Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:06 AM JST

PDB ID	:	4UB6 / pdb_00004ub6
Title	:	Native structure of photosystem II (dataset-1) 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 ⓘ 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 ⓘ) were used in the production of this report:

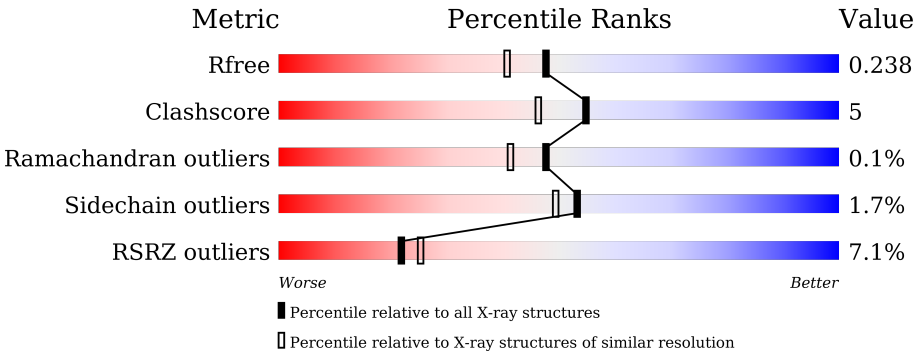
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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.



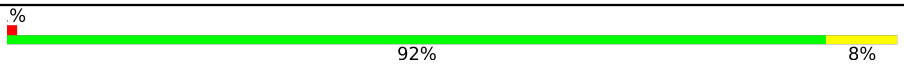
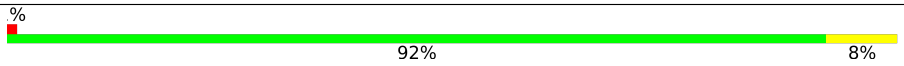
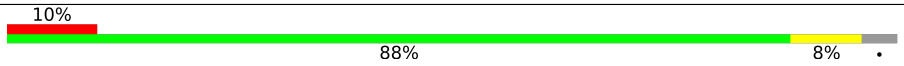
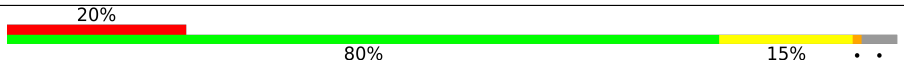
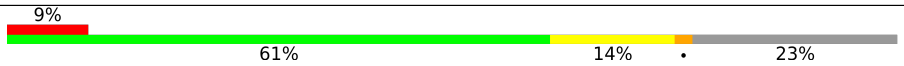
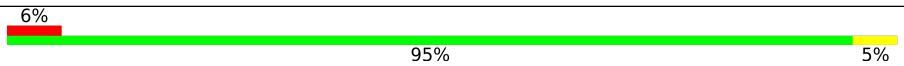
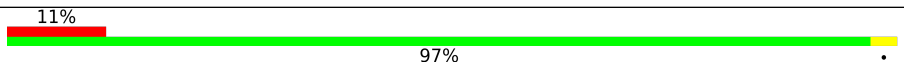
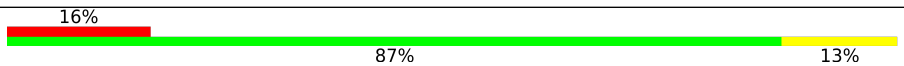
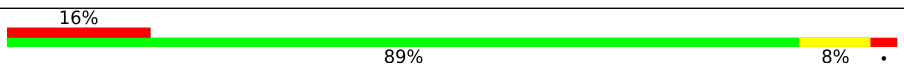
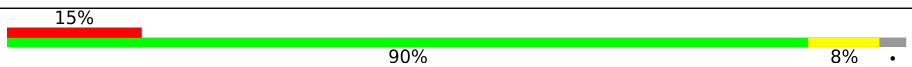
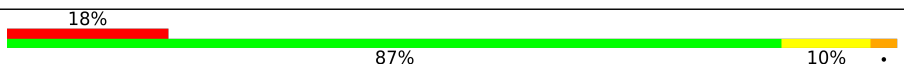
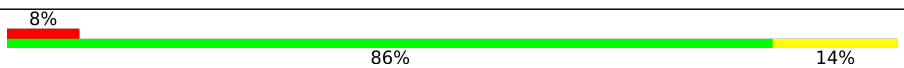
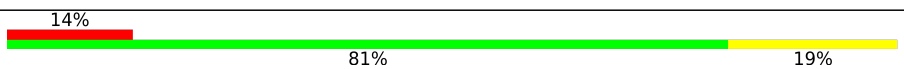
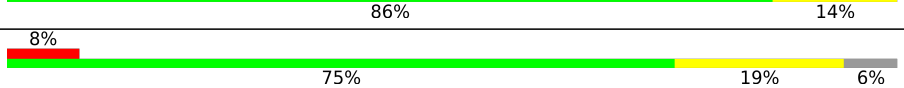
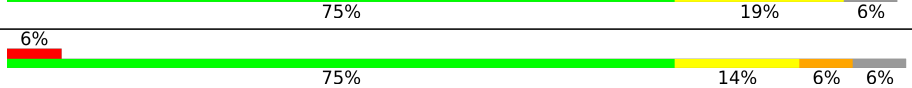
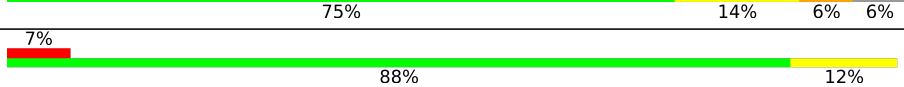
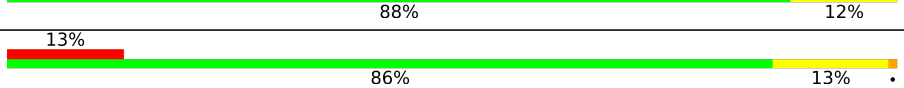
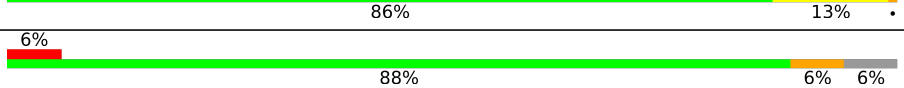
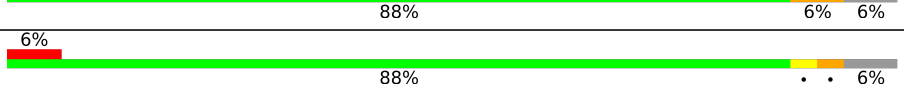
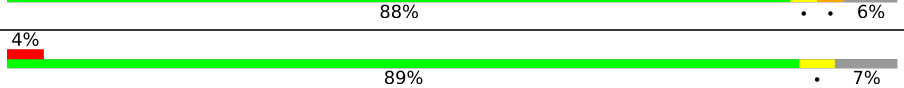
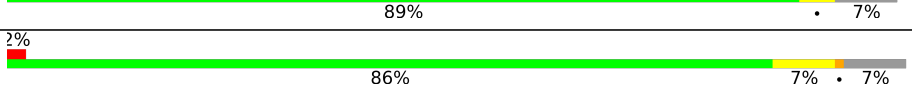
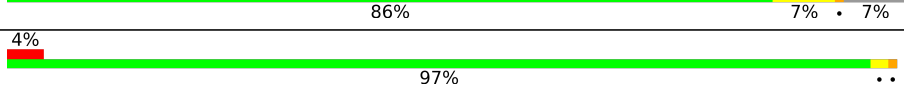
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	2% 91% 6%
1	a	344	3% 86% 11%
2	B	505	4% 92% 8%
2	b	505	6% 91% 8%
3	C	455	4% 90% 9%
3	c	455	4% 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	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	4% 93% 7%
17	Y	30	33% 77% 20%
17	y	30	47% 67% 27%
18	X	40	20% 95%
18	x	40	18% 98%
19	Z	62	34% 85% 15%
19	z	62	45% 90% 10%
20	R	34	79% 88% 9%

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	-
22	CL	v	201	-	-	X	-
40	HEC	V	201	X	-	-	-
40	HEC	v	202	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 54195 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
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	6	0
			2645	1737	432	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	11	0
			4027	2643	668	703	13			
2	b	504	Total	C	N	O	S	0	12	0
			4033	2650	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	4	0
			3501	2291	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	1	0
			2729	1807	445	465	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 670	C 439	N 107	O 124	0	2	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 280	C 187	N 43	O 48	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 1903	C 1191	N 315	O 392	S 5	0	8	0
13	o	243	Total 1891	C 1183	N 315	O 388	S 5	0	5	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	0	0
			287	191	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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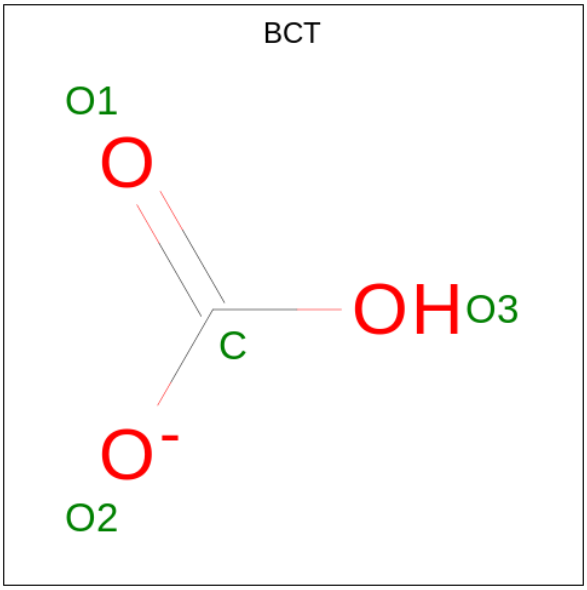
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	a	1	Total Fe 1 1	0	0

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

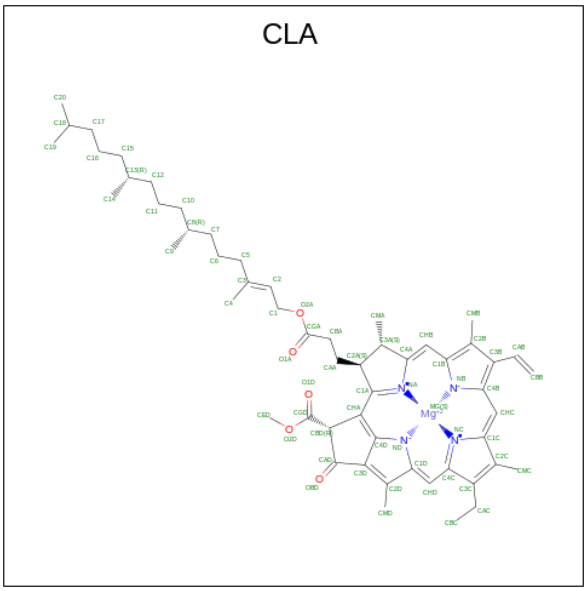
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	2	Total Cl 2 2	0	0
22	U	1	Total Cl 1 1	0	0
22	a	2	Total Cl 2 2	0	0
22	v	1	Total Cl 1 1	0	0

- 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	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		

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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	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	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		

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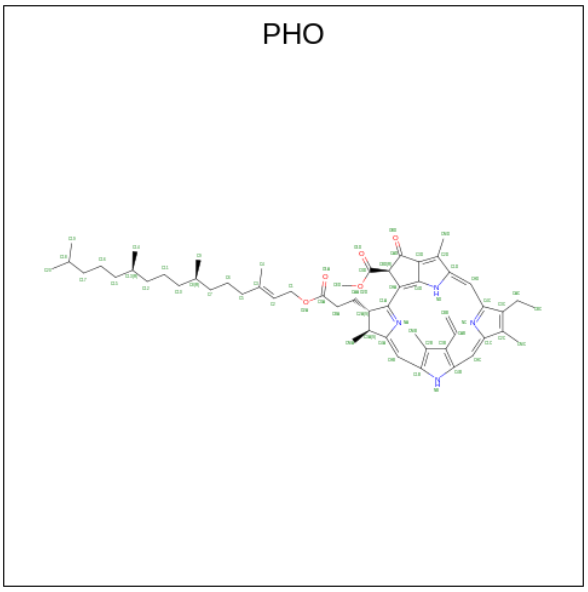
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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	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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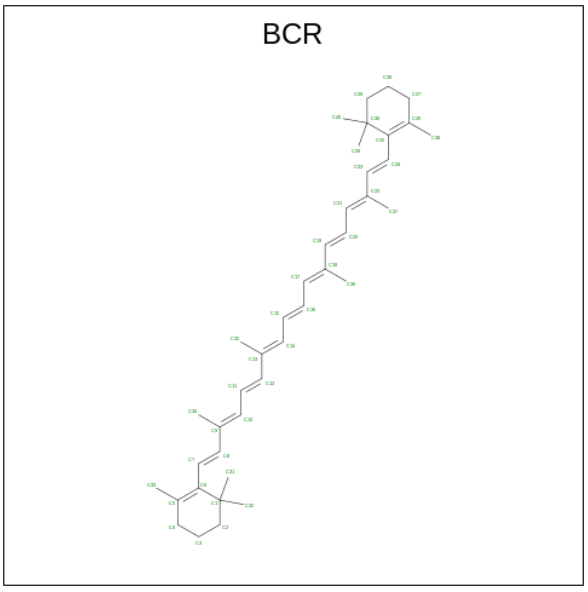
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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	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: $C_{55}H_{74}N_4O_5$).



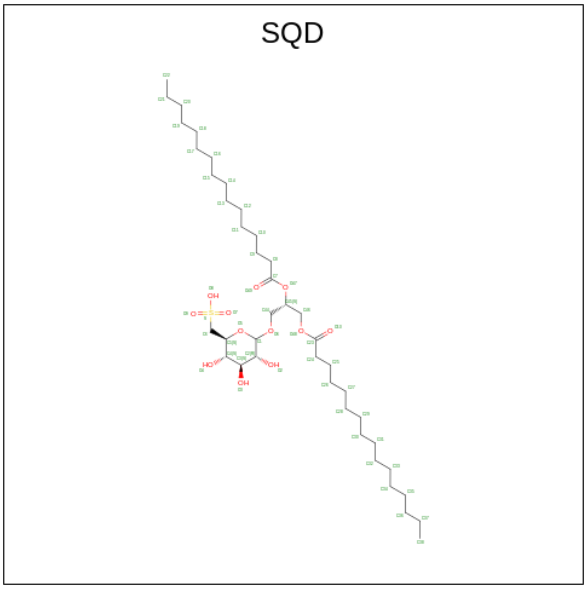
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



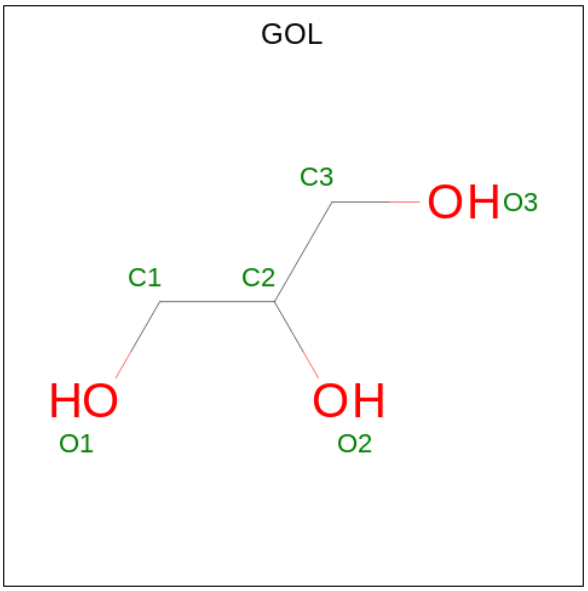
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total 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	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	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	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		
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		

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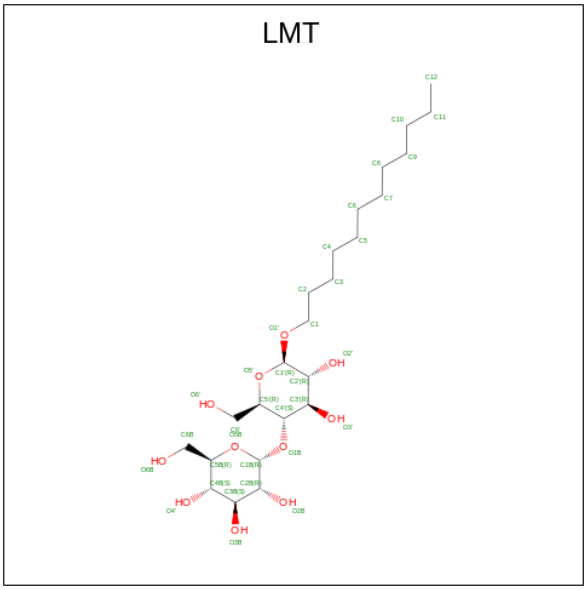
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28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

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



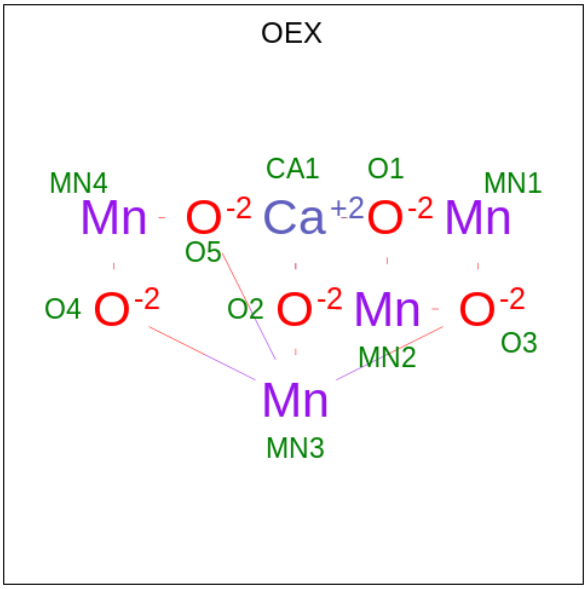
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 35 24 11	0	0
29	B	1	Total C O 35 24 11	0	0
29	B	1	Total C O 25 19 6	0	0
29	C	1	Total C O 35 24 11	0	0
29	E	1	Total C O 35 24 11	0	0
29	M	1	Total C O 35 24 11	0	0
29	a	1	Total C O 35 24 11	0	0
29	b	1	Total C O 25 19 6	0	0
29	b	1	Total C O 25 19 6	0	0

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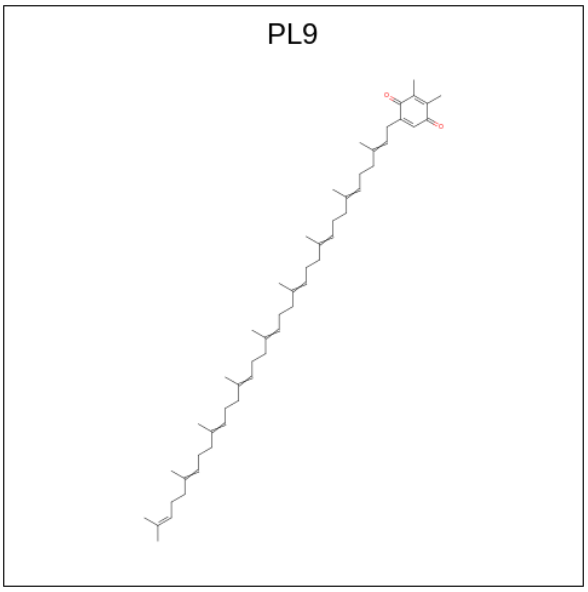
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	c	1	Total C O 35 24 11	0	0
29	f	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

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



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

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 28 23 5	0	0
32	B	1	Total C O 33 28 5	0	0
32	D	2	Total C O 57 51 6	0	0
32	I	1	Total C O 40 35 5	0	0
32	J	1	Total C 10 10	0	0
32	K	1	Total C O 34 29 5	0	0
32	M	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0

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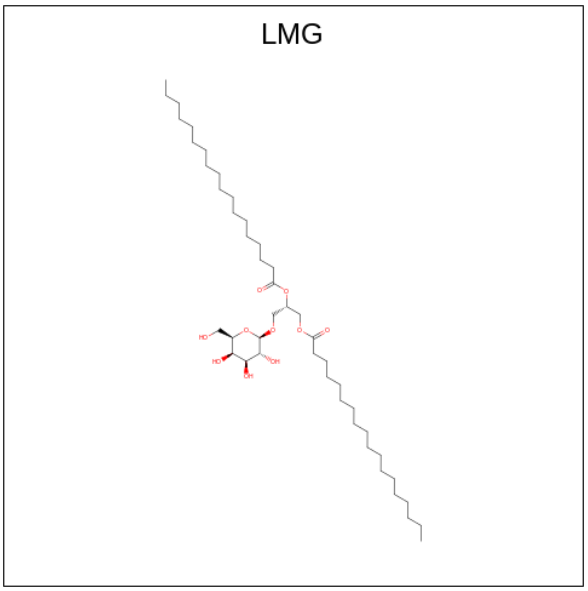
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	3	Total C O 71 63 8	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	0	0

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

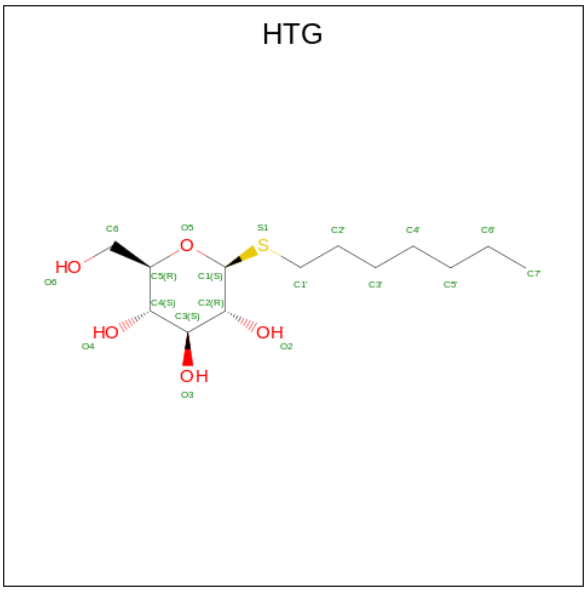
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	f	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0

- 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	a	1	Total C O 51 41 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	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: $C_{13}H_{26}O_5S$).



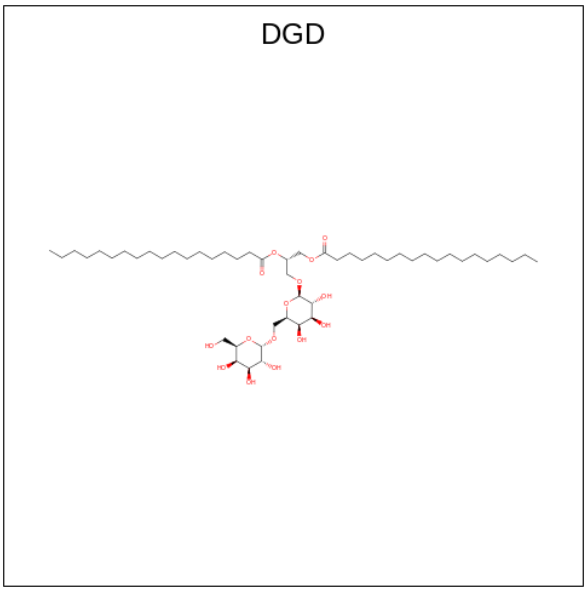
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	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: $C_{51}H_{96}O_{15}$).



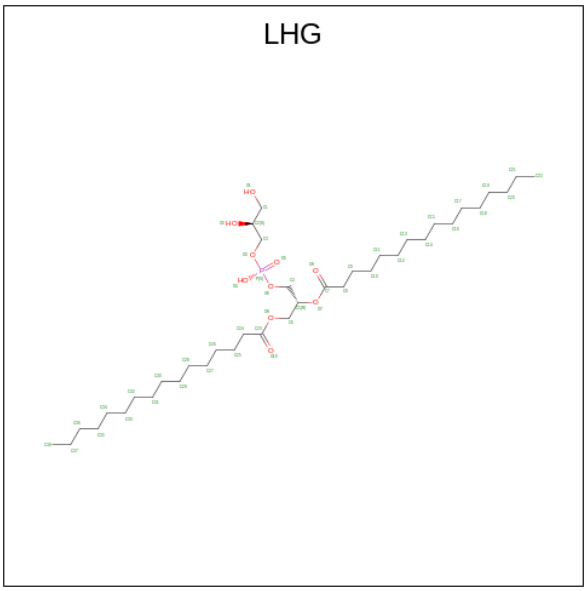
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	D	1	Total C O 62 47 15	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0

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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: $C_{38}H_{75}O_{10}P$).



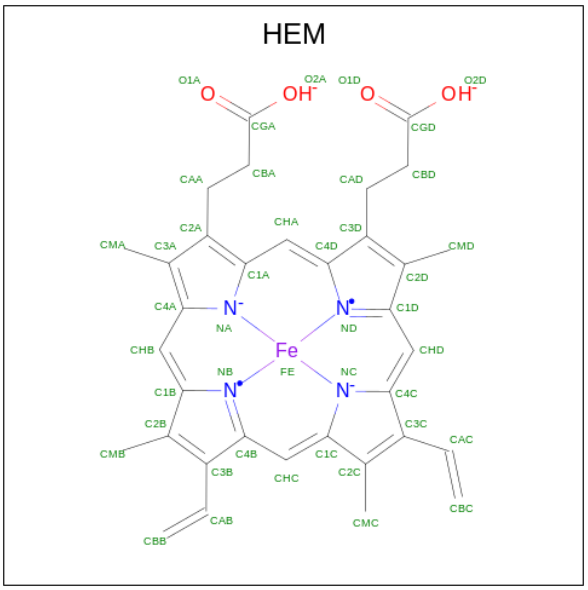
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	E	1	Total C O P 42 31 10 1	0	0
37	L	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 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: $C_{34}H_{32}FeN_4O_4$).

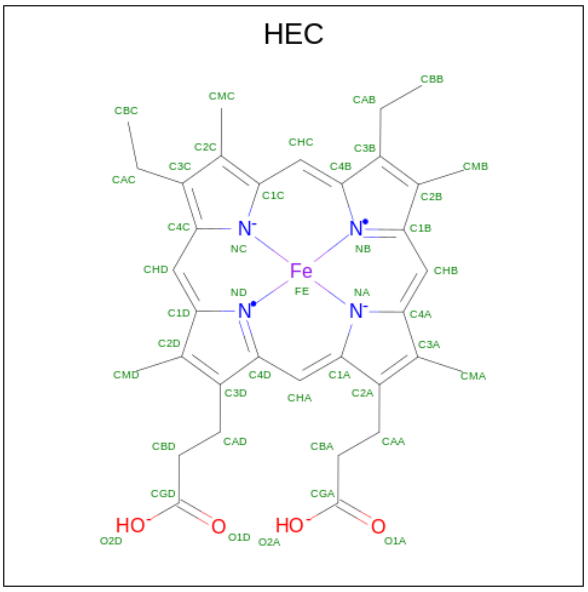


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	165	Total	O	0	2
			167	167		
41	B	289	Total	O	0	4
			293	293		
41	C	233	Total	O	0	2
			235	235		
41	D	138	Total	O	0	5
			143	143		
41	E	31	Total	O	0	0
			31	31		
41	F	9	Total	O	0	0
			9	9		
41	H	48	Total	O	0	1
			49	49		
41	I	4	Total	O	0	0
			4	4		
41	J	13	Total	O	0	0
			13	13		
41	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	16	Total O 17 17	0	1
41	M	8	Total O 8 8	0	0
41	O	188	Total O 191 191	0	3
41	T	16	Total O 17 17	0	1
41	U	81	Total O 81 81	0	0
41	V	116	Total O 118 118	0	2
41	Y	4	Total O 4 4	0	0
41	X	9	Total O 9 9	0	0
41	Z	1	Total O 1 1	0	0
41	a	153	Total O 154 154	0	1
41	b	261	Total O 264 264	0	3
41	c	197	Total O 199 199	0	2
41	d	132	Total O 137 137	0	5
41	e	17	Total O 17 17	0	0
41	f	5	Total O 5 5	0	0
41	h	41	Total O 41 41	0	0
41	i	6	Total O 6 6	0	0
41	j	7	Total O 7 7	0	0
41	k	6	Total O 6 6	0	0
41	l	10	Total O 10 10	0	0
41	m	18	Total O 18 18	0	0

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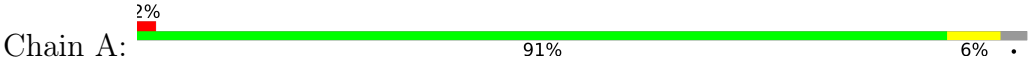
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	o	154	Total O 155 155	0	1
41	t	12	Total O 12 12	0	0
41	u	97	Total O 97 97	0	0
41	v	89	Total O 90 90	0	1
41	y	4	Total O 4 4	0	0
41	x	4	Total O 4 4	0	0

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

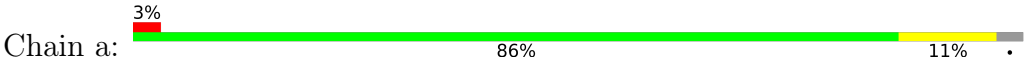
Chain A:

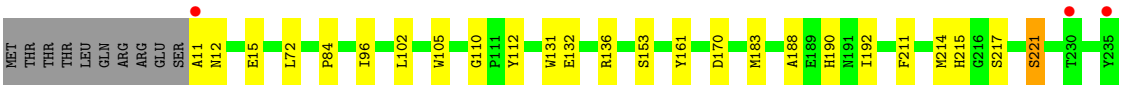


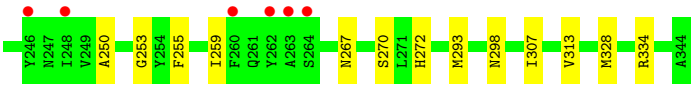


• Molecule 1: Photosystem Q(B) protein

Chain a:

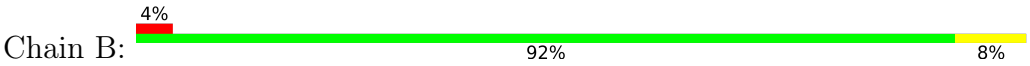


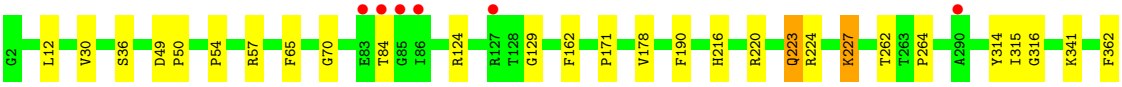


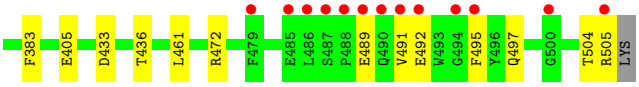


• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

Chain B:

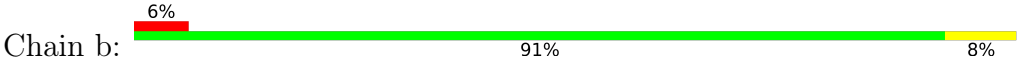




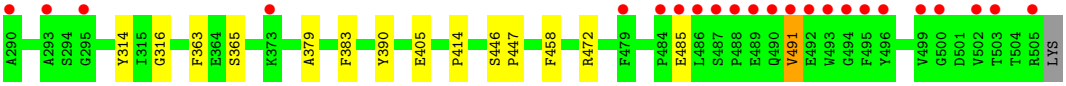


• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

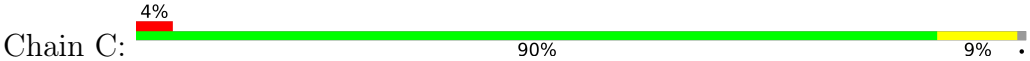
Chain b:

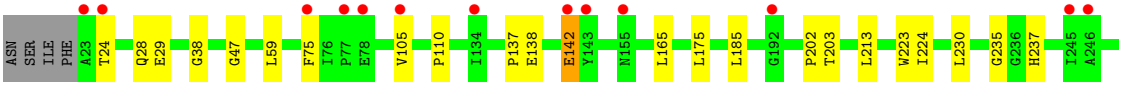


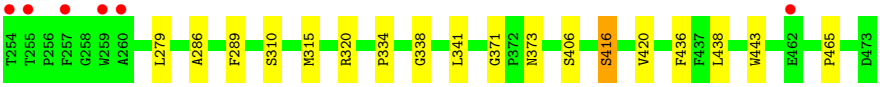




• Molecule 3: Photosystem II 44 kDa reaction center protein

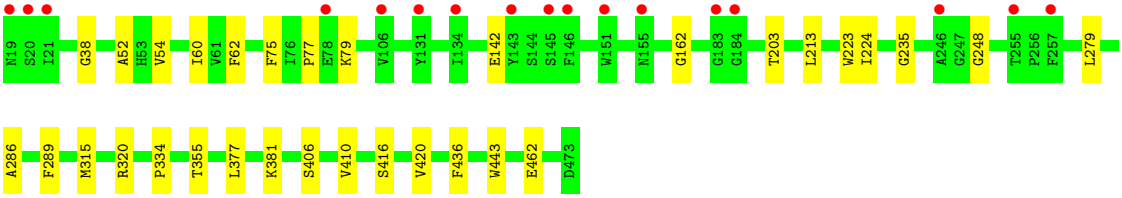




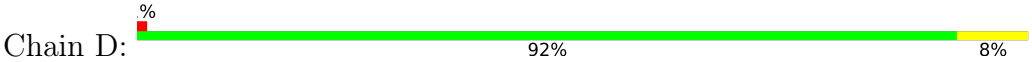


• Molecule 3: Photosystem II 44 kDa reaction center protein



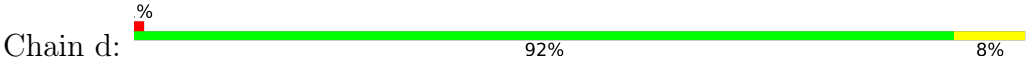


• Molecule 4: Photosystem II D2 protein



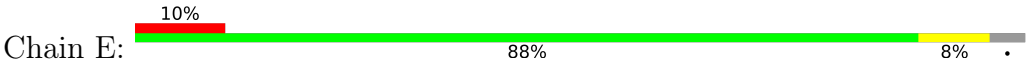


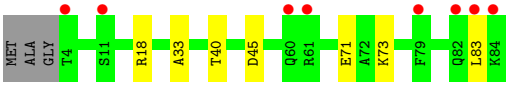
• Molecule 4: Photosystem II D2 protein



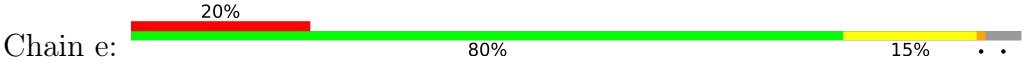


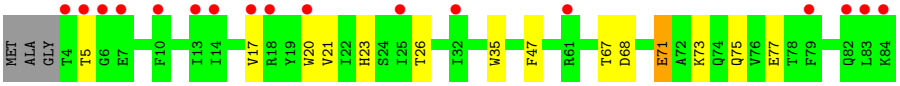
• Molecule 5: Cytochrome b559 subunit alpha





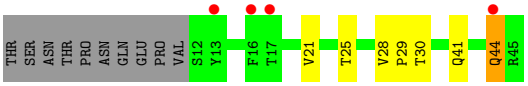
• Molecule 5: Cytochrome b559 subunit alpha





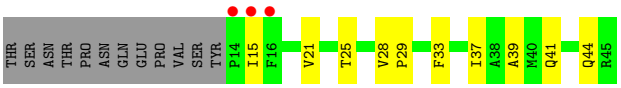
• Molecule 6: Cytochrome b559 subunit beta



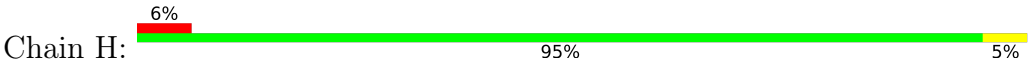


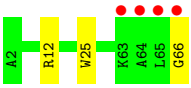
• Molecule 6: Cytochrome b559 subunit beta





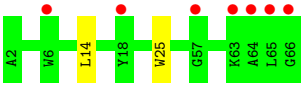
• Molecule 7: Photosystem II reaction center protein H



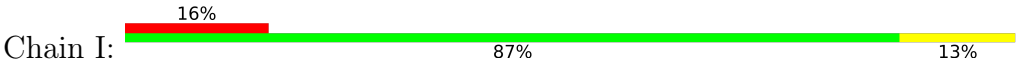


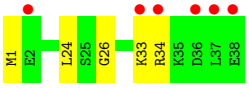
• Molecule 7: Photosystem II reaction center protein H



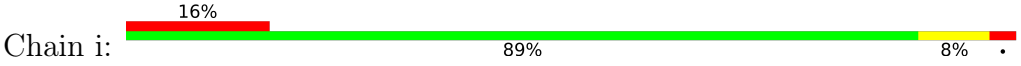


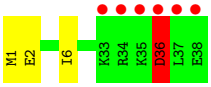
• Molecule 8: Photosystem II reaction center protein I





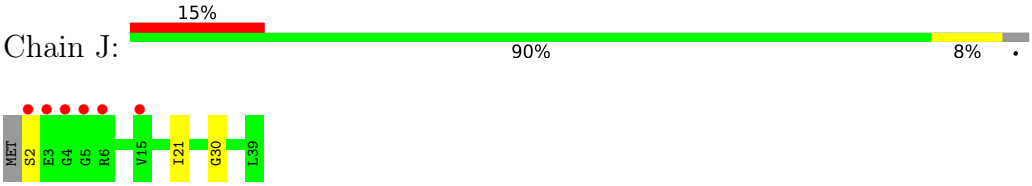
• Molecule 8: Photosystem II reaction center protein I





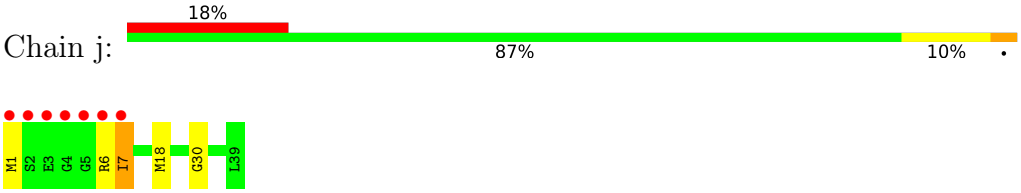
• Molecule 9: Photosystem II reaction center protein J

Chain J:



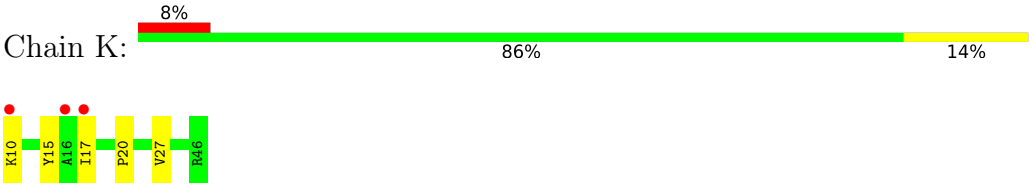
• Molecule 9: Photosystem II reaction center protein J

Chain j:



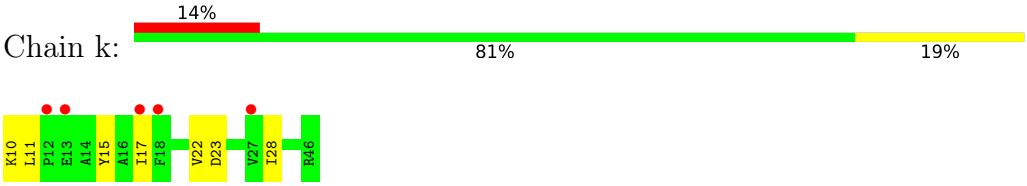
• Molecule 10: Photosystem II reaction center protein K

Chain K:



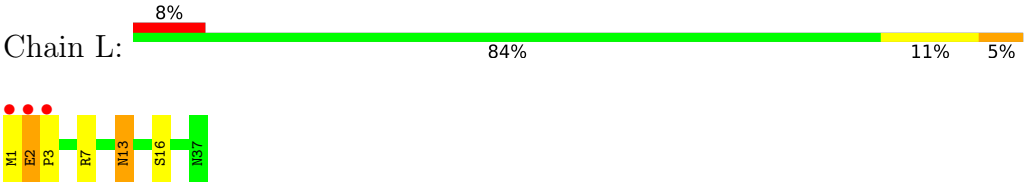
• Molecule 10: Photosystem II reaction center protein K

Chain k:



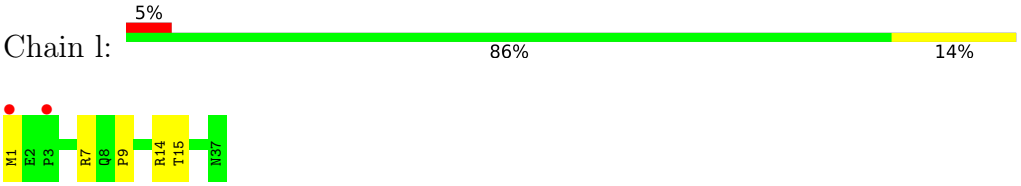
• Molecule 11: Photosystem II reaction center protein L

Chain L:



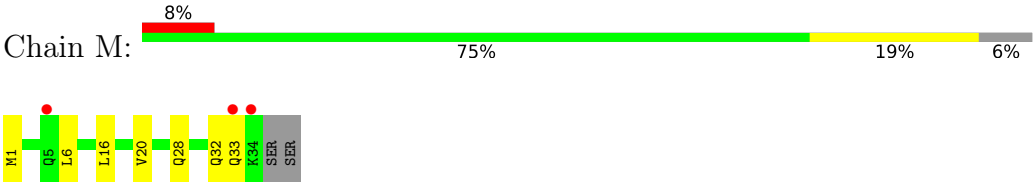
• Molecule 11: Photosystem II reaction center protein L

Chain l:



• Molecule 12: Photosystem II reaction center protein M

Chain M:



• Molecule 12: Photosystem II reaction center protein M

Chain m:

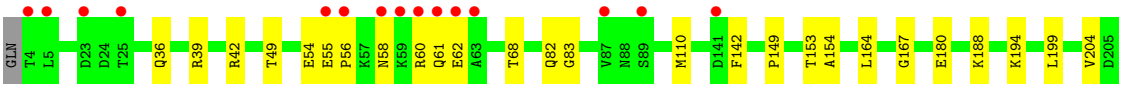


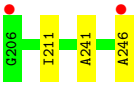


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



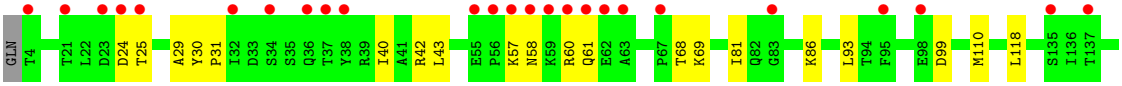


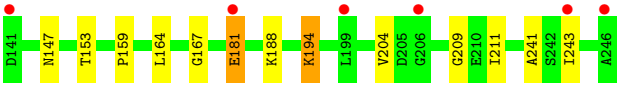


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



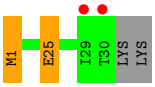




• Molecule 14: Photosystem II reaction center protein T

Chain T:

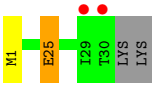




• Molecule 14: Photosystem II reaction center protein T

Chain t:

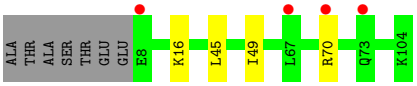




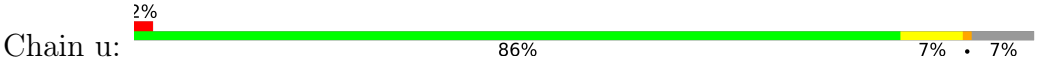
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:





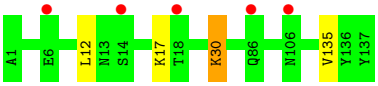
• Molecule 15: Photosystem II 12 kDa extrinsic protein





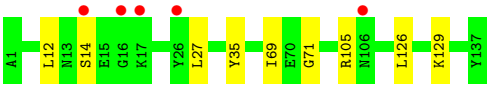
• Molecule 16: Cytochrome c-550



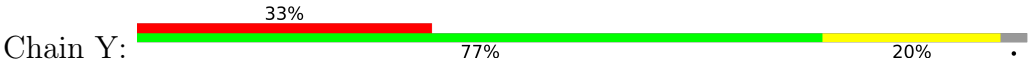


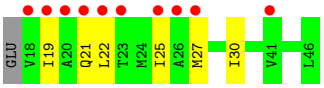
• Molecule 16: Cytochrome c-550





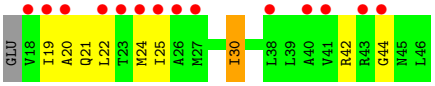
• Molecule 17: Photosystem II reaction center protein Ycf12





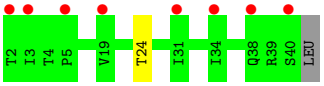
• Molecule 17: Photosystem II reaction center protein Ycf12





• Molecule 18: Photosystem II reaction center protein X

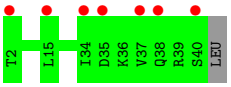




• Molecule 18: Photosystem II reaction center protein X

Chain x:

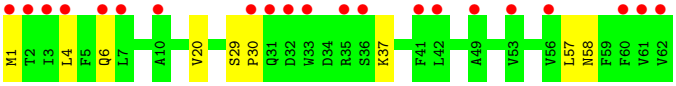




• Molecule 19: Photosystem II reaction center protein Z

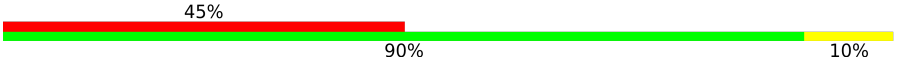
Chain Z:

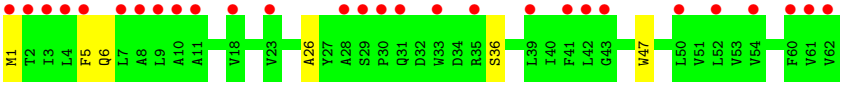




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

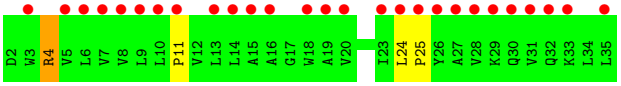




• Molecule 20: Photosystem II protein Y

Chain R:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.74Å 229.99Å 288.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.29 – 1.95 62.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (62.29-1.95) 92.2 (62.29-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.67 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.198 , 0.238 0.198 , 0.238	Depositor DCC
R_{free} test set	29338 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	54195	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: HTG, PL9, HEM, FME, SQD, LMG, HEC, BCT, CL, UNL, LHG, PHO, OEX, LMT, CA, FE2, GOL, DGD, BCR, CLA, MG

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	0.66	0/2728	0.85	0/3719
1	a	0.65	0/2748	0.84	0/3746
2	B	0.60	0/4200	0.82	0/5721
2	b	0.57	0/4209	0.83	2/5734 (0.0%)
3	C	0.56	1/3626 (0.0%)	0.83	2/4936 (0.0%)
3	c	0.56	1/3676 (0.0%)	0.82	0/5004
4	D	0.65	0/2827	0.84	0/3852
4	d	0.63	0/2818	0.83	4/3840 (0.1%)
5	E	0.47	0/693	0.87	1/944 (0.1%)
5	e	0.45	0/695	0.78	0/948
6	F	0.52	0/284	0.79	0/387
6	f	0.56	0/265	0.85	0/360
7	H	0.51	0/535	0.84	0/728
7	h	0.47	0/524	0.78	0/713
8	I	0.43	0/311	0.85	0/419
8	i	0.48	0/311	0.79	0/419
9	J	0.53	0/278	0.81	0/376
9	j	0.51	0/286	0.86	2/386 (0.5%)
10	K	0.47	0/303	0.80	0/416
10	k	0.57	0/303	0.78	0/416
11	L	0.58	0/319	0.73	0/433
11	l	0.53	0/319	0.75	0/433
12	M	0.61	0/270	0.89	0/368
12	m	0.74	0/262	0.95	0/357
13	O	0.50	0/1958	0.82	3/2654 (0.1%)
13	o	0.48	0/1937	0.81	0/2625
14	T	0.63	0/266	0.81	0/362
14	t	0.69	0/266	0.71	0/362
15	U	0.54	0/785	0.80	0/1064
15	u	0.52	0/785	0.77	0/1064
16	V	0.56	0/1096	0.80	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.51	0/1085	0.82	1/1473 (0.1%)
17	Y	0.46	0/216	0.80	0/289
17	y	0.45	0/216	0.85	0/289
18	X	0.46	0/290	0.73	0/392
18	x	0.42	0/290	0.76	0/392
19	Z	0.43	0/490	0.76	0/669
19	z	0.45	0/490	0.85	0/669
20	R	0.38	0/279	0.73	0/383
All	All	0.57	2/43239 (0.0%)	0.82	15/58829 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	410	VAL	CA-CB	5.56	1.59	1.54
3	C	310	SER	C-O	5.41	1.30	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	v	105	ARG	N-CA-C	6.89	119.63	111.71
2	b	221	PRO	O-C-N	6.03	123.98	121.15
4	d	170	ALA	CA-C-N	-5.69	114.07	119.76
4	d	170	ALA	C-N-CA	-5.69	114.07	119.76
4	d	55	VAL	N-CA-C	5.51	116.92	108.71
3	C	371	GLY	CA-C-N	5.50	125.84	119.47
3	C	371	GLY	C-N-CA	5.50	125.84	119.47
9	j	7	ILE	CA-C-N	5.32	125.62	119.93
9	j	7	ILE	C-N-CA	5.32	125.62	119.93
4	d	330	ALA	N-CA-C	5.21	120.02	113.25
5	E	83	LEU	N-CA-C	-5.17	107.49	112.97
13	O	55	GLU	CA-C-N	5.09	125.02	119.78
13	O	55	GLU	C-N-CA	5.09	125.02	119.78
13	O	154	ALA	N-CA-C	5.03	117.49	111.71
2	b	414	PRO	N-CA-C	5.03	116.83	110.70

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	2634	0	2546	13	0
1	a	2645	0	2567	29	0
2	B	4027	0	3906	27	0
2	b	4033	0	3921	35	0
3	C	3501	0	3428	26	0
3	c	3544	0	3480	22	0
4	D	2729	0	2632	22	0
4	d	2720	0	2626	21	0
5	E	668	0	658	6	0
5	e	670	0	664	11	0
6	F	275	0	282	5	0
6	f	257	0	269	5	0
7	H	519	0	545	4	0
7	h	511	0	532	5	0
8	I	314	0	328	4	0
8	i	314	0	328	2	0
9	J	272	0	279	3	0
9	j	280	0	291	4	0
10	K	293	0	305	5	0
10	k	293	0	305	5	0
11	L	309	0	327	5	0
11	l	309	0	327	5	0
12	M	274	0	299	7	0
12	m	269	0	288	8	0
13	O	1903	0	1886	16	0
13	o	1891	0	1870	18	0
14	T	264	0	267	2	0
14	t	264	0	267	1	0
15	U	774	0	773	2	0
15	u	774	0	773	5	0
16	V	1072	0	1086	3	0
16	v	1064	0	1073	6	0
17	Y	215	0	246	3	0
17	y	215	0	246	5	0
18	X	287	0	317	1	0
18	x	287	0	317	0	0
19	Z	479	0	516	5	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	U	1	0	0	3	0
22	a	2	0	0	0	0
22	v	1	0	0	2	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	260	0	288	8	0
24	B	1040	0	1152	28	0
24	C	845	0	936	29	0
24	D	130	0	144	3	0
24	a	195	0	216	5	0
24	b	1040	0	1152	23	0
24	c	845	0	936	25	0
24	d	195	0	216	5	0
25	A	128	0	148	1	0
25	a	128	0	148	1	0
26	A	40	0	56	1	0
26	B	120	0	168	7	0
26	C	80	0	112	1	0
26	D	40	0	56	2	0
26	H	40	0	56	3	0
26	K	80	0	112	4	0
26	T	40	0	56	4	0
26	a	40	0	56	3	0
26	b	120	0	168	6	0
26	c	40	0	56	2	0
26	d	40	0	56	4	0
26	h	40	0	56	2	0
26	k	80	0	112	6	0
26	t	40	0	56	7	0
26	y	40	0	56	2	0
27	A	108	0	156	7	0
27	B	54	0	78	3	0
27	F	43	0	52	3	0
27	L	54	0	78	2	0
27	a	108	0	156	4	0
27	f	43	0	53	0	0
28	A	18	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	42	0	56	4	0
28	C	12	0	16	2	0
28	F	6	0	7	0	0
28	O	6	0	8	0	0
28	T	12	0	16	4	0
28	V	24	0	32	0	0
28	a	18	0	24	2	0
28	b	36	0	48	4	0
28	c	12	0	16	2	0
28	f	6	0	6	1	0
28	o	6	0	8	0	0
28	t	6	0	8	0	0
28	v	18	0	24	2	0
29	A	35	0	46	0	0
29	B	60	0	81	2	0
29	C	35	0	46	2	0
29	E	35	0	46	1	0
29	M	35	0	46	3	0
29	a	35	0	46	2	0
29	b	50	0	70	4	0
29	c	35	0	46	1	0
29	f	35	0	46	1	0
29	m	105	0	138	7	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	55	0	80	5	0
31	D	55	0	80	1	0
31	a	55	0	80	5	0
31	d	55	0	80	1	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	D	57	0	0	0	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	K	34	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	71	0	0	0	0
32	i	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	j	10	0	0	0	0
32	m	10	0	0	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	3	0
34	Z	37	0	44	3	0
34	a	51	0	72	3	0
34	b	51	0	72	2	0
34	c	102	0	144	2	0
34	j	51	0	72	5	0
34	z	39	0	48	2	0
35	B	95	0	130	3	0
35	C	38	0	52	1	0
35	D	16	0	17	3	0
35	O	19	0	26	1	0
35	V	19	0	26	0	0
35	b	76	0	104	0	0
35	c	38	0	52	1	0
35	d	16	0	17	2	0
36	C	186	0	246	8	0
36	D	62	0	82	5	0
36	H	62	0	82	1	0
36	c	186	0	246	5	0
36	d	62	0	82	6	0
36	h	62	0	82	0	0
37	D	147	0	222	9	0
37	E	42	0	57	2	0
37	L	49	0	74	1	0
37	d	147	0	222	8	0
37	e	42	0	57	1	0
37	l	49	0	74	2	0
38	E	43	0	30	0	0
38	e	43	0	30	2	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	167	0	0	0	0
41	B	293	0	0	2	0
41	C	235	0	0	1	0
41	D	143	0	0	2	0
41	E	31	0	0	0	0
41	F	9	0	0	0	0
41	H	49	0	0	0	0
41	I	4	0	0	0	0
41	J	13	0	0	1	0
41	K	8	0	0	1	0
41	L	17	0	0	0	0
41	M	8	0	0	0	0
41	O	191	0	0	4	0
41	T	17	0	0	0	0
41	U	81	0	0	3	0
41	V	118	0	0	1	0
41	X	9	0	0	0	0
41	Y	4	0	0	0	0
41	Z	1	0	0	1	0
41	a	154	0	0	3	0
41	b	264	0	0	2	0
41	c	199	0	0	1	0
41	d	137	0	0	2	0
41	e	17	0	0	0	0
41	f	5	0	0	0	0
41	h	41	0	0	0	0
41	i	6	0	0	0	0
41	j	7	0	0	0	0
41	k	6	0	0	0	0
41	l	10	0	0	0	0
41	m	18	0	0	0	0
41	o	155	0	0	0	0
41	t	12	0	0	0	0
41	u	97	0	0	2	0
41	v	90	0	0	0	0
41	x	4	0	0	0	0
41	y	4	0	0	1	0
All	All	54195	0	52838	501	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 5.

All (501) 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	31:A:419:PL9:H102	1.48	0.95
5:e:67:THR:H	5:e:75:GLN:HE22	1.13	0.94
12:M:16[C]:LEU:HD23	12:m:16:LEU:HD12	1.55	0.88
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.55	0.87
1:a:214:MET:HG2	31:a:417:PL9:H102	1.55	0.85
22:U:201:CL:CL	41:U:305:HOH:O	2.35	0.82
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.63	0.81
24:C:514:CLA:H202	34:C:521:LMG:H402	1.66	0.76
26:T:102:BCR:H19C	26:b:622:BCR:H363	1.67	0.76
12:M:6:LEU:HD11	29:m:102:LMT:H21	1.68	0.76
28:a:414:GOL:H11	12:m:1:FME:HG2	1.69	0.73
28:A:414:GOL:H11	12:M:1:FME:HG2	1.71	0.73
41:b:754:HOH:O	22:v:201:CL:CL	2.43	0.73
14:T:25[A]:GLU:HG3	28:T:101:GOL:H2	1.70	0.72
37:D:408:LHG:H372	37:D:408:LHG:H132	1.72	0.72
34:j:101:LMG:H342	34:j:101:LMG:H241	1.72	0.72
22:U:201:CL:CL	41:V:407:HOH:O	2.46	0.70
2:B:223[B]:GLN:NE2	41:B:943:HOH:O	2.23	0.70
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.23	0.69
3:C:286:ALA:HB2	24:C:503:CLA:HMD1	1.75	0.69
27:A:412:SQD:H251	37:D:408:LHG:H131	1.74	0.68
36:D:405:DGD:O1B	36:D:405:DGD:O2D	2.11	0.68
5:E:45:ASP:OD2	20:R:4:ARG:NH2	2.27	0.68
34:j:101:LMG:H321	34:j:101:LMG:H221	1.75	0.68
3:c:279:LEU:HD22	24:c:910:CLA:HED2	1.75	0.68
22:U:201:CL:CL	41:U:331:HOH:O	2.49	0.67
36:C:519:DGD:HA32	34:J:101:LMG:H121	1.77	0.67
24:c:903:CLA:H61	24:c:913:CLA:H42	1.76	0.66
28:T:103:GOL:H2	29:b:601:LMT:H2'	1.76	0.66
2:b:266:GLU:HB3	28:b:633:GOL:H11	1.78	0.66
24:C:509:CLA:H92	37:D:408:LHG:H371	1.77	0.65
34:c:920:LMG:H391	34:c:920:LMG:H232	1.77	0.65
41:u:242:HOH:O	22:v:201:CL:CL	2.52	0.65
4:D:139:ARG:NH2	41:D:629:HOH:O	2.30	0.65
24:b:615:CLA:H142	37:l:101:LHG:H361	1.78	0.65
26:K:102:BCR:H321	26:K:102:BCR:HC8	1.80	0.64
26:H:101:BCR:HC8	26:H:101:BCR:H331	1.79	0.63
13:o:40:ILE:HG12	13:o:243:ILE:HD13	1.80	0.63
15:U:16:LYS:NZ	41:U:347:HOH:O	2.30	0.62
24:a:409:CLA:H152	24:c:907:CLA:H142	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:j:101:LMG:H292	34:j:101:LMG:H142	1.81	0.61
11:L:2:GLU:HG2	11:L:3:PRO:HD2	1.82	0.61
24:c:911:CLA:H41	37:d:409:LHG:H383	1.83	0.61
2:b:224:ARG:HH11	29:b:625:LMT:H1'	1.66	0.61
4:d:192:THR:HG23	24:d:402:CLA:HBC2	1.83	0.61
2:b:224:ARG:NH1	29:b:625:LMT:H1'	2.15	0.60
16:v:71:GLY:HA2	28:v:203:GOL:H32	1.83	0.60
6:F:30:THR:HG21	34:J:101:LMG:H412	1.82	0.60
12:M:16[C]:LEU:CD2	12:m:16:LEU:HD12	2.29	0.60
36:D:405:DGD:HD4	5:E:45:ASP:HB3	1.83	0.60
28:a:414:GOL:O1	41:a:523:HOH:O	2.16	0.59
1:A:121[B]:LEU:HD11	24:C:506:CLA:H122	1.85	0.59
12:M:16[C]:LEU:HD23	12:m:16:LEU:CD1	2.28	0.59
24:C:507:CLA:HMC2	24:C:508:CLA:H102	1.83	0.58
28:T:103:GOL:H12	29:m:104:LMT:H12	1.85	0.58
24:b:613:CLA:HHC	24:b:613:CLA:HBB1	1.84	0.58
1:a:298:ASN:ND2	41:a:578:HOH:O	2.33	0.58
12:m:6:LEU:HD11	29:m:104:LMT:H11	1.84	0.58
1:a:211:PHE:CE2	31:a:417:PL9:H13	2.38	0.58
24:C:503:CLA:H61	24:C:513:CLA:H42	1.85	0.58
29:B:636:LMT:H2'	28:B:637:GOL:H2	1.85	0.57
36:D:405:DGD:HA42	36:D:405:DGD:HB22	1.86	0.57
16:V:12:LEU:HD23	16:V:17:LYS:HD3	1.85	0.57
24:b:619:CLA:H2	24:b:620:CLA:HBB2	1.86	0.57
24:B:602:CLA:H12	24:B:602:CLA:H71	1.85	0.57
24:B:616:CLA:H71	24:B:617:CLA:H192	1.85	0.57
3:c:443:TRP:CE2	24:c:909:CLA:HMD2	2.40	0.57
3:c:54:VAL:HG22	24:c:914:CLA:HBB1	1.87	0.57
24:C:510:CLA:HMB1	24:C:510:CLA:HBB1	1.87	0.56
4:d:101:PHE:HB3	36:d:406:DGD:HG2	1.86	0.56
11:L:13:ASN:C	11:L:13:ASN:HD22	2.14	0.56
2:b:234:ILE:HB	28:b:632:GOL:H31	1.86	0.56
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.87	0.56
36:d:406:DGD:O1B	36:d:406:DGD:O2D	2.25	0.55
3:c:320:ARG:HB2	28:c:925:GOL:H32	1.88	0.55
3:C:320:ARG:HB2	28:C:525:GOL:H32	1.88	0.55
11:L:13:ASN:ND2	11:L:16:SER:H	2.03	0.55
24:B:605:CLA:HBB1	24:B:605:CLA:HMB1	1.89	0.55
28:B:637:GOL:H12	29:m:102:LMT:H11	1.88	0.55
3:C:406:SER:HA	3:C:420:VAL:HG23	1.89	0.55
16:v:14:SER:OG	28:v:203:GOL:O1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.89	0.55
24:B:617:CLA:H121	26:B:620:BCR:H12C	1.89	0.55
37:d:409:LHG:H381	37:d:409:LHG:H122	1.88	0.55
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.41	0.55
31:a:417:PL9:H28	37:e:101:LHG:H222	1.89	0.55
34:C:501:LMG:H161	36:C:517:DGD:HA62	1.89	0.55
34:c:920:LMG:H321	26:k:101:BCR:H342	1.87	0.54
24:c:907:CLA:HMC2	24:c:908:CLA:H102	1.89	0.54
8:i:36:ASP:OD1	8:i:36:ASP:N	2.38	0.54
28:B:637:GOL:H31	29:m:102:LMT:H6D	1.88	0.54
27:L:102:SQD:H1	27:L:102:SQD:H462	1.88	0.54
26:y:101:BCR:H321	26:y:101:BCR:HC8	1.89	0.54
25:A:409:PHO:HBC3	4:D:279:LEU:HD22	1.90	0.54
13:O:82:GLN:NE2	41:O:566:HOH:O	2.40	0.53
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.89	0.53
28:f:101:GOL:H11	16:v:27:LEU:HD21	1.90	0.53
24:A:410:CLA:H193	24:C:507:CLA:H93	1.91	0.53
1:A:84:PRO:HA	1:A:112:TYR:CG	2.44	0.53
4:d:103:ARG:HH21	5:e:77:GLU:HG3	1.73	0.53
24:C:509:CLA:HBC3	24:C:511:CLA:H71	1.90	0.53
29:M:101:LMT:H6'1	11:l:9:PRO:HB3	1.91	0.53
3:C:465:PRO:HG3	8:I:33:LYS:HE2	1.91	0.52
3:c:334:PRO:HA	13:o:153:THR:OG1	2.10	0.52
35:B:633:HTG:H61	1:a:102:LEU:HD12	1.90	0.52
26:H:101:BCR:H331	26:H:101:BCR:C8	2.37	0.52
34:B:622:LMG:HC5	29:m:102:LMT:H12	1.91	0.52
24:A:410:CLA:H171	24:C:507:CLA:H142	1.90	0.52
24:c:913:CLA:O2D	24:c:914:CLA:HBB2	2.10	0.52
24:C:511:CLA:H43	37:D:408:LHG:H383	1.92	0.52
34:J:101:LMG:H152	34:J:101:LMG:H292	1.92	0.52
28:b:631:GOL:H11	15:u:22:GLY:HA2	1.92	0.52
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.91	0.52
31:A:419:PL9:H502	4:D:39:PRO:HG3	1.93	0.51
34:C:501:LMG:H382	36:C:517:DGD:HB51	1.91	0.51
3:C:438:LEU:HD11	24:C:506:CLA:HBB1	1.92	0.51
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.91	0.51
3:c:213[B]:LEU:HD11	26:c:915:BCR:H373	1.93	0.51
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.10	0.51
24:B:609:CLA:HBB2	4:D:150:ILE:HD12	1.91	0.51
13:O:60:ARG:NH1	2:b:405:GLU:O	2.44	0.51
4:D:123:ILE:HD11	36:H:102:DGD:HAE1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	1.93	0.51
29:f:103:LMT:O3'	29:f:103:LMT:O2B	2.27	0.51
24:C:511:CLA:H192	24:C:511:CLA:HBC3	1.92	0.51
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.93	0.51
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.45	0.51
26:B:619:BCR:H363	26:t:101:BCR:H19C	1.93	0.50
2:b:145:LEU:HD22	24:b:608:CLA:H192	1.92	0.50
29:M:101:LMT:H6'2	12:m:32:GLN:HG2	1.92	0.50
8:i:2:GLU:O	8:i:6:ILE:HG12	2.12	0.50
26:B:620:BCR:H331	26:B:620:BCR:C8	2.42	0.50
2:b:86[B]:ILE:HD13	2:b:86[B]:ILE:H	1.76	0.50
36:d:406:DGD:HBT2	5:e:47:PHE:HZ	1.76	0.50
27:A:412:SQD:H381	9:J:21:ILE:HD11	1.93	0.50
2:B:162:PHE:O	24:B:607:CLA:HHD	2.11	0.50
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.92	0.50
4:d:139:ARG:NH2	41:d:627:HOH:O	2.43	0.50
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.50
3:C:279:LEU:HD22	24:C:510:CLA:HED2	1.93	0.50
3:c:443:TRP:CD2	24:c:909:CLA:HMD2	2.46	0.50
3:C:223:TRP:CG	3:C:224:ILE:H	2.30	0.50
29:B:623:LMT:O6'	4:D:16:ASP:OD2	2.30	0.50
2:b:201:HIS:HB2	24:b:606:CLA:CHB	2.42	0.49
24:c:902:CLA:C4D	24:c:904:CLA:H2	2.42	0.49
6:F:21:VAL:O	6:F:25:THR:HG23	2.12	0.49
2:b:491:VAL:HG13	4:d:136:VAL:HG13	1.95	0.49
3:c:381:LYS:NZ	13:o:99:ASP:OD2	2.42	0.49
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.46	0.49
2:b:216:HIS:HE1	24:b:613:CLA:C1A	2.25	0.49
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.48	0.49
1:a:267:ASN:HB3	1:a:270[B]:SER:OG	2.13	0.49
17:y:20:ALA:O	17:y:24:MET:HG2	2.13	0.49
2:B:497:GLN:HB2	2:B:504:THR:HB	1.95	0.49
2:b:12:LEU:HB2	24:b:616:CLA:HMC2	1.94	0.49
13:o:181[A]:GLU:H	13:o:181[A]:GLU:CD	2.20	0.49
1:A:38:ILE:HG12	27:A:416:SQD:H142	1.94	0.49
24:c:910:CLA:H191	24:c:913:CLA:HAC1	1.95	0.48
4:D:103:ARG:HG3	5:E:73:LYS:HE2	1.96	0.48
13:o:58:ASN:HD21	13:o:61:GLN:HB2	1.76	0.48
2:B:49:ASP:OD1	13:o:57:LYS:NZ	2.44	0.48
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.48	0.48
26:d:404:BCR:HC22	36:d:406:DGD:HA71	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:D:408:LHG:H382	37:D:408:LHG:H112	1.96	0.48
12:M:20:VAL:HG22	12:m:20:VAL:HG11	1.95	0.48
27:B:621:SQD:H462	27:B:621:SQD:H1	1.94	0.48
19:z:47:TRP:CE2	34:z:101:LMG:H241	2.48	0.48
3:C:185:LEU:HB2	3:C:230:LEU:HD13	1.95	0.48
29:C:522:LMT:H6'1	8:I:26:GLY:HA3	1.95	0.48
25:a:420:PHO:NC	25:a:420:PHO:ND	2.61	0.48
26:b:622:BCR:H331	26:b:622:BCR:C8	2.44	0.48
13:O:42:ARG:O	13:O:241:ALA:HA	2.14	0.48
27:a:411:SQD:H321	24:c:909:CLA:H71	1.95	0.48
24:c:903:CLA:H193	35:c:922:HTG:H3'1	1.95	0.48
36:d:406:DGD:HE3	36:d:406:DGD:HD4	1.96	0.48
37:d:409:LHG:H302	37:d:409:LHG:H332	1.38	0.48
13:o:42:ARG:O	13:o:241:ALA:HA	2.14	0.48
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.96	0.47
24:a:406:CLA:HBB1	24:a:406:CLA:HMB3	1.95	0.47
35:O:303:HTG:HO6	2:b:76[A]:SER:HG	1.63	0.47
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.27	0.47
26:k:102:BCR:H24C	26:k:102:BCR:H371	1.64	0.47
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.96	0.47
27:a:411:SQD:H251	37:d:409:LHG:H132	1.95	0.47
36:c:917:DGD:HB61	36:c:917:DGD:HB32	1.62	0.47
26:d:404:BCR:H381	34:j:101:LMG:H232	1.96	0.47
5:e:35:TRP:CD2	6:f:39:ALA:HB2	2.50	0.47
4:D:49:LEU:HD13	26:D:403:BCR:C15	2.44	0.47
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.97	0.47
35:d:412:HTG:H1	7:h:25:TRP:CD1	2.49	0.47
17:y:44:GLY:O	41:y:203:HOH:O	2.20	0.47
9:j:6:ARG:HA	9:j:6:ARG:NH2	2.30	0.47
1:a:132:GLU:O	1:a:136:ARG:HG2	2.15	0.47
9:j:18:MET:HE1	17:y:30:ILE:HD12	1.97	0.47
27:a:402:SQD:H142	26:t:101:BCR:HC41	1.96	0.47
16:v:12:LEU:HD12	16:v:69:ILE:HB	1.97	0.47
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.96	0.47
3:C:24:THR:HB	3:C:138:GLU:OE1	2.15	0.47
13:O:68:THR:HG22	13:O:110[B]:MET:HG2	1.97	0.47
26:T:102:BCR:HC8	26:T:102:BCR:H311	1.96	0.47
37:d:409:LHG:H331	37:d:409:LHG:H361	1.67	0.47
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.50	0.46
3:C:203:THR:O	3:C:235:GLY:HA3	2.15	0.46
4:D:27:PHE:HD1	37:E:101:LHG:HC12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.50	0.46
29:C:522:LMT:H31	8:I:24:LEU:HD13	1.98	0.46
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.51	0.46
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.96	0.46
4:d:101:PHE:HB2	36:d:406:DGD:HA41	1.97	0.46
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.98	0.46
1:a:153:SER:HB2	24:a:406:CLA:H43	1.97	0.46
36:C:518:DGD:HA81	36:C:518:DGD:HAE2	1.61	0.46
34:C:520:LMG:H192	10:K:27:VAL:HG11	1.97	0.46
34:C:521:LMG:HC1	34:C:521:LMG:HC8	1.74	0.46
1:a:84:PRO:HA	1:a:112:TYR:CG	2.51	0.46
13:o:30:TYR:CD1	13:o:209:GLY:HA2	2.51	0.46
27:A:412:SQD:O7	3:C:28:GLN:NE2	2.30	0.46
3:C:59:LEU:HD21	26:K:103:BCR:H372	1.97	0.46
24:D:402:CLA:HAC1	27:F:101:SQD:H383	1.98	0.46
26:K:103:BCR:H24C	26:K:103:BCR:H371	1.73	0.46
24:d:403:CLA:H142	24:d:403:CLA:H112	1.71	0.46
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.98	0.46
1:a:183:MET:HA	24:a:406:CLA:HMD1	1.98	0.46
19:z:47:TRP:CE3	34:z:101:LMG:H221	2.51	0.46
37:D:406:LHG:H101	37:D:406:LHG:H351	1.98	0.46
11:L:13:ASN:HD22	11:L:16:SER:H	1.64	0.46
1:a:131:TRP:CH2	24:c:906:CLA:HAA2	2.51	0.46
3:C:38:GLY:HA3	24:C:512:CLA:HMD2	1.98	0.45
27:L:102:SQD:H62	11:l:7:ARG:NH1	2.31	0.45
4:d:223:PHE:CZ	4:d:245:SER:HB2	2.51	0.45
4:d:341:PHE:O	41:d:614:HOH:O	2.21	0.45
26:h:101:BCR:H24C	26:h:101:BCR:H371	1.70	0.45
31:A:419:PL9:H251	31:A:419:PL9:H271	1.62	0.45
24:B:614:CLA:H143	24:B:614:CLA:H111	1.84	0.45
4:D:304:ARG:NH1	41:D:504:HOH:O	2.29	0.45
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.76	0.45
2:b:156:PHE:HB3	2:b:162:PHE:HB3	1.98	0.45
24:b:605:CLA:H202	26:h:101:BCR:H353	1.97	0.45
3:c:62:PHE:HZ	10:k:28:ILE:HD12	1.80	0.45
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.50	0.45
3:C:436:PHE:CE1	24:C:505:CLA:H161	2.51	0.45
29:E:102:LMT:O3'	29:E:102:LMT:O2B	2.30	0.45
1:a:72:LEU:HD11	29:a:401:LMT:H52	1.98	0.45
37:d:408:LHG:HC62	11:l:15:THR:HG23	1.99	0.45
37:d:409:LHG:H151	37:d:409:LHG:H342	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:C:518:DGD:HA31	36:C:518:DGD:HA62	1.80	0.45
24:b:619:CLA:H2	24:b:620:CLA:CBB	2.46	0.45
15:u:45:LEU:HD21	15:u:71:GLN:HB3	1.98	0.45
2:B:220:ARG:NH1	41:B:703:HOH:O	2.44	0.45
24:B:616:CLA:H112	24:B:616:CLA:H152	1.63	0.45
19:Z:30:PRO:HD2	41:Z:201:HOH:O	2.16	0.45
3:c:406:SER:HA	3:c:420:VAL:HG23	1.97	0.45
1:A:132:GLU:O	1:A:136:ARG:HG2	2.17	0.45
13:o:29:ALA:O	13:o:31:PRO:HD3	2.17	0.45
1:A:200:LEU:HG	36:C:519:DGD:HAT2	1.98	0.45
24:A:410:CLA:H61	24:A:410:CLA:H41	1.76	0.45
2:B:171:PRO:HD3	7:H:66:GLY:HA2	1.99	0.45
26:T:102:BCR:HC8	26:T:102:BCR:H321	1.99	0.45
15:U:45:LEU:O	15:U:49:ILE:HG13	2.17	0.45
3:C:47:GLY:HA3	3:C:137:PRO:O	2.17	0.45
24:C:508:CLA:H92	24:C:508:CLA:H61	1.84	0.45
28:C:525:GOL:H2	41:C:708:HOH:O	2.16	0.45
2:b:172:TYR:CE1	2:b:283:GLU:HB2	2.52	0.45
24:c:909:CLA:H92	37:d:409:LHG:H371	1.99	0.45
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.98	0.45
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.52	0.45
4:D:13:GLY:HA3	35:D:411:HTG:H62	1.99	0.45
10:K:10:LYS:N	41:K:204:HOH:O	2.50	0.45
3:c:223:TRP:CG	3:c:224:ILE:H	2.34	0.45
35:D:411:HTG:H1	7:H:25:TRP:CD1	2.52	0.45
27:F:101:SQD:H331	18:X:24:THR:HA	1.99	0.45
2:b:363:PHE:HB3	2:b:365:SER:O	2.16	0.45
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.99	0.45
2:B:65:PHE:HE1	24:B:605:CLA:HED2	1.83	0.44
27:B:621:SQD:H383	27:B:621:SQD:H352	1.78	0.44
4:D:14:TRP:CD1	35:D:411:HTG:HO6	2.35	0.44
4:D:192:THR:HG23	24:D:401:CLA:HBC2	1.99	0.44
4:d:49:LEU:HD13	26:d:404:BCR:C15	2.46	0.44
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.52	0.44
12:M:28:GLN:O	12:M:32:GLN:HG3	2.18	0.44
3:c:79:LYS:HD2	16:v:35:TYR:HE1	1.82	0.44
24:c:911:CLA:H161	24:c:911:CLA:H121	1.88	0.44
11:l:14:ARG:HB3	14:t:25[A]:GLU:HG2	1.99	0.44
13:o:68:THR:HG22	13:o:110[B]:MET:HG2	1.98	0.44
26:t:101:BCR:H24C	26:t:101:BCR:H371	1.82	0.44
26:B:619:BCR:H331	26:B:619:BCR:C8	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:C:520:LMG:H172	17:Y:25:ILE:HG12	2.00	0.44
13:O:39:ARG:HG3	13:O:83:GLY:O	2.18	0.44
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.99	0.44
24:b:610:CLA:H162	24:b:610:CLA:H122	1.43	0.44
24:c:902:CLA:H202	24:c:908:CLA:HBB1	2.00	0.44
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.53	0.44
3:c:38:GLY:HA3	24:c:912:CLA:HMD2	1.98	0.44
2:B:124:ARG:HD2	2:B:129:GLY:O	2.18	0.44
2:B:461:LEU:HD22	37:D:406:LHG:H301	1.99	0.44
13:O:36:GLN:O	41:O:557:HOH:O	2.20	0.44
35:B:633:HTG:O2	35:B:634:HTG:S1	2.58	0.44
24:C:502:CLA:H192	24:C:507:CLA:C1B	2.47	0.44
34:a:412:LMG:H172	34:a:412:LMG:H201	1.73	0.44
24:c:906:CLA:H112	24:c:906:CLA:H72	1.83	0.44
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.99	0.44
1:a:105:TRP:NE1	1:a:110:GLY:HA3	2.33	0.44
1:a:334:ARG:NH2	13:o:159:PRO:HA	2.33	0.44
4:d:85:MET:CE	4:d:96:GLU:HG2	2.48	0.44
2:B:50:PRO:HB2	28:B:631:GOL:H12	2.00	0.44
3:C:334:PRO:HA	13:O:153:THR:OG1	2.18	0.44
4:D:102:THR:OG1	36:D:405:DGD:HG31	2.18	0.44
26:a:410:BCR:H24C	26:a:410:BCR:H371	1.73	0.44
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.99	0.44
5:e:23:HIS:CD2	38:e:102:HEM:NC	2.84	0.44
26:t:101:BCR:H331	26:t:101:BCR:HC7	1.55	0.44
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.99	0.44
24:C:507:CLA:HBB1	24:C:507:CLA:HMB3	2.00	0.43
36:C:517:DGD:HAH1	36:C:517:DGD:HAT2	1.78	0.43
24:b:612:CLA:HAB	4:d:123:ILE:HG12	2.00	0.43
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	2.00	0.43
6:F:44:GLN:HE21	6:F:44:GLN:HB2	1.60	0.43
13:O:204:VAL:HG22	13:O:211:ILE:HG22	2.00	0.43
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.00	0.43
26:y:101:BCR:H15C	26:y:101:BCR:H351	1.78	0.43
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.43
3:c:203:THR:O	3:c:235:GLY:HA3	2.17	0.43
4:d:103:ARG:HG3	5:e:73:LYS:HG3	2.00	0.43
26:k:101:BCR:H24C	26:k:101:BCR:H371	1.72	0.43
5:E:40:THR:HB	20:R:4:ARG:HG2	1.99	0.43
2:b:201:HIS:HB2	24:b:606:CLA:C1B	2.48	0.43
26:t:101:BCR:H321	26:t:101:BCR:HC8	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:VAL:HG12	4:D:136:VAL:HG13	2.00	0.43
24:B:603:CLA:H203	24:B:603:CLA:H162	1.83	0.43
13:O:164:LEU:HB2	13:O:188:LYS:HB2	2.01	0.43
13:O:180:GLU:CD	13:O:180:GLU:H	2.26	0.43
26:a:410:BCR:H15C	26:a:410:BCR:H351	1.91	0.43
36:c:917:DGD:HBE1	36:c:917:DGD:HBF2	1.62	0.43
26:B:618:BCR:H11C	26:B:618:BCR:H341	1.89	0.43
2:b:30:VAL:HG12	24:b:609:CLA:HHD	1.99	0.43
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.53	0.43
24:C:510:CLA:H191	24:C:513:CLA:HAC1	2.01	0.43
26:T:102:BCR:H331	26:T:102:BCR:HC7	1.51	0.43
34:a:412:LMG:H201	36:c:916:DGD:HA81	2.01	0.43
2:b:446:SER:HB2	2:b:447:PRO:HD2	2.00	0.43
36:c:917:DGD:HA81	36:c:917:DGD:HAF1	2.01	0.43
27:A:412:SQD:H171	37:D:408:LHG:H181	2.01	0.43
6:f:21:VAL:O	6:f:25:THR:HG23	2.19	0.43
26:k:101:BCR:H11C	26:k:101:BCR:H341	1.91	0.43
12:m:28:GLN:O	12:m:32:GLN:HG3	2.19	0.43
26:t:101:BCR:H23C	26:t:101:BCR:H382	2.00	0.43
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.01	0.43
3:C:202:PRO:HD2	35:C:524:HTG:H62	1.99	0.43
13:O:54:GLU:O	13:O:56:PRO:HD3	2.19	0.43
20:R:24:LEU:N	20:R:25:PRO:HD2	2.34	0.43
1:a:153:SER:CB	24:a:406:CLA:H43	2.48	0.43
2:b:137:LYS:HD2	7:h:14:LEU:O	2.19	0.43
4:D:343:GLU:HG2	16:V:135:VAL:HG11	2.00	0.43
5:E:33:ALA:HB2	20:R:11:PRO:HB2	2.00	0.43
34:b:624:LMG:H421	37:l:101:LHG:H371	2.01	0.43
4:d:272:LEU:C	4:d:272:LEU:HD23	2.43	0.43
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.54	0.42
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.01	0.42
15:u:27:LEU:HD22	15:u:49:ILE:HG21	2.00	0.42
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.53	0.42
5:e:68:ASP:OD1	5:e:71:GLU:HB2	2.19	0.42
10:k:15:TYR:CZ	19:z:5:PHE:HZ	2.37	0.42
17:y:22:LEU:HA	17:y:25:ILE:HG22	2.01	0.42
28:T:103:GOL:H32	29:m:104:LMT:H21	2.01	0.42
1:a:215:HIS:HA	31:a:417:PL9:O1	2.19	0.42
24:d:402:CLA:H201	34:j:101:LMG:H222	2.00	0.42
15:u:86:GLU:HG2	41:u:293:HOH:O	2.18	0.42
24:A:405:CLA:CBD	24:A:406:CLA:HAC2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:609:CLA:H162	24:D:402:CLA:H3A	2.01	0.42
24:B:610:CLA:HHC	24:B:610:CLA:HBB1	2.02	0.42
3:C:110:PRO:HG3	34:C:521:LMG:H121	2.01	0.42
31:a:417:PL9:H251	31:a:417:PL9:H272	1.87	0.42
24:b:618:CLA:H41	24:b:618:CLA:H62	1.64	0.42
3:C:373:ASN:HB3	41:O:558:HOH:O	2.19	0.42
26:a:410:BCR:H11C	26:a:410:BCR:H341	1.94	0.42
24:b:605:CLA:H93	24:b:605:CLA:H111	1.88	0.42
2:B:190:PHE:CZ	24:B:603:CLA:HBB1	2.54	0.42
24:C:514:CLA:HBA1	24:C:514:CLA:H3A	1.67	0.42
24:C:514:CLA:HBC1	34:Z:101:LMG:H171	2.02	0.42
1:a:170:ASP:CG	41:a:527:HOH:O	2.61	0.42
2:b:221:PRO:HA	24:b:613:CLA:HED3	2.02	0.42
24:b:609:CLA:HHC	24:b:609:CLA:HBB1	2.02	0.42
6:f:33:PHE:O	6:f:37:ILE:HG13	2.20	0.42
26:C:515:BCR:H24C	26:C:515:BCR:H371	1.88	0.42
4:D:27:PHE:CD1	37:E:101:LHG:HC12	2.54	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.51	0.42
4:d:186:GLN:HB2	24:d:402:CLA:HBC1	2.01	0.42
24:A:406:CLA:H203	24:A:406:CLA:H162	1.80	0.42
31:A:419:PL9:H28	31:A:419:PL9:H321	1.87	0.42
2:B:433:ASP:OD1	2:B:436:THR:OG1	2.36	0.42
24:B:608:CLA:C4A	24:B:608:CLA:HBA2	2.49	0.42
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.54	0.42
24:b:607:CLA:CGA	24:b:607:CLA:H3A	2.50	0.42
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.02	0.42
4:d:202:ALA:HB2	31:d:405:PL9:H353	2.01	0.42
24:d:401:CLA:H203	24:d:401:CLA:H162	1.73	0.42
5:e:17:VAL:O	5:e:21:VAL:HG23	2.20	0.42
24:A:406:CLA:C4A	24:A:406:CLA:HBA1	2.49	0.42
26:K:103:BCR:H15C	26:K:103:BCR:H351	1.90	0.42
27:a:411:SQD:H312	27:a:411:SQD:H342	1.69	0.42
26:b:623:BCR:H15C	26:b:623:BCR:H351	1.92	0.42
3:c:286:ALA:HB2	24:c:903:CLA:HMD2	2.02	0.42
26:c:915:BCR:H15C	26:c:915:BCR:H351	1.87	0.42
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.54	0.42
13:o:86:LYS:O	13:o:93:LEU:HA	2.20	0.42
13:o:147:ASN:ND2	13:o:194:LYS:HE2	2.34	0.42
24:B:614:CLA:H162	24:B:614:CLA:H121	1.67	0.42
5:E:18:ARG:H	9:J:2:SER:N	2.18	0.42
24:b:605:CLA:C1B	24:b:605:CLA:H143	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:621:BCR:H24C	26:b:621:BCR:H371	1.77	0.42
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.19	0.41
24:B:617:CLA:H91	24:B:617:CLA:H112	1.60	0.41
24:C:506:CLA:HAA1	24:C:506:CLA:HBD	2.02	0.41
41:J:206:HOH:O	16:V:30:LYS:HE3	2.20	0.41
13:O:142:PHE:HB2	13:O:199:LEU:HD12	2.02	0.41
14:T:1:FME:HCN	29:b:601:LMT:H11	2.01	0.41
24:b:619:CLA:H112	24:b:619:CLA:H152	1.80	0.41
28:c:925:GOL:H2	41:c:1107:HOH:O	2.19	0.41
26:A:411:BCR:H24C	26:A:411:BCR:H371	1.80	0.41
24:B:602:CLA:C4A	24:B:602:CLA:HBA2	2.50	0.41
35:B:625:HTG:H2'2	35:B:625:HTG:H1	1.88	0.41
34:a:412:LMG:H211	34:a:412:LMG:H241	1.77	0.41
24:c:914:CLA:C4B	26:k:101:BCR:H383	2.50	0.41
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.55	0.41
24:C:508:CLA:H61	24:C:508:CLA:H41	1.87	0.41
13:O:58:ASN:HD21	13:O:61:GLN:HB2	1.86	0.41
2:b:125:ASP:HA	2:b:126:PRO:HD3	1.93	0.41
26:b:621:BCR:H12C	34:b:624:LMG:C43	2.51	0.41
4:d:26:ARG:HA	5:e:5:THR:HB	2.03	0.41
10:k:10:LYS:HD2	10:k:10:LYS:N	2.35	0.41
31:A:419:PL9:H512	27:F:101:SQD:H302	2.02	0.41
36:C:517:DGD:HAE1	36:C:517:DGD:HA81	1.79	0.41
2:b:26:HIS:CE1	24:b:616:CLA:HMA2	2.56	0.41
27:A:412:SQD:H152	27:A:412:SQD:H122	1.61	0.41
4:D:85:MET:CE	4:D:96:GLU:HG2	2.51	0.41
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.55	0.41
5:e:26:THR:HB	38:e:102:HEM:HAB	2.03	0.41
13:o:164:LEU:HB2	13:o:188:LYS:HB2	2.02	0.41
24:B:602:CLA:H142	24:B:602:CLA:H112	1.80	0.41
3:C:142:GLU:CD	3:C:142:GLU:H	2.28	0.41
3:C:165:LEU:HD21	24:C:507:CLA:CAB	2.51	0.41
3:C:338:GLY:HA3	3:C:341:LEU:O	2.20	0.41
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.55	0.41
13:O:149:PRO:HB2	41:O:409:HOH:O	2.21	0.41
1:a:11:ALA:HA	1:a:15:GLU:OE2	2.20	0.41
35:d:412:HTG:H1	7:h:25:TRP:CG	2.56	0.41
24:B:607:CLA:H122	24:B:607:CLA:H161	1.81	0.41
26:D:403:BCR:H11C	26:D:403:BCR:H341	1.93	0.41
34:Z:101:LMG:H111	34:Z:101:LMG:HC8	1.64	0.41
28:b:632:GOL:H32	41:b:961:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:614:CLA:H122	34:B:622:LMG:H232	2.02	0.41
24:C:506:CLA:H93	24:C:506:CLA:H111	1.87	0.41
24:C:508:CLA:HAA2	24:C:508:CLA:HBD	2.02	0.41
13:O:39:ARG:HB2	13:O:246:ALA:HB2	2.02	0.41
3:c:52:ALA:HB2	24:c:912:CLA:HMA2	2.02	0.41
4:d:47:GLY:C	4:d:114:ILE:HD11	2.46	0.41
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.03	0.41
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.02	0.41
2:B:223[A]:GLN:OE1	2:B:227:LYS:HD2	2.21	0.41
24:B:602:CLA:HAA1	24:B:602:CLA:HBD	2.02	0.41
24:B:612:CLA:H142	37:L:101:LHG:H362	2.02	0.41
24:B:617:CLA:H152	24:B:617:CLA:H111	1.75	0.41
36:D:405:DGD:HBT1	36:D:405:DGD:HBH1	1.85	0.41
37:D:408:LHG:H112	37:D:408:LHG:C38	2.51	0.41
1:a:217:SER:O	1:a:221[A]:SER:HB3	2.20	0.41
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.21	0.41
2:b:458:PHE:HB3	24:b:608:CLA:HBC2	2.02	0.41
3:c:436:PHE:CE1	24:c:905:CLA:H161	2.55	0.41
36:c:917:DGD:HA81	36:c:917:DGD:HAE2	1.80	0.41
29:c:921:LMT:H72	29:c:921:LMT:H102	1.89	0.41
26:k:101:BCR:H351	26:k:101:BCR:H15C	1.78	0.41
24:B:604:CLA:CGA	24:B:604:CLA:H3A	2.51	0.41
3:C:443:TRP:CE2	24:C:509:CLA:HMD2	2.56	0.41
10:K:10:LYS:N	10:K:10:LYS:HD2	2.36	0.41
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.88	0.41
1:a:72:LEU:HD13	29:a:401:LMT:H11	2.02	0.41
3:c:75:PHE:CZ	3:c:77:PRO:HA	2.55	0.41
5:e:20:TRP:HD1	9:j:7:ILE:HD12	1.85	0.41
2:B:262:THR:C	2:B:264:PRO:HD3	2.45	0.40
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.02	0.40
24:b:605:CLA:H142	24:b:605:CLA:H112	1.80	0.40
3:c:213[A]:LEU:HG	24:c:907:CLA:H202	2.03	0.40
26:B:619:BCR:H371	26:B:619:BCR:H24C	1.77	0.40
19:Z:37:LYS:NZ	34:Z:101:LMG:HC61	2.36	0.40
2:b:86[A]:ILE:H	2:b:86[A]:ILE:HG13	1.77	0.40
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.55	0.40
26:d:404:BCR:H15C	26:d:404:BCR:H351	1.85	0.40
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.04	0.40
24:A:406:CLA:H192	27:A:416:SQD:H223	2.02	0.40
27:B:621:SQD:O8	11:L:7:ARG:HD3	2.21	0.40
24:C:513:CLA:H101	24:C:514:CLA:H141	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:623:BCR:C8	26:b:623:BCR:H331	2.51	0.40
31:D:404:PL9:H422	31:D:404:PL9:H401	1.74	0.40
29:M:101:LMT:H6D	11:l:9:PRO:HA	2.03	0.40
1:a:161:TYR:OH	1:a:190:HIS:NE2	2.35	0.40
3:c:60:ILE:HG22	24:c:904:CLA:HHD	2.03	0.40
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.53	0.40
26:t:101:BCR:H11C	26:t:101:BCR:H341	1.97	0.40
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.21	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%)	331 (99%)	3 (1%)	1 (0%)	36	28
1	a	338/344 (98%)	333 (98%)	4 (1%)	1 (0%)	36	28
2	B	513/505 (102%)	506 (99%)	7 (1%)	0	100	100
2	b	514/505 (102%)	506 (98%)	8 (2%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	30	21
3	c	459/455 (101%)	445 (97%)	12 (3%)	2 (0%)	30	21
4	D	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	79 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (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	249/244 (102%)	240 (96%)	8 (3%)	1 (0%)	30	21
13	o	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	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%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5290/5384 (98%)	5170 (98%)	112 (2%)	8 (0%)	48	36

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER

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Mol	Chain	Res	Type
3	c	416[A]	SER
3	c	416[B]	SER
13	O	62	GLU
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	275/279 (99%)	272 (99%)	3 (1%)	65 64
2	B	413/403 (102%)	404 (98%)	9 (2%)	45 40
2	b	414/403 (103%)	409 (99%)	5 (1%)	63 61
3	C	356/356 (100%)	349 (98%)	7 (2%)	48 43
3	c	362/356 (102%)	356 (98%)	6 (2%)	53 49
4	D	278/277 (100%)	275 (99%)	3 (1%)	65 64
4	d	277/277 (100%)	274 (99%)	3 (1%)	65 64
5	E	74/73 (101%)	73 (99%)	1 (1%)	59 56
5	e	74/73 (101%)	73 (99%)	1 (1%)	59 56
6	F	28/38 (74%)	27 (96%)	1 (4%)	31 21
6	f	26/38 (68%)	24 (92%)	2 (8%)	12 3
7	H	55/54 (102%)	53 (96%)	2 (4%)	31 21
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%)	33 (97%)	1 (3%)	37 29
9	J	26/27 (96%)	26 (100%)	0	100 100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30 20
10	K	30/30 (100%)	29 (97%)	1 (3%)	33 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	k	30/30 (100%)	29 (97%)	1 (3%)	33 24
11	L	36/35 (103%)	33 (92%)	3 (8%)	10 3
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 30
12	M	31/32 (97%)	30 (97%)	1 (3%)	34 25
12	m	30/32 (94%)	28 (93%)	2 (7%)	15 5
13	O	214/207 (103%)	211 (99%)	3 (1%)	59 56
13	o	211/207 (102%)	204 (97%)	7 (3%)	33 24
14	T	27/28 (96%)	25 (93%)	2 (7%)	13 4
14	t	27/28 (96%)	25 (93%)	2 (7%)	13 4
15	U	84/89 (94%)	83 (99%)	1 (1%)	63 61
15	u	84/89 (94%)	83 (99%)	1 (1%)	63 61
16	V	118/117 (101%)	117 (99%)	1 (1%)	73 74
16	v	117/117 (100%)	117 (100%)	0	100 100
17	Y	22/23 (96%)	19 (86%)	3 (14%)	3 0
17	y	22/23 (96%)	19 (86%)	3 (14%)	3 0
18	X	32/33 (97%)	32 (100%)	0	100 100
18	x	32/33 (97%)	32 (100%)	0	100 100
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18 7
19	z	52/52 (100%)	50 (96%)	2 (4%)	29 19
20	R	29/29 (100%)	28 (97%)	1 (3%)	32 23
All	All	4395/4403 (100%)	4312 (98%)	83 (2%)	53 45

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	84	THR
2	B	223[A]	GLN
2	B	223[B]	GLN
2	B	227	LYS
2	B	315	ILE
2	B	362	PHE
2	B	472	ARG
2	B	492	GLU
2	B	505	ARG
3	C	29	GLU

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Mol	Chain	Res	Type
3	C	142	GLU
3	C	213	LEU
3	C	289	PHE
3	C	315	MET
3	C	416[A]	SER
3	C	416[B]	SER
4	D	90	LEU
4	D	150	ILE
4	D	329	MET
5	E	71	GLU
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
10	K	17	ILE
11	L	1	MET
11	L	2	GLU
11	L	13	ASN
12	M	33	GLN
13	O	49[A]	THR
13	O	49[B]	THR
13	O	194	LYS
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	70	ARG
16	V	30	LYS
17	Y	19	ILE
17	Y	27	MET
17	Y	30	ILE
19	Z	1	MET
19	Z	6	GLN
19	Z	20	VAL
20	R	4	ARG
1	a	12	ASN
1	a	221[A]	SER
1	a	221[B]	SER
2	b	14	ASN
2	b	84	THR
2	b	472	ARG
2	b	485	GLU
2	b	491	VAL
3	c	142	GLU
3	c	289	PHE

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Mol	Chain	Res	Type
3	c	315	MET
3	c	355	THR
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	90	LEU
4	d	150	ILE
4	d	329	MET
5	e	71	GLU
6	f	15	ILE
6	f	44	GLN
8	i	36	ASP
9	j	1	MET
10	k	17	ILE
11	l	1	MET
12	m	16	LEU
12	m	33	GLN
13	o	24	ASP
13	o	25	THR
13	o	69	LYS
13	o	118	LEU
13	o	181[A]	GLU
13	o	181[B]	GLU
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
15	u	86	GLU
17	y	19	ILE
17	y	30	ILE
17	y	42	ARG
19	z	1	MET
19	z	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
3	C	418	ASN
4	D	83	ASN
4	D	301	GLN
4	D	332	GLN
6	F	44	GLN
11	L	13	ASN

