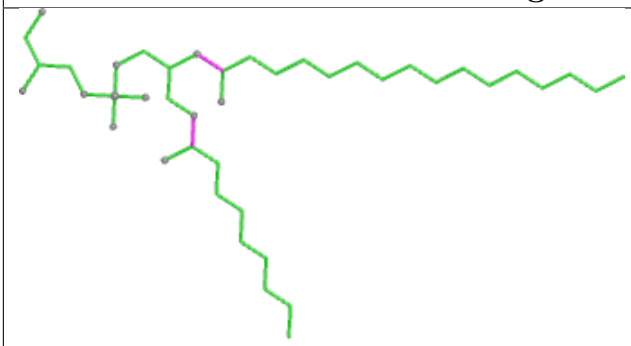


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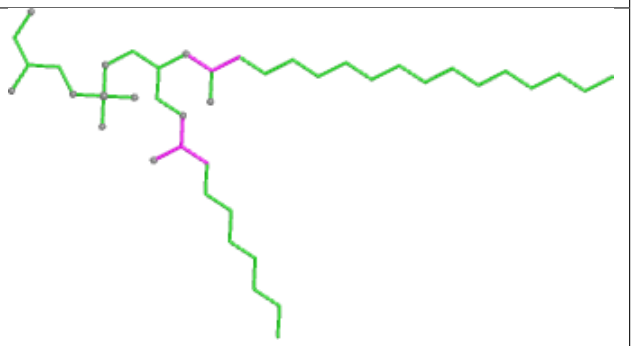


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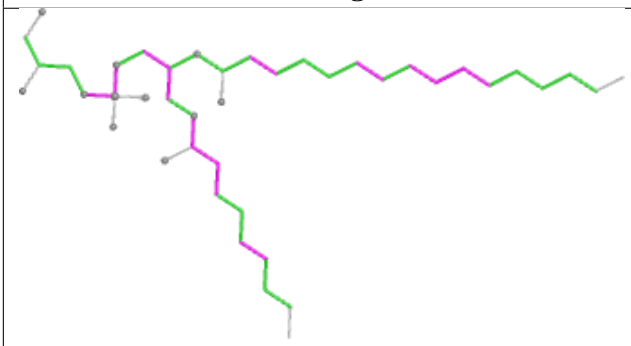
Ligand LHG e 101



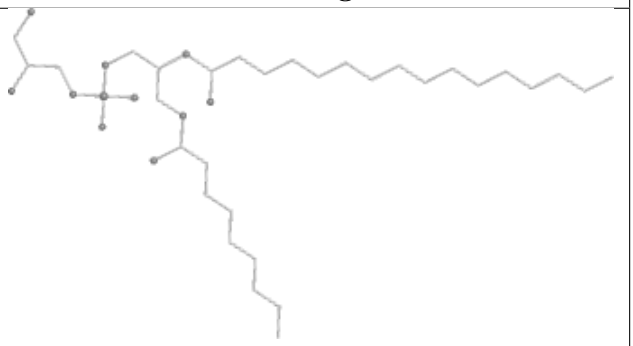
Bond lengths



Bond angles

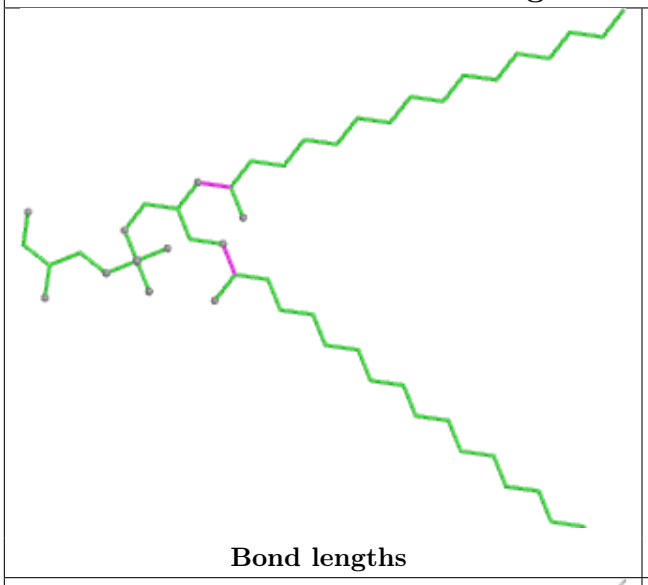


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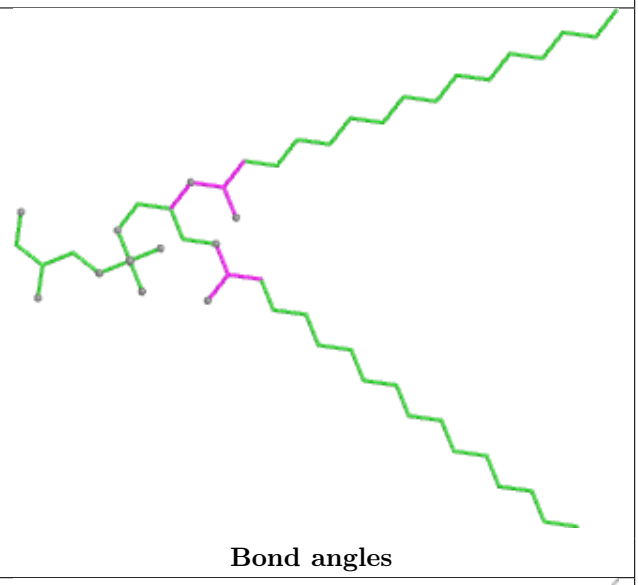


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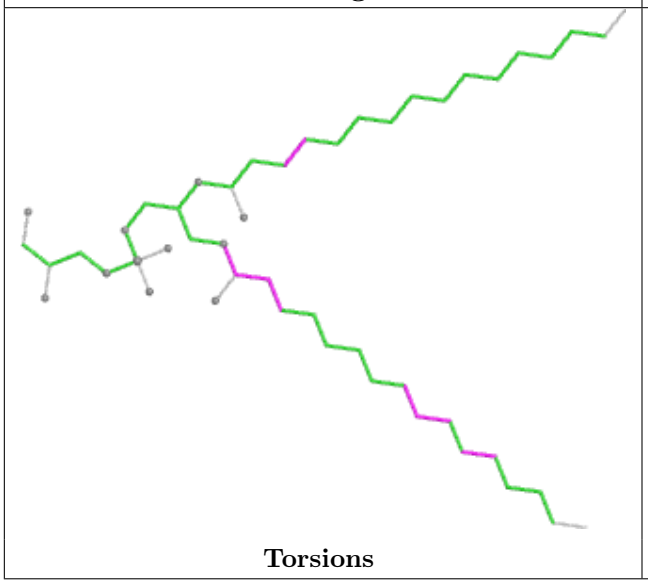
Ligand LHG d 408



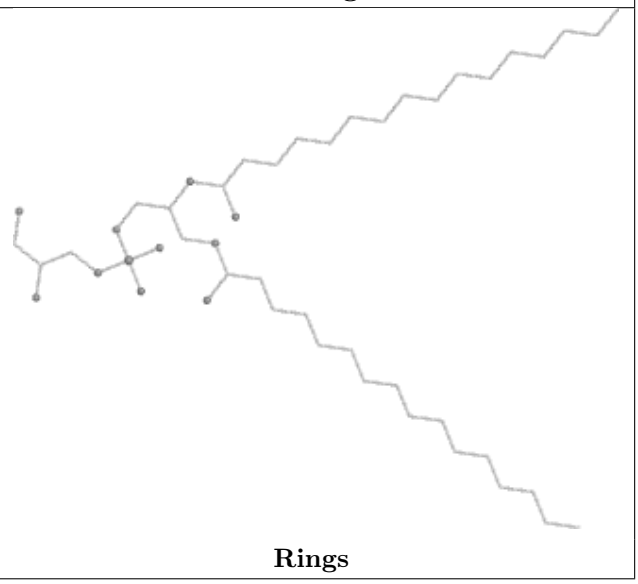
Bond lengths



Bond angles

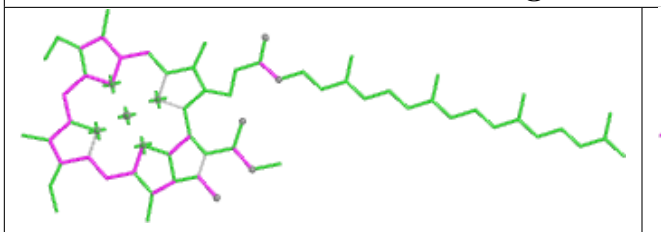


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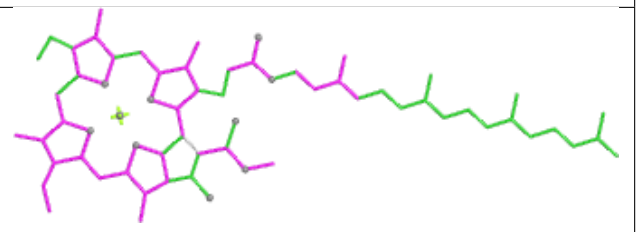


Rings

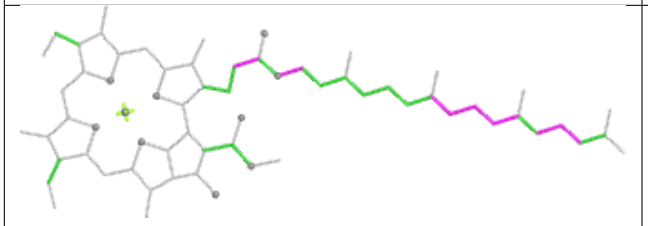
Ligand CLA B 614



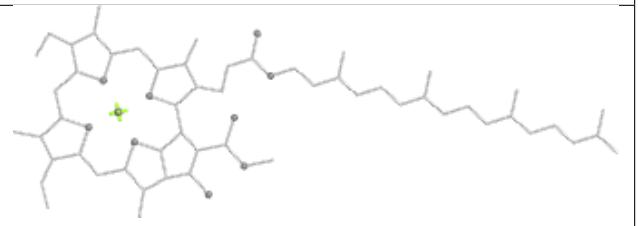
Bond lengths



Bond angles

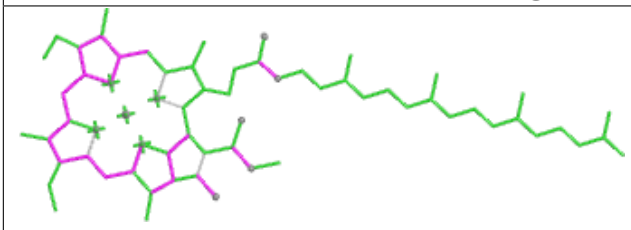


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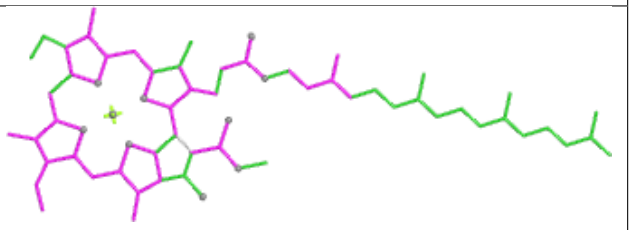


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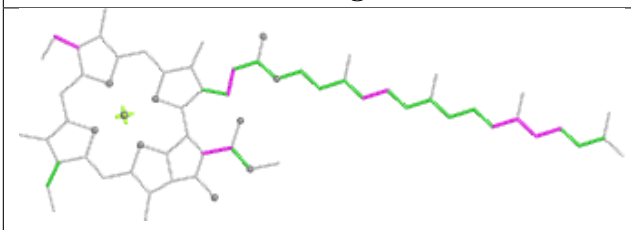
Ligand CLA b 611



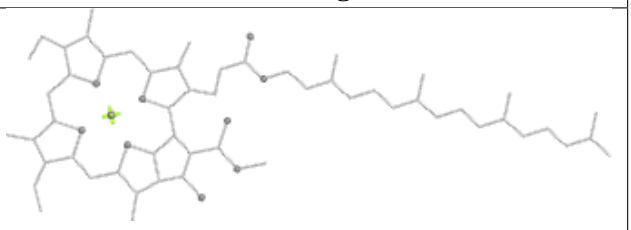
Bond lengths



Bond angles

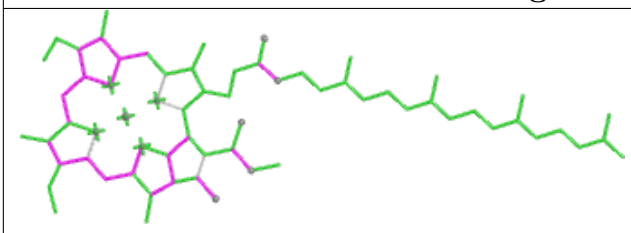


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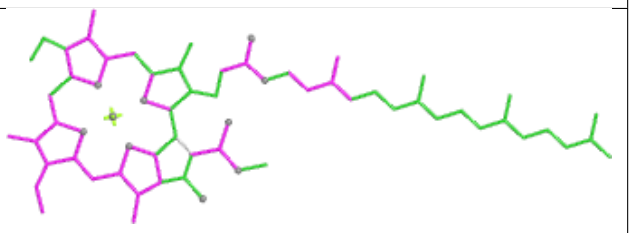


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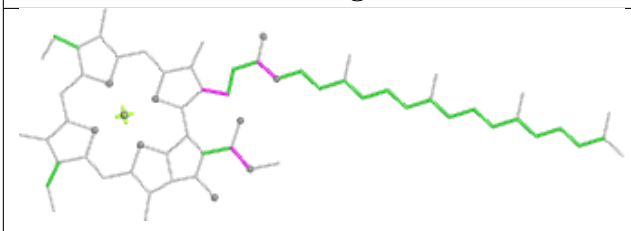
Ligand CLA c 513



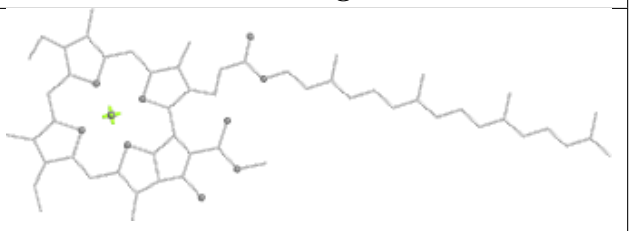
Bond lengths



Bond angles

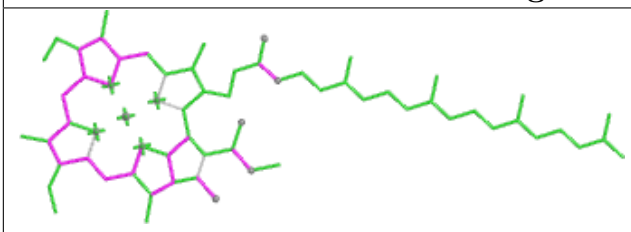


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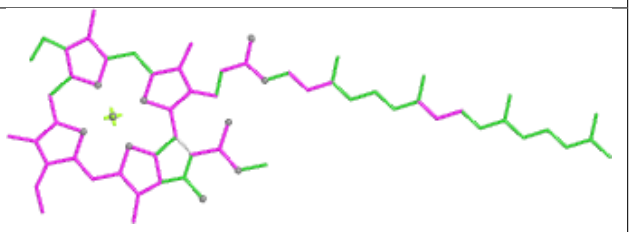


Rings

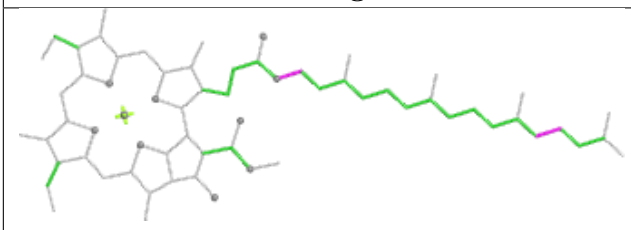
Ligand CLA b 613



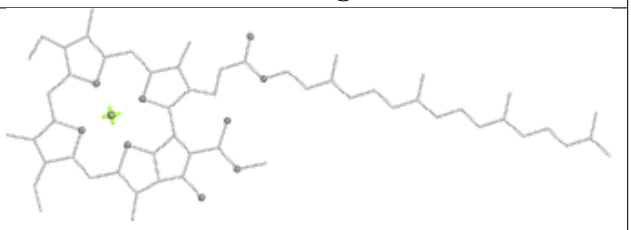
Bond lengths



Bond angles

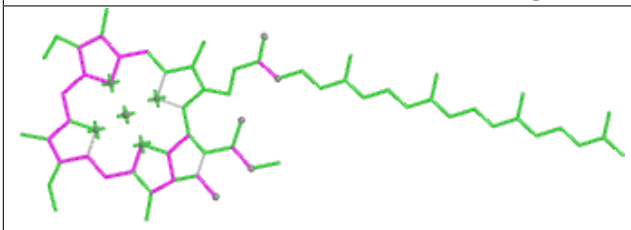


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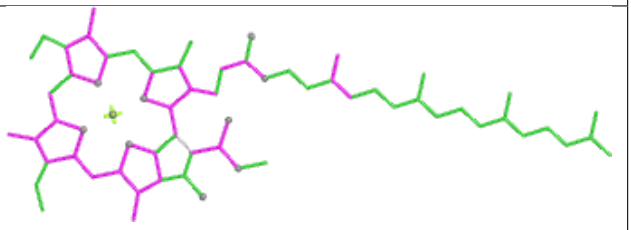


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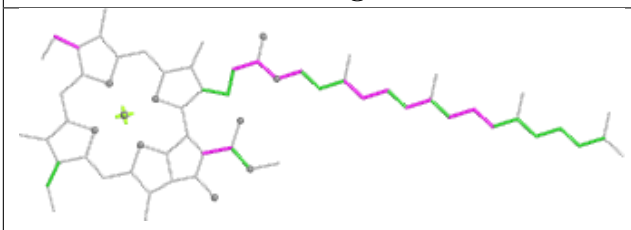
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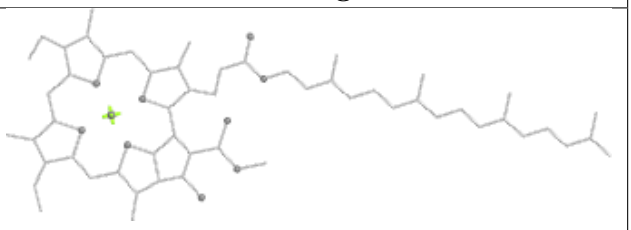
Bond lengths



Bond angles



Torsions

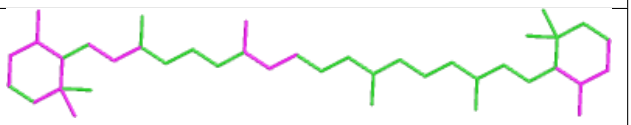


Rings

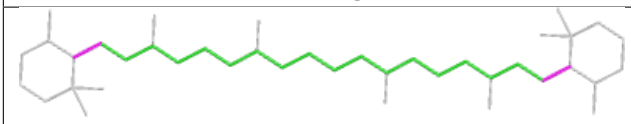
Ligand BCR c 516



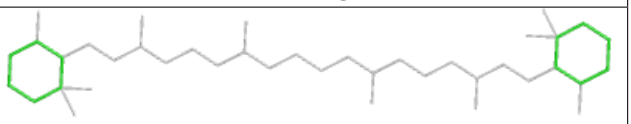
Bond lengths



Bond angles

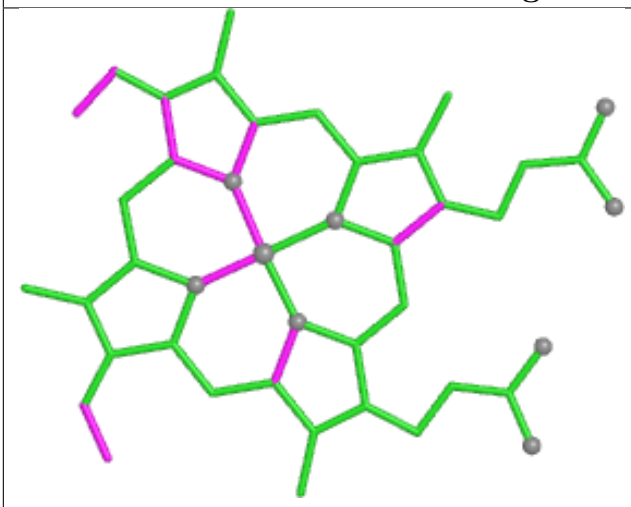


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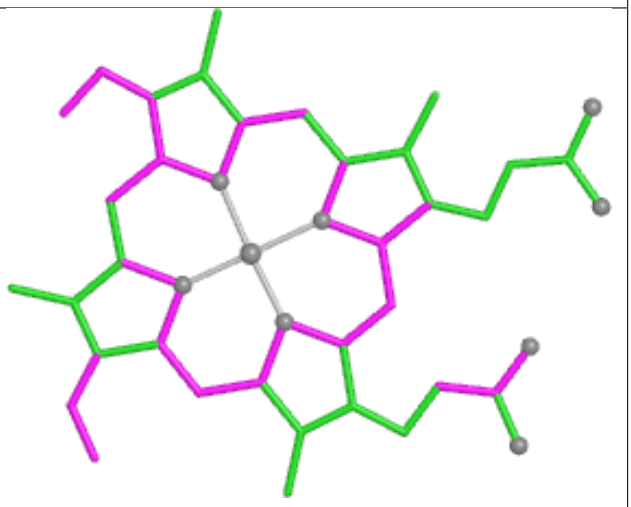


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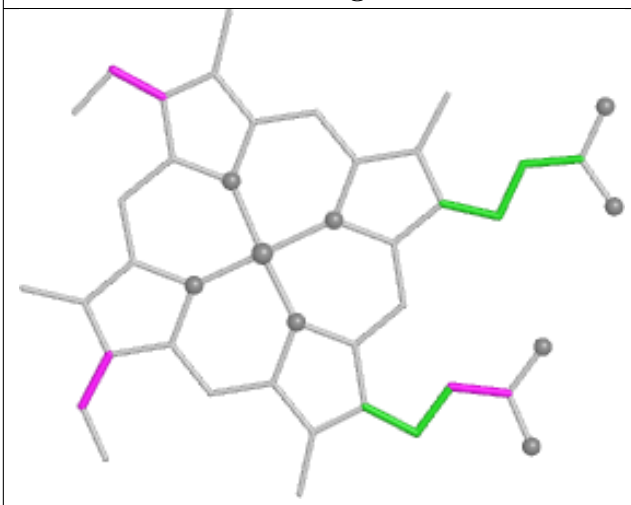
Ligand HEC V 203



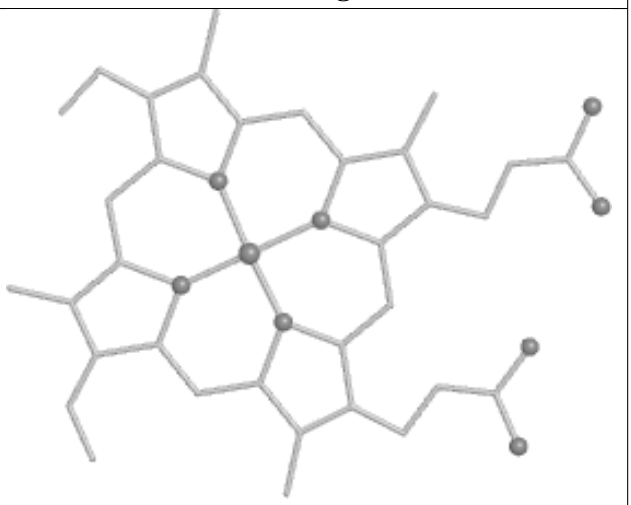
Bond lengths



Bond angles

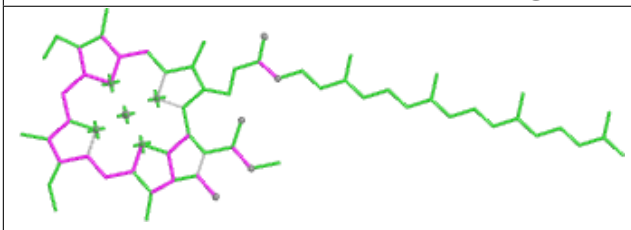


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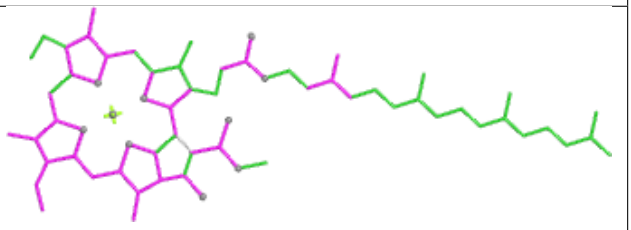


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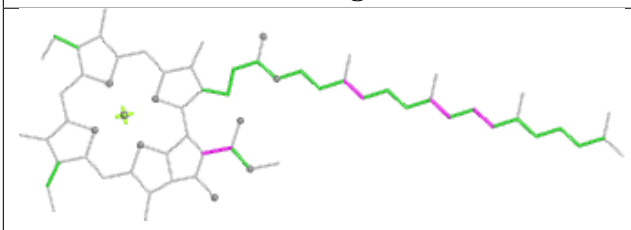
Ligand CLA b 610



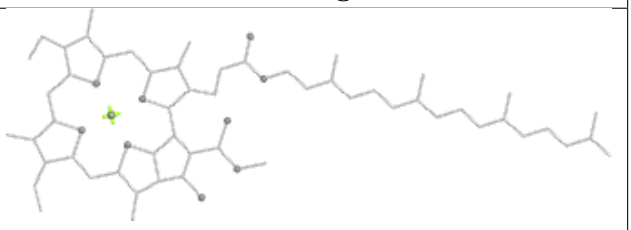
Bond lengths



Bond angles

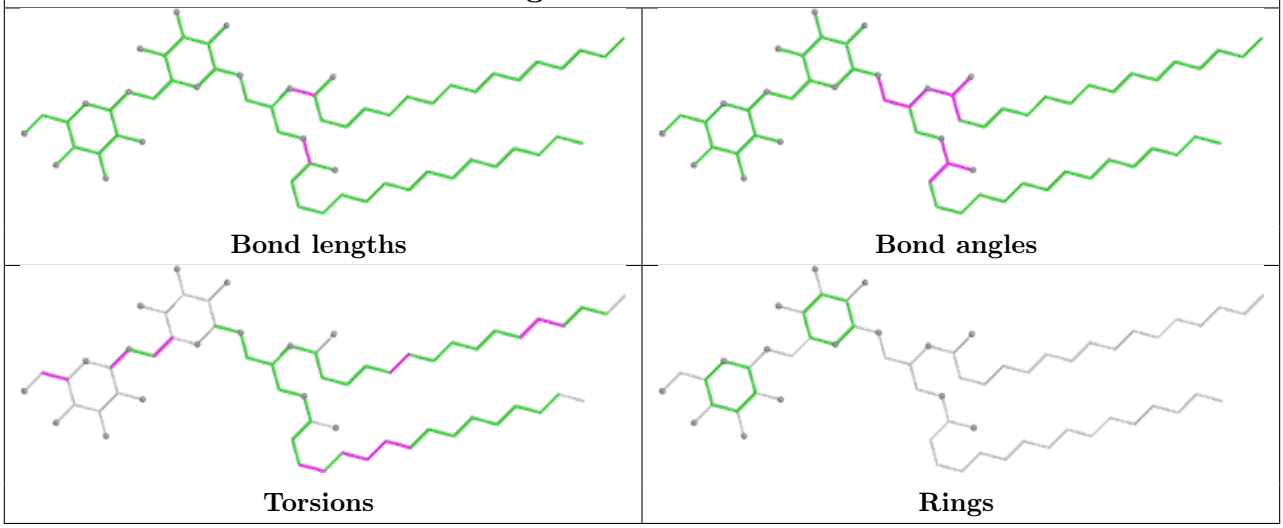


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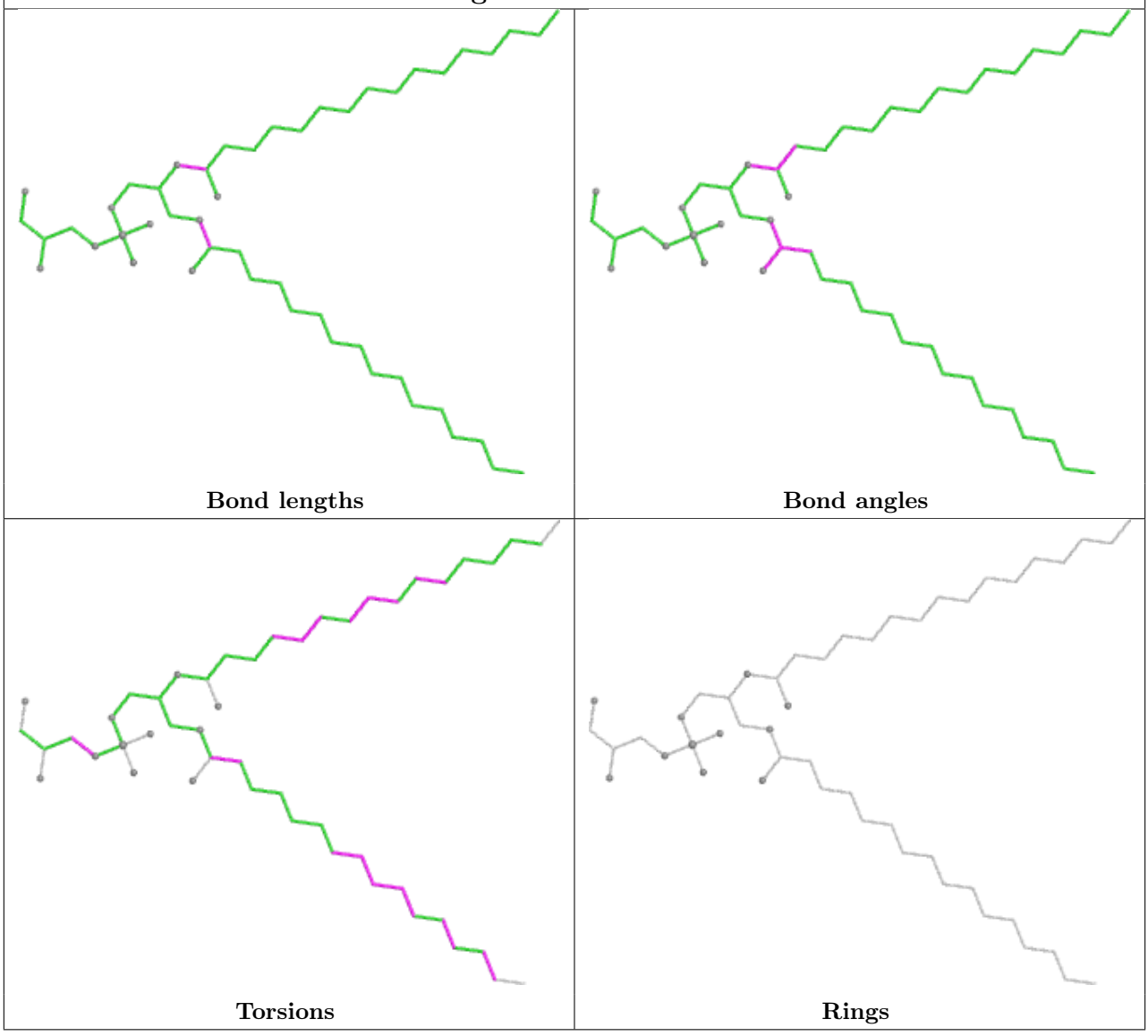


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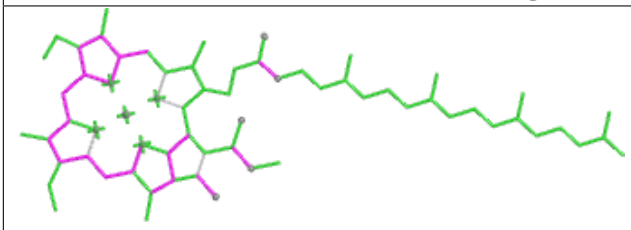
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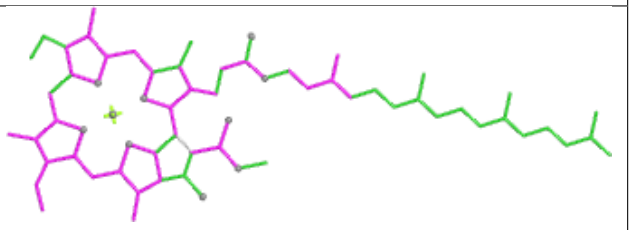
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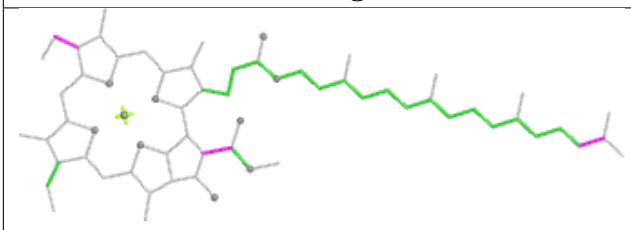
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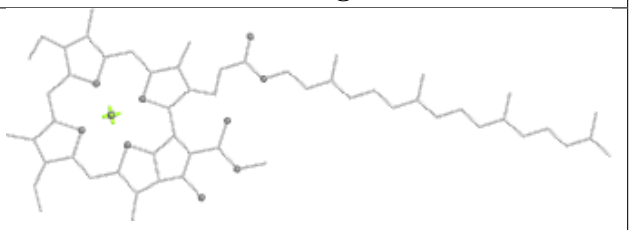
Bond lengths



Bond angles

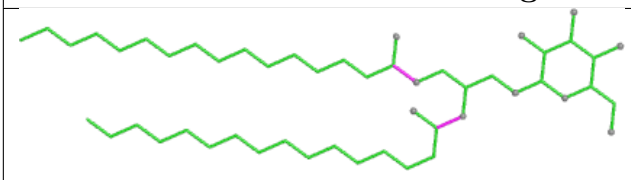


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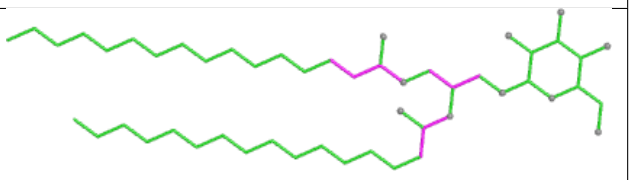


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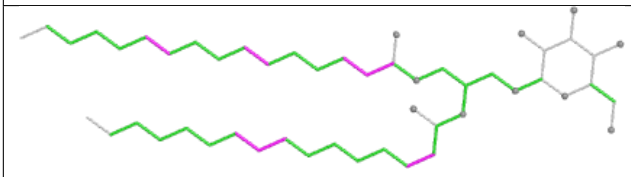
Ligand LMG B 621



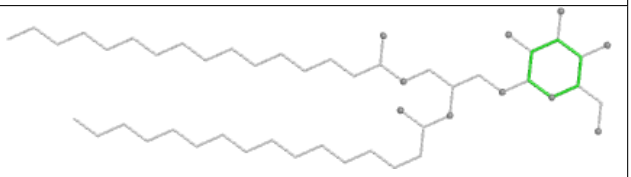
Bond lengths



Bond angles

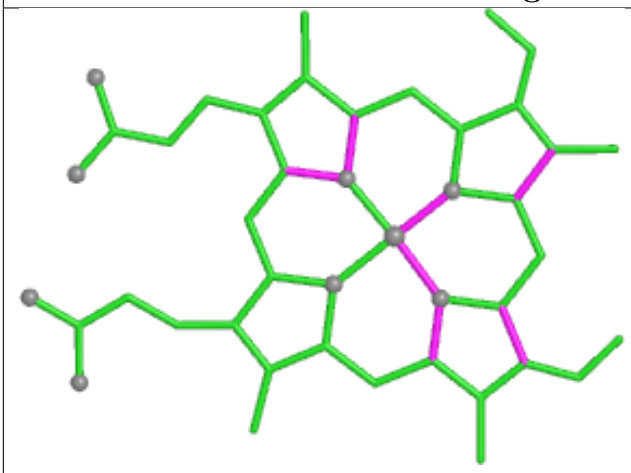


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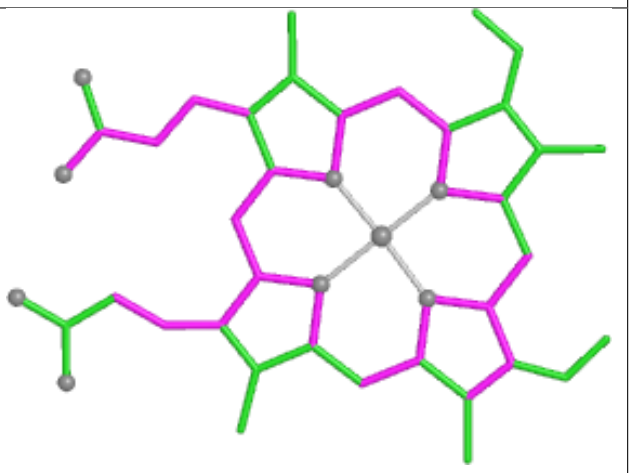


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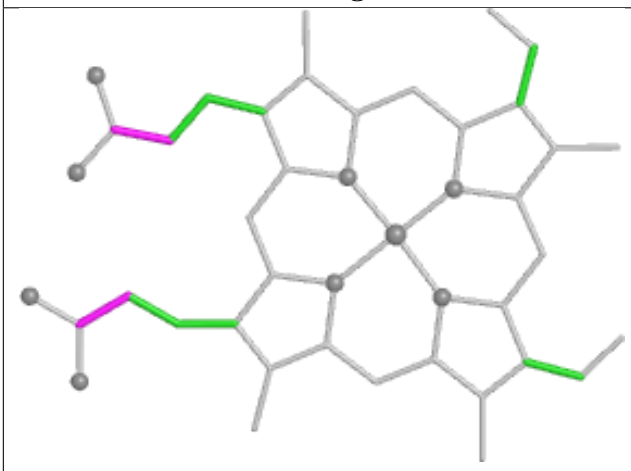
Ligand HEM e 102



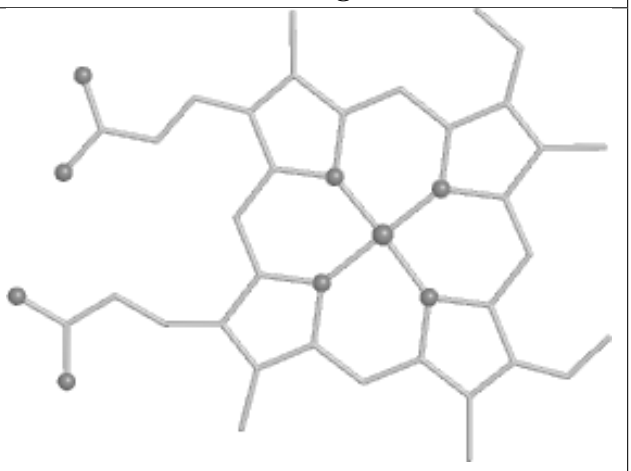
Bond lengths



Bond angles

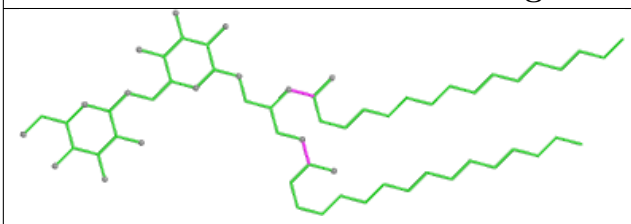


Torsions

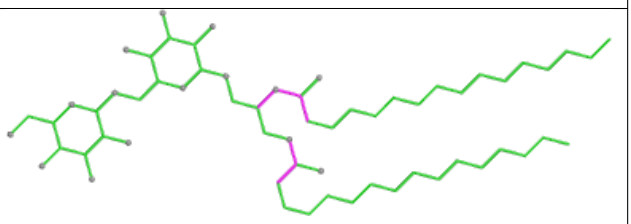


Rings

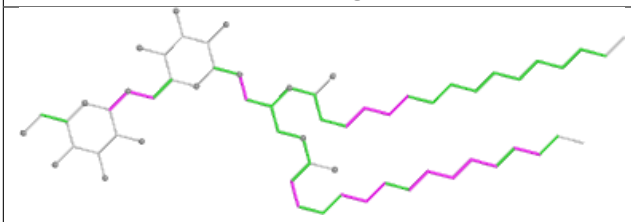
Ligand DGD c 518



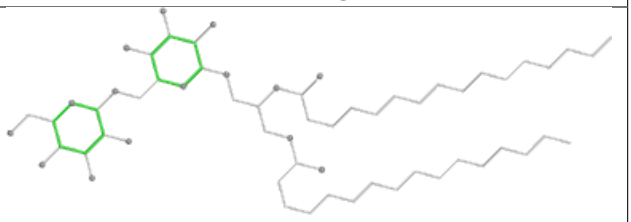
Bond lengths



Bond angles

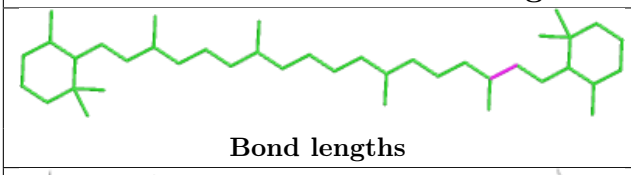


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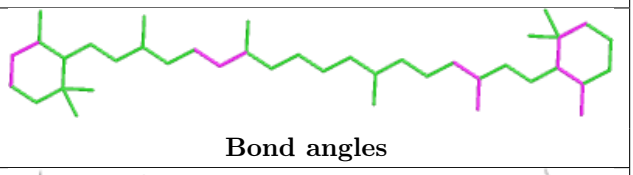


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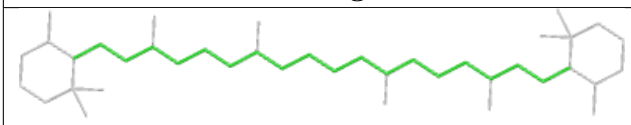
Ligand BCR b 623



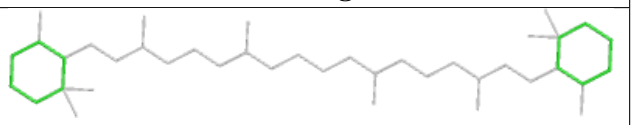
Bond lengths



Bond angles

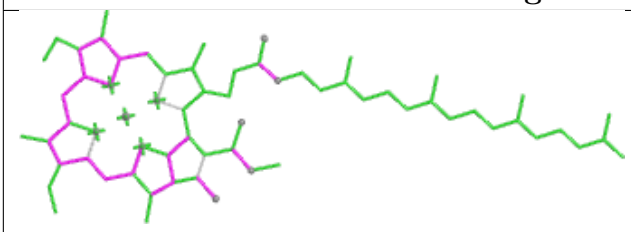


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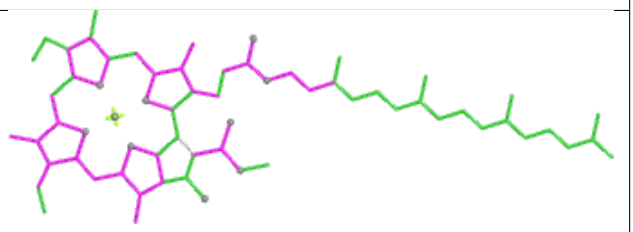


Rings

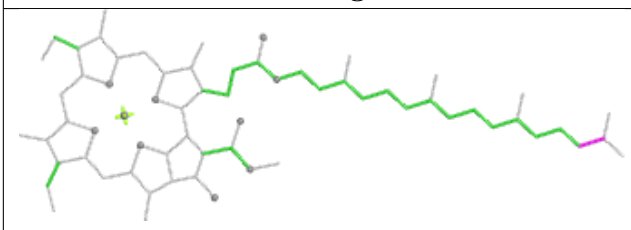
Ligand CLA B 609



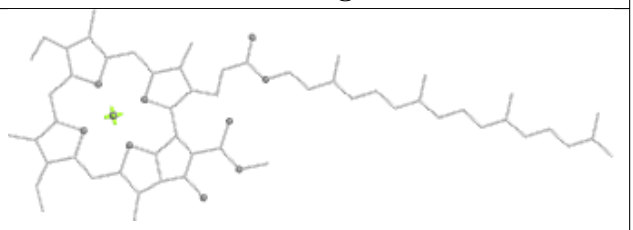
Bond lengths



Bond angles

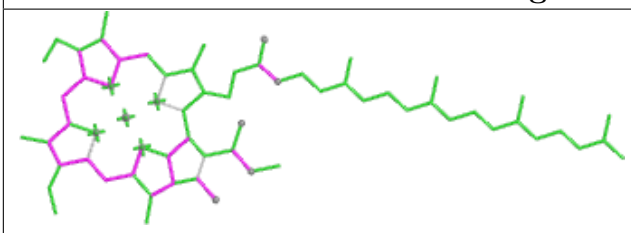


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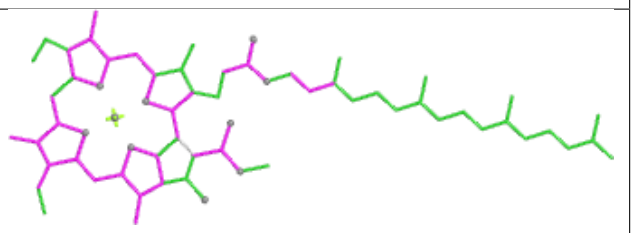


Rings

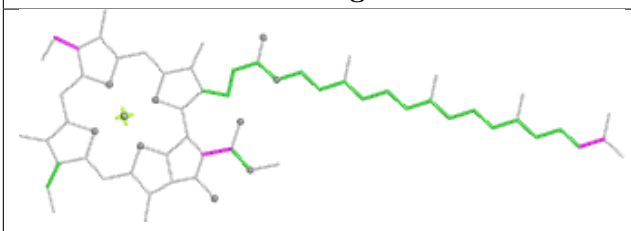
Ligand CLA c 504



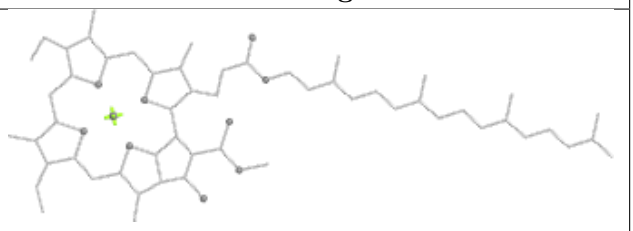
Bond lengths



Bond angles

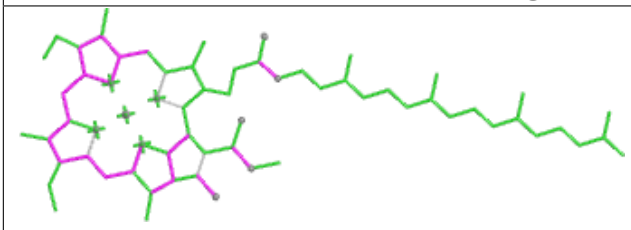


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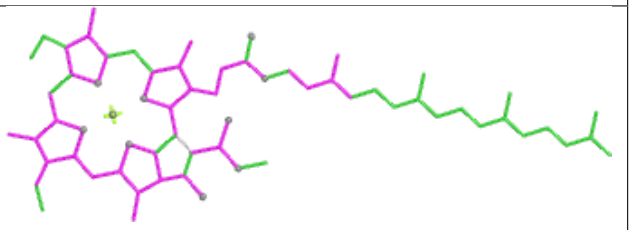


Rings

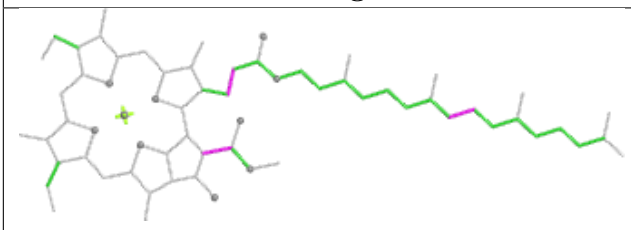
Ligand CLA B 611



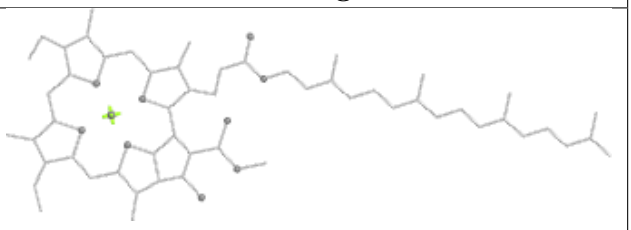
Bond lengths



Bond angles



Torsions

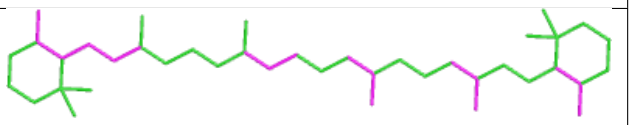


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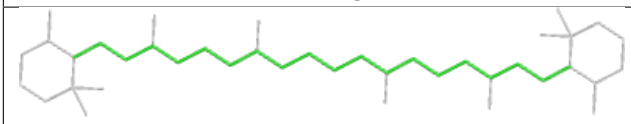
Ligand BCR A 410



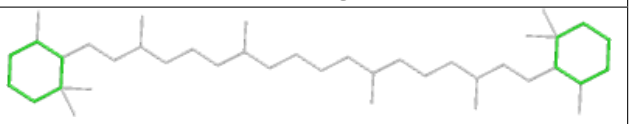
Bond lengths



Bond angles

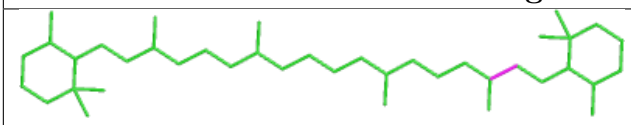


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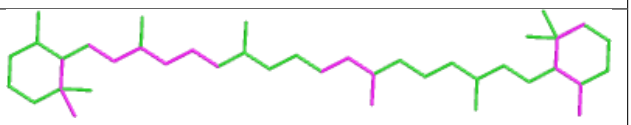


Rings

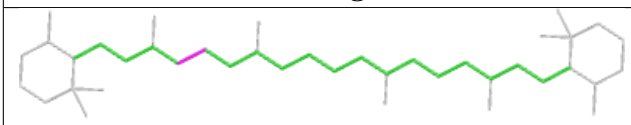
Ligand BCR h 101



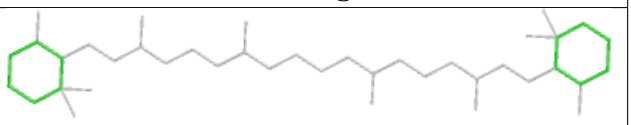
Bond lengths



Bond angles

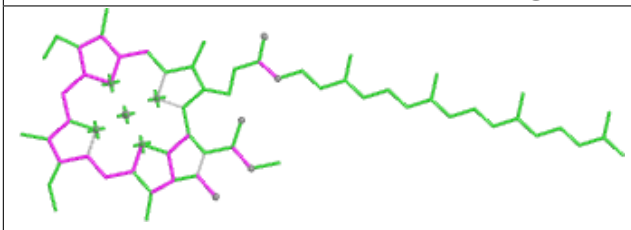


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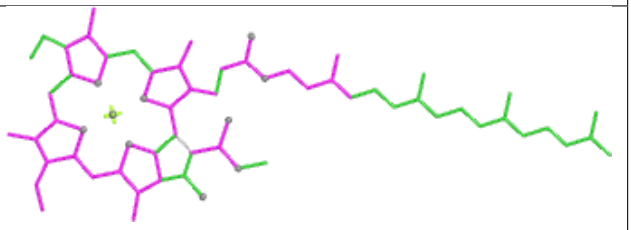


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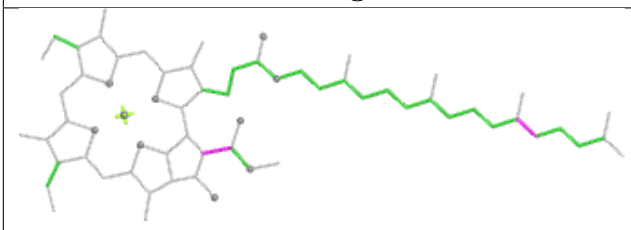
Ligand CLA b 607



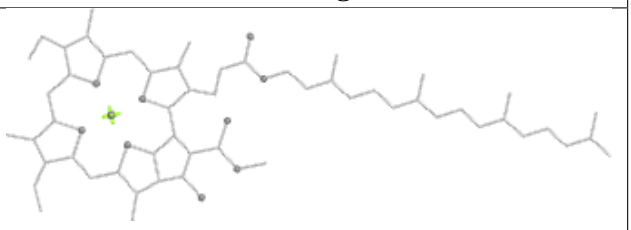
Bond lengths



Bond angles

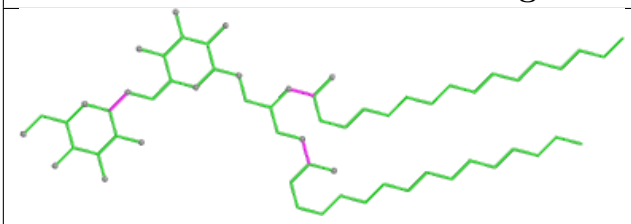


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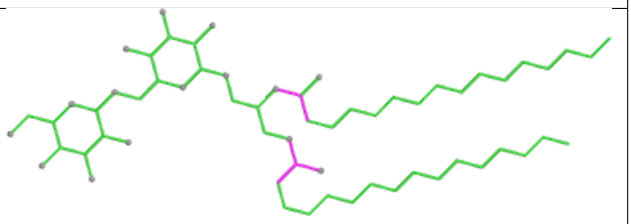


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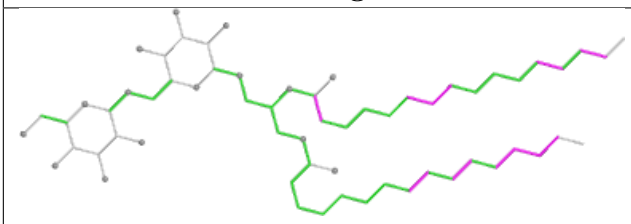
Ligand DGD H 102



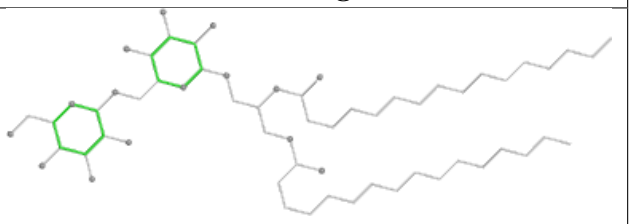
Bond lengths



Bond angles

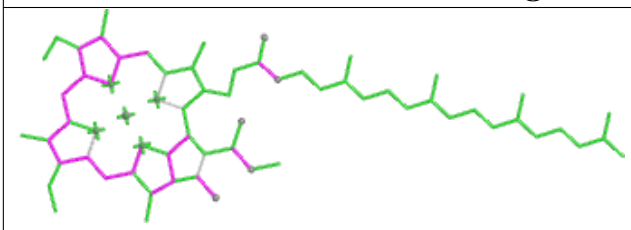


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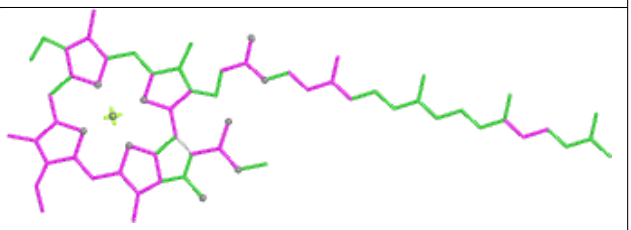


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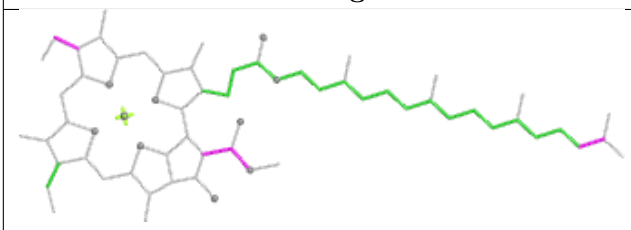
Ligand CLA C 503



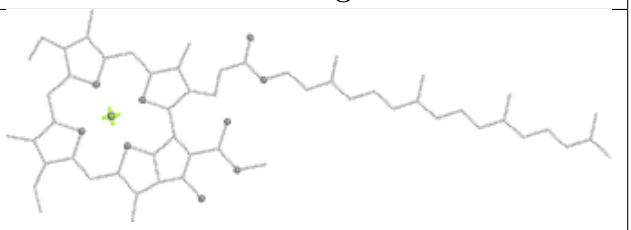
Bond lengths



Bond angles

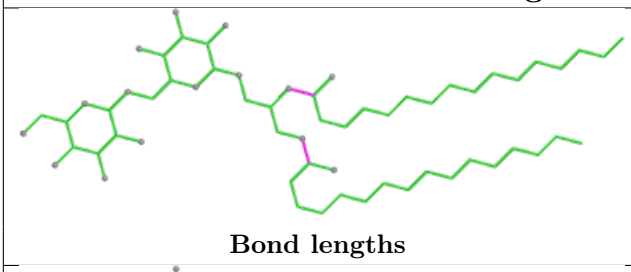


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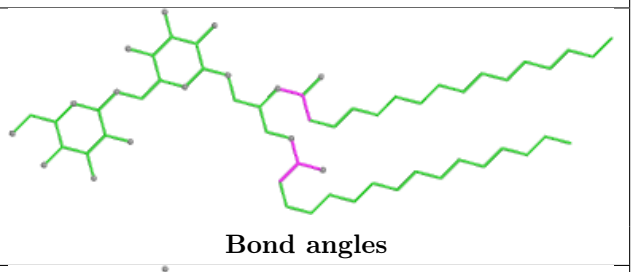


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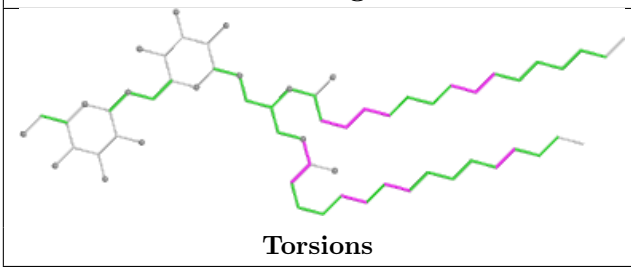
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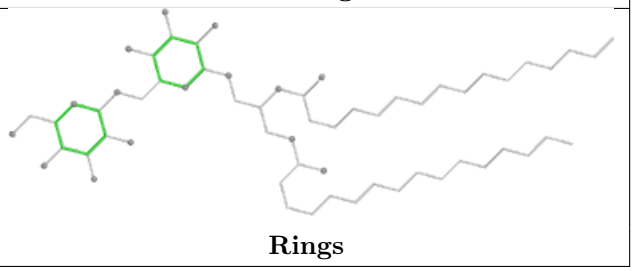
Bond lengths



Bond angles

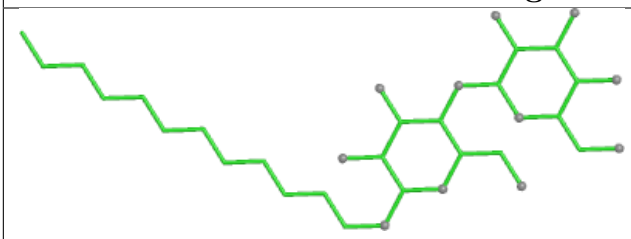


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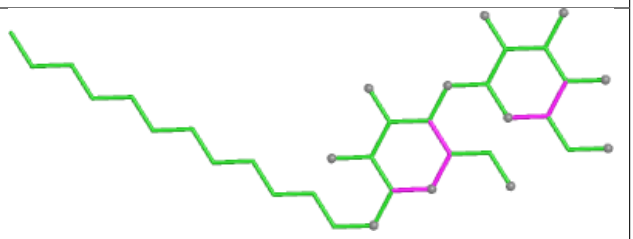


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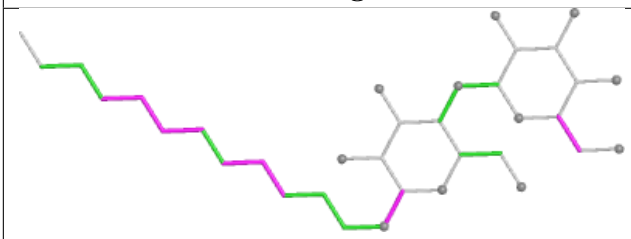
Ligand LMT a 401



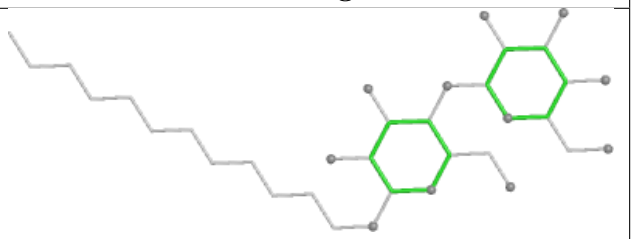
Bond lengths



Bond angles

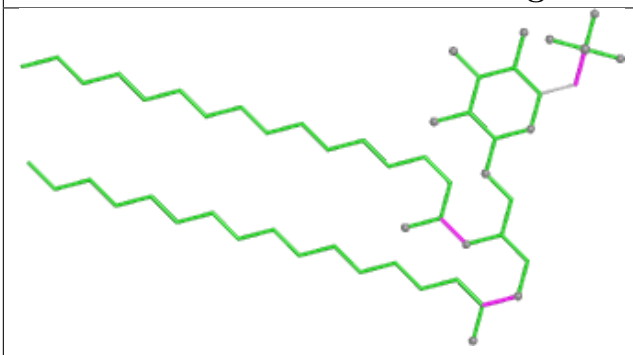


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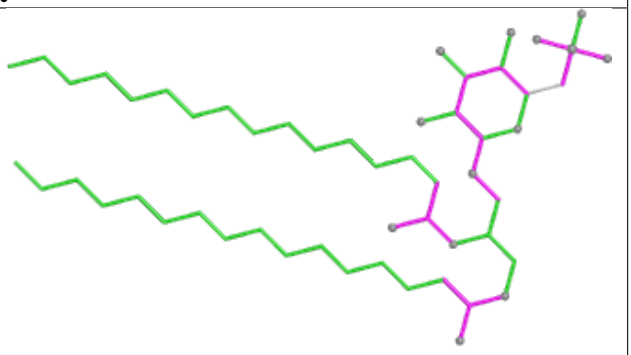


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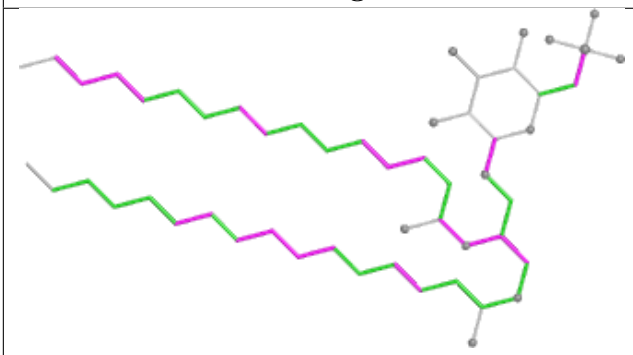
Ligand SQD b 601



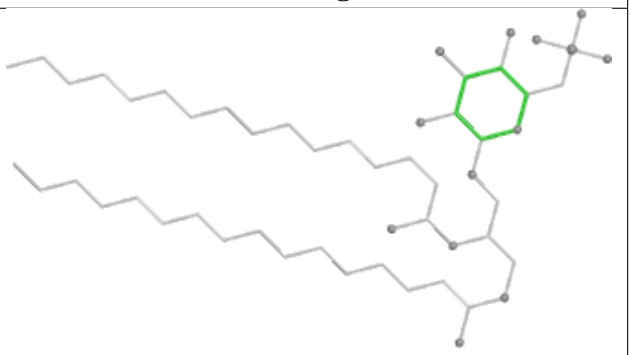
Bond lengths



Bond angles

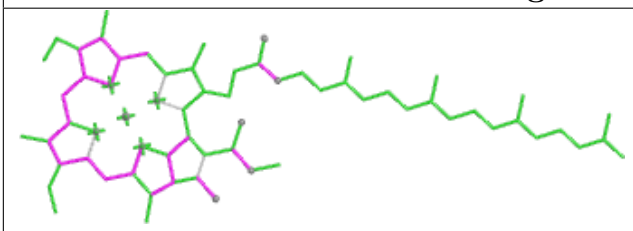


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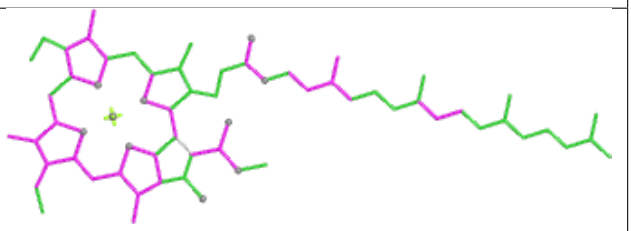


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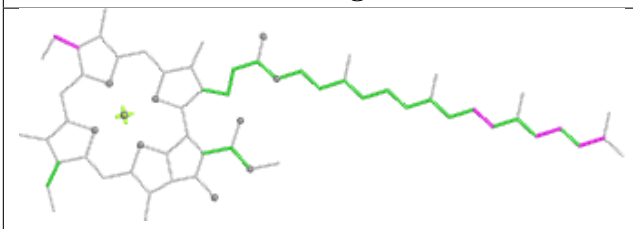
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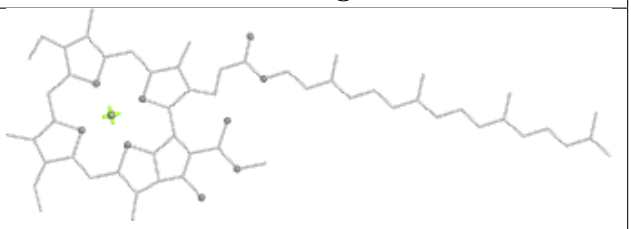
Bond lengths



Bond angles

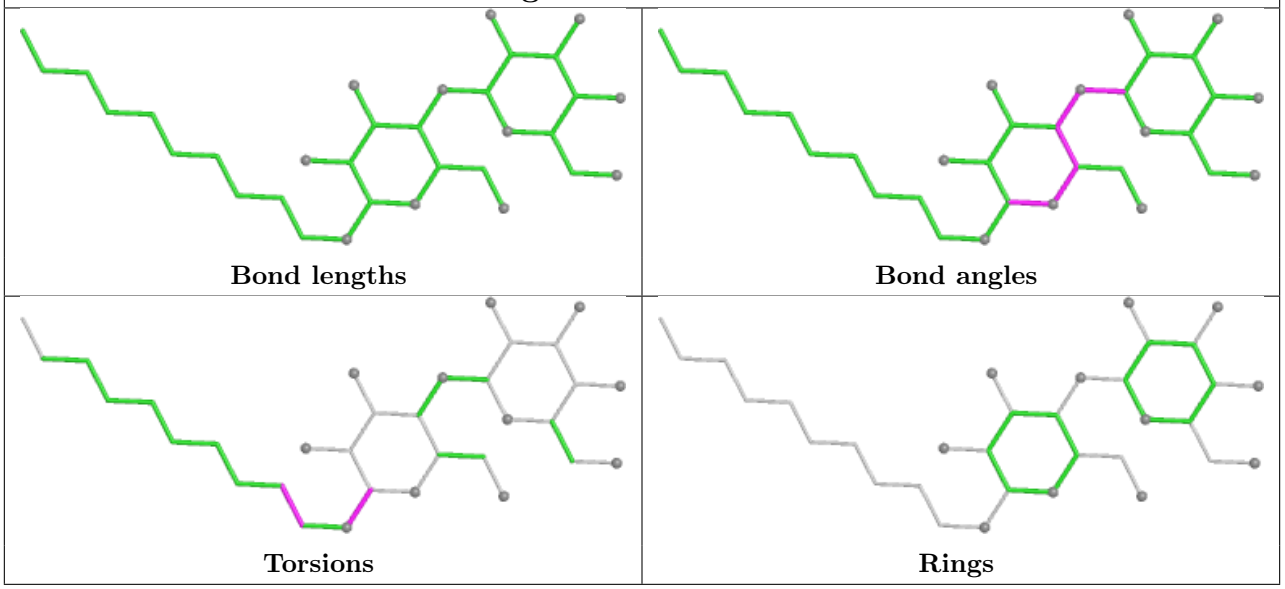


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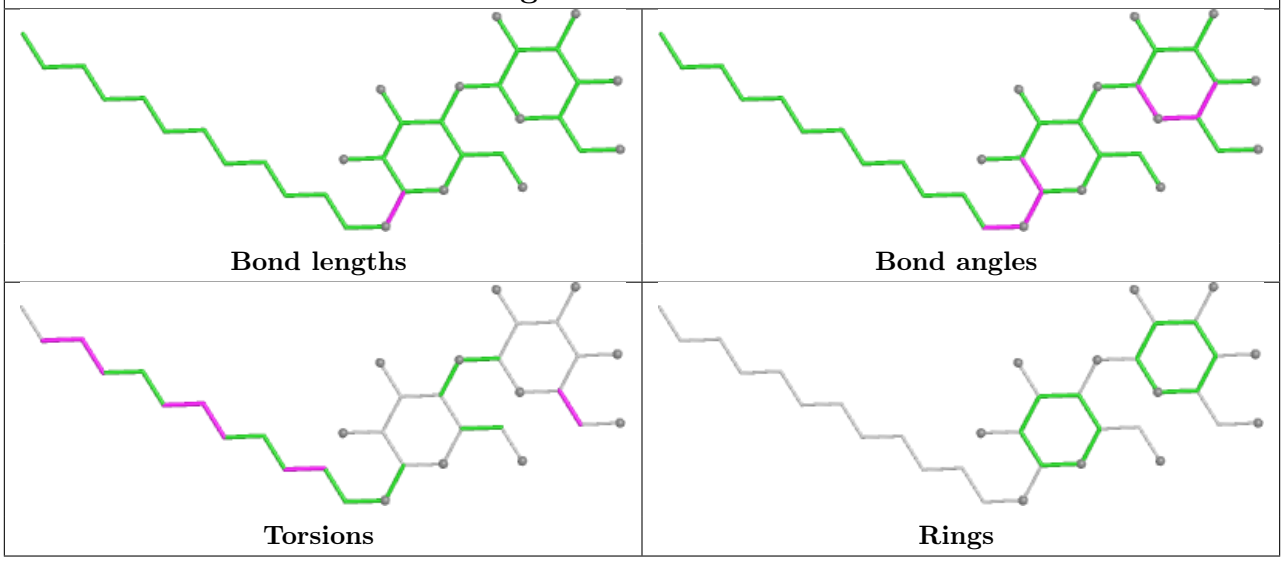


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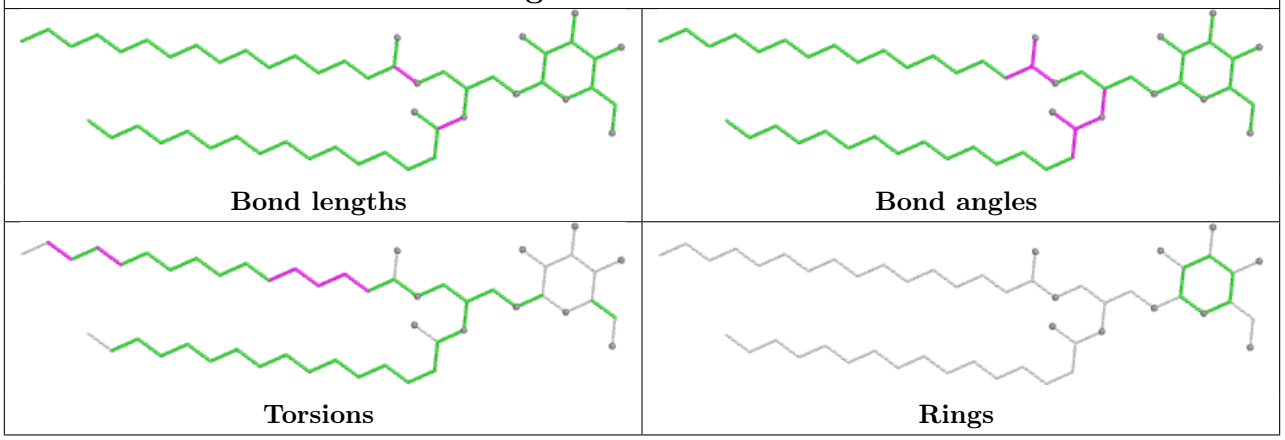
Ligand LMT A 417



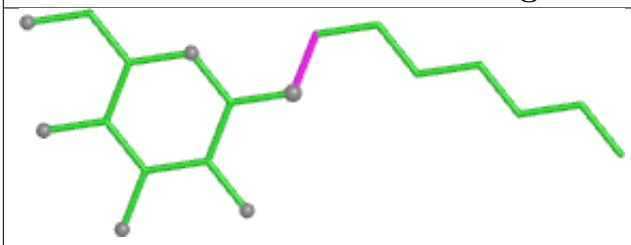
Ligand LMT m 103



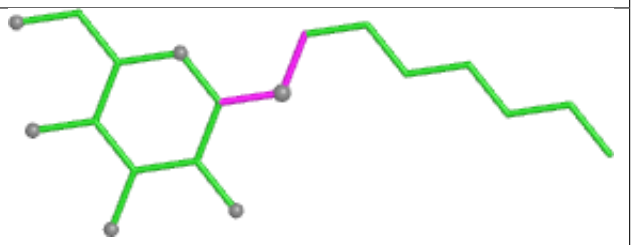
Ligand LMG c 521



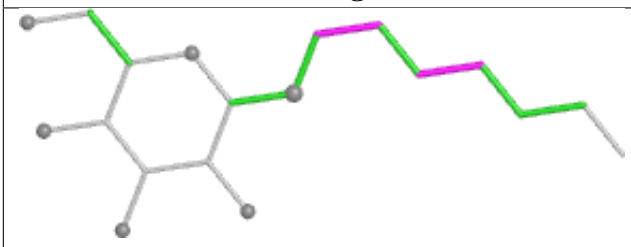
Ligand HTG O 303



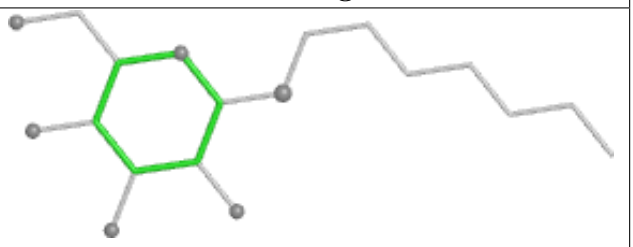
Bond lengths



Bond angles

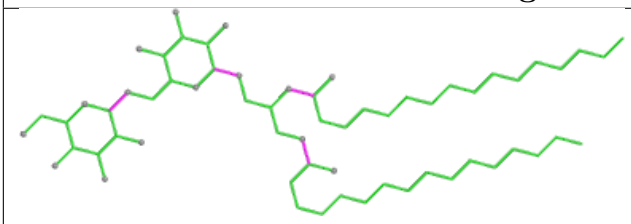


Torsions

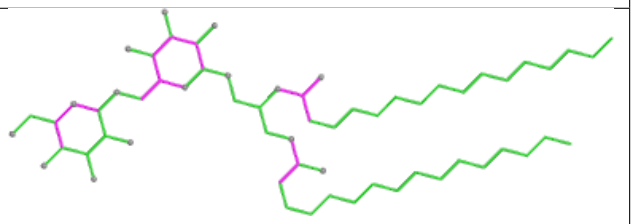


Rings

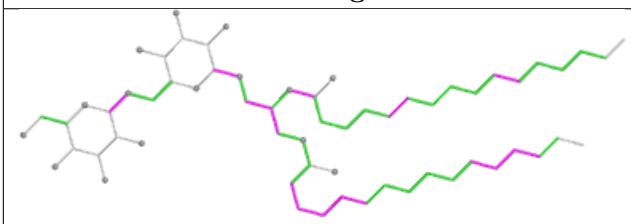
Ligand DGD D 407



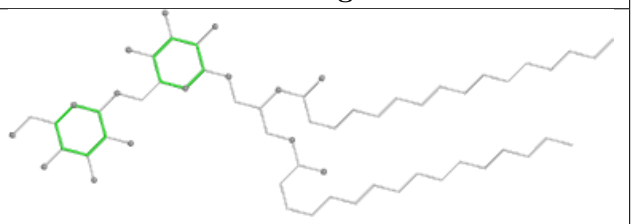
Bond lengths



Bond angles

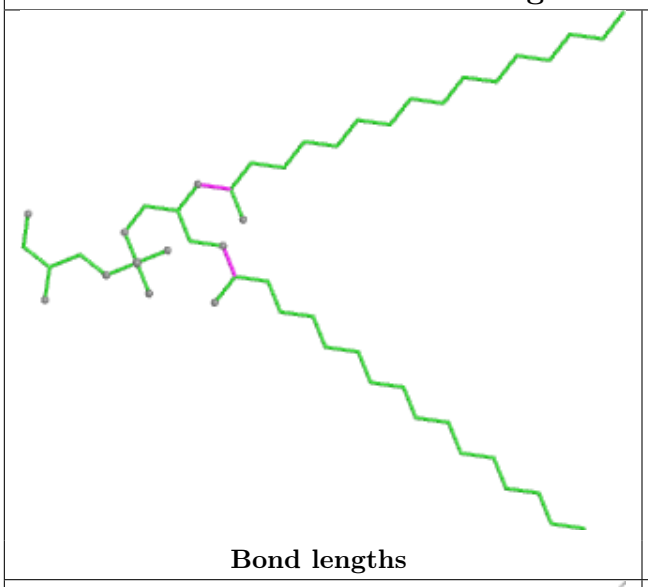


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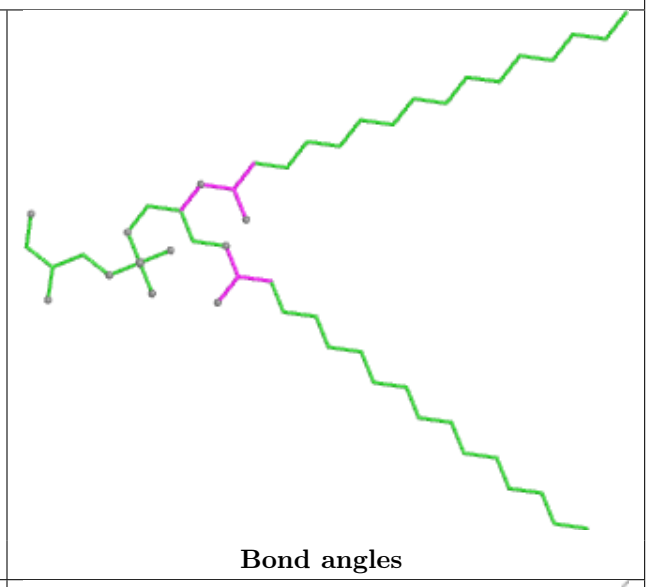


Rings

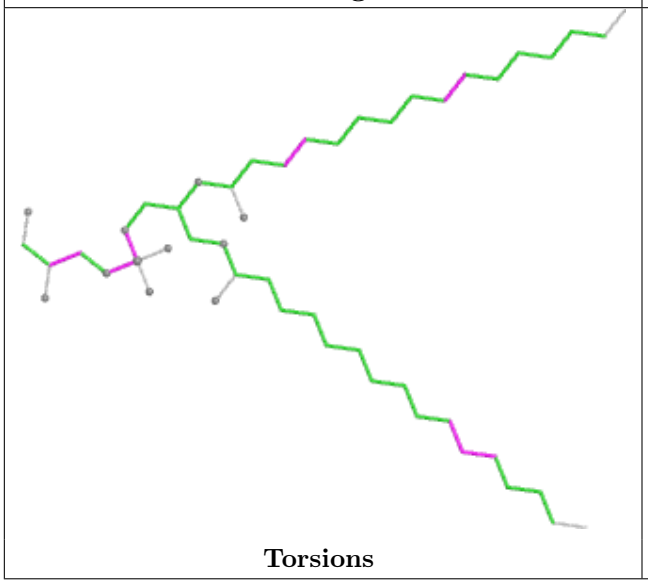
Ligand LHG d 409



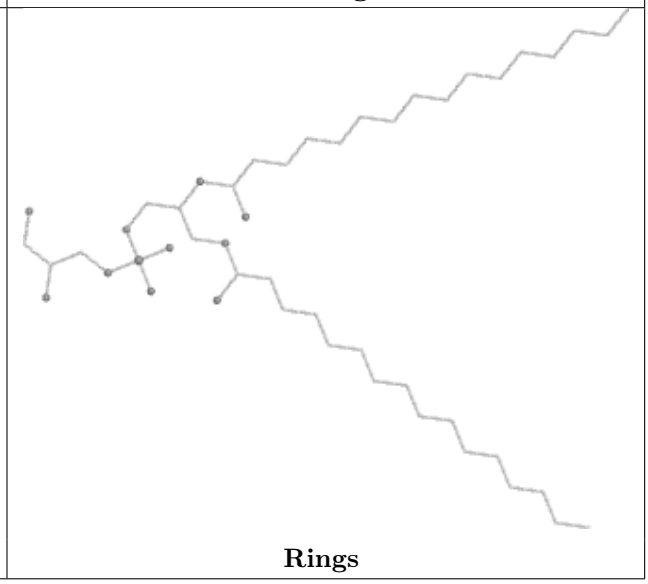
Bond lengths



Bond angles



Torsions

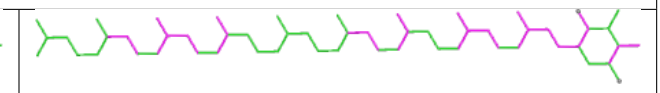


Rings

Ligand PL9 d 406



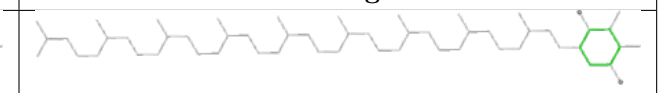
Bond lengths



Bond angles

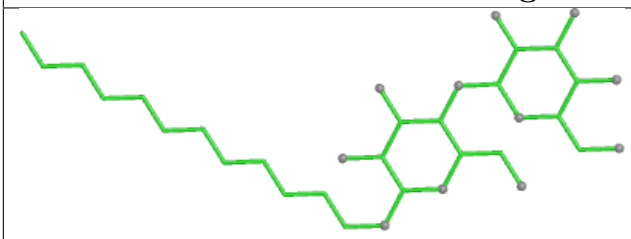


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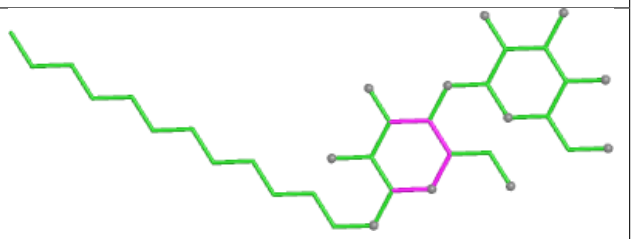


Rings

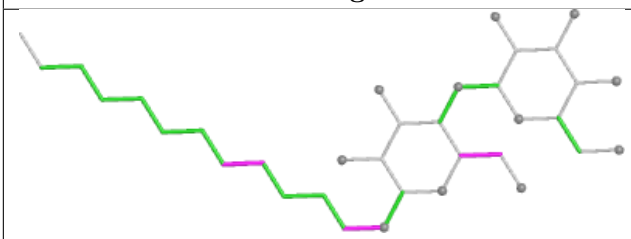
Ligand LMT m 102



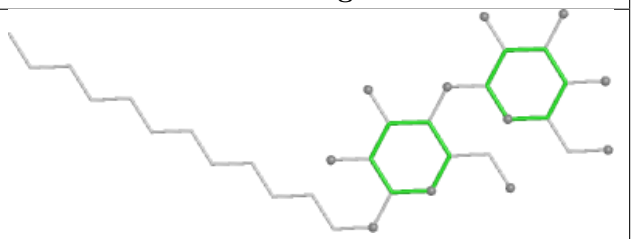
Bond lengths



Bond angles

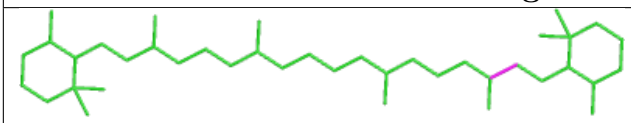


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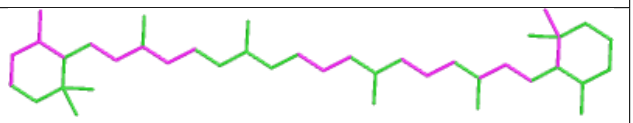


Rings

Ligand BCR C 516



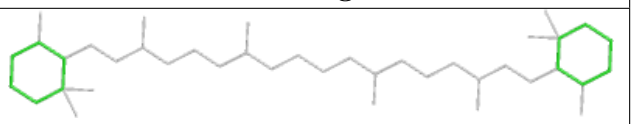
Bond lengths



Bond angles

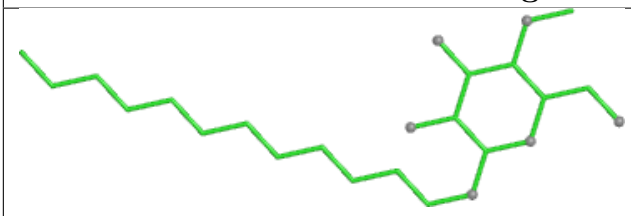


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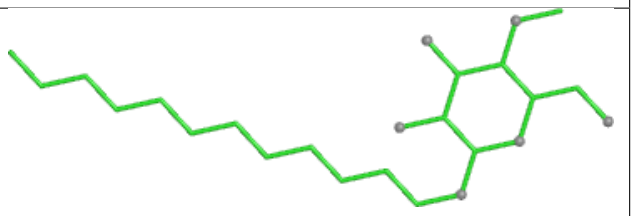


Rings

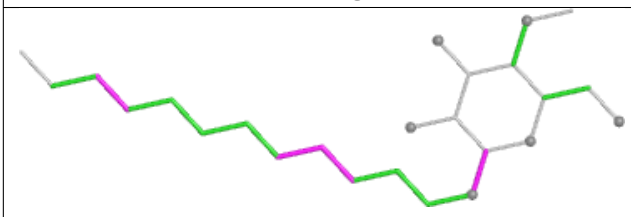
Ligand LMT B 634



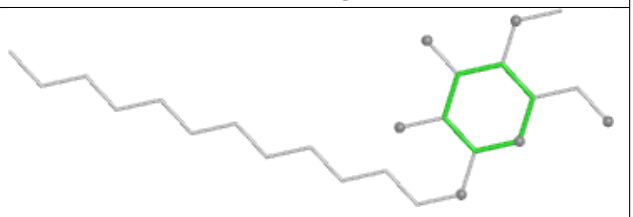
Bond lengths



Bond angles

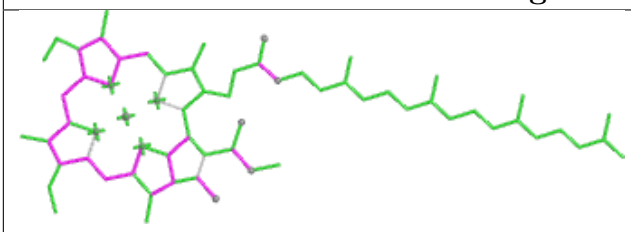


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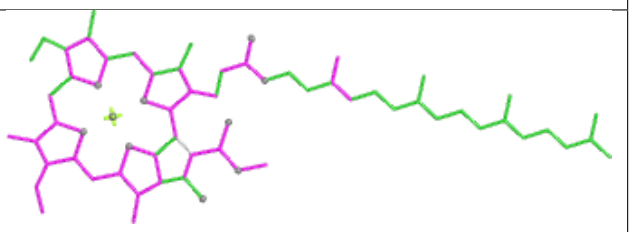


Rings

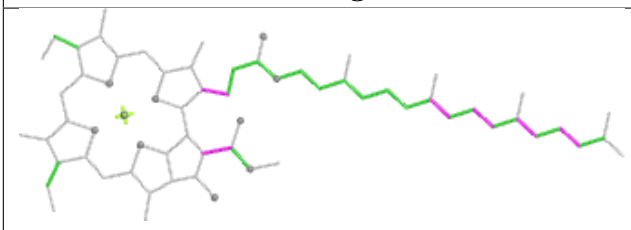
Ligand CLA c 508



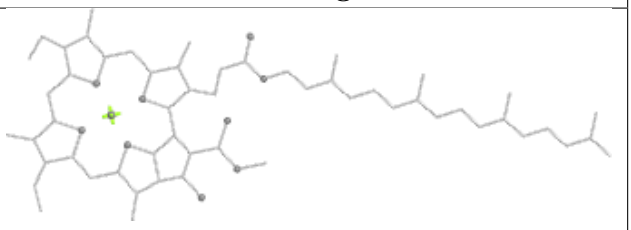
Bond lengths



Bond angles

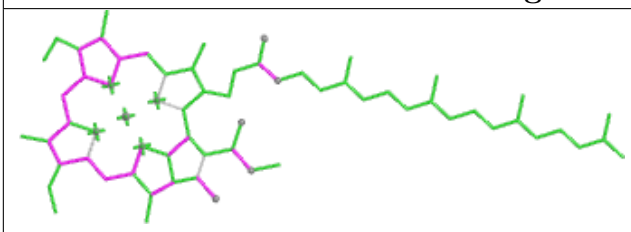


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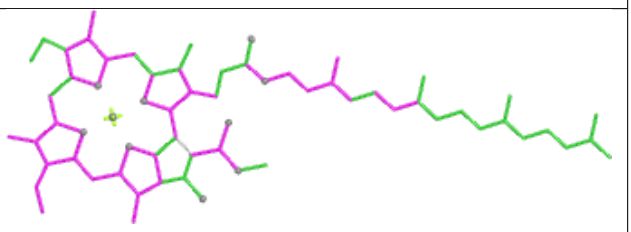