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Mol	Chain	Res	Type
13	O	124	ASN
13	O	147	ASN
19	Z	31	GLN
19	Z	58	ASN
1	a	165	GLN
1	a	296	ASN
2	b	53	ASN
2	b	490	GLN
3	c	201	ASN
3	c	373	ASN
4	d	83	ASN
4	d	186	GLN
4	d	332	GLN
4	d	350	ASN
5	e	75	GLN
6	f	44	GLN
10	k	40	GLN
11	l	6	ASN
13	o	124	ASN
13	o	147	ASN
13	o	155	ASN
16	v	118	HIS
19	z	6	GLN
19	z	31	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	FME	m	1	12	8,9,10	0.72	0	7,9,11	1.11	1 (14%)
14	FME	T	1	14	8,9,10	0.64	0	7,9,11	1.56	1 (14%)
12	FME	M	1	12	8,9,10	0.65	0	7,9,11	1.11	0
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	2.10	4 (57%)
8	FME	i	1	8	8,9,10	0.69	0	7,9,11	1.37	1 (14%)
8	FME	I	1	8	8,9,10	0.57	0	7,9,11	1.32	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	C-CA-N	3.07	115.27	109.73
14	T	1	FME	C-CA-N	2.67	114.55	109.73
14	t	1	FME	O-C-CA	-2.63	117.88	124.78
14	t	1	FME	CA-N-CN	-2.56	118.89	122.82
8	I	1	FME	O-C-CA	-2.36	118.59	124.78
8	i	1	FME	CA-N-CN	-2.29	119.30	122.82
8	I	1	FME	CA-N-CN	-2.19	119.45	122.82
12	m	1	FME	O-C-CA	-2.16	119.12	124.78
14	t	1	FME	CE-SD-CG	-2.00	93.52	100.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 251 ligands modelled in this entry, 17 are monoatomic and 18 are unknown - leaving 216 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	C	512	3	69,73,73	2.05	22 (31%)	83,113,113	2.74	29 (34%)
29	LMT	m	102	-	36,36,36	0.48	0	47,47,47	0.91	1 (2%)
35	HTG	B	624	-	19,19,19	1.13	1 (5%)	23,24,24	1.39	1 (4%)
36	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	0.93	4 (5%)
29	LMT	A	417	-	36,36,36	0.50	1 (2%)	47,47,47	1.06	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	HEC	V	201	16	50,50,50	1.70	10 (20%)	68,82,82	1.79	17 (25%)
24	CLA	b	607	2	69,73,73	2.06	20 (28%)	83,113,113	2.86	32 (38%)
35	HTG	c	922	-	19,19,19	0.90	1 (5%)	23,24,24	1.34	1 (4%)
24	CLA	a	409	1	69,73,73	2.02	19 (27%)	83,113,113	2.74	35 (42%)
34	LMG	b	624	-	51,51,55	0.91	3 (5%)	59,59,63	1.05	3 (5%)
24	CLA	c	914	3	69,73,73	2.05	21 (30%)	83,113,113	2.84	30 (36%)
26	BCR	T	102	-	41,41,41	0.97	1 (2%)	56,56,56	1.38	11 (19%)
24	CLA	A	405	1	69,73,73	2.03	19 (27%)	83,113,113	2.82	26 (31%)
34	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.07	4 (6%)
29	LMT	c	921	-	36,36,36	0.45	0	47,47,47	0.82	1 (2%)
24	CLA	b	613	2	69,73,73	2.02	19 (27%)	83,113,113	2.81	31 (37%)
24	CLA	b	617	2	69,73,73	2.01	21 (30%)	83,113,113	2.75	34 (40%)
35	HTG	C	523	-	19,19,19	0.98	2 (10%)	23,24,24	1.37	2 (8%)
29	LMT	C	522	-	36,36,36	0.48	0	47,47,47	1.27	5 (10%)
31	PL9	d	405	-	55,55,55	0.73	2 (3%)	68,69,69	1.55	14 (20%)
34	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.22	7 (11%)
35	HTG	d	412	-	16,16,19	1.11	2 (12%)	20,21,24	1.38	1 (5%)
35	HTG	b	602	-	19,19,19	1.14	2 (10%)	23,24,24	1.22	1 (4%)
34	LMG	B	622	-	51,51,55	0.92	2 (3%)	59,59,63	1.16	3 (5%)
24	CLA	c	903	3	69,73,73	2.03	19 (27%)	83,113,113	2.78	29 (34%)
35	HTG	B	633	-	19,19,19	1.12	2 (10%)	23,24,24	1.30	1 (4%)
26	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.37	7 (12%)
24	CLA	B	602	41	69,73,73	2.05	20 (28%)	83,113,113	2.86	30 (36%)
28	GOL	f	101	33	5,5,5	0.37	0	5,5,5	0.40	0
28	GOL	C	526	-	5,5,5	0.22	0	5,5,5	0.43	0
26	BCR	b	622	-	41,41,41	1.06	1 (2%)	56,56,56	1.27	5 (8%)
28	GOL	b	629	-	5,5,5	0.34	0	5,5,5	0.15	0
34	LMG	Z	101	-	37,37,55	0.99	2 (5%)	45,45,63	1.31	6 (13%)
34	LMG	a	412	-	51,51,55	0.91	2 (3%)	59,59,63	1.15	6 (10%)
24	CLA	A	407	41	69,73,73	2.08	19 (27%)	83,113,113	2.87	33 (39%)
26	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.39	7 (12%)
25	PHO	a	420	-	58,69,69	2.82	13 (22%)	56,99,99	2.74	15 (26%)
24	CLA	C	511	3	69,73,73	2.06	20 (28%)	83,113,113	2.69	29 (34%)
28	GOL	T	101	-	5,5,5	0.41	0	5,5,5	0.31	0
24	CLA	c	906	3	69,73,73	2.01	19 (27%)	83,113,113	2.74	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	K	103	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	6 (10%)
24	CLA	A	410	1	69,73,73	2.06	18 (26%)	83,113,113	2.80	30 (36%)
28	GOL	B	631	-	5,5,5	0.42	0	5,5,5	0.47	0
29	LMT	b	601	-	25,25,36	0.46	0	30,30,47	1.35	3 (10%)
37	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.09	3 (6%)
24	CLA	b	618	2	69,73,73	2.03	20 (28%)	83,113,113	2.94	33 (39%)
35	HTG	B	625	-	19,19,19	0.83	1 (5%)	23,24,24	1.18	2 (8%)
24	CLA	B	613	2	69,73,73	2.00	20 (28%)	83,113,113	2.69	25 (30%)
24	CLA	B	617	2	69,73,73	1.99	20 (28%)	83,113,113	2.80	29 (34%)
35	HTG	b	626	-	19,19,19	0.89	1 (5%)	23,24,24	1.46	3 (13%)
34	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.46	7 (14%)
26	BCR	C	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.33	4 (7%)
37	LHG	D	406	-	48,48,48	0.86	2 (4%)	51,54,54	1.09	5 (9%)
37	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	1.06	4 (7%)
24	CLA	B	614	2	69,73,73	2.00	19 (27%)	83,113,113	2.83	31 (37%)
24	CLA	a	407	41	69,73,73	2.07	20 (28%)	83,113,113	2.86	34 (40%)
25	PHO	A	408	-	58,69,69	2.75	11 (18%)	56,99,99	2.90	13 (23%)
24	CLA	c	908	41	69,73,73	2.01	20 (28%)	83,113,113	2.80	30 (36%)
28	GOL	V	206	-	5,5,5	0.32	0	5,5,5	0.30	0
24	CLA	C	510	3	69,73,73	2.10	20 (28%)	83,113,113	2.81	34 (40%)
28	GOL	v	203	-	5,5,5	0.28	0	5,5,5	0.61	0
35	HTG	C	524	-	19,19,19	1.03	2 (10%)	23,24,24	1.64	4 (17%)
35	HTG	b	627	-	19,19,19	1.09	2 (10%)	23,24,24	1.97	4 (17%)
27	SQD	B	621	-	53,54,54	1.05	4 (7%)	62,65,65	1.48	9 (14%)
35	HTG	V	202	-	19,19,19	1.01	2 (10%)	23,24,24	1.54	3 (13%)
24	CLA	C	513	3	69,73,73	2.00	19 (27%)	83,113,113	2.86	32 (38%)
28	GOL	B	637	-	5,5,5	0.40	0	5,5,5	0.30	0
26	BCR	B	620	-	41,41,41	1.09	1 (2%)	56,56,56	1.22	4 (7%)
34	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.06	4 (6%)
28	GOL	B	630	-	5,5,5	0.33	0	5,5,5	0.36	0
28	GOL	c	925	-	5,5,5	0.36	0	5,5,5	0.56	0
26	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.23	5 (8%)
26	BCR	D	403	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	14 (25%)
24	CLA	B	612	2	69,73,73	2.02	20 (28%)	83,113,113	2.87	31 (37%)
24	CLA	C	514	3	69,73,73	2.02	20 (28%)	83,113,113	2.81	30 (36%)
24	CLA	D	401	4	69,73,73	1.99	19 (27%)	83,113,113	2.75	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	GOL	o	302	-	5,5,5	0.39	0	5,5,5	0.48	0
35	HTG	B	634	-	19,19,19	1.04	2 (10%)	23,24,24	1.59	3 (13%)
31	PL9	a	417	-	55,55,55	0.63	2 (3%)	68,69,69	1.91	18 (26%)
40	HEC	v	202	16	50,50,50	1.69	7 (14%)	68,82,82	1.78	15 (22%)
36	DGD	d	406	-	63,63,67	0.93	3 (4%)	77,77,81	1.22	6 (7%)
28	GOL	T	103	-	5,5,5	0.39	0	5,5,5	0.19	0
24	CLA	B	603	2	69,73,73	2.04	20 (28%)	83,113,113	2.92	34 (40%)
35	HTG	O	303	-	19,19,19	0.95	1 (5%)	23,24,24	0.71	0
23	BCT	A	404	21	2,3,3	0.88	0	2,3,3	0.45	0
28	GOL	V	205	-	5,5,5	0.36	0	5,5,5	0.38	0
36	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	b	612	2	69,73,73	2.08	20 (28%)	83,113,113	2.74	29 (34%)
24	CLA	b	610	2	69,73,73	1.98	19 (27%)	83,113,113	2.91	30 (36%)
24	CLA	C	505	41	69,73,73	2.07	20 (28%)	83,113,113	2.89	28 (33%)
24	CLA	c	905	41	69,73,73	2.03	20 (28%)	83,113,113	2.83	31 (37%)
24	CLA	c	912	3	69,73,73	2.05	21 (30%)	83,113,113	2.73	29 (34%)
24	CLA	d	403	4	69,73,73	2.01	20 (28%)	83,113,113	2.82	30 (36%)
25	PHO	a	408	-	58,69,69	2.66	12 (20%)	56,99,99	2.81	13 (23%)
24	CLA	b	609	2	69,73,73	2.02	19 (27%)	83,113,113	2.92	30 (36%)
27	SQD	a	411	-	53,54,54	0.95	3 (5%)	62,65,65	1.60	10 (16%)
24	CLA	b	614	41	69,73,73	2.06	20 (28%)	83,113,113	2.76	34 (40%)
26	BCR	b	623	-	41,41,41	0.99	1 (2%)	56,56,56	1.43	9 (16%)
29	LMT	B	623	-	36,36,36	0.43	0	47,47,47	1.40	5 (10%)
24	CLA	B	616	2	69,73,73	1.98	21 (30%)	83,113,113	2.83	32 (38%)
24	CLA	B	606	2	69,73,73	2.00	20 (28%)	83,113,113	2.74	30 (36%)
35	HTG	c	923	-	19,19,19	1.14	2 (10%)	23,24,24	1.84	5 (21%)
26	BCR	c	915	-	41,41,41	1.07	1 (2%)	56,56,56	1.43	9 (16%)
24	CLA	b	620	2	69,73,73	2.02	21 (30%)	83,113,113	2.74	26 (31%)
24	CLA	C	506	3	69,73,73	2.06	20 (28%)	83,113,113	2.74	30 (36%)
27	SQD	A	412	-	53,54,54	0.99	3 (5%)	62,65,65	1.77	12 (19%)
24	CLA	c	911	3	69,73,73	2.07	20 (28%)	83,113,113	2.63	31 (37%)
35	HTG	B	626	-	19,19,19	1.00	1 (5%)	23,24,24	1.71	2 (8%)
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.61	12 (21%)
24	CLA	b	619	2	69,73,73	2.01	19 (27%)	83,113,113	2.76	30 (36%)
34	LMG	C	501	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	c	907	3	69,73,73	2.03	20 (28%)	83,113,113	2.72	31 (37%)
35	HTG	D	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.00	1 (5%)
29	LMT	M	101	-	36,36,36	0.41	0	47,47,47	0.90	1 (2%)
28	GOL	b	632	-	5,5,5	0.37	0	5,5,5	0.56	0
24	CLA	b	611	41	69,73,73	2.03	20 (28%)	83,113,113	2.88	30 (36%)
24	CLA	C	504	3	69,73,73	2.02	20 (28%)	83,113,113	2.87	28 (33%)
28	GOL	b	630	-	5,5,5	0.32	0	5,5,5	0.52	0
24	CLA	b	606	2	69,73,73	2.02	21 (30%)	83,113,113	2.86	30 (36%)
24	CLA	b	615	2	69,73,73	2.00	20 (28%)	83,113,113	2.89	29 (34%)
29	LMT	B	636	-	25,25,36	0.43	0	30,30,47	0.65	0
24	CLA	D	402	4	69,73,73	2.03	19 (27%)	83,113,113	2.78	27 (32%)
29	LMT	b	625	-	25,25,36	0.52	1 (4%)	30,30,47	0.60	0
24	CLA	C	507	3	69,73,73	2.07	20 (28%)	83,113,113	2.75	33 (39%)
28	GOL	V	203	-	5,5,5	0.38	0	5,5,5	0.15	0
27	SQD	F	101	-	42,43,54	1.16	3 (7%)	51,54,65	1.96	10 (19%)
30	OEX	a	416	1,3,41	0,14,14	-	-	-		
36	DGD	c	916	-	63,63,67	0.83	2 (3%)	77,77,81	1.11	6 (7%)
24	CLA	B	608	41	69,73,73	2.02	20 (28%)	83,113,113	2.68	27 (32%)
24	CLA	c	904	3	69,73,73	2.03	20 (28%)	83,113,113	2.76	29 (34%)
28	GOL	t	102	-	5,5,5	0.40	0	5,5,5	0.23	0
28	GOL	B	628	-	5,5,5	0.27	0	5,5,5	0.42	0
30	OEX	A	418	1,3,41	0,14,14	-	-	-		
28	GOL	b	631	-	5,5,5	0.33	0	5,5,5	0.46	0
27	SQD	a	402	-	53,54,54	1.06	3 (5%)	62,65,65	1.16	7 (11%)
23	BCT	a	419	21	2,3,3	0.96	0	2,3,3	0.22	0
36	DGD	c	917	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	2 (2%)
34	LMG	j	101	39	51,51,55	0.89	2 (3%)	59,59,63	0.99	4 (6%)
37	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	4 (7%)
29	LMT	m	103	-	36,36,36	0.48	0	47,47,47	0.99	1 (2%)
28	GOL	B	629	-	5,5,5	0.41	0	5,5,5	0.56	0
28	GOL	A	415	-	5,5,5	0.42	0	5,5,5	0.27	0
24	CLA	B	611	41	69,73,73	2.09	20 (28%)	83,113,113	2.74	33 (39%)
28	GOL	b	633	-	5,5,5	0.36	0	5,5,5	0.35	0
28	GOL	c	924	-	5,5,5	0.37	0	5,5,5	0.31	0
26	BCR	k	101	-	41,41,41	1.10	1 (2%)	56,56,56	1.46	10 (17%)
28	GOL	a	413	-	5,5,5	0.31	0	5,5,5	0.65	0
26	BCR	a	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	5 (8%)
27	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.57	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	GOL	C	525	-	5,5,5	0.37	0	5,5,5	0.61	0
36	DGD	C	517	-	63,63,67	0.86	3 (4%)	77,77,81	1.04	4 (5%)
35	HTG	b	603	-	19,19,19	1.03	2 (10%)	23,24,24	1.47	3 (13%)
24	CLA	B	604	2	69,73,73	2.05	20 (28%)	83,113,113	2.90	29 (34%)
28	GOL	V	204	-	5,5,5	0.43	0	5,5,5	0.44	0
36	DGD	C	519	-	63,63,67	0.84	3 (4%)	77,77,81	0.95	5 (6%)
38	HEM	E	103	6,5	50,50,50	1.50	6 (12%)	66,82,82	1.79	16 (24%)
24	CLA	c	902	3	69,73,73	1.98	19 (27%)	83,113,113	2.74	28 (33%)
28	GOL	a	415	-	5,5,5	0.40	0	5,5,5	0.46	0
34	LMG	J	101	39	51,51,55	0.88	2 (3%)	59,59,63	0.89	3 (5%)
24	CLA	B	605	2	69,73,73	1.93	19 (27%)	83,113,113	2.76	28 (33%)
24	CLA	c	913	3	69,73,73	1.99	20 (28%)	83,113,113	2.90	32 (38%)
27	SQD	f	102	-	42,43,54	1.17	3 (7%)	51,54,65	1.45	8 (15%)
24	CLA	C	502	3	69,73,73	2.01	20 (28%)	83,113,113	2.85	31 (37%)
31	PL9	D	404	-	55,55,55	0.73	2 (3%)	68,69,69	1.58	14 (20%)
34	LMG	c	919	-	51,51,55	0.97	3 (5%)	59,59,63	1.01	2 (3%)
26	BCR	A	411	-	41,41,41	1.02	1 (2%)	56,56,56	1.22	5 (8%)
29	LMT	m	104	-	36,36,36	0.51	0	47,47,47	1.01	2 (4%)
36	DGD	c	918	-	63,63,67	0.86	2 (3%)	77,77,81	0.95	4 (5%)
26	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	7 (12%)
36	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.98	6 (7%)
28	GOL	A	413	-	5,5,5	0.25	0	5,5,5	0.52	0
24	CLA	C	503	3	69,73,73	2.06	20 (28%)	83,113,113	2.70	31 (37%)
25	PHO	A	409	-	58,69,69	2.83	15 (25%)	56,99,99	2.81	14 (25%)
28	GOL	O	302	-	5,5,5	0.32	0	5,5,5	0.44	0
27	SQD	A	416	-	53,54,54	1.03	3 (5%)	62,65,65	1.21	6 (9%)
24	CLA	B	610	2	69,73,73	1.98	18 (26%)	83,113,113	2.80	31 (37%)
24	CLA	B	615	2	69,73,73	2.04	20 (28%)	83,113,113	2.99	32 (38%)
28	GOL	A	414	-	5,5,5	0.44	0	5,5,5	0.34	0
28	GOL	B	627	-	5,5,5	0.41	0	5,5,5	0.57	0
24	CLA	A	406	41	69,73,73	1.99	19 (27%)	83,113,113	3.05	33 (39%)
26	BCR	t	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	7 (12%)
29	LMT	E	102	-	36,36,36	0.48	0	47,47,47	0.86	0
31	PL9	A	419	-	55,55,55	0.63	2 (3%)	68,69,69	1.83	21 (30%)
37	LHG	L	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.03	4 (7%)
26	BCR	C	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	d	404	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	16 (28%)
24	CLA	C	508	41	69,73,73	2.01	20 (28%)	83,113,113	2.68	28 (33%)
24	CLA	d	402	4	69,73,73	1.96	21 (30%)	83,113,113	2.91	29 (34%)
28	GOL	v	205	-	5,5,5	0.39	0	5,5,5	0.35	0
24	CLA	c	910	3	69,73,73	2.08	20 (28%)	83,113,113	2.80	30 (36%)
28	GOL	F	103	33	5,5,5	0.32	0	5,5,5	0.30	0
29	LMT	f	103	-	36,36,36	0.54	1 (2%)	47,47,47	0.93	4 (8%)
24	CLA	b	616	2	69,73,73	2.02	19 (27%)	83,113,113	2.81	30 (36%)
37	LHG	d	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	4 (7%)
26	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.29	5 (8%)
24	CLA	d	401	41	69,73,73	2.05	20 (28%)	83,113,113	2.85	31 (37%)
37	LHG	d	407	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	4 (7%)
24	CLA	C	509	3	69,73,73	2.03	20 (28%)	83,113,113	2.84	30 (36%)
26	BCR	b	621	-	41,41,41	1.12	1 (2%)	56,56,56	1.19	2 (3%)
38	HEM	e	102	6,5	50,50,50	1.57	8 (16%)	66,82,82	1.77	17 (25%)
28	GOL	v	204	-	5,5,5	0.37	0	5,5,5	0.37	0
24	CLA	b	608	2	69,73,73	2.04	20 (28%)	83,113,113	2.70	27 (32%)
24	CLA	c	909	3	69,73,73	2.03	20 (28%)	83,113,113	2.75	28 (33%)
36	DGD	D	405	-	63,63,67	0.98	3 (4%)	77,77,81	1.24	7 (9%)
24	CLA	b	605	41	69,73,73	2.07	19 (27%)	83,113,113	2.78	26 (31%)
28	GOL	B	632	-	5,5,5	0.35	0	5,5,5	0.36	0
29	LMT	a	401	-	36,36,36	0.52	1 (2%)	47,47,47	0.94	2 (4%)
26	BCR	B	618	-	41,41,41	1.09	1 (2%)	56,56,56	1.22	8 (14%)
24	CLA	B	607	2	69,73,73	2.04	20 (28%)	83,113,113	2.92	32 (38%)
28	GOL	b	628	-	5,5,5	0.36	0	5,5,5	0.30	0
37	LHG	d	408	-	48,48,48	0.88	2 (4%)	51,54,54	0.91	3 (5%)
37	LHG	e	101	-	41,41,48	1.01	2 (4%)	44,47,54	0.97	2 (4%)
24	CLA	B	609	2	69,73,73	2.07	21 (30%)	83,113,113	2.78	32 (38%)
37	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	0.85	2 (3%)
28	GOL	a	414	-	5,5,5	0.39	0	5,5,5	0.43	0
24	CLA	a	406	1	69,73,73	2.04	20 (28%)	83,113,113	2.78	34 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	512	3	-	2/39/115/115	-
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
35	HTG	B	624	-	-	1/10/30/30	0/1/1/1
36	DGD	H	102	-	-	9/51/91/95	0/2/2/2
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
40	HEC	V	201	16	1/1/3/7	4/14/54/54	-
24	CLA	b	607	2	-	8/39/115/115	-
35	HTG	c	922	-	-	4/10/30/30	0/1/1/1
24	CLA	a	409	1	-	7/39/115/115	-
34	LMG	b	624	-	-	14/46/66/70	0/1/1/1
24	CLA	c	914	3	-	12/39/115/115	-
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
24	CLA	A	405	1	-	2/39/115/115	-
34	LMG	C	521	-	-	12/46/66/70	0/1/1/1
29	LMT	c	921	-	-	4/21/61/61	0/2/2/2
24	CLA	b	613	2	-	2/39/115/115	-
24	CLA	b	617	2	-	4/39/115/115	-
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
29	LMT	C	522	-	-	9/21/61/61	0/2/2/2
31	PL9	d	405	-	-	5/53/73/73	0/1/1/1
34	LMG	c	920	-	-	4/46/66/70	0/1/1/1
35	HTG	d	412	-	-	0/7/27/30	0/1/1/1
35	HTG	b	602	-	-	1/10/30/30	0/1/1/1
34	LMG	B	622	-	-	12/46/66/70	0/1/1/1
24	CLA	c	903	3	-	6/39/115/115	-
35	HTG	B	633	-	-	3/10/30/30	0/1/1/1
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2
28	GOL	f	101	33	-	4/4/4/4	-
28	GOL	C	526	-	-	0/4/4/4	-
26	BCR	b	622	-	-	1/29/63/63	0/2/2/2
28	GOL	b	629	-	-	0/4/4/4	-
34	LMG	Z	101	-	-	13/31/51/70	0/1/1/1
34	LMG	a	412	-	-	10/46/66/70	0/1/1/1
24	CLA	A	407	41	-	2/39/115/115	-
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
25	PHO	a	420	-	-	2/37/103/103	0/5/6/6
24	CLA	C	511	3	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	T	101	-	-	0/4/4/4	-
24	CLA	c	906	3	-	6/39/115/115	-
26	BCR	K	103	-	-	2/29/63/63	0/2/2/2
24	CLA	A	410	1	-	9/39/115/115	-
28	GOL	B	631	-	-	4/4/4/4	-
29	LMT	b	601	-	-	8/17/37/61	0/1/1/2
37	LHG	E	101	-	-	21/46/46/53	-
24	CLA	b	618	2	-	17/39/115/115	-
35	HTG	B	625	-	-	3/10/30/30	0/1/1/1
24	CLA	B	613	2	-	4/39/115/115	-
24	CLA	B	617	2	-	9/39/115/115	-
35	HTG	b	626	-	-	1/10/30/30	0/1/1/1
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
37	LHG	D	406	-	-	6/53/53/53	-
37	LHG	D	408	-	-	11/53/53/53	-
24	CLA	B	614	2	-	9/39/115/115	-
24	CLA	a	407	41	-	6/39/115/115	-
25	PHO	A	408	-	-	5/37/103/103	0/5/6/6
24	CLA	c	908	41	-	4/39/115/115	-
28	GOL	V	206	-	-	1/4/4/4	-
24	CLA	C	510	3	-	7/39/115/115	-
28	GOL	v	203	-	-	4/4/4/4	-
35	HTG	C	524	-	-	2/10/30/30	0/1/1/1
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
27	SQD	B	621	-	-	24/49/69/69	0/1/1/1
35	HTG	V	202	-	-	5/10/30/30	0/1/1/1
24	CLA	C	513	3	-	12/39/115/115	-
28	GOL	B	637	-	-	2/4/4/4	-
26	BCR	B	620	-	-	2/29/63/63	0/2/2/2
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
28	GOL	B	630	-	-	0/4/4/4	-
28	GOL	c	925	-	-	0/4/4/4	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	D	403	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	612	2	-	2/39/115/115	-
24	CLA	C	514	3	-	2/39/115/115	-
24	CLA	D	401	4	-	2/39/115/115	-
28	GOL	o	302	-	-	2/4/4/4	-
35	HTG	B	634	-	-	2/10/30/30	0/1/1/1
31	PL9	a	417	-	-	12/53/73/73	0/1/1/1
40	HEC	v	202	16	1/1/3/7	4/14/54/54	-
36	DGD	d	406	-	-	28/51/91/95	0/2/2/2
28	GOL	T	103	-	-	4/4/4/4	-
24	CLA	B	603	2	-	7/39/115/115	-
35	HTG	O	303	-	-	1/10/30/30	0/1/1/1
28	GOL	V	205	-	-	1/4/4/4	-
36	DGD	C	518	-	-	15/51/91/95	0/2/2/2
24	CLA	b	612	2	-	4/39/115/115	-
24	CLA	b	610	2	-	18/39/115/115	-
24	CLA	C	505	41	-	5/39/115/115	-
24	CLA	c	905	41	-	5/39/115/115	-
24	CLA	c	912	3	-	5/39/115/115	-
24	CLA	d	403	4	-	7/39/115/115	-
25	PHO	a	408	-	-	2/37/103/103	0/5/6/6
24	CLA	b	609	2	-	9/39/115/115	-
27	SQD	a	411	-	-	11/49/69/69	0/1/1/1
24	CLA	b	614	41	-	3/39/115/115	-
26	BCR	b	623	-	-	3/29/63/63	0/2/2/2
29	LMT	B	623	-	-	7/21/61/61	0/2/2/2
24	CLA	B	616	2	-	11/39/115/115	-
24	CLA	B	606	2	-	7/39/115/115	-
35	HTG	c	923	-	-	0/10/30/30	0/1/1/1
26	BCR	c	915	-	-	4/29/63/63	0/2/2/2
24	CLA	b	620	2	-	9/39/115/115	-
24	CLA	C	506	3	-	8/39/115/115	-
27	SQD	A	412	-	-	11/49/69/69	0/1/1/1
24	CLA	c	911	3	-	9/39/115/115	-
35	HTG	B	626	-	-	4/10/30/30	0/1/1/1
26	BCR	y	101	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	619	2	-	4/39/115/115	-
34	LMG	C	501	-	-	19/46/66/70	0/1/1/1
24	CLA	c	907	3	-	9/39/115/115	-
35	HTG	D	411	-	-	1/7/27/30	0/1/1/1
29	LMT	M	101	-	-	6/21/61/61	0/2/2/2
28	GOL	b	632	-	-	2/4/4/4	-
24	CLA	b	611	41	-	4/39/115/115	-
24	CLA	C	504	3	-	7/39/115/115	-
28	GOL	b	630	-	-	0/4/4/4	-
24	CLA	b	606	2	-	3/39/115/115	-
24	CLA	b	615	2	-	5/39/115/115	-
29	LMT	B	636	-	-	8/17/37/61	0/1/1/2
24	CLA	D	402	4	-	11/39/115/115	-
29	LMT	b	625	-	-	4/17/37/61	0/1/1/2
24	CLA	C	507	3	-	11/39/115/115	-
28	GOL	V	203	-	-	4/4/4/4	-
27	SQD	F	101	-	-	14/38/58/69	0/1/1/1
36	DGD	c	916	-	-	10/51/91/95	0/2/2/2
24	CLA	B	608	41	-	2/39/115/115	-
24	CLA	c	904	3	-	5/39/115/115	-
28	GOL	t	102	-	-	0/4/4/4	-
28	GOL	B	628	-	-	2/4/4/4	-
28	GOL	b	631	-	-	2/4/4/4	-
27	SQD	a	402	-	-	17/49/69/69	0/1/1/1
24	CLA	a	406	1	-	2/39/115/115	-
37	LHG	l	101	-	-	15/53/53/53	-
36	DGD	c	917	-	-	14/51/91/95	0/2/2/2
34	LMG	j	101	39	-	11/46/66/70	0/1/1/1
29	LMT	m	103	-	-	3/21/61/61	0/2/2/2
28	GOL	B	629	-	-	2/4/4/4	-
28	GOL	A	415	-	-	2/4/4/4	-
24	CLA	B	611	41	-	7/39/115/115	-
28	GOL	b	633	-	-	2/4/4/4	-
28	GOL	c	924	-	-	0/4/4/4	-
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	a	413	-	-	0/4/4/4	-
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
27	SQD	L	102	-	-	25/49/69/69	0/1/1/1
28	GOL	C	525	-	-	0/4/4/4	-
36	DGD	C	517	-	-	15/51/91/95	0/2/2/2
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
24	CLA	B	604	2	-	6/39/115/115	-
28	GOL	V	204	-	-	2/4/4/4	-
36	DGD	C	519	-	-	8/51/91/95	0/2/2/2
38	HEM	E	103	6,5	-	4/14/54/54	-
24	CLA	c	902	3	-	5/39/115/115	-
28	GOL	a	415	-	-	2/4/4/4	-
34	LMG	J	101	39	-	13/46/66/70	0/1/1/1
24	CLA	B	605	2	-	4/39/115/115	-
24	CLA	c	913	3	-	9/39/115/115	-
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
24	CLA	C	502	3	-	9/39/115/115	-
31	PL9	D	404	-	-	3/53/73/73	0/1/1/1
34	LMG	c	919	-	-	16/46/66/70	0/1/1/1
26	BCR	A	411	-	-	1/29/63/63	0/2/2/2
29	LMT	m	104	-	-	7/21/61/61	0/2/2/2
36	DGD	c	918	-	-	17/51/91/95	0/2/2/2
26	BCR	K	102	-	-	6/29/63/63	0/2/2/2
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
28	GOL	A	413	-	-	2/4/4/4	-
24	CLA	C	503	3	-	6/39/115/115	-
25	PHO	A	409	-	-	0/37/103/103	0/5/6/6
28	GOL	O	302	-	-	2/4/4/4	-
27	SQD	A	416	-	-	16/49/69/69	0/1/1/1
24	CLA	B	610	2	-	3/39/115/115	-
24	CLA	B	615	2	-	18/39/115/115	-
28	GOL	A	414	-	-	2/4/4/4	-
28	GOL	B	627	-	-	1/4/4/4	-
24	CLA	A	406	41	-	4/39/115/115	-
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
29	LMT	E	102	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PL9	A	419	-	-	7/53/73/73	0/1/1/1
37	LHG	L	101	-	-	15/53/53/53	-
26	BCR	C	516	-	-	2/29/63/63	0/2/2/2
26	BCR	d	404	-	-	4/29/63/63	0/2/2/2
24	CLA	C	508	41	-	6/39/115/115	-
24	CLA	d	402	4	-	2/39/115/115	-
28	GOL	v	205	-	-	2/4/4/4	-
24	CLA	c	910	3	-	9/39/115/115	-
28	GOL	F	103	33	-	2/4/4/4	-
29	LMT	f	103	-	-	9/21/61/61	0/2/2/2
24	CLA	b	616	2	-	1/39/115/115	-
37	LHG	d	409	-	-	12/53/53/53	-
26	BCR	h	101	-	-	3/29/63/63	0/2/2/2
24	CLA	d	401	41	-	7/39/115/115	-
37	LHG	d	407	-	-	9/53/53/53	-
24	CLA	C	509	3	-	7/39/115/115	-
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2
38	HEM	e	102	6,5	-	4/14/54/54	-
28	GOL	v	204	-	-	3/4/4/4	-
24	CLA	b	608	2	-	9/39/115/115	-
24	CLA	c	909	3	-	3/39/115/115	-
36	DGD	D	405	-	-	22/51/91/95	0/2/2/2
24	CLA	b	605	41	-	12/39/115/115	-
28	GOL	B	632	-	-	2/4/4/4	-
29	LMT	a	401	-	-	11/21/61/61	0/2/2/2
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	B	607	2	-	7/39/115/115	-
28	GOL	b	628	-	-	2/4/4/4	-
37	LHG	d	408	-	-	11/53/53/53	-
37	LHG	e	101	-	-	10/46/46/53	-
24	CLA	B	609	2	-	0/39/115/115	-
37	LHG	D	407	-	-	5/53/53/53	-
28	GOL	a	414	-	-	2/4/4/4	-
24	CLA	B	602	41	-	16/39/115/115	-

All (1630) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	408	PHO	C1D-C2D	9.19	1.49	1.39
25	A	409	PHO	C1B-C2B	9.14	1.49	1.39
25	a	420	PHO	C1B-C2B	9.04	1.49	1.39
25	A	408	PHO	C1B-C2B	8.77	1.49	1.39
25	a	408	PHO	C1B-C2B	8.63	1.49	1.39
25	a	420	PHO	C1D-C2D	8.48	1.49	1.39
25	A	408	PHO	C1D-C2D	8.21	1.48	1.39
25	A	409	PHO	C1D-C2D	8.00	1.48	1.39
25	A	409	PHO	C3B-C4B	7.54	1.50	1.41
25	A	408	PHO	C3B-C4B	7.40	1.50	1.41
25	a	420	PHO	C4D-CHA	7.26	1.51	1.39
25	a	420	PHO	C3B-C4B	7.21	1.49	1.41
25	a	420	PHO	C3B-C2B	6.72	1.49	1.40
25	A	409	PHO	C3B-C2B	6.62	1.49	1.40
25	A	408	PHO	C4D-CHA	6.58	1.50	1.39
25	a	408	PHO	C3B-C4B	6.32	1.48	1.41
25	A	409	PHO	C4D-CHA	6.28	1.49	1.39
25	A	408	PHO	C3B-C2B	6.21	1.49	1.40
25	A	408	PHO	C3C-C2C	6.06	1.49	1.36
25	a	408	PHO	C3B-C2B	5.96	1.48	1.40
25	a	408	PHO	C4D-CHA	5.88	1.49	1.39
24	B	611	CLA	C3C-C2C	5.77	1.49	1.36
25	A	409	PHO	C3C-C2C	5.72	1.48	1.36
25	A	409	PHO	C3D-C2D	5.72	1.49	1.39
24	b	605	CLA	C3C-C2C	5.71	1.48	1.36
24	A	407	CLA	C3C-C2C	5.65	1.48	1.36
24	C	504	CLA	C3C-C2C	5.55	1.48	1.36
24	b	618	CLA	C3C-C2C	5.52	1.48	1.36
24	d	401	CLA	C1D-ND	5.50	1.44	1.37
24	C	507	CLA	C3C-C2C	5.50	1.48	1.36
24	c	910	CLA	C1D-ND	5.50	1.44	1.37
24	C	510	CLA	C1D-ND	5.50	1.44	1.37
24	b	612	CLA	C3C-C2C	5.50	1.48	1.36
25	a	420	PHO	C3C-C2C	5.49	1.48	1.36
24	D	402	CLA	C3C-C2C	5.49	1.48	1.36
24	a	406	CLA	C1D-ND	5.49	1.44	1.37
24	B	609	CLA	C3C-C2C	5.47	1.48	1.36
38	e	102	HEM	FE-NB	5.47	2.11	1.94
24	C	511	CLA	C3C-C2C	5.47	1.48	1.36
25	a	420	PHO	C3D-C2D	5.45	1.49	1.39
24	C	513	CLA	C3C-C2C	5.45	1.48	1.36
24	b	614	CLA	C3C-C2C	5.44	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C3C-C2C	5.43	1.48	1.36
24	B	614	CLA	C3C-C2C	5.42	1.48	1.36
24	a	407	CLA	C1D-ND	5.42	1.44	1.37
24	d	401	CLA	C3C-C2C	5.40	1.48	1.36
24	C	507	CLA	C1D-ND	5.40	1.44	1.37
24	C	506	CLA	C3C-C2C	5.39	1.48	1.36
24	C	514	CLA	C3C-C2C	5.39	1.48	1.36
24	b	607	CLA	C3C-C2C	5.38	1.48	1.36
24	a	406	CLA	C3C-C2C	5.37	1.48	1.36
40	V	201	HEC	FE-NB	5.36	2.11	1.94
24	c	913	CLA	C3C-C2C	5.35	1.48	1.36
24	c	909	CLA	C3C-C2C	5.35	1.48	1.36
24	b	617	CLA	O2D-CGD	5.34	1.46	1.33
24	b	612	CLA	C1D-ND	5.33	1.44	1.37
24	A	410	CLA	C3C-C2C	5.33	1.48	1.36
24	c	911	CLA	C3C-C2C	5.33	1.48	1.36
24	a	409	CLA	C3C-C2C	5.31	1.48	1.36
24	B	616	CLA	C1D-ND	5.31	1.44	1.37
24	c	904	CLA	C1D-ND	5.31	1.44	1.37
24	C	503	CLA	C3C-C2C	5.30	1.48	1.36
24	B	604	CLA	C1D-ND	5.29	1.44	1.37
24	C	505	CLA	C3C-C2C	5.29	1.48	1.36
25	a	408	PHO	C3C-C2C	5.28	1.48	1.36
24	A	405	CLA	C1D-ND	5.28	1.44	1.37
24	B	603	CLA	C3C-C2C	5.28	1.47	1.36
24	B	611	CLA	C1D-ND	5.26	1.44	1.37
24	c	903	CLA	C3C-C2C	5.25	1.47	1.36
24	c	907	CLA	O2D-CGD	5.25	1.46	1.33
24	A	406	CLA	C1D-ND	5.25	1.44	1.37
40	v	202	HEC	FE-NB	5.24	2.11	1.94
24	c	907	CLA	C1D-ND	5.24	1.44	1.37
24	c	904	CLA	C3C-C2C	5.23	1.47	1.36
24	B	615	CLA	C1D-ND	5.23	1.44	1.37
24	c	903	CLA	C1D-ND	5.23	1.44	1.37
24	b	616	CLA	C3C-C2C	5.22	1.47	1.36
24	b	605	CLA	C1D-ND	5.22	1.44	1.37
24	C	510	CLA	O2D-CGD	5.22	1.45	1.33
24	A	407	CLA	O2D-CGD	5.21	1.45	1.33
24	b	611	CLA	C3C-C2C	5.21	1.47	1.36
24	B	608	CLA	C3C-C2C	5.20	1.47	1.36
24	A	405	CLA	C3C-C2C	5.20	1.47	1.36
24	c	912	CLA	C3C-C2C	5.19	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	O2D-CGD	5.18	1.45	1.33
24	B	603	CLA	O2D-CGD	5.18	1.45	1.33
24	c	914	CLA	C3C-C2C	5.17	1.47	1.36
24	a	409	CLA	O2D-CGD	5.17	1.45	1.33
24	c	909	CLA	C1D-ND	5.16	1.44	1.37
24	b	620	CLA	C3C-C2C	5.16	1.47	1.36
24	A	410	CLA	C1D-ND	5.15	1.44	1.37
24	c	912	CLA	C1D-ND	5.14	1.44	1.37
24	B	617	CLA	C3C-C2C	5.13	1.47	1.36
24	b	613	CLA	O2D-CGD	5.12	1.45	1.33
24	a	407	CLA	C3C-C2C	5.11	1.47	1.36
24	A	410	CLA	O2D-CGD	5.11	1.45	1.33
24	A	406	CLA	C3C-C2C	5.11	1.47	1.36
24	c	908	CLA	C3C-C2C	5.11	1.47	1.36
24	b	617	CLA	C3C-C2C	5.11	1.47	1.36
24	B	612	CLA	C1D-ND	5.10	1.44	1.37
24	B	602	CLA	O2D-CGD	5.10	1.45	1.33
24	B	610	CLA	C3C-C2C	5.10	1.47	1.36
24	c	905	CLA	O2D-CGD	5.10	1.45	1.33
26	k	101	BCR	C23-C22	-5.10	1.35	1.45
24	b	606	CLA	O2D-CGD	5.10	1.45	1.33
24	c	910	CLA	C3C-C2C	5.10	1.47	1.36
24	C	514	CLA	C1D-ND	5.10	1.44	1.37
24	d	403	CLA	C3C-C2C	5.09	1.47	1.36
24	C	506	CLA	O2D-CGD	5.09	1.45	1.33
24	B	605	CLA	C3C-C2C	5.09	1.47	1.36
24	c	905	CLA	C3C-C2C	5.09	1.47	1.36
24	D	402	CLA	C1D-ND	5.08	1.44	1.37
24	C	503	CLA	O2D-CGD	5.08	1.45	1.33
38	E	103	HEM	FE-NB	5.07	2.10	1.94
24	b	616	CLA	O2D-CGD	5.07	1.45	1.33
24	B	602	CLA	C1D-ND	5.07	1.44	1.37
24	b	617	CLA	C1D-ND	5.07	1.44	1.37
24	B	602	CLA	C3C-C2C	5.06	1.47	1.36
26	t	101	BCR	C23-C22	-5.06	1.35	1.45
24	C	509	CLA	C3C-C2C	5.06	1.47	1.36
24	C	503	CLA	C1D-ND	5.06	1.44	1.37
25	a	420	PHO	O2D-CGD	5.05	1.45	1.33
24	c	902	CLA	C3C-C2C	5.05	1.47	1.36
24	A	407	CLA	CHC-C1C	5.04	1.48	1.38
24	b	618	CLA	C1D-ND	5.04	1.44	1.37
24	B	612	CLA	C3C-C2C	5.04	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	910	CLA	O2D-CGD	5.03	1.45	1.33
24	b	606	CLA	C3C-C2C	5.03	1.47	1.36
24	d	403	CLA	C1D-ND	5.03	1.44	1.37
24	B	615	CLA	C3C-C2C	5.03	1.47	1.36
24	b	609	CLA	C3C-C2C	5.03	1.47	1.36
24	b	610	CLA	C3C-C2C	5.03	1.47	1.36
24	b	613	CLA	C1D-ND	5.03	1.44	1.37
24	c	906	CLA	O2D-CGD	5.02	1.45	1.33
24	C	504	CLA	C1D-ND	5.02	1.44	1.37
24	C	509	CLA	O2D-CGD	5.02	1.45	1.33
24	B	603	CLA	C1D-ND	5.01	1.43	1.37
24	c	907	CLA	C3C-C2C	5.01	1.47	1.36
24	C	510	CLA	C3C-C2C	5.01	1.47	1.36
24	C	505	CLA	C1D-ND	5.01	1.43	1.37
26	B	620	BCR	C23-C22	-5.01	1.35	1.45
24	a	407	CLA	CHC-C1C	5.00	1.48	1.38
24	b	607	CLA	O2D-CGD	5.00	1.45	1.33
24	b	606	CLA	C1D-ND	5.00	1.43	1.37
26	b	622	BCR	C23-C22	-4.99	1.35	1.45
24	B	608	CLA	O2D-CGD	4.99	1.45	1.33
24	D	402	CLA	O2D-CGD	4.99	1.45	1.33
24	C	511	CLA	C1D-ND	4.99	1.43	1.37
24	b	615	CLA	O2D-CGD	4.98	1.45	1.33
24	b	609	CLA	C1D-ND	4.97	1.43	1.37
24	C	512	CLA	C1D-ND	4.97	1.43	1.37
24	C	508	CLA	C3C-C2C	4.97	1.47	1.36
24	C	512	CLA	O2D-CGD	4.97	1.45	1.33
25	a	408	PHO	C3D-C2D	4.95	1.48	1.39
24	B	613	CLA	C3C-C2C	4.95	1.47	1.36
24	B	607	CLA	C3C-C2C	4.95	1.47	1.36
24	B	606	CLA	C3C-C2C	4.95	1.47	1.36
24	b	620	CLA	O2D-CGD	4.95	1.45	1.33
24	A	407	CLA	C1D-ND	4.94	1.43	1.37
24	c	911	CLA	C1D-ND	4.94	1.43	1.37
26	k	102	BCR	C23-C22	-4.94	1.35	1.45
24	B	613	CLA	O2D-CGD	4.94	1.45	1.33
24	B	607	CLA	O2D-CGD	4.94	1.45	1.33
24	c	914	CLA	CHC-C1C	4.93	1.48	1.38
24	b	615	CLA	C1D-ND	4.93	1.43	1.37
24	b	608	CLA	C3C-C2C	4.92	1.47	1.36
24	B	612	CLA	O2D-CGD	4.92	1.45	1.33
24	B	606	CLA	O2D-CGD	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C1D-ND	4.91	1.43	1.37
24	B	616	CLA	O2D-CGD	4.91	1.45	1.33
25	A	408	PHO	OBD-CAD	4.90	1.29	1.22
24	D	401	CLA	C1D-ND	4.90	1.43	1.37
24	c	914	CLA	C1D-ND	4.90	1.43	1.37
24	b	611	CLA	CHC-C1C	4.90	1.48	1.38
24	C	513	CLA	CHC-C1C	4.90	1.48	1.38
24	C	512	CLA	C3C-C2C	4.90	1.47	1.36
24	c	906	CLA	C3C-C2C	4.89	1.47	1.36
24	D	401	CLA	C3C-C2C	4.89	1.47	1.36
24	d	402	CLA	C3C-C2C	4.89	1.47	1.36
24	C	513	CLA	O2D-CGD	4.89	1.45	1.33
24	c	909	CLA	O2D-CGD	4.88	1.45	1.33
24	b	616	CLA	C1D-ND	4.88	1.43	1.37
24	d	403	CLA	O2D-CGD	4.88	1.45	1.33
25	A	408	PHO	O2D-CGD	4.88	1.45	1.33
24	b	618	CLA	CHC-C1C	4.87	1.48	1.38
24	B	616	CLA	C3C-C2C	4.87	1.47	1.36
24	b	608	CLA	O2D-CGD	4.87	1.45	1.33
24	c	911	CLA	CHC-C1C	4.86	1.48	1.38
24	b	619	CLA	O2D-CGD	4.86	1.45	1.33
24	c	914	CLA	O2D-CGD	4.85	1.45	1.33
24	C	502	CLA	C3C-C2C	4.85	1.47	1.36
24	C	502	CLA	C1D-ND	4.85	1.43	1.37
24	c	908	CLA	C1D-ND	4.85	1.43	1.37
24	c	913	CLA	O2D-CGD	4.84	1.45	1.33
24	b	609	CLA	O2D-CGD	4.84	1.45	1.33
24	C	508	CLA	C1D-ND	4.84	1.43	1.37
26	d	404	BCR	C23-C22	-4.83	1.35	1.45
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	c	906	CLA	C1D-ND	4.83	1.43	1.37
26	D	403	BCR	C23-C22	-4.83	1.35	1.45
24	b	620	CLA	C1D-ND	4.83	1.43	1.37
24	C	502	CLA	O2D-CGD	4.83	1.45	1.33
24	c	903	CLA	CHC-C1C	4.83	1.48	1.38
24	A	405	CLA	CHC-C1C	4.82	1.48	1.38
24	c	912	CLA	O2D-CGD	4.82	1.45	1.33
24	c	913	CLA	CHC-C1C	4.82	1.48	1.38
24	c	911	CLA	O2D-CGD	4.82	1.45	1.33
24	b	616	CLA	CHC-C1C	4.81	1.48	1.38
24	B	605	CLA	C1D-ND	4.81	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C1D-ND	4.81	1.43	1.37
24	D	402	CLA	CHC-C1C	4.80	1.48	1.38
24	B	609	CLA	O2D-CGD	4.80	1.44	1.33
26	C	515	BCR	C23-C22	-4.79	1.35	1.45
24	B	614	CLA	O2D-CGD	4.79	1.44	1.33
24	B	604	CLA	O2D-CGD	4.79	1.44	1.33
24	b	619	CLA	C3C-C2C	4.79	1.46	1.36
26	C	516	BCR	C23-C22	-4.78	1.35	1.45
24	b	614	CLA	C1D-ND	4.78	1.43	1.37
24	c	904	CLA	CHC-C1C	4.78	1.48	1.38
24	c	908	CLA	O2D-CGD	4.78	1.44	1.33
24	b	613	CLA	CHC-C1C	4.77	1.48	1.38
25	A	409	PHO	OBD-CAD	4.77	1.29	1.22
24	A	406	CLA	O2D-CGD	4.77	1.44	1.33
24	B	614	CLA	CHC-C1C	4.76	1.48	1.38
24	b	614	CLA	O2D-CGD	4.76	1.44	1.33
24	C	505	CLA	CHC-C1C	4.76	1.48	1.38
24	C	513	CLA	C1D-ND	4.76	1.43	1.37
24	b	608	CLA	C1D-ND	4.75	1.43	1.37
24	b	612	CLA	CHC-C1C	4.75	1.48	1.38
24	b	615	CLA	C3C-C2C	4.74	1.46	1.36
26	h	101	BCR	C23-C22	-4.74	1.35	1.45
24	B	607	CLA	C1D-ND	4.74	1.43	1.37
24	b	607	CLA	C1D-ND	4.73	1.43	1.37
25	A	408	PHO	C3D-C2D	4.73	1.47	1.39
24	C	507	CLA	O2D-CGD	4.72	1.44	1.33
24	B	604	CLA	CHC-C1C	4.72	1.48	1.38
26	b	623	BCR	C23-C22	-4.71	1.35	1.45
24	b	610	CLA	O2D-CGD	4.71	1.44	1.33
24	c	903	CLA	O2D-CGD	4.71	1.44	1.33
26	K	103	BCR	C23-C22	-4.70	1.35	1.45
24	b	607	CLA	CHC-C1C	4.70	1.48	1.38
25	A	409	PHO	O2D-CGD	4.69	1.44	1.33
24	B	617	CLA	O2D-CGD	4.68	1.44	1.33
24	B	610	CLA	CHC-C1C	4.68	1.48	1.38
24	B	603	CLA	CHC-C1C	4.68	1.48	1.38
24	C	509	CLA	C1D-ND	4.67	1.43	1.37
24	B	617	CLA	C1D-ND	4.67	1.43	1.37
24	B	609	CLA	C1D-ND	4.67	1.43	1.37
24	b	608	CLA	CHC-C1C	4.66	1.48	1.38
24	b	613	CLA	C3C-C2C	4.66	1.46	1.36
24	c	910	CLA	CHC-C1C	4.66	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	CLA	O2D-CGD	4.65	1.44	1.33
24	C	506	CLA	C1D-ND	4.65	1.43	1.37
24	B	613	CLA	CHC-C1C	4.65	1.48	1.38
24	B	602	CLA	CHC-C1C	4.64	1.48	1.38
24	B	611	CLA	O2D-CGD	4.64	1.44	1.33
24	C	507	CLA	CHD-C1D	4.64	1.47	1.38
24	C	511	CLA	O2D-CGD	4.64	1.44	1.33
24	b	611	CLA	O2D-CGD	4.63	1.44	1.33
24	C	504	CLA	O2D-CGD	4.63	1.44	1.33
24	c	912	CLA	CHC-C1C	4.63	1.47	1.38
26	y	101	BCR	C23-C22	-4.63	1.36	1.45
24	B	615	CLA	O2D-CGD	4.63	1.44	1.33
24	c	905	CLA	C1D-ND	4.63	1.43	1.37
24	b	605	CLA	CHC-C1C	4.62	1.47	1.38
26	b	621	BCR	C23-C22	-4.62	1.36	1.45
24	c	902	CLA	O2D-CGD	4.61	1.44	1.33
24	b	609	CLA	CHC-C1C	4.61	1.47	1.38
37	E	101	LHG	O8-C23	4.61	1.46	1.33
24	C	503	CLA	CHD-C1D	4.60	1.47	1.38
24	b	614	CLA	CHD-C1D	4.60	1.47	1.38
24	B	603	CLA	CHD-C1D	4.60	1.47	1.38
24	c	908	CLA	O2A-CGA	4.60	1.46	1.33
24	B	612	CLA	CHC-C1C	4.59	1.47	1.38
36	D	405	DGD	O1G-C1A	4.59	1.46	1.33
24	b	619	CLA	C1D-ND	4.59	1.43	1.37
24	a	406	CLA	O2D-CGD	4.59	1.44	1.33
24	b	618	CLA	O2D-CGD	4.58	1.44	1.33
24	a	409	CLA	C1D-ND	4.58	1.43	1.37
26	H	101	BCR	C23-C22	-4.58	1.36	1.45
24	C	505	CLA	O2A-CGA	4.58	1.46	1.33
24	C	511	CLA	CHD-C1D	4.56	1.47	1.38
24	b	608	CLA	CHD-C1D	4.56	1.47	1.38
24	b	614	CLA	CHC-C1C	4.55	1.47	1.38
24	b	617	CLA	CHC-C1C	4.55	1.47	1.38
24	C	508	CLA	CHC-C1C	4.54	1.47	1.38
24	A	405	CLA	O2D-CGD	4.54	1.44	1.33
24	B	610	CLA	O2D-CGD	4.54	1.44	1.33
24	a	407	CLA	O2D-CGD	4.53	1.44	1.33
24	c	910	CLA	CHD-C1D	4.53	1.47	1.38
26	c	915	BCR	C23-C22	-4.53	1.36	1.45
24	B	615	CLA	O2A-CGA	4.53	1.46	1.33
24	C	506	CLA	CHC-C1C	4.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	C1D-ND	4.53	1.43	1.37
24	B	605	CLA	O2D-CGD	4.52	1.44	1.33
27	B	621	SQD	O47-C7	4.52	1.47	1.34
24	b	611	CLA	O2A-CGA	4.52	1.46	1.33
27	a	402	SQD	O48-C23	4.52	1.46	1.33
34	z	101	LMG	O8-C28	4.52	1.46	1.33
24	B	613	CLA	CHD-C1D	4.51	1.47	1.38
24	C	510	CLA	O2A-CGA	4.51	1.46	1.33
24	b	610	CLA	CHC-C1C	4.51	1.47	1.38
24	b	607	CLA	CHD-C1D	4.50	1.47	1.38
26	T	102	BCR	C23-C22	-4.50	1.36	1.45
24	B	616	CLA	CHC-C1C	4.49	1.47	1.38
24	c	904	CLA	CHD-C1D	4.49	1.47	1.38
24	b	620	CLA	CHC-C1C	4.49	1.47	1.38
34	c	919	LMG	O8-C28	4.49	1.46	1.33
26	A	411	BCR	C23-C22	-4.48	1.36	1.45
24	c	905	CLA	CHC-C1C	4.48	1.47	1.38
24	C	506	CLA	CHD-C1D	4.48	1.47	1.38
27	f	102	SQD	O47-C7	4.48	1.46	1.34
24	b	606	CLA	CHC-C1C	4.48	1.47	1.38
24	c	913	CLA	C1D-ND	4.47	1.43	1.37
25	a	408	PHO	O2D-CGD	4.47	1.44	1.33
24	C	509	CLA	CHD-C1D	4.47	1.47	1.38
24	d	401	CLA	CHD-C1D	4.47	1.47	1.38
27	F	101	SQD	O47-C7	4.47	1.46	1.34
24	d	403	CLA	CHC-C1C	4.47	1.47	1.38
24	B	602	CLA	O2A-CGA	4.46	1.46	1.33
24	d	402	CLA	C1D-ND	4.45	1.43	1.37
24	B	608	CLA	OBD-CAD	4.45	1.30	1.22
24	B	606	CLA	C1D-ND	4.45	1.43	1.37
24	C	505	CLA	O2D-CGD	4.45	1.44	1.33
24	C	514	CLA	CHC-C1C	4.45	1.47	1.38
26	B	619	BCR	C23-C22	-4.45	1.36	1.45
24	B	615	CLA	CHC-C1C	4.45	1.47	1.38
24	c	906	CLA	CHD-C1D	4.44	1.47	1.38
34	C	520	LMG	O8-C28	4.44	1.46	1.33
24	a	406	CLA	CHB-C1B	4.44	1.49	1.39
24	b	607	CLA	O2A-CGA	4.44	1.46	1.33
26	a	410	BCR	C23-C22	-4.44	1.36	1.45
24	c	902	CLA	C1D-ND	4.43	1.43	1.37
24	A	410	CLA	CHC-C1C	4.43	1.47	1.38
24	b	609	CLA	O2A-CGA	4.42	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	CHC-C1C	4.42	1.47	1.38
24	c	908	CLA	CHC-C1C	4.41	1.47	1.38
24	d	402	CLA	O2A-CGA	4.41	1.46	1.33
24	b	619	CLA	CHD-C1D	4.41	1.46	1.38
24	a	409	CLA	CHC-C1C	4.41	1.47	1.38
24	d	402	CLA	O2D-CGD	4.40	1.43	1.33
24	C	511	CLA	CHC-C1C	4.40	1.47	1.38
24	C	509	CLA	C3D-C2D	4.40	1.51	1.39
24	c	907	CLA	CHD-C1D	4.40	1.46	1.38
24	b	611	CLA	CHD-C1D	4.39	1.46	1.38
24	C	510	CLA	CHD-C1D	4.38	1.46	1.38
24	b	620	CLA	CHD-C1D	4.38	1.46	1.38
24	c	902	CLA	CHC-C1C	4.38	1.47	1.38
24	B	605	CLA	CHC-C1C	4.38	1.47	1.38
24	C	503	CLA	CHC-C1C	4.37	1.47	1.38
24	c	914	CLA	CHD-C1D	4.37	1.46	1.38
24	B	608	CLA	CHC-C1C	4.37	1.47	1.38
24	B	617	CLA	CHC-C1C	4.37	1.47	1.38
24	C	507	CLA	CHC-C1C	4.36	1.47	1.38
24	C	508	CLA	O2D-CGD	4.36	1.43	1.33
24	C	512	CLA	CHD-C1D	4.36	1.46	1.38
24	c	911	CLA	CHD-C1D	4.36	1.46	1.38
24	B	609	CLA	CHD-C1D	4.36	1.46	1.38
24	c	911	CLA	CHB-C1B	4.36	1.49	1.39
24	c	906	CLA	CHC-C1C	4.35	1.47	1.38
24	c	904	CLA	O2D-CGD	4.35	1.43	1.33
26	K	102	BCR	C23-C22	-4.34	1.36	1.45
24	B	611	CLA	CHD-C1D	4.34	1.46	1.38
24	C	504	CLA	CHC-C1C	4.34	1.47	1.38
24	B	607	CLA	O2A-CGA	4.33	1.46	1.33
24	b	619	CLA	C3D-C2D	4.33	1.51	1.39
36	D	405	DGD	O2G-C1B	4.32	1.46	1.34
24	C	513	CLA	O2A-CGA	4.32	1.46	1.33
24	D	401	CLA	O2D-CGD	4.32	1.43	1.33
34	C	521	LMG	O7-C10	4.31	1.46	1.34
36	d	406	DGD	O2G-C1B	4.31	1.46	1.34
24	B	610	CLA	CHD-C1D	4.31	1.46	1.38
24	B	610	CLA	O2A-CGA	4.30	1.45	1.33
24	b	612	CLA	CHD-C1D	4.30	1.46	1.38
37	d	409	LHG	O8-C23	4.30	1.45	1.33
34	C	501	LMG	O7-C10	4.30	1.46	1.34
24	C	510	CLA	CHC-C1C	4.30	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	CLA	CHD-C1D	4.30	1.46	1.38
24	b	619	CLA	O2A-CGA	4.29	1.45	1.33
24	c	914	CLA	O2A-CGA	4.29	1.45	1.33
34	b	624	LMG	O8-C28	4.29	1.45	1.33
34	C	501	LMG	O8-C28	4.28	1.45	1.33
24	d	401	CLA	CHC-C1C	4.28	1.47	1.38
24	B	607	CLA	CHD-C1D	4.28	1.46	1.38
24	C	502	CLA	O2A-CGA	4.28	1.45	1.33
24	D	402	CLA	CHD-C1D	4.27	1.46	1.38
34	c	920	LMG	O8-C28	4.27	1.45	1.33
34	Z	101	LMG	O7-C10	4.27	1.46	1.34
24	B	606	CLA	CHD-C1D	4.27	1.46	1.38
24	c	914	CLA	CHD-C4C	4.27	1.49	1.39
27	A	416	SQD	O47-C7	4.26	1.46	1.34
24	c	909	CLA	O2A-CGA	4.26	1.45	1.33
24	b	605	CLA	O2A-CGA	4.26	1.45	1.33
24	B	611	CLA	CHC-C1C	4.26	1.47	1.38
24	b	615	CLA	CHC-C1C	4.26	1.47	1.38
24	D	402	CLA	O2A-CGA	4.26	1.45	1.33
24	C	502	CLA	CHC-C1C	4.26	1.47	1.38
24	A	406	CLA	C3D-C2D	4.25	1.50	1.39
35	b	602	HTG	C1'-S1	-4.25	1.76	1.81
24	C	506	CLA	OBD-CAD	4.25	1.29	1.22
24	a	406	CLA	CHC-C1C	4.25	1.47	1.38
24	b	618	CLA	CHB-C1B	4.25	1.48	1.39
24	C	508	CLA	O2A-CGA	4.25	1.45	1.33
24	B	606	CLA	O2A-CGA	4.25	1.45	1.33
24	b	612	CLA	O2A-CGA	4.25	1.45	1.33
24	c	906	CLA	O2A-CGA	4.24	1.45	1.33
35	B	624	HTG	C1'-S1	-4.24	1.76	1.81
24	B	609	CLA	O2A-CGA	4.24	1.45	1.33
40	v	202	HEC	FE-NC	4.24	2.09	1.95
25	a	408	PHO	O2A-CGA	4.24	1.45	1.33
24	B	609	CLA	C3D-C2D	4.24	1.50	1.39
36	d	406	DGD	O1G-C1A	4.24	1.45	1.33
27	L	102	SQD	O47-C7	4.24	1.46	1.34
24	b	610	CLA	O2A-CGA	4.23	1.45	1.33
34	C	521	LMG	O8-C28	4.23	1.45	1.33
24	b	610	CLA	CHD-C1D	4.23	1.46	1.38
24	B	608	CLA	CHD-C1D	4.23	1.46	1.38
24	c	902	CLA	CHD-C1D	4.23	1.46	1.38
24	C	502	CLA	CHD-C1D	4.23	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	e	101	LHG	O8-C23	4.23	1.45	1.33
27	A	412	SQD	O48-C23	4.23	1.45	1.33
24	C	509	CLA	CHC-C1C	4.23	1.47	1.38
24	C	514	CLA	CHD-C1D	4.23	1.46	1.38
24	c	909	CLA	CHC-C1C	4.23	1.47	1.38
24	b	613	CLA	CHD-C1D	4.23	1.46	1.38
24	d	402	CLA	CHD-C1D	4.23	1.46	1.38
34	B	622	LMG	O8-C28	4.23	1.45	1.33
24	B	602	CLA	CHD-C1D	4.23	1.46	1.38
24	c	910	CLA	O2A-CGA	4.23	1.45	1.33
24	A	410	CLA	O2A-CGA	4.22	1.45	1.33
27	A	416	SQD	O48-C23	4.22	1.45	1.33
24	c	912	CLA	CHD-C1D	4.22	1.46	1.38
24	D	401	CLA	CHC-C1C	4.22	1.47	1.38
24	C	511	CLA	CHC-C4B	4.22	1.48	1.39
36	h	102	DGD	O2G-C1B	4.22	1.46	1.34
24	a	407	CLA	CHD-C1D	4.22	1.46	1.38
24	d	403	CLA	CHD-C1D	4.22	1.46	1.38
24	b	606	CLA	CHD-C1D	4.21	1.46	1.38
24	b	618	CLA	O2A-CGA	4.21	1.45	1.33
40	V	201	HEC	FE-NC	4.20	2.09	1.95
24	C	512	CLA	O2A-CGA	4.20	1.45	1.33
24	b	620	CLA	O2A-CGA	4.20	1.45	1.33
25	a	420	PHO	O2A-CGA	4.20	1.45	1.33
27	F	101	SQD	O48-C23	4.20	1.45	1.33
24	b	615	CLA	CHB-C1B	4.20	1.48	1.39
24	B	615	CLA	CHB-C1B	4.20	1.48	1.39
24	B	603	CLA	O2A-CGA	4.20	1.45	1.33
27	a	411	SQD	O48-C23	4.20	1.45	1.33
24	C	507	CLA	O2A-CGA	4.20	1.45	1.33
24	a	407	CLA	O2A-CGA	4.19	1.45	1.33
24	c	913	CLA	O2A-CGA	4.19	1.45	1.33
24	C	504	CLA	CHD-C1D	4.19	1.46	1.38
24	C	505	CLA	CHD-C1D	4.19	1.46	1.38
34	c	920	LMG	O7-C10	4.18	1.46	1.34
27	f	102	SQD	O48-C23	4.18	1.45	1.33
24	a	406	CLA	CHD-C4C	4.18	1.48	1.39
24	b	619	CLA	CHC-C1C	4.18	1.47	1.38
24	b	605	CLA	CHD-C1D	4.17	1.46	1.38
24	c	902	CLA	CHB-C1B	4.17	1.48	1.39
24	C	505	CLA	OBD-CAD	4.17	1.29	1.22
24	c	912	CLA	O2A-CGA	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	O2A-CGA	4.16	1.45	1.33
24	A	407	CLA	CHD-C4C	4.16	1.48	1.39
24	C	503	CLA	C3D-C2D	4.15	1.50	1.39
24	b	616	CLA	O2A-CGA	4.15	1.45	1.33
24	B	611	CLA	CHB-C1B	4.15	1.48	1.39
24	c	908	CLA	CHD-C1D	4.15	1.46	1.38
24	B	617	CLA	O2A-CGA	4.14	1.45	1.33
24	a	406	CLA	CHD-C1D	4.14	1.46	1.38
24	c	902	CLA	O2A-CGA	4.14	1.45	1.33
24	D	401	CLA	O2A-CGA	4.14	1.45	1.33
24	b	605	CLA	CHD-C4C	4.13	1.48	1.39
34	a	412	LMG	O8-C28	4.13	1.45	1.33
24	C	507	CLA	CHB-C1B	4.13	1.48	1.39
24	A	405	CLA	O2A-CGA	4.12	1.45	1.33
24	B	607	CLA	CHC-C1C	4.11	1.46	1.38
24	a	409	CLA	CHD-C1D	4.11	1.46	1.38
24	B	602	CLA	CHD-C4C	4.11	1.48	1.39
24	B	608	CLA	O2A-CGA	4.11	1.45	1.33
24	B	612	CLA	O2A-CGA	4.10	1.45	1.33
37	l	101	LHG	O7-C7	4.10	1.45	1.34
24	D	401	CLA	CHB-C1B	4.10	1.48	1.39
37	e	101	LHG	O7-C7	4.10	1.45	1.34
24	c	907	CLA	CHC-C1C	4.09	1.46	1.38
24	b	612	CLA	CHC-C4B	4.09	1.48	1.39
24	B	609	CLA	CHC-C1C	4.09	1.46	1.38
27	L	102	SQD	O48-C23	4.09	1.45	1.33
24	B	616	CLA	O2A-CGA	4.08	1.45	1.33
24	c	903	CLA	O2A-CGA	4.08	1.45	1.33
24	b	605	CLA	C3D-C2D	4.08	1.50	1.39
24	C	505	CLA	CHB-C1B	4.08	1.48	1.39
37	D	408	LHG	O7-C7	4.08	1.45	1.34
24	c	904	CLA	O2A-CGA	4.07	1.45	1.33
24	B	608	CLA	C1D-ND	4.07	1.42	1.37
24	B	615	CLA	CHD-C1D	4.06	1.46	1.38
38	E	103	HEM	FE-NC	4.06	2.08	1.95
24	c	905	CLA	O2A-CGA	4.06	1.45	1.33
37	d	407	LHG	O8-C23	4.06	1.45	1.33
24	C	508	CLA	CHD-C1D	4.05	1.46	1.38
24	B	604	CLA	O2A-CGA	4.05	1.45	1.33
24	d	401	CLA	O2A-CGA	4.05	1.45	1.33
24	B	602	CLA	C3D-C2D	4.05	1.50	1.39
38	e	102	HEM	FE-NC	4.05	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	CHD-C4C	4.05	1.48	1.39
24	C	511	CLA	CHB-C1B	4.04	1.48	1.39
24	B	605	CLA	CHB-C1B	4.04	1.48	1.39
24	d	403	CLA	O2A-CGA	4.04	1.45	1.33
24	C	510	CLA	C3D-C2D	4.04	1.50	1.39
24	B	611	CLA	O2A-CGA	4.04	1.45	1.33
24	C	512	CLA	CHD-C4C	4.04	1.48	1.39
24	B	606	CLA	CHC-C1C	4.03	1.46	1.38
24	b	618	CLA	CHD-C1D	4.03	1.46	1.38
24	A	407	CLA	CHC-C4B	4.03	1.48	1.39
24	A	410	CLA	CHD-C1D	4.03	1.46	1.38
24	c	909	CLA	C3D-C2D	4.03	1.50	1.39
24	C	511	CLA	C3D-C2D	4.03	1.50	1.39
24	B	616	CLA	C3D-C2D	4.03	1.50	1.39
24	b	614	CLA	CHD-C4C	4.03	1.48	1.39
37	E	101	LHG	O7-C7	4.03	1.45	1.34
24	c	905	CLA	C3D-C2D	4.02	1.50	1.39
34	z	101	LMG	O7-C10	4.02	1.45	1.34
24	A	410	CLA	C3D-C2D	4.02	1.50	1.39
24	B	613	CLA	C1D-ND	4.02	1.42	1.37
24	c	905	CLA	CHD-C1D	4.02	1.46	1.38
24	B	617	CLA	CHD-C1D	4.02	1.46	1.38
24	C	508	CLA	CHD-C4C	4.01	1.48	1.39
24	D	401	CLA	CHD-C1D	4.01	1.46	1.38
24	C	507	CLA	CHD-C4C	4.01	1.48	1.39
24	b	615	CLA	O2A-CGA	4.01	1.45	1.33
24	c	907	CLA	O2A-CGA	4.01	1.45	1.33
24	b	611	CLA	C1D-ND	4.01	1.42	1.37
24	C	503	CLA	CHD-C4C	4.01	1.48	1.39
26	B	618	BCR	C23-C22	-4.01	1.37	1.45
24	d	401	CLA	C3D-C2D	4.01	1.50	1.39
24	C	504	CLA	CHD-C4C	4.01	1.48	1.39
27	a	402	SQD	O47-C7	4.01	1.45	1.34
24	c	907	CLA	CHD-C4C	4.00	1.48	1.39
24	A	406	CLA	CHC-C1C	4.00	1.46	1.38
24	a	409	CLA	C3D-C2D	4.00	1.50	1.39
24	a	407	CLA	CHD-C4C	4.00	1.48	1.39
36	c	918	DGD	O1G-C1A	3.99	1.45	1.33
36	c	917	DGD	O1G-C1A	3.99	1.45	1.33
34	B	622	LMG	O7-C10	3.99	1.45	1.34
24	b	608	CLA	CHD-C4C	3.99	1.48	1.39
24	a	409	CLA	O2A-CGA	3.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C3D-C2D	3.99	1.50	1.39
40	v	202	HEC	CBC-CAC	-3.98	1.33	1.51
24	C	512	CLA	CHB-C1B	3.98	1.48	1.39
24	c	912	CLA	CHD-C4C	3.98	1.48	1.39
24	b	614	CLA	O2A-CGA	3.98	1.45	1.33
34	C	520	LMG	O7-C10	3.98	1.45	1.34
24	c	903	CLA	CHD-C1D	3.97	1.46	1.38
35	c	923	HTG	C1'-S1	-3.97	1.76	1.81
24	A	410	CLA	CHD-C4C	3.97	1.48	1.39
24	b	616	CLA	CHB-C1B	3.96	1.48	1.39
24	A	406	CLA	CHD-C4C	3.96	1.48	1.39
24	b	618	CLA	CHD-C4C	3.96	1.48	1.39
25	A	408	PHO	O2A-CGA	3.96	1.44	1.33
24	C	503	CLA	CHB-C1B	3.96	1.48	1.39
24	B	605	CLA	CHD-C1D	3.96	1.46	1.38
34	a	412	LMG	O7-C10	3.96	1.45	1.34
24	d	402	CLA	CHC-C1C	3.95	1.46	1.38
24	c	904	CLA	CHD-C4C	3.95	1.48	1.39
24	B	612	CLA	CHC-C4B	3.95	1.48	1.39
36	H	102	DGD	O2G-C1B	3.95	1.45	1.34
24	c	911	CLA	O2A-CGA	3.95	1.44	1.33
24	C	504	CLA	O2A-CGA	3.95	1.44	1.33
37	d	409	LHG	O7-C7	3.95	1.45	1.34
24	A	410	CLA	OBD-CAD	3.94	1.29	1.22
34	c	919	LMG	O7-C10	3.94	1.45	1.34
24	c	910	CLA	C3D-C2D	3.94	1.49	1.39
24	C	509	CLA	CHD-C4C	3.94	1.48	1.39
24	B	611	CLA	CHD-C4C	3.93	1.48	1.39
24	B	609	CLA	OBD-CAD	3.93	1.29	1.22
24	b	611	CLA	OBD-CAD	3.93	1.29	1.22
24	c	908	CLA	CHD-C4C	3.93	1.48	1.39
24	C	511	CLA	CHD-C4C	3.93	1.48	1.39
24	c	910	CLA	CHD-C4C	3.93	1.48	1.39
24	C	505	CLA	CHD-C4C	3.92	1.48	1.39
24	A	405	CLA	CHB-C1B	3.92	1.48	1.39
24	B	609	CLA	CHD-C4C	3.92	1.48	1.39
24	B	615	CLA	CHD-C4C	3.92	1.48	1.39
27	B	621	SQD	O48-C23	3.92	1.44	1.33
24	B	606	CLA	CHB-C1B	3.92	1.48	1.39
24	b	613	CLA	CHB-C1B	3.91	1.48	1.39
36	H	102	DGD	O1G-C1A	3.91	1.44	1.33
24	B	617	CLA	OBD-CAD	3.91	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C3D-C2D	3.91	1.49	1.39
24	B	612	CLA	CHD-C4C	3.91	1.48	1.39
24	C	506	CLA	O2A-CGA	3.91	1.44	1.33
24	C	513	CLA	C3D-C2D	3.91	1.49	1.39
24	b	608	CLA	O2A-CGA	3.90	1.44	1.33
24	c	907	CLA	C3D-C2D	3.90	1.49	1.39
24	B	606	CLA	C3D-C2D	3.90	1.49	1.39
24	B	611	CLA	C3D-C2D	3.90	1.49	1.39
36	C	519	DGD	O1G-C1A	3.90	1.44	1.33
37	L	101	LHG	O8-C23	3.90	1.44	1.33
24	b	613	CLA	CHC-C4B	3.90	1.48	1.39
24	c	905	CLA	OBD-CAD	3.89	1.29	1.22
24	C	510	CLA	CHB-C1B	3.89	1.48	1.39
24	B	608	CLA	CHD-C4C	3.89	1.48	1.39
35	B	633	HTG	C1'-S1	-3.89	1.76	1.81
24	b	609	CLA	CHD-C4C	3.89	1.48	1.39
24	b	620	CLA	CHB-C1B	3.89	1.48	1.39
36	c	917	DGD	O2G-C1B	3.89	1.45	1.34
24	B	612	CLA	CHD-C1D	3.89	1.45	1.38
24	C	507	CLA	C3D-C2D	3.89	1.49	1.39
24	b	620	CLA	C3D-C2D	3.89	1.49	1.39
36	C	518	DGD	O1G-C1A	3.88	1.44	1.33
24	B	610	CLA	CHB-C1B	3.88	1.48	1.39
34	j	101	LMG	O8-C28	3.88	1.44	1.33
24	B	617	CLA	CHB-C1B	3.88	1.48	1.39
24	c	911	CLA	CHC-C4B	3.88	1.48	1.39
24	C	506	CLA	CHD-C4C	3.88	1.48	1.39
37	D	406	LHG	O8-C23	3.88	1.44	1.33
37	d	408	LHG	O7-C7	3.88	1.45	1.34
36	c	916	DGD	O1G-C1A	3.88	1.44	1.33
40	V	201	HEC	CBC-CAC	-3.88	1.34	1.51
24	c	903	CLA	C3D-C2D	3.87	1.49	1.39
24	C	503	CLA	O2A-CGA	3.87	1.44	1.33
37	l	101	LHG	O8-C23	3.87	1.44	1.33
24	A	410	CLA	CHC-C4B	3.87	1.48	1.39
24	c	903	CLA	CHB-C1B	3.87	1.48	1.39
24	c	913	CLA	CHD-C1D	3.87	1.45	1.38
25	a	420	PHO	OBD-CAD	3.87	1.27	1.22
24	c	911	CLA	CHD-C4C	3.87	1.48	1.39
24	d	403	CLA	CHB-C1B	3.87	1.48	1.39
24	B	604	CLA	CHD-C1D	3.86	1.45	1.38
24	B	614	CLA	CHD-C1D	3.86	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	CHD-C4C	3.86	1.48	1.39
24	B	605	CLA	CHD-C4C	3.86	1.48	1.39
24	c	903	CLA	CHD-C4C	3.86	1.48	1.39
24	b	617	CLA	O2A-CGA	3.86	1.44	1.33
24	B	605	CLA	O2A-CGA	3.86	1.44	1.33
24	C	509	CLA	O2A-CGA	3.85	1.44	1.33
24	b	614	CLA	CHB-C1B	3.85	1.48	1.39
36	h	102	DGD	O1G-C1A	3.85	1.44	1.33
34	j	101	LMG	O7-C10	3.85	1.45	1.34
24	D	401	CLA	C3D-C2D	3.85	1.49	1.39
36	C	519	DGD	O2G-C1B	3.85	1.45	1.34
24	d	401	CLA	OBD-CAD	3.85	1.29	1.22
24	B	612	CLA	C3D-C2D	3.85	1.49	1.39
24	A	407	CLA	O2A-CGA	3.85	1.44	1.33
24	b	612	CLA	CHD-C4C	3.85	1.48	1.39
24	b	606	CLA	CHB-C1B	3.85	1.48	1.39
24	C	508	CLA	C3D-C2D	3.85	1.49	1.39
24	B	614	CLA	C3D-C2D	3.85	1.49	1.39
24	b	609	CLA	CHB-C1B	3.85	1.48	1.39
24	A	407	CLA	C3D-C2D	3.85	1.49	1.39
24	C	506	CLA	CHC-C4B	3.84	1.48	1.39
24	c	910	CLA	CHC-C4B	3.84	1.48	1.39
24	b	615	CLA	CHD-C1D	3.84	1.45	1.38
24	C	514	CLA	C3D-C2D	3.84	1.49	1.39
24	b	609	CLA	OBD-CAD	3.84	1.29	1.22
36	c	918	DGD	O2G-C1B	3.84	1.45	1.34
24	d	403	CLA	C3D-C2D	3.84	1.49	1.39
27	A	412	SQD	O47-C7	3.84	1.45	1.34
34	J	101	LMG	O8-C28	3.84	1.44	1.33
24	a	407	CLA	CHC-C4B	3.84	1.48	1.39
24	B	613	CLA	O2A-CGA	3.84	1.44	1.33
24	B	616	CLA	CHD-C1D	3.84	1.45	1.38
24	A	405	CLA	C3D-C2D	3.83	1.49	1.39
37	D	407	LHG	O7-C7	3.83	1.45	1.34
24	c	912	CLA	CHB-C1B	3.83	1.48	1.39
24	B	612	CLA	CHB-C1B	3.83	1.48	1.39
24	c	906	CLA	CHB-C1B	3.83	1.48	1.39
24	C	502	CLA	CHD-C4C	3.83	1.48	1.39
24	B	613	CLA	OBD-CAD	3.83	1.29	1.22
36	C	517	DGD	O2G-C1B	3.83	1.45	1.34
24	b	619	CLA	OBD-CAD	3.83	1.29	1.22
24	c	909	CLA	CHD-C1D	3.83	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	CHB-C1B	3.83	1.48	1.39
24	b	608	CLA	CHC-C4B	3.83	1.48	1.39
24	B	614	CLA	O2A-CGA	3.83	1.44	1.33
35	D	411	HTG	C1'-S1	-3.83	1.76	1.81
24	c	907	CLA	CHB-C1B	3.82	1.48	1.39
24	A	406	CLA	CHD-C1D	3.82	1.45	1.38
24	c	903	CLA	CHC-C4B	3.82	1.48	1.39
24	B	607	CLA	OBD-CAD	3.82	1.29	1.22
24	c	908	CLA	CHB-C1B	3.82	1.48	1.39
34	J	101	LMG	O7-C10	3.82	1.45	1.34
24	c	903	CLA	OBD-CAD	3.82	1.29	1.22
25	A	409	PHO	O2A-CGA	3.82	1.44	1.33
24	b	610	CLA	C3D-C2D	3.82	1.49	1.39
24	b	617	CLA	C3D-C2D	3.81	1.49	1.39
24	B	611	CLA	CHC-C4B	3.81	1.48	1.39
24	C	512	CLA	OBD-CAD	3.81	1.29	1.22
37	L	101	LHG	O7-C7	3.81	1.45	1.34
24	d	401	CLA	CHB-C1B	3.81	1.48	1.39
24	C	510	CLA	CHD-C4C	3.81	1.47	1.39
24	b	613	CLA	CHD-C4C	3.81	1.47	1.39
24	b	617	CLA	CHD-C1D	3.81	1.45	1.38
36	C	517	DGD	O1G-C1A	3.80	1.44	1.33
24	b	615	CLA	C3D-C2D	3.80	1.49	1.39
24	c	913	CLA	CHC-C4B	3.80	1.47	1.39
24	C	511	CLA	O2A-CGA	3.80	1.44	1.33
24	C	514	CLA	CHB-C1B	3.80	1.47	1.39
24	A	405	CLA	CHD-C1D	3.79	1.45	1.38
24	B	617	CLA	C3D-C2D	3.79	1.49	1.39
25	a	408	PHO	OBD-CAD	3.79	1.27	1.22
24	d	402	CLA	C1B-NB	-3.79	1.33	1.37
24	a	406	CLA	C3D-C2D	3.79	1.49	1.39
24	b	605	CLA	CHC-C4B	3.79	1.47	1.39
24	B	606	CLA	OBD-CAD	3.79	1.29	1.22
24	C	504	CLA	C3D-C2D	3.79	1.49	1.39
24	c	912	CLA	C3D-C2D	3.79	1.49	1.39
40	v	202	HEC	CBB-CAB	-3.79	1.34	1.51
24	b	606	CLA	C3D-C2D	3.78	1.49	1.39
24	A	407	CLA	OBD-CAD	3.78	1.29	1.22
24	C	505	CLA	C3D-C2D	3.78	1.49	1.39
24	C	502	CLA	C3D-C2D	3.78	1.49	1.39
24	a	407	CLA	C3D-C2D	3.78	1.49	1.39
24	c	908	CLA	C3D-C2D	3.78	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	CHB-C1B	3.78	1.47	1.39
24	b	616	CLA	CHD-C1D	3.78	1.45	1.38
24	c	913	CLA	C3D-C2D	3.77	1.49	1.39
24	a	409	CLA	OBD-CAD	3.77	1.29	1.22
36	c	916	DGD	O2G-C1B	3.77	1.44	1.34
24	B	603	CLA	C3D-C2D	3.77	1.49	1.39
24	A	405	CLA	CHC-C4B	3.77	1.47	1.39
24	D	402	CLA	CHB-C1B	3.77	1.47	1.39
24	b	609	CLA	CHD-C1D	3.77	1.45	1.38
24	C	502	CLA	CHC-C4B	3.76	1.47	1.39
24	c	904	CLA	CHC-C4B	3.76	1.47	1.39
24	c	902	CLA	C3D-C2D	3.76	1.49	1.39
24	b	617	CLA	CHB-C1B	3.76	1.47	1.39
35	B	634	HTG	C1'-S1	-3.76	1.76	1.81
36	C	518	DGD	O2G-C1B	3.76	1.44	1.34
24	A	407	CLA	CHB-C1B	3.76	1.47	1.39
35	b	627	HTG	C1'-S1	-3.76	1.76	1.81
24	c	905	CLA	CHB-C1B	3.75	1.47	1.39
24	C	514	CLA	CHD-C4C	3.75	1.47	1.39
24	b	612	CLA	C3D-C2D	3.75	1.49	1.39
34	b	624	LMG	O7-C10	3.75	1.44	1.34
24	C	513	CLA	CHD-C1D	3.75	1.45	1.38
24	c	904	CLA	C3D-C2D	3.75	1.49	1.39
24	C	506	CLA	C1B-NB	-3.75	1.33	1.37
24	B	603	CLA	CHD-C4C	3.74	1.47	1.39
24	b	614	CLA	C3D-C2D	3.74	1.49	1.39
24	d	403	CLA	CHD-C4C	3.74	1.47	1.39
24	c	906	CLA	CHD-C4C	3.74	1.47	1.39
24	b	619	CLA	CHD-C4C	3.74	1.47	1.39
24	d	401	CLA	CHD-C4C	3.74	1.47	1.39
27	a	411	SQD	O47-C7	3.74	1.44	1.34
24	c	913	CLA	CHD-C4C	3.74	1.47	1.39
24	b	620	CLA	CHD-C4C	3.73	1.47	1.39
24	B	604	CLA	C3D-C2D	3.73	1.49	1.39
24	B	613	CLA	CHB-C1B	3.73	1.47	1.39
24	B	615	CLA	OBD-CAD	3.73	1.28	1.22
24	b	613	CLA	O2A-CGA	3.73	1.44	1.33
24	B	607	CLA	CHD-C4C	3.73	1.47	1.39
24	b	606	CLA	O2A-CGA	3.72	1.44	1.33
24	B	602	CLA	CHC-C4B	3.72	1.47	1.39
24	B	617	CLA	C4B-NB	-3.72	1.33	1.37
24	b	614	CLA	OBD-CAD	3.72	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	O2A-CGA	3.72	1.44	1.33
40	V	201	HEC	CBB-CAB	-3.72	1.34	1.51
24	c	911	CLA	C3D-C2D	3.72	1.49	1.39
24	B	604	CLA	CHC-C4B	3.71	1.47	1.39
24	a	406	CLA	OBD-CAD	3.71	1.28	1.22
24	B	614	CLA	CHB-C1B	3.71	1.47	1.39
24	b	609	CLA	CHC-C4B	3.70	1.47	1.39
24	b	614	CLA	CHC-C4B	3.70	1.47	1.39
24	C	502	CLA	OBD-CAD	3.70	1.28	1.22
24	C	508	CLA	CHC-C4B	3.70	1.47	1.39
24	b	611	CLA	CHB-C1B	3.70	1.47	1.39
24	c	906	CLA	OBD-CAD	3.70	1.28	1.22
24	c	912	CLA	OBD-CAD	3.70	1.28	1.22
24	b	612	CLA	CHB-C1B	3.69	1.47	1.39
24	b	616	CLA	CHC-C4B	3.69	1.47	1.39
24	B	615	CLA	C3D-C2D	3.68	1.49	1.39
24	B	610	CLA	OBD-CAD	3.68	1.28	1.22
24	c	910	CLA	CHB-C1B	3.68	1.47	1.39
24	B	608	CLA	CHC-C4B	3.68	1.47	1.39
24	C	502	CLA	CHB-C1B	3.68	1.47	1.39
24	b	608	CLA	CHB-C1B	3.67	1.47	1.39
24	b	606	CLA	CHD-C4C	3.67	1.47	1.39
24	c	907	CLA	C1B-NB	-3.67	1.33	1.37
24	C	513	CLA	CHC-C4B	3.67	1.47	1.39
24	C	510	CLA	CHC-C4B	3.67	1.47	1.39
24	B	616	CLA	CHD-C4C	3.66	1.47	1.39
24	B	605	CLA	CHC-C4B	3.66	1.47	1.39
24	c	911	CLA	OBD-CAD	3.66	1.28	1.22
24	B	608	CLA	CHB-C1B	3.66	1.47	1.39
24	B	610	CLA	CHD-C4C	3.66	1.47	1.39
24	b	607	CLA	CHC-C4B	3.66	1.47	1.39
24	B	610	CLA	CHC-C4B	3.66	1.47	1.39
24	D	402	CLA	C3D-C2D	3.65	1.49	1.39
24	a	409	CLA	CHD-C4C	3.65	1.47	1.39
24	c	909	CLA	CHD-C4C	3.65	1.47	1.39
24	B	607	CLA	C1B-NB	-3.65	1.33	1.37
24	c	910	CLA	OBD-CAD	3.65	1.28	1.22
24	C	509	CLA	CHC-C4B	3.65	1.47	1.39
24	d	402	CLA	C3D-C2D	3.65	1.49	1.39
37	d	407	LHG	O7-C7	3.65	1.44	1.34
24	C	512	CLA	C3D-C2D	3.64	1.49	1.39
24	B	614	CLA	CHD-C4C	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C3D-C2D	3.64	1.49	1.39
24	c	909	CLA	OBD-CAD	3.64	1.28	1.22
24	C	508	CLA	CHB-C1B	3.64	1.47	1.39
24	B	603	CLA	CHC-C4B	3.63	1.47	1.39
24	C	512	CLA	C4B-NB	-3.63	1.33	1.37
24	B	614	CLA	CHC-C4B	3.63	1.47	1.39
24	c	914	CLA	C3D-C2D	3.63	1.49	1.39
24	c	904	CLA	CHB-C1B	3.63	1.47	1.39
24	b	611	CLA	CHC-C4B	3.63	1.47	1.39
24	C	513	CLA	CHD-C4C	3.63	1.47	1.39
24	B	612	CLA	OBD-CAD	3.62	1.28	1.22
24	a	407	CLA	CHB-C1B	3.62	1.47	1.39
24	A	410	CLA	CHB-C1B	3.62	1.47	1.39
24	B	604	CLA	CHD-C4C	3.62	1.47	1.39
24	C	503	CLA	CHC-C4B	3.62	1.47	1.39
24	D	402	CLA	CHC-C4B	3.62	1.47	1.39
24	b	605	CLA	CHB-C1B	3.61	1.47	1.39
24	c	902	CLA	CHD-C4C	3.61	1.47	1.39
24	B	616	CLA	CHC-C4B	3.61	1.47	1.39
24	C	508	CLA	OBD-CAD	3.61	1.28	1.22
24	b	608	CLA	C3D-C2D	3.61	1.49	1.39
24	c	912	CLA	CHC-C4B	3.61	1.47	1.39
24	b	613	CLA	OBD-CAD	3.61	1.28	1.22
24	B	613	CLA	CHC-C4B	3.61	1.47	1.39
24	d	402	CLA	CHC-C4B	3.60	1.47	1.39
24	D	402	CLA	CHD-C4C	3.60	1.47	1.39
24	A	406	CLA	CHC-C4B	3.60	1.47	1.39
38	e	102	HEM	C4D-ND	-3.59	1.34	1.40
24	a	406	CLA	O2A-CGA	3.59	1.43	1.33
37	d	408	LHG	O8-C23	3.59	1.43	1.33
24	C	505	CLA	CHC-C4B	3.59	1.47	1.39
37	D	408	LHG	O8-C23	3.58	1.43	1.33
24	C	504	CLA	CHC-C4B	3.58	1.47	1.39
24	B	607	CLA	CHB-C1B	3.58	1.47	1.39
24	c	914	CLA	OBD-CAD	3.58	1.28	1.22
24	B	607	CLA	C3D-C2D	3.58	1.48	1.39
24	C	506	CLA	CHB-C1B	3.58	1.47	1.39
24	d	402	CLA	CHD-C4C	3.57	1.47	1.39
24	B	604	CLA	CHB-C1B	3.57	1.47	1.39
24	b	612	CLA	OBD-CAD	3.57	1.28	1.22
24	b	616	CLA	OBD-CAD	3.57	1.28	1.22
24	d	402	CLA	CHB-C1B	3.57	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	CLA	CHC-C4B	3.57	1.47	1.39
24	c	914	CLA	CHC-C4B	3.56	1.47	1.39
24	D	401	CLA	CHD-C4C	3.56	1.47	1.39
24	d	403	CLA	OBD-CAD	3.56	1.28	1.22
24	b	618	CLA	CHC-C4B	3.55	1.47	1.39
24	b	615	CLA	CHD-C4C	3.54	1.47	1.39
24	B	607	CLA	C4B-NB	-3.54	1.33	1.37
24	C	513	CLA	CHB-C1B	3.54	1.47	1.39
24	b	617	CLA	CHC-C4B	3.54	1.47	1.39
24	b	609	CLA	C3D-C2D	3.54	1.48	1.39
24	B	613	CLA	CHD-C4C	3.54	1.47	1.39
24	B	609	CLA	C4B-NB	-3.54	1.33	1.37
24	b	615	CLA	CHC-C4B	3.53	1.47	1.39
24	B	615	CLA	C4B-NB	-3.53	1.33	1.37
24	b	611	CLA	C3D-C2D	3.53	1.48	1.39
24	B	602	CLA	OBD-CAD	3.52	1.28	1.22
24	c	908	CLA	OBD-CAD	3.52	1.28	1.22
24	a	407	CLA	OBD-CAD	3.52	1.28	1.22
24	c	909	CLA	CHC-C4B	3.52	1.47	1.39
24	B	609	CLA	C1B-NB	-3.52	1.33	1.37
24	c	905	CLA	CHD-C4C	3.52	1.47	1.39
24	B	611	CLA	C1B-NB	-3.51	1.33	1.37
24	B	606	CLA	CHC-C4B	3.51	1.47	1.39
24	A	405	CLA	CHD-C4C	3.51	1.47	1.39
24	c	909	CLA	CHB-C1B	3.51	1.47	1.39
24	B	604	CLA	OBD-CAD	3.51	1.28	1.22
24	b	606	CLA	OBD-CAD	3.51	1.28	1.22
24	C	504	CLA	OBD-CAD	3.51	1.28	1.22
35	b	603	HTG	C1'-S1	-3.50	1.76	1.81
24	b	605	CLA	OBD-CAD	3.50	1.28	1.22
37	D	407	LHG	O8-C23	3.50	1.43	1.33
24	b	618	CLA	OBD-CAD	3.50	1.28	1.22
24	d	403	CLA	CHC-C4B	3.50	1.47	1.39
24	B	608	CLA	C3D-C2D	3.50	1.48	1.39
24	b	618	CLA	C3D-C2D	3.49	1.48	1.39
24	b	613	CLA	C1B-NB	-3.49	1.33	1.37
35	C	524	HTG	C1'-S1	-3.49	1.77	1.81
24	c	913	CLA	CHB-C1B	3.49	1.47	1.39
35	d	412	HTG	C1'-S1	-3.49	1.77	1.81
24	b	617	CLA	OBD-CAD	3.48	1.28	1.22
35	B	626	HTG	C1'-S1	-3.47	1.77	1.81
24	a	409	CLA	CHB-C1B	3.47	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C3D-C2D	3.47	1.48	1.39
24	b	607	CLA	C3D-C2D	3.47	1.48	1.39
24	b	617	CLA	CHD-C4C	3.47	1.47	1.39
24	b	611	CLA	C1B-NB	-3.46	1.33	1.37
24	C	507	CLA	OBD-CAD	3.45	1.28	1.22
24	b	606	CLA	CHC-C4B	3.45	1.47	1.39
24	b	615	CLA	OBD-CAD	3.45	1.28	1.22
24	b	611	CLA	CHD-C4C	3.44	1.47	1.39
24	b	610	CLA	CHC-C4B	3.44	1.47	1.39
24	b	620	CLA	CHC-C4B	3.44	1.47	1.39
24	C	514	CLA	CHC-C4B	3.44	1.47	1.39
24	d	401	CLA	CHC-C4B	3.44	1.47	1.39
24	c	914	CLA	CHB-C1B	3.44	1.47	1.39
24	b	610	CLA	OBD-CAD	3.44	1.28	1.22
24	b	607	CLA	CHB-C1B	3.43	1.47	1.39
24	c	905	CLA	C4B-NB	-3.43	1.33	1.37
24	D	401	CLA	OBD-CAD	3.43	1.28	1.22
24	c	905	CLA	CHC-C4B	3.43	1.47	1.39
24	b	607	CLA	C1B-NB	-3.42	1.33	1.37
35	V	202	HTG	C1'-S1	-3.42	1.77	1.81
24	b	619	CLA	CHB-C1B	3.42	1.47	1.39
24	a	409	CLA	CHC-C4B	3.41	1.47	1.39
24	c	907	CLA	CHC-C4B	3.41	1.47	1.39
24	D	402	CLA	OBD-CAD	3.41	1.28	1.22
24	B	602	CLA	CHB-C1B	3.40	1.47	1.39
40	v	202	HEC	C1D-ND	-3.40	1.34	1.40
24	B	603	CLA	OBD-CAD	3.40	1.28	1.22
24	C	513	CLA	OBD-CAD	3.40	1.28	1.22
24	c	907	CLA	OBD-CAD	3.39	1.28	1.22
24	C	506	CLA	C3D-C2D	3.39	1.48	1.39
38	E	103	HEM	C4D-ND	-3.39	1.34	1.40
24	c	911	CLA	C1B-NB	-3.36	1.33	1.37
24	B	609	CLA	CHC-C4B	3.36	1.46	1.39
24	d	401	CLA	C1B-C2B	3.35	1.51	1.43
24	c	913	CLA	OBD-CAD	3.35	1.28	1.22
35	C	523	HTG	C1'-S1	-3.34	1.77	1.81
24	C	514	CLA	OBD-CAD	3.34	1.28	1.22
24	b	615	CLA	C1B-C2B	3.34	1.51	1.43
24	c	906	CLA	C3D-C2D	3.33	1.48	1.39
24	B	607	CLA	CHC-C4B	3.33	1.46	1.39
24	B	614	CLA	OBD-CAD	3.33	1.28	1.22
24	C	514	CLA	C4B-NB	-3.32	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	CLA	CHC-C4B	3.32	1.46	1.39
24	b	619	CLA	CHC-C4B	3.31	1.46	1.39
24	C	510	CLA	C4B-NB	-3.31	1.33	1.37
24	A	406	CLA	C4B-NB	-3.30	1.33	1.37
24	B	617	CLA	CHC-C4B	3.30	1.46	1.39
24	c	908	CLA	C4B-NB	-3.30	1.33	1.37
24	c	912	CLA	C4B-NB	-3.30	1.33	1.37
24	b	620	CLA	OBD-CAD	3.29	1.28	1.22
24	C	507	CLA	CHC-C4B	3.29	1.46	1.39
24	c	904	CLA	OBD-CAD	3.28	1.28	1.22
24	C	510	CLA	OBD-CAD	3.28	1.28	1.22
24	B	604	CLA	C4B-NB	-3.28	1.33	1.37
24	c	902	CLA	C1B-NB	-3.28	1.33	1.37
24	C	509	CLA	OBD-CAD	3.28	1.28	1.22
24	d	401	CLA	C1B-NB	-3.27	1.33	1.37
24	b	619	CLA	C1B-C2B	3.27	1.50	1.43
35	O	303	HTG	C1'-S1	-3.26	1.77	1.81
24	C	504	CLA	C4B-NB	-3.26	1.33	1.37
24	b	605	CLA	C3B-C4B	3.26	1.50	1.42
24	b	610	CLA	CHB-C1B	3.26	1.46	1.39
24	b	608	CLA	OBD-CAD	3.25	1.28	1.22
35	b	626	HTG	C1'-S1	-3.25	1.77	1.81
24	B	617	CLA	CHD-C4C	3.25	1.46	1.39
38	E	103	HEM	C1B-NB	-3.24	1.34	1.40
24	c	912	CLA	C1B-NB	-3.23	1.33	1.37
24	b	611	CLA	C1B-C2B	3.23	1.50	1.43
24	c	906	CLA	C1B-C2B	3.23	1.50	1.43
24	C	508	CLA	C4B-NB	-3.23	1.33	1.37
37	D	406	LHG	O7-C7	3.23	1.43	1.34
24	C	503	CLA	OBD-CAD	3.23	1.28	1.22
24	B	605	CLA	C3D-C2D	3.23	1.47	1.39
24	c	908	CLA	CHC-C4B	3.22	1.46	1.39
24	c	902	CLA	OBD-CAD	3.21	1.28	1.22
24	C	504	CLA	CHB-C1B	3.21	1.46	1.39
24	C	512	CLA	CHC-C4B	3.20	1.46	1.39
24	A	407	CLA	C3B-C4B	3.20	1.50	1.42
24	B	615	CLA	CHC-C4B	3.20	1.46	1.39
24	C	507	CLA	C4B-NB	-3.20	1.33	1.37
24	B	616	CLA	C1B-NB	-3.20	1.33	1.37
24	a	409	CLA	C4B-NB	-3.20	1.33	1.37
24	A	406	CLA	C1B-NB	-3.19	1.33	1.37
24	c	902	CLA	CHC-C4B	3.18	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	CHD-C4C	3.18	1.46	1.39
24	B	613	CLA	C1B-NB	-3.18	1.33	1.37
24	b	610	CLA	C1B-NB	-3.18	1.33	1.37
24	C	512	CLA	C1B-C2B	3.17	1.50	1.43
24	b	616	CLA	CHD-C4C	3.17	1.46	1.39
24	b	607	CLA	OBD-CAD	3.16	1.27	1.22
24	a	407	CLA	C3B-C4B	3.16	1.50	1.42
24	c	914	CLA	C1B-NB	-3.16	1.33	1.37
24	c	910	CLA	C1B-NB	-3.16	1.33	1.37
24	B	606	CLA	C1B-NB	-3.15	1.33	1.37
24	A	405	CLA	OBD-CAD	3.15	1.27	1.22
24	C	510	CLA	C1B-NB	-3.15	1.33	1.37
24	a	409	CLA	C1B-NB	-3.14	1.33	1.37
40	V	201	HEC	C1D-ND	-3.14	1.34	1.40
35	B	625	HTG	C1'-S1	-3.14	1.77	1.81
24	b	605	CLA	C1B-NB	-3.13	1.33	1.37
24	B	602	CLA	C4B-NB	-3.13	1.33	1.37
24	b	616	CLA	C4B-NB	-3.13	1.33	1.37
24	B	616	CLA	CHB-C1B	3.12	1.46	1.39
24	b	613	CLA	C3B-C4B	3.12	1.50	1.42
24	C	511	CLA	C1B-NB	-3.12	1.33	1.37
24	c	906	CLA	CHC-C4B	3.12	1.46	1.39
24	D	402	CLA	C3B-C4B	3.12	1.50	1.42
25	A	409	PHO	CHA-CBD	-3.12	1.47	1.51
24	C	511	CLA	OBD-CAD	3.11	1.27	1.22
24	b	608	CLA	C4C-C3C	3.11	1.50	1.45
24	B	609	CLA	CHB-C1B	3.11	1.46	1.39
24	b	618	CLA	C1B-NB	-3.11	1.34	1.37
24	b	607	CLA	C3B-C4B	3.10	1.50	1.42
24	D	401	CLA	C1B-C2B	3.10	1.50	1.43
24	c	913	CLA	C3B-C4B	3.10	1.50	1.42
24	b	620	CLA	C4B-NB	-3.10	1.34	1.37
24	c	909	CLA	C1B-C2B	3.09	1.50	1.43
27	a	402	SQD	C6-S	-3.08	1.66	1.77
24	A	405	CLA	C1B-NB	-3.08	1.34	1.37
24	A	406	CLA	CHB-C1B	3.08	1.46	1.39
24	a	407	CLA	C4B-NB	-3.07	1.34	1.37
38	e	102	HEM	C1B-NB	-3.07	1.35	1.40
24	C	505	CLA	C1B-NB	-3.07	1.34	1.37
24	B	602	CLA	C3B-C4B	3.07	1.49	1.42
24	b	617	CLA	C4B-NB	-3.06	1.34	1.37
24	C	507	CLA	C1B-NB	-3.05	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C1B-C2B	3.05	1.50	1.43
24	c	907	CLA	C4B-NB	-3.05	1.34	1.37
24	B	608	CLA	C4C-C3C	3.05	1.50	1.45
24	b	616	CLA	C1B-NB	-3.05	1.34	1.37
24	b	608	CLA	C1C-C2C	3.04	1.50	1.44
24	D	402	CLA	C1B-C2B	3.04	1.50	1.43
24	d	403	CLA	C1B-NB	-3.04	1.34	1.37
24	B	608	CLA	C1B-NB	-3.04	1.34	1.37
24	a	409	CLA	C1B-C2B	3.03	1.50	1.43
24	b	614	CLA	C1B-NB	-3.03	1.34	1.37
24	c	906	CLA	C4C-C3C	3.02	1.50	1.45
24	A	410	CLA	C1B-NB	-3.02	1.34	1.37
24	b	610	CLA	C1C-C2C	3.02	1.50	1.44
24	A	406	CLA	OBD-CAD	3.01	1.27	1.22
40	V	201	HEC	C4B-NB	-3.01	1.35	1.40
24	b	610	CLA	C1B-C2B	3.01	1.50	1.43
24	b	612	CLA	C3B-C4B	3.00	1.49	1.42
24	c	903	CLA	C1B-NB	-3.00	1.34	1.37
24	B	605	CLA	OBD-CAD	2.99	1.27	1.22
24	C	503	CLA	C1B-NB	-2.98	1.34	1.37
24	b	615	CLA	C1B-NB	-2.98	1.34	1.37
24	b	606	CLA	C1B-C2B	2.98	1.50	1.43
35	c	922	HTG	C1'-S1	-2.98	1.77	1.81
24	B	604	CLA	C1B-NB	-2.97	1.34	1.37
24	B	614	CLA	C4D-CHA	2.97	1.48	1.38
24	B	611	CLA	C4D-CHA	2.96	1.48	1.38
24	c	910	CLA	C4B-NB	-2.96	1.34	1.37
24	C	513	CLA	C1B-NB	-2.96	1.34	1.37
24	C	510	CLA	C4C-C3C	2.96	1.50	1.45
24	b	612	CLA	C1B-NB	-2.95	1.34	1.37
24	b	619	CLA	C4D-CHA	2.95	1.48	1.38
24	C	507	CLA	C1B-C2B	2.94	1.50	1.43
24	B	610	CLA	C3B-C4B	2.94	1.49	1.42
24	b	609	CLA	C3B-C4B	2.94	1.49	1.42
24	B	606	CLA	C1B-C2B	2.94	1.50	1.43
27	f	102	SQD	C6-S	-2.94	1.66	1.77
24	C	508	CLA	C1B-C2B	2.94	1.50	1.43
24	d	403	CLA	C1B-C2B	2.94	1.50	1.43
24	c	906	CLA	C1B-NB	-2.93	1.34	1.37
24	b	613	CLA	C1C-C2C	2.93	1.50	1.44
24	b	618	CLA	C1B-C2B	2.93	1.50	1.43
24	C	505	CLA	C3B-C4B	2.93	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	C3B-C4B	2.92	1.49	1.42
24	C	514	CLA	C1B-NB	-2.92	1.34	1.37
24	b	619	CLA	C4B-NB	-2.92	1.34	1.37
27	A	416	SQD	C6-S	-2.92	1.66	1.77
24	C	509	CLA	C4C-C3C	2.92	1.50	1.45
24	c	902	CLA	C4B-NB	-2.92	1.34	1.37
24	b	609	CLA	C1C-C2C	2.91	1.50	1.44
24	c	908	CLA	C4D-CHA	2.91	1.48	1.38
24	C	502	CLA	C1B-NB	-2.91	1.34	1.37
24	c	908	CLA	C1B-C2B	2.90	1.50	1.43
25	a	420	PHO	C3A-C2A	-2.90	1.52	1.54
24	A	410	CLA	C4B-NB	-2.90	1.34	1.37
24	B	604	CLA	C3B-C4B	2.90	1.49	1.42
24	C	504	CLA	C1B-NB	-2.90	1.34	1.37
24	A	410	CLA	C1B-C2B	2.89	1.50	1.43
24	C	513	CLA	C1C-C2C	2.89	1.50	1.44
24	B	617	CLA	C1B-NB	-2.89	1.34	1.37
24	B	611	CLA	OBD-CAD	2.89	1.27	1.22
24	c	913	CLA	C1B-NB	-2.89	1.34	1.37
24	C	503	CLA	C1B-C2B	2.89	1.50	1.43
24	D	401	CLA	C4C-C3C	2.88	1.50	1.45
24	B	603	CLA	C4B-NB	-2.88	1.34	1.37
24	B	611	CLA	C4B-NB	-2.88	1.34	1.37
24	C	503	CLA	C4D-CHA	2.88	1.48	1.38
24	C	508	CLA	C1B-NB	-2.88	1.34	1.37
24	a	407	CLA	C4D-CHA	2.88	1.48	1.38
40	v	202	HEC	C4B-NB	-2.87	1.35	1.40
24	C	505	CLA	C4B-NB	-2.87	1.34	1.37
24	C	511	CLA	C3B-C4B	2.87	1.49	1.42
24	b	614	CLA	C3B-C4B	2.87	1.49	1.42
24	C	506	CLA	C4C-C3C	2.87	1.50	1.45
24	A	406	CLA	C4D-CHA	2.86	1.48	1.38
24	C	509	CLA	C1B-NB	-2.86	1.34	1.37
24	C	503	CLA	C3B-C4B	2.86	1.49	1.42
24	B	611	CLA	C3B-C4B	2.86	1.49	1.42
24	c	905	CLA	C1C-C2C	2.86	1.50	1.44
24	c	905	CLA	C1B-NB	-2.86	1.34	1.37
24	b	619	CLA	C1B-NB	-2.85	1.34	1.37
24	b	608	CLA	C4D-CHA	2.85	1.48	1.38
24	B	607	CLA	C4C-C3C	2.85	1.49	1.45
24	c	909	CLA	C1B-NB	-2.85	1.34	1.37
24	b	608	CLA	C1B-C2B	2.84	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C4B-NB	-2.84	1.34	1.37
24	b	616	CLA	C3B-C4B	2.84	1.49	1.42
24	c	906	CLA	C4B-NB	-2.84	1.34	1.37
24	B	603	CLA	C1B-NB	-2.84	1.34	1.37
24	C	505	CLA	C1B-C2B	2.84	1.49	1.43
24	B	602	CLA	C1B-NB	-2.84	1.34	1.37
24	A	410	CLA	C4D-CHA	2.83	1.48	1.38
24	A	407	CLA	C1B-NB	-2.82	1.34	1.37
24	c	909	CLA	C4C-C3C	2.82	1.49	1.45
24	B	616	CLA	OBD-CAD	2.82	1.27	1.22
24	b	609	CLA	C4D-CHA	2.82	1.48	1.38
24	B	615	CLA	C1B-C2B	2.82	1.49	1.43
24	B	612	CLA	C1B-C2B	2.82	1.49	1.43
24	C	511	CLA	C1C-C2C	2.82	1.50	1.44
24	c	904	CLA	C1B-NB	-2.82	1.34	1.37
24	c	914	CLA	C3B-C4B	2.81	1.49	1.42
24	B	613	CLA	C1C-C2C	2.81	1.50	1.44
24	b	612	CLA	C1B-C2B	2.81	1.49	1.43
24	C	510	CLA	C4D-CHA	2.81	1.48	1.38
24	C	505	CLA	C1C-C2C	2.80	1.50	1.44
24	C	503	CLA	C1C-C2C	2.80	1.50	1.44
24	B	615	CLA	C1B-NB	-2.80	1.34	1.37
24	B	608	CLA	C4D-CHA	2.80	1.48	1.38
24	C	504	CLA	C1C-C2C	2.80	1.50	1.44
24	C	510	CLA	C1B-C2B	2.80	1.49	1.43
24	B	610	CLA	C1B-C2B	2.80	1.49	1.43
24	c	911	CLA	C1B-C2B	2.80	1.49	1.43
24	a	406	CLA	C1B-C2B	2.79	1.49	1.43
24	b	620	CLA	C1B-NB	-2.79	1.34	1.37
24	A	410	CLA	C3B-C4B	2.79	1.49	1.42
24	B	615	CLA	C4D-CHA	2.79	1.48	1.38
24	B	603	CLA	C1C-C2C	2.79	1.50	1.44
24	c	904	CLA	C4C-C3C	2.79	1.49	1.45
24	b	606	CLA	C1B-NB	-2.79	1.34	1.37
24	d	402	CLA	C4B-NB	-2.79	1.34	1.37
24	B	606	CLA	C4C-C3C	2.78	1.49	1.45
24	a	406	CLA	C4C-C3C	2.78	1.49	1.45
24	A	405	CLA	C3B-C4B	2.78	1.49	1.42
24	B	606	CLA	C4B-NB	-2.78	1.34	1.37
24	c	905	CLA	C3B-C4B	2.77	1.49	1.42
24	a	407	CLA	C3D-C4D	-2.77	1.37	1.44
24	B	612	CLA	C4C-C3C	2.76	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	C4D-CHA	2.76	1.48	1.38
24	D	402	CLA	C4C-C3C	2.76	1.49	1.45
24	B	612	CLA	C1B-NB	-2.76	1.34	1.37
24	c	913	CLA	C1C-C2C	2.75	1.49	1.44
24	c	902	CLA	C4D-CHA	2.75	1.48	1.38
24	c	910	CLA	C4D-CHA	2.75	1.48	1.38
24	B	606	CLA	C3B-C4B	2.75	1.49	1.42
24	B	617	CLA	C1B-C2B	2.75	1.49	1.43
24	B	607	CLA	C1C-C2C	2.75	1.49	1.44
24	b	620	CLA	C1B-C2B	2.75	1.49	1.43
24	b	606	CLA	C4B-NB	-2.75	1.34	1.37
24	B	616	CLA	C1B-C2B	2.74	1.49	1.43
24	C	504	CLA	C3B-C4B	2.74	1.49	1.42
24	B	616	CLA	C3B-C4B	2.74	1.49	1.42
24	c	911	CLA	C3B-C4B	2.74	1.49	1.42
24	C	514	CLA	C1B-C2B	2.74	1.49	1.43
24	d	402	CLA	C4C-C3C	2.74	1.49	1.45
24	C	502	CLA	C1C-C2C	2.74	1.49	1.44
24	C	512	CLA	C1B-NB	-2.74	1.34	1.37
24	D	401	CLA	C3B-C4B	2.74	1.49	1.42
24	c	902	CLA	C1B-C2B	2.73	1.49	1.43
24	C	503	CLA	C4C-C3C	2.73	1.49	1.45
24	d	403	CLA	C4B-NB	-2.73	1.34	1.37
24	C	512	CLA	C4D-CHA	2.73	1.48	1.38
36	H	102	DGD	O5D-C1E	2.73	1.44	1.40
24	d	402	CLA	OBD-CAD	2.73	1.27	1.22
24	b	609	CLA	C1B-C2B	2.73	1.49	1.43
24	c	910	CLA	C1C-C2C	2.73	1.49	1.44
24	B	605	CLA	C1B-NB	-2.73	1.34	1.37
24	C	506	CLA	C4B-NB	-2.73	1.34	1.37
24	b	611	CLA	C1C-C2C	2.73	1.49	1.44
24	B	614	CLA	C1C-C2C	2.72	1.49	1.44
24	C	513	CLA	C3B-C4B	2.72	1.49	1.42
24	b	606	CLA	C3B-C4B	2.72	1.49	1.42
27	a	411	SQD	C6-S	-2.72	1.67	1.77
24	c	903	CLA	C3B-C4B	2.72	1.49	1.42
24	B	614	CLA	C4B-NB	-2.72	1.34	1.37
24	D	401	CLA	C4D-CHA	2.71	1.48	1.38
24	C	502	CLA	C1B-C2B	2.71	1.49	1.43
24	c	913	CLA	C1B-C2B	2.71	1.49	1.43
24	B	615	CLA	C1C-C2C	2.71	1.49	1.44
24	c	909	CLA	C4D-CHA	2.71	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	C1B-NB	-2.71	1.34	1.37
24	c	914	CLA	C1B-C2B	2.70	1.49	1.43
24	B	612	CLA	C4D-CHA	2.70	1.48	1.38
24	a	409	CLA	C4D-CHA	2.70	1.48	1.38
27	A	412	SQD	C6-S	-2.70	1.67	1.77
24	B	617	CLA	C4D-CHA	2.70	1.48	1.38
24	C	504	CLA	C4C-C3C	2.70	1.49	1.45
24	A	405	CLA	C4B-NB	-2.70	1.34	1.37
24	b	607	CLA	C4B-NB	-2.70	1.34	1.37
24	B	603	CLA	C3D-C4D	-2.69	1.38	1.44
24	c	905	CLA	C1B-C2B	2.69	1.49	1.43
24	A	405	CLA	C1B-C2B	2.69	1.49	1.43
24	b	617	CLA	C4D-CHA	2.68	1.47	1.38
24	b	608	CLA	C3B-C4B	2.68	1.49	1.42
24	b	618	CLA	C3B-C4B	2.68	1.49	1.42
24	C	502	CLA	C4D-CHA	2.68	1.47	1.38
24	C	509	CLA	C4B-NB	-2.68	1.34	1.37
24	b	615	CLA	C3B-C4B	2.68	1.49	1.42
24	c	907	CLA	C4D-CHA	2.68	1.47	1.38
34	Z	101	LMG	O8-C28	2.67	1.46	1.33
24	C	510	CLA	C1C-C2C	2.67	1.49	1.44
24	b	614	CLA	C1B-C2B	2.67	1.49	1.43
24	C	502	CLA	C4B-NB	-2.67	1.34	1.37
24	D	401	CLA	C1B-NB	-2.67	1.34	1.37
24	A	407	CLA	C1B-C2B	2.67	1.49	1.43
24	b	610	CLA	C4B-NB	-2.67	1.34	1.37
24	c	911	CLA	C4B-NB	-2.66	1.34	1.37
24	c	906	CLA	C4D-CHA	2.66	1.47	1.38
24	C	507	CLA	C4C-C3C	2.66	1.49	1.45
24	C	511	CLA	C1B-C2B	2.66	1.49	1.43
24	B	602	CLA	C4D-CHA	2.66	1.47	1.38
24	B	603	CLA	C4D-CHA	2.66	1.47	1.38
24	b	616	CLA	C1C-C2C	2.66	1.49	1.44
24	C	506	CLA	C1B-C2B	2.65	1.49	1.43
24	C	511	CLA	C4D-CHA	2.65	1.47	1.38
24	b	617	CLA	C1C-C2C	2.65	1.49	1.44
24	B	614	CLA	C4C-C3C	2.65	1.49	1.45
35	c	923	HTG	C1-S1	-2.65	1.76	1.80
24	c	914	CLA	C1C-C2C	2.65	1.49	1.44
31	A	419	PL9	C6-C5	2.65	1.49	1.35
24	a	407	CLA	C1B-NB	-2.65	1.34	1.37
31	a	417	PL9	C6-C5	2.65	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	C3B-C4B	2.64	1.49	1.42
24	B	609	CLA	C1C-C2C	2.64	1.49	1.44
24	b	606	CLA	C1C-C2C	2.64	1.49	1.44
24	b	617	CLA	C1B-C2B	2.64	1.49	1.43
24	c	912	CLA	C1B-C2B	2.64	1.49	1.43
40	V	201	HEC	C4B-C3B	2.64	1.49	1.45
24	B	608	CLA	C3B-C4B	2.64	1.48	1.42
24	B	613	CLA	C1B-C2B	2.63	1.49	1.43
24	b	610	CLA	C4D-CHA	2.63	1.47	1.38
24	c	911	CLA	C4D-CHA	2.63	1.47	1.38
24	c	910	CLA	C1B-C2B	2.63	1.49	1.43
24	B	605	CLA	C1C-C2C	2.63	1.49	1.44
24	b	609	CLA	C3D-C4D	-2.62	1.38	1.44
24	c	909	CLA	C3B-C4B	2.62	1.48	1.42
24	d	402	CLA	C4D-CHA	2.62	1.47	1.38
24	c	910	CLA	C3B-C4B	2.62	1.48	1.42
24	c	911	CLA	C1C-C2C	2.62	1.49	1.44
24	B	614	CLA	C3B-C2B	2.62	1.50	1.41
24	A	407	CLA	C4D-CHA	2.62	1.47	1.38
24	d	401	CLA	C4B-NB	-2.62	1.34	1.37
24	b	607	CLA	C4D-CHA	2.62	1.47	1.38
24	B	611	CLA	C4C-C3C	2.62	1.49	1.45
24	B	604	CLA	C1C-C2C	2.61	1.49	1.44
24	D	401	CLA	C3D-C4D	-2.61	1.38	1.44
24	b	611	CLA	C4D-CHA	2.61	1.47	1.38
24	c	913	CLA	C4D-CHA	2.61	1.47	1.38
24	B	609	CLA	C4C-C3C	2.61	1.49	1.45
31	d	405	PL9	C6-C5	2.61	1.48	1.35
24	c	904	CLA	C4B-NB	-2.61	1.34	1.37
31	D	404	PL9	C6-C5	2.61	1.48	1.35
24	b	605	CLA	C4D-CHA	2.61	1.47	1.38
35	B	633	HTG	C1-S1	-2.61	1.76	1.80
24	D	402	CLA	C1C-C2C	2.61	1.49	1.44
24	c	906	CLA	C1C-C2C	2.61	1.49	1.44
24	B	609	CLA	C4D-CHA	2.60	1.47	1.38
24	B	613	CLA	C4B-NB	-2.60	1.34	1.37
24	c	903	CLA	C4B-NB	-2.60	1.34	1.37
24	C	513	CLA	C1B-C2B	2.60	1.49	1.43
24	B	607	CLA	C4D-CHA	2.60	1.47	1.38
27	B	621	SQD	C6-S	-2.60	1.67	1.77
24	c	905	CLA	C4D-CHA	2.60	1.47	1.38
24	b	607	CLA	C3D-C4D	-2.59	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	904	CLA	C1C-C2C	2.59	1.49	1.44
24	C	508	CLA	C4D-CHA	2.58	1.47	1.38
24	c	902	CLA	C1C-C2C	2.58	1.49	1.44
24	B	606	CLA	C3D-C4D	-2.58	1.38	1.44
24	C	509	CLA	C1C-C2C	2.58	1.49	1.44
24	b	618	CLA	C1C-C2C	2.58	1.49	1.44
24	b	612	CLA	C4B-NB	-2.58	1.34	1.37
24	c	904	CLA	C4D-CHA	2.58	1.47	1.38
24	b	619	CLA	C4C-C3C	2.57	1.49	1.45
24	d	403	CLA	C4D-CHA	2.57	1.47	1.38
24	b	614	CLA	C4B-NB	-2.57	1.34	1.37
24	A	405	CLA	C4D-CHA	2.57	1.47	1.38
24	b	614	CLA	C4D-CHA	2.57	1.47	1.38
27	L	102	SQD	C6-S	-2.57	1.67	1.77
24	C	509	CLA	C4D-CHA	2.56	1.47	1.38
25	A	409	PHO	C3A-C2A	-2.56	1.52	1.54
24	b	607	CLA	C4C-C3C	2.56	1.49	1.45
24	c	908	CLA	C1B-NB	-2.56	1.34	1.37
24	b	616	CLA	C1B-C2B	2.56	1.49	1.43
24	B	614	CLA	C1B-NB	-2.56	1.34	1.37
24	a	409	CLA	C3B-C4B	2.56	1.48	1.42
24	B	604	CLA	C1B-C2B	2.56	1.49	1.43
24	C	511	CLA	C4B-NB	-2.55	1.34	1.37
24	b	616	CLA	C4D-CHA	2.55	1.47	1.38
24	b	611	CLA	C3B-C4B	2.55	1.48	1.42
24	c	903	CLA	C1B-C2B	2.55	1.49	1.43
24	c	909	CLA	C4B-NB	-2.55	1.34	1.37
24	B	603	CLA	C4C-C3C	2.55	1.49	1.45
24	B	610	CLA	C4D-CHA	2.55	1.47	1.38
24	B	605	CLA	C4D-CHA	2.55	1.47	1.38
24	B	616	CLA	C4D-CHA	2.54	1.47	1.38
24	C	506	CLA	C1C-C2C	2.54	1.49	1.44
24	C	506	CLA	C3D-C4D	-2.54	1.38	1.44
24	a	406	CLA	C1B-NB	-2.54	1.34	1.37
24	A	410	CLA	C1C-C2C	2.54	1.49	1.44
24	b	607	CLA	C1C-C2C	2.54	1.49	1.44
36	h	102	DGD	O5D-C1E	2.53	1.44	1.40
24	b	620	CLA	C4D-CHA	2.53	1.47	1.38
24	b	609	CLA	C1B-NB	-2.53	1.34	1.37
24	C	511	CLA	C4C-C3C	2.53	1.49	1.45
24	b	612	CLA	C4C-C3C	2.53	1.49	1.45
24	d	402	CLA	C1B-C2B	2.53	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C4B-NB	-2.53	1.34	1.37
24	C	502	CLA	C4C-C3C	2.52	1.49	1.45
24	B	613	CLA	C3B-C4B	2.52	1.48	1.42
24	c	913	CLA	C4B-NB	-2.52	1.34	1.37
24	D	402	CLA	C4D-CHA	2.52	1.47	1.38
24	B	605	CLA	C1B-C2B	2.52	1.49	1.43
24	b	620	CLA	C3B-C2B	2.52	1.49	1.41
24	B	602	CLA	C1B-C2B	2.52	1.49	1.43
24	b	615	CLA	C4B-NB	-2.52	1.34	1.37
24	B	608	CLA	C1B-C2B	2.52	1.49	1.43
24	a	406	CLA	C3B-C2B	2.52	1.49	1.41
24	C	509	CLA	C3B-C4B	2.52	1.48	1.42
24	B	617	CLA	C3B-C2B	2.51	1.49	1.41
24	a	406	CLA	C4B-NB	-2.51	1.34	1.37
24	c	904	CLA	C3B-C4B	2.51	1.48	1.42
24	B	607	CLA	C1B-C2B	2.51	1.49	1.43
24	b	620	CLA	C3B-C4B	2.51	1.48	1.42
24	c	907	CLA	C1B-C2B	2.51	1.49	1.43
24	C	503	CLA	C3D-C4D	-2.51	1.38	1.44
24	c	904	CLA	C3D-C4D	-2.51	1.38	1.44
24	b	606	CLA	C4D-CHA	2.50	1.47	1.38
24	C	507	CLA	C4D-CHA	2.50	1.47	1.38
24	c	906	CLA	C3D-C4D	-2.50	1.38	1.44
24	B	606	CLA	C1C-C2C	2.50	1.49	1.44
24	c	906	CLA	C3B-C4B	2.50	1.48	1.42
24	b	615	CLA	C4C-C3C	2.50	1.49	1.45
24	b	611	CLA	C3D-C4D	-2.50	1.38	1.44
24	c	914	CLA	C4B-NB	-2.50	1.34	1.37
24	b	616	CLA	C3D-C4D	-2.50	1.38	1.44
24	c	903	CLA	C1C-C2C	2.50	1.49	1.44
24	B	610	CLA	C1C-C2C	2.50	1.49	1.44
24	C	509	CLA	C1B-C2B	2.49	1.49	1.43
24	C	505	CLA	C4D-CHA	2.49	1.47	1.38
24	B	610	CLA	C1B-NB	-2.49	1.34	1.37
24	b	614	CLA	C4C-C3C	2.49	1.49	1.45
24	c	902	CLA	C4C-C3C	2.49	1.49	1.45
24	C	510	CLA	C3D-C4D	-2.49	1.38	1.44
35	d	412	HTG	C1-S1	-2.49	1.76	1.80
24	c	903	CLA	C4D-CHA	2.49	1.47	1.38
24	c	908	CLA	C4C-C3C	2.49	1.49	1.45
24	c	914	CLA	C4D-CHA	2.48	1.47	1.38
24	b	607	CLA	C1B-C2B	2.48	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	C4D-CHA	2.48	1.47	1.38
24	C	512	CLA	C4C-C3C	2.48	1.49	1.45
24	C	512	CLA	C3B-C4B	2.48	1.48	1.42
24	c	910	CLA	C3B-C2B	2.48	1.49	1.41
24	C	502	CLA	C3B-C4B	2.48	1.48	1.42
24	d	402	CLA	C1C-C2C	2.48	1.49	1.44
24	c	913	CLA	C4C-C3C	2.48	1.49	1.45
25	A	408	PHO	CHA-CBD	-2.48	1.48	1.51
27	F	101	SQD	C6-S	-2.48	1.68	1.77
24	A	407	CLA	C3D-C4D	-2.48	1.38	1.44
24	b	618	CLA	C4B-NB	-2.47	1.34	1.37
24	b	618	CLA	C4D-CHA	2.47	1.47	1.38
24	a	406	CLA	C4D-CHA	2.47	1.47	1.38
24	C	508	CLA	C3B-C4B	2.47	1.48	1.42
24	C	505	CLA	C4C-C3C	2.47	1.49	1.45
24	C	514	CLA	C3B-C4B	2.47	1.48	1.42
24	C	513	CLA	C4D-CHA	2.47	1.47	1.38
24	B	613	CLA	C4D-CHA	2.47	1.47	1.38
24	B	604	CLA	C4D-CHA	2.47	1.47	1.38
24	B	612	CLA	C3B-C4B	2.46	1.48	1.42
24	D	402	CLA	C1B-NB	-2.46	1.34	1.37
24	c	908	CLA	C1C-C2C	2.46	1.49	1.44
24	B	616	CLA	C3D-C4D	-2.46	1.38	1.44
24	d	403	CLA	C4C-C3C	2.46	1.49	1.45
24	C	504	CLA	C4D-CHA	2.46	1.47	1.38
24	B	604	CLA	C3B-C2B	2.46	1.49	1.41
24	b	614	CLA	C1C-C2C	2.46	1.49	1.44
24	b	617	CLA	C4C-C3C	2.46	1.49	1.45
24	b	615	CLA	C3D-C4D	-2.46	1.38	1.44
24	C	508	CLA	C1C-C2C	2.46	1.49	1.44
24	C	510	CLA	C3B-C2B	2.45	1.49	1.41
24	C	510	CLA	C3B-C4B	2.45	1.48	1.42
24	B	612	CLA	C4B-NB	-2.45	1.34	1.37
38	e	102	HEM	C1C-C2C	-2.45	1.40	1.45
24	C	514	CLA	C3B-C2B	2.45	1.49	1.41
24	C	506	CLA	C3B-C4B	2.44	1.48	1.42
24	b	613	CLA	C4D-CHA	2.44	1.47	1.38
24	c	903	CLA	C3D-C4D	-2.44	1.38	1.44
24	C	506	CLA	C4D-CHA	2.44	1.47	1.38
24	a	407	CLA	C1B-C2B	2.44	1.49	1.43
24	B	604	CLA	C3D-C4D	-2.44	1.38	1.44
24	c	905	CLA	C4C-C3C	2.44	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	C4D-CHA	2.43	1.47	1.38
24	b	612	CLA	C1C-C2C	2.43	1.49	1.44
24	C	511	CLA	C3B-C2B	2.43	1.49	1.41
24	b	608	CLA	C3B-C2B	2.43	1.49	1.41
24	c	904	CLA	C1B-C2B	2.42	1.49	1.43
24	b	608	CLA	C1B-NB	-2.42	1.34	1.37
24	c	902	CLA	C3D-C4D	-2.42	1.38	1.44
24	B	613	CLA	C3B-C2B	2.42	1.49	1.41
24	c	914	CLA	C4C-C3C	2.42	1.49	1.45
29	a	401	LMT	O1'-C1'	2.42	1.44	1.40
24	b	606	CLA	C4C-C3C	2.42	1.49	1.45
24	c	911	CLA	C4C-C3C	2.42	1.49	1.45
24	b	608	CLA	C3D-C4D	-2.42	1.38	1.44
24	b	605	CLA	C1B-C2B	2.41	1.48	1.43
24	B	603	CLA	C3B-C4B	2.41	1.48	1.42
24	B	605	CLA	C3B-C2B	2.41	1.49	1.41
24	a	407	CLA	C1C-C2C	2.41	1.49	1.44
25	a	408	PHO	C1D-ND	-2.40	1.34	1.38
24	A	406	CLA	C3B-C4B	2.40	1.48	1.42
24	B	617	CLA	C3D-C4D	-2.40	1.38	1.44
24	D	401	CLA	C1C-C2C	2.39	1.49	1.44
24	C	513	CLA	C4B-NB	-2.39	1.34	1.37
24	A	405	CLA	C4C-C3C	2.39	1.49	1.45
36	D	405	DGD	O3G-C1D	2.39	1.44	1.40
24	A	406	CLA	C1B-C2B	2.39	1.48	1.43
24	c	912	CLA	C4D-CHA	2.39	1.46	1.38
24	C	513	CLA	C3D-C4D	-2.39	1.38	1.44
24	B	611	CLA	C3D-C4D	-2.39	1.38	1.44
24	B	605	CLA	C3B-C4B	2.38	1.48	1.42
24	C	514	CLA	C3D-C4D	-2.38	1.38	1.44
24	b	612	CLA	C3D-C4D	-2.38	1.38	1.44
24	B	603	CLA	C1B-C2B	2.38	1.48	1.43
24	d	403	CLA	C3D-C4D	-2.38	1.38	1.44
24	C	504	CLA	C1B-C2B	2.38	1.48	1.43
24	b	605	CLA	C4B-NB	-2.38	1.34	1.37
24	b	618	CLA	C4C-C3C	2.37	1.49	1.45
24	c	909	CLA	C1C-C2C	2.37	1.49	1.44
24	b	619	CLA	C3B-C2B	2.37	1.49	1.41
24	B	616	CLA	C4B-NB	-2.37	1.34	1.37
24	B	605	CLA	C4B-NB	-2.37	1.34	1.37
24	c	909	CLA	C3B-C2B	2.37	1.49	1.41
24	c	912	CLA	C1D-C2D	2.37	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C3B-C2B	2.37	1.49	1.41
24	b	618	CLA	C3D-C4D	-2.37	1.38	1.44
24	c	911	CLA	C3D-C4D	-2.36	1.38	1.44
24	c	913	CLA	C3D-C4D	-2.36	1.38	1.44
24	C	512	CLA	C1C-C2C	2.36	1.49	1.44
24	C	512	CLA	C1C-NC	-2.36	1.34	1.37
24	c	912	CLA	C3B-C4B	2.36	1.48	1.42
24	b	615	CLA	C1C-C2C	2.36	1.49	1.44
24	B	609	CLA	C3B-C2B	2.36	1.49	1.41
24	d	403	CLA	C3B-C2B	2.36	1.49	1.41
24	c	905	CLA	C3D-C4D	-2.35	1.38	1.44
24	B	615	CLA	C3B-C4B	2.35	1.48	1.42
24	c	907	CLA	C3D-C4D	-2.35	1.38	1.44
24	a	409	CLA	C1C-C2C	2.35	1.49	1.44
24	b	620	CLA	C4C-C3C	2.34	1.49	1.45
24	d	401	CLA	C4D-CHA	2.34	1.46	1.38
24	b	614	CLA	C3B-C2B	2.34	1.49	1.41
40	v	202	HEC	C4B-C3B	2.34	1.49	1.45
24	b	619	CLA	C3B-C4B	2.34	1.48	1.42
24	b	617	CLA	C3B-C2B	2.34	1.49	1.41
24	B	615	CLA	C3D-C4D	-2.34	1.38	1.44
24	A	405	CLA	C1C-C2C	2.33	1.49	1.44
24	B	607	CLA	C3B-C2B	2.33	1.49	1.41
24	C	508	CLA	C3D-C4D	-2.32	1.38	1.44
24	B	614	CLA	C1B-C2B	2.32	1.48	1.43
24	b	605	CLA	C1C-C2C	2.32	1.49	1.44
24	C	507	CLA	C3B-C4B	2.32	1.48	1.42
24	A	407	CLA	C1C-C2C	2.32	1.49	1.44
24	B	609	CLA	C1B-C2B	2.32	1.48	1.43
27	B	621	SQD	O6-C1	2.32	1.44	1.40
24	b	617	CLA	C3D-C4D	-2.31	1.39	1.44
24	B	616	CLA	C1C-C2C	2.31	1.49	1.44
24	A	407	CLA	C4B-NB	-2.31	1.34	1.37
38	E	103	HEM	C1C-C2C	-2.31	1.40	1.45
35	V	202	HTG	C1-S1	-2.30	1.77	1.80
24	a	407	CLA	C4C-C3C	2.30	1.49	1.45
24	A	406	CLA	C3D-C4D	-2.30	1.39	1.44
38	e	102	HEM	C1D-ND	-2.30	1.34	1.38
24	b	615	CLA	C3B-C2B	2.30	1.49	1.41
24	C	511	CLA	C3D-C4D	-2.30	1.39	1.44
24	c	910	CLA	C4C-C3C	2.30	1.49	1.45
24	c	902	CLA	C3B-C2B	2.30	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	CLA	C4C-C3C	2.29	1.49	1.45
24	B	612	CLA	C3B-C2B	2.29	1.48	1.41
40	V	201	HEC	C1B-NB	-2.29	1.34	1.38
24	A	406	CLA	C3B-C2B	2.29	1.48	1.41
24	B	617	CLA	C3B-C4B	2.29	1.48	1.42
24	a	406	CLA	C1C-C2C	2.28	1.49	1.44
24	C	504	CLA	C3D-C4D	-2.28	1.39	1.44
24	C	509	CLA	C3B-C2B	2.28	1.48	1.41
24	B	606	CLA	C4D-CHA	2.28	1.46	1.38
24	c	907	CLA	C4C-C3C	2.28	1.49	1.45
24	a	406	CLA	C3B-C4B	2.28	1.48	1.42
24	C	507	CLA	C1C-C2C	2.27	1.49	1.44
24	c	912	CLA	C3B-C2B	2.27	1.48	1.41
24	C	507	CLA	C3D-C4D	-2.27	1.39	1.44
24	d	401	CLA	C1D-C2D	2.27	1.49	1.45
24	b	606	CLA	C3D-C4D	-2.27	1.39	1.44
24	B	614	CLA	C3B-C4B	2.27	1.48	1.42
24	B	609	CLA	C3D-C4D	-2.27	1.39	1.44
24	c	909	CLA	C3D-C4D	-2.26	1.39	1.44
24	b	610	CLA	C3D-C4D	-2.26	1.39	1.44
24	c	914	CLA	C1D-C2D	2.26	1.49	1.45
35	b	602	HTG	C1-S1	-2.26	1.77	1.80
24	c	907	CLA	C3B-C4B	2.26	1.48	1.42
24	b	606	CLA	C3B-C2B	2.26	1.48	1.41
24	b	613	CLA	C3D-C4D	-2.25	1.39	1.44
35	D	411	HTG	C1-S1	-2.25	1.77	1.80
24	B	607	CLA	C3D-C4D	-2.25	1.39	1.44
24	b	609	CLA	C4B-NB	-2.25	1.35	1.37
24	d	402	CLA	C3B-C4B	2.25	1.48	1.42
25	A	409	PHO	C1D-ND	-2.25	1.34	1.38
29	A	417	LMT	O1'-C1'	2.24	1.44	1.40
24	b	613	CLA	C1B-C2B	2.24	1.48	1.43
24	B	609	CLA	C1C-NC	-2.24	1.34	1.37
24	b	620	CLA	C1C-C2C	2.24	1.48	1.44
24	B	613	CLA	C3D-C4D	-2.24	1.39	1.44
24	c	914	CLA	C3D-C4D	-2.24	1.39	1.44
24	C	508	CLA	C4C-C3C	2.24	1.48	1.45
24	B	607	CLA	C3B-C4B	2.24	1.48	1.42
24	c	910	CLA	C3D-C4D	-2.23	1.39	1.44
24	B	617	CLA	C1C-NC	-2.23	1.34	1.37
24	b	607	CLA	C3B-C2B	2.23	1.48	1.41
24	B	605	CLA	C3D-C4D	-2.23	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C3B-C2B	2.23	1.48	1.41
24	C	514	CLA	C1C-C2C	2.23	1.48	1.44
35	b	603	HTG	C1-S1	-2.22	1.77	1.80
24	c	908	CLA	C3B-C4B	2.22	1.48	1.42
24	B	612	CLA	C3D-C4D	-2.22	1.39	1.44
24	B	602	CLA	C1C-C2C	2.22	1.48	1.44
24	C	512	CLA	C3B-C2B	2.21	1.48	1.41
25	A	409	PHO	CBD-CGD	-2.21	1.49	1.52
24	B	602	CLA	C4C-C3C	2.21	1.48	1.45
24	B	603	CLA	C3B-C2B	2.21	1.48	1.41
24	B	611	CLA	C3B-C2B	2.21	1.48	1.41
40	V	201	HEC	C4A-C3A	-2.21	1.41	1.45
24	b	611	CLA	C4C-C3C	2.21	1.48	1.45
24	C	512	CLA	C3D-C4D	-2.21	1.39	1.44
24	c	907	CLA	C3B-C2B	2.20	1.48	1.41
24	B	608	CLA	C3B-C2B	2.20	1.48	1.41
24	A	410	CLA	C3B-C2B	2.20	1.48	1.41
25	a	408	PHO	C4B-NB	-2.20	1.34	1.38
24	C	504	CLA	C3B-C2B	2.20	1.48	1.41
24	b	613	CLA	C4B-NB	-2.20	1.35	1.37
24	c	907	CLA	C1C-C2C	2.20	1.48	1.44
35	C	523	HTG	C1-S1	-2.20	1.77	1.80
24	b	616	CLA	C4C-C3C	2.20	1.48	1.45
24	B	611	CLA	C1C-NC	-2.19	1.34	1.37
24	b	612	CLA	C3B-C2B	2.18	1.48	1.41
24	c	912	CLA	C3D-C4D	-2.18	1.39	1.44
24	C	502	CLA	C3D-C4D	-2.18	1.39	1.44
38	E	103	HEM	C1D-ND	-2.18	1.34	1.38
24	b	614	CLA	C3D-C4D	-2.18	1.39	1.44
24	d	401	CLA	C3D-C4D	-2.18	1.39	1.44
24	b	617	CLA	C1C-NC	-2.18	1.34	1.37
24	C	513	CLA	C3B-C2B	2.18	1.48	1.41
24	b	613	CLA	C4C-C3C	2.18	1.48	1.45
24	A	407	CLA	C4C-C3C	2.17	1.48	1.45
24	b	611	CLA	C3B-C2B	2.17	1.48	1.41
24	D	401	CLA	C3B-C2B	2.17	1.48	1.41
24	a	409	CLA	C3D-C4D	-2.17	1.39	1.44
24	d	402	CLA	C3D-C4D	-2.17	1.39	1.44
24	c	911	CLA	C3B-C2B	2.16	1.48	1.41
24	B	616	CLA	C4C-C3C	2.16	1.48	1.45
24	d	403	CLA	C1C-C2C	2.16	1.48	1.44
35	C	524	HTG	C1-S1	-2.16	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	C3B-C4B	2.15	1.47	1.42
24	b	617	CLA	C3B-C4B	2.15	1.47	1.42
31	a	417	PL9	C2-C3	2.15	1.40	1.34
26	a	410	BCR	C12-C13	2.14	1.50	1.45
24	C	505	CLA	C3B-C2B	2.14	1.48	1.41
24	c	912	CLA	C1C-C2C	2.14	1.48	1.44
24	B	608	CLA	C1C-C2C	2.14	1.48	1.44
38	e	102	HEM	C3C-C4C	-2.14	1.42	1.46
24	C	509	CLA	C3D-C4D	-2.14	1.39	1.44
35	b	627	HTG	C1-S1	-2.14	1.77	1.80
24	b	610	CLA	C3B-C2B	2.14	1.48	1.41
24	d	402	CLA	C3B-C2B	2.13	1.48	1.41
24	c	905	CLA	C3B-C2B	2.13	1.48	1.41
25	A	409	PHO	C4B-NB	-2.13	1.34	1.38
24	A	405	CLA	C3B-C2B	2.12	1.48	1.41
24	c	908	CLA	C3B-C2B	2.12	1.48	1.41
24	c	912	CLA	C4C-C3C	2.12	1.48	1.45
24	B	612	CLA	C1C-C2C	2.12	1.48	1.44
24	b	605	CLA	C3B-C2B	2.12	1.48	1.41
36	C	517	DGD	O5D-C1E	2.12	1.43	1.40
31	D	404	PL9	C2-C3	2.11	1.40	1.34
24	a	406	CLA	C3D-C4D	-2.11	1.39	1.44
24	c	914	CLA	C3B-C2B	2.11	1.48	1.41
24	b	605	CLA	C3D-C4D	-2.10	1.39	1.44
24	B	615	CLA	C1C-NC	-2.10	1.34	1.37
24	B	608	CLA	C3D-C4D	-2.10	1.39	1.44
24	C	505	CLA	C3D-C4D	-2.10	1.39	1.44
24	c	904	CLA	C3B-C2B	2.09	1.48	1.41
24	B	616	CLA	C1C-NC	-2.09	1.34	1.37
24	B	602	CLA	C3D-C4D	-2.09	1.39	1.44
38	e	102	HEM	C3B-C4B	2.09	1.49	1.44
24	b	609	CLA	C3B-C2B	2.09	1.48	1.41
24	a	409	CLA	C1C-NC	-2.09	1.34	1.37
24	d	401	CLA	C4C-C3C	2.08	1.48	1.45
24	c	908	CLA	C3D-C4D	-2.08	1.39	1.44
24	C	506	CLA	C3B-C2B	2.08	1.48	1.41
34	b	624	LMG	O7-C8	-2.08	1.41	1.46
35	B	634	HTG	C1-S1	-2.08	1.77	1.80
24	C	503	CLA	C3B-C2B	2.08	1.48	1.41
24	D	402	CLA	C4B-NB	-2.07	1.35	1.37
24	b	606	CLA	C1C-NC	-2.07	1.34	1.37
24	B	613	CLA	C4C-C3C	2.07	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C3B-C2B	2.07	1.48	1.41
25	a	420	PHO	C4B-NB	-2.07	1.34	1.38
24	a	407	CLA	C3B-C2B	2.07	1.48	1.41
24	b	608	CLA	C4B-NB	-2.07	1.35	1.37
24	D	402	CLA	C3D-C4D	-2.07	1.39	1.44
36	d	406	DGD	O5D-C1E	2.06	1.43	1.40
31	A	419	PL9	C2-C3	2.06	1.40	1.34
24	d	401	CLA	C3B-C4B	2.06	1.47	1.42
24	b	618	CLA	C3B-C2B	2.06	1.48	1.41
24	b	620	CLA	C1C-NC	-2.06	1.34	1.37
24	B	616	CLA	C3B-C2B	2.06	1.48	1.41
25	a	420	PHO	CHA-CBD	-2.05	1.49	1.51
24	b	611	CLA	C1A-CHA	2.05	1.51	1.43
24	B	610	CLA	C4C-C3C	2.04	1.48	1.45
24	b	620	CLA	C3D-C4D	-2.04	1.39	1.44
29	f	103	LMT	O1'-C1'	2.04	1.43	1.40
24	b	619	CLA	C3D-C4D	-2.03	1.39	1.44
31	d	405	PL9	C2-C3	2.03	1.40	1.34
36	C	519	DGD	O2G-C2G	-2.03	1.41	1.46
29	b	625	LMT	O1'-C1'	2.03	1.43	1.40
24	B	617	CLA	C1C-C2C	2.03	1.48	1.44
24	d	402	CLA	CHB-C4A	-2.02	1.32	1.37
24	d	401	CLA	C3B-C2B	2.02	1.48	1.41
40	V	201	HEC	C4D-C3D	2.02	1.48	1.45
24	B	610	CLA	C3D-C4D	-2.02	1.39	1.44
24	B	602	CLA	C1C-NC	-2.01	1.34	1.37
24	C	512	CLA	C1D-C2D	2.01	1.49	1.45
24	A	406	CLA	C1C-C2C	2.01	1.48	1.44
24	B	604	CLA	C4C-C3C	2.01	1.48	1.45
34	c	919	LMG	O1-C1	2.01	1.43	1.40
24	c	903	CLA	C4C-C3C	2.00	1.48	1.45
24	B	606	CLA	C3B-C2B	2.00	1.48	1.41
24	c	913	CLA	C3B-C2B	2.00	1.48	1.41
24	B	615	CLA	C3B-C2B	2.00	1.48	1.41