Rings

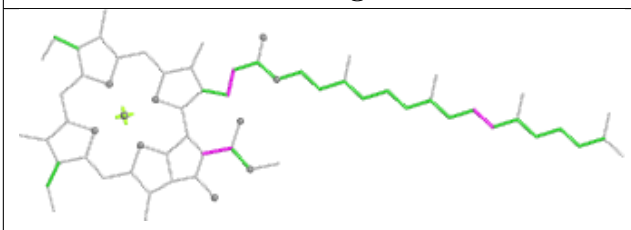
Ligand CLA B 607



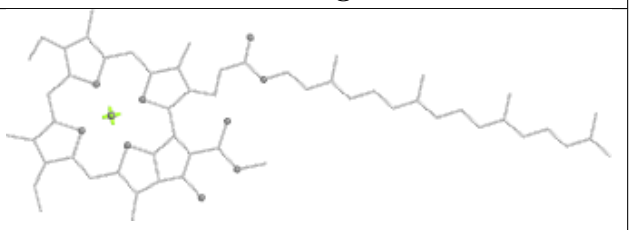
Bond lengths



Bond angles

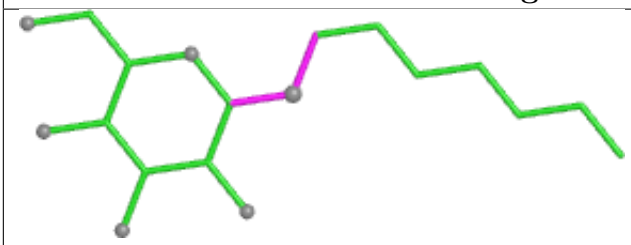


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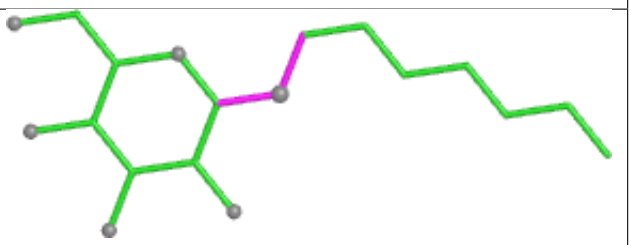


Rings

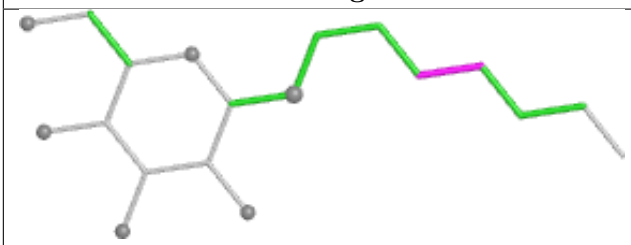
Ligand HTG B 630



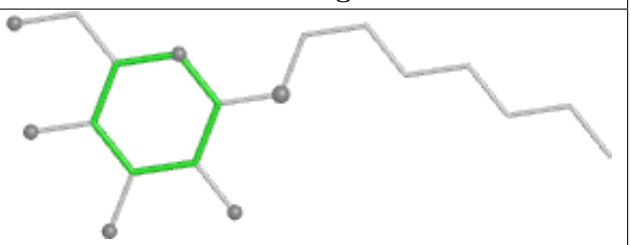
Bond lengths



Bond angles

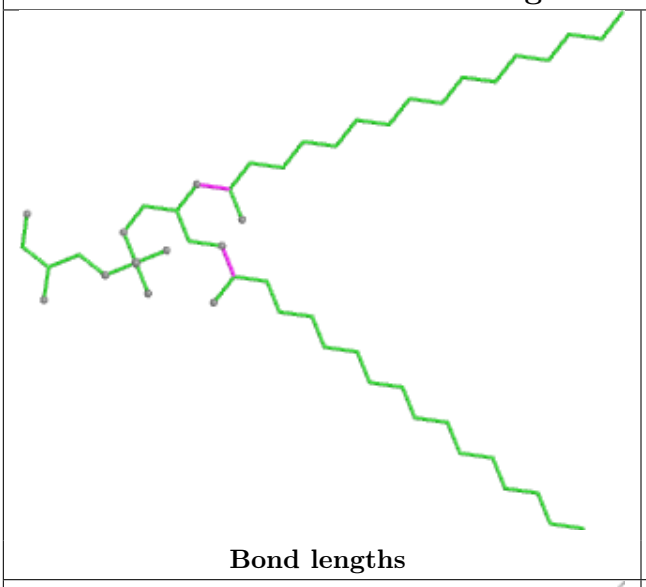


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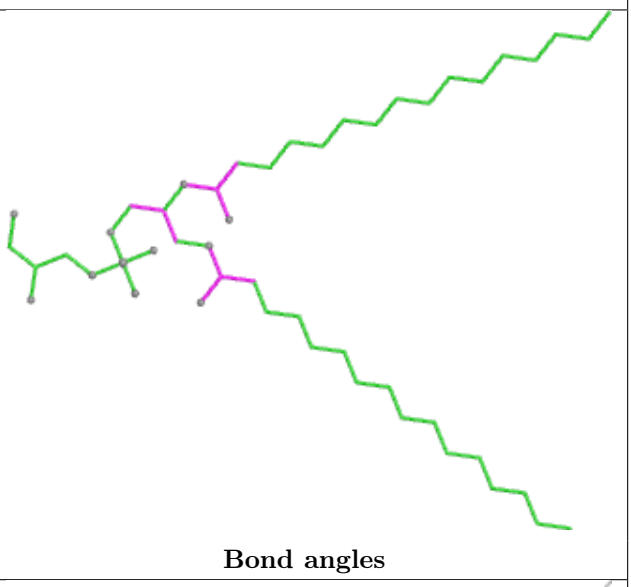


Rings

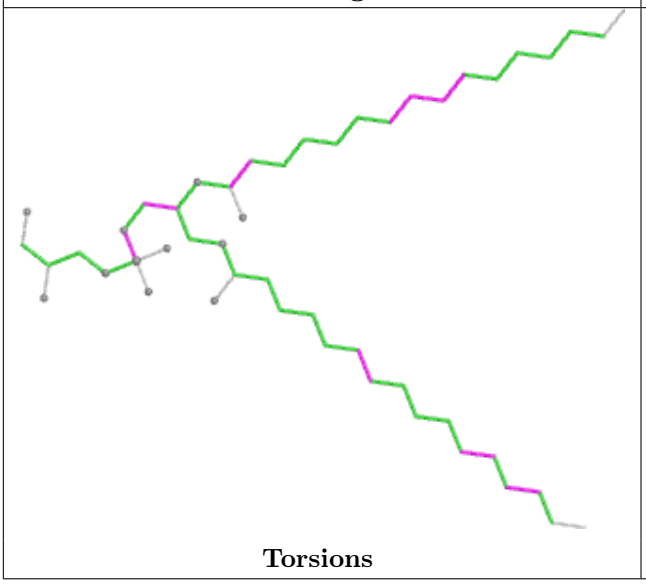
Ligand LHG L 101



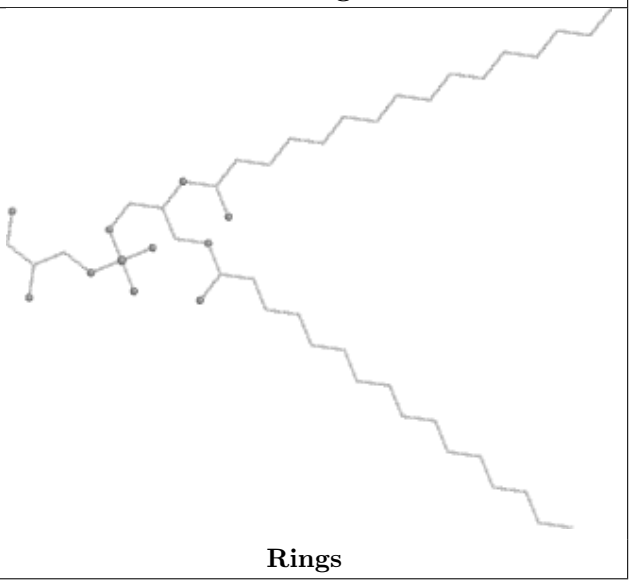
Bond lengths



Bond angles

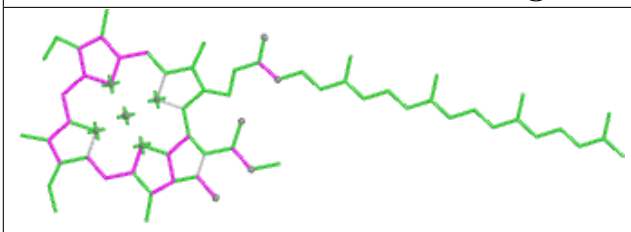


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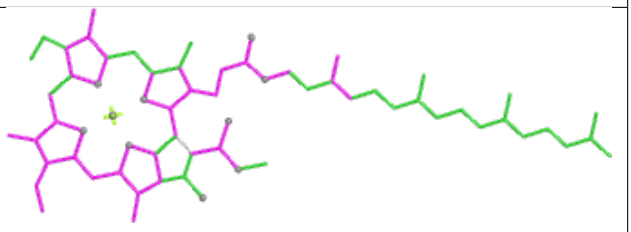


Rings

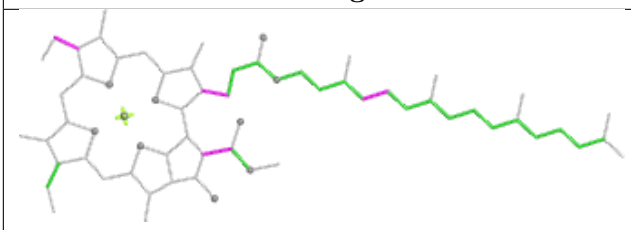
Ligand CLA b 612



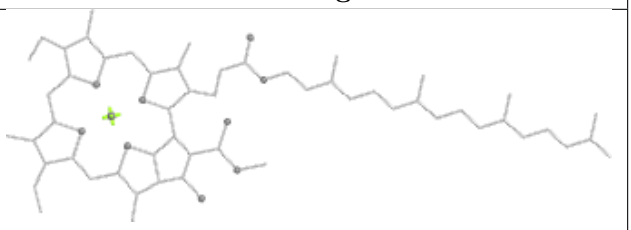
Bond lengths



Bond angles

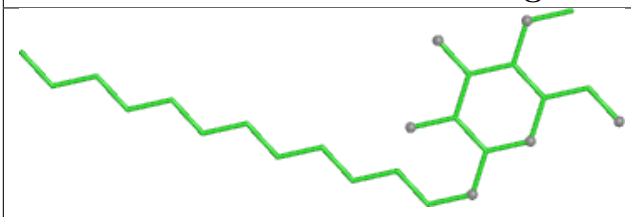


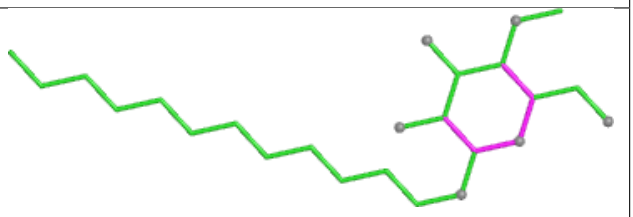
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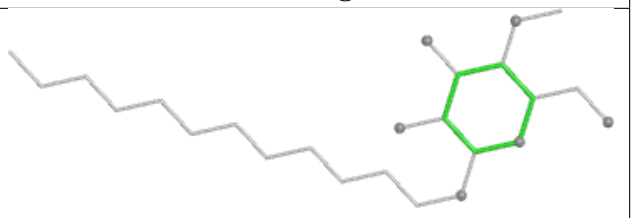
Rings

Ligand LMT b 602

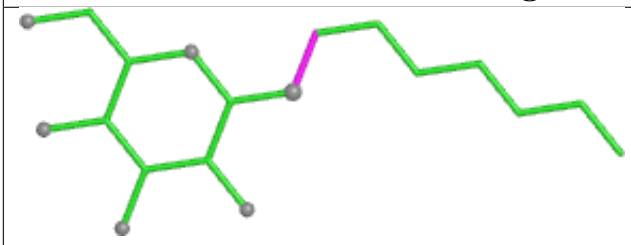

Bond lengths

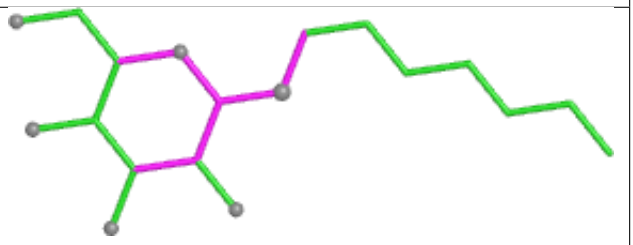

Bond angles

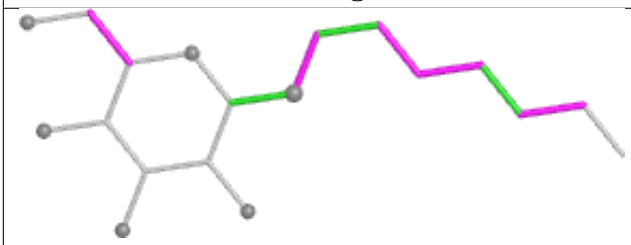

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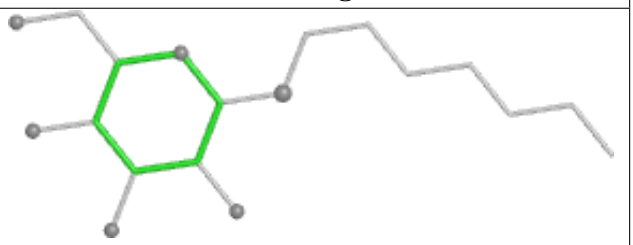

Rings

Ligand HTG B 623

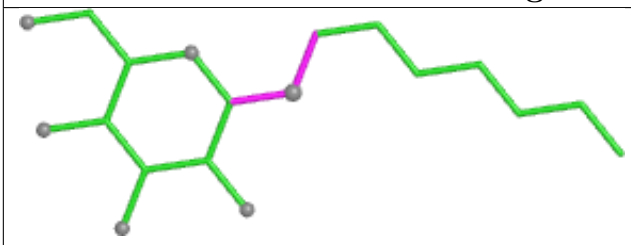

Bond lengths

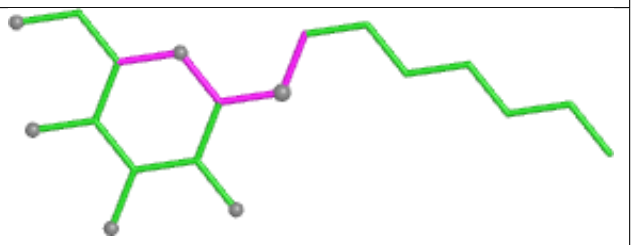

Bond angles

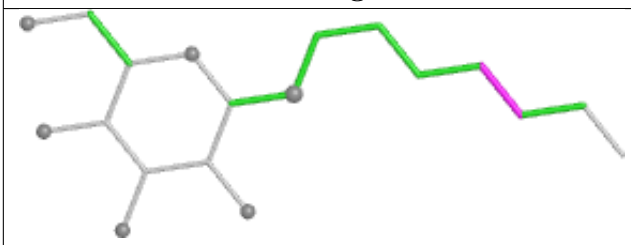

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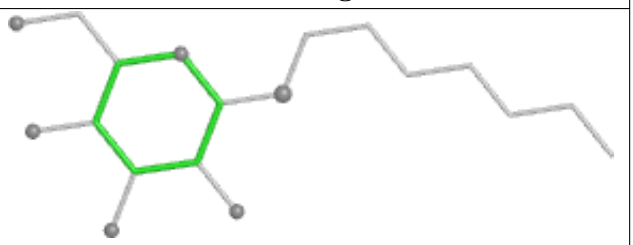

Rings

Ligand HTG c 522

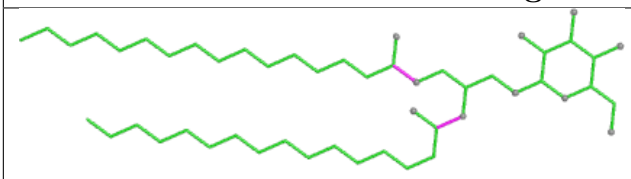

Bond lengths


Bond angles

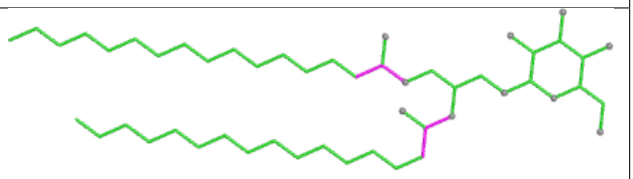

Torsions


Rings

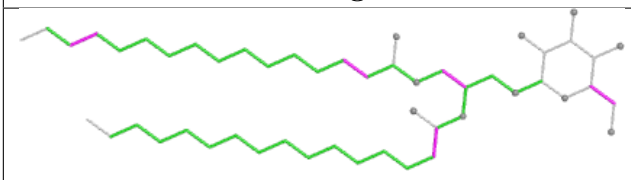
Ligand LMG c 520



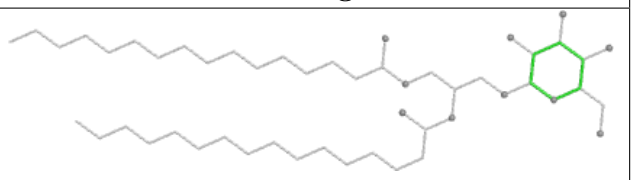
Bond lengths



Bond angles

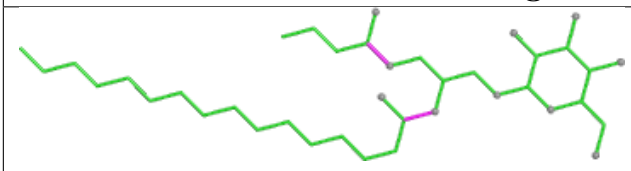


Torsions

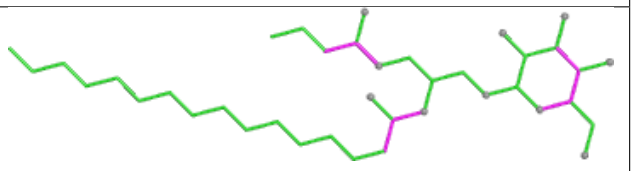


Rings

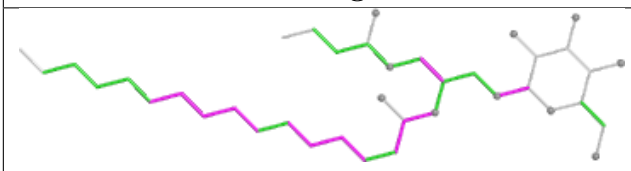
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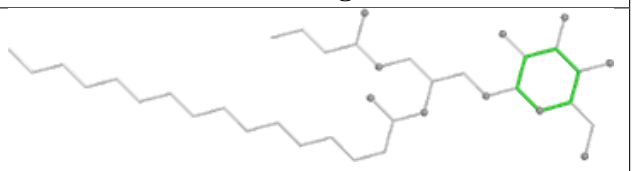
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Bond angles

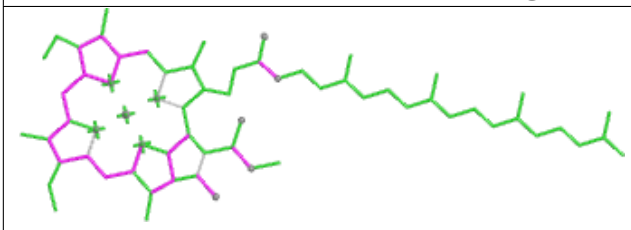


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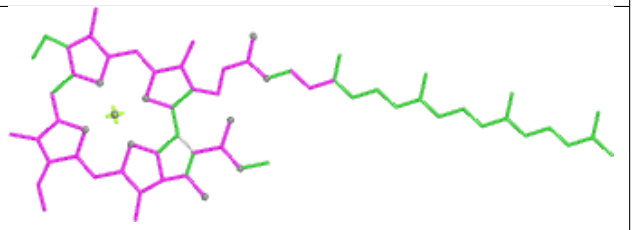


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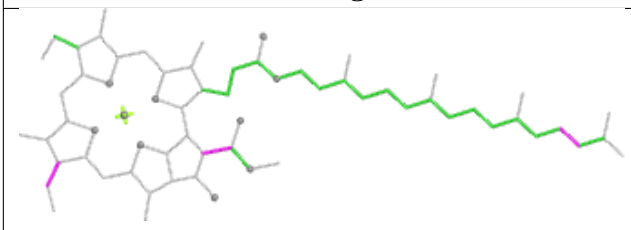
Ligand CLA D 401



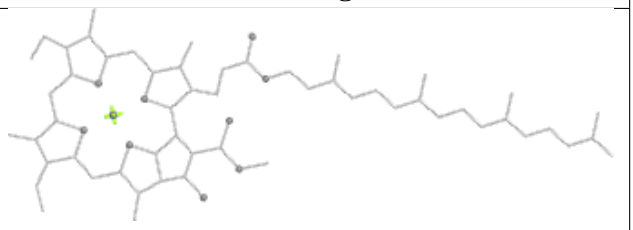
Bond lengths



Bond angles

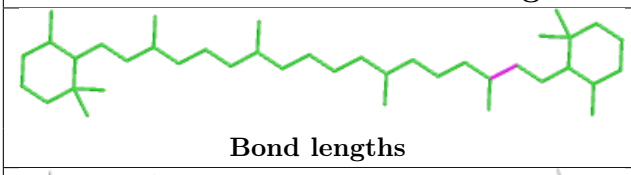


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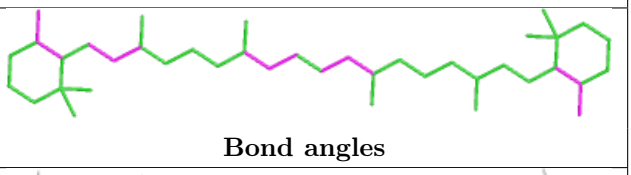


Rings

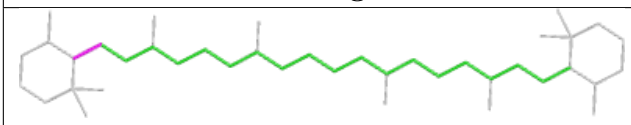
Ligand BCR C 515



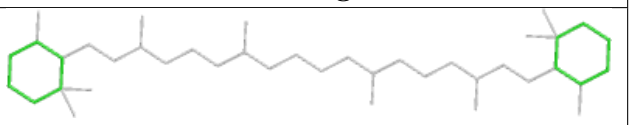
Bond lengths



Bond angles

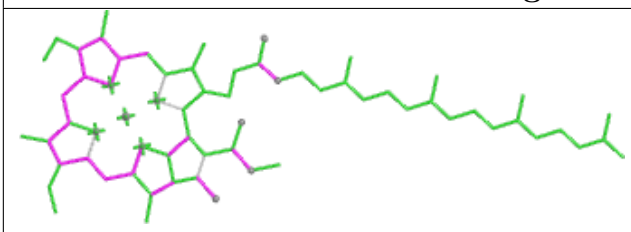


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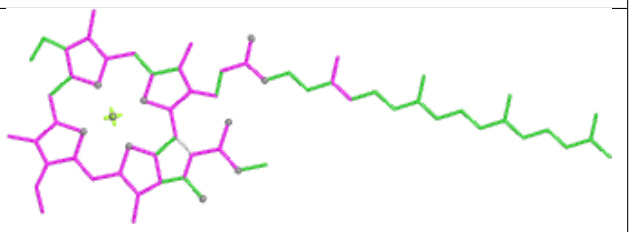


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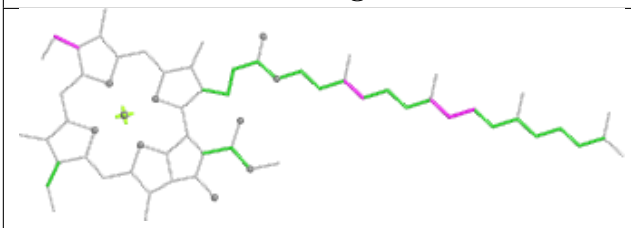
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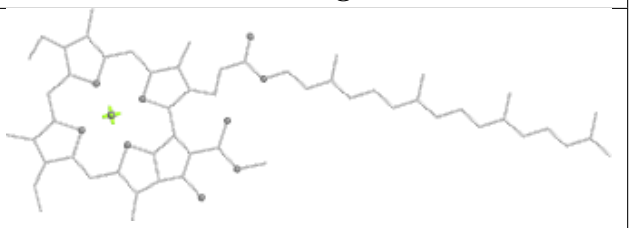
Bond lengths



Bond angles

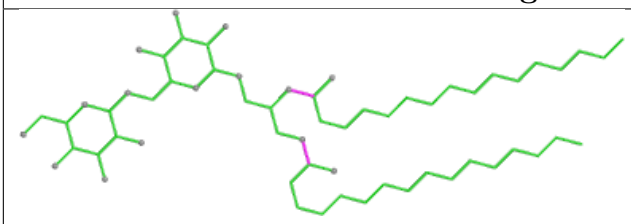


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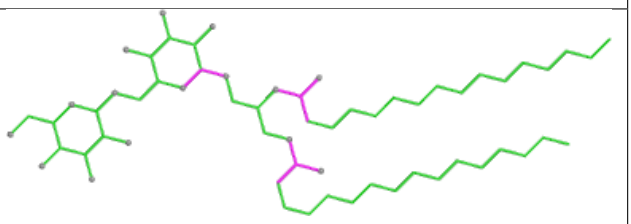


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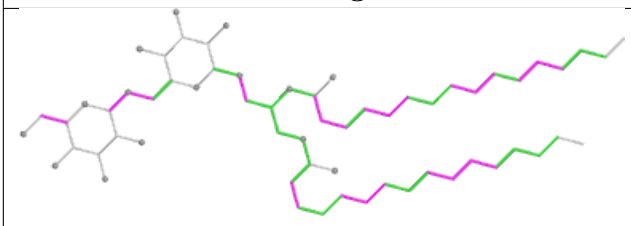
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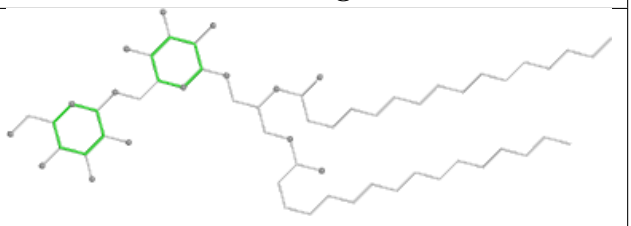
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Bond angles

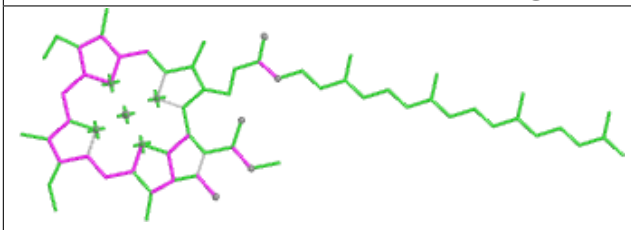


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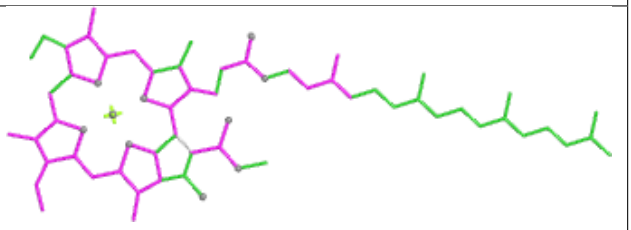


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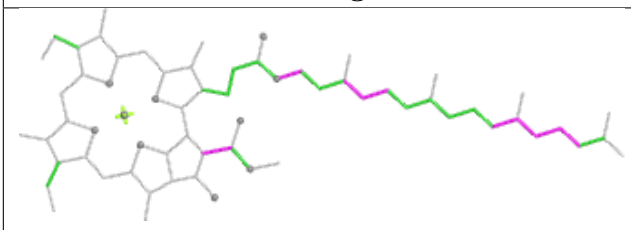
Ligand CLA b 619



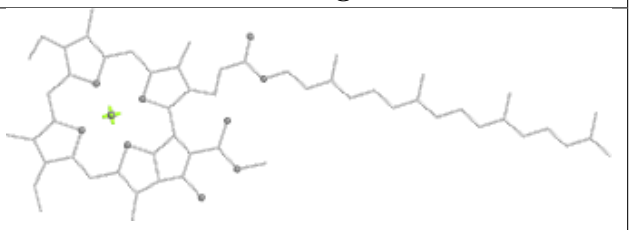
Bond lengths



Bond angles

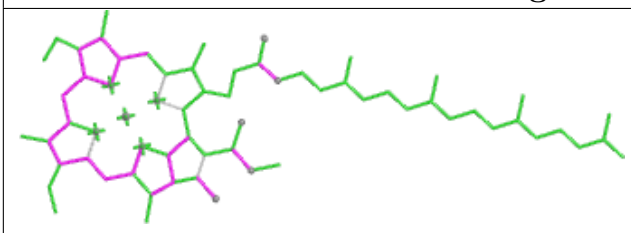


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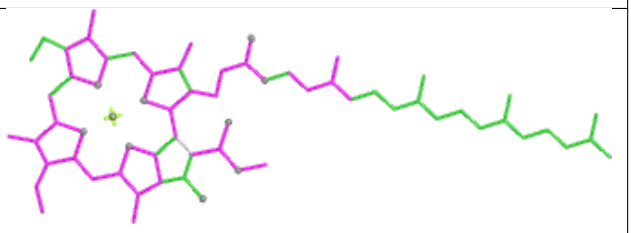


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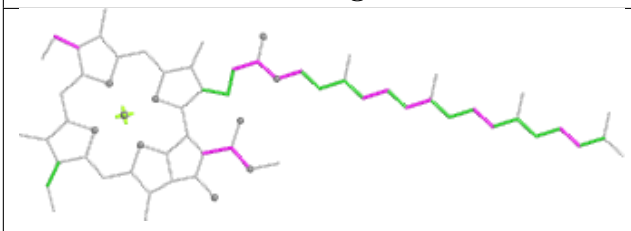
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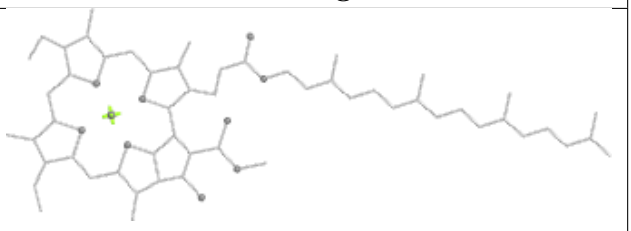
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Bond angles

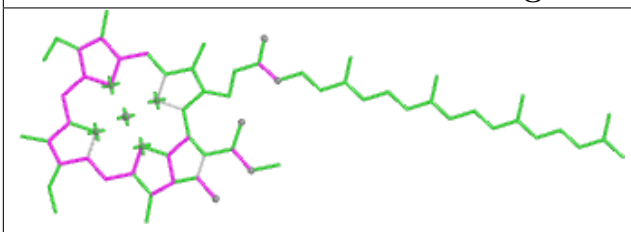


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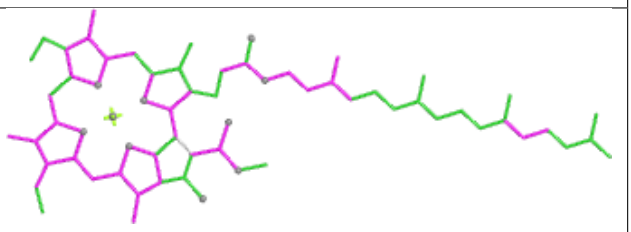


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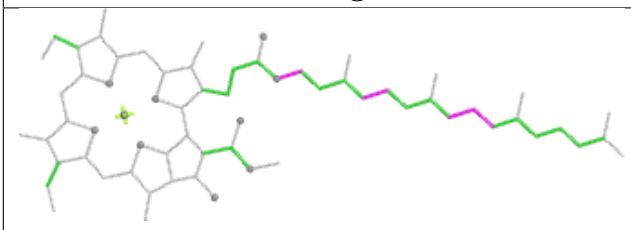
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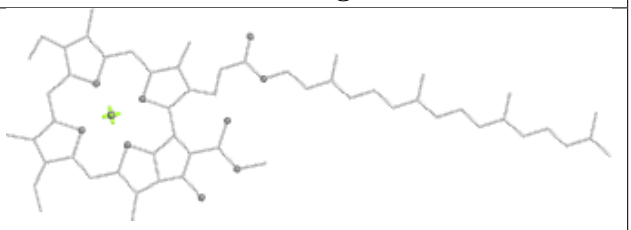
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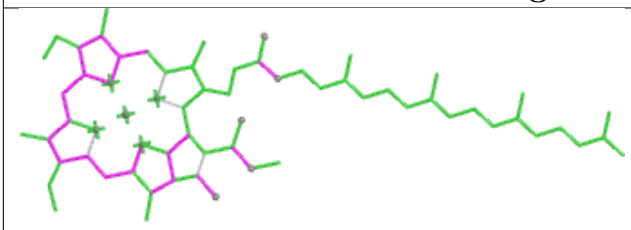


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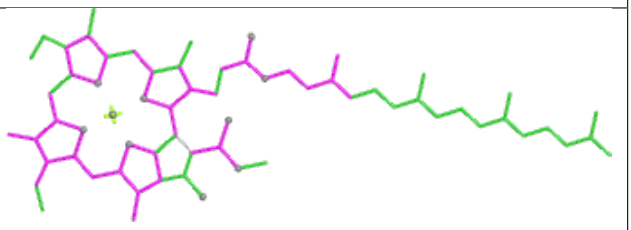


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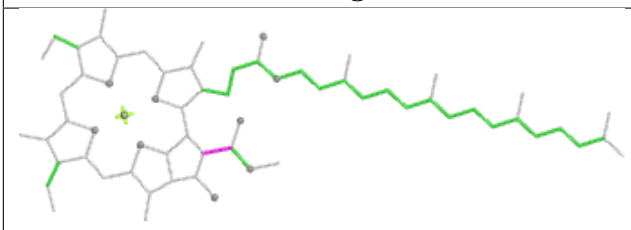
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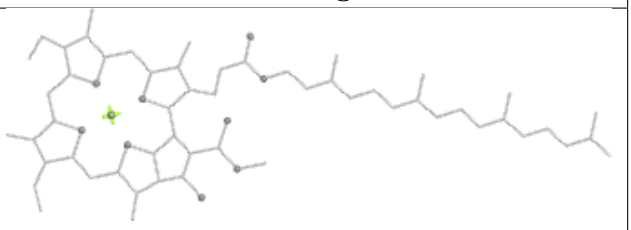
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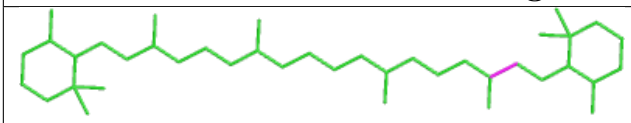


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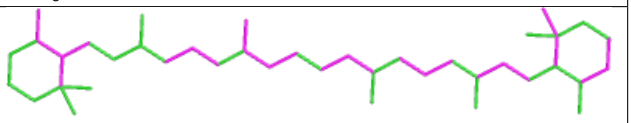


Rings

Ligand BCR y 101



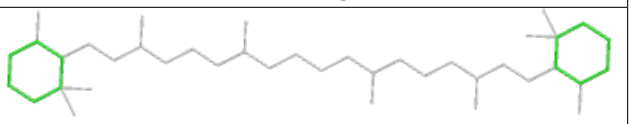
Bond lengths



Bond angles

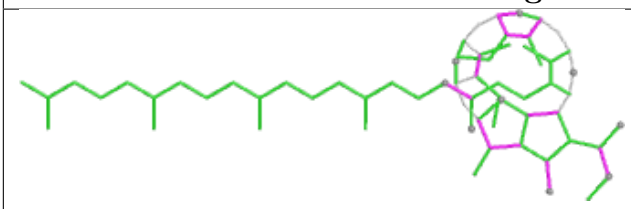


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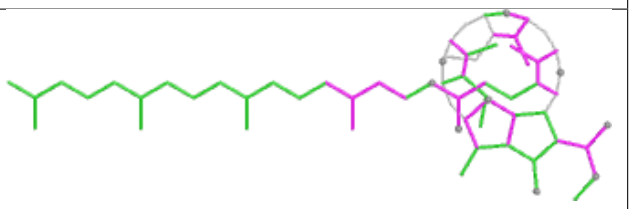


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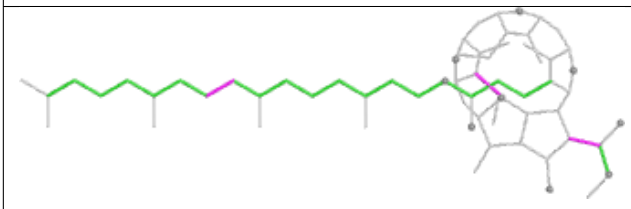
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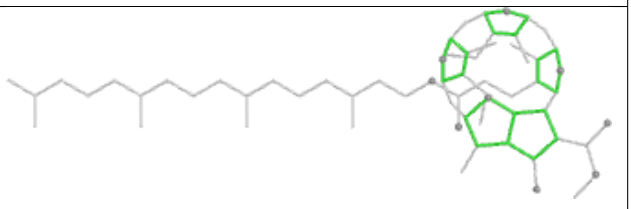
Bond lengths



Bond angles

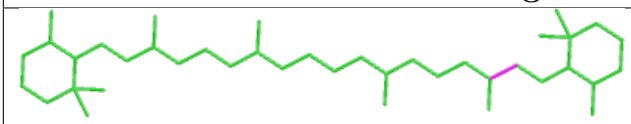


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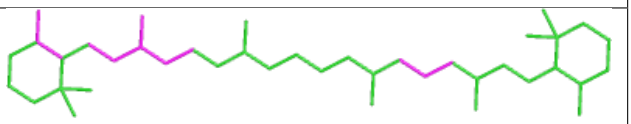


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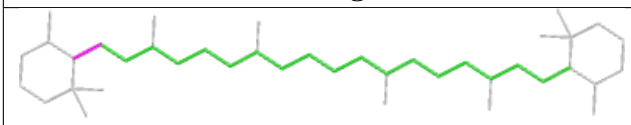
Ligand BCR B 618



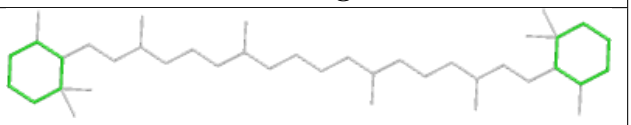
Bond lengths



Bond angles

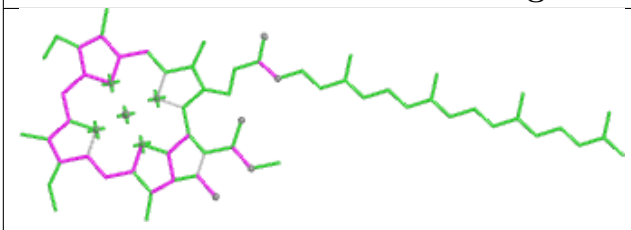


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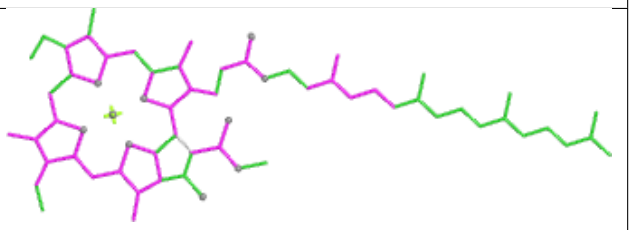


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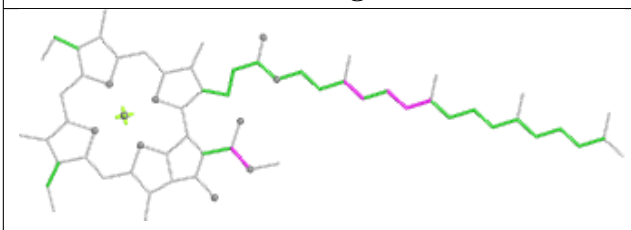
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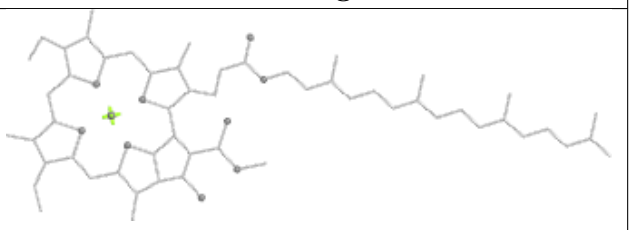
Bond lengths



Bond angles

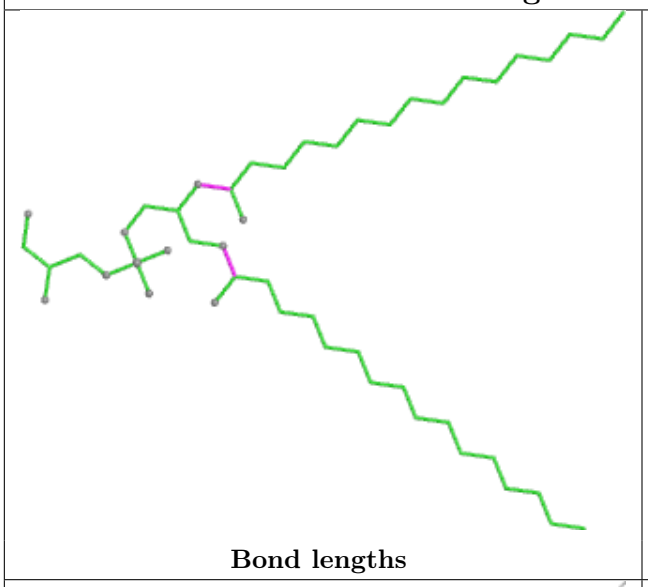


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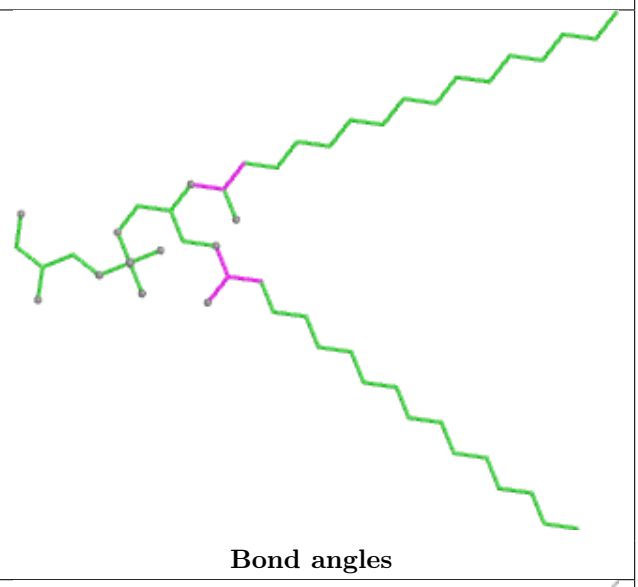


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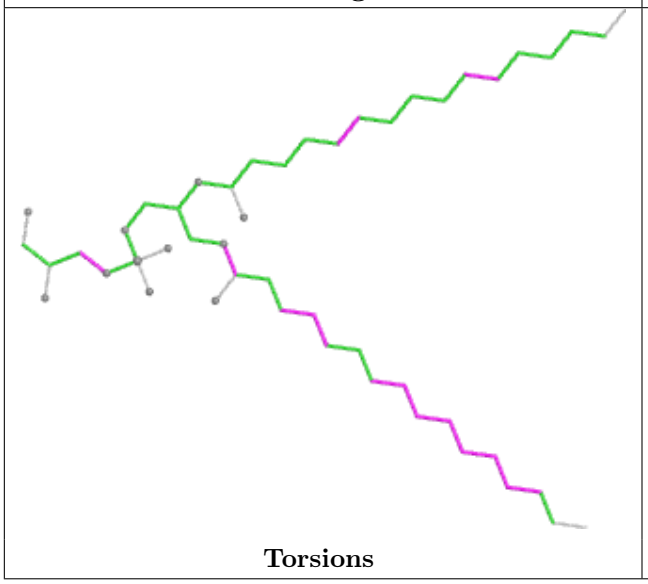
Ligand LHG D 410



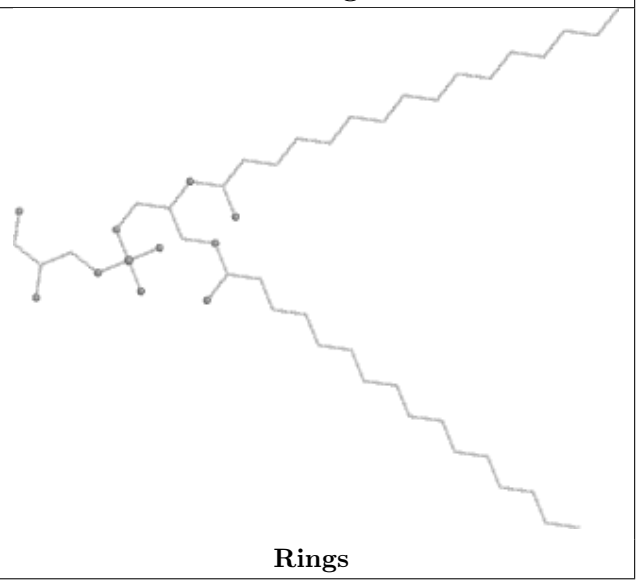
Bond lengths



Bond angles



Torsions

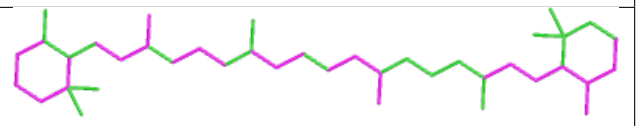


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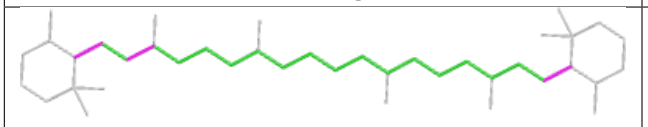
Ligand BCR B 620



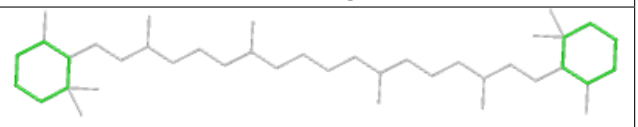
Bond lengths



Bond angles

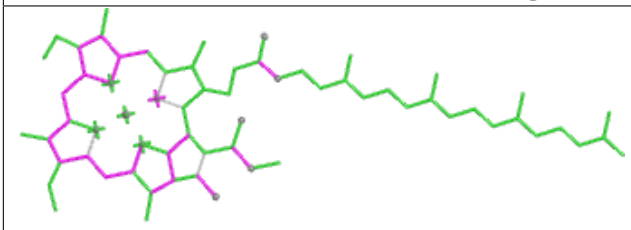


Torsions

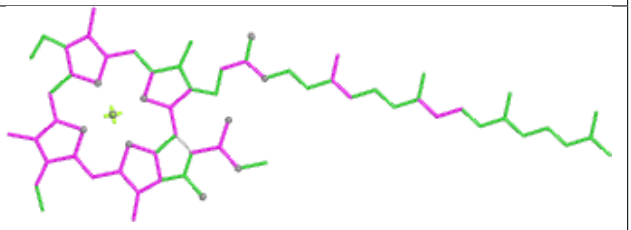


Rings

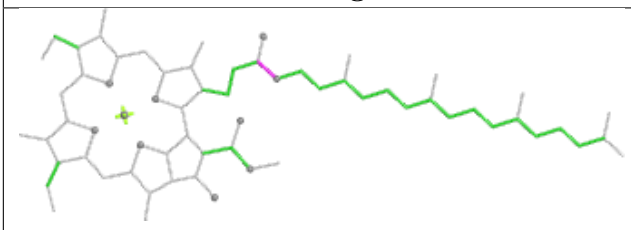
Ligand CLA B 613



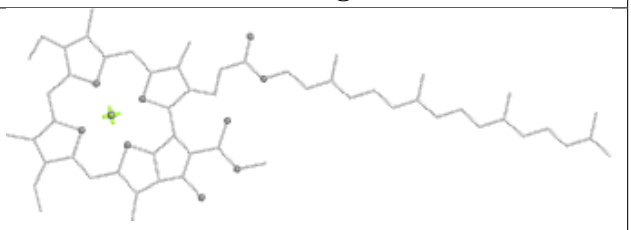
Bond lengths



Bond angles

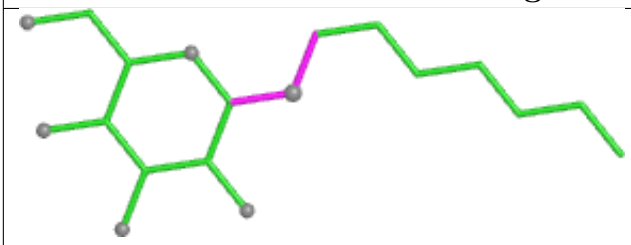


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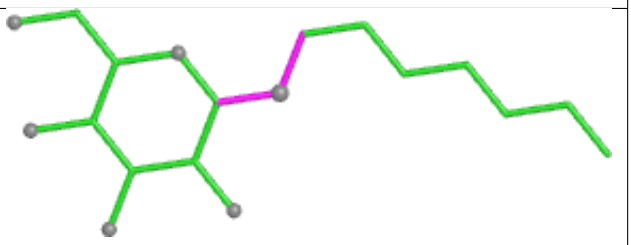


Rings

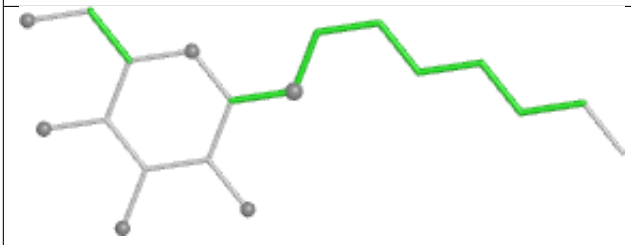
Ligand HTG b 603



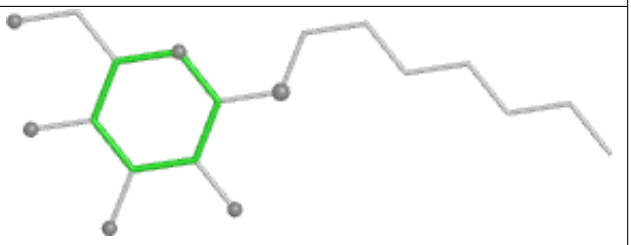
Bond lengths



Bond angles

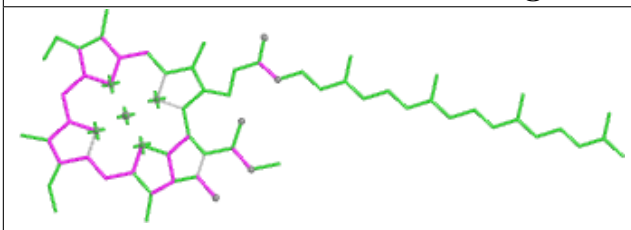


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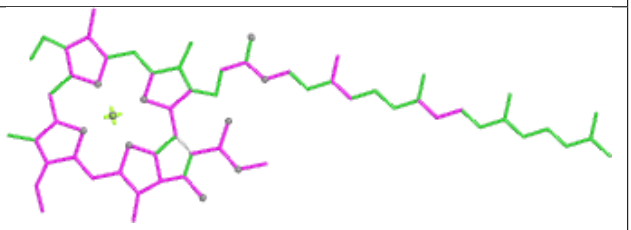


Rings

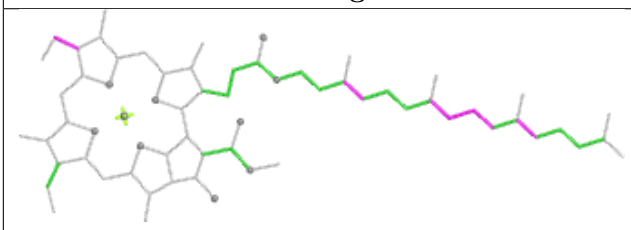
Ligand CLA B 616



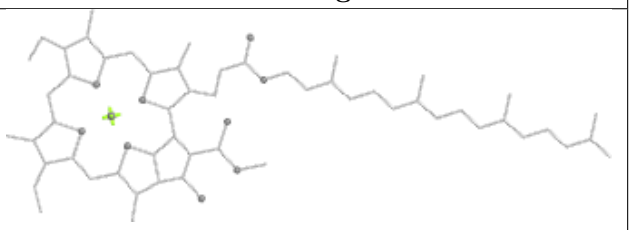
Bond lengths



Bond angles

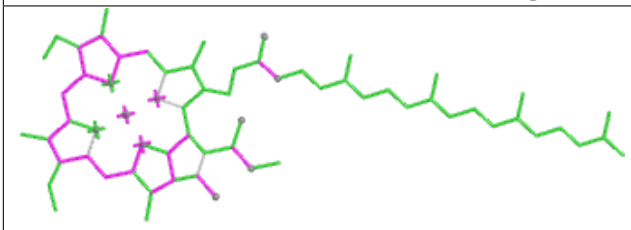


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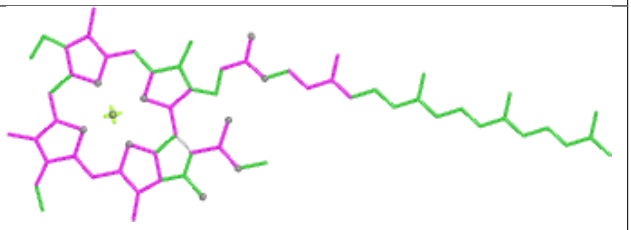


Rings

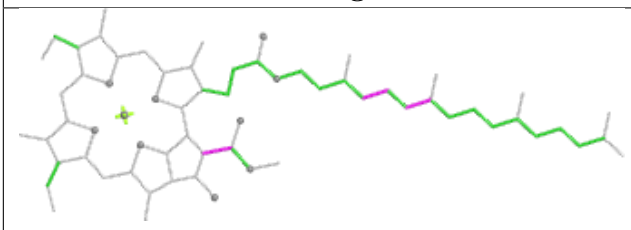
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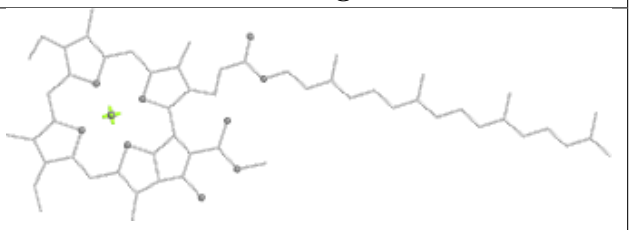
Bond lengths



Bond angles

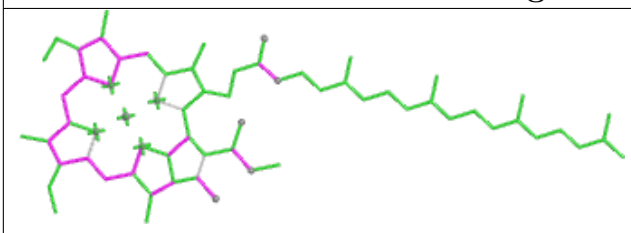


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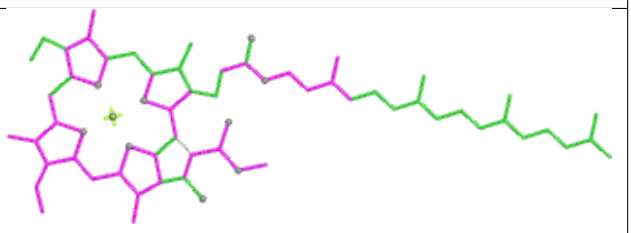


Rings

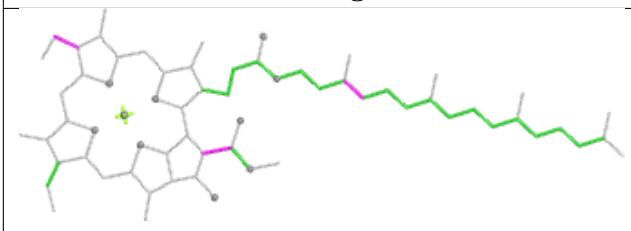
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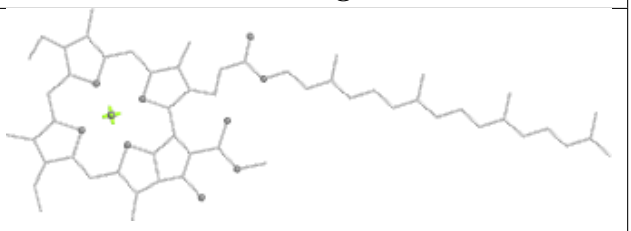
Bond lengths



Bond angles

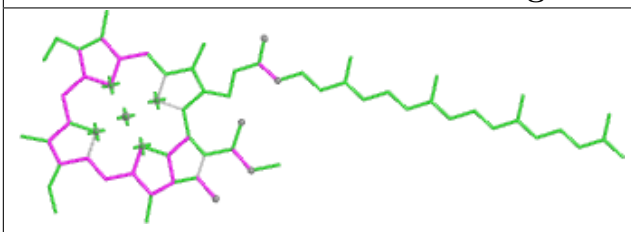


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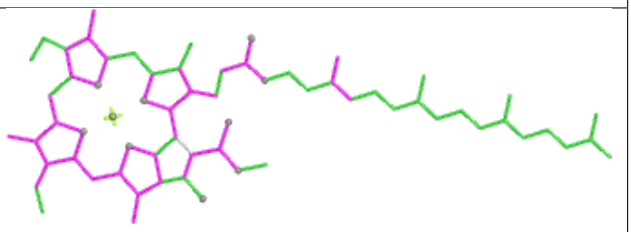


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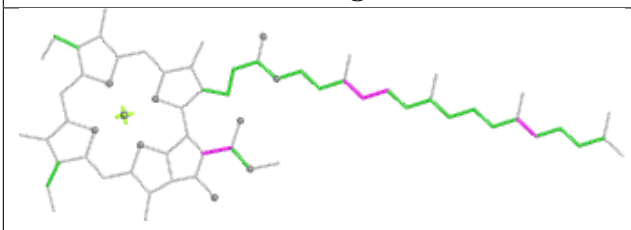
Ligand CLA d 404



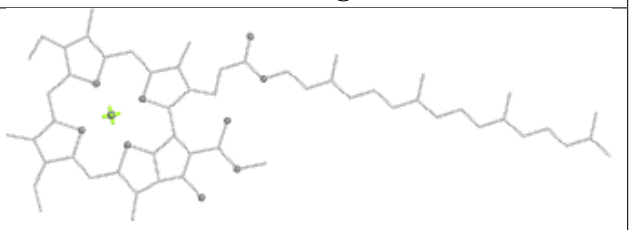
Bond lengths



Bond angles

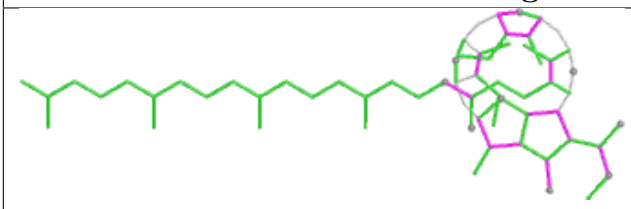


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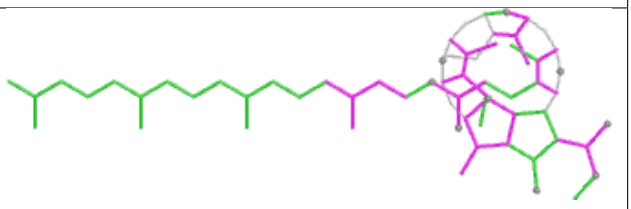


Rings

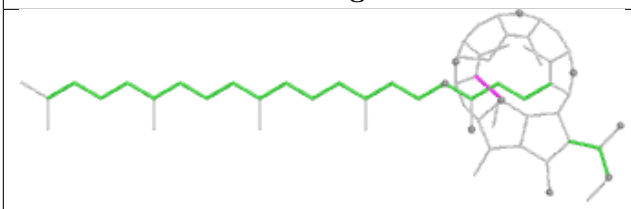
Ligand PHO A 408



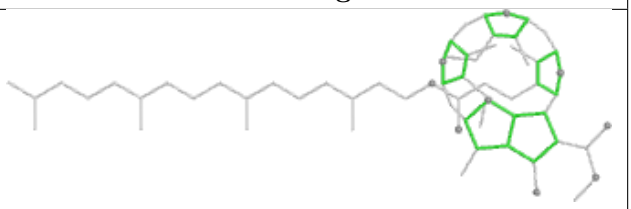
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Bond angles

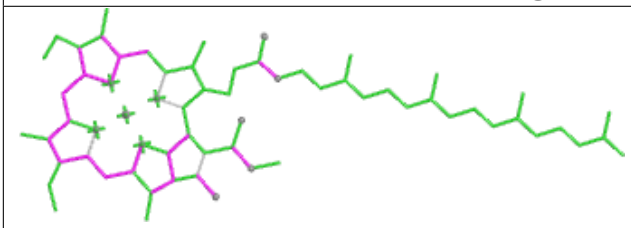


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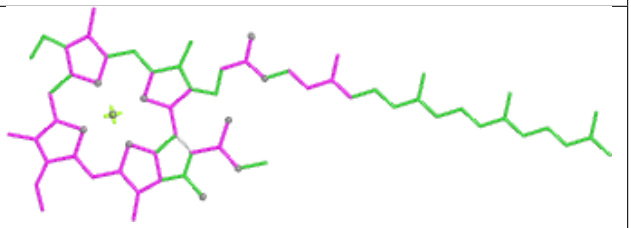


Rings

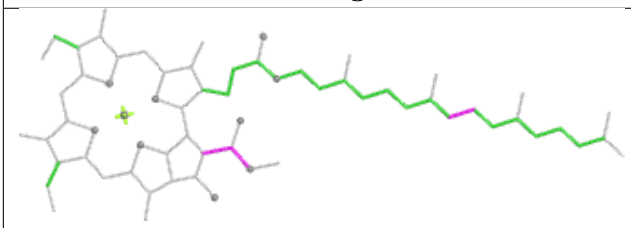
Ligand CLA c 505



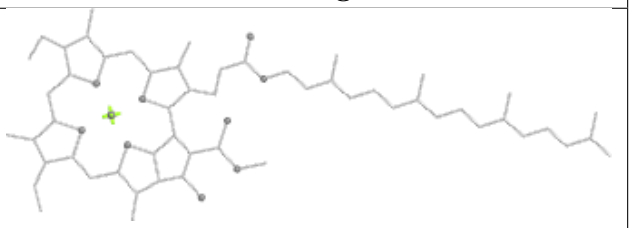
Bond lengths



Bond angles

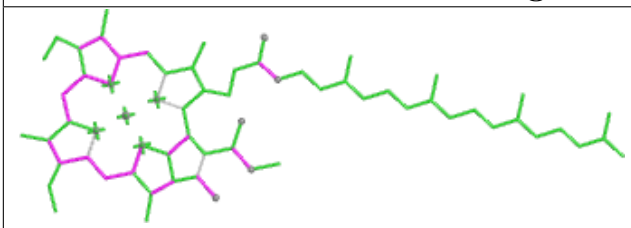


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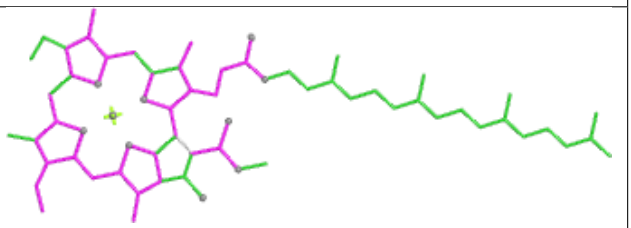


Rings

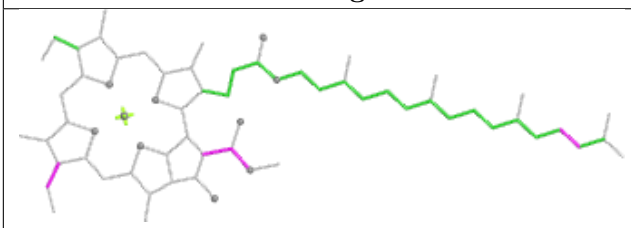
Ligand CLA d 401



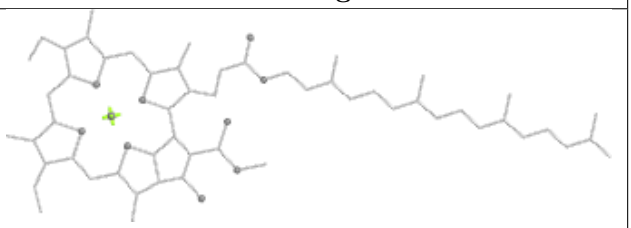
Bond lengths



Bond angles

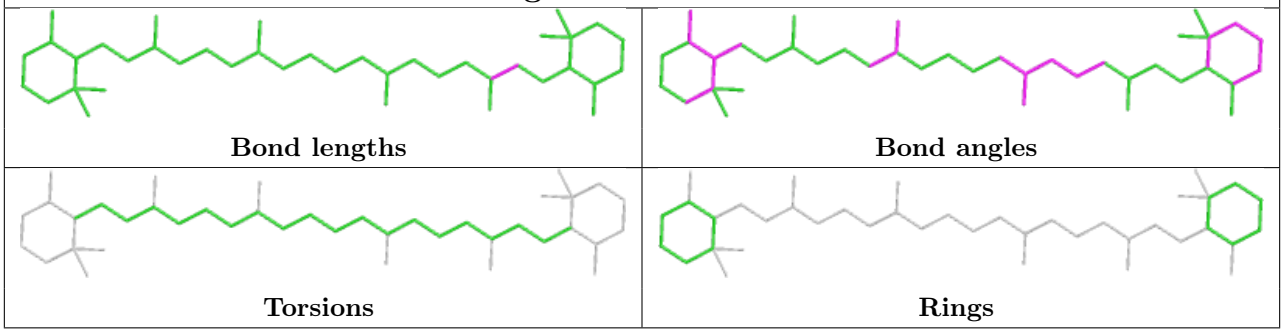


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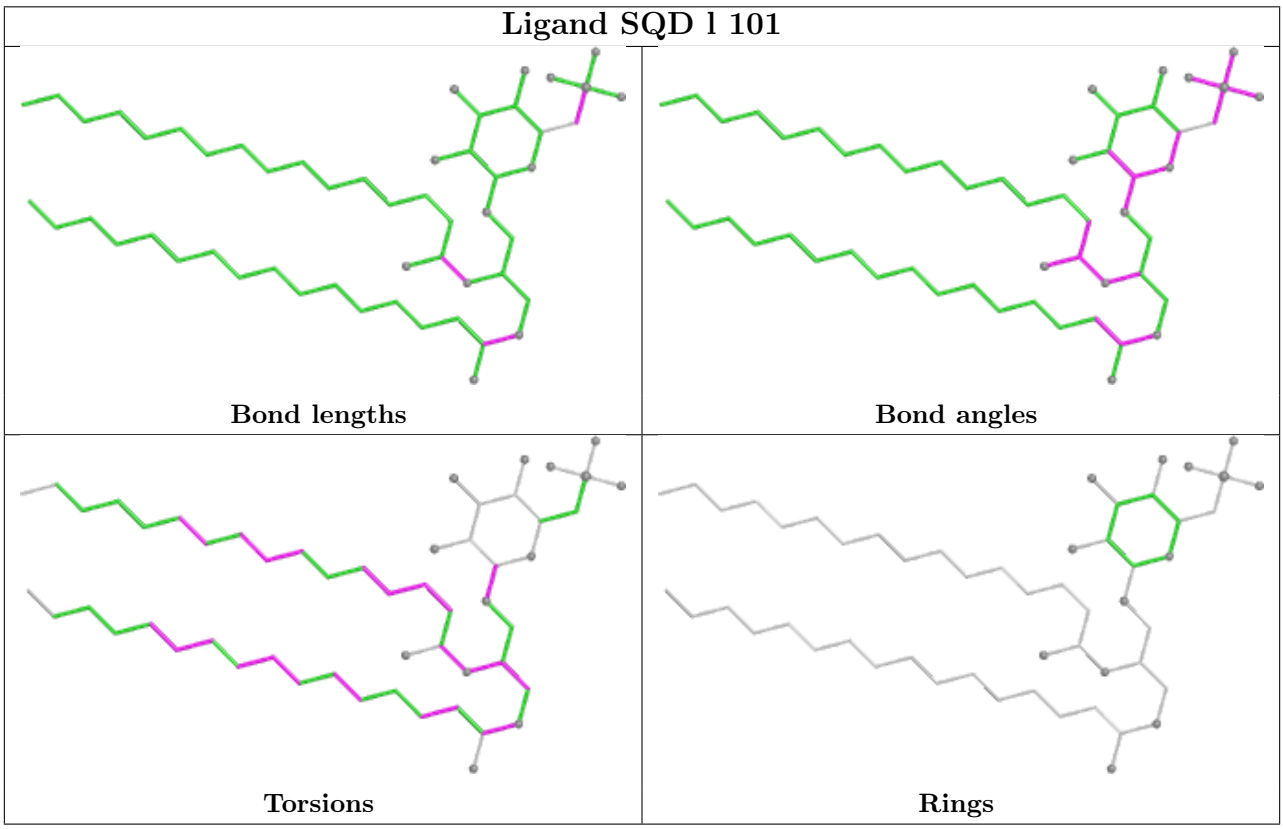


Rings

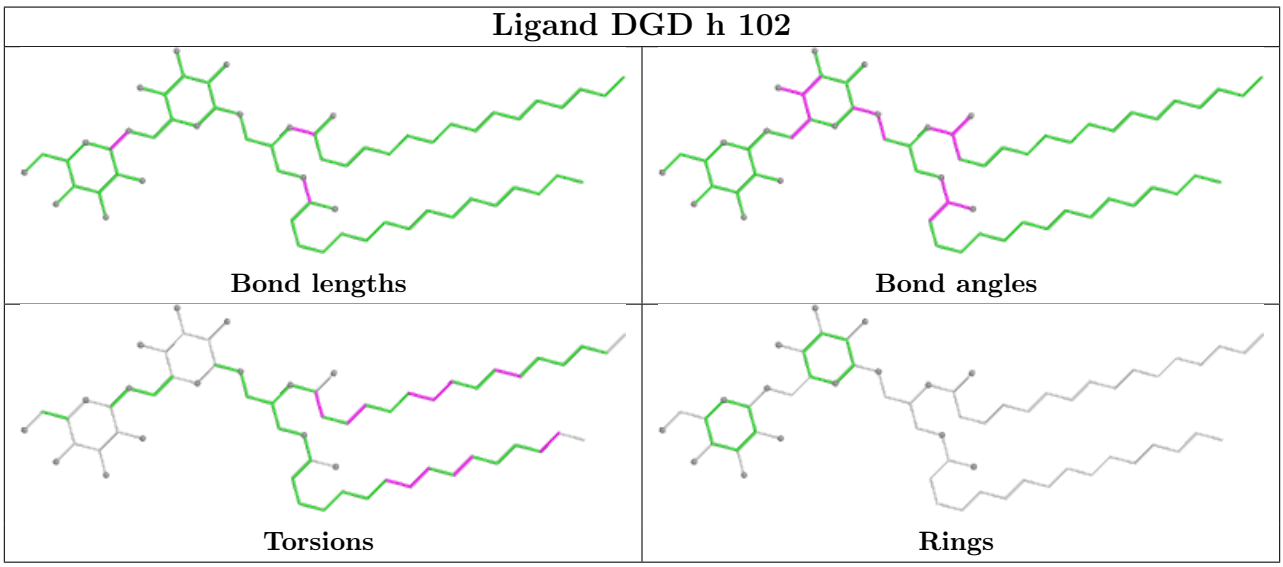
Ligand BCR T 102



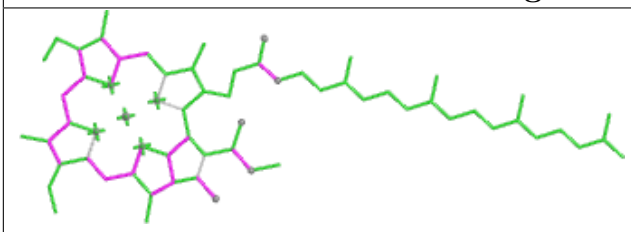
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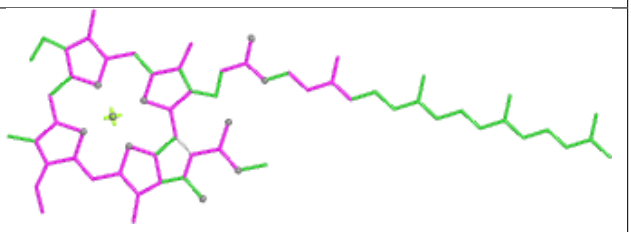
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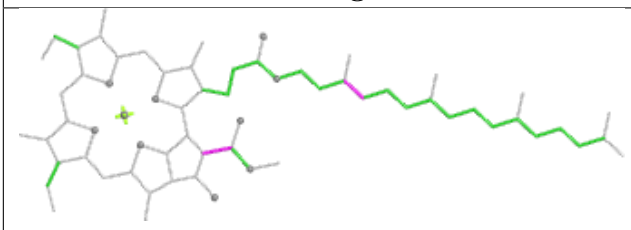
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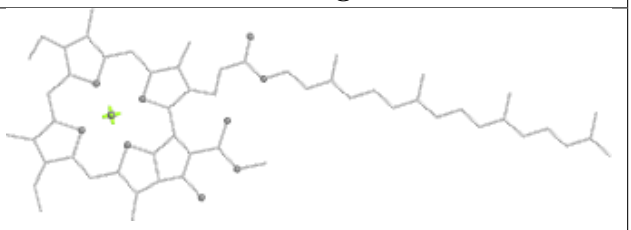
Bond lengths



Bond angles

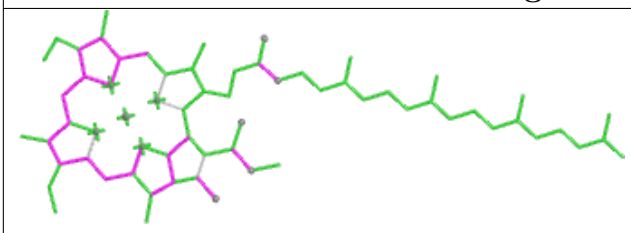


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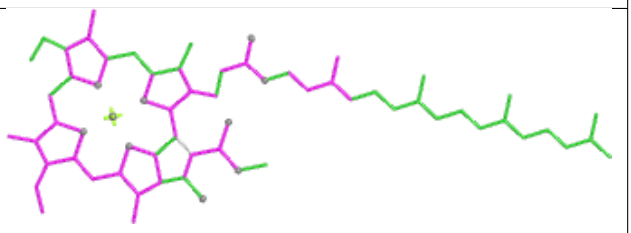


Rings

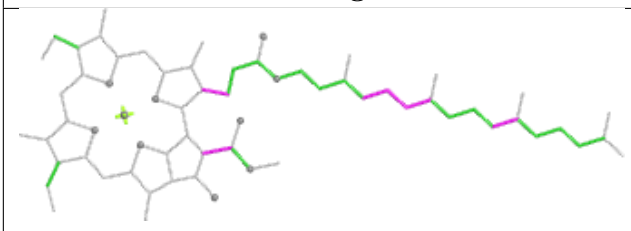
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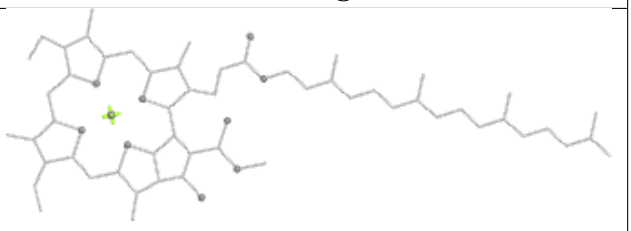
Bond lengths



Bond angles

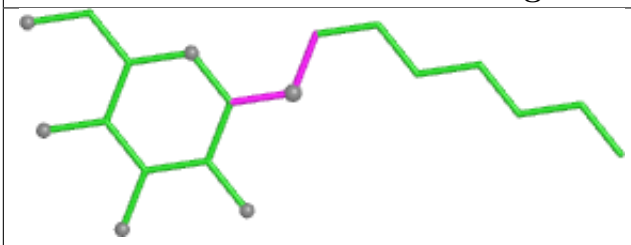


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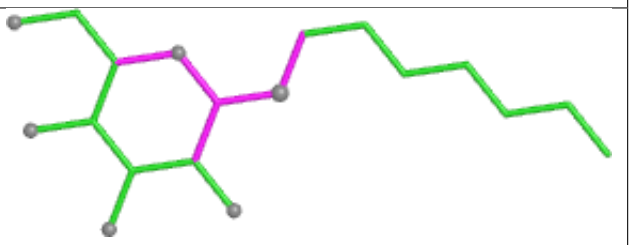


Rings

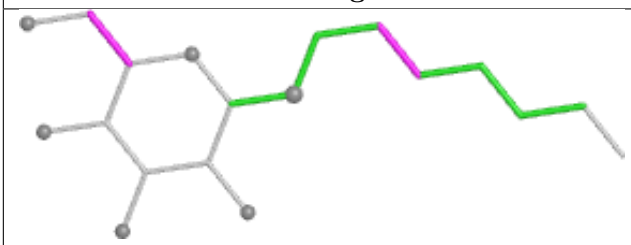
Ligand HTG b 628



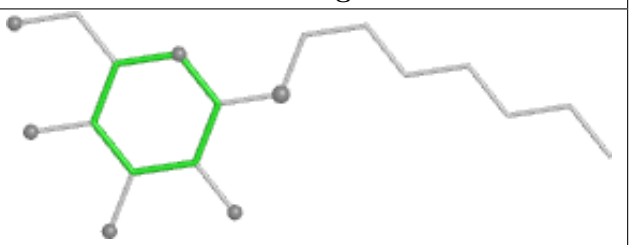
Bond lengths



Bond angles

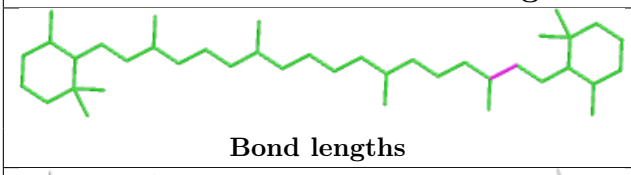


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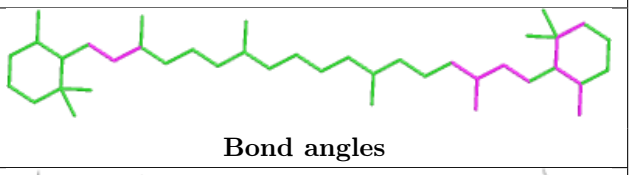


Rings

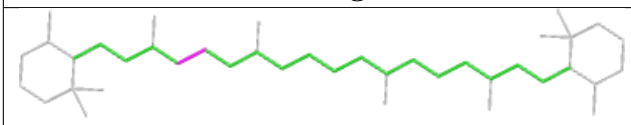
Ligand BCR H 101



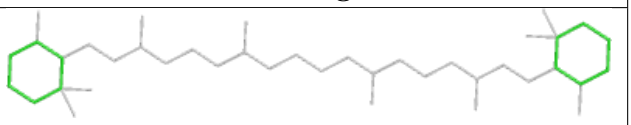
Bond lengths



Bond angles

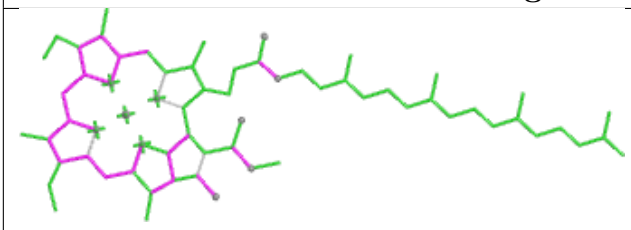


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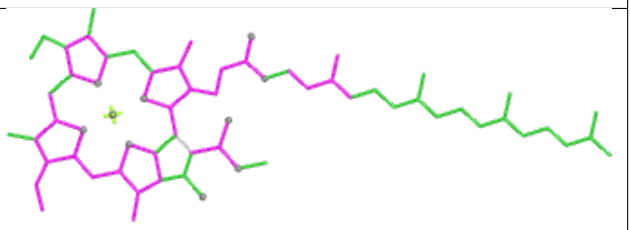


Rings

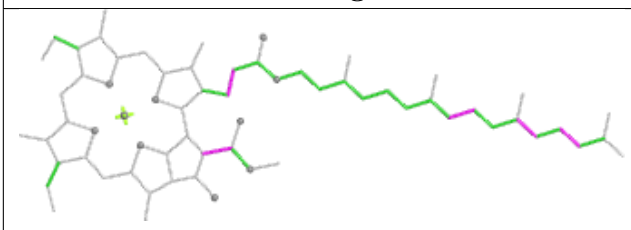
Ligand CLA B 603



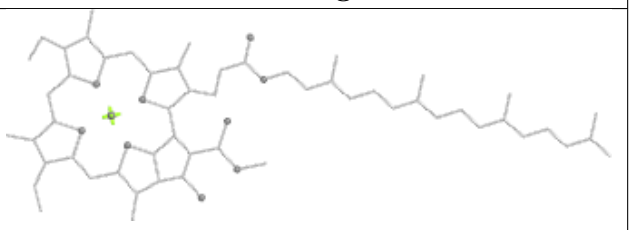
Bond lengths



Bond angles

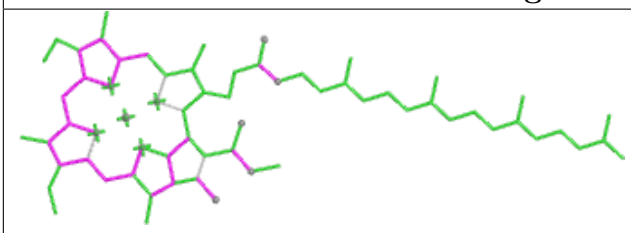


Torsions

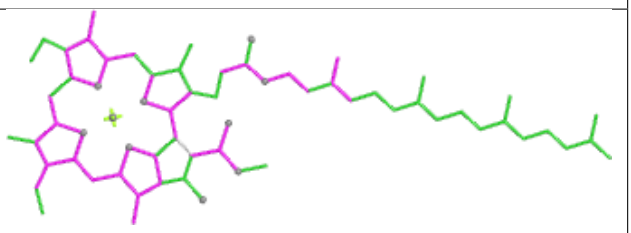


Rings

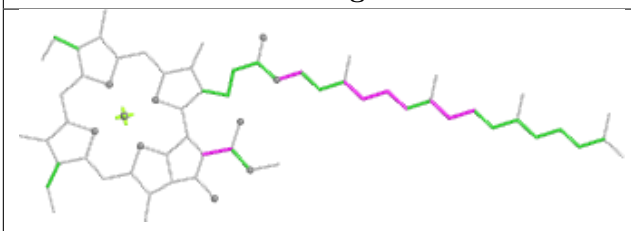
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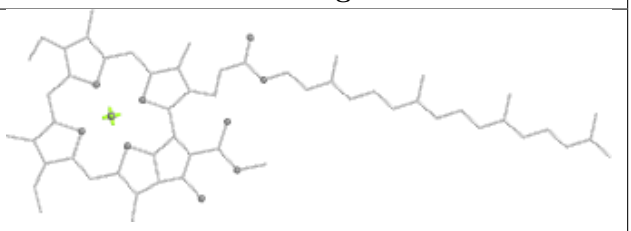
Bond lengths



Bond angles

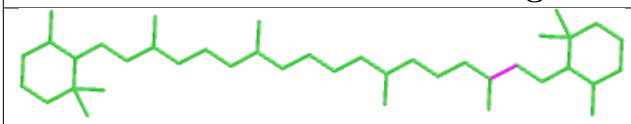


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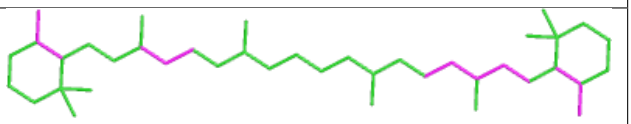


Rings

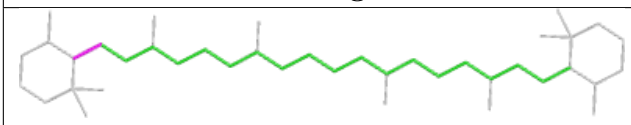
Ligand BCR k 103



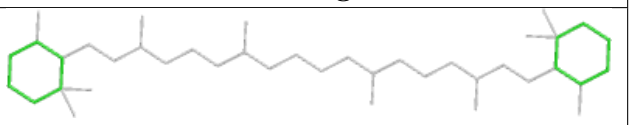
Bond lengths



Bond angles

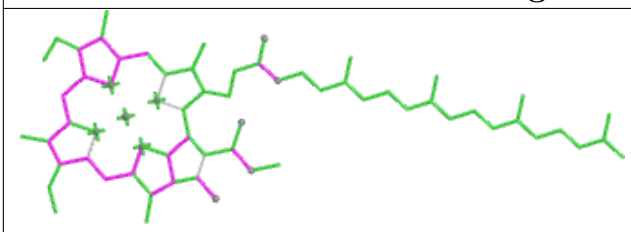


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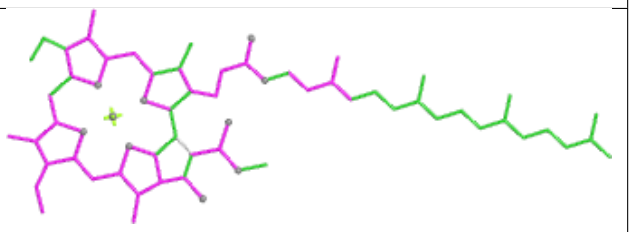


Rings

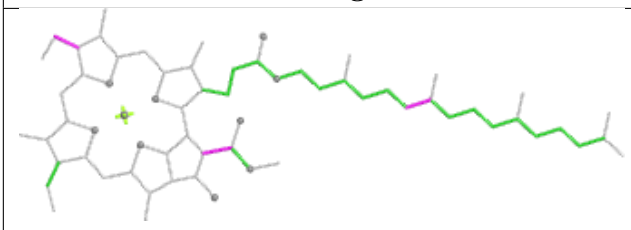
Ligand CLA a 407



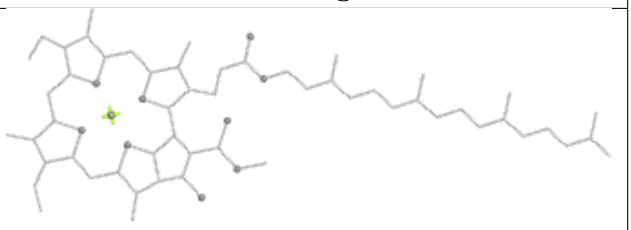
Bond lengths



Bond angles

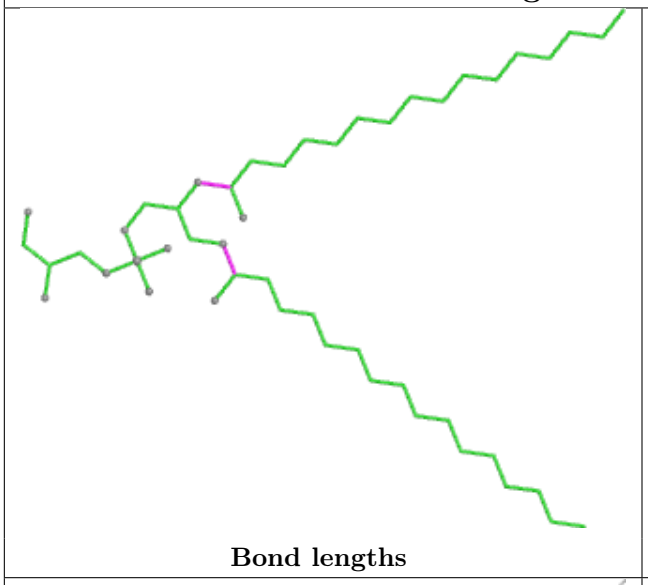


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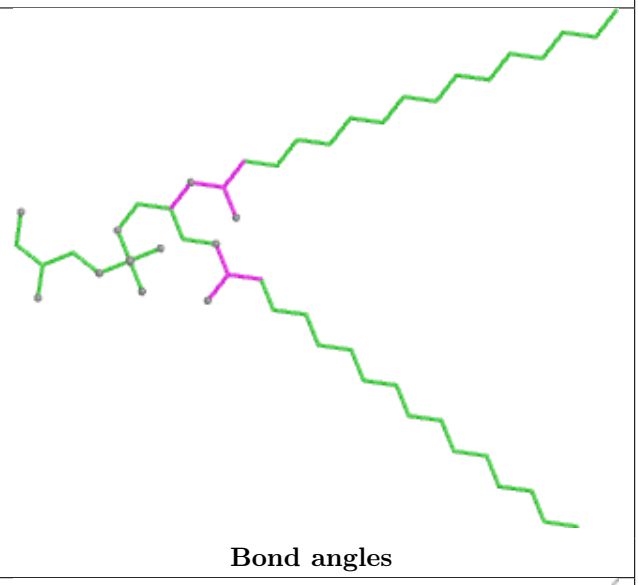