All (2741) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	408	PHO	C2D-C1D-ND	12.74	118.32	109.53
25	A	408	PHO	C2D-C1D-ND	11.97	117.79	109.53
25	A	409	PHO	C2D-C1D-ND	11.44	117.42	109.53
25	a	420	PHO	C2D-C1D-ND	11.35	117.36	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	C1D-ND-C4D	-10.00	99.23	106.33
24	C	505	CLA	C1D-ND-C4D	-9.97	99.26	106.33
24	B	615	CLA	C1D-ND-C4D	-9.86	99.33	106.33
24	c	914	CLA	C1D-ND-C4D	-9.84	99.34	106.33
24	C	504	CLA	C1D-ND-C4D	-9.73	99.43	106.33
24	A	406	CLA	C1D-ND-C4D	-9.59	99.52	106.33
24	b	609	CLA	C1D-ND-C4D	-9.58	99.53	106.33
24	b	618	CLA	C1D-ND-C4D	-9.57	99.54	106.33
24	B	603	CLA	C1D-ND-C4D	-9.56	99.54	106.33
24	B	605	CLA	C1D-ND-C4D	-9.55	99.55	106.33
24	B	610	CLA	C1D-ND-C4D	-9.52	99.57	106.33
24	A	407	CLA	C1D-ND-C4D	-9.51	99.58	106.33
24	c	913	CLA	C1D-ND-C4D	-9.48	99.60	106.33
24	b	611	CLA	C1D-ND-C4D	-9.42	99.64	106.33
24	C	514	CLA	C1D-ND-C4D	-9.41	99.65	106.33
24	B	602	CLA	C1D-ND-C4D	-9.38	99.67	106.33
24	D	402	CLA	C1D-ND-C4D	-9.36	99.68	106.33
24	d	402	CLA	C1D-ND-C4D	-9.36	99.69	106.33
24	A	406	CLA	C2D-C1D-ND	9.36	117.00	110.10
24	B	604	CLA	C1D-ND-C4D	-9.34	99.70	106.33
24	b	615	CLA	C1D-ND-C4D	-9.33	99.71	106.33
24	b	616	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	b	613	CLA	C1D-ND-C4D	-9.31	99.72	106.33
24	a	406	CLA	C1D-ND-C4D	-9.21	99.79	106.33
24	c	909	CLA	C1D-ND-C4D	-9.11	99.86	106.33
24	B	614	CLA	C1D-ND-C4D	-9.10	99.87	106.33
24	b	605	CLA	C1D-ND-C4D	-9.09	99.88	106.33
24	C	513	CLA	C1D-ND-C4D	-9.06	99.90	106.33
24	A	410	CLA	C1D-ND-C4D	-9.03	99.92	106.33
24	c	912	CLA	C1D-ND-C4D	-9.02	99.92	106.33
24	c	910	CLA	C1D-ND-C4D	-9.01	99.94	106.33
24	d	403	CLA	C1D-ND-C4D	-9.00	99.94	106.33
24	C	502	CLA	C1D-ND-C4D	-8.97	99.97	106.33
24	C	509	CLA	C1D-ND-C4D	-8.91	100.01	106.33
24	C	512	CLA	C1D-ND-C4D	-8.87	100.03	106.33
24	B	617	CLA	C1D-ND-C4D	-8.86	100.04	106.33
24	C	505	CLA	C2D-C1D-ND	8.86	116.63	110.10
24	d	401	CLA	C1D-ND-C4D	-8.85	100.05	106.33
24	b	606	CLA	C1D-ND-C4D	-8.83	100.06	106.33
24	C	513	CLA	C2D-C1D-ND	8.83	116.61	110.10
24	B	609	CLA	C1D-ND-C4D	-8.82	100.07	106.33
24	A	405	CLA	C1D-ND-C4D	-8.81	100.08	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	902	CLA	C1D-ND-C4D	-8.81	100.08	106.33
24	c	905	CLA	C1D-ND-C4D	-8.79	100.09	106.33
24	c	913	CLA	C2D-C1D-ND	8.77	116.57	110.10
24	B	615	CLA	C2D-C1D-ND	8.75	116.55	110.10
24	a	407	CLA	C1D-ND-C4D	-8.74	100.13	106.33
24	c	903	CLA	C1D-ND-C4D	-8.70	100.16	106.33
24	b	609	CLA	C2D-C1D-ND	8.68	116.50	110.10
24	b	615	CLA	C2D-C1D-ND	8.66	116.49	110.10
24	B	612	CLA	C2D-C1D-ND	8.65	116.48	110.10
25	A	408	PHO	O2D-CGD-CBD	8.64	121.95	111.00
24	b	610	CLA	C1D-ND-C4D	-8.58	100.24	106.33
24	B	614	CLA	C2D-C1D-ND	8.58	116.42	110.10
24	b	614	CLA	C1D-ND-C4D	-8.57	100.25	106.33
24	c	906	CLA	C1D-ND-C4D	-8.56	100.25	106.33
24	c	904	CLA	C1D-ND-C4D	-8.56	100.26	106.33
24	B	603	CLA	C2D-C1D-ND	8.56	116.41	110.10
24	c	911	CLA	C1D-ND-C4D	-8.53	100.27	106.33
24	B	616	CLA	C1D-ND-C4D	-8.53	100.28	106.33
24	C	510	CLA	C1D-ND-C4D	-8.53	100.28	106.33
24	D	401	CLA	C1D-ND-C4D	-8.52	100.28	106.33
24	D	402	CLA	C2D-C1D-ND	8.47	116.35	110.10
24	B	606	CLA	C1D-ND-C4D	-8.46	100.32	106.33
24	b	611	CLA	C2D-C1D-ND	8.44	116.32	110.10
24	B	608	CLA	C1D-ND-C4D	-8.42	100.35	106.33
24	b	620	CLA	C1D-ND-C4D	-8.42	100.35	106.33
24	C	507	CLA	C1D-ND-C4D	-8.42	100.36	106.33
24	B	610	CLA	C2D-C1D-ND	8.35	116.26	110.10
24	b	616	CLA	C2D-C1D-ND	8.33	116.24	110.10
24	B	605	CLA	C2D-C1D-ND	8.33	116.24	110.10
24	b	612	CLA	C1D-ND-C4D	-8.32	100.42	106.33
24	c	905	CLA	C2D-C1D-ND	8.32	116.23	110.10
24	b	618	CLA	C2D-C1D-ND	8.31	116.22	110.10
24	d	402	CLA	C2D-C1D-ND	8.29	116.21	110.10
24	b	620	CLA	C2D-C1D-ND	8.29	116.21	110.10
24	C	514	CLA	C2D-C1D-ND	8.28	116.21	110.10
24	c	908	CLA	C1D-ND-C4D	-8.28	100.45	106.33
24	C	504	CLA	C2D-C1D-ND	8.28	116.21	110.10
24	A	406	CLA	C2B-C1B-NB	8.27	115.78	110.23
24	C	506	CLA	C1D-ND-C4D	-8.27	100.46	106.33
24	A	410	CLA	C2D-C1D-ND	8.26	116.19	110.10
24	B	617	CLA	C2D-C1D-ND	8.26	116.19	110.10
24	B	602	CLA	C2B-C1B-NB	8.24	115.76	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	617	CLA	C1D-ND-C4D	-8.24	100.48	106.33
24	c	908	CLA	C2D-C1D-ND	8.23	116.17	110.10
24	c	909	CLA	C2D-C1D-ND	8.23	116.17	110.10
24	B	602	CLA	C2D-C1D-ND	8.21	116.15	110.10
24	B	607	CLA	C1D-ND-C4D	-8.21	100.51	106.33
24	c	902	CLA	C2D-C1D-ND	8.19	116.14	110.10
24	C	511	CLA	C1D-ND-C4D	-8.18	100.53	106.33
24	C	503	CLA	C1D-ND-C4D	-8.16	100.54	106.33
24	B	608	CLA	C2D-C1D-ND	8.15	116.11	110.10
24	C	508	CLA	C1D-ND-C4D	-8.14	100.55	106.33
24	B	616	CLA	C2D-C1D-ND	8.13	116.09	110.10
24	b	607	CLA	C1D-ND-C4D	-8.08	100.60	106.33
24	B	613	CLA	C1D-ND-C4D	-8.04	100.62	106.33
25	a	420	PHO	O2D-CGD-CBD	8.02	121.16	111.00
24	C	504	CLA	C2B-C1B-NB	8.00	115.60	110.23
24	c	913	CLA	C2B-C1B-NB	8.00	115.59	110.23
24	B	609	CLA	C2B-C1B-NB	7.99	115.59	110.23
24	b	619	CLA	C1D-ND-C4D	-7.96	100.68	106.33
24	c	910	CLA	C2D-C1D-ND	7.95	115.96	110.10
24	b	610	CLA	C2D-C1D-ND	7.94	115.96	110.10
24	b	606	CLA	C2D-C1D-ND	7.94	115.95	110.10
24	A	407	CLA	C2D-C1D-ND	7.92	115.94	110.10
24	a	409	CLA	C1D-ND-C4D	-7.91	100.71	106.33
24	A	405	CLA	C2D-C1D-ND	7.90	115.92	110.10
24	d	403	CLA	C2D-C1D-ND	7.89	115.92	110.10
24	C	513	CLA	C2B-C1B-NB	7.88	115.52	110.23
24	c	914	CLA	C2D-C1D-ND	7.88	115.91	110.10
24	b	617	CLA	C2D-C1D-ND	7.87	115.91	110.10
24	b	613	CLA	C2D-C1D-ND	7.87	115.91	110.10
24	a	407	CLA	C2B-C1B-NB	7.84	115.49	110.23
24	C	502	CLA	C2D-C1D-ND	7.84	115.88	110.10
24	b	608	CLA	C1D-ND-C4D	-7.82	100.78	106.33
24	B	604	CLA	C2D-C1D-ND	7.81	115.86	110.10
24	b	607	CLA	C2B-C1B-NB	7.80	115.46	110.23
24	B	607	CLA	C4A-NA-C1A	-7.78	103.21	106.71
24	C	512	CLA	C2D-C1D-ND	7.77	115.83	110.10
24	C	509	CLA	C2D-C1D-ND	7.77	115.83	110.10
24	B	606	CLA	C2D-C1D-ND	7.77	115.83	110.10
24	c	907	CLA	C1D-ND-C4D	-7.72	100.85	106.33
24	B	604	CLA	C2B-C1B-NB	7.72	115.41	110.23
24	B	611	CLA	C1D-ND-C4D	-7.70	100.86	106.33
24	A	407	CLA	C2B-C1B-NB	7.67	115.38	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	605	CLA	C2D-C1D-ND	7.67	115.76	110.10
24	b	619	CLA	C2D-C1D-ND	7.65	115.74	110.10
24	c	903	CLA	C2D-C1D-ND	7.63	115.73	110.10
24	C	503	CLA	C2D-C1D-ND	7.61	115.71	110.10
24	C	510	CLA	C2D-C1D-ND	7.60	115.71	110.10
24	B	609	CLA	C2D-C1D-ND	7.60	115.70	110.10
24	d	402	CLA	C4A-NA-C1A	-7.52	103.33	106.71
24	A	410	CLA	C2B-C1B-NB	7.52	115.27	110.23
24	B	616	CLA	C2B-C1B-NB	7.52	115.27	110.23
24	b	610	CLA	C2B-C1B-NB	7.51	115.27	110.23
24	c	903	CLA	C2B-C1B-NB	7.51	115.27	110.23
24	D	401	CLA	C2D-C1D-ND	7.50	115.63	110.10
24	c	904	CLA	C2D-C1D-ND	7.49	115.63	110.10
24	b	614	CLA	C2D-C1D-ND	7.48	115.61	110.10
24	d	401	CLA	C2D-C1D-ND	7.47	115.61	110.10
24	A	405	CLA	C2B-C1B-NB	7.46	115.23	110.23
24	a	407	CLA	C2D-C1D-ND	7.45	115.60	110.10
24	b	605	CLA	C2B-C1B-NB	7.44	115.22	110.23
24	c	914	CLA	C2B-C1B-NB	7.44	115.22	110.23
24	c	904	CLA	C2B-C1B-NB	7.41	115.20	110.23
24	a	409	CLA	C2B-C1B-NB	7.41	115.20	110.23
24	B	603	CLA	C2B-C1B-NB	7.40	115.19	110.23
24	b	612	CLA	C2B-C1B-NB	7.38	115.18	110.23
24	B	607	CLA	CMD-C2D-C1D	7.36	137.68	124.71
24	C	508	CLA	C2D-C1D-ND	7.36	115.53	110.10
24	a	406	CLA	C2D-C1D-ND	7.33	115.51	110.10
24	c	907	CLA	C2D-C1D-ND	7.31	115.49	110.10
24	b	613	CLA	C4A-NA-C1A	-7.29	103.43	106.71
24	B	611	CLA	C2D-C1D-ND	7.27	115.46	110.10
24	c	905	CLA	C2B-C1B-NB	7.25	115.09	110.23
24	C	507	CLA	C2D-C1D-ND	7.23	115.44	110.10
24	B	614	CLA	C2B-C1B-NB	7.23	115.08	110.23
24	c	912	CLA	C2B-C1B-NB	7.23	115.08	110.23
24	a	409	CLA	C2D-C1D-ND	7.23	115.43	110.10
24	C	503	CLA	C2B-C1B-NB	7.23	115.08	110.23
24	B	613	CLA	C2D-C1D-ND	7.22	115.43	110.10
24	b	609	CLA	C2B-C1B-NB	7.21	115.07	110.23
24	c	910	CLA	C2B-C1B-NB	7.20	115.06	110.23
25	a	408	PHO	C4D-ND-C1D	-7.19	101.52	108.83
24	B	616	CLA	C4A-NA-C1A	-7.09	103.52	106.71
24	b	606	CLA	C2B-C1B-NB	7.09	114.98	110.23
24	C	502	CLA	C2B-C1B-NB	7.08	114.98	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	611	CLA	CMD-C2D-C1D	7.07	137.18	124.71
24	B	607	CLA	C2D-C1D-ND	7.07	115.31	110.10
24	B	607	CLA	C2B-C1B-NB	7.05	114.96	110.23
24	c	909	CLA	C2B-C1B-NB	7.02	114.94	110.23
24	C	506	CLA	CMD-C2D-C1D	7.02	137.09	124.71
24	C	511	CLA	C2B-C1B-NB	7.02	114.94	110.23
24	C	514	CLA	C2B-C1B-NB	7.02	114.94	110.23
24	D	402	CLA	C2B-C1B-NB	7.00	114.92	110.23
24	a	407	CLA	CMD-C2D-C1D	7.00	137.04	124.71
24	C	511	CLA	C2D-C1D-ND	6.97	115.24	110.10
24	c	912	CLA	C2D-C1D-ND	6.97	115.24	110.10
25	A	408	PHO	C4D-ND-C1D	-6.96	101.75	108.83
24	b	619	CLA	C2B-C1B-NB	6.96	114.90	110.23
24	d	403	CLA	C2B-C1B-NB	6.94	114.88	110.23
24	A	405	CLA	C4A-NA-C1A	-6.94	103.59	106.71
24	c	906	CLA	C2B-C1B-NB	6.93	114.88	110.23
24	B	613	CLA	C2B-C1B-NB	6.93	114.88	110.23
24	C	510	CLA	CMD-C2D-C1D	6.92	136.91	124.71
24	B	615	CLA	CMD-C2D-C1D	6.91	136.89	124.71
24	c	908	CLA	O2D-CGD-CBD	6.91	123.54	111.27
24	c	911	CLA	C2D-C1D-ND	6.89	115.18	110.10
25	A	409	PHO	C4D-ND-C1D	-6.84	101.87	108.83
24	B	606	CLA	C2C-C1C-NC	6.83	116.37	109.97
24	c	914	CLA	CHD-C1D-ND	-6.82	118.19	124.45
24	b	616	CLA	C2B-C1B-NB	6.82	114.81	110.23
24	B	612	CLA	C2B-C1B-NB	6.81	114.80	110.23
24	b	608	CLA	C2B-C1B-NB	6.80	114.79	110.23
24	C	506	CLA	C2B-C1B-NB	6.79	114.79	110.23
24	b	612	CLA	C2D-C1D-ND	6.79	115.11	110.10
24	B	605	CLA	C2B-C1B-NB	6.78	114.78	110.23
24	B	615	CLA	C2B-C1B-NB	6.78	114.78	110.23
24	C	509	CLA	C2B-C1B-NB	6.77	114.77	110.23
24	b	620	CLA	C2B-C1B-NB	6.76	114.76	110.23
24	C	509	CLA	C4A-NA-C1A	-6.75	103.67	106.71
25	a	408	PHO	O2D-CGD-CBD	6.75	119.55	111.00
24	c	914	CLA	CMD-C2D-C1D	6.75	136.60	124.71
24	b	618	CLA	C2B-C1B-NB	6.74	114.75	110.23
24	C	505	CLA	C2B-C1B-NB	6.74	114.75	110.23
24	c	906	CLA	C2D-C1D-ND	6.73	115.06	110.10
24	b	607	CLA	C4A-NA-C1A	-6.72	103.68	106.71
24	b	609	CLA	CHD-C4C-C3C	-6.72	114.96	124.84
24	b	618	CLA	CMD-C2D-C1D	6.70	136.52	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	C2B-C1B-NB	6.69	114.72	110.23
24	C	502	CLA	CMD-C2D-C1D	6.68	136.48	124.71
24	b	615	CLA	C2B-C1B-NB	6.67	114.70	110.23
24	b	611	CLA	CHD-C4C-C3C	-6.67	115.04	124.84
27	F	101	SQD	O6-C1-C2	6.65	118.69	108.30
24	C	513	CLA	CHD-C4C-C3C	-6.64	115.08	124.84
24	d	402	CLA	C2B-C1B-NB	6.64	114.68	110.23
24	b	617	CLA	C2B-C1B-NB	6.62	114.67	110.23
24	B	615	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
24	C	512	CLA	C2B-C1B-NB	6.61	114.66	110.23
24	b	607	CLA	CMD-C2D-C1D	6.60	136.34	124.71
24	C	512	CLA	CMD-C2D-C1D	6.60	136.34	124.71
24	C	507	CLA	C2B-C1B-NB	6.59	114.65	110.23
24	C	510	CLA	C2B-C1B-NB	6.59	114.65	110.23
35	B	626	HTG	C1'-S1-C1	6.58	112.39	100.09
24	B	607	CLA	C2C-C1C-NC	6.56	116.12	109.97
24	B	611	CLA	CMD-C2D-C1D	6.52	136.21	124.71
24	b	612	CLA	CMD-C2D-C1D	6.51	136.19	124.71
24	C	505	CLA	CHD-C1D-ND	-6.51	118.47	124.45
24	b	608	CLA	C2D-C1D-ND	6.50	114.89	110.10
24	B	617	CLA	C2B-C1B-NB	6.49	114.58	110.23
24	b	610	CLA	C4A-NA-C1A	-6.48	103.79	106.71
24	d	403	CLA	CMD-C2D-C1D	6.48	136.14	124.71
24	B	617	CLA	CHD-C4C-C3C	-6.48	115.32	124.84
24	b	607	CLA	C2D-C1D-ND	6.47	114.87	110.10
24	D	401	CLA	C2C-C1C-NC	6.47	116.03	109.97
24	d	401	CLA	CMD-C2D-C1D	6.46	136.09	124.71
24	C	508	CLA	C2B-C1B-NB	6.46	114.56	110.23
24	b	605	CLA	CHD-C1D-ND	-6.45	118.52	124.45
24	a	406	CLA	C2C-C1C-NC	6.43	116.00	109.97
24	C	505	CLA	CMD-C2D-C1D	6.43	136.04	124.71
24	C	506	CLA	C4A-NA-C1A	-6.43	103.82	106.71
24	c	907	CLA	CMD-C2D-C1D	6.42	136.03	124.71
24	c	906	CLA	C2C-C1C-NC	6.41	115.98	109.97
24	b	608	CLA	CMD-C2D-C1D	6.41	136.01	124.71
24	a	407	CLA	C4A-NA-C1A	-6.40	103.83	106.71
24	b	605	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	C	507	CLA	CMD-C2D-C1D	6.39	135.98	124.71
24	B	606	CLA	C2B-C1B-NB	6.39	114.52	110.23
24	c	907	CLA	C2B-C1B-NB	6.38	114.51	110.23
25	a	420	PHO	C4D-ND-C1D	-6.38	102.34	108.83
24	b	617	CLA	C2C-C1C-NC	6.37	115.94	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	607	CLA	CHD-C1D-ND	-6.37	118.60	124.45
24	B	609	CLA	C2C-C1C-NC	6.37	115.94	109.97
24	c	905	CLA	CMD-C2D-C1D	6.36	135.92	124.71
24	b	615	CLA	CMD-C2D-C1D	6.36	135.91	124.71
24	b	615	CLA	CHD-C4C-C3C	-6.34	115.51	124.84
24	a	406	CLA	CMD-C2D-C1D	6.34	135.88	124.71
24	B	604	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
24	d	401	CLA	C2C-C1C-NC	6.31	115.89	109.97
24	d	403	CLA	C2C-C1C-NC	6.31	115.88	109.97
24	c	904	CLA	C4A-NA-C1A	-6.31	103.87	106.71
24	B	617	CLA	O2D-CGD-CBD	6.30	122.46	111.27
24	B	605	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
24	b	610	CLA	CMD-C2D-C1D	6.29	135.81	124.71
24	B	603	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
24	B	611	CLA	C2B-C1B-NB	6.28	114.44	110.23
25	a	408	PHO	C1C-C2C-C3C	-6.28	103.39	108.61
24	D	402	CLA	CMD-C2D-C1D	6.27	135.76	124.71
24	c	912	CLA	CMD-C2D-C1D	6.27	135.76	124.71
24	b	606	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
24	c	903	CLA	CMD-C2D-C1D	6.26	135.75	124.71
24	C	507	CLA	C2C-C1C-NC	6.26	115.83	109.97
24	A	405	CLA	CMD-C2D-C1D	6.25	135.73	124.71
24	A	405	CLA	C2C-C1C-NC	6.25	115.83	109.97
25	A	409	PHO	C2B-C1B-NB	6.24	113.84	109.53
25	A	409	PHO	C1C-C2C-C3C	-6.24	103.42	108.61
24	c	908	CLA	C2B-C1B-NB	6.24	114.41	110.23
24	B	604	CLA	CMD-C2D-C1D	6.24	135.70	124.71
24	B	610	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
24	C	509	CLA	C2C-C1C-NC	6.23	115.81	109.97
24	B	608	CLA	C2C-C1C-NC	6.23	115.80	109.97
24	d	401	CLA	C2B-C1B-NB	6.22	114.41	110.23
24	B	614	CLA	CMD-C2D-C1D	6.22	135.67	124.71
24	b	609	CLA	CMD-C2D-C1D	6.21	135.66	124.71
24	b	619	CLA	C4A-NA-C1A	-6.21	103.91	106.71
24	b	618	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
24	b	605	CLA	CMD-C2D-C1D	6.21	135.66	124.71
24	c	906	CLA	CMD-C2D-C1D	6.21	135.65	124.71
24	c	904	CLA	CMD-C2D-C1D	6.20	135.65	124.71
24	c	908	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	A	410	CLA	CHD-C1D-ND	-6.18	118.77	124.45
24	d	402	CLA	C2C-C1C-NC	6.18	115.76	109.97
24	b	610	CLA	CHD-C1D-ND	-6.18	118.77	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	CHD-C1D-ND	-6.18	118.78	124.45
24	C	504	CLA	CHD-C1D-ND	-6.18	118.78	124.45
24	B	616	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
24	a	409	CLA	CHD-C4C-C3C	-6.17	115.76	124.84
24	b	619	CLA	C2C-C1C-NC	6.17	115.76	109.97
24	c	911	CLA	C2B-C1B-NB	6.17	114.37	110.23
24	D	402	CLA	CHD-C1D-ND	-6.17	118.79	124.45
24	b	610	CLA	O2D-CGD-CBD	6.16	122.21	111.27
24	c	905	CLA	CHD-C1D-ND	-6.15	118.80	124.45
24	d	401	CLA	CHD-C1D-ND	-6.15	118.80	124.45
24	C	504	CLA	CMD-C2D-C1D	6.15	135.55	124.71
24	b	614	CLA	CMD-C2D-C1D	6.15	135.54	124.71
24	D	401	CLA	CMD-C2D-C1D	6.13	135.53	124.71
24	B	615	CLA	CHD-C1D-ND	-6.11	118.83	124.45
24	B	603	CLA	CHD-C1D-ND	-6.11	118.84	124.45
24	c	907	CLA	C2C-C1C-NC	6.11	115.70	109.97
24	b	613	CLA	C2B-C1B-NB	6.11	114.33	110.23
24	b	606	CLA	CMD-C2D-C1D	6.11	135.47	124.71
24	A	410	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
24	C	509	CLA	O2D-CGD-CBD	6.10	122.11	111.27
24	A	406	CLA	CHD-C4C-C3C	-6.10	115.88	124.84
24	B	609	CLA	C4A-NA-C1A	-6.10	103.97	106.71
24	b	613	CLA	CMD-C2D-C1D	6.08	135.44	124.71
24	C	504	CLA	C4A-NA-C1A	-6.08	103.97	106.71
24	B	612	CLA	CMD-C2D-C1D	6.06	135.40	124.71
24	c	902	CLA	CMD-C2D-C1D	6.06	135.39	124.71
24	a	406	CLA	C2B-C1B-NB	6.05	114.29	110.23
24	b	608	CLA	C2C-C1C-NC	6.05	115.64	109.97
24	d	402	CLA	CMD-C2D-C1D	6.05	135.38	124.71
24	c	908	CLA	CMD-C2D-C1D	6.05	135.37	124.71
24	c	913	CLA	CHD-C4C-C3C	-6.05	115.95	124.84
24	C	508	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
24	b	617	CLA	CMD-C2D-C1D	6.03	135.35	124.71
24	b	611	CLA	C2B-C1B-NB	6.02	114.27	110.23
24	A	410	CLA	CMD-C2D-C1D	6.02	135.32	124.71
24	b	616	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
24	D	401	CLA	C4A-NA-C1A	-6.01	104.00	106.71
35	B	634	HTG	C1'-S1-C1	6.01	111.33	100.09
24	B	608	CLA	C2B-C1B-NB	6.01	114.26	110.23
24	b	608	CLA	O2D-CGD-CBD	6.00	121.94	111.27
24	C	514	CLA	CMD-C2D-C1D	6.00	135.29	124.71
24	C	512	CLA	C2C-C1C-NC	6.00	115.59	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	614	CLA	CHD-C1D-ND	-6.00	118.94	124.45
24	b	614	CLA	C2C-C1C-NC	6.00	115.59	109.97
24	c	903	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
24	b	611	CLA	C2C-C1C-NC	5.99	115.59	109.97
24	C	506	CLA	C2D-C1D-ND	5.99	114.52	110.10
25	A	409	PHO	O2D-CGD-CBD	5.98	118.58	111.00
24	a	407	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
24	A	407	CLA	C4A-NA-C1A	-5.97	104.02	106.71
24	D	401	CLA	CHD-C1D-ND	-5.97	118.96	124.45
24	C	502	CLA	CHD-C1D-ND	-5.97	118.97	124.45
24	B	603	CLA	CMD-C2D-C1D	5.97	135.24	124.71
24	b	613	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
24	b	613	CLA	CHD-C1D-ND	-5.96	118.98	124.45
24	c	912	CLA	CHD-C1D-ND	-5.96	118.98	124.45
24	b	618	CLA	O2D-CGD-CBD	5.95	121.85	111.27
24	b	611	CLA	CHD-C1D-ND	-5.95	118.99	124.45
24	C	511	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
24	b	615	CLA	C2C-C1C-NC	5.94	115.54	109.97
24	c	910	CLA	CMD-C2D-C1D	5.93	135.16	124.71
24	b	617	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
24	B	613	CLA	O2D-CGD-CBD	5.92	121.79	111.27
24	B	608	CLA	C4A-NA-C1A	-5.91	104.05	106.71
24	b	612	CLA	C4A-NA-C1A	-5.91	104.05	106.71
24	c	902	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
24	C	507	CLA	CHD-C1D-ND	-5.91	119.03	124.45
24	C	510	CLA	C2C-C1C-NC	5.91	115.50	109.97
24	B	605	CLA	CMD-C2D-C1D	5.90	135.12	124.71
24	c	902	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	d	403	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
24	C	512	CLA	CHD-C4C-C3C	-5.89	116.17	124.84
24	B	602	CLA	CHD-C1D-ND	-5.89	119.04	124.45
25	A	408	PHO	C2B-C1B-NB	5.88	113.59	109.53
24	c	904	CLA	C2C-C1C-NC	5.88	115.48	109.97
24	c	911	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
24	b	610	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
24	C	504	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
24	b	607	CLA	O2D-CGD-CBD	5.86	121.68	111.27
24	D	402	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
24	d	402	CLA	CHD-C1D-ND	-5.85	119.08	124.45
24	c	912	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	A	405	CLA	CHD-C1D-ND	-5.85	119.08	124.45
24	C	502	CLA	C2C-C1C-NC	5.85	115.45	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	506	CLA	C2C-C1C-NC	5.83	115.44	109.97
24	c	910	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
24	C	511	CLA	O2D-CGD-CBD	5.83	121.63	111.27
24	B	602	CLA	CMD-C2D-C1D	5.83	134.99	124.71
24	C	505	CLA	O2D-CGD-CBD	5.82	121.62	111.27
24	A	407	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
24	b	616	CLA	CMD-C2D-C1D	5.82	134.97	124.71
24	B	611	CLA	C2C-C1C-NC	5.81	115.42	109.97
24	B	606	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	A	406	CLA	CHD-C1D-ND	-5.81	119.12	124.45
24	B	614	CLA	C2C-C1C-NC	5.80	115.41	109.97
24	B	613	CLA	C4A-NA-C1A	-5.79	104.10	106.71
24	b	620	CLA	C4A-NA-C1A	-5.79	104.10	106.71
24	B	608	CLA	CMD-C2D-C1D	5.79	134.91	124.71
24	C	514	CLA	CHD-C1D-ND	-5.79	119.14	124.45
24	B	616	CLA	CMD-C2D-C1D	5.78	134.91	124.71
24	C	508	CLA	CMD-C2D-C1D	5.78	134.89	124.71
24	c	909	CLA	C2C-C1C-NC	5.77	115.38	109.97
24	B	610	CLA	C4A-NA-C1A	-5.77	104.11	106.71
24	b	620	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
24	B	615	CLA	C2C-C1C-NC	5.76	115.37	109.97
24	c	904	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
24	c	905	CLA	O2D-CGD-CBD	5.75	121.48	111.27
24	C	508	CLA	C2C-C1C-NC	5.74	115.35	109.97
35	c	923	HTG	C1'-S1-C1	5.74	110.83	100.09
24	c	906	CLA	O2D-CGD-CBD	5.74	121.46	111.27
24	d	403	CLA	CHD-C1D-ND	-5.73	119.19	124.45
24	C	506	CLA	O2D-CGD-CBD	5.73	121.45	111.27
24	A	406	CLA	CMD-C2D-C1D	5.72	134.79	124.71
24	B	605	CLA	C2C-C1C-NC	5.71	115.32	109.97
24	B	603	CLA	C4A-NA-C1A	-5.71	104.14	106.71
24	B	612	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
24	C	503	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
24	c	908	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
24	b	612	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
24	a	409	CLA	C2C-C1C-NC	5.69	115.30	109.97
35	b	603	HTG	C1'-S1-C1	5.68	110.71	100.09
24	c	913	CLA	CMD-C2D-C1D	5.68	134.72	124.71
24	B	602	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
24	C	509	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
24	B	614	CLA	C4A-NA-C1A	-5.67	104.16	106.71
24	a	406	CLA	CHD-C1D-ND	-5.66	119.25	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	C2B-C1B-NB	5.65	114.02	110.23
24	A	405	CLA	CHD-C4C-C3C	-5.64	116.54	124.84
24	A	407	CLA	CMD-C2D-C1D	5.64	134.66	124.71
24	b	607	CLA	CHD-C1D-ND	-5.64	119.28	124.45
24	B	611	CLA	C4A-NA-C1A	-5.63	104.18	106.71
24	C	510	CLA	CHD-C1D-ND	-5.62	119.29	124.45
24	B	611	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
24	B	602	CLA	O2D-CGD-CBD	5.61	121.24	111.27
24	C	502	CLA	O2D-CGD-CBD	5.61	121.24	111.27
24	B	610	CLA	CMD-C2D-C1D	5.61	134.59	124.71
24	b	612	CLA	C2C-C1C-NC	5.60	115.22	109.97
24	c	914	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
24	B	617	CLA	CMD-C2D-C1D	5.60	134.58	124.71
24	C	503	CLA	C2C-C1C-NC	5.59	115.21	109.97
24	C	514	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
27	L	102	SQD	O7-S-C6	5.58	113.57	106.94
24	c	905	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
24	C	511	CLA	C4A-NA-C1A	-5.56	104.21	106.71
24	B	614	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
24	B	616	CLA	CHD-C1D-ND	-5.56	119.35	124.45
24	b	618	CLA	C2C-C1C-NC	5.55	115.17	109.97
24	c	902	CLA	CHD-C1D-ND	-5.54	119.36	124.45
24	c	905	CLA	C2C-C1C-NC	5.53	115.16	109.97
24	b	614	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
24	c	910	CLA	O2D-CGD-CBD	5.53	121.09	111.27
24	C	502	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
24	b	606	CLA	C4A-NA-C1A	-5.51	104.23	106.71
24	C	506	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
24	C	511	CLA	CMD-C2D-C1D	5.50	134.41	124.71
24	b	620	CLA	C2C-C1C-NC	5.50	115.12	109.97
24	C	505	CLA	C2C-C1C-NC	5.50	115.12	109.97
24	c	902	CLA	O2D-CGD-CBD	5.50	121.03	111.27
24	C	508	CLA	O2D-CGD-CBD	5.49	121.03	111.27
24	b	616	CLA	O2D-CGD-CBD	5.49	121.03	111.27
24	B	609	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
24	B	613	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
24	b	611	CLA	C3C-C4C-NC	5.48	116.72	110.57
24	B	603	CLA	C2C-C1C-NC	5.48	115.11	109.97
25	A	408	PHO	C1C-C2C-C3C	-5.48	104.05	108.61
24	c	906	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
24	C	509	CLA	CHD-C1D-ND	-5.47	119.43	124.45
24	c	909	CLA	CHD-C4C-C3C	-5.47	116.81	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	406	CLA	C2C-C1C-NC	5.46	115.09	109.97
24	c	903	CLA	C4A-NA-C1A	-5.46	104.25	106.71
24	b	616	CLA	C4A-NA-C1A	-5.46	104.25	106.71
24	c	911	CLA	CMD-C2D-C1D	5.46	134.33	124.71
24	c	907	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
24	A	406	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
25	a	408	PHO	C2B-C1B-NB	5.43	113.27	109.53
24	b	609	CLA	C2C-C1C-NC	5.42	115.05	109.97
24	b	609	CLA	CHD-C1D-ND	-5.42	119.47	124.45
24	c	910	CLA	CHD-C1D-ND	-5.42	119.47	124.45
24	b	618	CLA	C4A-NA-C1A	-5.42	104.27	106.71
24	c	912	CLA	C4A-NA-C1A	-5.42	104.27	106.71
24	C	510	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
24	C	512	CLA	CHD-C1D-ND	-5.42	119.48	124.45
24	b	606	CLA	O2D-CGD-CBD	5.42	120.89	111.27
24	B	610	CLA	CHD-C1D-ND	-5.41	119.48	124.45
25	a	420	PHO	C2B-C1B-NB	5.41	113.26	109.53
38	E	103	HEM	CHC-C4B-NB	5.41	130.29	124.42
24	c	913	CLA	CHD-C1D-ND	-5.40	119.49	124.45
24	B	612	CLA	C2C-C1C-NC	5.39	115.02	109.97
24	D	401	CLA	C2B-C1B-NB	5.38	113.84	110.23
24	d	401	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
24	B	602	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	c	910	CLA	C2C-C1C-NC	5.37	115.00	109.97
24	C	514	CLA	C2C-C1C-NC	5.36	115.00	109.97
24	B	604	CLA	CHD-C1D-ND	-5.36	119.53	124.45
24	C	504	CLA	C2C-C1C-NC	5.36	114.99	109.97
27	a	411	SQD	O47-C7-C8	5.35	123.03	111.50
24	B	607	CLA	O2D-CGD-CBD	5.35	120.77	111.27
24	b	612	CLA	CHD-C1D-ND	-5.35	119.54	124.45
24	b	619	CLA	CHD-C1D-ND	-5.34	119.55	124.45
24	b	614	CLA	C4A-NA-C1A	-5.34	104.31	106.71
24	b	605	CLA	O2D-CGD-CBD	5.34	120.76	111.27
24	A	407	CLA	CHD-C1D-ND	-5.33	119.55	124.45
35	b	626	HTG	C1'-S1-C1	5.33	110.06	100.09
27	a	411	SQD	O6-C1-C2	5.33	116.62	108.30
24	b	606	CLA	CHD-C1D-ND	-5.32	119.56	124.45
24	C	513	CLA	CMD-C2D-C1D	5.32	134.10	124.71
24	d	402	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
24	c	913	CLA	C4A-NA-C1A	-5.32	104.32	106.71
24	B	608	CLA	CHD-C1D-ND	-5.31	119.58	124.45
24	B	604	CLA	O2D-CGD-CBD	5.31	120.70	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	903	CLA	O2D-CGD-CBD	5.30	120.68	111.27
24	c	911	CLA	C2C-C1C-NC	5.29	114.93	109.97
24	B	615	CLA	O2D-CGD-CBD	5.29	120.67	111.27
24	b	609	CLA	O2D-CGD-CBD	5.29	120.67	111.27
24	B	606	CLA	C3C-C4C-NC	5.29	116.50	110.57
24	b	620	CLA	O2D-CGD-CBD	5.28	120.66	111.27
24	c	902	CLA	C2B-C1B-NB	5.28	113.77	110.23
24	B	615	CLA	C4A-NA-C1A	-5.28	104.33	106.71
24	B	607	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
24	b	614	CLA	CHD-C1D-ND	-5.27	119.61	124.45
24	c	907	CLA	CHD-C1D-ND	-5.27	119.61	124.45
24	b	607	CLA	C2C-C1C-NC	5.27	114.91	109.97
24	C	505	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
24	B	605	CLA	CHD-C1D-ND	-5.26	119.62	124.45
24	b	606	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	C	511	CLA	C2C-C1C-NC	5.24	114.88	109.97
27	A	412	SQD	O6-C1-C2	5.24	116.49	108.30
25	A	409	PHO	C3D-C4D-ND	5.24	114.86	107.72
24	C	505	CLA	C4A-NA-C1A	-5.24	104.35	106.71
24	B	616	CLA	C2C-C1C-NC	5.24	114.88	109.97
24	c	903	CLA	CHD-C1D-ND	-5.23	119.65	124.45
24	B	613	CLA	C2C-C1C-NC	5.23	114.87	109.97
24	B	612	CLA	C4A-NA-C1A	-5.22	104.36	106.71
24	b	605	CLA	C4A-NA-C1A	-5.22	104.36	106.71
24	B	609	CLA	CHD-C1D-ND	-5.22	119.66	124.45
24	b	615	CLA	CHD-C1D-ND	-5.22	119.66	124.45
35	c	922	HTG	C1'-S1-C1	5.21	109.84	100.09
24	b	610	CLA	C2C-C1C-NC	5.21	114.85	109.97
24	c	903	CLA	C2C-C1C-NC	5.21	114.85	109.97
24	c	913	CLA	O2D-CGD-CBD	5.20	120.51	111.27
24	B	604	CLA	C2C-C1C-NC	5.20	114.84	109.97
24	a	407	CLA	O2D-CGD-CBD	5.19	120.49	111.27
24	b	609	CLA	C4A-NA-C1A	-5.19	104.37	106.71
24	c	904	CLA	CHD-C1D-ND	-5.19	119.69	124.45
24	b	608	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
27	f	102	SQD	O47-C7-C8	5.18	122.67	111.50
24	B	603	CLA	O2D-CGD-CBD	5.17	120.46	111.27
24	C	510	CLA	O2D-CGD-CBD	5.17	120.46	111.27
24	C	513	CLA	C4A-NA-C1A	-5.17	104.38	106.71
24	a	409	CLA	CMD-C2D-C1D	5.17	133.82	124.71
24	c	914	CLA	C2C-C1C-NC	5.16	114.80	109.97
24	C	506	CLA	CHD-C1D-ND	-5.15	119.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	912	CLA	C3B-C2B-C1B	-5.14	100.96	107.16
27	A	412	SQD	O47-C7-C8	5.13	122.56	111.50
24	a	409	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
24	C	513	CLA	O2D-CGD-CBD	5.12	120.37	111.27
24	b	608	CLA	CHD-C1D-ND	-5.12	119.75	124.45
24	c	909	CLA	CMD-C2D-C1D	5.12	133.73	124.71
24	b	618	CLA	CHD-C1D-ND	-5.12	119.75	124.45
24	b	607	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
24	b	620	CLA	CMD-C2D-C1D	5.11	133.72	124.71
24	D	402	CLA	C2C-C1C-NC	5.11	114.76	109.97
24	B	611	CLA	CHD-C1D-ND	-5.10	119.76	124.45
24	b	616	CLA	C3C-C4C-NC	5.10	116.29	110.57
24	c	913	CLA	C2C-C1C-NC	5.09	114.74	109.97
24	b	615	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
24	C	507	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
24	b	615	CLA	C3C-C4C-NC	5.08	116.27	110.57
24	B	613	CLA	CMD-C2D-C1D	5.08	133.67	124.71
24	a	407	CLA	CHD-C1D-ND	-5.07	119.79	124.45
24	C	513	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
24	B	606	CLA	C4A-NA-C1A	-5.06	104.43	106.71
24	b	609	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
24	b	619	CLA	CHD-C4C-C3C	-5.06	117.41	124.84
24	B	610	CLA	C2C-C1C-NC	5.05	114.70	109.97
24	A	410	CLA	C3B-C2B-C1B	-5.05	101.06	107.16
24	A	410	CLA	C2C-C1C-NC	5.05	114.70	109.97
24	c	908	CLA	CHD-C1D-ND	-5.04	119.82	124.45
27	F	101	SQD	O47-C7-C8	5.04	122.37	111.50
24	C	514	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
36	d	406	DGD	O6E-C5E-C4E	5.04	118.85	109.69
24	C	508	CLA	C4A-NA-C1A	-5.04	104.44	106.71
24	B	617	CLA	C2C-C1C-NC	5.03	114.69	109.97
24	b	619	CLA	CMD-C2D-C1D	5.03	133.58	124.71
24	C	508	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
24	b	606	CLA	C3C-C4C-NC	5.03	116.21	110.57
24	c	912	CLA	C2C-C1C-NC	5.03	114.68	109.97
24	c	908	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
24	B	615	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
35	b	627	HTG	O5-C1-C2	5.02	116.62	110.31
24	c	910	CLA	C4A-NA-C1A	-5.01	104.45	106.71
24	B	616	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	b	618	CLA	C3C-C4C-NC	5.00	116.18	110.57
24	A	406	CLA	C3B-C2B-C1B	-5.00	101.12	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	905	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	B	609	CLA	CMD-C2D-C1D	4.99	133.52	124.71
25	a	408	PHO	C3D-C4D-ND	4.99	114.52	107.72
26	K	103	BCR	C7-C8-C9	-4.99	118.70	126.23
24	a	407	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
24	B	611	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
24	c	909	CLA	O2D-CGD-CBD	4.98	120.11	111.27
24	C	503	CLA	CMD-C2D-C1D	4.97	133.47	124.71
24	b	611	CLA	O2D-CGD-CBD	4.97	120.09	111.27
24	C	513	CLA	C3B-C2B-C1B	-4.96	101.17	107.16
24	A	405	CLA	C3C-C4C-NC	4.96	116.14	110.57
24	D	401	CLA	O2D-CGD-CBD	4.96	120.08	111.27
35	b	627	HTG	C1'-S1-C1	4.96	109.36	100.09
24	B	617	CLA	C3B-C2B-C1B	-4.96	101.18	107.16
24	D	402	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
25	a	420	PHO	C1C-C2C-C3C	-4.95	104.50	108.61
24	C	504	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
24	B	603	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
24	b	605	CLA	C2C-C1C-NC	4.95	114.61	109.97
24	B	603	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
24	B	604	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
24	B	609	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
24	b	620	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
24	B	606	CLA	O2D-CGD-CBD	4.93	120.03	111.27
24	b	615	CLA	O2D-CGD-CBD	4.93	120.03	111.27
24	b	615	CLA	C4A-NA-C1A	-4.92	104.50	106.71
24	D	401	CLA	CHD-C4C-C3C	-4.91	117.62	124.84
24	B	602	CLA	C3B-C2B-C1B	-4.91	101.24	107.16
35	C	523	HTG	C1'-S1-C1	4.90	109.26	100.09
24	B	606	CLA	CMD-C2D-C1D	4.90	133.35	124.71
24	C	508	CLA	CHD-C1D-ND	-4.90	119.95	124.45
24	B	604	CLA	C4A-NA-C1A	-4.90	104.50	106.71
24	C	511	CLA	CHD-C1D-ND	-4.89	119.96	124.45
24	B	615	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
35	C	524	HTG	C1'-S1-C1	4.88	109.22	100.09
24	d	402	CLA	O2D-CGD-CBD	4.87	119.93	111.27
24	C	505	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
24	b	611	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
24	C	514	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
24	B	610	CLA	CMB-C2B-C1B	4.86	132.78	125.37
24	c	913	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
24	d	401	CLA	C3B-C4B-NB	4.85	115.01	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	610	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
24	d	403	CLA	C3B-C2B-C1B	-4.84	101.31	107.16
24	d	403	CLA	C4A-NA-C1A	-4.84	104.53	106.71
35	d	412	HTG	C1'-S1-C1	4.84	109.15	100.09
24	c	908	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
24	C	513	CLA	CHD-C1D-ND	-4.84	120.01	124.45
24	d	403	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	C	513	CLA	C2C-C1C-NC	4.84	114.50	109.97
24	b	617	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
24	C	503	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
24	c	903	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
25	A	408	PHO	C3D-C4D-ND	4.83	114.31	107.72
27	B	621	SQD	O6-C1-C2	4.81	115.82	108.30
24	c	910	CLA	C3B-C2B-C1B	-4.81	101.35	107.16
24	c	913	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
24	C	512	CLA	C3B-C2B-C1B	-4.80	101.36	107.16
27	B	621	SQD	O47-C7-C8	4.80	121.85	111.50
24	b	606	CLA	C3B-C2B-C1B	-4.80	101.37	107.16
24	b	617	CLA	C3C-C4C-NC	4.80	115.95	110.57
24	b	619	CLA	C3B-C2B-C1B	-4.79	101.37	107.16
24	C	514	CLA	O2D-CGD-CBD	4.79	119.79	111.27
24	a	407	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	B	613	CLA	CHD-C1D-ND	-4.79	120.05	124.45
24	B	616	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
24	b	613	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	b	609	CLA	C3C-C4C-NC	4.79	115.94	110.57
24	c	905	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
24	B	608	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	C	510	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	C	510	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
24	b	606	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	B	607	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
24	B	613	CLA	C3C-C4C-NC	4.77	115.92	110.57
24	b	619	CLA	C3B-C4B-NB	4.76	114.93	110.52
24	c	914	CLA	C3D-C4D-ND	4.76	117.94	110.24
24	d	402	CLA	C3C-C4C-NC	4.76	115.91	110.57
24	c	907	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
24	c	914	CLA	C3B-C2B-C1B	-4.75	101.42	107.16
24	c	902	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
24	C	507	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
24	d	401	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
24	c	909	CLA	C3D-C2D-C1D	-4.74	99.36	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
26	D	403	BCR	C7-C8-C9	-4.73	119.08	126.23
24	b	616	CLA	CHD-C1D-ND	-4.73	120.11	124.45
24	b	614	CLA	O2D-CGD-CBD	4.73	119.68	111.27
24	b	610	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
24	b	612	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
24	A	410	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
24	B	614	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	c	906	CLA	C3C-C4C-NC	4.71	115.85	110.57
24	C	503	CLA	C4A-NA-C1A	-4.71	104.59	106.71
24	C	506	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
24	c	904	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
24	C	503	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
24	C	507	CLA	O2D-CGD-CBD	4.70	119.62	111.27
24	C	512	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
25	A	409	PHO	C1-C2-C3	-4.70	117.92	126.04
24	b	615	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
24	B	612	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
24	c	907	CLA	O2D-CGD-CBD	4.69	119.60	111.27
24	C	502	CLA	C4A-NA-C1A	-4.68	104.60	106.71
24	a	406	CLA	C1C-C2C-C3C	-4.68	102.03	106.96
24	b	620	CLA	CHD-C1D-ND	-4.68	120.16	124.45
29	b	601	LMT	C1'-O5'-C5'	4.68	122.87	113.69
24	B	617	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
24	a	407	CLA	C2C-C1C-NC	4.68	114.35	109.97
24	C	509	CLA	C3D-C4D-ND	4.67	117.80	110.24
24	A	405	CLA	C3B-C2B-C1B	-4.67	101.53	107.16
24	b	620	CLA	C3B-C2B-C1B	-4.67	101.53	107.16
24	c	904	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
24	b	617	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
24	A	407	CLA	O2D-CGD-CBD	4.65	119.53	111.27
24	b	608	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
24	d	401	CLA	O2D-CGD-CBD	4.64	119.52	111.27
24	a	409	CLA	O2D-CGD-CBD	4.64	119.52	111.27
24	B	612	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
24	c	902	CLA	O2D-CGD-O1D	-4.64	114.77	123.84
24	C	502	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	A	406	CLA	O2D-CGD-CBD	4.63	119.50	111.27
24	B	612	CLA	O2D-CGD-CBD	4.63	119.49	111.27
24	C	504	CLA	O2D-CGD-CBD	4.63	119.49	111.27
27	L	102	SQD	O47-C7-C8	4.62	121.47	111.50
24	c	911	CLA	C4A-NA-C1A	-4.62	104.63	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	502	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
35	B	633	HTG	C1'-S1-C1	4.62	108.73	100.09
24	b	609	CLA	C3B-C2B-C1B	-4.62	101.59	107.16
24	D	401	CLA	C3C-C4C-NC	4.62	115.75	110.57
24	C	507	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
24	A	406	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
36	D	405	DGD	O2G-C1B-C2B	4.61	121.44	111.50
24	b	620	CLA	C3C-C4C-NC	4.61	115.74	110.57
24	B	602	CLA	C3D-C2D-C1D	-4.61	99.55	105.83
24	B	605	CLA	C3C-C4C-NC	4.61	115.74	110.57
24	C	509	CLA	CMD-C2D-C1D	4.60	132.82	124.71
26	K	102	BCR	C33-C5-C6	-4.60	119.36	124.53
24	c	909	CLA	C3C-C4C-NC	4.60	115.73	110.57
24	B	613	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
24	c	906	CLA	CHD-C1D-ND	-4.60	120.23	124.45
24	C	504	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
25	A	408	PHO	C1A-C2A-C3A	-4.59	98.47	102.84
24	D	401	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
24	c	906	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
24	B	605	CLA	O2D-CGD-CBD	4.59	119.43	111.27
24	B	606	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
24	c	911	CLA	O2D-CGD-CBD	4.59	119.42	111.27
24	A	407	CLA	C3D-C4D-ND	4.59	117.66	110.24
24	B	617	CLA	C3C-C4C-NC	4.58	115.71	110.57
35	b	627	HTG	C1-O5-C5	4.58	121.02	112.58
27	L	102	SQD	O6-C1-C2	4.57	115.44	108.30
24	b	616	CLA	C2C-C1C-NC	4.57	114.26	109.97
24	c	909	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
24	c	903	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
24	B	615	CLA	C1D-CHD-C4C	-4.57	116.21	126.06
27	A	412	SQD	C45-O47-C7	-4.57	106.55	117.79
24	B	615	CLA	C1C-C2C-C3C	-4.57	102.16	106.96
24	b	613	CLA	O2D-CGD-CBD	4.55	119.36	111.27
24	B	607	CLA	C3C-C4C-NC	4.55	115.68	110.57
24	C	507	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
24	c	910	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
24	B	603	CLA	C3C-C4C-NC	4.55	115.67	110.57
24	b	616	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
24	b	618	CLA	C1-C2-C3	-4.55	118.18	126.04
24	B	602	CLA	C3D-C4D-ND	4.55	117.59	110.24
24	C	504	CLA	C3C-C4C-NC	4.54	115.67	110.57
24	B	606	CLA	C3D-C2D-C1D	-4.54	99.64	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	402	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	C	508	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	B	610	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
40	V	201	HEC	C4B-NB-C1B	4.53	109.75	105.07
24	B	604	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
24	B	604	CLA	C3C-C4C-NC	4.52	115.64	110.57
24	C	504	CLA	C3D-C4D-ND	4.52	117.55	110.24
24	c	908	CLA	C3C-C4C-NC	4.52	115.64	110.57
24	a	406	CLA	CHD-C4C-C3C	-4.52	118.20	124.84
24	B	605	CLA	C3B-C2B-C1B	-4.51	101.71	107.16
24	A	407	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
24	B	607	CLA	C1C-C2C-C3C	-4.50	102.22	106.96
24	a	409	CLA	C3C-C4C-NC	4.50	115.61	110.57
24	c	914	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
26	d	404	BCR	C28-C27-C26	-4.49	106.05	114.08
24	B	609	CLA	C3D-C4D-ND	4.49	117.51	110.24
24	B	605	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	C	503	CLA	C3C-C4C-NC	4.49	115.61	110.57
24	a	406	CLA	C3D-C4D-ND	4.49	117.50	110.24
24	B	610	CLA	C3D-C4D-ND	4.49	117.50	110.24
24	c	907	CLA	C4A-NA-C1A	-4.48	104.69	106.71
24	C	513	CLA	C3C-C4C-NC	4.48	115.59	110.57
26	C	516	BCR	C7-C8-C9	-4.48	119.47	126.23
34	c	920	LMG	O7-C10-C11	4.48	121.15	111.50
24	C	511	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
26	y	101	BCR	C33-C5-C6	-4.47	119.50	124.53
24	d	402	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	c	912	CLA	C3D-C4D-ND	4.47	117.47	110.24
24	B	608	CLA	CHD-C4C-C3C	-4.47	118.27	124.84
24	B	612	CLA	C3D-C4D-ND	4.47	117.47	110.24
24	a	406	CLA	C4A-NA-C1A	-4.47	104.70	106.71
24	b	616	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
24	B	608	CLA	O2D-CGD-CBD	4.46	119.20	111.27
24	B	614	CLA	C3C-C4C-NC	4.46	115.58	110.57
24	A	405	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
24	b	614	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
24	c	902	CLA	C3C-C4C-NC	4.46	115.57	110.57
24	A	407	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
24	B	614	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
24	b	605	CLA	C3D-C4D-ND	4.46	117.45	110.24
38	e	102	HEM	CHC-C4B-NB	4.45	129.25	124.42
34	z	101	LMG	C3-C4-C5	4.45	118.17	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	608	CLA	C4A-NA-C1A	-4.44	104.71	106.71
24	C	506	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	C	508	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	c	903	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	c	911	CLA	CHD-C1D-ND	-4.44	120.38	124.45
24	b	613	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	B	617	CLA	C4A-NA-C1A	-4.43	104.71	106.71
24	c	909	CLA	CHD-C1D-ND	-4.43	120.39	124.45
24	d	401	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
40	v	202	HEC	C4B-NB-C1B	4.42	109.64	105.07
24	B	609	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
24	C	505	CLA	C3D-C4D-ND	4.41	117.37	110.24
24	B	605	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
24	B	617	CLA	C1D-CHD-C4C	-4.40	116.56	126.06
24	C	509	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
24	A	410	CLA	C4A-NA-C1A	-4.40	104.73	106.71
24	B	610	CLA	C3C-C4C-NC	4.40	115.50	110.57
24	b	607	CLA	C3B-C2B-C1B	-4.40	101.86	107.16
24	B	607	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	D	402	CLA	C3B-C2B-C1B	-4.39	101.87	107.16
24	b	613	CLA	C3D-C2D-C1D	-4.39	99.85	105.83
24	b	608	CLA	C3C-C4C-NC	4.38	115.49	110.57
24	B	609	CLA	O2D-CGD-CBD	4.38	119.06	111.27
24	d	401	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
24	c	904	CLA	C1D-CHD-C4C	-4.38	116.61	126.06
24	b	605	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
24	b	618	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
24	b	619	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
24	c	914	CLA	C4A-NA-C1A	-4.37	104.74	106.71
24	a	407	CLA	C1D-CHD-C4C	-4.36	116.64	126.06
24	B	611	CLA	O2D-CGD-CBD	4.36	119.02	111.27
24	d	402	CLA	C3B-C2B-C1B	-4.36	101.89	107.16
24	C	512	CLA	C3B-C4B-NB	4.36	114.56	110.52
24	d	401	CLA	C3D-C4D-ND	4.36	117.29	110.24
24	c	906	CLA	C3B-C4B-NB	4.36	114.56	110.52
24	B	614	CLA	C3B-C4B-NB	4.35	114.55	110.52
36	d	406	DGD	O2G-C1B-C2B	4.35	120.88	111.50
24	B	602	CLA	C4A-NA-C1A	-4.35	104.75	106.71
24	d	401	CLA	C4A-NA-C1A	-4.35	104.75	106.71
25	a	420	PHO	O2D-CGD-O1D	-4.34	115.35	123.84
24	b	614	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
31	a	417	PL9	C15-C14-C16	4.34	122.57	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	402	CLA	C3D-C4D-ND	4.34	117.26	110.24
24	b	619	CLA	O2D-CGD-CBD	4.33	118.97	111.27
24	d	403	CLA	C3C-C4C-NC	4.33	115.43	110.57
34	C	521	LMG	O7-C10-C11	4.33	120.83	111.50
26	y	101	BCR	C15-C14-C13	-4.33	121.13	127.31
24	c	904	CLA	C3C-C4C-NC	4.33	115.42	110.57
24	c	909	CLA	C3D-C4D-ND	4.33	117.23	110.24
24	A	407	CLA	C2C-C1C-NC	4.32	114.02	109.97
24	c	905	CLA	C4A-NA-C1A	-4.32	104.76	106.71
24	C	514	CLA	C3D-C4D-ND	4.31	117.21	110.24
24	C	503	CLA	CHD-C1D-ND	-4.31	120.49	124.45
24	B	608	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
36	c	917	DGD	O2G-C1B-C2B	4.31	120.79	111.50
24	b	605	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
34	C	501	LMG	O7-C10-C11	4.29	120.76	111.50
24	C	505	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
26	t	101	BCR	C33-C5-C6	-4.29	119.71	124.53
24	B	604	CLA	C3D-C4D-ND	4.29	117.18	110.24
24	C	510	CLA	C4A-NA-C1A	-4.29	104.78	106.71
24	C	512	CLA	C4A-NA-C1A	-4.29	104.78	106.71
24	a	406	CLA	C3B-C2B-C1B	-4.28	101.99	107.16
24	C	514	CLA	C4A-NA-C1A	-4.28	104.78	106.71
24	b	610	CLA	C3C-C4C-NC	4.28	115.38	110.57
27	F	101	SQD	C44-O6-C1	-4.28	105.38	113.74
24	C	512	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	b	618	CLA	O2D-CGD-O1D	-4.27	115.48	123.84
31	a	417	PL9	C32-C33-C34	-4.27	117.38	127.66
24	b	610	CLA	CMC-C2C-C1C	4.27	131.54	125.04
24	c	905	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	a	409	CLA	C3D-C2D-C1D	-4.26	100.01	105.83
24	b	614	CLA	C3C-C4C-NC	4.26	115.35	110.57
24	B	611	CLA	C3C-C4C-NC	4.26	115.35	110.57
24	C	509	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
24	c	911	CLA	C3C-C4C-NC	4.24	115.33	110.57
24	c	909	CLA	C3B-C4B-NB	4.24	114.45	110.52
35	C	524	HTG	C1-O5-C5	4.24	120.40	112.58
24	b	612	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
24	b	613	CLA	C3D-C4D-ND	4.24	117.09	110.24
24	d	403	CLA	C3D-C4D-ND	4.24	117.09	110.24
24	C	511	CLA	C3C-C4C-NC	4.24	115.32	110.57
26	D	403	BCR	C24-C23-C22	-4.24	119.83	126.23
24	C	502	CLA	C3D-C4D-ND	4.24	117.09	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	913	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	D	402	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	a	409	CLA	CHD-C1D-ND	-4.23	120.57	124.45
24	B	610	CLA	O2D-CGD-CBD	4.22	118.77	111.27
24	b	619	CLA	CAC-C3C-C4C	4.22	130.28	124.81
24	C	506	CLA	C3D-C4D-ND	4.22	117.06	110.24
37	l	101	LHG	O7-C7-C8	4.22	120.59	111.50
24	A	406	CLA	C3D-C4D-ND	4.21	117.06	110.24
24	B	609	CLA	C3C-C4C-NC	4.21	115.30	110.57
24	B	615	CLA	C3D-C4D-ND	4.21	117.05	110.24
24	a	406	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
24	c	911	CLA	C3D-C4D-ND	4.21	117.05	110.24
24	d	401	CLA	CMB-C2B-C1B	4.21	131.78	125.37
24	A	406	CLA	C3B-C4B-NB	4.21	114.42	110.52
24	b	612	CLA	O2D-CGD-CBD	4.21	118.74	111.27
24	b	611	CLA	C3D-C4D-ND	4.20	117.04	110.24
24	c	907	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
29	B	623	LMT	O1B-C4'-C3'	4.19	118.44	107.28
24	B	604	CLA	C1D-CHD-C4C	-4.19	117.01	126.06
25	a	420	PHO	C3D-C4D-ND	4.19	113.43	107.72
24	D	401	CLA	C3D-C4D-ND	4.18	117.00	110.24
38	E	103	HEM	CAD-CBD-CGD	4.18	122.60	113.60
24	c	911	CLA	C1-C2-C3	-4.18	118.81	126.04
40	v	202	HEC	C4C-NC-C1C	4.18	109.44	105.35
24	B	603	CLA	C3D-C4D-ND	4.18	117.00	110.24
24	C	507	CLA	C4A-NA-C1A	-4.18	104.83	106.71
24	B	611	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
24	A	410	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
24	D	402	CLA	O2D-CGD-CBD	4.18	118.69	111.27
24	C	503	CLA	O2D-CGD-CBD	4.18	118.69	111.27
24	C	509	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
34	Z	101	LMG	O7-C10-C11	4.17	120.49	111.50
24	A	410	CLA	C3D-C4D-ND	4.17	116.98	110.24
24	c	905	CLA	C3D-C4D-ND	4.16	116.97	110.24
24	C	503	CLA	C1-C2-C3	-4.16	118.86	126.04
24	b	617	CLA	CHD-C1D-ND	-4.15	120.64	124.45
24	B	615	CLA	O2D-CGD-O1D	-4.15	115.72	123.84
24	b	609	CLA	C1D-CHD-C4C	-4.15	117.10	126.06
24	a	409	CLA	C1-C2-C3	-4.15	118.87	126.04
24	C	502	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
24	b	618	CLA	C3D-C4D-ND	4.15	116.94	110.24
24	C	509	CLA	C3D-C2D-C1D	-4.15	100.17	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	C3D-C4D-ND	4.15	116.94	110.24
24	A	406	CLA	C4-C3-C5	4.14	122.24	115.27
24	b	608	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
24	B	609	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
24	C	514	CLA	C3C-C4C-NC	4.13	115.21	110.57
24	D	401	CLA	C3B-C4B-NB	4.13	114.34	110.52
24	b	608	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
24	c	907	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
24	A	406	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
24	b	615	CLA	CAC-C3C-C4C	4.11	130.15	124.81
24	C	511	CLA	C3D-C4D-ND	4.11	116.89	110.24
34	a	412	LMG	O7-C10-C11	4.11	120.36	111.50
24	c	902	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
24	c	908	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
24	c	904	CLA	O2D-CGD-CBD	4.11	118.57	111.27
24	b	613	CLA	CMC-C2C-C1C	4.11	131.29	125.04
24	b	619	CLA	C3C-C4C-NC	4.11	115.17	110.57
24	b	610	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
24	c	905	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
35	V	202	HTG	C1'-S1-C1	4.10	107.76	100.09
24	B	606	CLA	C3D-C4D-ND	4.10	116.87	110.24
24	d	403	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
24	B	613	CLA	C3D-C4D-ND	4.10	116.87	110.24
24	B	606	CLA	O2D-CGD-O1D	-4.10	115.83	123.84
24	c	910	CLA	C3C-C4C-NC	4.09	115.16	110.57
34	B	622	LMG	O7-C10-C11	4.09	120.32	111.50
24	b	606	CLA	C3D-C4D-ND	4.09	116.86	110.24
24	D	402	CLA	CMB-C2B-C1B	4.09	131.60	125.37
24	b	609	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
24	c	908	CLA	C4A-NA-C1A	-4.09	104.87	106.71
24	C	509	CLA	C3C-C4C-NC	4.09	115.16	110.57
24	C	502	CLA	CBC-CAC-C3C	-4.09	101.16	112.43
27	F	101	SQD	O7-S-C6	4.09	111.80	106.94
24	c	903	CLA	C3D-C4D-ND	4.09	116.85	110.24
24	b	607	CLA	C3D-C2D-C1D	-4.09	100.26	105.83
24	c	902	CLA	C4A-NA-C1A	-4.08	104.87	106.71
24	c	912	CLA	C3C-C4C-NC	4.08	115.15	110.57
24	A	406	CLA	C4A-NA-C1A	-4.08	104.87	106.71
24	B	616	CLA	C3C-C4C-NC	4.08	115.14	110.57
24	C	508	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
31	A	419	PL9	C27-C28-C29	-4.07	117.86	127.66
24	A	406	CLA	CMA-C3A-C4A	-4.07	100.84	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	512	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
24	b	615	CLA	C3D-C4D-ND	4.07	116.81	110.24
35	c	923	HTG	C1-O5-C5	4.06	120.07	112.58
24	b	612	CLA	C3D-C4D-ND	4.06	116.81	110.24
24	C	510	CLA	C3C-C4C-NC	4.05	115.12	110.57
24	B	615	CLA	C3C-C4C-NC	4.05	115.12	110.57
24	B	611	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
24	C	505	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
31	a	417	PL9	C37-C38-C39	-4.05	117.92	127.66
24	c	912	CLA	C3D-C2D-C1D	-4.05	100.31	105.83
24	b	617	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	c	902	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	C	507	CLA	C3D-C4D-ND	4.04	116.77	110.24
24	c	906	CLA	C3D-C4D-ND	4.04	116.77	110.24
24	B	606	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
24	c	911	CLA	C3B-C2B-C1B	-4.03	102.29	107.16
24	B	605	CLA	C4A-NA-C1A	-4.03	104.89	106.71
24	d	403	CLA	C3B-C4B-NB	4.03	114.26	110.52
24	C	511	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
24	b	607	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
24	c	910	CLA	C3D-C4D-ND	4.03	116.76	110.24
31	A	419	PL9	C37-C38-C39	-4.03	117.96	127.66
24	A	407	CLA	C1D-CHD-C4C	-4.03	117.37	126.06
37	d	409	LHG	O7-C7-C8	4.02	120.17	111.50
36	C	517	DGD	O2G-C1B-C2B	4.02	120.17	111.50
24	B	614	CLA	C3D-C4D-ND	4.02	116.75	110.24
24	C	512	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	C	513	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
24	c	902	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	A	407	CLA	CBC-CAC-C3C	-4.02	101.35	112.43
24	B	613	CLA	C3D-C2D-C1D	-4.01	100.35	105.83
24	b	610	CLA	C3D-C4D-ND	4.01	116.73	110.24
38	E	103	HEM	CHD-C4C-NC	4.01	128.78	124.44
38	e	102	HEM	CAD-CBD-CGD	4.00	122.22	113.60
24	d	401	CLA	CHB-C1B-NB	-4.00	120.02	124.26
24	a	407	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	A	405	CLA	C3D-C4D-ND	4.00	116.70	110.24
27	B	621	SQD	O7-S-C6	3.99	111.68	106.94
24	b	609	CLA	C3D-C4D-ND	3.99	116.69	110.24
24	c	913	CLA	C3C-C4C-NC	3.99	115.05	110.57
24	d	402	CLA	O2D-CGD-O1D	-3.99	116.04	123.84
24	C	510	CLA	CAC-C3C-C4C	3.99	129.98	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	C3D-C4D-ND	3.99	116.69	110.24
26	c	915	BCR	C7-C8-C9	-3.99	120.21	126.23
24	d	402	CLA	CAC-C3C-C4C	3.98	129.98	124.81
24	b	611	CLA	C3B-C2B-C1B	-3.98	102.35	107.16
24	a	406	CLA	C3B-C4B-NB	3.98	114.21	110.52
24	C	504	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
24	c	906	CLA	CAC-C3C-C4C	3.98	129.97	124.81
24	B	617	CLA	CHD-C1D-ND	-3.98	120.80	124.45
26	T	102	BCR	C33-C5-C6	-3.98	120.06	124.53
24	C	505	CLA	C3C-C4C-NC	3.97	115.03	110.57
24	b	609	CLA	CMB-C2B-C1B	3.97	131.42	125.37
24	c	913	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
24	C	502	CLA	C3C-C4C-NC	3.97	115.02	110.57
24	c	914	CLA	C3C-C4C-NC	3.97	115.02	110.57
24	B	610	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
24	a	409	CLA	C1C-C2C-C3C	-3.97	102.79	106.96
24	b	608	CLA	CAC-C3C-C4C	3.96	129.95	124.81
24	a	407	CLA	C3D-C4D-ND	3.96	116.65	110.24
24	c	911	CLA	C1D-CHD-C4C	-3.96	117.53	126.06
26	C	515	BCR	C7-C8-C9	-3.95	120.26	126.23
24	b	607	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
24	a	409	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
29	C	522	LMT	C1'-O5'-C5'	3.95	121.43	113.69
24	b	612	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	b	607	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	c	908	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
24	B	606	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
24	B	614	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
24	C	508	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
27	A	412	SQD	C1-O5-C5	-3.94	105.96	113.69
24	b	619	CLA	C3D-C4D-ND	3.94	116.61	110.24
24	C	503	CLA	C3D-C4D-ND	3.94	116.61	110.24
24	b	608	CLA	C1-C2-C3	-3.93	119.24	126.04
26	D	403	BCR	C28-C27-C26	-3.93	107.06	114.08
24	C	513	CLA	C3D-C4D-ND	3.93	116.60	110.24
24	b	609	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	b	605	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	b	616	CLA	C3D-C4D-ND	3.92	116.58	110.24
24	B	606	CLA	CHD-C1D-ND	-3.92	120.85	124.45
24	C	510	CLA	C1-C2-C3	-3.91	119.27	126.04
24	c	912	CLA	O2D-CGD-CBD	3.91	118.22	111.27
24	c	906	CLA	C3D-C2D-C1D	-3.91	100.50	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	607	CLA	C3D-C4D-ND	3.91	116.56	110.24
24	c	907	CLA	C3B-C4B-NB	3.90	114.14	110.52
27	F	101	SQD	C1-C2-C3	-3.90	101.88	110.00
24	A	405	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
26	h	101	BCR	C38-C26-C25	-3.90	120.15	124.53
24	C	507	CLA	C3B-C4B-NB	3.89	114.12	110.52
24	B	617	CLA	C3D-C4D-ND	3.89	116.53	110.24
26	B	620	BCR	C38-C26-C25	-3.89	120.16	124.53
24	B	608	CLA	C3B-C2B-C1B	-3.89	102.47	107.16
38	e	102	HEM	C1B-NB-C4B	3.89	109.09	105.07
24	b	620	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
40	v	202	HEC	CHC-C4B-NB	3.87	129.15	124.37
24	B	608	CLA	C3C-C4C-NC	3.87	114.91	110.57
24	D	401	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
24	B	602	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
24	b	606	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
24	B	607	CLA	C3B-C4B-NB	3.86	114.09	110.52
24	b	618	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
24	B	607	CLA	C3D-C4D-ND	3.86	116.48	110.24
24	C	510	CLA	C3D-C4D-ND	3.85	116.47	110.24
24	B	613	CLA	CMC-C2C-C1C	3.85	130.91	125.04
24	c	904	CLA	C3D-C4D-ND	3.85	116.47	110.24
24	c	911	CLA	C3D-C2D-C1D	-3.85	100.58	105.83
24	B	602	CLA	C3C-C4C-NC	3.85	114.89	110.57
24	D	402	CLA	C4A-NA-C1A	-3.85	104.98	106.71
36	d	406	DGD	C3E-C4E-C5E	3.85	117.10	110.24
24	b	612	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	c	907	CLA	C3C-C4C-NC	3.84	114.88	110.57
38	e	102	HEM	C4C-NC-C1C	3.84	109.11	105.35
24	C	514	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
24	c	910	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
24	A	407	CLA	CMB-C2B-C1B	3.84	131.21	125.37
24	a	409	CLA	C3D-C4D-ND	3.84	116.44	110.24
24	b	615	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
24	b	620	CLA	C3B-C4B-NB	3.83	114.07	110.52
40	v	202	HEC	CBC-CAC-C3C	3.83	122.98	112.43
26	b	621	BCR	C33-C5-C6	-3.83	120.23	124.53
29	B	623	LMT	C3B-C4B-C5B	3.83	117.06	110.24
40	V	201	HEC	CBC-CAC-C3C	3.82	122.96	112.43
24	c	910	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
24	b	616	CLA	C4C-C3C-C2C	-3.82	101.33	106.90
24	B	604	CLA	C4-C3-C5	3.82	121.69	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	E	103	HEM	C1B-NB-C4B	3.82	109.01	105.07
25	a	420	PHO	C1-C2-C3	-3.81	119.45	126.04
24	b	606	CLA	CAA-C2A-C3A	-3.81	102.34	112.78
26	d	404	BCR	C7-C8-C9	-3.81	120.48	126.23
24	C	503	CLA	CMB-C2B-C1B	3.81	131.17	125.37
24	b	605	CLA	C3C-C4C-NC	3.81	114.84	110.57
24	A	405	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
24	C	508	CLA	C3D-C4D-ND	3.80	116.38	110.24
24	D	401	CLA	C1-C2-C3	-3.80	119.48	126.04
24	b	605	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
24	b	611	CLA	C4A-NA-C1A	-3.79	105.00	106.71
24	b	611	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	c	907	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
24	a	406	CLA	CAC-C3C-C4C	3.79	129.73	124.81
24	C	502	CLA	C3B-C4B-NB	3.79	114.03	110.52
29	C	522	LMT	O1B-C4'-C3'	3.79	117.36	107.28
24	b	614	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	b	606	CLA	C4C-C3C-C2C	-3.78	101.39	106.90
24	b	615	CLA	C3B-C4B-NB	3.78	114.02	110.52
24	B	613	CLA	CAC-C3C-C4C	3.78	129.72	124.81
24	b	620	CLA	C3D-C4D-ND	3.78	116.35	110.24
24	B	617	CLA	CAC-C3C-C4C	3.78	129.71	124.81
24	B	608	CLA	C3D-C4D-ND	3.78	116.35	110.24
24	B	611	CLA	C3B-C4B-NB	3.78	114.02	110.52
24	B	616	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
24	b	614	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
24	b	612	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
24	C	503	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
25	A	408	PHO	O1D-CGD-CBD	-3.77	118.47	124.74
37	D	408	LHG	O7-C7-C8	3.77	119.62	111.50
24	B	605	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
24	b	608	CLA	C3D-C4D-ND	3.76	116.32	110.24
24	C	510	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	B	603	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
24	A	405	CLA	CAA-C2A-C3A	-3.75	102.50	112.78
27	A	412	SQD	C1-C2-C3	-3.75	102.18	110.00
24	C	504	CLA	C1-C2-C3	-3.75	119.56	126.04
24	B	606	CLA	CMB-C2B-C1B	3.75	131.08	125.37
24	b	617	CLA	O2D-CGD-CBD	3.75	117.93	111.27
27	A	416	SQD	O47-C7-C8	3.74	119.57	111.50
24	B	617	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
24	c	914	CLA	C1C-C2C-C3C	-3.74	103.02	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	912	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
24	B	616	CLA	O2D-CGD-CBD	3.74	117.91	111.27
24	C	506	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
24	c	902	CLA	C3B-C4B-NB	3.74	113.98	110.52
35	B	624	HTG	C1'-S1-C1	3.73	107.08	100.09
24	B	602	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
24	c	904	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
24	C	503	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
24	b	610	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
35	b	602	HTG	C1'-S1-C1	3.72	107.05	100.09
34	z	101	LMG	O6-C5-C4	3.72	116.45	109.69
24	C	511	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
24	b	606	CLA	CAC-C3C-C4C	3.72	129.63	124.81
24	a	406	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
24	c	909	CLA	CAC-C3C-C4C	3.71	129.63	124.81
24	b	611	CLA	C3B-C4B-NB	3.70	113.95	110.52
24	C	514	CLA	C1-C2-C3	-3.69	119.66	126.04
24	c	913	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
34	z	101	LMG	O7-C10-C11	3.69	119.45	111.50
24	C	511	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	B	612	CLA	C3C-C4C-NC	3.69	114.71	110.57
24	b	617	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
24	C	502	CLA	CMC-C2C-C1C	3.69	130.65	125.04
36	c	918	DGD	O2G-C1B-C2B	3.68	119.44	111.50
24	a	409	CLA	CAA-C2A-C3A	-3.68	102.69	112.78
24	c	903	CLA	CMB-C2B-C1B	3.68	130.98	125.37
24	d	401	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
40	v	202	HEC	CHB-C1B-NB	3.68	128.42	124.42
24	C	513	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	C	505	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
24	c	910	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
24	b	620	CLA	CAC-C3C-C4C	3.68	129.58	124.81
27	L	102	SQD	C3-C4-C5	3.68	116.80	110.24
24	B	612	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
27	a	411	SQD	C1-O5-C5	-3.67	106.48	113.69
24	C	505	CLA	C1D-CHD-C4C	-3.66	118.15	126.06
24	c	914	CLA	O2D-CGD-CBD	3.66	117.78	111.27
24	b	607	CLA	CAA-C2A-C3A	-3.66	102.75	112.78
24	B	616	CLA	C3D-C4D-ND	3.66	116.16	110.24
24	B	611	CLA	C4C-C3C-C2C	-3.66	101.56	106.90
40	v	202	HEC	CHA-C4D-ND	3.66	128.39	124.42
38	e	102	HEM	CHD-C4C-NC	3.66	128.40	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k	102	BCR	C20-C21-C22	-3.66	122.09	127.31
24	A	406	CLA	CHD-C4C-NC	3.66	129.96	124.20
24	A	406	CLA	CBC-CAC-C3C	-3.65	102.36	112.43
26	B	618	BCR	C33-C5-C6	-3.65	120.42	124.53
24	b	610	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
24	B	617	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
24	B	609	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
24	d	403	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
24	c	908	CLA	C3D-C4D-ND	3.65	116.14	110.24
35	V	202	HTG	C1-C2-C3	-3.65	103.38	110.59
24	C	505	CLA	C3B-C4B-NB	3.65	113.90	110.52
24	d	403	CLA	O2D-CGD-CBD	3.65	117.75	111.27
31	a	417	PL9	C27-C28-C29	-3.65	118.88	127.66
24	C	509	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
24	B	617	CLA	C3B-C4B-NB	3.64	113.90	110.52
24	b	616	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
24	c	913	CLA	CMB-C2B-C1B	3.64	130.91	125.37
24	c	914	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
24	b	613	CLA	CAC-C3C-C4C	3.64	129.53	124.81
24	B	615	CLA	C3B-C4B-NB	3.64	113.89	110.52
24	A	410	CLA	CMC-C2C-C1C	3.64	130.58	125.04
24	B	603	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
25	A	408	PHO	C1-C2-C3	-3.63	119.77	126.04
24	A	410	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
26	H	101	BCR	C38-C26-C25	-3.62	120.46	124.53
24	B	607	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
24	a	407	CLA	CAC-C3C-C4C	3.62	129.50	124.81
24	c	903	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	c	906	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
24	b	613	CLA	C3B-C2B-C1B	-3.61	102.81	107.16
34	B	622	LMG	O8-C28-C29	3.61	123.22	111.91
24	b	607	CLA	C4-C3-C5	3.61	121.34	115.27
24	B	604	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
24	d	401	CLA	C3C-C4C-NC	3.60	114.61	110.57
24	c	906	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
24	C	507	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
24	b	618	CLA	C3B-C4B-NB	3.60	113.85	110.52
24	A	410	CLA	C3C-C4C-NC	3.60	114.61	110.57
24	B	609	CLA	C3B-C4B-NB	3.59	113.85	110.52
24	C	506	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
24	C	502	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
24	B	604	CLA	O2D-CGD-O1D	-3.59	116.82	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407	CLA	CAC-C3C-C4C	3.59	129.47	124.81
26	K	103	BCR	C20-C21-C22	-3.59	122.19	127.31
25	A	409	PHO	C1A-C2A-C3A	-3.58	99.43	102.84
24	b	611	CLA	CAA-C2A-C3A	-3.58	102.97	112.78
36	c	916	DGD	O2G-C1B-C2B	3.58	119.22	111.50
38	E	103	HEM	CBD-CAD-C3D	-3.58	102.69	112.63
26	D	403	BCR	C38-C26-C25	-3.58	120.51	124.53
27	a	411	SQD	C45-O47-C7	-3.57	108.99	117.79
36	D	405	DGD	C1D-C2D-C3D	3.57	117.44	110.00
40	V	201	HEC	C4C-NC-C1C	3.57	108.84	105.35
27	A	416	SQD	O48-C23-C24	3.57	123.10	111.91
24	b	619	CLA	C4-C3-C5	3.57	121.27	115.27
24	B	611	CLA	C3D-C4D-ND	3.56	116.00	110.24
26	k	101	BCR	C15-C14-C13	-3.56	122.23	127.31
24	B	612	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
37	E	101	LHG	O7-C7-C8	3.56	119.17	111.50
26	b	623	BCR	C3-C4-C5	-3.56	107.72	114.08
24	c	908	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
24	B	604	CLA	CAA-C2A-C3A	-3.56	103.04	112.78
29	b	601	LMT	O5'-C5'-C4'	3.56	117.25	109.75
38	E	103	HEM	C4C-NC-C1C	3.55	108.83	105.35
26	a	410	BCR	C7-C8-C9	-3.55	120.87	126.23
24	C	510	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
24	b	620	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
24	c	911	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
24	b	617	CLA	C3D-C4D-ND	3.55	115.97	110.24
24	b	619	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
24	c	903	CLA	O2D-CGD-O1D	-3.55	116.91	123.84
24	b	607	CLA	O2A-CGA-O1A	-3.55	114.64	123.59
24	c	903	CLA	C1D-CHD-C4C	-3.55	118.41	126.06
24	c	911	CLA	C3B-C4B-NB	3.55	113.80	110.52
27	F	101	SQD	C1-O5-C5	-3.54	106.73	113.69
24	C	510	CLA	C3B-C4B-NB	3.54	113.80	110.52
24	A	407	CLA	C3C-C4C-NC	3.54	114.54	110.57
24	b	619	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
34	c	919	LMG	O7-C10-C11	3.54	119.14	111.50
24	C	512	CLA	CAC-C3C-C4C	3.54	129.41	124.81
24	a	407	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
31	A	419	PL9	C7-C8-C9	-3.54	120.90	126.79
24	c	905	CLA	C3B-C4B-NB	3.54	113.80	110.52
24	c	907	CLA	C3D-C4D-ND	3.54	115.96	110.24
24	C	506	CLA	O2D-CGD-O1D	-3.53	116.93	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	CAC-C3C-C4C	3.53	129.39	124.81
24	c	907	CLA	C1-C2-C3	-3.53	119.94	126.04
24	d	402	CLA	C3B-C4B-NB	3.53	113.79	110.52
25	a	408	PHO	CMA-C3A-C4A	-3.52	106.66	114.38
24	b	618	CLA	C4C-C3C-C2C	-3.52	101.76	106.90
24	c	908	CLA	C3B-C4B-NB	3.52	113.78	110.52
24	C	512	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
24	C	511	CLA	C1-C2-C3	-3.52	119.95	126.04
24	b	608	CLA	CMC-C2C-C1C	3.52	130.40	125.04
24	b	607	CLA	C3B-C4B-NB	3.52	113.78	110.52
24	b	607	CLA	O2A-CGA-CBA	3.52	122.96	111.91
24	B	607	CLA	CMC-C2C-C1C	3.52	130.40	125.04
24	b	615	CLA	CMB-C2B-C1B	3.51	130.72	125.37
24	c	907	CLA	CBC-CAC-C3C	-3.51	102.75	112.43
37	e	101	LHG	O7-C7-C8	3.51	119.07	111.50
24	c	902	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
24	b	619	CLA	C1-C2-C3	-3.51	119.98	126.04
24	b	606	CLA	C3B-C4B-NB	3.51	113.77	110.52
24	C	514	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
24	B	615	CLA	CHD-C4C-NC	3.50	129.72	124.20
24	b	605	CLA	CHD-C4C-NC	3.50	129.72	124.20
31	D	404	PL9	C7-C8-C9	-3.50	120.96	126.79
24	B	612	CLA	CAC-C3C-C4C	3.50	129.35	124.81
24	A	407	CLA	C4-C3-C5	3.49	121.15	115.27
24	a	406	CLA	CAA-C2A-C3A	-3.49	103.21	112.78
24	c	909	CLA	C1-C2-C3	-3.49	120.01	126.04
24	B	611	CLA	CHC-C1C-C2C	-3.49	117.04	126.73
24	C	505	CLA	C4-C3-C5	3.49	121.14	115.27
24	b	615	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
24	a	406	CLA	CHC-C1C-C2C	-3.49	117.04	126.73
24	A	406	CLA	CAA-C2A-C3A	-3.49	103.23	112.78
40	V	201	HEC	CHC-C4B-NB	3.48	128.67	124.37
24	c	906	CLA	C4A-NA-C1A	-3.48	105.14	106.71
24	B	610	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
24	b	617	CLA	C3B-C4B-NB	3.48	113.74	110.52
31	a	417	PL9	C22-C23-C24	-3.48	119.29	127.66
24	B	608	CLA	CAA-C2A-C3A	-3.47	103.28	112.78
24	c	909	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
24	D	401	CLA	C3B-C2B-C1B	-3.47	102.97	107.16
25	a	420	PHO	C4-C3-C5	3.47	121.11	115.27
24	B	616	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
24	B	608	CLA	C3B-C4B-NB	3.46	113.73	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
24	C	506	CLA	C3D-C2D-C1D	-3.46	101.11	105.83
24	c	909	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
24	B	612	CLA	C3B-C4B-NB	3.46	113.72	110.52
24	d	402	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
24	B	610	CLA	C3B-C2B-C1B	-3.45	102.99	107.16
26	C	515	BCR	C38-C26-C25	-3.45	120.65	124.53
24	a	409	CLA	C4A-NA-C1A	-3.45	105.16	106.71
24	c	910	CLA	C1-C2-C3	-3.45	120.08	126.04
24	a	409	CLA	C3B-C4B-NB	3.45	113.71	110.52
24	b	607	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
24	C	506	CLA	CAC-C3C-C4C	3.44	129.28	124.81
24	b	619	CLA	CHC-C1C-C2C	-3.44	117.17	126.73
37	D	406	LHG	O8-C23-O10	-3.44	114.91	123.59
24	b	611	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
35	B	625	HTG	C1'-S1-C1	3.44	106.52	100.09
24	C	509	CLA	C3B-C4B-NB	3.43	113.70	110.52
24	B	603	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
26	c	915	BCR	C33-C5-C6	-3.43	120.68	124.53
29	B	623	LMT	C4B-C3B-C2B	3.43	116.81	110.82
31	d	405	PL9	C53-C6-C1	3.42	121.98	114.99
40	V	201	HEC	CHB-C1B-NB	3.42	128.13	124.42
24	C	511	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
24	d	402	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
24	A	406	CLA	O2A-CGA-O1A	-3.41	114.98	123.59
26	B	619	BCR	C29-C30-C25	3.41	115.73	110.48
24	A	405	CLA	C3B-C4B-NB	3.41	113.68	110.52
27	f	102	SQD	C1-O5-C5	3.41	120.38	113.69
24	c	909	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
24	C	504	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
34	C	520	LMG	O7-C10-C11	3.40	118.84	111.50
24	c	906	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
24	b	611	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
24	c	907	CLA	CAC-C3C-C4C	3.40	129.22	124.81
24	B	612	CLA	C1-C2-C3	-3.40	120.16	126.04
24	B	604	CLA	C3B-C4B-NB	3.40	113.67	110.52
24	b	616	CLA	CMB-C2B-C1B	3.40	130.54	125.37
24	C	504	CLA	C3B-C4B-NB	3.40	113.67	110.52
24	D	402	CLA	C4C-C3C-C2C	-3.40	101.95	106.90
24	C	502	CLA	CAC-C3C-C4C	3.40	129.22	124.81
24	b	616	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
24	C	502	CLA	O2D-CGD-O1D	-3.39	117.21	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	CMA-C3A-C4A	-3.39	102.66	111.77
34	c	920	LMG	C3-C4-C5	3.39	116.29	110.24
24	b	617	CLA	C4A-NA-C1A	-3.39	105.18	106.71
31	D	404	PL9	C53-C6-C1	3.39	121.92	114.99
24	B	613	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
24	B	606	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
24	B	614	CLA	C1-C2-C3	-3.38	120.19	126.04
26	k	102	BCR	C24-C23-C22	-3.38	121.13	126.23
24	b	617	CLA	C1-C2-C3	-3.38	120.20	126.04
24	A	410	CLA	CHD-C4C-NC	3.38	129.52	124.20
24	d	402	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
31	d	405	PL9	C10-C9-C11	3.36	120.93	115.27
34	C	520	LMG	O8-C28-C29	3.36	122.46	111.91
24	b	616	CLA	CAC-C3C-C4C	3.36	129.17	124.81
40	V	201	HEC	CHA-C1A-NA	3.36	128.07	124.44
24	B	611	CLA	CAC-C3C-C4C	3.36	129.17	124.81
24	B	616	CLA	CMB-C2B-C1B	3.36	130.48	125.37
24	B	605	CLA	C1-C2-C3	-3.36	120.24	126.04
24	C	506	CLA	CMB-C2B-C1B	3.36	130.48	125.37
25	a	408	PHO	C1A-C2A-C3A	-3.36	99.65	102.84
24	b	613	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
24	C	514	CLA	C3B-C4B-NB	3.35	113.62	110.52
24	C	509	CLA	C1-C2-C3	-3.35	120.25	126.04