Rings

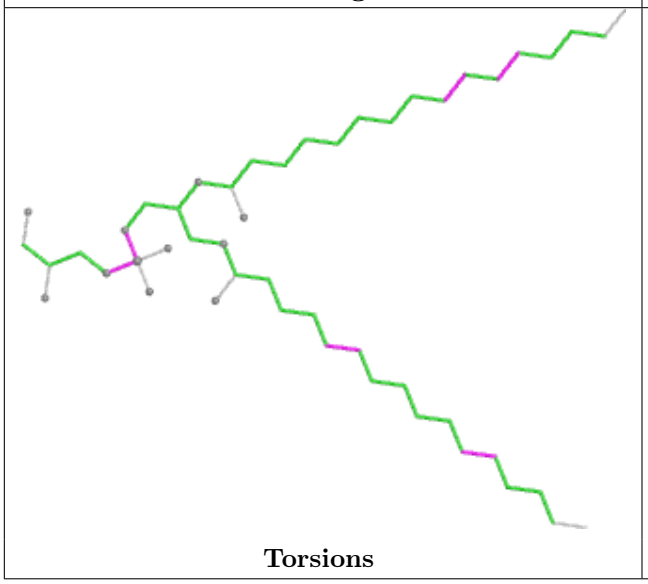
Ligand LHG D 409



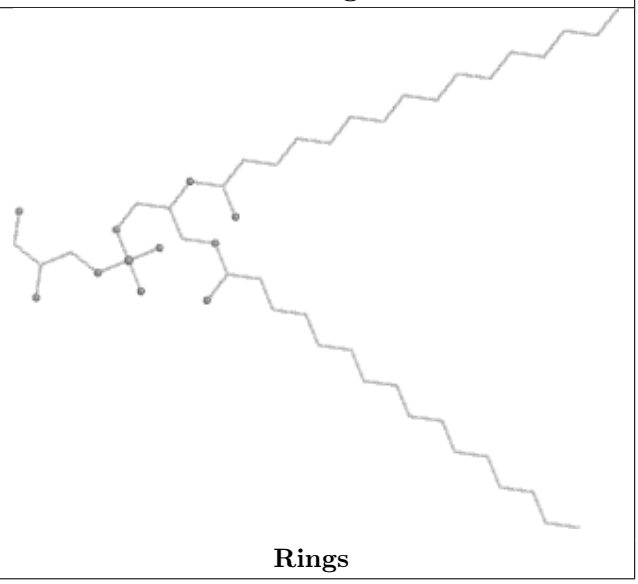
Bond lengths



Bond angles

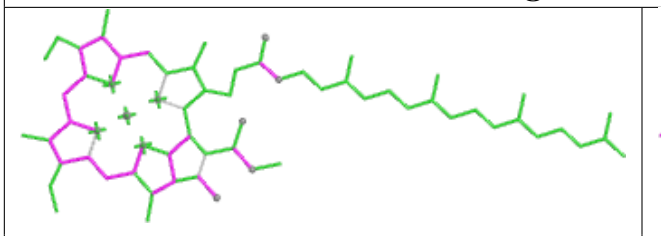


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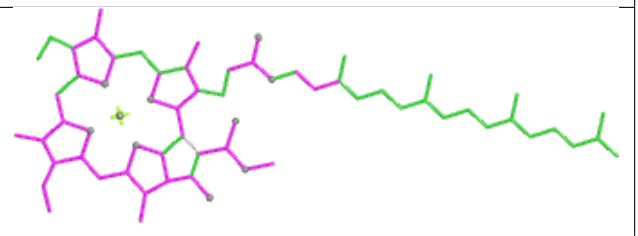


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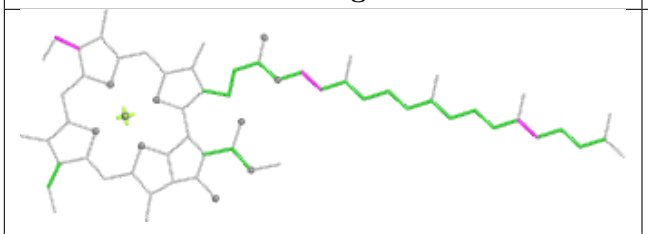
Ligand CLA D 403



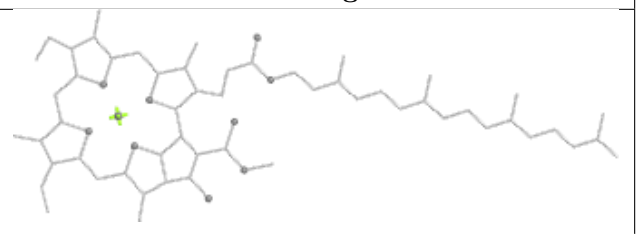
Bond lengths



Bond angles

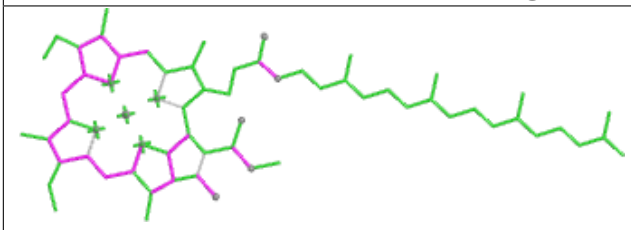


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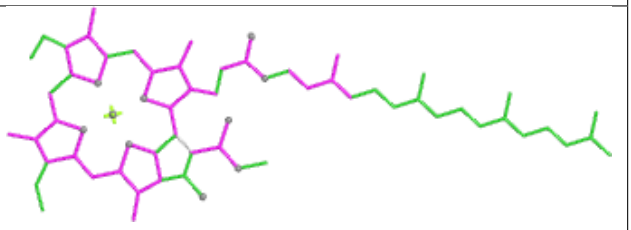


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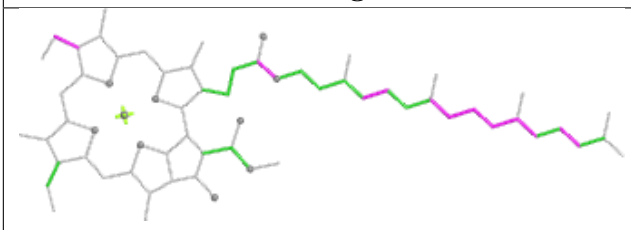
Ligand CLA A 409



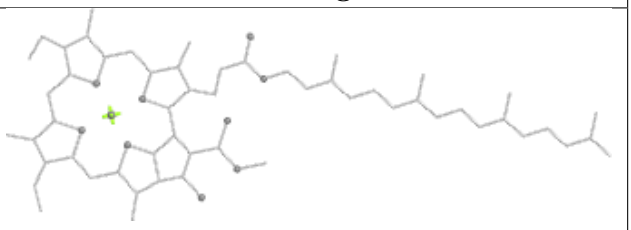
Bond lengths



Bond angles

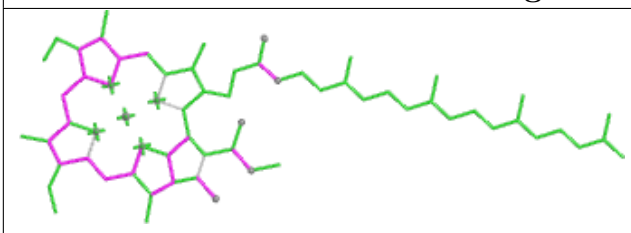


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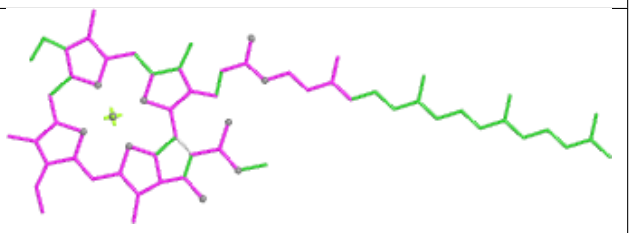


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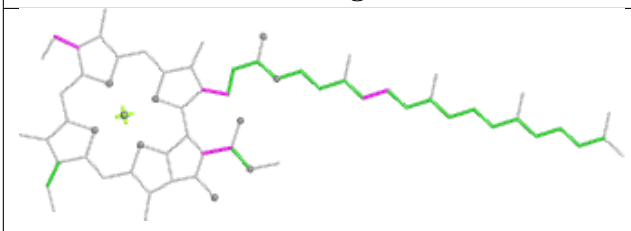
Ligand CLA B 608



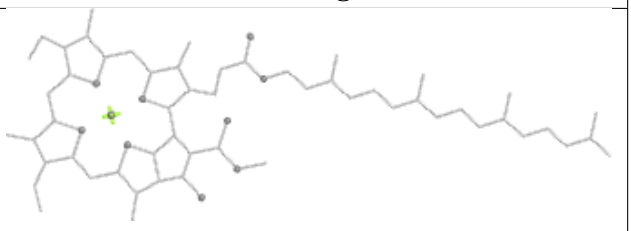
Bond lengths



Bond angles

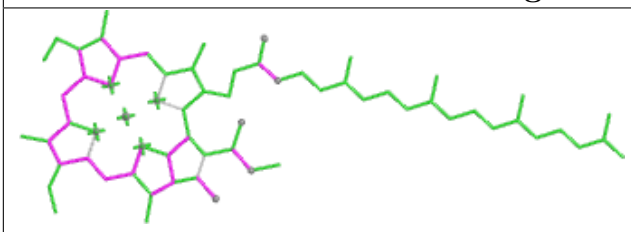


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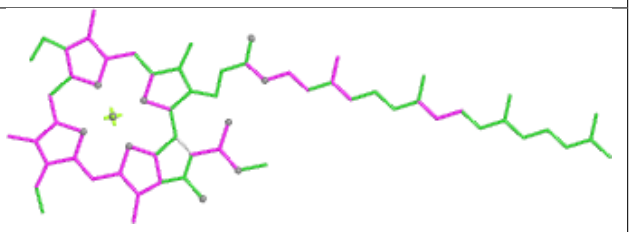


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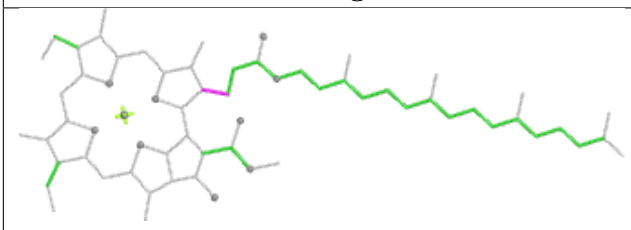
Ligand CLA C 512



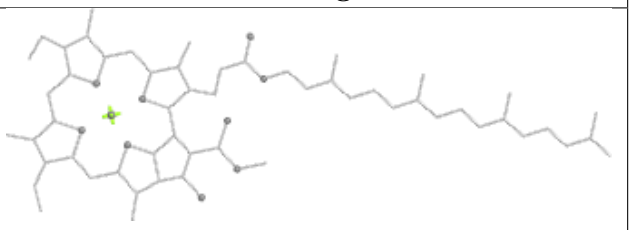
Bond lengths



Bond angles

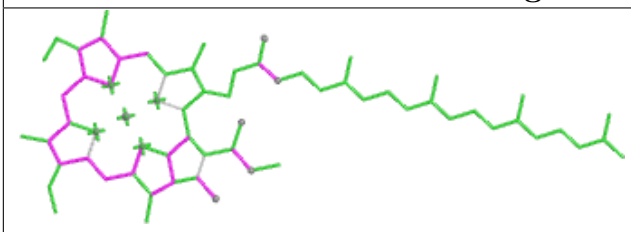


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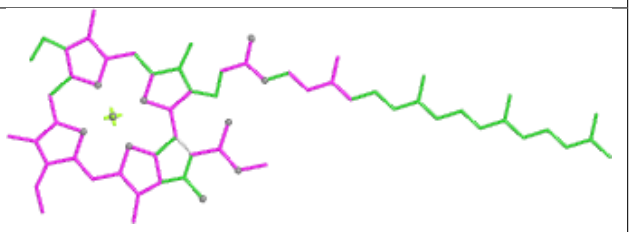


Rings

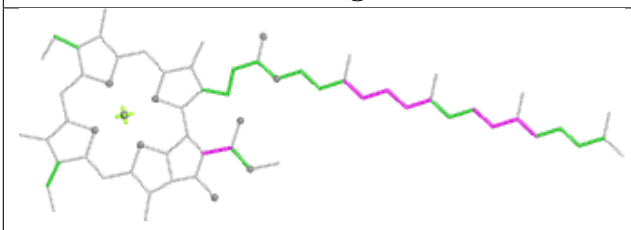
Ligand CLA B 615



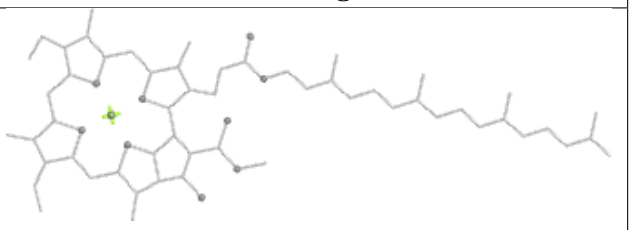
Bond lengths



Bond angles

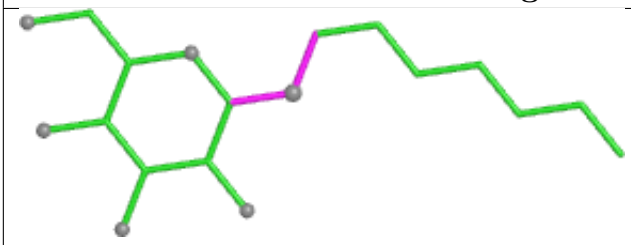


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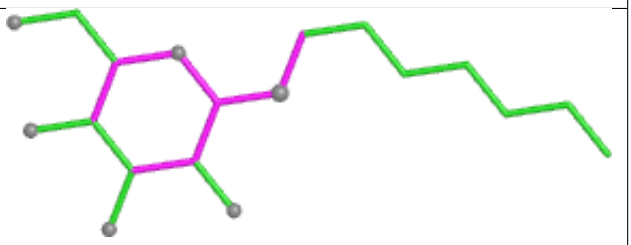


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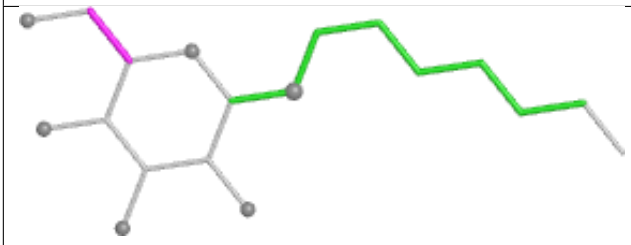
Ligand HTG C 523



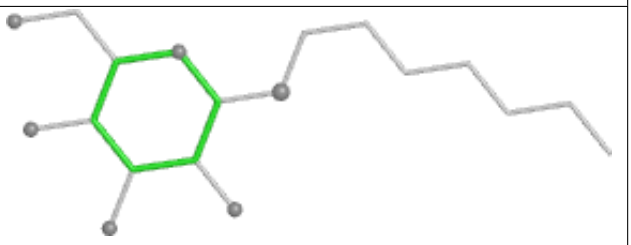
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Bond angles

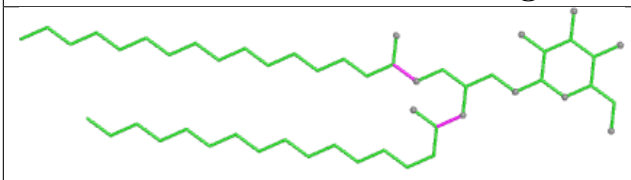


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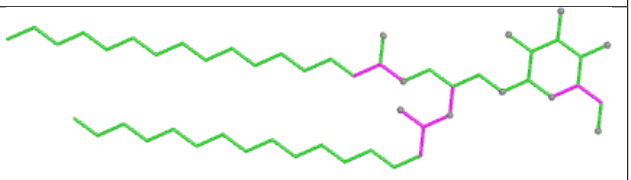


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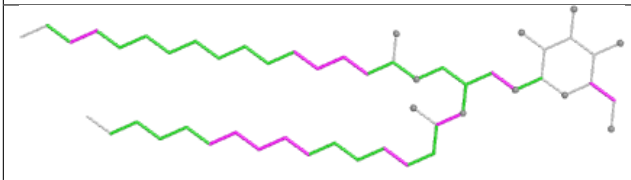
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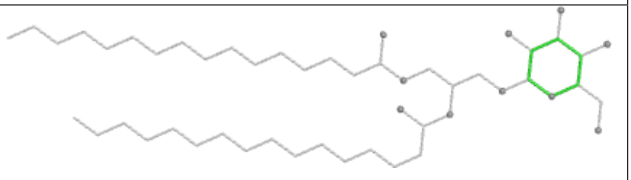
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Bond angles

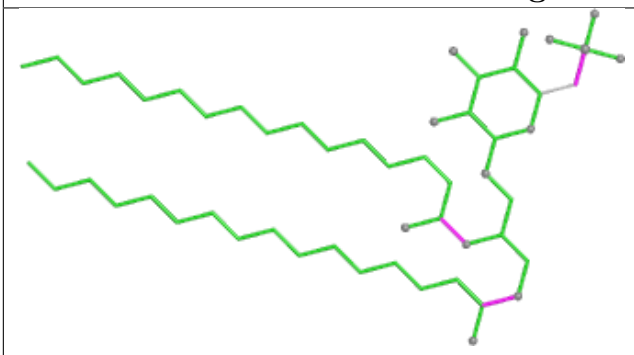


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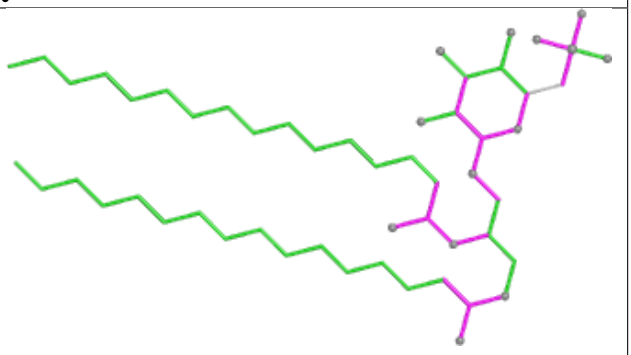


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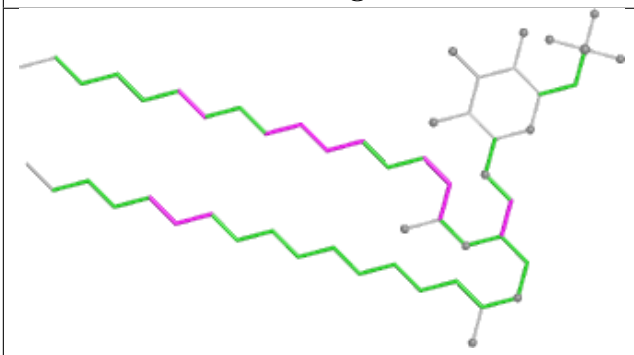
Ligand SQD a 411



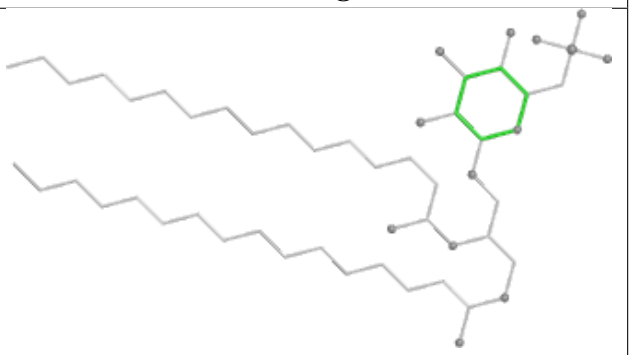
Bond lengths



Bond angles



Torsions

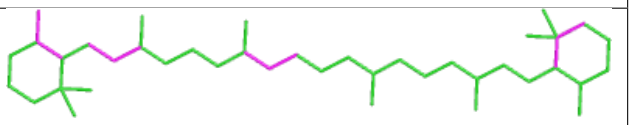


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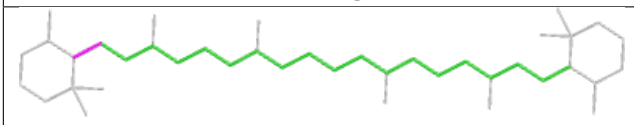
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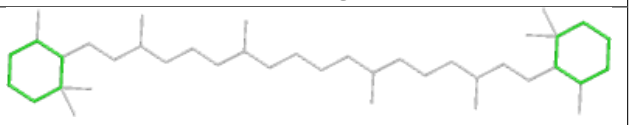
Bond lengths



Bond angles

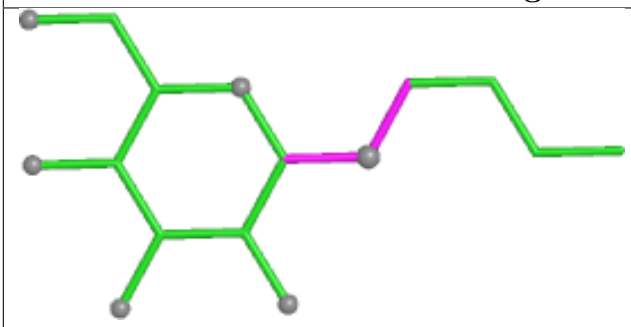


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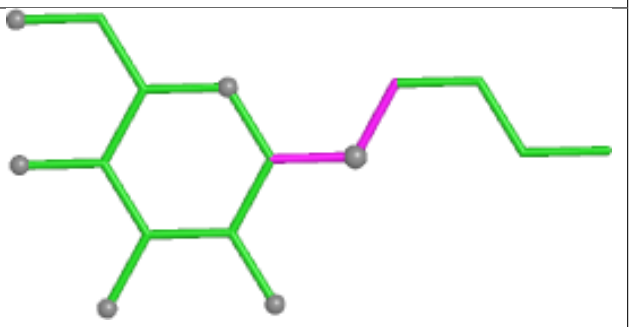


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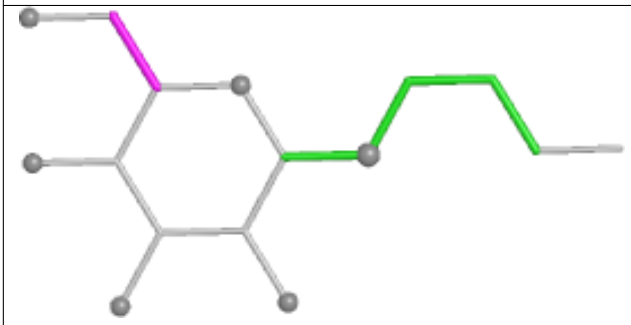
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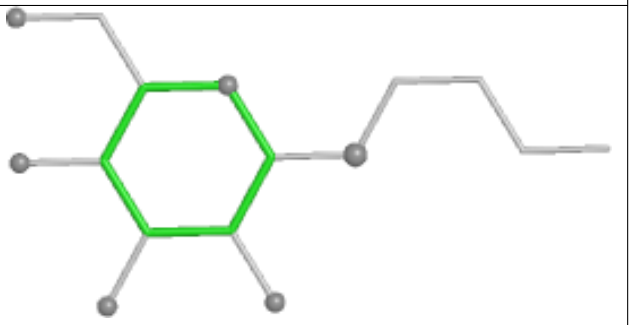
Bond lengths



Bond angles

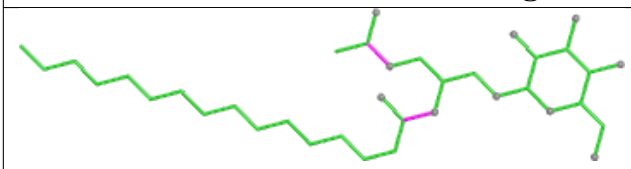


Torsions



Rings

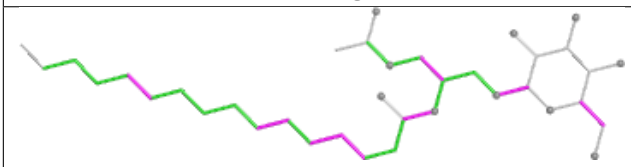
Ligand LMG Z 101



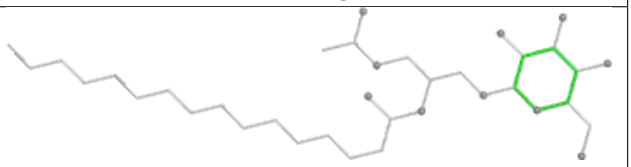
Bond lengths



Bond angles

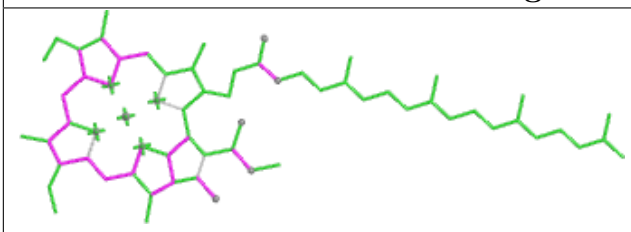


Torsions

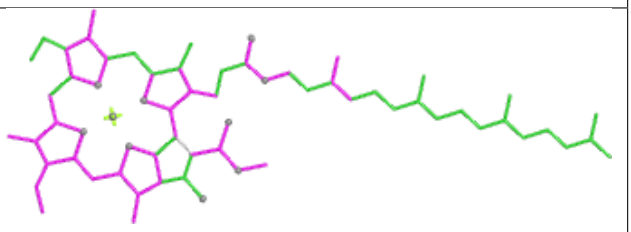


Rings

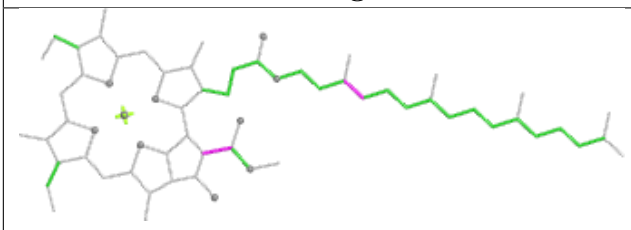
Ligand CLA B 606



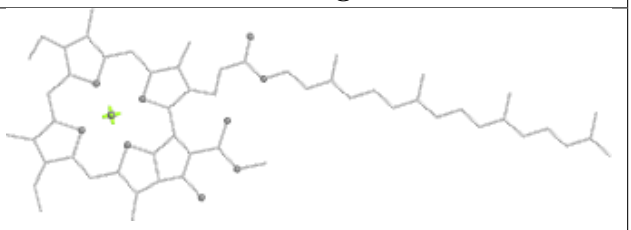
Bond lengths



Bond angles

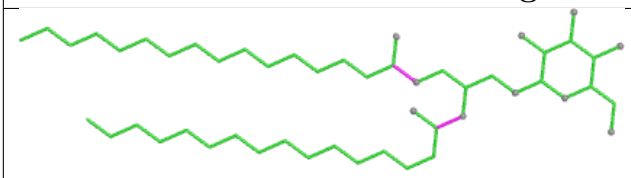


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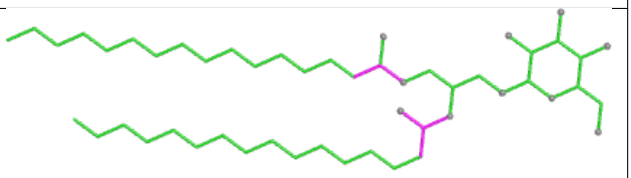


Rings

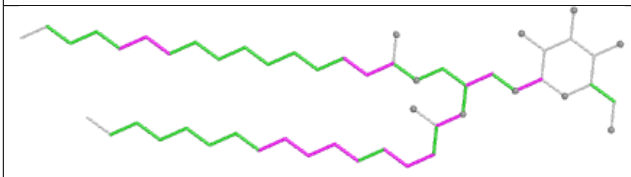
Ligand LMG C 501



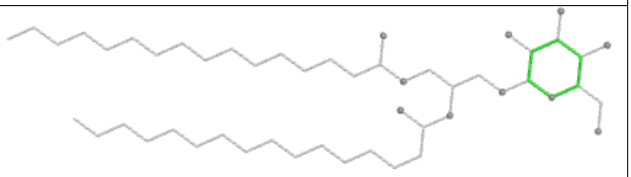
Bond lengths



Bond angles

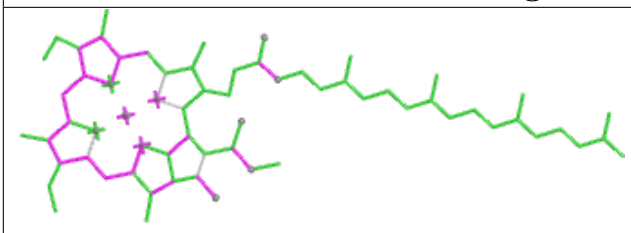


Torsions

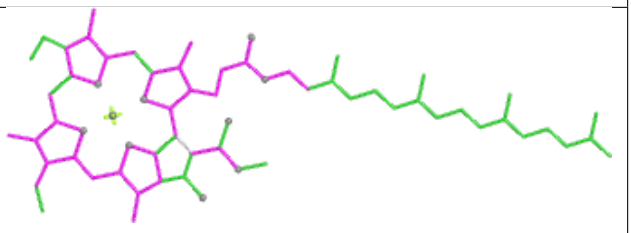


Rings

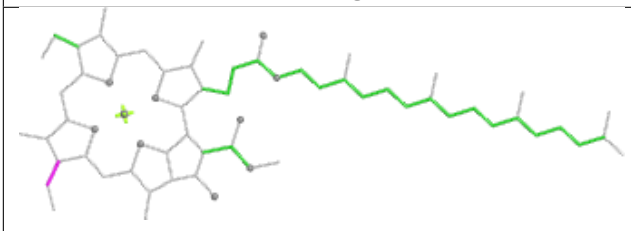
Ligand CLA A 405



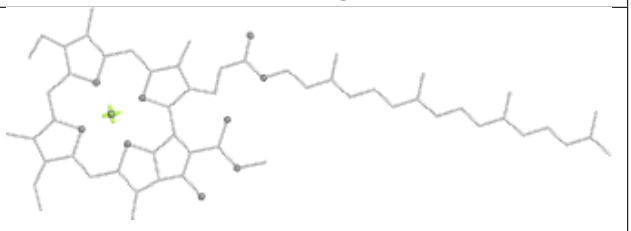
Bond lengths



Bond angles

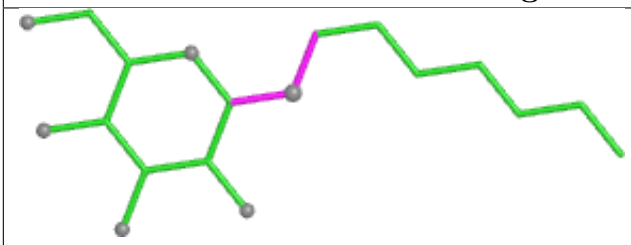


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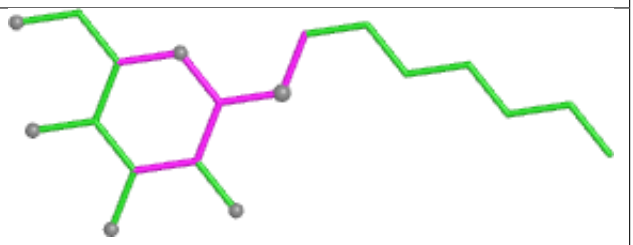


Rings

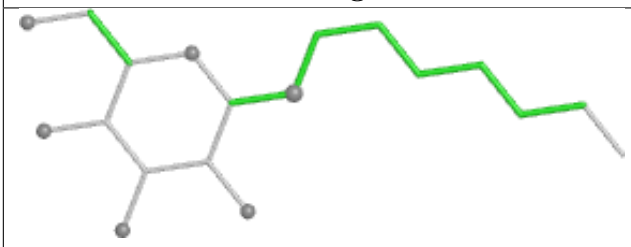
Ligand HTG B 624



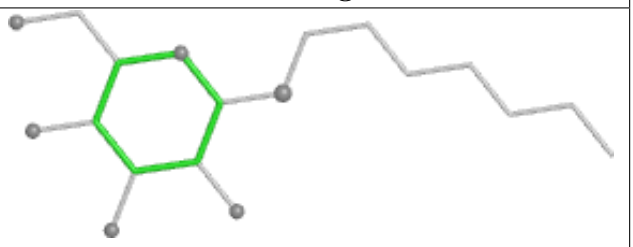
Bond lengths



Bond angles



Torsions

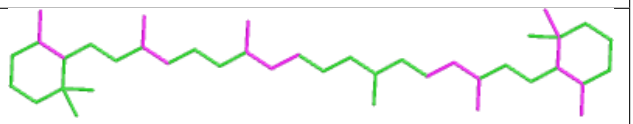


Rings

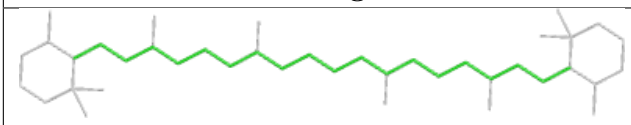
Ligand BCR a 410



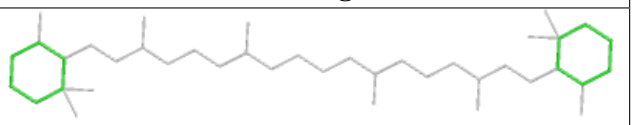
Bond lengths



Bond angles

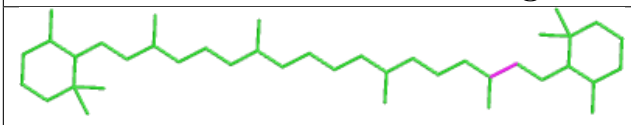


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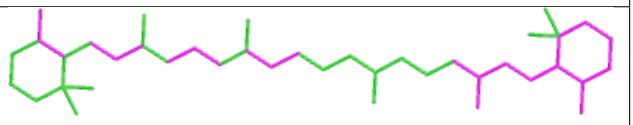


Rings

Ligand BCR D 405



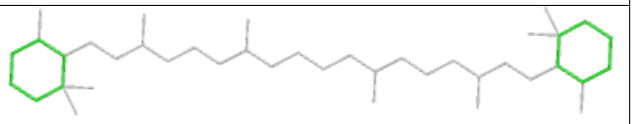
Bond lengths



Bond angles

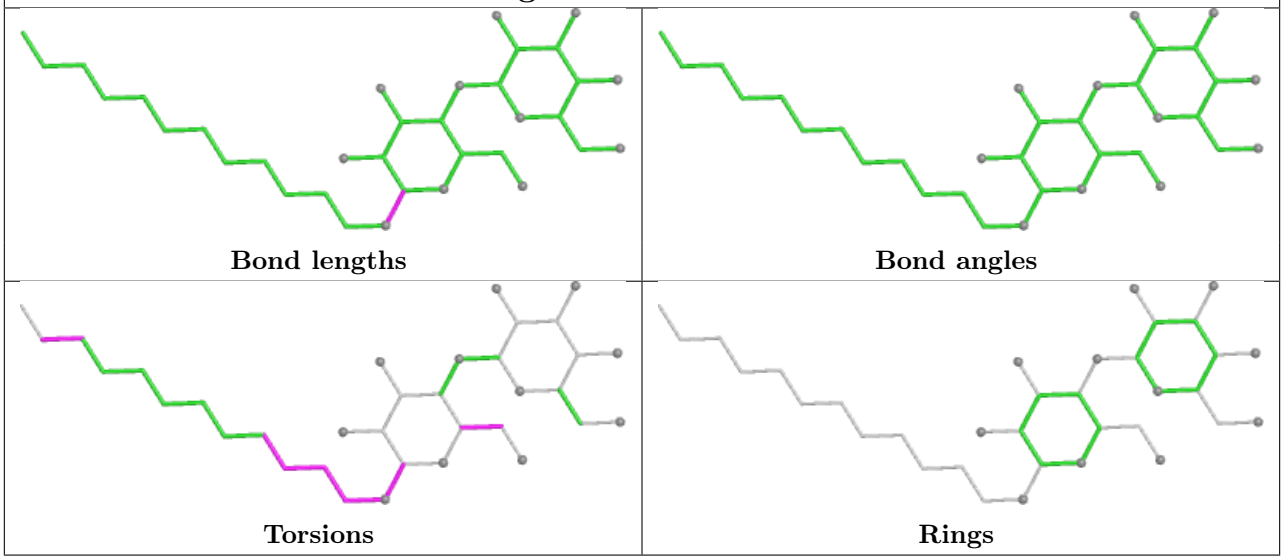


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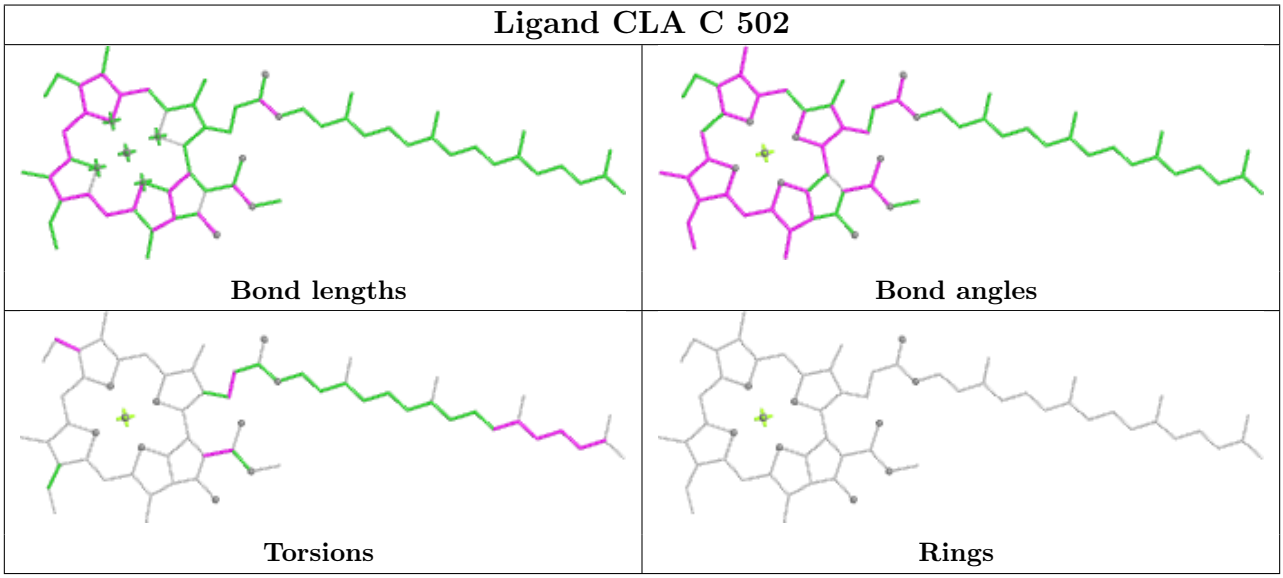


Rings

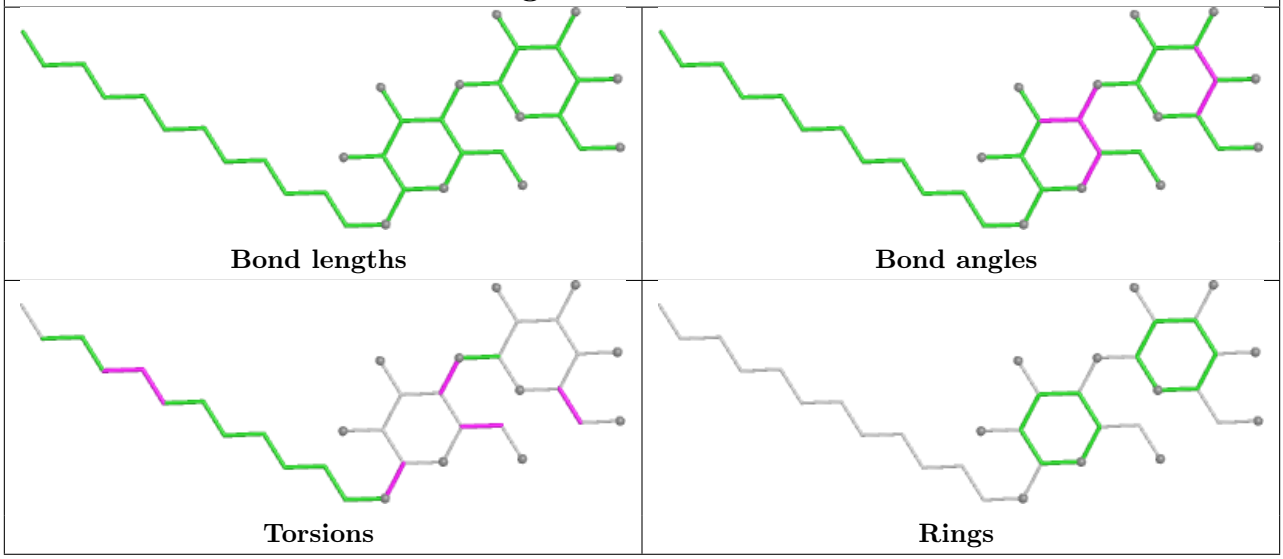
Ligand LMT M 101



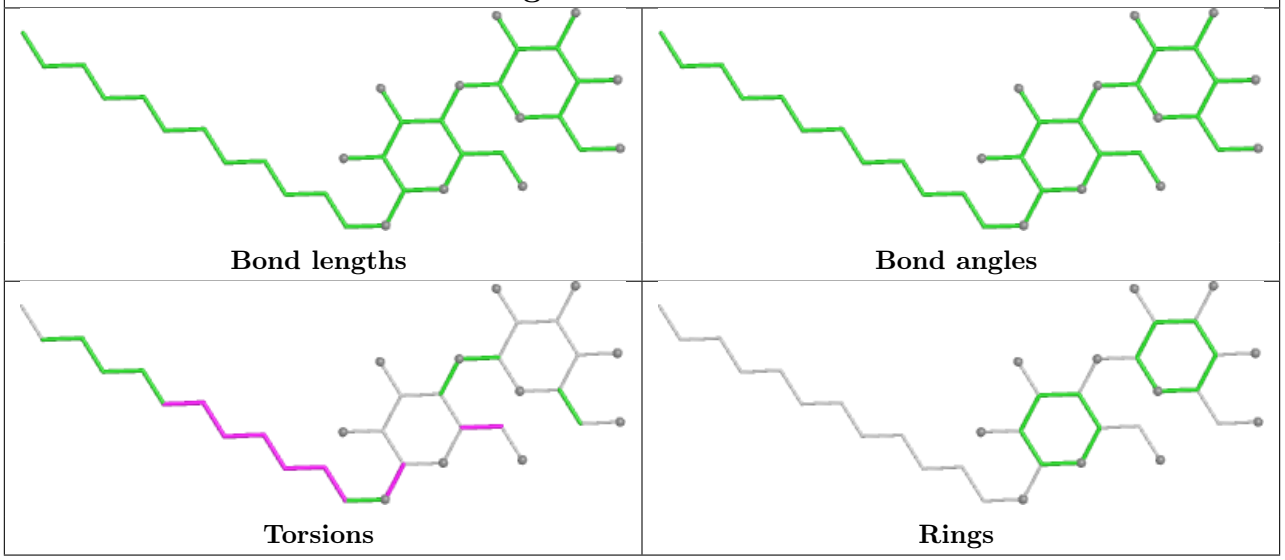
Ligand CLA C 502



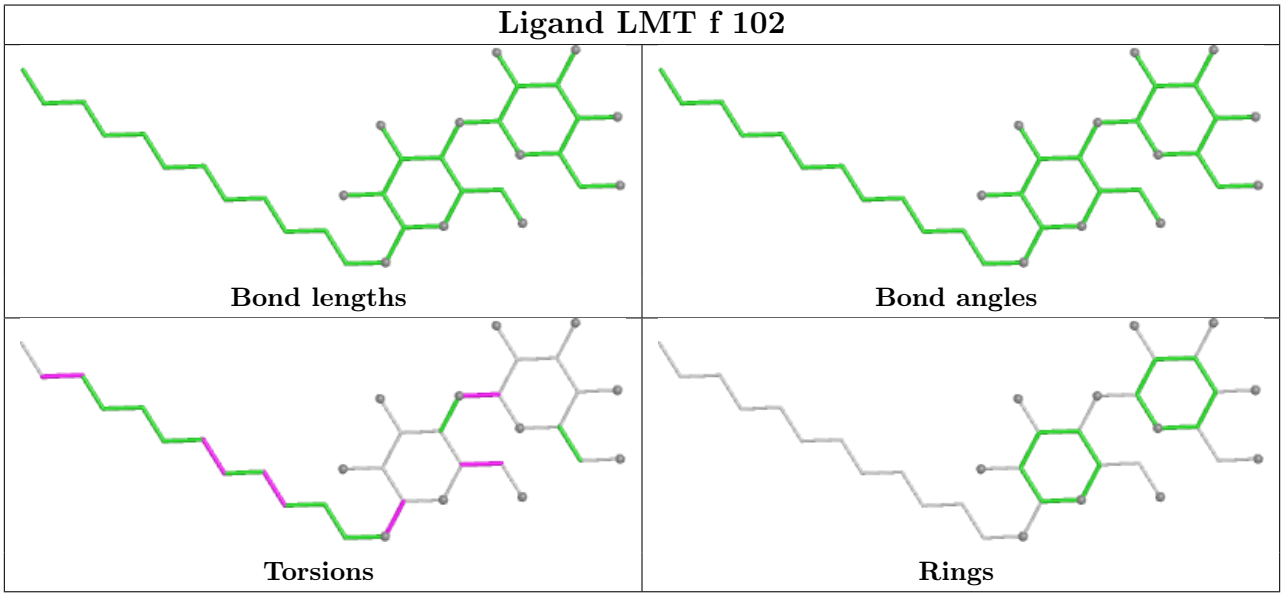
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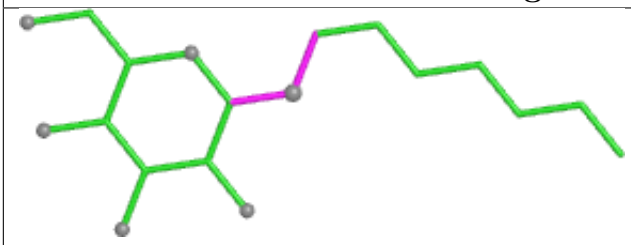
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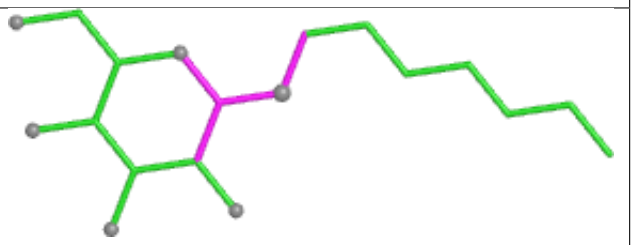
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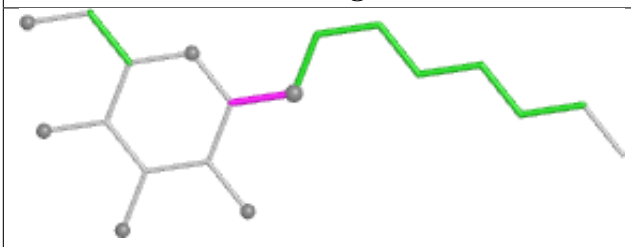
Ligand HTG b 604



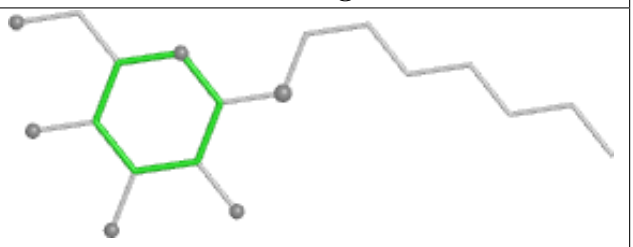
Bond lengths



Bond angles

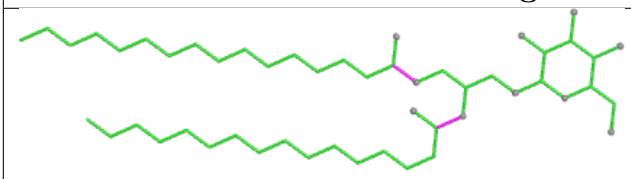


Torsions

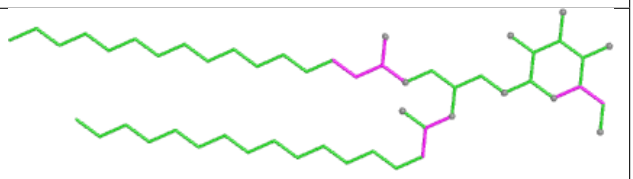


Rings

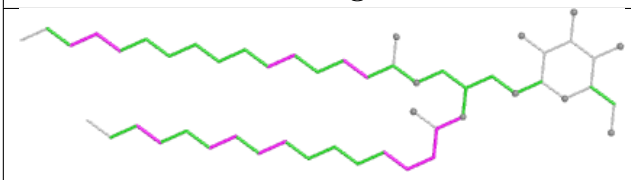
Ligand LMG C 520



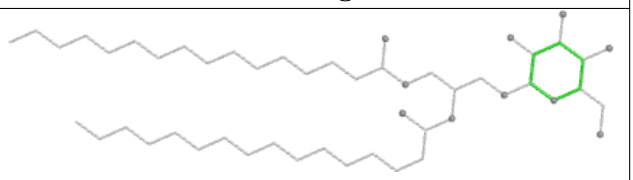
Bond lengths



Bond angles

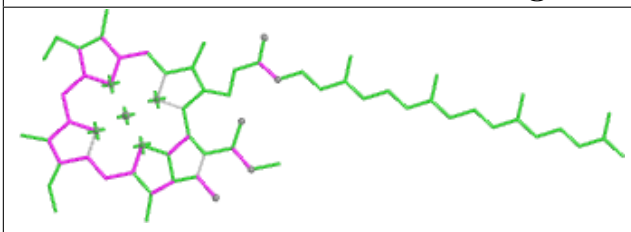


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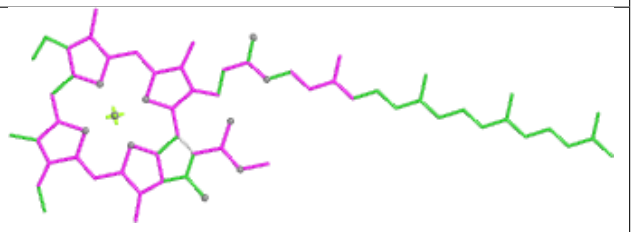


Rings

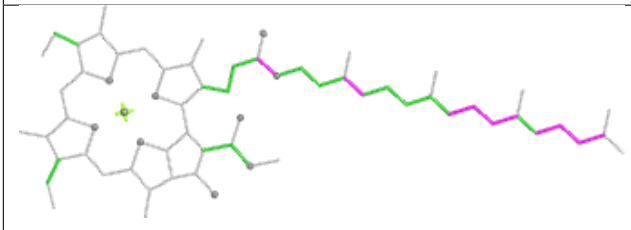
Ligand CLA a 409



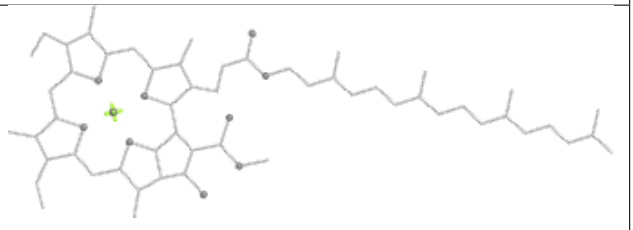
Bond lengths



Bond angles

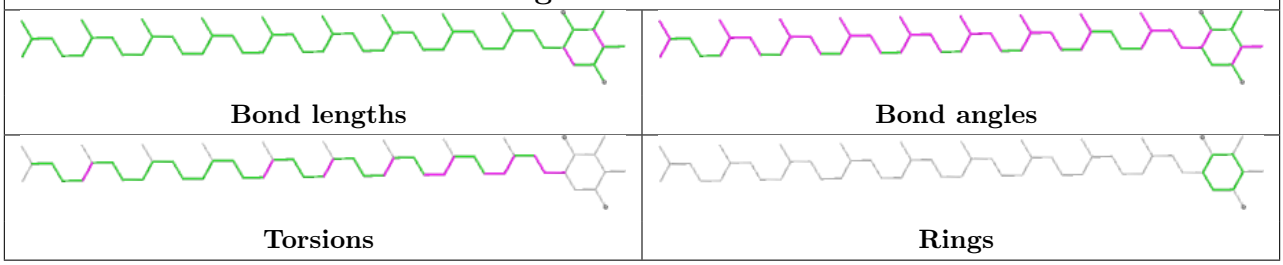


Torsions

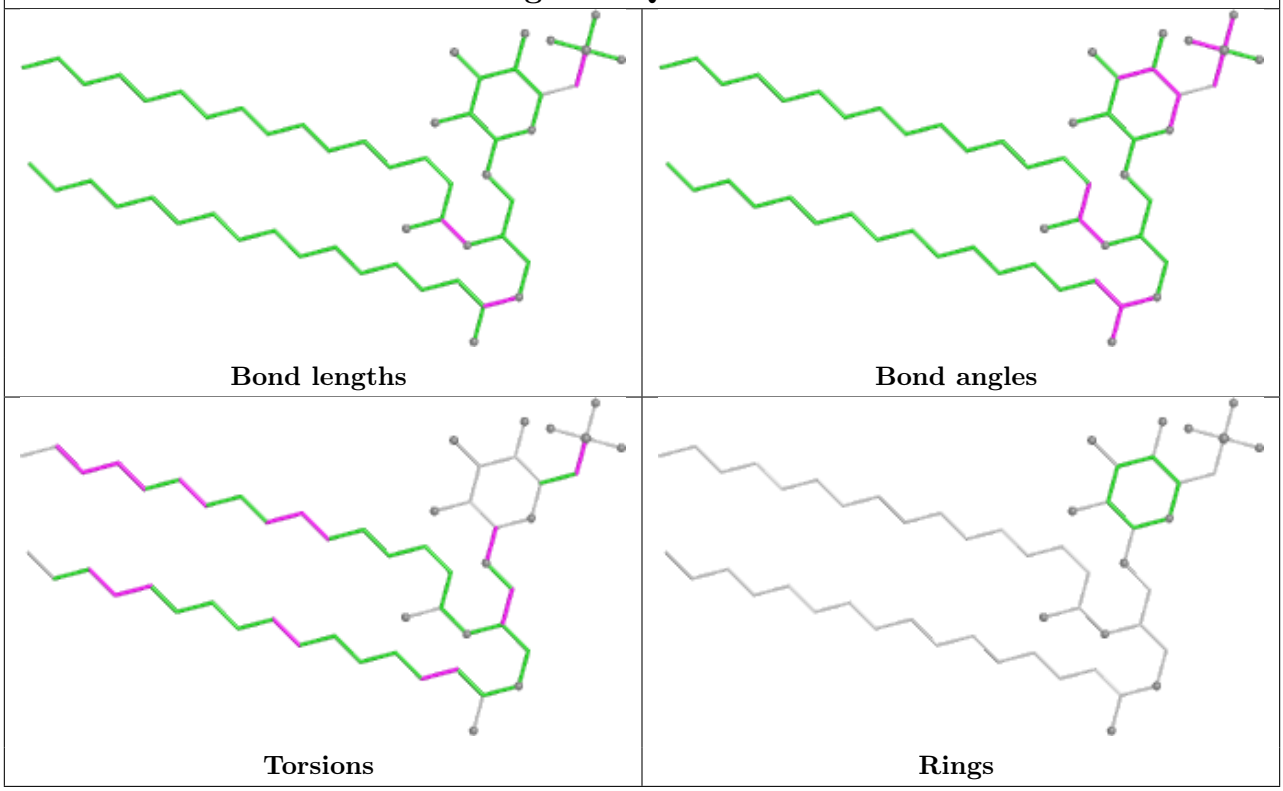


Rings

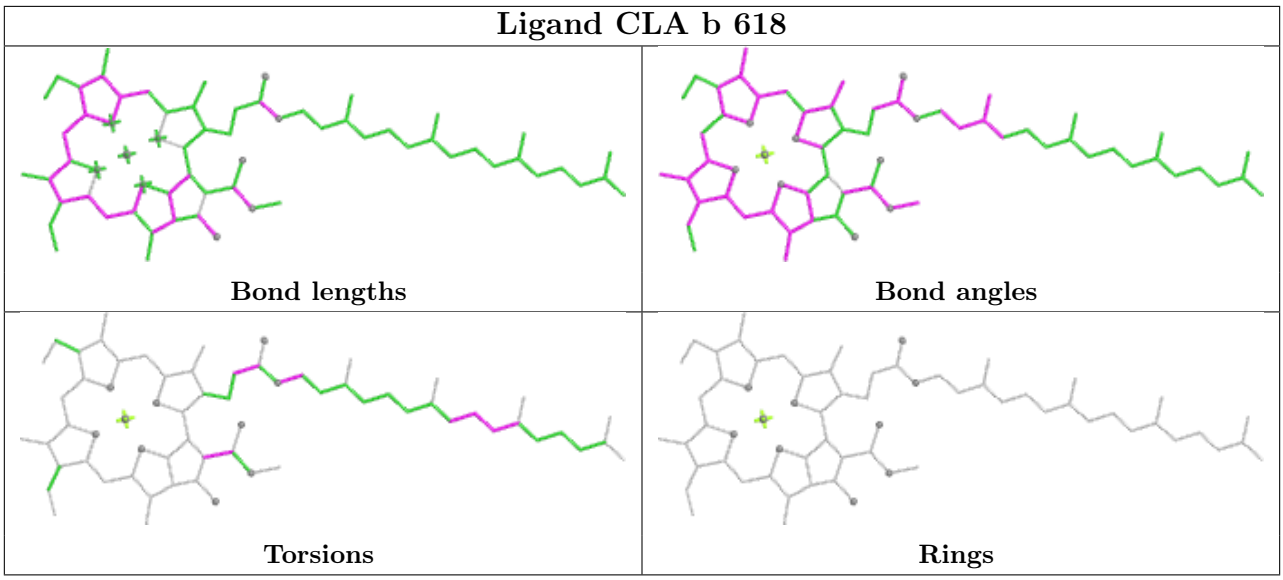
Ligand PL9 a 416



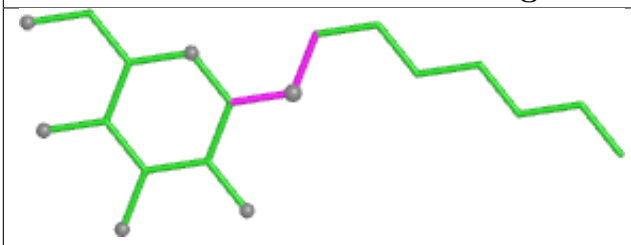
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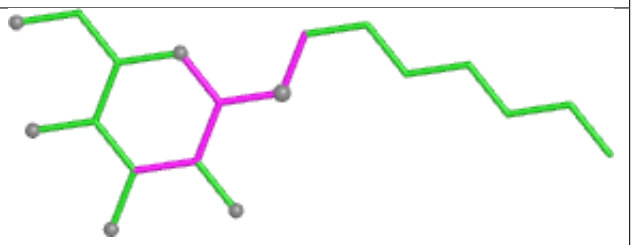
Ligand CLA b 618



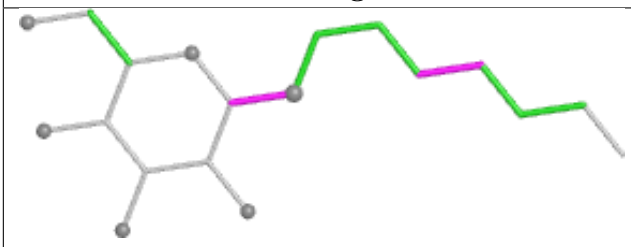
Ligand HTG V 204



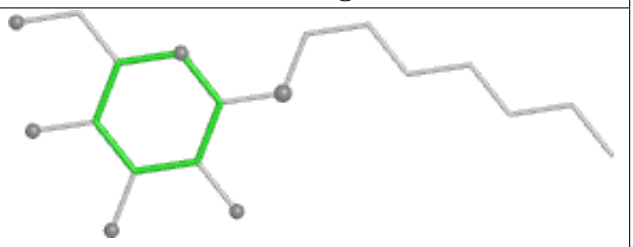
Bond lengths



Bond angles

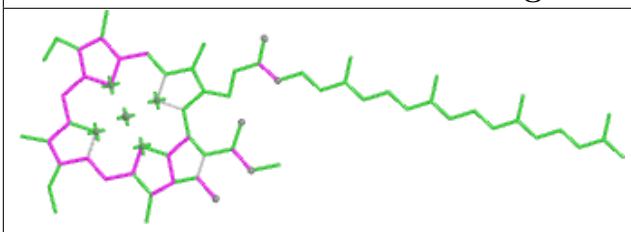


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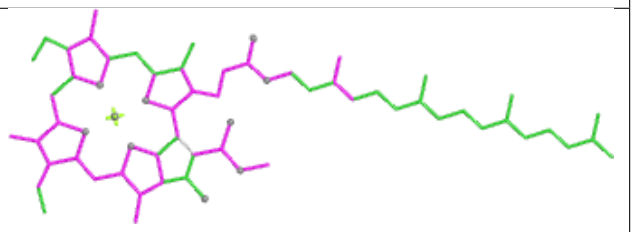


Rings

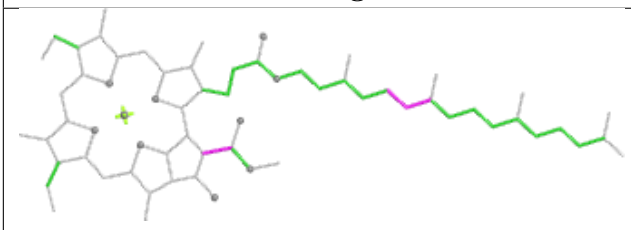
Ligand CLA B 604



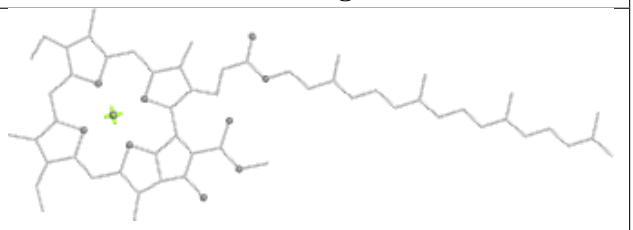
Bond lengths



Bond angles

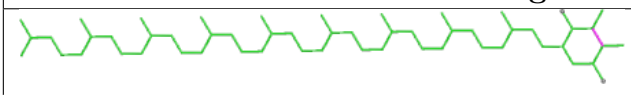


Torsions

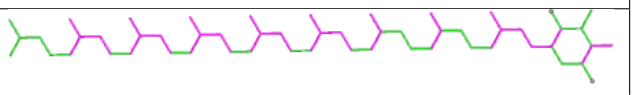


Rings

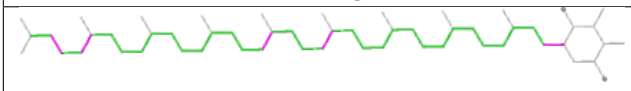
Ligand PL9 A 419



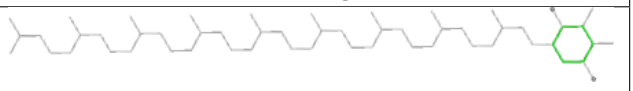
Bond lengths



Bond angles

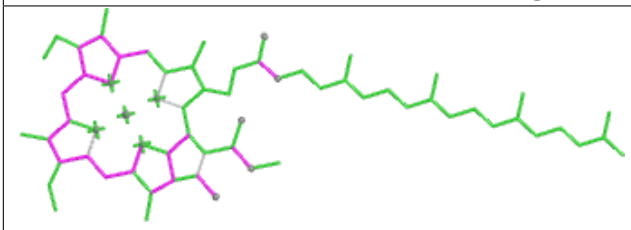


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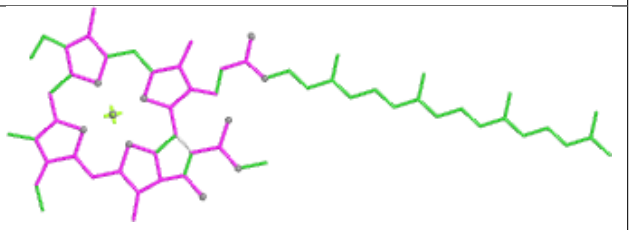


Rings

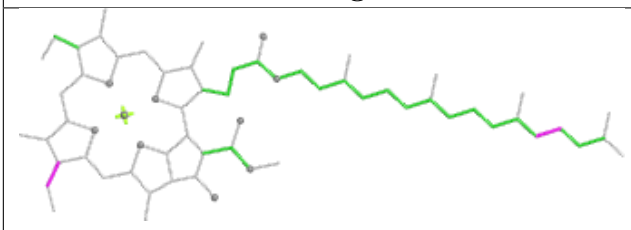
Ligand CLA a 406



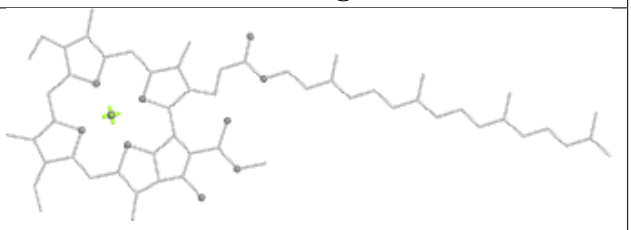
Bond lengths



Bond angles



Torsions

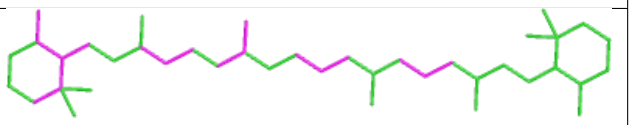


Rings

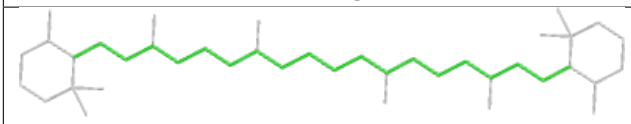
Ligand BCR t 101



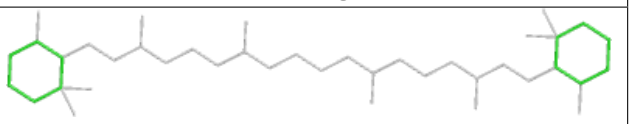
Bond lengths



Bond angles

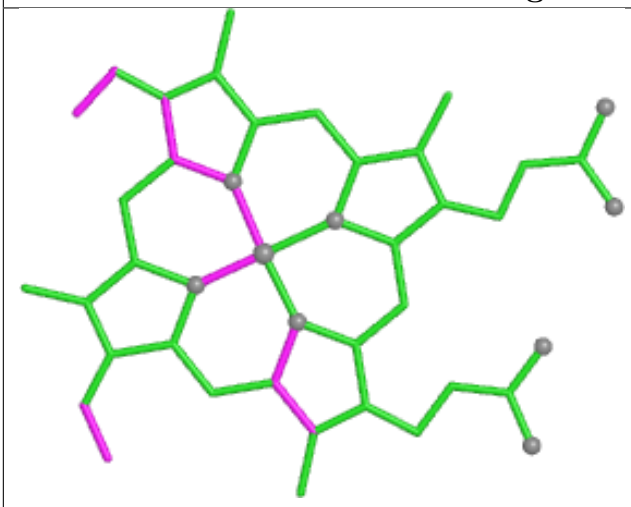


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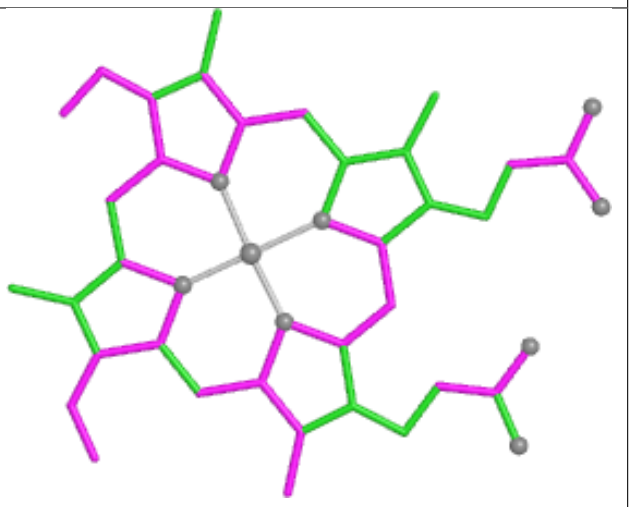


Rings

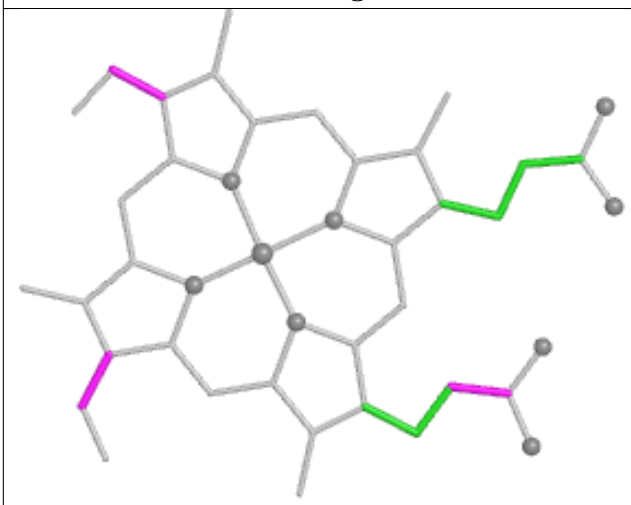
Ligand HEC v 202



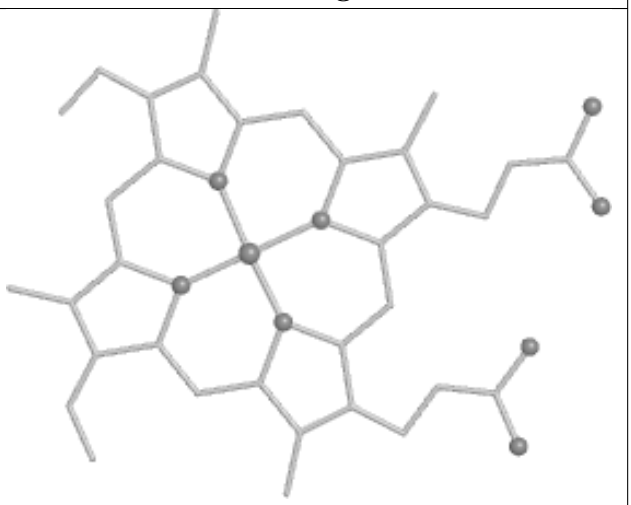
Bond lengths



Bond angles

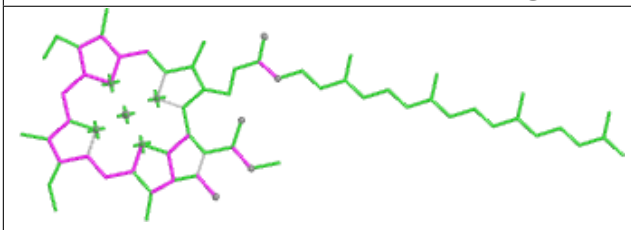


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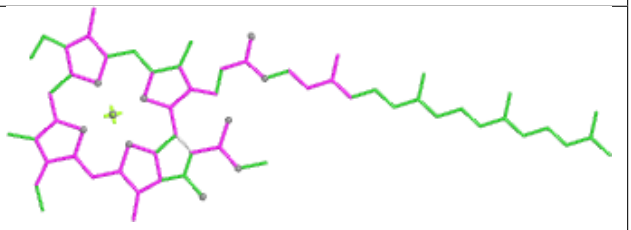


Rings

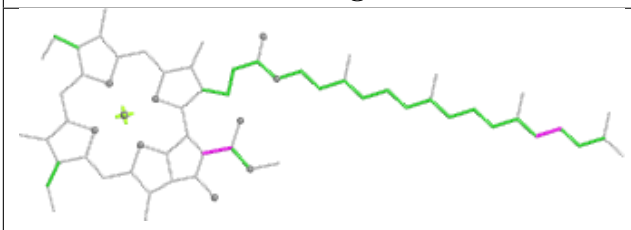
Ligand CLA C 509



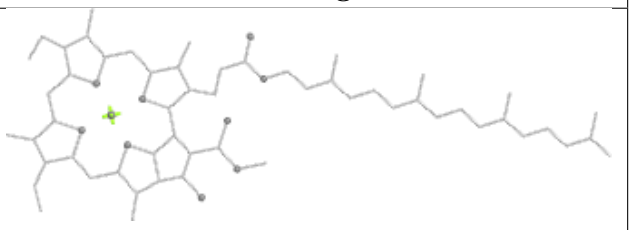
Bond lengths



Bond angles

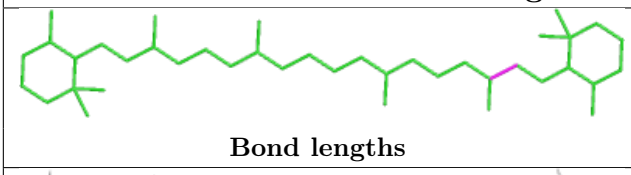


Torsions

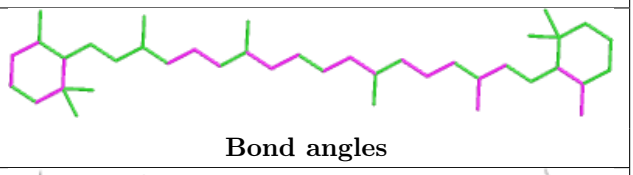


Rings

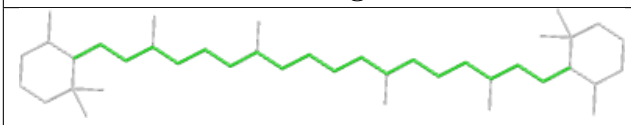
Ligand BCR b 624



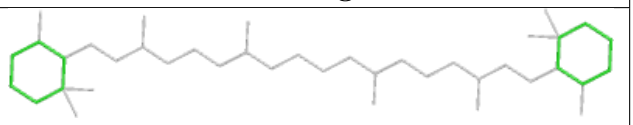
Bond lengths



Bond angles

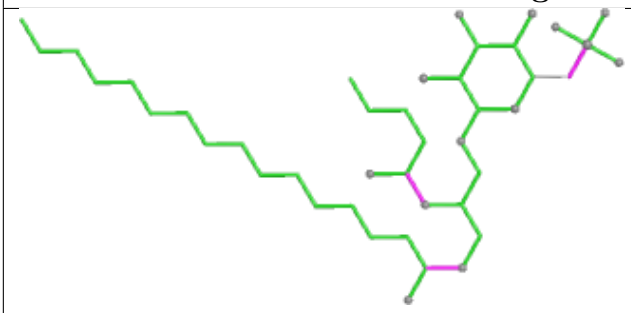


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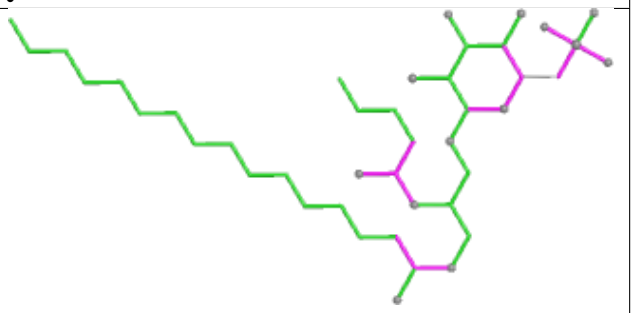


Rings

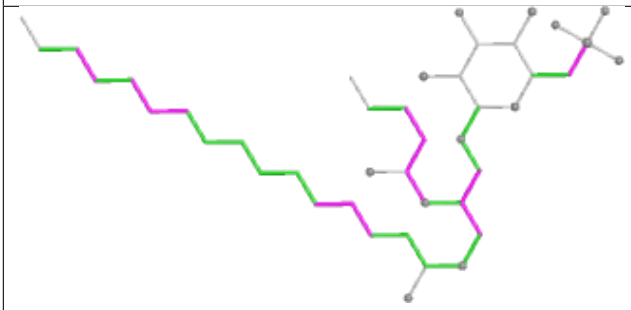
Ligand SQD f 101



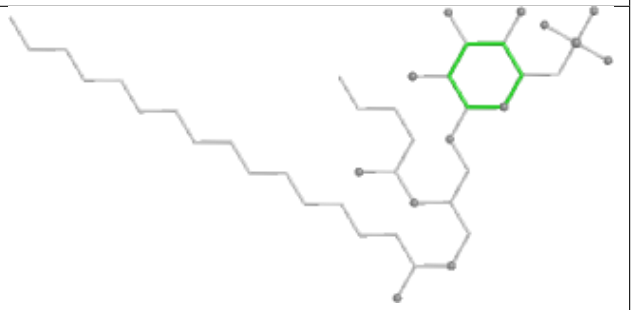
Bond lengths



Bond angles

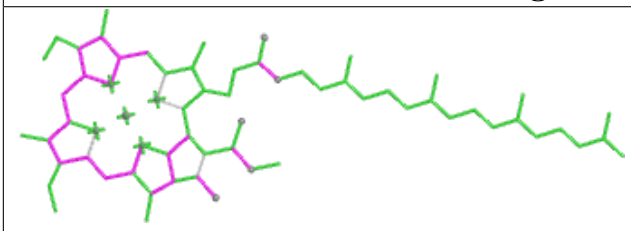


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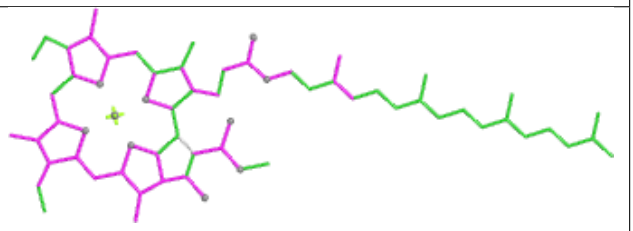


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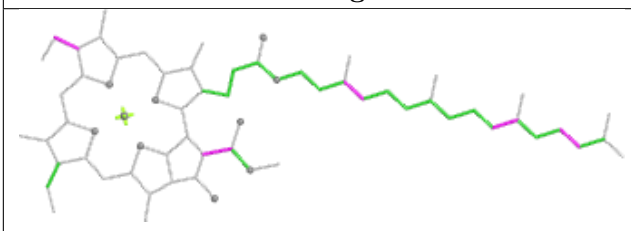
Ligand CLA c 506



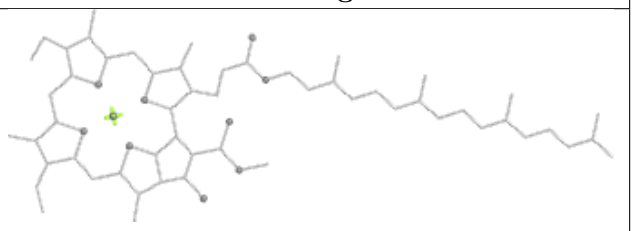
Bond lengths



Bond angles

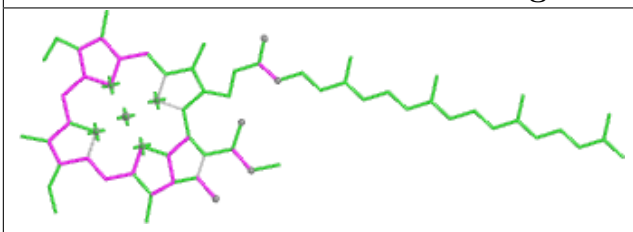


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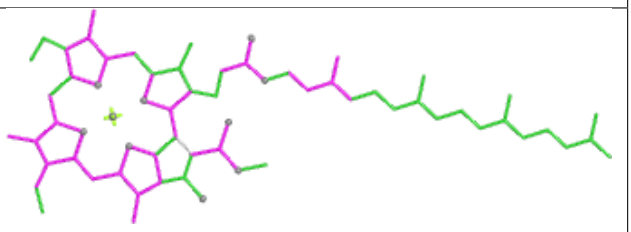


Rings

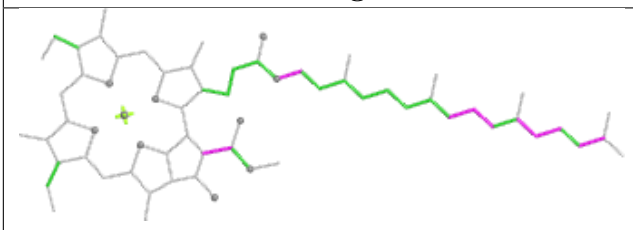
Ligand CLA c 511



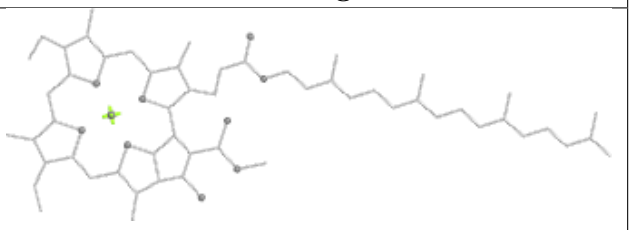
Bond lengths



Bond angles

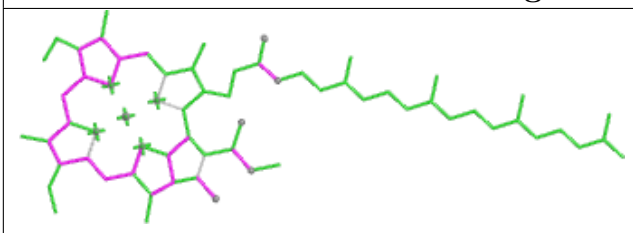


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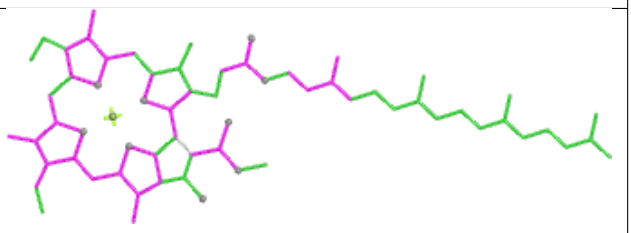


Rings

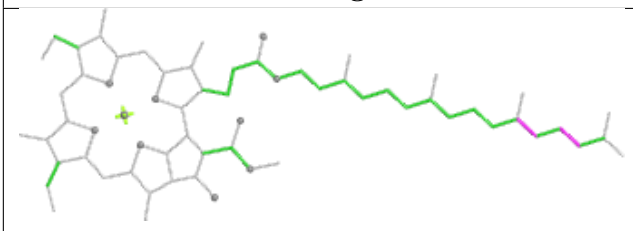
Ligand CLA B 612



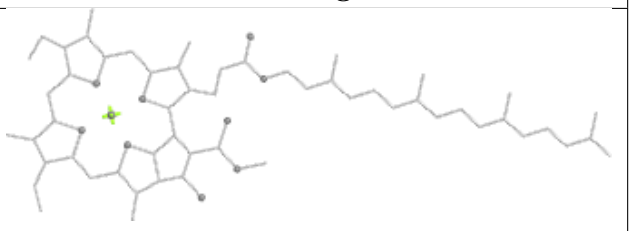
Bond lengths



Bond angles

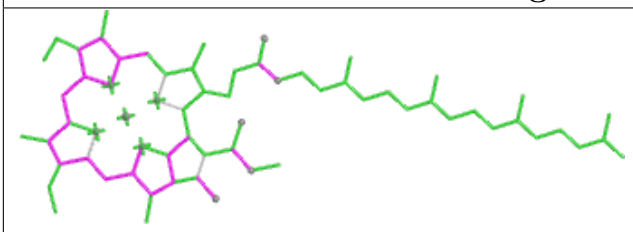


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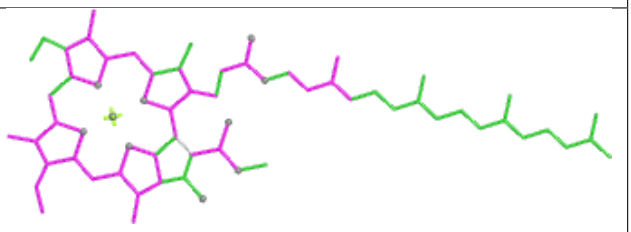


Rings

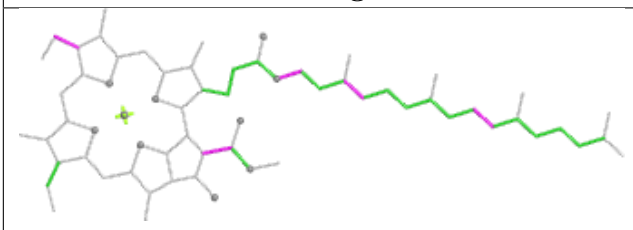
Ligand CLA c 515



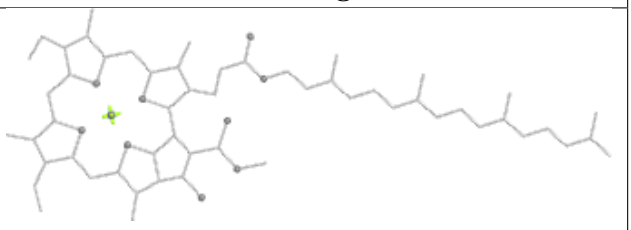
Bond lengths



Bond angles

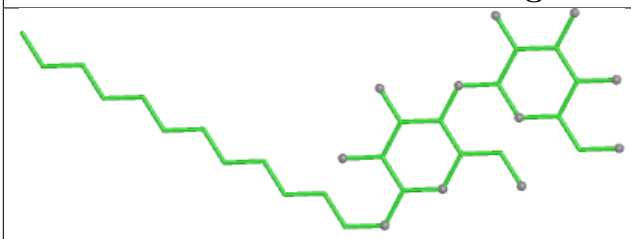


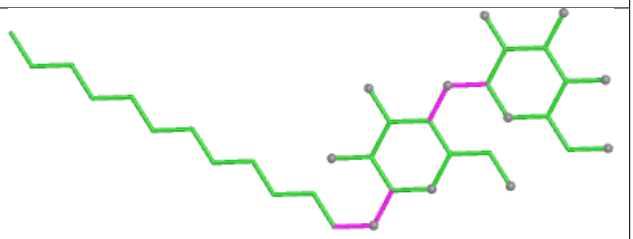
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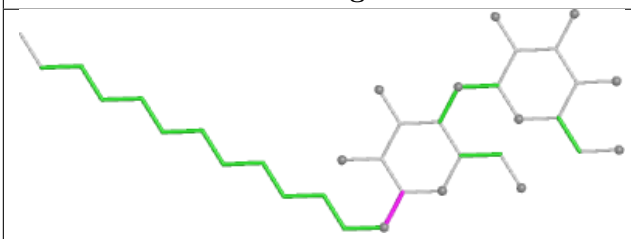


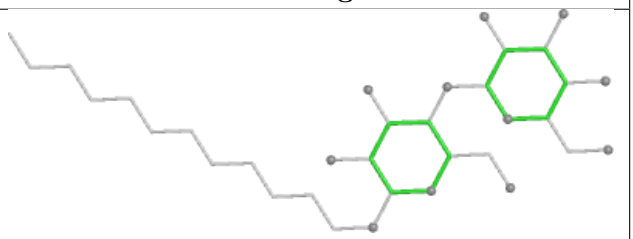
Rings

Ligand LMT a 417

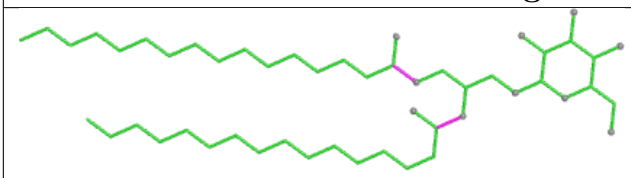

Bond lengths

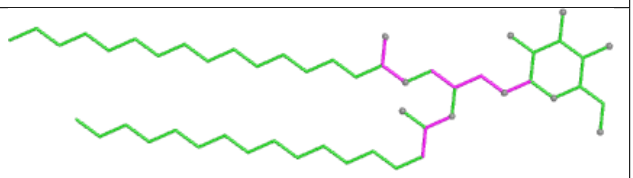

Bond angles

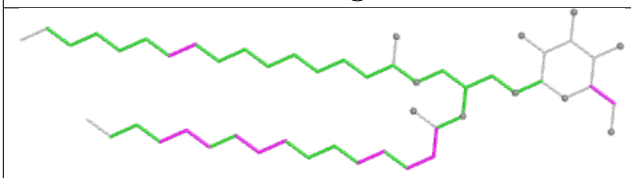

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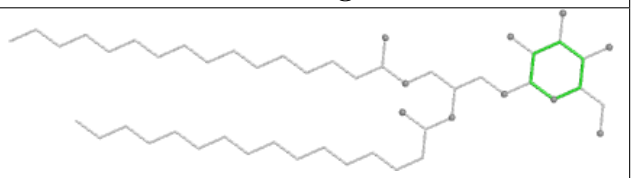

Rings

Ligand LMG J 101

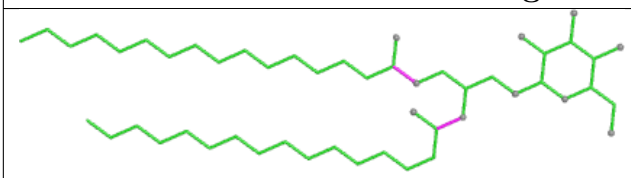

Bond lengths

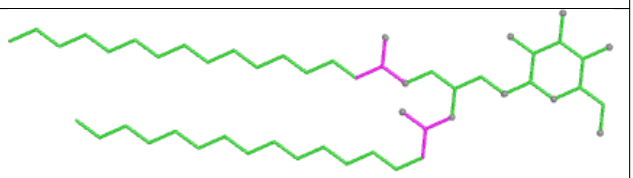

Bond angles

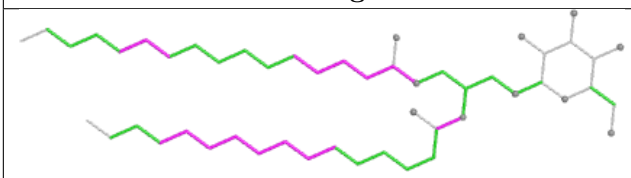

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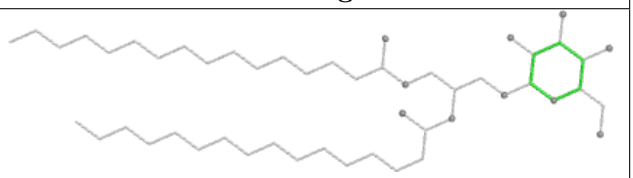