24	B	613	CLA	C3B-C4B-NB	3.35	113.62	110.52
24	b	615	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
27	a	411	SQD	O47-C7-O49	-3.35	115.61	123.70
24	b	610	CLA	C3B-C4B-NB	3.34	113.62	110.52
24	b	607	CLA	CAC-C3C-C4C	3.34	129.15	124.81
24	d	401	CLA	CHC-C1C-C2C	-3.34	117.44	126.73
24	C	507	CLA	CHC-C1C-C2C	-3.34	117.45	126.73
27	A	412	SQD	C44-O6-C1	-3.34	107.21	113.74
24	C	510	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
24	B	605	CLA	C3B-C4B-NB	3.34	113.61	110.52
31	d	405	PL9	C7-C8-C9	-3.34	121.24	126.79
24	c	910	CLA	C3B-C4B-NB	3.34	113.61	110.52
24	c	910	CLA	CMC-C2C-C1C	3.34	130.12	125.04
35	c	923	HTG	O5-C1-C2	3.33	114.50	110.31
24	c	904	CLA	CAC-C3C-C4C	3.33	129.13	124.81
24	b	618	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
26	K	102	BCR	C38-C26-C25	-3.33	120.79	124.53
26	b	623	BCR	C38-C26-C25	-3.32	120.80	124.53
24	C	507	CLA	C3C-C4C-NC	3.32	114.30	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	402	CLA	O2A-CGA-CBA	3.32	122.33	111.91
24	a	407	CLA	CBC-CAC-C3C	-3.32	103.28	112.43
24	D	402	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
24	c	914	CLA	CAC-C3C-C4C	3.31	129.11	124.81
26	d	404	BCR	C33-C5-C6	-3.31	120.81	124.53
24	C	507	CLA	CBC-CAC-C3C	-3.31	103.32	112.43
24	a	406	CLA	C3C-C4C-NC	3.30	114.27	110.57
31	A	419	PL9	C20-C19-C21	3.30	120.82	115.27
24	D	401	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
36	C	518	DGD	O2G-C1B-C2B	3.30	118.60	111.50
31	A	419	PL9	C53-C6-C1	3.29	121.72	114.99
24	b	609	CLA	CMC-C2C-C1C	3.28	130.04	125.04
27	a	402	SQD	O47-C7-C8	3.28	118.58	111.50
24	B	615	CLA	CMC-C2C-C1C	3.28	130.03	125.04
24	D	402	CLA	C4-C3-C5	3.27	120.78	115.27
24	c	912	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
24	C	504	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
24	b	619	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
24	b	610	CLA	C4-C3-C5	3.26	120.76	115.27
24	A	410	CLA	O2D-CGD-CBD	3.25	117.05	111.27
24	B	610	CLA	CMC-C2C-C1C	3.25	129.99	125.04
24	C	513	CLA	CHD-C4C-NC	3.25	129.33	124.20
24	c	906	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
34	c	919	LMG	O8-C28-C29	3.25	122.11	111.91
24	c	905	CLA	CMC-C2C-C1C	3.25	129.98	125.04
24	B	607	CLA	C4-C3-C5	3.24	120.72	115.27
31	A	419	PL9	C22-C23-C24	-3.24	119.86	127.66
24	B	613	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
24	C	511	CLA	C3B-C4B-NB	3.24	113.52	110.52
24	B	613	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
37	d	407	LHG	O7-C7-C8	3.24	118.47	111.50
24	B	610	CLA	C3B-C4B-NB	3.23	113.52	110.52
24	c	904	CLA	C3B-C4B-NB	3.23	113.52	110.52
31	a	417	PL9	C7-C8-C9	-3.23	121.41	126.79
24	b	613	CLA	C1-C2-C3	-3.23	120.45	126.04
24	c	908	CLA	CMB-C2B-C1B	3.23	130.29	125.37
24	b	613	CLA	C1D-CHD-C4C	-3.23	119.08	126.06
24	c	906	CLA	CMB-C2B-C1B	3.23	130.28	125.37
37	D	406	LHG	O8-C23-C24	3.22	122.03	111.91
24	B	607	CLA	CAC-C3C-C4C	3.22	128.99	124.81
24	c	907	CLA	CHC-C1C-C2C	-3.22	117.78	126.73
24	D	401	CLA	C4C-C3C-C2C	-3.22	102.20	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	905	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
37	D	407	LHG	O7-C7-C8	3.22	118.44	111.50
24	c	909	CLA	C4-C3-C5	3.22	120.68	115.27
24	D	402	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
24	b	609	CLA	C4-C3-C5	3.21	120.68	115.27
24	d	401	CLA	C2A-C1A-CHA	-3.21	118.24	123.86
27	A	412	SQD	O48-C23-C24	3.21	121.99	111.91
24	b	617	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
24	b	608	CLA	C1D-CHD-C4C	-3.21	119.14	126.06
24	C	512	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
24	d	403	CLA	CAC-C3C-C4C	3.21	128.97	124.81
24	B	602	CLA	C3B-C4B-NB	3.20	113.49	110.52
24	C	512	CLA	O2D-CGD-CBD	3.20	116.96	111.27
24	D	402	CLA	C3B-C4B-NB	3.20	113.48	110.52
24	c	906	CLA	CHC-C1C-C2C	-3.20	117.84	126.73
24	A	406	CLA	C3C-C4C-NC	3.20	114.16	110.57
26	D	403	BCR	C15-C14-C13	-3.20	122.75	127.31
24	B	602	CLA	CMB-C2B-C1B	3.20	130.24	125.37
24	C	507	CLA	CMB-C2B-C1B	3.20	130.24	125.37
38	e	102	HEM	CBA-CAA-C2A	-3.20	103.75	112.63
40	v	202	HEC	C1D-ND-C4D	3.19	108.37	105.07
27	f	102	SQD	O5-C5-C4	3.19	115.50	109.69
24	C	507	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
37	d	408	LHG	O7-C7-C8	3.19	118.38	111.50
24	A	410	CLA	C4-C3-C5	3.19	120.64	115.27
24	C	509	CLA	C2A-C1A-CHA	-3.19	118.28	123.86
24	b	616	CLA	C4-C3-C5	3.19	120.64	115.27
24	B	604	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
37	E	101	LHG	O8-C23-C24	3.19	121.91	111.91
24	c	914	CLA	CMC-C2C-C1C	3.19	129.89	125.04
26	d	404	BCR	C29-C30-C25	3.18	115.38	110.48
24	a	407	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	B	614	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
35	V	202	HTG	O5-C1-C2	-3.18	106.32	110.31
34	b	624	LMG	O8-C28-C29	3.17	121.86	111.91
24	B	602	CLA	O2A-CGA-CBA	3.17	121.86	111.91
24	C	507	CLA	C1-C2-C3	-3.17	120.56	126.04
24	A	405	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
24	c	905	CLA	C1-C2-C3	-3.17	120.56	126.04
27	a	402	SQD	O48-C23-C24	3.16	121.82	111.91
24	b	614	CLA	C3B-C4B-NB	3.16	113.44	110.52
24	b	612	CLA	O2A-CGA-CBA	3.16	121.81	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	617	CLA	CMC-C2C-C1C	3.16	129.84	125.04
27	A	412	SQD	O8-S-C6	3.15	110.77	105.74
24	B	616	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	C	514	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
27	f	102	SQD	O7-S-C6	3.15	110.69	106.94
24	A	406	CLA	CHC-C1C-C2C	-3.15	117.98	126.73
26	c	915	BCR	C38-C26-C25	-3.15	120.99	124.53
26	d	404	BCR	C3-C4-C5	-3.15	108.45	114.08
24	B	604	CLA	O2A-CGA-CBA	3.15	121.80	111.91
24	d	403	CLA	CHC-C1C-C2C	-3.15	117.98	126.73
24	A	407	CLA	CHD-C4C-NC	3.15	129.17	124.20
24	A	405	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	b	617	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	C	503	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	D	401	CLA	CHC-C1C-C2C	-3.15	117.99	126.73
24	C	505	CLA	CMC-C2C-C1C	3.15	129.83	125.04
24	B	608	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
24	c	906	CLA	CHB-C1B-NB	-3.14	120.93	124.26
24	b	618	CLA	CAC-C3C-C4C	3.14	128.89	124.81
24	B	611	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
31	a	417	PL9	C10-C9-C11	3.14	120.55	115.27
38	e	102	HEM	CHD-C1D-ND	3.14	127.83	124.42
24	A	410	CLA	C3B-C4B-NB	3.14	113.43	110.52
26	H	101	BCR	C37-C22-C21	-3.13	118.54	122.92
24	c	909	CLA	CHC-C1C-C2C	-3.13	118.04	126.73
24	A	410	CLA	CMB-C2B-C1B	3.12	130.13	125.37
24	a	406	CLA	C2A-C1A-CHA	-3.12	118.40	123.86
24	d	401	CLA	CBC-CAC-C3C	-3.12	103.83	112.43
24	A	407	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
24	B	616	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
24	C	506	CLA	C4C-C3C-C2C	-3.12	102.36	106.90
24	C	503	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
24	A	406	CLA	CMC-C2C-C1C	3.11	129.78	125.04
24	c	912	CLA	C3B-C4B-NB	3.11	113.40	110.52
24	a	406	CLA	O2A-CGA-O1A	-3.11	115.74	123.59
24	C	512	CLA	C4-C3-C5	3.11	120.50	115.27
24	b	609	CLA	CHD-C4C-NC	3.11	129.10	124.20
24	D	401	CLA	CMB-C2B-C1B	3.11	130.10	125.37
24	C	504	CLA	C4-C3-C5	3.11	120.50	115.27
31	a	417	PL9	C30-C29-C31	3.10	120.49	115.27
24	B	616	CLA	CHD-C4C-NC	3.10	129.09	124.20
24	c	910	CLA	CAC-C3C-C4C	3.10	128.83	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	V	201	HEC	C2A-C1A-NA	-3.10	107.31	110.32
24	B	605	CLA	O2A-CGA-O1A	-3.10	115.77	123.59
24	B	613	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
38	E	103	HEM	CHB-C1B-NB	3.10	128.19	124.37
24	d	402	CLA	CHC-C1C-C2C	-3.10	118.13	126.73
26	b	622	BCR	C28-C27-C26	-3.09	108.55	114.08
27	a	411	SQD	O8-S-C6	3.09	110.67	105.74
31	a	417	PL9	C17-C18-C19	-3.09	120.21	127.66
24	B	611	CLA	CMB-C2B-C1B	3.09	130.08	125.37
24	a	406	CLA	CAA-C2A-C1A	-3.09	101.85	111.97
24	C	508	CLA	CMB-C2B-C1B	3.09	130.07	125.37
29	m	104	LMT	C1'-O5'-C5'	3.09	119.75	113.69
31	A	419	PL9	C32-C33-C34	-3.09	120.23	127.66
24	a	406	CLA	O2A-CGA-CBA	3.09	121.59	111.91
24	b	607	CLA	C5-C3-C2	-3.08	114.88	121.12
24	B	603	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
24	C	504	CLA	CAC-C3C-C4C	3.08	128.81	124.81
24	b	619	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
24	A	407	CLA	C3B-C4B-NB	3.08	113.37	110.52
24	c	909	CLA	C4A-NA-C1A	-3.08	105.32	106.71
24	C	509	CLA	CHC-C1C-C2C	-3.08	118.19	126.73
24	a	407	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
31	D	404	PL9	C10-C9-C11	3.07	120.44	115.27
31	a	417	PL9	C42-C43-C44	-3.07	120.27	127.66
26	k	101	BCR	C33-C5-C6	-3.07	121.08	124.53
24	B	610	CLA	CAC-C3C-C4C	3.07	128.79	124.81
24	b	605	CLA	C4-C3-C5	3.07	120.43	115.27
24	B	610	CLA	O2A-CGA-CBA	3.07	121.53	111.91
24	b	614	CLA	CAC-C3C-C4C	3.07	128.79	124.81
24	b	616	CLA	C1-C2-C3	-3.07	120.74	126.04
24	C	508	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	c	912	CLA	CAC-C3C-C4C	3.06	128.79	124.81
24	c	912	CLA	C1-C2-C3	-3.06	120.74	126.04
24	b	608	CLA	C3B-C4B-NB	3.06	113.36	110.52
24	b	614	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
24	C	503	CLA	C3B-C4B-NB	3.06	113.35	110.52
24	C	509	CLA	C4-C3-C5	3.06	120.41	115.27
24	B	612	CLA	C4-C3-C5	3.06	120.41	115.27
24	b	618	CLA	C2A-C1A-CHA	-3.06	118.52	123.86
24	c	903	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
24	B	614	CLA	C4-C3-C5	3.05	120.41	115.27
24	C	514	CLA	O2D-CGD-O1D	-3.05	117.87	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	610	CLA	CBC-CAC-C3C	-3.05	104.02	112.43
24	c	908	CLA	CAC-C3C-C4C	3.05	128.76	124.81
24	B	608	CLA	CAC-C3C-C4C	3.04	128.76	124.81
24	c	913	CLA	CHD-C4C-NC	3.04	129.00	124.20
24	b	615	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	b	612	CLA	C3B-C4B-NB	3.04	113.33	110.52
24	c	903	CLA	CAC-C3C-C4C	3.03	128.75	124.81
26	y	101	BCR	C40-C30-C25	-3.03	105.38	110.30
24	C	513	CLA	C1-C2-C3	-3.03	120.80	126.04
24	c	908	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
24	B	616	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
29	C	522	LMT	C2'-C3'-C4'	-3.03	102.77	109.68
24	a	409	CLA	CMB-C2B-C1B	3.03	129.98	125.37
24	b	620	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
24	B	611	CLA	CAA-C2A-C3A	-3.03	104.49	112.78
24	b	605	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
26	d	404	BCR	C38-C26-C25	-3.02	121.13	124.53
24	B	617	CLA	CHD-C4C-NC	3.02	128.97	124.20
26	H	101	BCR	C16-C17-C18	-3.02	123.00	127.31
24	C	503	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
24	c	914	CLA	CMB-C2B-C1B	3.02	129.97	125.37
24	a	409	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
24	b	606	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	B	612	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
24	c	913	CLA	CMC-C2C-C1C	3.01	129.62	125.04
24	B	616	CLA	C11-C10-C8	-3.01	106.19	115.92
24	b	612	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
24	b	617	CLA	CMB-C2B-C1B	3.01	129.95	125.37
24	c	902	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
24	c	904	CLA	CMC-C2C-C1C	3.01	129.62	125.04
24	b	610	CLA	O2A-CGA-O1A	-3.00	116.01	123.59
36	H	102	DGD	O1G-C1A-O1A	-3.00	116.01	123.59
24	c	912	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
31	A	419	PL9	C15-C14-C16	3.00	120.32	115.27
24	b	616	CLA	C3B-C4B-NB	3.00	113.30	110.52
24	b	612	CLA	C1-C2-C3	-3.00	120.86	126.04
24	B	608	CLA	CHC-C1C-C2C	-3.00	118.41	126.73
38	e	102	HEM	C4A-NA-C1A	3.00	108.28	105.35
24	C	506	CLA	C4-C3-C5	3.00	120.31	115.27
24	B	614	CLA	O2A-CGA-CBA	3.00	121.31	111.91
25	A	409	PHO	C4-C3-C5	2.99	120.31	115.27
24	B	613	CLA	C2A-C1A-CHA	-2.99	118.62	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	615	CLA	CBC-CAC-C3C	-2.99	104.18	112.43
24	B	602	CLA	CAC-C3C-C4C	2.99	128.69	124.81
24	b	614	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
24	a	409	CLA	CBC-CAC-C3C	-2.99	104.19	112.43
24	b	615	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
31	d	405	PL9	C27-C28-C29	-2.99	120.46	127.66
24	D	401	CLA	CAC-C3C-C4C	2.99	128.69	124.81
24	b	614	CLA	O2A-CGA-CBA	2.99	121.28	111.91
24	A	407	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
24	d	401	CLA	CAA-C2A-C3A	-2.98	104.60	112.78
24	B	615	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
24	b	613	CLA	O2A-CGA-O1A	-2.98	116.06	123.59
24	c	911	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	b	612	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	c	911	CLA	CAC-C3C-C4C	2.98	128.68	124.81
24	B	606	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
26	h	101	BCR	C7-C8-C9	-2.98	121.74	126.23
24	a	407	CLA	CHD-C4C-NC	2.98	128.89	124.20
24	b	607	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
24	c	908	CLA	CHC-C1C-C2C	-2.98	118.47	126.73
24	c	902	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
24	C	510	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
37	D	406	LHG	O7-C7-C8	2.97	117.91	111.50
24	B	611	CLA	O2A-CGA-CBA	2.97	121.24	111.91
26	b	623	BCR	C37-C22-C23	2.97	122.75	118.08
24	B	602	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
24	C	505	CLA	CAC-C3C-C4C	2.97	128.66	124.81
24	A	407	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
24	B	616	CLA	C3B-C4B-NB	2.96	113.26	110.52
24	C	512	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
26	b	622	BCR	C29-C30-C25	2.96	115.04	110.48
24	C	514	CLA	C4-C3-C5	2.96	120.25	115.27
31	D	404	PL9	C27-C28-C29	-2.96	120.53	127.66
24	C	514	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
24	b	612	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
24	B	609	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
24	C	506	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
37	L	101	LHG	O7-C7-C8	2.95	117.87	111.50
24	C	502	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
24	c	913	CLA	C3B-C4B-NB	2.95	113.25	110.52
24	c	905	CLA	CAC-C3C-C4C	2.95	128.64	124.81
24	B	616	CLA	CBC-CAC-C3C	-2.95	104.30	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	605	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
24	b	615	CLA	C1-C2-C3	-2.95	120.94	126.04
24	A	405	CLA	CAA-C2A-C1A	-2.95	102.31	111.97
35	D	411	HTG	C1'-S1-C1	2.95	105.61	100.09
24	C	513	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
24	C	507	CLA	CAC-C3C-C4C	2.95	128.63	124.81
24	b	613	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
24	a	406	CLA	O2D-CGD-CBD	2.95	116.50	111.27
24	d	401	CLA	CAC-C3C-C4C	2.94	128.63	124.81
24	c	914	CLA	O2A-CGA-CBA	2.94	121.14	111.91
24	b	611	CLA	CMC-C2C-C1C	2.94	129.52	125.04
24	B	603	CLA	C3B-C4B-NB	2.94	113.24	110.52
24	c	913	CLA	CBC-CAC-C3C	-2.94	104.32	112.43
24	B	605	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
24	c	907	CLA	CMC-C2C-C1C	2.94	129.52	125.04
25	A	408	PHO	CMA-C3A-C4A	-2.94	107.94	114.38
24	B	610	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	b	615	CLA	CMC-C2C-C1C	2.94	129.51	125.04
24	C	510	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
24	C	508	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
24	b	620	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
24	C	513	CLA	C3B-C4B-NB	2.94	113.24	110.52
24	b	608	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
24	C	503	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
24	c	909	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	c	914	CLA	C3B-C4B-NB	2.93	113.23	110.52
24	B	610	CLA	CHD-C4C-NC	2.93	128.82	124.20
24	C	508	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	c	905	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
24	a	409	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
24	b	613	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
24	B	603	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
24	B	614	CLA	C1D-CHD-C4C	-2.92	119.75	126.06
24	b	609	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	C	509	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
31	A	419	PL9	C10-C9-C11	2.92	120.19	115.27
24	B	604	CLA	CHD-C4C-NC	2.92	128.81	124.20
24	a	409	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
24	c	904	CLA	CMB-C2B-C1B	2.92	129.81	125.37
24	a	409	CLA	CHB-C4A-NA	2.92	128.55	124.51
31	a	417	PL9	C53-C6-C1	2.92	120.96	114.99
24	C	513	CLA	C1-O2A-CGA	2.92	124.10	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	CHD-C4C-NC	2.92	128.80	124.20
24	b	617	CLA	CHB-C1B-NB	-2.92	121.17	124.26
24	C	514	CLA	CAC-C3C-C4C	2.91	128.59	124.81
26	B	620	BCR	C24-C23-C22	-2.91	121.83	126.23
26	C	516	BCR	C15-C14-C13	-2.91	123.15	127.31
29	f	103	LMT	C1B-O5B-C5B	2.91	119.40	113.69
24	C	511	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	d	403	CLA	CMC-C2C-C1C	2.91	129.46	125.04
24	D	401	CLA	O2A-CGA-CBA	2.90	121.02	111.91
29	A	417	LMT	O5'-C5'-C4'	2.90	115.87	109.75
24	A	405	CLA	CMC-C2C-C1C	2.90	129.46	125.04
36	D	405	DGD	C4D-C3D-C2D	2.90	115.88	110.82
24	b	614	CLA	CMB-C2B-C1B	2.90	129.78	125.37
26	b	621	BCR	C7-C8-C9	-2.89	121.86	126.23
24	B	617	CLA	CMB-C2B-C1B	2.89	129.77	125.37
24	b	617	CLA	O2A-CGA-CBA	2.89	120.98	111.91
24	c	907	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	B	607	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
24	c	911	CLA	C4-C3-C5	2.89	120.13	115.27
24	c	904	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
26	t	101	BCR	C15-C16-C17	-2.88	117.56	123.47
25	a	420	PHO	C1A-C2A-C3A	-2.88	100.10	102.84
36	C	519	DGD	O3G-C3G-C2G	-2.88	103.95	110.90
24	B	602	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
29	C	522	LMT	C1B-O5B-C5B	2.88	119.34	113.69
34	J	101	LMG	O7-C10-C11	2.88	117.70	111.50
24	C	505	CLA	CBC-CAC-C3C	-2.87	104.51	112.43
26	d	404	BCR	C16-C17-C18	-2.87	123.21	127.31
35	B	626	HTG	O5-C1-C2	2.87	113.93	110.31
24	B	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	B	609	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	B	603	CLA	CHD-C4C-NC	2.87	128.72	124.20
24	B	609	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
36	h	102	DGD	O2G-C1B-C2B	2.87	117.68	111.50
24	b	614	CLA	C1-C2-C3	-2.87	121.08	126.04
26	C	516	BCR	C33-C5-C6	-2.87	121.31	124.53
24	B	616	CLA	CMC-C2C-C1C	2.87	129.40	125.04
24	C	511	CLA	CMC-C2C-C1C	2.87	129.40	125.04
24	B	615	CLA	C2A-C1A-CHA	-2.87	118.85	123.86
24	c	902	CLA	CAC-C3C-C4C	2.86	128.53	124.81
24	b	620	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
36	h	102	DGD	O1G-C1A-C2A	2.86	120.89	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	C	517	DGD	O3G-C3G-C2G	-2.86	103.99	110.90
24	B	611	CLA	C4-C3-C5	2.86	120.08	115.27
24	A	410	CLA	CBC-CAC-C3C	-2.86	104.54	112.43
24	d	403	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
31	D	404	PL9	C40-C39-C41	2.86	120.08	115.27
24	a	407	CLA	O2A-CGA-CBA	2.86	120.87	111.91
24	b	612	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
27	A	416	SQD	O48-C23-O10	-2.85	116.39	123.59
24	c	912	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
24	a	407	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
31	D	404	PL9	C42-C43-C44	-2.85	120.79	127.66
24	b	611	CLA	CAA-CBA-CGA	2.85	121.58	113.25
24	c	913	CLA	C1-C2-C3	-2.85	121.12	126.04
24	C	503	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
24	B	617	CLA	CHC-C1C-C2C	-2.85	118.83	126.73
24	b	618	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
24	B	612	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
40	V	201	HEC	CHD-C1D-ND	2.84	127.88	124.37
24	B	609	CLA	O2A-CGA-CBA	2.84	120.83	111.91
24	d	402	CLA	C1-C2-C3	-2.84	121.13	126.04
37	D	408	LHG	O8-C23-O10	-2.84	116.43	123.59
34	a	412	LMG	C8-O7-C10	-2.84	110.81	117.79
24	b	611	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
24	b	620	CLA	C1-C2-C3	-2.84	121.14	126.04
24	B	605	CLA	CHD-C4C-NC	2.84	128.67	124.20
24	b	610	CLA	CMB-C2B-C1B	2.84	129.69	125.37
24	A	407	CLA	CED-O2D-CGD	2.83	122.35	115.94
24	b	608	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	B	621	SQD	O48-C23-C24	2.83	120.79	111.91
37	d	407	LHG	O8-C23-C24	2.83	120.79	111.91
31	D	404	PL9	C20-C19-C21	2.83	120.03	115.27
24	c	913	CLA	C4-C3-C5	2.83	120.02	115.27
24	C	503	CLA	C4-C3-C5	2.82	120.02	115.27
36	H	102	DGD	O2G-C1B-C2B	2.82	117.58	111.50
31	a	417	PL9	C7-C3-C4	2.82	119.17	116.88
24	B	612	CLA	CMC-C2C-C1C	2.82	129.33	125.04
24	B	612	CLA	CMB-C2B-C1B	2.82	129.66	125.37
24	B	615	CLA	C4-C3-C5	2.82	120.01	115.27
24	b	607	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
24	c	902	CLA	CMC-C2C-C1C	2.82	129.33	125.04
24	B	610	CLA	CHC-C1C-C2C	-2.81	118.91	126.73
24	c	902	CLA	C1-O2A-CGA	2.81	123.82	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	O2A-CGA-CBA	2.81	120.73	111.91
40	V	201	HEC	CHA-C4D-ND	2.81	127.47	124.42
24	b	609	CLA	C3B-C4B-NB	2.81	113.12	110.52
24	A	406	CLA	CED-O2D-CGD	2.81	122.30	115.94
24	A	405	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
24	C	512	CLA	C1-O2A-CGA	2.81	123.81	116.44
24	c	904	CLA	C4-C3-C5	2.81	120.00	115.27
24	a	406	CLA	C4-C3-C5	2.81	119.99	115.27
24	B	614	CLA	CHC-C1C-C2C	-2.80	118.94	126.73
24	B	615	CLA	O2A-CGA-CBA	2.80	120.71	111.91
24	a	409	CLA	CHD-C4C-NC	2.80	128.62	124.20
24	B	606	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
25	A	409	PHO	CMB-C2B-C3B	2.80	129.92	124.68
24	B	602	CLA	CHD-C4C-NC	2.80	128.62	124.20
37	L	101	LHG	O8-C23-C24	2.80	120.69	111.91
24	d	402	CLA	C4-C3-C5	2.80	119.98	115.27
26	b	622	BCR	C38-C26-C25	-2.80	121.39	124.53
34	a	412	LMG	C7-O1-C1	-2.80	108.28	113.74
40	V	201	HEC	C1D-ND-C4D	2.80	107.96	105.07
24	c	912	CLA	CHD-C4C-NC	2.80	128.61	124.20
24	B	616	CLA	C1-C2-C3	-2.80	121.21	126.04
24	c	911	CLA	CMC-C2C-C1C	2.80	129.30	125.04
24	B	606	CLA	C3B-C4B-NB	2.80	113.11	110.52
38	e	102	HEM	CHB-C1B-NB	2.79	127.82	124.37
24	c	905	CLA	C4-C3-C5	2.79	119.97	115.27
24	c	914	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
24	d	402	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
24	c	911	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
24	C	508	CLA	C3B-C4B-NB	2.79	113.10	110.52
24	B	614	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
31	a	417	PL9	C25-C24-C26	2.79	119.96	115.27
24	A	407	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
24	c	905	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
24	D	402	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
24	c	904	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
24	c	912	CLA	O2A-CGA-CBA	2.78	120.64	111.91
24	c	914	CLA	C2A-C1A-CHA	-2.78	118.99	123.86
24	b	616	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
26	d	404	BCR	C38-C26-C27	2.78	118.95	113.62
24	a	407	CLA	CMB-C2B-C1B	2.78	129.60	125.37
24	c	908	CLA	O2A-CGA-CBA	2.78	120.62	111.91
24	C	510	CLA	CMB-C2B-C1B	2.78	129.60	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	c	910	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	B	616	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
24	b	611	CLA	C4-C3-C5	2.77	119.93	115.27
24	B	602	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	c	903	CLA	O2A-CGA-CBA	2.77	120.60	111.91
24	D	401	CLA	O2A-CGA-O1A	-2.77	116.60	123.59
24	c	907	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
24	C	509	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	B	606	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
24	A	406	CLA	CHB-C1B-NB	-2.76	121.33	124.26
34	c	920	LMG	O6-C5-C4	2.76	114.71	109.69
24	c	914	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
29	m	102	LMT	O5'-C5'-C4'	2.76	115.57	109.75
25	A	408	PHO	CMB-C2B-C3B	2.76	129.84	124.68
24	A	410	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
24	b	612	CLA	CHD-C4C-NC	2.75	128.54	124.20
24	C	504	CLA	CHC-C1C-C2C	-2.75	119.08	126.73
24	B	614	CLA	CED-O2D-CGD	2.75	122.16	115.94
24	c	904	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
34	b	624	LMG	O7-C10-C11	2.75	117.42	111.50
24	b	613	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
24	A	406	CLA	CHB-C4A-NA	2.75	128.31	124.51
31	A	419	PL9	C7-C3-C4	2.75	119.11	116.88
24	C	502	CLA	C1-C2-C3	-2.74	121.30	126.04
31	a	417	PL9	C20-C19-C21	2.74	119.89	115.27
24	b	606	CLA	CMB-C2B-C1B	2.74	129.55	125.37
38	E	103	HEM	C4A-NA-C1A	2.74	108.03	105.35
24	C	508	CLA	CBC-CAC-C3C	-2.74	104.87	112.43
27	a	402	SQD	O5-C5-C4	2.74	114.67	109.69
27	a	411	SQD	C44-O6-C1	-2.74	108.38	113.74
24	b	606	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
36	c	916	DGD	O5D-C6D-C5D	-2.74	103.98	109.05
24	c	905	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
24	b	610	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
26	b	623	BCR	C2-C1-C6	2.74	114.69	110.48
24	C	513	CLA	CHC-C1C-C2C	-2.74	119.13	126.73
24	C	506	CLA	C3B-C4B-NB	2.74	113.05	110.52
24	b	606	CLA	CHC-C1C-C2C	-2.74	119.13	126.73
34	J	101	LMG	O8-C28-O10	-2.73	116.69	123.59
26	B	619	BCR	C2-C1-C6	2.73	114.69	110.48
24	c	907	CLA	C4-C3-C5	2.73	119.87	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	910	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
24	b	610	CLA	O2A-CGA-CBA	2.73	120.48	111.91
26	h	101	BCR	C24-C23-C22	-2.73	122.11	126.23
24	b	616	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
27	F	101	SQD	C3-C4-C5	2.73	115.11	110.24
24	b	614	CLA	C4-C3-C5	2.73	119.86	115.27
24	b	620	CLA	O2A-CGA-CBA	2.73	120.47	111.91
24	b	616	CLA	O2A-CGA-CBA	2.73	120.47	111.91
24	A	405	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
24	b	615	CLA	CHB-C1B-NB	-2.73	121.37	124.26
31	A	419	PL9	C25-C24-C26	2.72	119.86	115.27
24	b	605	CLA	O2A-CGA-CBA	2.72	120.46	111.91
24	c	903	CLA	CHC-C1C-C2C	-2.72	119.16	126.73
24	a	406	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	C	513	CLA	CMC-C2C-C1C	2.72	129.18	125.04
31	A	419	PL9	C42-C43-C44	-2.72	121.11	127.66
24	B	606	CLA	C1-O2A-CGA	2.72	123.58	116.44
24	C	510	CLA	CHB-C1B-NB	-2.72	121.38	124.26
24	b	608	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
24	B	617	CLA	CHB-C1B-NB	-2.71	121.38	124.26
34	z	101	LMG	O8-C28-C29	2.71	120.42	111.91
24	c	908	CLA	CMC-C2C-C1C	2.71	129.17	125.04
24	C	508	CLA	CHD-C4C-NC	2.71	128.47	124.20
34	C	521	LMG	C8-O7-C10	-2.71	111.12	117.79
24	c	903	CLA	CMC-C2C-C1C	2.71	129.16	125.04
24	c	909	CLA	CHB-C1B-NB	-2.71	121.39	124.26
24	c	911	CLA	CHD-C4C-NC	2.71	128.47	124.20
40	V	201	HEC	C3B-C4B-NB	-2.71	107.15	110.17
36	D	405	DGD	O1G-C1A-C2A	2.70	120.40	111.91
24	b	617	CLA	CMA-C3A-C4A	-2.70	104.50	111.77
24	C	504	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
31	d	405	PL9	C15-C14-C16	2.70	119.82	115.27
24	C	512	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	C	511	CLA	C4-C3-C5	2.70	119.81	115.27
24	c	910	CLA	CHC-C1C-C2C	-2.70	119.23	126.73
24	d	401	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	B	610	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
24	C	507	CLA	C4-C3-C5	2.70	119.81	115.27
31	A	419	PL9	C35-C34-C36	2.70	119.81	115.27
40	v	202	HEC	C3C-C4C-NC	-2.70	107.13	110.15
24	b	608	CLA	O2A-CGA-CBA	2.69	120.36	111.91
24	c	913	CLA	C4C-C3C-C2C	-2.69	102.97	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
27	L	102	SQD	O48-C23-C24	2.69	120.35	111.91
38	e	102	HEM	CHA-C1A-NA	2.69	128.79	123.85
24	B	609	CLA	CHC-C1C-C2C	-2.69	119.26	126.73
24	B	611	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	B	615	CLA	CMB-C2B-C1B	2.69	129.46	125.37
27	f	102	SQD	O48-C23-C24	2.69	120.34	111.91
24	b	612	CLA	CAC-C3C-C4C	2.68	128.29	124.81
24	B	607	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	a	407	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
24	c	914	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
24	B	609	CLA	CMA-C3A-C4A	-2.68	104.57	111.77
24	d	401	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
24	c	903	CLA	CHD-C4C-NC	2.68	128.42	124.20
36	d	406	DGD	C1E-O6E-C5E	2.68	118.94	113.69
34	c	920	LMG	O8-C28-C29	2.67	120.30	111.91
24	c	913	CLA	CED-O2D-CGD	2.67	121.98	115.94
24	C	505	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
24	d	402	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
24	a	409	CLA	CMA-C3A-C4A	-2.67	104.60	111.77
26	D	403	BCR	C29-C30-C25	2.67	114.59	110.48
24	C	513	CLA	C4-C3-C5	2.67	119.76	115.27
24	c	913	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	A	407	CLA	C1-C2-C3	-2.67	121.43	126.04
24	b	610	CLA	CHD-C4C-NC	2.67	128.40	124.20
24	b	605	CLA	C4C-C3C-C2C	-2.66	103.01	106.90
26	k	101	BCR	C24-C23-C22	-2.66	122.21	126.23
24	B	608	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
38	e	102	HEM	CHA-C4D-ND	2.66	127.66	124.37
26	B	619	BCR	C37-C22-C21	-2.66	119.20	122.92
26	d	404	BCR	C21-C20-C19	-2.66	114.92	123.22
24	b	605	CLA	C3B-C4B-NB	2.66	112.98	110.52
34	Z	101	LMG	O6-C5-C4	2.66	114.52	109.69
24	C	510	CLA	CMC-C2C-C1C	2.66	129.09	125.04
27	A	412	SQD	O47-C7-O49	-2.66	117.28	123.70
24	B	605	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
27	A	412	SQD	O9-S-C6	2.65	110.09	106.94
34	B	622	LMG	O8-C28-O10	-2.65	116.89	123.59
24	B	614	CLA	CAC-C3C-C4C	2.65	128.25	124.81
24	b	613	CLA	CHD-C4C-NC	2.65	128.38	124.20
24	C	514	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
24	d	403	CLA	CHD-C4C-NC	2.65	128.38	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	602	CLA	C1-C2-C3	-2.65	121.46	126.04
24	c	913	CLA	CHC-C1C-C2C	-2.65	119.38	126.73
24	B	612	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
36	h	102	DGD	O1G-C1A-O1A	-2.64	116.92	123.59
24	B	607	CLA	C1-C2-C3	-2.64	121.48	126.04
24	B	611	CLA	C1-C2-C3	-2.64	121.48	126.04
24	c	906	CLA	C1-O2A-CGA	2.64	123.37	116.44
24	b	616	CLA	CMC-C2C-C1C	2.64	129.06	125.04
24	C	512	CLA	CMB-C2B-C1B	2.64	129.39	125.37
31	d	405	PL9	C45-C44-C46	2.64	119.71	115.27
24	c	905	CLA	CMB-C2B-C1B	2.64	129.39	125.37
24	C	505	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
24	d	402	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
31	a	417	PL9	C40-C39-C41	2.64	119.71	115.27
24	C	510	CLA	C4-C3-C5	2.64	119.71	115.27
24	b	609	CLA	CHC-C1C-C2C	-2.63	119.41	126.73
31	A	419	PL9	C45-C44-C46	2.63	119.70	115.27
24	c	914	CLA	CHD-C4C-NC	2.63	128.35	124.20
24	C	511	CLA	CHC-C1C-C2C	-2.63	119.42	126.73
24	c	906	CLA	CMC-C2C-C1C	2.63	129.04	125.04
24	b	608	CLA	CMB-C2B-C1B	2.63	129.38	125.37
24	c	912	CLA	C4-C3-C5	2.63	119.69	115.27
26	A	411	BCR	C33-C5-C6	-2.63	121.58	124.53
24	b	617	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
31	D	404	PL9	C7-C3-C4	2.63	119.01	116.88
24	C	509	CLA	CHD-C4C-NC	2.63	128.34	124.20
24	b	607	CLA	C2A-C1A-CHA	-2.63	119.27	123.86
24	B	604	CLA	CHC-C1C-C2C	-2.63	119.44	126.73
24	c	903	CLA	C3B-C4B-NB	2.63	112.95	110.52
24	C	511	CLA	O2A-CGA-CBA	2.62	120.14	111.91
26	T	102	BCR	C21-C20-C19	-2.62	115.03	123.22
24	b	609	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
24	B	617	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
24	C	507	CLA	CHD-C4C-NC	2.62	128.33	124.20
26	K	103	BCR	C15-C14-C13	-2.62	123.57	127.31
24	D	402	CLA	CAC-C3C-C4C	2.62	128.21	124.81
24	d	401	CLA	CMA-C3A-C2A	-2.62	103.27	113.83
24	A	410	CLA	O2A-CGA-CBA	2.62	120.12	111.91
24	b	609	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
24	B	606	CLA	C4-C3-C5	2.62	119.67	115.27
29	A	417	LMT	C1'-O5'-C5'	2.62	118.82	113.69
31	d	405	PL9	C42-C43-C44	-2.62	121.36	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	D	402	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
26	c	915	BCR	C3-C4-C5	-2.61	109.41	114.08
24	c	906	CLA	C1-C2-C3	-2.61	121.53	126.04
24	A	410	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
24	B	605	CLA	O2A-CGA-CBA	2.61	120.09	111.91
35	B	634	HTG	C1-O5-C5	2.61	117.39	112.58
24	c	904	CLA	O2A-CGA-CBA	2.61	120.09	111.91
24	c	907	CLA	O2A-CGA-O1A	-2.61	117.02	123.59
26	T	102	BCR	C7-C6-C5	-2.60	115.15	121.46
24	b	618	CLA	CMC-C2C-C1C	2.60	129.00	125.04
26	b	623	BCR	C15-C14-C13	-2.60	123.59	127.31
24	B	607	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
24	b	617	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
24	c	903	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
34	J	101	LMG	O8-C28-C29	2.60	120.06	111.91
24	B	606	CLA	O2A-CGA-CBA	2.60	120.06	111.91
24	a	409	CLA	C4-C3-C5	2.60	119.64	115.27
24	B	613	CLA	CHC-C1C-C2C	-2.60	119.52	126.73
31	a	417	PL9	C37-C36-C34	-2.60	104.44	112.98
27	F	101	SQD	O48-C23-C24	2.59	120.04	111.91
24	B	614	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	b	606	CLA	C4-C3-C5	2.59	119.62	115.27
24	c	914	CLA	C4-C3-C5	2.59	119.62	115.27
26	t	101	BCR	C1-C6-C7	2.59	123.10	115.78
37	D	408	LHG	O8-C23-C24	2.59	120.02	111.91
24	c	902	CLA	CHD-C4C-NC	2.58	128.27	124.20
37	L	101	LHG	O8-C23-O10	-2.58	117.08	123.59
24	d	402	CLA	CMB-C2B-C1B	2.58	129.30	125.37
31	d	405	PL9	C40-C39-C41	2.58	119.61	115.27
24	B	604	CLA	CBC-CAC-C3C	-2.58	105.32	112.43
24	b	606	CLA	CMC-C2C-C1C	2.58	128.96	125.04
24	B	609	CLA	CHB-C4A-NA	2.58	128.07	124.51
26	k	101	BCR	C7-C8-C9	-2.58	122.34	126.23
24	C	511	CLA	O2A-CGA-O1A	-2.57	117.09	123.59
24	C	508	CLA	CAC-C3C-C4C	2.57	128.15	124.81
24	c	907	CLA	CHD-C4C-NC	2.57	128.26	124.20
35	C	524	HTG	O5-C1-C2	2.57	113.55	110.31
24	b	619	CLA	CMB-C2B-C1B	2.57	129.28	125.37
34	z	101	LMG	C7-O1-C1	-2.57	108.72	113.74
24	c	902	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
24	C	502	CLA	CHD-C4C-NC	2.57	128.25	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	406	CLA	CMA-C3A-C2A	-2.57	103.47	113.83
24	c	912	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
38	e	102	HEM	C4D-ND-C1D	2.57	107.72	105.07
24	c	902	CLA	CMB-C2B-C1B	2.56	129.27	125.37
26	K	102	BCR	C16-C17-C18	-2.56	123.65	127.31
24	C	510	CLA	C1-O2A-CGA	2.56	123.17	116.44
40	v	202	HEC	CHA-C1A-NA	2.56	127.21	124.44
25	a	408	PHO	CBC-CAC-C3C	-2.56	109.13	112.88
24	c	903	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
24	b	611	CLA	CHD-C4C-NC	2.56	128.23	124.20
24	B	609	CLA	CAC-C3C-C4C	2.56	128.13	124.81
24	b	617	CLA	C4-C3-C5	2.56	119.57	115.27
34	c	920	LMG	C8-O7-C10	-2.56	111.50	117.79
24	B	613	CLA	C4-C3-C5	2.55	119.57	115.27
24	A	407	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
24	c	910	CLA	C4-C3-C5	2.55	119.56	115.27
24	B	605	CLA	CMC-C2C-C1C	2.55	128.93	125.04
26	k	101	BCR	C38-C26-C25	-2.55	121.66	124.53
24	B	608	CLA	C4-C3-C5	2.55	119.56	115.27
26	y	101	BCR	C35-C13-C14	-2.55	119.35	122.92
36	D	405	DGD	C3D-C4D-C5D	2.55	114.78	110.24
24	C	508	CLA	CMC-C2C-C1C	2.55	128.92	125.04
26	a	410	BCR	C2-C1-C6	2.55	114.40	110.48
26	D	403	BCR	C33-C5-C6	-2.55	121.67	124.53
24	b	615	CLA	CHD-C4C-NC	2.54	128.21	124.20
24	b	615	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
24	b	612	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
24	B	603	CLA	CMB-C2B-C1B	2.54	129.24	125.37
26	y	101	BCR	C10-C11-C12	-2.54	115.29	123.22
24	C	509	CLA	CAC-C3C-C4C	2.54	128.11	124.81
24	B	603	CLA	CMA-C3A-C4A	-2.54	104.95	111.77
24	d	401	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
26	d	404	BCR	C15-C14-C13	-2.54	123.69	127.31
24	c	907	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
24	b	618	CLA	CMB-C2B-C1B	2.54	129.23	125.37
24	B	608	CLA	C2A-C1A-CHA	-2.54	119.43	123.86
24	c	910	CLA	O2A-CGA-CBA	2.53	119.86	111.91
35	b	627	HTG	C1-C2-C3	2.53	115.59	110.59
24	C	513	CLA	CMB-C2B-C1B	2.53	129.22	125.37
36	c	918	DGD	O1G-C1A-C2A	2.53	119.85	111.91
24	b	610	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
24	b	609	CLA	O2A-CGA-CBA	2.53	119.84	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	617	CLA	O2A-CGA-CBA	2.53	119.84	111.91
24	B	604	CLA	CMC-C2C-C1C	2.53	128.89	125.04
24	b	618	CLA	CHB-C1B-NB	-2.53	121.58	124.26
24	c	903	CLA	C1-C2-C3	-2.53	121.67	126.04
26	K	102	BCR	C24-C23-C22	-2.53	122.42	126.23
24	c	909	CLA	CMB-C2B-C1B	2.53	129.22	125.37
24	C	506	CLA	CMD-C2D-C3D	-2.52	121.81	127.61
24	c	904	CLA	CHD-C4C-NC	2.52	128.18	124.20
26	B	618	BCR	C37-C22-C21	-2.52	119.39	122.92
38	E	103	HEM	CBA-CAA-C2A	-2.52	105.62	112.63
26	c	915	BCR	C15-C14-C13	-2.52	123.71	127.31
26	t	101	BCR	C29-C28-C27	-2.52	105.75	111.38
24	d	401	CLA	C4C-C3C-C2C	-2.52	103.22	106.90
24	c	913	CLA	O2A-CGA-CBA	2.52	119.81	111.91
24	a	407	CLA	C1-C2-C3	-2.52	121.69	126.04
24	b	610	CLA	CHC-C1C-C2C	-2.52	119.73	126.73
27	B	621	SQD	O8-S-C6	2.52	109.75	105.74
24	B	611	CLA	OBD-CAD-C3D	-2.52	122.46	128.52
27	L	102	SQD	C1-C2-C3	-2.52	104.75	110.00
24	C	514	CLA	CHD-C4C-NC	2.52	128.17	124.20
40	v	202	HEC	CBB-CAB-C3B	2.51	119.36	112.43
24	b	607	CLA	CMC-C2C-C1C	2.51	128.87	125.04
26	k	102	BCR	C33-C5-C6	-2.51	121.70	124.53
25	a	420	PHO	CMB-C2B-C3B	2.51	129.38	124.68
24	a	409	CLA	CAC-C3C-C4C	2.51	128.07	124.81
36	H	102	DGD	O1G-C1A-C2A	2.51	119.79	111.91
36	d	406	DGD	O1G-C1A-C2A	2.51	119.79	111.91
26	t	101	BCR	C7-C6-C5	-2.51	115.38	121.46
24	B	607	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
24	b	616	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
26	K	103	BCR	C38-C26-C25	-2.51	121.71	124.53
26	k	101	BCR	C35-C13-C14	-2.51	119.41	122.92
38	E	103	HEM	CHD-C1D-ND	2.51	127.14	124.42
24	C	503	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
24	B	612	CLA	O2A-CGA-CBA	2.51	119.77	111.91
34	a	412	LMG	O8-C28-C29	2.51	119.77	111.91
24	b	606	CLA	CHD-C4C-NC	2.50	128.15	124.20
37	d	409	LHG	O8-C23-C24	2.50	119.76	111.91
36	C	519	DGD	O2G-C1B-C2B	2.50	116.90	111.50
24	C	503	CLA	OBD-CAD-C3D	-2.50	122.50	128.52
26	D	403	BCR	C29-C28-C27	-2.50	105.79	111.38
24	b	616	CLA	OBD-CAD-C3D	-2.50	122.50	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	503	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
24	C	513	CLA	O2A-CGA-CBA	2.50	119.75	111.91
24	a	407	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
26	y	101	BCR	C28-C27-C26	-2.50	109.62	114.08
24	b	609	CLA	OBD-CAD-C3D	-2.50	122.51	128.52
24	B	602	CLA	C4-C3-C5	2.50	119.47	115.27
38	E	103	HEM	C4D-ND-C1D	2.50	107.65	105.07
24	B	604	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
40	V	201	HEC	C4A-NA-C1A	2.50	107.79	105.35
26	H	101	BCR	C7-C8-C9	-2.50	122.46	126.23
26	d	404	BCR	C24-C23-C22	-2.49	122.47	126.23
24	B	603	CLA	CBC-CAC-C3C	-2.49	105.55	112.43
26	y	101	BCR	C16-C17-C18	-2.49	123.75	127.31
27	f	102	SQD	O47-C7-O49	-2.49	117.67	123.70
24	A	406	CLA	CMA-C3A-C2A	-2.49	103.77	113.83
24	C	502	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
24	B	608	CLA	C1-O2A-CGA	2.49	122.98	116.44
24	B	614	CLA	CMA-C3A-C4A	-2.49	105.08	111.77
29	m	103	LMT	C1'-C2'-C3'	2.49	115.18	110.00
24	c	905	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
37	d	408	LHG	O8-C23-O10	-2.49	117.31	123.59
25	A	409	PHO	C4A-C3A-C2A	-2.49	100.47	102.84
24	C	503	CLA	CMC-C2C-C1C	2.49	128.82	125.04
24	B	615	CLA	C4C-C3C-C2C	-2.49	103.28	106.90
24	c	911	CLA	O2A-CGA-CBA	2.48	119.70	111.91
24	A	405	CLA	CMB-C2B-C1B	2.48	129.15	125.37
24	A	405	CLA	O2A-CGA-CBA	2.48	119.70	111.91
26	C	515	BCR	C33-C5-C6	-2.48	121.74	124.53
24	d	403	CLA	CHB-C1B-NB	-2.48	121.63	124.26
24	d	403	CLA	CMB-C2B-C1B	2.48	129.15	125.37
24	a	409	CLA	CMC-C2C-C1C	2.48	128.82	125.04
24	B	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
34	j	101	LMG	O8-C28-O10	-2.48	117.34	123.59
24	D	402	CLA	CHD-C4C-NC	2.48	128.11	124.20
29	m	104	LMT	O5'-C5'-C4'	2.48	114.98	109.75
24	C	504	CLA	CHD-C4C-NC	2.48	128.11	124.20
24	B	603	CLA	C4-C3-C5	2.48	119.44	115.27
24	B	609	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
24	C	505	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
26	b	623	BCR	C16-C15-C14	-2.48	118.40	123.47
26	T	102	BCR	C1-C6-C7	2.47	122.78	115.78
24	b	606	CLA	O2A-CGA-CBA	2.47	119.67	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Z	101	LMG	C8-O7-C10	-2.47	111.70	117.79
24	C	513	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
24	b	618	CLA	CHD-C4C-NC	2.47	128.10	124.20
38	E	103	HEM	C4B-C3B-C2B	-2.47	105.15	107.11
31	A	419	PL9	C8-C7-C3	2.47	118.97	111.98
31	d	405	PL9	C35-C34-C36	2.47	119.43	115.27
24	B	607	CLA	C1-O2A-CGA	2.47	122.93	116.44
27	A	412	SQD	O48-C23-O10	-2.47	117.36	123.59
35	c	923	HTG	O5-C5-C4	2.47	114.17	109.69
24	C	503	CLA	O2A-CGA-CBA	2.46	119.64	111.91
25	A	409	PHO	O2D-CGD-O1D	-2.46	119.02	123.84
35	C	524	HTG	O5-C5-C4	2.46	114.17	109.69
24	b	613	CLA	O2A-CGA-CBA	2.46	119.64	111.91
24	b	618	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
26	T	102	BCR	C11-C10-C9	-2.46	123.80	127.31
24	b	617	CLA	CHB-C4A-NA	2.46	127.92	124.51
24	a	409	CLA	O2A-CGA-CBA	2.46	119.62	111.91
29	a	401	LMT	O5'-C5'-C4'	2.45	114.92	109.75
24	B	611	CLA	CHD-C4C-NC	2.45	128.06	124.20
31	d	405	PL9	C20-C19-C21	2.45	119.39	115.27
24	C	506	CLA	CMC-C2C-C1C	2.45	128.77	125.04
24	b	613	CLA	CHC-C1C-C2C	-2.45	119.92	126.73
26	B	618	BCR	C34-C9-C10	-2.45	119.49	122.92
24	b	615	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
24	B	608	CLA	CMC-C2C-C1C	2.44	128.76	125.04
24	B	604	CLA	CAC-C3C-C4C	2.44	127.98	124.81
24	C	507	CLA	CMC-C2C-C1C	2.44	128.76	125.04
24	D	401	CLA	C1D-CHD-C4C	-2.44	120.79	126.06
24	a	407	CLA	CMC-C2C-C1C	2.44	128.76	125.04
27	L	102	SQD	O47-C7-O49	-2.44	117.81	123.70
24	b	608	CLA	C4-C3-C5	2.44	119.37	115.27
36	d	406	DGD	O5D-C1E-C2E	2.44	112.11	108.30
26	a	410	BCR	C3-C4-C5	-2.43	109.73	114.08
36	c	916	DGD	C2G-O2G-C1B	-2.43	111.80	117.79
25	a	420	PHO	O2A-CGA-CBA	2.43	119.55	111.91
24	b	611	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
24	a	407	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
40	v	202	HEC	C3B-C4B-NB	-2.43	107.46	110.17
25	A	408	PHO	C4-C3-C5	2.43	119.36	115.27
31	a	417	PL9	C51-C49-C50	2.43	119.97	114.60
24	b	606	CLA	C1-C2-C3	-2.43	121.84	126.04
24	b	612	CLA	CMC-C2C-C1C	2.43	128.74	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	617	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
36	C	519	DGD	O1G-C1A-C2A	2.43	119.53	111.91
24	B	604	CLA	C5-C3-C2	-2.43	116.21	121.12
24	C	508	CLA	O2A-CGA-CBA	2.43	119.52	111.91
24	A	410	CLA	CMA-C3A-C4A	-2.43	105.25	111.77
24	B	603	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
24	c	913	CLA	CBA-CAA-C2A	-2.42	106.71	113.86
26	B	619	BCR	C28-C27-C26	-2.42	109.75	114.08
26	D	403	BCR	C10-C11-C12	-2.42	115.67	123.22
24	b	610	CLA	CAC-C3C-C4C	2.42	127.95	124.81
24	B	605	CLA	CMB-C2B-C1B	2.42	129.05	125.37
35	B	634	HTG	O5-C5-C4	2.41	114.08	109.69
24	c	909	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
29	f	103	LMT	O5B-C5B-C4B	2.41	114.08	109.69
24	C	510	CLA	CHD-C4C-NC	2.41	128.00	124.20
38	e	102	HEM	CBD-CAD-C3D	-2.41	105.93	112.63
26	B	618	BCR	C7-C8-C9	-2.41	122.59	126.23
24	c	908	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
24	C	512	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
24	b	618	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
26	t	101	BCR	C21-C20-C19	-2.40	115.71	123.22
24	c	910	CLA	CHB-C1B-NB	-2.40	121.71	124.26
24	B	605	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
37	l	101	LHG	O7-C7-O9	-2.40	117.89	123.70
24	a	407	CLA	C3B-C4B-NB	2.40	112.74	110.52
31	d	405	PL9	C32-C33-C34	-2.40	121.88	127.66
27	a	411	SQD	O48-C23-C24	2.40	119.44	111.91
24	c	905	CLA	CHD-C4C-NC	2.40	127.99	124.20
24	c	904	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
24	b	605	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
26	h	101	BCR	C10-C11-C12	-2.40	115.73	123.22
37	d	409	LHG	O7-C7-O9	-2.40	117.90	123.70
31	A	419	PL9	C30-C29-C31	2.40	119.30	115.27
37	l	101	LHG	O8-C23-C24	2.40	119.43	111.91
24	c	911	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
24	C	512	CLA	CHB-C1B-NB	-2.39	121.72	124.26
26	B	620	BCR	C39-C30-C25	-2.39	106.42	110.30
24	C	502	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
31	d	405	PL9	C31-C32-C33	-2.39	104.02	111.88
27	F	101	SQD	O9-S-C6	2.39	109.78	106.94
24	B	610	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
24	C	513	CLA	O2D-CGD-O1D	-2.39	119.17	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	L	102	SQD	C44-O6-C1	-2.39	109.07	113.74
24	C	504	CLA	CMC-C2C-C1C	2.39	128.68	125.04
24	B	611	CLA	CHB-C1B-NB	-2.39	121.73	124.26
26	y	101	BCR	C21-C20-C19	-2.39	115.77	123.22
24	C	507	CLA	C4C-C3C-C2C	-2.39	103.42	106.90
24	C	514	CLA	O2A-CGA-CBA	2.38	119.39	111.91
24	A	405	CLA	O2D-CGD-CBD	2.38	115.50	111.27
24	B	603	CLA	O2A-CGA-CBA	2.38	119.39	111.91
24	B	603	CLA	CAA-CBA-CGA	-2.38	106.30	113.25
24	B	614	CLA	O2D-CGD-CBD	2.38	115.50	111.27
31	D	404	PL9	C25-C24-C26	2.38	119.27	115.27
24	B	610	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
24	b	618	CLA	OBD-CAD-C3D	-2.38	122.80	128.52
31	d	405	PL9	C37-C38-C39	-2.38	121.94	127.66
24	b	605	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
24	b	615	CLA	O2A-CGA-CBA	2.38	119.37	111.91
26	c	915	BCR	C15-C16-C17	-2.38	118.61	123.47
24	b	616	CLA	CHC-C1C-C2C	-2.38	120.13	126.73
24	C	504	CLA	CMB-C2B-C1B	2.38	128.99	125.37
24	c	912	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
25	a	408	PHO	CBA-CAA-C2A	-2.37	106.87	113.81
24	B	615	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
24	c	907	CLA	CGD-CBD-CAD	-2.37	103.05	110.73
24	B	617	CLA	C1-O2A-CGA	2.37	122.66	116.44
24	b	614	CLA	CHD-C4C-NC	2.37	127.94	124.20
24	b	614	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
24	B	609	CLA	CHD-C4C-NC	2.37	127.94	124.20
24	B	610	CLA	CMA-C3A-C4A	-2.37	105.41	111.77
27	B	621	SQD	C1-C2-C3	-2.37	105.07	110.00
24	C	503	CLA	CHD-C4C-NC	2.37	127.93	124.20
34	z	101	LMG	O1-C1-C2	2.37	112.00	108.30
24	B	610	CLA	CGD-CBD-CAD	-2.37	103.07	110.73
29	b	601	LMT	O5'-C1'-C2'	2.36	115.35	110.35
24	C	504	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
27	A	416	SQD	C3-C4-C5	2.36	114.45	110.24
27	F	101	SQD	O47-C7-O49	-2.36	117.99	123.70
24	c	909	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
24	d	403	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
24	b	611	CLA	CAC-C3C-C4C	2.36	127.87	124.81
24	d	403	CLA	C4-C3-C5	2.36	119.24	115.27
26	D	403	BCR	C16-C17-C18	-2.36	123.94	127.31
24	b	620	CLA	C4-C3-C5	2.36	119.24	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	608	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
24	b	617	CLA	CHD-C4C-NC	2.36	127.92	124.20
24	C	513	CLA	CMA-C3A-C4A	-2.35	105.44	111.77
24	C	509	CLA	O2A-CGA-CBA	2.35	119.29	111.91
24	B	612	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
31	D	404	PL9	C22-C23-C24	-2.35	121.99	127.66
24	B	612	CLA	CHB-C1B-NB	-2.35	121.77	124.26
24	C	502	CLA	C4-C3-C5	2.35	119.23	115.27
38	E	103	HEM	O2A-CGA-CBA	2.35	121.59	114.03
24	A	406	CLA	CAA-CBA-CGA	2.35	120.12	113.25
24	B	602	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
24	C	511	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
24	b	614	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
24	C	502	CLA	O2A-CGA-CBA	2.35	119.28	111.91
24	C	507	CLA	CHB-C1B-NB	-2.35	121.77	124.26
24	b	609	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
24	C	502	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
24	B	607	CLA	O2A-CGA-CBA	2.34	119.26	111.91
24	B	607	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
24	b	620	CLA	CHD-C4C-NC	2.34	127.89	124.20
31	D	404	PL9	C12-C13-C14	-2.34	122.02	127.66
24	B	614	CLA	CHB-C1B-NB	-2.34	121.78	124.26
29	B	623	LMT	O1B-C4'-C5'	-2.34	103.04	109.45
29	B	623	LMT	C1-O1'-C1'	-2.34	109.96	113.84
24	C	509	CLA	CMC-C2C-C1C	2.34	128.60	125.04
24	B	615	CLA	C1-C2-C3	-2.34	122.00	126.04
24	b	619	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
24	c	908	CLA	CHD-C4C-NC	2.33	127.88	124.20
24	b	606	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
24	D	401	CLA	CMC-C2C-C1C	2.33	128.59	125.04
36	c	918	DGD	O1G-C1A-O1A	-2.33	117.71	123.59
36	C	518	DGD	O1G-C1A-C2A	2.33	119.22	111.91
24	b	617	CLA	C6-C7-C8	-2.33	108.39	115.92
24	c	910	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
40	v	202	HEC	CAB-C3B-C4B	2.33	127.83	124.81
24	C	505	CLA	CHD-C4C-NC	2.33	127.87	124.20
40	V	201	HEC	CAB-C3B-C4B	2.33	127.83	124.81
24	C	506	CLA	CHB-C1B-NB	-2.32	121.80	124.26
26	A	411	BCR	C37-C22-C21	-2.32	119.67	122.92
24	a	409	CLA	CMA-C3A-C2A	-2.32	104.47	113.83
24	C	502	CLA	CHB-C1B-NB	-2.32	121.80	124.26
35	b	626	HTG	O5-C1-C2	2.32	113.23	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	v	202	HEC	CHD-C1D-ND	2.31	127.23	124.37
26	k	102	BCR	C36-C18-C19	2.31	121.72	118.08
24	B	603	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
24	D	401	CLA	CBC-CAC-C3C	-2.31	106.05	112.43
35	b	603	HTG	C1-O5-C5	2.31	116.84	112.58
24	A	410	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
24	d	403	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
24	C	511	CLA	C6-C7-C8	-2.31	108.46	115.92
24	b	613	CLA	CMA-C3A-C2A	-2.31	104.52	113.83
26	B	618	BCR	C29-C30-C25	2.31	114.03	110.48
31	A	419	PL9	C40-C39-C41	2.30	119.15	115.27
24	B	607	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
24	B	609	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
26	d	404	BCR	C40-C30-C25	-2.30	106.56	110.30
24	A	407	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
24	C	507	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
24	a	407	CLA	OBD-CAD-C3D	-2.30	122.98	128.52
24	b	612	CLA	CMB-C2B-C1B	2.30	128.87	125.37
25	a	408	PHO	CMC-C2C-C1C	2.30	129.07	124.73
26	d	404	BCR	C30-C25-C26	-2.30	119.38	122.61
26	C	516	BCR	C3-C4-C5	-2.30	109.97	114.08
24	A	407	CLA	CMA-C3A-C2A	-2.30	104.56	113.83
24	b	606	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
24	A	406	CLA	CAC-C3C-C4C	2.30	127.79	124.81
24	C	506	CLA	O2A-CGA-CBA	2.30	119.11	111.91
27	A	416	SQD	O5-C5-C4	2.30	113.86	109.69
31	D	404	PL9	C51-C49-C50	2.29	119.67	114.60
24	C	508	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
26	c	915	BCR	C37-C22-C21	-2.29	119.71	122.92
24	B	613	CLA	CMB-C2B-C1B	2.29	128.86	125.37
36	D	405	DGD	O6D-C5D-C6D	2.29	111.29	106.67
37	l	101	LHG	C6-C5-C4	-2.29	106.37	111.79
24	a	409	CLA	CHB-C1B-NB	-2.29	121.83	124.26
24	B	617	CLA	OBD-CAD-C3D	-2.29	123.02	128.52
24	A	410	CLA	CAC-C3C-C4C	2.29	127.78	124.81
24	C	513	CLA	CHB-C4A-NA	2.28	127.67	124.51
31	D	404	PL9	C37-C38-C39	-2.28	122.16	127.66
24	B	602	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	b	612	CLA	C11-C10-C8	-2.28	108.54	115.92
24	b	614	CLA	C11-C12-C13	-2.28	108.54	115.92
26	k	102	BCR	C2-C1-C6	2.28	113.99	110.48
34	C	520	LMG	C8-O7-C10	-2.28	112.17	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	406	LHG	O7-C7-O9	-2.28	118.19	123.70
24	A	407	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
24	b	614	CLA	CHB-C4A-NA	2.28	127.66	124.51
24	b	616	CLA	CHB-C1B-NB	-2.28	121.84	124.26
24	C	510	CLA	C16-C15-C13	-2.28	108.56	115.92
24	b	608	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
24	a	407	CLA	C4-C3-C5	2.27	119.09	115.27
26	y	101	BCR	C37-C22-C21	-2.27	119.74	122.92
26	B	620	BCR	C3-C4-C5	-2.27	110.03	114.08
24	d	402	CLA	C1-O2A-CGA	2.27	122.39	116.44
34	a	412	LMG	O1-C1-C2	2.27	111.84	108.30
24	A	410	CLA	CMA-C3A-C2A	-2.27	104.68	113.83
24	B	615	CLA	CAC-C3C-C4C	2.27	127.75	124.81
24	B	605	CLA	C2A-C1A-CHA	-2.27	119.90	123.86
24	c	902	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
24	B	608	CLA	O2A-CGA-CBA	2.26	119.01	111.91
24	B	602	CLA	CMC-C2C-C1C	2.26	128.49	125.04
24	c	911	CLA	CMA-C3A-C4A	-2.26	105.69	111.77
24	B	612	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
24	b	617	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
25	a	408	PHO	O1D-CGD-CBD	-2.26	120.97	124.74
34	z	101	LMG	C8-O7-C10	-2.26	112.23	117.79
24	c	911	CLA	CMB-C2B-C1B	2.26	128.81	125.37
24	a	406	CLA	C4C-C3C-C2C	-2.26	103.61	106.90
24	c	912	CLA	C1-O2A-CGA	2.26	122.37	116.44
24	C	512	CLA	CMC-C2C-C1C	2.26	128.47	125.04
24	B	611	CLA	CAA-CBA-CGA	-2.26	106.66	113.25
26	d	404	BCR	C37-C22-C23	2.26	121.63	118.08
26	C	515	BCR	C2-C1-C6	2.25	113.95	110.48
24	b	613	CLA	C3B-C4B-NB	2.25	112.61	110.52
24	b	610	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
27	f	102	SQD	C3-C4-C5	2.25	114.26	110.24
24	B	617	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
24	B	614	CLA	CHD-C4C-NC	2.25	127.75	124.20
26	b	623	BCR	C10-C11-C12	-2.25	116.19	123.22
24	B	616	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	C	510	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
26	B	618	BCR	C37-C22-C23	2.25	121.62	118.08
24	b	618	CLA	C4-C3-C5	2.25	119.06	115.27
24	A	410	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
24	C	505	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
24	D	402	CLA	C1-C2-C3	-2.25	122.16	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	619	BCR	C15-C16-C17	-2.25	118.87	123.47
26	y	101	BCR	C38-C26-C25	-2.25	122.00	124.53
36	C	518	DGD	O6E-C5E-C6E	2.25	112.02	106.44
27	a	411	SQD	O9-S-C6	2.24	109.61	106.94
26	k	101	BCR	C21-C20-C19	-2.24	116.22	123.22
37	D	406	LHG	O4-P-O5	2.24	123.32	112.24
24	c	912	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
24	B	616	CLA	CHA-C1A-NA	-2.24	121.27	126.40
37	e	101	LHG	O8-C23-C24	2.24	118.93	111.91
24	B	614	CLA	CMB-C2B-C1B	2.24	128.77	125.37
24	C	511	CLA	CAC-C3C-C4C	2.24	127.71	124.81
29	a	401	LMT	C1'-O5'-C5'	2.24	118.08	113.69
35	b	626	HTG	C1-C2-C3	2.23	115.00	110.59
24	b	619	CLA	O2A-CGA-CBA	2.23	118.92	111.91
24	C	509	CLA	CMB-C2B-C1B	2.23	128.77	125.37
24	b	611	CLA	CMB-C2B-C1B	2.23	128.77	125.37
24	B	607	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
24	C	514	CLA	C1-O2A-CGA	2.23	122.30	116.44
24	a	407	CLA	CHB-C1B-C2B	-2.23	120.93	127.24
24	d	401	CLA	CAA-CBA-CGA	2.23	119.78	113.25
36	C	518	DGD	C6D-C5D-C4D	2.23	116.75	112.09
24	C	504	CLA	O2A-CGA-CBA	2.23	118.91	111.91
24	B	616	CLA	CED-O2D-CGD	2.23	120.98	115.94
24	D	401	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
24	B	612	CLA	CHB-C4A-NA	2.23	127.60	124.51
24	B	615	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
35	B	625	HTG	C1-C2-C3	2.23	114.99	110.59
25	a	408	PHO	O2D-CGD-O1D	-2.23	119.48	123.84
24	B	607	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
24	b	619	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
24	C	510	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
37	d	407	LHG	O8-C23-O10	-2.22	117.98	123.59
26	d	404	BCR	C35-C13-C12	2.22	121.58	118.08
24	C	512	CLA	CED-O2D-CGD	2.22	120.97	115.94
24	b	616	CLA	CHD-C4C-NC	2.22	127.71	124.20
24	A	410	CLA	CHB-C4A-NA	2.22	127.59	124.51
38	E	103	HEM	CHA-C4D-ND	2.22	127.11	124.37
34	b	624	LMG	O8-C28-O10	-2.22	117.99	123.59
24	C	513	CLA	CAA-C2A-C1A	2.22	119.25	111.97
24	b	613	CLA	CMB-C2B-C1B	2.22	128.75	125.37
24	b	609	CLA	C1-C2-C3	-2.22	122.20	126.04
27	B	621	SQD	C3-C4-C5	2.22	114.20	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	613	CLA	C1-C2-C3	-2.22	122.21	126.04
24	C	514	CLA	CMB-C2B-C1B	2.22	128.75	125.37
24	b	614	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
24	B	611	CLA	CMA-C3A-C4A	-2.22	105.82	111.77
24	C	506	CLA	CHD-C4C-NC	2.21	127.69	124.20
24	B	603	CLA	CMC-C2C-C1C	2.21	128.41	125.04
24	A	405	CLA	CHB-C1B-NB	-2.21	121.91	124.26
24	C	512	CLA	C11-C10-C8	-2.21	108.77	115.92
29	M	101	LMT	O5B-C5B-C6B	2.21	111.93	106.44
24	C	510	CLA	C11-C12-C13	-2.21	108.77	115.92
34	Z	101	LMG	C1-O6-C5	2.21	118.02	113.69
24	b	607	CLA	CHD-C4C-NC	2.21	127.68	124.20
24	d	401	CLA	O2A-CGA-CBA	2.21	118.84	111.91
24	a	407	CLA	C1-O2A-CGA	2.21	122.24	116.44
26	b	623	BCR	C7-C8-C9	-2.21	122.90	126.23
26	K	102	BCR	C15-C14-C13	-2.20	124.16	127.31
27	a	411	SQD	C1-C2-C3	-2.20	105.41	110.00
24	c	914	CLA	CED-O2D-CGD	2.20	120.92	115.94
24	a	407	CLA	CMA-C3A-C2A	-2.20	104.94	113.83
26	K	102	BCR	C10-C11-C12	-2.20	116.34	123.22
24	b	617	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
24	c	903	CLA	CHB-C1B-NB	-2.20	121.93	124.26
24	B	603	CLA	C1-C2-C3	-2.20	122.24	126.04
24	c	905	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
24	c	905	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
37	D	407	LHG	O8-C23-O10	-2.20	118.04	123.59
25	A	408	PHO	O2D-CGD-O1D	-2.20	119.54	123.84
24	C	504	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
24	c	908	CLA	CHB-C4A-NA	2.20	127.55	124.51
24	C	503	CLA	CHB-C1B-NB	-2.20	121.93	124.26
24	B	606	CLA	CMC-C2C-C1C	2.20	128.38	125.04
24	B	611	CLA	CHC-C1C-NC	2.19	127.53	124.20
26	T	102	BCR	C37-C22-C23	2.19	121.53	118.08
26	A	411	BCR	C8-C7-C6	-2.19	121.05	127.20
24	D	401	CLA	CED-O2D-CGD	2.19	120.89	115.94
24	c	914	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
26	k	101	BCR	C16-C17-C18	-2.19	124.18	127.31
34	c	920	LMG	O7-C10-O9	-2.19	118.41	123.70
24	d	403	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	b	619	CLA	CMC-C2C-C1C	2.19	128.37	125.04
40	v	202	HEC	O2A-CGA-O1A	-2.19	117.85	123.30
26	D	403	BCR	C30-C25-C24	2.19	121.97	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	911	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
24	c	908	CLA	CBC-CAC-C3C	-2.18	106.41	112.43
24	B	610	CLA	C1-O2A-CGA	2.18	122.17	116.44
26	H	101	BCR	C20-C21-C22	-2.18	124.19	127.31
24	b	605	CLA	CAC-C3C-C2C	2.18	131.26	127.53
24	A	407	CLA	C1-O2A-CGA	2.18	122.17	116.44
24	c	910	CLA	OBD-CAD-C3D	-2.18	123.27	128.52
26	b	623	BCR	C21-C20-C19	-2.18	116.41	123.22
24	c	913	CLA	C1-O2A-CGA	2.18	122.16	116.44
26	T	102	BCR	C37-C22-C21	-2.18	119.87	122.92
40	V	201	HEC	C1A-CHA-C4D	-2.18	121.36	126.06
27	A	416	SQD	O8-S-C6	2.18	109.21	105.74
24	C	514	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
24	B	617	CLA	C4-C3-C5	2.18	118.93	115.27
24	C	507	CLA	O2A-CGA-CBA	2.18	118.74	111.91
26	A	411	BCR	C16-C17-C18	-2.18	124.20	127.31
26	D	403	BCR	C38-C26-C27	2.18	117.80	113.62
24	C	506	CLA	C1-O2A-CGA	2.17	122.15	116.44
34	a	412	LMG	O7-C10-O9	-2.17	118.45	123.70
24	C	506	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	b	619	CLA	CHA-C1A-NA	-2.17	121.42	126.40
24	b	606	CLA	CMA-C3A-C2A	-2.17	105.07	113.83
24	B	603	CLA	CAC-C3C-C4C	2.17	127.63	124.81
24	B	607	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	b	607	CLA	CHB-C4A-NA	2.17	127.51	124.51
35	b	603	HTG	O5-C1-C2	2.17	113.04	110.31
24	B	612	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
31	D	404	PL9	C36-C37-C38	-2.17	104.76	111.88
24	C	509	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
36	C	517	DGD	C2G-O2G-C1B	-2.17	112.46	117.79
24	c	905	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
24	B	606	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
26	y	101	BCR	C37-C22-C23	2.16	121.49	118.08
24	D	402	CLA	O2A-CGA-CBA	2.16	118.70	111.91
24	B	614	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
34	Z	101	LMG	C7-O1-C1	-2.16	109.51	113.74
26	T	102	BCR	C29-C28-C27	-2.16	106.55	111.38
24	C	502	CLA	C1-O2A-CGA	2.16	122.12	116.44
26	K	102	BCR	C37-C22-C23	2.16	121.48	118.08
27	a	402	SQD	O9-S-C6	2.16	109.51	106.94
24	B	615	CLA	C1-O2A-CGA	2.16	122.11	116.44
24	B	603	CLA	O2A-CGA-O1A	-2.16	118.14	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	402	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
29	C	522	LMT	O5'-C5'-C4'	2.16	114.31	109.75
27	a	402	SQD	O6-C1-C2	2.16	111.67	108.30
24	b	611	CLA	C1-O2A-CGA	2.16	122.10	116.44
36	C	519	DGD	O1G-C1A-O1A	-2.16	118.15	123.59
24	C	507	CLA	CGD-CBD-CAD	-2.16	103.75	110.73
24	c	904	CLA	C1-C2-C3	-2.15	122.32	126.04
36	h	102	DGD	C3B-C2B-C1B	-2.15	105.79	113.62
27	a	402	SQD	O48-C23-O10	-2.15	118.16	123.59
24	a	409	CLA	OBD-CAD-C3D	-2.15	123.34	128.52
26	D	403	BCR	C37-C22-C23	2.15	121.47	118.08
40	V	201	HEC	CAD-C3D-C4D	2.15	128.42	124.66
27	a	402	SQD	C3-C4-C5	2.15	114.08	110.24
24	C	508	CLA	C4-C3-C5	2.15	118.89	115.27
38	e	102	HEM	O2D-CGD-CBD	2.15	120.93	114.03
34	Z	101	LMG	C9-O8-C28	2.15	122.50	117.10
26	h	101	BCR	C7-C6-C5	2.15	126.66	121.46
25	A	409	PHO	O2A-CGA-CBA	2.14	118.62	111.91
40	V	201	HEC	O2D-CGD-CBD	2.14	120.91	114.03
24	B	616	CLA	C1-O2A-CGA	2.14	122.05	116.44
24	b	620	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
24	C	514	CLA	CHB-C1B-NB	-2.14	121.99	124.26
38	e	102	HEM	C2A-C1A-NA	-2.14	107.76	110.15
37	d	407	LHG	O7-C7-O9	-2.14	118.54	123.70
24	d	401	CLA	CED-O2D-CGD	2.14	120.77	115.94
27	B	621	SQD	O47-C7-O49	-2.14	118.54	123.70
36	C	519	DGD	C4D-C3D-C2D	-2.13	107.10	110.82
26	k	102	BCR	C37-C22-C21	-2.13	119.94	122.92
27	L	102	SQD	C45-O47-C7	-2.13	112.54	117.79
24	b	607	CLA	OBD-CAD-C3D	-2.13	123.39	128.52
24	c	908	CLA	C4-C3-C5	2.13	118.86	115.27
24	C	512	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
24	b	611	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
26	T	102	BCR	C15-C16-C17	-2.13	119.11	123.47
26	k	102	BCR	C29-C30-C25	2.13	113.76	110.48
34	C	521	LMG	O7-C10-O9	-2.13	118.56	123.70
26	t	101	BCR	C31-C1-C6	2.13	113.75	110.30
24	b	613	CLA	C7-C6-C5	-2.12	107.59	113.36
24	a	406	CLA	C11-C10-C8	-2.12	109.05	115.92
35	c	923	HTG	C4-C3-C2	-2.12	107.12	110.82
24	b	609	CLA	CAC-C3C-C4C	2.12	127.56	124.81
24	b	618	CLA	C4D-CHA-C1A	-2.12	118.67	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	c	916	DGD	O6E-C5E-C4E	2.12	113.55	109.69
24	A	406	CLA	C4C-C3C-C2C	-2.12	103.81	106.90
24	C	502	CLA	CMB-C2B-C1B	2.12	128.60	125.37
24	c	911	CLA	CHB-C1B-NB	-2.12	122.01	124.26
24	a	406	CLA	C11-C12-C13	-2.12	109.07	115.92
24	B	605	CLA	CHB-C1B-NB	-2.12	122.02	124.26
31	A	419	PL9	C17-C18-C19	-2.12	122.56	127.66
37	D	408	LHG	O4-P-O5	2.12	122.71	112.24
31	A	419	PL9	C16-C17-C18	-2.12	104.92	111.88
26	b	622	BCR	C11-C10-C9	-2.12	124.29	127.31
38	E	103	HEM	CHA-C1A-NA	2.12	127.74	123.85
24	b	618	CLA	CHB-C4A-NA	2.12	127.44	124.51
24	B	610	CLA	C7-C6-C5	-2.12	107.61	113.36
37	E	101	LHG	C5-O7-C7	-2.11	112.58	117.79
24	b	614	CLA	CED-O2D-CGD	2.11	120.72	115.94
24	C	514	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
24	a	409	CLA	CED-O2D-CGD	2.11	120.72	115.94
26	c	915	BCR	C39-C30-C25	-2.11	106.87	110.30
36	c	918	DGD	O2G-C1B-O1B	-2.11	118.59	123.70
24	B	614	CLA	CMC-C2C-C1C	2.11	128.26	125.04
25	a	420	PHO	OBD-CAD-C3D	-2.11	124.47	127.98
24	a	406	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
24	c	913	CLA	CAC-C3C-C4C	2.11	127.55	124.81
25	a	420	PHO	C4-C3-C2	-2.11	118.27	123.68
24	C	505	CLA	C1-O2A-CGA	2.11	121.97	116.44
24	c	904	CLA	OBD-CAD-C3D	-2.11	123.45	128.52
24	b	617	CLA	CED-O2D-CGD	2.11	120.70	115.94
34	c	920	LMG	O8-C28-O10	-2.11	118.27	123.59
24	c	908	CLA	CAA-C2A-C1A	2.11	118.88	111.97
24	d	403	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
26	B	618	BCR	C21-C20-C19	-2.11	116.65	123.22
35	C	523	HTG	C1-O5-C5	2.10	116.46	112.58
37	d	408	LHG	O8-C23-C24	2.10	118.51	111.91
24	C	510	CLA	OBD-CAD-C3D	-2.10	123.46	128.52
24	b	620	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
36	C	517	DGD	O1G-C1A-O1A	-2.10	118.28	123.59
24	D	401	CLA	C4-C3-C5	2.10	118.81	115.27
24	c	908	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
34	C	501	LMG	O8-C28-C29	2.10	118.50	111.91
24	B	611	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	B	609	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
27	A	412	SQD	C3-C4-C5	2.10	113.99	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	621	SQD	C25-C24-C23	-2.10	105.98	113.62
34	C	501	LMG	O6-C5-C4	2.10	113.51	109.69
24	c	911	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
38	e	102	HEM	CMD-C2D-C1D	2.10	128.24	125.04
26	k	101	BCR	C11-C10-C9	-2.10	124.31	127.31
24	c	907	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
24	b	617	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
26	T	102	BCR	C3-C4-C5	-2.10	110.33	114.08
24	c	910	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
26	d	404	BCR	C35-C13-C14	-2.10	119.99	122.92
24	B	605	CLA	C4-C3-C5	2.09	118.80	115.27
24	B	609	CLA	C1-C2-C3	-2.09	122.42	126.04
24	c	904	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
24	B	603	CLA	CHB-C4A-NA	2.09	127.41	124.51
24	A	406	CLA	O2A-CGA-CBA	2.09	118.47	111.91
40	V	201	HEC	CHB-C1B-C2B	-2.09	121.71	124.98
24	C	509	CLA	C7-C6-C5	-2.09	107.68	113.36
24	c	909	CLA	O2A-CGA-CBA	2.09	118.47	111.91
24	c	912	CLA	CED-O2D-CGD	2.09	120.66	115.94
24	c	913	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
24	a	409	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
24	B	606	CLA	CHB-C1B-NB	-2.09	122.05	124.26
26	a	410	BCR	C38-C26-C25	-2.09	122.18	124.53
24	b	614	CLA	CMC-C2C-C1C	2.08	128.21	125.04
26	a	410	BCR	C16-C17-C18	-2.08	124.34	127.31
26	b	622	BCR	C20-C21-C22	-2.08	124.34	127.31
29	c	921	LMT	C1B-O1B-C4'	-2.08	112.81	117.96
24	c	914	CLA	CBC-CAC-C3C	-2.08	106.69	112.43
26	H	101	BCR	C24-C23-C22	-2.08	123.09	126.23
24	c	907	CLA	CAA-CBA-CGA	2.08	119.33	113.25
24	A	406	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
36	c	916	DGD	O2G-C1B-O1B	-2.08	118.68	123.70
34	C	501	LMG	C8-O7-C10	-2.08	112.67	117.79
24	C	510	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
26	y	101	BCR	C8-C7-C6	-2.08	121.37	127.20
24	c	907	CLA	CED-O2D-CGD	2.08	120.64	115.94
24	b	610	CLA	C11-C10-C8	-2.08	109.21	115.92
31	A	419	PL9	C37-C36-C34	-2.08	106.15	112.98
26	A	411	BCR	C11-C10-C9	-2.07	124.35	127.31
26	K	103	BCR	C33-C5-C6	-2.07	122.20	124.53
24	d	403	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
36	D	405	DGD	C1E-O6E-C5E	2.07	117.75	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	508	CLA	C1-C2-C3	-2.07	122.46	126.04
24	b	607	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
26	T	102	BCR	C7-C8-C9	-2.07	123.11	126.23
24	c	909	CLA	CHD-C4C-NC	2.07	127.46	124.20
34	j	101	LMG	O7-C10-C11	2.07	115.96	111.50
24	B	611	CLA	CHA-C1A-NA	-2.07	121.66	126.40
40	v	202	HEC	O2D-CGD-CBD	2.07	120.67	114.03
36	c	916	DGD	C3G-C2G-C1G	-2.07	106.90	111.79
25	A	409	PHO	C4D-CHA-CBD	2.07	109.45	108.52
24	C	506	CLA	CHA-C1A-NA	-2.07	121.67	126.40
24	b	615	CLA	C7-C6-C5	-2.07	107.75	113.36
24	d	402	CLA	CHB-C1B-NB	-2.06	122.07	124.26
24	C	513	CLA	CHA-C1A-NA	-2.06	121.68	126.40
36	C	518	DGD	C2G-O2G-C1B	-2.06	112.72	117.79
24	d	403	CLA	O2A-CGA-CBA	2.06	118.37	111.91
37	d	409	LHG	O8-C23-O10	-2.06	118.39	123.59
24	c	914	CLA	CHB-C4A-NA	2.06	127.36	124.51
24	b	611	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
26	B	618	BCR	C16-C17-C18	-2.06	124.38	127.31
24	b	607	CLA	CMA-C3A-C2A	-2.05	105.54	113.83
36	h	102	DGD	C3E-C4E-C5E	-2.05	106.58	110.24
24	C	513	CLA	CBA-CAA-C2A	-2.05	107.80	113.86
24	c	905	CLA	O2A-CGA-CBA	2.05	118.35	111.91
24	c	911	CLA	C4-C3-C2	-2.05	118.42	123.68
24	a	406	CLA	CMC-C2C-C1C	2.05	128.16	125.04
24	a	406	CLA	CHD-C4C-NC	2.05	127.43	124.20
24	B	608	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
34	C	520	LMG	O6-C5-C6	2.05	111.52	106.44
36	H	102	DGD	O6E-C5E-C6E	2.05	111.52	106.44
24	b	614	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
24	b	614	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
24	B	609	CLA	CMB-C2B-C3B	2.04	131.54	126.59
24	b	605	CLA	CMB-C2B-C1B	2.04	128.48	125.37
31	a	417	PL9	C45-C44-C46	2.04	118.71	115.27
24	B	609	CLA	CHB-C1B-C2B	-2.04	121.47	127.24
24	B	606	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
26	c	915	BCR	C20-C21-C22	-2.04	124.40	127.31
24	b	612	CLA	C4-C3-C5	2.04	118.70	115.27
24	c	902	CLA	O2A-CGA-CBA	2.04	118.30	111.91
24	b	619	CLA	CHD-C4C-NC	2.04	127.42	124.20
24	C	511	CLA	CMB-C2B-C1B	2.04	128.47	125.37
24	B	616	CLA	C6-C7-C8	-2.04	109.33	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	H	101	BCR	C29-C30-C25	2.04	113.62	110.48
29	f	103	LMT	O1B-C1B-C2B	2.04	113.38	108.10
24	b	611	CLA	CED-O2D-CGD	2.04	120.54	115.94
31	d	405	PL9	C30-C29-C31	2.03	118.69	115.27
24	C	507	CLA	CMA-C3A-C2A	-2.03	105.62	113.83
29	f	103	LMT	O5'-C5'-C4'	2.03	114.03	109.75
26	k	101	BCR	C20-C21-C22	-2.03	124.41	127.31
27	f	102	SQD	O48-C23-O10	-2.03	118.47	123.59
24	a	406	CLA	C5-C3-C2	-2.03	117.01	121.12
24	a	406	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
24	B	602	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
34	j	101	LMG	O8-C28-C29	2.03	118.26	111.91
38	e	102	HEM	C4C-CHD-C1D	-2.03	121.69	126.06
36	h	102	DGD	O4E-C4E-C5E	2.02	114.33	109.30
24	b	619	CLA	C11-C10-C8	-2.02	109.37	115.92
24	B	616	CLA	O2A-CGA-CBA	2.02	118.26	111.91
26	K	103	BCR	C2-C1-C6	2.02	113.60	110.48
37	L	101	LHG	C6-C5-C4	-2.02	107.00	111.79
26	C	516	BCR	C11-C10-C9	-2.02	124.42	127.31
27	L	102	SQD	O48-C23-O10	-2.02	118.49	123.59
24	c	910	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	b	613	CLA	CED-O2D-CGD	2.02	120.50	115.94
27	L	102	SQD	O8-S-C6	2.02	108.96	105.74
24	c	906	CLA	CHB-C4A-NA	2.02	127.30	124.51
36	C	518	DGD	O6D-C1D-O3G	-2.02	105.20	109.97
24	C	510	CLA	O2A-CGA-CBA	2.02	118.23	111.91
24	B	609	CLA	C4-C3-C5	2.02	118.66	115.27
24	c	913	CLA	CHB-C4A-NA	2.02	127.30	124.51
24	D	402	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
24	c	902	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
34	j	101	LMG	O6-C5-C4	2.01	113.35	109.69
36	c	917	DGD	O2G-C1B-O1B	-2.01	118.84	123.70
31	A	419	PL9	C12-C13-C14	-2.01	122.82	127.66
24	c	905	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
38	E	103	HEM	CMD-C2D-C1D	2.01	128.10	125.04
24	c	912	CLA	CMB-C2B-C1B	2.01	128.43	125.37
26	D	403	BCR	C11-C10-C9	-2.01	124.44	127.31
34	C	521	LMG	O8-C28-C29	2.01	118.21	111.91
24	c	903	CLA	O2A-C1-C2	2.01	113.91	108.64
24	B	603	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
24	A	407	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
25	a	420	PHO	CAC-C3C-C4C	2.01	129.35	124.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	613	CLA	C4-C3-C5	2.00	118.64	115.27
24	B	615	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
24	C	507	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	A	407	CLA	CMC-C2C-C1C	2.00	128.09	125.04
24	c	906	CLA	CHD-C4C-NC	2.00	127.36	124.20
24	C	505	CLA	CAA-CBA-CGA	2.00	119.11	113.25
24	B	607	CLA	CMB-C2B-C1B	2.00	128.42	125.37

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	201	HEC	NA
40	v	202	HEC	NA

All (1295) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	410	CLA	C2-C3-C5-C6
24	A	410	CLA	C4-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	506	CLA	C2B-C3B-CAB-CBB
24	C	506	CLA	C4B-C3B-CAB-CBB
24	C	508	CLA	CHA-CBD-CGD-O2D
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	b	609	CLA	C2-C3-C5-C6
24	b	609	CLA	C4-C3-C5-C6
24	b	610	CLA	C2B-C3B-CAB-CBB
24	b	610	CLA	C4B-C3B-CAB-CBB
24	b	610	CLA	CHA-CBD-CGD-O1D
24	b	610	CLA	CHA-CBD-CGD-O2D
24	b	618	CLA	CHA-CBD-CGD-O1D
24	b	618	CLA	CHA-CBD-CGD-O2D
24	b	618	CLA	CAD-CBD-CGD-O1D
24	b	618	CLA	CAD-CBD-CGD-O2D
24	b	618	CLA	C2-C3-C5-C6
24	b	618	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	c	909	CLA	CHA-CBD-CGD-O1D
24	c	909	CLA	CHA-CBD-CGD-O2D
24	c	914	CLA	C2B-C3B-CAB-CBB
24	c	914	CLA	C4B-C3B-CAB-CBB
26	D	403	BCR	C21-C22-C23-C24
26	D	403	BCR	C37-C22-C23-C24
26	H	101	BCR	C7-C8-C9-C10
26	K	102	BCR	C5-C6-C7-C8
26	K	102	BCR	C21-C22-C23-C24
26	K	102	BCR	C37-C22-C23-C24
26	d	404	BCR	C21-C22-C23-C24
26	d	404	BCR	C37-C22-C23-C24
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
27	A	416	SQD	O6-C44-C45-O47
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
27	F	101	SQD	O49-C7-O47-C45
27	F	101	SQD	C8-C7-O47-C45
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
27	L	102	SQD	C5-C6-S-O7
27	L	102	SQD	C5-C6-S-O8
27	L	102	SQD	C5-C6-S-O9
27	a	402	SQD	O6-C44-C45-O47
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8
27	f	102	SQD	C5-C6-S-O9
28	A	414	GOL	C1-C2-C3-O3
28	A	414	GOL	O2-C2-C3-O3
28	A	415	GOL	O1-C1-C2-C3
28	B	629	GOL	O1-C1-C2-C3
28	B	631	GOL	O1-C1-C2-C3
28	B	637	GOL	O1-C1-C2-C3
28	F	103	GOL	O1-C1-C2-C3
28	O	302	GOL	O1-C1-C2-C3
28	T	103	GOL	O1-C1-C2-C3
28	V	203	GOL	O1-C1-C2-C3
28	V	203	GOL	C1-C2-C3-O3
28	a	415	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
28	b	631	GOL	O1-C1-C2-C3
28	b	633	GOL	O1-C1-C2-O2
28	f	101	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
28	v	205	GOL	O1-C1-C2-C3
29	B	636	LMT	C2'-C1'-O1'-C1
29	B	636	LMT	O5'-C1'-O1'-C1
29	C	522	LMT	C2'-C1'-O1'-C1
29	C	522	LMT	O5'-C1'-O1'-C1
29	E	102	LMT	C2'-C1'-O1'-C1
29	E	102	LMT	O5'-C1'-O1'-C1
29	b	601	LMT	C2'-C1'-O1'-C1
29	b	601	LMT	O5'-C1'-O1'-C1
29	b	625	LMT	C2'-C1'-O1'-C1
29	b	625	LMT	O5'-C1'-O1'-C1
29	m	102	LMT	O5'-C1'-O1'-C1
29	m	102	LMT	C2-C1-O1'-C1'
31	a	417	PL9	C9-C11-C12-C13
31	a	417	PL9	C13-C14-C16-C17
31	a	417	PL9	C15-C14-C16-C17
34	Z	101	LMG	O6-C1-O1-C7
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
34	z	101	LMG	O9-C10-O7-C8
34	z	101	LMG	C11-C10-O7-C8
35	B	625	HTG	C2'-C1'-S1-C1
35	V	202	HTG	C2-C1-S1-C1'
35	V	202	HTG	O5-C1-S1-C1'
35	c	922	HTG	C2'-C1'-S1-C1
36	D	405	DGD	C2B-C1B-O2G-C2G
36	D	405	DGD	C2D-C1D-O3G-C3G
36	D	405	DGD	O6D-C1D-O3G-C3G
36	D	405	DGD	O6E-C1E-O5D-C6D
36	d	406	DGD	C2B-C1B-O2G-C2G
36	d	406	DGD	O1B-C1B-O2G-C2G
36	d	406	DGD	C2E-C1E-O5D-C6D
36	d	406	DGD	O6E-C1E-O5D-C6D
37	D	407	LHG	C3-O3-P-O6
37	E	101	LHG	C24-C23-O8-C6
37	L	101	LHG	C4-O6-P-O4
37	L	101	LHG	C4-O6-P-O5
37	d	408	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
37	d	408	LHG	C4-O6-P-O4
37	l	101	LHG	C4-O6-P-O3
37	l	101	LHG	C4-O6-P-O4
37	l	101	LHG	C4-O6-P-O5
29	B	623	LMT	C3'-C4'-O1B-C1B
29	C	522	LMT	C3'-C4'-O1B-C1B
37	E	101	LHG	O10-C23-O8-C6
37	e	101	LHG	O10-C23-O8-C6
37	e	101	LHG	C24-C23-O8-C6
36	D	405	DGD	O1B-C1B-O2G-C2G
24	B	605	CLA	C3-C5-C6-C7
27	L	102	SQD	C8-C7-O47-C45
24	c	902	CLA	CBD-CGD-O2D-CED
24	B	604	CLA	C4-C3-C5-C6
24	B	615	CLA	C4-C3-C5-C6
24	b	607	CLA	C4-C3-C5-C6
24	b	607	CLA	C2-C3-C5-C6
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C2A-CAA-CBA-CGA
24	B	615	CLA	C3-C5-C6-C7
29	B	623	LMT	O5B-C5B-C6B-O6B
24	d	401	CLA	CBD-CGD-O2D-CED
24	b	618	CLA	C3-C5-C6-C7
37	E	101	LHG	C8-C7-O7-C5
24	B	617	CLA	C3-C5-C6-C7
29	f	103	LMT	O5'-C5'-C6'-O6'
35	B	633	HTG	O5-C5-C6-O6
31	A	419	PL9	C25-C24-C26-C27
35	V	202	HTG	C4-C5-C6-O6
24	B	615	CLA	C2-C3-C5-C6
31	A	419	PL9	C23-C24-C26-C27
29	m	102	LMT	C4'-C5'-C6'-O6'
34	C	521	LMG	O6-C5-C6-O5
24	C	510	CLA	C3-C5-C6-C7
24	d	403	CLA	C3-C5-C6-C7
29	B	623	LMT	C4B-C5B-C6B-O6B
37	E	101	LHG	O6-C4-C5-O7
24	a	409	CLA	C5-C6-C7-C8
27	B	621	SQD	C7-C8-C9-C10
27	F	101	SQD	C7-C8-C9-C10
34	Z	101	LMG	C2-C1-O1-C7
36	D	405	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
24	D	402	CLA	C4-C3-C5-C6
24	B	604	CLA	C2-C3-C5-C6
24	B	617	CLA	C6-C7-C8-C9
24	C	502	CLA	C11-C12-C13-C14
24	C	513	CLA	C6-C7-C8-C9
24	a	407	CLA	C14-C13-C15-C16
24	c	907	CLA	C6-C7-C8-C9
24	c	911	CLA	C11-C12-C13-C14
24	C	510	CLA	C8-C10-C11-C12
26	D	403	BCR	C7-C8-C9-C34
26	H	101	BCR	C7-C8-C9-C34
26	K	103	BCR	C7-C8-C9-C34
26	b	623	BCR	C37-C22-C23-C24
35	B	633	HTG	C4-C5-C6-O6
24	B	604	CLA	C5-C6-C7-C8
24	B	615	CLA	C5-C6-C7-C8
24	c	907	CLA	C10-C11-C12-C13
24	C	509	CLA	C10-C11-C12-C13
24	a	409	CLA	C8-C10-C11-C12
24	b	610	CLA	C10-C11-C12-C13
24	b	620	CLA	C15-C16-C17-C18
24	c	911	CLA	C8-C10-C11-C12
35	B	626	HTG	O5-C5-C6-O6
24	B	602	CLA	C5-C6-C7-C8
24	b	607	CLA	C5-C6-C7-C8
24	b	618	CLA	C15-C16-C17-C18
29	a	401	LMT	C3-C4-C5-C6
28	B	629	GOL	O1-C1-C2-O2
28	B	631	GOL	O1-C1-C2-O2
28	T	103	GOL	O1-C1-C2-O2
28	b	632	GOL	O2-C2-C3-O3
28	v	203	GOL	O1-C1-C2-O2
27	A	416	SQD	C23-C24-C25-C26
29	m	104	LMT	O5'-C5'-C6'-O6'
35	V	202	HTG	O5-C5-C6-O6
24	a	409	CLA	C15-C16-C17-C18
37	d	409	LHG	C30-C31-C32-C33
29	m	103	LMT	O5'-C5'-C6'-O6'
37	E	101	LHG	O9-C7-O7-C5
34	C	521	LMG	C11-C10-O7-C8
24	B	617	CLA	C10-C11-C12-C13
24	A	410	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	A	410	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C10-C8-C7
24	b	610	CLA	C12-C13-C15-C16
24	C	507	CLA	C13-C15-C16-C17
24	b	618	CLA	C10-C11-C12-C13
34	b	624	LMG	C30-C31-C32-C33
24	b	610	CLA	CBD-CGD-O2D-CED
29	f	103	LMT	C4'-C5'-C6'-O6'
29	f	103	LMT	O5'-C1'-O1'-C1
24	D	402	CLA	C5-C6-C7-C8
34	C	520	LMG	C28-C29-C30-C31
29	C	522	LMT	O5B-C5B-C6B-O6B
24	c	907	CLA	C15-C16-C17-C18
29	m	102	LMT	O5'-C5'-C6'-O6'
24	b	605	CLA	C8-C10-C11-C12
37	E	101	LHG	C4-O6-P-O3
37	L	101	LHG	C4-O6-P-O3
37	e	101	LHG	C3-O3-P-O6
35	C	524	HTG	O5-C5-C6-O6
24	c	907	CLA	C3-C5-C6-C7
27	F	101	SQD	C23-C24-C25-C26
34	C	521	LMG	O9-C10-O7-C8
24	B	615	CLA	C10-C11-C12-C13
36	c	917	DGD	C3B-C4B-C5B-C6B
24	C	508	CLA	C2A-CAA-CBA-CGA
36	d	406	DGD	C4E-C5E-C6E-O5E
37	D	407	LHG	C32-C33-C34-C35
27	L	102	SQD	C30-C31-C32-C33
29	b	601	LMT	C3-C4-C5-C6
37	d	407	LHG	C27-C28-C29-C30
34	C	501	LMG	C11-C10-O7-C8
29	M	101	LMT	O5'-C5'-C6'-O6'
24	B	602	CLA	C3-C5-C6-C7
27	L	102	SQD	C14-C15-C16-C17
27	a	411	SQD	C25-C26-C27-C28
34	B	622	LMG	C31-C32-C33-C34
36	H	102	DGD	C7A-C8A-C9A-CAA
24	a	409	CLA	C16-C17-C18-C19
24	b	605	CLA	CBA-CGA-O2A-C1
27	a	402	SQD	C10-C11-C12-C13
27	f	102	SQD	C29-C30-C31-C32
34	Z	101	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
36	C	519	DGD	C2A-C3A-C4A-C5A
37	L	101	LHG	C12-C13-C14-C15
34	C	501	LMG	O9-C10-O7-C8
34	c	919	LMG	O9-C10-O7-C8
36	D	405	DGD	C1A-C2A-C3A-C4A
27	a	411	SQD	C9-C10-C11-C12
29	C	522	LMT	C4-C5-C6-C7
34	C	501	LMG	C37-C38-C39-C40
35	B	625	HTG	C2'-C3'-C4'-C5'
36	c	918	DGD	C5A-C6A-C7A-C8A
37	D	408	LHG	C29-C30-C31-C32
27	L	102	SQD	C26-C27-C28-C29
27	a	411	SQD	C34-C35-C36-C37
34	J	101	LMG	C20-C21-C22-C23
34	j	101	LMG	C17-C18-C19-C20
36	C	517	DGD	C3B-C4B-C5B-C6B
36	H	102	DGD	CCB-CDB-CEB-CFB
36	c	918	DGD	C2B-C3B-C4B-C5B
37	d	407	LHG	C32-C33-C34-C35
27	A	412	SQD	C9-C10-C11-C12
27	B	621	SQD	C31-C32-C33-C34
34	C	520	LMG	C17-C18-C19-C20
34	b	624	LMG	C38-C39-C40-C41
29	a	401	LMT	C2'-C1'-O1'-C1
29	c	921	LMT	C2'-C1'-O1'-C1
29	f	103	LMT	C2'-C1'-O1'-C1
29	m	102	LMT	C2'-C1'-O1'-C1
36	d	406	DGD	C2D-C1D-O3G-C3G
27	a	411	SQD	C30-C31-C32-C33
36	C	517	DGD	C4B-C5B-C6B-C7B
24	C	507	CLA	C16-C17-C18-C20
24	c	903	CLA	C16-C17-C18-C20
24	c	902	CLA	O1D-CGD-O2D-CED
25	A	408	PHO	C4-C3-C5-C6
27	A	412	SQD	C32-C33-C34-C35
27	f	102	SQD	C25-C26-C27-C28
34	J	101	LMG	C14-C15-C16-C17
36	c	917	DGD	C9B-CAB-CBB-CCB
37	L	101	LHG	C13-C14-C15-C16
24	A	410	CLA	C14-C13-C15-C16
24	B	605	CLA	C6-C7-C8-C9
24	b	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	c	912	CLA	C6-C7-C8-C9
24	d	403	CLA	C14-C13-C15-C16
36	c	916	DGD	O6D-C5D-C6D-O5D
36	c	918	DGD	C1A-C2A-C3A-C4A
27	L	102	SQD	C34-C35-C36-C37
34	C	501	LMG	C12-C13-C14-C15
34	c	919	LMG	C13-C14-C15-C16
37	l	101	LHG	C25-C26-C27-C28
29	a	401	LMT	C4B-C5B-C6B-O6B
26	c	915	BCR	C7-C8-C9-C34
34	z	101	LMG	C15-C16-C17-C18
36	d	406	DGD	C8B-C9B-CAB-CBB
37	d	409	LHG	C29-C30-C31-C32
28	A	413	GOL	O1-C1-C2-C3
28	B	627	GOL	O1-C1-C2-C3
28	B	632	GOL	O1-C1-C2-C3
28	T	103	GOL	C1-C2-C3-O3
28	V	204	GOL	O1-C1-C2-C3
28	V	205	GOL	O1-C1-C2-C3
28	b	628	GOL	C1-C2-C3-O3
28	b	632	GOL	C1-C2-C3-O3
28	b	633	GOL	O1-C1-C2-C3
28	f	101	GOL	C1-C2-C3-O3
28	o	302	GOL	O1-C1-C2-C3
26	b	623	BCR	C21-C22-C23-C24
24	C	513	CLA	C3-C5-C6-C7
24	b	605	CLA	C3-C5-C6-C7
24	C	502	CLA	C15-C16-C17-C18
34	c	919	LMG	C11-C10-O7-C8
29	B	636	LMT	C3-C4-C5-C6
34	C	520	LMG	C12-C13-C14-C15
36	c	918	DGD	C3B-C4B-C5B-C6B
36	D	405	DGD	C1B-C2B-C3B-C4B
27	B	621	SQD	C11-C10-C9-C8
27	L	102	SQD	C28-C29-C30-C31
34	z	101	LMG	C12-C13-C14-C15
36	D	405	DGD	C2A-C3A-C4A-C5A
36	H	102	DGD	CBA-CCA-CDA-CEA
36	H	102	DGD	CAB-CBB-CCB-CDB
36	c	918	DGD	C2A-C3A-C4A-C5A
36	h	102	DGD	CBB-CCB-CDB-CEB
37	E	101	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
37	E	101	LHG	C25-C26-C27-C28
37	L	101	LHG	C14-C15-C16-C17
37	l	101	LHG	C13-C14-C15-C16
34	J	101	LMG	O6-C5-C6-O5
34	j	101	LMG	O6-C5-C6-O5
35	b	627	HTG	O5-C5-C6-O6
24	D	401	CLA	C4B-C3B-CAB-CBB
29	a	401	LMT	O5'-C1'-O1'-C1
29	c	921	LMT	O5'-C1'-O1'-C1
36	d	406	DGD	O6D-C1D-O3G-C3G
27	a	411	SQD	C16-C17-C18-C19
34	C	501	LMG	C14-C15-C16-C17
36	C	518	DGD	CAB-CBB-CCB-CDB
36	d	406	DGD	C2A-C3A-C4A-C5A
36	h	102	DGD	C5B-C6B-C7B-C8B
37	E	101	LHG	C24-C25-C26-C27
27	f	102	SQD	C26-C27-C28-C29
29	B	636	LMT	C6-C7-C8-C9
36	c	917	DGD	C2B-C3B-C4B-C5B
37	e	101	LHG	C9-C10-C11-C12
24	B	614	CLA	C13-C15-C16-C17
27	F	101	SQD	C32-C33-C34-C35
34	C	520	LMG	C11-C12-C13-C14
36	C	518	DGD	CAA-CBA-CCA-CDA
37	d	409	LHG	C15-C16-C17-C18
37	l	101	LHG	C33-C34-C35-C36
24	B	602	CLA	CBA-CGA-O2A-C1
24	d	401	CLA	O1D-CGD-O2D-CED
24	b	612	CLA	C13-C15-C16-C17
24	c	910	CLA	C13-C15-C16-C17
34	B	622	LMG	C30-C31-C32-C33
34	J	101	LMG	C16-C17-C18-C19
27	a	402	SQD	C16-C17-C18-C19
34	C	501	LMG	C11-C12-C13-C14
34	J	101	LMG	C11-C12-C13-C14
36	c	918	DGD	CBA-CCA-CDA-CEA
36	C	517	DGD	O6D-C5D-C6D-O5D
24	b	608	CLA	C3-C5-C6-C7
29	m	102	LMT	O1'-C1-C2-C3
37	D	408	LHG	C13-C14-C15-C16
40	V	201	HEC	C2C-C3C-CAC-CBC
31	A	419	PL9	C30-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
25	A	408	PHO	C2-C3-C5-C6
31	A	419	PL9	C28-C29-C31-C32
34	j	101	LMG	C16-C17-C18-C19
28	A	415	GOL	O1-C1-C2-O2
28	B	637	GOL	O1-C1-C2-O2
28	F	103	GOL	O1-C1-C2-O2
28	O	302	GOL	O1-C1-C2-O2
28	T	103	GOL	O2-C2-C3-O3
28	a	415	GOL	O1-C1-C2-O2
28	f	101	GOL	O2-C2-C3-O3
28	v	205	GOL	O1-C1-C2-O2
34	C	521	LMG	C11-C12-C13-C14
37	D	406	LHG	C28-C29-C30-C31
37	E	101	LHG	C23-C24-C25-C26
36	d	406	DGD	C9B-CAB-CBB-CCB
24	D	401	CLA	C2B-C3B-CAB-CBB
24	c	913	CLA	C2B-C3B-CAB-CBB
27	L	102	SQD	C12-C13-C14-C15
24	c	913	CLA	CBD-CGD-O2D-CED
27	a	411	SQD	C10-C11-C12-C13
34	J	101	LMG	C35-C36-C37-C38
35	V	202	HTG	C2'-C3'-C4'-C5'
24	B	617	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C2-C1-O2A-CGA
24	b	605	CLA	C2-C1-O2A-CGA
34	j	101	LMG	C32-C33-C34-C35
35	B	626	HTG	C3'-C4'-C5'-C6'
24	C	502	CLA	C13-C15-C16-C17
24	b	610	CLA	C13-C15-C16-C17
24	b	605	CLA	O1A-CGA-O2A-C1
36	D	405	DGD	C4A-C5A-C6A-C7A
36	d	406	DGD	CAA-CBA-CCA-CDA
36	h	102	DGD	CAA-CBA-CCA-CDA
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
26	H	101	BCR	C5-C6-C7-C8
26	K	102	BCR	C1-C6-C7-C8
26	b	621	BCR	C1-C6-C7-C8
26	b	621	BCR	C5-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C26
26	h	101	BCR	C23-C24-C25-C30
27	B	621	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
34	c	919	LMG	C20-C21-C22-C23
36	C	517	DGD	C7A-C8A-C9A-CAA
36	c	918	DGD	C6A-C7A-C8A-C9A
24	B	602	CLA	O1A-CGA-O2A-C1
29	M	101	LMT	C4B-C5B-C6B-O6B
24	B	607	CLA	C10-C11-C12-C13
37	l	101	LHG	C14-C15-C16-C17
24	B	606	CLA	C4-C3-C5-C6
24	c	911	CLA	C4-C3-C5-C6
24	B	606	CLA	C2-C3-C5-C6
24	B	616	CLA	C11-C12-C13-C15
24	C	511	CLA	C6-C7-C8-C10
24	D	402	CLA	C2-C3-C5-C6
24	a	407	CLA	C12-C13-C15-C16
24	b	608	CLA	C11-C12-C13-C15
24	b	610	CLA	C11-C10-C8-C7
24	c	907	CLA	C11-C10-C8-C7
24	c	911	CLA	C11-C12-C13-C15
24	d	403	CLA	C12-C13-C15-C16
35	C	524	HTG	S1-C1'-C2'-C3'
24	b	620	CLA	C3-C5-C6-C7
24	A	405	CLA	C2C-C3C-CAC-CBC
36	d	406	DGD	C7A-C8A-C9A-CAA
37	d	407	LHG	C28-C29-C30-C31
36	H	102	DGD	C9B-CAB-CBB-CCB
35	B	625	HTG	C1'-C2'-C3'-C4'
34	Z	101	LMG	C10-C11-C12-C13
38	e	102	HEM	C2B-C3B-CAB-CBB
29	E	102	LMT	C4'-C5'-C6'-O6'
34	j	101	LMG	C14-C15-C16-C17
36	h	102	DGD	CCA-CDA-CEA-CFA
37	l	101	LHG	C12-C13-C14-C15
24	b	619	CLA	C10-C11-C12-C13
36	d	406	DGD	C3A-C4A-C5A-C6A
24	a	406	CLA	C2C-C3C-CAC-CBC
27	a	402	SQD	C31-C32-C33-C34
35	c	922	HTG	S1-C1'-C2'-C3'
34	C	521	LMG	C16-C17-C18-C19
37	d	407	LHG	C30-C31-C32-C33
36	H	102	DGD	C5B-C6B-C7B-C8B
36	h	102	DGD	C8A-C9A-CAA-CBA
24	B	607	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	M	101	LMT	O5B-C5B-C6B-O6B
34	Z	101	LMG	O6-C5-C6-O5
27	L	102	SQD	C15-C16-C17-C18
34	a	412	LMG	C29-C30-C31-C32
24	C	507	CLA	C16-C17-C18-C19
24	a	409	CLA	C16-C17-C18-C20
24	B	616	CLA	C2-C3-C5-C6
24	C	511	CLA	C2-C3-C5-C6
24	c	911	CLA	C2-C3-C5-C6
31	A	419	PL9	C4-C3-C7-C8
31	a	417	PL9	C4-C3-C7-C8
24	A	410	CLA	C6-C7-C8-C9
24	B	615	CLA	C14-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C9
24	b	608	CLA	C11-C12-C13-C14
24	b	618	CLA	C6-C7-C8-C9
24	c	907	CLA	C11-C10-C8-C9
27	a	402	SQD	C25-C26-C27-C28
37	d	409	LHG	C32-C33-C34-C35
27	F	101	SQD	C31-C32-C33-C34
29	f	103	LMT	C5-C6-C7-C8
36	c	917	DGD	C1A-C2A-C3A-C4A
29	m	104	LMT	C2-C3-C4-C5
37	l	101	LHG	C31-C32-C33-C34
36	C	517	DGD	O6E-C5E-C6E-O5E
24	c	903	CLA	C16-C17-C18-C19
29	B	623	LMT	C5-C6-C7-C8
34	b	624	LMG	C17-C18-C19-C20
37	L	101	LHG	C32-C33-C34-C35
24	b	620	CLA	C10-C11-C12-C13
24	c	904	CLA	C8-C10-C11-C12
29	A	417	LMT	O1'-C1-C2-C3
29	b	601	LMT	C2-C3-C4-C5
36	c	917	DGD	CAA-CBA-CCA-CDA
34	C	521	LMG	C17-C18-C19-C20
36	C	517	DGD	C5B-C6B-C7B-C8B
29	a	401	LMT	C7-C8-C9-C10
34	C	520	LMG	C16-C17-C18-C19
27	F	101	SQD	C30-C31-C32-C33
36	c	916	DGD	CAA-CBA-CCA-CDA
29	a	401	LMT	C1-C2-C3-C4
24	b	619	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	a	412	LMG	C35-C36-C37-C38
36	d	406	DGD	O6D-C5D-C6D-O5D
36	C	517	DGD	C4D-C5D-C6D-O5D
24	B	616	CLA	C4-C3-C5-C6
24	C	511	CLA	C4-C3-C5-C6
24	d	403	CLA	C4-C3-C5-C6
27	B	621	SQD	C34-C35-C36-C37
24	c	905	CLA	C8-C10-C11-C12
29	B	636	LMT	C5-C6-C7-C8
27	B	621	SQD	O10-C23-O48-C46
27	B	621	SQD	C35-C36-C37-C38
29	b	601	LMT	C4-C5-C6-C7
24	b	618	CLA	C16-C17-C18-C20
34	c	919	LMG	C7-C8-C9-O8
36	D	405	DGD	O1G-C1G-C2G-C3G
34	C	521	LMG	C8-C7-O1-C1
36	C	518	DGD	C2G-C3G-O3G-C1D
36	C	518	DGD	C5D-C6D-O5D-C1E
36	c	917	DGD	C2G-C3G-O3G-C1D
36	c	917	DGD	C5D-C6D-O5D-C1E
34	C	520	LMG	C21-C22-C23-C24
29	f	103	LMT	C2B-C1B-O1B-C4'
36	H	102	DGD	CDB-CEB-CFB-CGB
36	c	918	DGD	C7A-C8A-C9A-CAA
29	c	921	LMT	C6-C7-C8-C9
24	A	410	CLA	C3-C5-C6-C7
24	B	616	CLA	C16-C17-C18-C20
27	f	102	SQD	C32-C33-C34-C35
28	V	203	GOL	O1-C1-C2-O2
28	V	203	GOL	O2-C2-C3-O3
28	b	628	GOL	O2-C2-C3-O3
28	b	631	GOL	O1-C1-C2-O2
28	f	101	GOL	O1-C1-C2-O2
28	o	302	GOL	O1-C1-C2-O2
35	B	633	HTG	C4'-C5'-C6'-C7'
34	a	412	LMG	C28-C29-C30-C31
34	C	520	LMG	C22-C23-C24-C25
27	A	416	SQD	C26-C27-C28-C29
35	O	303	HTG	C3'-C4'-C5'-C6'
36	c	916	DGD	O6E-C5E-C6E-O5E
24	b	605	CLA	C2-C3-C5-C6
36	C	519	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
29	C	522	LMT	O5'-C5'-C6'-O6'
36	C	519	DGD	CBA-CCA-CDA-CEA
24	B	603	CLA	C15-C16-C17-C18
24	b	614	CLA	C15-C16-C17-C18
34	a	412	LMG	C21-C22-C23-C24
34	b	624	LMG	C15-C16-C17-C18
34	Z	101	LMG	C29-C28-O8-C9
34	C	521	LMG	C15-C16-C17-C18
24	C	510	CLA	C10-C11-C12-C13
24	b	605	CLA	C5-C6-C7-C8
36	H	102	DGD	O2G-C1B-C2B-C3B
40	V	201	HEC	C4C-C3C-CAC-CBC
37	E	101	LHG	C7-C8-C9-C10
27	a	411	SQD	C31-C32-C33-C34
29	m	103	LMT	C4'-C5'-C6'-O6'
24	C	508	CLA	C5-C6-C7-C8
24	b	618	CLA	C13-C15-C16-C17
24	C	510	CLA	C15-C16-C17-C18
24	B	602	CLA	CAA-CBA-CGA-O2A
29	b	601	LMT	C7-C8-C9-C10
37	L	101	LHG	C24-C25-C26-C27
36	c	916	DGD	C5A-C6A-C7A-C8A
24	b	605	CLA	C4-C3-C5-C6
34	B	622	LMG	C34-C35-C36-C37
24	B	615	CLA	C11-C12-C13-C15
24	B	615	CLA	C12-C13-C15-C16
24	C	502	CLA	C12-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C15
24	C	507	CLA	C6-C7-C8-C10
24	C	513	CLA	C11-C10-C8-C7
24	D	402	CLA	C11-C10-C8-C7
24	b	618	CLA	C6-C7-C8-C10
24	b	620	CLA	C11-C12-C13-C15
24	c	910	CLA	C12-C13-C15-C16
29	c	921	LMT	C7-C8-C9-C10
24	B	602	CLA	C11-C10-C8-C9
24	B	611	CLA	C14-C13-C15-C16
24	B	615	CLA	C11-C10-C8-C9
24	C	502	CLA	C14-C13-C15-C16
24	C	507	CLA	C6-C7-C8-C9
24	C	513	CLA	C11-C10-C8-C9
24	b	609	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	b	610	CLA	C14-C13-C15-C16
24	b	620	CLA	C11-C12-C13-C14
24	c	910	CLA	C14-C13-C15-C16
34	C	501	LMG	C13-C14-C15-C16
37	D	406	LHG	C25-C26-C27-C28
24	B	616	CLA	C10-C11-C12-C13
36	c	916	DGD	C4D-C5D-C6D-O5D
24	B	616	CLA	C16-C17-C18-C19
34	a	412	LMG	C33-C34-C35-C36
26	K	103	BCR	C7-C8-C9-C10
24	B	614	CLA	C10-C11-C12-C13
37	D	406	LHG	C34-C35-C36-C37
36	d	406	DGD	C2A-C1A-O1G-C1G
37	L	101	LHG	C26-C27-C28-C29
24	B	603	CLA	C4B-C3B-CAB-CBB
24	C	503	CLA	C4B-C3B-CAB-CBB
24	b	611	CLA	C4B-C3B-CAB-CBB
24	c	903	CLA	C4B-C3B-CAB-CBB
24	c	906	CLA	C4B-C3B-CAB-CBB
24	c	913	CLA	C4B-C3B-CAB-CBB
37	E	101	LHG	O6-C4-C5-C6
37	l	101	LHG	O6-C4-C5-C6
31	a	417	PL9	C14-C16-C17-C18
29	b	625	LMT	C3'-C4'-O1B-C1B
27	A	412	SQD	C15-C16-C17-C18
24	c	911	CLA	CBA-CGA-O2A-C1
24	B	616	CLA	C13-C15-C16-C17
24	b	610	CLA	C15-C16-C17-C18
36	C	517	DGD	C6A-C7A-C8A-C9A
36	C	519	DGD	O1A-C1A-O1G-C1G
27	F	101	SQD	C34-C35-C36-C37
29	a	401	LMT	C2-C3-C4-C5
24	b	618	CLA	C16-C17-C18-C19
27	F	101	SQD	C29-C30-C31-C32
37	d	408	LHG	C26-C27-C28-C29
24	A	410	CLA	CBA-CGA-O2A-C1
27	f	102	SQD	C23-C24-C25-C26
34	c	919	LMG	C10-C11-C12-C13
24	C	514	CLA	C3A-C2A-CAA-CBA
27	A	412	SQD	C13-C14-C15-C16
27	A	416	SQD	O6-C44-C45-C46
27	a	402	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	C44-C45-C46-O48
36	d	406	DGD	O1G-C1G-C2G-C3G
37	E	101	LHG	C4-C5-C6-O8
37	e	101	LHG	C4-C5-C6-O8
29	b	601	LMT	O1'-C1-C2-C3
27	F	101	SQD	C24-C25-C26-C27
36	C	519	DGD	C9B-CAB-CBB-CCB
34	a	412	LMG	C22-C23-C24-C25
37	D	408	LHG	C28-C29-C30-C31
37	d	408	LHG	C4-O6-P-O3
27	a	402	SQD	C23-C24-C25-C26
29	a	401	LMT	O5B-C5B-C6B-O6B
24	d	401	CLA	C15-C16-C17-C18
29	E	102	LMT	C2-C3-C4-C5
36	h	102	DGD	C6A-C7A-C8A-C9A
24	c	912	CLA	CBA-CGA-O2A-C1
27	a	402	SQD	C24-C23-O48-C46
34	C	501	LMG	C38-C39-C40-C41
24	C	506	CLA	C10-C11-C12-C13
27	a	402	SQD	C27-C28-C29-C30
35	c	922	HTG	C3'-C4'-C5'-C6'
24	B	603	CLA	C2B-C3B-CAB-CBB
24	C	503	CLA	C2B-C3B-CAB-CBB
24	c	903	CLA	C2B-C3B-CAB-CBB
37	d	408	LHG	O2-C2-C3-O3
34	J	101	LMG	C13-C14-C15-C16
24	c	911	CLA	O1A-CGA-O2A-C1
36	h	102	DGD	CDA-CEA-CFA-CGA
27	A	412	SQD	O6-C44-C45-O47
27	B	621	SQD	O47-C45-C46-O48
27	F	101	SQD	O47-C45-C46-O48
27	L	102	SQD	O47-C45-C46-O48
34	C	501	LMG	O1-C7-C8-O7
34	c	919	LMG	O1-C7-C8-O7
34	c	919	LMG	O7-C8-C9-O8
34	z	101	LMG	O1-C7-C8-O7
36	D	405	DGD	O2G-C2G-C3G-O3G
34	C	501	LMG	C16-C17-C18-C19
36	C	517	DGD	O6E-C1E-O5D-C6D
24	B	614	CLA	C2-C1-O2A-CGA
24	c	912	CLA	C2-C1-O2A-CGA
24	c	914	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C6-C7-C8-C9
24	a	407	CLA	C11-C12-C13-C14
24	c	914	CLA	C6-C7-C8-C9
34	B	622	LMG	C36-C37-C38-C39
34	c	919	LMG	C39-C40-C41-C42
29	A	417	LMT	C4B-C5B-C6B-O6B
24	b	610	CLA	C8-C10-C11-C12
24	b	617	CLA	C5-C6-C7-C8
37	D	408	LHG	C2-C3-O3-P
34	b	624	LMG	C32-C33-C34-C35
37	d	408	LHG	C34-C35-C36-C37
26	D	403	BCR	C23-C24-C25-C26
26	D	403	BCR	C23-C24-C25-C30
26	c	915	BCR	C5-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C26
26	d	404	BCR	C23-C24-C25-C30
24	B	612	CLA	C8-C10-C11-C12
29	m	104	LMT	C9-C10-C11-C12
36	c	916	DGD	C8A-C9A-CAA-CBA
37	l	101	LHG	C30-C31-C32-C33
26	D	403	BCR	C7-C8-C9-C10
26	c	915	BCR	C7-C8-C9-C10
36	d	406	DGD	C4D-C5D-C6D-O5D
27	L	102	SQD	C9-C10-C11-C12
37	L	101	LHG	C7-C8-C9-C10
24	c	913	CLA	O1D-CGD-O2D-CED
36	D	405	DGD	C8B-C9B-CAB-CBB
36	c	917	DGD	C7A-C8A-C9A-CAA
37	d	407	LHG	C25-C26-C27-C28
24	b	609	CLA	C10-C11-C12-C13
37	L	101	LHG	C11-C12-C13-C14
24	C	507	CLA	C8-C10-C11-C12
34	J	101	LMG	C10-C11-C12-C13
24	A	405	CLA	C4C-C3C-CAC-CBC
34	J	101	LMG	C15-C16-C17-C18
24	B	605	CLA	C6-C7-C8-C10
24	B	607	CLA	C11-C10-C8-C7
24	B	611	CLA	C12-C13-C15-C16
24	C	505	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
24	c	905	CLA	C12-C13-C15-C16
24	c	912	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	B	614	CLA	C15-C16-C17-C18
26	h	101	BCR	C9-C10-C11-C12
36	D	405	DGD	CDA-CEA-CFA-CGA
37	d	407	LHG	C23-C24-C25-C26
36	d	406	DGD	O1A-C1A-O1G-C1G
34	b	624	LMG	C36-C37-C38-C39
34	z	101	LMG	C16-C17-C18-C19
35	b	626	HTG	C2'-C1'-S1-C1
29	f	103	LMT	O5B-C1B-O1B-C4'
34	C	501	LMG	C17-C18-C19-C20
36	c	918	DGD	CAB-CBB-CCB-CDB
36	C	518	DGD	C8A-C9A-CAA-CBA
34	j	101	LMG	C18-C19-C20-C21
36	C	517	DGD	C5A-C6A-C7A-C8A
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	b	620	CLA	CAD-CBD-CGD-O2D
24	c	904	CLA	CAD-CBD-CGD-O2D
24	c	911	CLA	CAD-CBD-CGD-O2D
24	c	913	CLA	CAD-CBD-CGD-O2D
24	c	914	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
27	B	621	SQD	C46-C45-O47-C7
27	L	102	SQD	C46-C45-O47-C7
38	E	103	HEM	C2C-C3C-CAC-CBC
25	a	420	PHO	C2C-C3C-CAC-CBC
24	d	401	CLA	C2C-C3C-CAC-CBC
27	L	102	SQD	C31-C32-C33-C34
27	a	411	SQD	C26-C27-C28-C29
24	C	512	CLA	CBA-CGA-O2A-C1
36	d	406	DGD	C5A-C6A-C7A-C8A
36	C	518	DGD	O6E-C1E-O5D-C6D
36	c	917	DGD	O6E-C1E-O5D-C6D
34	B	622	LMG	C10-C11-C12-C13
27	B	621	SQD	C44-C45-C46-O48
27	L	102	SQD	C44-C45-C46-O48
34	c	919	LMG	O1-C7-C8-C9
34	z	101	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
36	h	102	DGD	O1G-C1G-C2G-C3G
24	c	912	CLA	O1A-CGA-O2A-C1
37	l	101	LHG	O6-C4-C5-O7
27	L	102	SQD	C27-C28-C29-C30
37	l	101	LHG	C35-C36-C37-C38
38	e	102	HEM	C4B-C3B-CAB-CBB
35	B	624	HTG	S1-C1'-C2'-C3'
29	A	417	LMT	C7-C8-C9-C10
24	C	512	CLA	O1A-CGA-O2A-C1
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	505	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	b	605	CLA	CHA-CBD-CGD-O1D
24	b	605	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O1D
24	b	609	CLA	CHA-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	CBD-CGD-O2D-CED
24	A	410	CLA	O1A-CGA-O2A-C1
27	A	416	SQD	C19-C20-C21-C22
27	L	102	SQD	C13-C14-C15-C16
27	F	101	SQD	C2-C1-O6-C44
34	C	501	LMG	C2-C1-O1-C7
31	A	419	PL9	C2-C3-C7-C8
29	E	102	LMT	C5-C6-C7-C8
36	d	406	DGD	C2B-C3B-C4B-C5B
36	h	102	DGD	CDB-CEB-CFB-CGB
37	d	409	LHG	C9-C10-C11-C12
27	f	102	SQD	O47-C45-C46-O48
36	d	406	DGD	O1G-C1G-C2G-O2G
37	E	101	LHG	O7-C5-C6-O8
28	B	628	GOL	O1-C1-C2-O2
28	B	632	GOL	O1-C1-C2-O2
28	v	204	GOL	O1-C1-C2-O2
36	c	918	DGD	C4B-C5B-C6B-C7B
24	c	913	CLA	C15-C16-C17-C18
27	a	402	SQD	O10-C23-O48-C46
29	b	625	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
34	B	622	LMG	O9-C10-O7-C8
24	B	607	CLA	C11-C10-C8-C9
24	C	509	CLA	C11-C10-C8-C9
24	b	608	CLA	C6-C7-C8-C9
24	c	905	CLA	C14-C13-C15-C16
34	C	521	LMG	C4-C5-C6-O5
27	A	416	SQD	C17-C18-C19-C20
29	b	601	LMT	C11-C10-C9-C8
29	m	104	LMT	C11-C10-C9-C8
37	d	409	LHG	C17-C18-C19-C20
29	m	104	LMT	C6-C7-C8-C9
29	B	636	LMT	C4'-C5'-C6'-O6'
35	B	634	HTG	C4-C5-C6-O6
36	h	102	DGD	O2G-C1B-C2B-C3B
26	y	101	BCR	C36-C18-C19-C20
28	B	628	GOL	O1-C1-C2-C3
34	j	101	LMG	C19-C20-C21-C22
36	d	406	DGD	C1A-C2A-C3A-C4A
34	B	622	LMG	C32-C33-C34-C35
27	B	621	SQD	C9-C10-C11-C12
34	C	520	LMG	C37-C38-C39-C40
36	C	518	DGD	C9A-CAA-CBA-CCA
37	e	101	LHG	C11-C12-C13-C14
37	D	406	LHG	C27-C28-C29-C30
37	d	409	LHG	C2-C3-O3-P
24	d	403	CLA	C2-C3-C5-C6
35	B	634	HTG	C4'-C5'-C6'-C7'
24	D	402	CLA	C4B-C3B-CAB-CBB
37	D	407	LHG	C3-O3-P-O4
37	E	101	LHG	C4-O6-P-O5
37	d	408	LHG	C3-O3-P-O4
37	d	408	LHG	C4-O6-P-O5
37	e	101	LHG	C3-O3-P-O5
24	b	615	CLA	C16-C17-C18-C20
34	c	919	LMG	O6-C1-O1-C7
34	B	622	LMG	C37-C38-C39-C40
37	D	407	LHG	C33-C34-C35-C36
37	D	408	LHG	C12-C13-C14-C15
25	a	408	PHO	C8-C10-C11-C12
29	a	401	LMT	C6-C7-C8-C9
36	C	519	DGD	C6B-C7B-C8B-C9B
24	B	602	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	606	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	b	605	CLA	CAD-CBD-CGD-O1D
24	b	609	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
24	c	903	CLA	CAD-CBD-CGD-O1D
27	B	621	SQD	C5-C6-S-O7
34	a	412	LMG	C10-C11-C12-C13
36	c	918	DGD	C1B-C2B-C3B-C4B
24	B	606	CLA	C8-C10-C11-C12
27	B	621	SQD	C32-C33-C34-C35
34	J	101	LMG	C36-C37-C38-C39
37	d	407	LHG	C33-C34-C35-C36
24	B	615	CLA	C16-C17-C18-C20
24	B	602	CLA	C12-C13-C15-C16
24	B	616	CLA	C12-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C10
24	B	617	CLA	C12-C13-C15-C16
24	C	502	CLA	C11-C12-C13-C15
24	C	506	CLA	C12-C13-C15-C16
24	D	402	CLA	C12-C13-C15-C16
24	a	407	CLA	C11-C12-C13-C15
24	c	907	CLA	C6-C7-C8-C10
35	b	627	HTG	C2-C1-S1-C1'
29	a	401	LMT	O1'-C1-C2-C3
34	B	622	LMG	C11-C10-O7-C8
27	a	411	SQD	C15-C16-C17-C18
34	C	521	LMG	C18-C19-C20-C21
24	b	607	CLA	CBD-CGD-O2D-CED
24	b	609	CLA	CBD-CGD-O2D-CED
24	B	611	CLA	C16-C17-C18-C20
27	a	402	SQD	C34-C35-C36-C37
34	C	501	LMG	C10-C11-C12-C13
34	C	501	LMG	O1-C7-C8-C9
34	Z	101	LMG	O1-C7-C8-O7
37	e	101	LHG	O7-C5-C6-O8
27	a	402	SQD	C19-C20-C21-C22
36	C	518	DGD	C3A-C4A-C5A-C6A
36	C	519	DGD	C2B-C3B-C4B-C5B
27	A	416	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
34	B	622	LMG	C16-C17-C18-C19
27	B	621	SQD	C27-C28-C29-C30
24	B	616	CLA	C14-C13-C15-C16
24	B	617	CLA	C14-C13-C15-C16
24	C	505	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C14
24	b	607	CLA	C6-C7-C8-C9
24	b	615	CLA	C16-C17-C18-C19
36	c	918	DGD	C4A-C5A-C6A-C7A
34	C	501	LMG	O6-C1-O1-C7
24	C	511	CLA	O1A-CGA-O2A-C1
28	A	413	GOL	O1-C1-C2-O2
24	A	406	CLA	C15-C16-C17-C18
35	D	411	HTG	O5-C5-C6-O6
27	A	416	SQD	C15-C16-C17-C18
27	A	416	SQD	C24-C23-O48-C46
27	F	101	SQD	C11-C10-C9-C8
36	c	918	DGD	CCB-CDB-CEB-CFB
36	d	406	DGD	CAB-CBB-CCB-CDB
24	C	504	CLA	C2B-C3B-CAB-CBB
24	C	513	CLA	C2B-C3B-CAB-CBB
24	D	402	CLA	C2B-C3B-CAB-CBB
24	b	608	CLA	C2B-C3B-CAB-CBB
24	b	611	CLA	C2B-C3B-CAB-CBB
24	c	904	CLA	C2B-C3B-CAB-CBB
24	c	906	CLA	C2B-C3B-CAB-CBB
24	d	402	CLA	C2B-C3B-CAB-CBB
37	d	409	LHG	O10-C23-O8-C6
27	B	621	SQD	C12-C13-C14-C15
27	A	416	SQD	O10-C23-O48-C46
37	D	408	LHG	O10-C23-O8-C6
24	b	610	CLA	O1D-CGD-O2D-CED
24	b	619	CLA	C16-C17-C18-C19
27	L	102	SQD	C18-C19-C20-C21
34	a	412	LMG	C13-C14-C15-C16
29	B	636	LMT	C11-C10-C9-C8
34	J	101	LMG	C34-C35-C36-C37
36	C	517	DGD	CDB-CEB-CFB-CGB
24	a	406	CLA	C4C-C3C-CAC-CBC
24	B	611	CLA	C16-C17-C18-C19
31	a	417	PL9	C2-C3-C7-C8
27	a	402	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
37	d	407	LHG	C26-C27-C28-C29
24	C	511	CLA	CBA-CGA-O2A-C1
24	D	402	CLA	C8-C10-C11-C12
34	c	920	LMG	C28-C29-C30-C31
26	c	915	BCR	C1-C6-C7-C8
27	A	412	SQD	O49-C7-O47-C45
24	b	609	CLA	O1D-CGD-O2D-CED
36	C	517	DGD	C1B-C2B-C3B-C4B
37	D	408	LHG	C24-C23-O8-C6
27	A	412	SQD	C8-C7-O47-C45
24	C	507	CLA	C5-C6-C7-C8
24	B	602	CLA	C2A-CAA-CBA-CGA
31	D	404	PL9	C39-C41-C42-C43
34	c	919	LMG	C2-C1-O1-C7
36	C	517	DGD	C2E-C1E-O5D-C6D
36	C	518	DGD	C2E-C1E-O5D-C6D
36	c	917	DGD	C2E-C1E-O5D-C6D
27	A	416	SQD	C24-C25-C26-C27
34	c	920	LMG	O7-C8-C9-O8
36	D	405	DGD	O1G-C1G-C2G-O2G
27	L	102	SQD	C35-C36-C37-C38
24	b	616	CLA	C3-C5-C6-C7
35	B	626	HTG	C2'-C3'-C4'-C5'
35	b	627	HTG	C1'-C2'-C3'-C4'
35	B	626	HTG	C4-C5-C6-O6
24	A	407	CLA	C12-C13-C15-C16
24	B	602	CLA	C11-C10-C8-C7
24	b	608	CLA	C6-C7-C8-C10
24	B	615	CLA	C11-C12-C13-C14
24	D	402	CLA	C11-C10-C8-C9
24	b	618	CLA	C11-C12-C13-C14
34	j	101	LMG	C13-C14-C15-C16
34	Z	101	LMG	O10-C28-O8-C9
27	B	621	SQD	C19-C20-C21-C22
36	c	917	DGD	C4B-C5B-C6B-C7B
28	B	631	GOL	C1-C2-C3-O3
28	v	204	GOL	C1-C2-C3-O3
24	A	406	CLA	C2C-C3C-CAC-CBC
36	c	916	DGD	C4B-C5B-C6B-C7B
28	V	204	GOL	O1-C1-C2-O2
24	C	513	CLA	CBA-CGA-O2A-C1
34	C	520	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	b	624	LMG	C29-C28-O8-C9
37	d	409	LHG	C24-C23-O8-C6
24	C	507	CLA	C10-C11-C12-C13
27	A	412	SQD	C34-C35-C36-C37
24	B	614	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	CBD-CGD-O2D-CED
29	B	623	LMT	C3-C4-C5-C6
24	C	511	CLA	C8-C10-C11-C12
24	c	907	CLA	C13-C15-C16-C17
34	C	520	LMG	O10-C28-O8-C9
36	c	916	DGD	C5B-C6B-C7B-C8B
24	C	513	CLA	C4B-C3B-CAB-CBB
24	b	608	CLA	C4B-C3B-CAB-CBB
24	c	904	CLA	C4B-C3B-CAB-CBB
24	c	908	CLA	C4B-C3B-CAB-CBB
24	d	402	CLA	C4B-C3B-CAB-CBB
29	M	101	LMT	C4'-C5'-C6'-O6'
36	D	405	DGD	C7B-C8B-C9B-CAB
29	B	623	LMT	C4-C5-C6-C7
24	C	513	CLA	O1A-CGA-O2A-C1
34	B	622	LMG	C20-C21-C22-C23
37	L	101	LHG	C31-C32-C33-C34
24	c	910	CLA	C16-C17-C18-C19
36	h	102	DGD	C7A-C8A-C9A-CAA
24	b	615	CLA	C2-C3-C5-C6
31	d	405	PL9	C13-C14-C16-C17
24	b	617	CLA	C2-C1-O2A-CGA
24	B	604	CLA	C16-C17-C18-C20
36	C	517	DGD	CBA-CCA-CDA-CEA
24	B	617	CLA	C8-C10-C11-C12
24	B	603	CLA	C2A-CAA-CBA-CGA
24	B	611	CLA	C2A-CAA-CBA-CGA
24	b	614	CLA	C2A-CAA-CBA-CGA
24	c	902	CLA	C2A-CAA-CBA-CGA
36	d	406	DGD	C6A-C7A-C8A-C9A
24	B	602	CLA	C3A-C2A-CAA-CBA
27	a	411	SQD	C13-C14-C15-C16
38	e	102	HEM	CAA-CBA-CGA-O1A
29	B	636	LMT	O5'-C5'-C6'-O6'
29	C	522	LMT	C1-C2-C3-C4
37	D	406	LHG	C33-C34-C35-C36
24	B	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	C	506	CLA	C14-C13-C15-C16
24	b	619	CLA	C16-C17-C18-C20
36	c	918	DGD	C8B-C9B-CAB-CBB
36	c	917	DGD	C1B-C2B-C3B-C4B
34	a	412	LMG	C15-C16-C17-C18
34	J	101	LMG	C30-C31-C32-C33
34	C	521	LMG	O1-C7-C8-C9
29	m	104	LMT	C1-C2-C3-C4
24	B	602	CLA	CAA-CBA-CGA-O1A
36	c	918	DGD	C2A-C1A-O1G-C1G
29	M	101	LMT	O5'-C1'-O1'-C1
37	d	407	LHG	C11-C10-C9-C8
38	E	103	HEM	CAD-CBD-CGD-O1D
27	B	621	SQD	C17-C18-C19-C20
34	c	920	LMG	C29-C30-C31-C32
36	d	406	DGD	CCA-CDA-CEA-CFA
34	b	624	LMG	C10-C11-C12-C13
24	B	612	CLA	C15-C16-C17-C18
24	a	409	CLA	C4-C3-C5-C6
24	b	615	CLA	C4-C3-C5-C6
31	a	417	PL9	C45-C44-C46-C47
24	C	514	CLA	C1A-C2A-CAA-CBA
24	B	617	CLA	C11-C12-C13-C15
24	b	607	CLA	C6-C7-C8-C10
24	b	610	CLA	C11-C12-C13-C15
37	d	409	LHG	C33-C34-C35-C36
40	v	202	HEC	CAD-CBD-CGD-O1D
29	A	417	LMT	C1-C2-C3-C4
37	L	101	LHG	C25-C26-C27-C28
34	C	501	LMG	C21-C22-C23-C24
37	D	408	LHG	C10-C11-C12-C13
24	b	605	CLA	CAA-CBA-CGA-O2A
40	V	201	HEC	CAD-CBD-CGD-O2D
29	B	623	LMT	C6-C7-C8-C9
36	d	406	DGD	C4A-C5A-C6A-C7A
25	a	420	PHO	C8-C10-C11-C12
36	C	518	DGD	C4E-C5E-C6E-O5E
38	e	102	HEM	CAA-CBA-CGA-O2A
34	j	101	LMG	C29-C30-C31-C32
27	L	102	SQD	C11-C10-C9-C8
36	c	917	DGD	CBB-CCB-CDB-CEB
24	c	908	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
40	V	201	HEC	CAD-CBD-CGD-O1D
24	B	603	CLA	C13-C15-C16-C17
29	A	417	LMT	O5B-C5B-C6B-O6B
34	b	624	LMG	C18-C19-C20-C21
37	D	408	LHG	C30-C31-C32-C33
29	E	102	LMT	C2B-C1B-O1B-C4'
27	a	411	SQD	O6-C44-C45-O47
29	C	522	LMT	C5-C6-C7-C8
29	a	401	LMT	C9-C10-C11-C12
34	b	624	LMG	C40-C41-C42-C43
34	c	919	LMG	C36-C37-C38-C39
26	t	101	BCR	C13-C14-C15-C16
34	C	501	LMG	C15-C16-C17-C18
36	D	405	DGD	CAA-CBA-CCA-CDA
31	d	405	PL9	C39-C41-C42-C43
31	a	417	PL9	C20-C19-C21-C22
34	Z	101	LMG	C11-C12-C13-C14
24	c	910	CLA	C2-C1-O2A-CGA
35	C	523	HTG	O5-C5-C6-O6
24	d	401	CLA	C4C-C3C-CAC-CBC
24	b	608	CLA	C11-C10-C8-C9
24	C	504	CLA	C8-C10-C11-C12
34	b	624	LMG	O10-C28-O8-C9
36	c	918	DGD	O1A-C1A-O1G-C1G
35	b	602	HTG	C4'-C5'-C6'-C7'
40	v	202	HEC	CAD-CBD-CGD-O2D
24	C	504	CLA	C5-C6-C7-C8
37	E	101	LHG	C17-C18-C19-C20
26	B	620	BCR	C23-C24-C25-C30
26	C	516	BCR	C1-C6-C7-C8
26	K	102	BCR	C23-C24-C25-C30
26	b	622	BCR	C23-C24-C25-C30
26	b	623	BCR	C23-C24-C25-C30
26	k	101	BCR	C1-C6-C7-C8
26	k	102	BCR	C1-C6-C7-C8
27	A	412	SQD	C12-C13-C14-C15
34	c	919	LMG	C21-C22-C23-C24
28	v	203	GOL	C1-C2-C3-O3
28	v	204	GOL	O1-C1-C2-C3
29	f	103	LMT	C4-C5-C6-C7
34	c	919	LMG	C32-C33-C34-C35
24	c	914	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	a	417	PL9	C12-C11-C9-C10
34	C	501	LMG	C18-C19-C20-C21
36	H	102	DGD	O1B-C1B-C2B-C3B
24	B	615	CLA	C16-C17-C18-C19
24	C	504	CLA	C4B-C3B-CAB-CBB
34	C	520	LMG	C29-C30-C31-C32
34	j	101	LMG	C21-C22-C23-C24
34	j	101	LMG	C36-C37-C38-C39
24	b	620	CLA	C4-C3-C5-C6
31	D	404	PL9	C40-C39-C41-C42
24	B	610	CLA	C2-C3-C5-C6
24	a	409	CLA	C2-C3-C5-C6
24	b	618	CLA	C11-C12-C13-C15
24	c	914	CLA	C2-C3-C5-C6
25	A	408	PHO	C8-C10-C11-C12
36	D	405	DGD	CBA-CCA-CDA-CEA
27	A	416	SQD	C16-C17-C18-C19
36	c	916	DGD	C7A-C8A-C9A-CAA
37	d	408	LHG	O10-C23-O8-C6
36	C	518	DGD	CCB-CDB-CEB-CFB
27	B	621	SQD	C30-C31-C32-C33
29	f	103	LMT	C9-C10-C11-C12
29	m	104	LMT	C3-C4-C5-C6
24	b	612	CLA	C4-C3-C5-C6
24	B	602	CLA	C15-C16-C17-C18
31	d	405	PL9	C28-C29-C31-C32
34	z	101	LMG	O7-C10-C11-C12
36	D	405	DGD	CAB-CBB-CCB-CDB
24	A	407	CLA	C14-C13-C15-C16
24	B	602	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	D	402	CLA	C14-C13-C15-C16
24	a	407	CLA	C6-C7-C8-C9
24	c	910	CLA	C11-C10-C8-C9
37	d	409	LHG	C28-C29-C30-C31
24	B	608	CLA	C3A-C2A-CAA-CBA
24	B	610	CLA	C3A-C2A-CAA-CBA
38	E	103	HEM	CAD-CBD-CGD-O2D
24	B	604	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	608	CLA	CAD-CBD-CGD-O2D
24	c	902	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	c	906	CLA	CAD-CBD-CGD-O2D
24	d	403	CLA	CAD-CBD-CGD-O2D
27	B	621	SQD	C18-C19-C20-C21
24	C	502	CLA	C2A-CAA-CBA-CGA
24	b	612	CLA	C2-C1-O2A-CGA
37	d	409	LHG	C25-C26-C27-C28
40	v	202	HEC	C2B-C3B-CAB-CBB
37	L	101	LHG	C23-C24-C25-C26
34	c	919	LMG	C37-C38-C39-C40
31	d	405	PL9	C30-C29-C31-C32
31	a	417	PL9	C18-C19-C21-C22
31	a	417	PL9	C43-C44-C46-C47
24	C	513	CLA	CAA-CBA-CGA-O2A
36	d	406	DGD	O2G-C1B-C2B-C3B
37	E	101	LHG	C18-C19-C20-C21
24	c	914	CLA	O1A-CGA-O2A-C1
31	a	417	PL9	C39-C41-C42-C43
27	F	101	SQD	C44-C45-C46-O48
34	Z	101	LMG	O1-C7-C8-C9
36	D	405	DGD	C1G-C2G-C3G-O3G
27	A	412	SQD	C14-C15-C16-C17
37	D	408	LHG	C24-C25-C26-C27
24	B	614	CLA	O2A-C1-C2-C3
24	D	402	CLA	O2A-C1-C2-C3
24	c	910	CLA	O2A-C1-C2-C3
25	a	408	PHO	O2A-C1-C2-C3
37	D	407	LHG	C17-C18-C19-C20
38	E	103	HEM	C4C-C3C-CAC-CBC
24	b	618	CLA	C8-C10-C11-C12
24	c	913	CLA	CAA-CBA-CGA-O2A
27	f	102	SQD	O47-C7-C8-C9
34	c	920	LMG	C30-C31-C32-C33
37	d	408	LHG	C13-C14-C15-C16
24	B	611	CLA	C15-C16-C17-C18
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	b	609	CLA	CHA-CBD-CGD-O2D
24	b	611	CLA	CHA-CBD-CGD-O1D
24	c	903	CLA	CHA-CBD-CGD-O1D
24	c	905	CLA	CHA-CBD-CGD-O1D
24	c	910	CLA	CHA-CBD-CGD-O1D
24	c	910	CLA	CHA-CBD-CGD-O2D
24	c	913	CLA	CHA-CBD-CGD-O2D
24	d	401	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O2D
36	c	918	DGD	CBB-CCB-CDB-CEB
27	A	416	SQD	C25-C26-C27-C28
24	B	614	CLA	CAA-CBA-CGA-O2A
37	l	101	LHG	C11-C12-C13-C14
37	E	101	LHG	O8-C23-C24-C25
25	A	408	PHO	CHA-CBD-CGD-O1D
28	B	631	GOL	O2-C2-C3-O3
28	a	414	GOL	O2-C2-C3-O3
28	v	203	GOL	O2-C2-C3-O3
24	B	613	CLA	CBA-CGA-O2A-C1
37	d	408	LHG	C24-C23-O8-C6
29	E	102	LMT	O5'-C5'-C6'-O6'
24	B	606	CLA	O1D-CGD-O2D-CED
24	c	914	CLA	C12-C13-C15-C16
34	B	622	LMG	O8-C28-C29-C30
24	b	610	CLA	C11-C12-C13-C14
24	b	620	CLA	C2B-C3B-CAB-CBB
35	c	922	HTG	C2'-C3'-C4'-C5'
24	B	613	CLA	CAA-CBA-CGA-O2A
37	e	101	LHG	O8-C23-C24-C25
27	A	416	SQD	C5-C6-S-O8
27	B	621	SQD	C5-C6-S-O8
27	a	402	SQD	C5-C6-S-O8
27	L	102	SQD	C29-C30-C31-C32
24	B	613	CLA	O1A-CGA-O2A-C1
24	c	904	CLA	C2A-CAA-CBA-CGA
29	C	522	LMT	O1'-C1-C2-C3
24	c	911	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
36	D	405	DGD	O1G-C1A-C2A-C3A
24	c	909	CLA	C13-C15-C16-C17
37	D	408	LHG	C9-C10-C11-C12
34	z	101	LMG	O9-C10-C11-C12
24	B	606	CLA	C16-C17-C18-C19
24	b	610	CLA	C16-C17-C18-C19
37	L	101	LHG	C16-C17-C18-C19
28	V	206	GOL	C1-C2-C3-O3
28	a	414	GOL	C1-C2-C3-O3
24	b	620	CLA	C2-C3-C5-C6
24	C	509	CLA	C1A-C2A-CAA-CBA
29	M	101	LMT	C7-C8-C9-C10
34	C	501	LMG	C36-C37-C38-C39
36	C	518	DGD	CDA-CEA-CFA-CGA
27	B	621	SQD	C28-C29-C30-C31
36	h	102	DGD	C5A-C6A-C7A-C8A
27	A	412	SQD	O6-C44-C45-C46
24	B	604	CLA	C16-C17-C18-C19
27	f	102	SQD	O49-C7-C8-C9
31	d	405	PL9	C15-C14-C16-C17
24	C	506	CLA	CAA-CBA-CGA-O2A
24	b	617	CLA	CAA-CBA-CGA-O2A
24	c	913	CLA	CAA-CBA-CGA-O1A
36	d	406	DGD	O1B-C1B-C2B-C3B
36	c	917	DGD	C9A-CAA-CBA-CCA
24	c	914	CLA	C10-C11-C12-C13
27	f	102	SQD	C34-C35-C36-C37
24	B	616	CLA	C4B-C3B-CAB-CBB
24	c	902	CLA	C4B-C3B-CAB-CBB
24	C	511	CLA	C16-C17-C18-C19
36	h	102	DGD	O1G-C1G-C2G-O2G
24	B	613	CLA	CAA-CBA-CGA-O1A
37	l	101	LHG	O7-C7-C8-C9
24	c	914	CLA	CBA-CGA-O2A-C1
26	B	620	BCR	C23-C24-C25-C26
26	C	516	BCR	C5-C6-C7-C8
26	K	102	BCR	C23-C24-C25-C26
31	A	419	PL9	C19-C21-C22-C23
24	C	503	CLA	C13-C15-C16-C17
24	d	403	CLA	C10-C11-C12-C13
34	J	101	LMG	C32-C33-C34-C35
24	C	511	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	b	606	CLA	C2A-CAA-CBA-CGA
24	C	513	CLA	CAA-CBA-CGA-O1A
24	C	504	CLA	C4-C3-C5-C6
24	B	608	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	b	613	CLA	CAD-CBD-CGD-O1D
24	c	905	CLA	CAD-CBD-CGD-O1D
24	c	907	CLA	CAD-CBD-CGD-O1D
27	A	416	SQD	C5-C6-S-O7
27	A	416	SQD	C5-C6-S-O9
27	B	621	SQD	O5-C5-C6-S
27	a	402	SQD	C5-C6-S-O7
27	a	402	SQD	C5-C6-S-O9
37	e	101	LHG	O10-C23-C24-C25
34	b	624	LMG	O8-C28-C29-C30
24	B	616	CLA	C11-C12-C13-C14
24	c	906	CLA	C11-C12-C13-C14
24	c	914	CLA	C14-C13-C15-C16
36	C	518	DGD	CBB-CCB-CDB-CEB
37	E	101	LHG	O7-C7-C8-C9
34	C	521	LMG	C39-C40-C41-C42
37	E	101	LHG	O10-C23-C24-C25
36	C	518	DGD	C5A-C6A-C7A-C8A
24	c	906	CLA	CAA-CBA-CGA-O2A
36	C	518	DGD	O2G-C1B-C2B-C3B
36	C	519	DGD	O1G-C1A-C2A-C3A
24	C	504	CLA	C15-C16-C17-C18
31	D	404	PL9	C35-C34-C36-C37
24	C	509	CLA	C5-C6-C7-C8
24	C	513	CLA	C6-C7-C8-C10
24	a	407	CLA	C6-C7-C8-C10
24	b	612	CLA	C11-C10-C8-C7
24	b	613	CLA	C2-C3-C5-C6
34	b	624	LMG	C39-C40-C41-C42
36	C	517	DGD	C2A-C3A-C4A-C5A
34	b	624	LMG	C31-C32-C33-C34
37	D	406	LHG	C11-C12-C13-C14
26	A	411	BCR	C17-C18-C19-C20
26	T	102	BCR	C13-C14-C15-C16
36	c	916	DGD	C2A-C3A-C4A-C5A
34	C	520	LMG	O7-C10-C11-C12
29	m	103	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
27	a	402	SQD	C13-C14-C15-C16
24	B	614	CLA	CAA-CBA-CGA-O1A
24	c	906	CLA	CAA-CBA-CGA-O1A
37	E	101	LHG	O9-C7-C8-C9
34	a	412	LMG	C31-C32-C33-C34
40	v	202	HEC	C4B-C3B-CAB-CBB
27	L	102	SQD	O48-C23-C24-C25
34	Z	101	LMG	O7-C10-C11-C12
24	b	615	CLA	C8-C10-C11-C12
36	D	405	DGD	O1A-C1A-C2A-C3A

There are no ring outliers.

157 monomers are involved in 303 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	512	CLA	1	0
29	m	102	LMT	4	0
36	H	102	DGD	1	0
24	b	607	CLA	1	0
35	c	922	HTG	1	0
24	a	409	CLA	1	0
34	b	624	LMG	2	0
24	c	914	CLA	3	0
26	T	102	BCR	4	0
24	A	405	CLA	2	0
34	C	521	LMG	3	0
29	c	921	LMT	1	0
24	b	613	CLA	3	0
29	C	522	LMT	2	0
31	d	405	PL9	1	0
34	c	920	LMG	2	0
35	d	412	HTG	2	0
34	B	622	LMG	2	0
24	c	903	CLA	3	0
35	B	633	HTG	2	0
26	k	102	BCR	1	0
24	B	602	CLA	4	0
28	f	101	GOL	1	0
26	b	622	BCR	2	0
34	Z	101	LMG	3	0
34	a	412	LMG	3	0
26	H	101	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	420	PHO	1	0
24	C	511	CLA	3	0
28	T	101	GOL	1	0
24	c	906	CLA	2	0
26	K	103	BCR	3	0
24	A	410	CLA	3	0
28	B	631	GOL	1	0
29	b	601	LMT	2	0
37	E	101	LHG	2	0
24	b	618	CLA	1	0
35	B	625	HTG	1	0
24	B	613	CLA	1	0
24	B	617	CLA	5	0
34	z	101	LMG	2	0
26	C	515	BCR	1	0
37	D	406	LHG	2	0
37	D	408	LHG	7	0
24	B	614	CLA	3	0
24	c	908	CLA	2	0
24	C	510	CLA	3	0
28	v	203	GOL	2	0
35	C	524	HTG	1	0
27	B	621	SQD	3	0
24	C	513	CLA	3	0
28	B	637	GOL	3	0
26	B	620	BCR	2	0
34	C	520	LMG	2	0
28	c	925	GOL	2	0
26	B	619	BCR	4	0
26	D	403	BCR	2	0
24	B	612	CLA	1	0
24	C	514	CLA	4	0
24	D	401	CLA	1	0
35	B	634	HTG	1	0
31	a	417	PL9	5	0
36	d	406	DGD	6	0
28	T	103	GOL	3	0
24	B	603	CLA	2	0
35	O	303	HTG	1	0
36	C	518	DGD	2	0
24	b	612	CLA	1	0
24	b	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	505	CLA	1	0
24	c	905	CLA	1	0
24	c	912	CLA	2	0
24	d	403	CLA	1	0
24	b	609	CLA	2	0
27	a	411	SQD	3	0
26	b	623	BCR	2	0
29	B	623	LMT	1	0
24	B	616	CLA	2	0
24	B	606	CLA	1	0
26	c	915	BCR	2	0
24	b	620	CLA	2	0
24	C	506	CLA	4	0
27	A	412	SQD	5	0
24	c	911	CLA	2	0
26	y	101	BCR	2	0
24	b	619	CLA	3	0
34	C	501	LMG	2	0
24	c	907	CLA	3	0
35	D	411	HTG	3	0
29	M	101	LMT	3	0
28	b	632	GOL	2	0
24	b	606	CLA	2	0
24	b	615	CLA	1	0
29	B	636	LMT	1	0
24	D	402	CLA	2	0
29	b	625	LMT	2	0
24	C	507	CLA	6	0
27	F	101	SQD	3	0
36	c	916	DGD	1	0
24	B	608	CLA	1	0
24	c	904	CLA	2	0
28	b	631	GOL	1	0
27	a	402	SQD	1	0
36	c	917	DGD	4	0
34	j	101	LMG	5	0
37	l	101	LHG	2	0
28	b	633	GOL	1	0
26	k	101	BCR	5	0
26	a	410	BCR	3	0
27	L	102	SQD	2	0
28	C	525	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	C	517	DGD	4	0
24	B	604	CLA	1	0
36	C	519	DGD	2	0
24	c	902	CLA	2	0
34	J	101	LMG	3	0
24	B	605	CLA	2	0
24	c	913	CLA	3	0
24	C	502	CLA	1	0
31	D	404	PL9	1	0
26	A	411	BCR	1	0
29	m	104	LMT	3	0
26	K	102	BCR	1	0
24	C	503	CLA	2	0
25	A	409	PHO	1	0
27	A	416	SQD	2	0
24	B	610	CLA	2	0
28	A	414	GOL	1	0
24	A	406	CLA	4	0
26	t	101	BCR	7	0
29	E	102	LMT	1	0
31	A	419	PL9	5	0
37	L	101	LHG	1	0
26	d	404	BCR	4	0
24	C	508	CLA	4	0
24	d	402	CLA	3	0
24	c	910	CLA	2	0
29	f	103	LMT	1	0
24	b	616	CLA	2	0
37	d	409	LHG	7	0
26	h	101	BCR	2	0
24	d	401	CLA	1	0
24	C	509	CLA	3	0
26	b	621	BCR	2	0
38	e	102	HEM	2	0
24	b	608	CLA	2	0
24	c	909	CLA	4	0
36	D	405	DGD	5	0
24	b	605	CLA	4	0
29	a	401	LMT	2	0
26	B	618	BCR	1	0
24	B	607	CLA	2	0
37	d	408	LHG	1	0

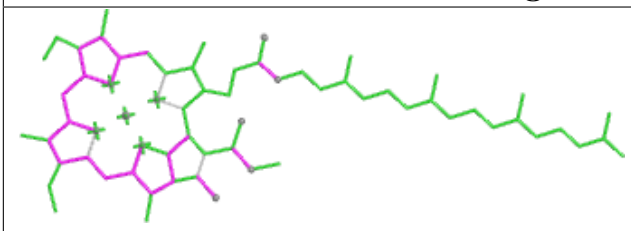
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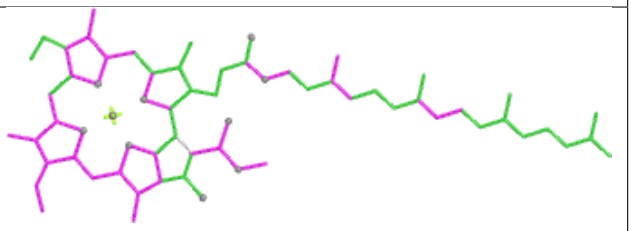
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	e	101	LHG	1	0
24	B	609	CLA	2	0
28	a	414	GOL	2	0
24	a	406	CLA	4	0

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.

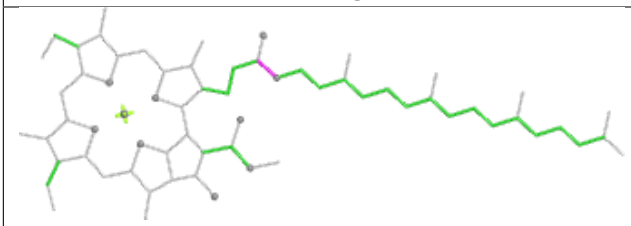
Ligand CLA C 512



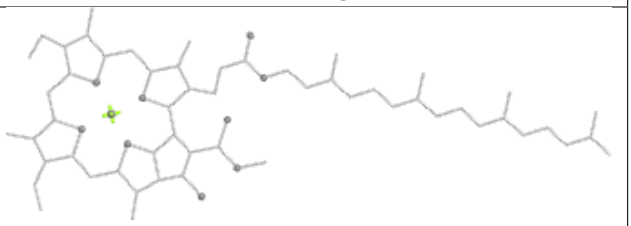
Bond lengths



Bond angles

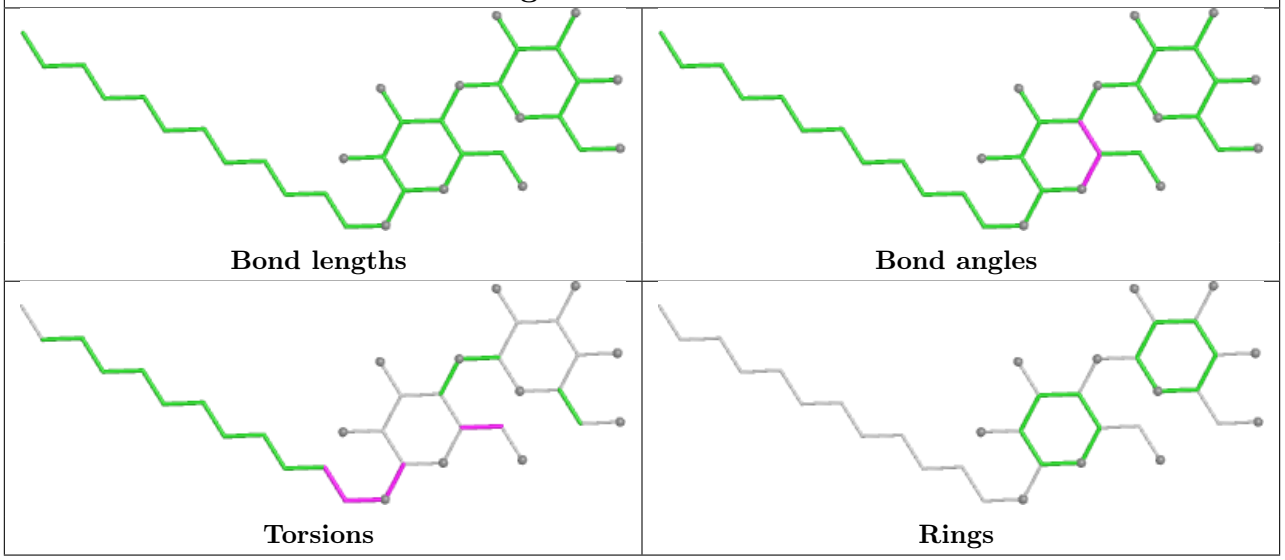


Torsions

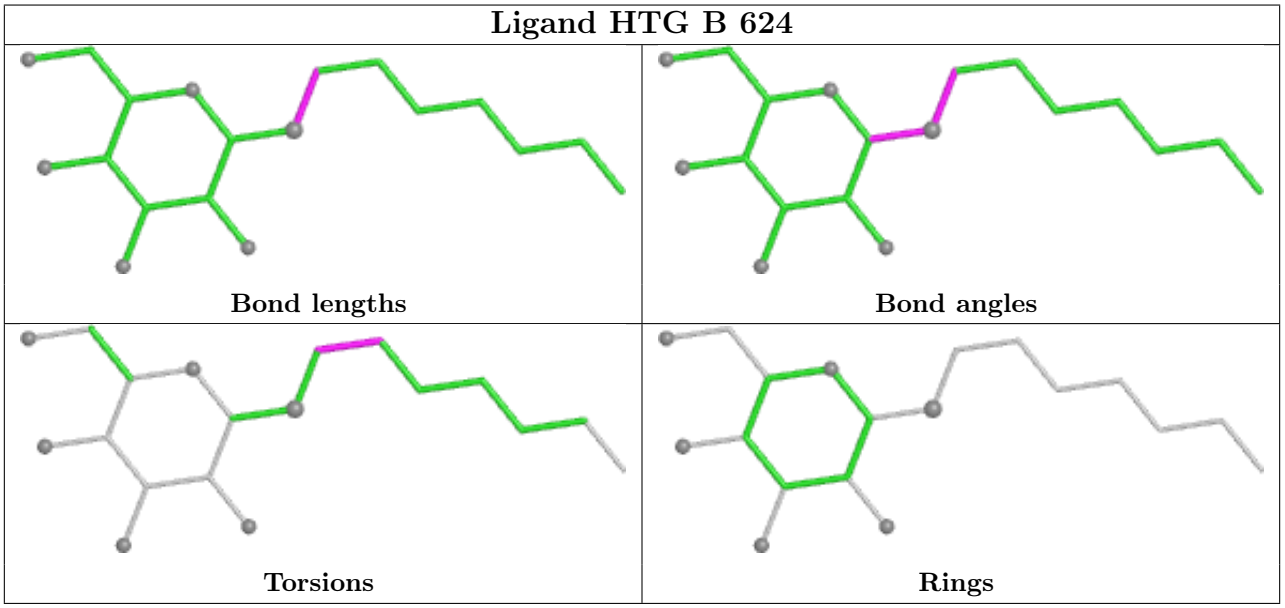


Rings

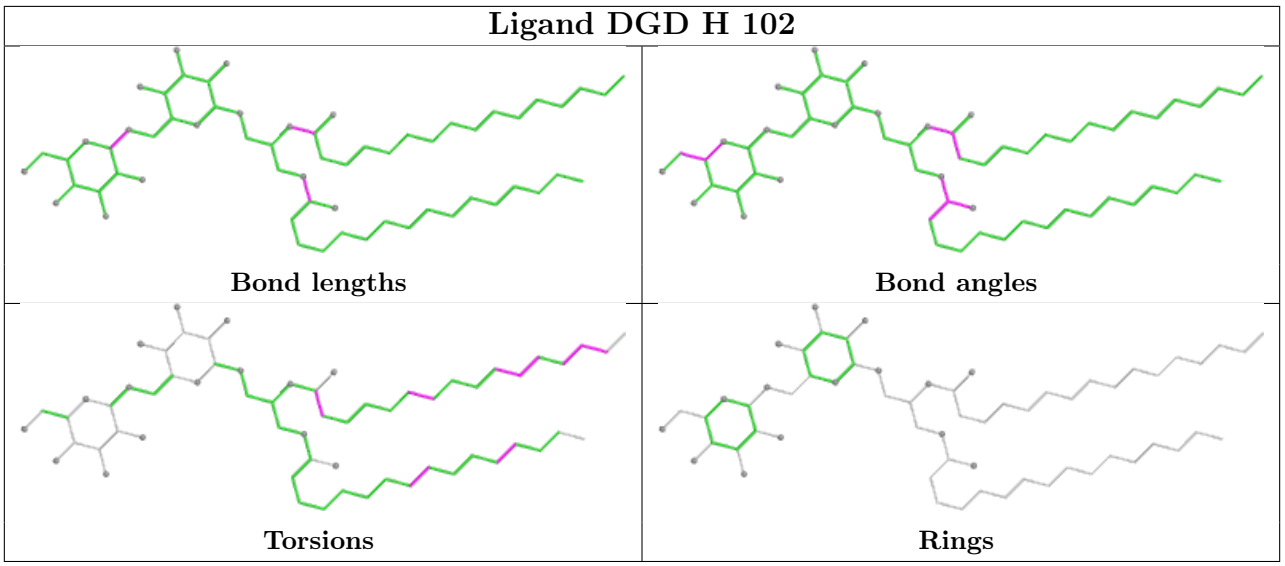
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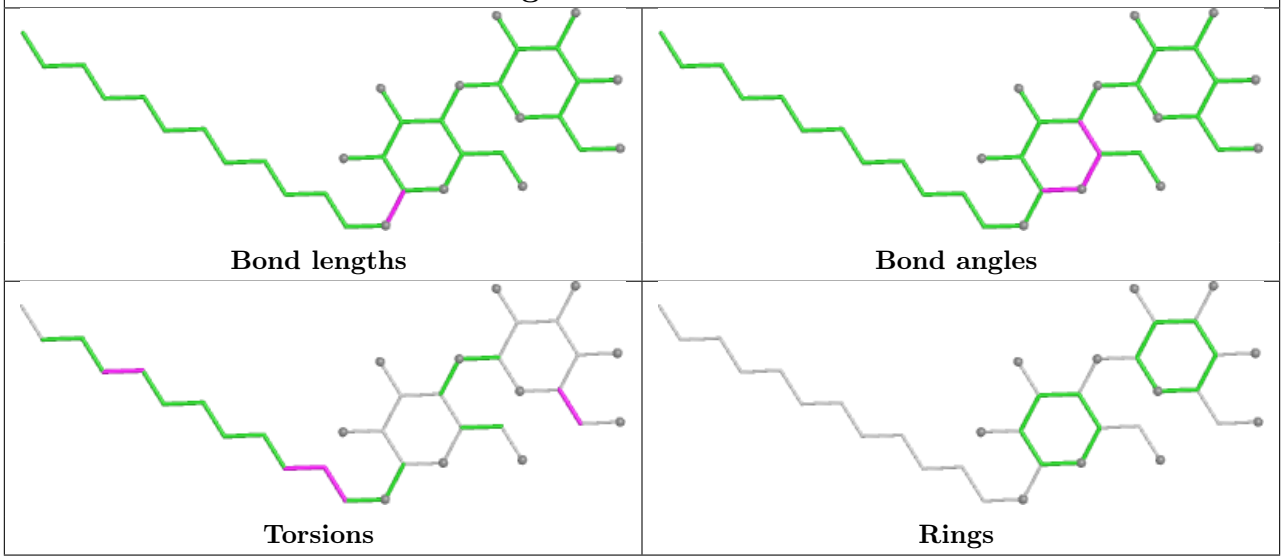
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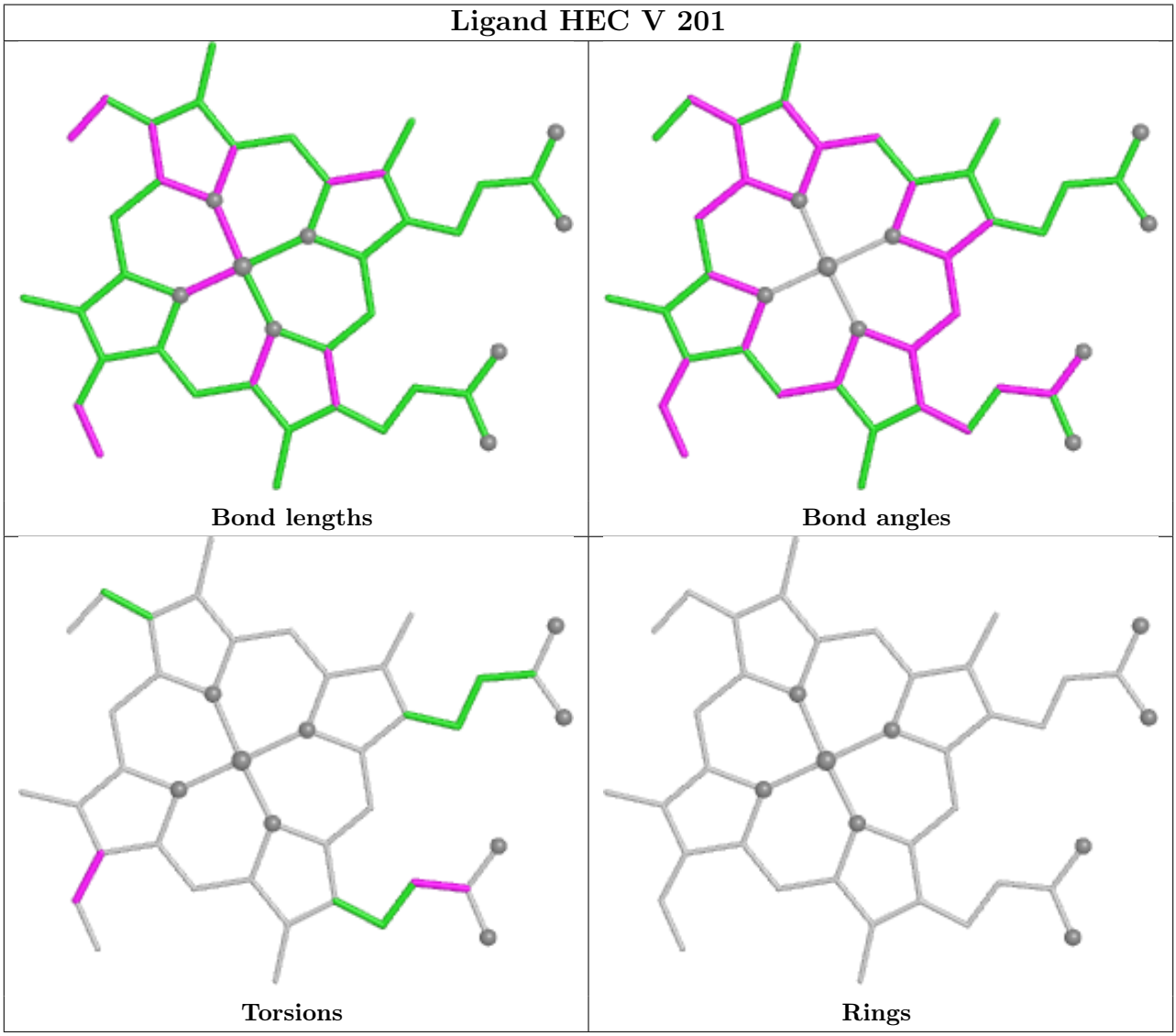
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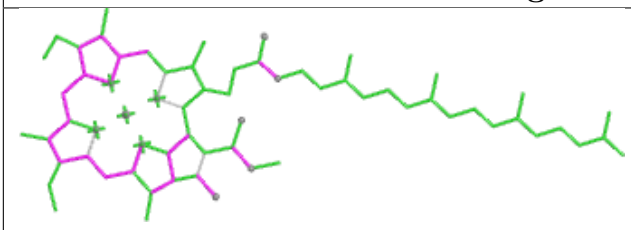
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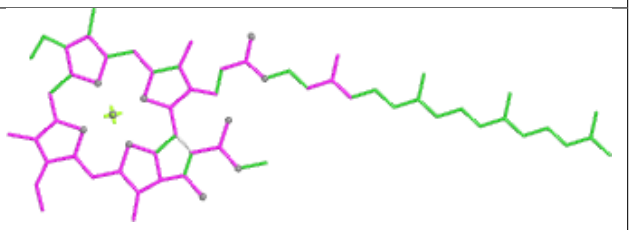
Ligand HEC V 201



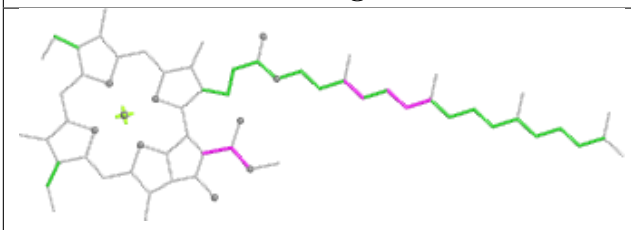
Ligand CLA b 607



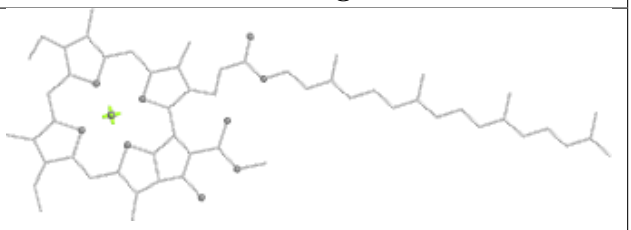
Bond lengths



Bond angles

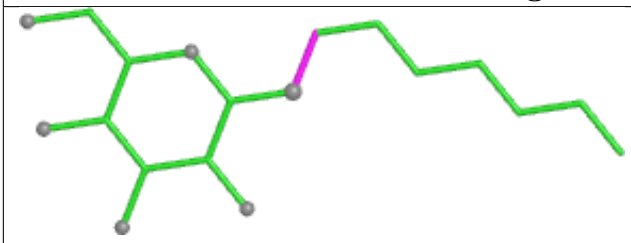


Torsions

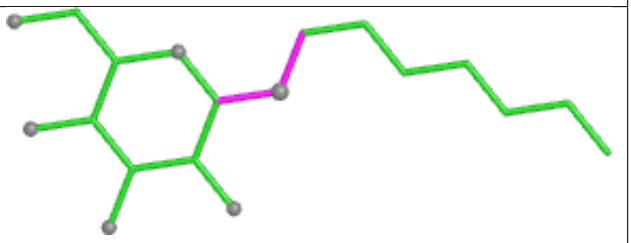


Rings

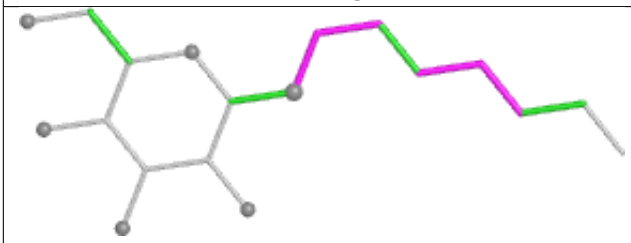
Ligand HTG c 922



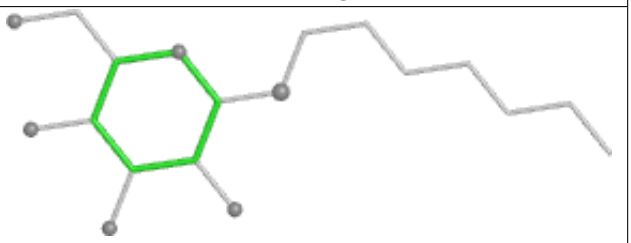
Bond lengths



Bond angles

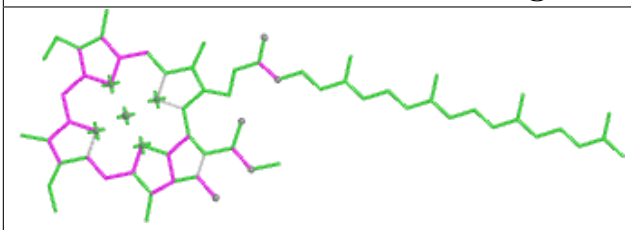


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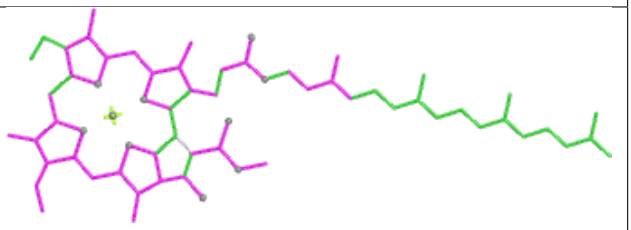


Rings

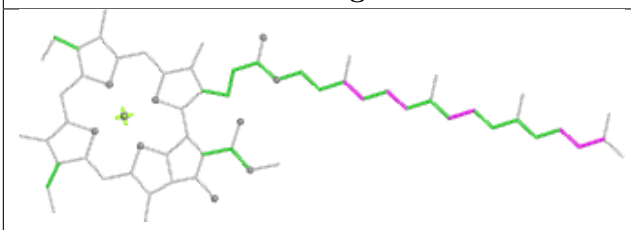
Ligand CLA a 409



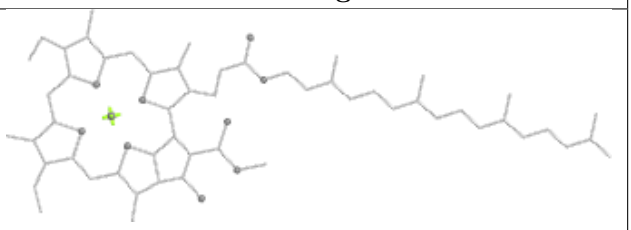
Bond lengths



Bond angles

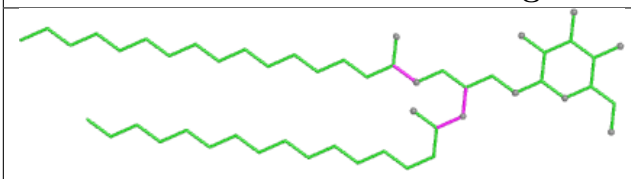


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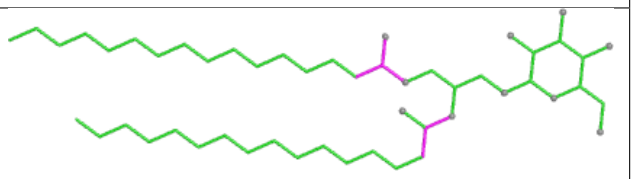


Rings

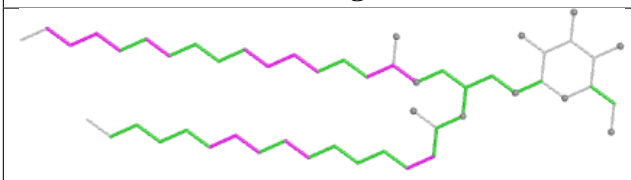
Ligand LMG b 624



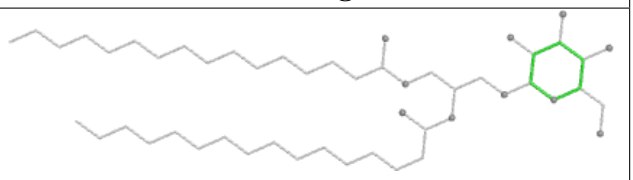
Bond lengths



Bond angles

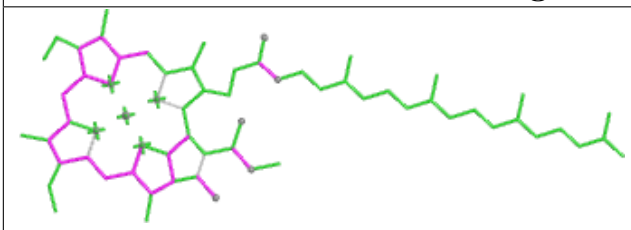


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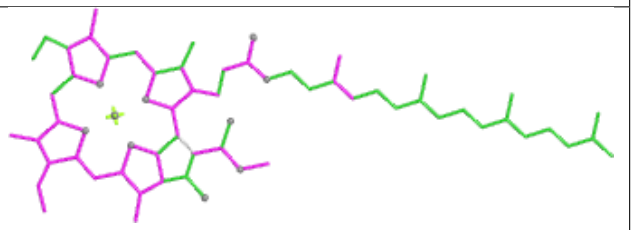


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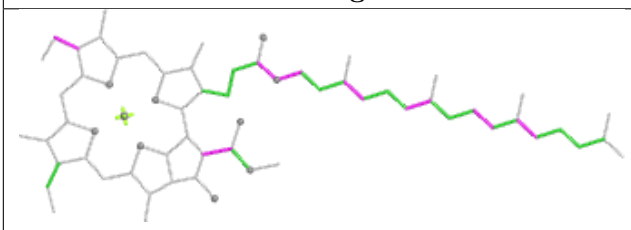
Ligand CLA c 914



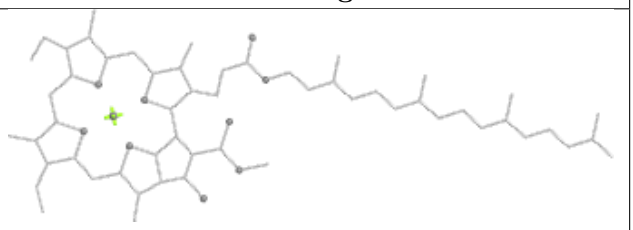
Bond lengths



Bond angles



Torsions

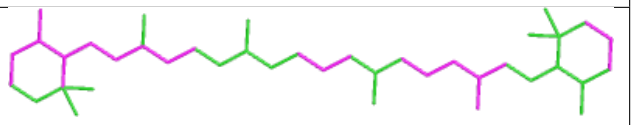


Rings

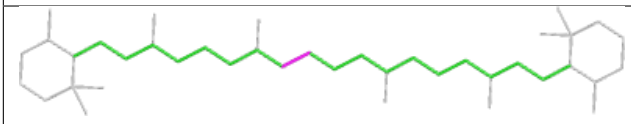
Ligand BCR T 102



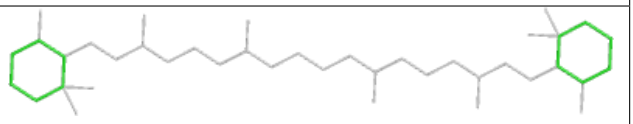
Bond lengths



Bond angles

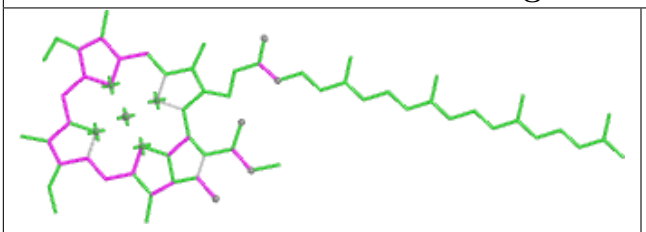


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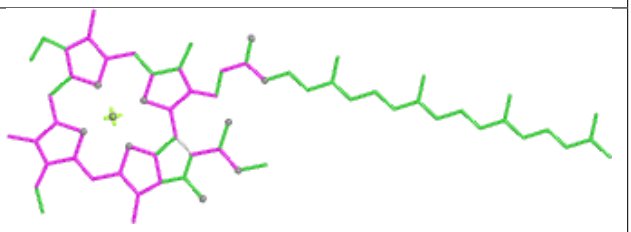


Rings

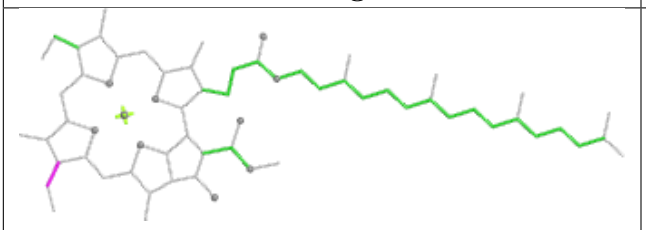
Ligand CLA A 405



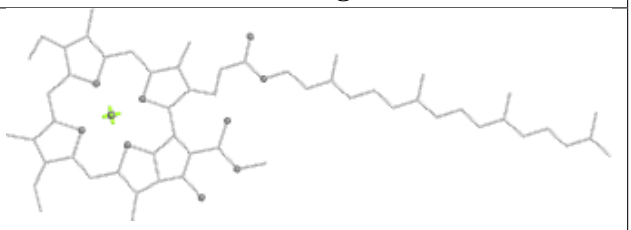
Bond lengths



Bond angles

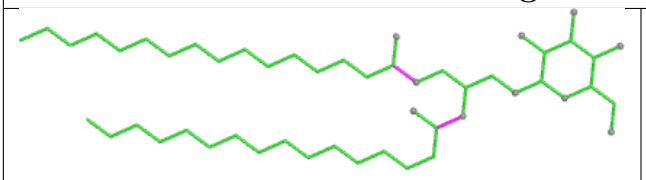


Torsions

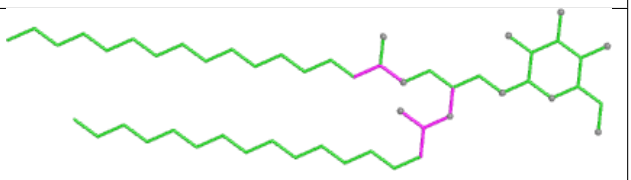


Rings

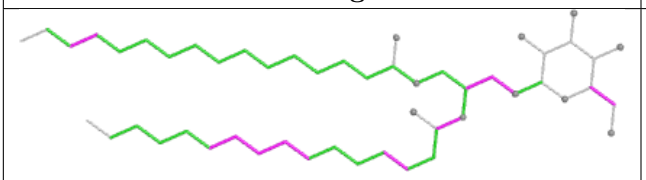
Ligand LMG C 521



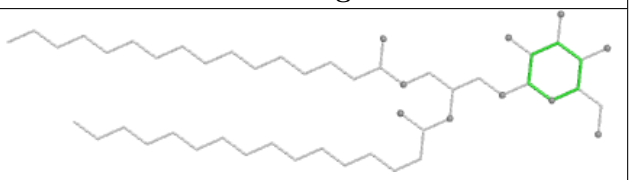
Bond lengths



Bond angles

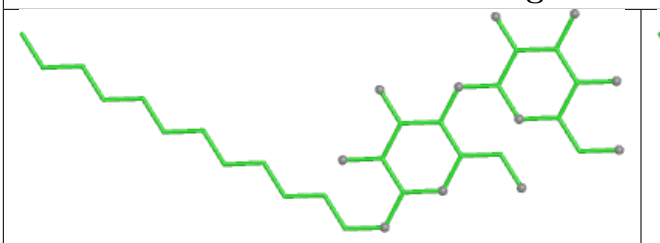


Torsions

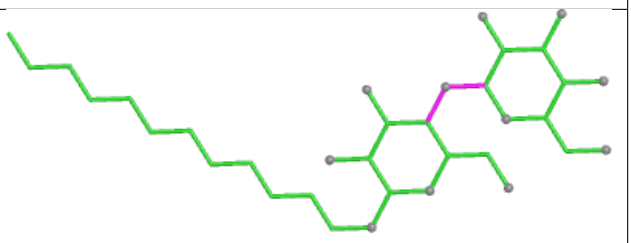


Rings

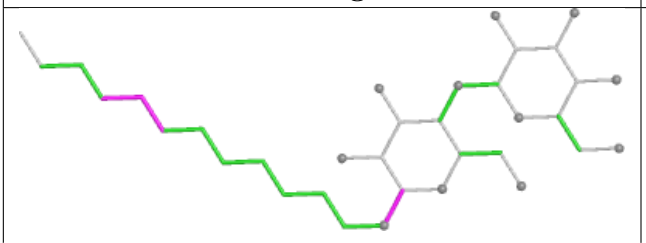
Ligand LMT c 921



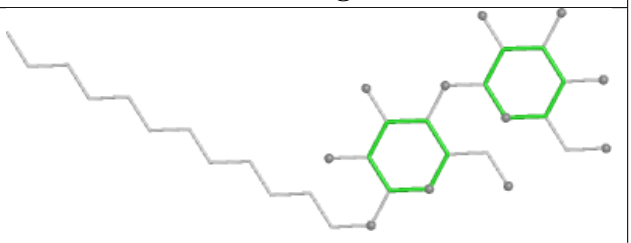
Bond lengths



Bond angles

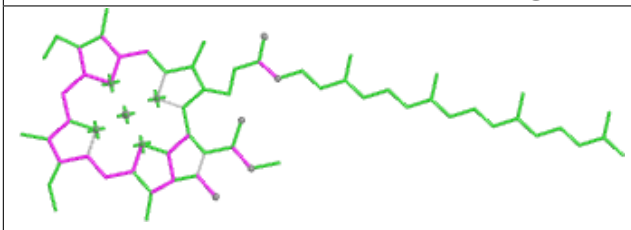


Torsions

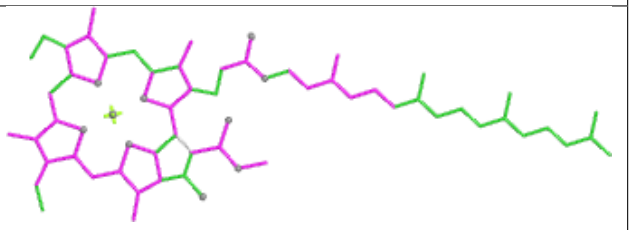


Rings

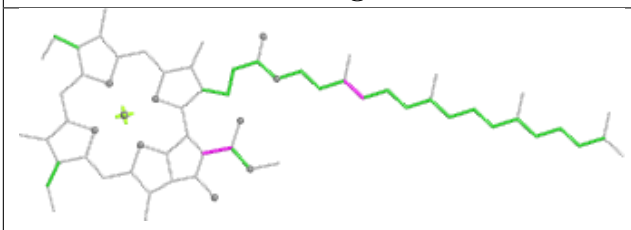
Ligand CLA b 613



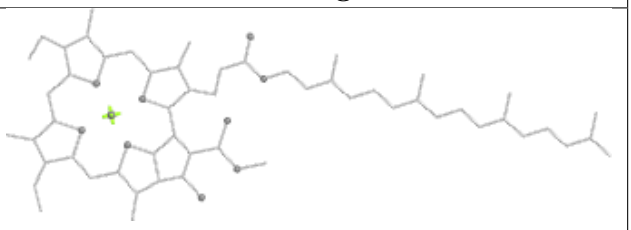
Bond lengths



Bond angles

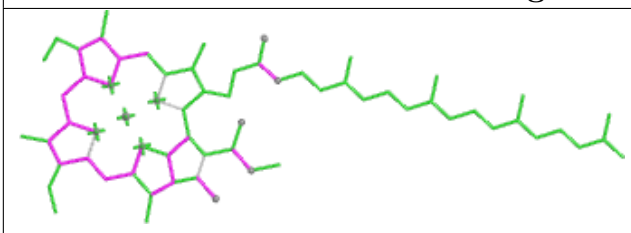


Torsions

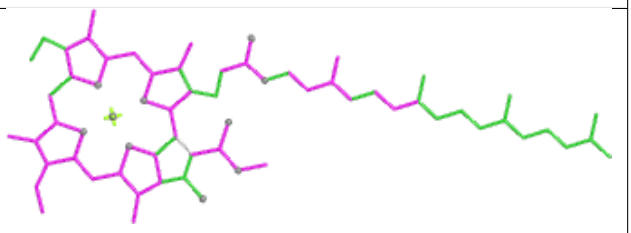


Rings

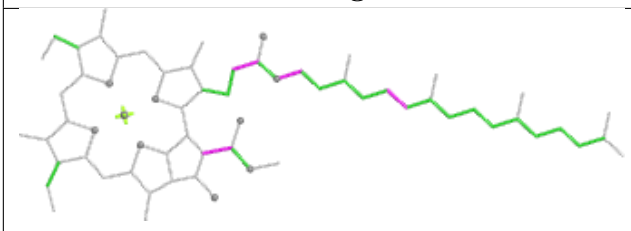
Ligand CLA b 617



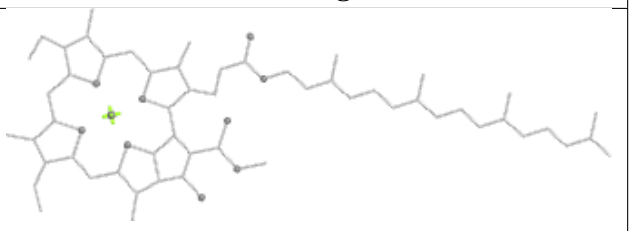
Bond lengths



Bond angles

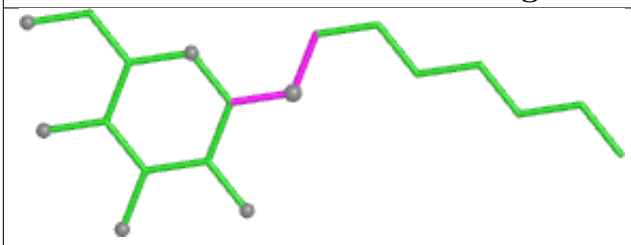


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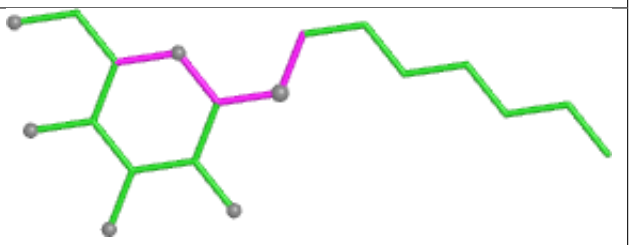


Rings

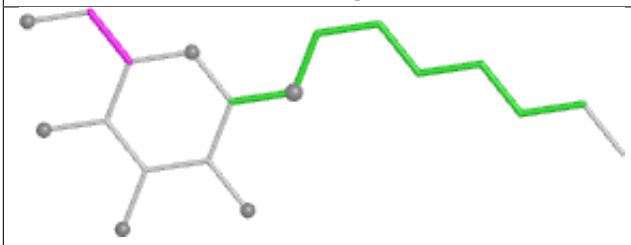
Ligand HTG C 523



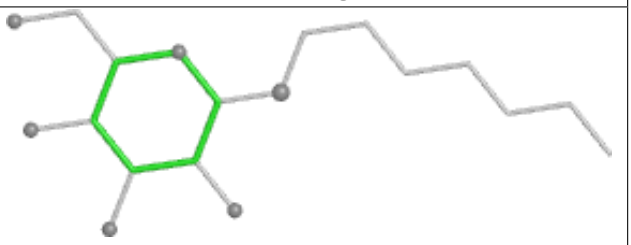
Bond lengths



Bond angles

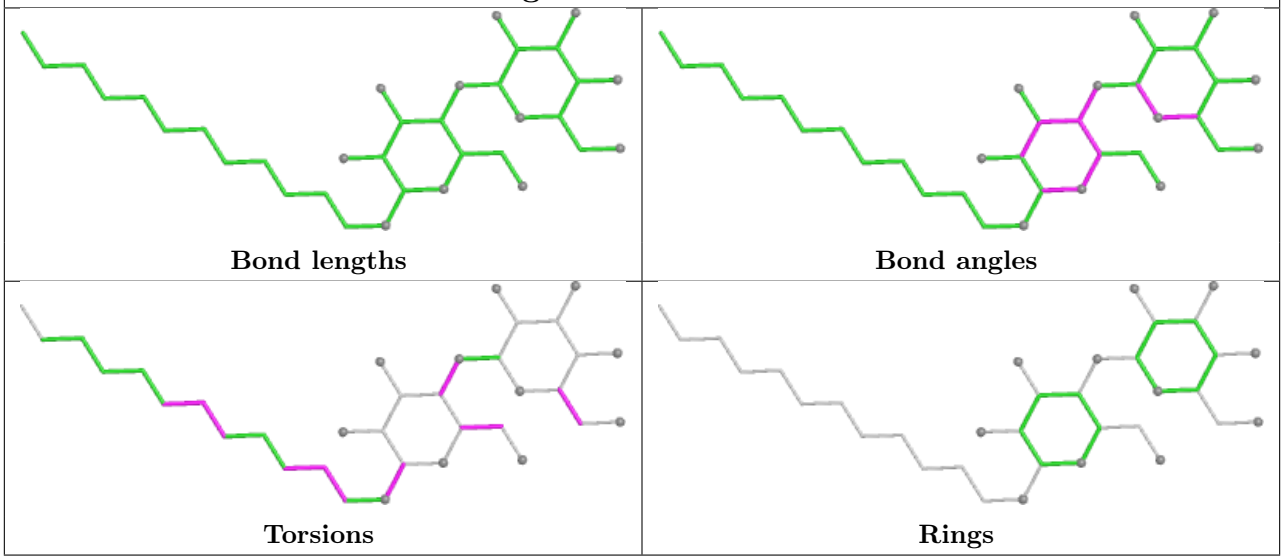


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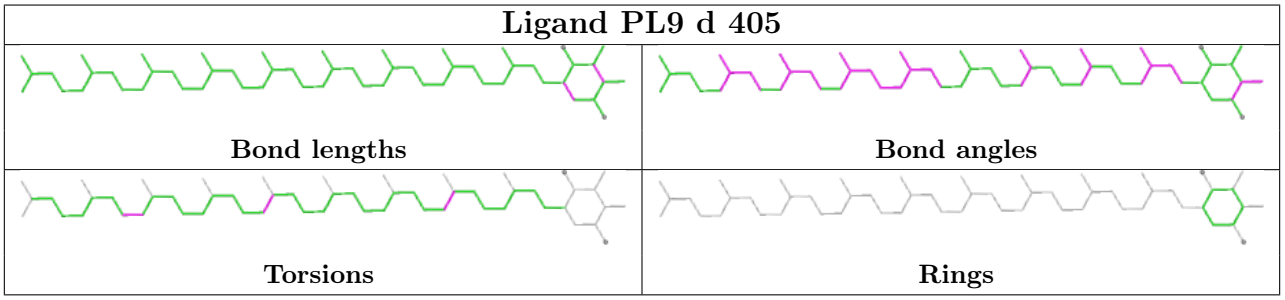