Rings

Ligand LMG b 625

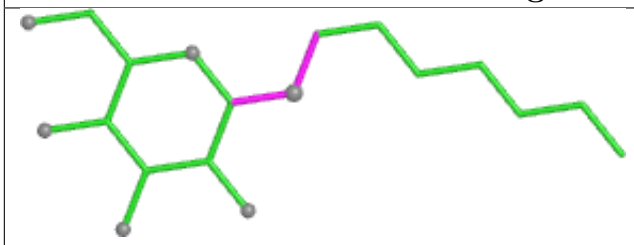

Bond lengths


Bond angles

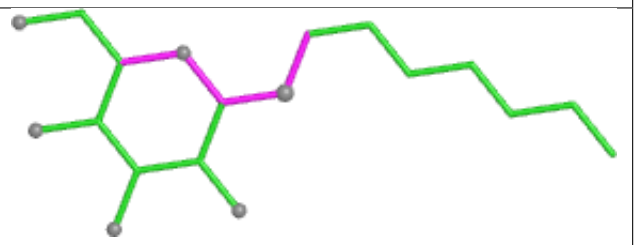

Torsions


Rings

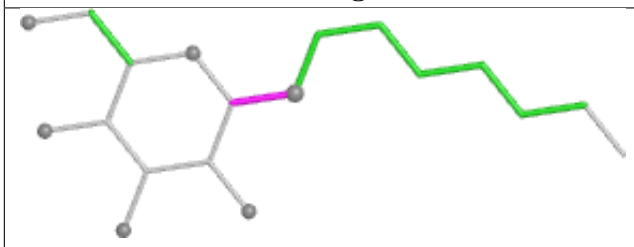
Ligand HTG c 523



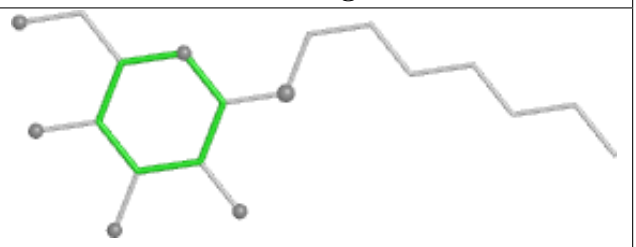
Bond lengths



Bond angles

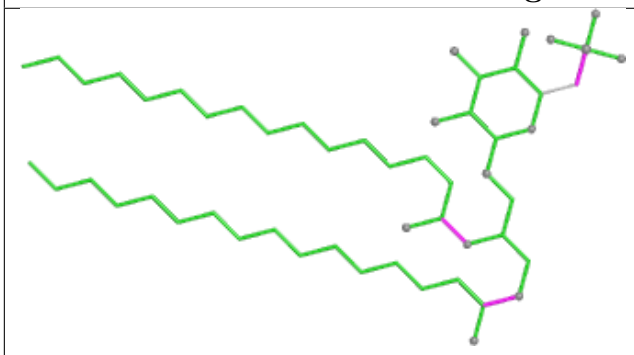


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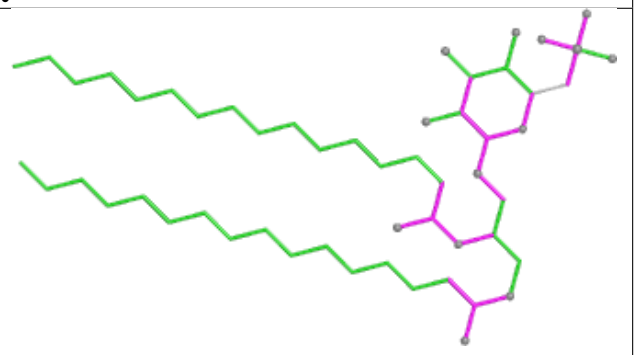


Rings

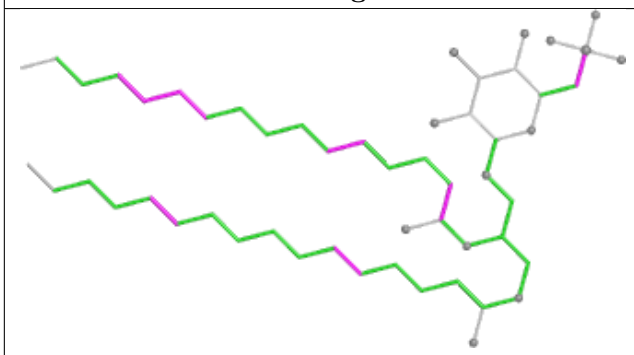
Ligand SQD A 411



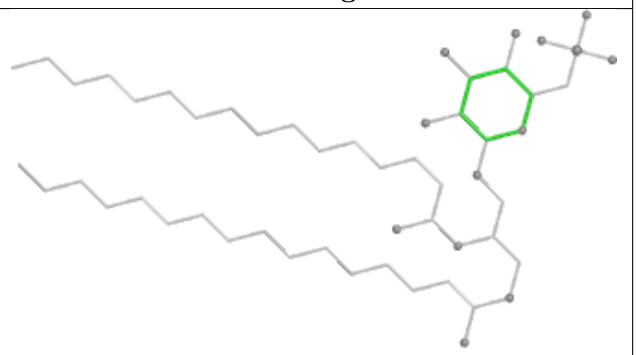
Bond lengths



Bond angles

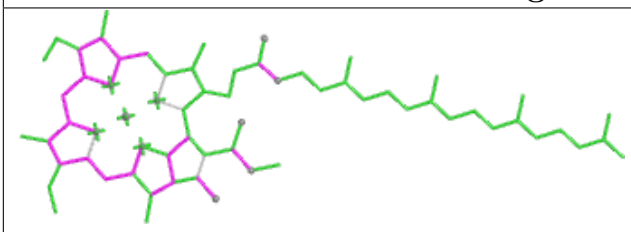


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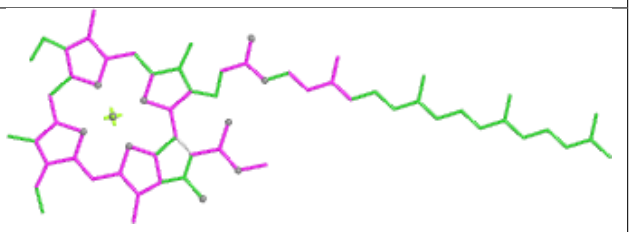


Rings

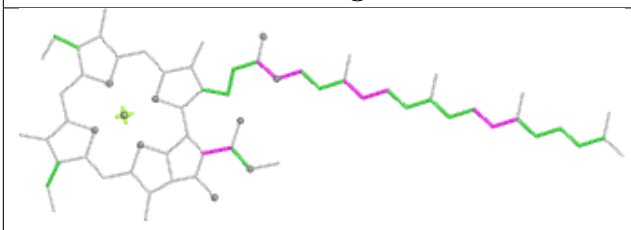
Ligand CLA b 621



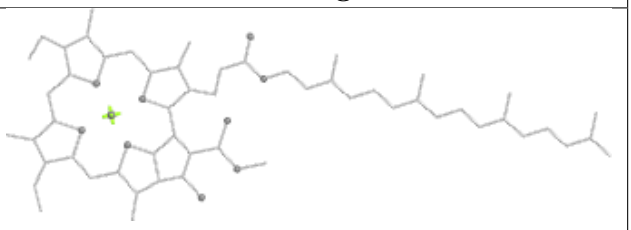
Bond lengths



Bond angles

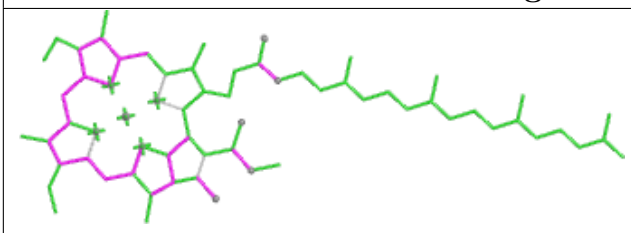


Torsions

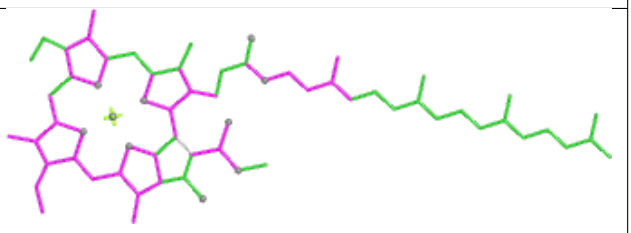


Rings

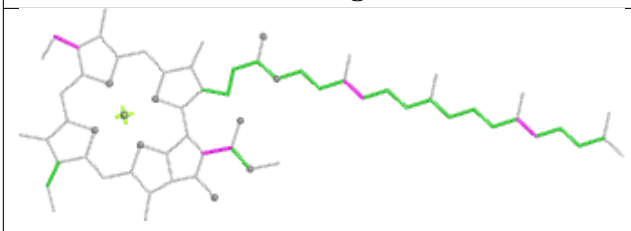
Ligand CLA C 505



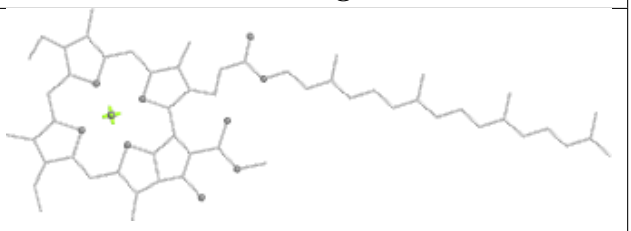
Bond lengths



Bond angles

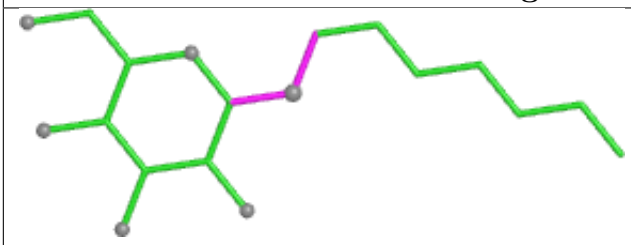


Torsions

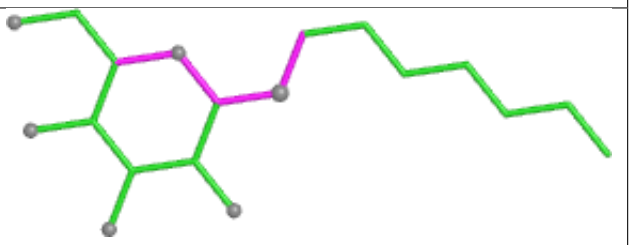


Rings

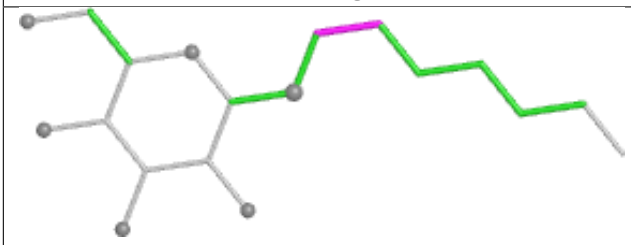
Ligand HTG B 631



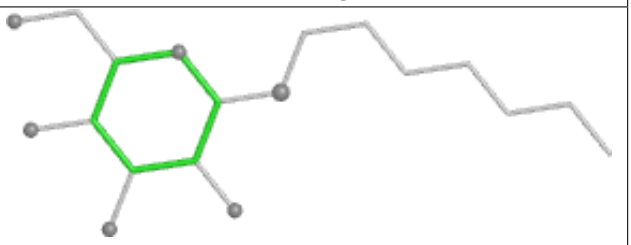
Bond lengths



Bond angles

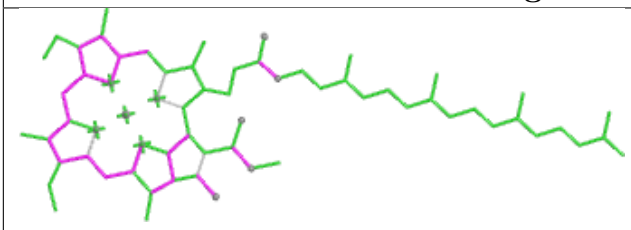


Torsions

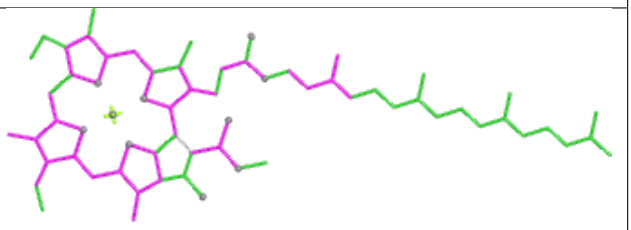


Rings

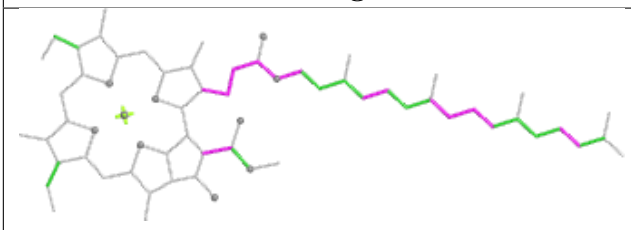
Ligand CLA B 602



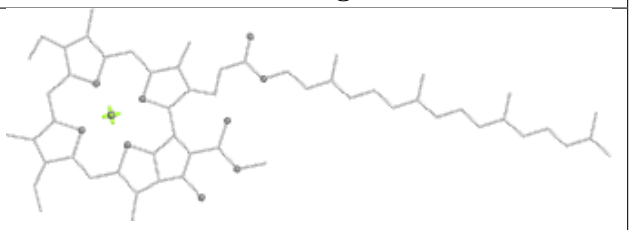
Bond lengths



Bond angles

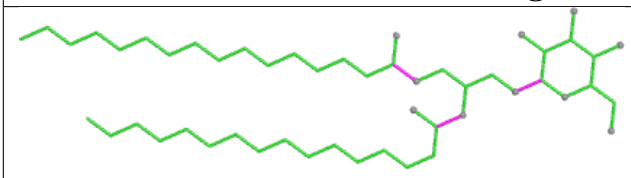


Torsions

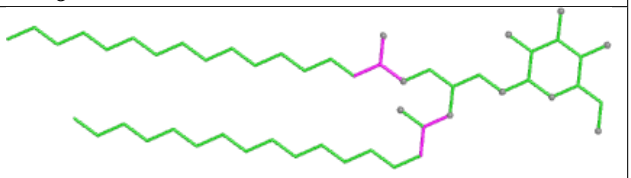


Rings

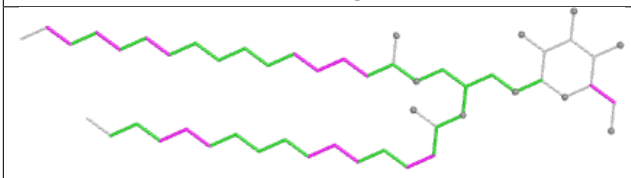
Ligand LMG j 101



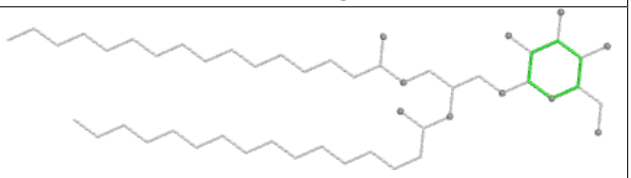
Bond lengths



Bond angles

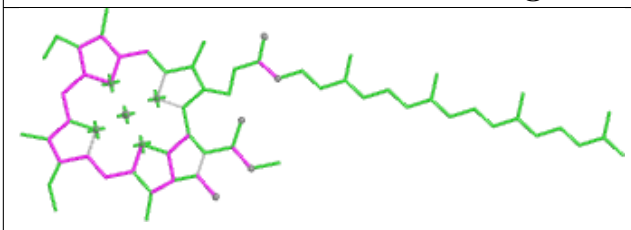


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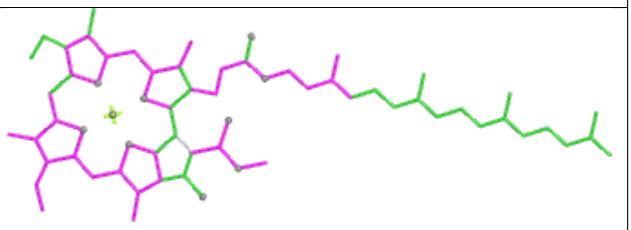


Rings

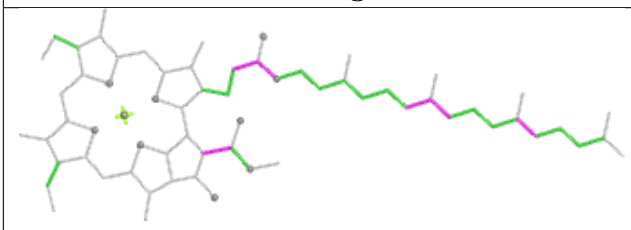
Ligand CLA C 513



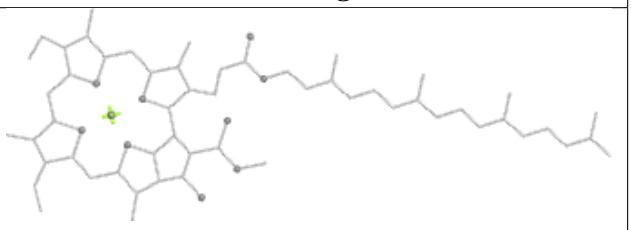
Bond lengths



Bond angles

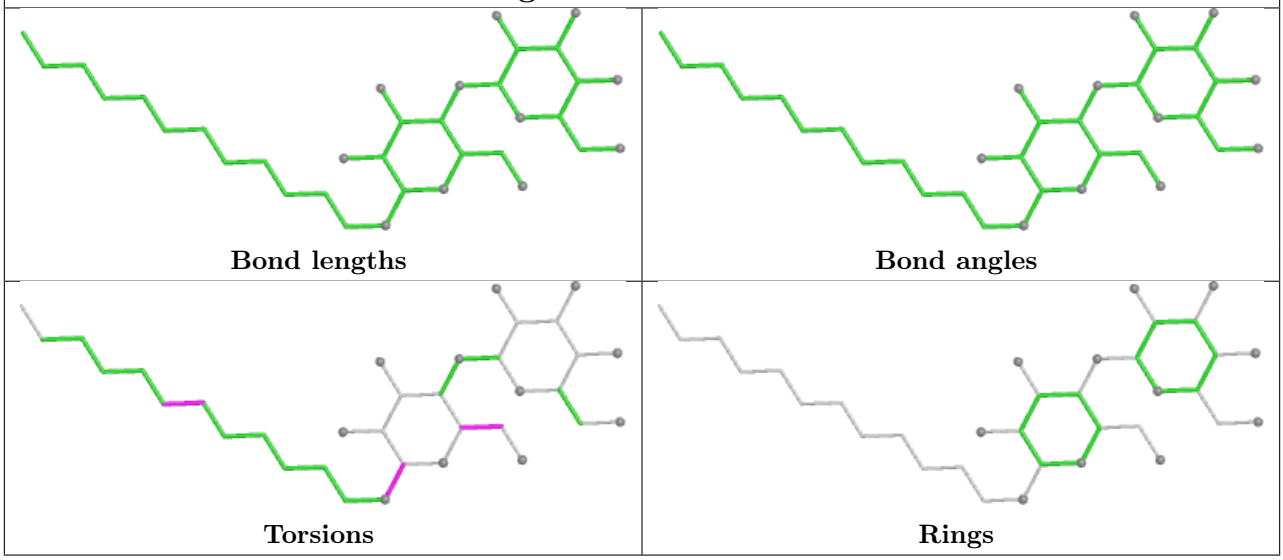


Torsions

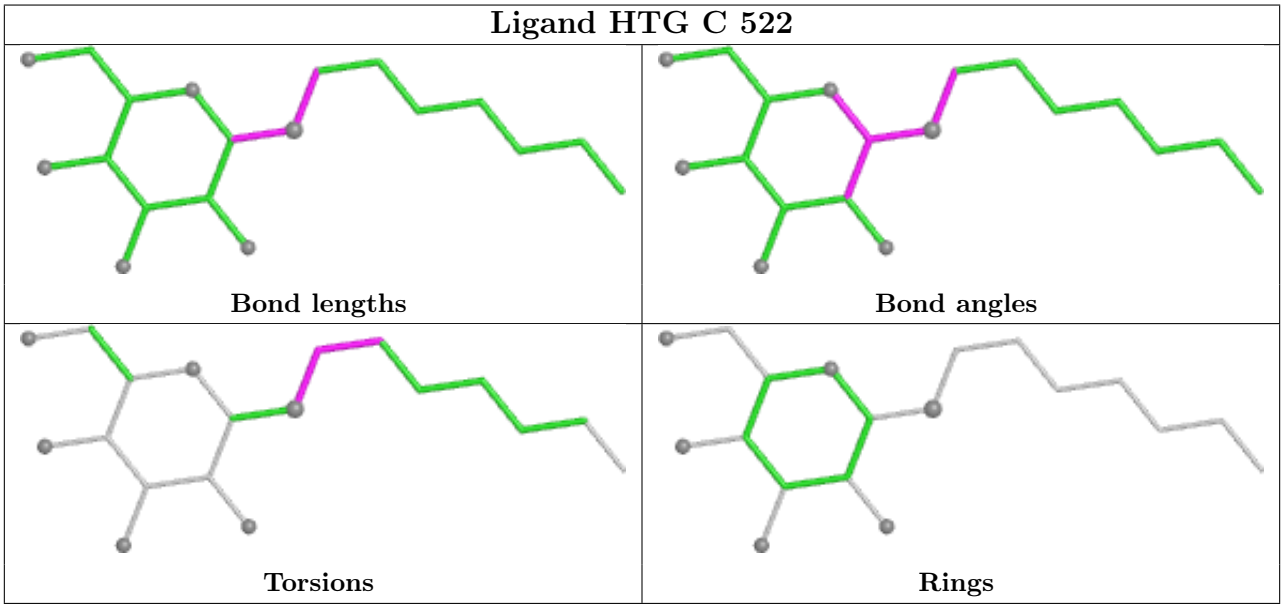


Rings

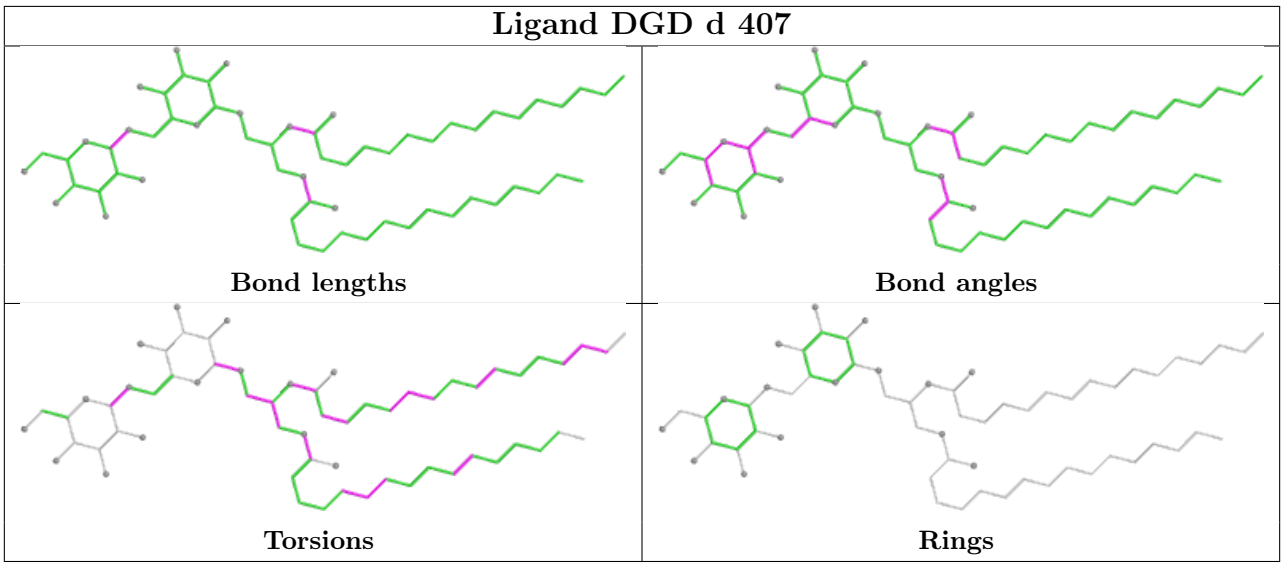
Ligand LMT M 102



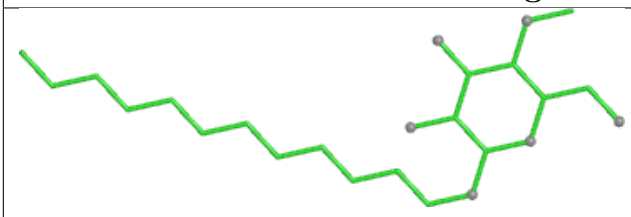
Ligand HTG C 522



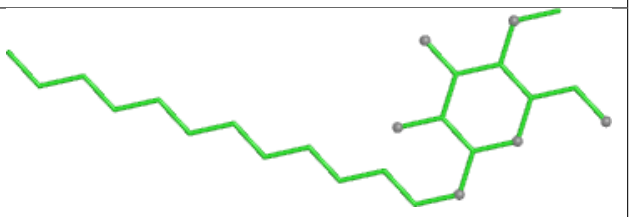
Ligand DGD d 407



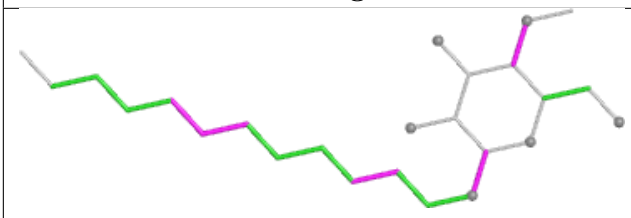
Ligand LMT b 626



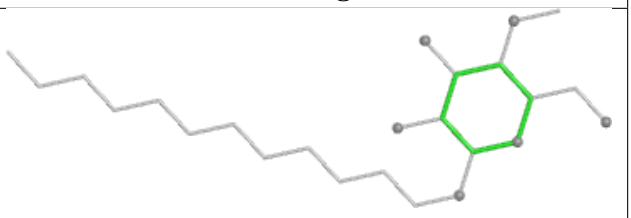
Bond lengths



Bond angles

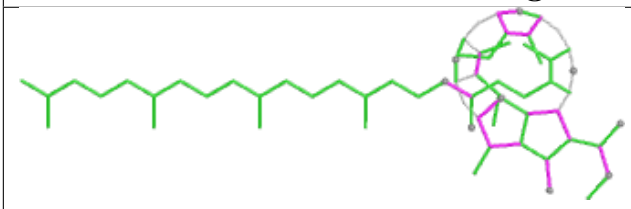


Torsions

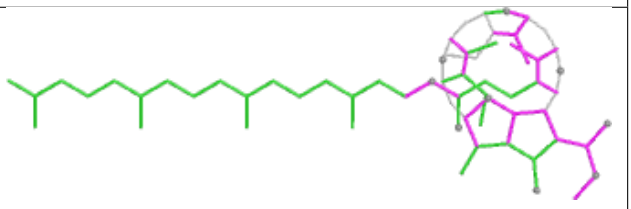


Rings

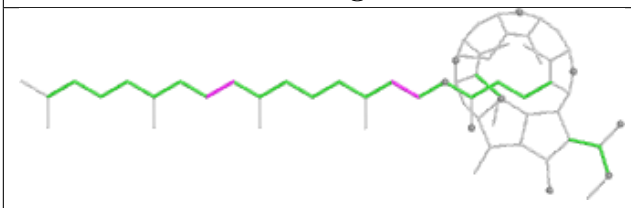
Ligand PHO a 408



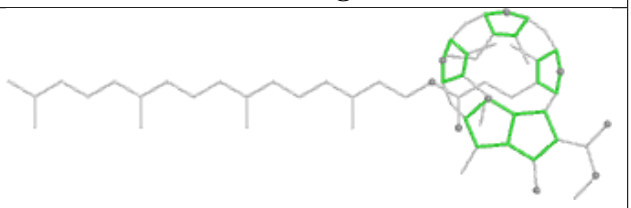
Bond lengths



Bond angles

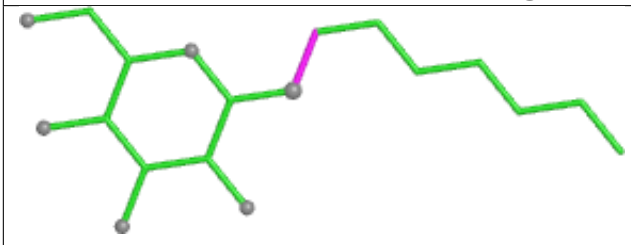


Torsions

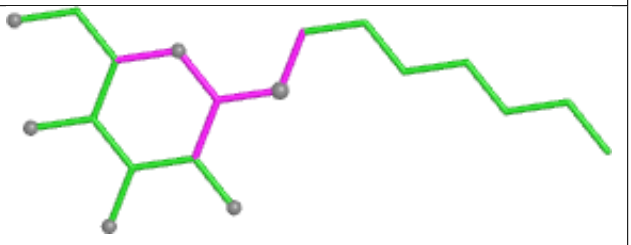


Rings

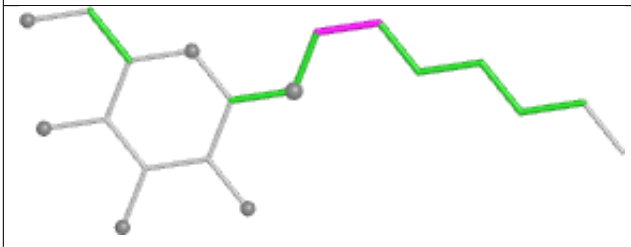
Ligand HTG B 622



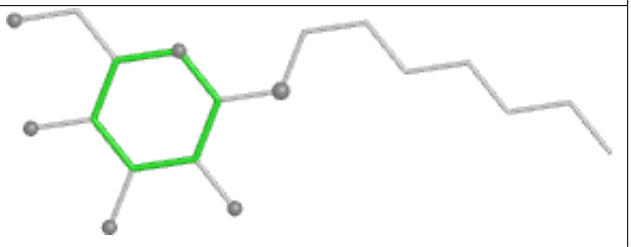
Bond lengths



Bond angles

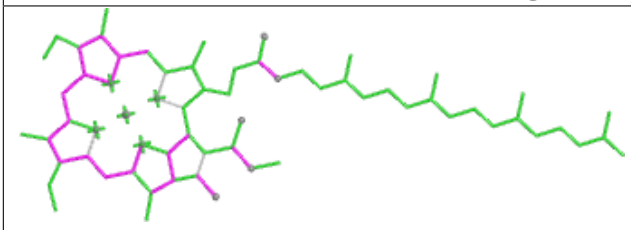


Torsions

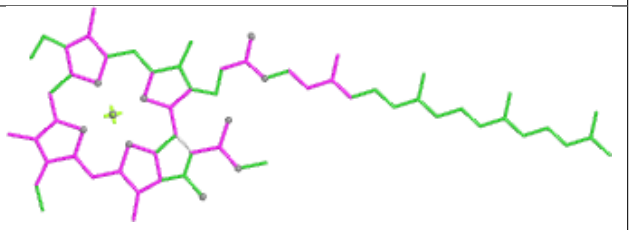


Rings

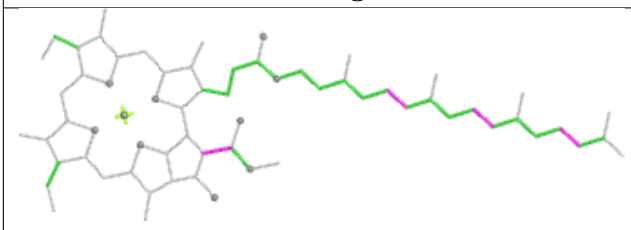
Ligand CLA C 504



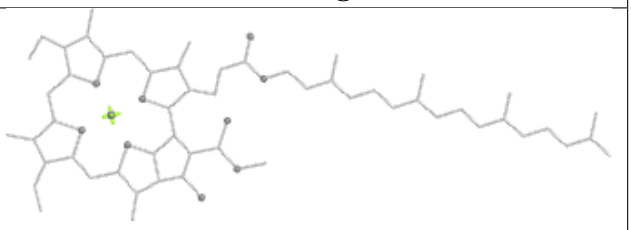
Bond lengths



Bond angles

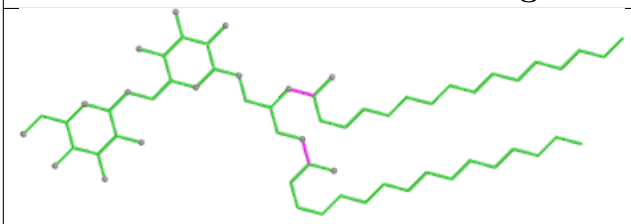


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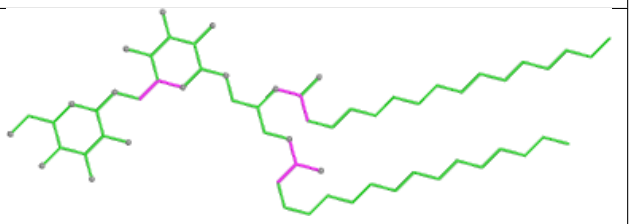


Rings

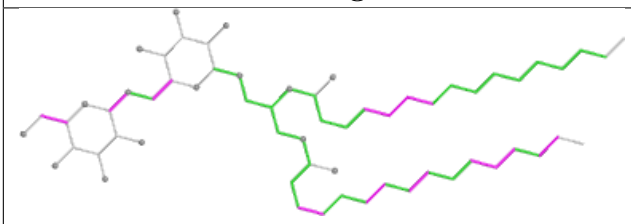
Ligand DGD C 517



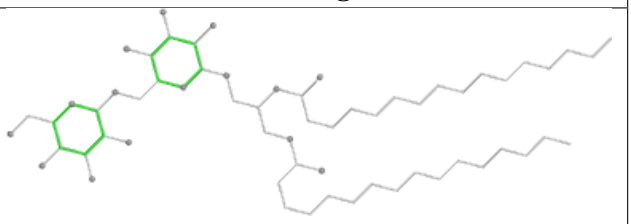
Bond lengths



Bond angles

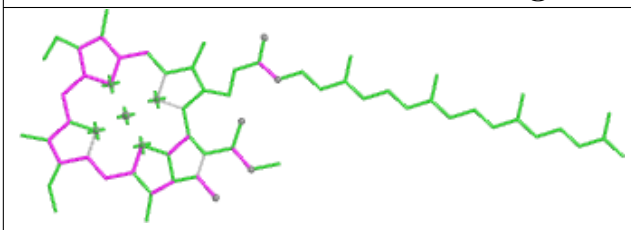


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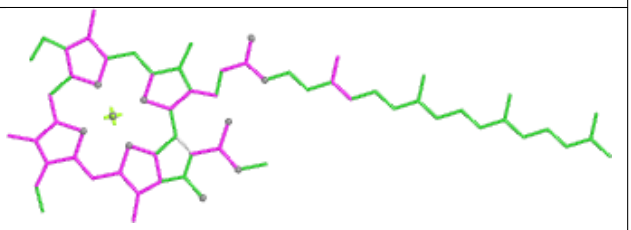


Rings

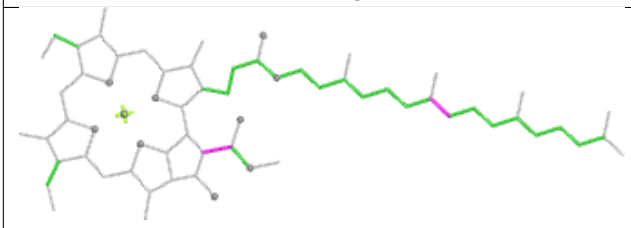
Ligand CLA c 509



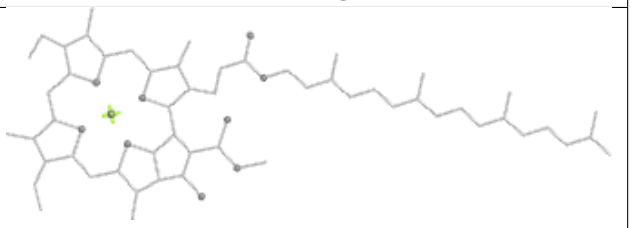
Bond lengths



Bond angles

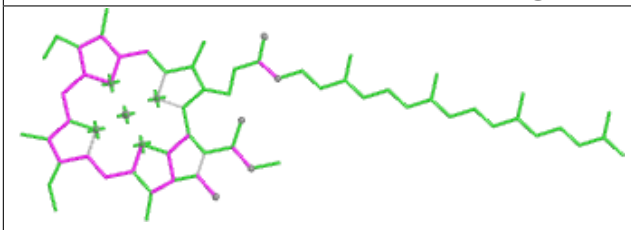


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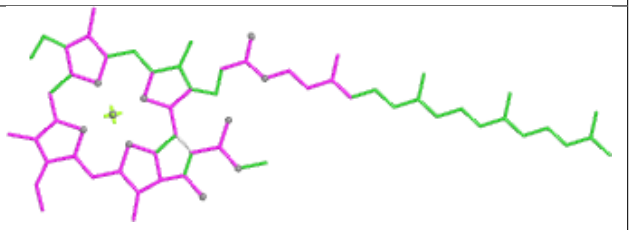


Rings

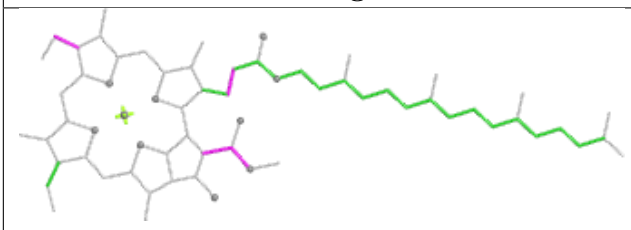
Ligand CLA c 503



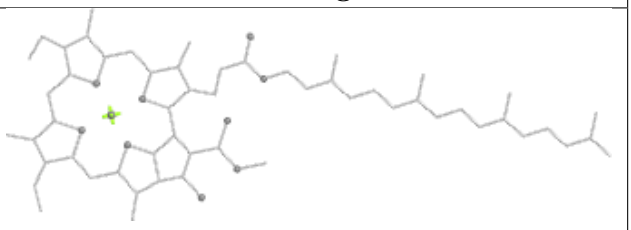
Bond lengths



Bond angles



Torsions

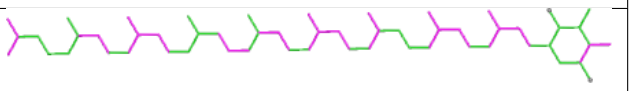


Rings

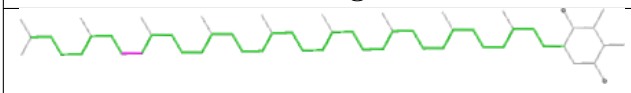
Ligand PL9 D 406



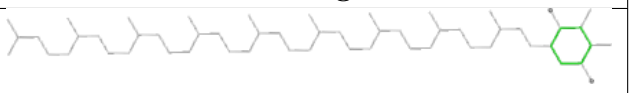
Bond lengths



Bond angles

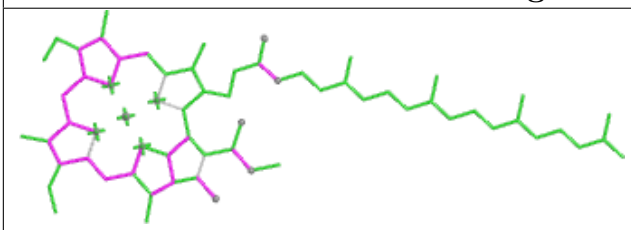


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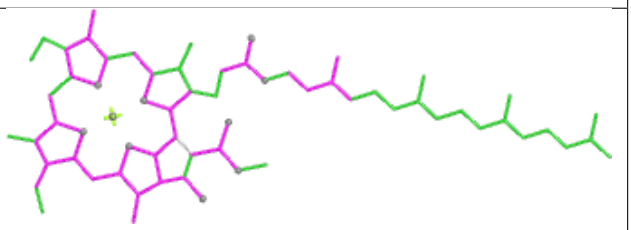


Rings

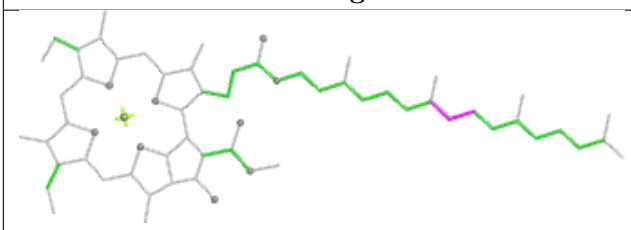
Ligand CLA b 617



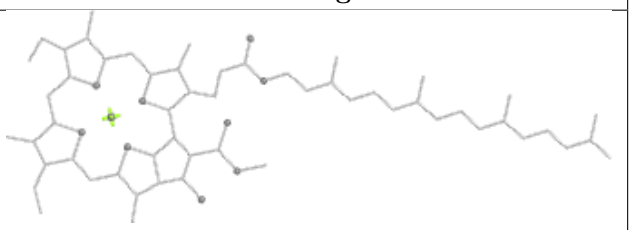
Bond lengths



Bond angles

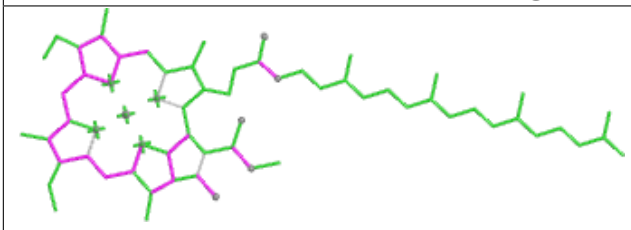


Torsions

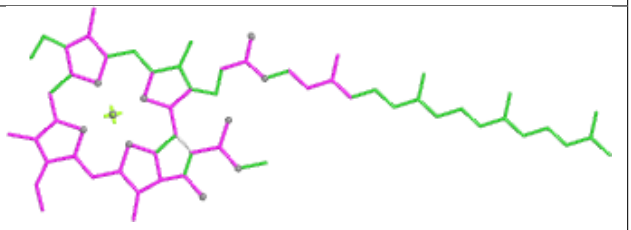


Rings

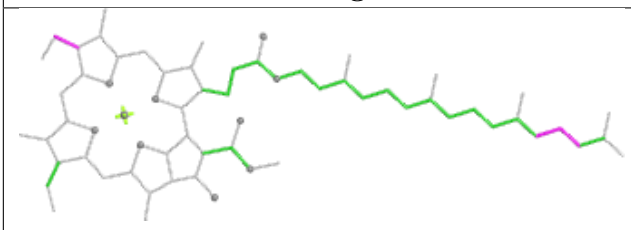
Ligand CLA b 616



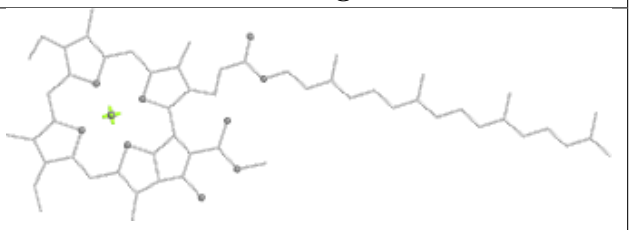
Bond lengths



Bond angles

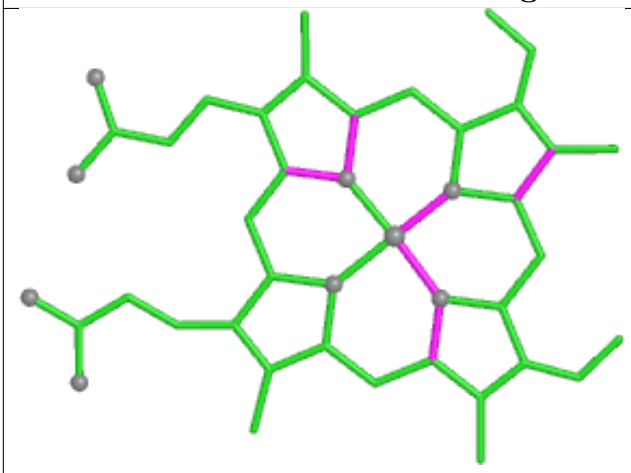


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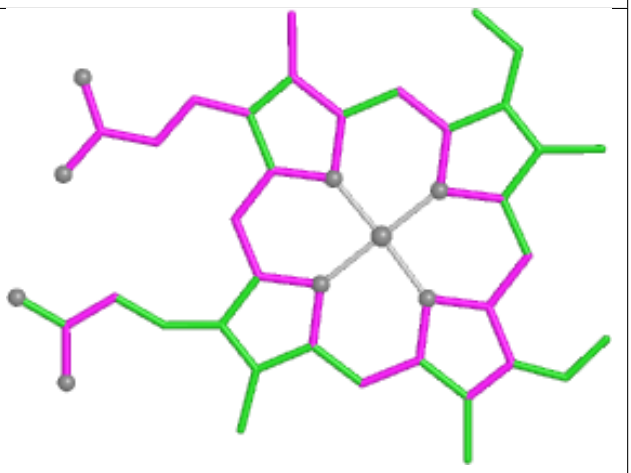


Rings

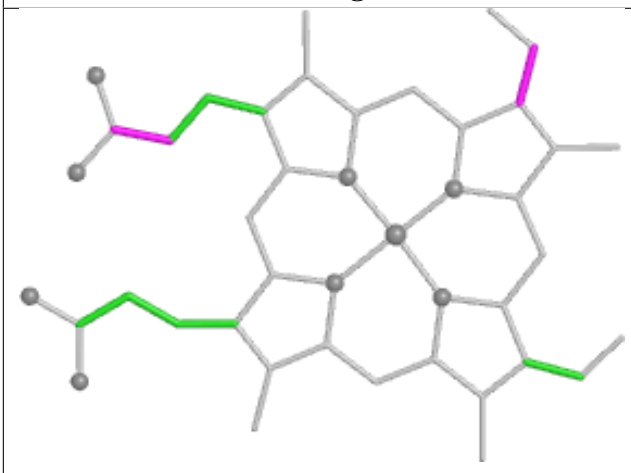
Ligand HEM E 103



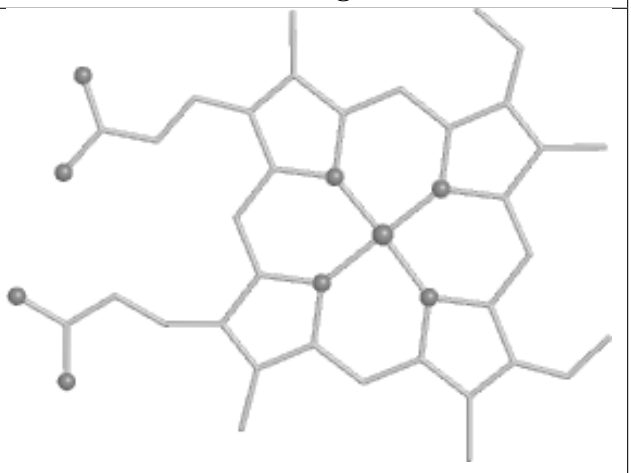
Bond lengths



Bond angles

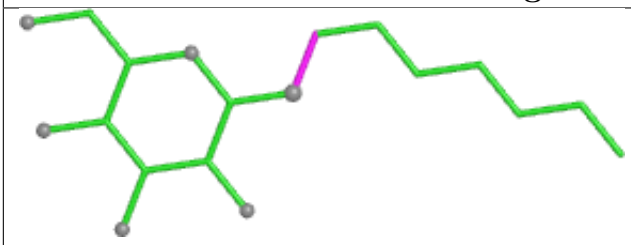


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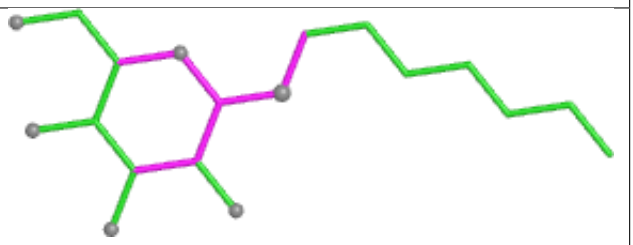


Rings

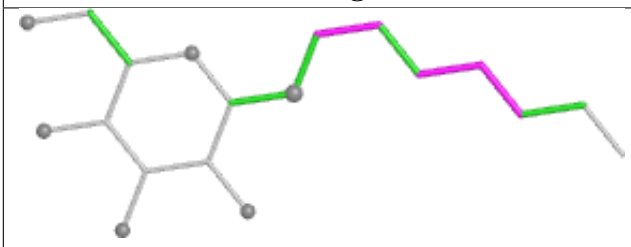
Ligand HTG b 627



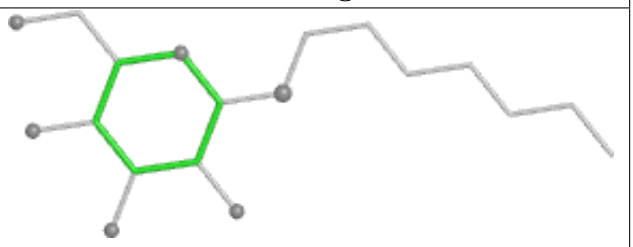
Bond lengths



Bond angles

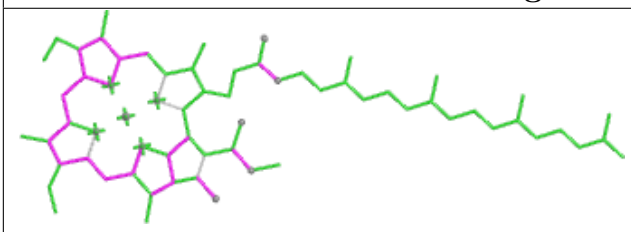


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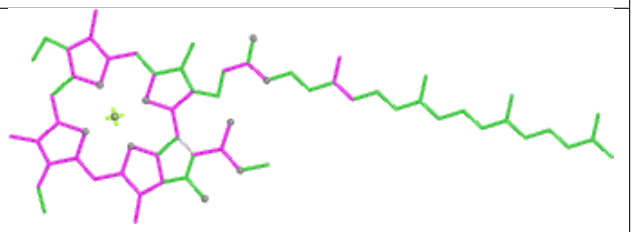


Rings

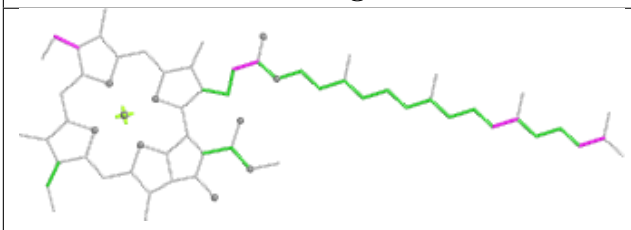
Ligand CLA C 506



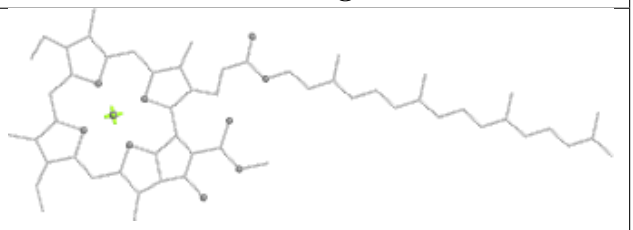
Bond lengths



Bond angles

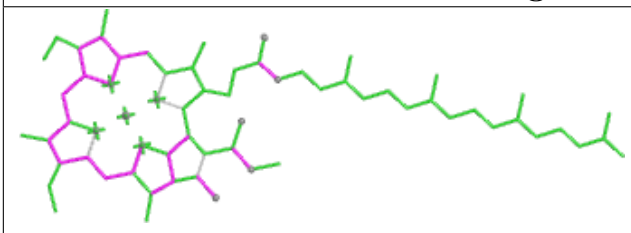


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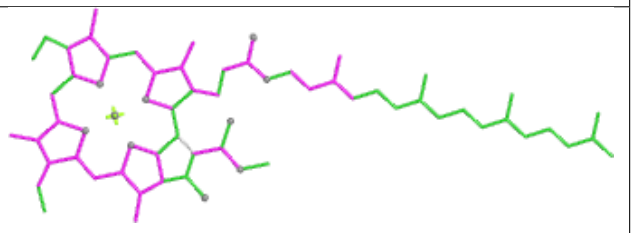


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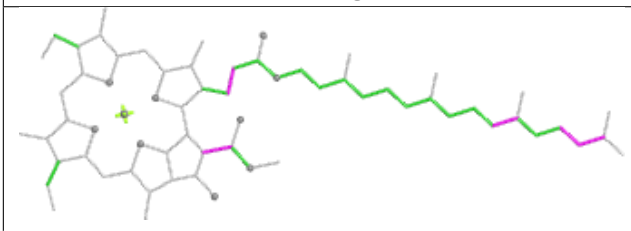
Ligand CLA b 615



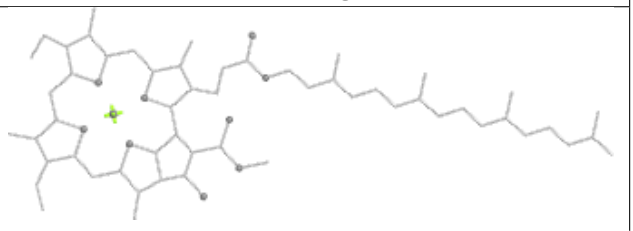
Bond lengths



Bond angles

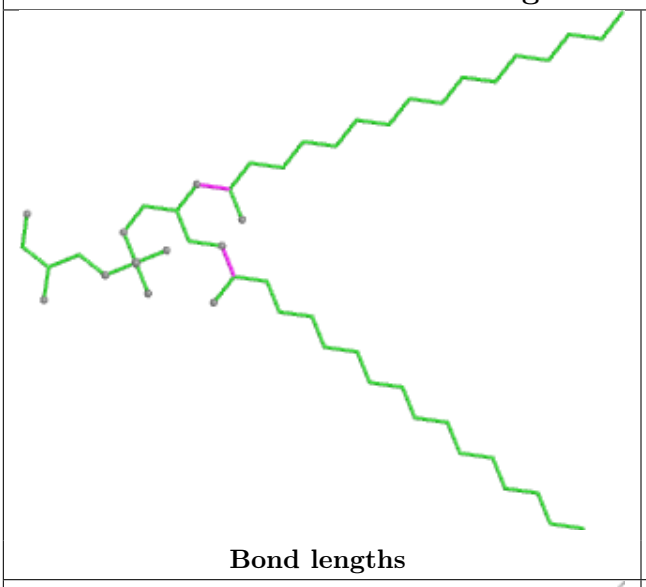


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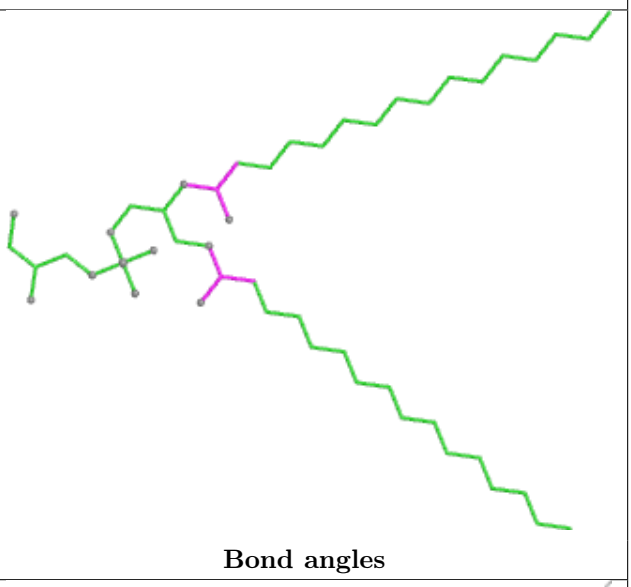


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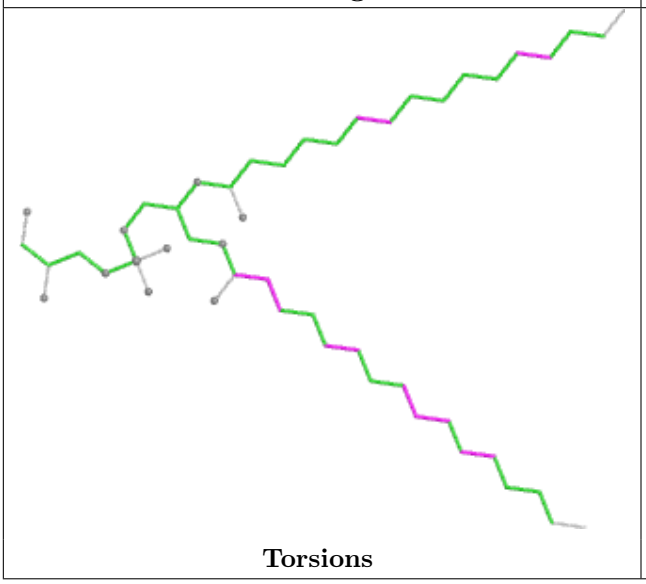
Ligand LHG D 408



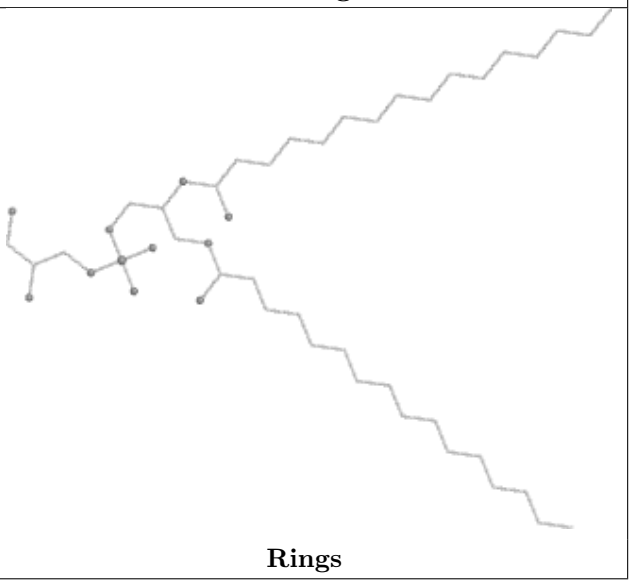
Bond lengths



Bond angles

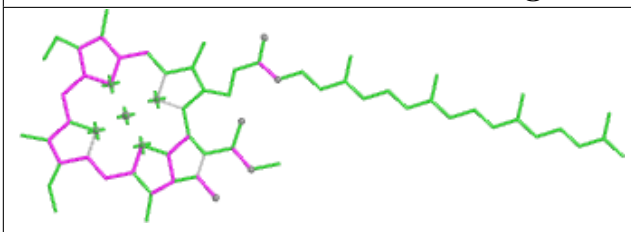


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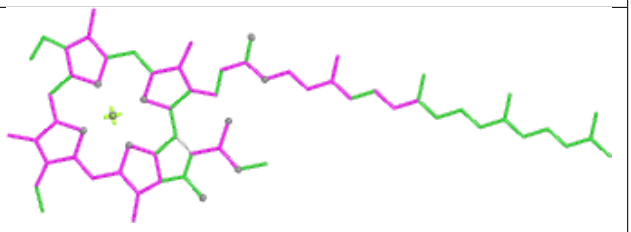


Rings

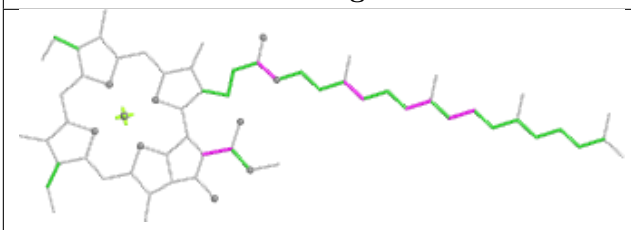
Ligand CLA C 511



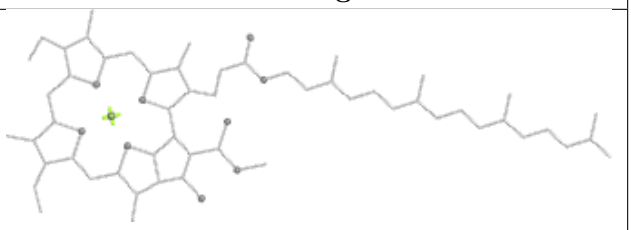
Bond lengths



Bond angles

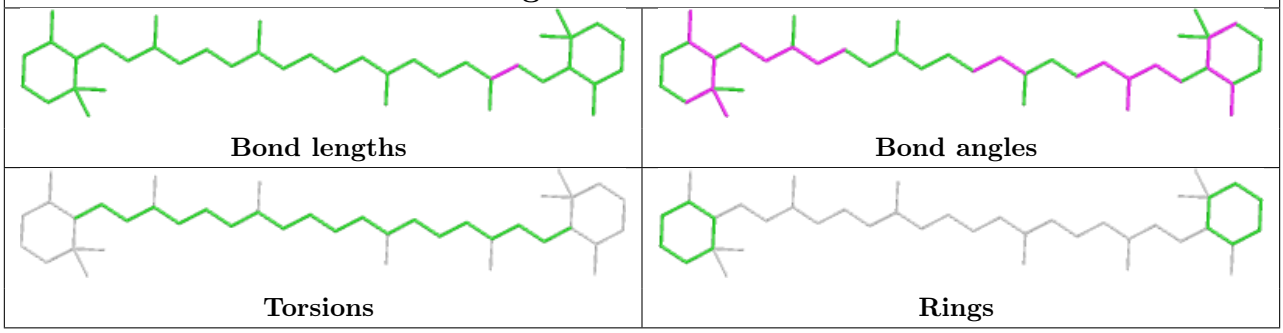


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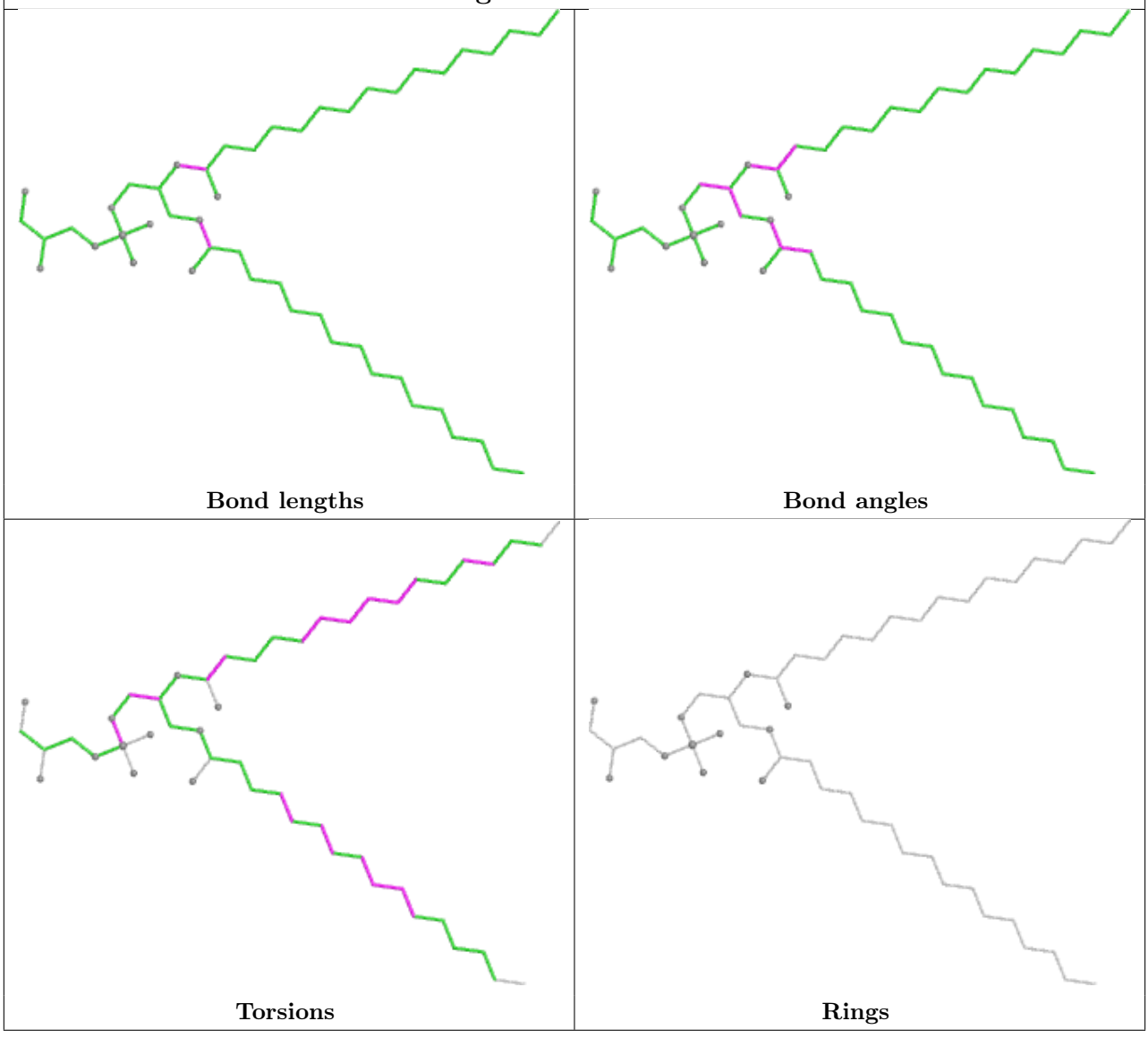


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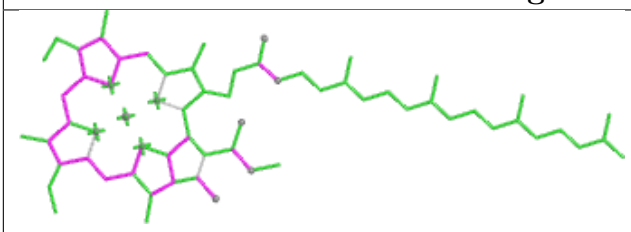
Ligand BCR K 101



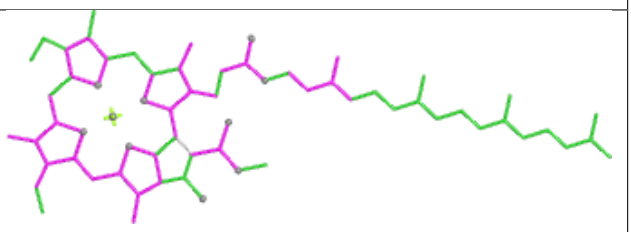
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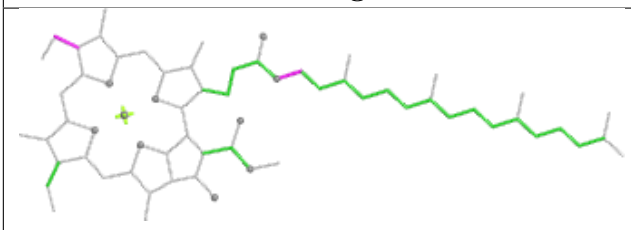
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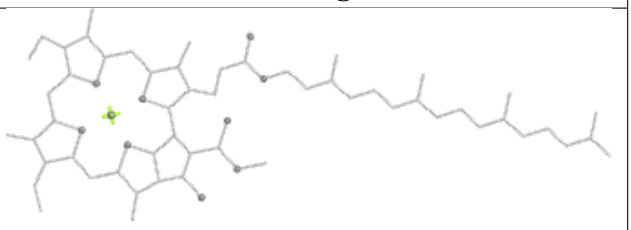
Bond lengths



Bond angles

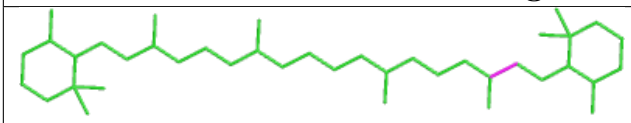


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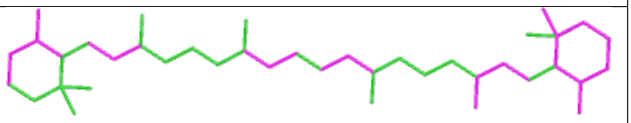


Rings

Ligand BCR d 405



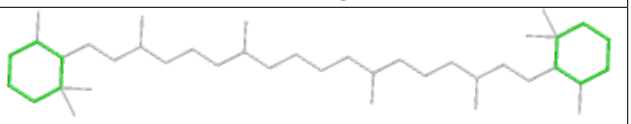
Bond lengths



Bond angles

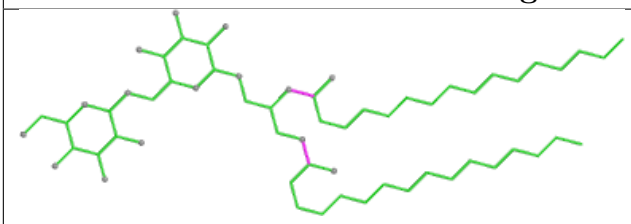


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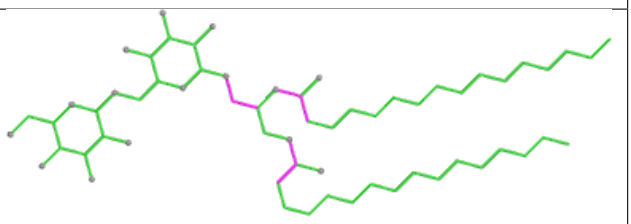


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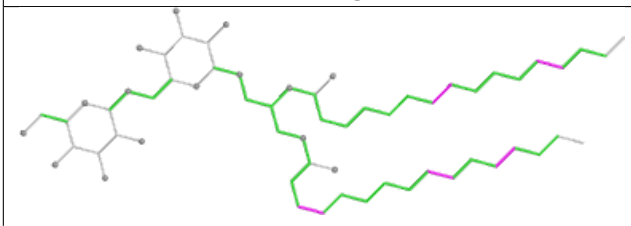
Ligand DGD C 519



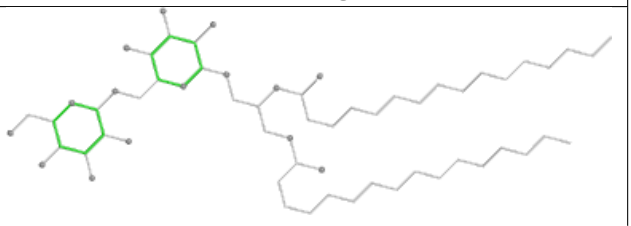
Bond lengths



Bond angles

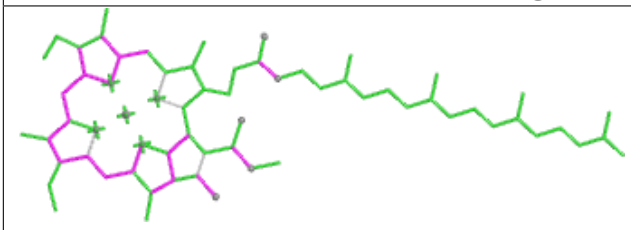


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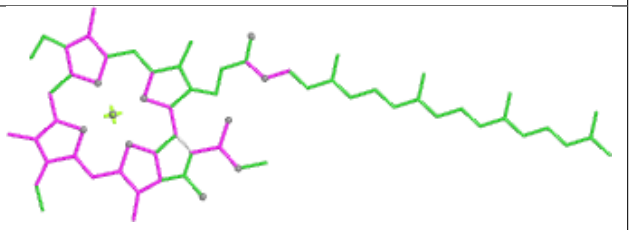


Rings

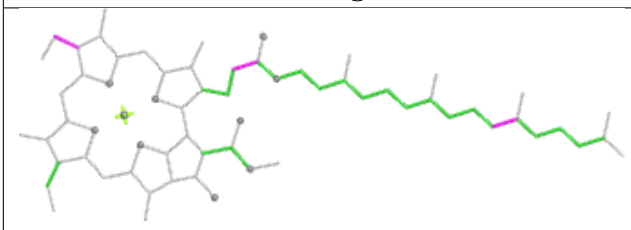
Ligand CLA c 507



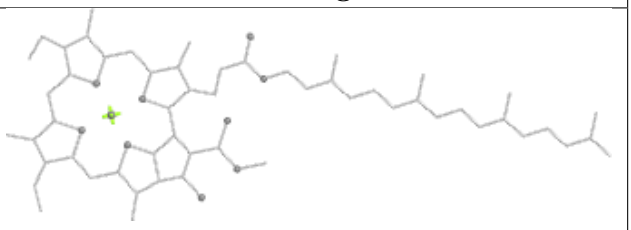
Bond lengths



Bond angles



Torsions

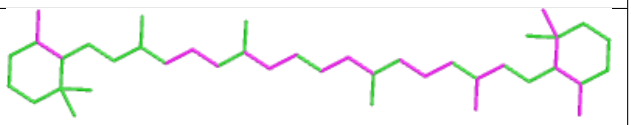


Rings

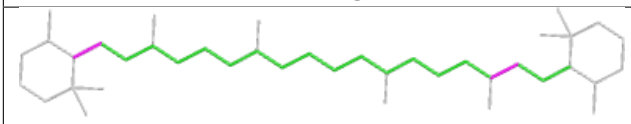
Ligand BCR Y 101



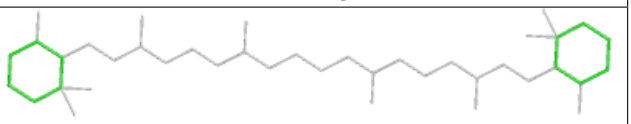
Bond lengths



Bond angles

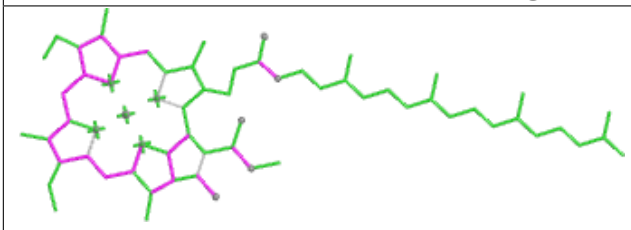


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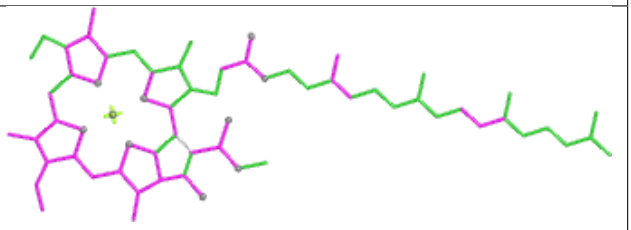


Rings

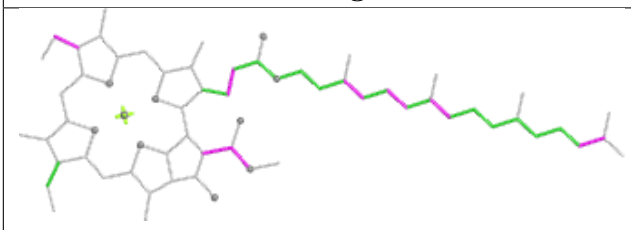
Ligand CLA C 508



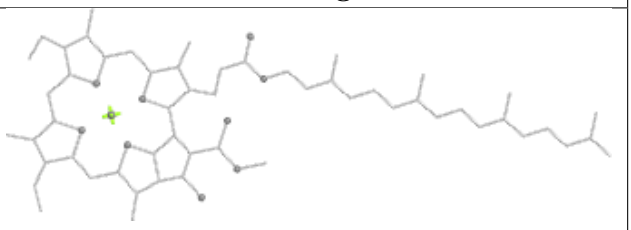
Bond lengths



Bond angles

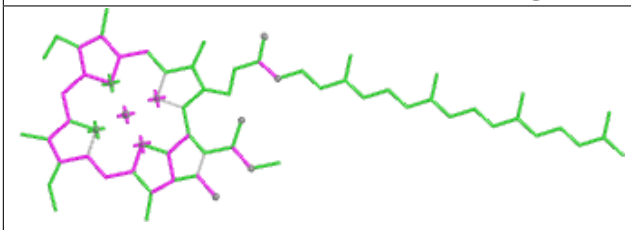


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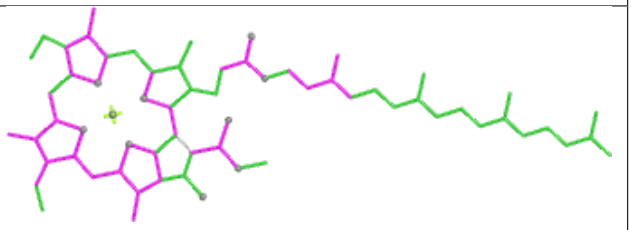


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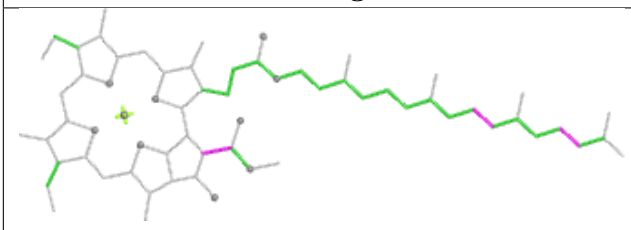
Ligand CLA b 609



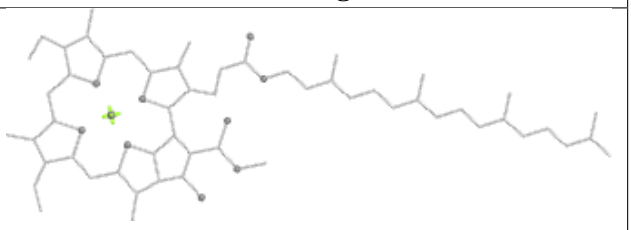
Bond lengths



Bond angles

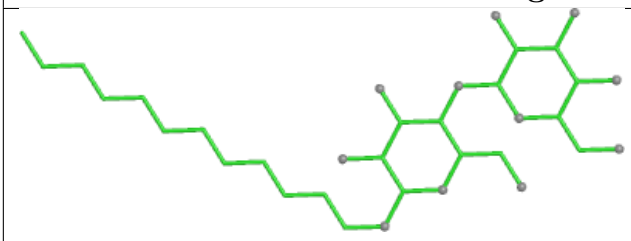


Torsions

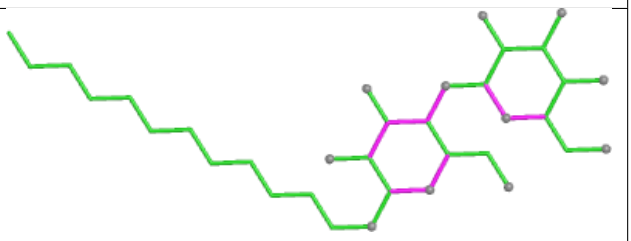


Rings

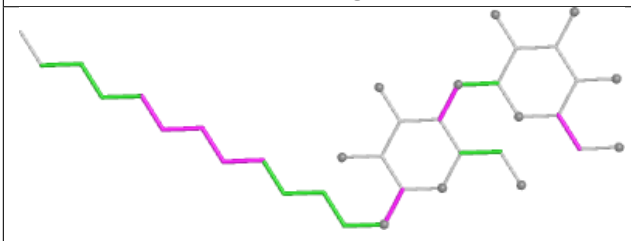
Ligand LMT I 102



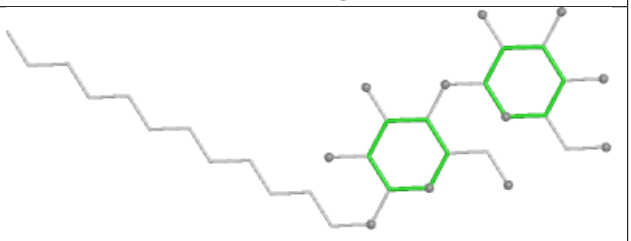
Bond lengths



Bond angles

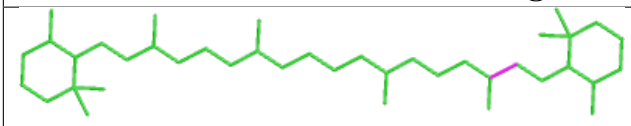


Torsions

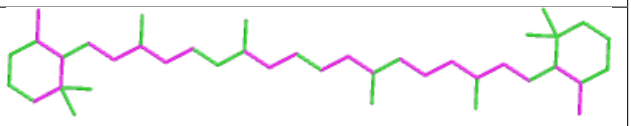


Rings

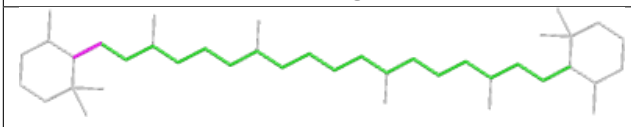
Ligand BCR c 526



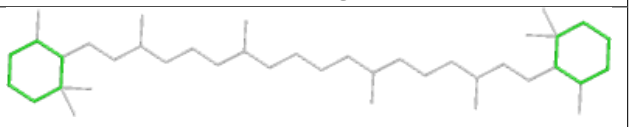
Bond lengths



Bond angles

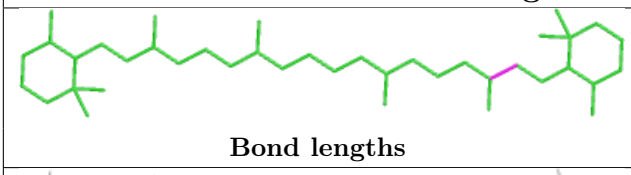


Torsions

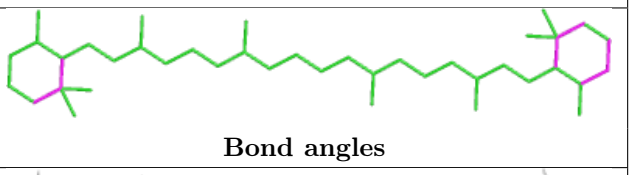


Rings

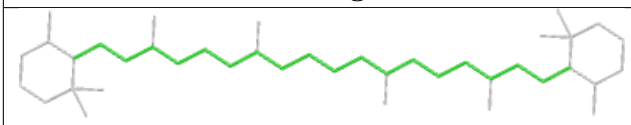
Ligand BCR B 619



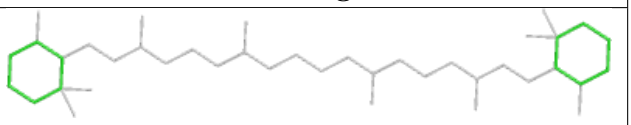
Bond lengths



Bond angles

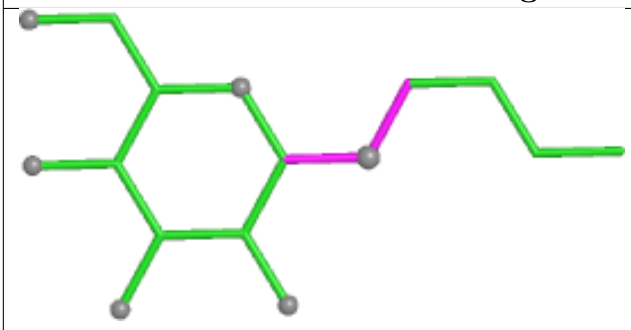


Torsions

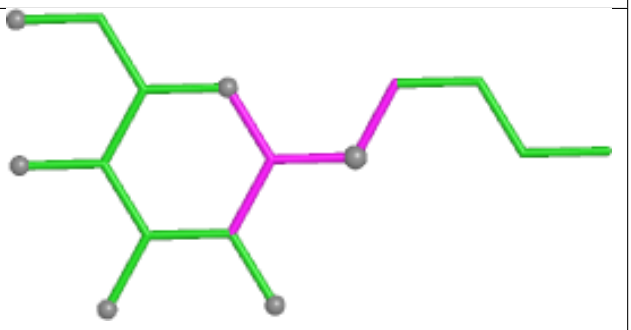


Rings

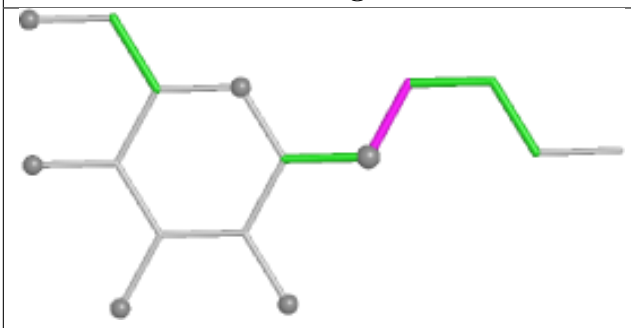
Ligand HTG D 411



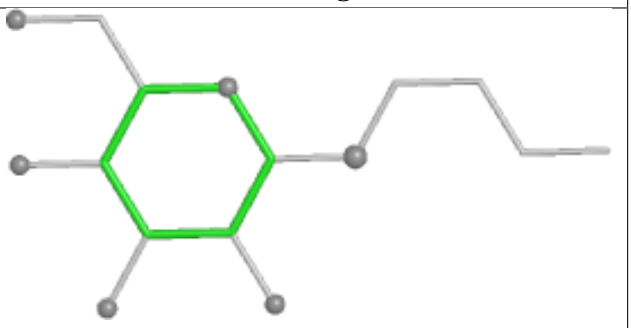
Bond lengths



Bond angles

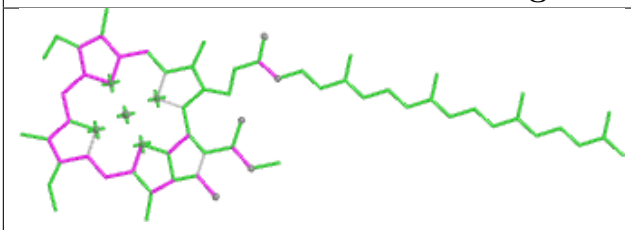


Torsions

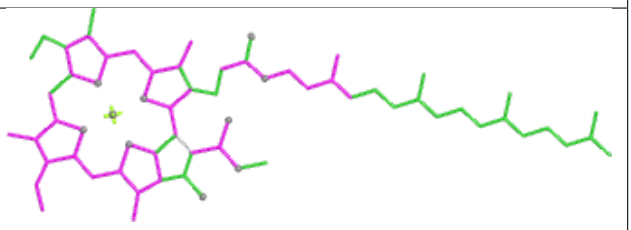


Rings

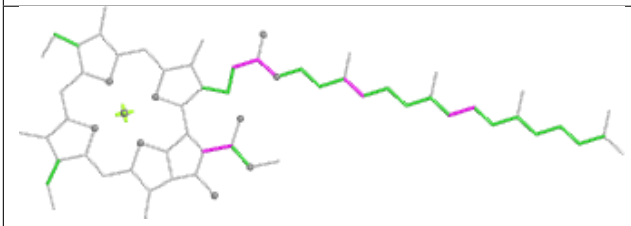
Ligand CLA c 512



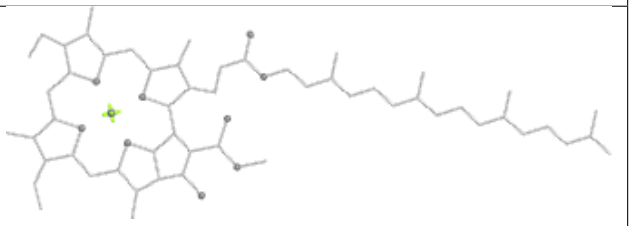
Bond lengths



Bond angles

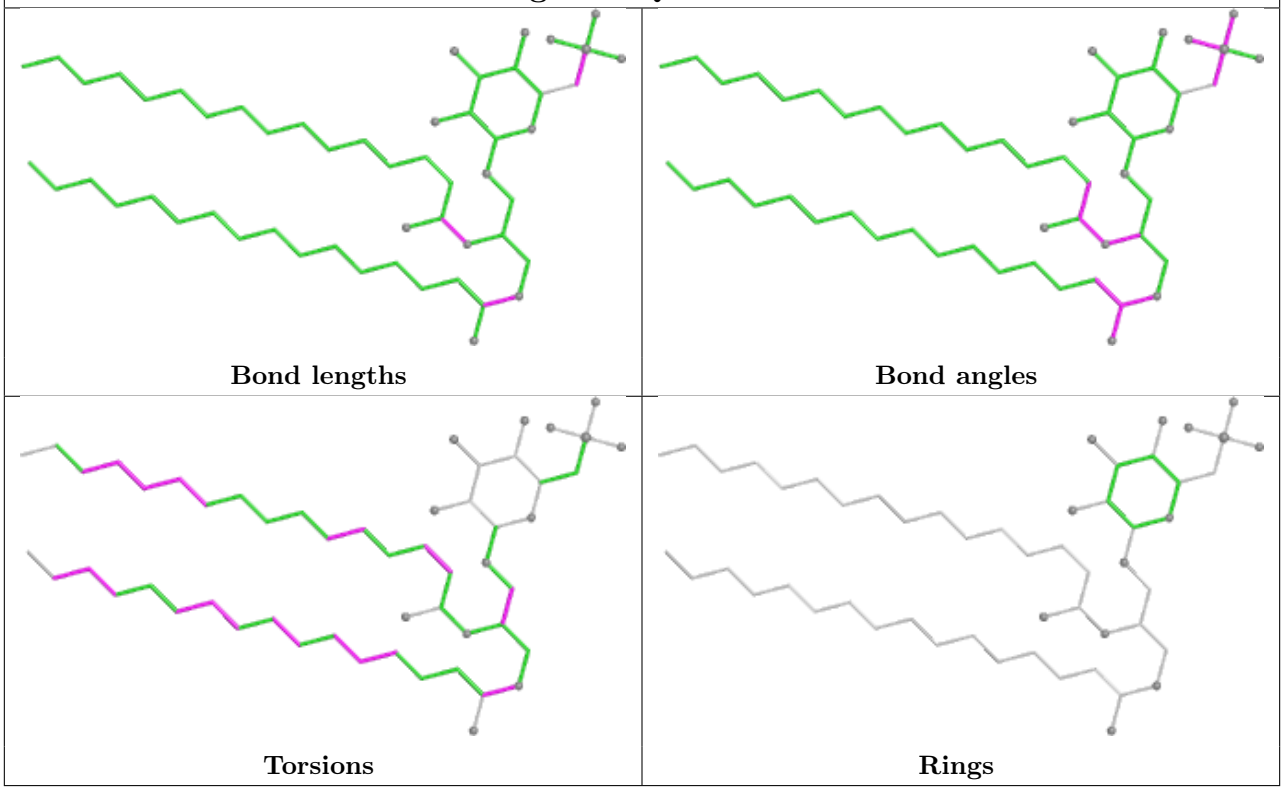


Torsions

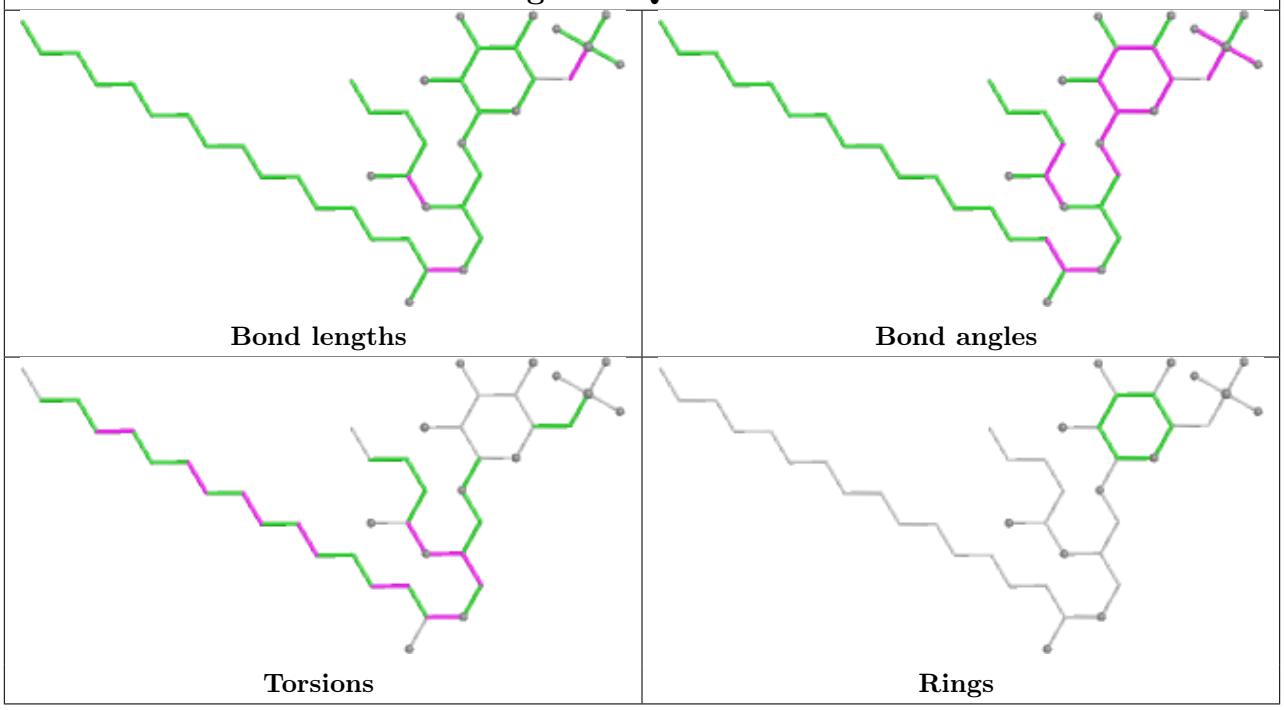


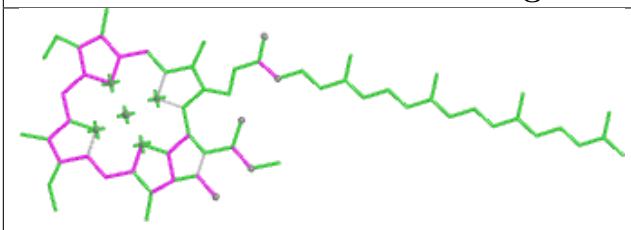
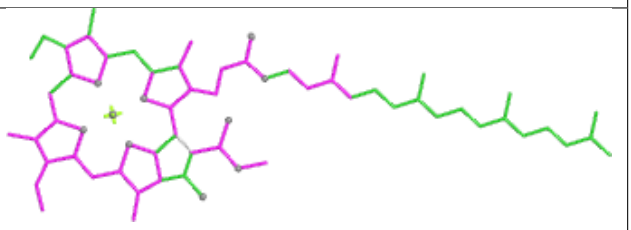
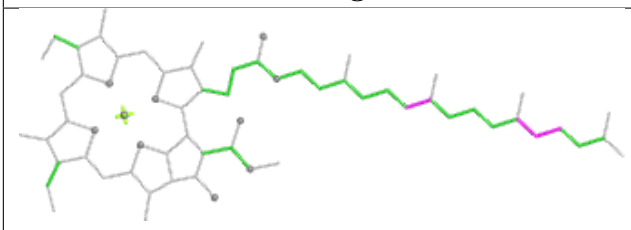
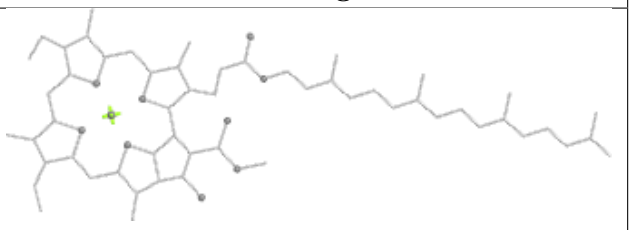
Rings