Rings

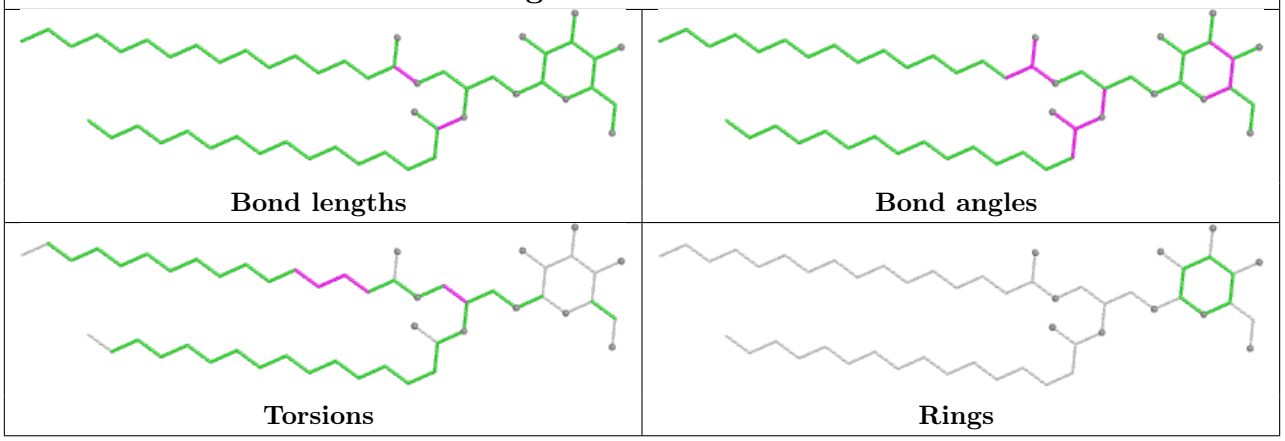
Ligand LMT C 522



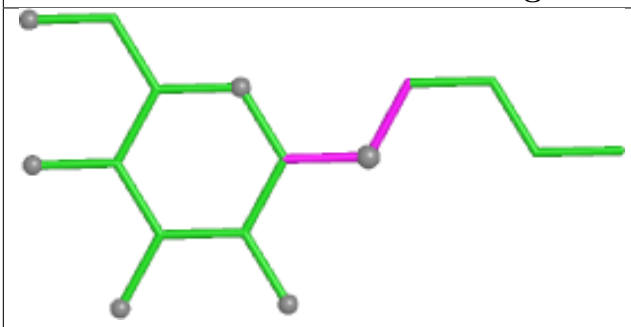
Ligand PL9 d 405



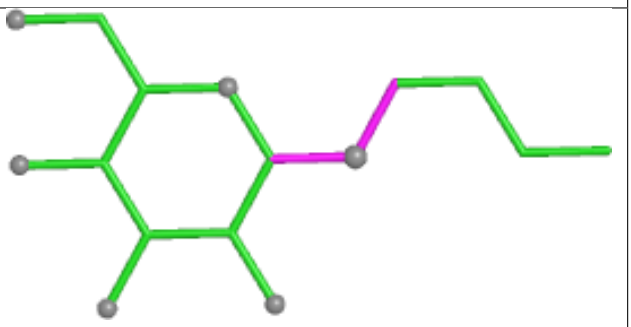
Ligand LMG c 920



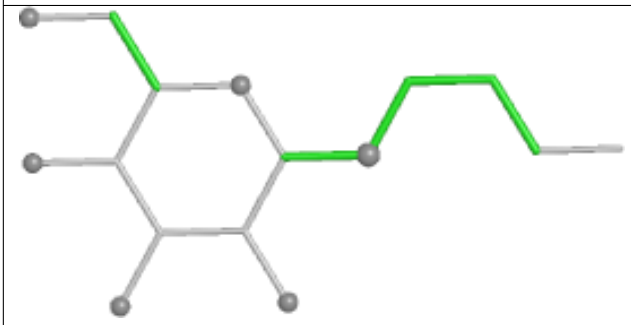
Ligand HTG d 412



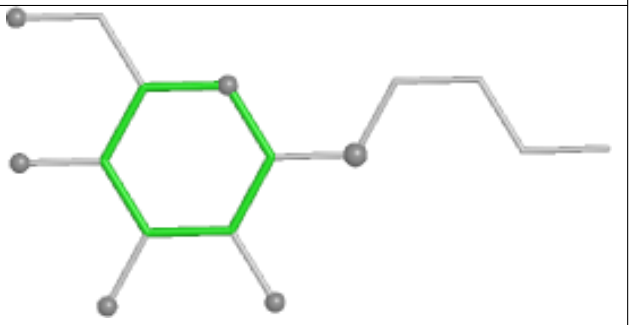
Bond lengths



Bond angles

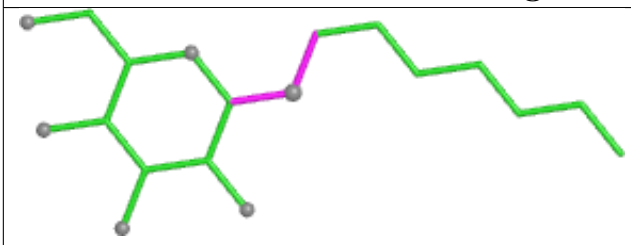


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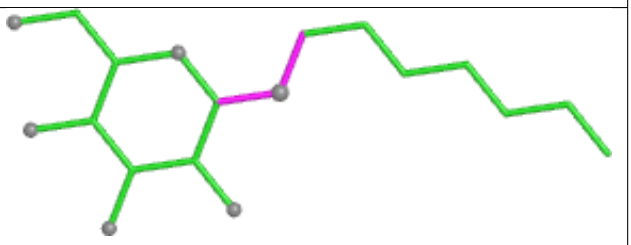


Rings

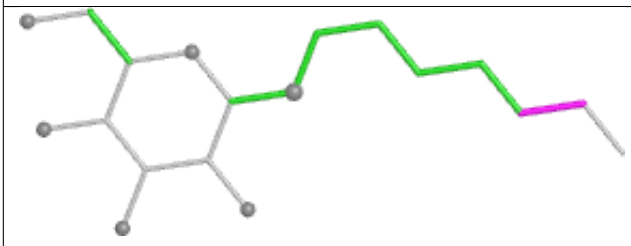
Ligand HTG b 602



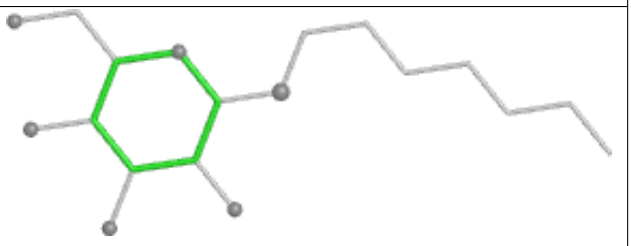
Bond lengths



Bond angles

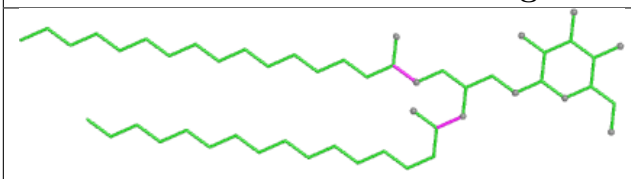


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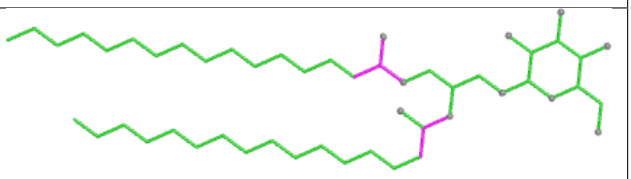


Rings

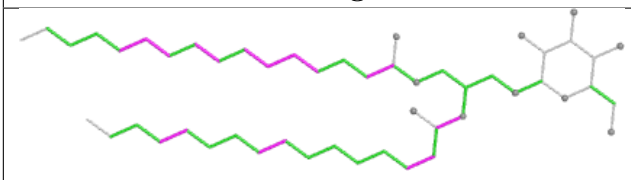
Ligand LMG B 622



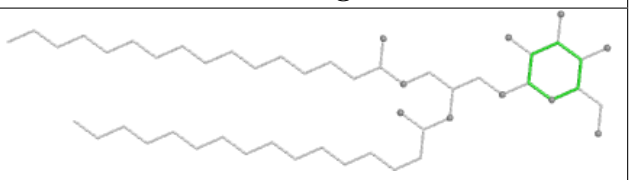
Bond lengths



Bond angles

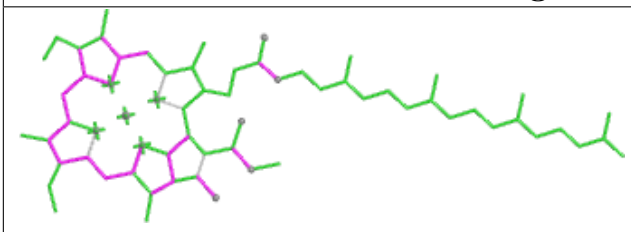


Torsions

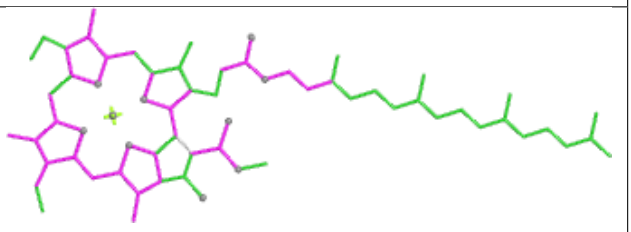


Rings

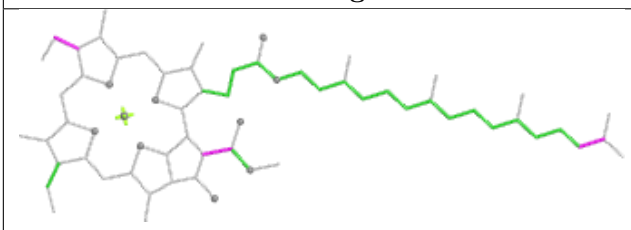
Ligand CLA c 903



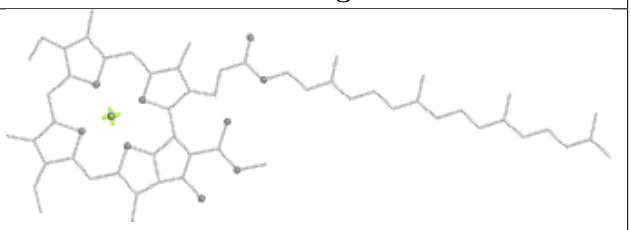
Bond lengths



Bond angles

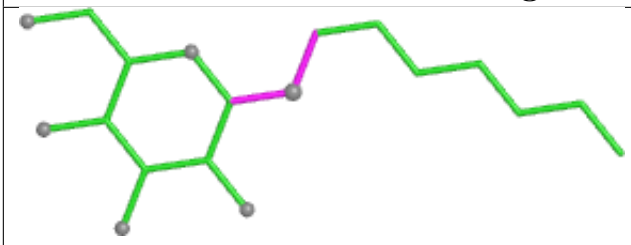


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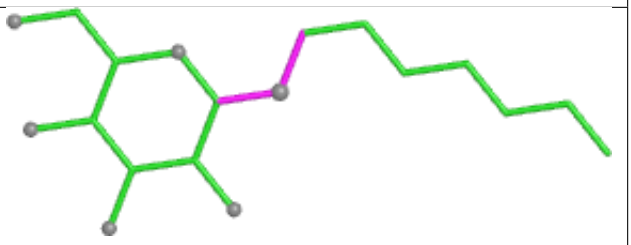


Rings

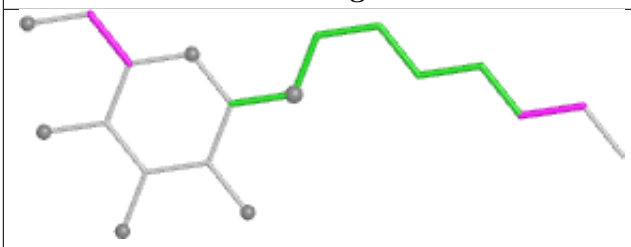
Ligand HTG B 633



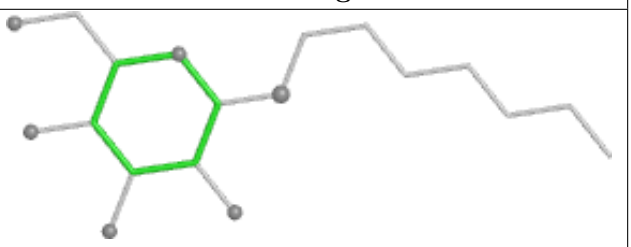
Bond lengths



Bond angles

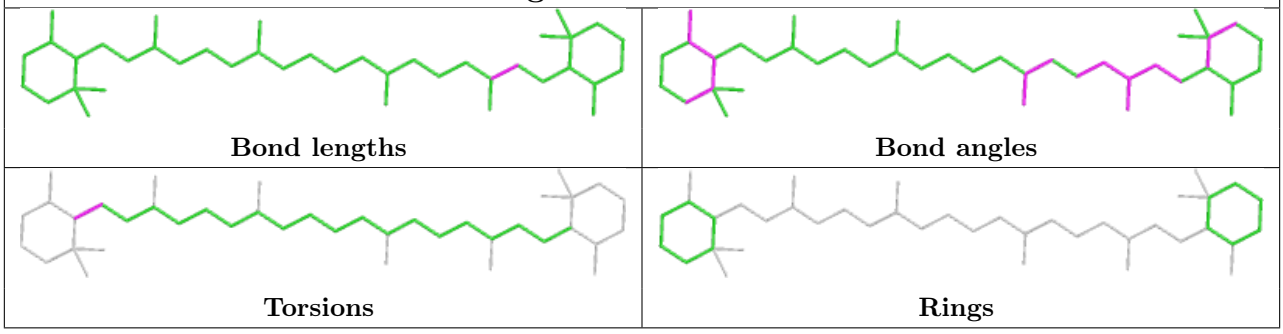


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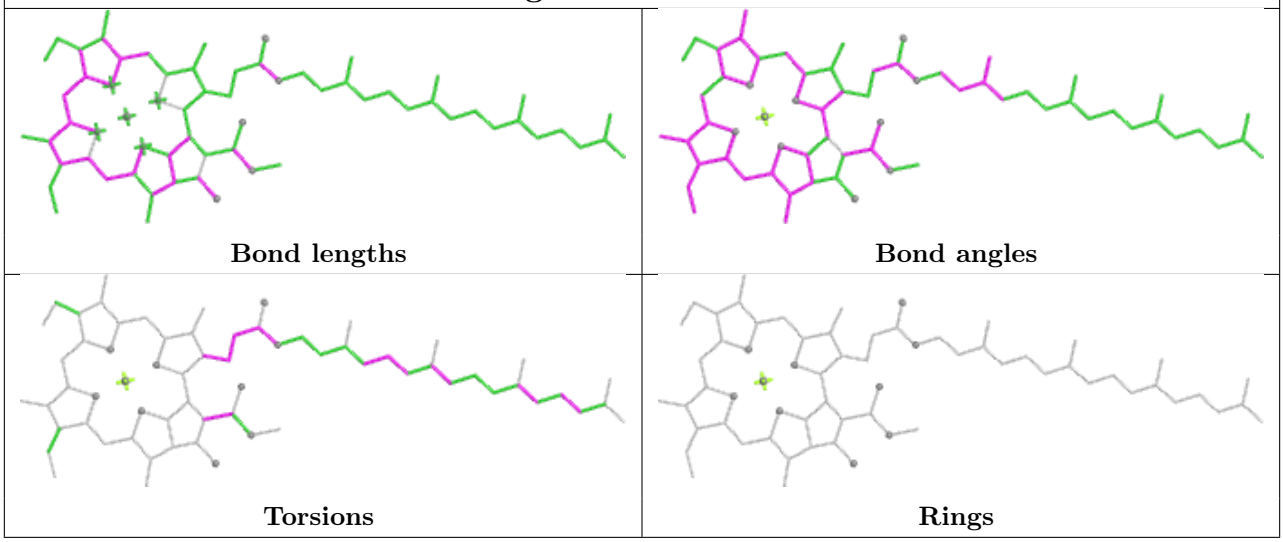


Rings

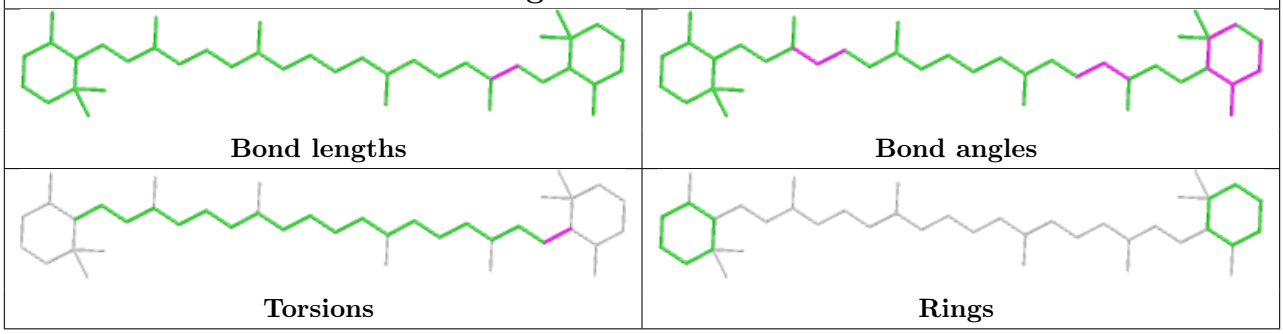
Ligand BCR k 102



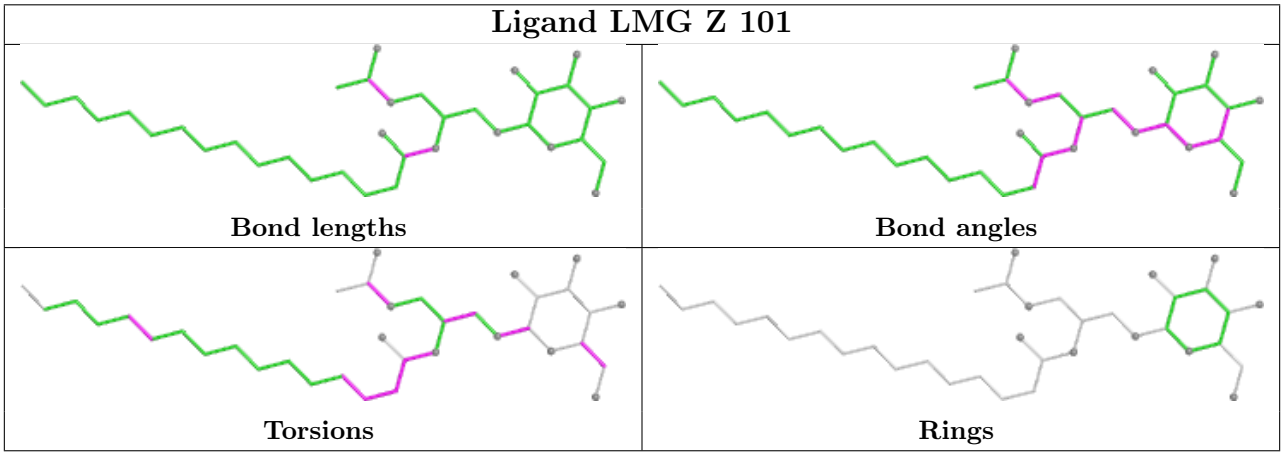
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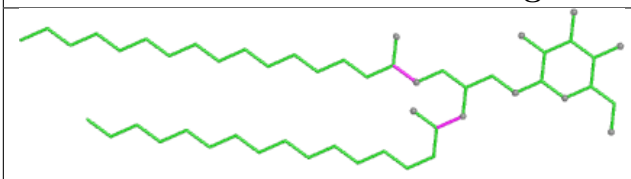
Ligand BCR b 622



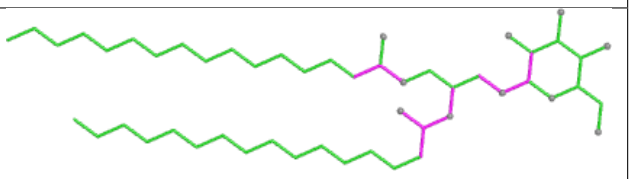
Ligand LMG Z 101



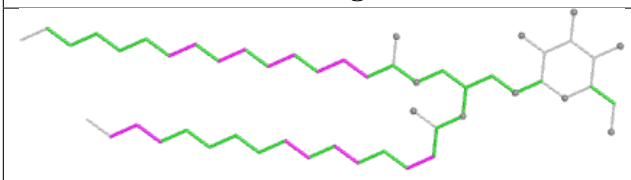
Ligand LMG a 412



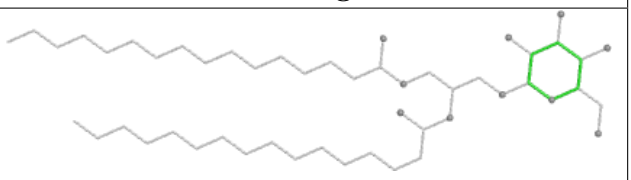
Bond lengths



Bond angles

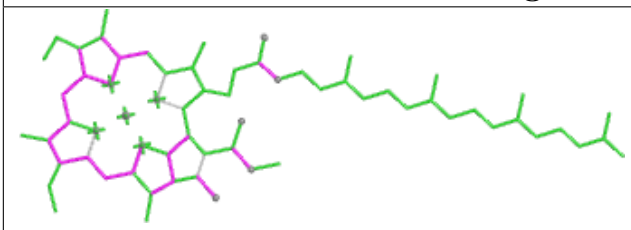


Torsions

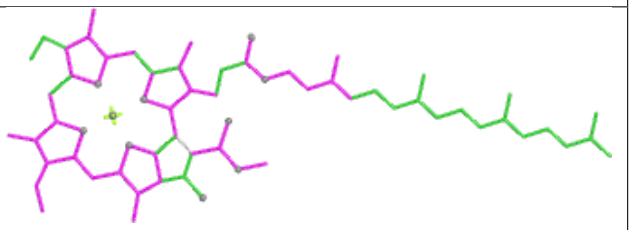


Rings

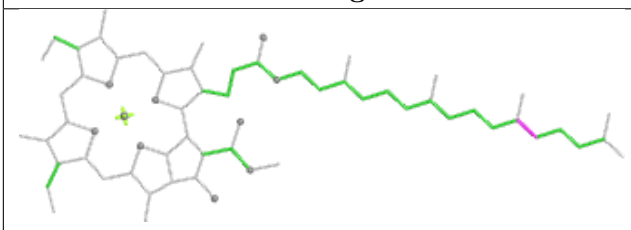
Ligand CLA A 407



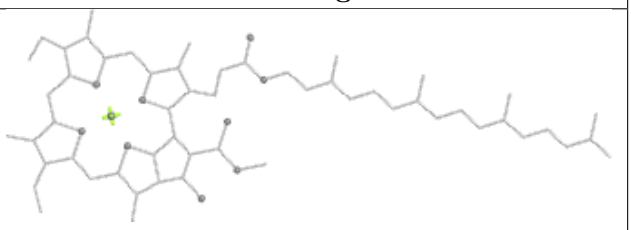
Bond lengths



Bond angles



Torsions

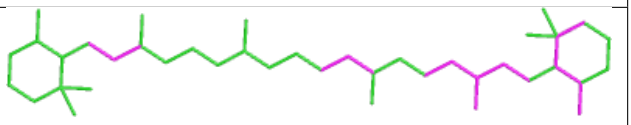


Rings

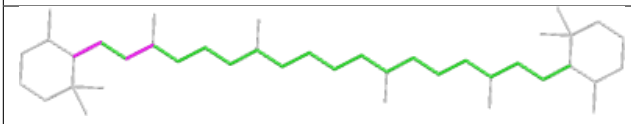
Ligand BCR H 101



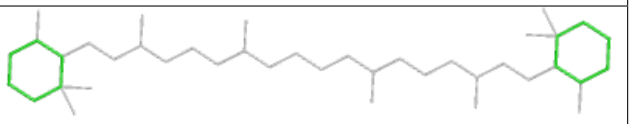
Bond lengths



Bond angles

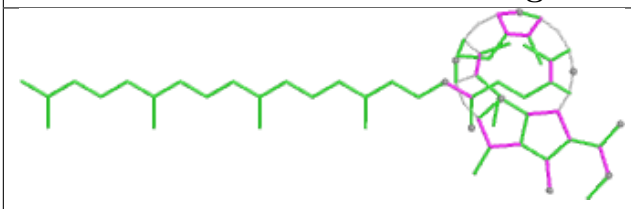


Torsions

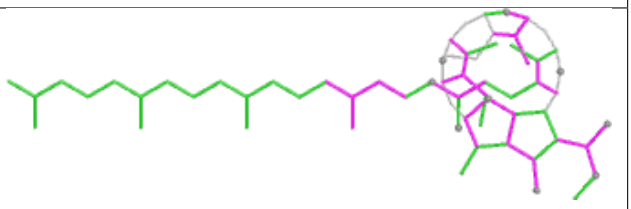


Rings

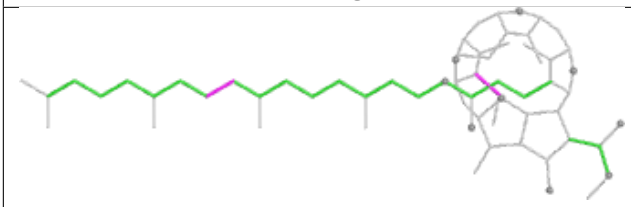
Ligand PHO a 420



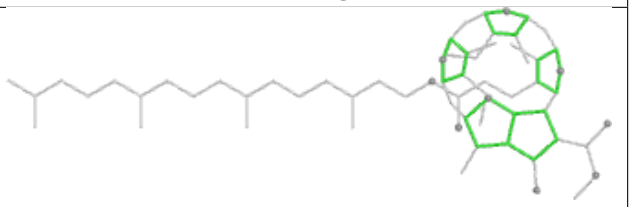
Bond lengths



Bond angles

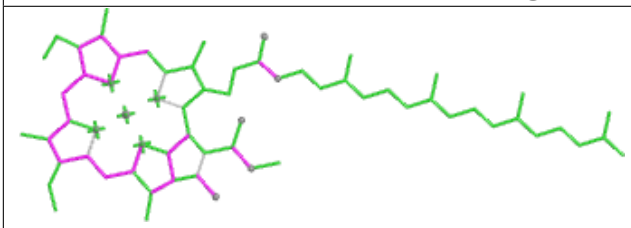


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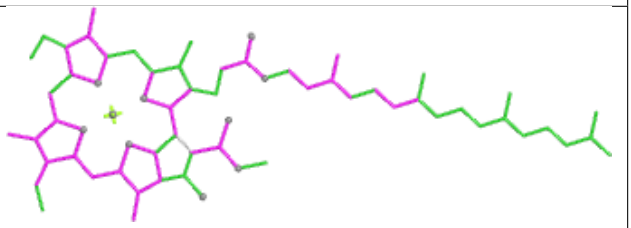


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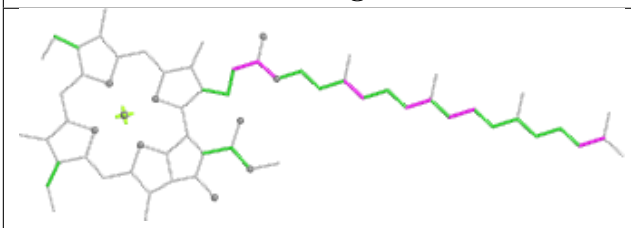
Ligand CLA C 511



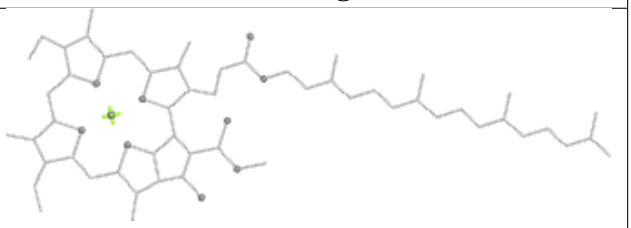
Bond lengths



Bond angles

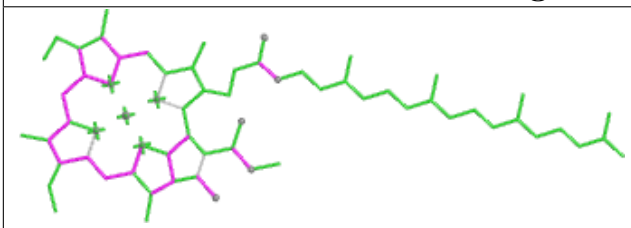


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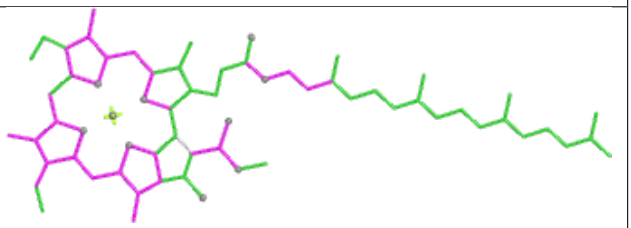


Rings

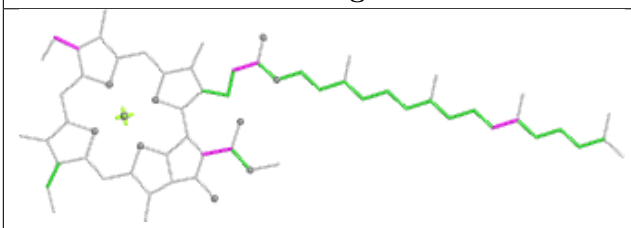
Ligand CLA c 906



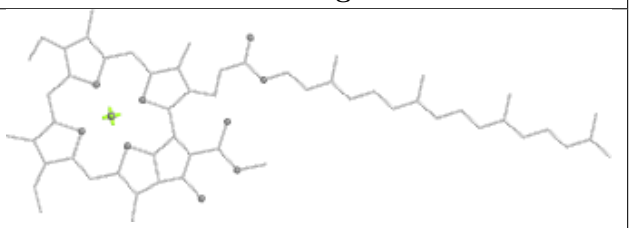
Bond lengths



Bond angles

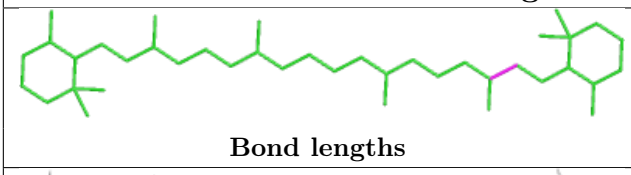


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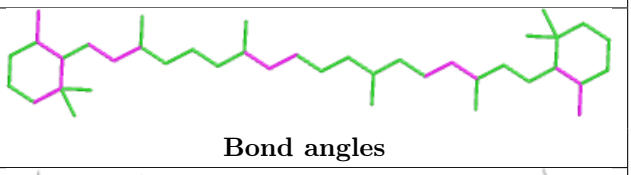


Rings

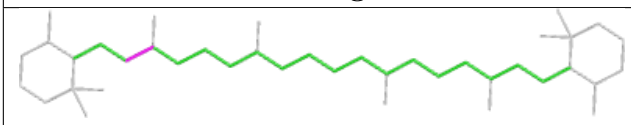
Ligand BCR K 103



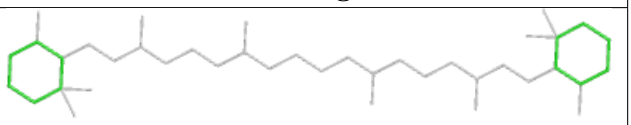
Bond lengths



Bond angles

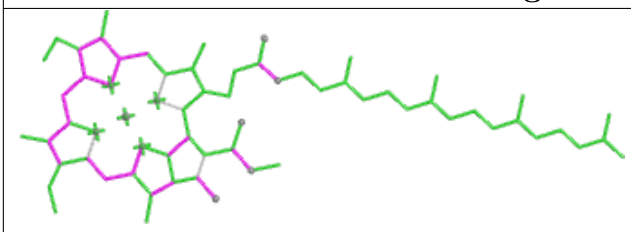


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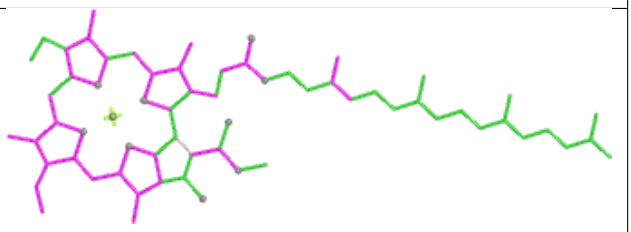


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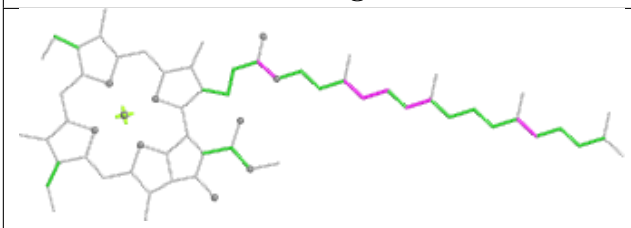
Ligand CLA A 410



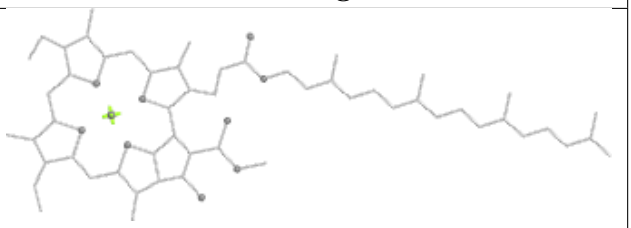
Bond lengths



Bond angles

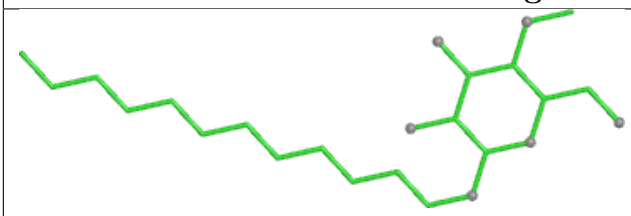


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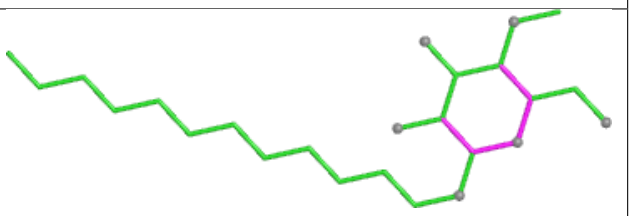


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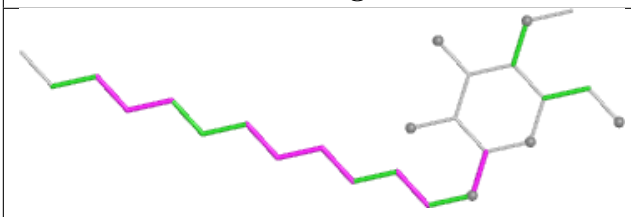
Ligand LMT b 601



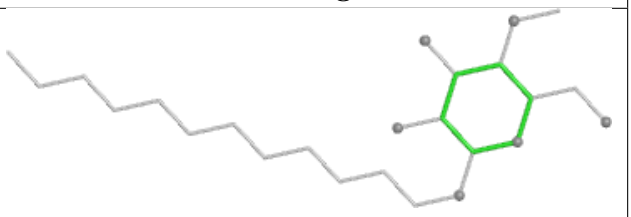
Bond lengths



Bond angles

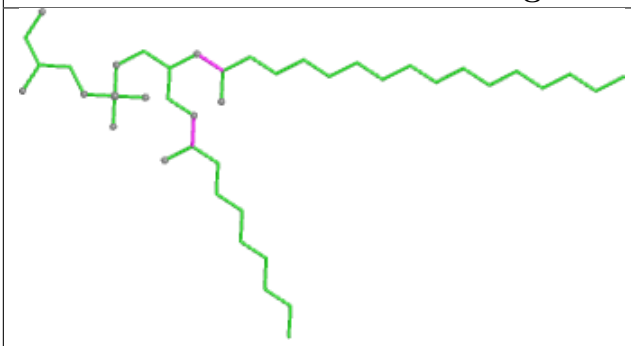


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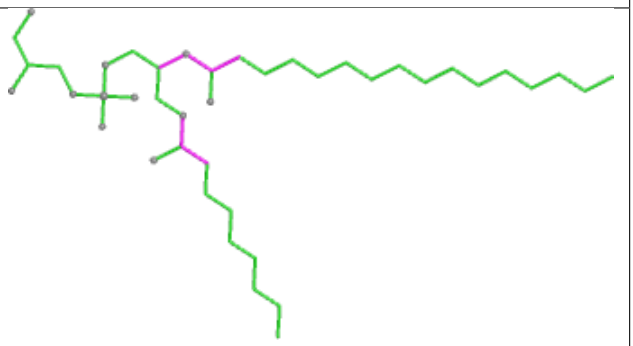


Rings

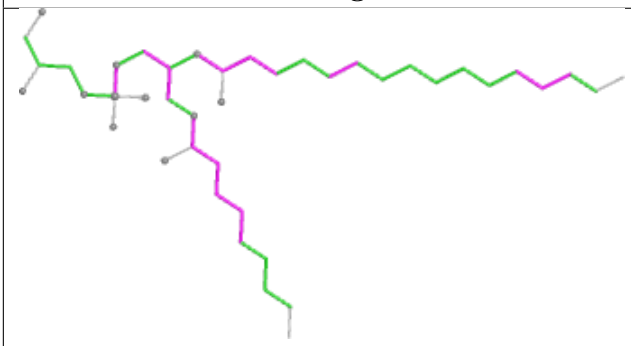
Ligand LHG E 101



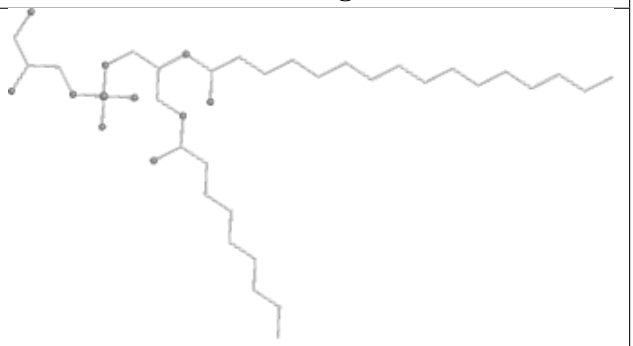
Bond lengths



Bond angles

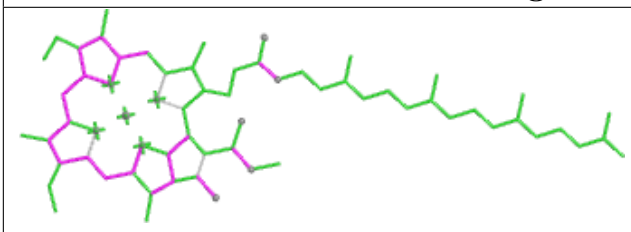


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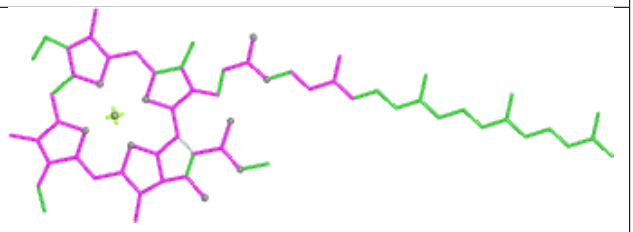


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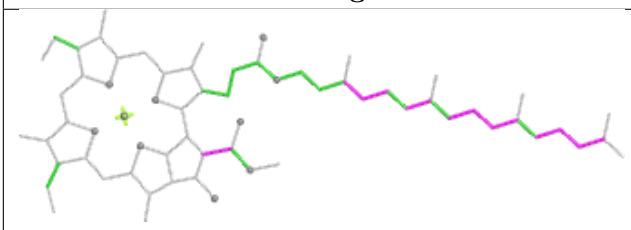
Ligand CLA b 618



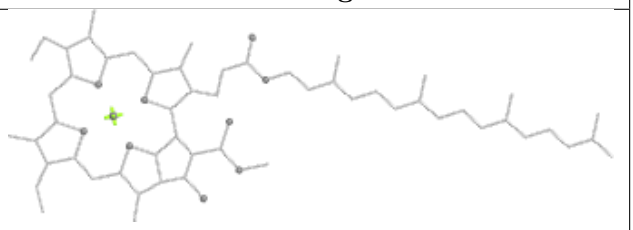
Bond lengths



Bond angles

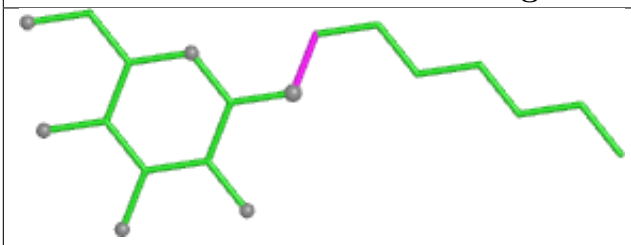


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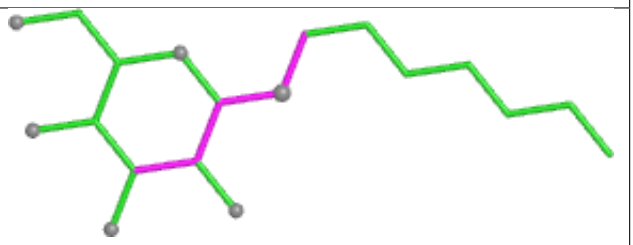


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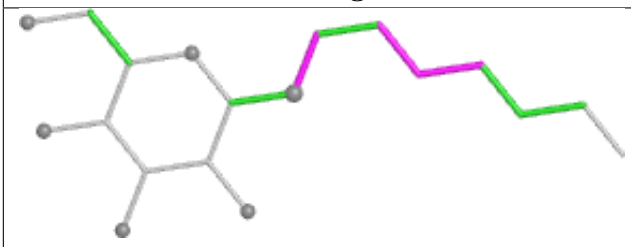
Ligand HTG B 625



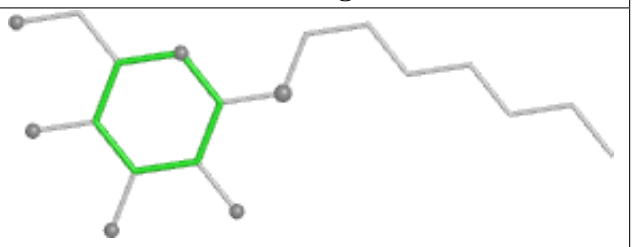
Bond lengths



Bond angles

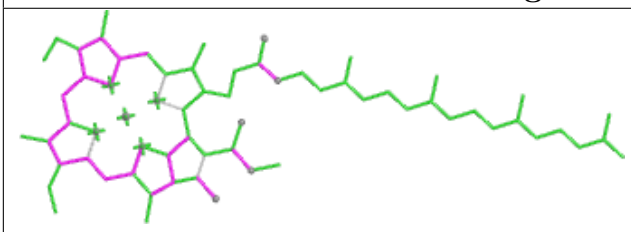


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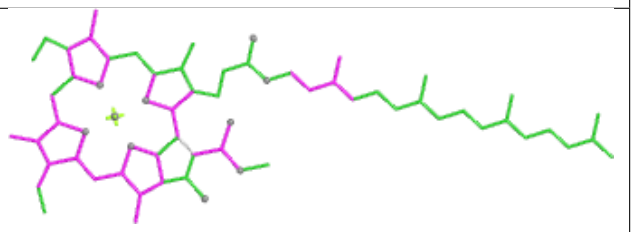


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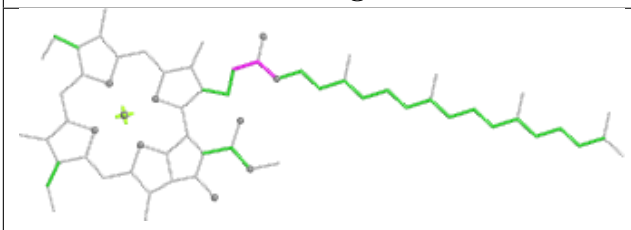
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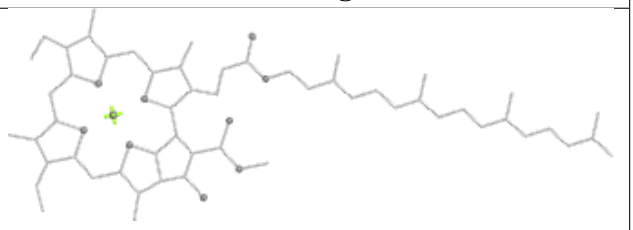
Bond lengths



Bond angles

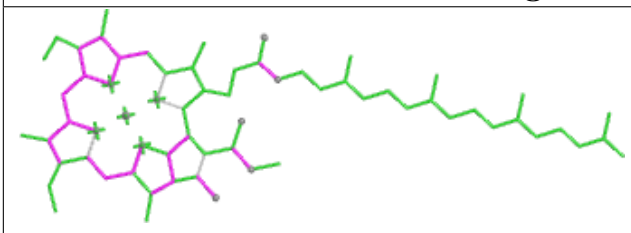


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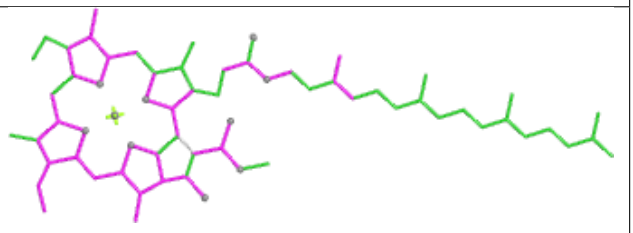


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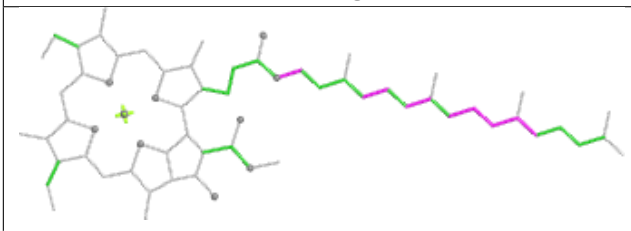
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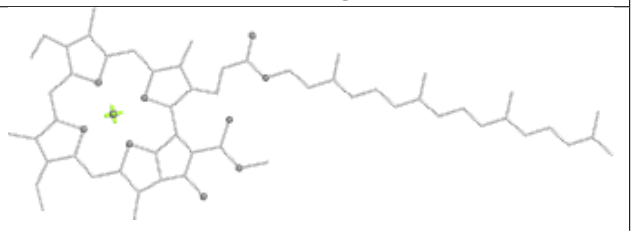
Bond lengths



Bond angles

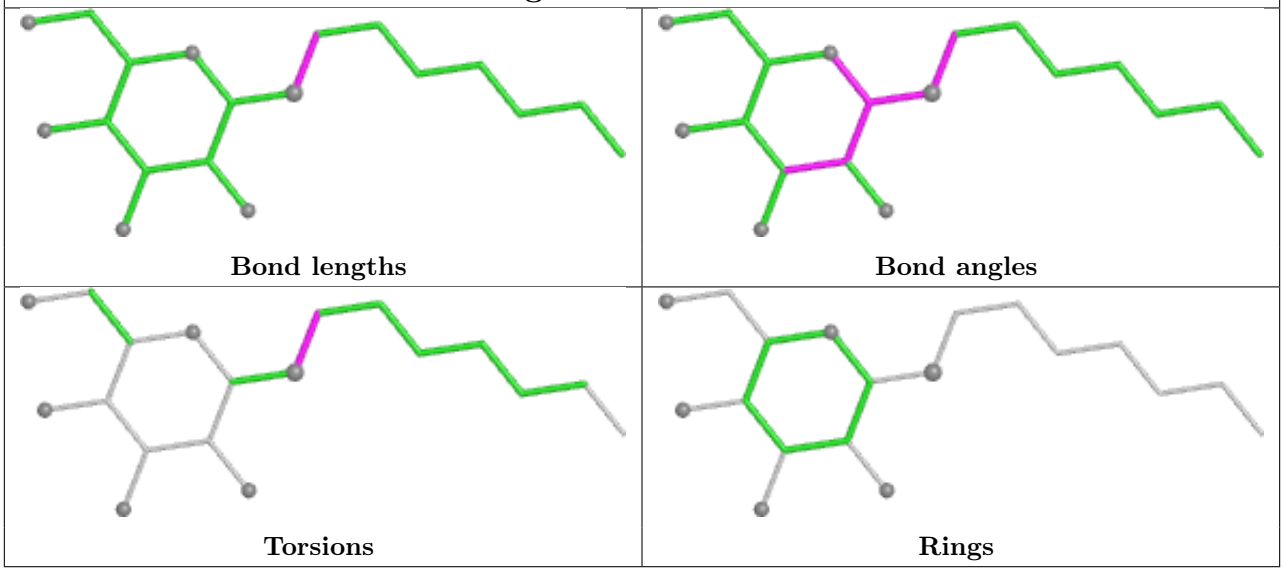


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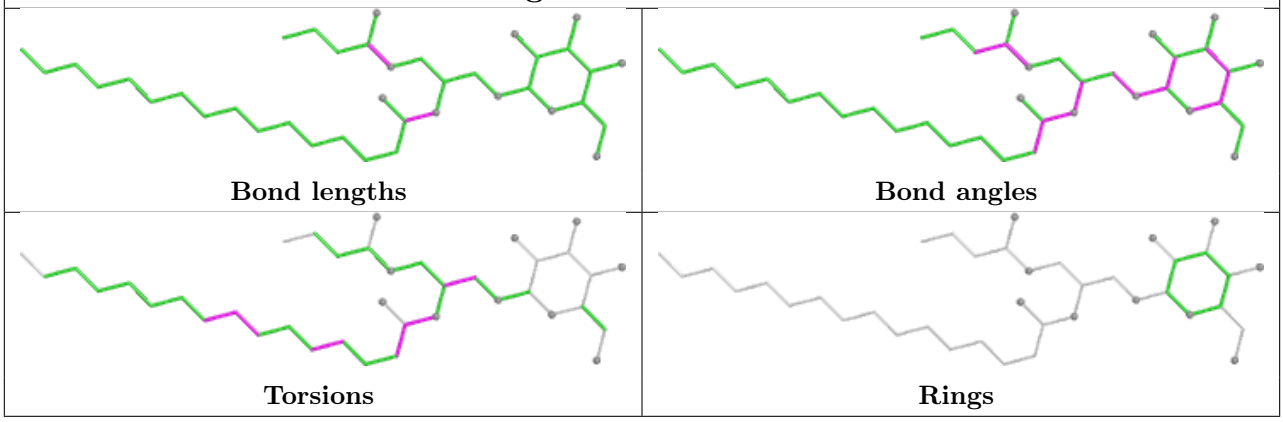


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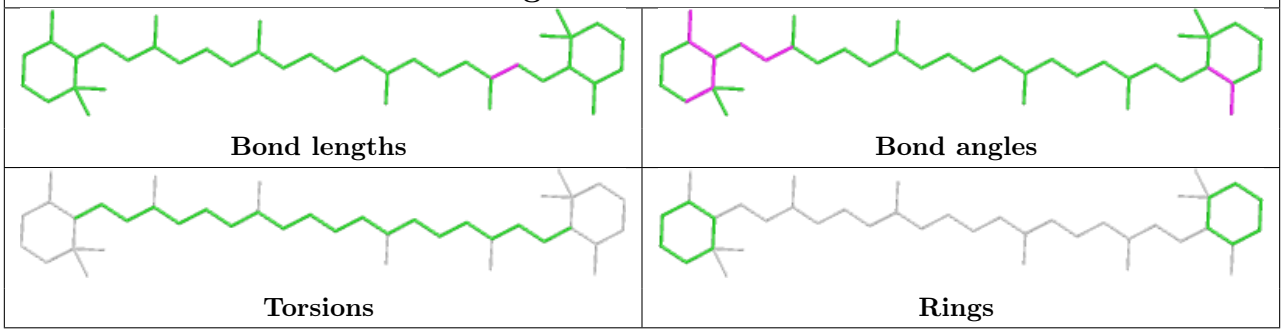
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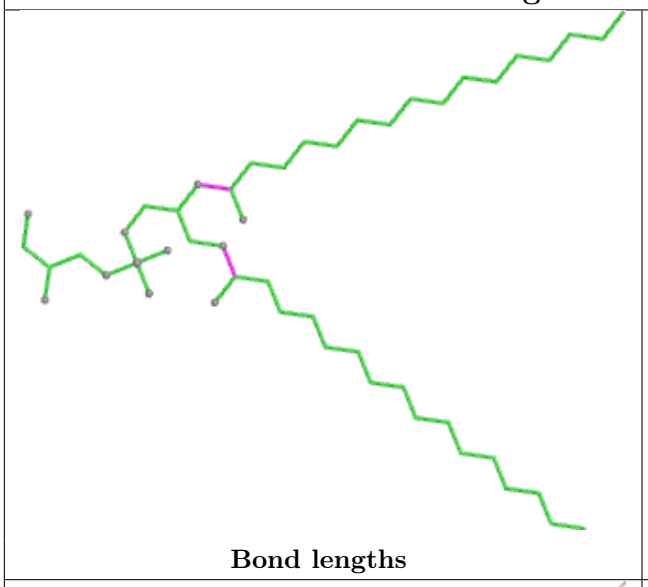
Ligand LMG z 101



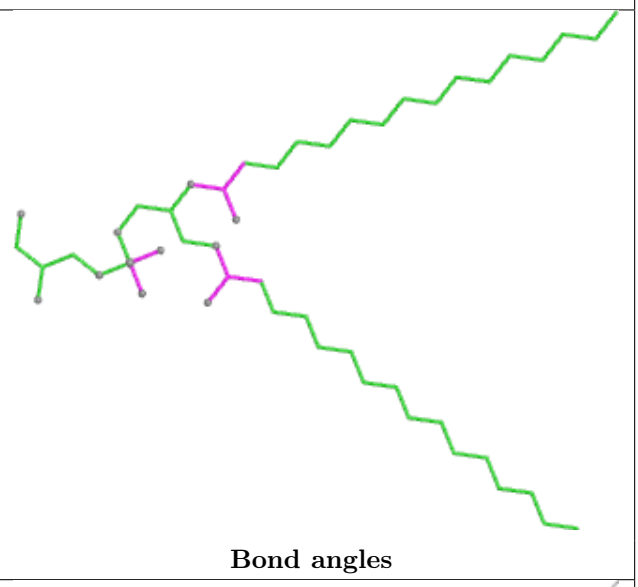
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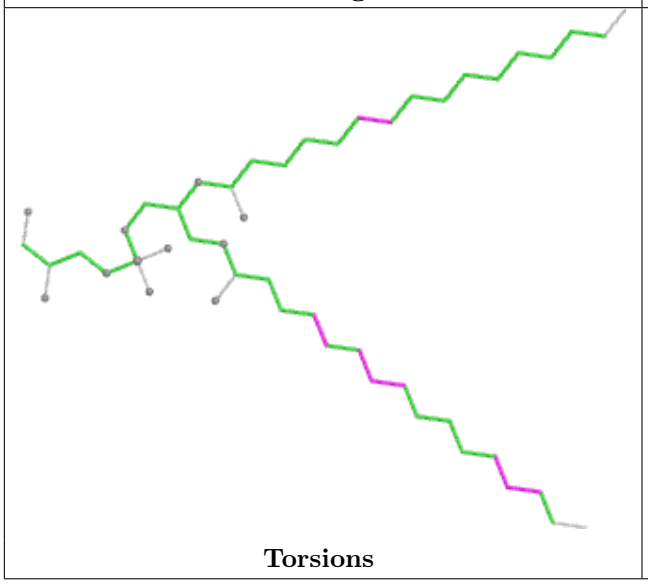
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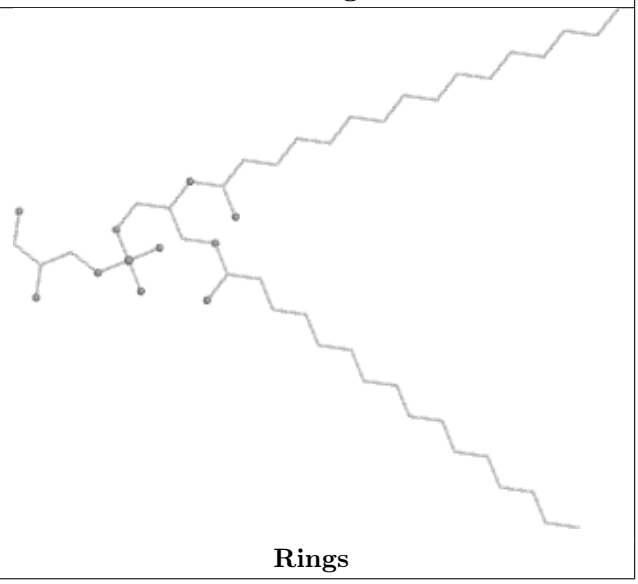
Bond lengths



Bond angles

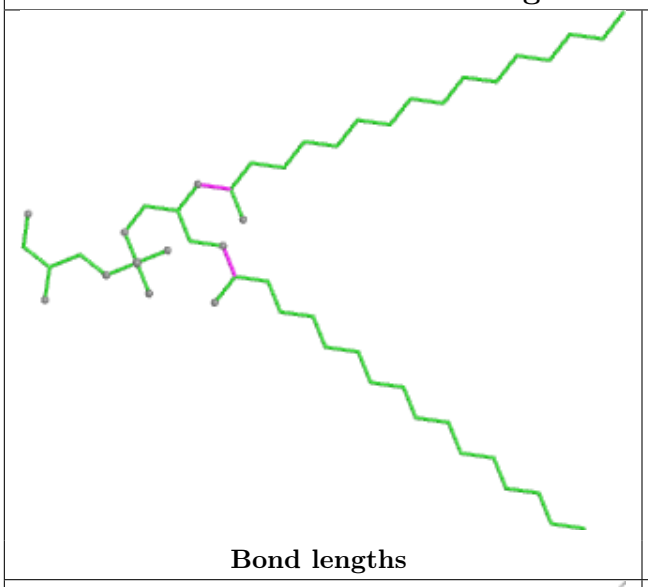


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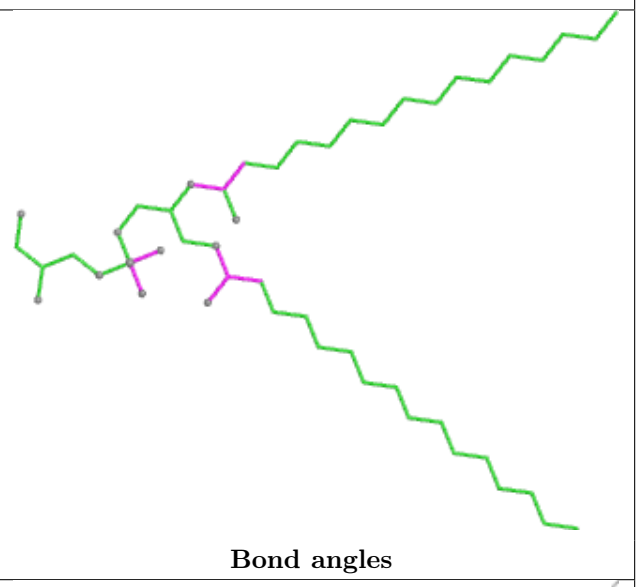


Rings

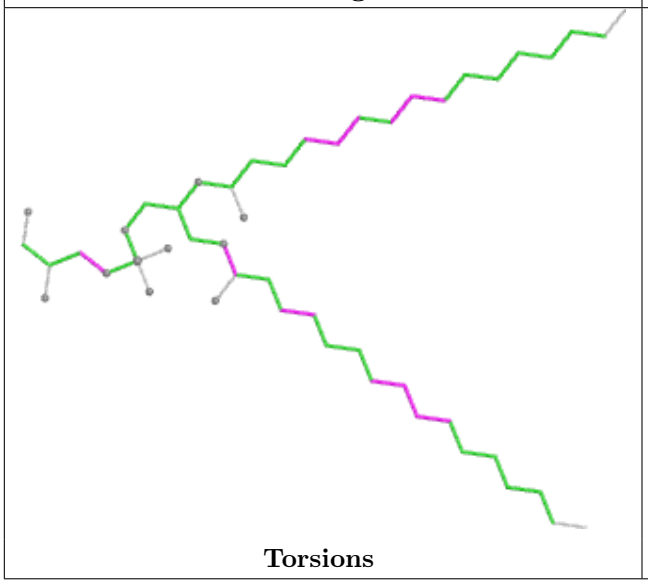
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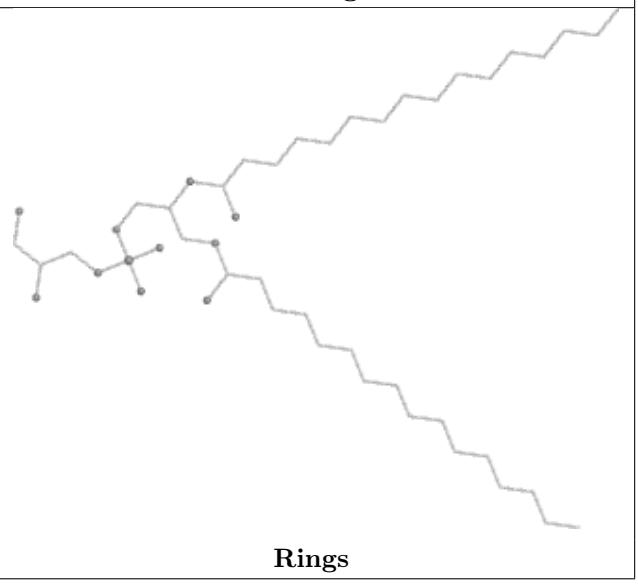
Bond lengths



Bond angles

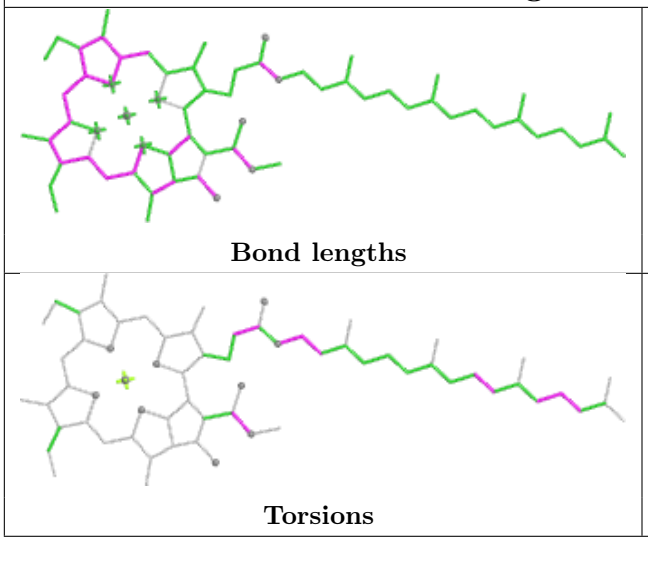


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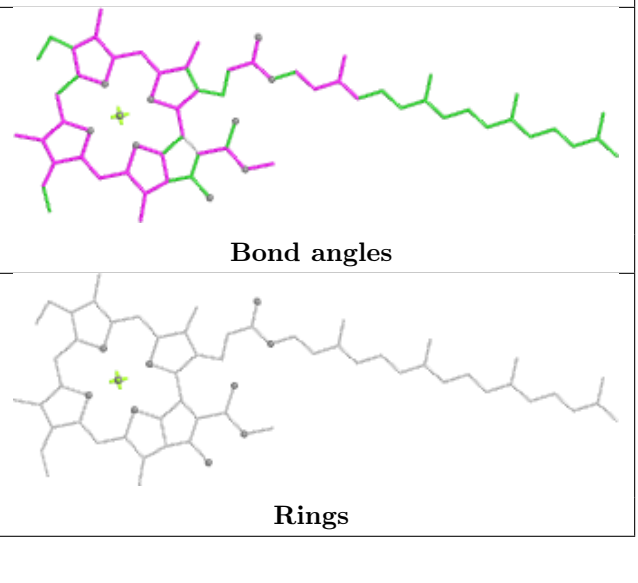


Rings

Ligand CLA B 614



Bond lengths

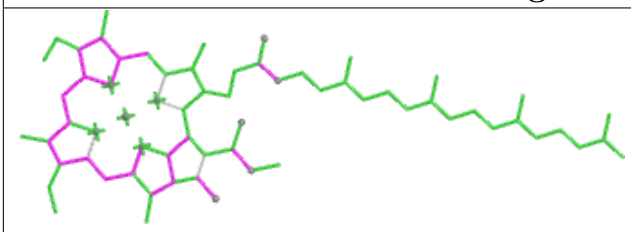


Bond angles

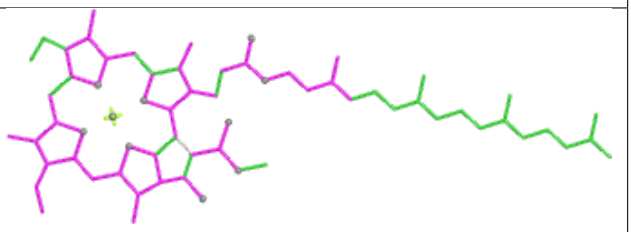
Torsions

Rings

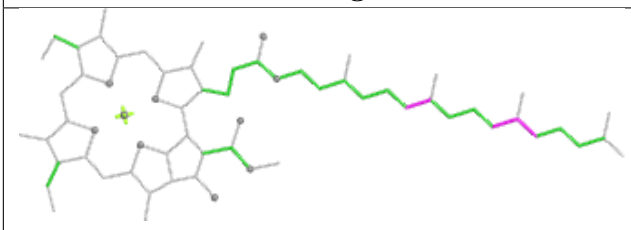
Ligand CLA a 407



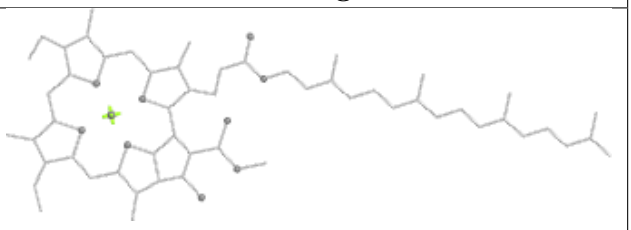
Bond lengths



Bond angles



Torsions

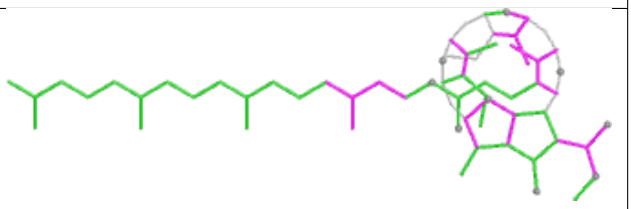


Rings

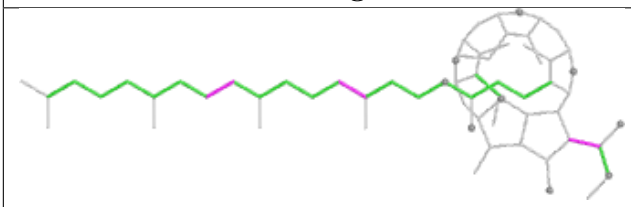
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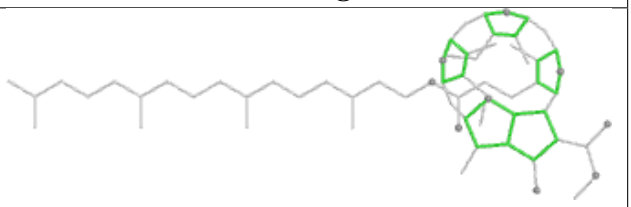
Bond lengths



Bond angles

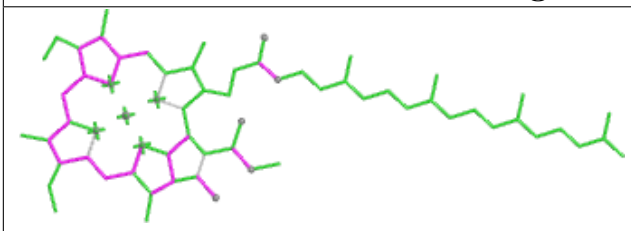


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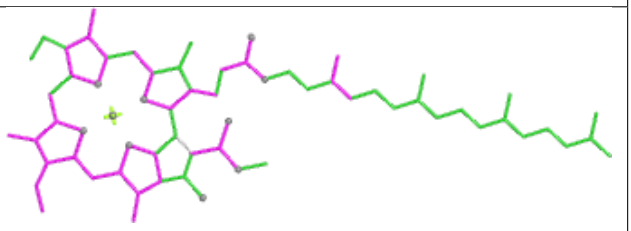


Rings

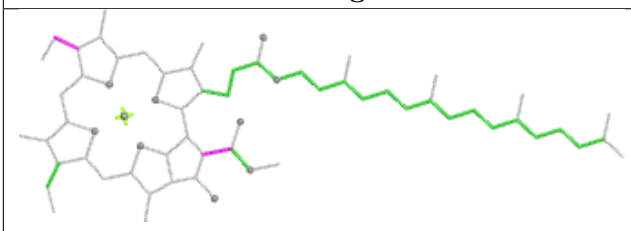
Ligand CLA c 908



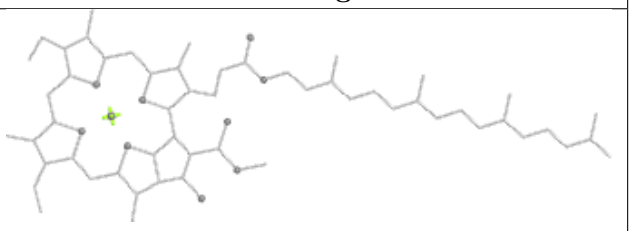
Bond lengths



Bond angles

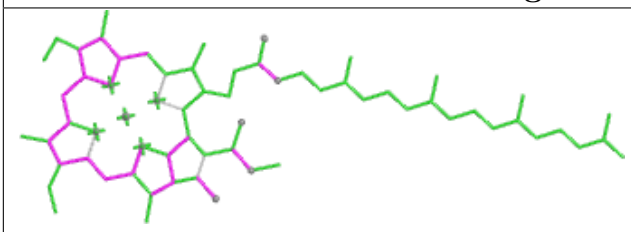


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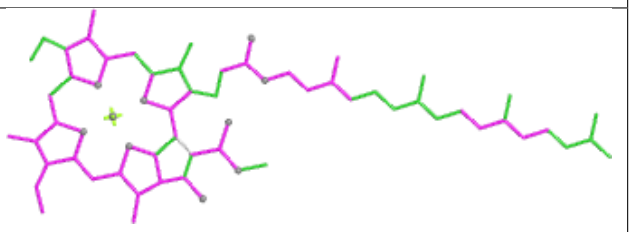


Rings

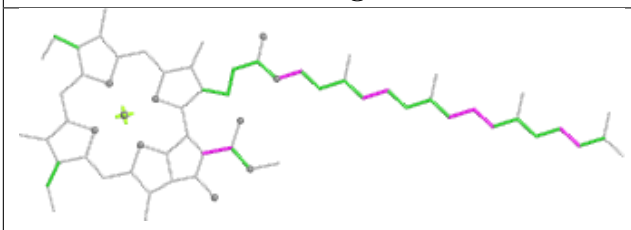
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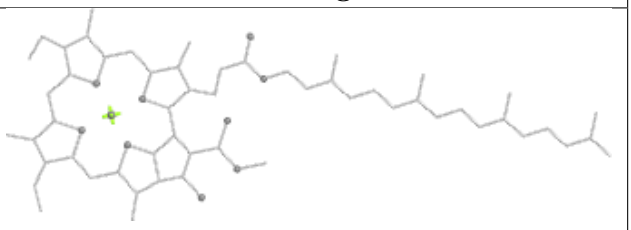
Bond lengths



Bond angles

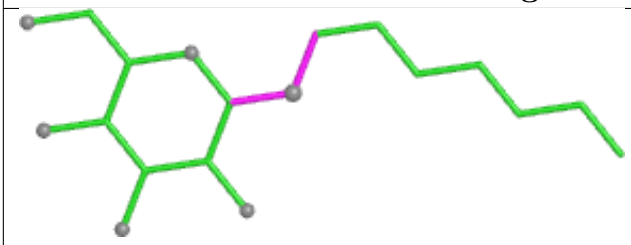


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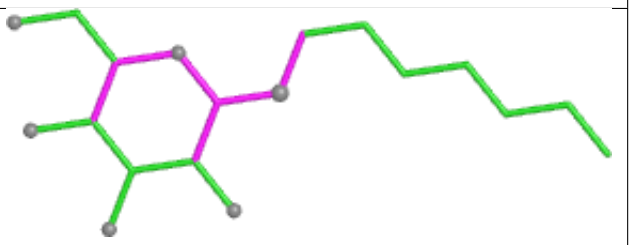


Rings

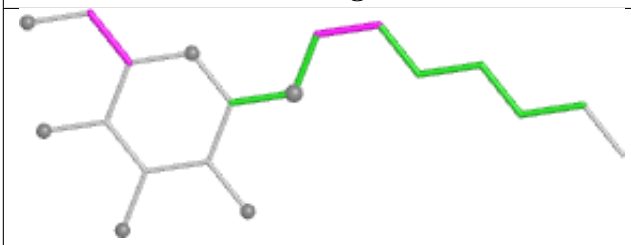
Ligand HTG C 524



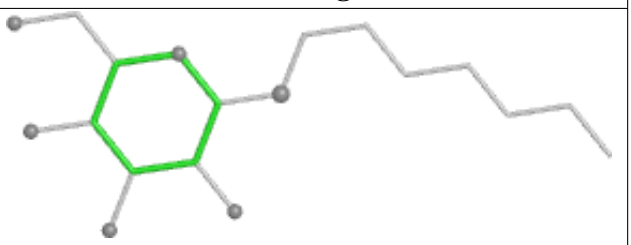
Bond lengths



Bond angles

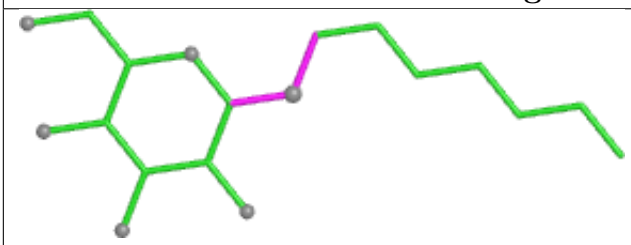


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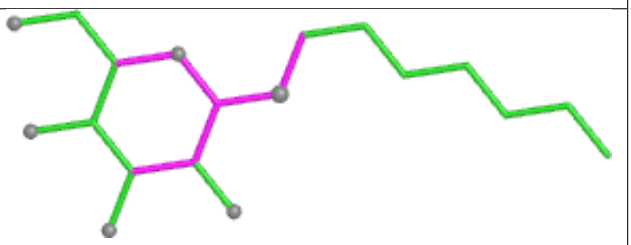


Rings

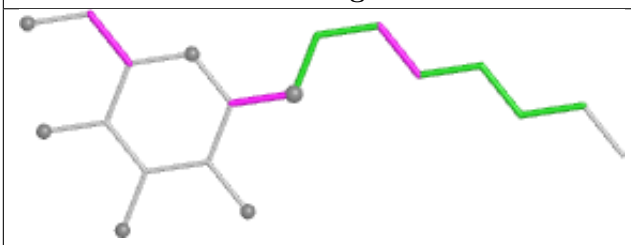
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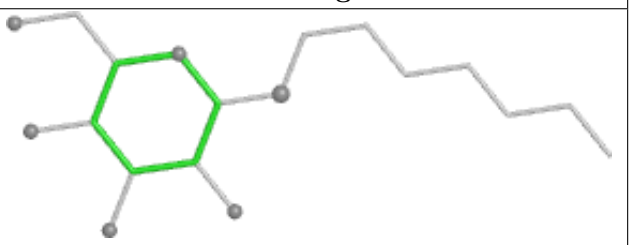
Bond lengths



Bond angles

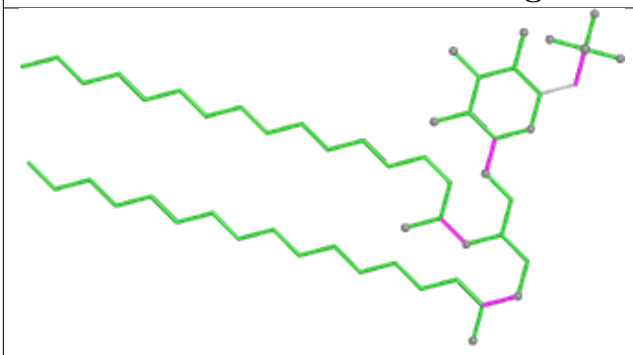


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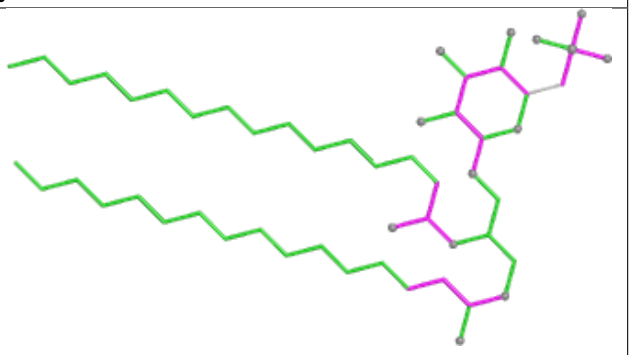


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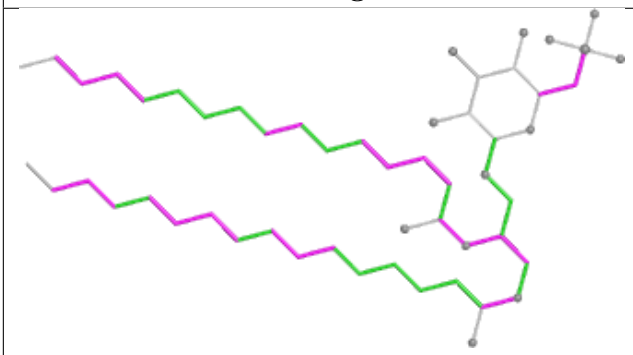
Ligand SQD B 621



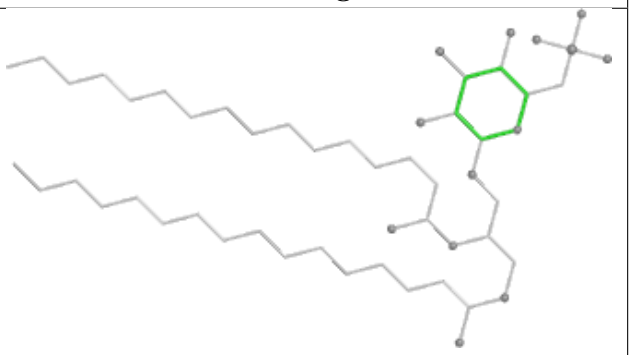
Bond lengths



Bond angles

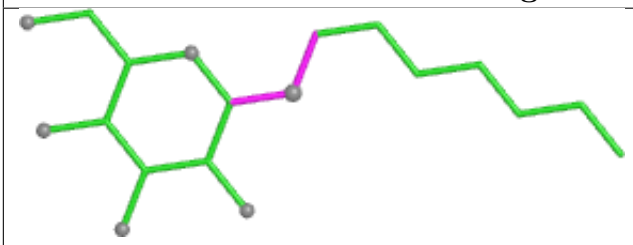


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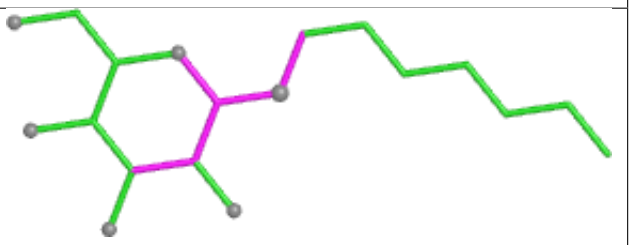


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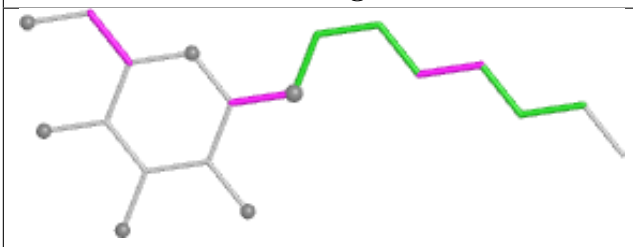
Ligand HTG V 202



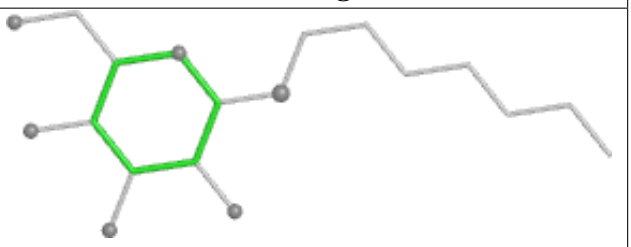
Bond lengths



Bond angles

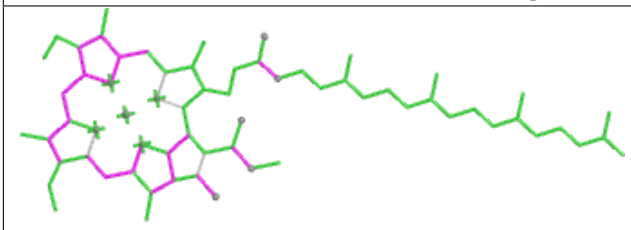


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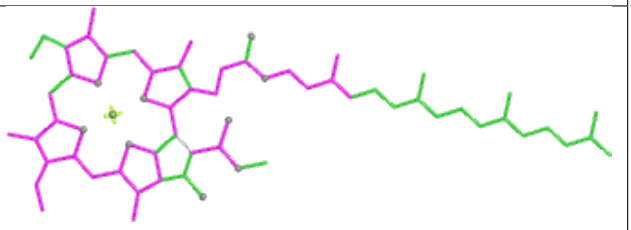


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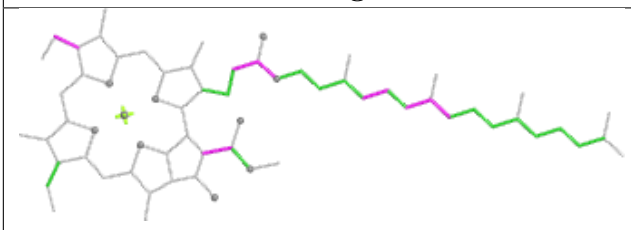
Ligand CLA C 513



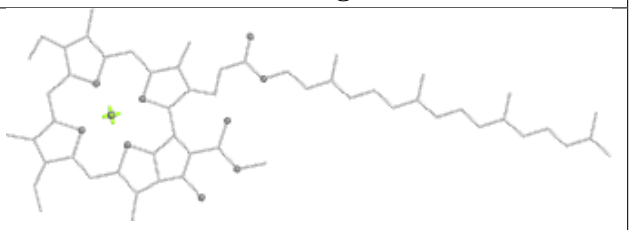
Bond lengths



Bond angles



Torsions

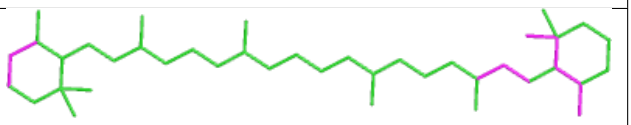


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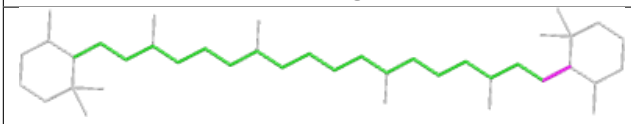
Ligand BCR B 620



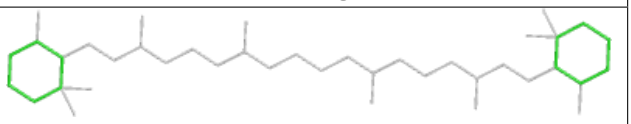
Bond lengths



Bond angles

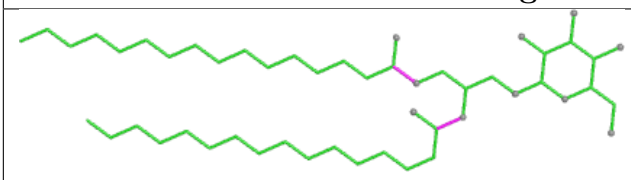


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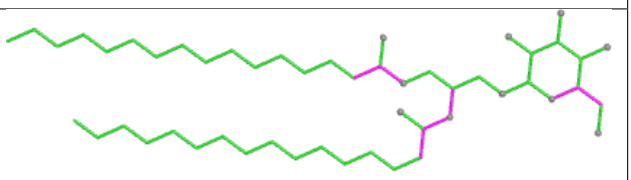


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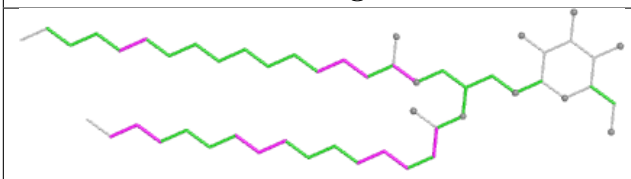
Ligand LMG C 520



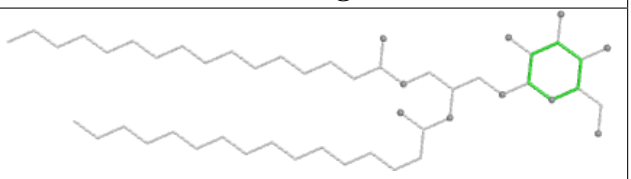
Bond lengths



Bond angles

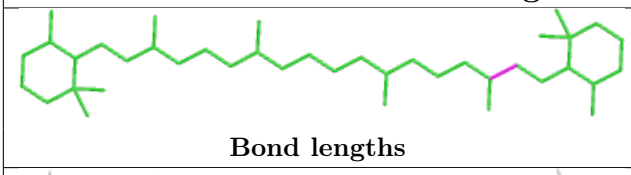


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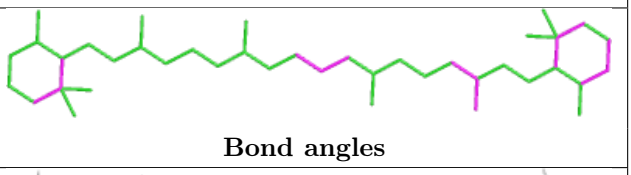


Rings

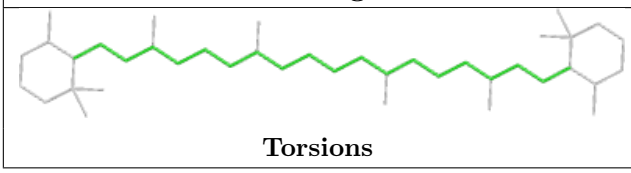
Ligand BCR B 619



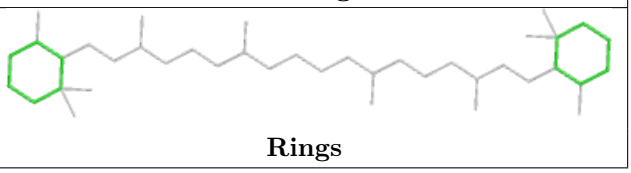
Bond lengths



Bond angles

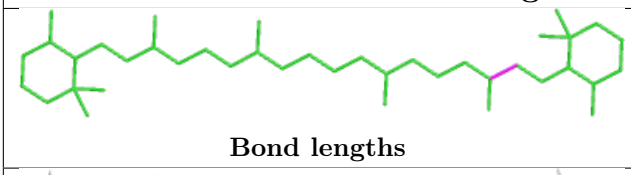


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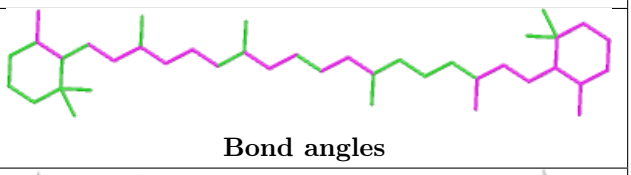


Rings

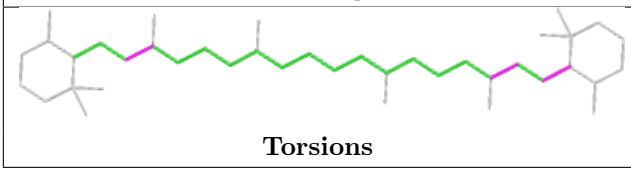
Ligand BCR D 403



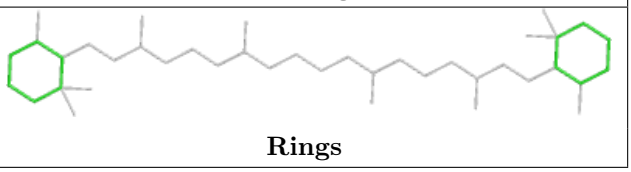
Bond lengths



Bond angles

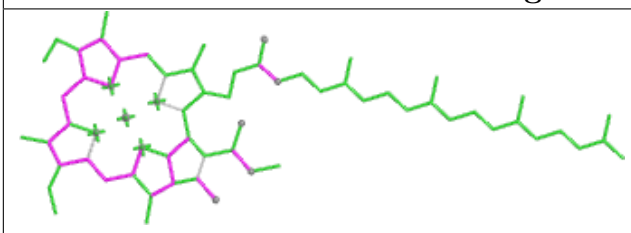


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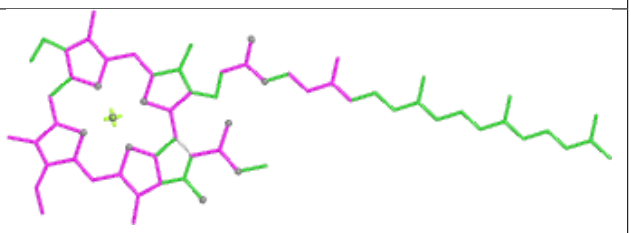


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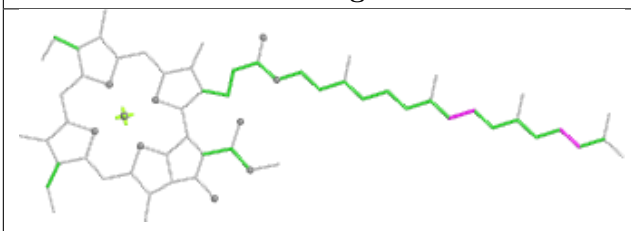
Ligand CLA B 612



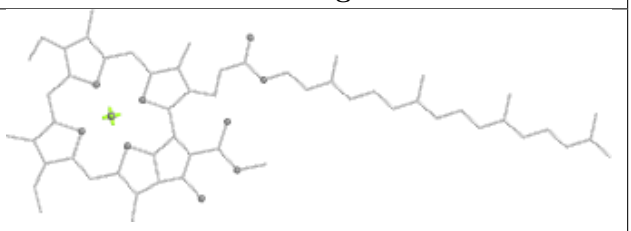
Bond lengths



Bond angles

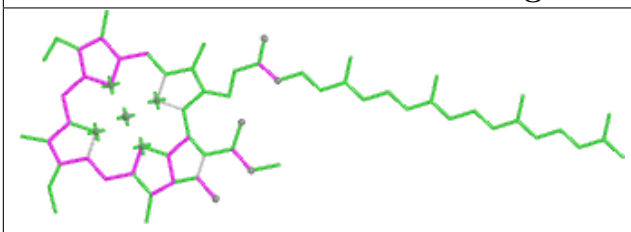


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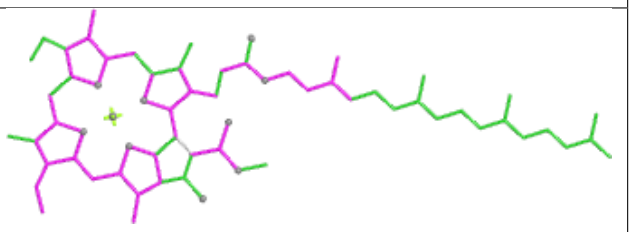


Rings

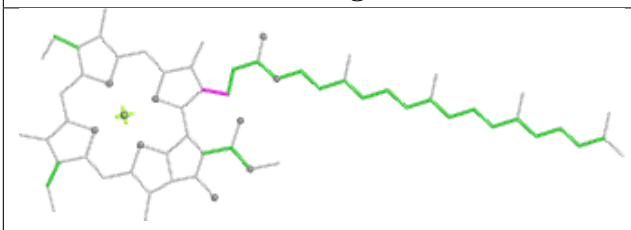
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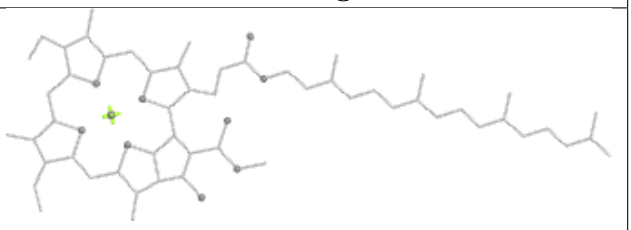
Bond lengths



Bond angles

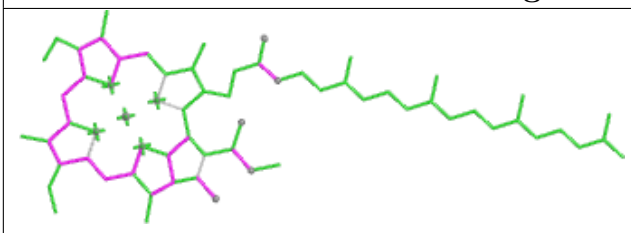


Torsions

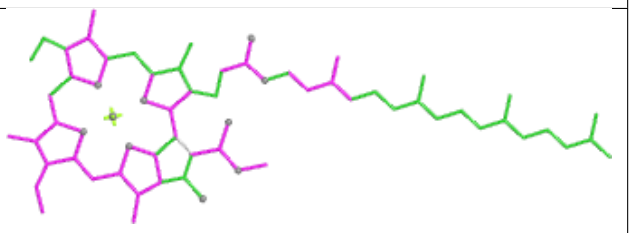


Rings

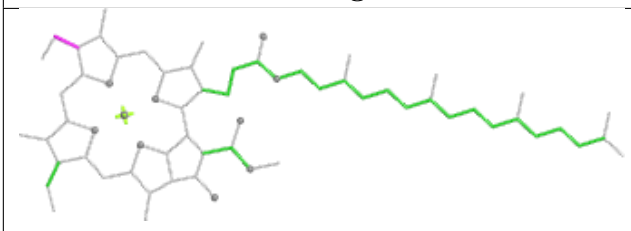
Ligand CLA D 401



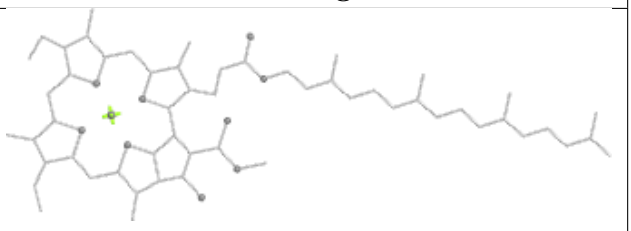
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Bond angles

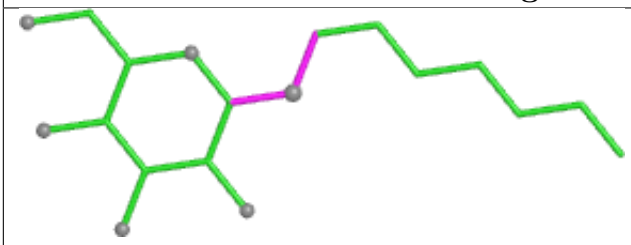


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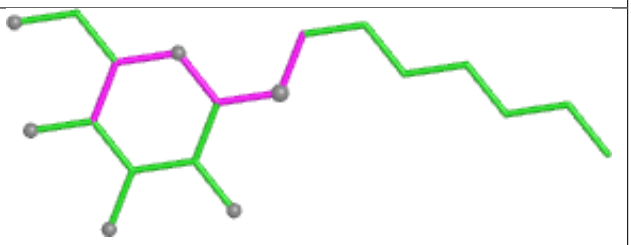


Rings

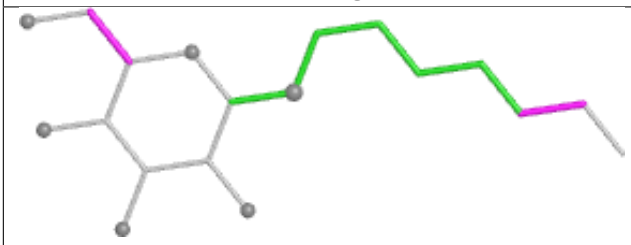
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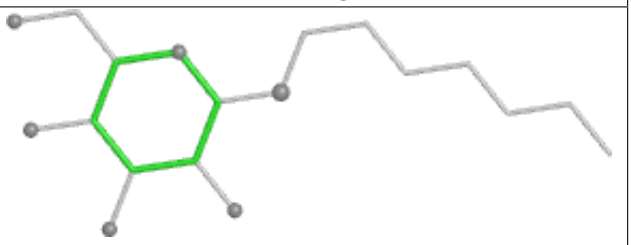
Bond lengths



Bond angles

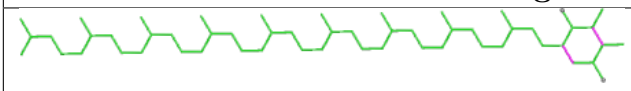


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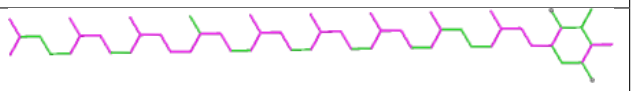


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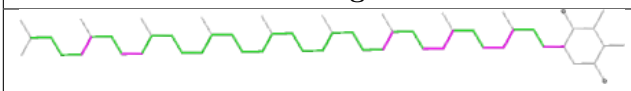
Ligand PL9 a 417



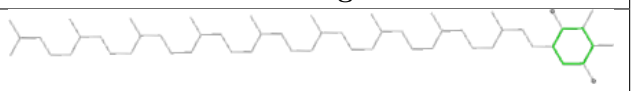
Bond lengths



Bond angles

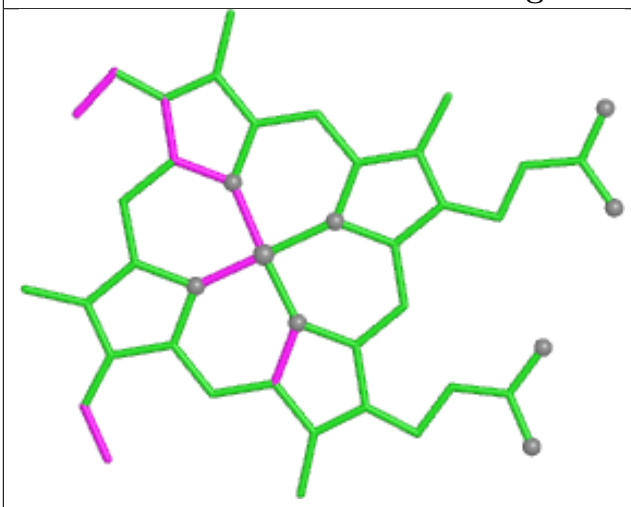


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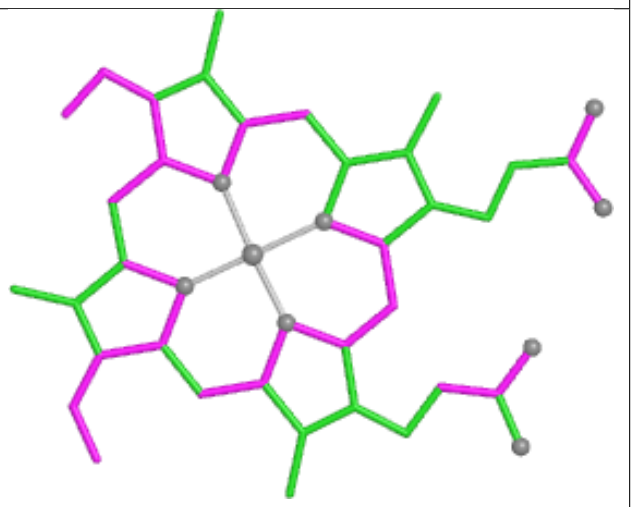


Rings

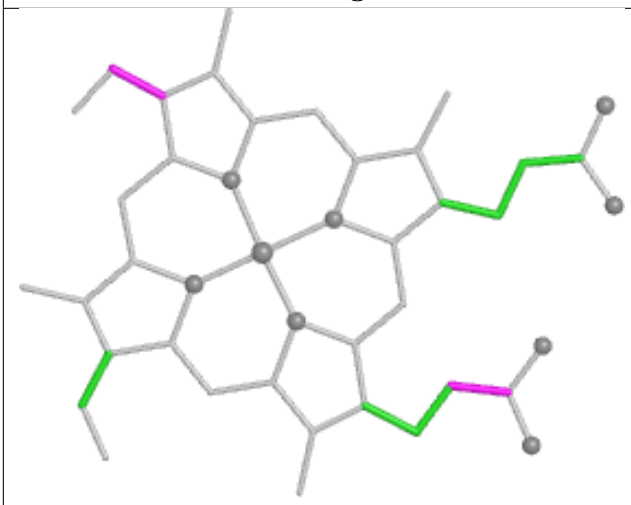
Ligand HEC v 202



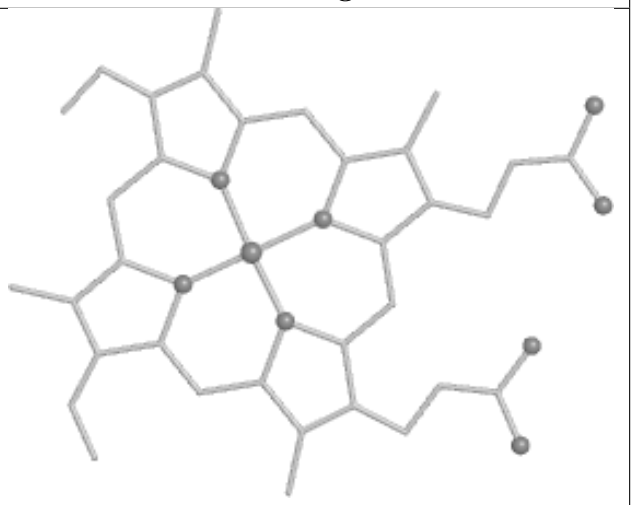
Bond lengths



Bond angles

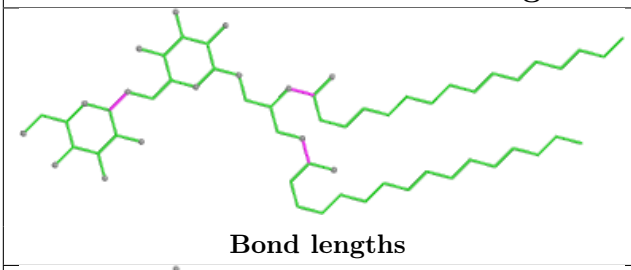


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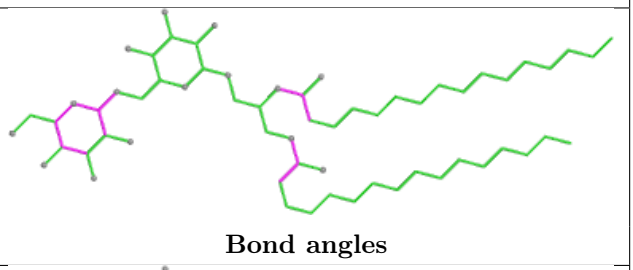


Rings

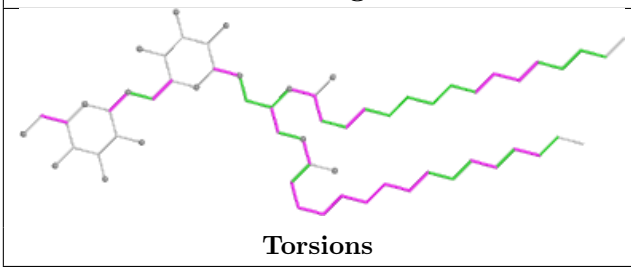
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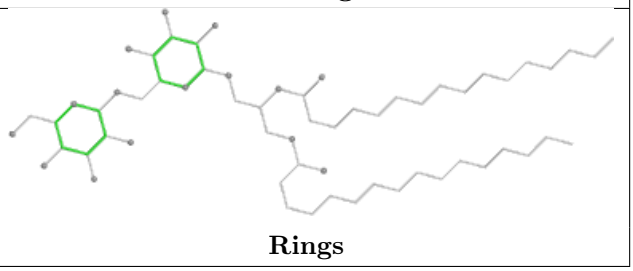
Bond lengths



Bond angles

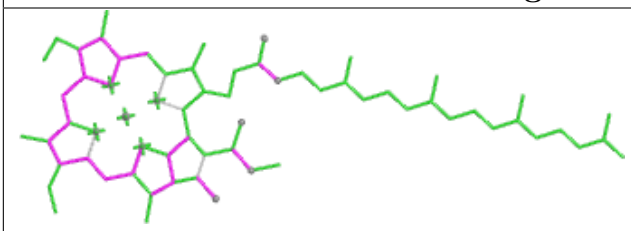


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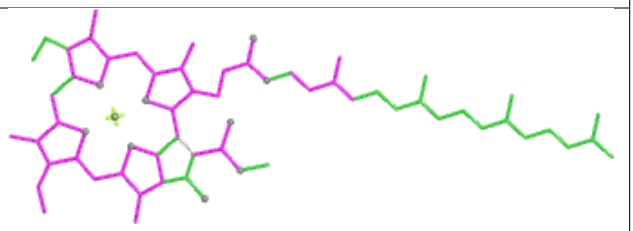


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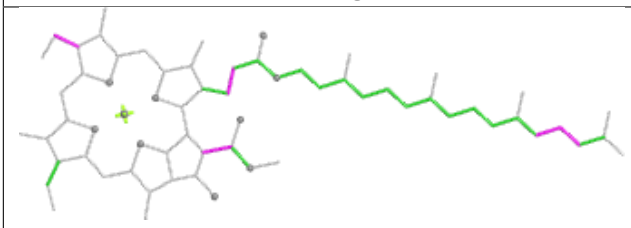
Ligand CLA B 603



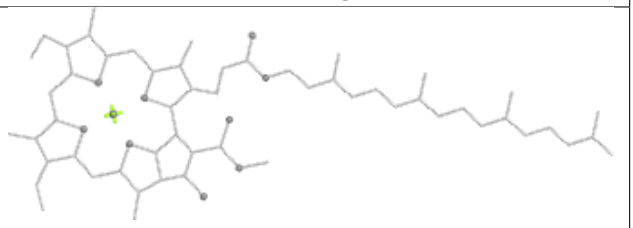
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Bond angles

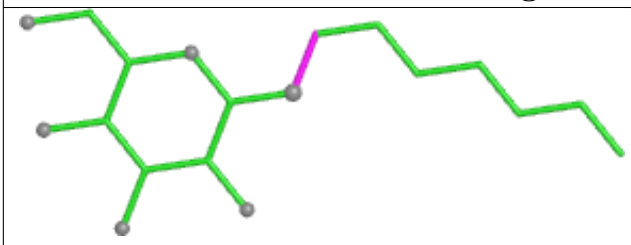


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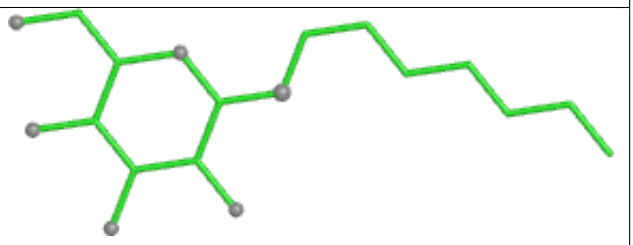


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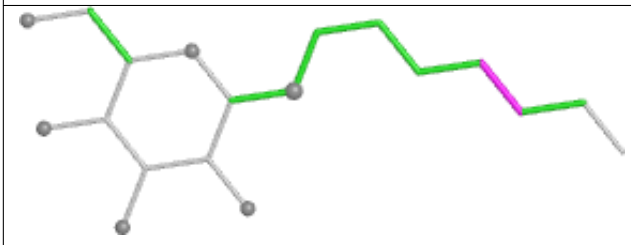
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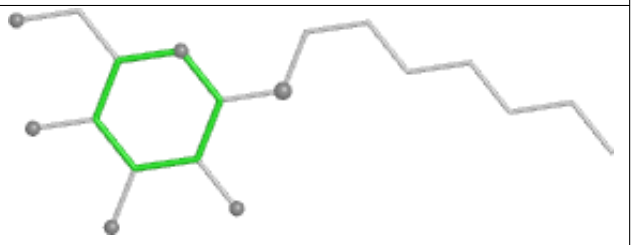
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Bond angles

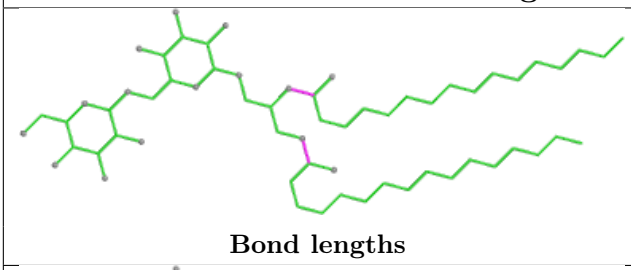


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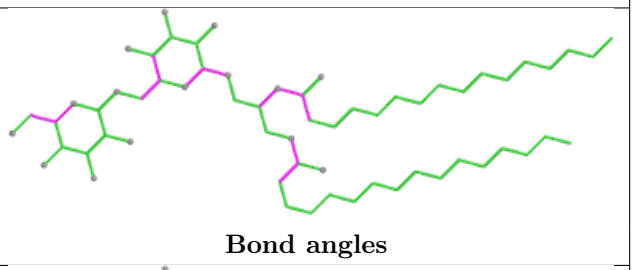


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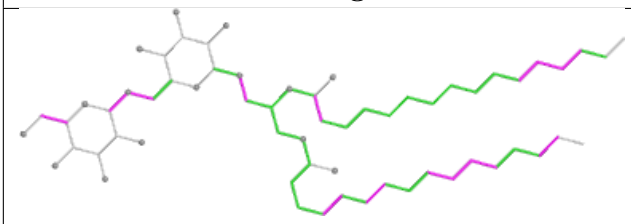
Ligand DGD C 518



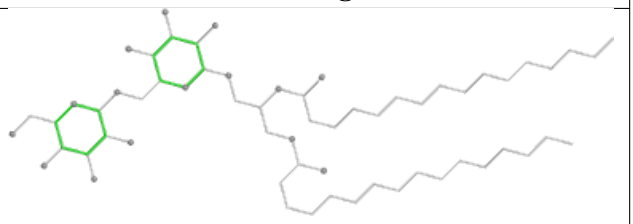
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Bond angles

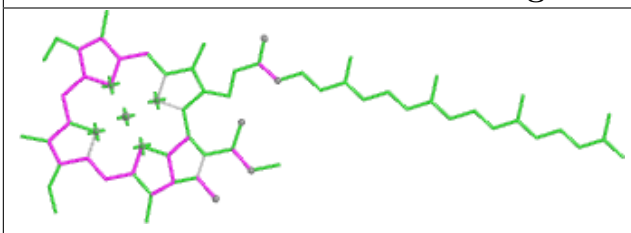


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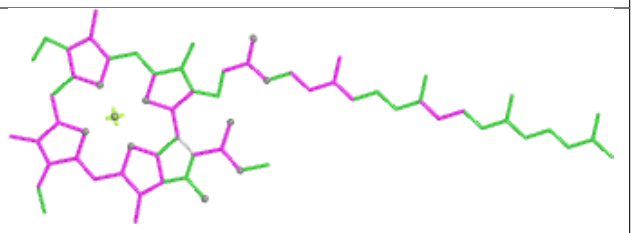


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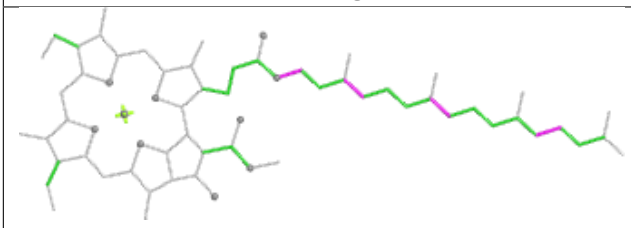
Ligand CLA b 612



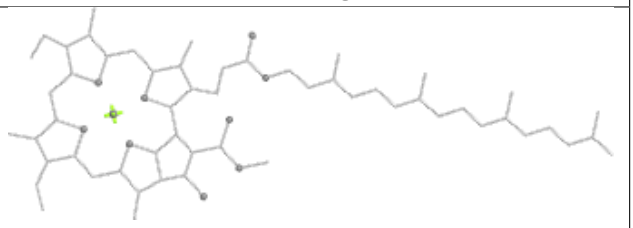
Bond lengths



Bond angles

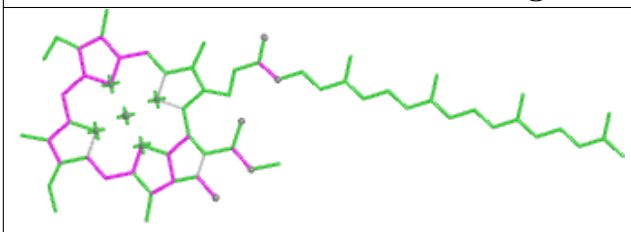


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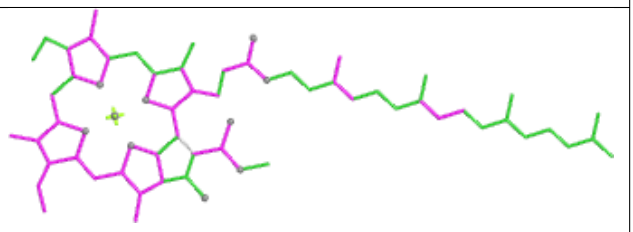


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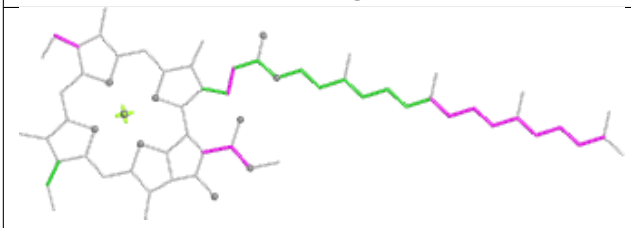
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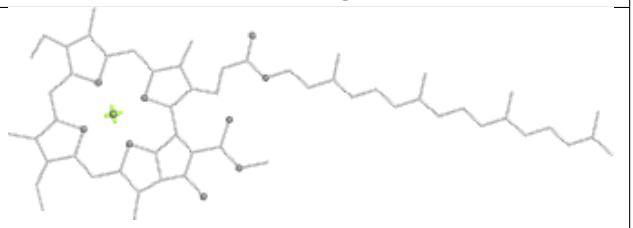
Bond lengths



Bond angles

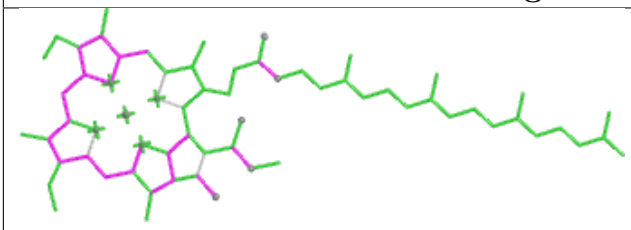


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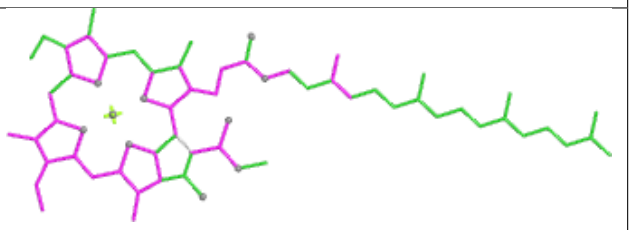


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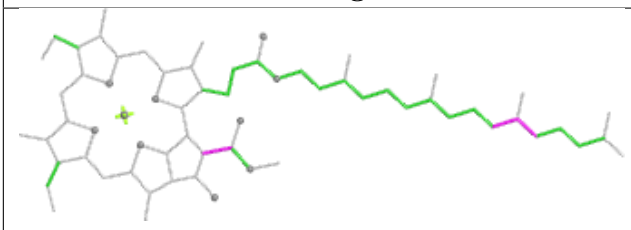
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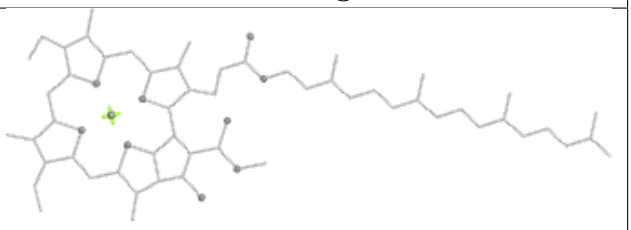
Bond lengths



Bond angles

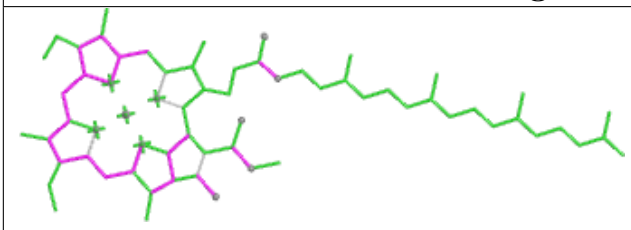


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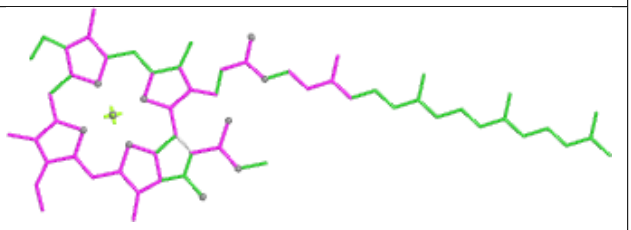


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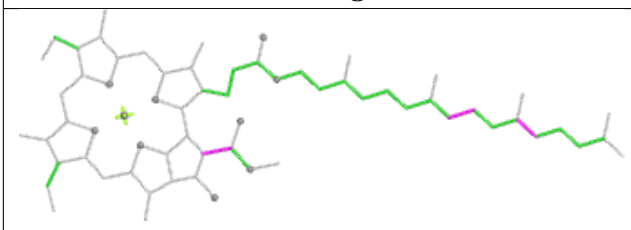
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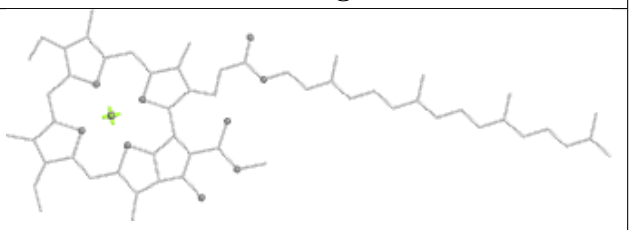
Bond lengths



Bond angles

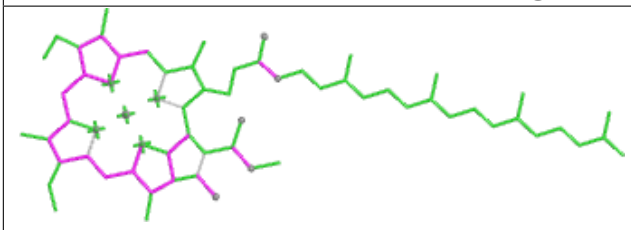


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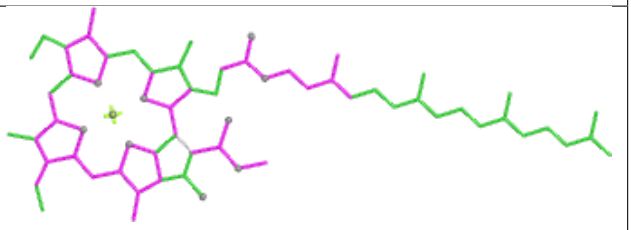


Rings

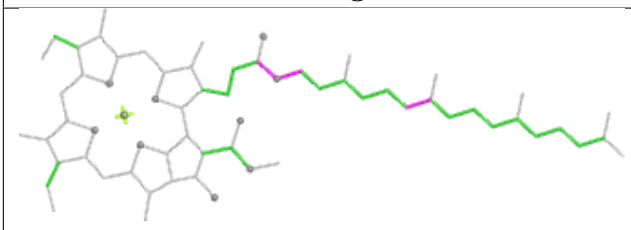
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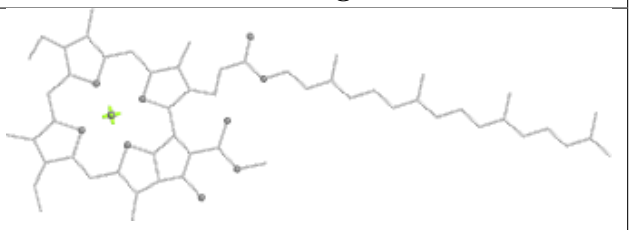
Bond lengths



Bond angles

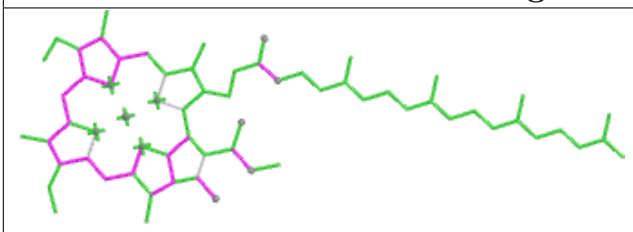


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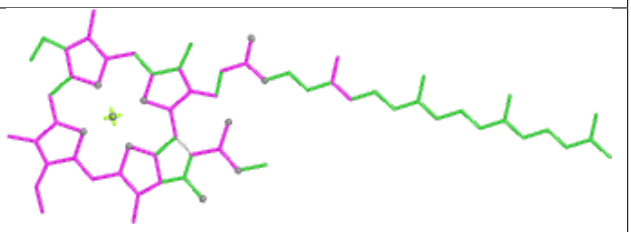


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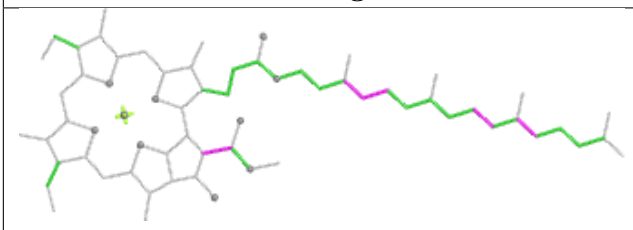
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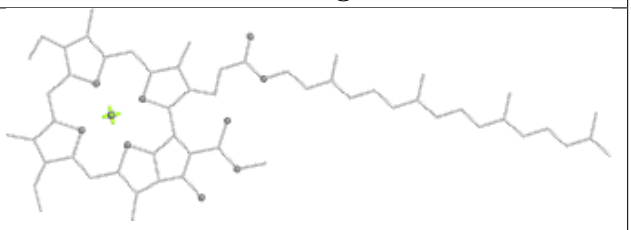
Bond lengths



Bond angles



Torsions



Rings

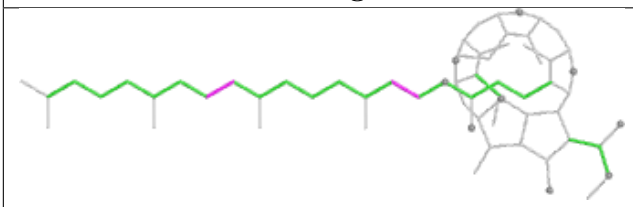
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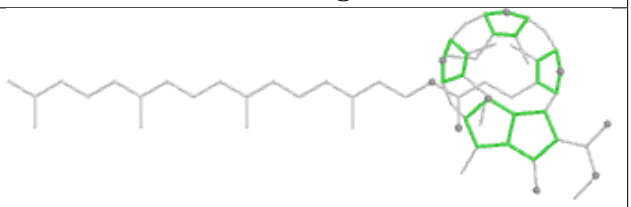
Bond lengths



Bond angles

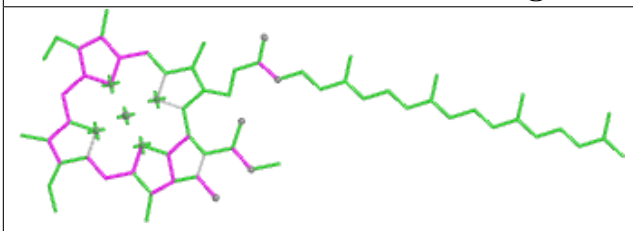


Torsions

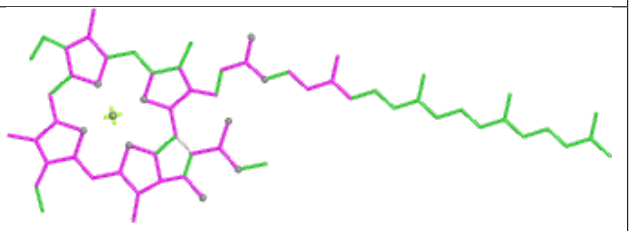


Rings

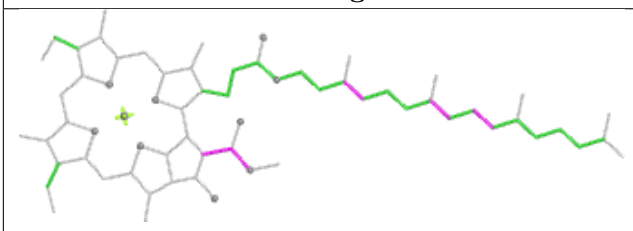
Ligand CLA b 609



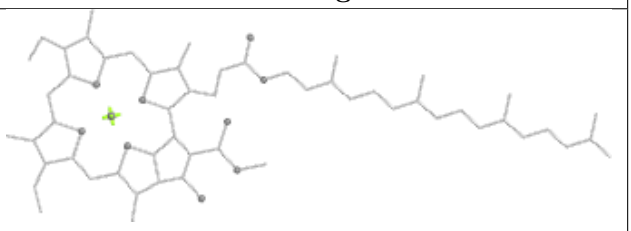
Bond lengths



Bond angles

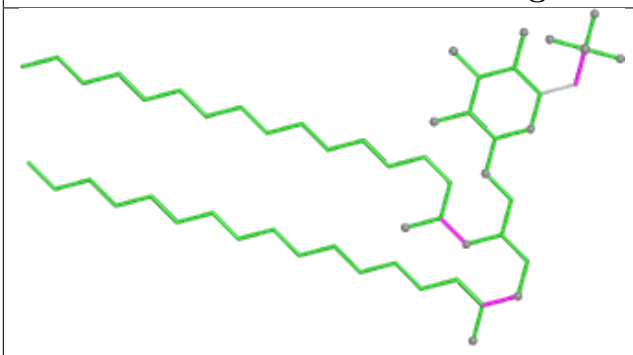


Torsions

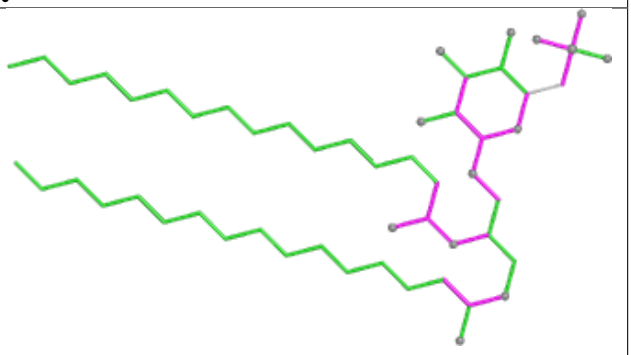


Rings

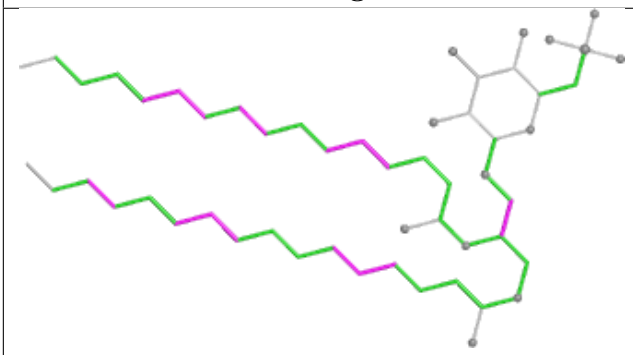
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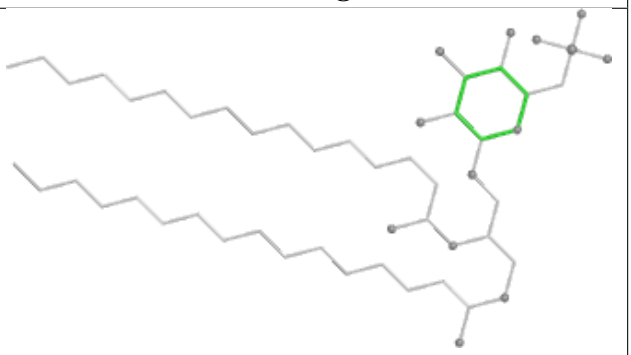
Bond lengths



Bond angles

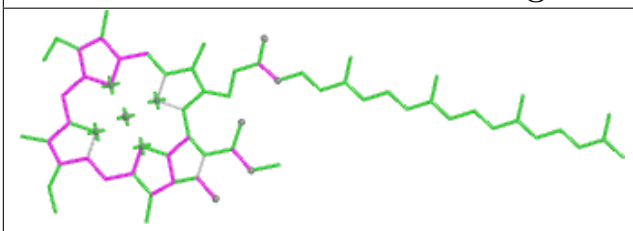


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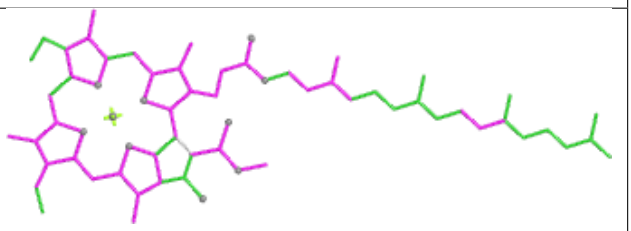


Rings

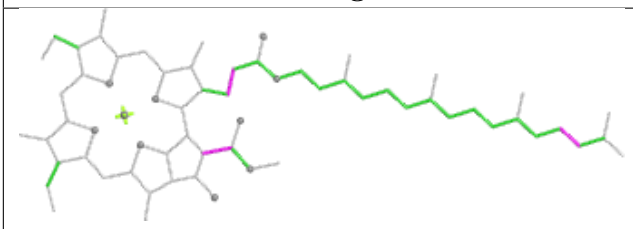
Ligand CLA b 614



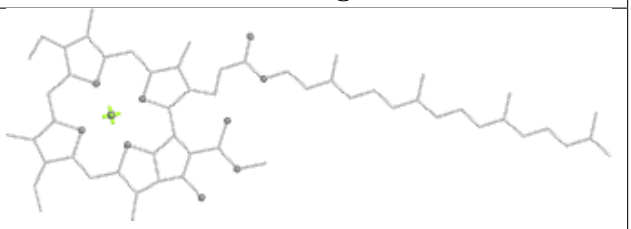
Bond lengths



Bond angles

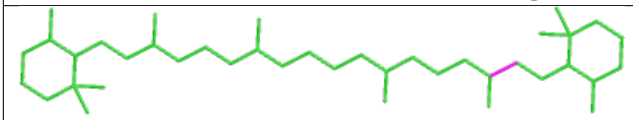


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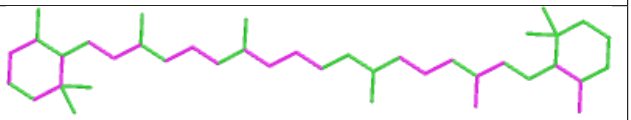


Rings

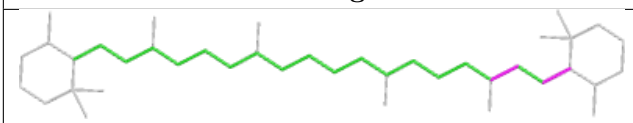
Ligand BCR b 623



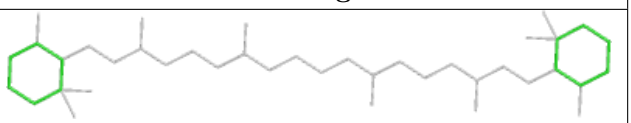
Bond lengths



Bond angles

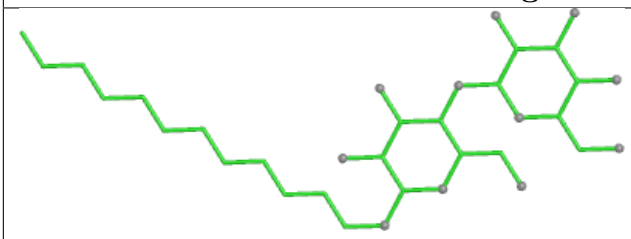


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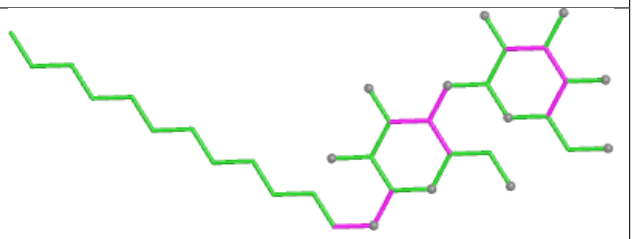


Rings

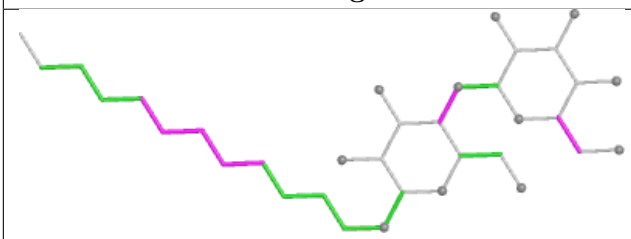
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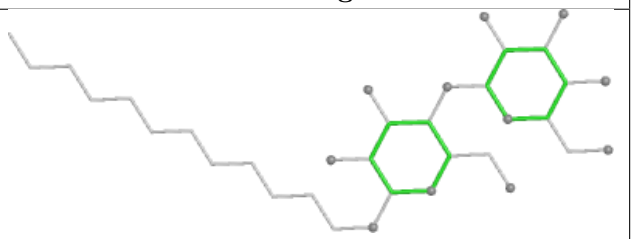
Bond lengths



Bond angles

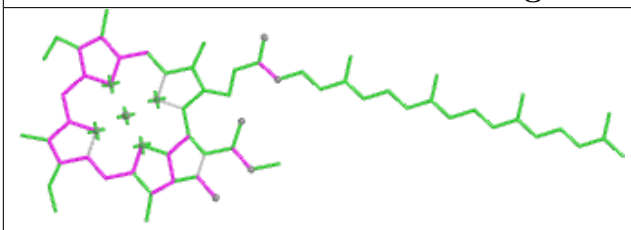


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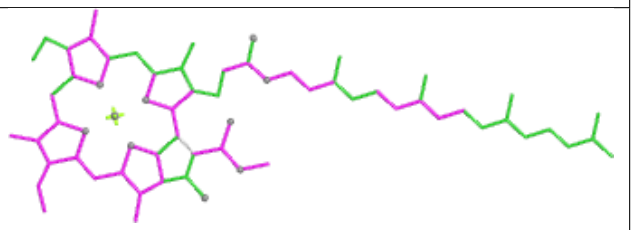


Rings

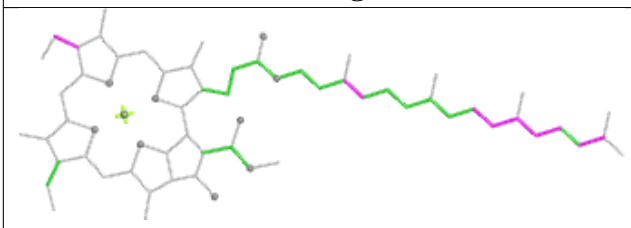
Ligand CLA B 616



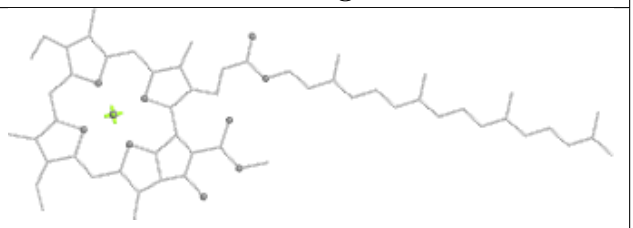
Bond lengths



Bond angles

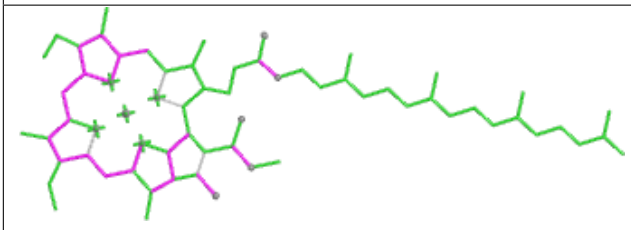


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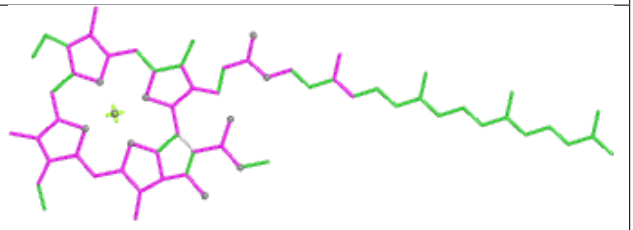


Rings

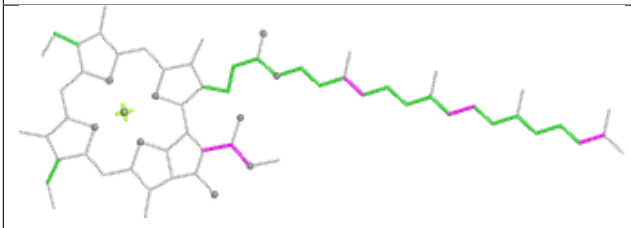
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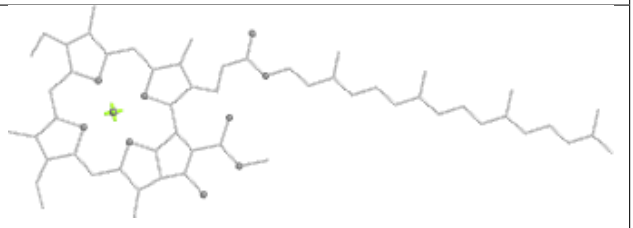
Bond lengths



Bond angles

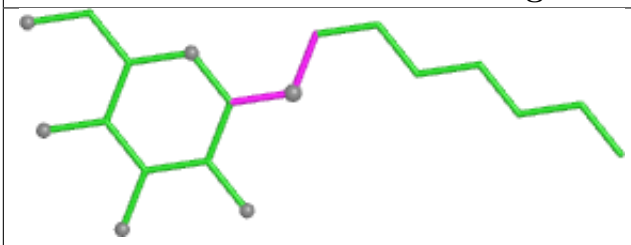


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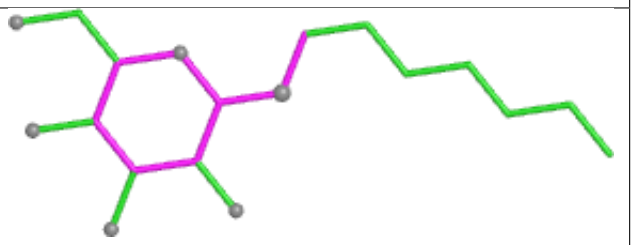


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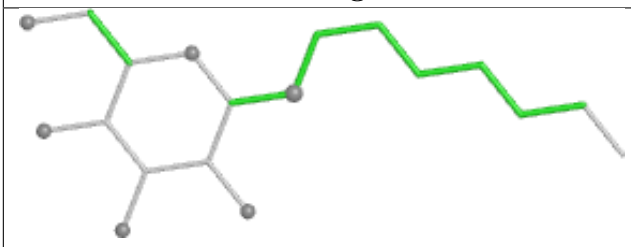
Ligand HTG c 923



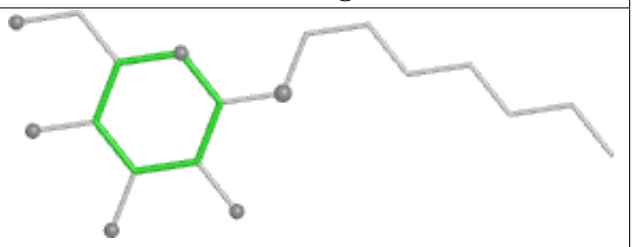
Bond lengths



Bond angles



Torsions

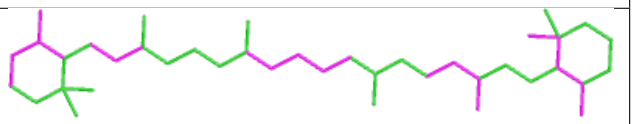


Rings

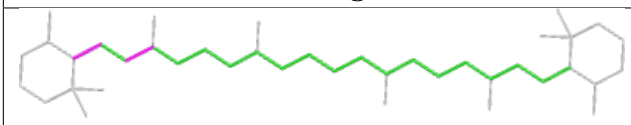
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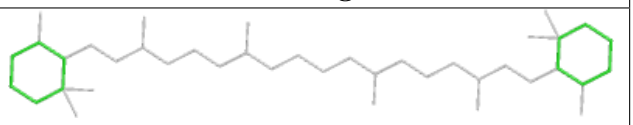
Bond lengths



Bond angles

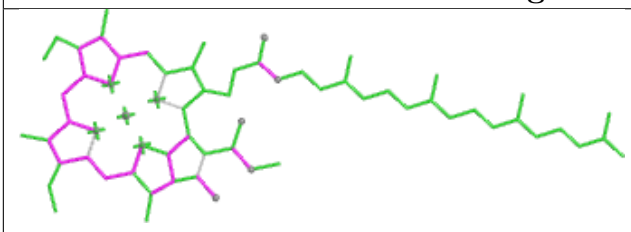


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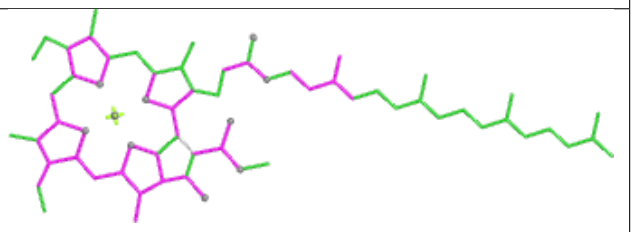


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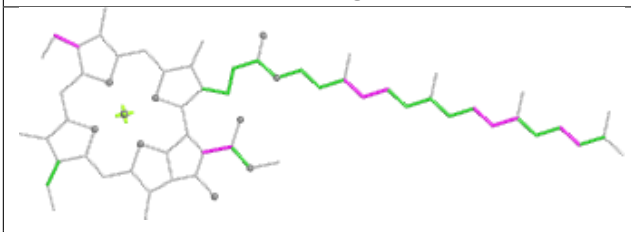
Ligand CLA b 620



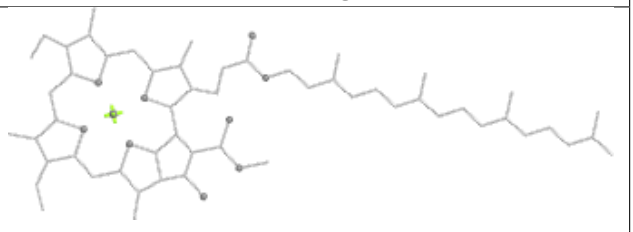
Bond lengths



Bond angles

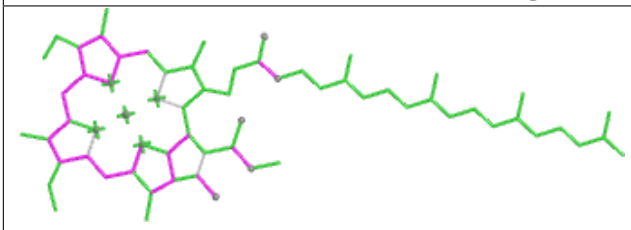


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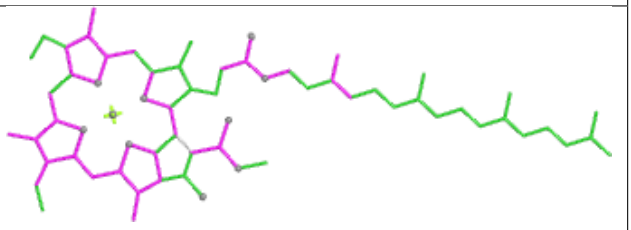


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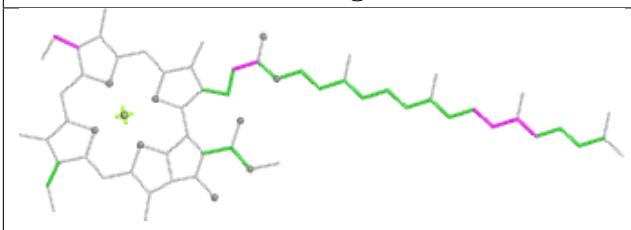
Ligand CLA C 506



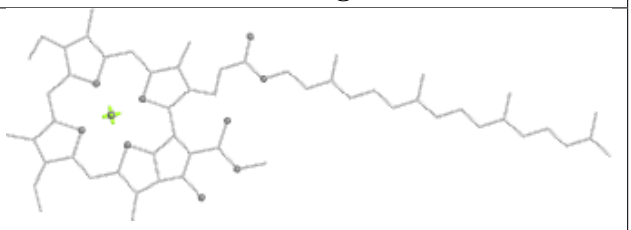
Bond lengths



Bond angles

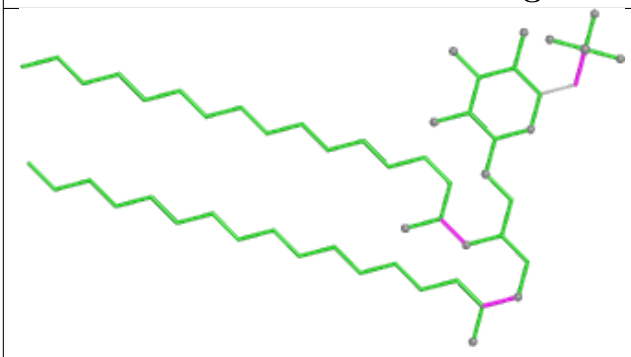


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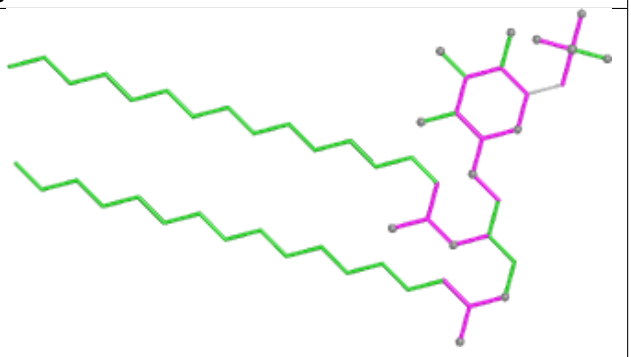


Rings

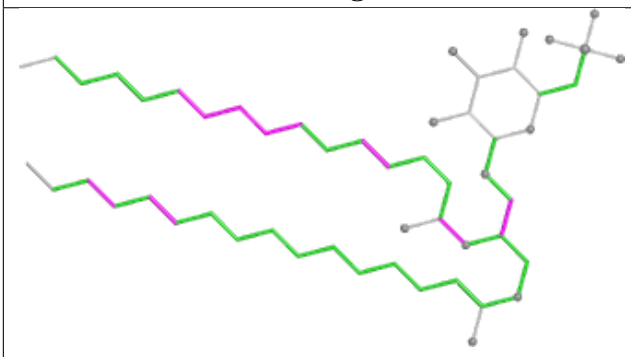
Ligand SQD A 412



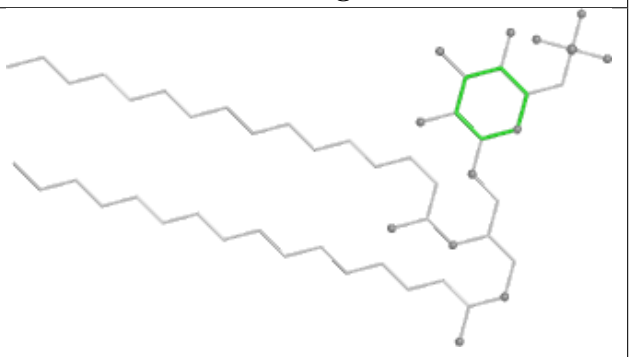
Bond lengths



Bond angles

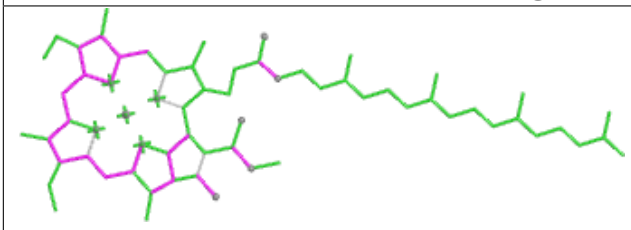


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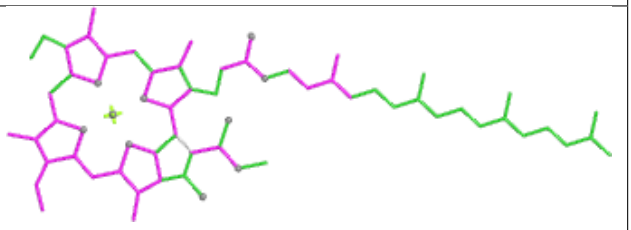


Rings

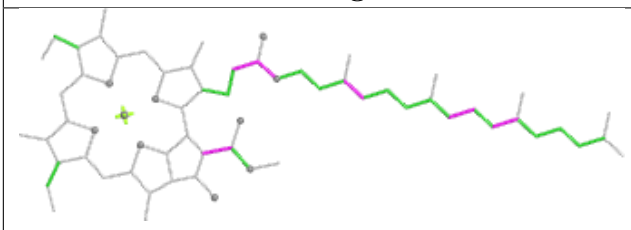
Ligand CLA c 911



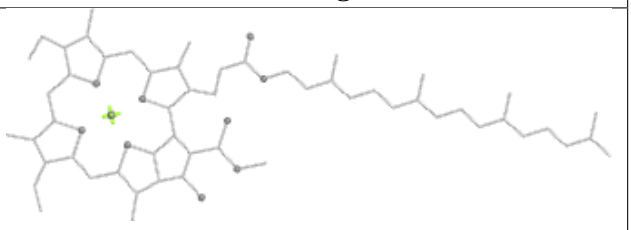
Bond lengths



Bond angles

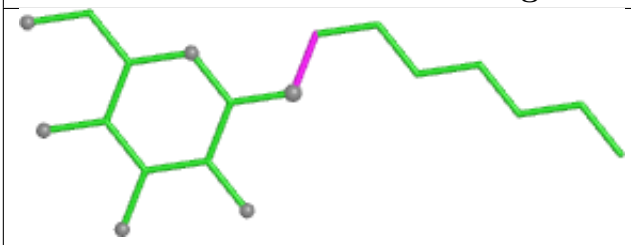


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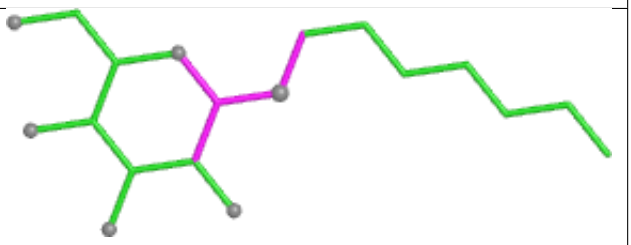


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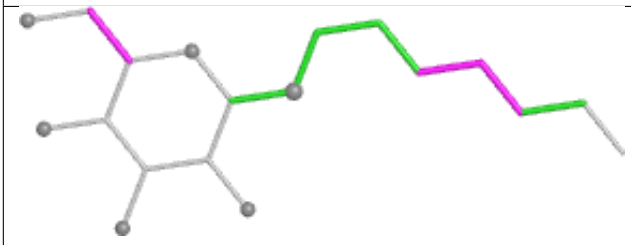
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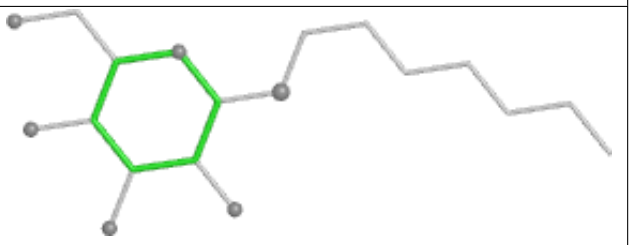
Bond lengths



Bond angles

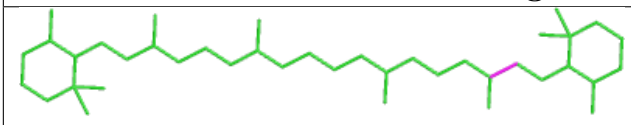


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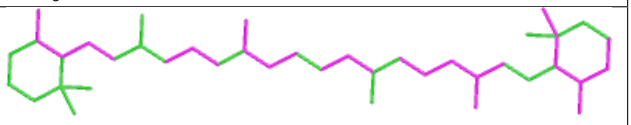


Rings

Ligand BCR y 101



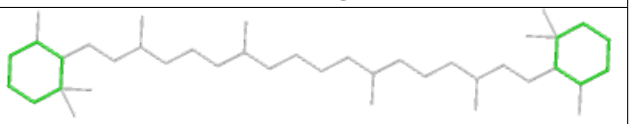
Bond lengths



Bond angles

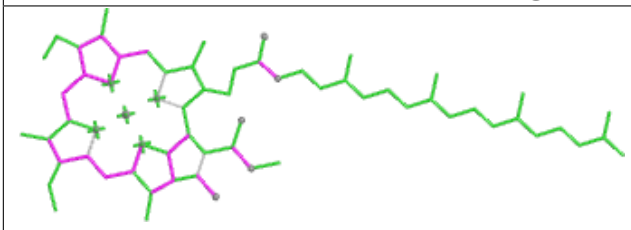


Torsions

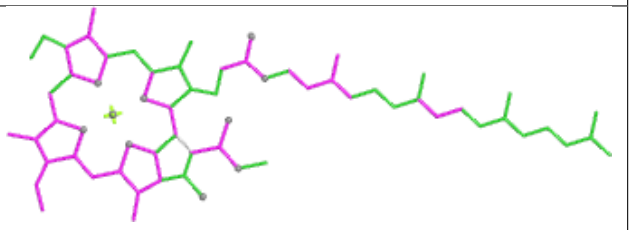


Rings

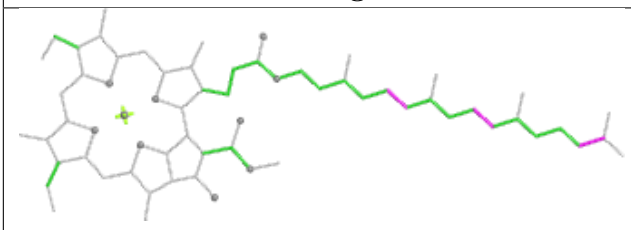
Ligand CLA b 619



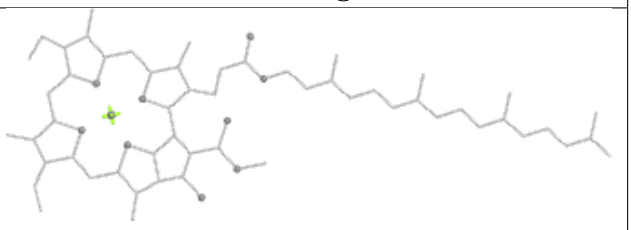
Bond lengths



Bond angles

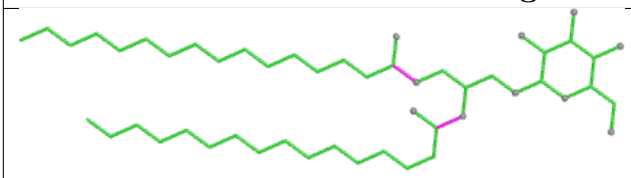


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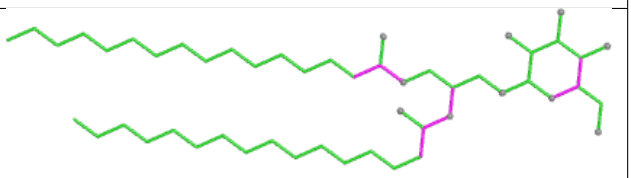


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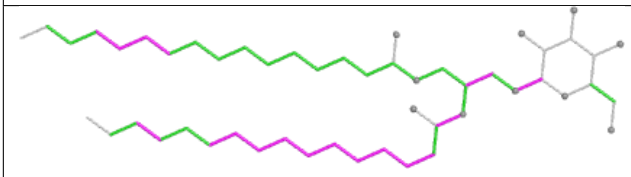
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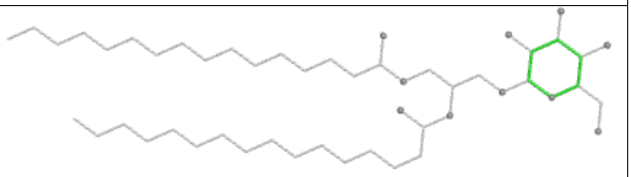
Bond lengths



Bond angles

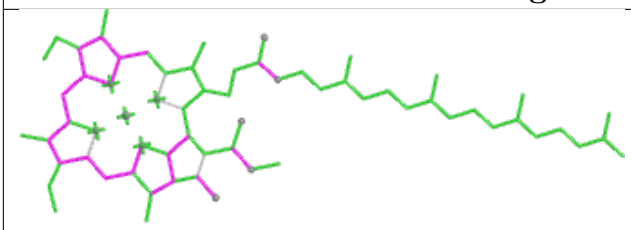


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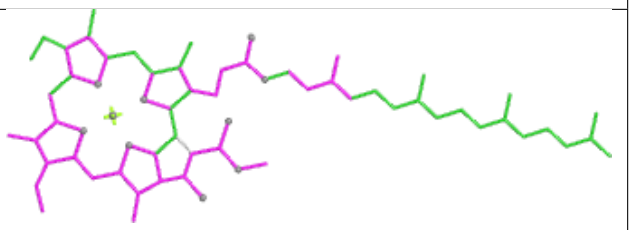


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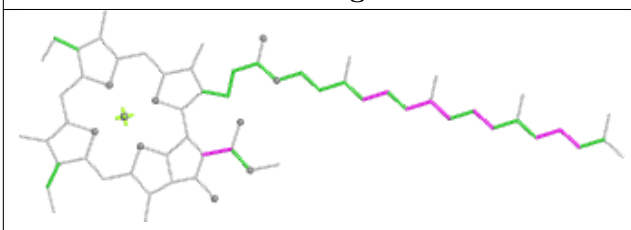
Ligand CLA c 907



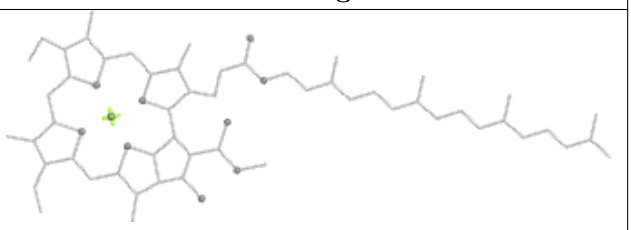
Bond lengths



Bond angles

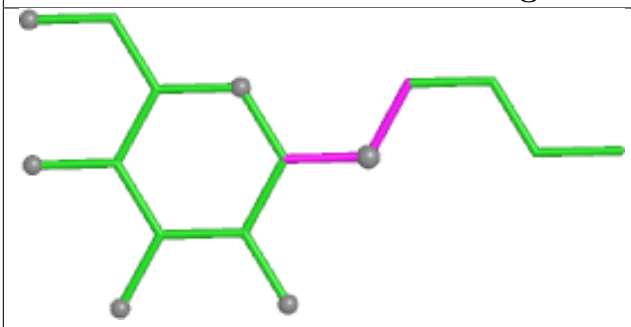


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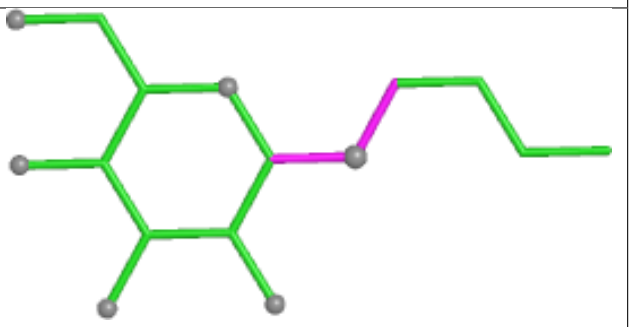


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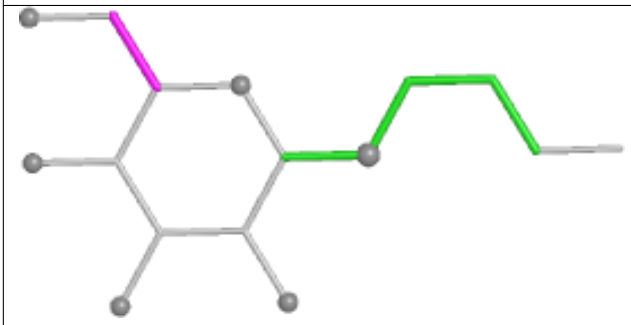
Ligand HTG D 411



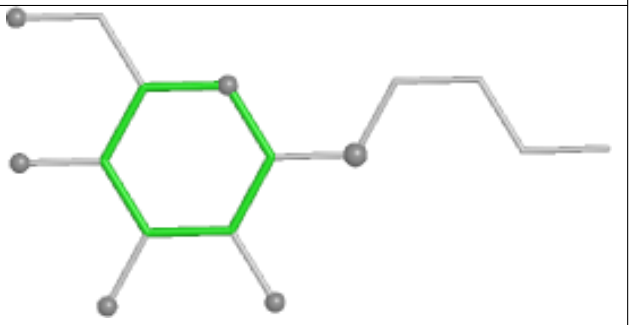
Bond lengths



Bond angles

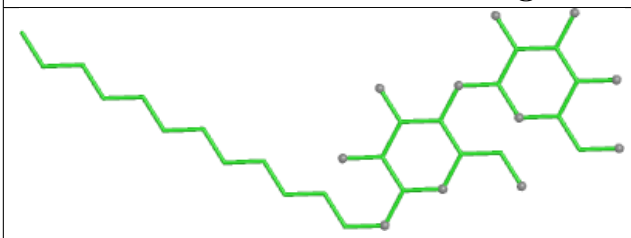


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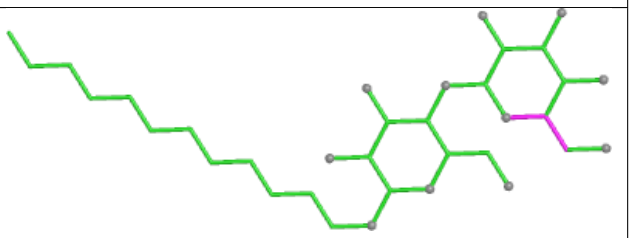


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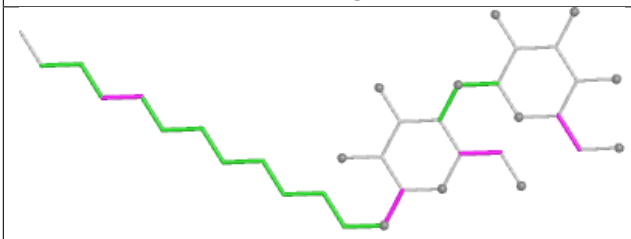
Ligand LMT M 101



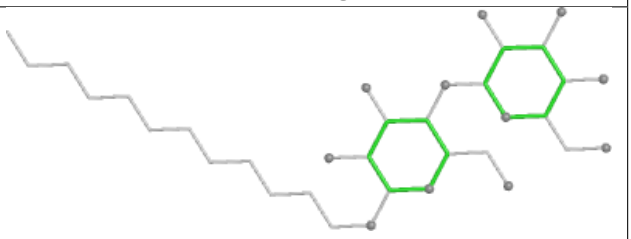
Bond lengths



Bond angles

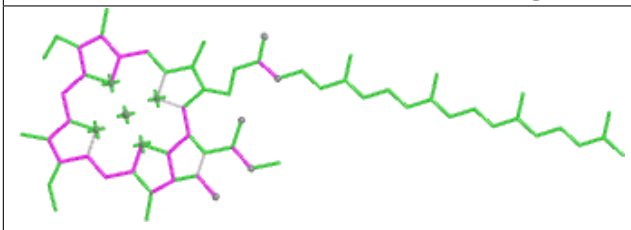


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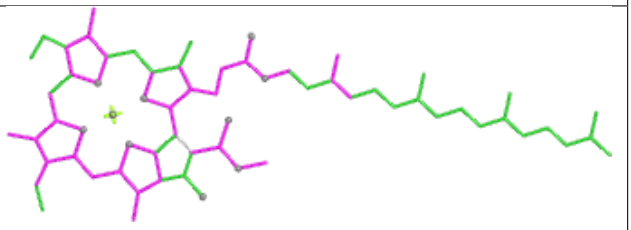


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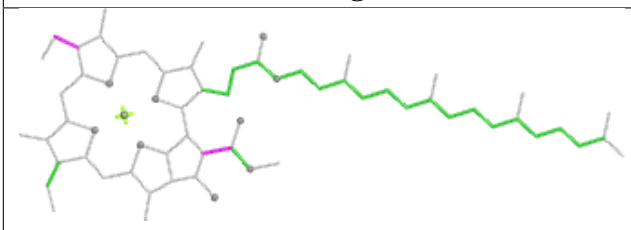
Ligand CLA b 611



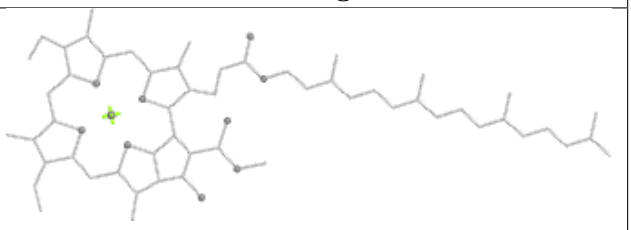
Bond lengths



Bond angles

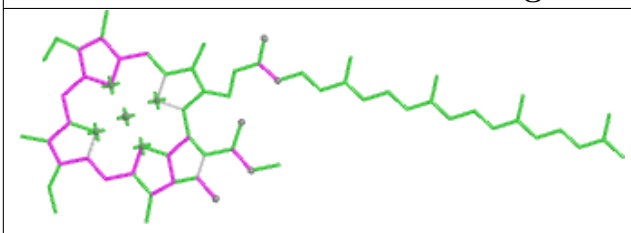


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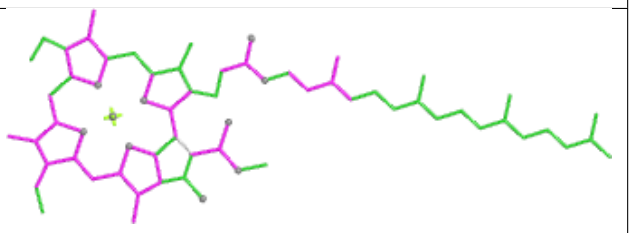


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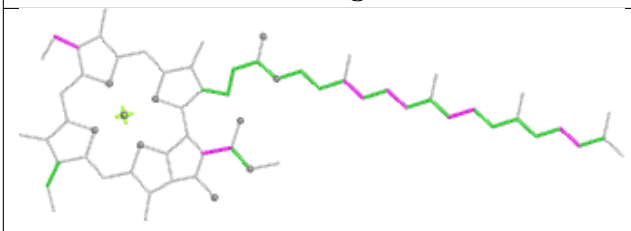
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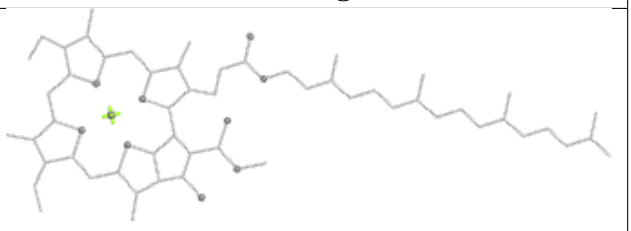
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Bond angles

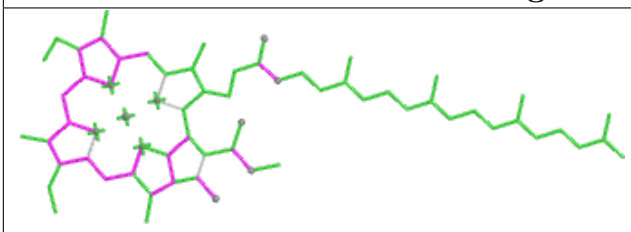


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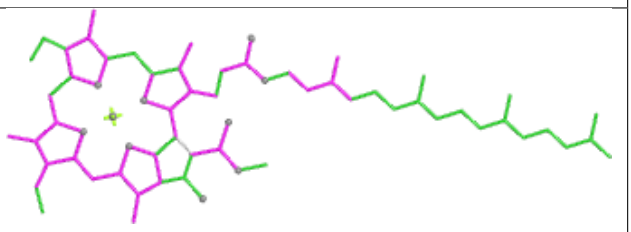


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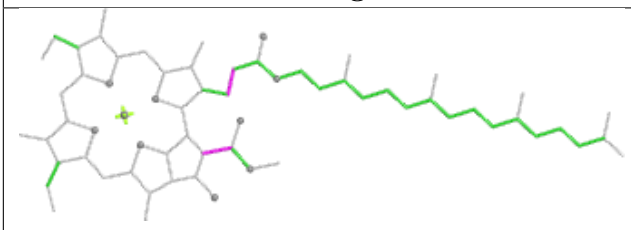
Ligand CLA b 606



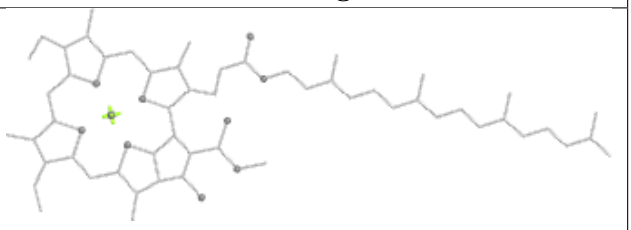
Bond lengths



Bond angles

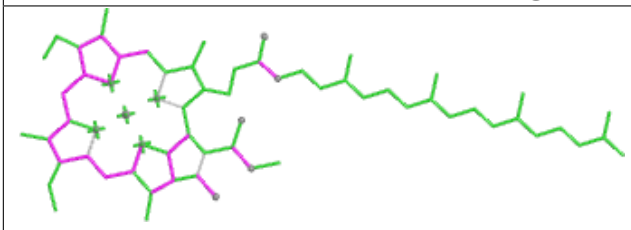


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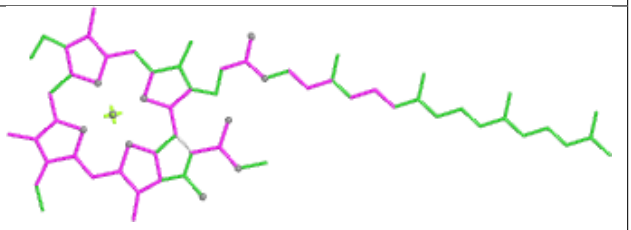


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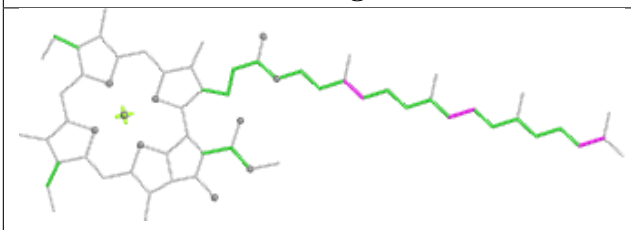
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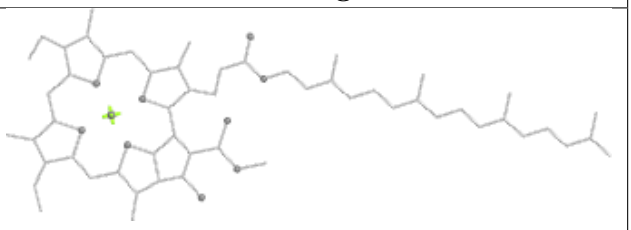
Bond lengths



Bond angles



Torsions

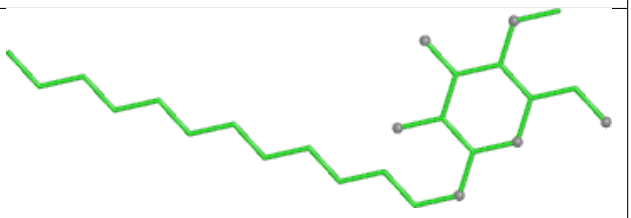


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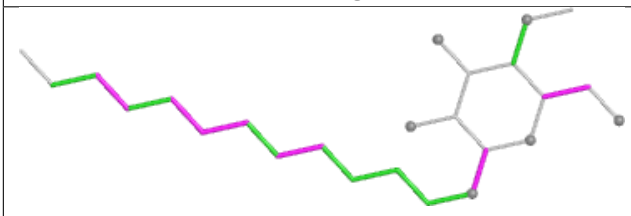
Ligand LMT B 636



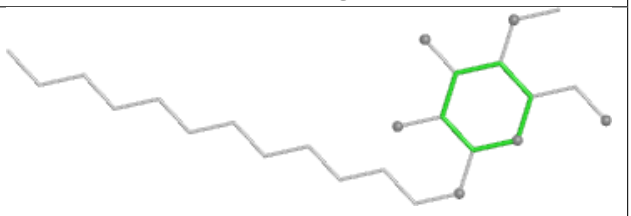
Bond lengths



Bond angles

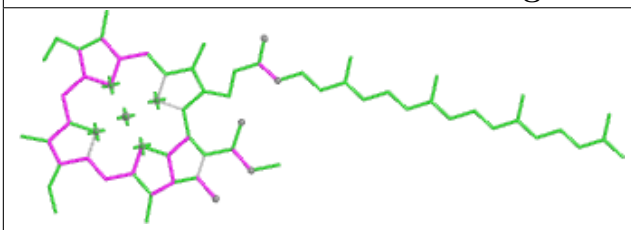


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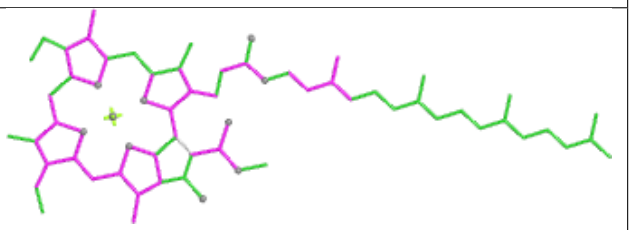


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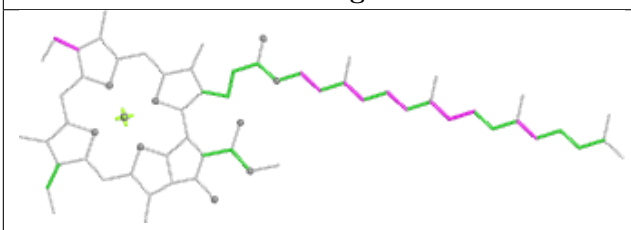
Ligand CLA D 402



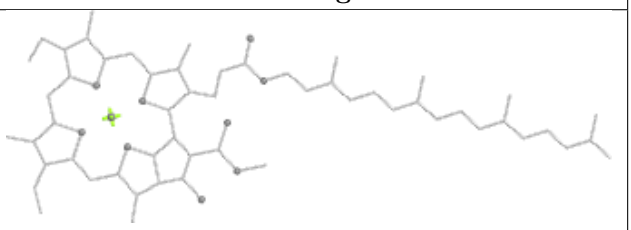
Bond lengths



Bond angles

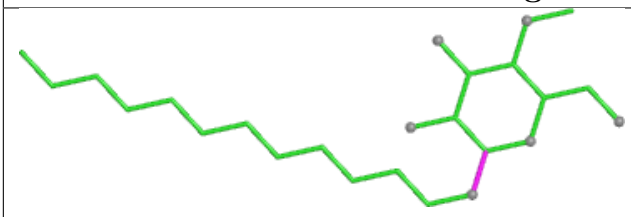


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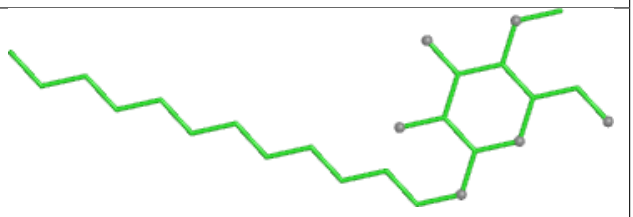


Rings

Ligand LMT b 625



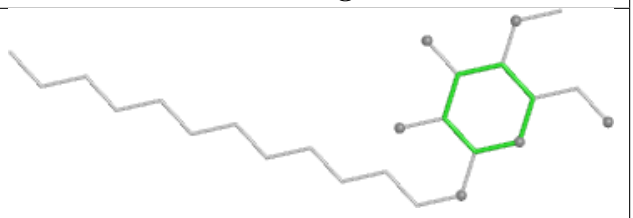
Bond lengths



Bond angles

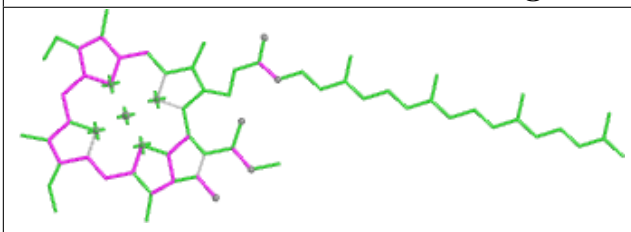


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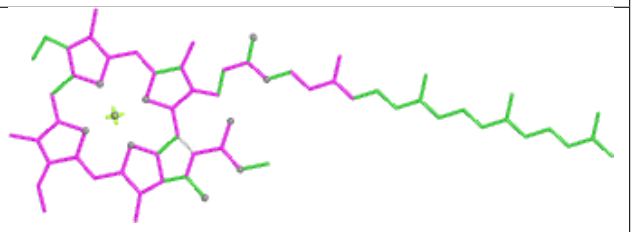


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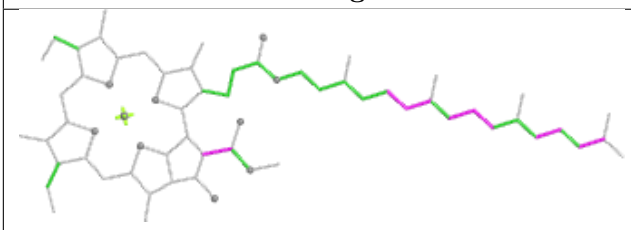
Ligand CLA C 507



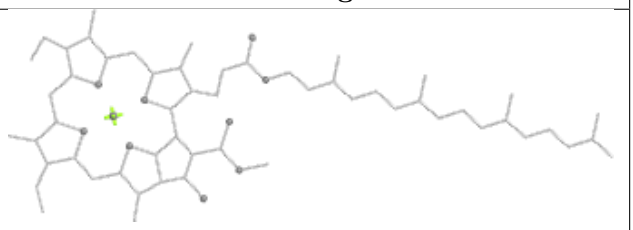
Bond lengths



Bond angles

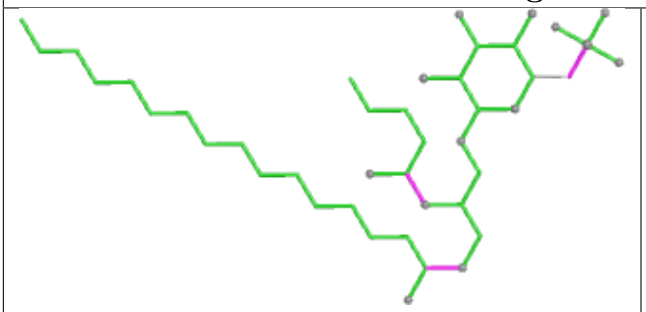


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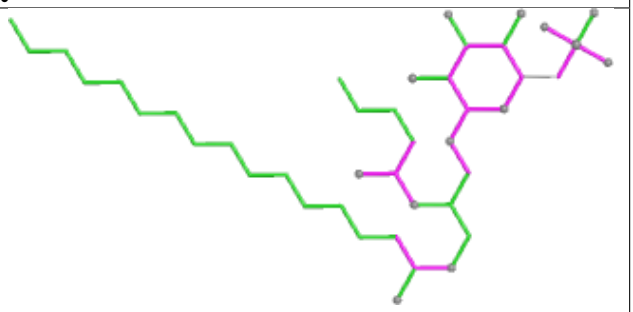


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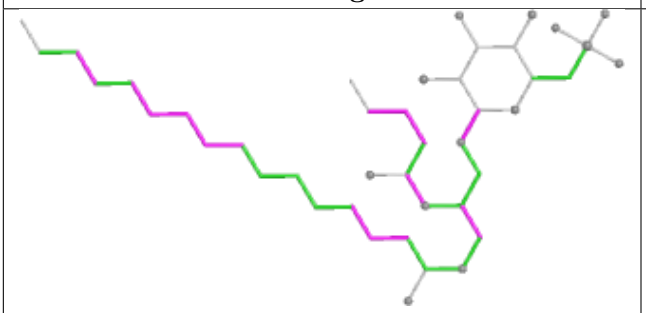
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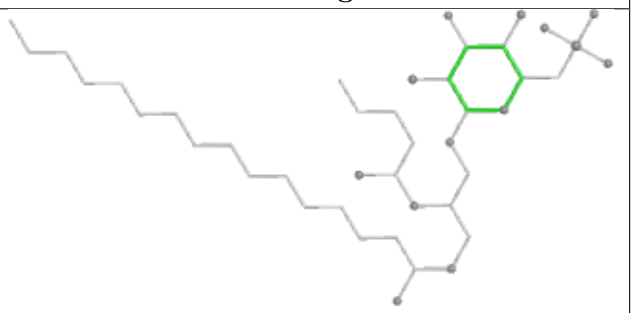
Bond lengths



Bond angles

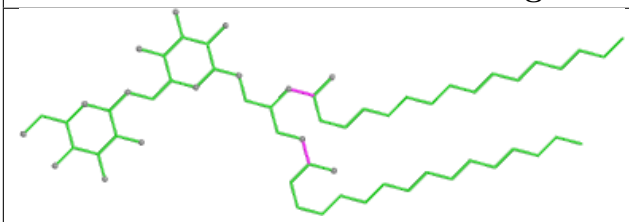


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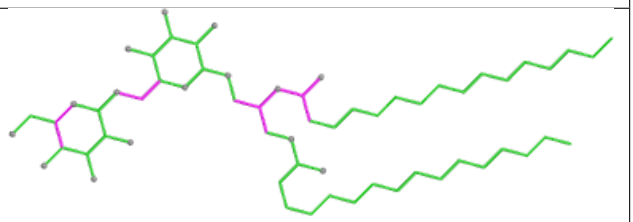


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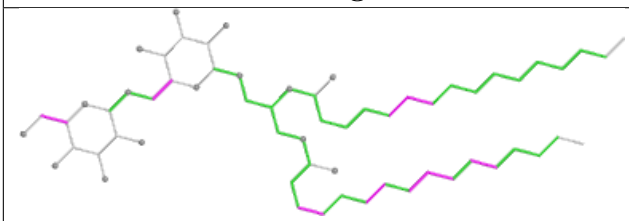
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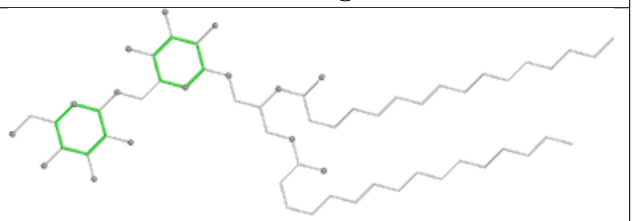
Bond lengths



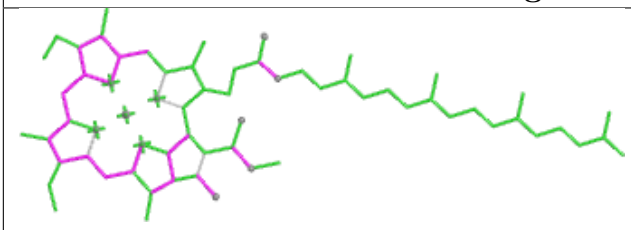
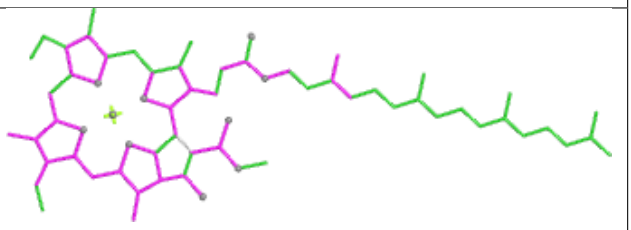
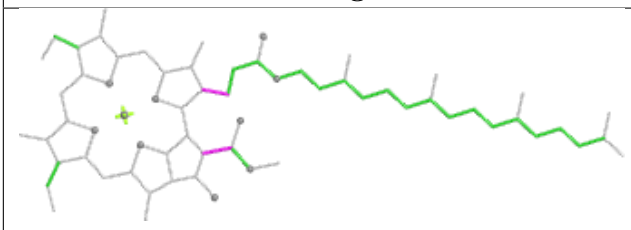
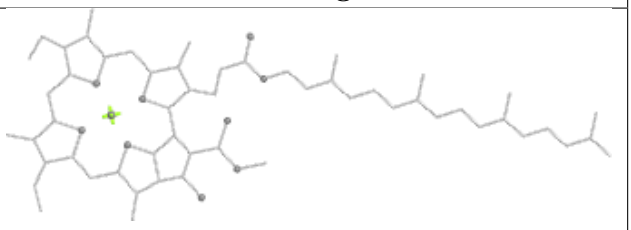
Bond angles

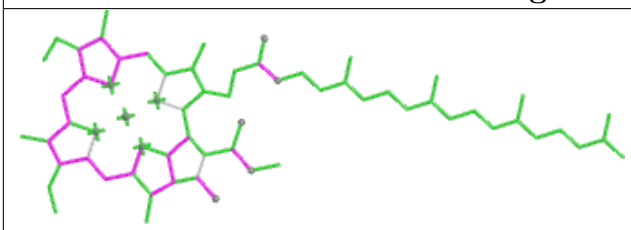
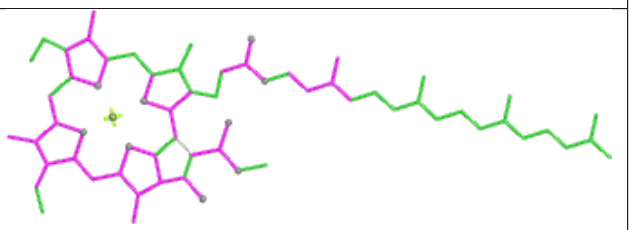
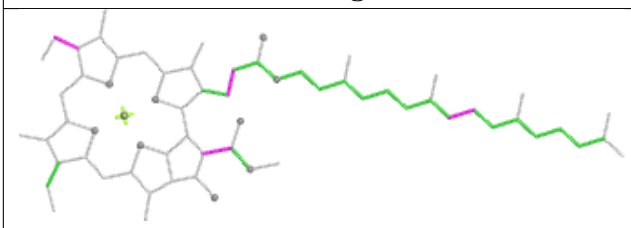
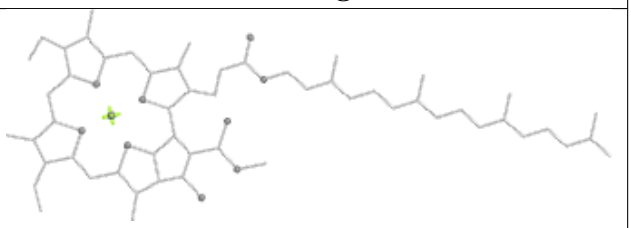


Torsions

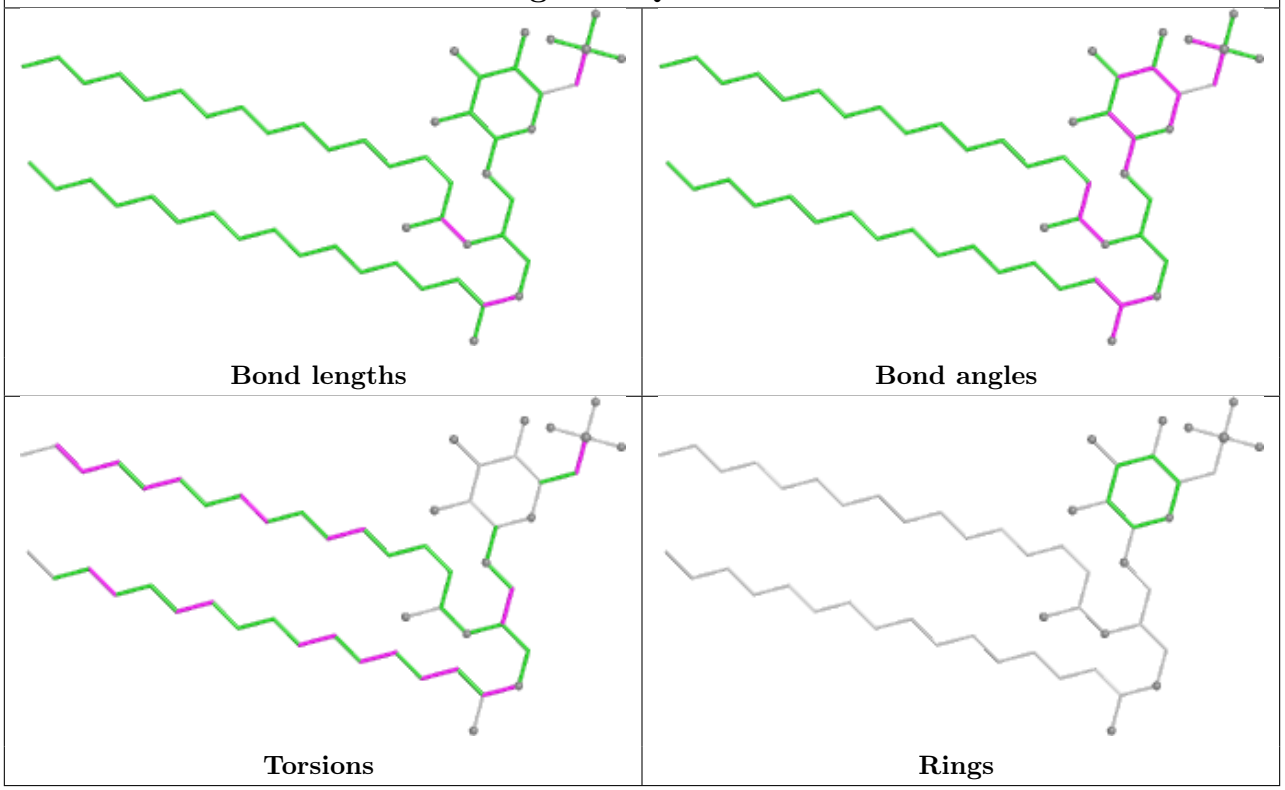


Rings

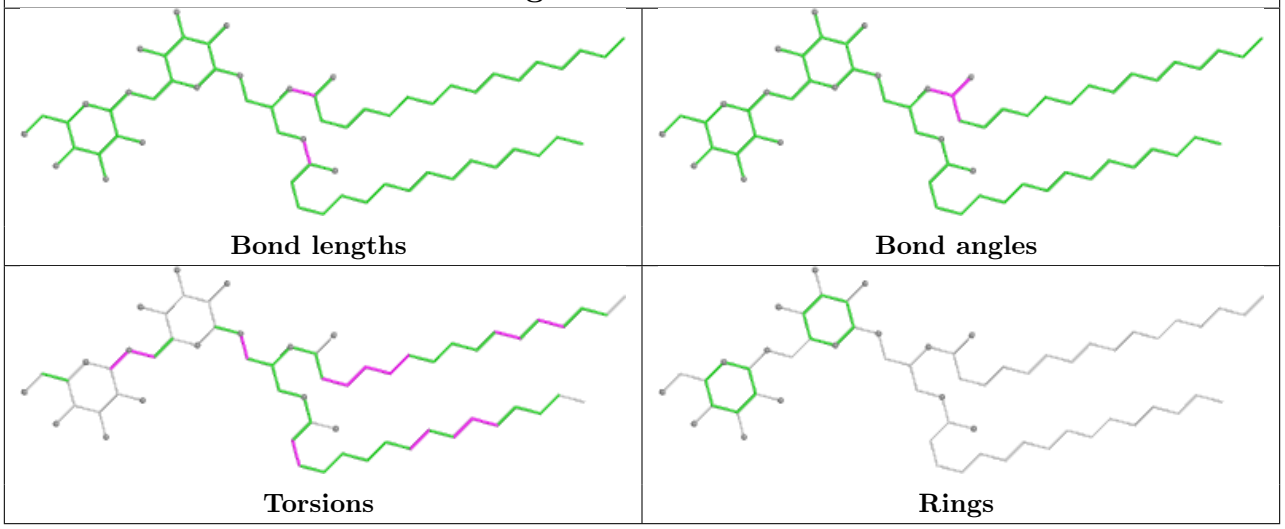
Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 904	
	
Bond lengths	Bond angles
	
Torsions	Rings

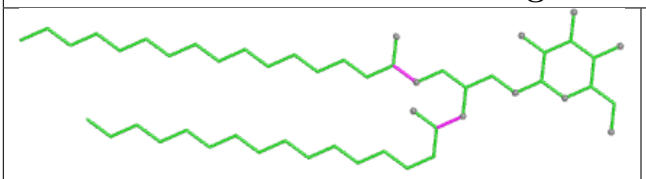
Ligand SQD a 402



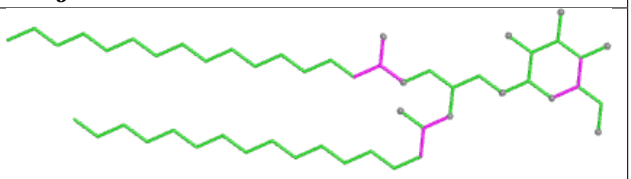
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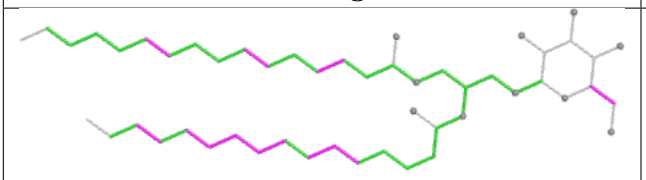
Ligand LMG j 101



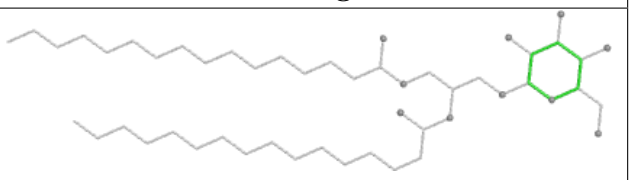
Bond lengths



Bond angles

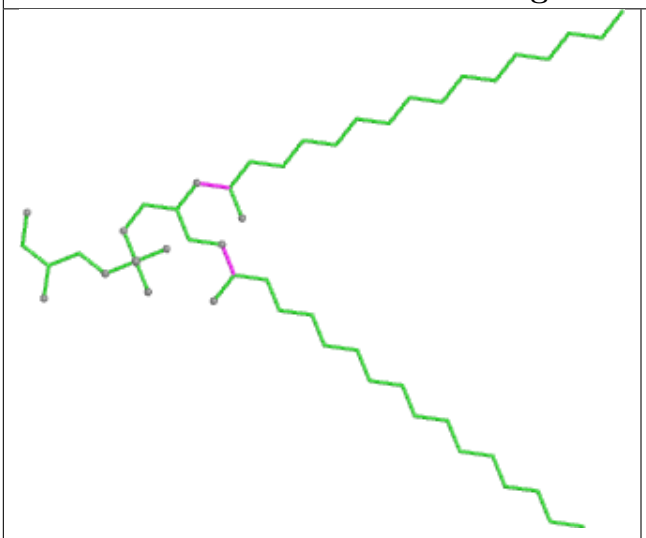


Torsions

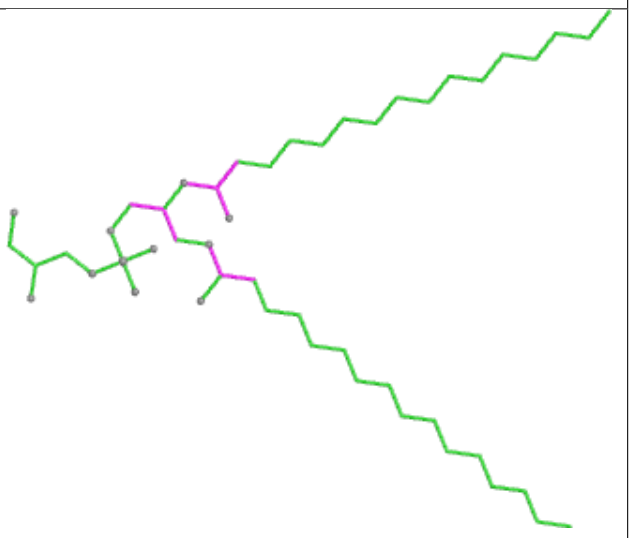


Rings

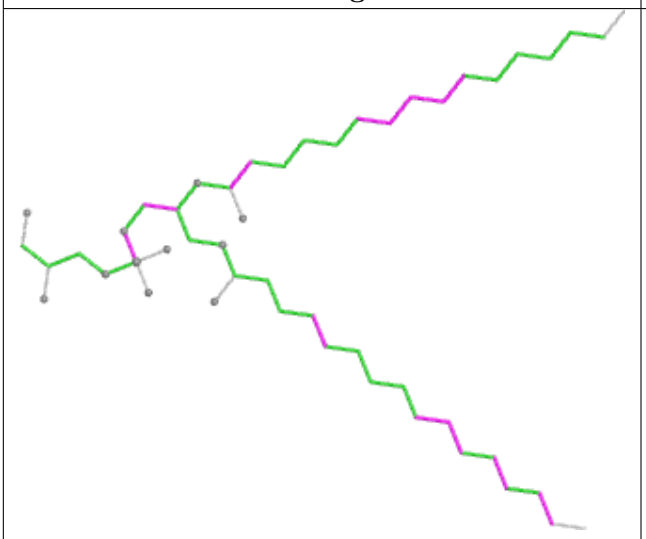
Ligand LHG l 101



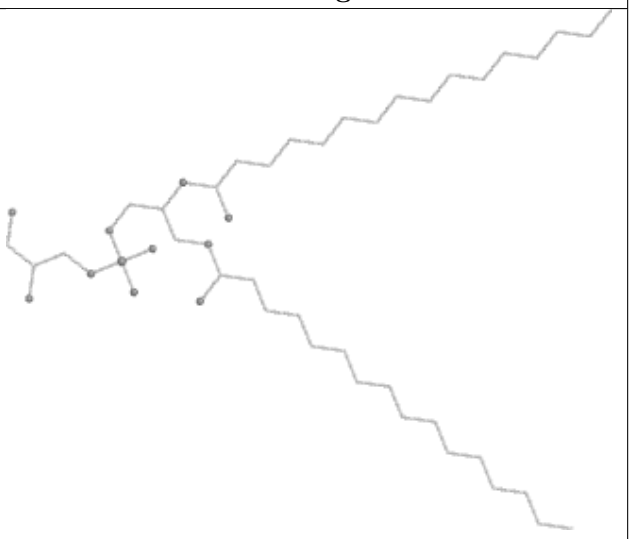
Bond lengths



Bond angles

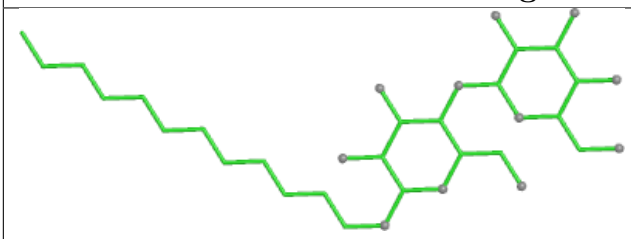


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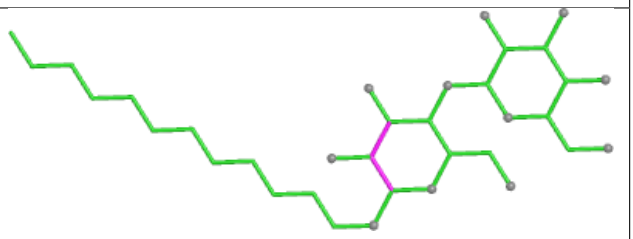


Rings

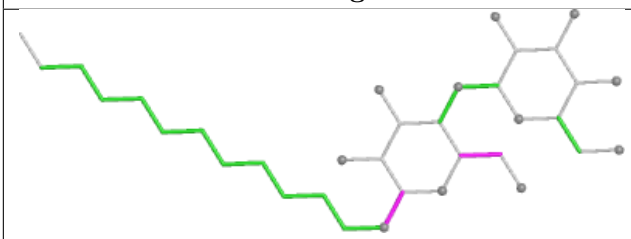
Ligand LMT m 103



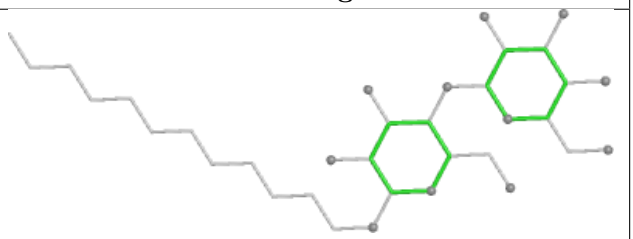
Bond lengths



Bond angles

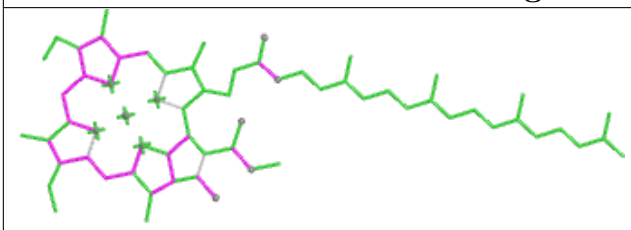


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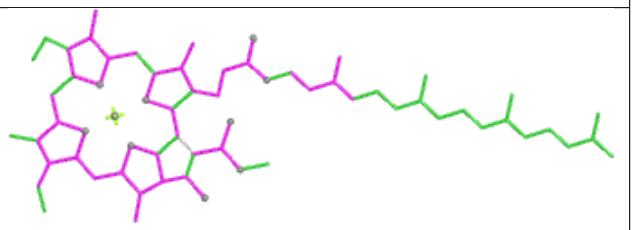


Rings

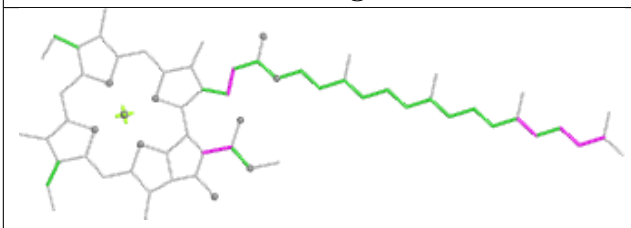
Ligand CLA B 611



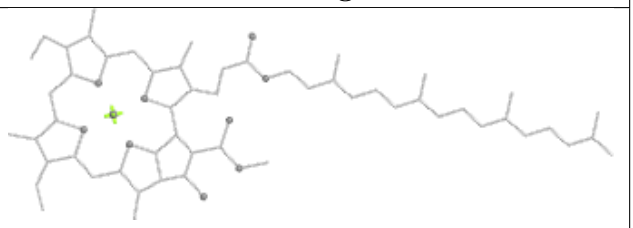
Bond lengths



Bond angles



Torsions

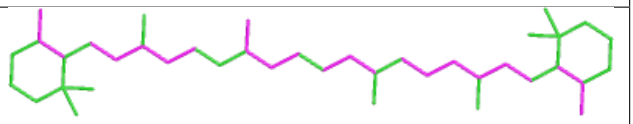


Rings

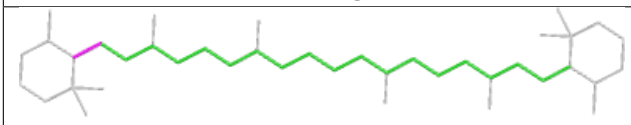
Ligand BCR k 101



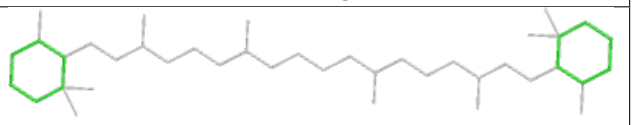
Bond lengths



Bond angles



Torsions

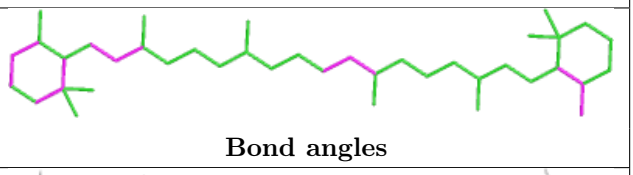


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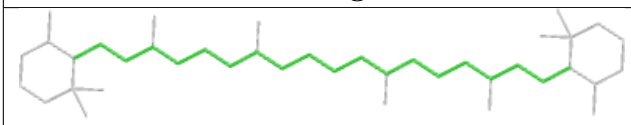
Ligand BCR a 410



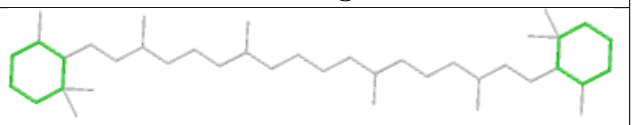
Bond lengths



Bond angles

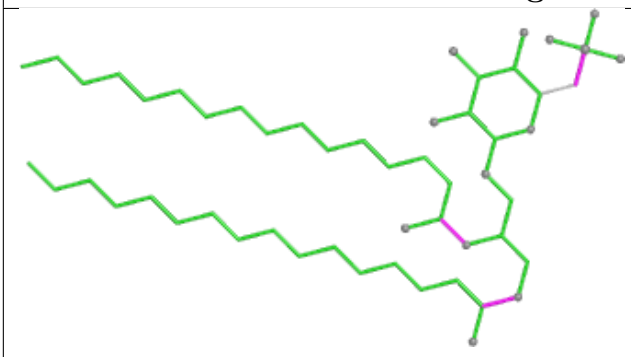


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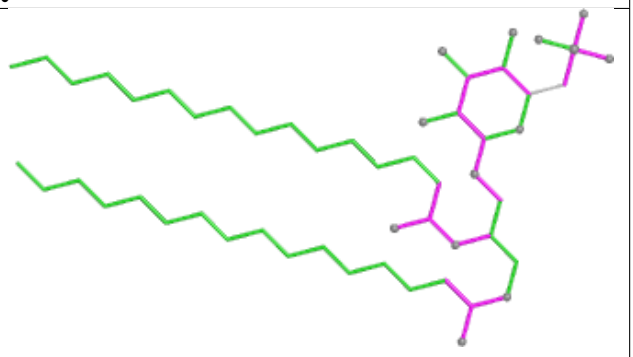


Rings

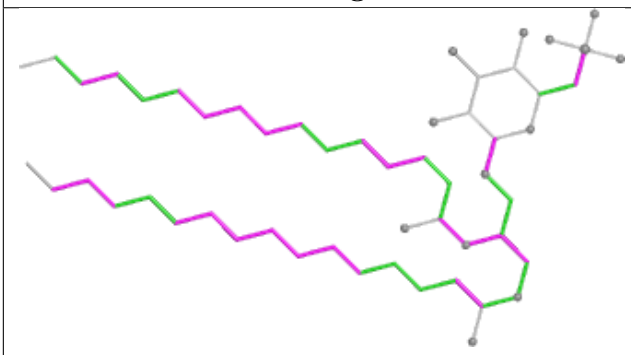
Ligand SQD L 102



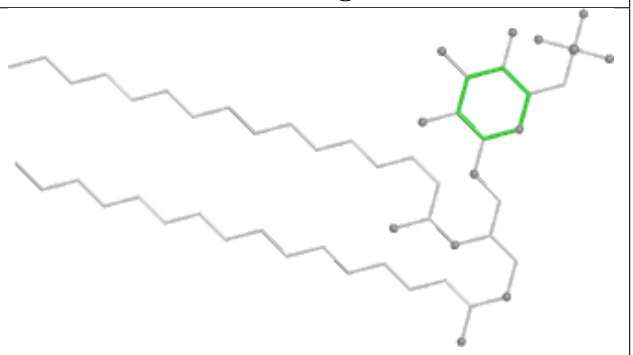
Bond lengths



Bond angles

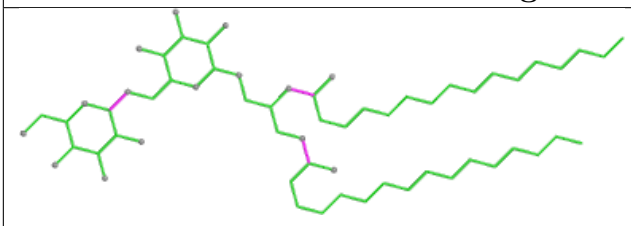


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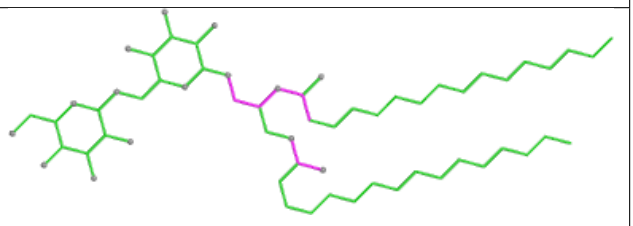


Rings

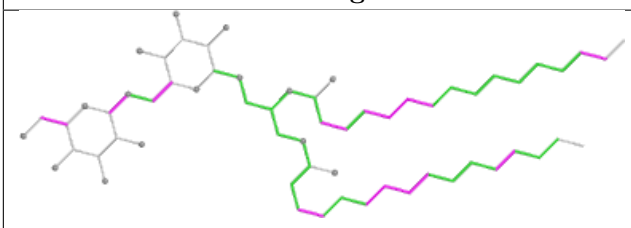
Ligand DGD C 517



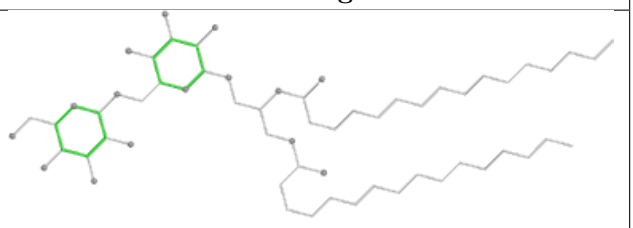
Bond lengths



Bond angles

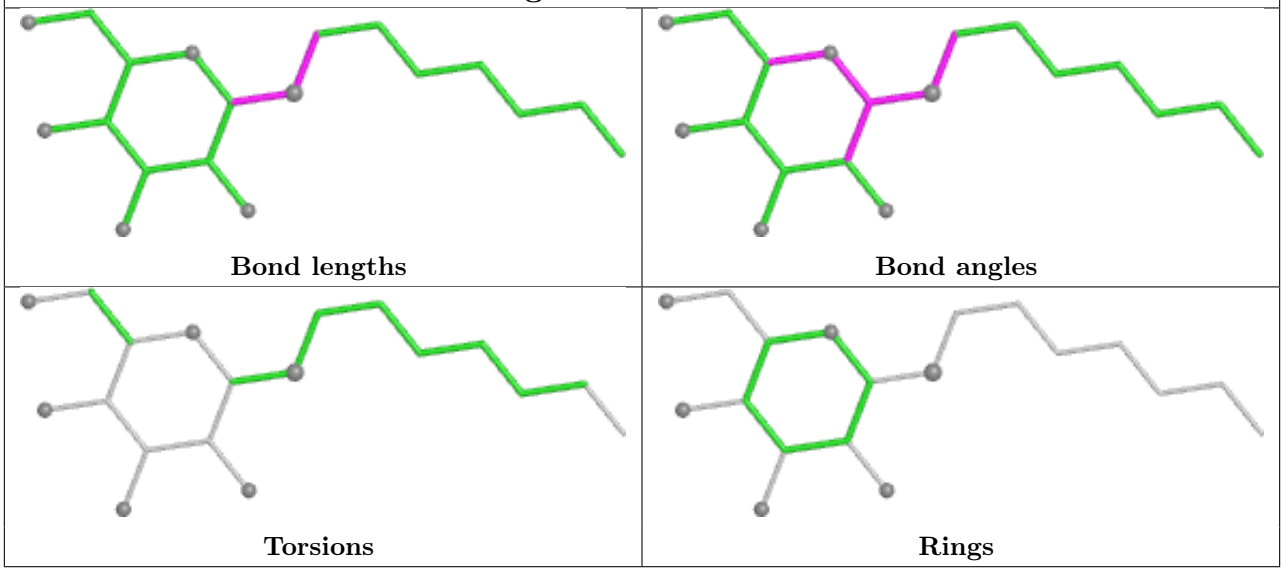


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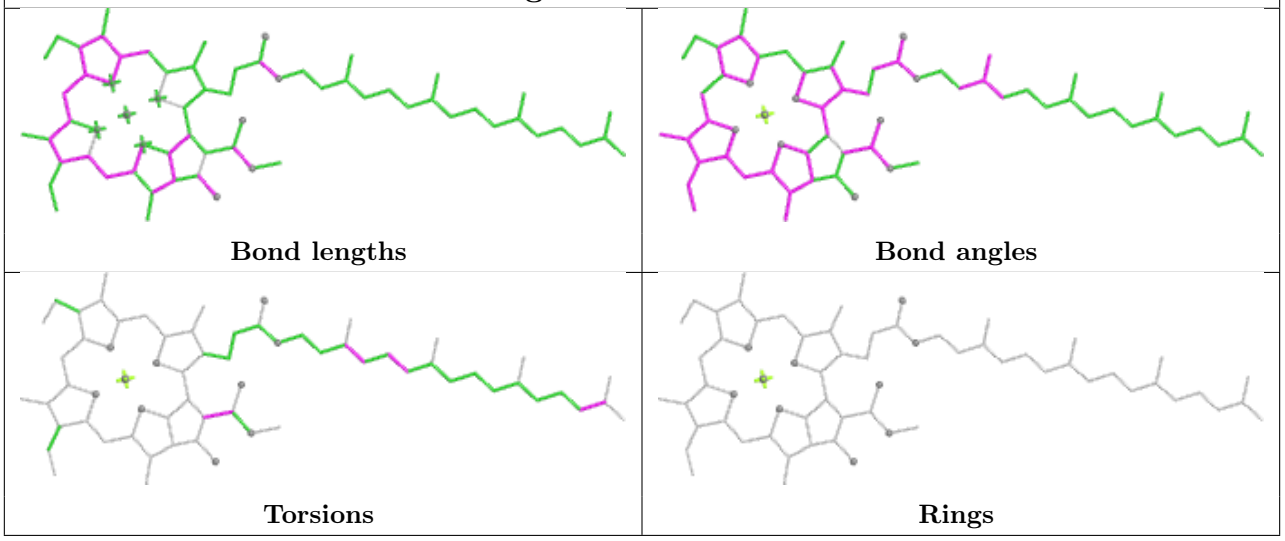


Rings

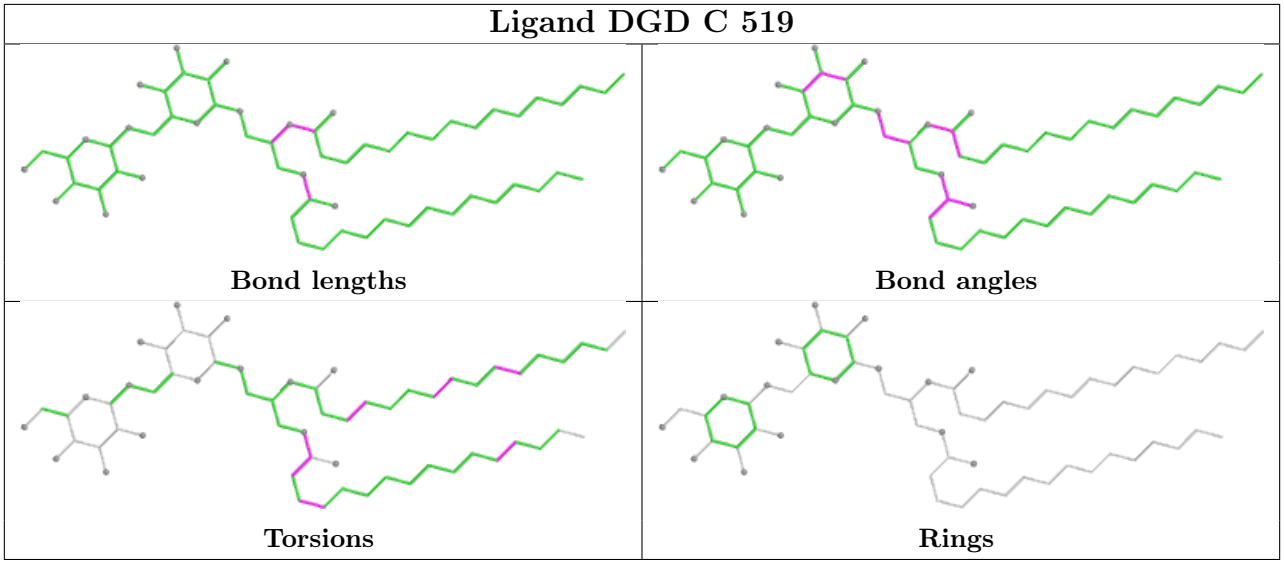
Ligand HTG b 603



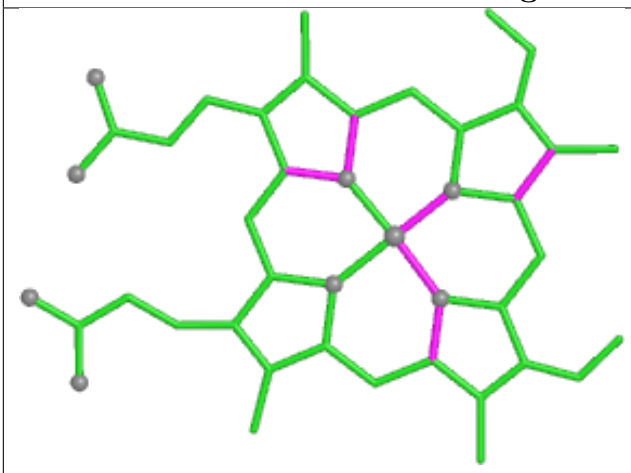
Ligand CLA B 604



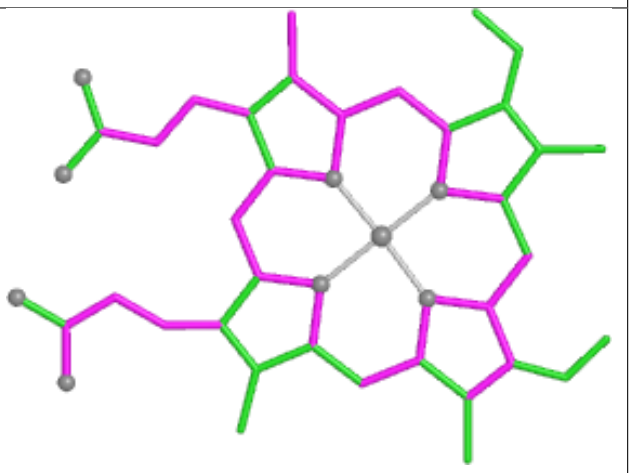
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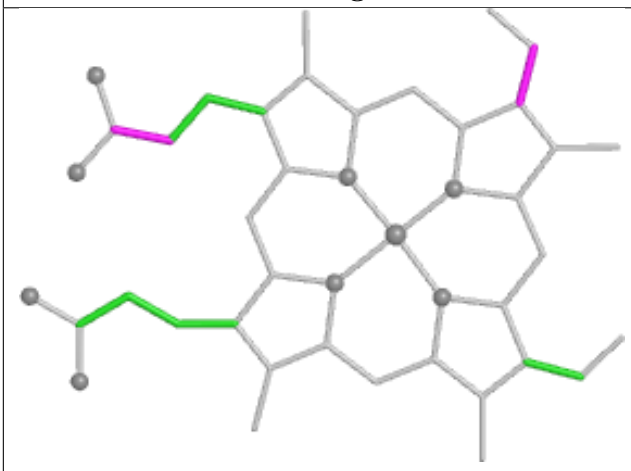
Ligand HEM E 103