Ligand SQD a 402



Ligand SQD F 101



Ligand CLA A 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.11	5 (1%)	72	78	15, 23, 42, 79	3 (0%)
1	a	334/344 (97%)	-0.06	8 (2%)	59	66	17, 24, 48, 82	4 (1%)
2	B	504/505 (99%)	0.07	16 (3%)	50	56	13, 27, 51, 90	10 (1%)
2	b	504/505 (99%)	0.17	24 (4%)	35	41	17, 29, 60, 108	11 (2%)
3	C	451/455 (99%)	0.20	8 (1%)	67	75	19, 32, 49, 89	5 (1%)
3	c	455/455 (100%)	0.30	8 (1%)	67	75	18, 35, 50, 87	6 (1%)
4	D	342/342 (100%)	-0.15	3 (0%)	81	85	15, 24, 40, 114	0
4	d	341/342 (99%)	-0.12	4 (1%)	76	82	14, 26, 42, 90	1 (0%)
5	E	81/84 (96%)	0.92	9 (11%)	10	12	23, 40, 68, 97	2 (2%)
5	e	81/84 (96%)	0.97	9 (11%)	10	12	32, 45, 77, 97	0
6	F	34/44 (77%)	0.51	3 (8%)	15	18	26, 35, 56, 64	0
6	f	32/44 (72%)	0.69	3 (9%)	14	16	31, 37, 84, 99	0
7	H	65/65 (100%)	0.47	3 (4%)	37	43	20, 34, 52, 97	1 (1%)
7	h	65/65 (100%)	0.65	6 (9%)	14	16	28, 37, 58, 113	0
8	I	37/38 (97%)	0.85	6 (16%)	4	5	30, 34, 91, 101	0
8	i	37/38 (97%)	0.82	4 (10%)	11	12	29, 34, 79, 102	0
9	J	38/39 (97%)	0.78	7 (18%)	3	3	26, 38, 85, 109	0
9	j	38/39 (97%)	0.77	5 (13%)	7	8	30, 41, 84, 85	0
10	K	37/37 (100%)	0.52	3 (8%)	18	21	31, 38, 55, 64	0
10	k	37/37 (100%)	0.81	1 (2%)	56	62	33, 42, 56, 66	0
11	L	37/37 (100%)	0.02	3 (8%)	18	21	12, 20, 66, 91	1 (2%)
11	l	37/37 (100%)	0.06	3 (8%)	18	21	12, 21, 61, 91	1 (2%)
12	M	33/36 (91%)	0.00	2 (6%)	27	31	14, 23, 44, 100	1 (3%)
12	m	33/36 (91%)	0.01	1 (3%)	52	59	19, 23, 44, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.34	15 (6%) 26 31	16, 34, 65, 113	4 (1%)
13	o	243/244 (99%)	0.48	19 (7%) 19 22	17, 35, 75, 122	3 (1%)
14	T	29/31 (93%)	0.02	2 (6%) 23 26	17, 22, 48, 85	1 (3%)
14	t	29/31 (93%)	0.09	2 (6%) 23 26	17, 23, 49, 85	1 (3%)
15	U	97/104 (93%)	0.23	2 (2%) 63 70	22, 33, 53, 85	0
15	u	97/104 (93%)	0.13	1 (1%) 79 84	25, 34, 51, 85	0
16	V	137/137 (100%)	0.19	6 (4%) 39 45	17, 33, 54, 70	1 (0%)
16	v	137/137 (100%)	0.32	5 (3%) 46 53	26, 38, 57, 72	0
17	Y	29/30 (96%)	1.92	10 (34%) 1 0	38, 50, 91, 107	0
17	y	29/30 (96%)	1.80	9 (31%) 1 1	40, 54, 91, 107	0
18	X	39/40 (97%)	1.25	9 (23%) 2 2	31, 42, 80, 92	1 (2%)
18	x	39/40 (97%)	1.18	6 (15%) 5 5	35, 45, 93, 96	0
19	Z	62/62 (100%)	1.59	20 (32%) 1 0	40, 52, 87, 98	0
19	z	62/62 (100%)	1.72	21 (33%) 1 0	44, 53, 87, 98	0
20	R	34/34 (100%)	3.68	30 (88%) 0 0	69, 93, 111, 118	0
All	All	5293/5382 (98%)	0.28	301 (5%) 29 34	12, 31, 63, 122	57 (1%)

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	i	37	LEU	7.1
17	Y	18	VAL	7.0
20	R	18	TRP	6.5
2	b	486	LEU	6.2
7	h	65	LEU	6.2
8	I	38	GLU	5.8
20	R	10	LEU	5.7
19	Z	62	VAL	5.6
20	R	3	TRP	5.6
13	o	58	ASN	5.5
19	z	62	VAL	5.5
17	y	18	VAL	5.5
8	I	37	LEU	5.4
18	X	2	THR	5.3
2	b	491	VAL	5.3
17	Y	19	ILE	5.3
2	b	85	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
7	h	66	GLY	5.1
2	B	479	PHE	5.0
2	b	495	PHE	5.0
2	b	502	VAL	5.0
5	e	4	THR	5.0
12	m	34	LYS	5.0
7	H	65	LEU	5.0
13	O	58	ASN	4.9
18	x	2	THR	4.9
2	B	85	GLY	4.9
20	R	6	LEU	4.8
20	R	12	VAL	4.8
20	R	16	ALA	4.8
6	f	14	PRO	4.8
18	x	34	ILE	4.8
20	R	15	ALA	4.7
20	R	19	ALA	4.6
17	y	19	ILE	4.6
20	R	28	VAL	4.6
18	x	37	VAL	4.5
7	H	66	GLY	4.5
20	R	9	LEU	4.5
19	Z	7	LEU	4.5
6	f	16	PHE	4.4
17	Y	25	ILE	4.4
19	z	3	ILE	4.4
20	R	31	VAL	4.4
17	Y	22	LEU	4.3
19	z	5	PHE	4.3
5	e	5	THR	4.2
2	B	84	THR	4.2
14	t	30	THR	4.2
19	z	4	LEU	4.2
20	R	14	LEU	4.2
2	B	86[A]	ILE	4.1
1	a	11	ALA	4.1
20	R	34	LEU	4.1
2	B	494	GLY	4.1
2	b	493	TRP	4.1
20	R	5	VAL	4.1
3	C	23	ALA	4.1
20	R	11	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
20	R	20	VAL	4.0
18	x	38	GLN	4.0
1	A	230	THR	3.9
20	R	24	LEU	3.9
1	A	11	ALA	3.9
2	b	86	ILE	3.9
17	Y	21	GLN	3.9
6	f	15	ILE	3.9
20	R	25	PRO	3.9
6	F	16	PHE	3.9
20	R	13	LEU	3.8
2	B	495	PHE	3.8
2	b	499	VAL	3.8
2	b	487	SER	3.8
20	R	35	LEU	3.7
17	Y	20	ALA	3.7
2	b	490	GLN	3.7
20	R	27	ALA	3.7
18	X	3	ILE	3.7
19	Z	61	VAL	3.7
3	c	134	ILE	3.6
13	o	56	PRO	3.6
1	A	13	LEU	3.6
17	y	20	ALA	3.5
16	v	19	ILE	3.5
13	o	246	ALA	3.5
19	Z	60	PHE	3.5
7	h	64	ALA	3.5
2	B	489	GLU	3.5
9	J	4	GLY	3.5
14	T	30	THR	3.4
19	Z	2	THR	3.4
9	J	2	SER	3.4
3	C	262	ARG	3.4
19	Z	41	PHE	3.4
2	b	496	TYR	3.4
3	C	257	PHE	3.4
16	V	24	LYS	3.3
5	E	6	GLY	3.3
16	V	106	ASN	3.3
13	O	60	ARG	3.3
19	z	41	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
13	o	4	THR	3.3
12	M	33	GLN	3.3
5	e	6	GLY	3.3
9	J	5	GLY	3.3
17	y	25	ILE	3.3
19	Z	31	GLN	3.3
1	a	260	PHE	3.3
13	o	36	GLN	3.2
9	j	5	GLY	3.2
19	Z	36	SER	3.2
3	c	21	ILE	3.2
19	Z	10	ALA	3.2
13	O	57	LYS	3.2
18	X	31	ILE	3.2
4	D	238	THR	3.2
20	R	26	TYR	3.2
2	B	488	PRO	3.2
20	R	8	VAL	3.2
5	e	84	LYS	3.2
12	M	34	LYS	3.2
13	o	57	LYS	3.2
18	X	15[A]	LEU	3.2
9	j	4	GLY	3.2
5	E	61	ARG	3.1
13	o	59	LYS	3.1
6	F	15	ILE	3.1
10	k	12	PRO	3.1
19	Z	3	ILE	3.1
1	a	265	PHE	3.1
5	E	84	LYS	3.1
2	b	84	THR	3.1
13	o	61	GLN	3.1
2	b	484	PRO	3.1
13	O	56	PRO	3.1
2	b	488	PRO	3.0
8	I	33	LYS	3.0
8	i	35	LYS	3.0
2	B	499	VAL	3.0
5	E	4	THR	3.0
13	O	4	THR	3.0
2	b	500	GLY	3.0
9	J	3	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
17	y	22	LEU	2.9
2	B	490	GLN	2.9
13	o	23	ASP	2.9
19	Z	33	TRP	2.9
1	a	263	ALA	2.9
19	Z	42	LEU	2.9
13	o	206	GLY	2.9
13	o	194	LYS	2.9
1	a	248	ILE	2.9
19	Z	32	ASP	2.9
11	l	1	MET	2.9
19	z	61	VAL	2.9
3	c	19	ASN	2.9
2	b	293	ALA	2.9
18	X	19	VAL	2.8
4	D	11	GLU	2.8
19	z	33	TRP	2.8
2	b	494	GLY	2.8
16	v	17	LYS	2.8
17	Y	23	THR	2.8
11	L	2	GLU	2.8
20	R	7	VAL	2.8
4	D	12	ARG	2.8
20	R	30	GLN	2.8
19	Z	4	LEU	2.8
19	Z	39	LEU	2.8
16	V	19	ILE	2.8
13	o	62	GLU	2.7
4	d	237	PRO	2.7
7	H	64	ALA	2.7
2	b	126	PRO	2.7
1	a	264	SER	2.7
4	d	12	ARG	2.7
20	R	32	GLN	2.7
19	z	60	PHE	2.7
11	l	3	PRO	2.7
1	a	262	TYR	2.6
2	B	505	ARG	2.6
8	i	34	ARG	2.6
3	c	20	SER	2.6
20	R	29	LYS	2.6
8	I	36	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
13	O	207	ARG	2.6
19	z	31	GLN	2.6
1	A	235	TYR	2.6
3	C	134	ILE	2.6
20	R	23	ILE	2.6
5	e	61	ARG	2.6
19	z	2	THR	2.6
19	z	42	LEU	2.6
18	X	34	ILE	2.6
2	B	487	SER	2.6
16	v	106	ASN	2.6
2	b	497	GLN	2.5
2	b	413	ASP	2.5
13	O	89	SER	2.5
3	C	24	THR	2.5
19	Z	1	MET	2.5
20	R	22	ASN	2.5
13	o	25	THR	2.5
8	I	35	LYS	2.5
18	x	15	LEU	2.5
19	z	9	LEU	2.5
13	o	89	SER	2.5
15	U	8	GLU	2.5
13	o	63	ALA	2.5
13	o	33	ASP	2.5
13	O	61	GLN	2.4
16	v	110	LYS	2.4
17	y	23	THR	2.4
19	z	30	PRO	2.4
2	B	486	LEU	2.4
2	b	479	PHE	2.4
3	C	152	LYS	2.4
3	c	252	ILE	2.4
6	F	18	VAL	2.4
16	V	86	GLN	2.4
13	O	59	LYS	2.4
14	t	29	ILE	2.4
10	K	16	ALA	2.4
13	o	98	GLU	2.4
5	E	60	GLN	2.4
17	y	21	GLN	2.4
18	X	38	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
17	y	27	MET	2.4
17	Y	24	MET	2.3
10	K	24	VAL	2.3
5	e	20	TRP	2.3
15	u	8	GLU	2.3
5	E	79	PHE	2.3
9	J	23	ILE	2.3
18	x	40	SER	2.3
11	l	2	GLU	2.3
7	h	30	LEU	2.3
19	z	52	LEU	2.3
2	B	127	ARG	2.3
10	K	17	ILE	2.3
16	v	16	GLY	2.3
16	V	14	SER	2.3
3	C	143	TYR	2.2
5	e	81	GLU	2.2
8	I	6	ILE	2.2
13	O	36	GLN	2.2
9	J	6	ARG	2.2
13	o	60	ARG	2.2
19	z	7	LEU	2.2
16	V	16	GLY	2.2
3	c	143	TYR	2.2
9	J	7	ILE	2.2
17	Y	30	ILE	2.2
20	R	21	ARG	2.2
13	O	87	VAL	2.2
18	X	37	VAL	2.2
11	L	8	GLN	2.2
13	O	246	ALA	2.2
1	a	235	TYR	2.2
2	b	127	ARG	2.2
2	b	492	GLU	2.2
4	d	25	ASP	2.2
19	z	29	SER	2.2
7	h	57	GLY	2.2
3	c	77	PRO	2.2
5	E	29	ALA	2.2
19	Z	35	ARG	2.2
19	Z	27	TYR	2.1
9	j	7	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
19	Z	6	GLN	2.1
15	U	66	GLY	2.1
13	o	31	PRO	2.1
3	C	246	ALA	2.1
19	z	26	ALA	2.1
17	y	30	ILE	2.1
19	z	32	ASP	2.1
18	X	40	SER	2.1
1	A	253	GLY	2.1
2	b	82	GLY	2.1
5	e	17	VAL	2.1
9	j	6	ARG	2.1
5	E	73	LYS	2.1
13	O	67	PRO	2.1
13	O	93	LEU	2.1
19	z	39	LEU	2.1
8	i	36	ASP	2.1
2	B	373	LYS	2.0
5	e	79	PHE	2.0
14	T	29	ILE	2.0
19	Z	5	PHE	2.0
9	j	2	SER	2.0
3	c	183	GLY	2.0
13	O	28	GLY	2.0
4	d	136	VAL	2.0
19	z	46	LEU	2.0
11	L	1	MET	2.0
17	Y	34	MET	2.0
2	B	496	TYR	2.0
7	h	18	TYR	2.0
5	E	21	VAL	2.0
19	z	35	ARG	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	FME	j	1	10/11	0.76	0.23	53,71,94,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	t	1	10/11	0.92	0.10	13,22,33,65	0
12	FME	m	1	10/11	0.93	0.12	25,31,61,62	0
12	FME	M	1	10/11	0.94	0.11	23,34,56,61	0
14	FME	T	1	10/11	0.95	0.08	21,27,45,56	0
8	FME	i	1	10/11	0.96	0.09	23,34,37,42	0
8	FME	I	1	10/11	0.97	0.07	22,34,37,40	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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
36	DGD	D	407	62/66	0.65	0.23	44,89,114,119	0
28	GOL	B	635	6/6	0.66	0.28	82,91,97,98	0
36	DGD	d	407	62/66	0.68	0.21	41,88,117,122	0
29	UNL	k	101	32/-	0.69	0.22	42,75,105,108	0
30	LMT	E	102	35/35	0.71	0.18	43,81,105,107	0
30	LMT	f	102	35/35	0.71	0.18	56,83,109,113	0
30	LMT	b	626	25/35	0.74	0.19	33,67,110,115	0
29	UNL	j	103	10/-	0.74	0.23	44,61,67,73	0
28	GOL	O	302	6/6	0.74	0.16	52,61,64,70	0
29	UNL	i	101	40/-	0.74	0.23	36,64,96,108	0
28	GOL	v	203	6/6	0.75	0.20	50,69,71,78	0
29	UNL	I	101	40/-	0.75	0.23	27,63,114,119	0
35	HTG	d	411	16/19	0.75	0.18	54,73,84,87	0
29	UNL	k	102	10/-	0.75	0.37	54,83,94,102	0
28	GOL	T	103	6/6	0.75	0.22	63,76,80,81	0
37	LHG	e	101	42/49	0.75	0.18	49,87,117,128	0
35	HTG	B	624	19/19	0.76	0.15	38,95,102,121	0
35	HTG	B	631	19/19	0.76	0.16	25,84,104,120	0
35	HTG	V	204	19/19	0.76	0.19	40,65,99,175	0
35	HTG	b	628	19/19	0.76	0.17	48,90,106,124	0
35	HTG	c	523	19/19	0.76	0.16	60,84,93,98	0
28	GOL	t	102	6/6	0.76	0.22	29,60,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	LMT	M	101	35/35	0.76	0.16	35,60,79,85	0
29	UNL	a	414	30/-	0.76	0.18	45,65,86,89	0
28	GOL	v	204	6/6	0.76	0.19	47,64,70,92	0
30	LMT	a	417	35/35	0.77	0.17	52,76,90,94	0
27	SQD	a	402	54/54	0.77	0.16	34,61,79,100	0
35	HTG	D	411	16/19	0.77	0.17	38,100,111,113	0
29	UNL	b	634	33/-	0.77	0.22	42,71,112,116	0
34	LMG	Z	101	37/55	0.77	0.21	32,81,104,105	0
29	UNL	A	415	28/-	0.78	0.20	55,65,84,90	0
29	UNL	B	632	33/-	0.78	0.20	32,70,105,113	0
30	LMT	I	102	35/35	0.78	0.18	59,81,95,100	0
29	UNL	C	526	34/-	0.78	0.19	46,71,82,84	0
37	LHG	E	101	42/49	0.78	0.19	38,73,93,103	0
34	LMG	z	101	39/55	0.78	0.18	47,74,94,101	0
30	LMT	m	103	35/35	0.79	0.16	30,60,86,90	0
32	PL9	a	416	55/55	0.79	0.23	50,76,94,95	0
28	GOL	a	413	6/6	0.79	0.18	38,67,69,71	0
28	GOL	c	525	6/6	0.79	0.18	43,46,61,62	0
27	SQD	l	101	54/54	0.79	0.18	31,67,98,101	0
28	GOL	b	632	6/6	0.80	0.20	40,46,68,69	0
30	LMT	B	634	25/35	0.80	0.20	32,63,105,111	0
30	LMT	D	402	35/35	0.80	0.15	32,75,96,97	0
29	UNL	M	103	10/-	0.81	0.17	34,42,59,64	0
34	LMG	c	521	51/55	0.81	0.17	35,79,91,98	0
29	UNL	d	413	36/-	0.81	0.17	35,58,94,99	0
29	UNL	J	103	10/-	0.81	0.21	38,53,73,75	0
29	UNL	m	101	10/-	0.81	0.18	37,51,60,62	0
29	UNL	x	101	10/-	0.81	0.19	35,44,57,58	0
34	LMG	C	521	51/55	0.81	0.17	31,74,90,96	0
30	LMT	b	602	25/35	0.82	0.18	22,63,102,106	0
35	HTG	c	522	19/19	0.82	0.15	63,69,80,85	0
32	PL9	A	419	55/55	0.82	0.21	38,66,87,92	0
27	SQD	f	101	43/54	0.82	0.19	55,82,109,117	0
33	CA	b	605	1/1	0.82	0.14	95,95,95,95	0
35	HTG	C	523	19/19	0.82	0.16	46,75,97,109	0
29	UNL	D	413	40/-	0.82	0.20	33,55,105,108	0
30	LMT	m	102	35/35	0.82	0.14	16,51,73,79	0
28	GOL	C	524	6/6	0.83	0.16	39,45,57,60	0
27	SQD	F	101	43/54	0.83	0.18	39,70,96,105	0
27	SQD	A	416	54/54	0.83	0.15	28,52,75,76	0
35	HTG	b	604	19/19	0.83	0.16	50,80,106,112	0
28	GOL	A	414	6/6	0.83	0.19	40,60,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	SQD	b	601	54/54	0.83	0.16	36,58,91,95	0
30	LMT	a	401	35/35	0.84	0.15	28,61,79,86	0
28	GOL	V	205	6/6	0.84	0.15	37,54,59,72	0
28	GOL	A	413	6/6	0.84	0.14	35,38,41,42	0
30	LMT	A	417	33/35	0.84	0.16	27,65,78,85	0
28	GOL	B	627	6/6	0.84	0.16	31,35,43,44	0
34	LMG	C	520	51/55	0.84	0.18	26,61,82,87	0
35	HTG	b	627	19/19	0.86	0.17	27,44,80,80	0
33	CA	B	601	1/1	0.86	0.09	79,79,79,79	0
35	HTG	B	623	19/19	0.86	0.17	29,42,64,71	0
29	UNL	d	412	17/-	0.87	0.17	31,48,79,85	0
29	UNL	X	101	10/-	0.87	0.12	29,37,41,42	0
34	LMG	c	501	51/55	0.87	0.15	39,60,77,85	0
30	LMT	M	102	35/35	0.87	0.12	22,50,66,76	0
28	GOL	B	628	6/6	0.87	0.17	35,46,67,70	0
34	LMG	C	501	51/55	0.87	0.14	37,54,74,82	0
28	GOL	F	103	6/6	0.87	0.15	52,59,65,68	0
28	GOL	b	631	6/6	0.88	0.12	39,46,48,60	0
34	LMG	c	520	51/55	0.88	0.16	33,63,86,88	0
35	HTG	C	522	19/19	0.89	0.15	53,65,89,95	0
28	GOL	V	206	6/6	0.89	0.15	21,38,44,48	0
27	SQD	a	411	54/54	0.89	0.15	32,56,75,78	0
28	GOL	T	101	6/6	0.89	0.16	35,60,64,65	0
24	CLA	c	515	65/65	0.89	0.13	37,51,79,88	0
35	HTG	B	630	19/19	0.89	0.13	30,54,78,81	0
28	GOL	B	633	6/6	0.89	0.11	27,36,40,41	0
28	GOL	B	626	6/6	0.90	0.10	32,37,40,59	0
26	BCR	c	526	40/40	0.90	0.12	39,48,59,63	0
24	CLA	b	606	65/65	0.90	0.12	30,46,82,98	0
34	LMG	B	621	51/55	0.90	0.12	20,35,52,64	0
28	GOL	V	208	6/6	0.90	0.10	41,56,62,63	0
28	GOL	c	527	6/6	0.91	0.12	36,57,61,63	0
34	LMG	b	625	51/55	0.91	0.12	24,39,59,71	0
26	BCR	C	515	40/40	0.91	0.10	31,42,49,53	0
26	BCR	H	101	40/40	0.91	0.10	21,32,48,52	0
26	BCR	Y	101	40/40	0.91	0.10	28,35,49,50	0
24	CLA	C	507	65/65	0.91	0.12	28,42,81,88	0
26	BCR	h	101	40/40	0.91	0.10	27,35,46,49	0
28	GOL	b	630	6/6	0.91	0.12	37,48,50,52	0
27	SQD	A	411	54/54	0.91	0.14	26,51,71,78	0
24	CLA	c	514	65/65	0.91	0.11	34,43,67,76	0
28	GOL	b	633	6/6	0.91	0.13	32,54,63,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	C	514	65/65	0.91	0.11	32,42,69,72	0
26	BCR	D	405	40/40	0.92	0.10	22,31,61,77	0
28	GOL	B	629	6/6	0.92	0.14	24,40,61,78	0
26	BCR	k	103	40/40	0.92	0.10	32,40,48,52	0
24	CLA	B	602	65/65	0.92	0.11	24,39,82,104	0
28	GOL	b	629	6/6	0.92	0.10	32,40,48,57	0
35	HTG	b	603	19/19	0.92	0.11	34,44,64,67	0
26	BCR	T	102	40/40	0.92	0.08	14,28,36,42	0
29	UNL	D	412	17/-	0.92	0.12	24,45,74,78	0
24	CLA	b	621	65/65	0.92	0.12	21,35,82,84	0
28	GOL	B	625	6/6	0.92	0.12	28,43,48,55	0
24	CLA	c	508	65/65	0.92	0.12	30,41,65,70	0
34	LMG	j	101	51/55	0.92	0.12	26,39,70,82	0
26	BCR	d	405	40/40	0.92	0.11	29,35,63,64	0
36	DGD	H	102	62/66	0.92	0.10	20,29,42,58	0
28	GOL	V	201	6/6	0.92	0.10	27,29,40,41	0
36	DGD	h	102	62/66	0.92	0.10	23,35,52,69	0
37	LHG	D	408	49/49	0.92	0.10	16,31,43,54	0
32	PL9	d	406	55/55	0.92	0.09	16,23,35,47	0
37	LHG	d	408	49/49	0.92	0.11	26,34,46,50	0
28	GOL	f	104	6/6	0.92	0.10	45,51,59,61	0
24	CLA	b	620	65/65	0.93	0.09	22,31,51,74	0
28	GOL	V	207	6/6	0.93	0.14	35,38,41,44	0
24	CLA	C	508	65/65	0.93	0.09	25,35,48,57	0
28	GOL	a	412	6/6	0.93	0.11	22,37,41,45	0
28	GOL	A	412	6/6	0.93	0.08	29,31,34,37	0
24	CLA	c	505	65/65	0.93	0.09	29,35,46,60	0
26	BCR	a	410	40/40	0.93	0.07	16,24,31,33	0
32	PL9	D	406	55/55	0.93	0.08	14,23,36,43	0
26	BCR	b	624	40/40	0.93	0.09	20,32,46,52	0
26	BCR	c	516	40/40	0.93	0.09	29,36,47,57	0
24	CLA	c	506	65/65	0.93	0.09	26,33,51,61	0
24	CLA	c	507	65/65	0.93	0.09	22,31,52,62	0
24	CLA	C	509	65/65	0.93	0.10	21,29,78,80	0
24	CLA	C	512	65/65	0.93	0.09	26,32,41,48	0
26	BCR	t	101	40/40	0.93	0.09	15,24,45,49	0
36	DGD	C	518	62/66	0.93	0.11	22,32,76,92	0
28	GOL	v	201	6/6	0.93	0.10	31,40,49,50	0
26	BCR	y	101	40/40	0.93	0.09	31,40,53,60	0
36	DGD	c	518	62/66	0.93	0.11	24,35,79,94	0
24	CLA	C	513	65/65	0.93	0.10	29,42,67,74	0
25	PHO	d	403	64/64	0.93	0.07	20,25,34,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	B	620	40/40	0.93	0.08	22,29,42,47	0
24	CLA	C	502	65/65	0.93	0.09	25,32,47,58	0
26	BCR	C	516	40/40	0.93	0.09	25,34,43,46	0
37	LHG	d	410	49/49	0.93	0.14	23,35,85,104	0
22	CL	u	201	1/1	0.93	0.07	63,63,63,63	0
37	LHG	l	102	49/49	0.93	0.10	19,30,48,57	0
26	BCR	B	619	40/40	0.94	0.08	17,25,44,46	0
24	CLA	b	612	65/65	0.94	0.07	14,23,30,36	0
24	CLA	b	613	65/65	0.94	0.07	22,29,38,42	0
24	CLA	b	614	65/65	0.94	0.08	24,31,41,50	0
24	CLA	b	619	65/65	0.94	0.10	15,25,72,77	0
24	CLA	B	604	65/65	0.94	0.08	18,25,32,40	0
26	BCR	K	101	40/40	0.94	0.09	27,33,42,47	0
24	CLA	B	607	65/65	0.94	0.09	18,26,51,75	0
24	CLA	c	503	65/65	0.94	0.09	29,34,45,54	0
24	CLA	B	612	65/65	0.94	0.08	15,21,37,41	0
26	BCR	b	622	40/40	0.94	0.07	16,26,33,36	0
33	CA	f	103	1/1	0.94	0.07	72,72,72,72	0
24	CLA	B	615	65/65	0.94	0.10	15,24,67,78	0
23	BCT	a	418	4/4	0.94	0.10	30,33,42,44	0
36	DGD	C	517	62/66	0.94	0.10	22,33,75,83	0
24	CLA	C	504	65/65	0.94	0.08	24,33,42,48	0
24	CLA	c	509	65/65	0.94	0.09	27,34,49,58	0
34	LMG	J	101	51/55	0.94	0.12	20,37,78,86	0
36	DGD	c	517	62/66	0.94	0.10	23,32,68,76	0
24	CLA	c	512	65/65	0.94	0.08	26,32,44,59	0
36	DGD	c	519	62/66	0.94	0.09	26,34,65,72	0
24	CLA	c	513	65/65	0.94	0.09	30,39,50,54	0
28	GOL	v	205	6/6	0.94	0.11	25,39,52,58	0
24	CLA	C	505	65/65	0.94	0.09	22,29,59,77	0
37	LHG	D	410	49/49	0.94	0.14	20,33,91,95	0
24	CLA	b	607	65/65	0.94	0.08	23,30,38,41	0
24	CLA	b	611	65/65	0.94	0.09	19,31,58,74	0
26	BCR	A	410	40/40	0.94	0.08	16,26,33,35	0
35	HTG	B	622	19/19	0.94	0.10	26,30,44,56	0
26	BCR	B	618	40/40	0.94	0.07	15,23,33,41	0
24	CLA	b	616	65/65	0.95	0.07	18,26,38,52	0
24	CLA	b	617	65/65	0.95	0.07	18,26,36,50	0
24	CLA	A	405	65/65	0.95	0.07	15,18,26,50	0
24	CLA	B	608	65/65	0.95	0.07	13,20,31,35	0
24	CLA	B	609	65/65	0.95	0.06	17,22,32,36	0
24	CLA	B	610	65/65	0.95	0.07	19,26,36,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	HTG	O	303	19/19	0.95	0.09	24,32,47,48	0
24	CLA	c	504	65/65	0.95	0.09	26,32,45,55	0
24	CLA	C	510	65/65	0.95	0.09	25,32,51,57	0
28	GOL	C	525	6/6	0.95	0.08	20,24,26,27	0
26	BCR	b	623	40/40	0.95	0.07	15,27,40,46	0
24	CLA	C	511	65/65	0.95	0.08	23,29,41,62	0
24	CLA	B	611	65/65	0.95	0.07	19,26,36,39	0
23	BCT	A	404	4/4	0.95	0.07	27,30,39,40	0
33	CA	F	102	1/1	0.95	0.07	72,72,72,72	0
24	CLA	B	613	65/65	0.95	0.07	15,23,32,35	0
24	CLA	c	510	65/65	0.95	0.09	24,31,70,87	0
36	DGD	C	519	62/66	0.95	0.09	20,30,58,63	0
24	CLA	c	511	65/65	0.95	0.08	29,36,49,55	0
24	CLA	a	409	65/65	0.95	0.12	20,27,83,88	0
24	CLA	B	603	65/65	0.95	0.07	18,25,32,38	0
24	CLA	B	616	65/65	0.95	0.09	19,28,48,60	0
24	CLA	b	608	65/65	0.95	0.07	22,29,38,42	0
24	CLA	d	402	65/65	0.95	0.07	18,22,38,46	0
24	CLA	d	404	65/65	0.95	0.10	27,34,74,81	0
25	PHO	A	407	64/64	0.95	0.06	15,18,23,28	0
24	CLA	b	610	65/65	0.95	0.07	18,24,37,42	0
24	CLA	B	617	65/65	0.95	0.11	19,28,88,91	0
22	CL	V	202	1/1	0.95	0.07	63,63,63,63	0
37	LHG	d	409	49/49	0.95	0.08	17,26,39,55	0
24	CLA	C	503	65/65	0.95	0.07	22,28,40,51	0
24	CLA	B	606	65/65	0.95	0.07	16,22,34,38	0
24	CLA	b	615	65/65	0.95	0.08	21,28,39,46	0
38	HEM	e	102	43/43	0.95	0.11	38,48,65,84	0
24	CLA	C	506	65/65	0.96	0.08	21,29,45,53	0
25	PHO	A	408	64/64	0.96	0.06	16,22,30,32	0
25	PHO	a	408	64/64	0.96	0.06	16,21,29,37	0
24	CLA	b	618	65/65	0.96	0.07	15,23,48,56	0
24	CLA	b	609	65/65	0.96	0.08	16,25,56,66	0
24	CLA	D	401	65/65	0.96	0.07	13,18,30,32	0
37	LHG	D	409	49/49	0.96	0.08	17,27,48,60	0
24	CLA	D	403	65/65	0.96	0.06	14,19,36,42	0
33	CA	o	301	1/1	0.96	0.05	62,62,62,62	0
37	LHG	L	101	49/49	0.96	0.08	15,29,47,58	0
24	CLA	D	404	65/65	0.96	0.09	21,28,73,84	0
24	CLA	a	407	65/65	0.96	0.09	19,25,72,79	0
24	CLA	B	605	65/65	0.96	0.08	15,22,51,63	0
24	CLA	d	401	65/65	0.96	0.06	16,19,26,42	0

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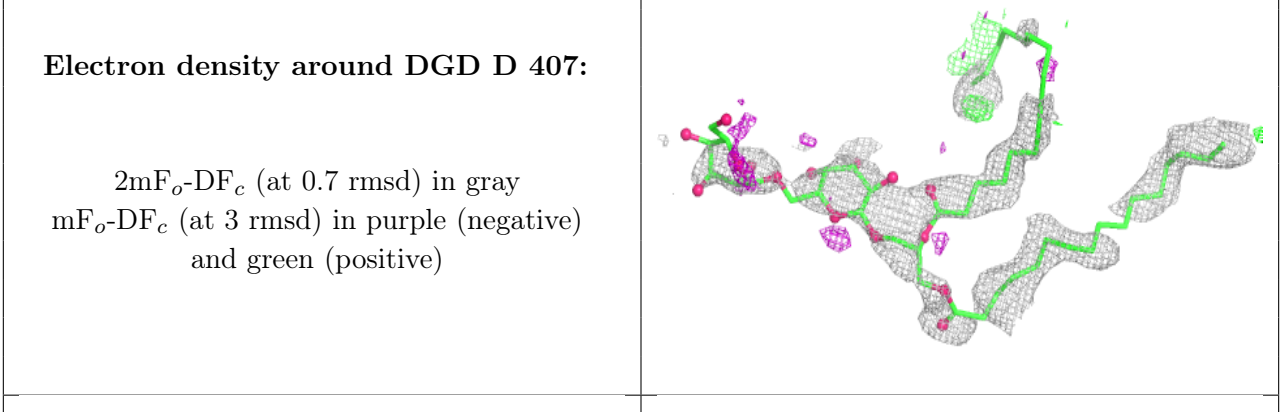
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	614	65/65	0.96	0.07	14,22,45,52	0
24	CLA	A	409	65/65	0.96	0.10	18,27,83,92	0
24	CLA	a	406	65/65	0.97	0.06	17,20,35,51	0
28	GOL	c	524	6/6	0.97	0.06	25,28,30,34	0
38	HEM	E	103	43/43	0.97	0.08	27,38,50,56	0
24	CLA	A	406	65/65	0.97	0.08	15,19,84,88	0
39	MG	j	102	1/1	0.97	0.12	34,34,34,34	0
39	MG	J	102	1/1	0.98	0.07	28,28,28,28	0
33	CA	O	301	1/1	0.98	0.04	56,56,56,56	0
40	HEC	V	203	43/43	0.98	0.06	23,26,31,36	0
40	HEC	v	202	43/43	0.98	0.07	29,33,40,48	0
21	FE2	a	403	1/1	0.99	0.06	30,30,30,30	0
22	CL	A	402	1/1	0.99	0.03	19,19,19,19	0
22	CL	A	403	1/1	0.99	0.05	23,23,23,23	0
31	OEX	A	418	10/10	0.99	0.04	16,23,28,32	0
31	OEX	a	415	10/10	0.99	0.04	20,24,35,37	0
33	CA	c	502	1/1	0.99	0.03	44,44,44,44	0
21	FE2	A	401	1/1	0.99	0.03	27,27,27,27	0
22	CL	a	404	1/1	0.99	0.05	20,20,20,20	0
22	CL	a	405	1/1	0.99	0.04	26,26,26,26	0

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

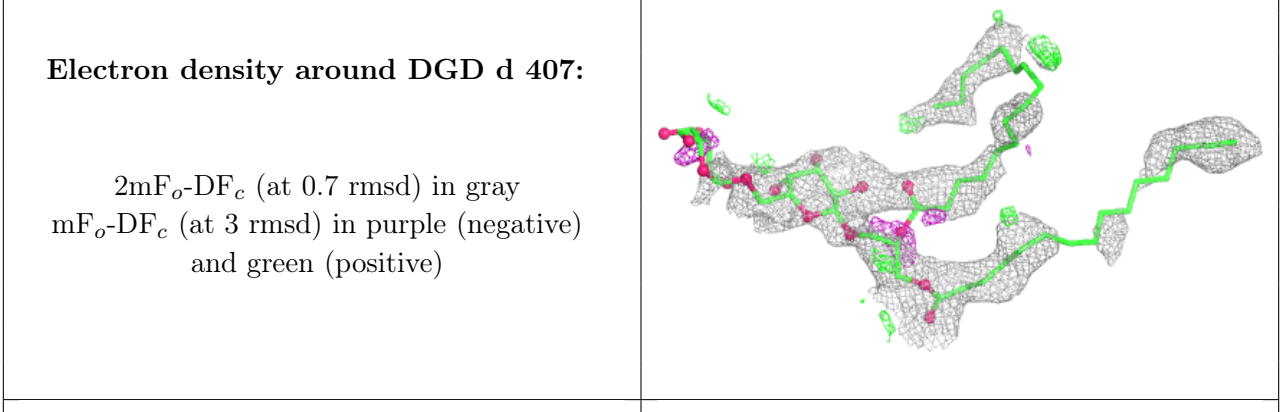
Electron density around DGD D 407:

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



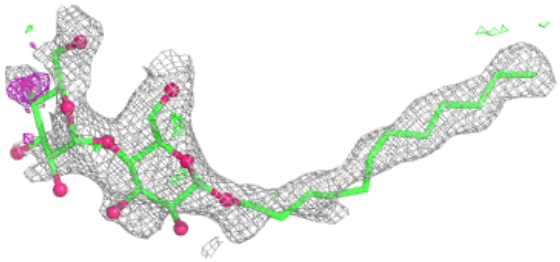
Electron density around DGD d 407:

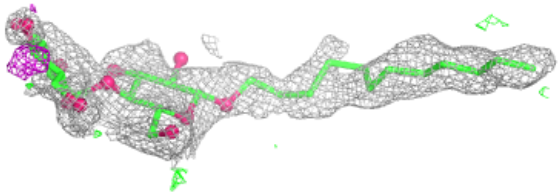
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

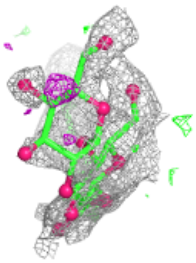


Electron density around LMT E 102:

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

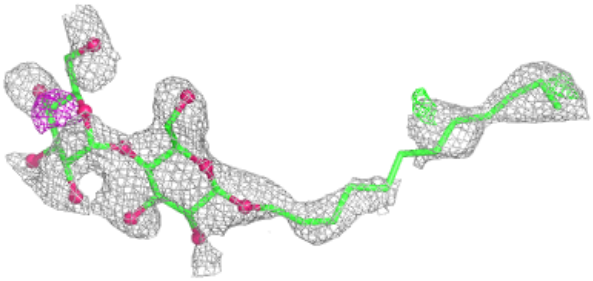


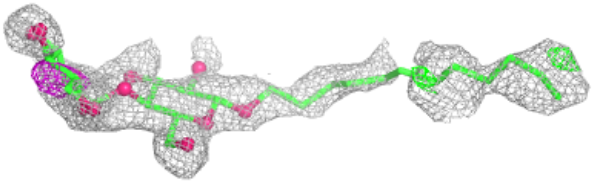


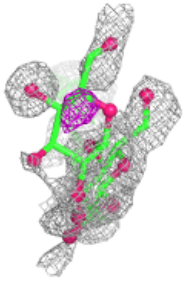


Electron density around LMT f 102:

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

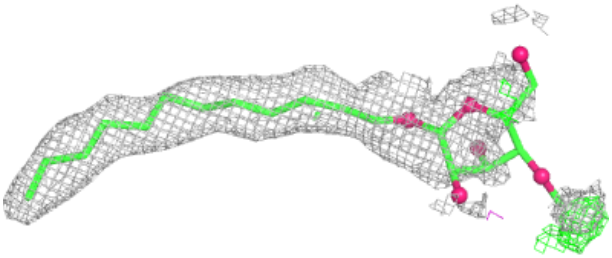


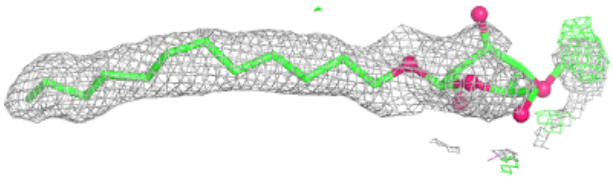


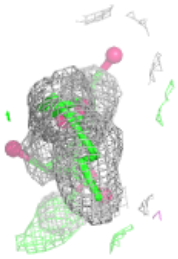


Electron density around LMT b 626:

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



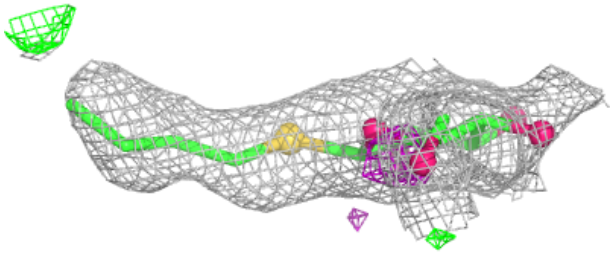


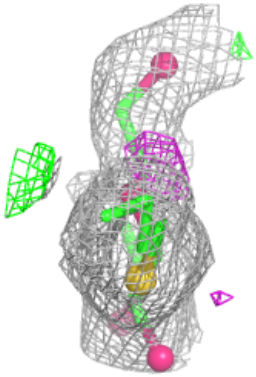


Electron density around HTG d 411:

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

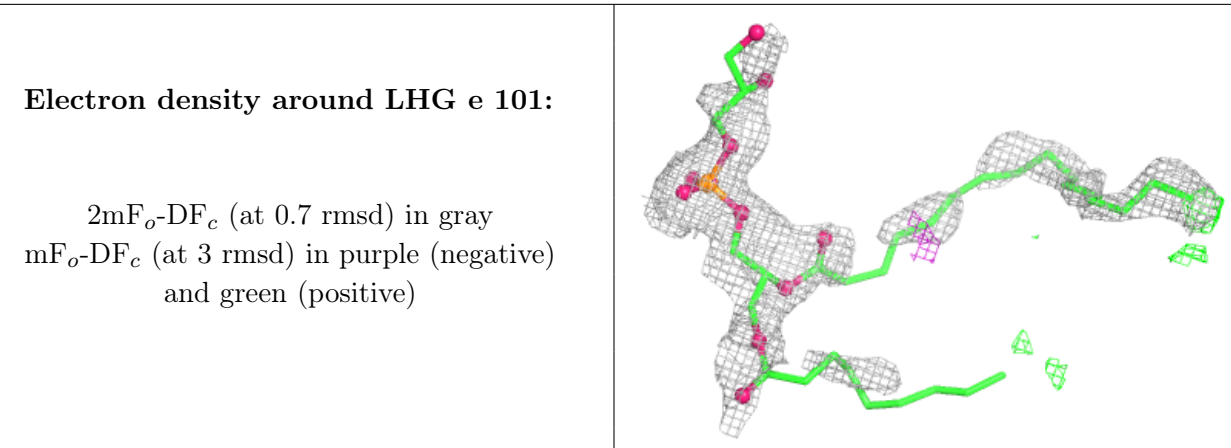






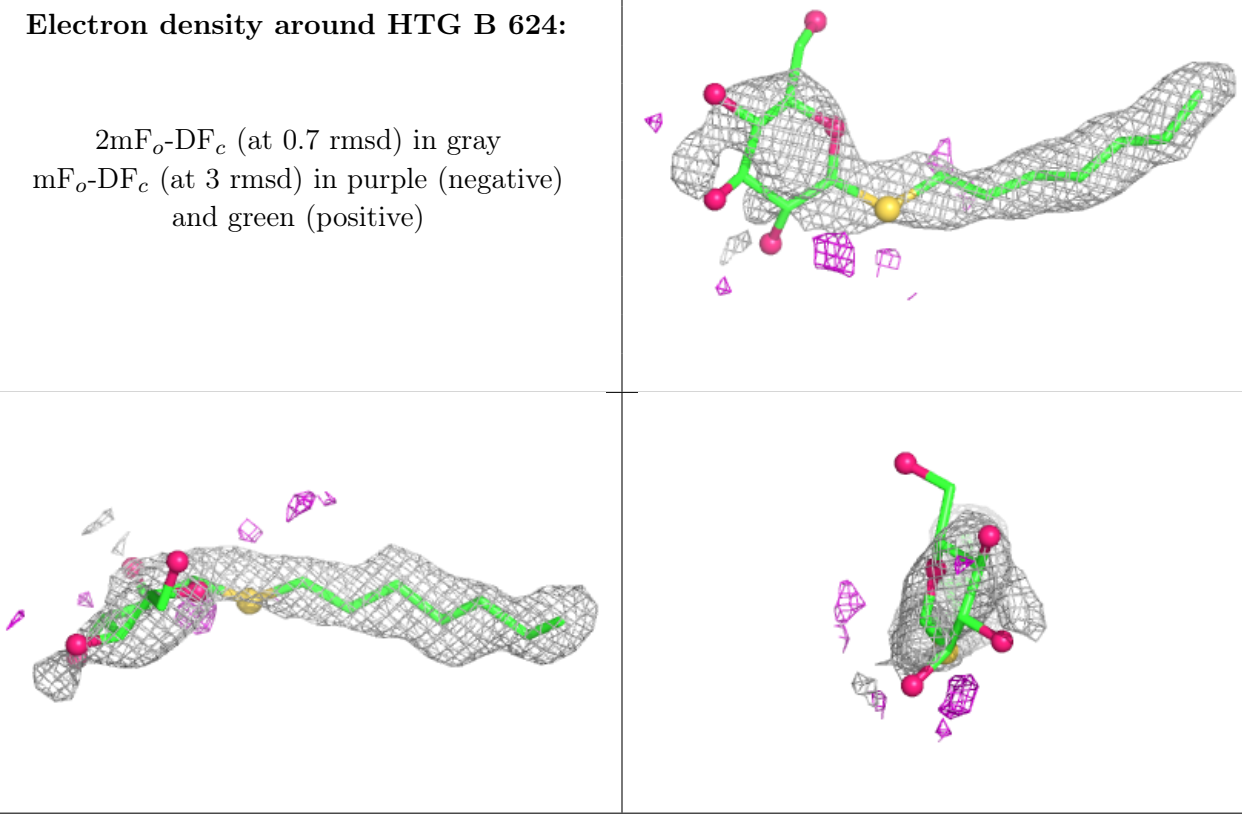
Electron density around LHG e 101:

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



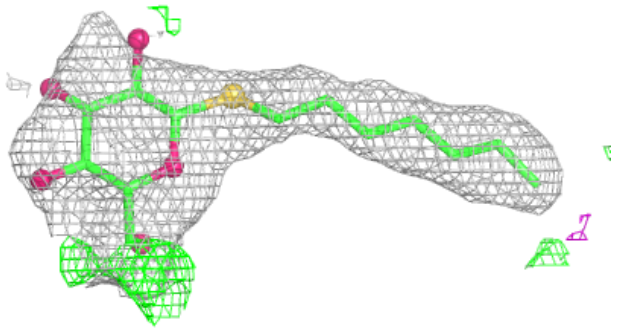
Electron density around HTG B 624:

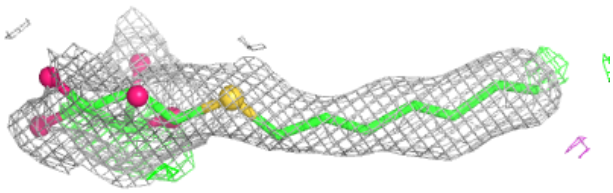
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

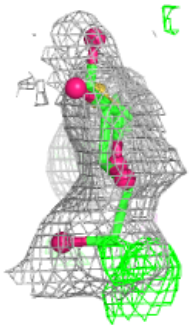


Electron density around HTG B 631:

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

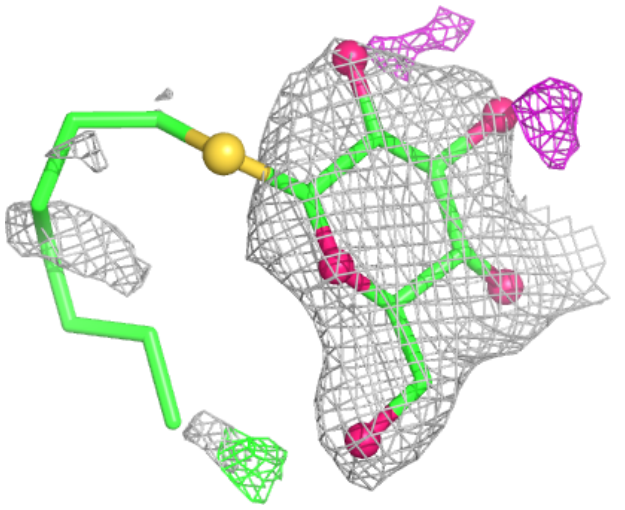


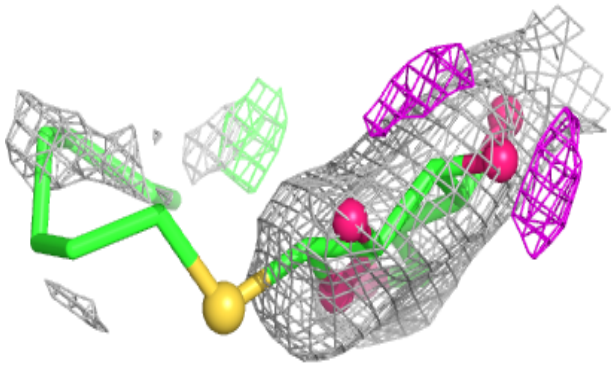


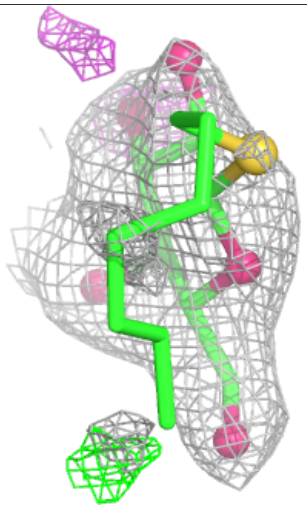


Electron density around HTG V 204:

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

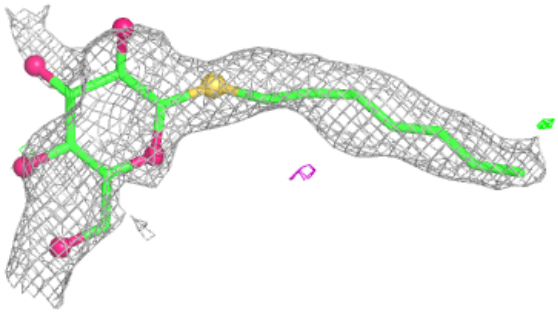


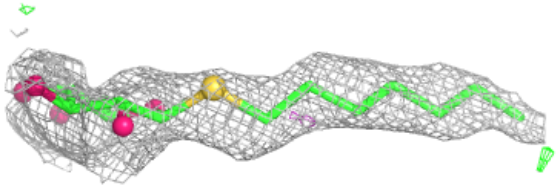


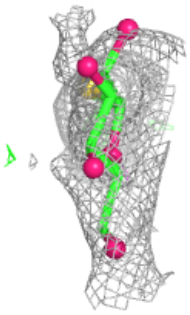


Electron density around HTG b 628:

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

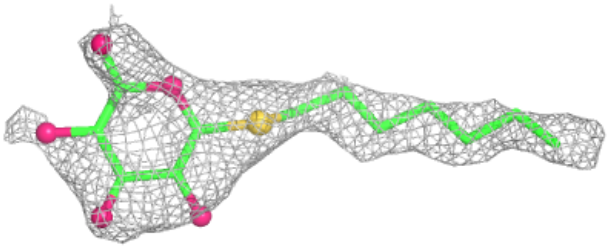


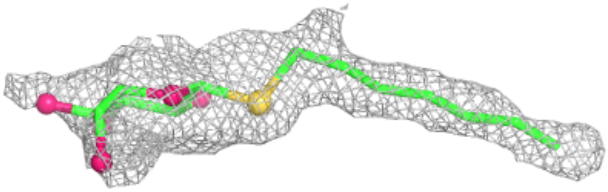


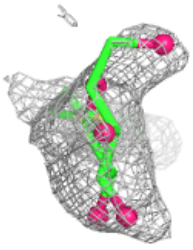


Electron density around HTG c 523:

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

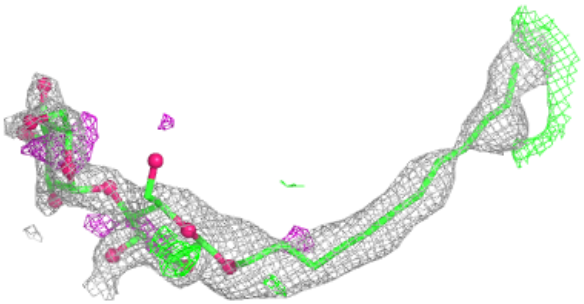


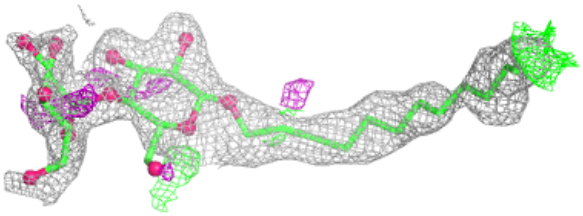


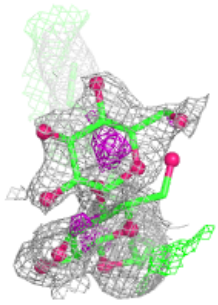


Electron density around LMT M 101:

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

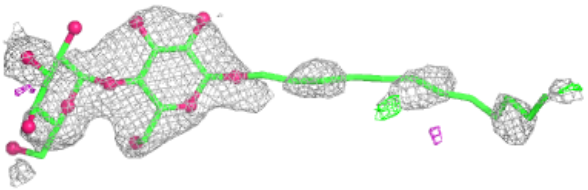


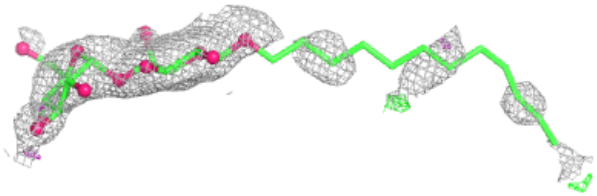


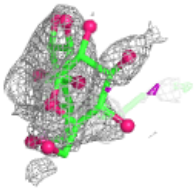


Electron density around LMT a 417:

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

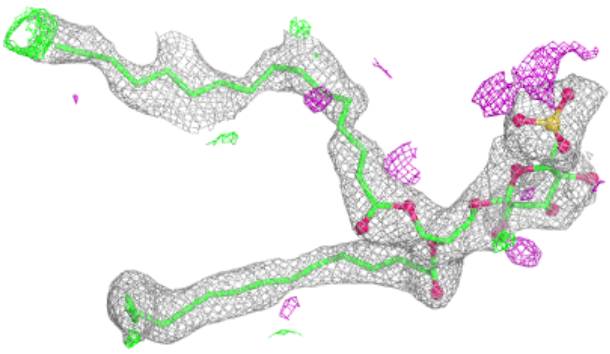


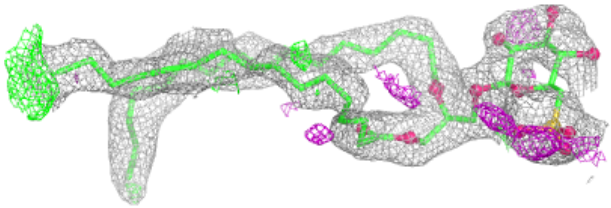




Electron density around SQD a 402:

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

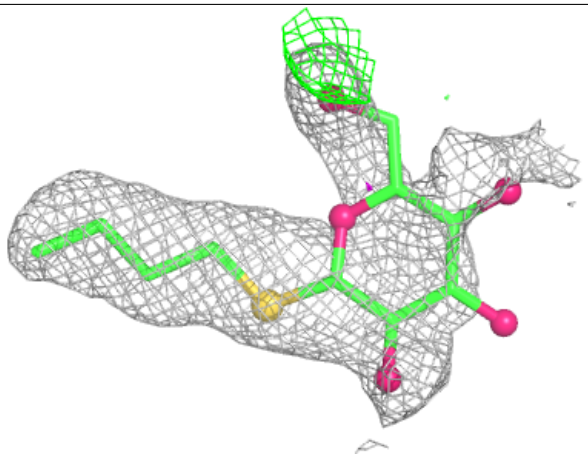


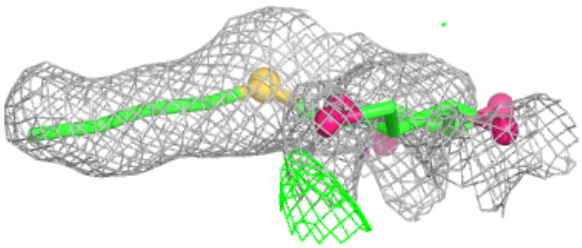


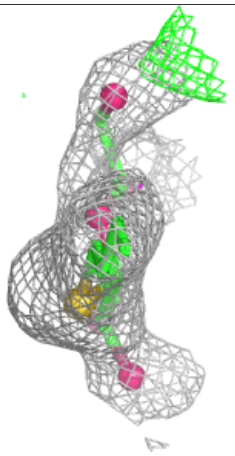


Electron density around HTG D 411:

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

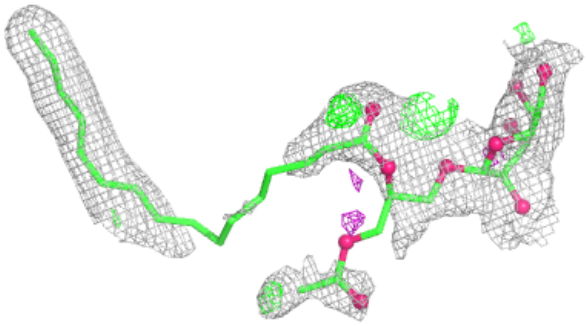


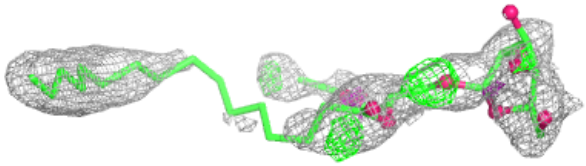


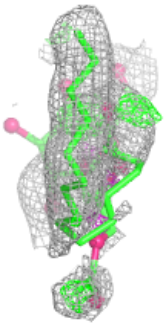


Electron density around LMG Z 101:

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

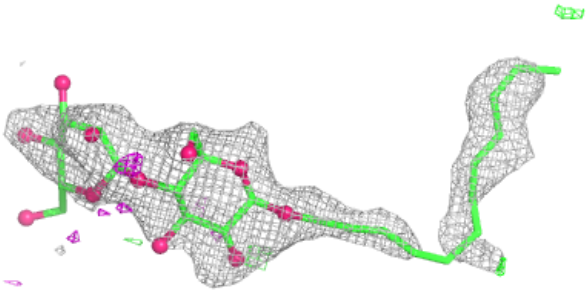


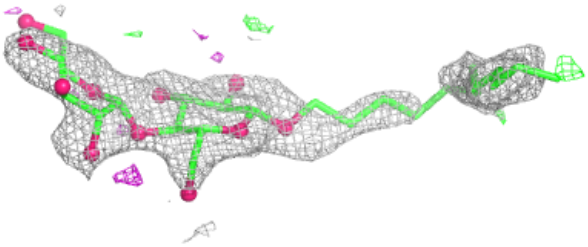


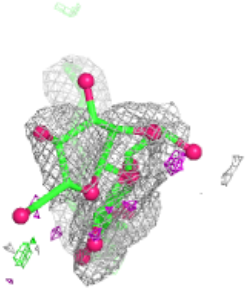


Electron density around LMT I 102:

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

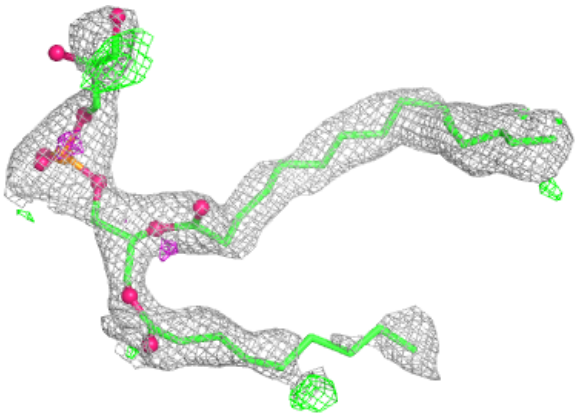


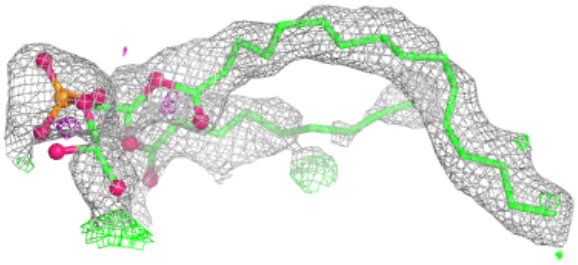




Electron density around LHG E 101:

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

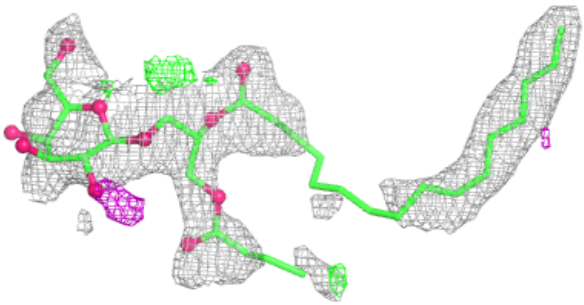


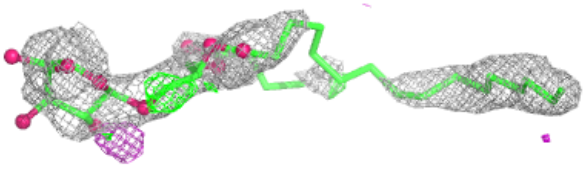


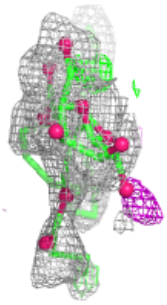


Electron density around LMG z 101:

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

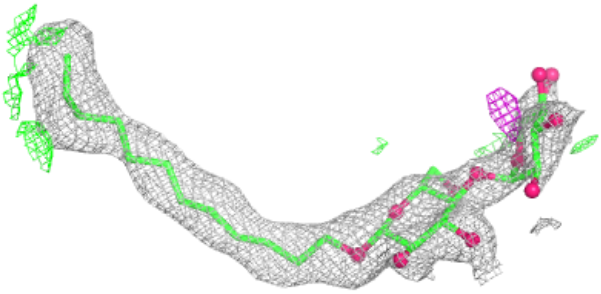


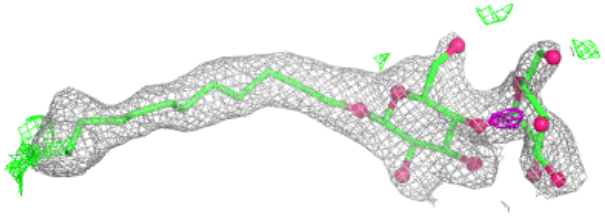


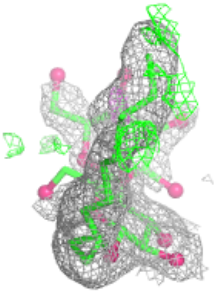


Electron density around LMT m 103:

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

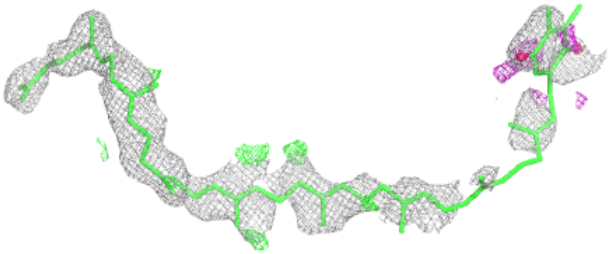


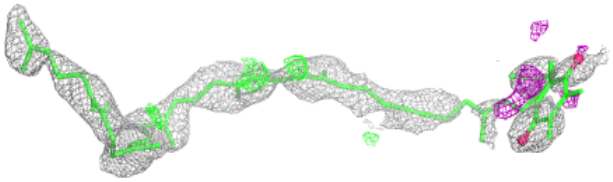


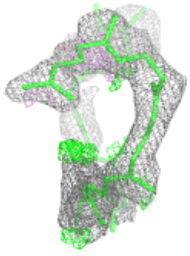


Electron density around PL9 a 416:

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

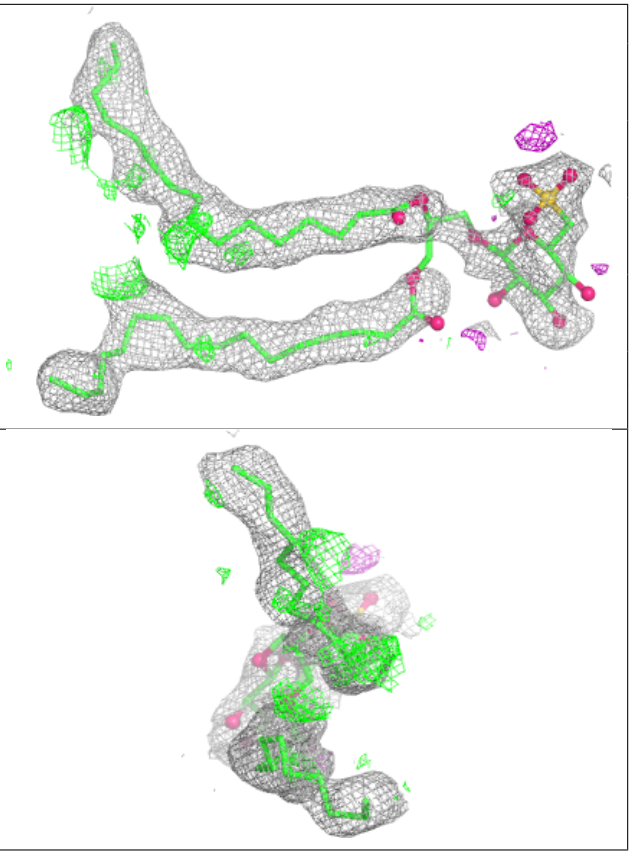






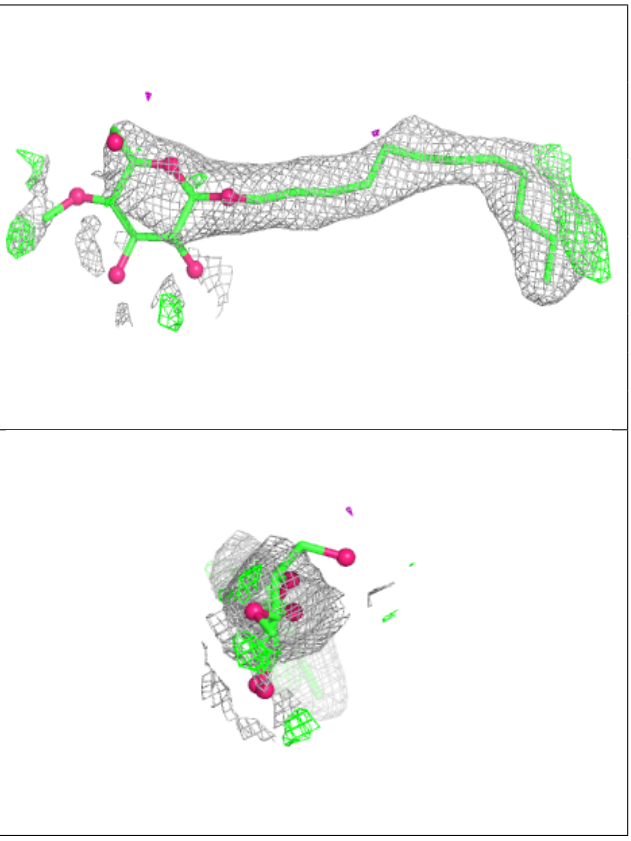
Electron density around SQD l 101:

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



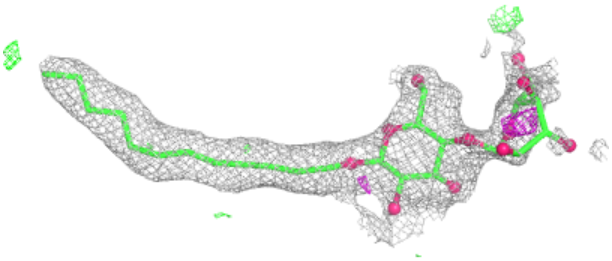
Electron density around LMT B 634:

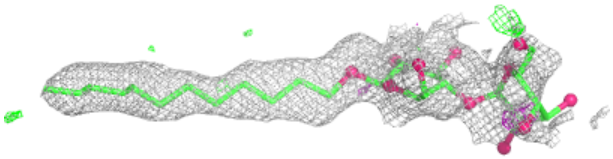
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

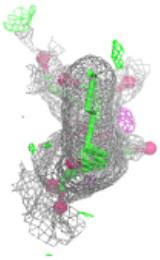


Electron density around LMT D 402:

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

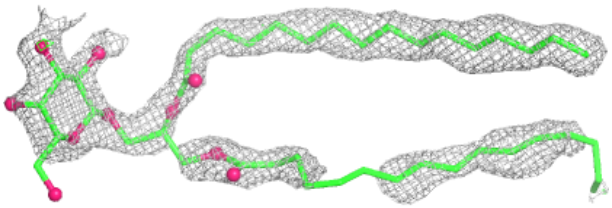


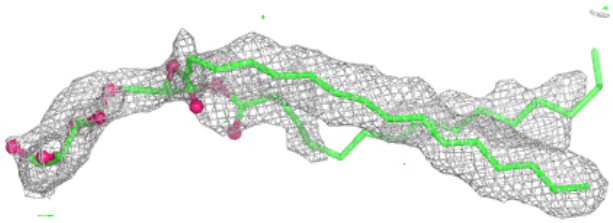


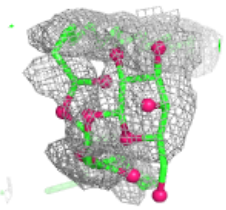


Electron density around LMG c 521:

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

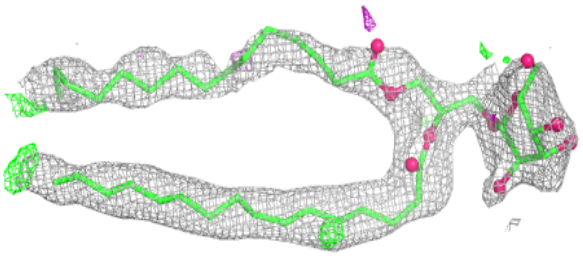


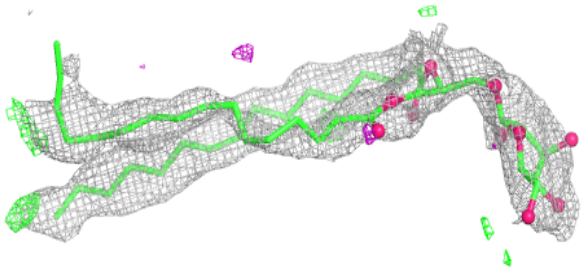


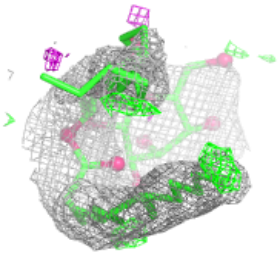


Electron density around LMG C 521:

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

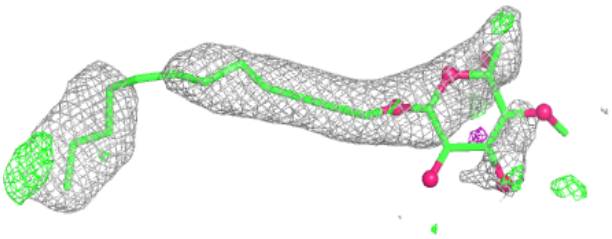


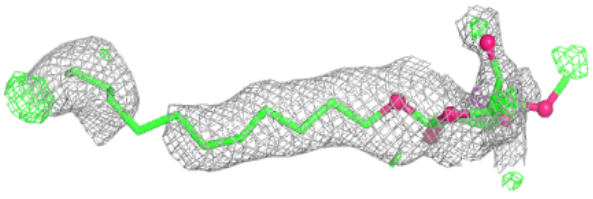


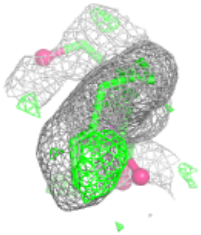


Electron density around LMT b 602:

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

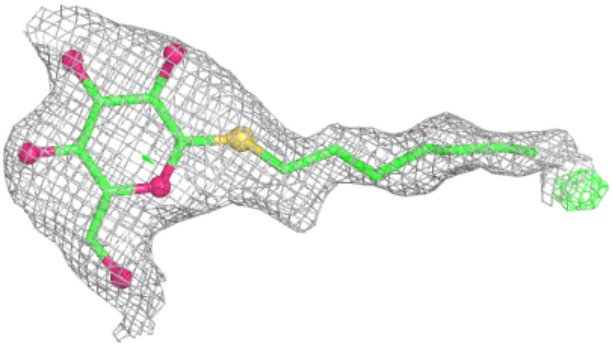


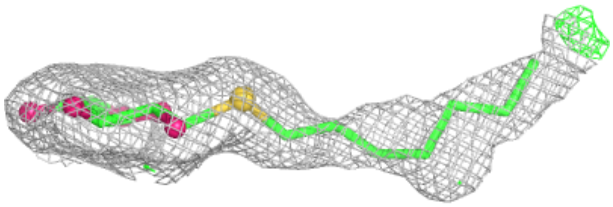


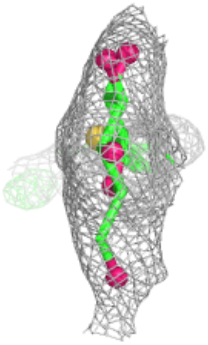


Electron density around HTG c 522:

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

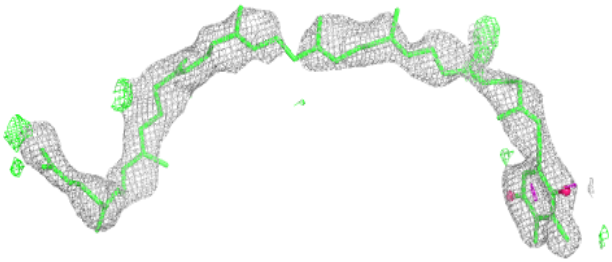


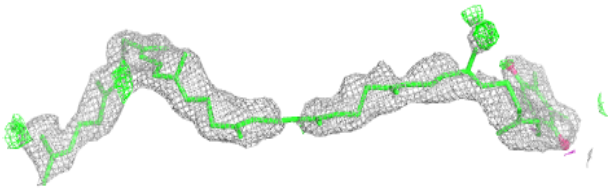


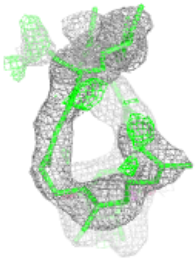


Electron density around PL9 A 419:

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

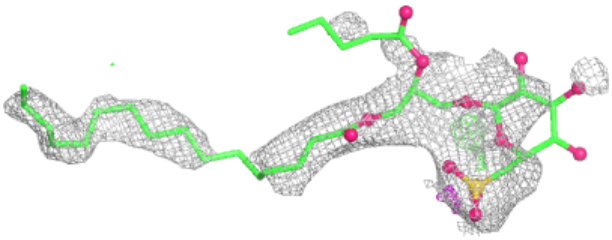


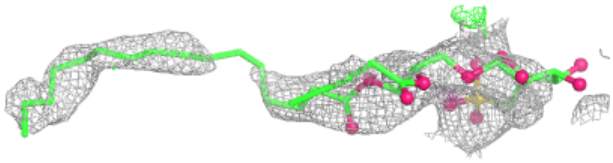


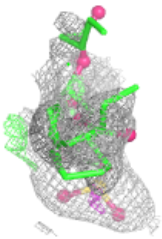


Electron density around SQD f 101:

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

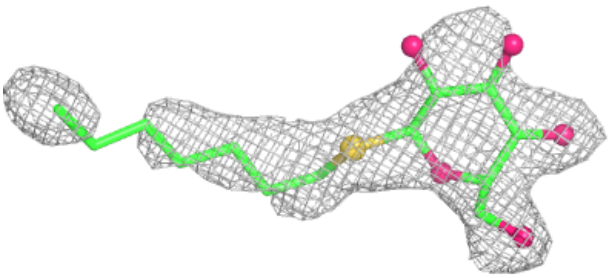


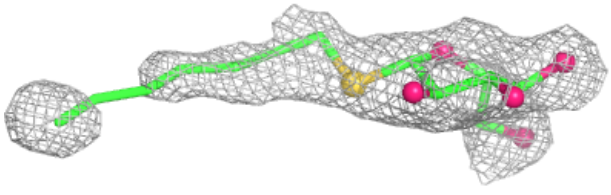


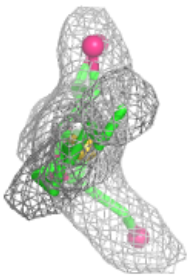


Electron density around HTG C 523:

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

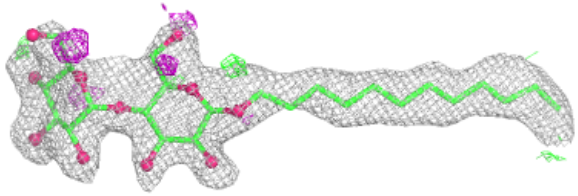


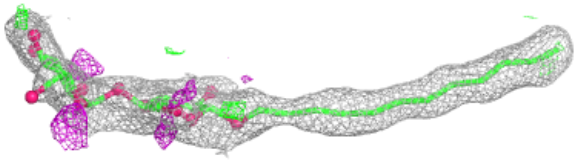


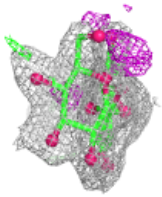


Electron density around LMT m 102:

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

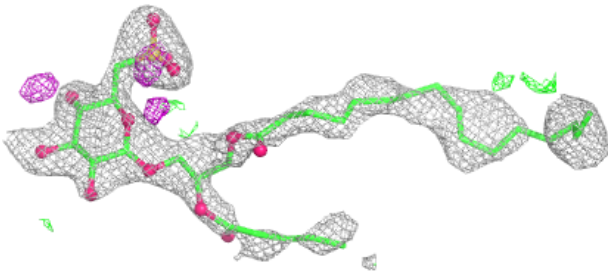


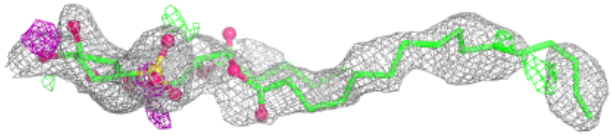


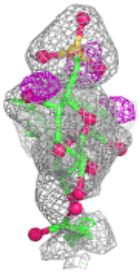


Electron density around SQD F 101:

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

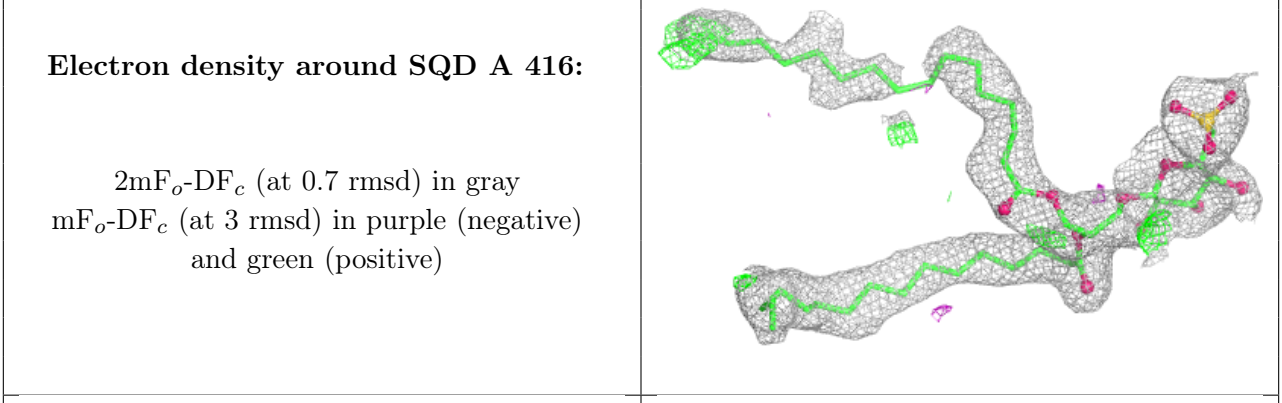






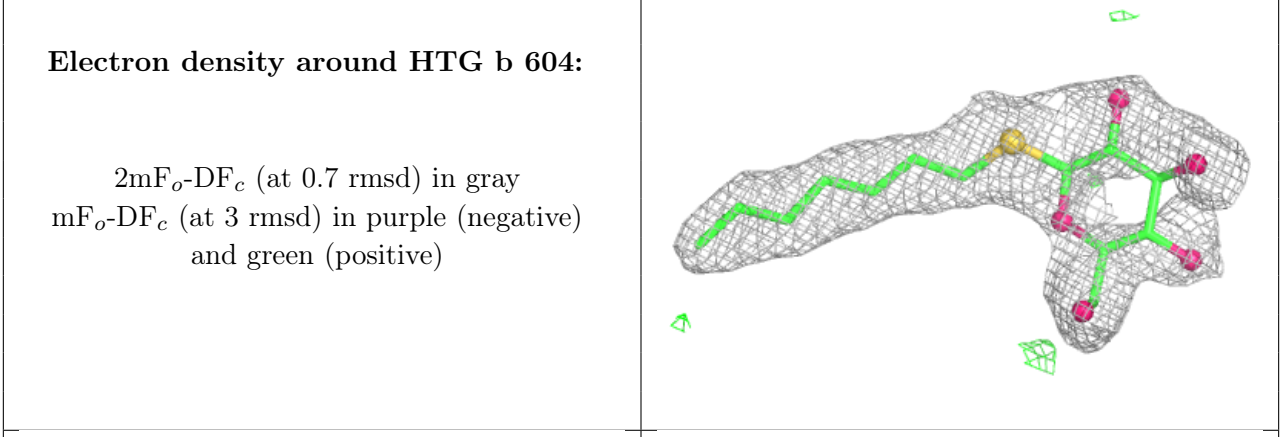
Electron density around SQD A 416:

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



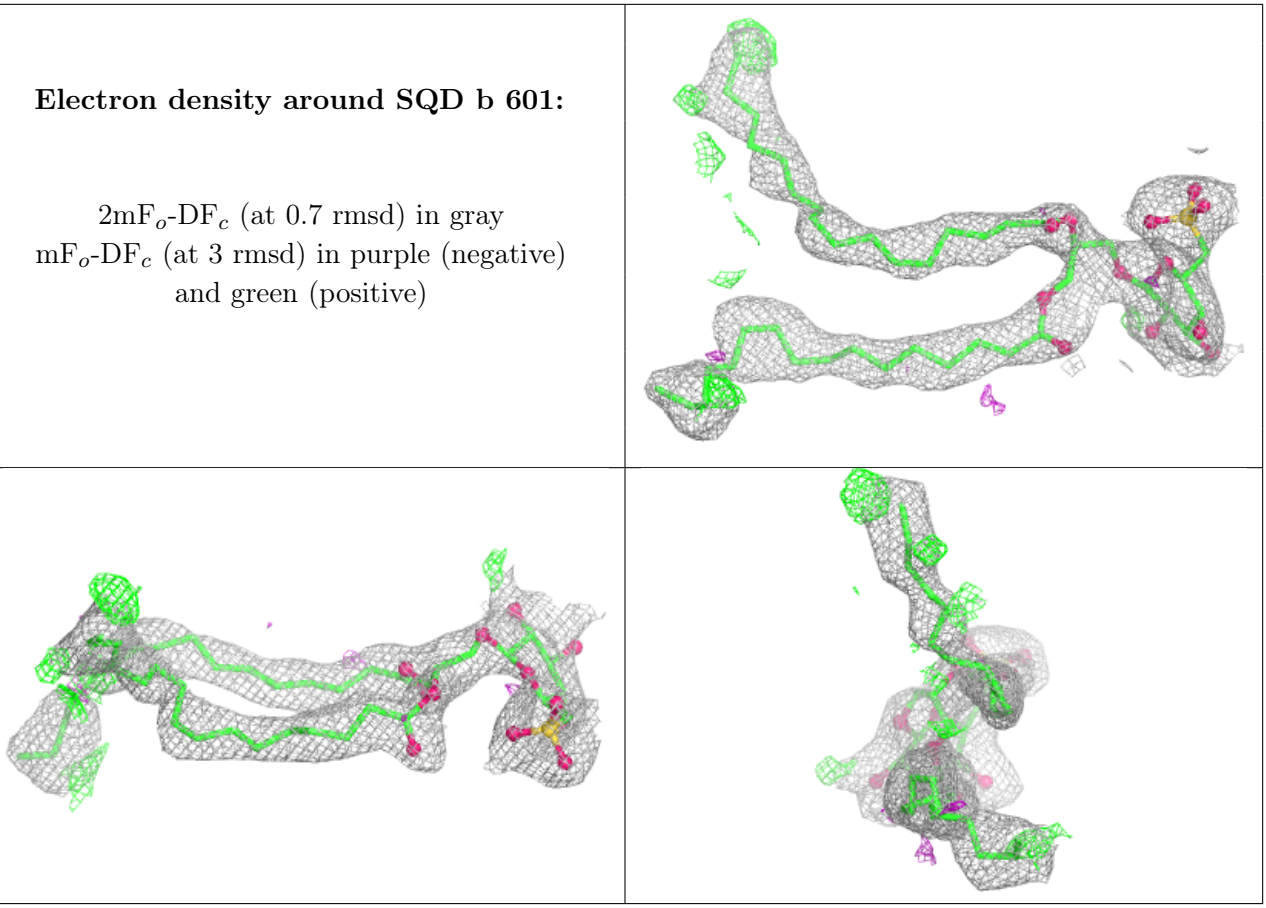
Electron density around HTG b 604:

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



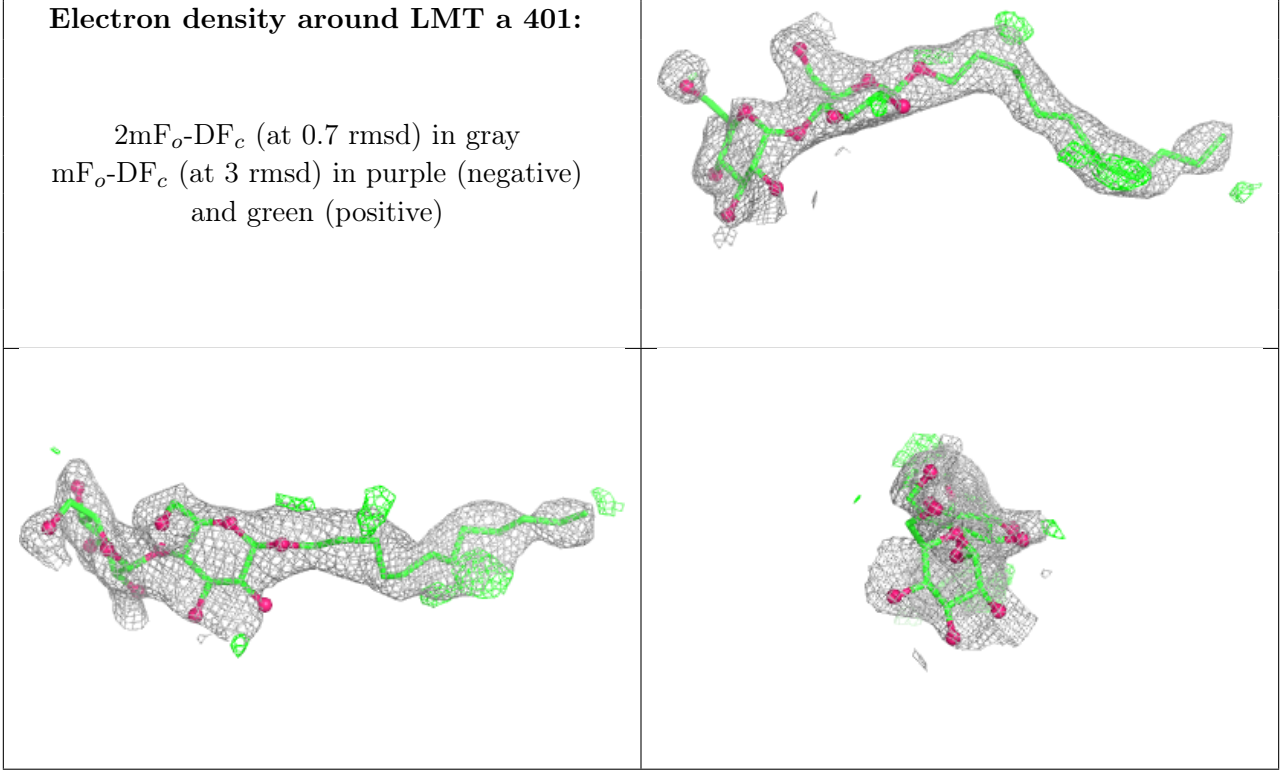
Electron density around SQD b 601:

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



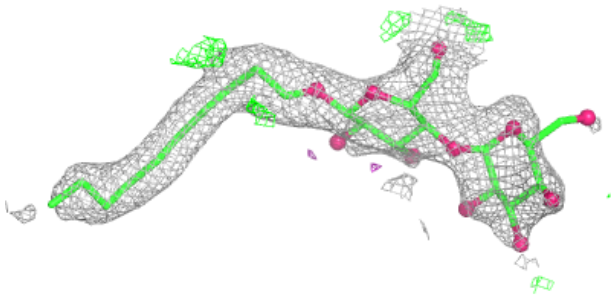
Electron density around LMT a 401:

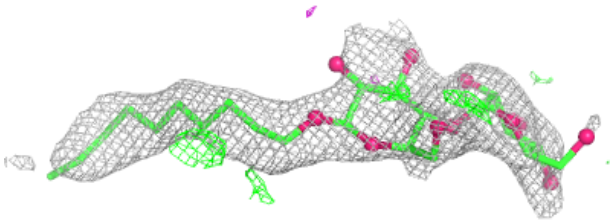
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

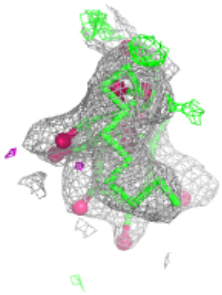


Electron density around LMT A 417:

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

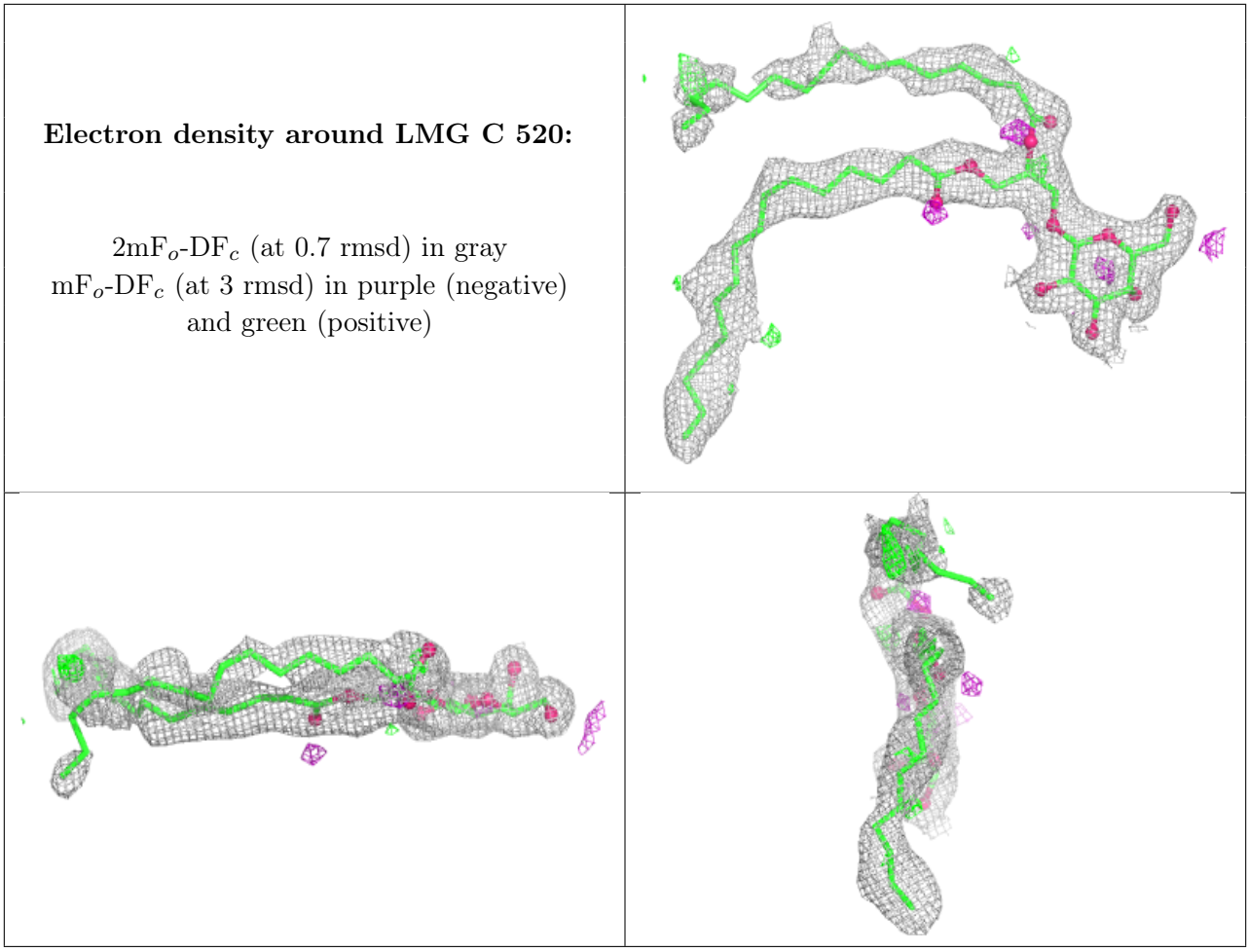






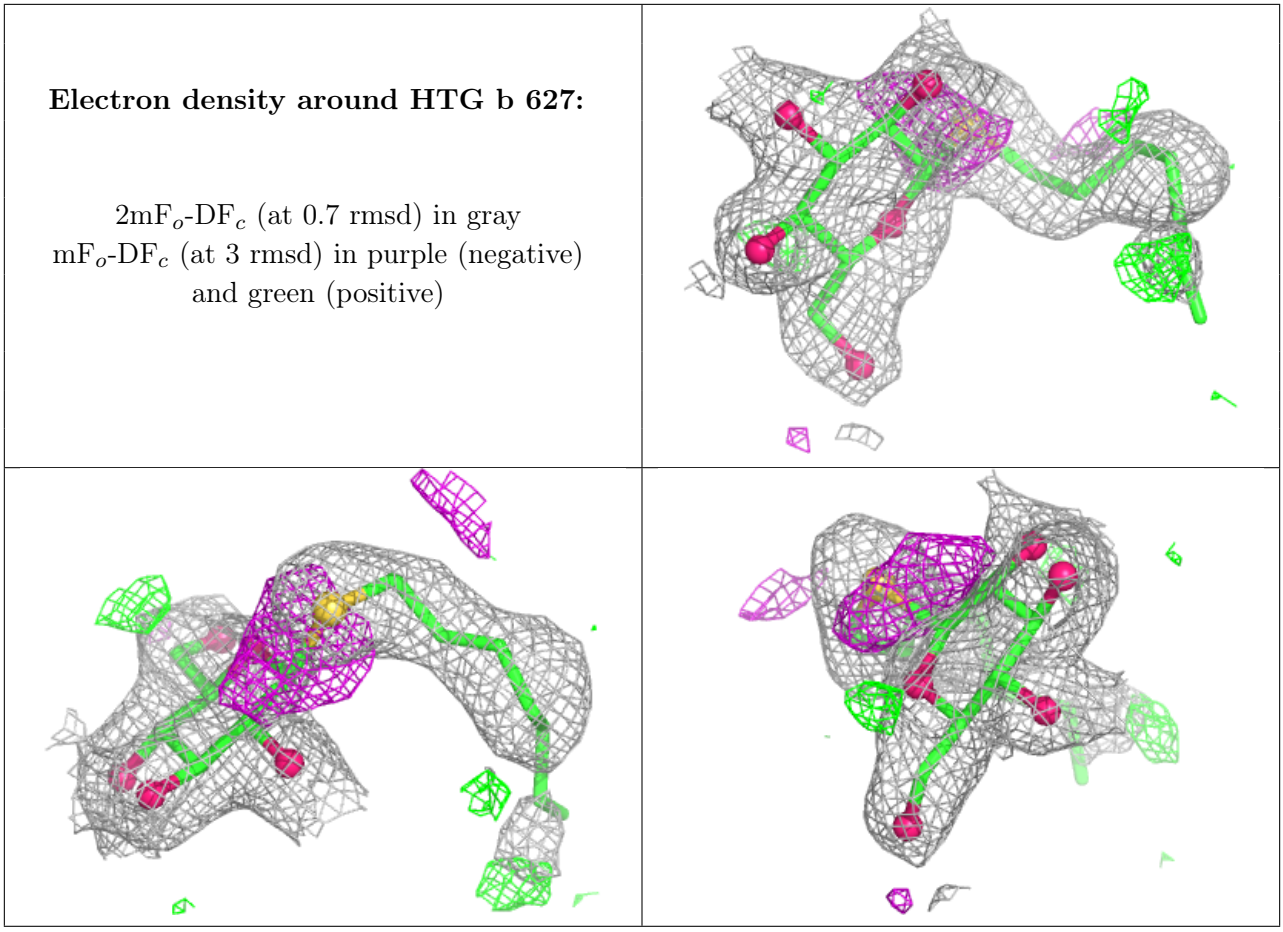
Electron density around LMG C 520:

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



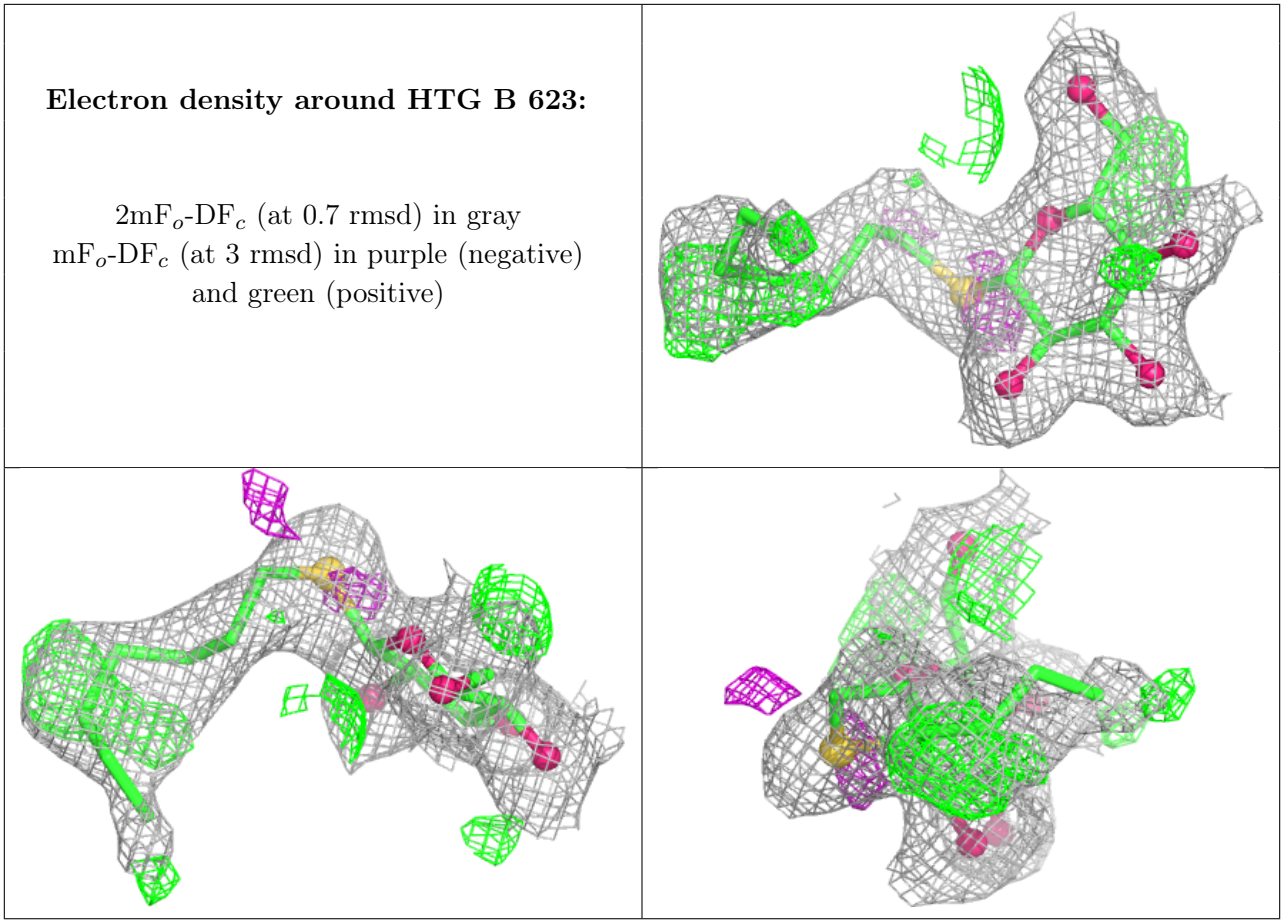
Electron density around HTG b 627:

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



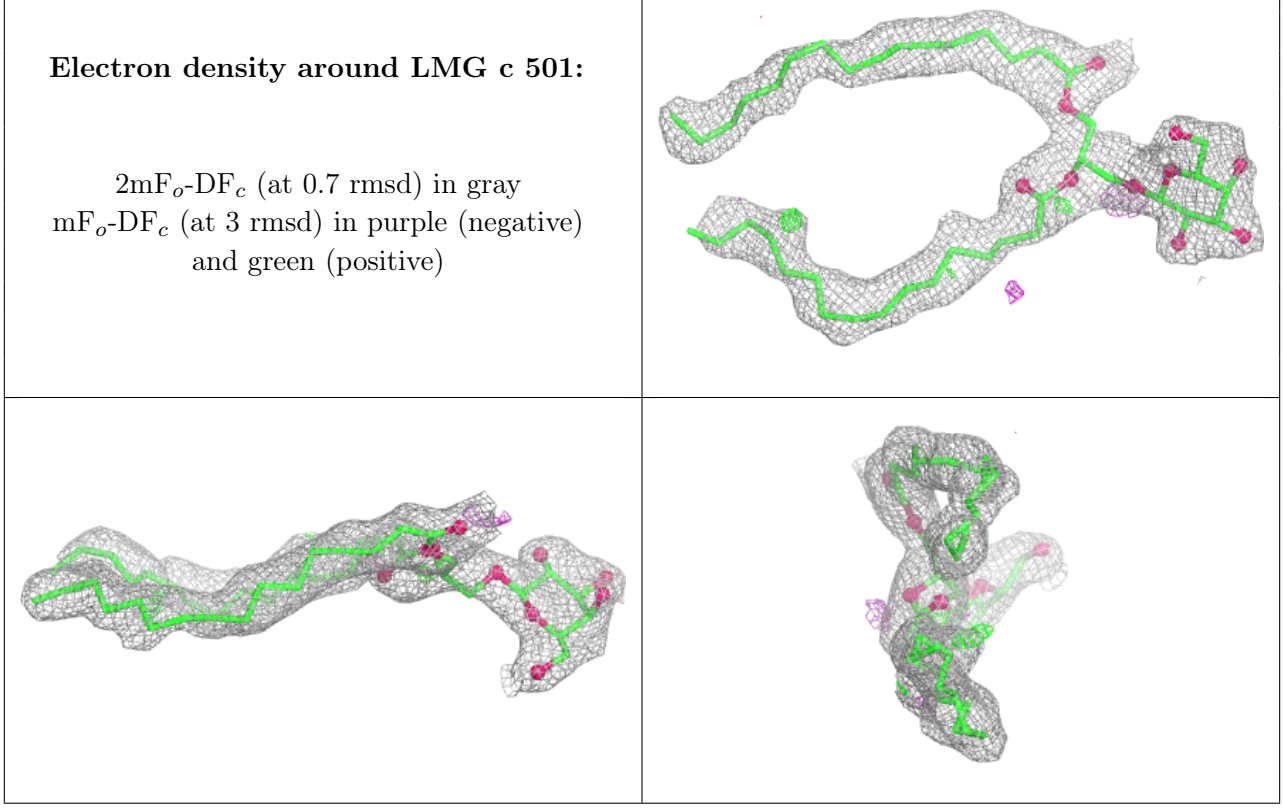
Electron density around HTG B 623:

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



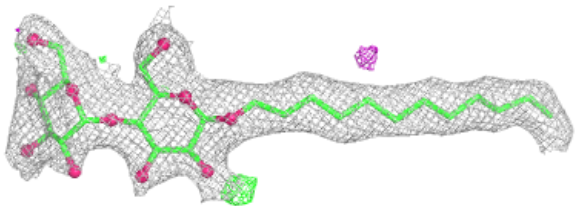
Electron density around LMG c 501:

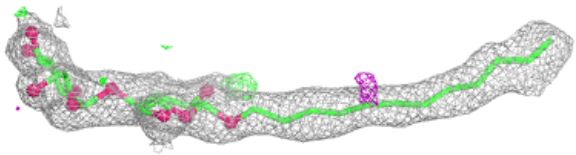
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

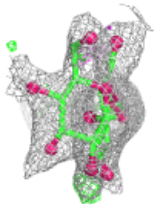


Electron density around LMT M 102:

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

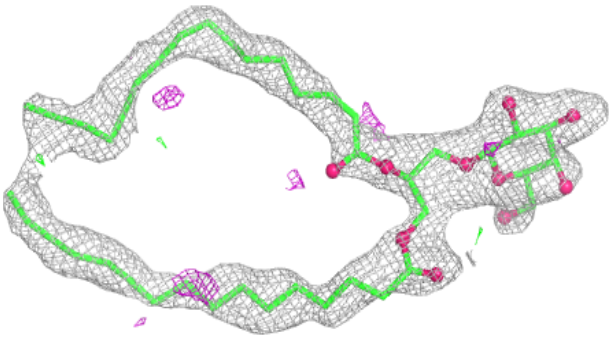


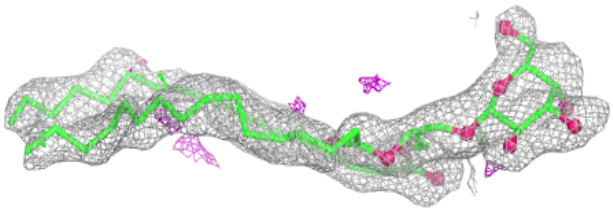


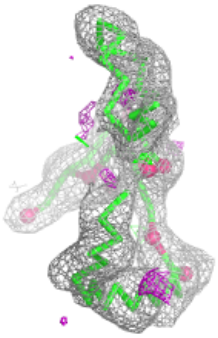


Electron density around LMG C 501:

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

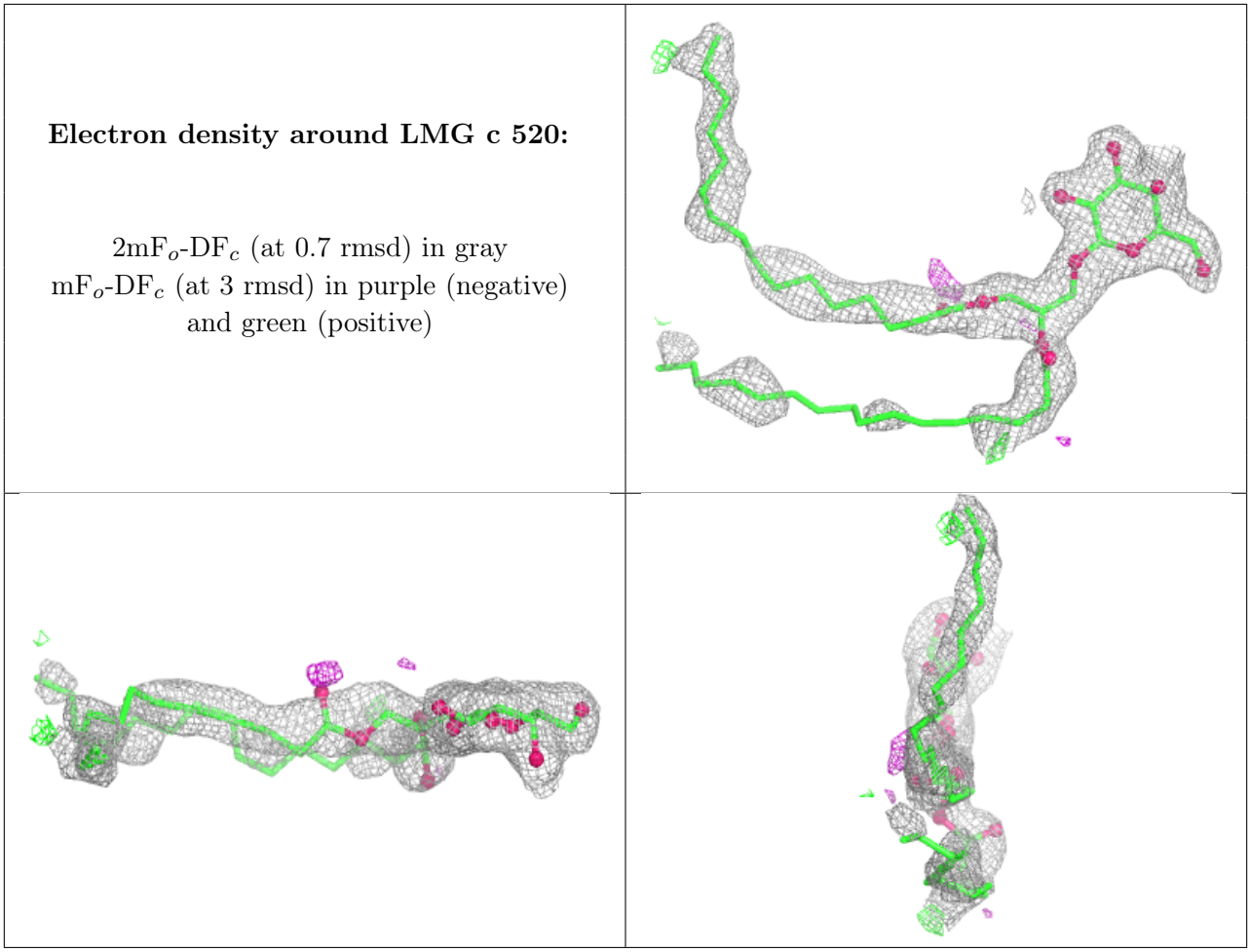






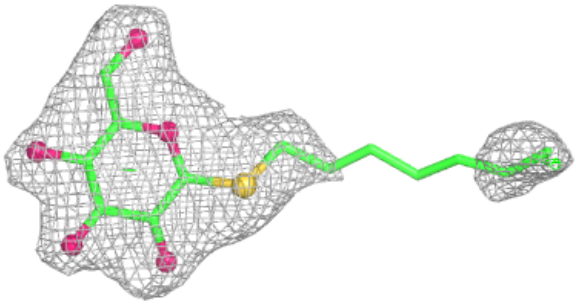
Electron density around LMG c 520:

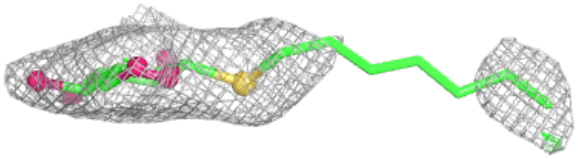
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

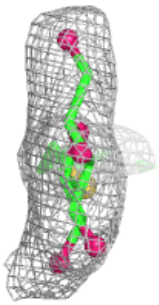


Electron density around HTG C 522:

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

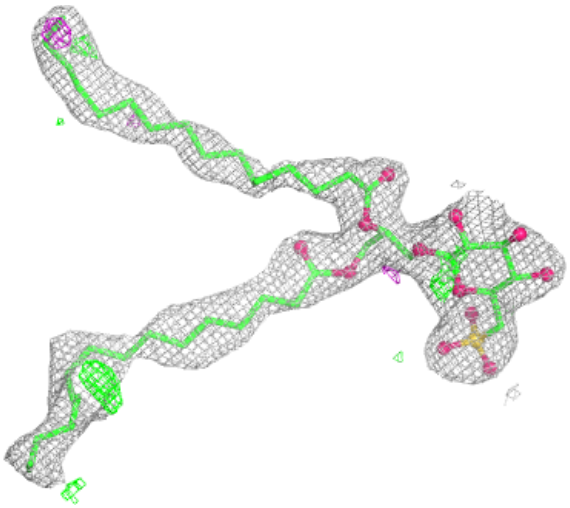


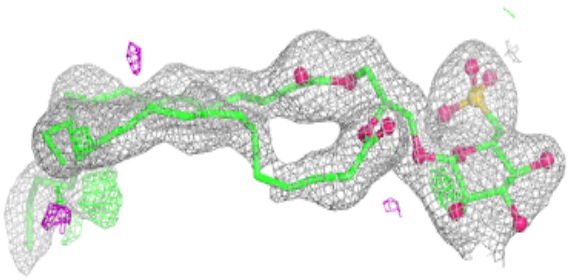


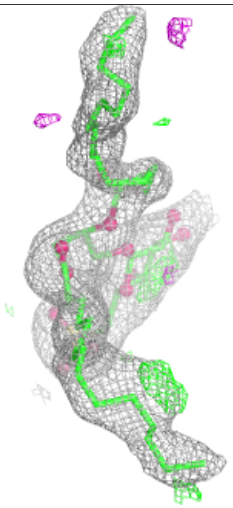


Electron density around SQD a 411:

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

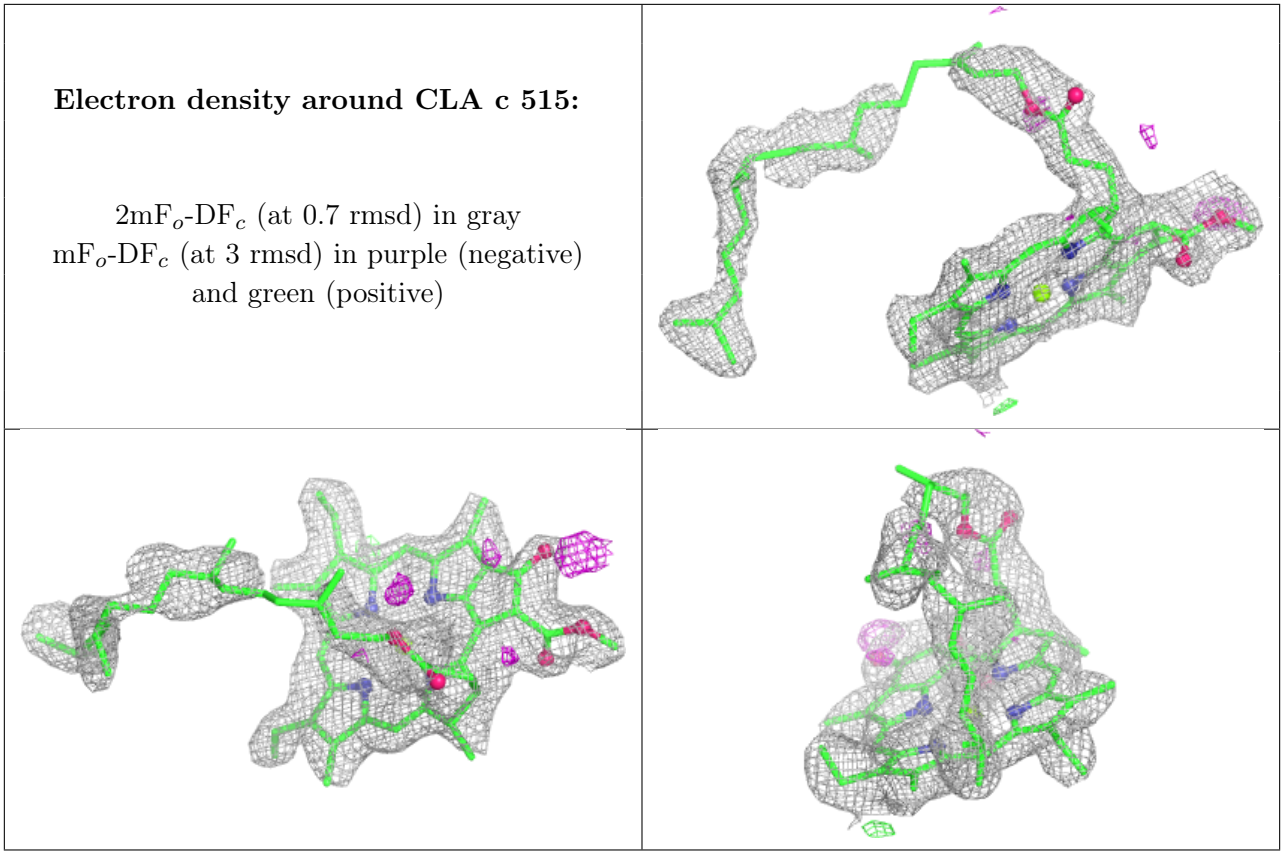






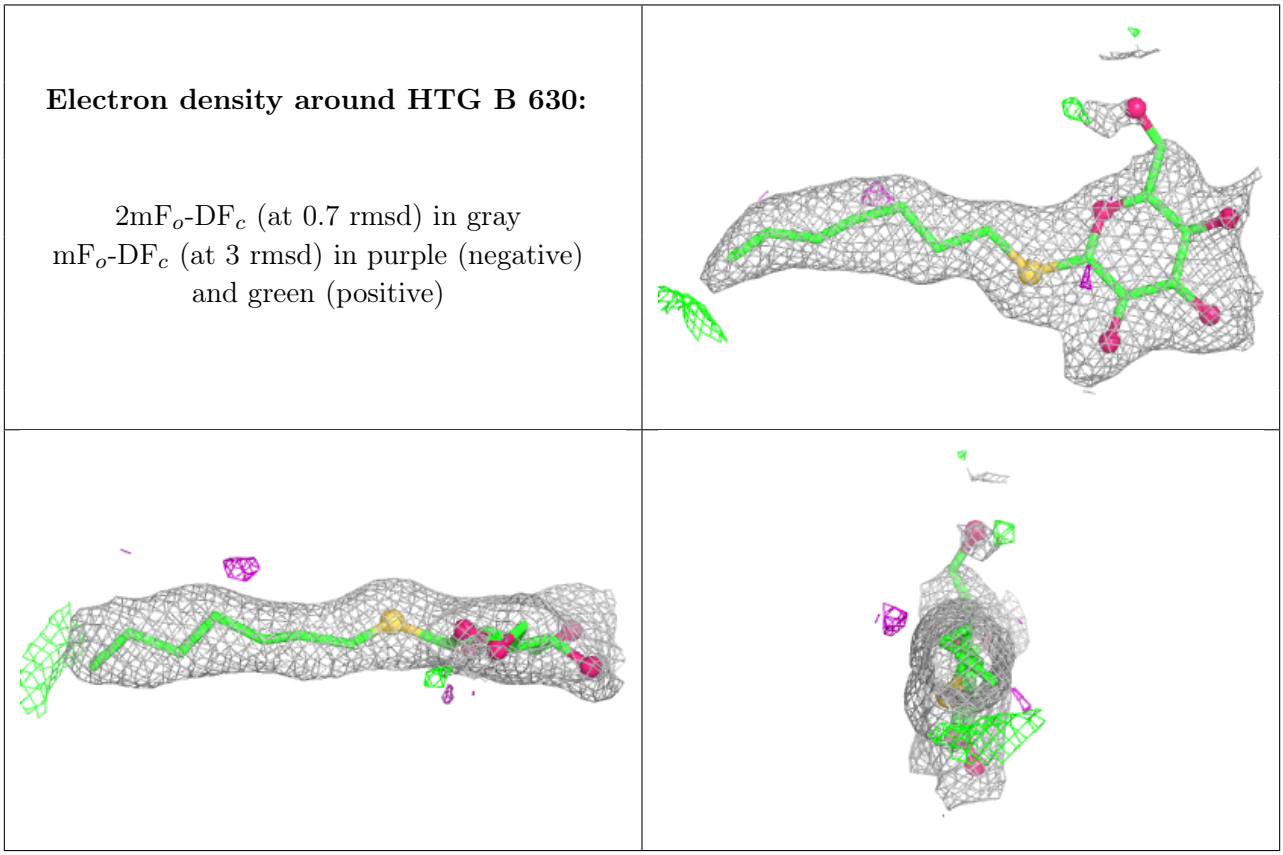
Electron density around CLA c 515:

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



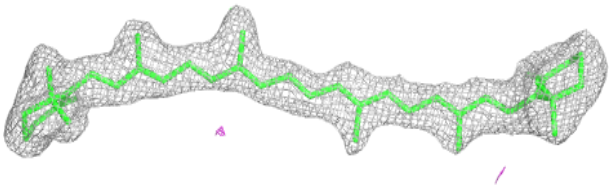
Electron density around HTG B 630:

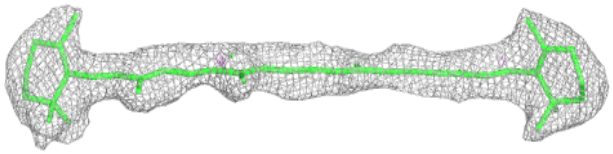
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

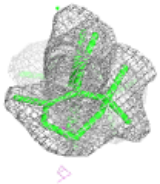


Electron density around BCR c 526:

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

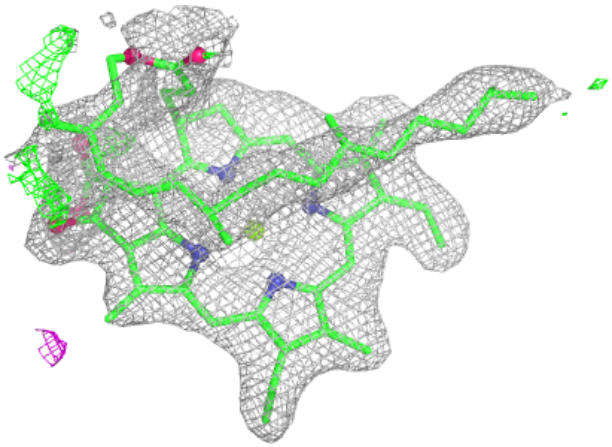


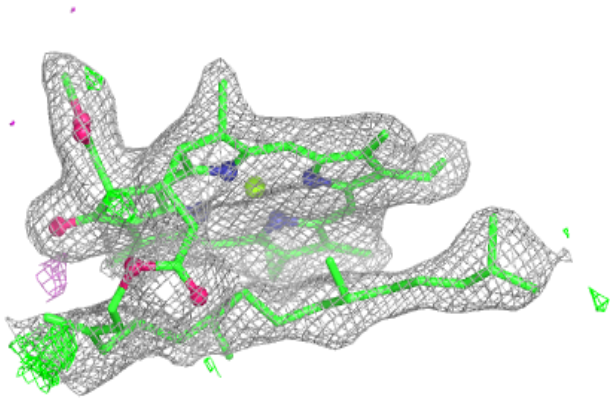


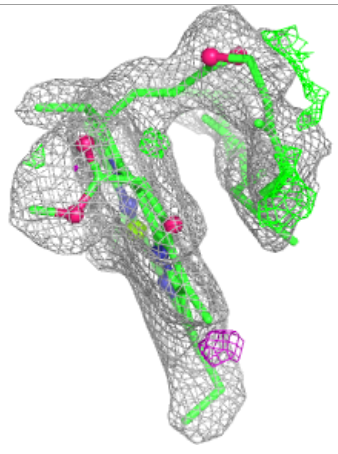


Electron density around CLA b 606:

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

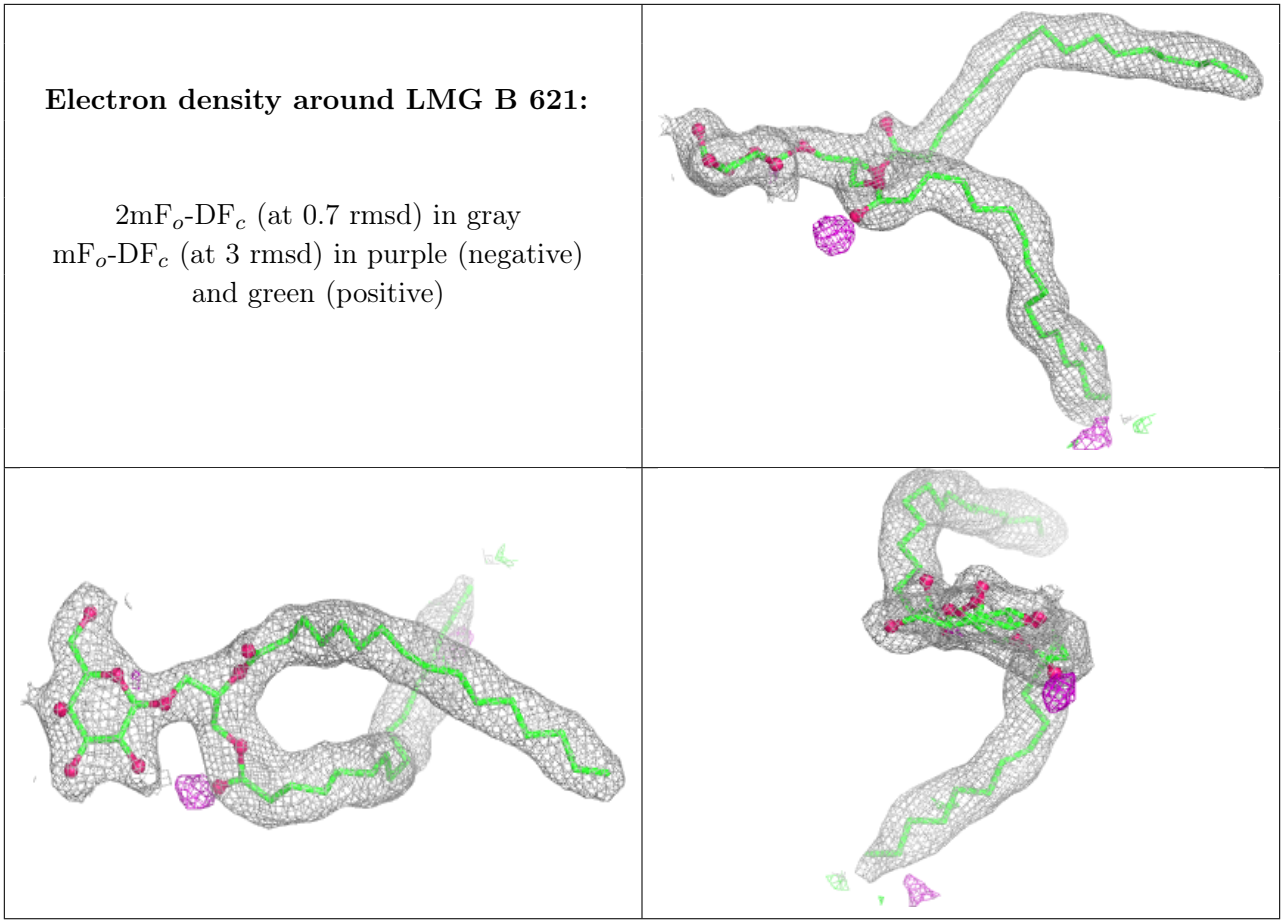






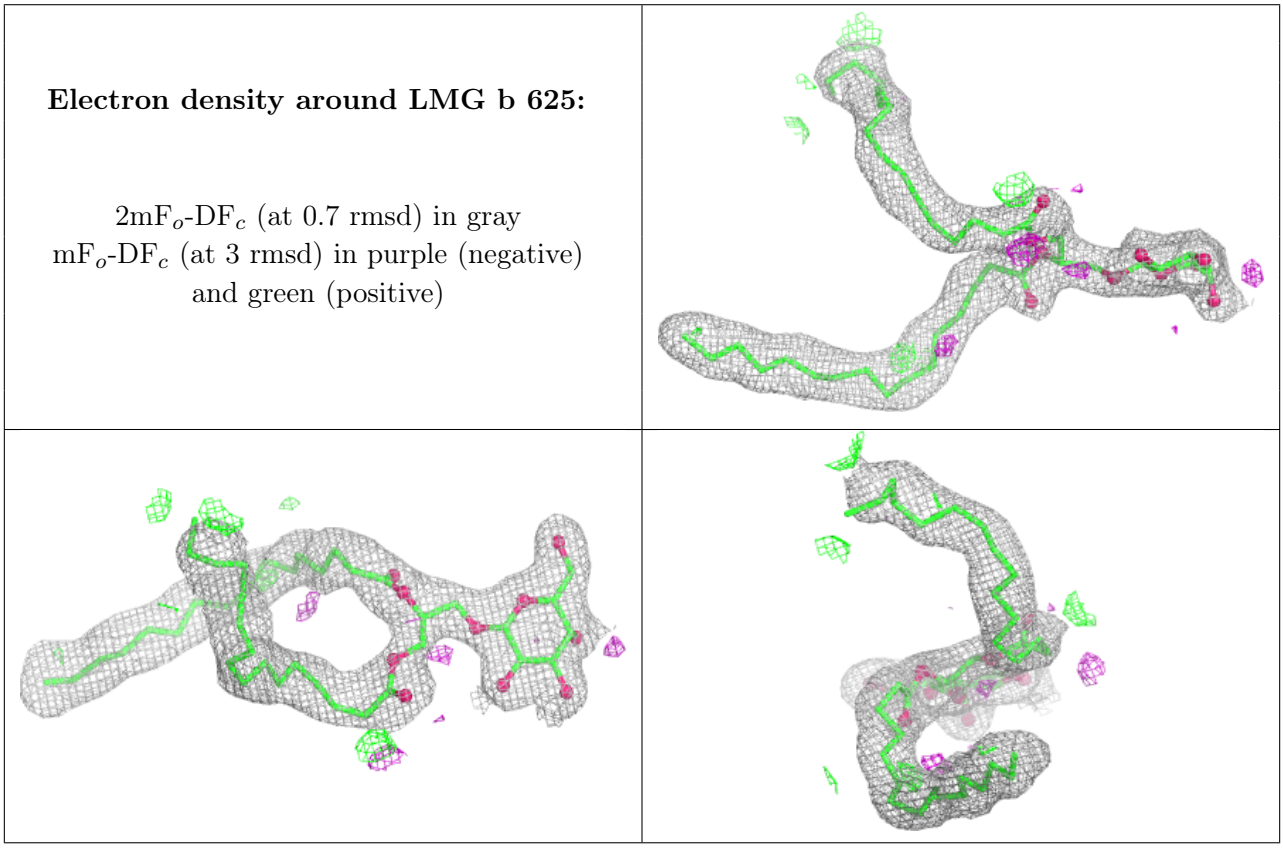
Electron density around LMG B 621:

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



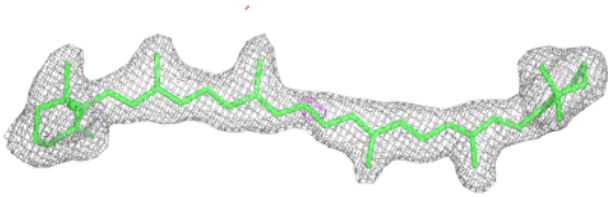
Electron density around LMG b 625:

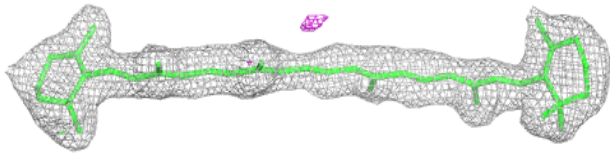
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

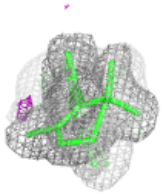


Electron density around BCR C 515:

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

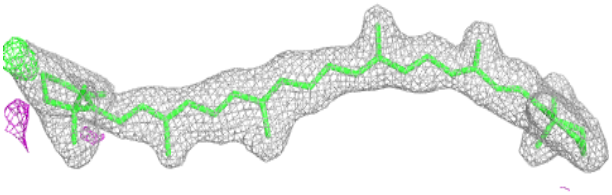


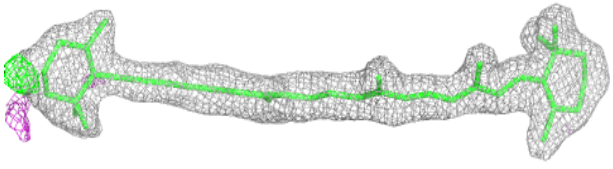


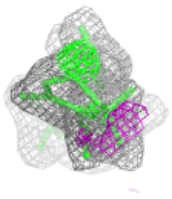


Electron density around BCR H 101:

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

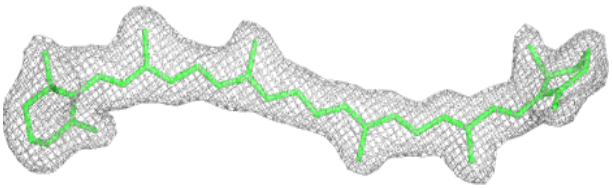


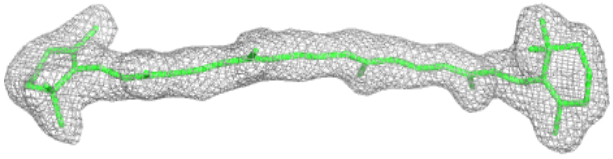


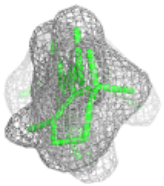


Electron density around BCR Y 101:

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

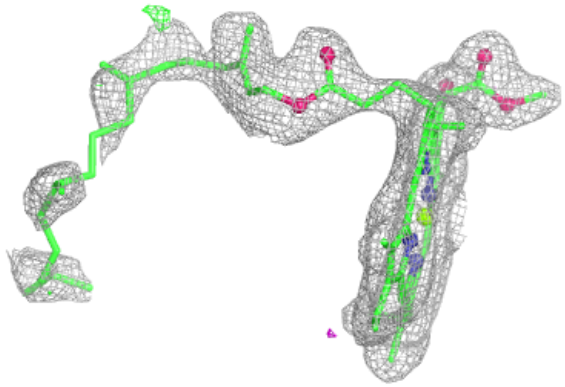


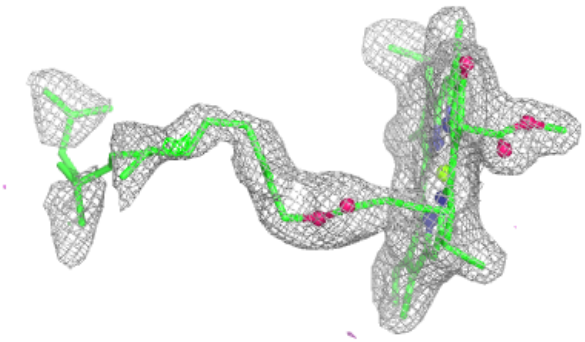


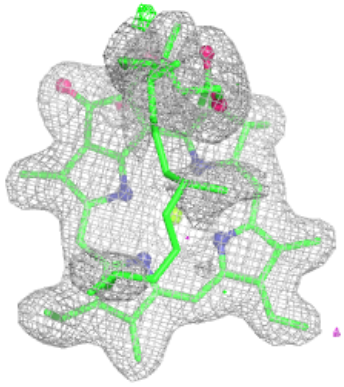


Electron density around CLA C 507:

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

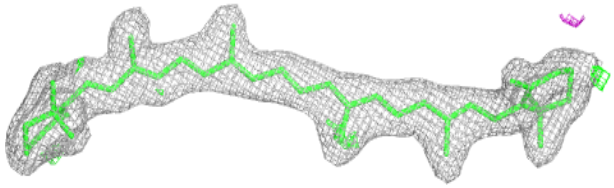


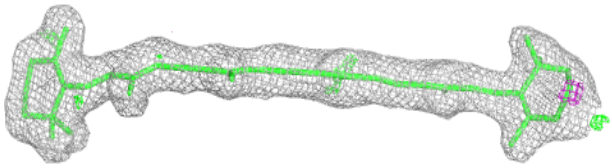


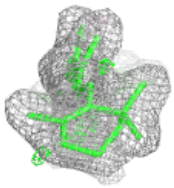


Electron density around BCR h 101:

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

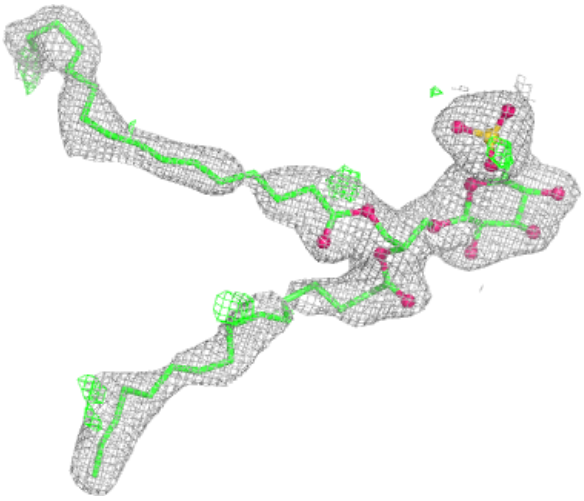


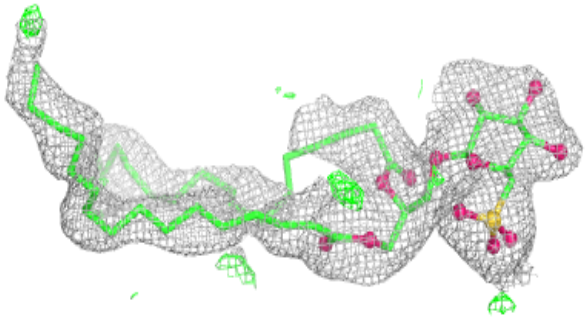


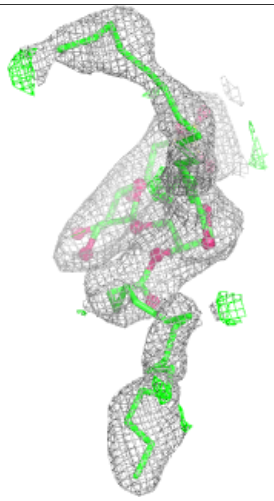


Electron density around SQD A 411:

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

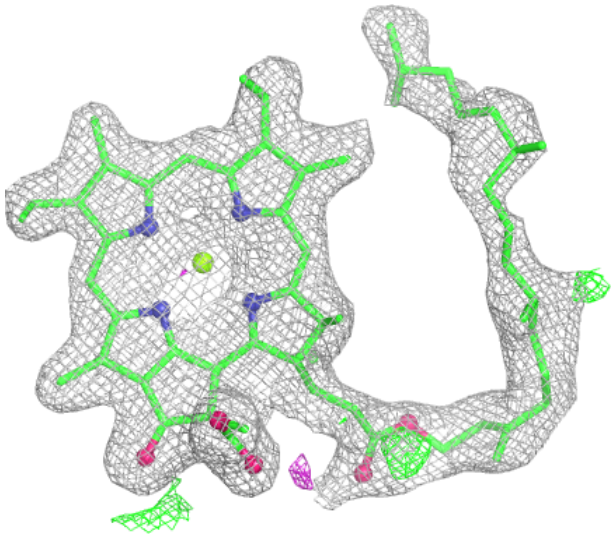


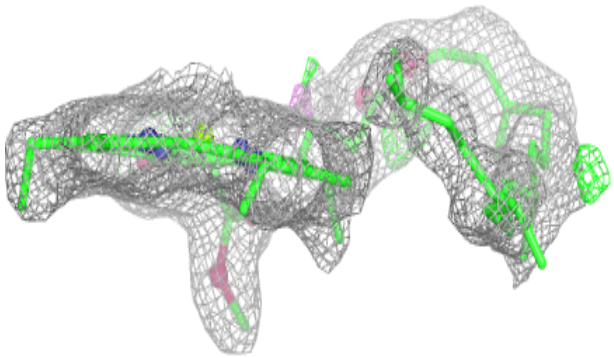


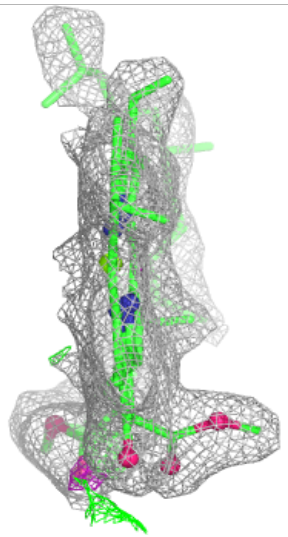


Electron density around CLA c 514:

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

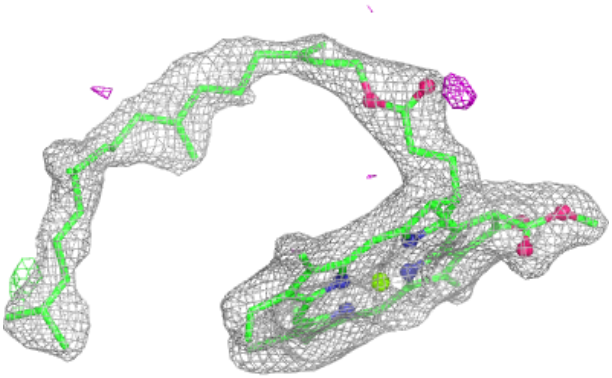


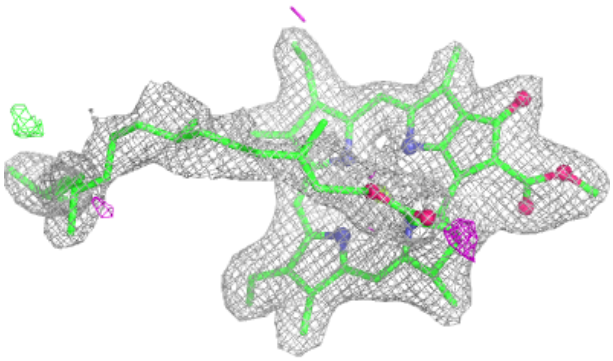


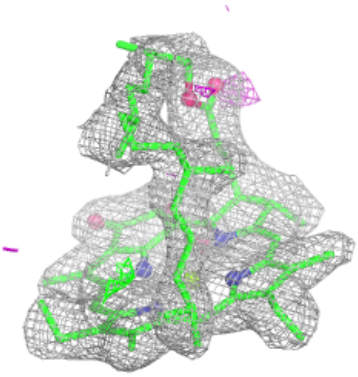


Electron density around CLA C 514:

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

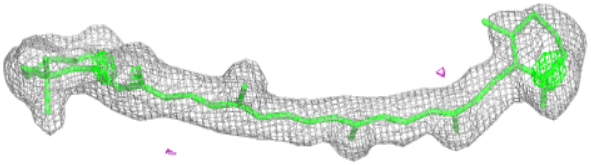


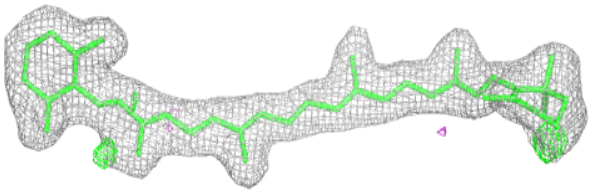


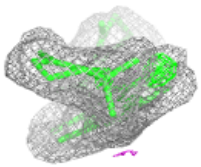


Electron density around BCR D 405:

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

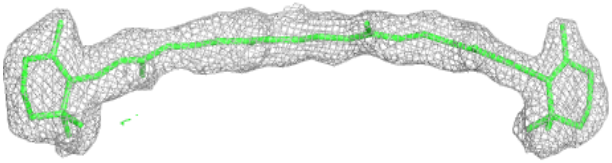


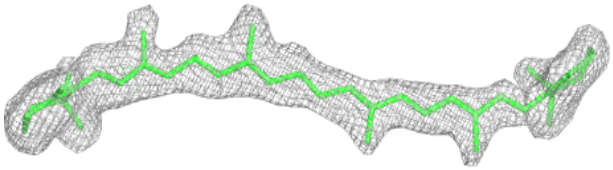


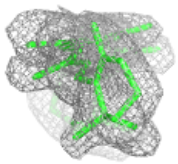


Electron density around BCR k 103:

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

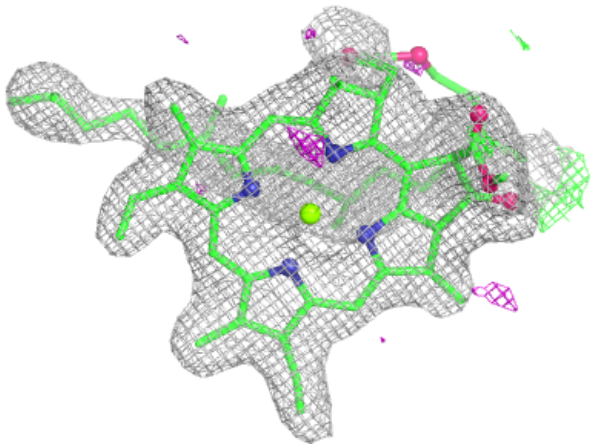


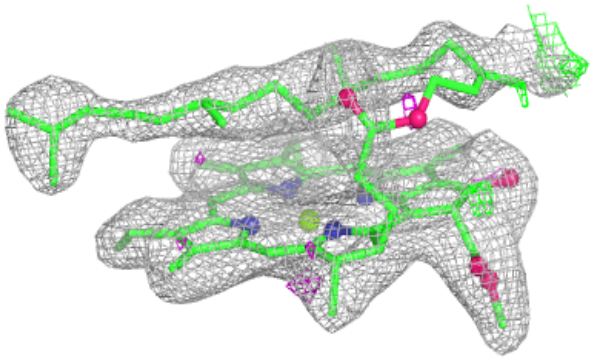


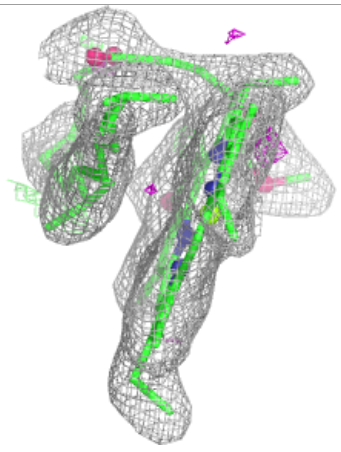


Electron density around CLA B 602:

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

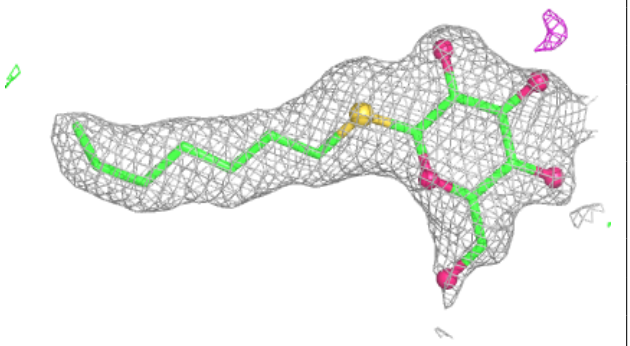


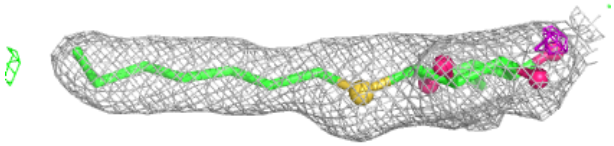


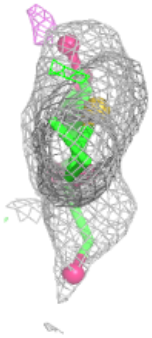


Electron density around HTG b 603:

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

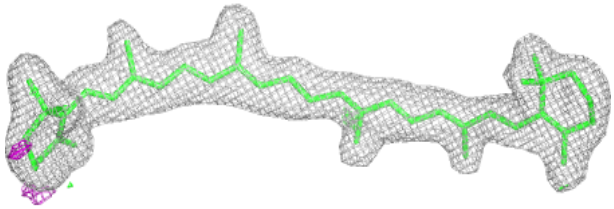


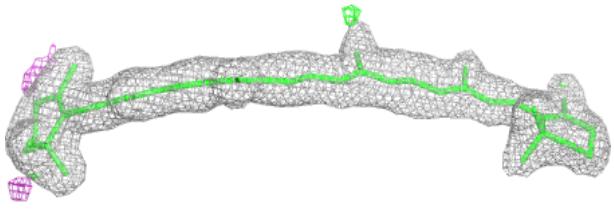


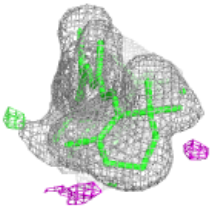


Electron density around BCR T 102:

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

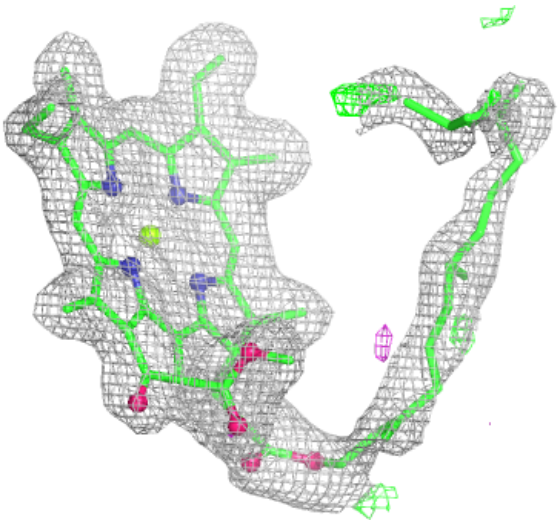


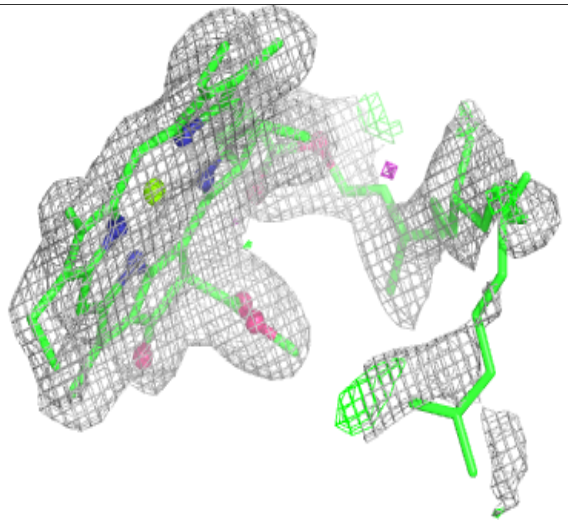


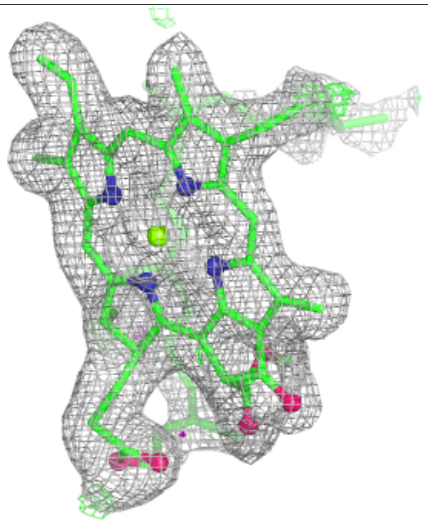


Electron density around CLA b 621:

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

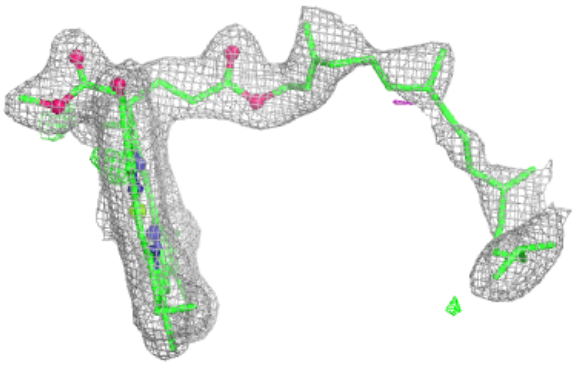


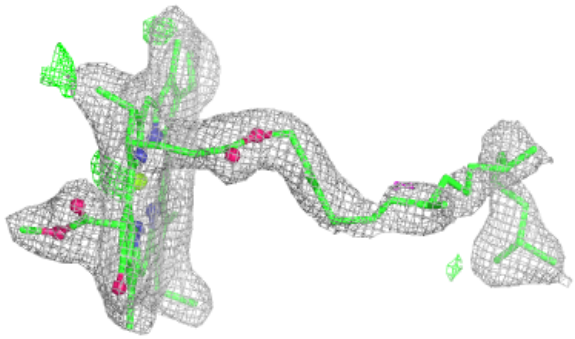


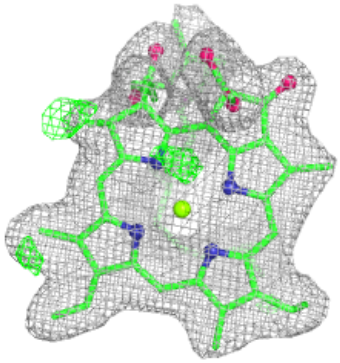


Electron density around CLA c 508:

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

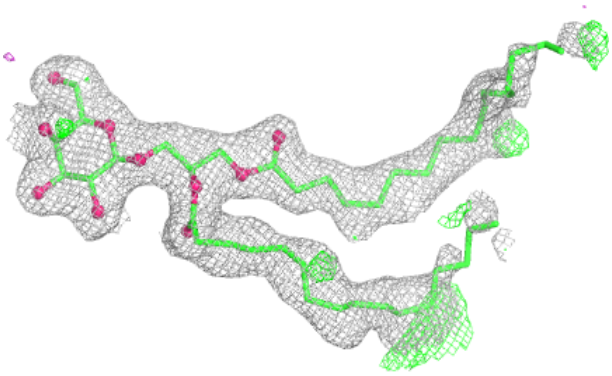


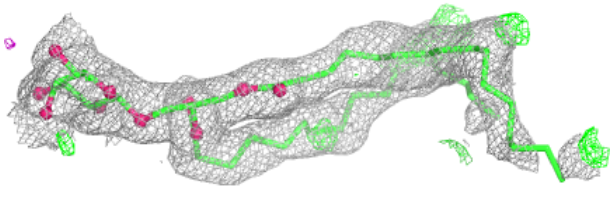


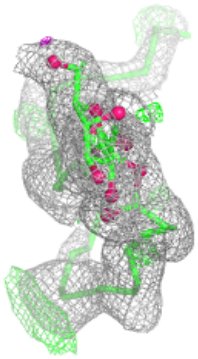


Electron density around LMG j 101:

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

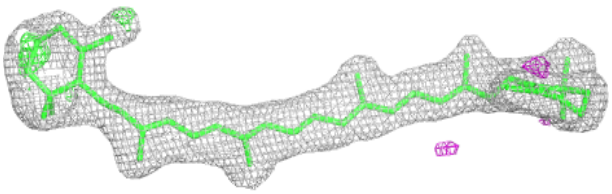


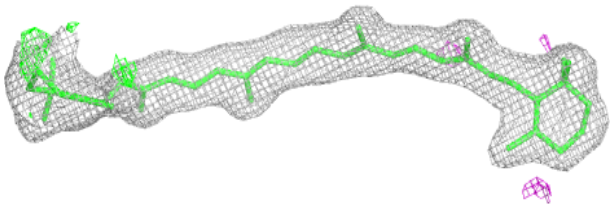


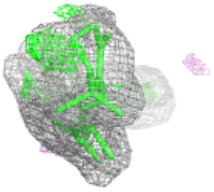


Electron density around BCR d 405:

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

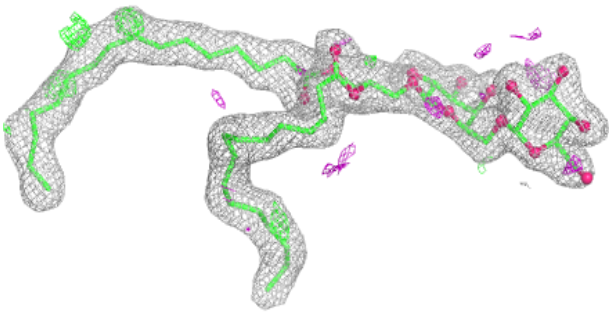


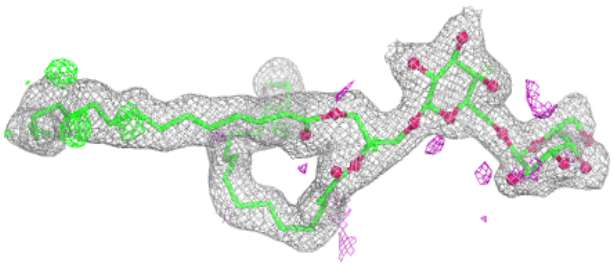


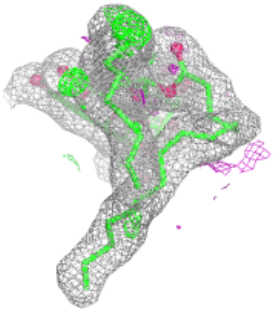


Electron density around DGD H 102:

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

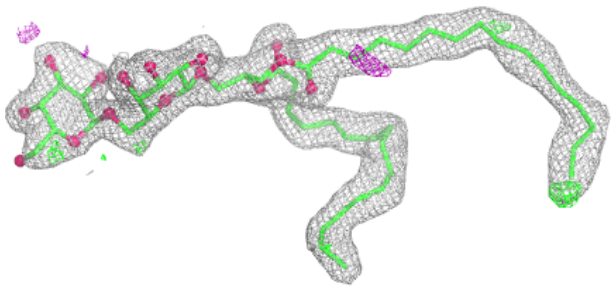


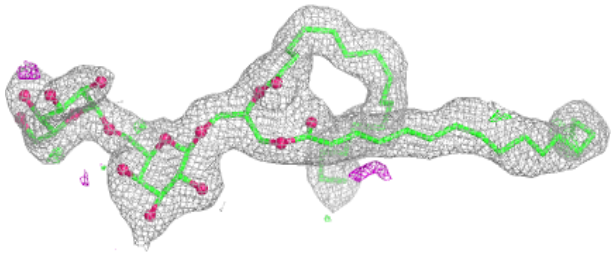


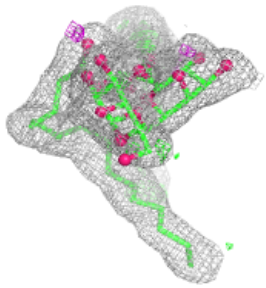


Electron density around DGD h 102:

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

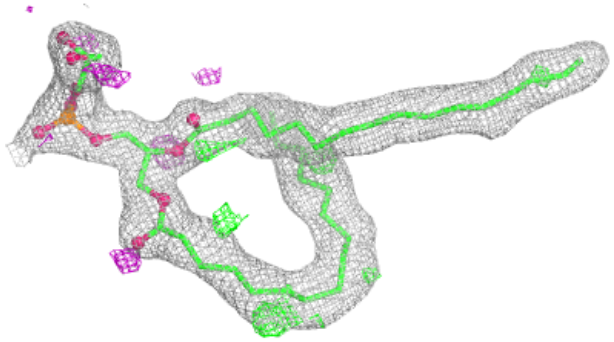


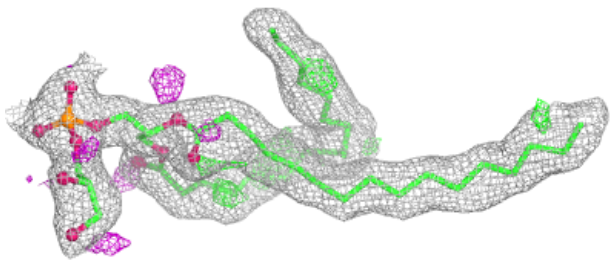


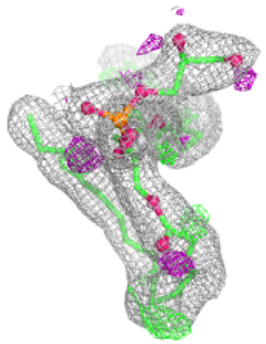


Electron density around LHG D 408:

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

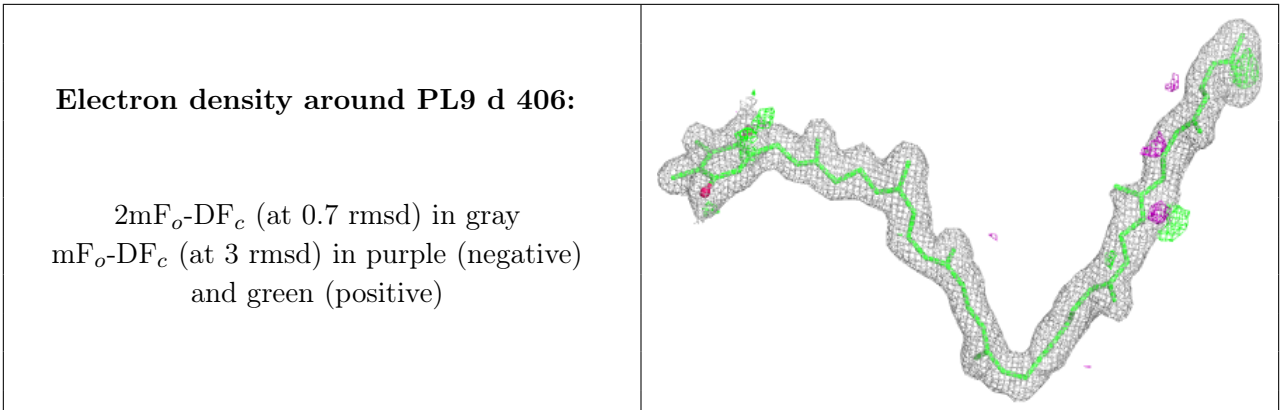






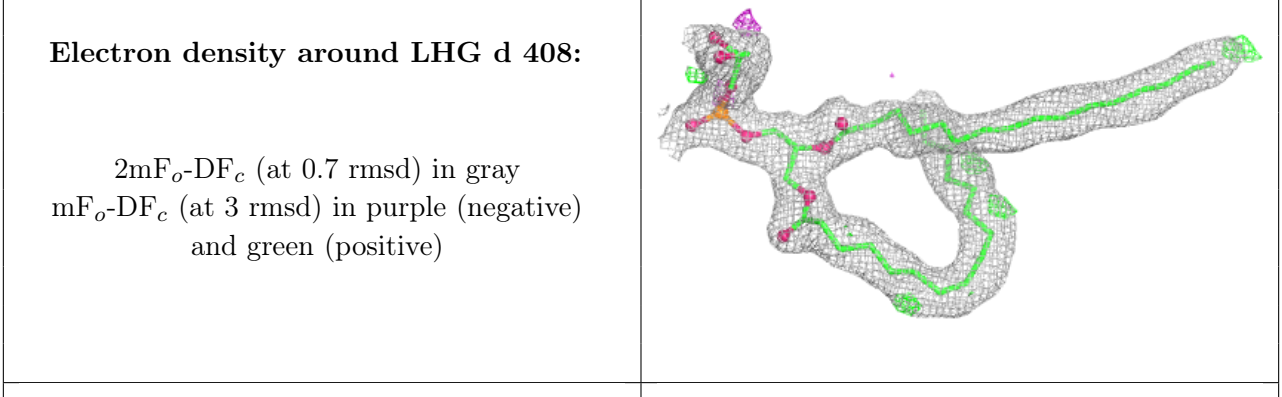
Electron density around PL9 d 406:

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



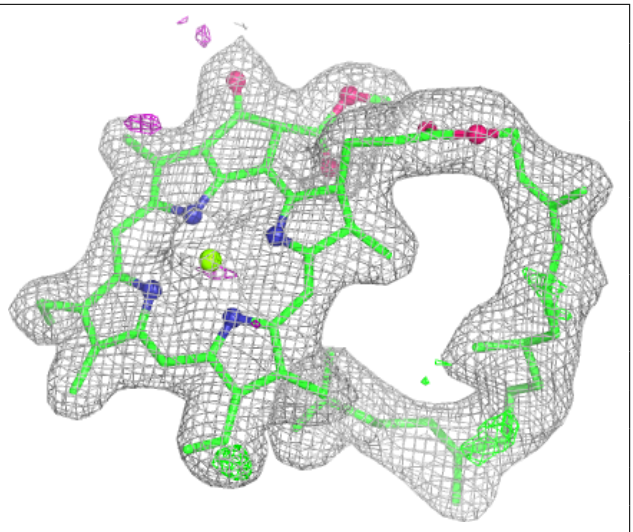
Electron density around LHG d 408:

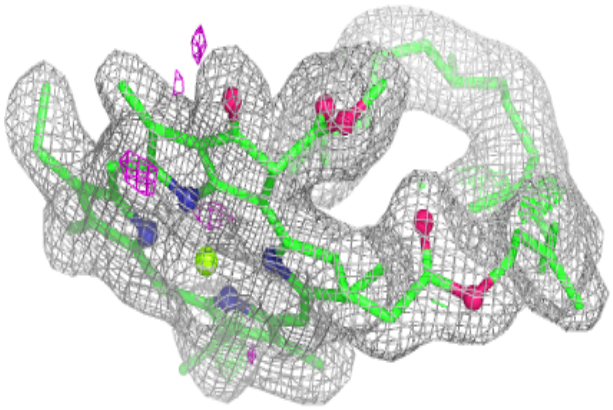
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

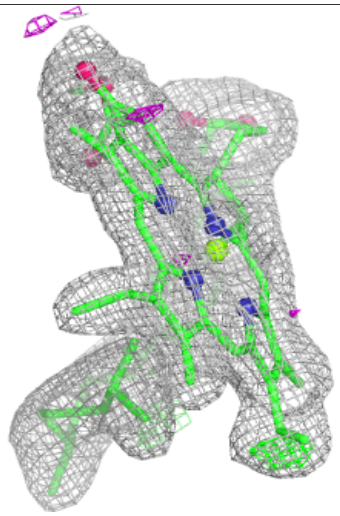


Electron density around CLA b 620:

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

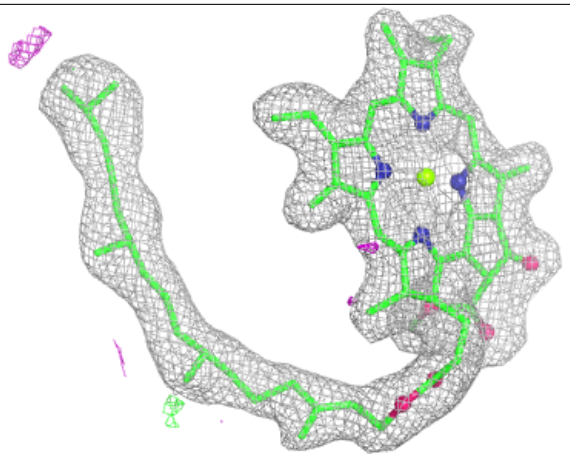


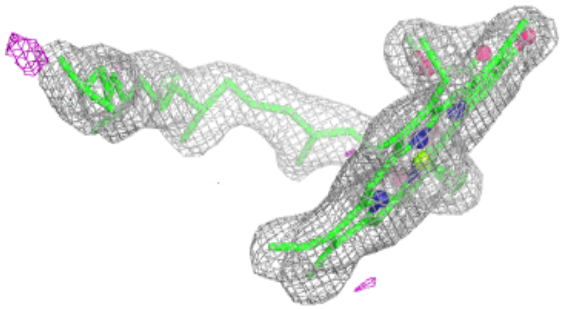


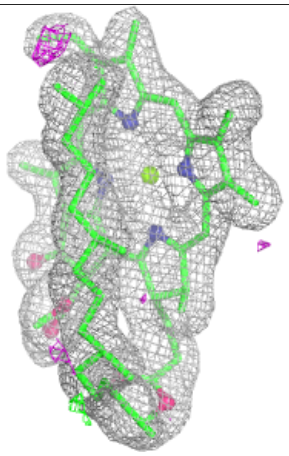


Electron density around CLA C 508:

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

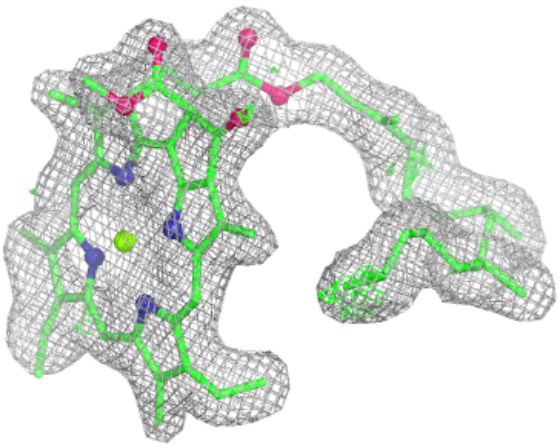


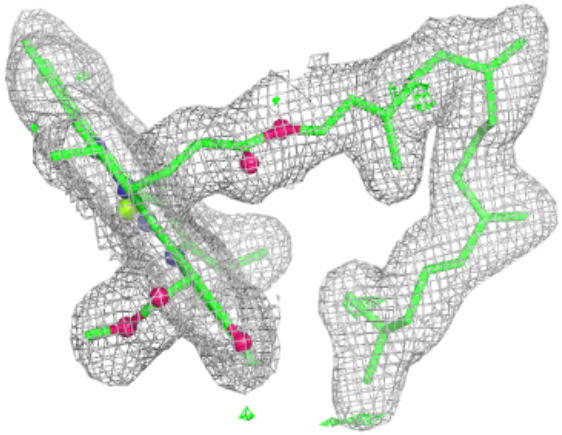


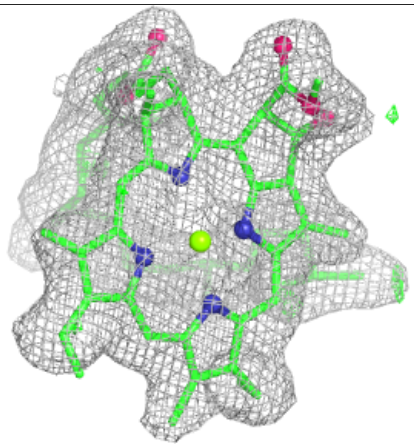


Electron density around CLA c 505:

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

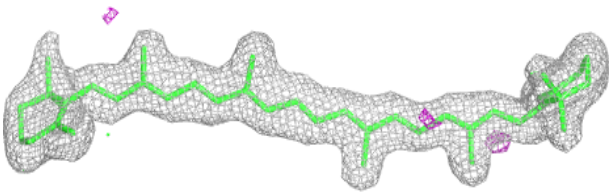


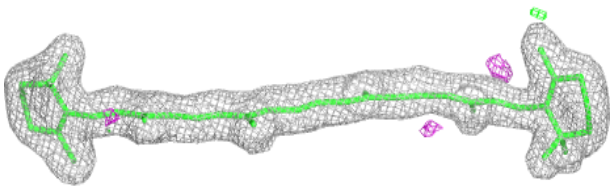


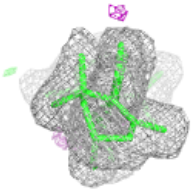


Electron density around BCR a 410:

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

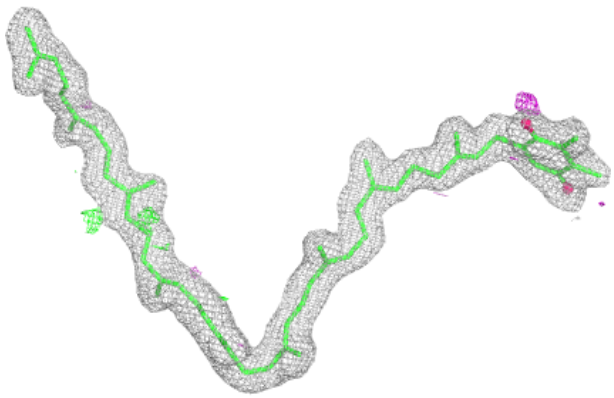


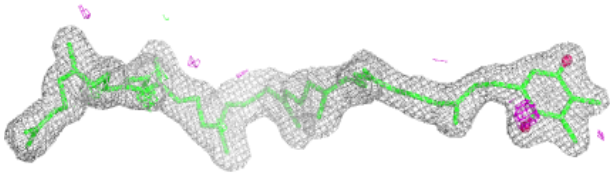


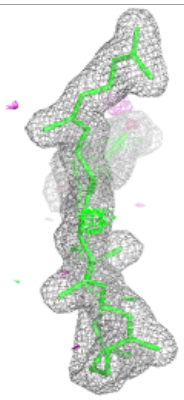


Electron density around PL9 D 406:

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

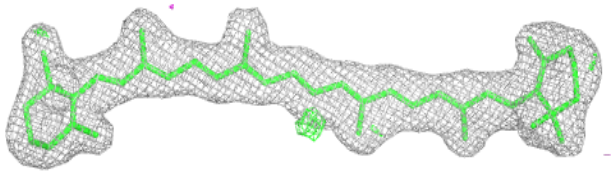


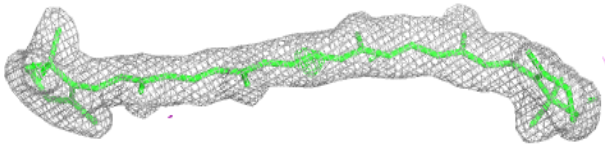


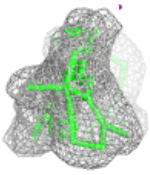


Electron density around BCR b 624:

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

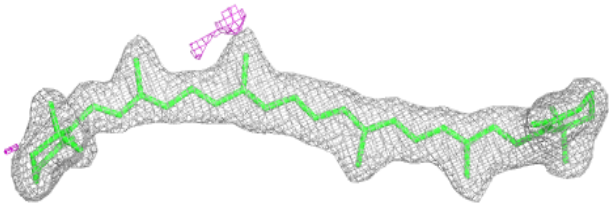


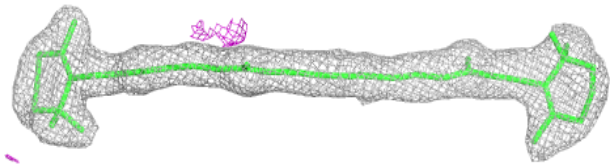


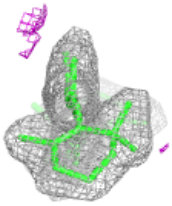


Electron density around BCR c 516:

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

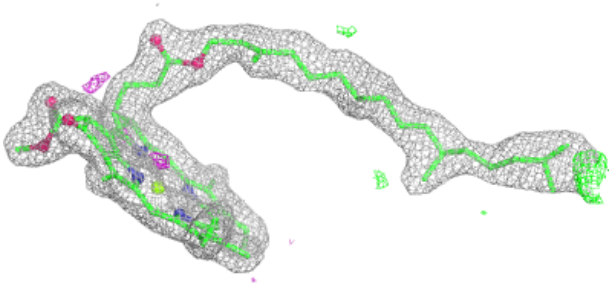


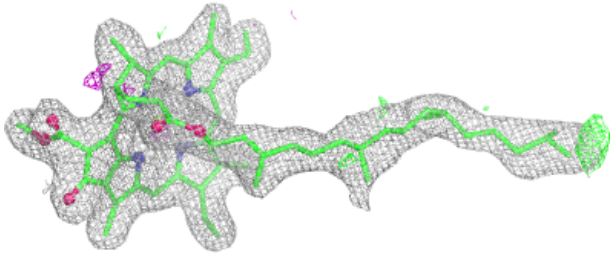


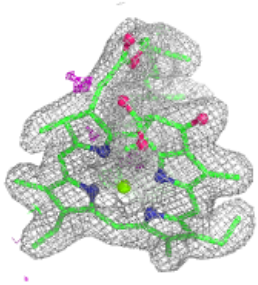


Electron density around CLA c 506:

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

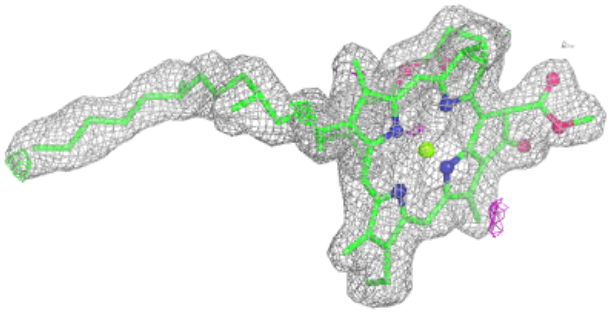


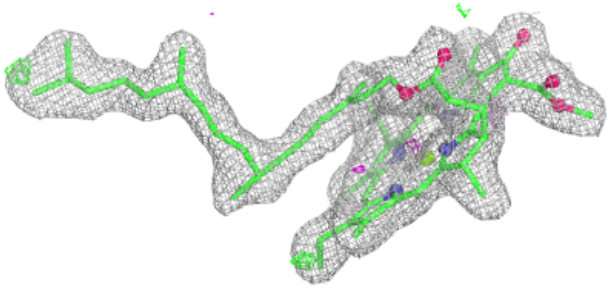


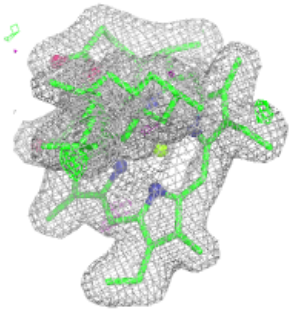


Electron density around CLA c 507:

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

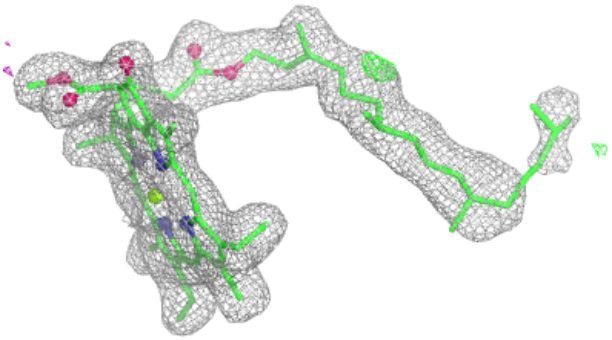


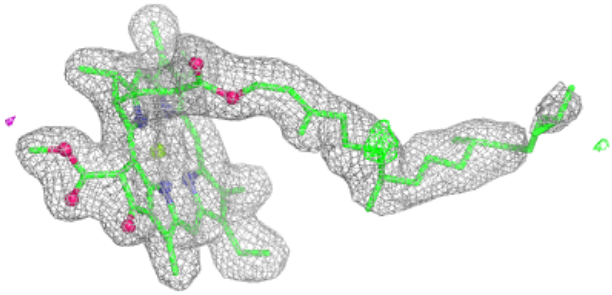


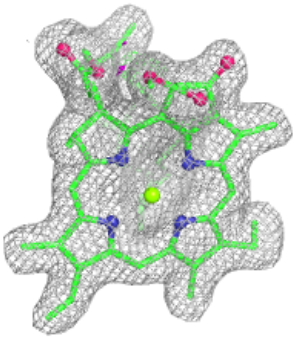


Electron density around CLA C 509:

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

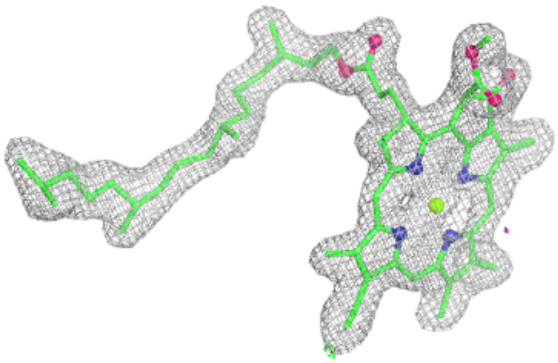


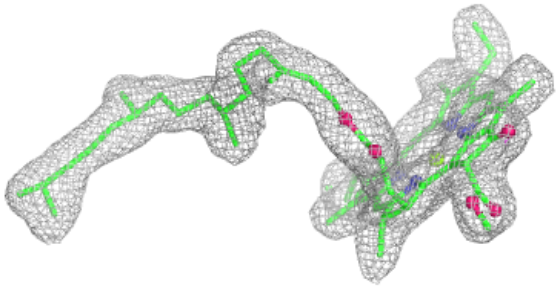


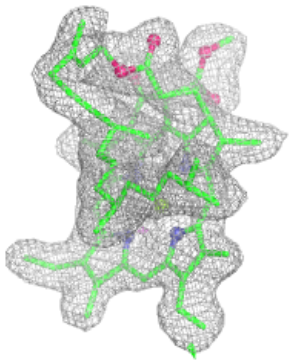


Electron density around CLA C 512:

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

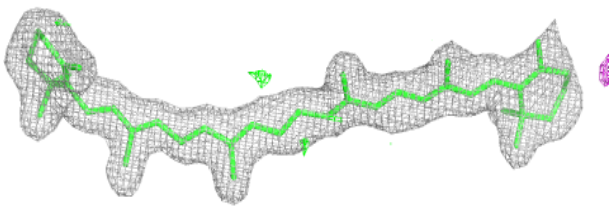


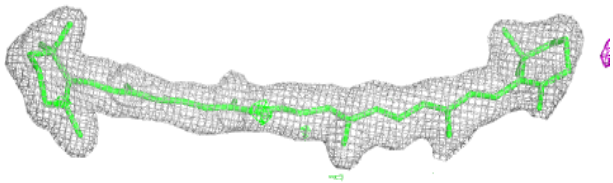


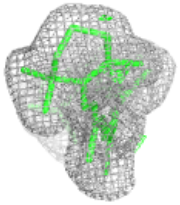


Electron density around BCR t 101:

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

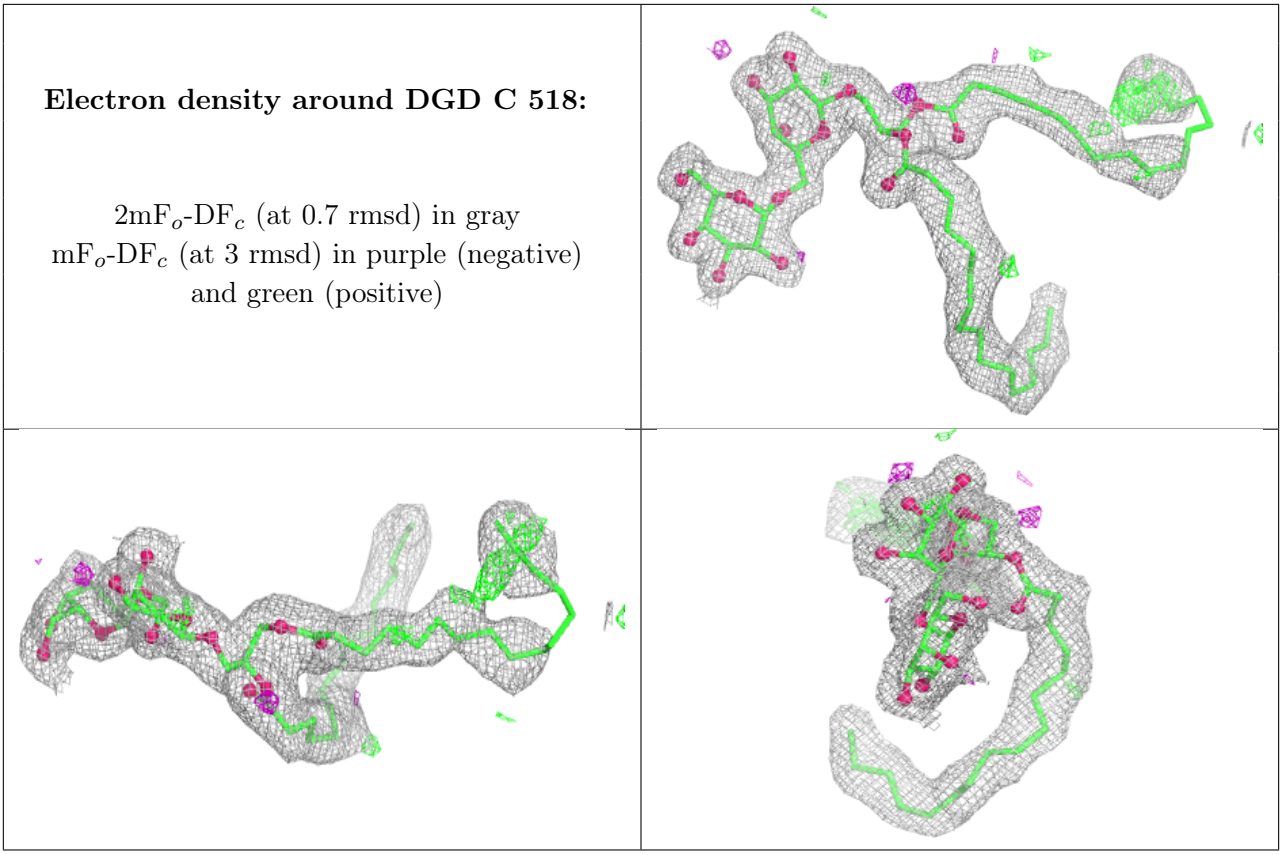






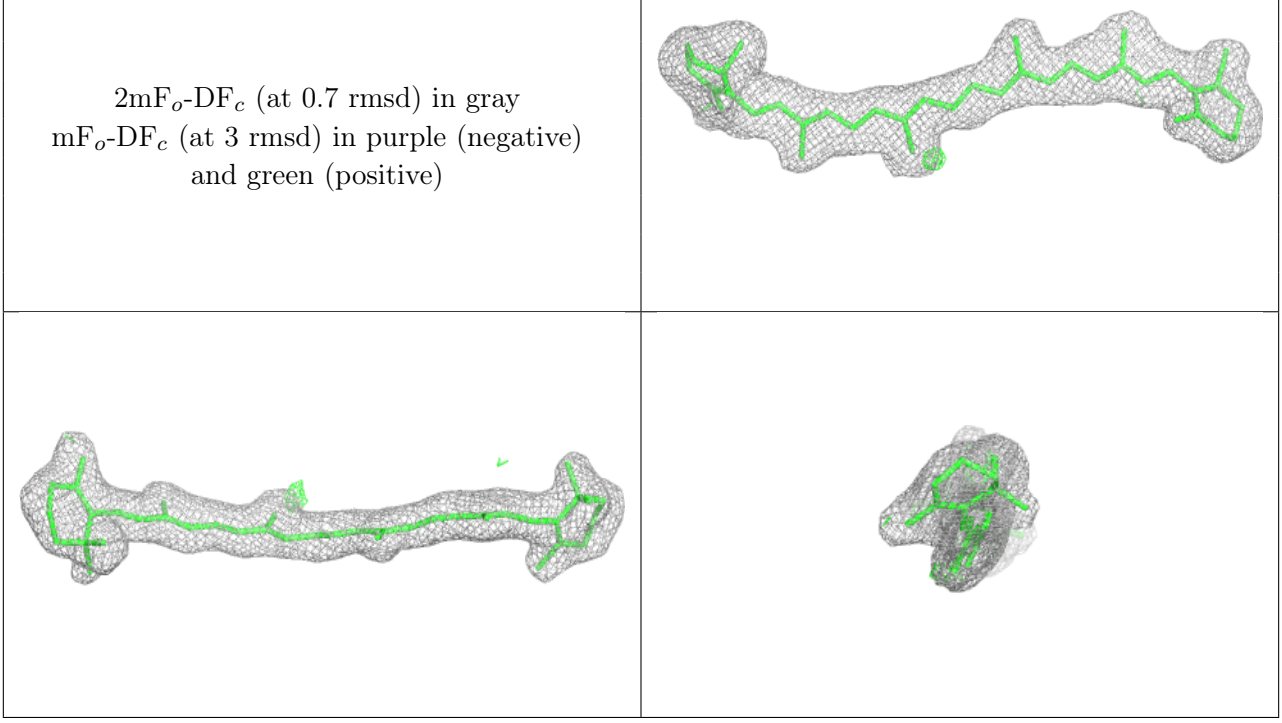
Electron density around DGD C 518:

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



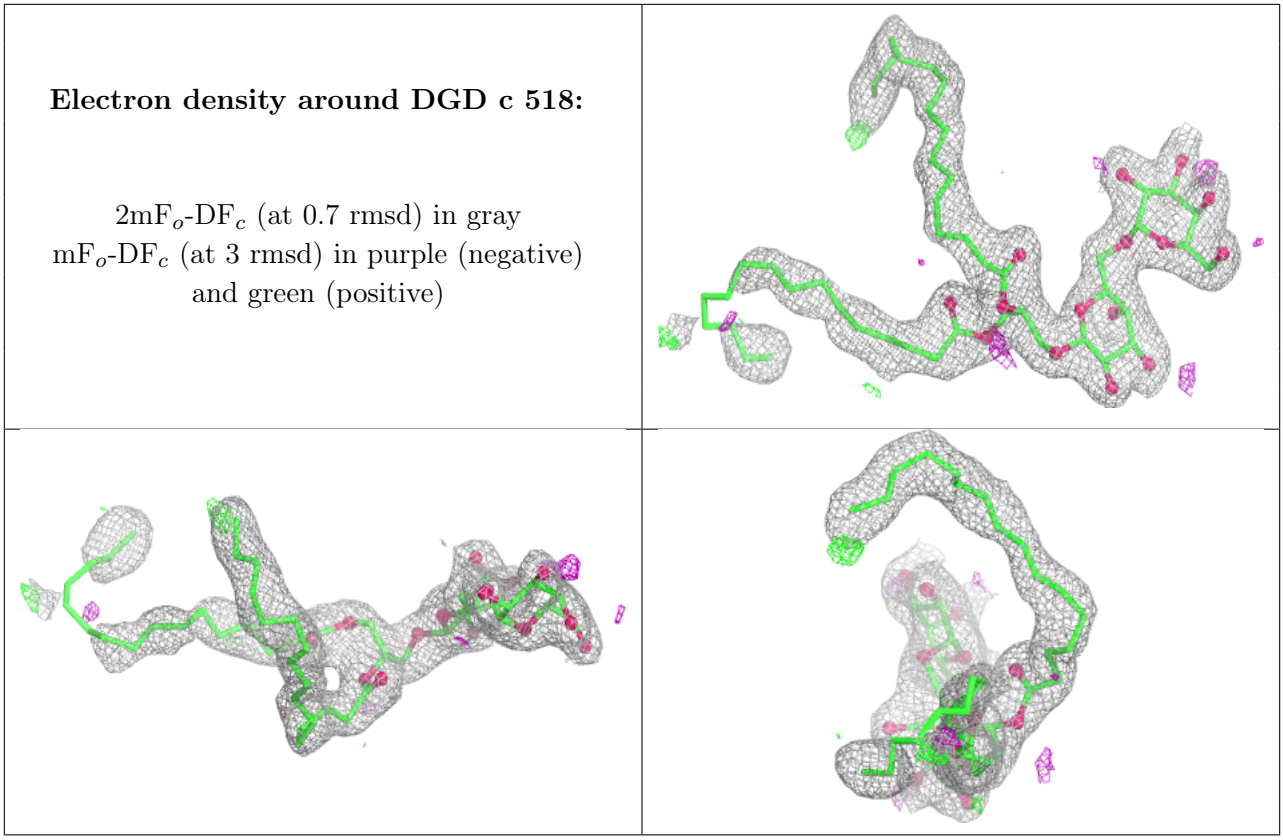
Electron density around BCR y 101:

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



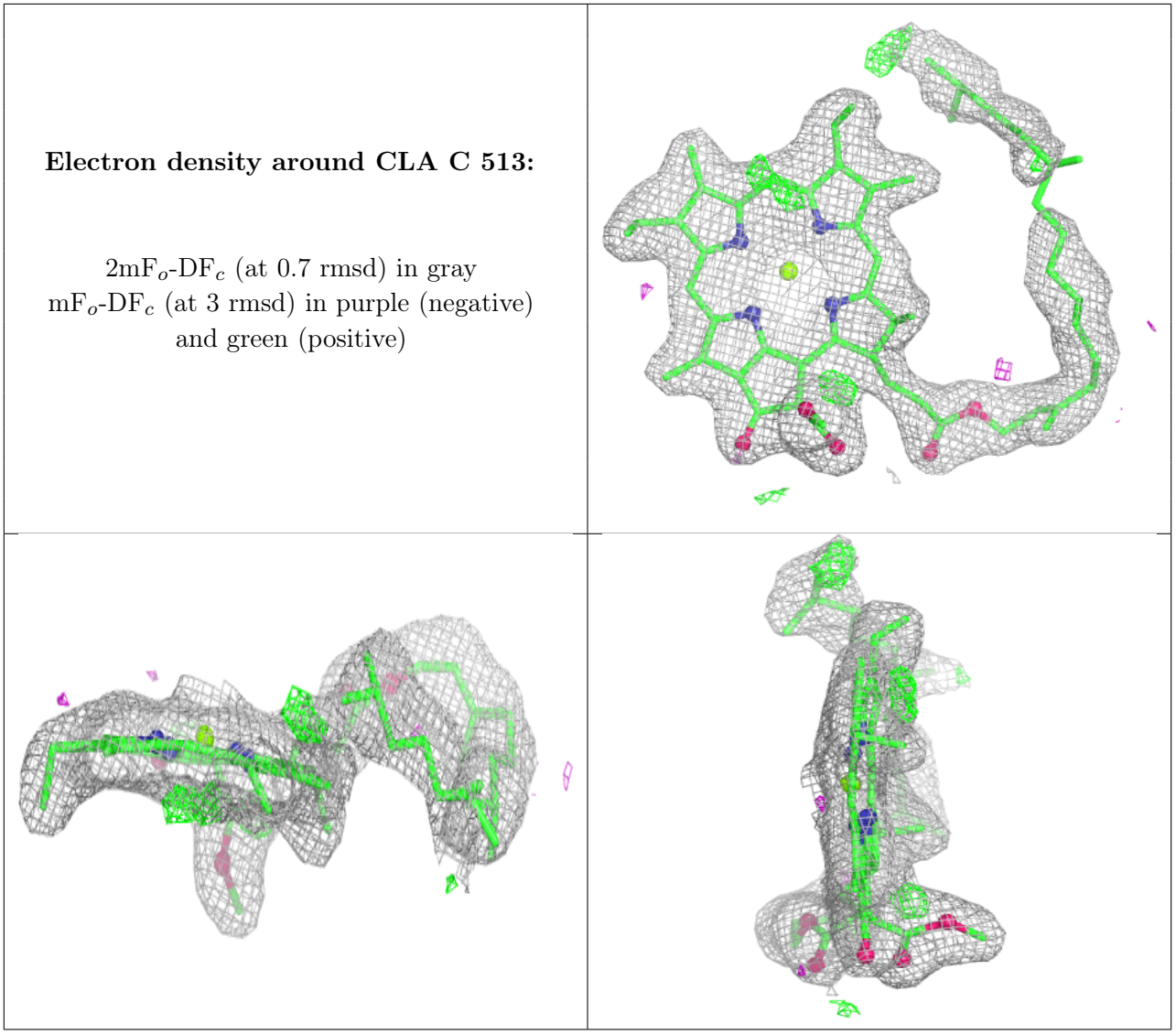
Electron density around DGD c 518:

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



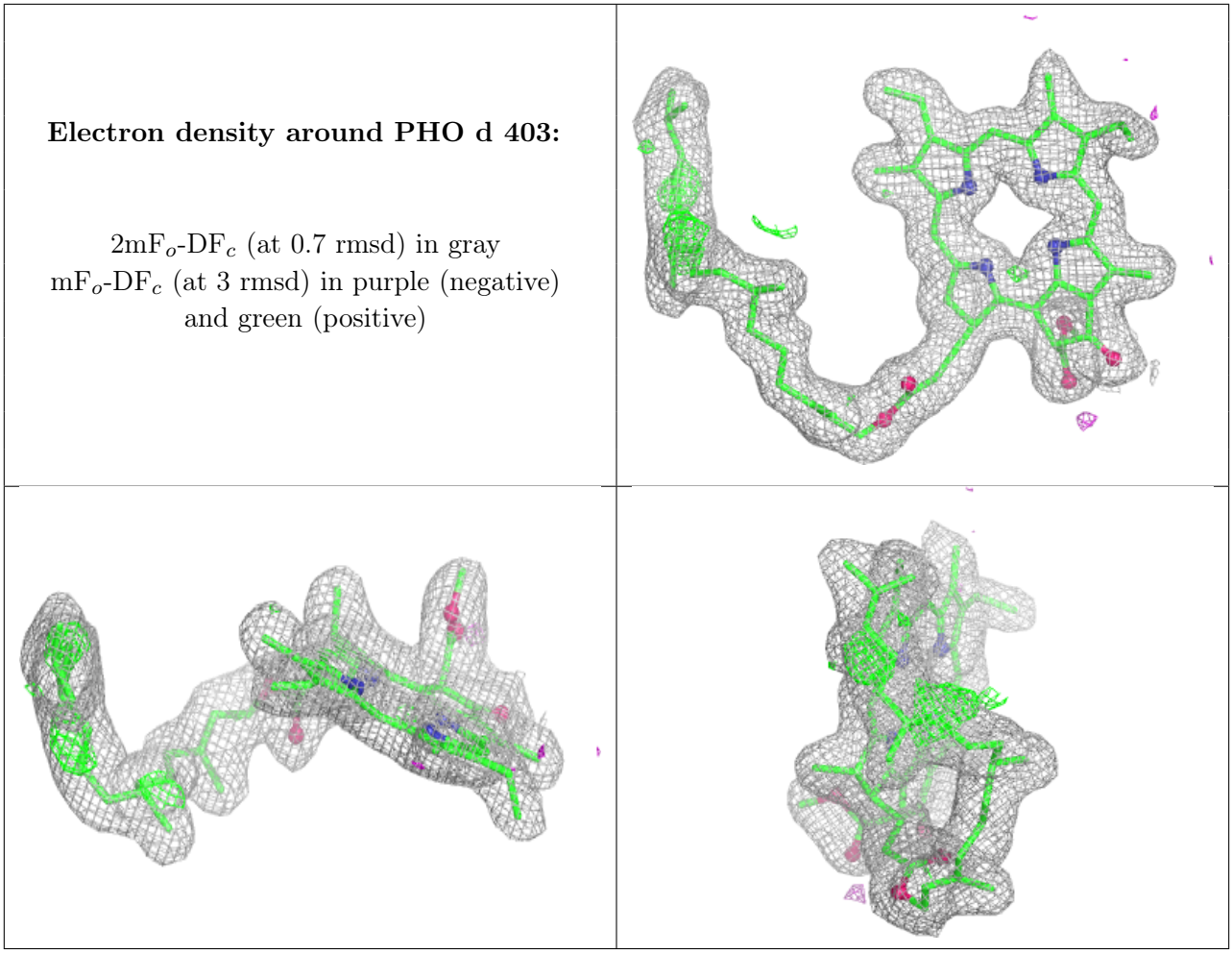
Electron density around CLA C 513:

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



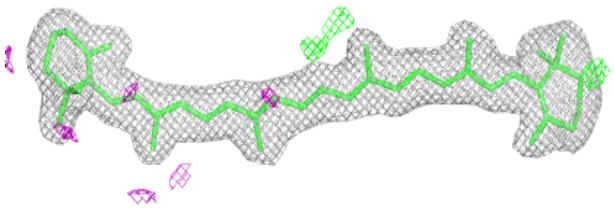
Electron density around PHO d 403:

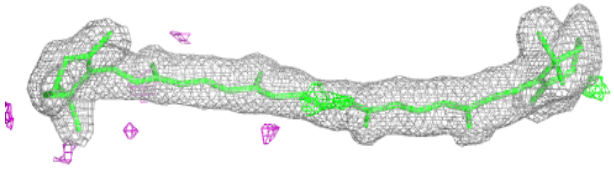
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

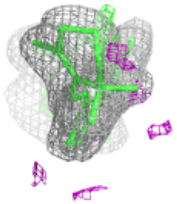


Electron density around BCR B 620:

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

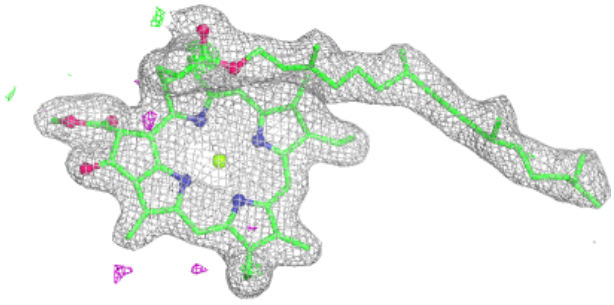


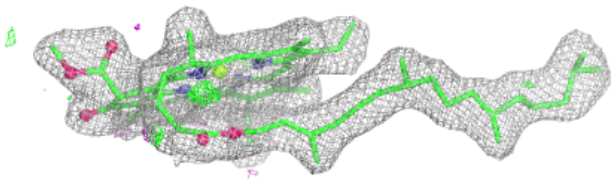


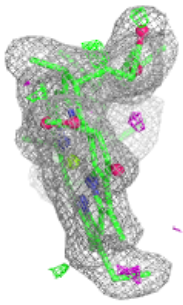


Electron density around CLA C 502:

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

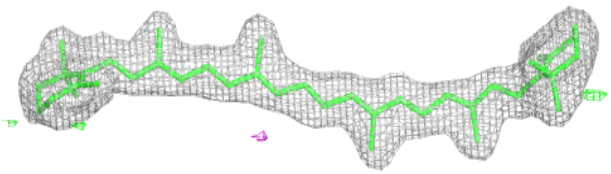


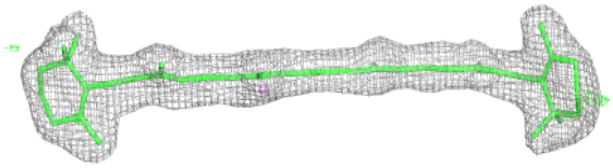


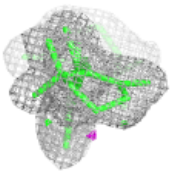


Electron density around BCR C 516:

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

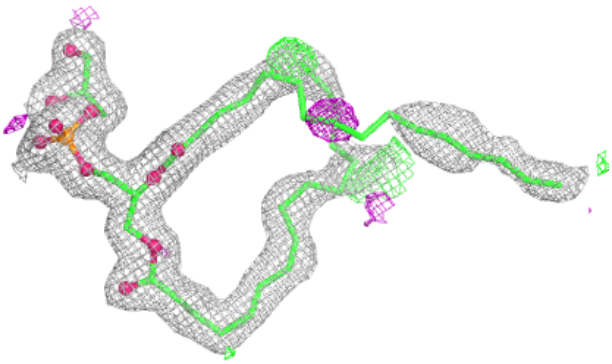


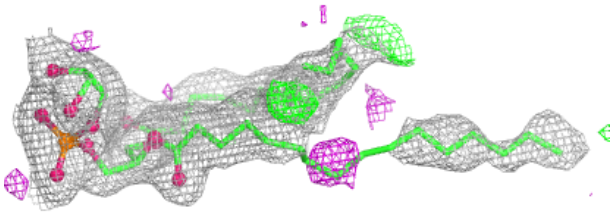


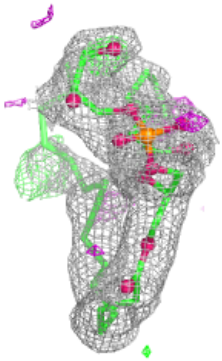


Electron density around LHG d 410:

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

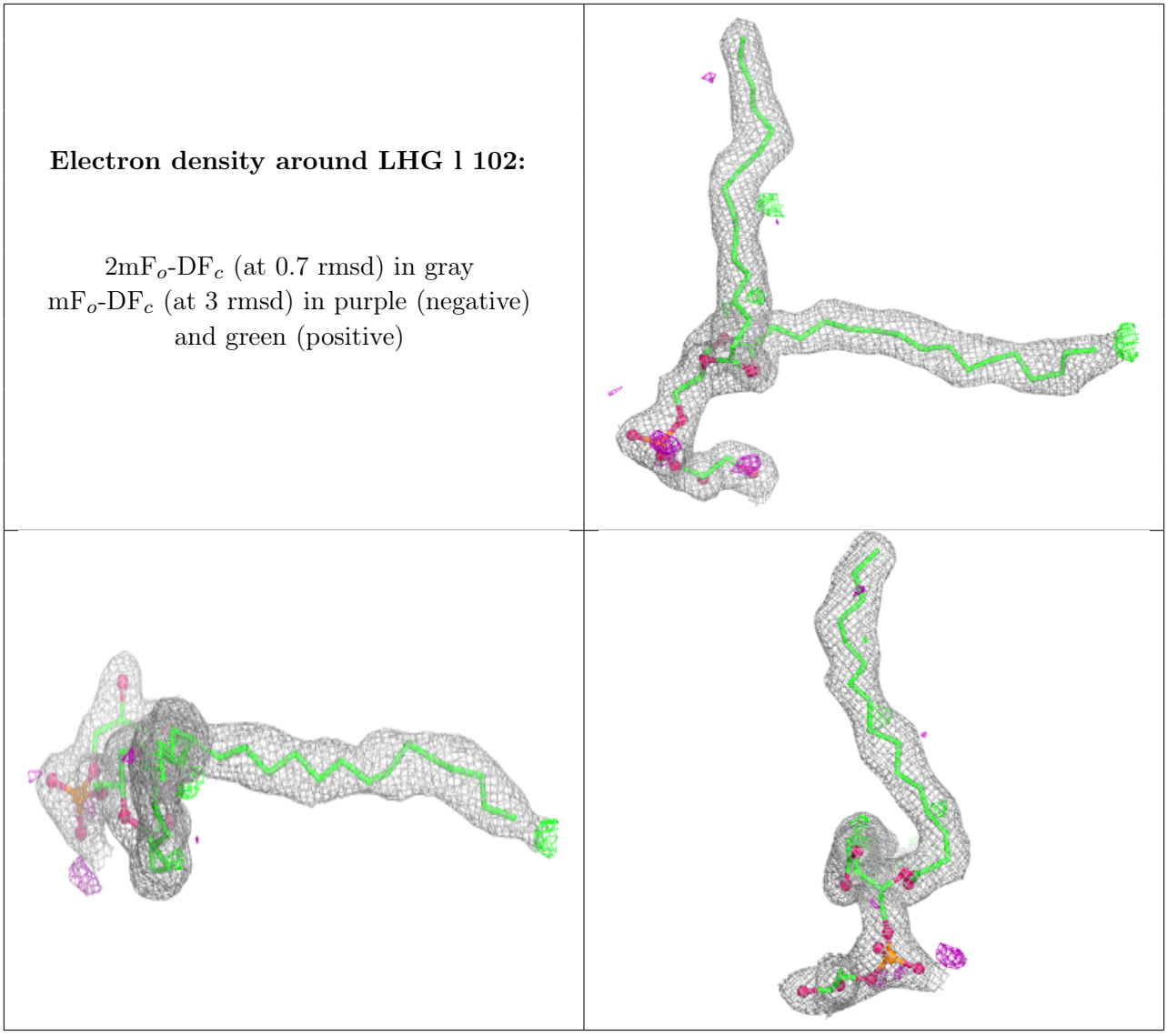






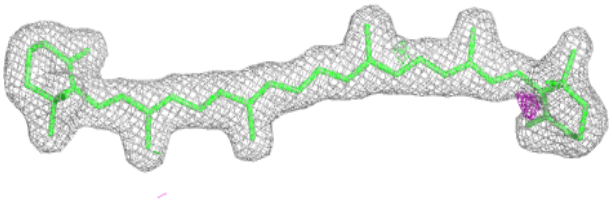
Electron density around LHG l 102:

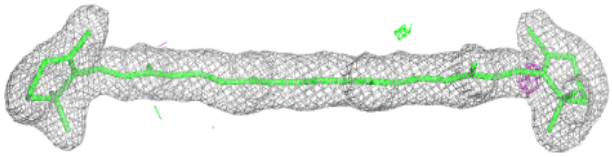
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

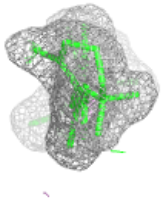


Electron density around BCR B 619:

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

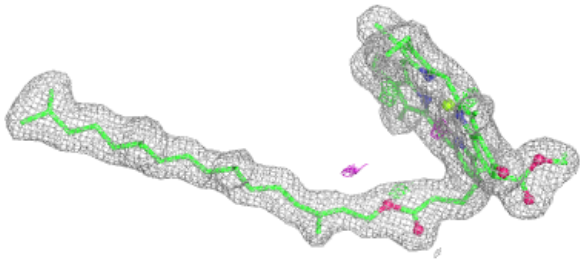


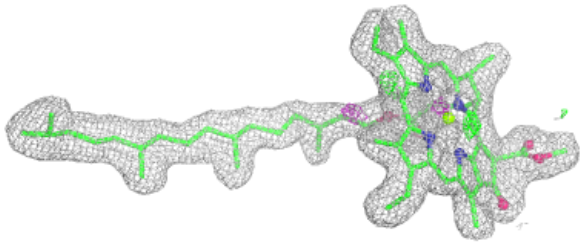


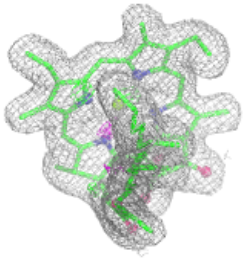


Electron density around CLA b 612:

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

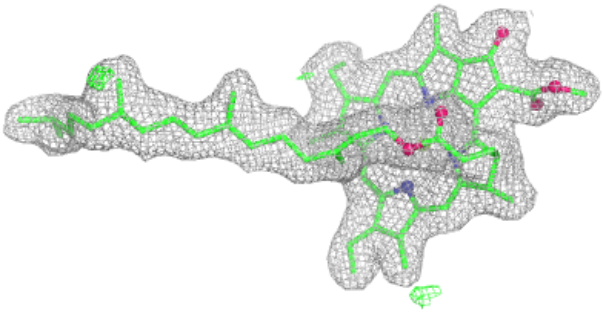


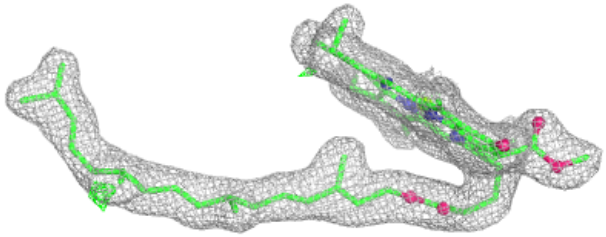


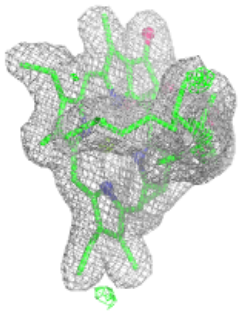


Electron density around CLA b 613:

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

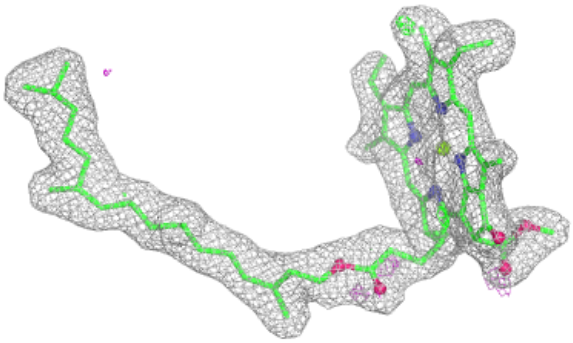


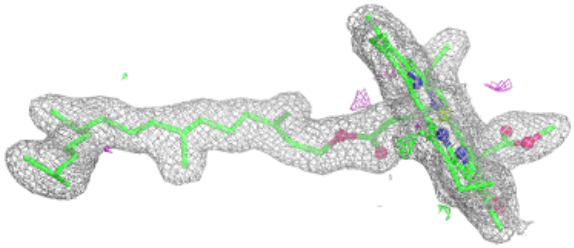


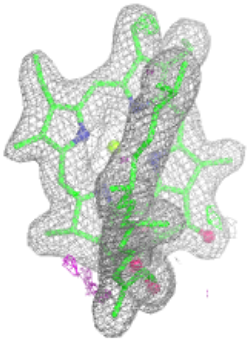


Electron density around CLA b 614:

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

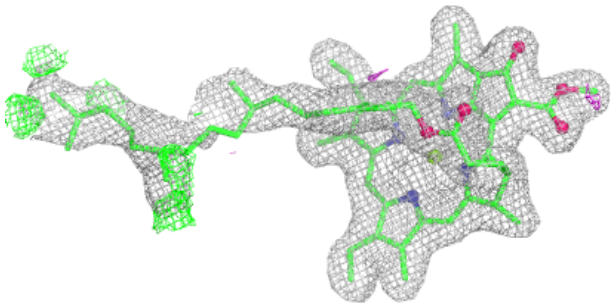


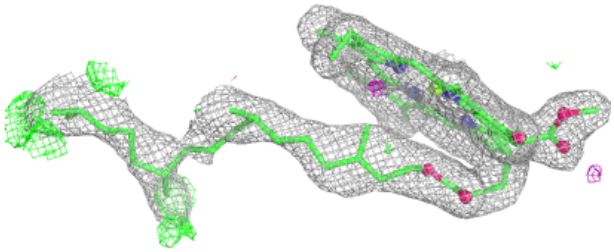


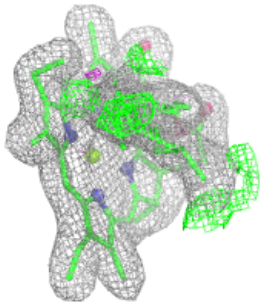


Electron density around CLA b 619:

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

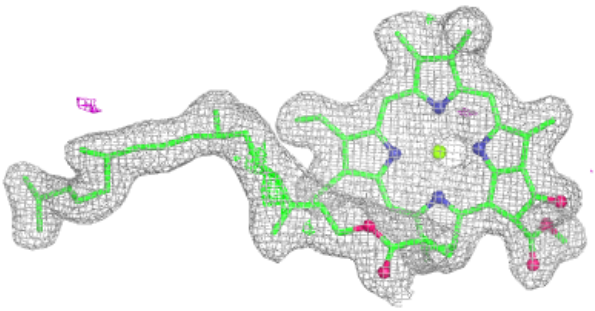


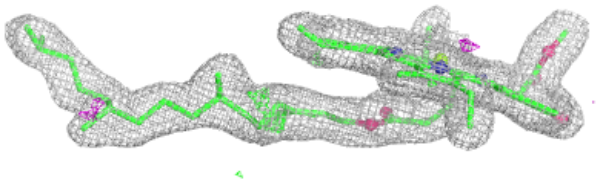


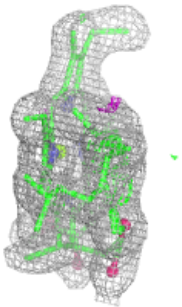


Electron density around CLA B 604:

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

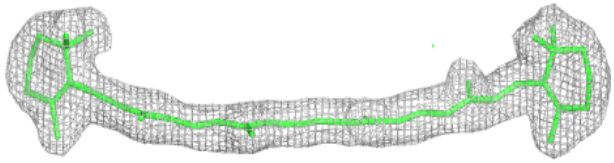


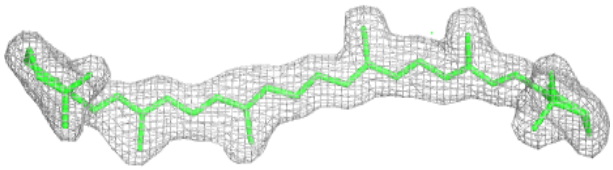


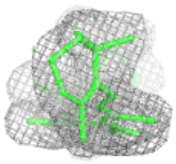


Electron density around BCR K 101:

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

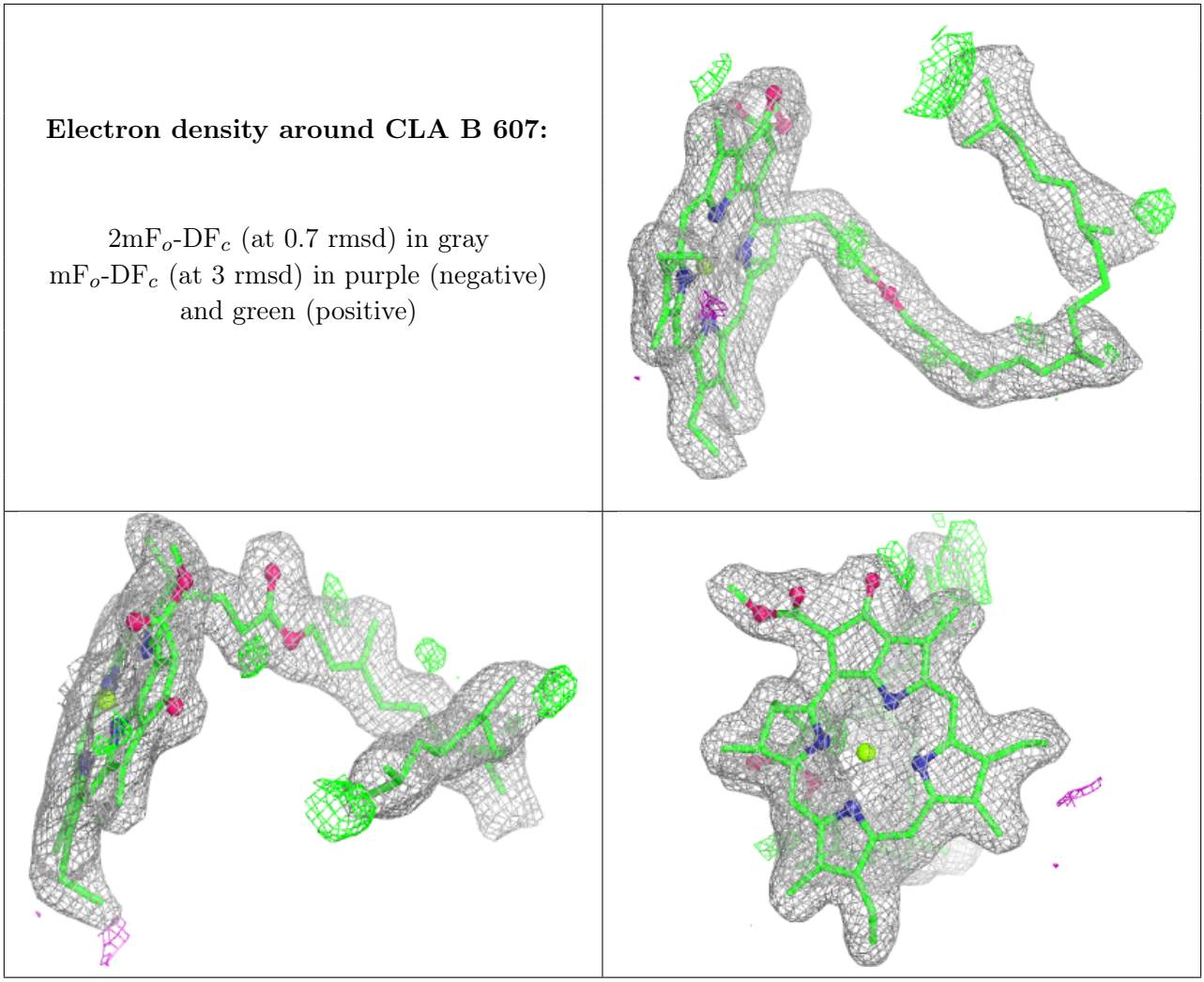






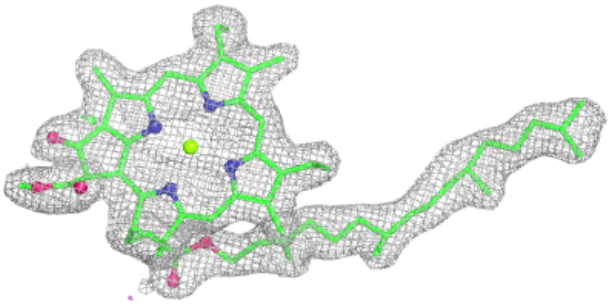
Electron density around CLA B 607:

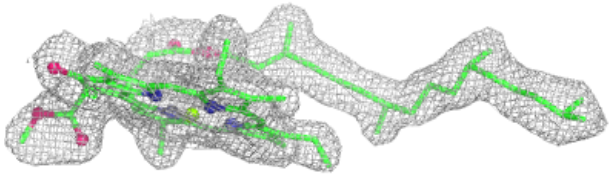
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

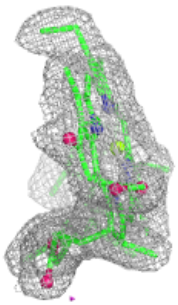


Electron density around CLA c 503:

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

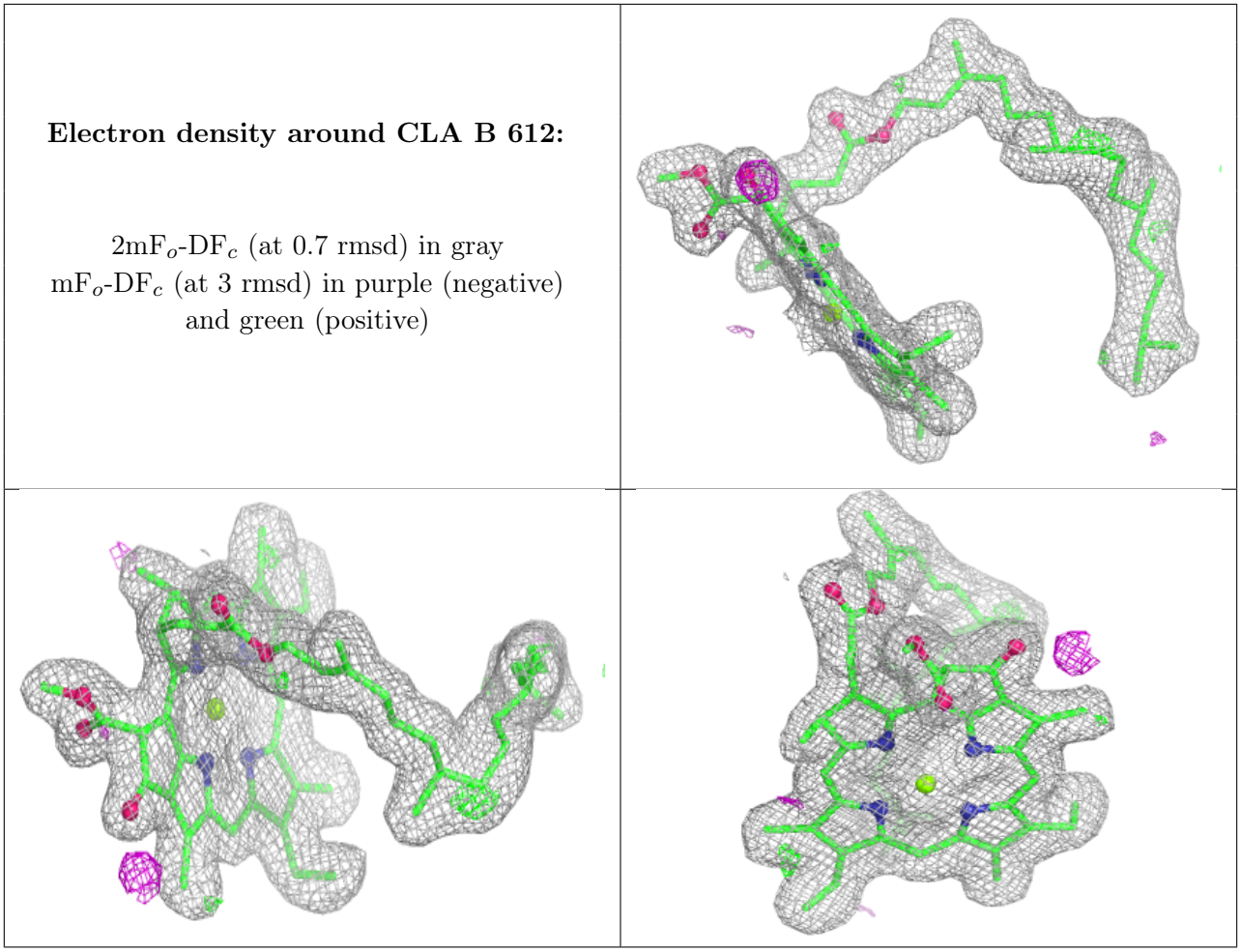






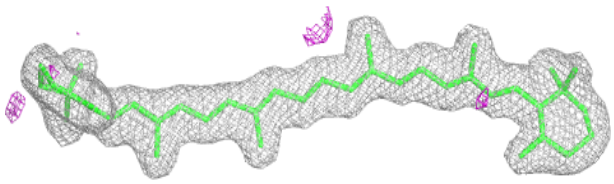
Electron density around CLA B 612:

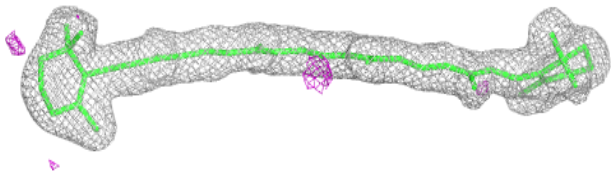
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

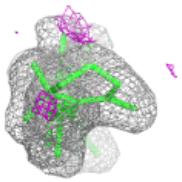


Electron density around BCR b 622:

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

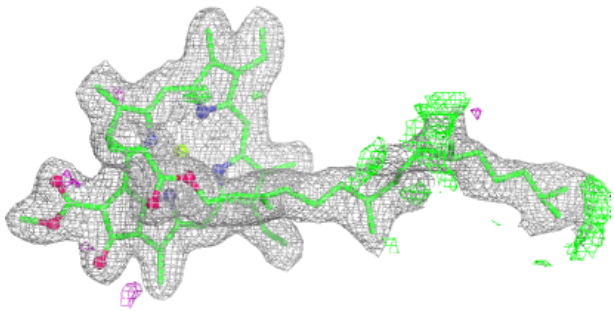


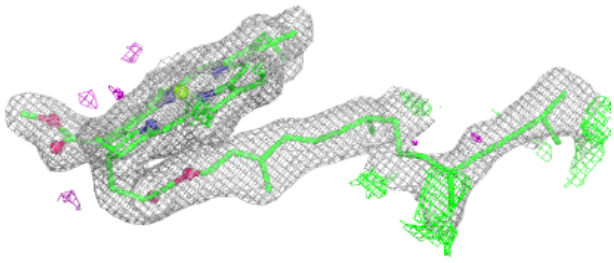


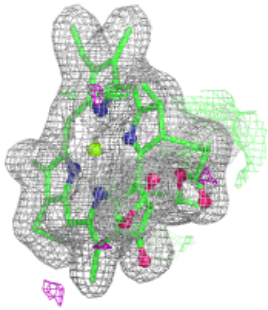


Electron density around CLA B 615:

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

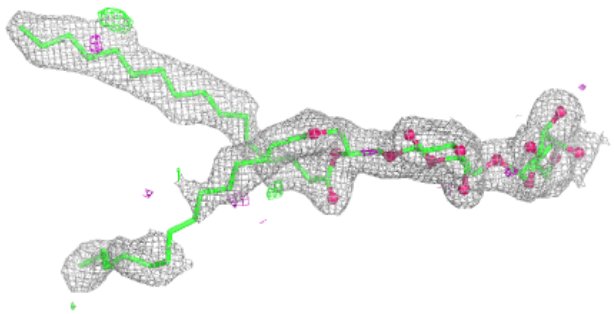


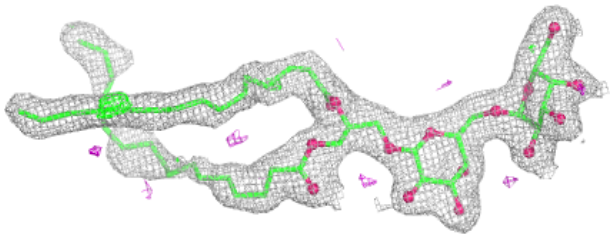


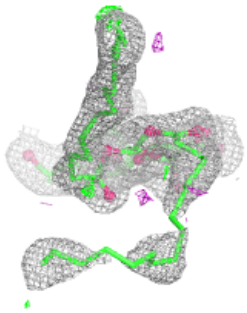


Electron density around DGD C 517:

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

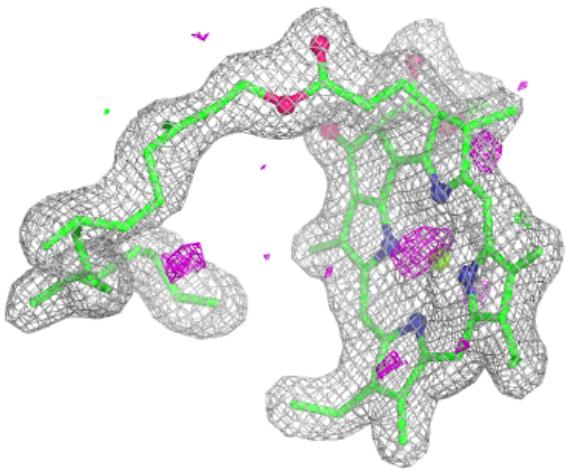


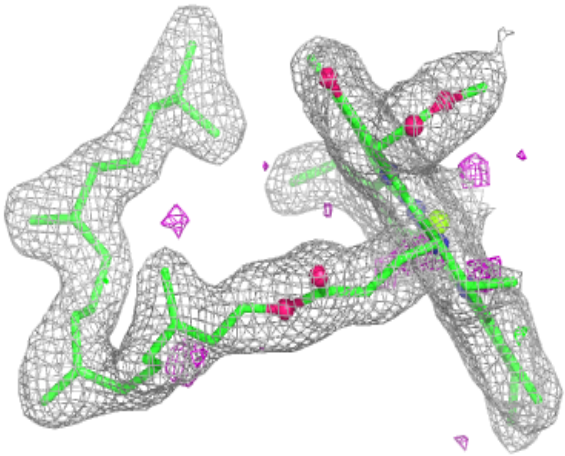


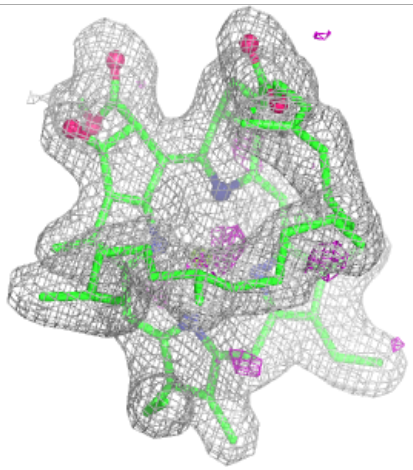


Electron density around CLA C 504:

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

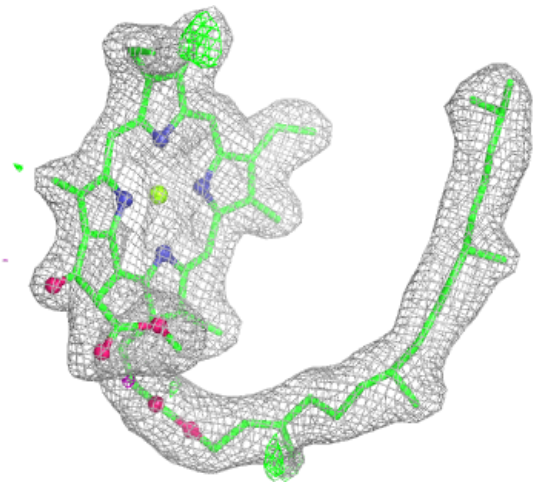


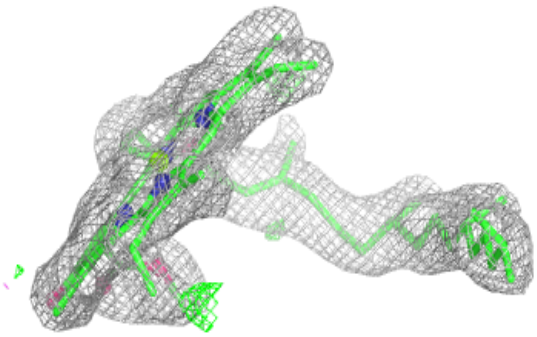


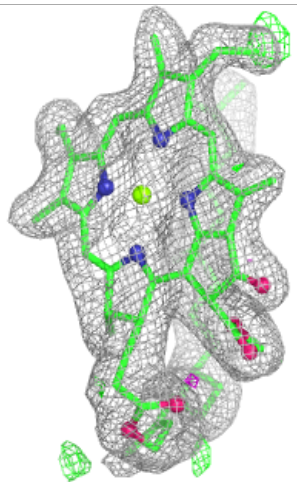


Electron density around CLA c 509:

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

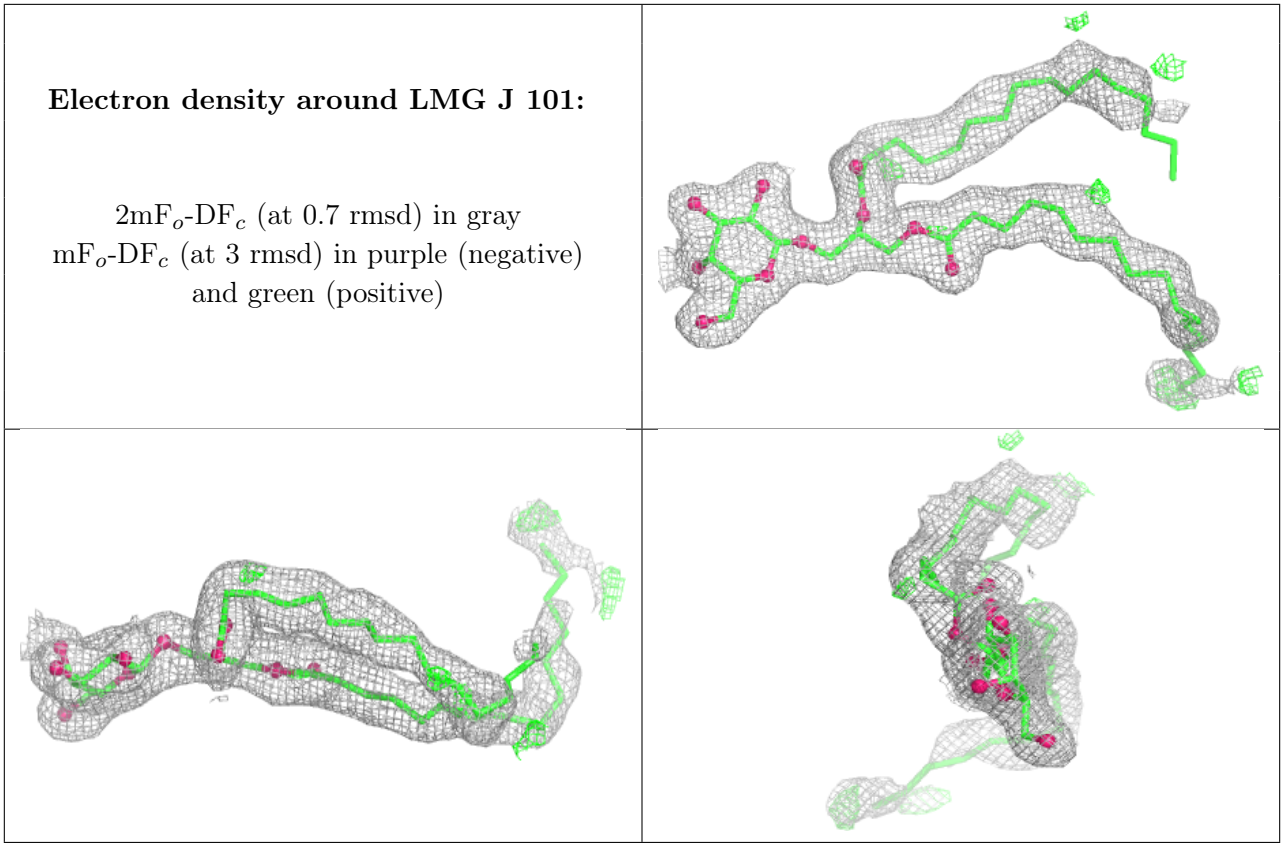






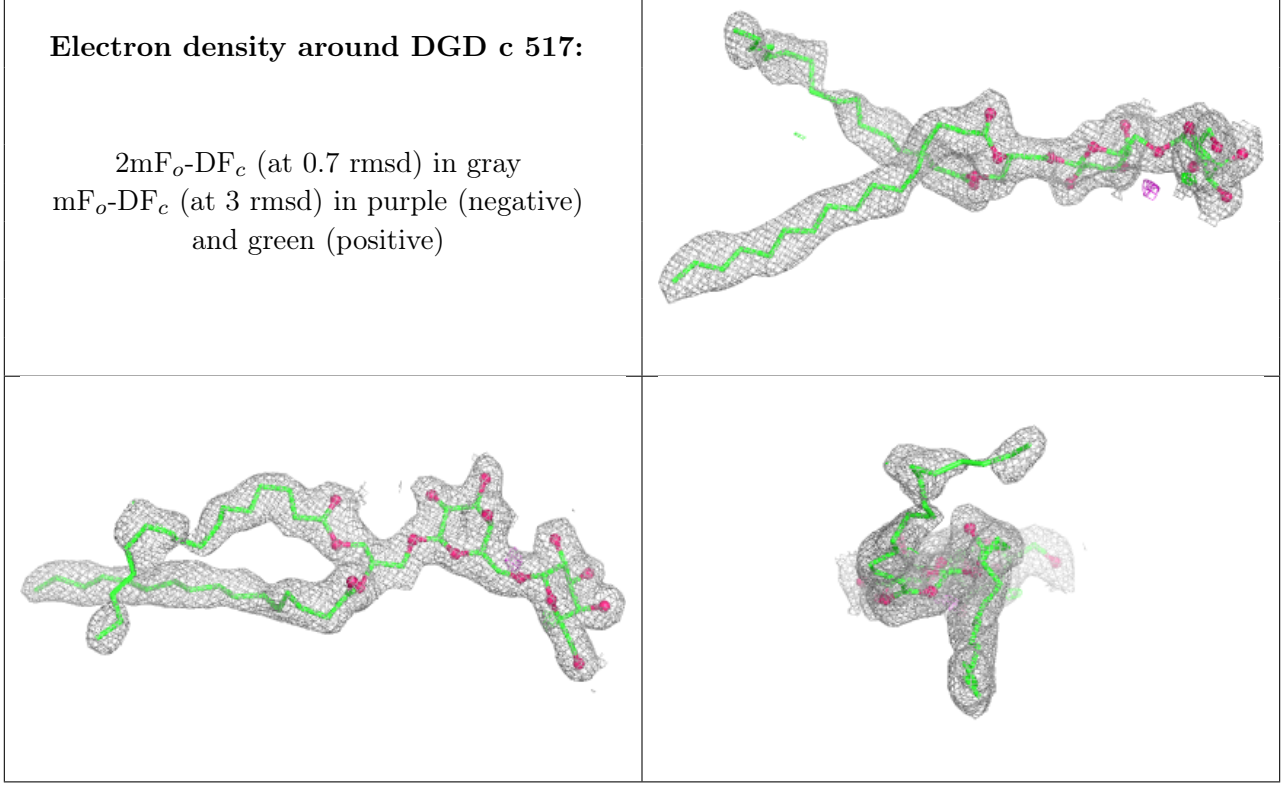
Electron density around LMG J 101:

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



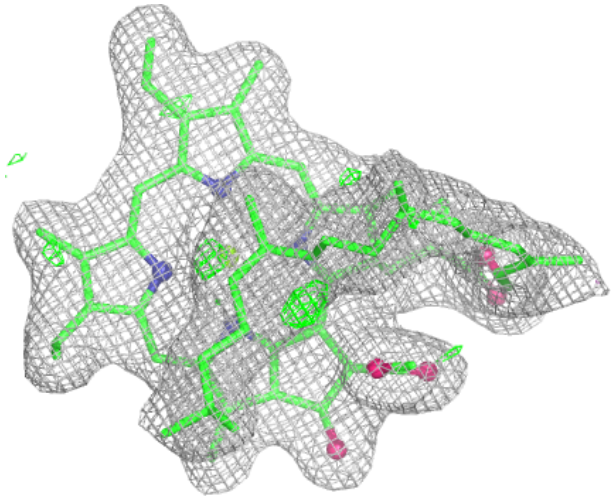
Electron density around DGD c 517:

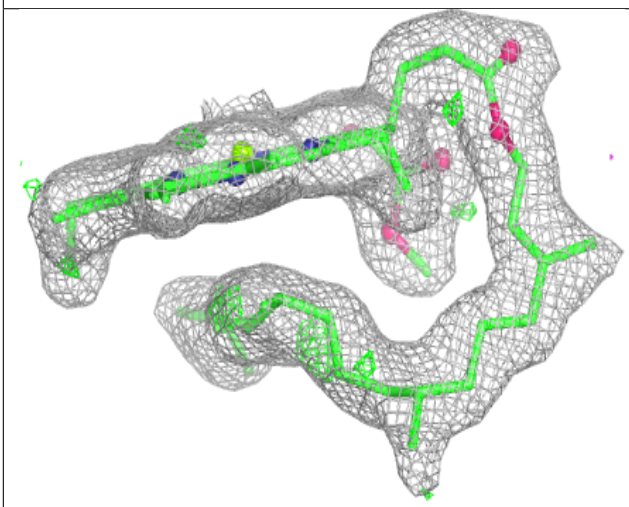
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 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)

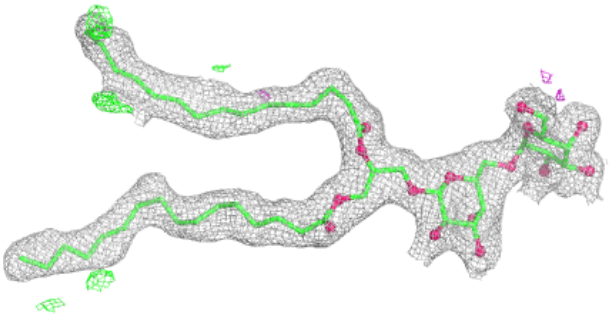


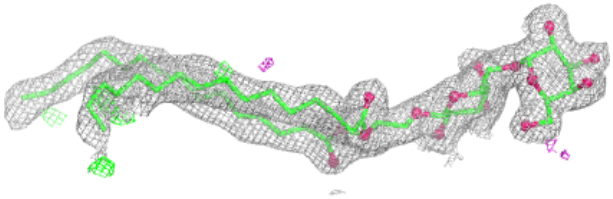


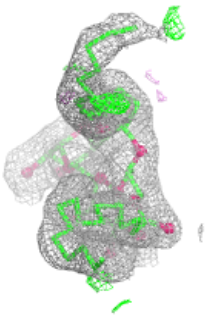


Electron density around DGD c 519:

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

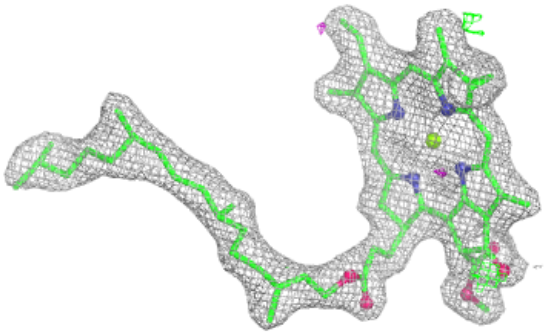


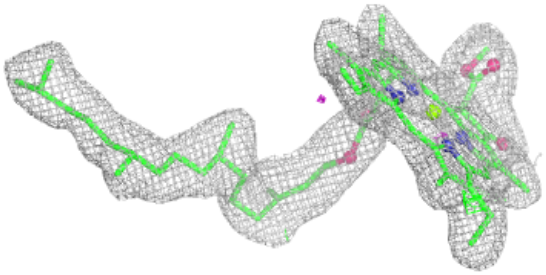


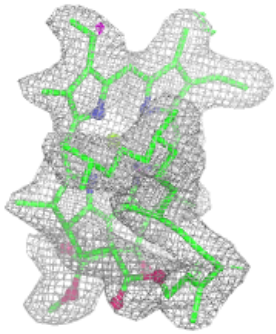


Electron density around CLA c 513:

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

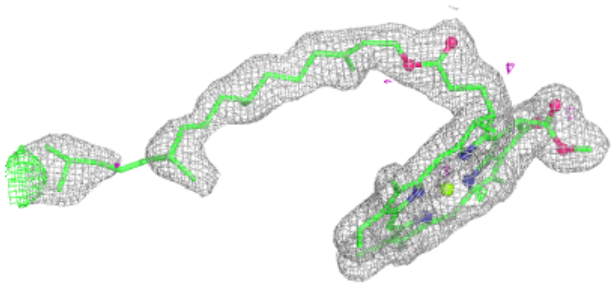


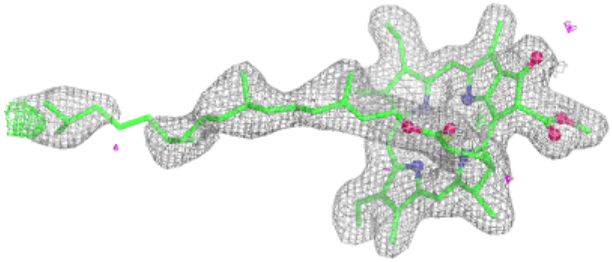


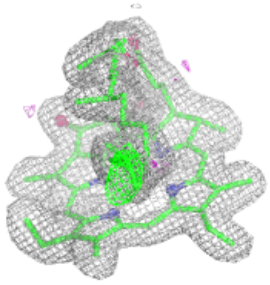


Electron density around CLA C 505:

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

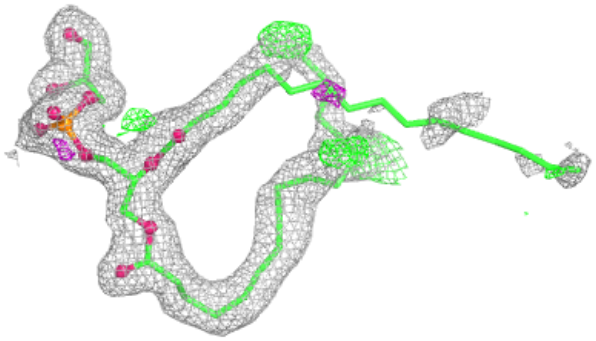


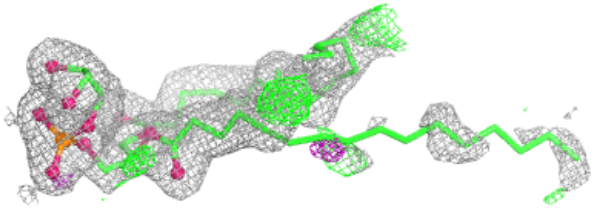


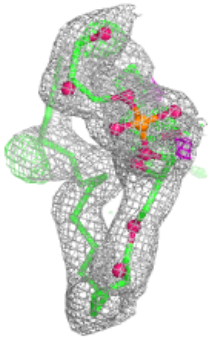


Electron density around LHG D 410:

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

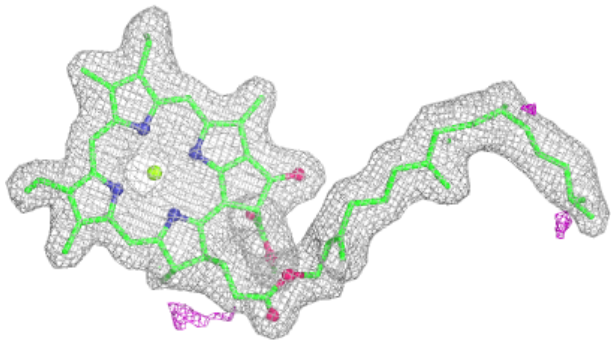


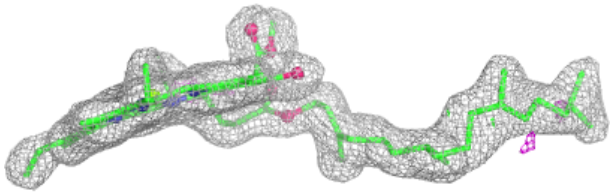


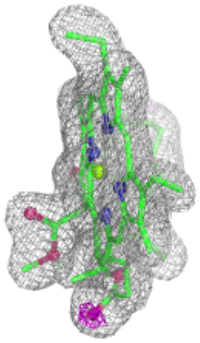


Electron density around CLA b 607:

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

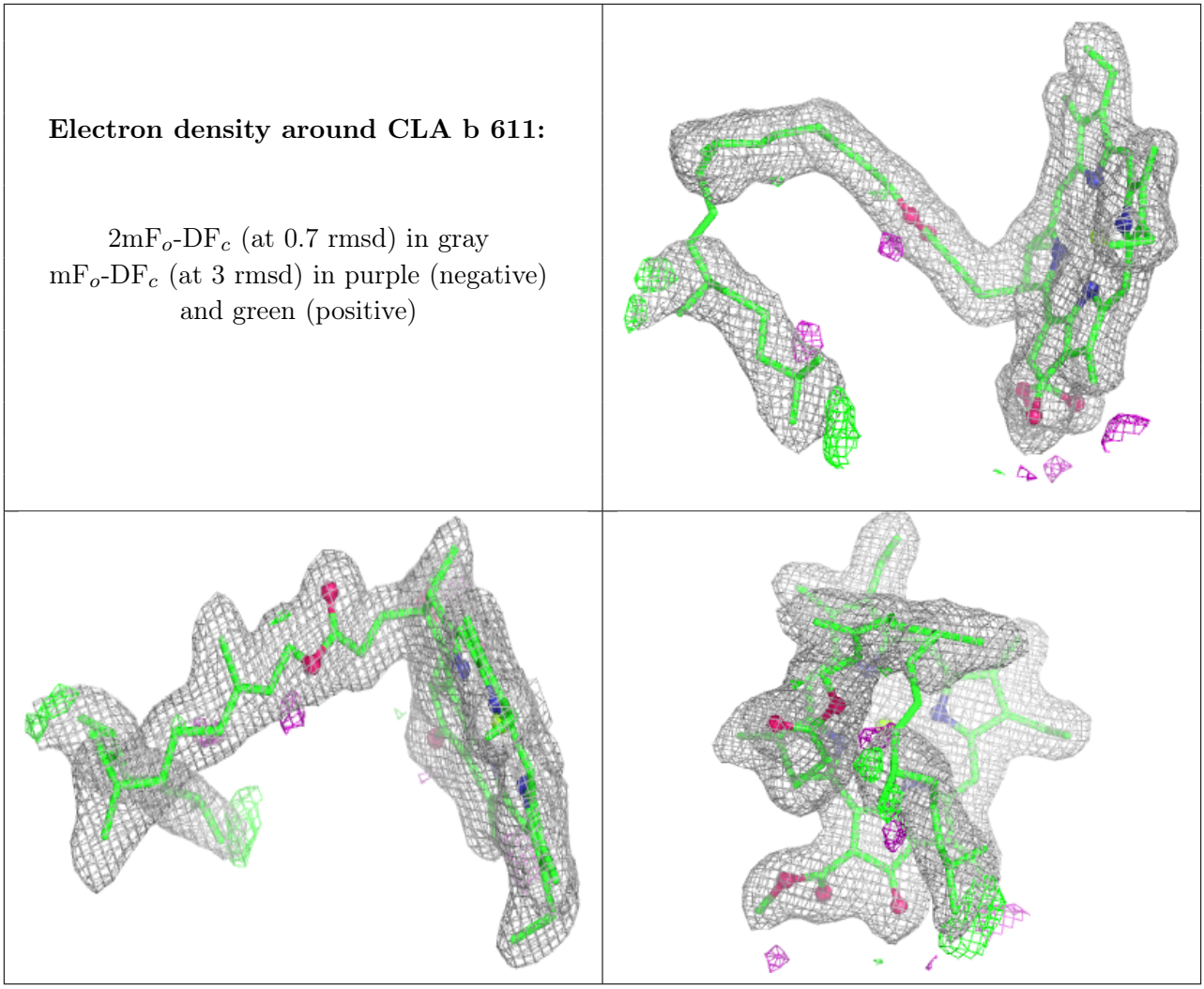






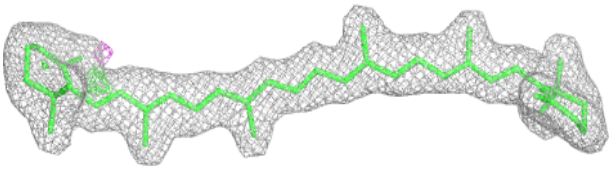
Electron density around CLA b 611:

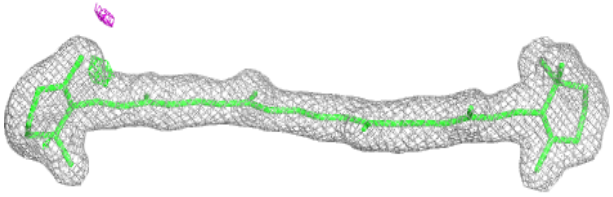
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

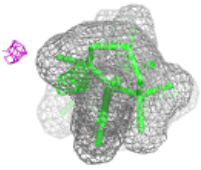


Electron density around BCR A 410:

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

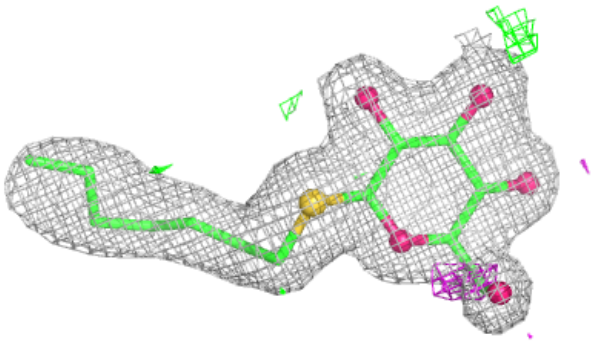


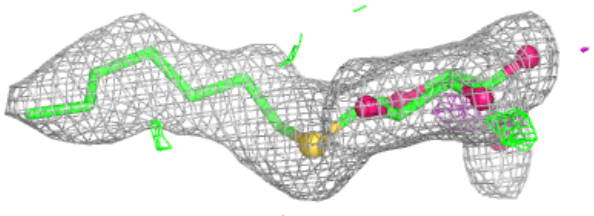


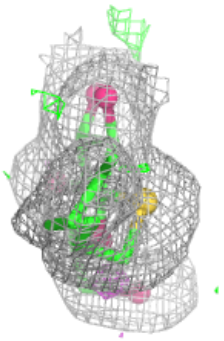


Electron density around HTG B 622:

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

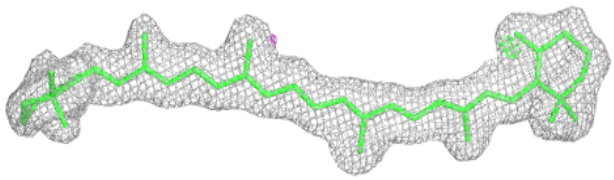


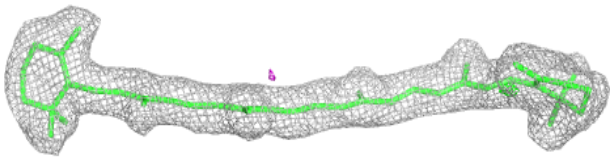


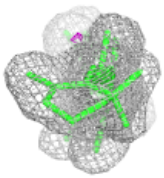


Electron density around BCR B 618:

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

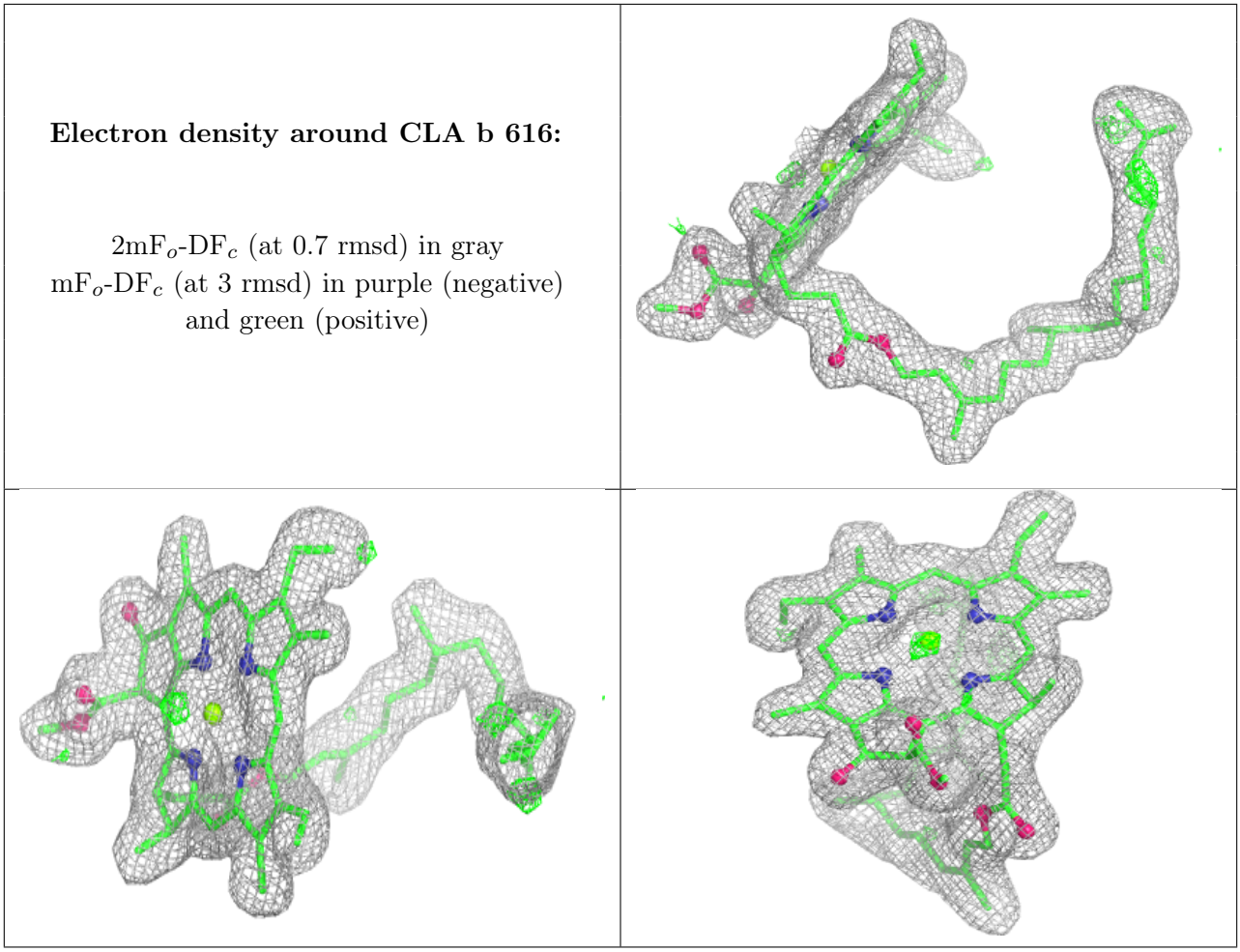






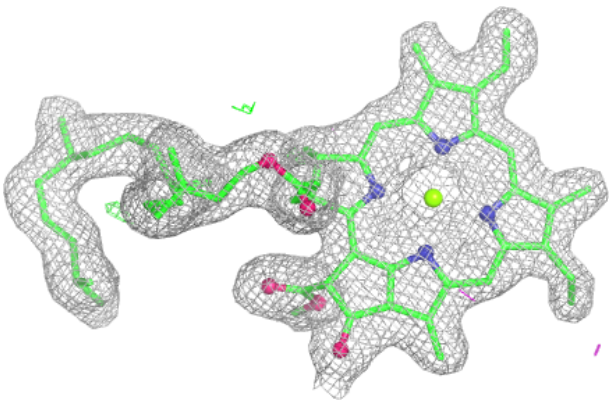
Electron density around CLA b 616:

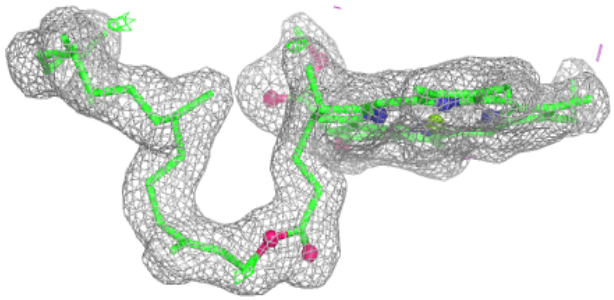
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 617:

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

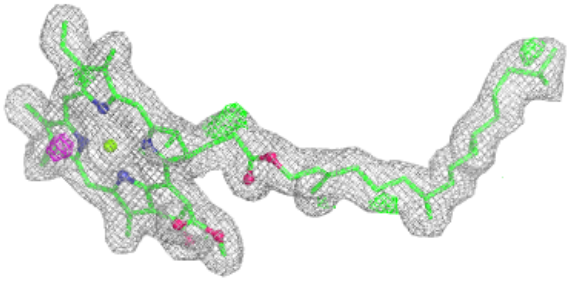


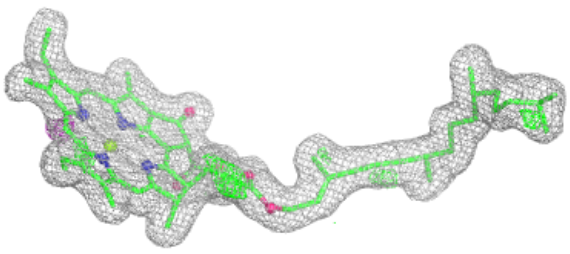


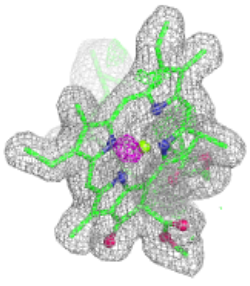


Electron density around CLA A 405:

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

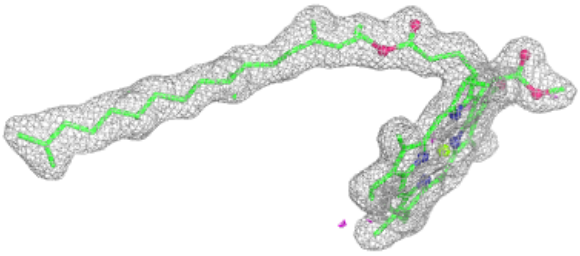


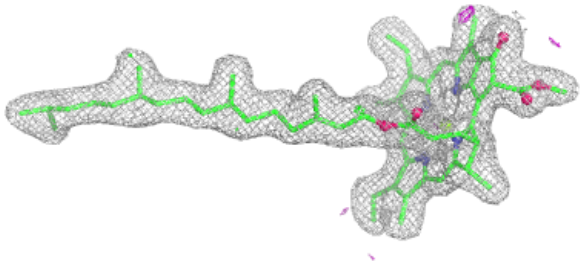


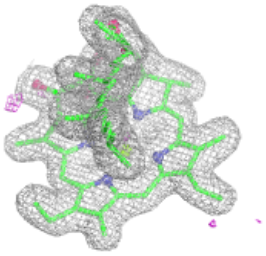


Electron density around CLA B 608:

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

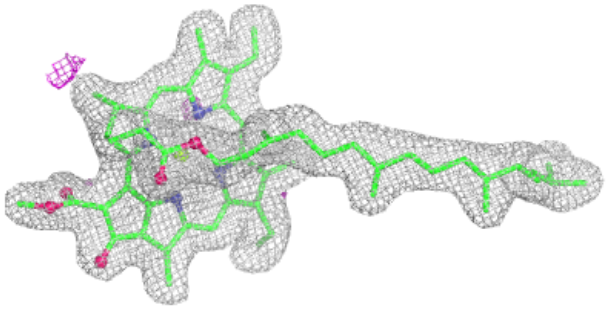


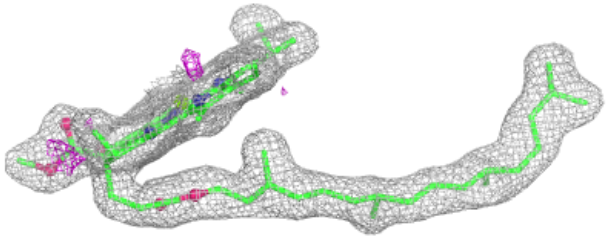


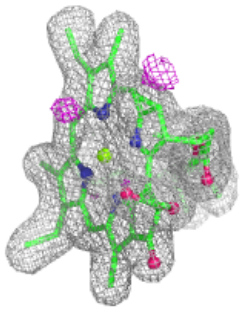


Electron density around CLA B 609:

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

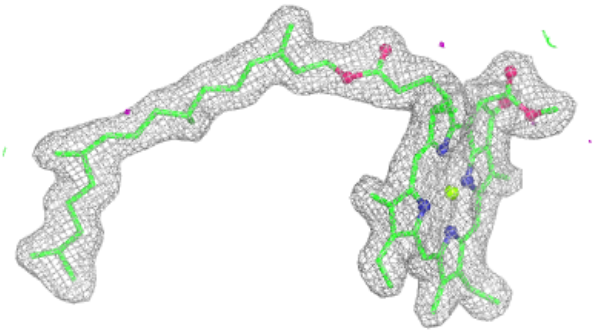


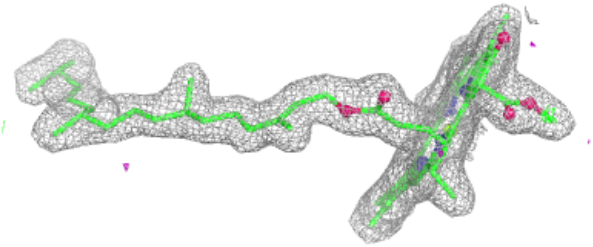


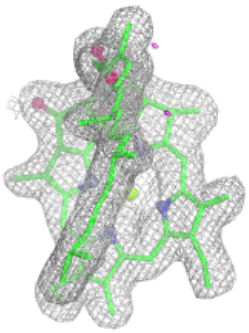


Electron density around CLA B 610:

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

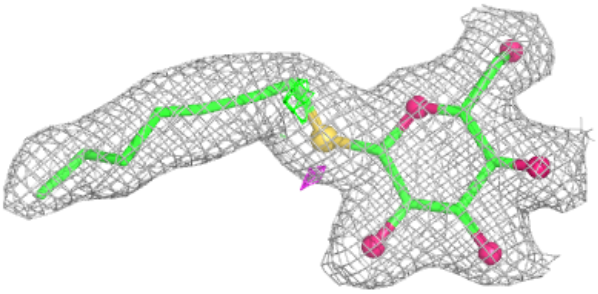


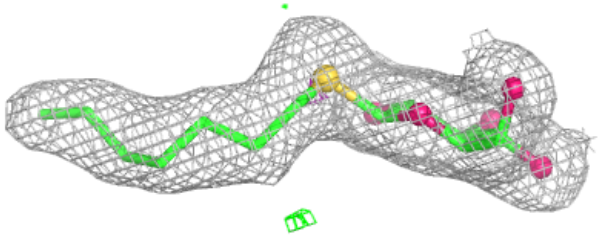


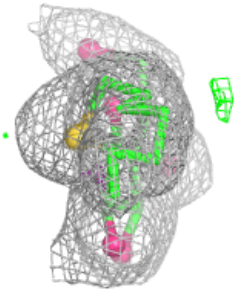


Electron density around HTG O 303:

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

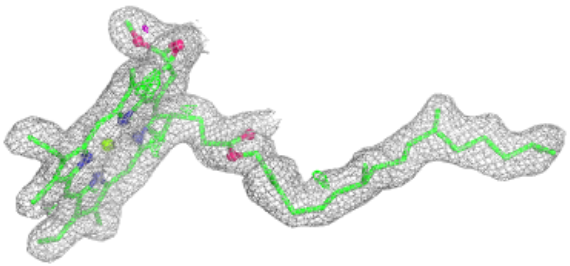


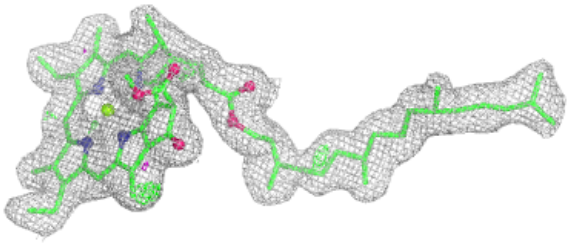


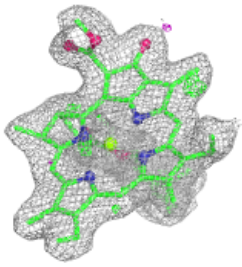


Electron density around CLA c 504:

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

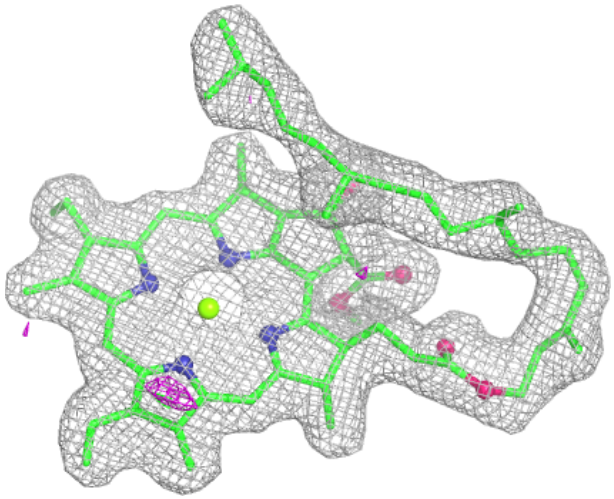


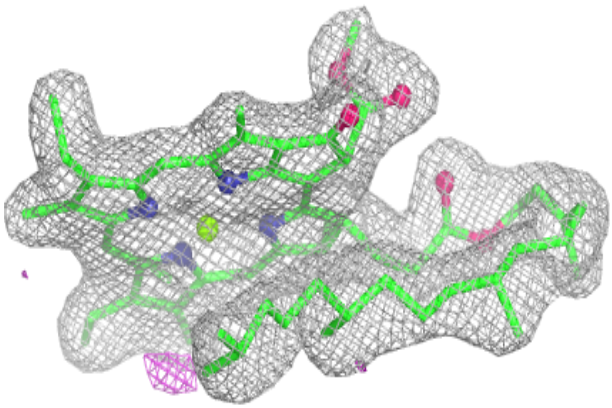


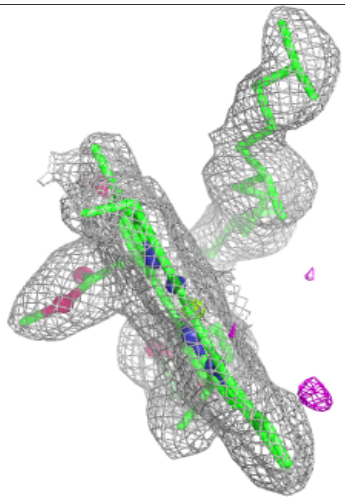


Electron density around CLA C 510:

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

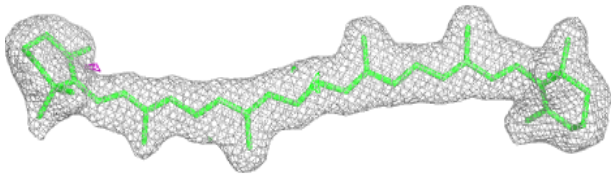


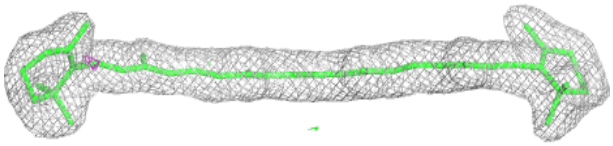


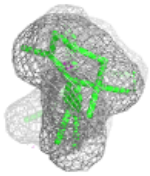


Electron density around BCR b 623:

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

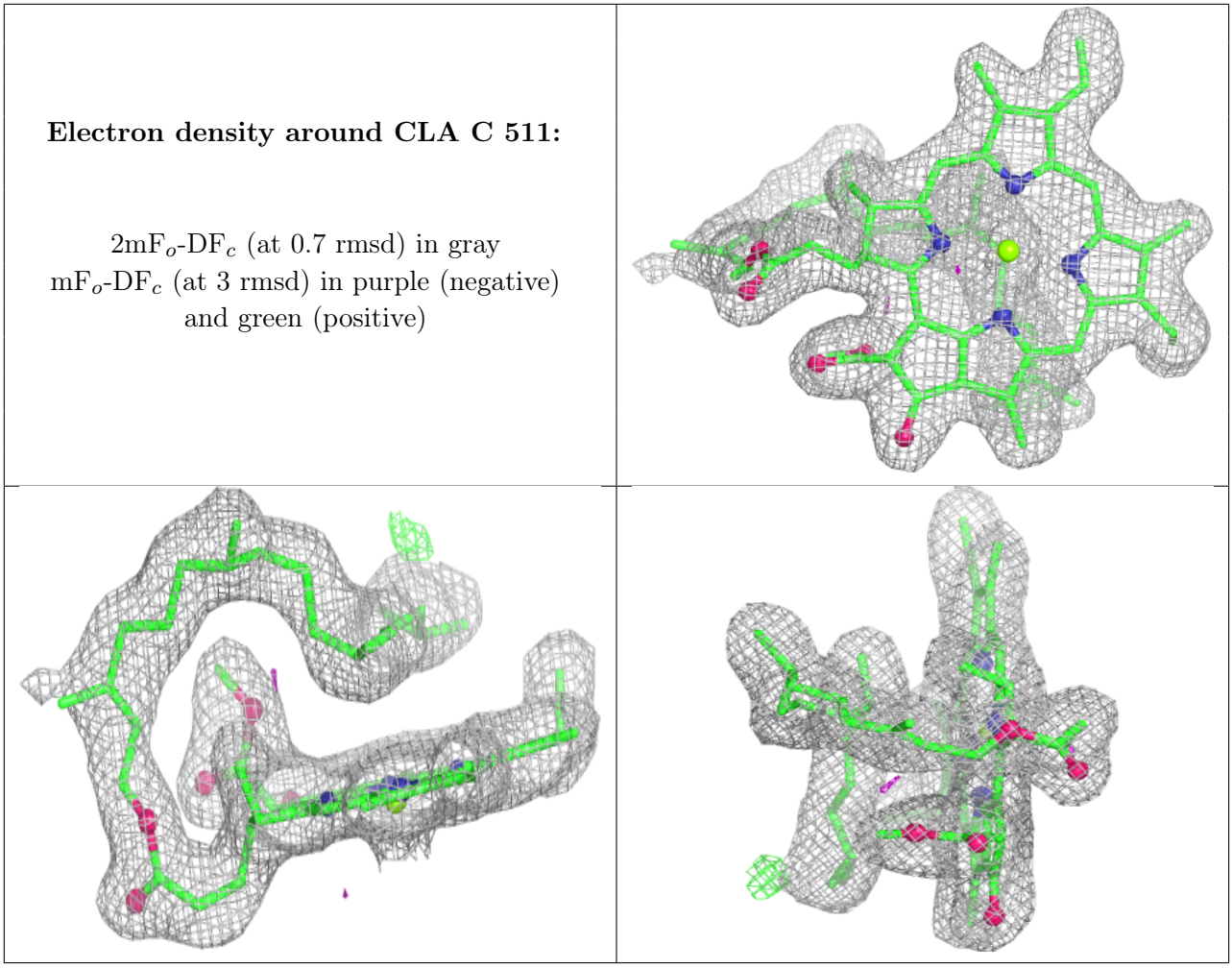






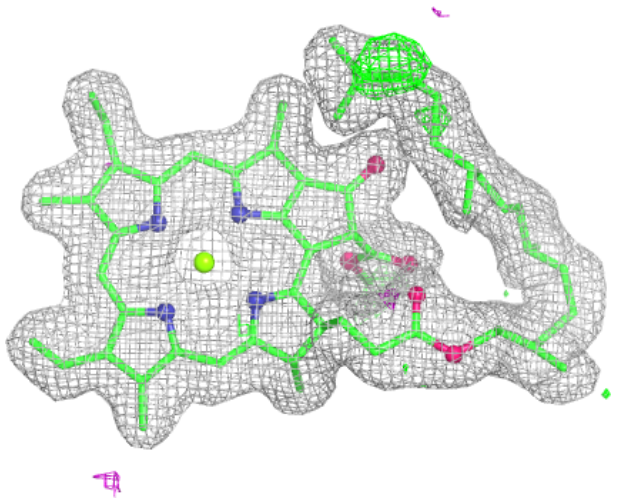
Electron density around CLA C 511:

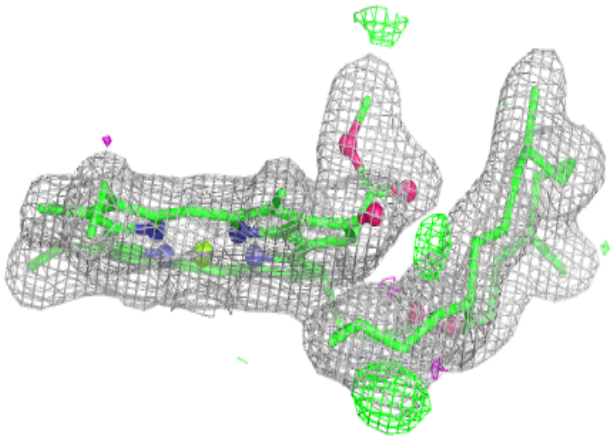
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

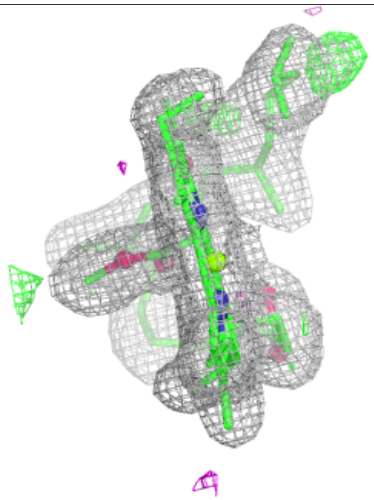


Electron density around CLA B 611:

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

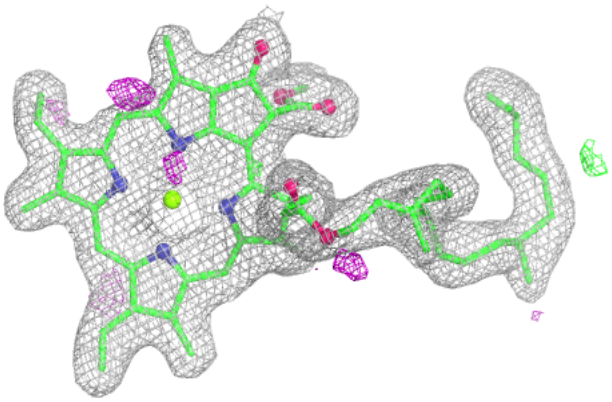


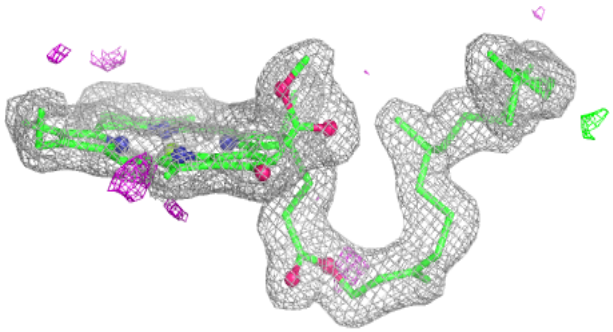


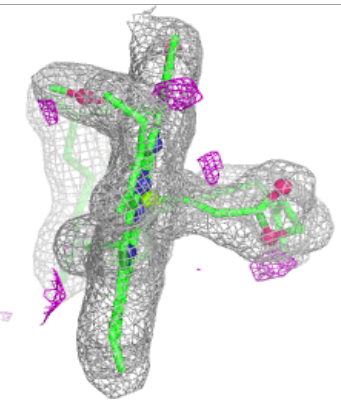


Electron density around CLA B 613:

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

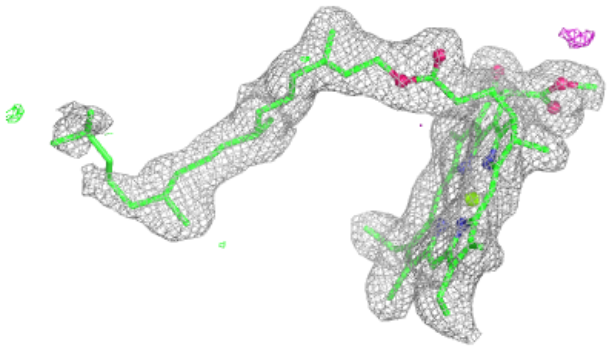


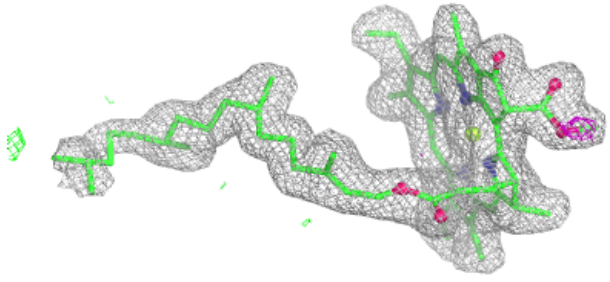


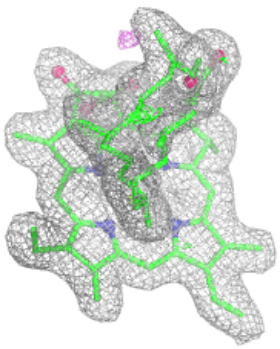


Electron density around CLA c 510:

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

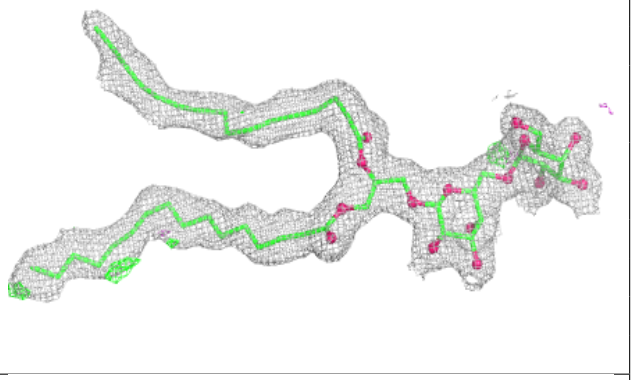


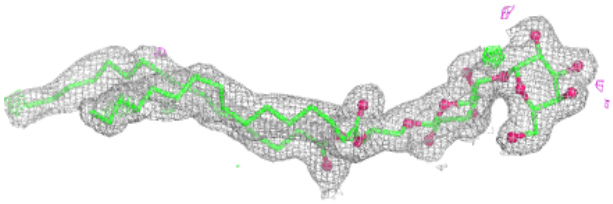




Electron density around DGD C 519:

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

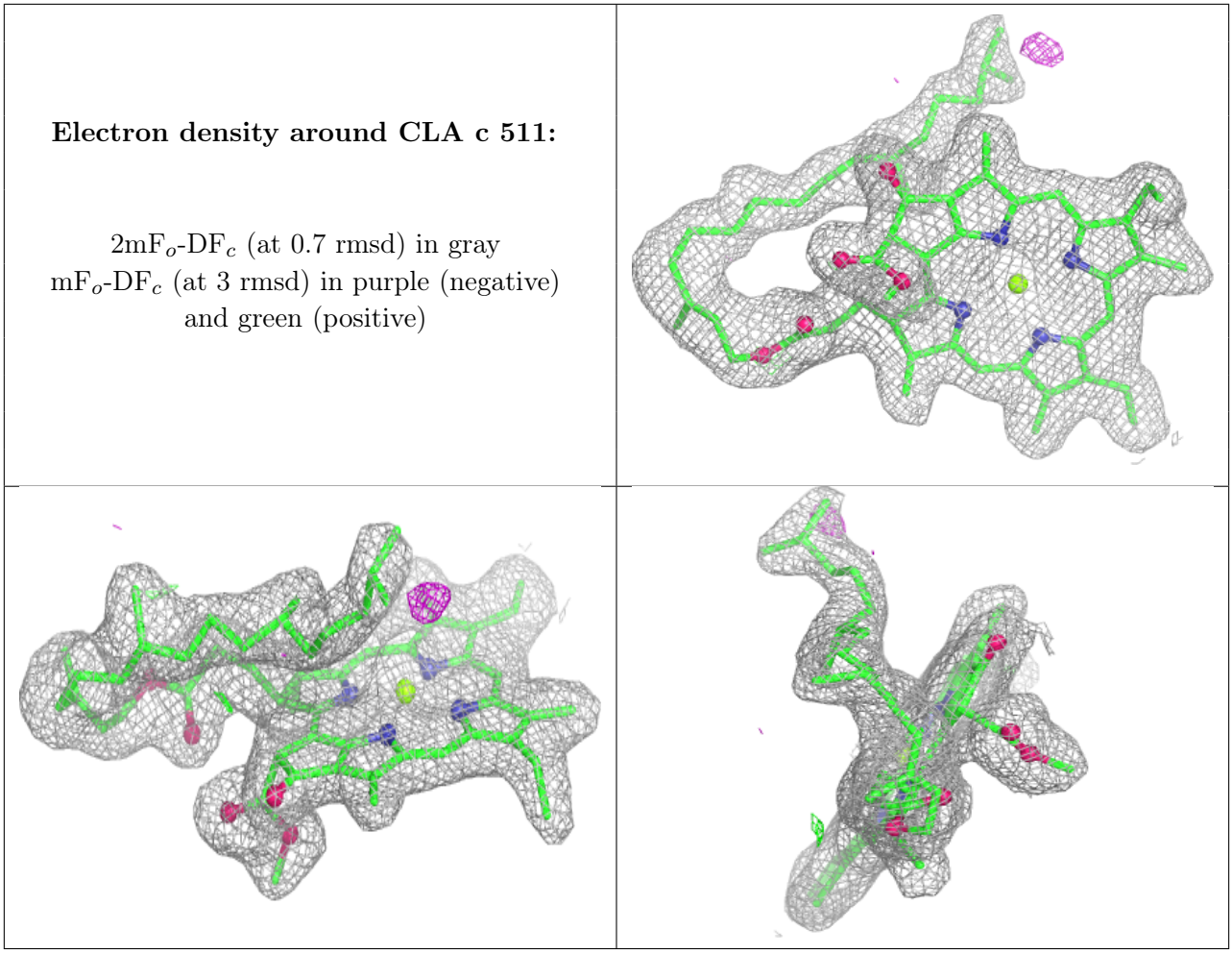






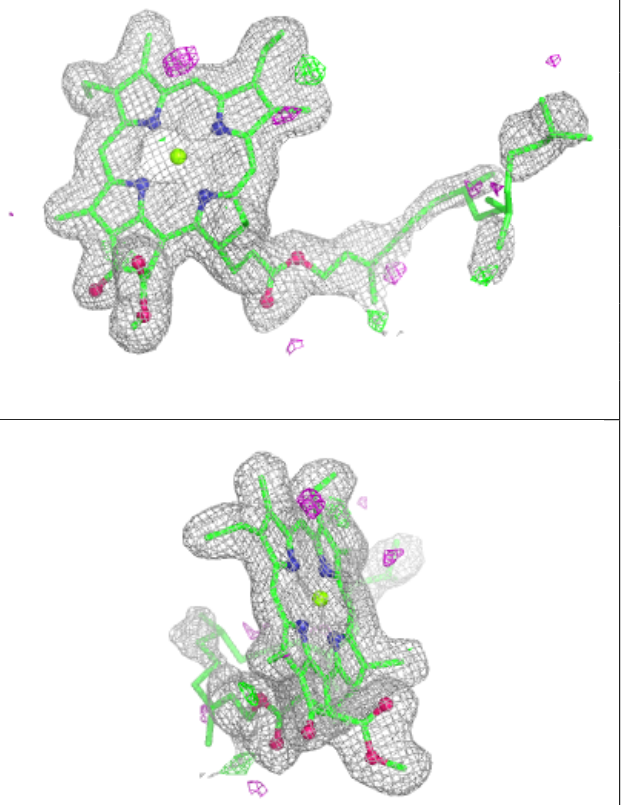
Electron density around CLA c 511:

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



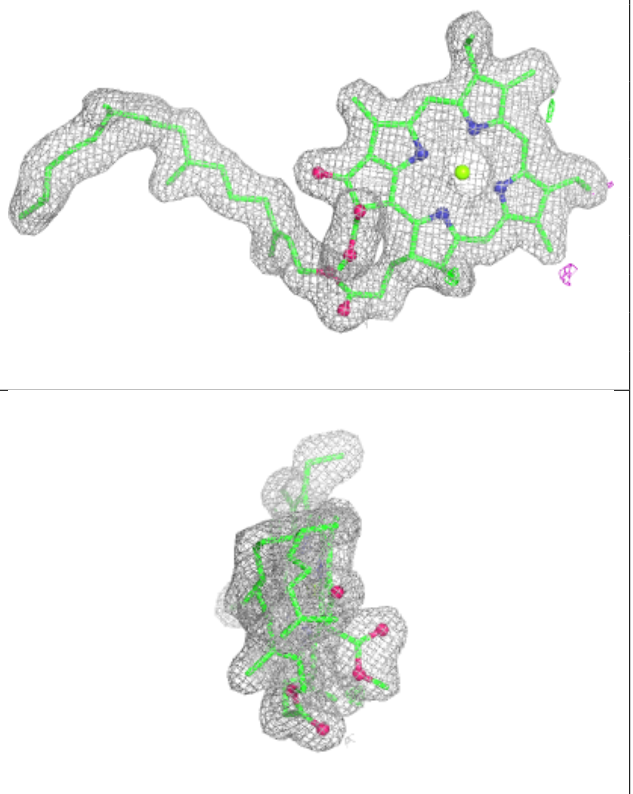
Electron density around CLA a 409:

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



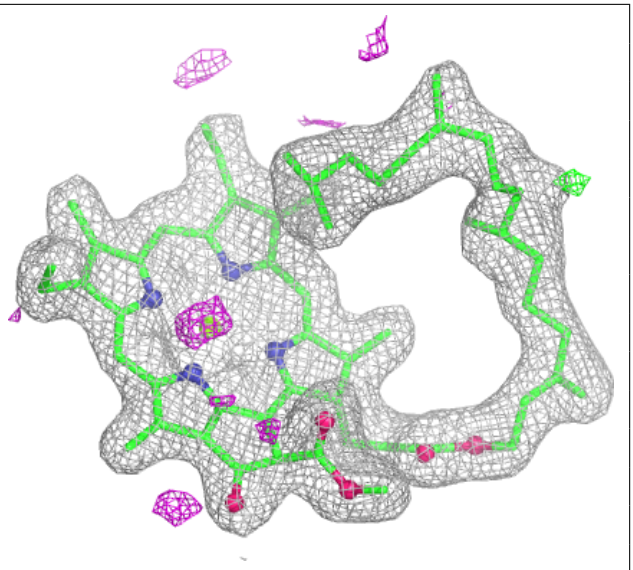
Electron density around CLA B 603:

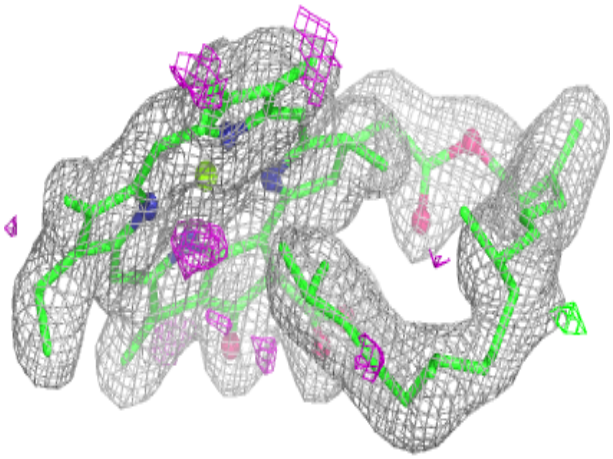
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

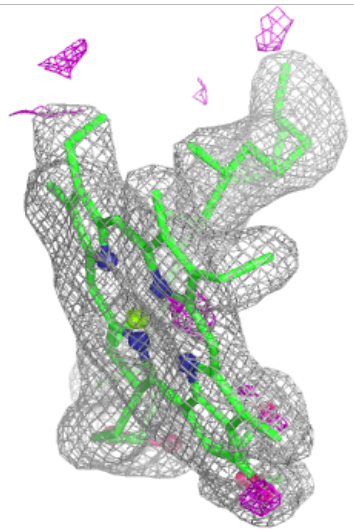


Electron density around CLA B 616:

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

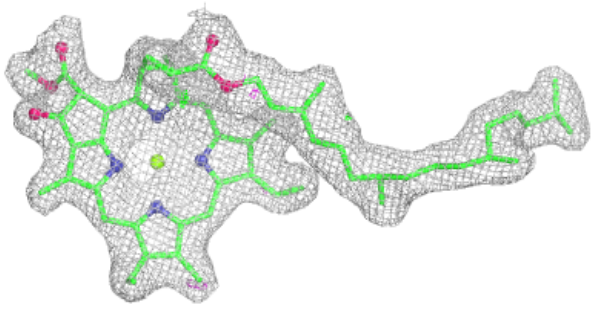


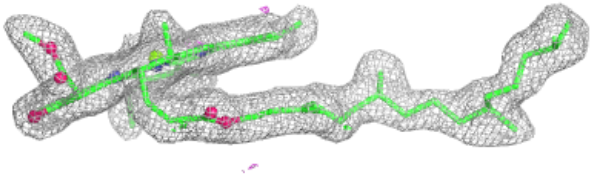


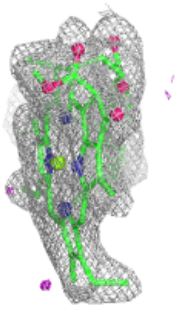


Electron density around CLA b 608:

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

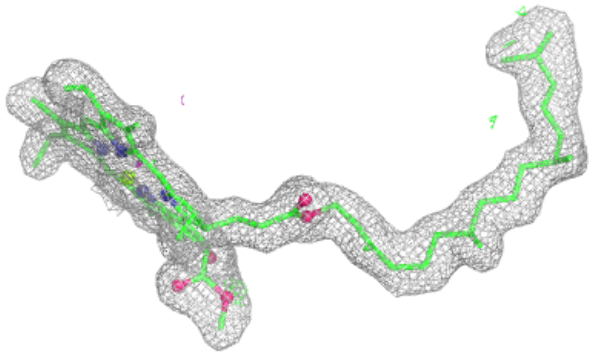


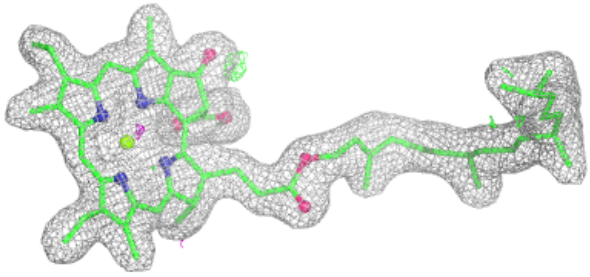


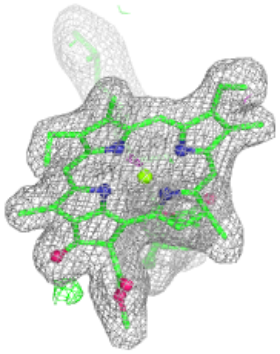


Electron density around CLA d 402:

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

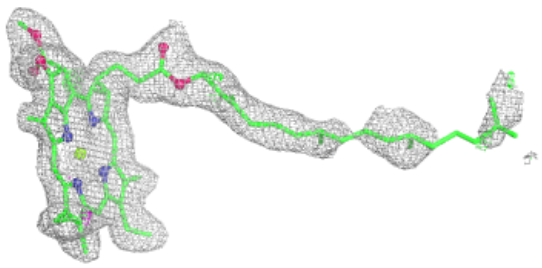


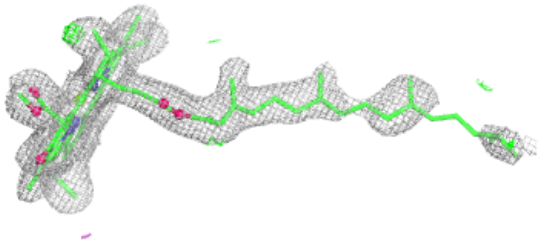


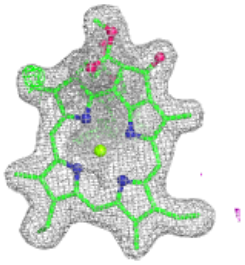


Electron density around CLA d 404:

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

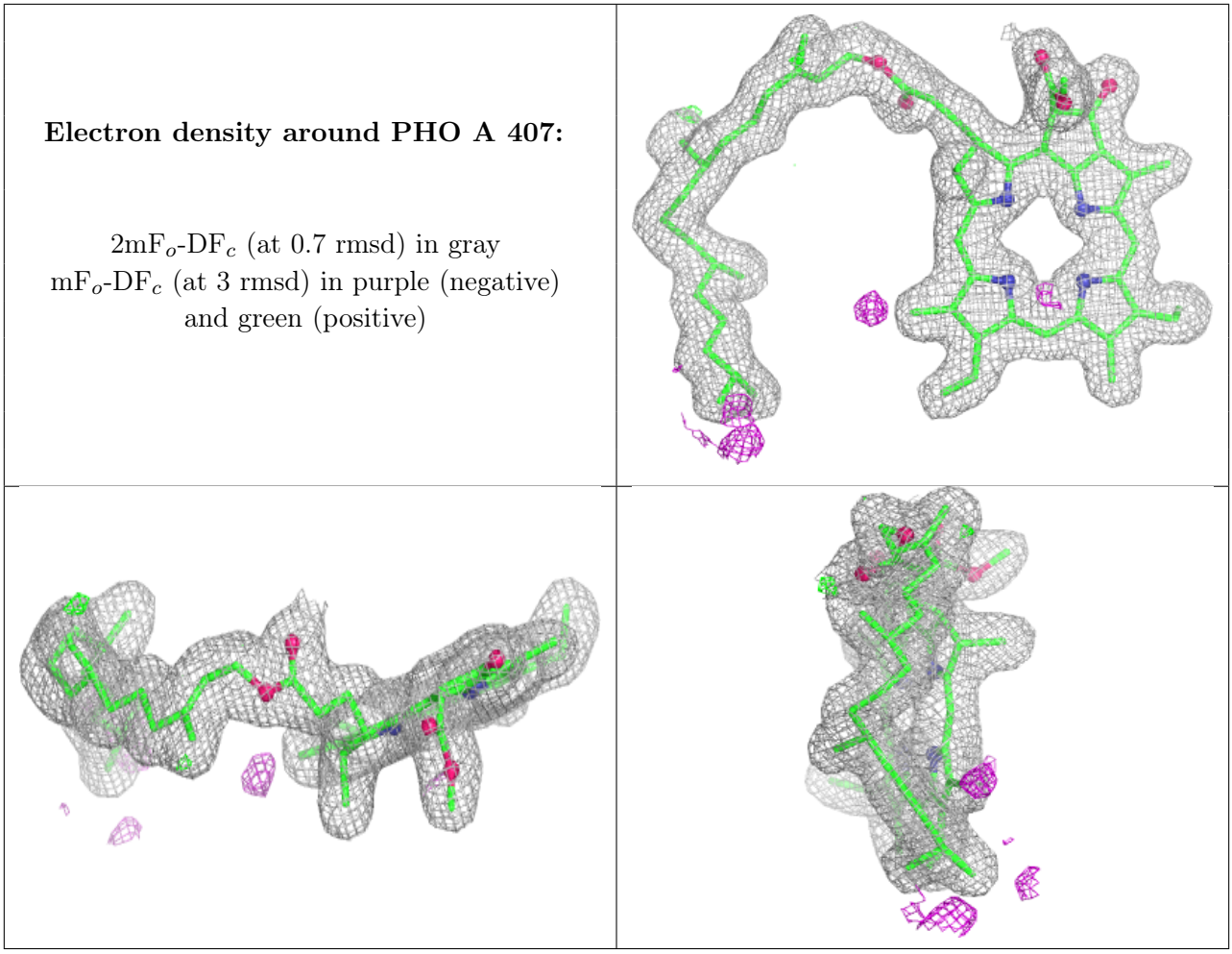






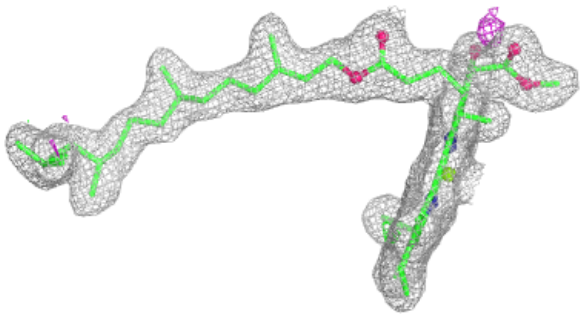
Electron density around PHO A 407:

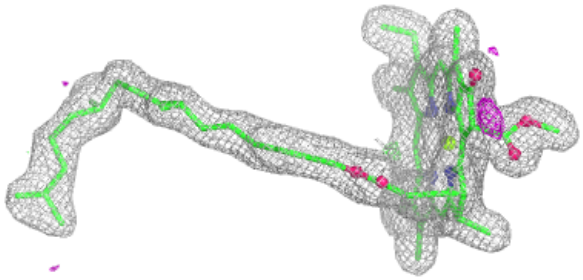
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

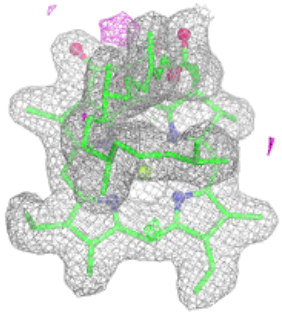


Electron density around CLA b 610:

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

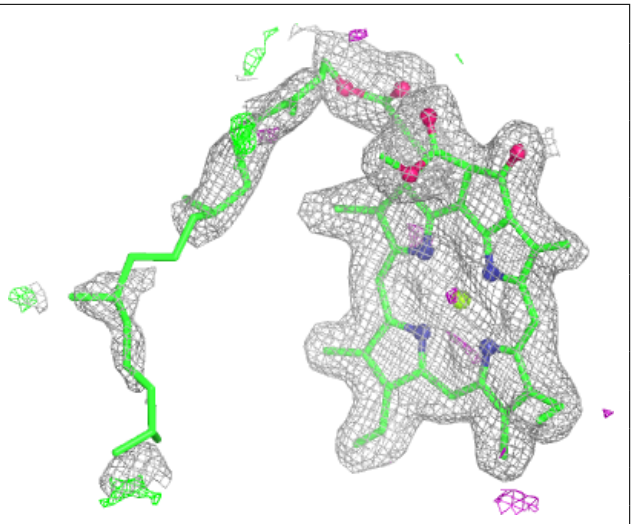


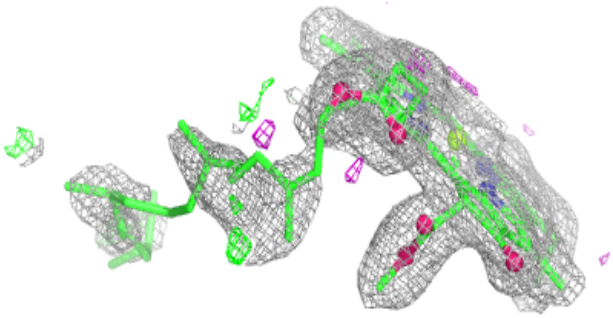




Electron density around CLA B 617:

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

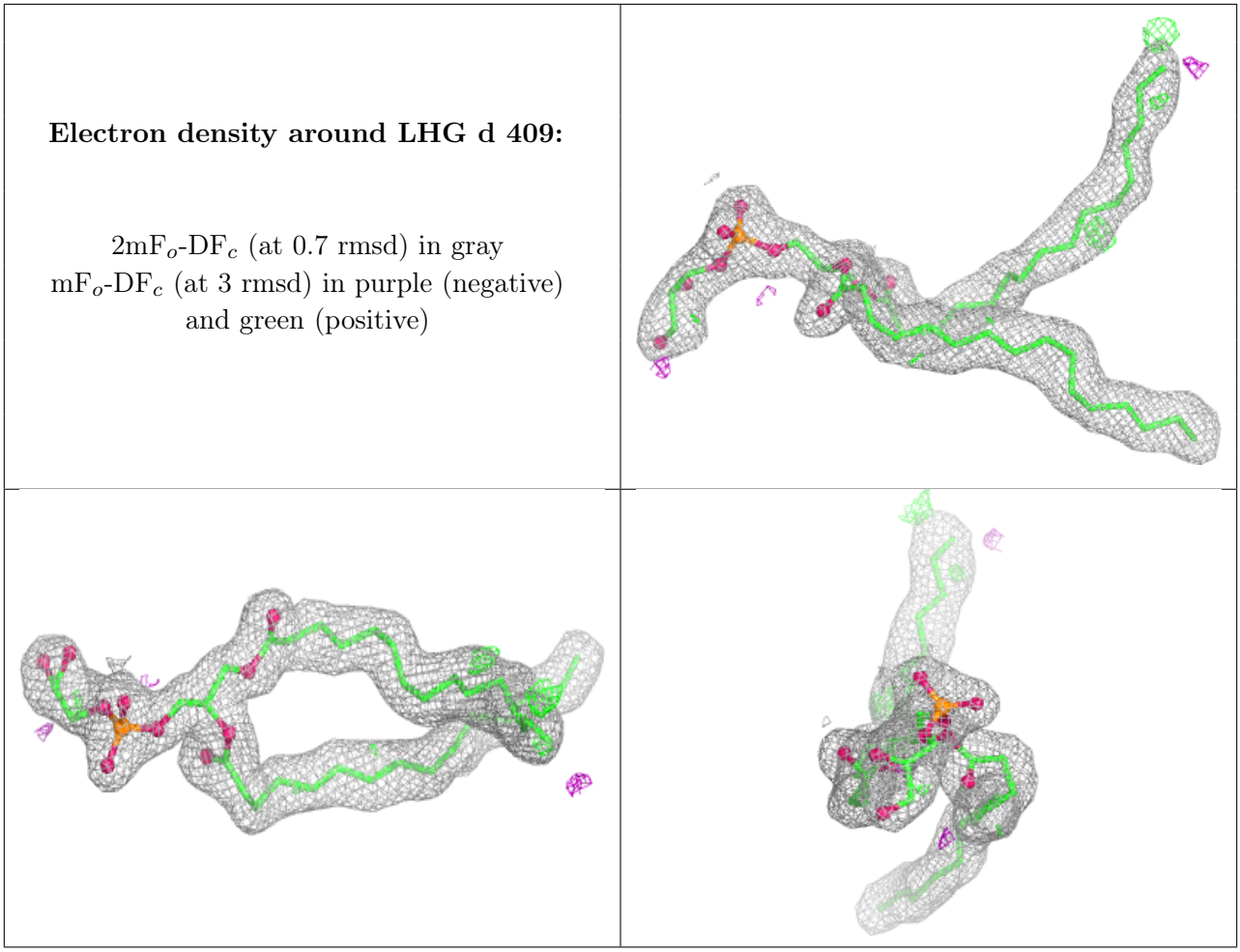






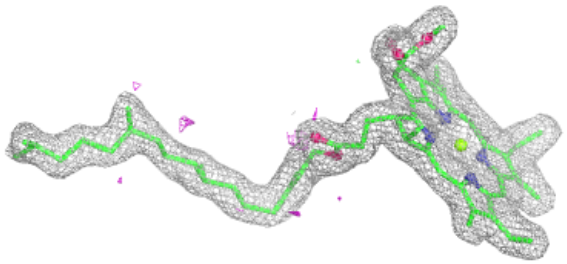
Electron density around LHG d 409:

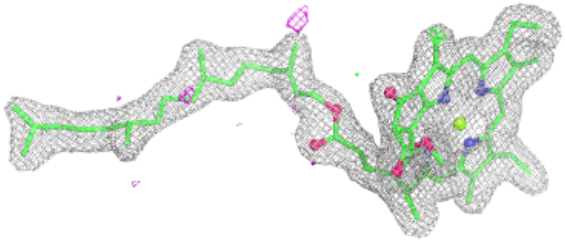
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

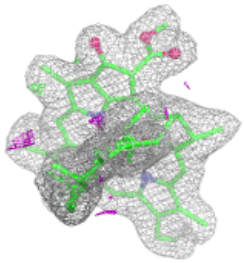


Electron density around CLA C 503:

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

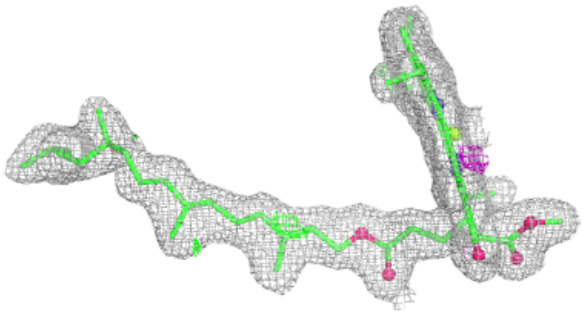


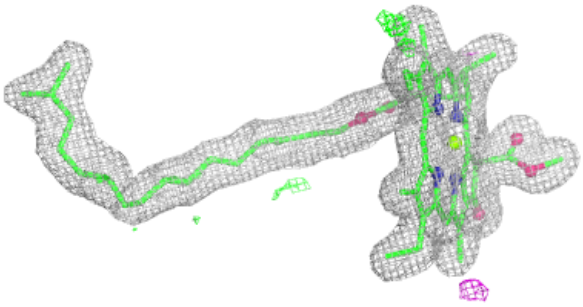


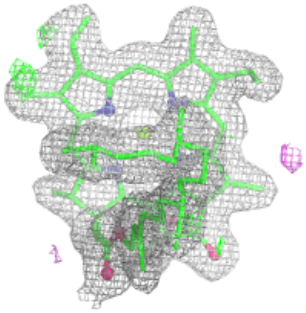


Electron density around CLA B 606:

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

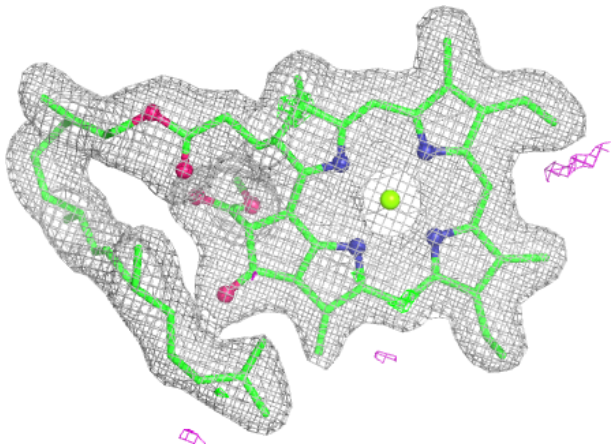


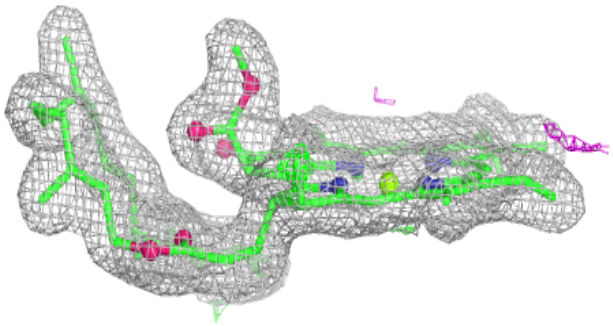


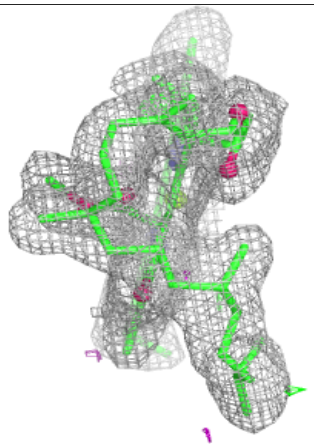


Electron density around CLA b 615:

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

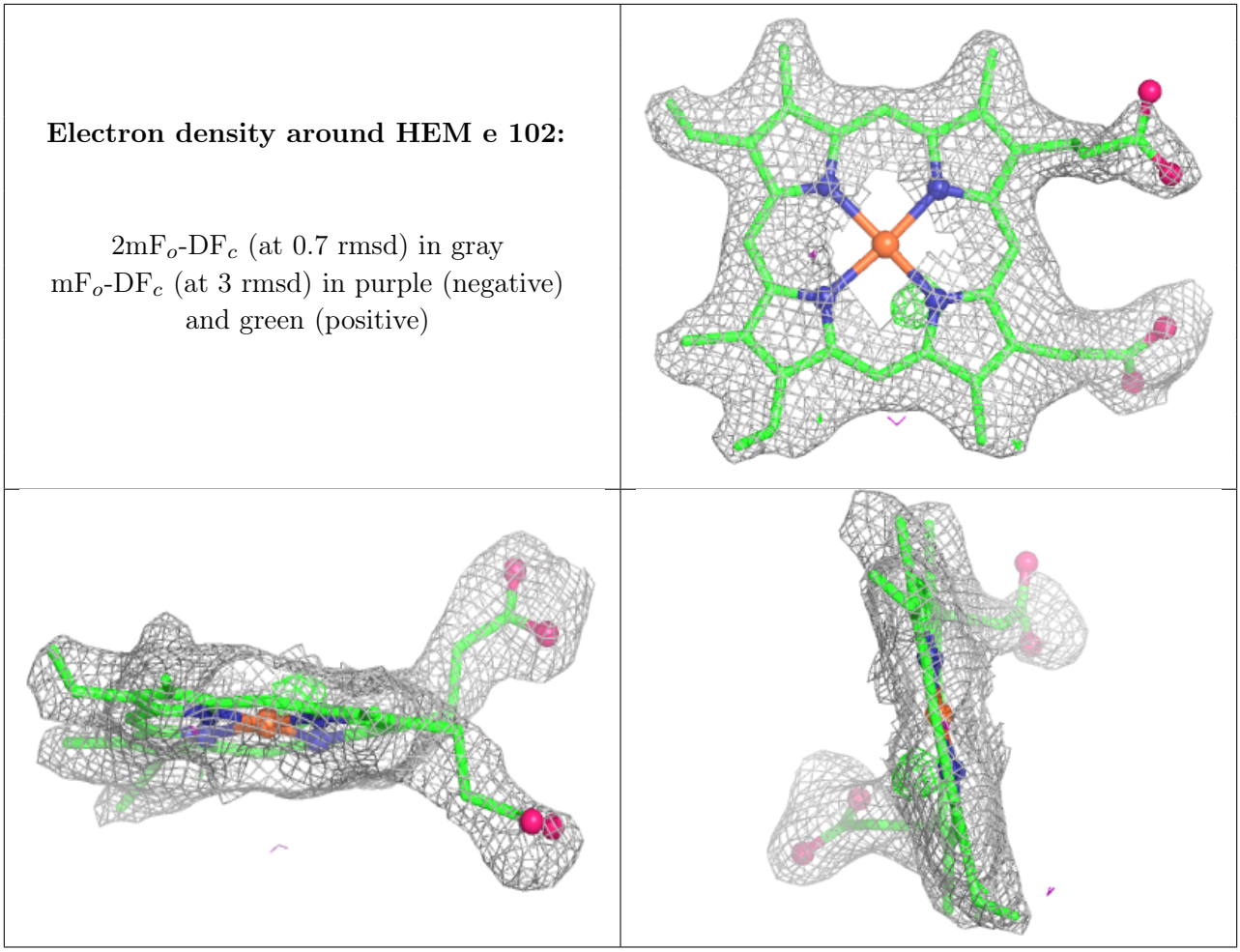






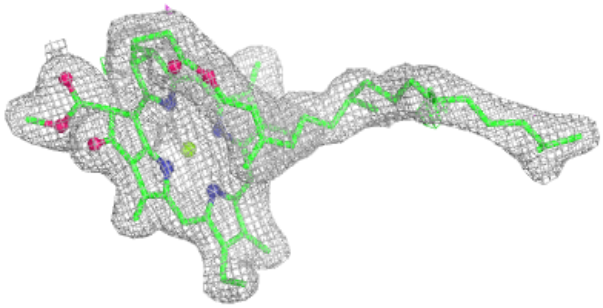
Electron density around HEM e 102:

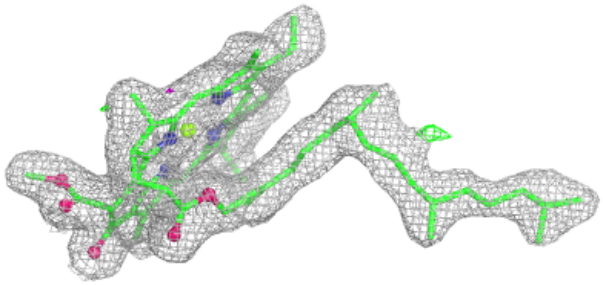
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

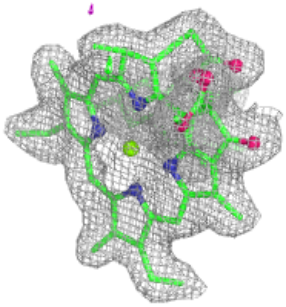


Electron density around CLA C 506:

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

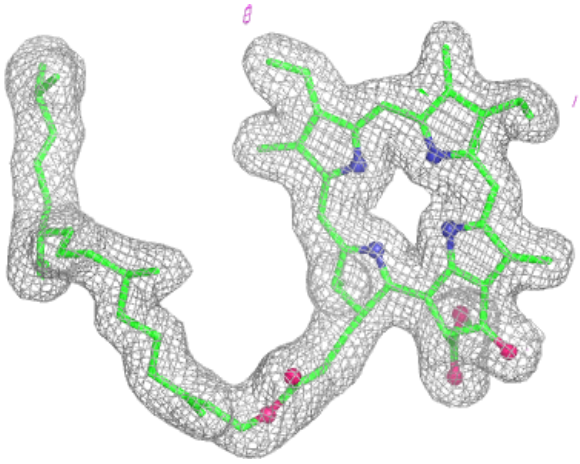


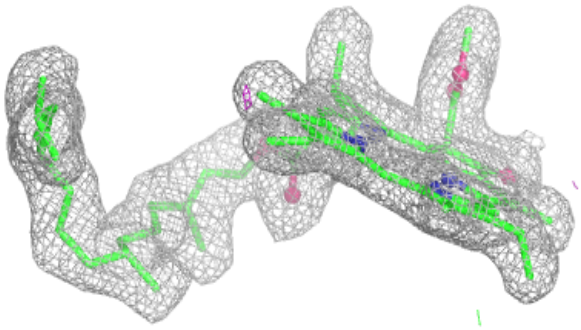


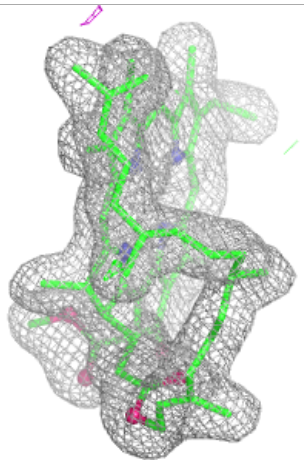


Electron density around PHO A 408:

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

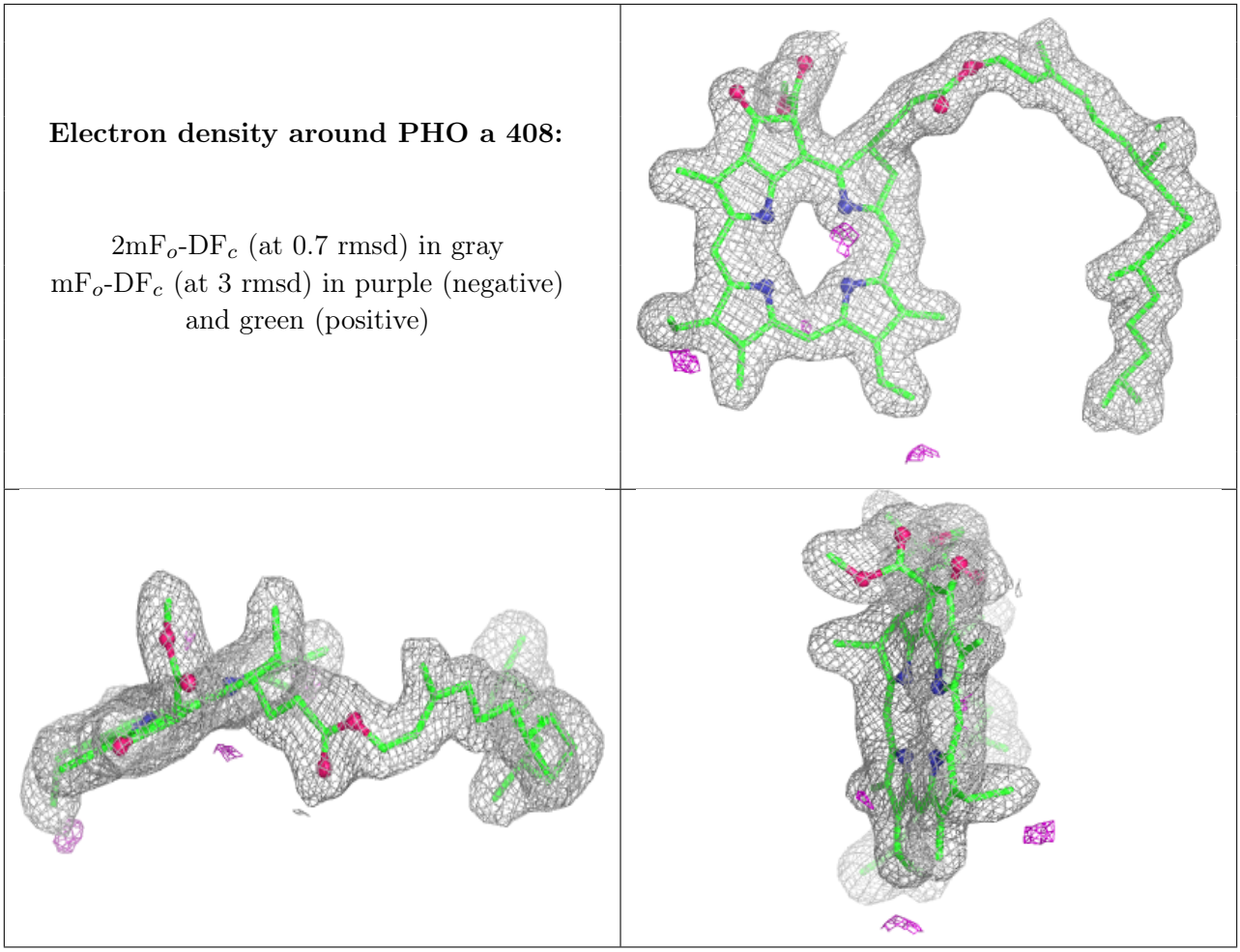






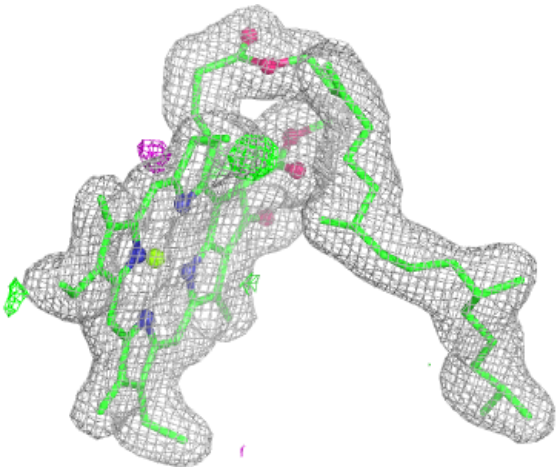
Electron density around PHO a 408:

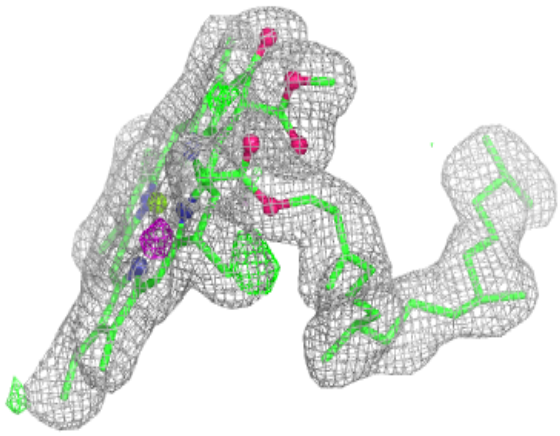
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

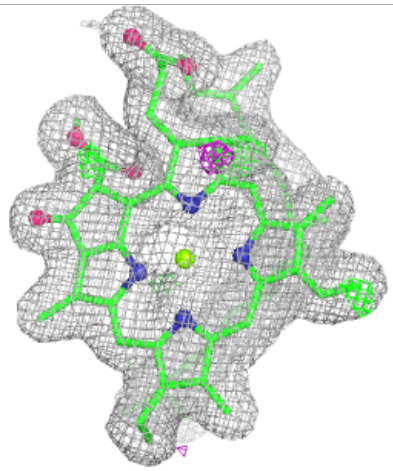


Electron density around CLA b 618:

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

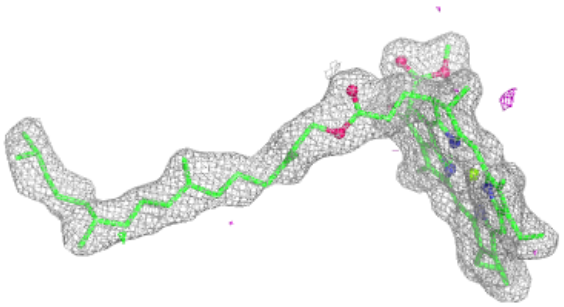


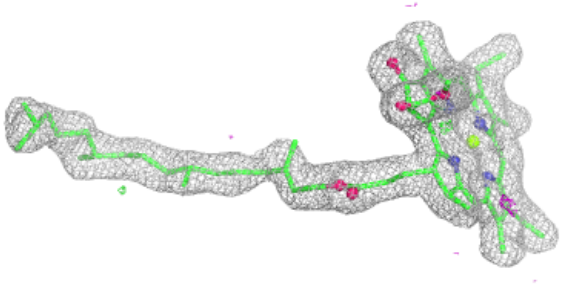


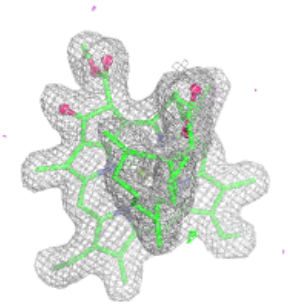


Electron density around CLA b 609:

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

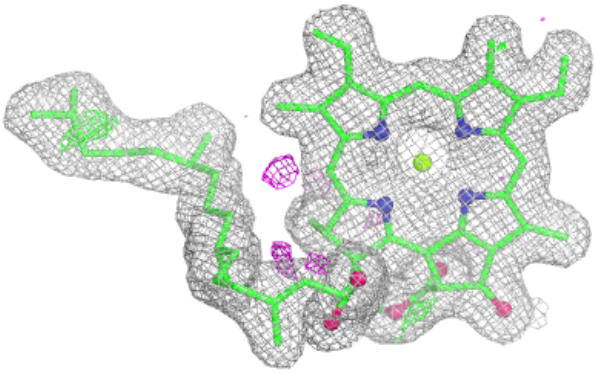


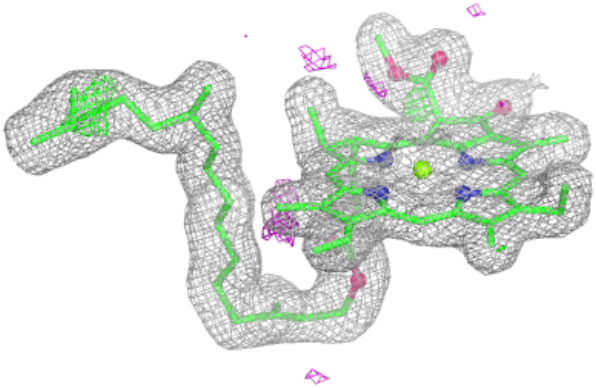


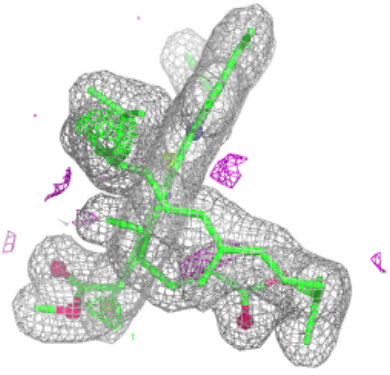


Electron density around CLA D 401:

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

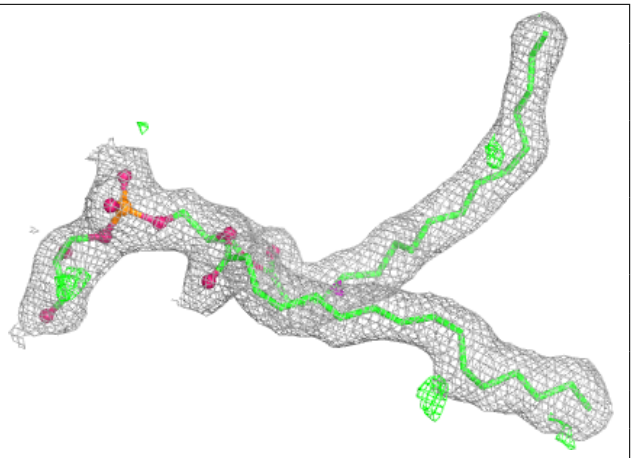


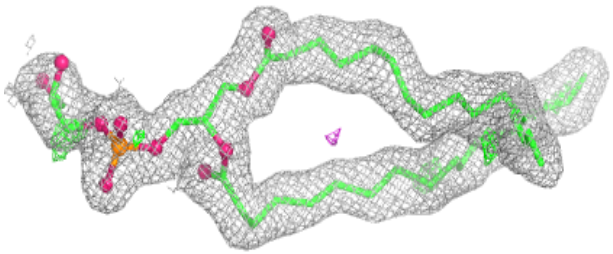


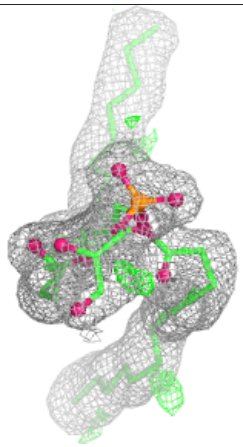


Electron density around LHG D 409:

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

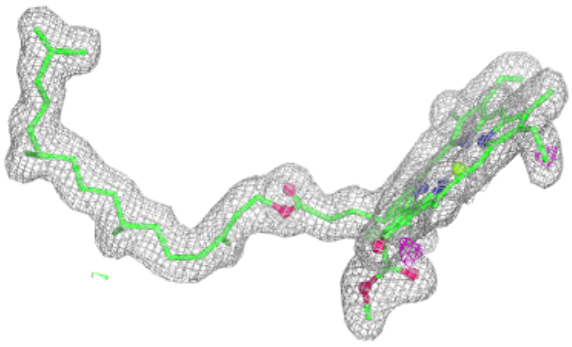


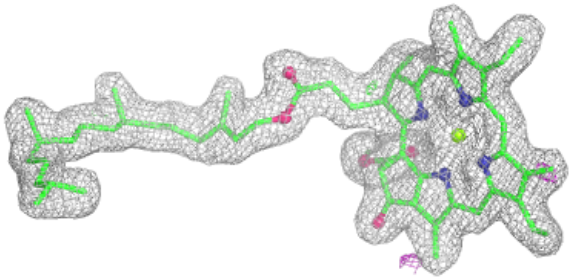


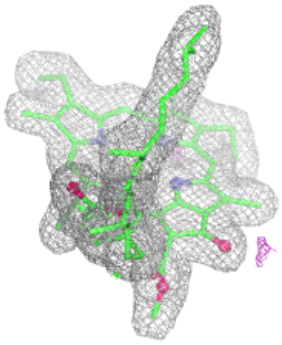


Electron density around CLA D 403:

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

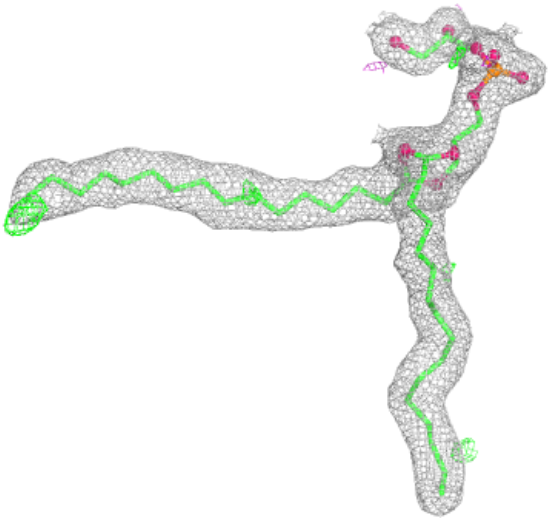


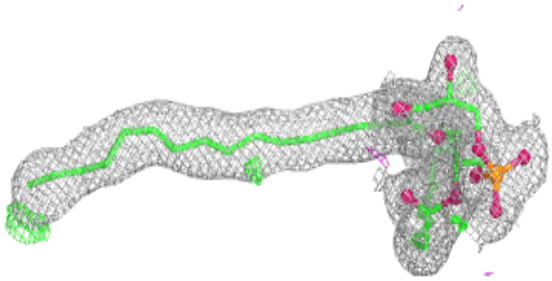


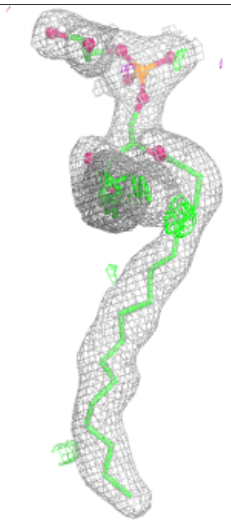


Electron density around LHG L 101:

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

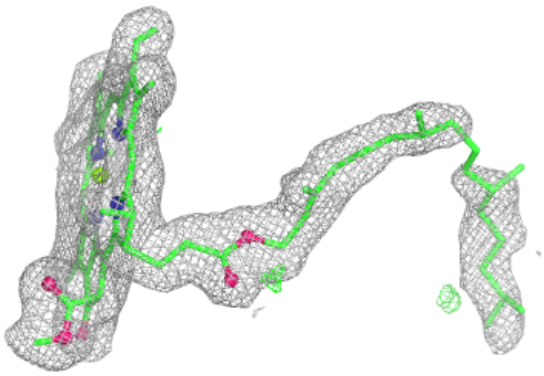


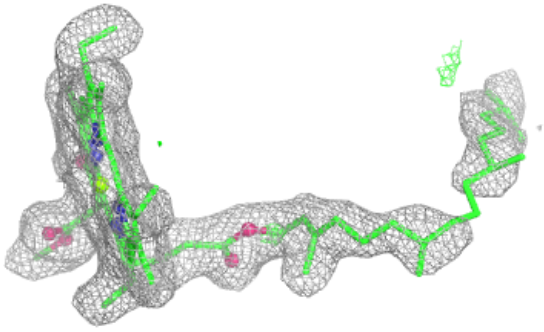


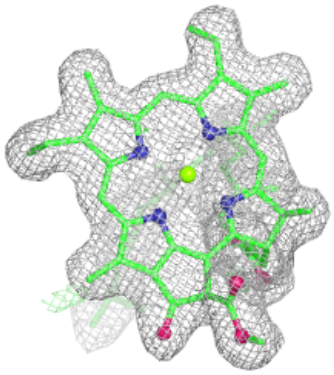


Electron density around CLA D 404:

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

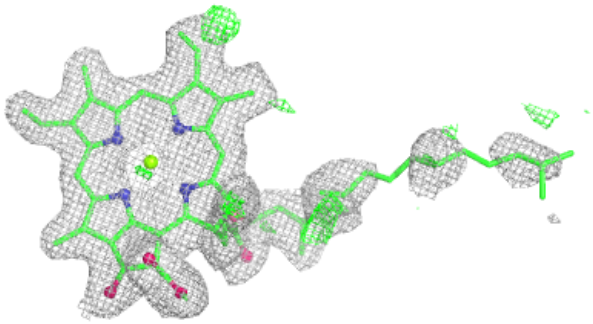


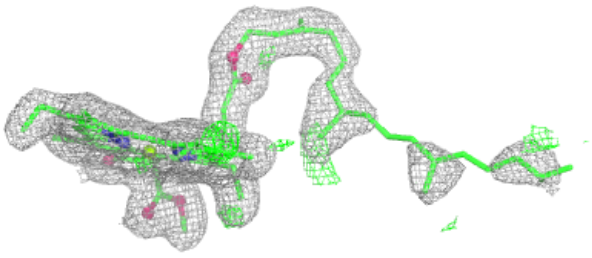


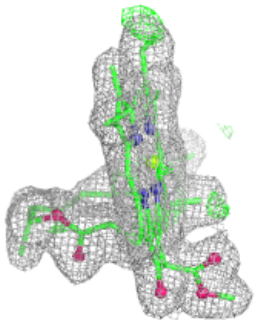


Electron density around CLA a 407:

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

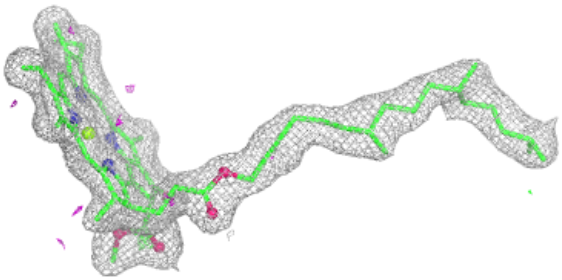


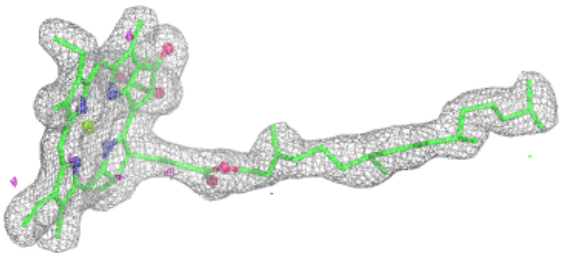


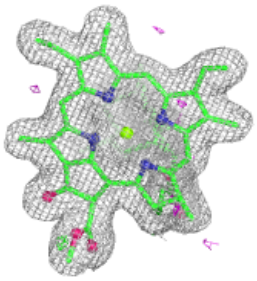


Electron density around CLA B 605:

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

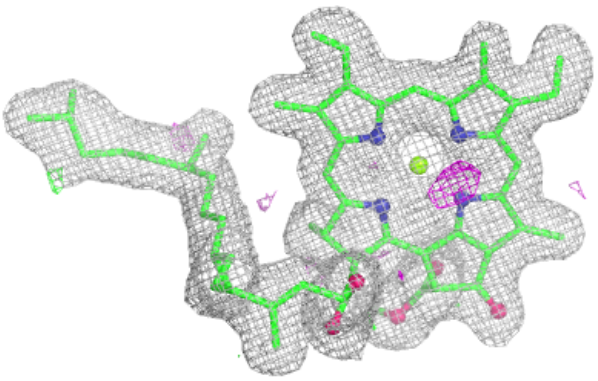


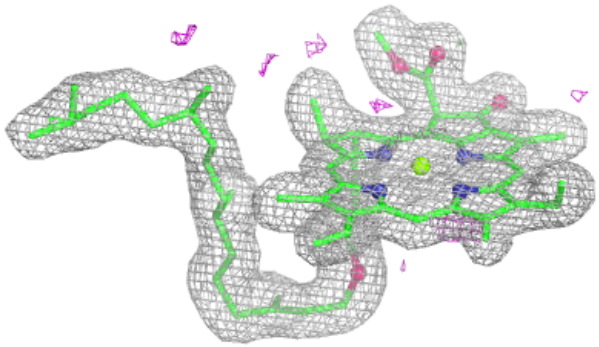


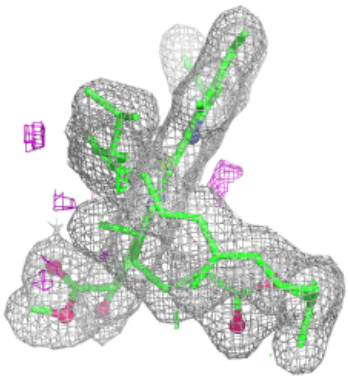


Electron density around CLA d 401:

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

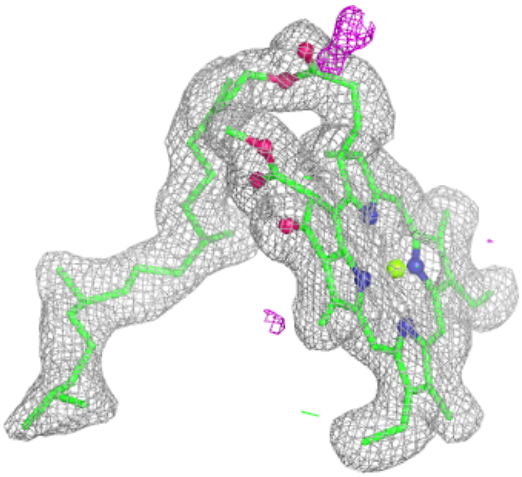


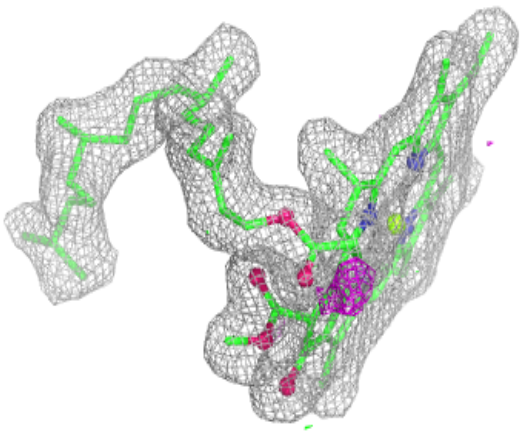


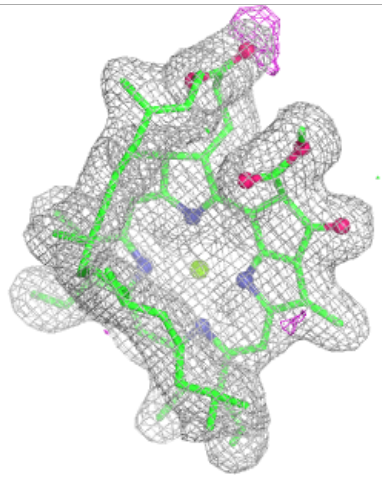


Electron density around CLA B 614:

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

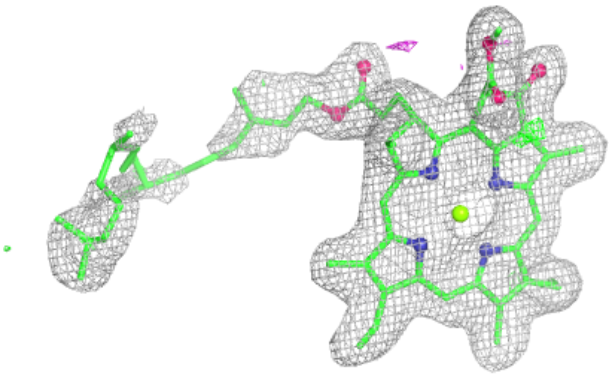


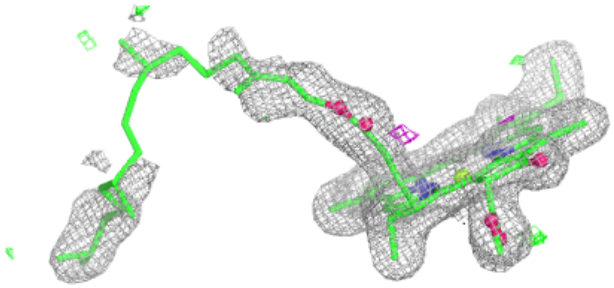


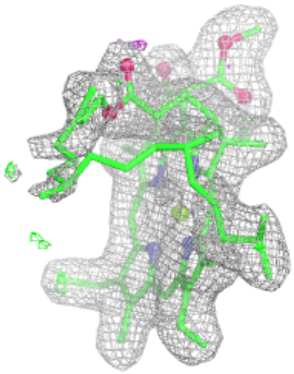


Electron density around CLA A 409:

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

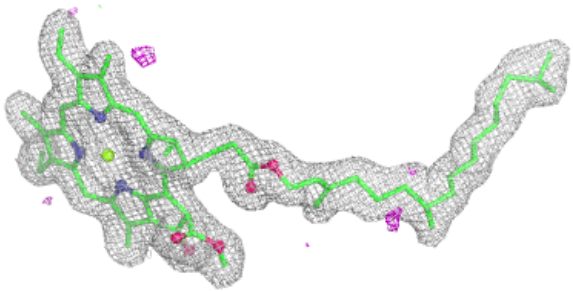


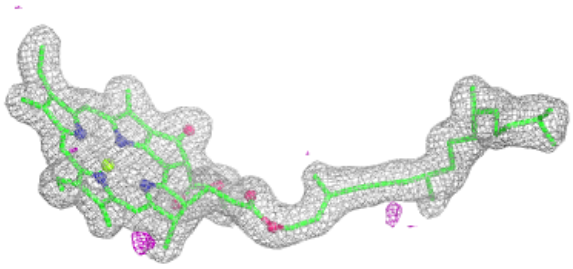


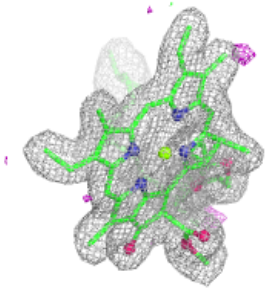


Electron density around CLA a 406:

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

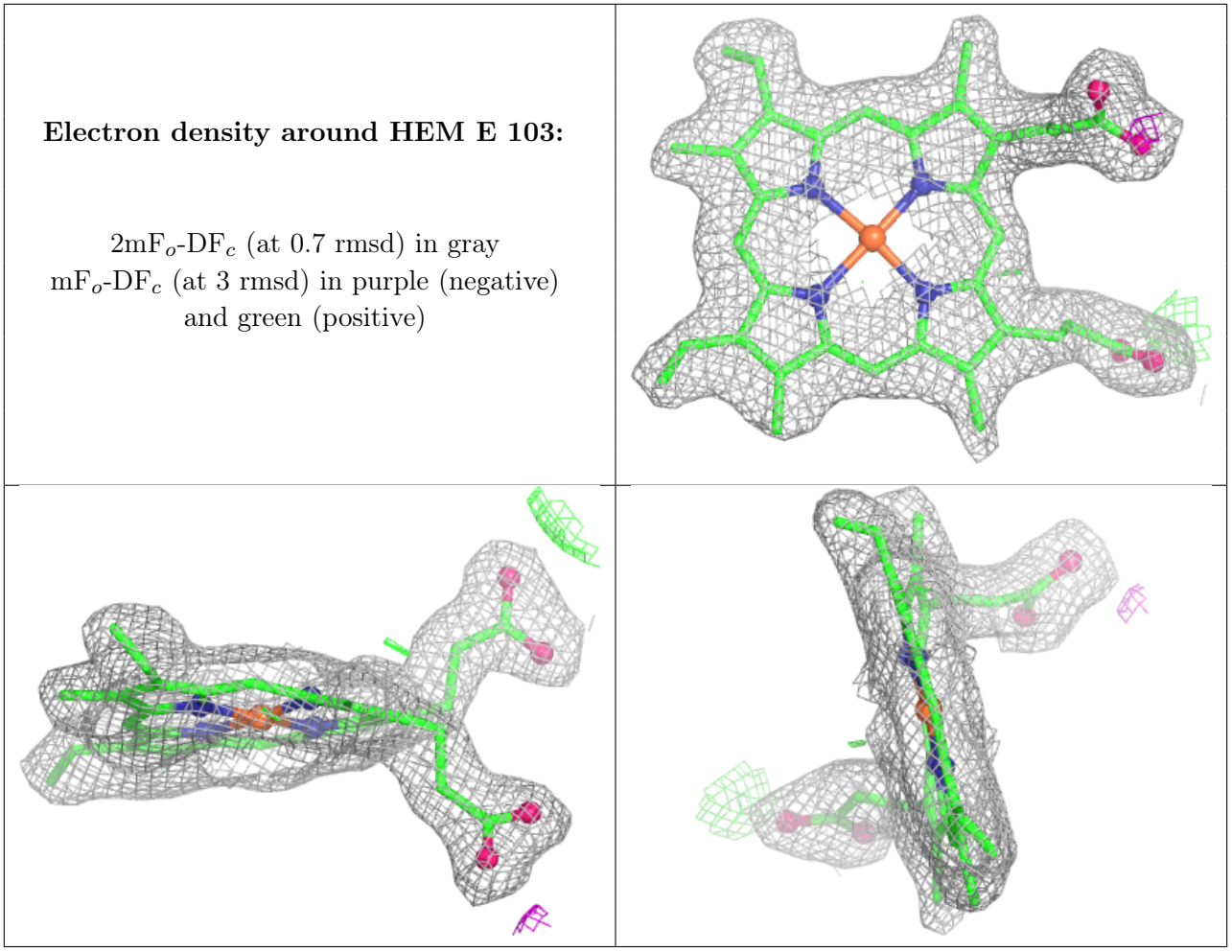






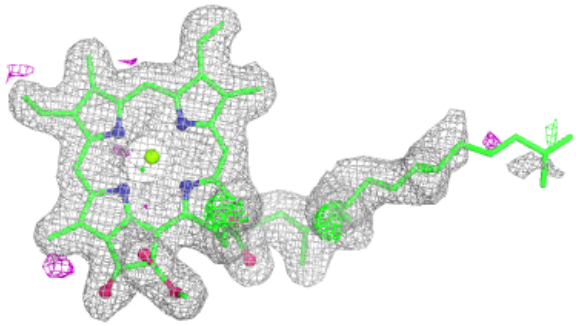
Electron density around HEM E 103:

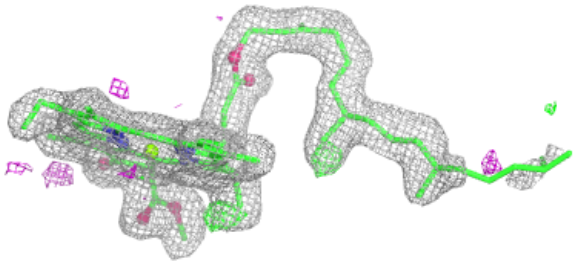
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

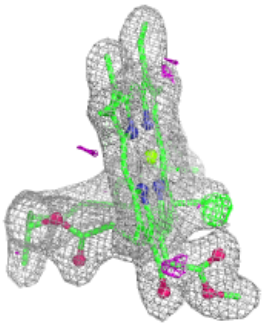


Electron density around CLA A 406:

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

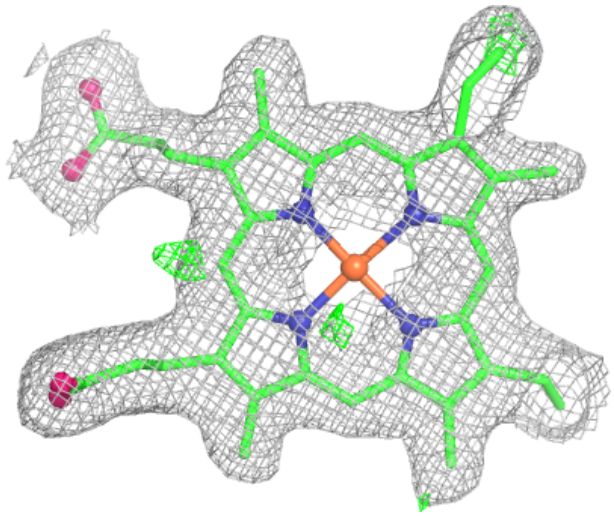


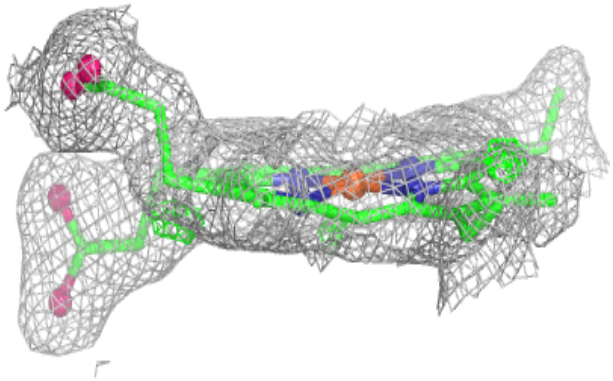


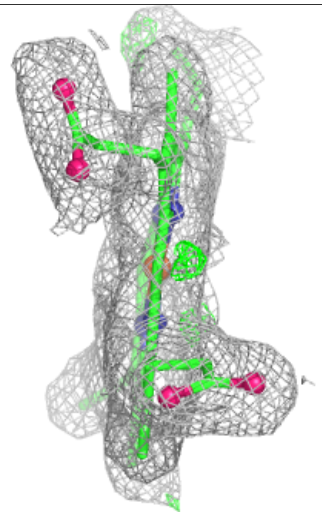


Electron density around HEC V 203:

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

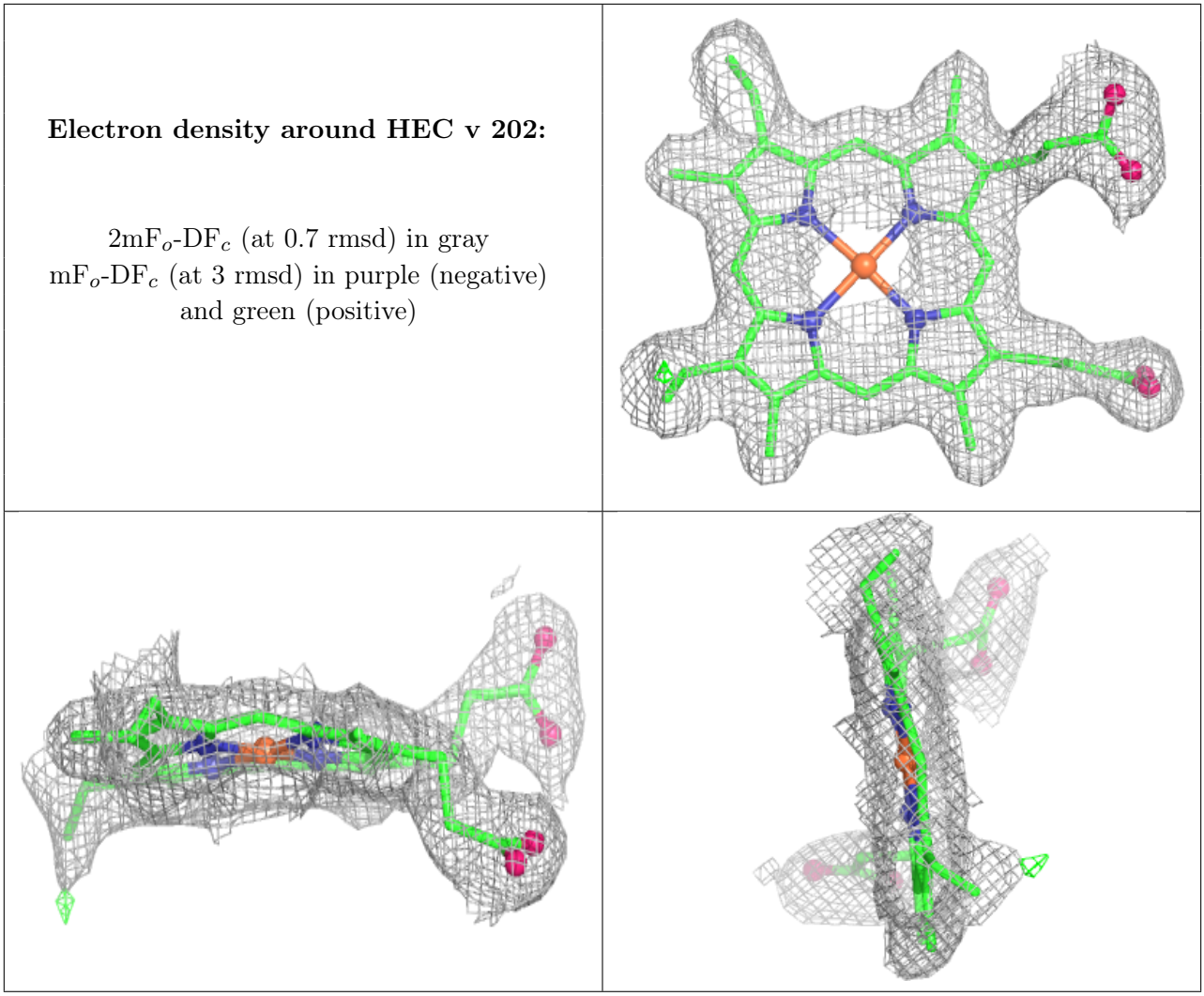






Electron density around HEC v 202:

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



6.5 Other polymers

There are no such residues in this entry.