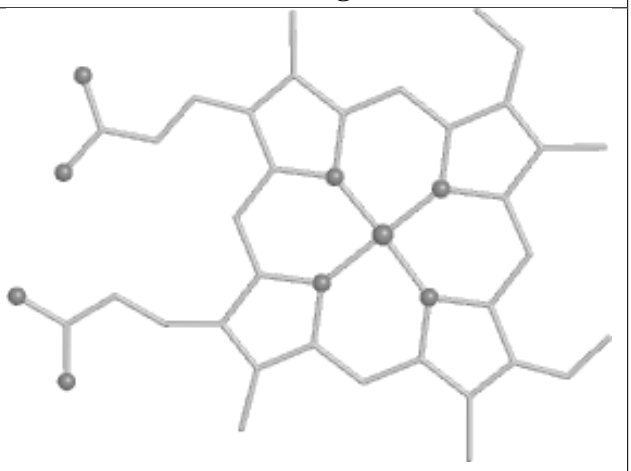
Bond lengths



Bond angles

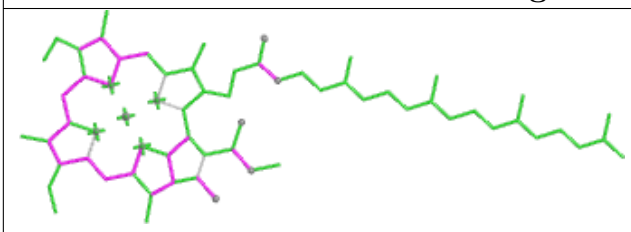


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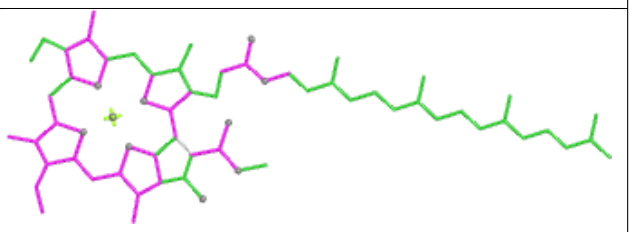


Rings

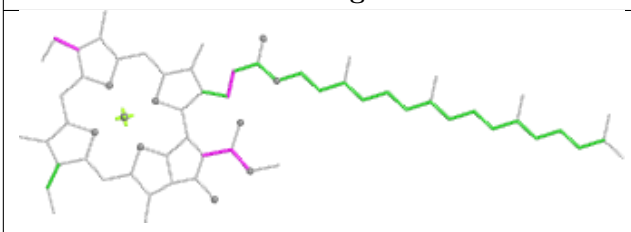
Ligand CLA c 902



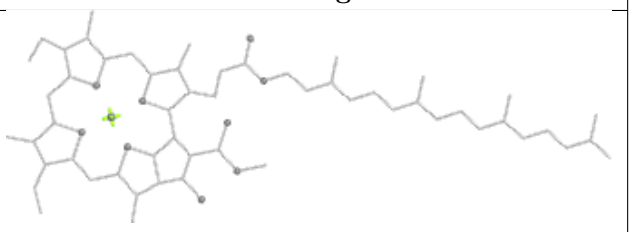
Bond lengths



Bond angles

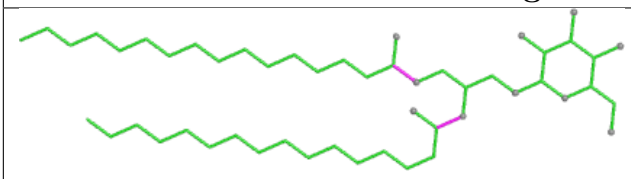


Torsions

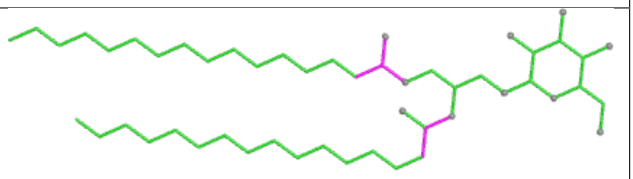


Rings

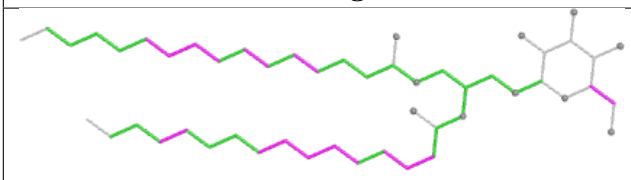
Ligand LMG J 101



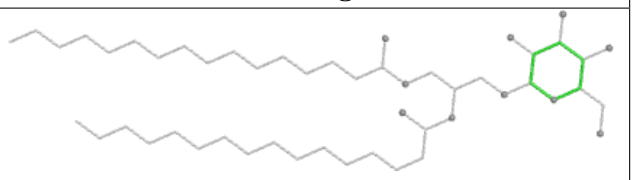
Bond lengths



Bond angles

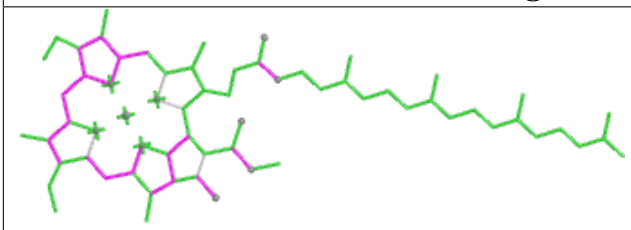


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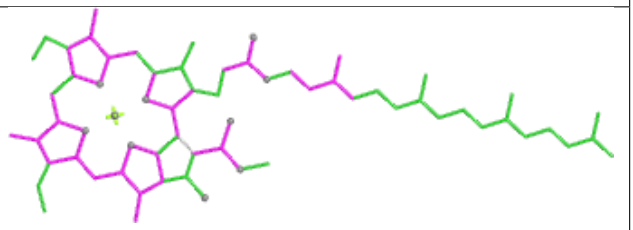


Rings

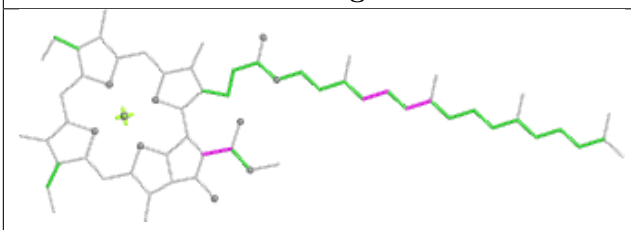
Ligand CLA B 605



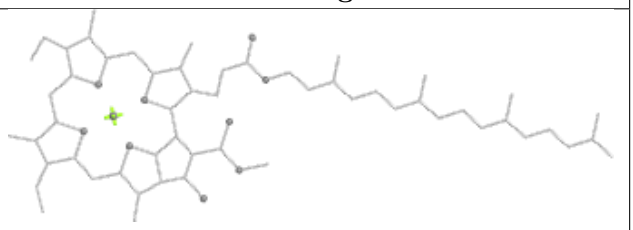
Bond lengths



Bond angles

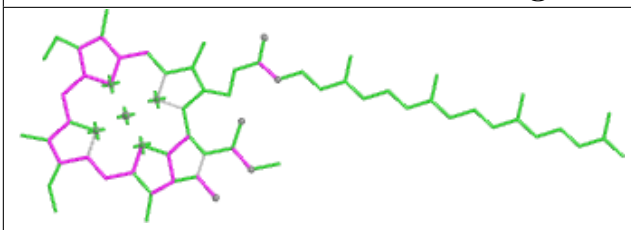


Torsions

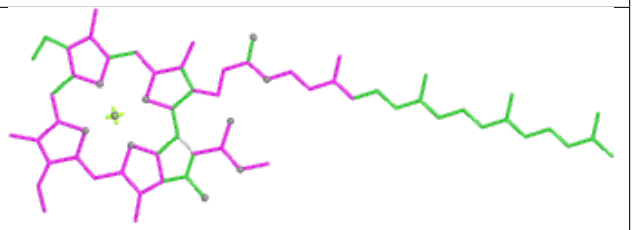


Rings

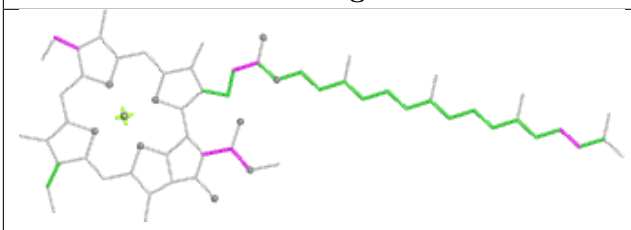
Ligand CLA c 913



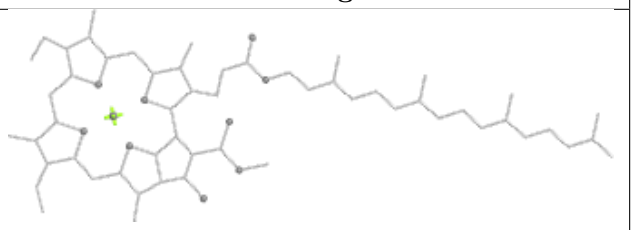
Bond lengths



Bond angles

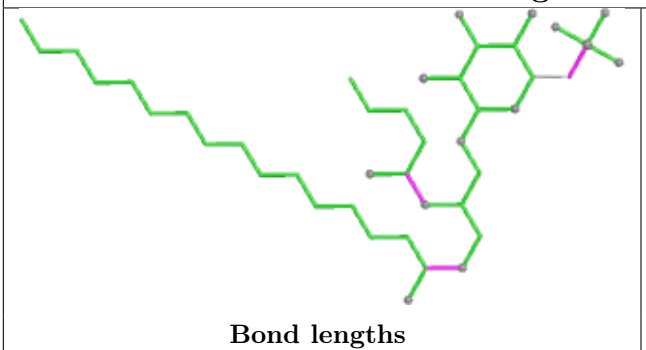


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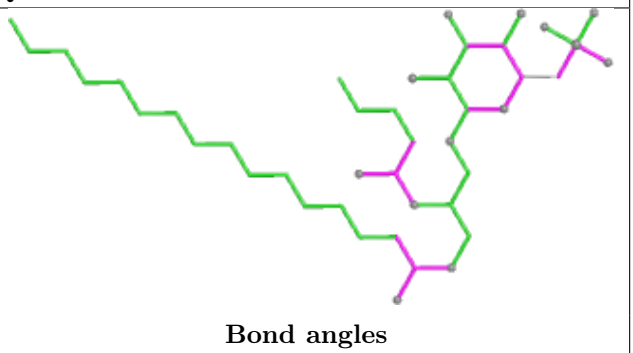


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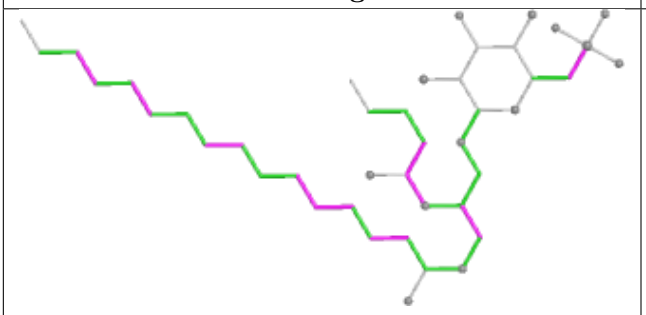
Ligand SQD f 102



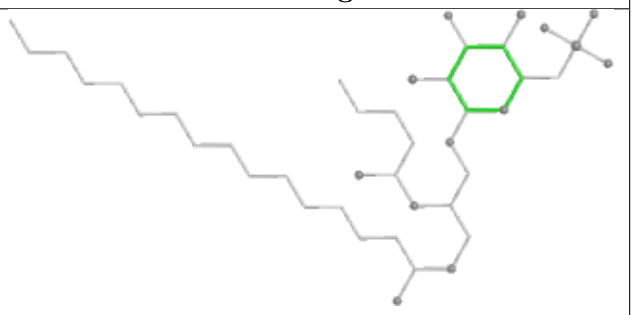
Bond lengths



Bond angles

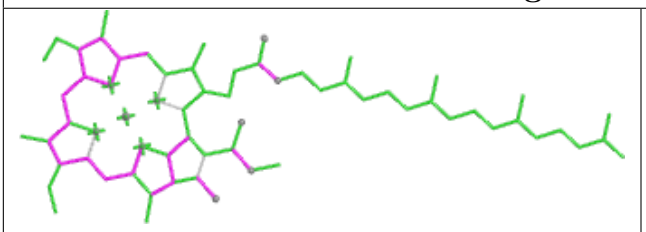


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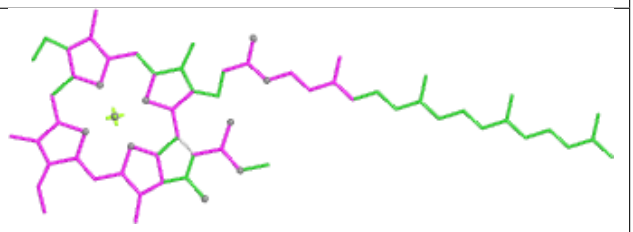


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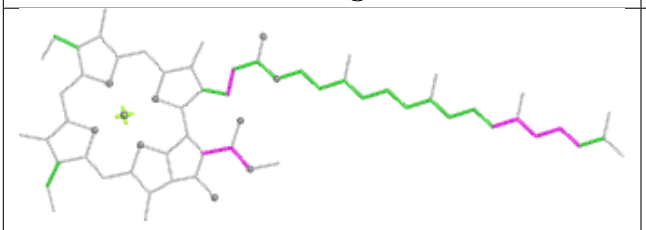
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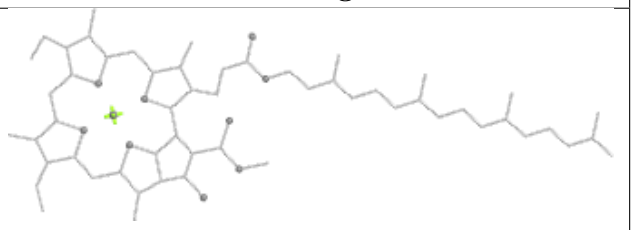
Bond lengths



Bond angles

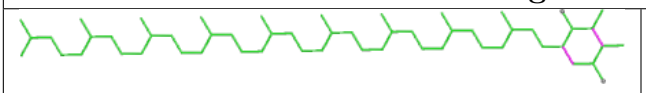


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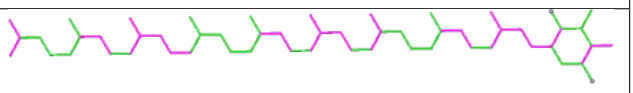


Rings

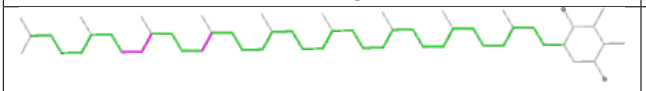
Ligand PL9 D 404



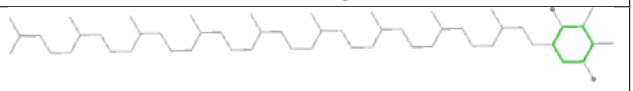
Bond lengths



Bond angles

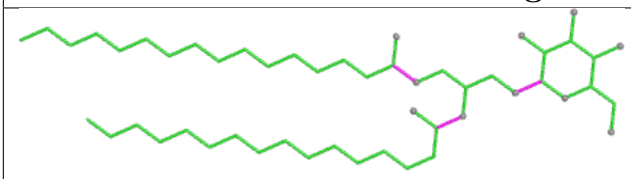


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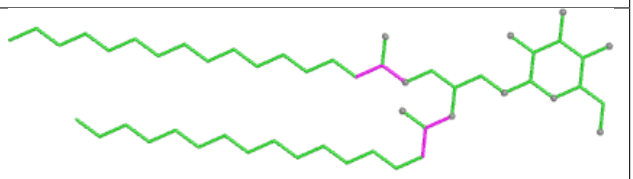


Rings

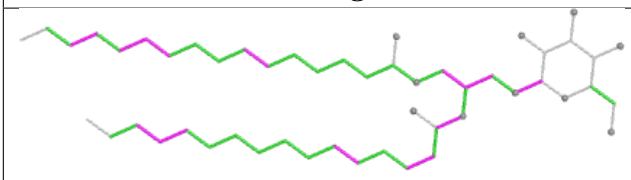
Ligand LMG c 919



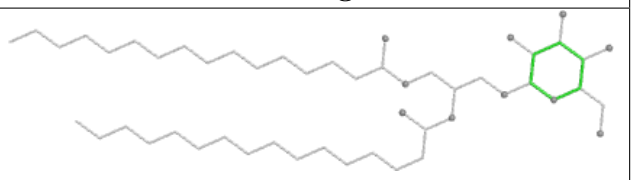
Bond lengths



Bond angles

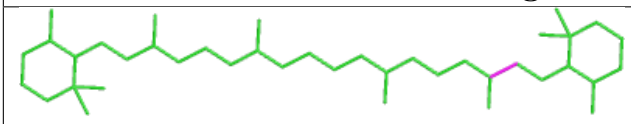


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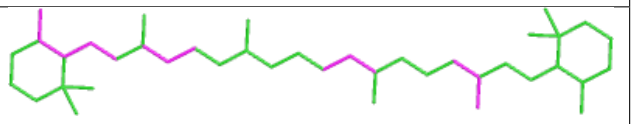


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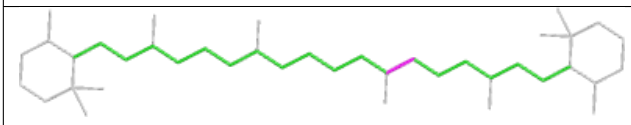
Ligand BCR A 411



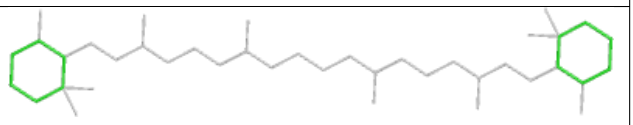
Bond lengths



Bond angles

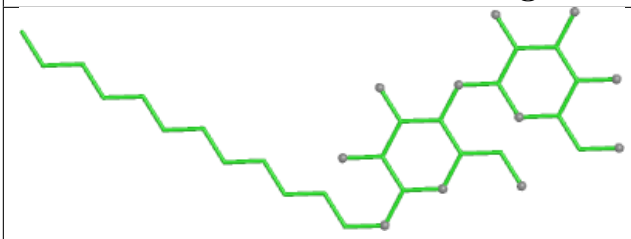


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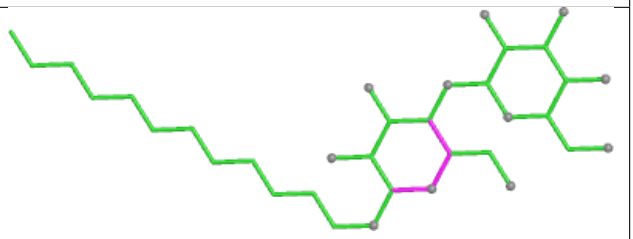


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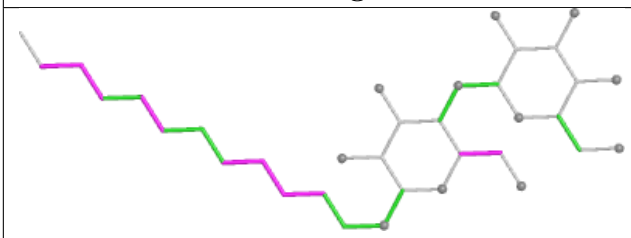
Ligand LMT m 104



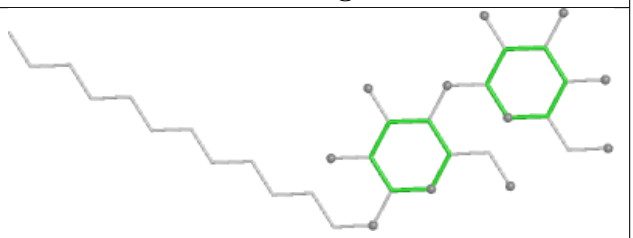
Bond lengths



Bond angles

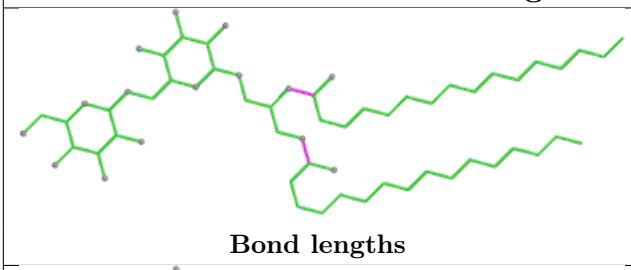


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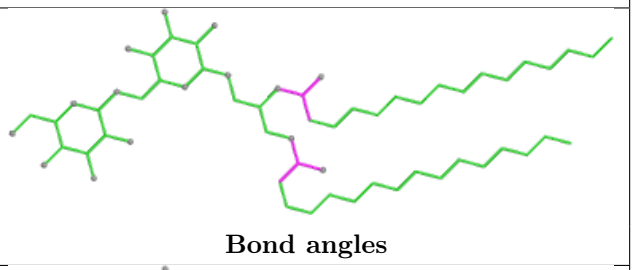


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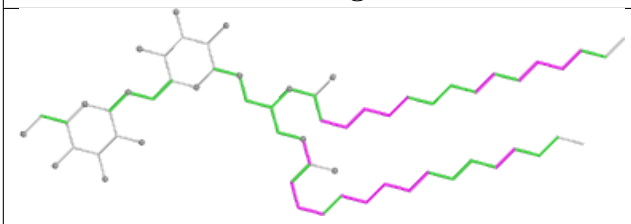
Ligand DGD c 918



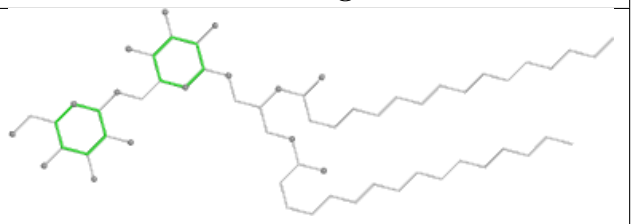
Bond lengths



Bond angles

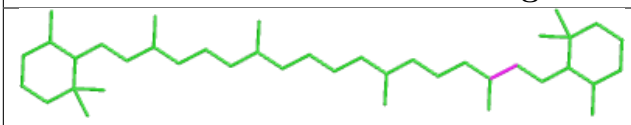


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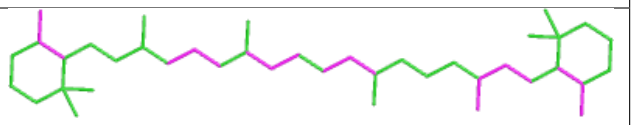


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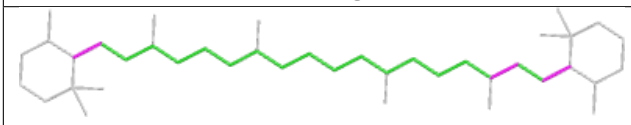
Ligand BCR K 102



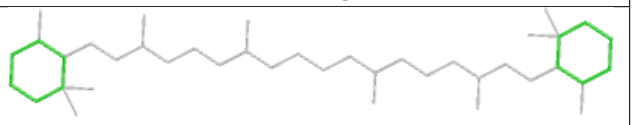
Bond lengths



Bond angles

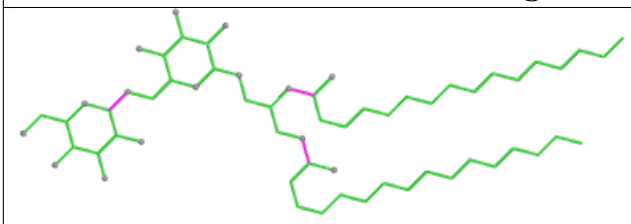


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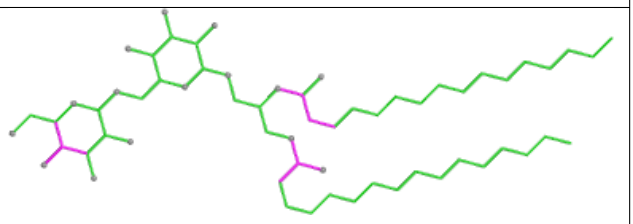


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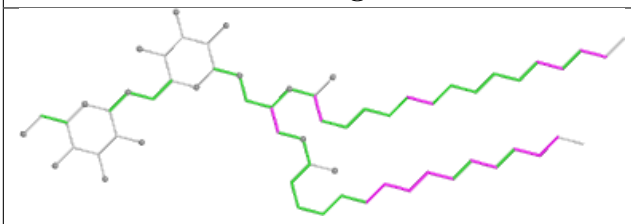
Ligand DGD h 102



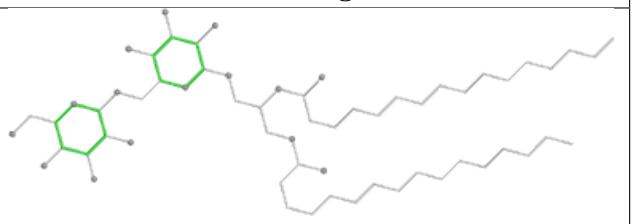
Bond lengths



Bond angles

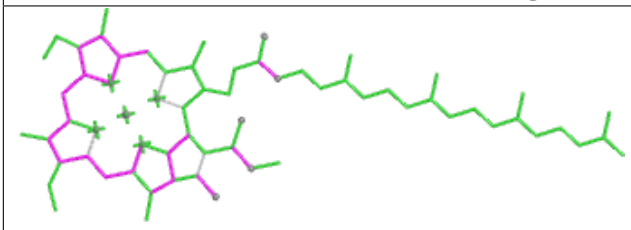


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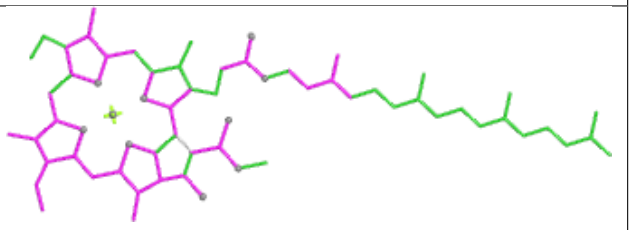


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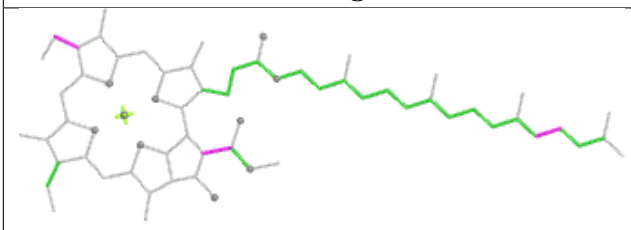
Ligand CLA C 503



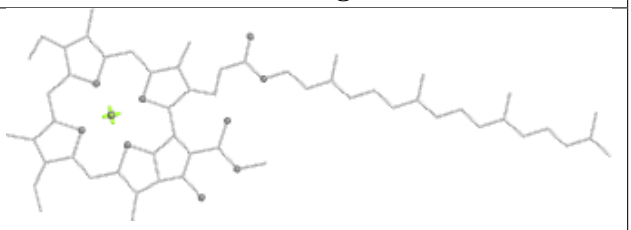
Bond lengths



Bond angles



Torsions

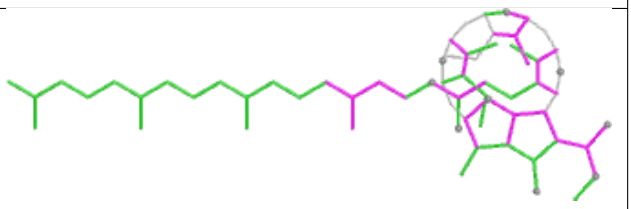


Rings

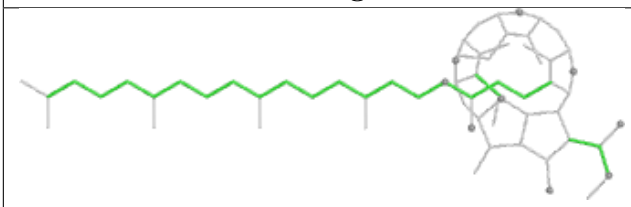
Ligand PHO A 409



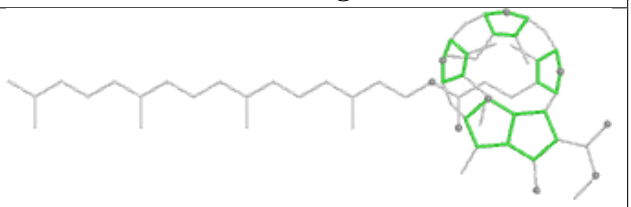
Bond lengths



Bond angles

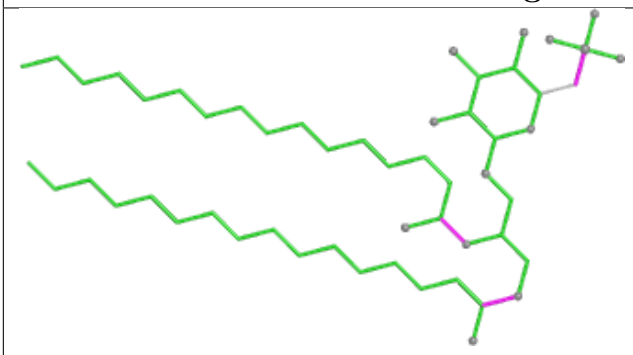


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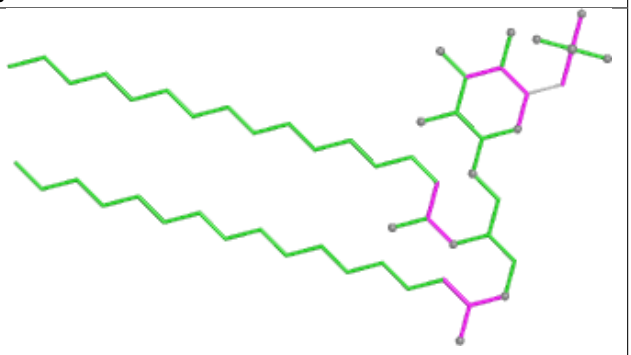


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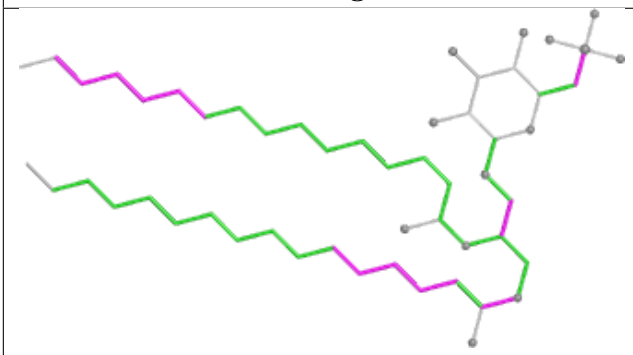
Ligand SQD A 416



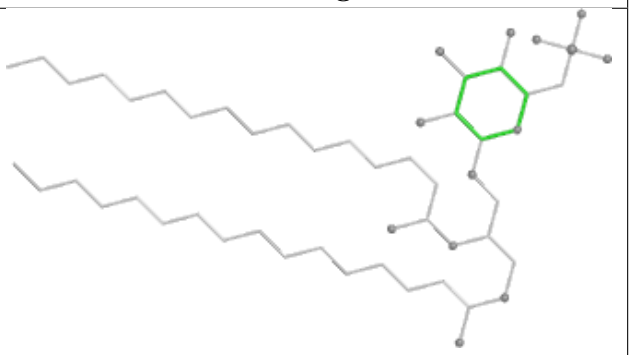
Bond lengths



Bond angles

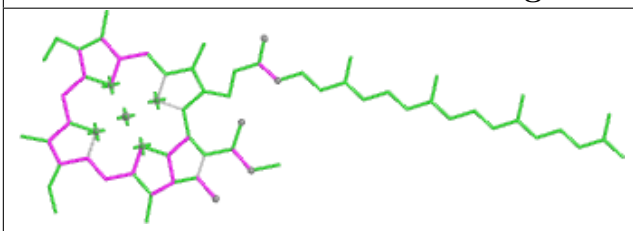


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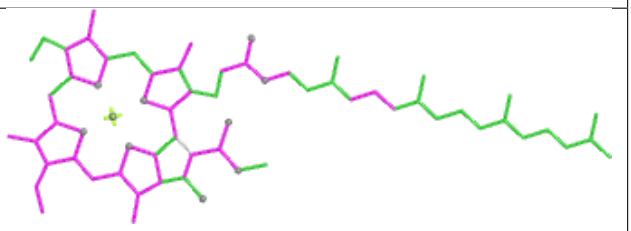


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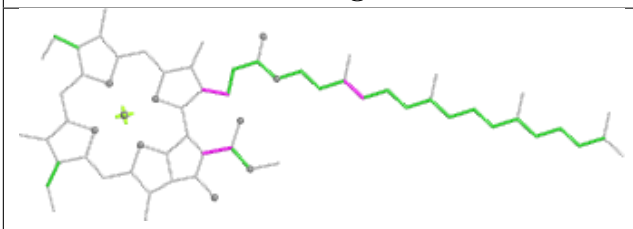
Ligand CLA B 610



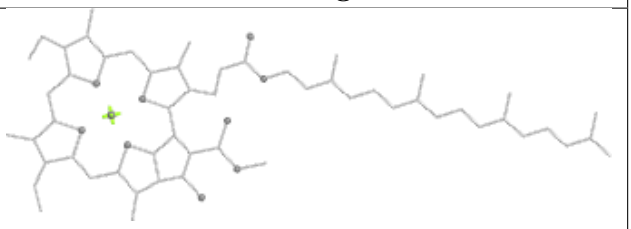
Bond lengths



Bond angles

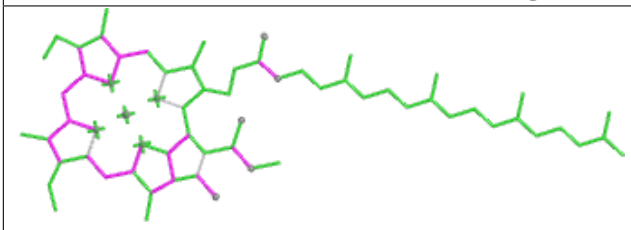


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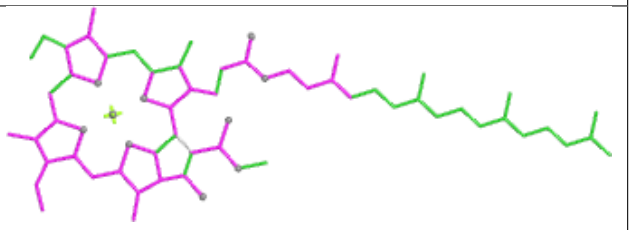


Rings

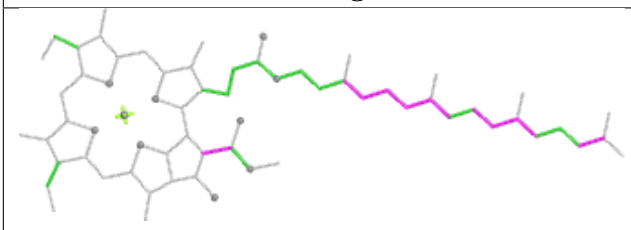
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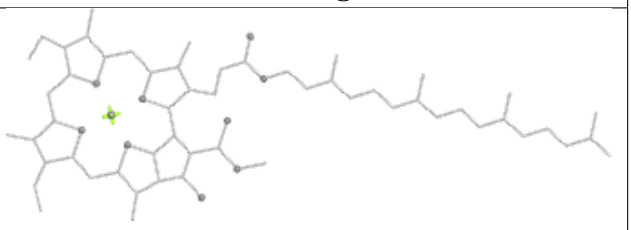
Bond lengths



Bond angles

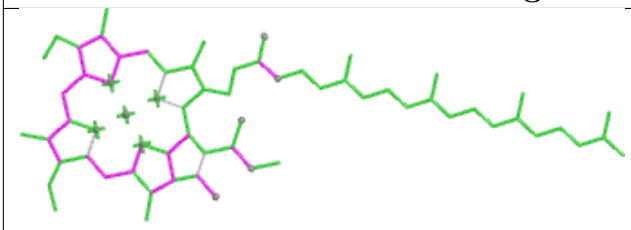


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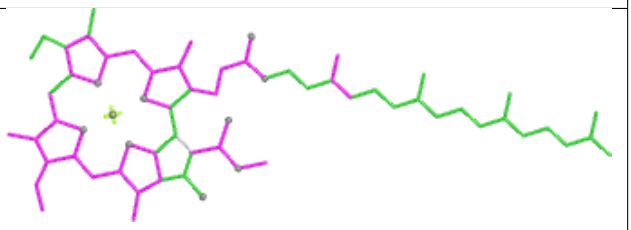


Rings

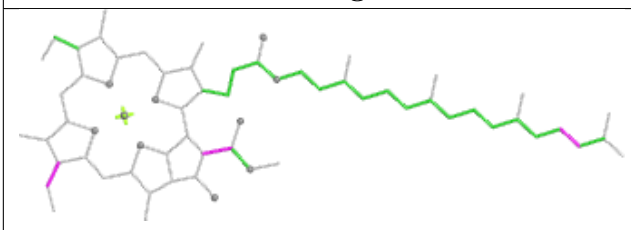
Ligand CLA A 406



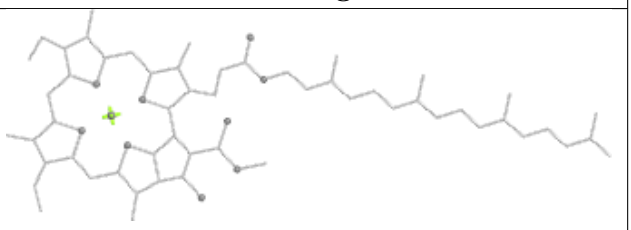
Bond lengths



Bond angles



Torsions

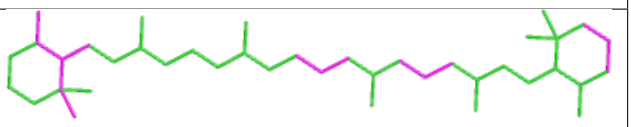


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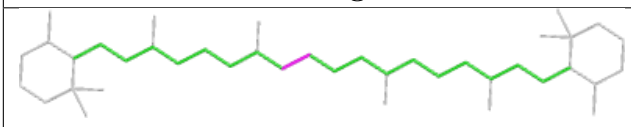
Ligand BCR t 101



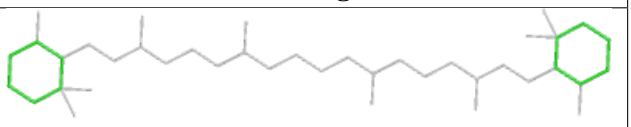
Bond lengths



Bond angles

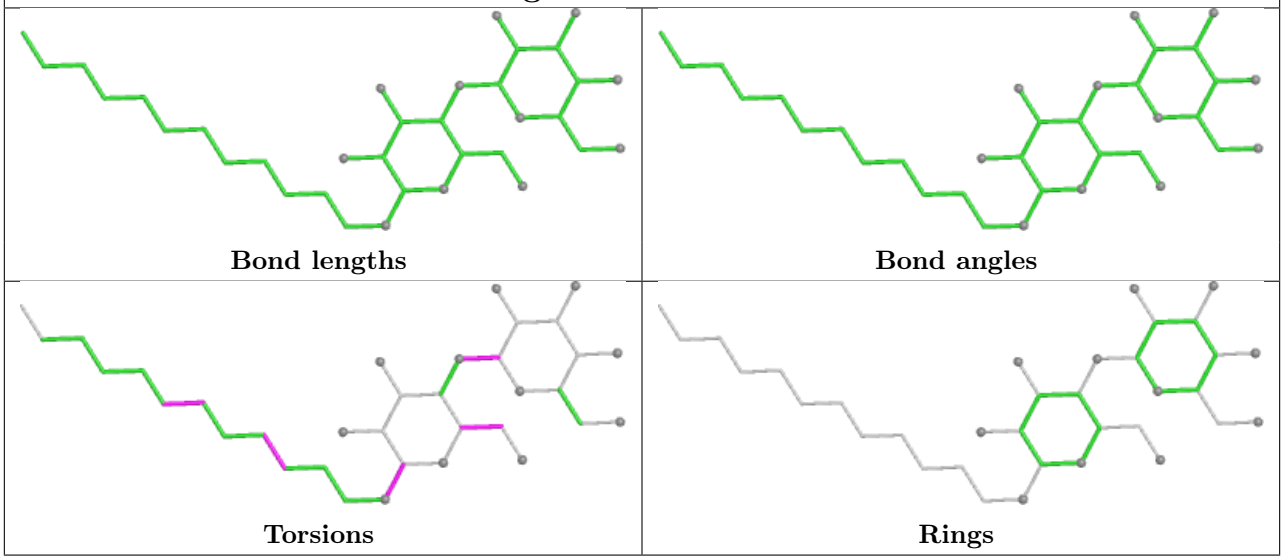


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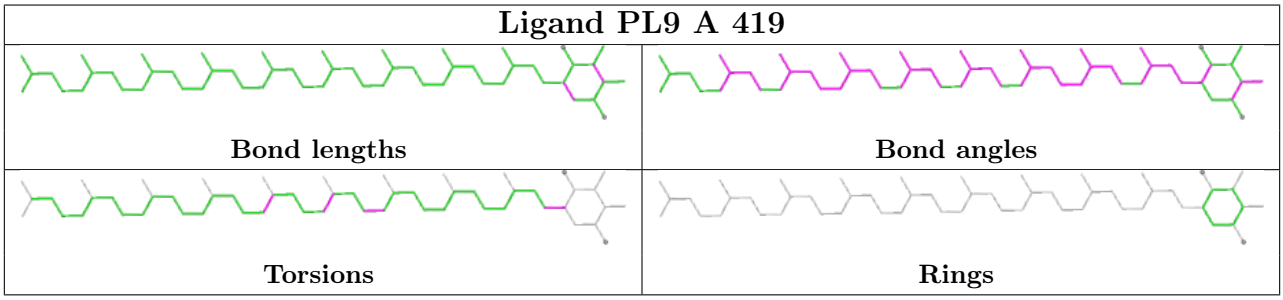


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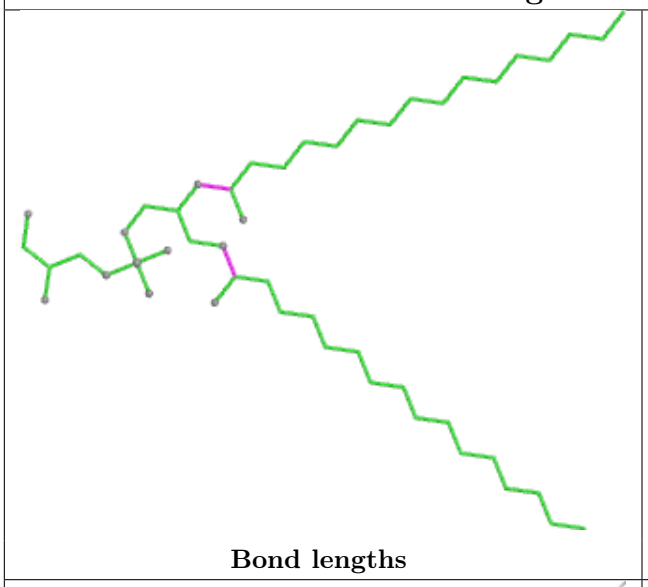
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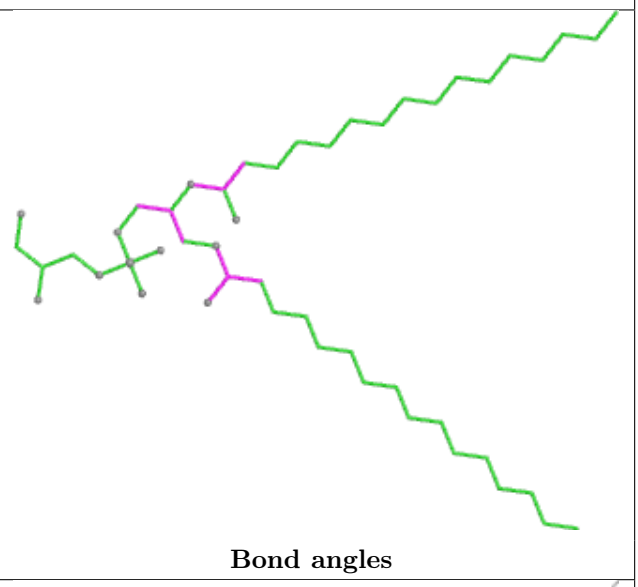
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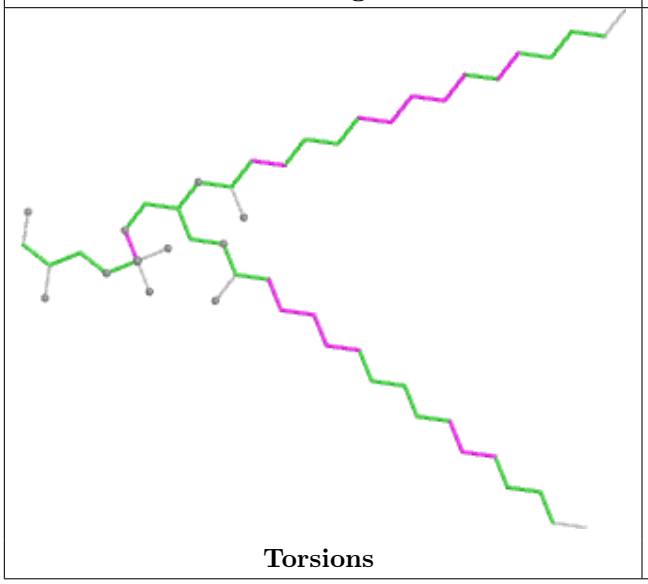
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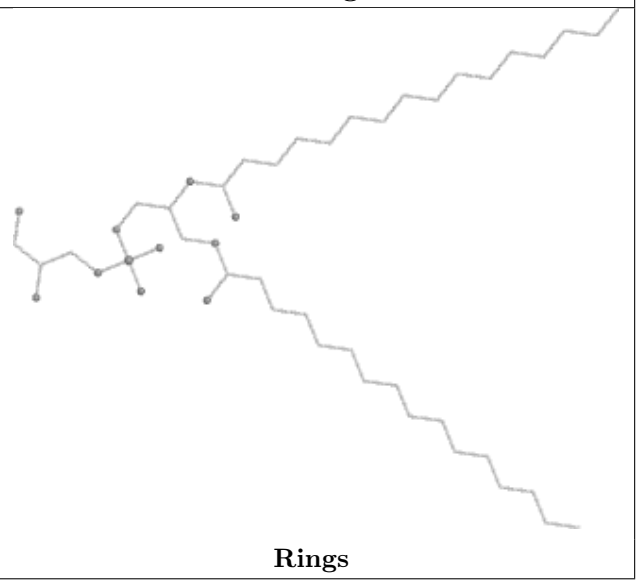
Bond lengths



Bond angles



Torsions

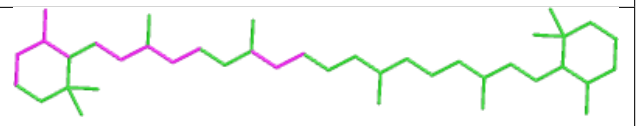


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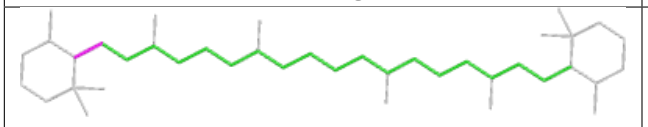
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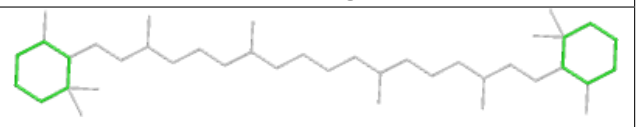
Bond lengths



Bond angles

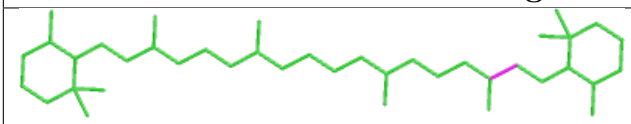


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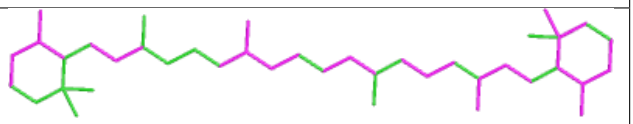


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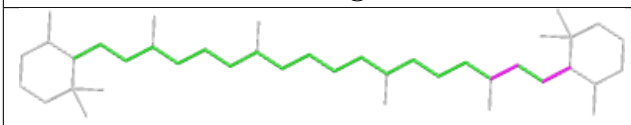
Ligand BCR d 404



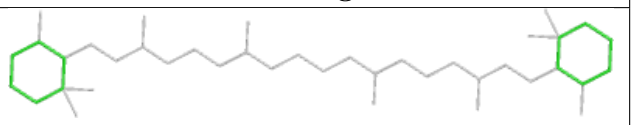
Bond lengths



Bond angles

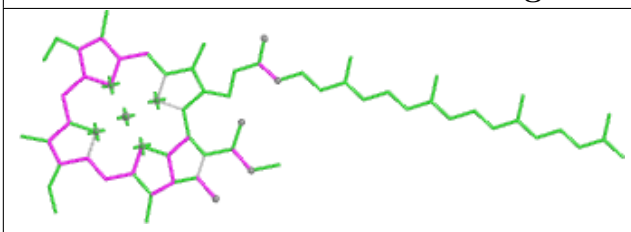


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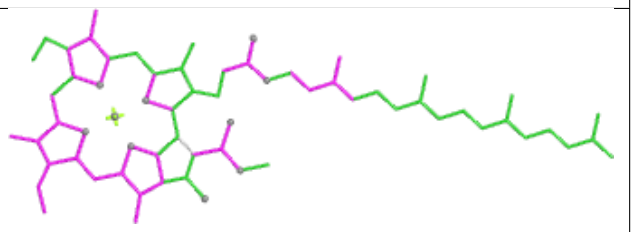


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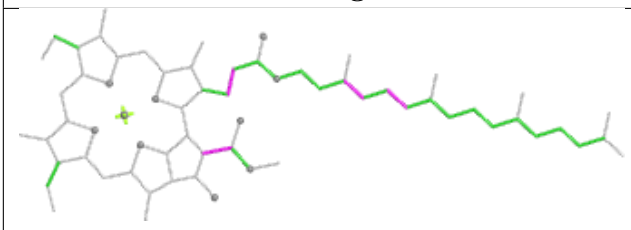
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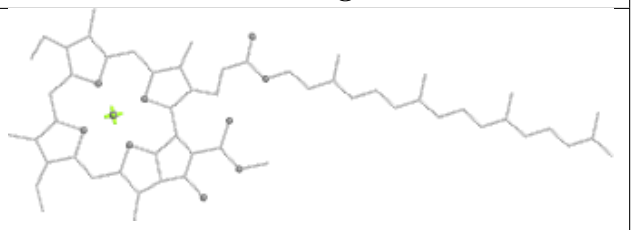
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Bond angles

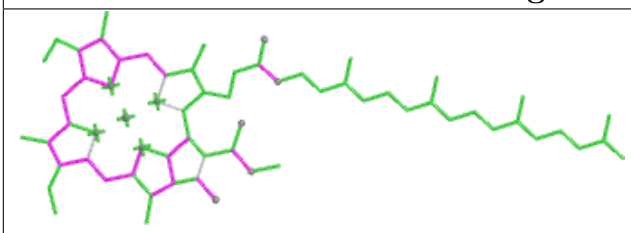


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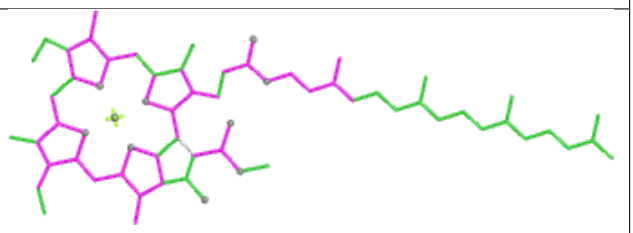


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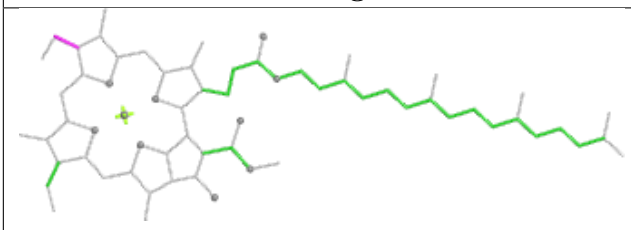
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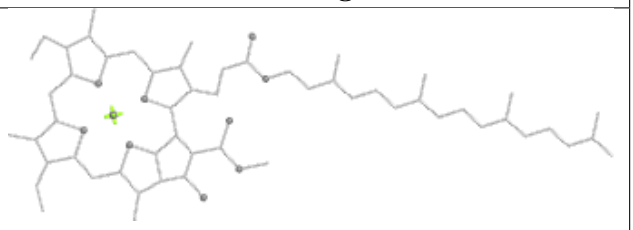
Bond lengths



Bond angles

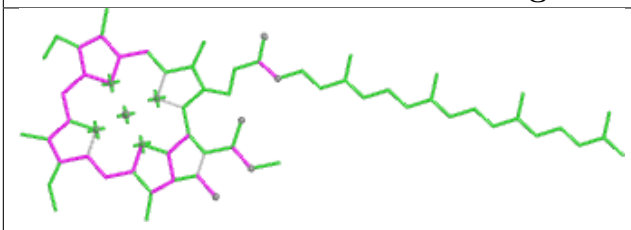


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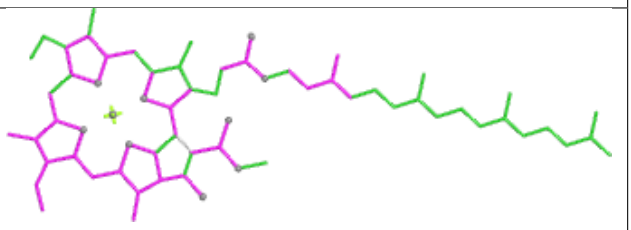


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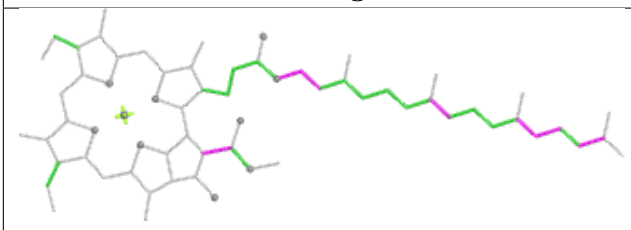
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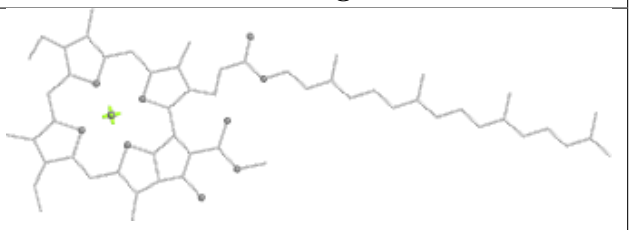
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Bond angles

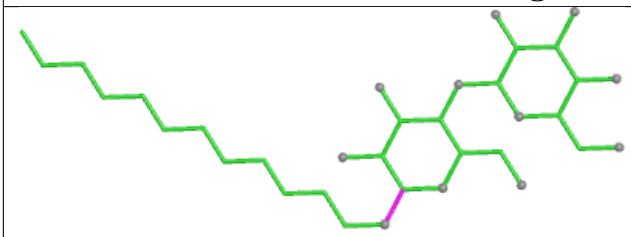


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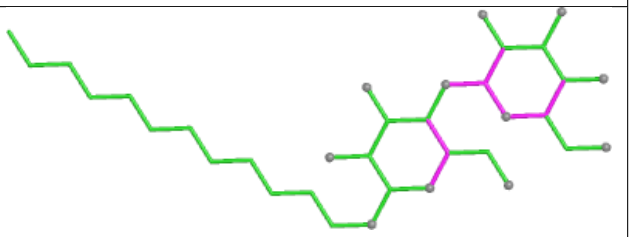


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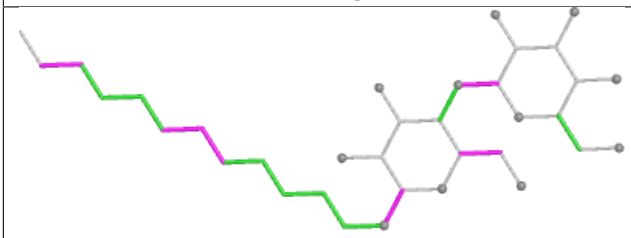
Ligand LMT f 103



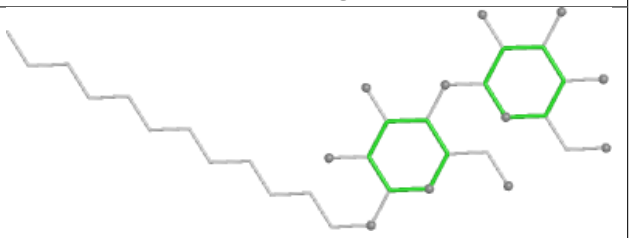
Bond lengths



Bond angles

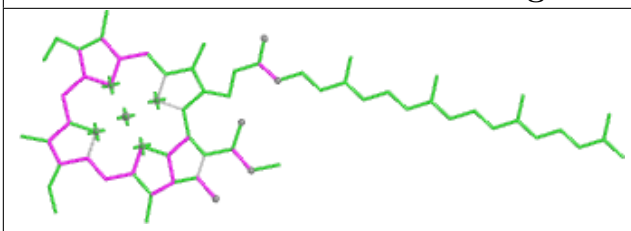


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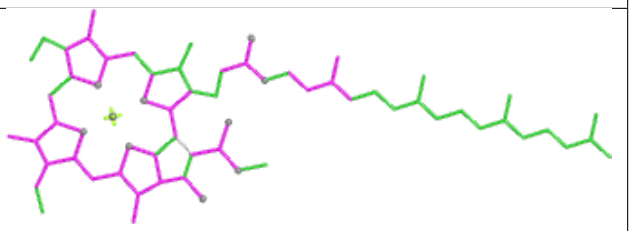


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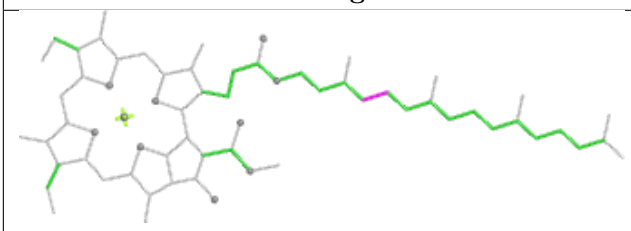
Ligand CLA b 616



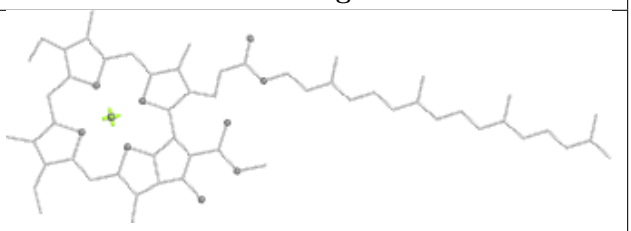
Bond lengths



Bond angles

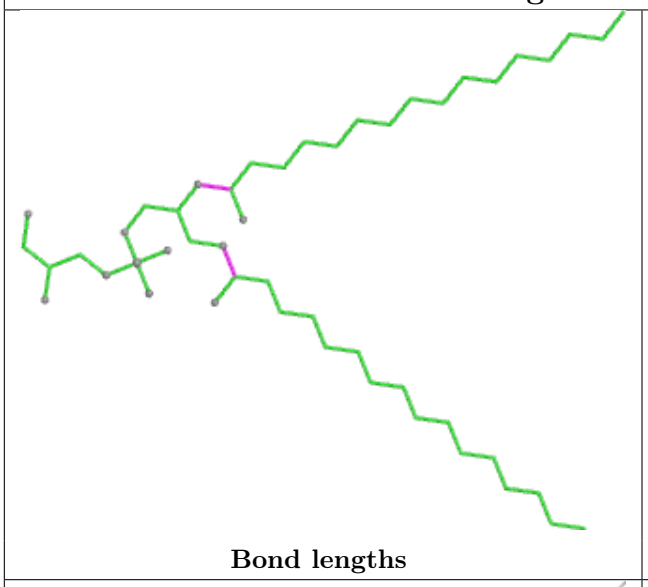


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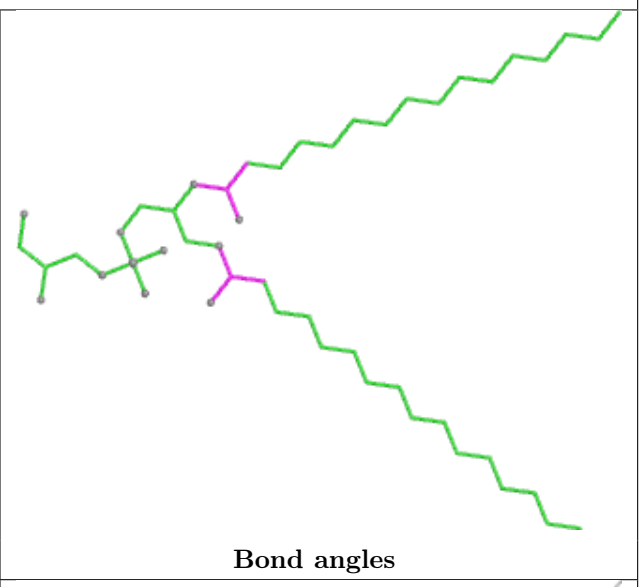


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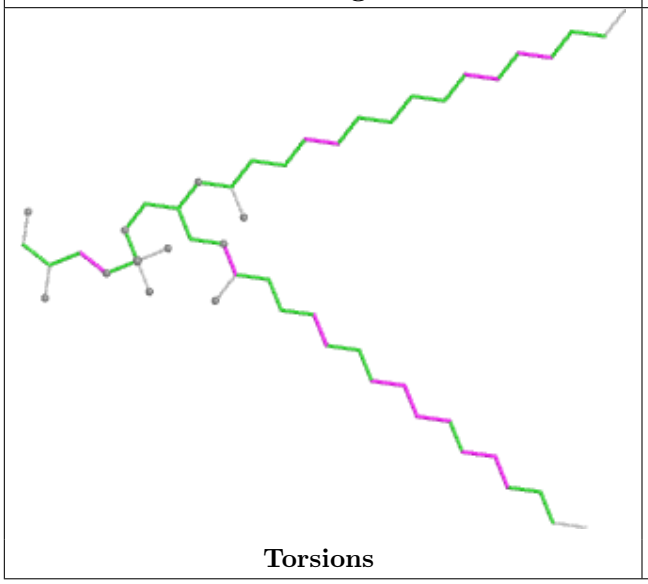
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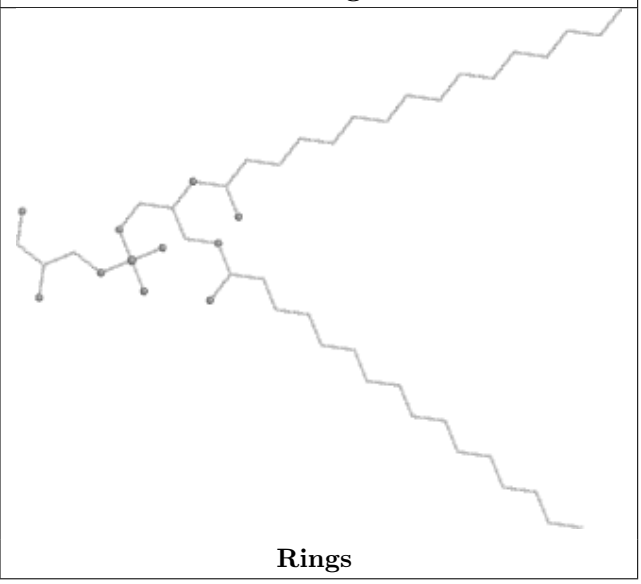
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR h 101



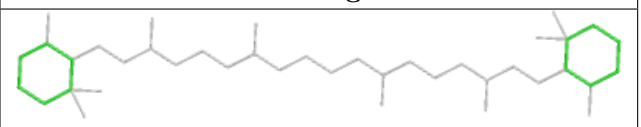
Bond lengths



Bond angles

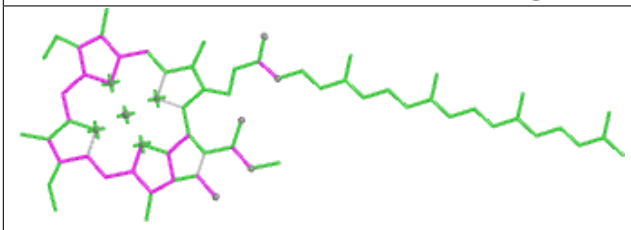


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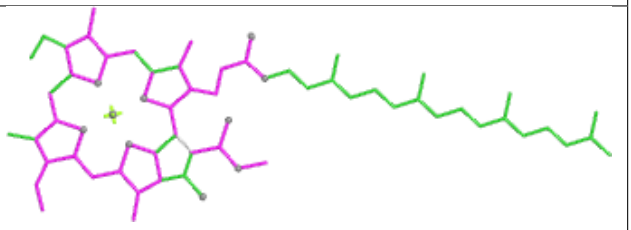


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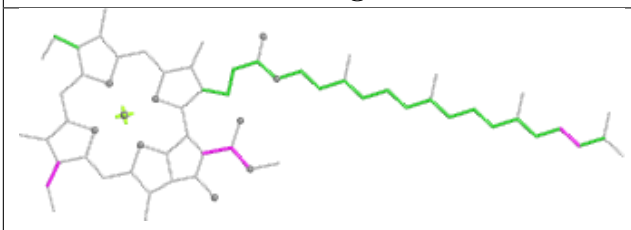
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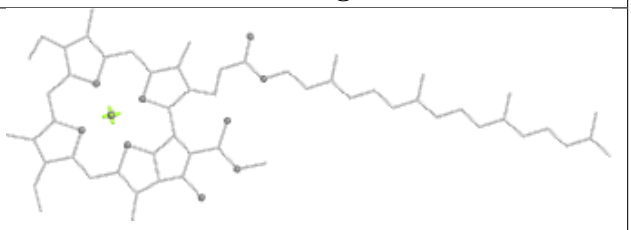
Bond lengths



Bond angles

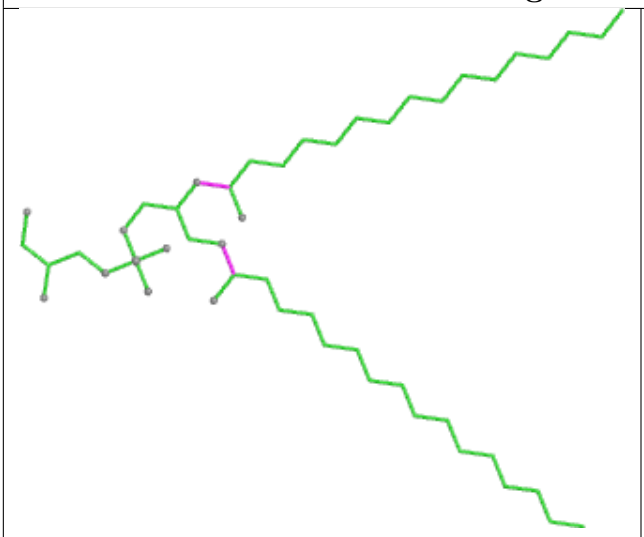


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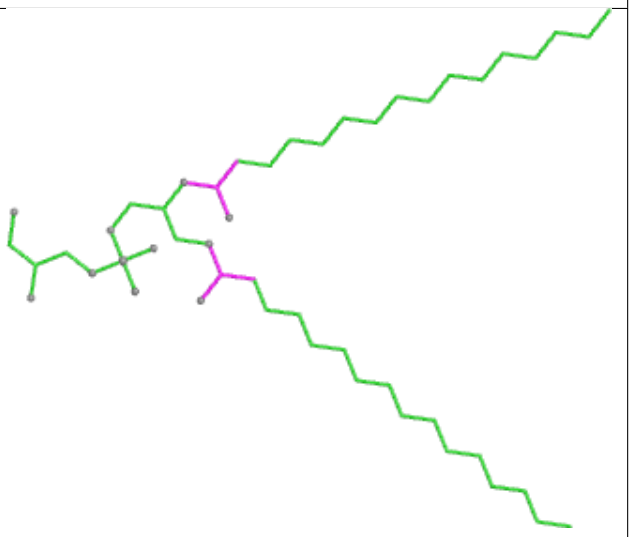


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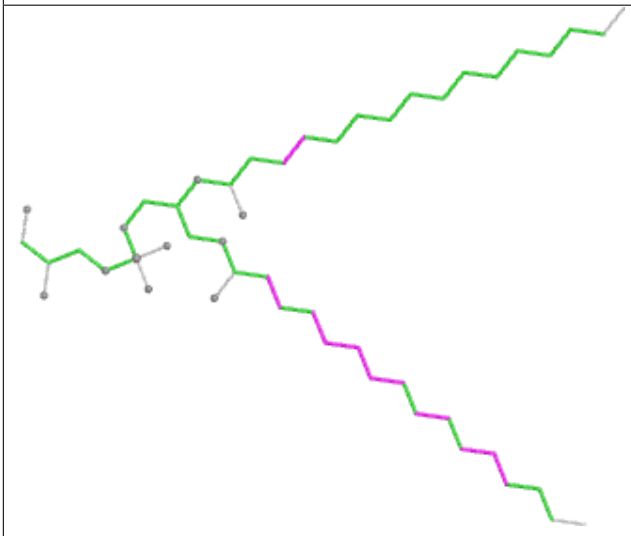
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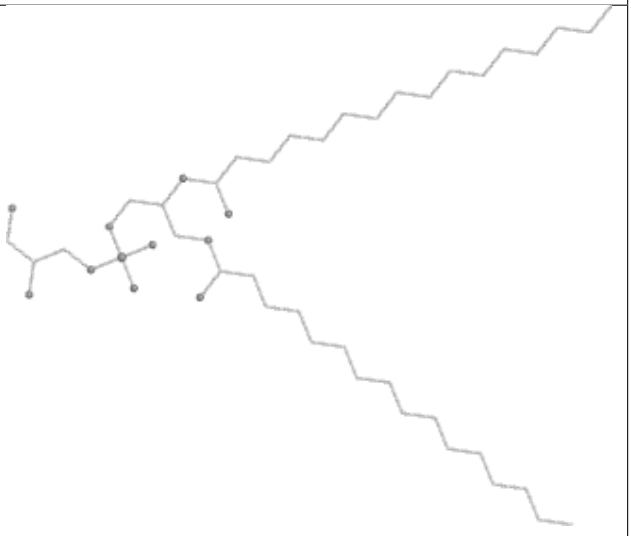
Bond lengths



Bond angles

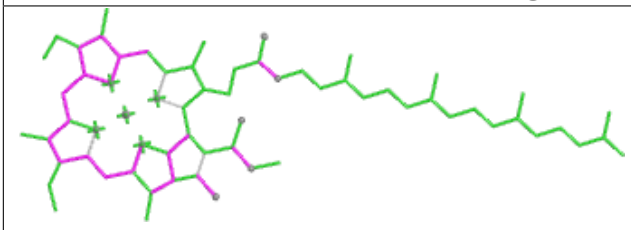


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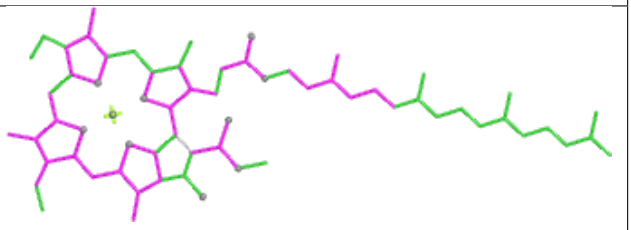


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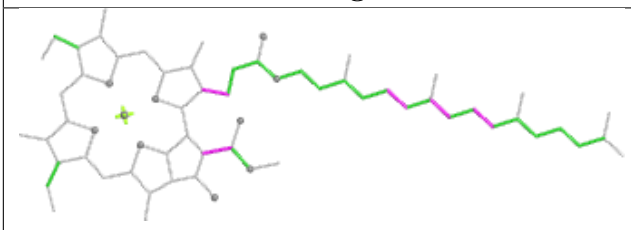
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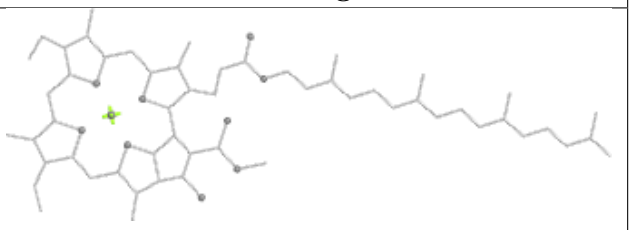
Bond lengths



Bond angles



Torsions

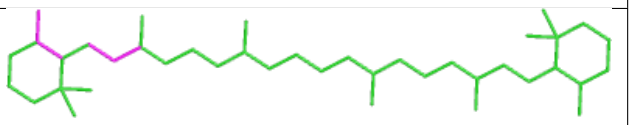


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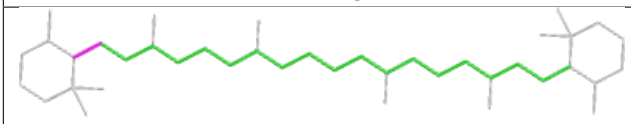
Ligand BCR b 621



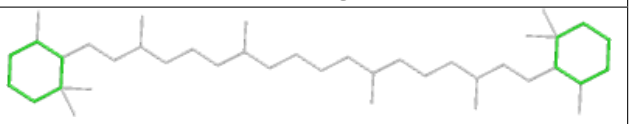
Bond lengths



Bond angles

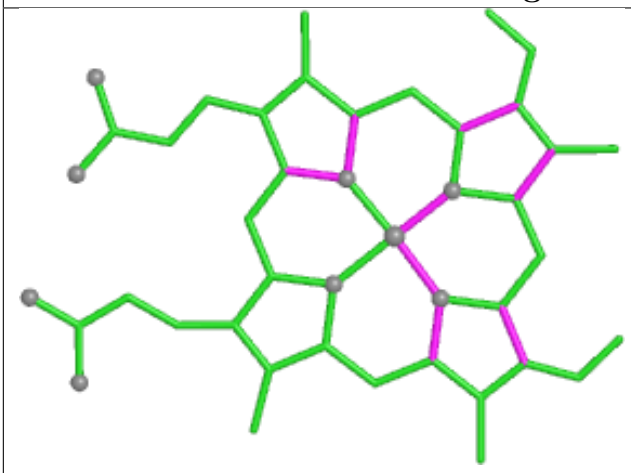


Torsions

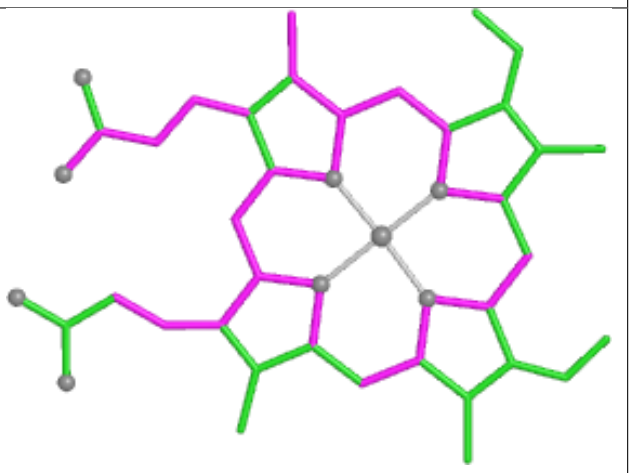


Rings

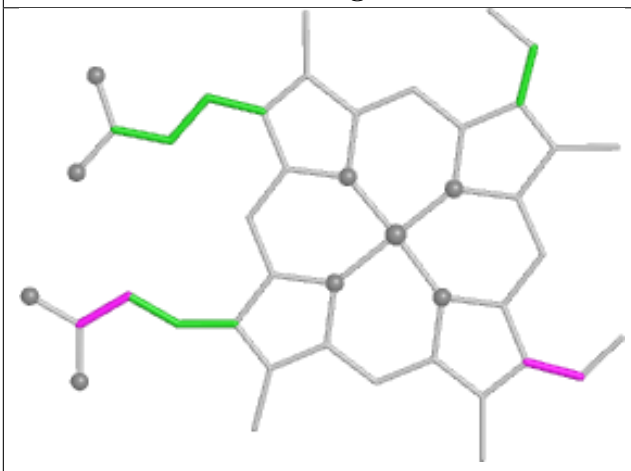
Ligand HEM e 102



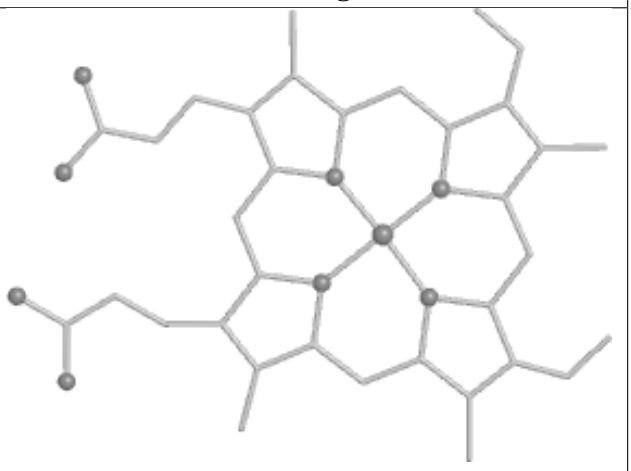
Bond lengths



Bond angles

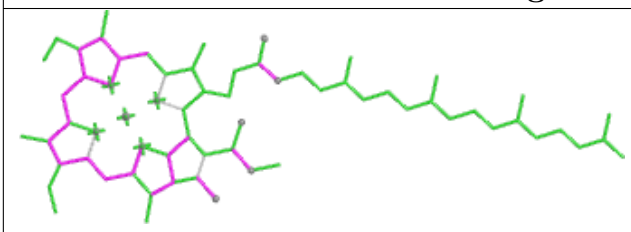


Torsions

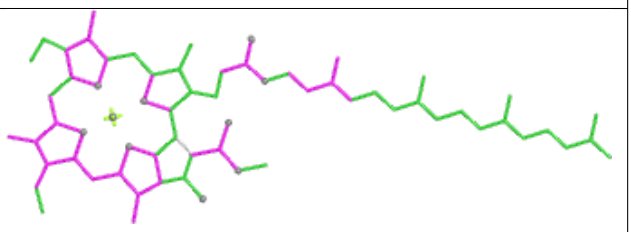


Rings

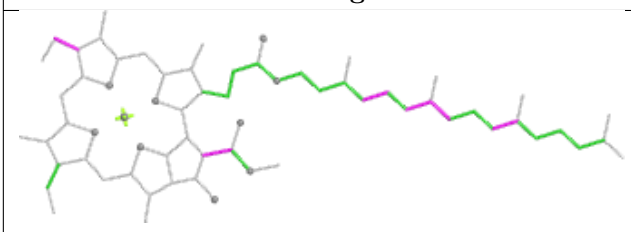
Ligand CLA b 608



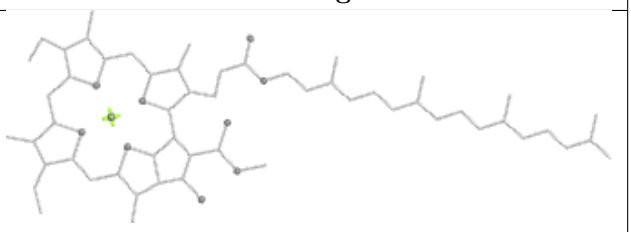
Bond lengths



Bond angles

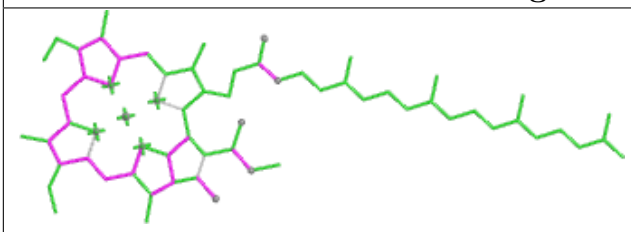


Torsions

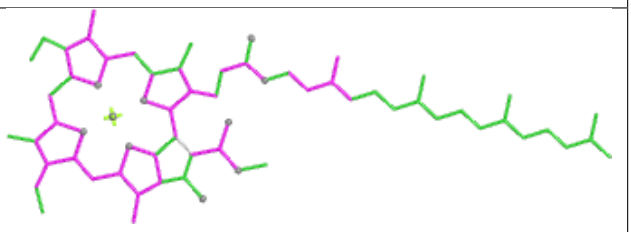


Rings

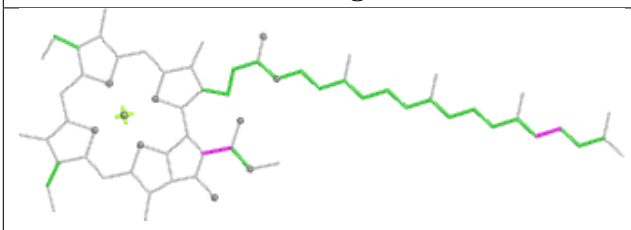
Ligand CLA c 909



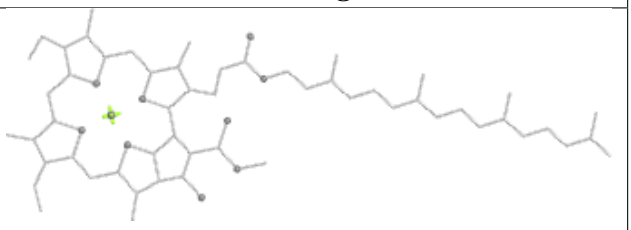
Bond lengths



Bond angles

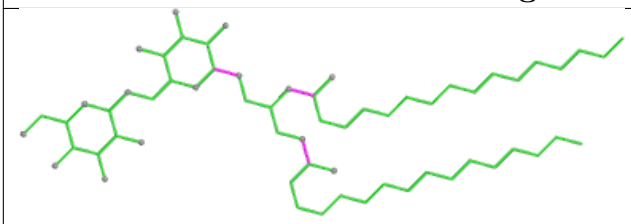


Torsions

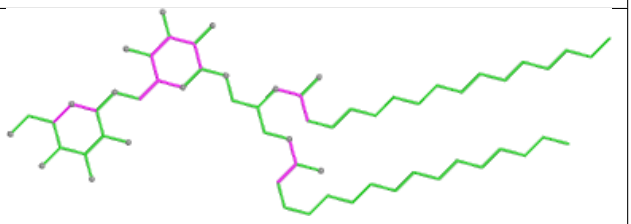


Rings

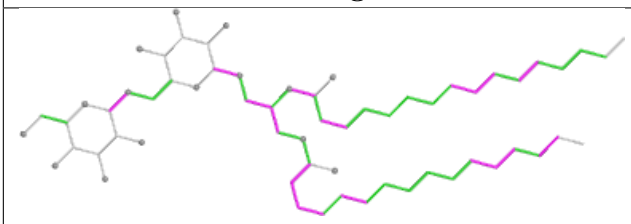
Ligand DGD D 405



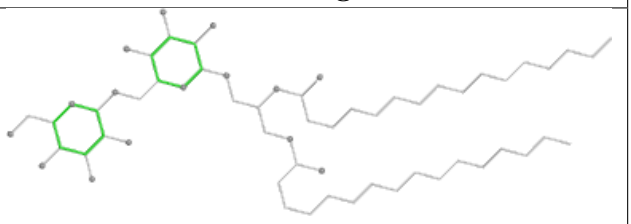
Bond lengths



Bond angles

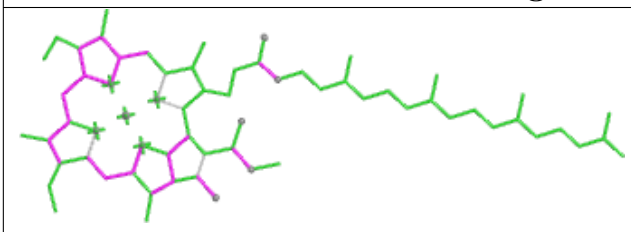


Torsions

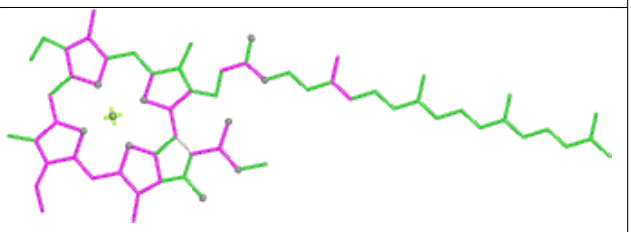


Rings

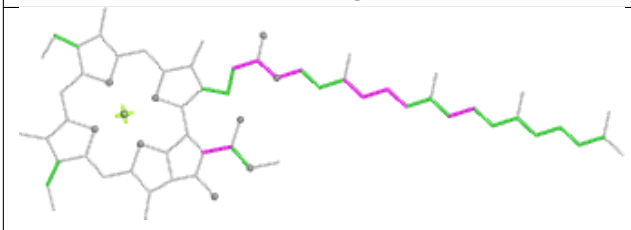
Ligand CLA b 605



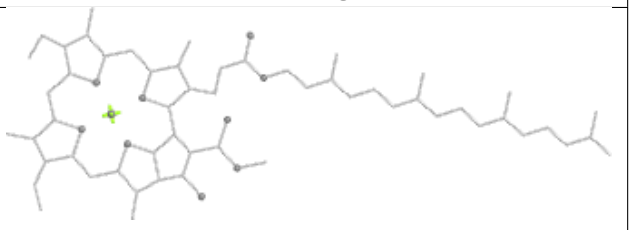
Bond lengths



Bond angles

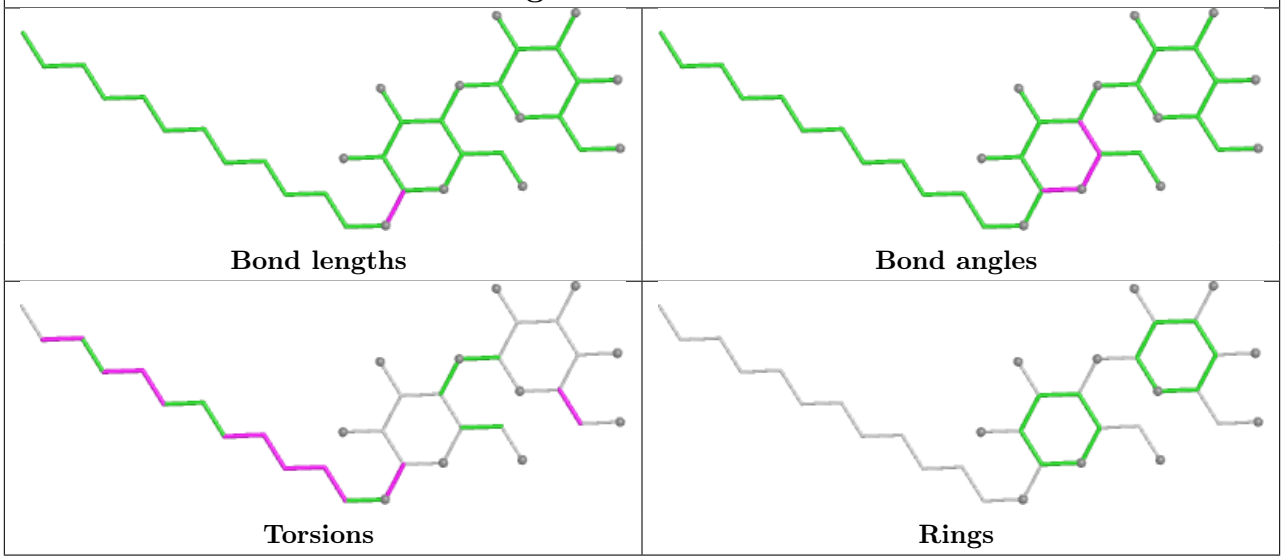


Torsions

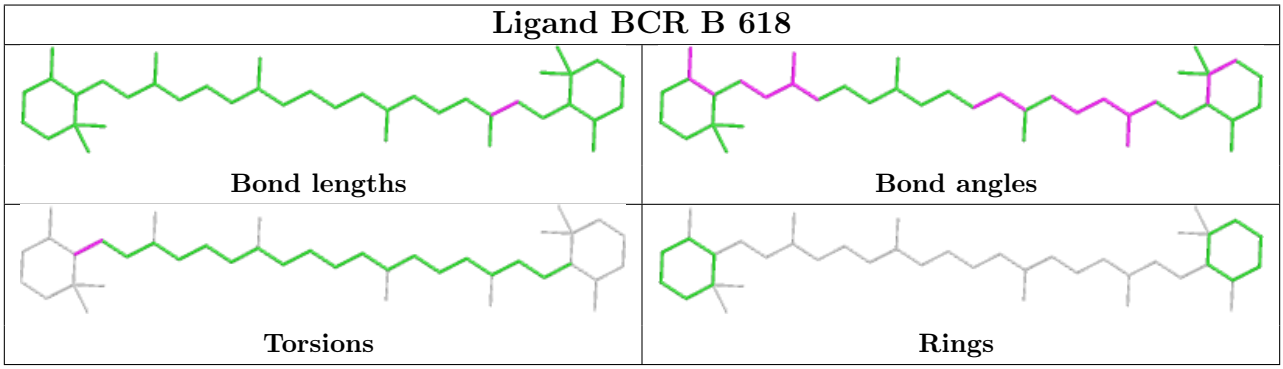


Rings

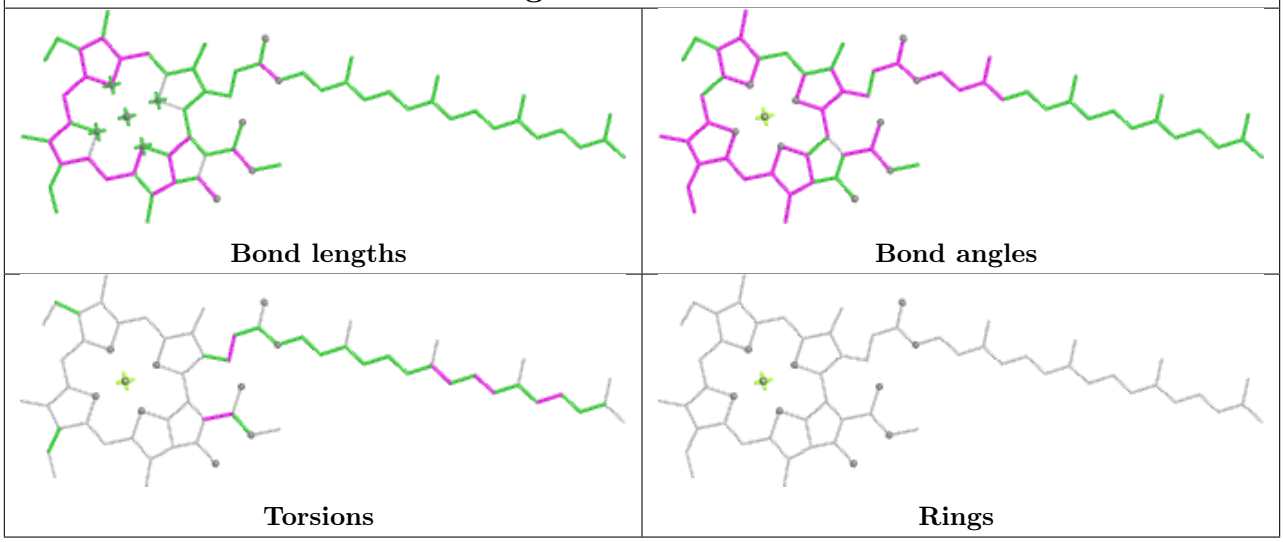
Ligand LMT a 401



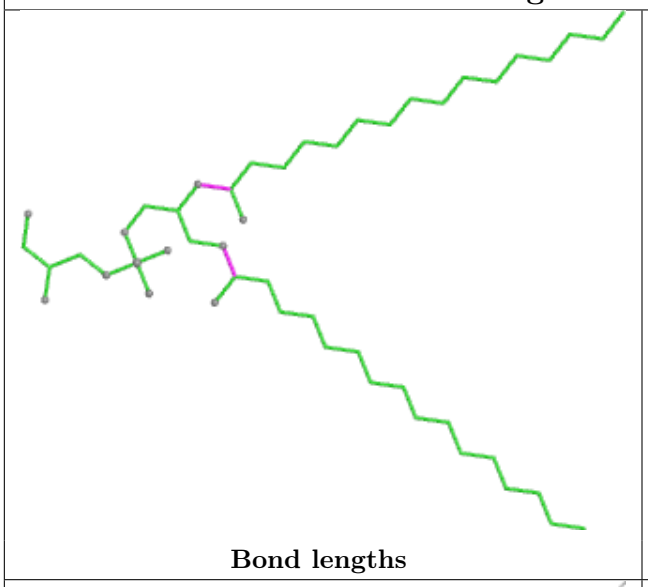
Ligand BCR B 618



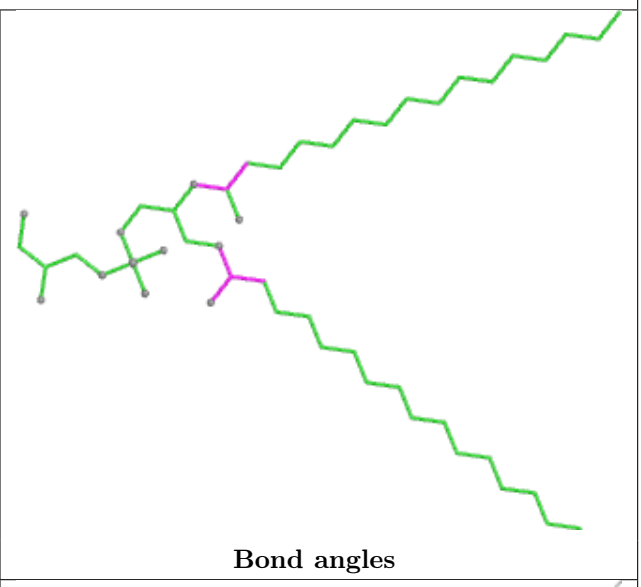
Ligand CLA B 607



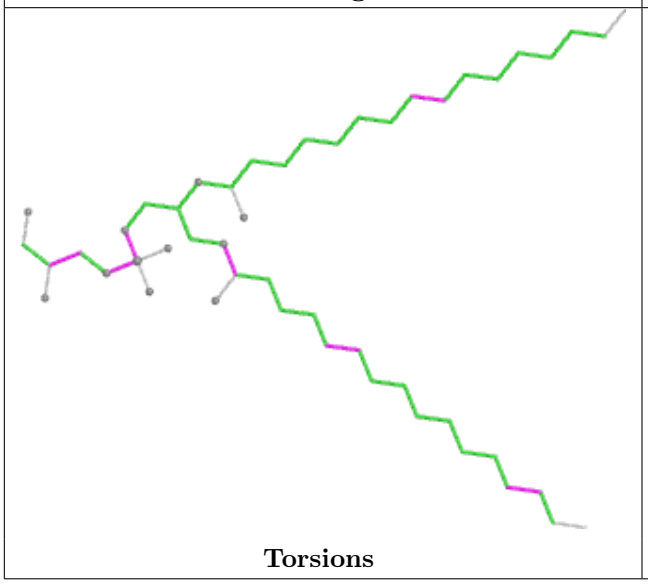
Ligand LHG d 408



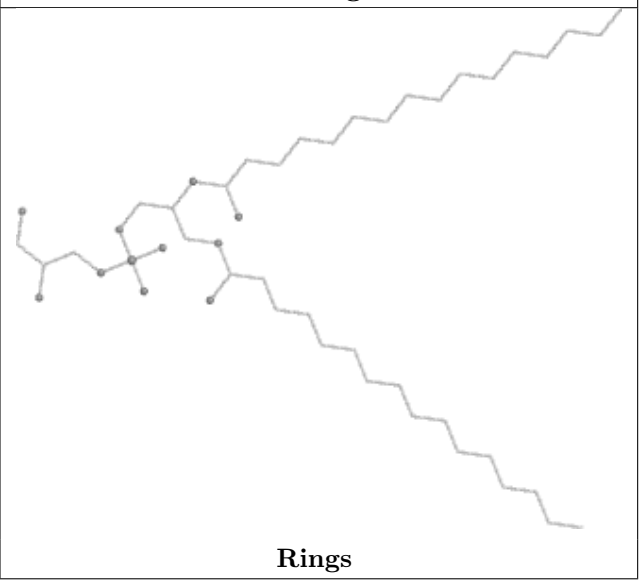
Bond lengths



Bond angles

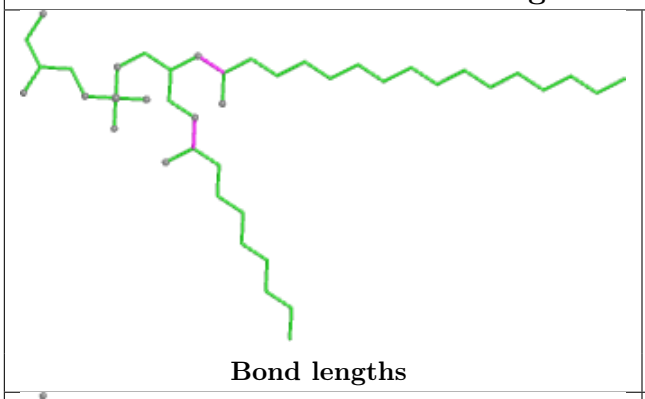


Torsions

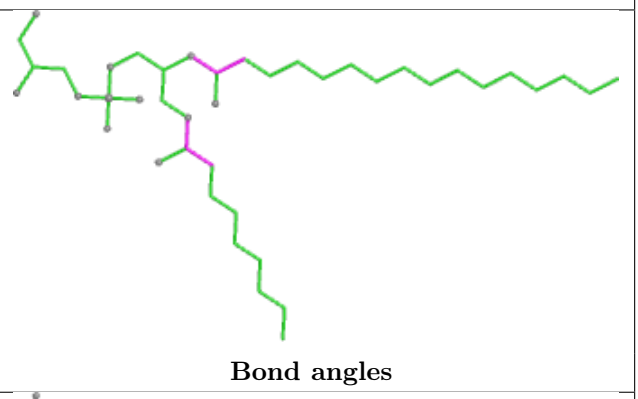


Rings

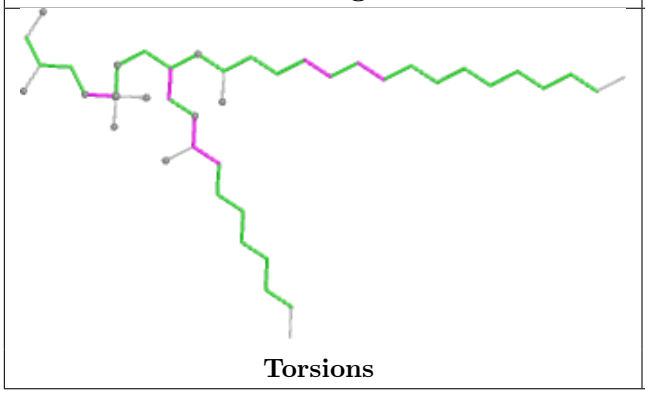
Ligand LHG e 101



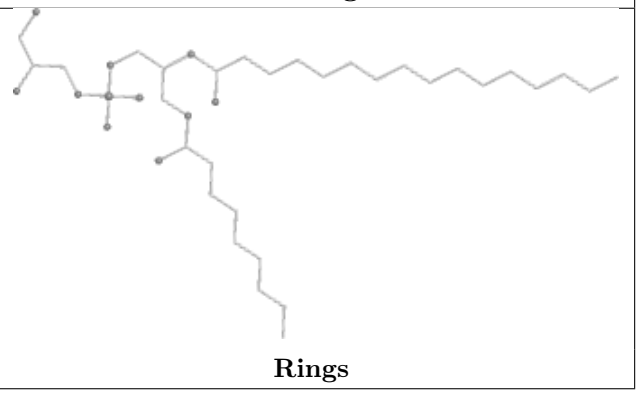
Bond lengths



Bond angles

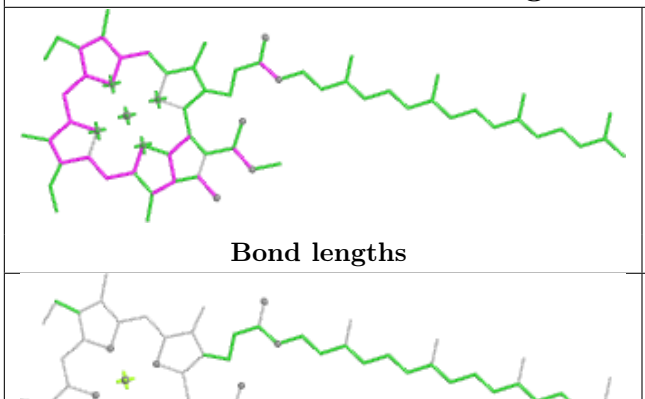


Torsions

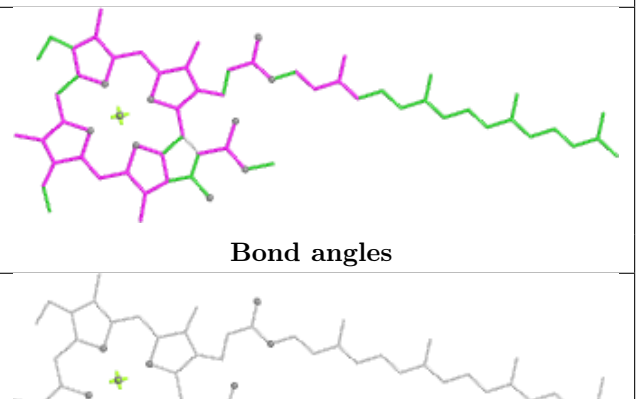


Rings

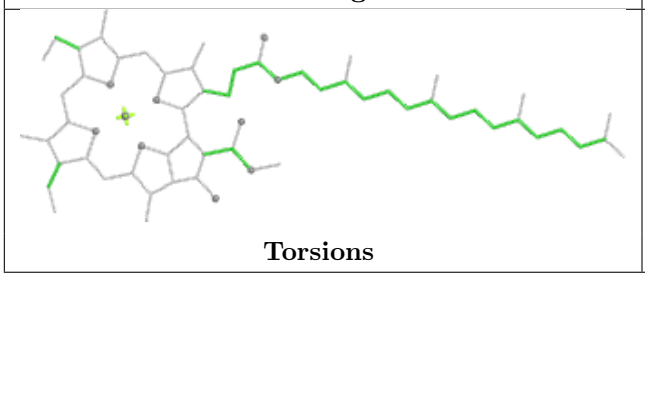
Ligand CLA B 609



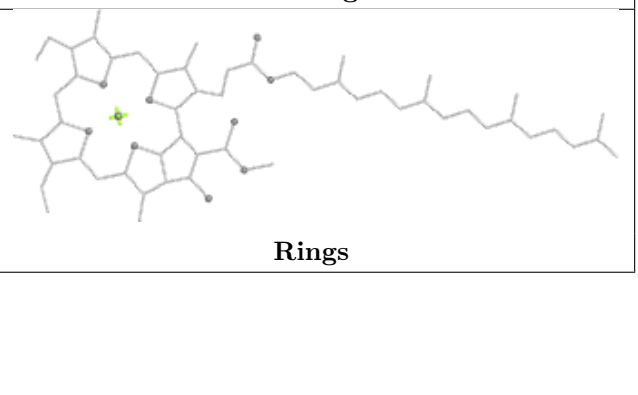
Bond lengths



Bond angles

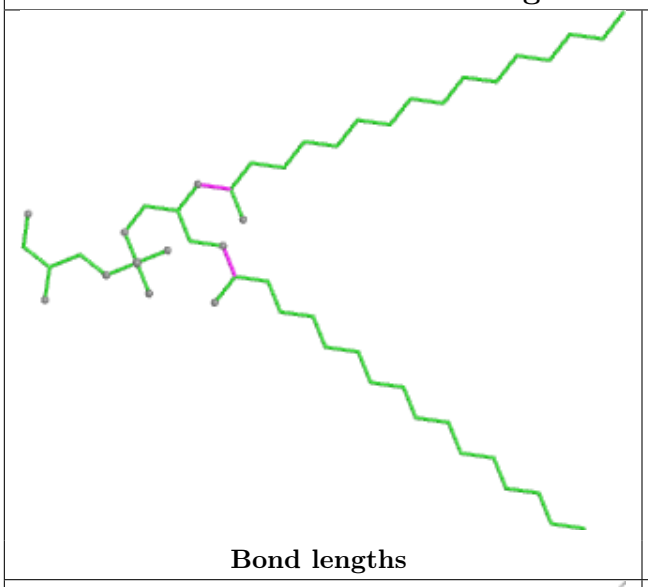


Torsions

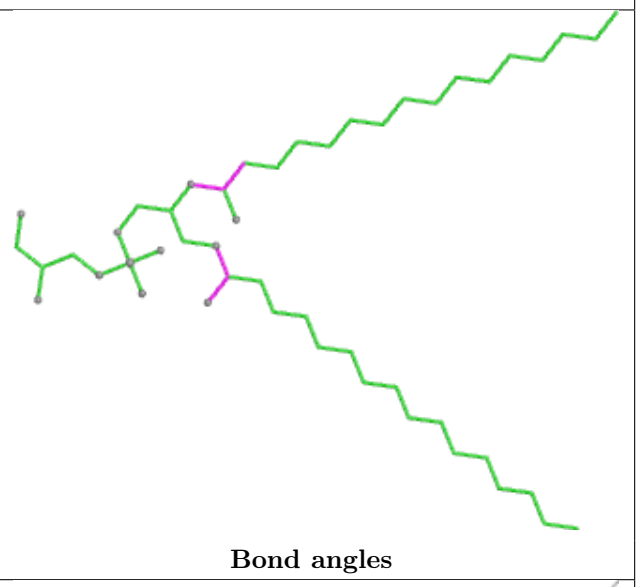


Rings

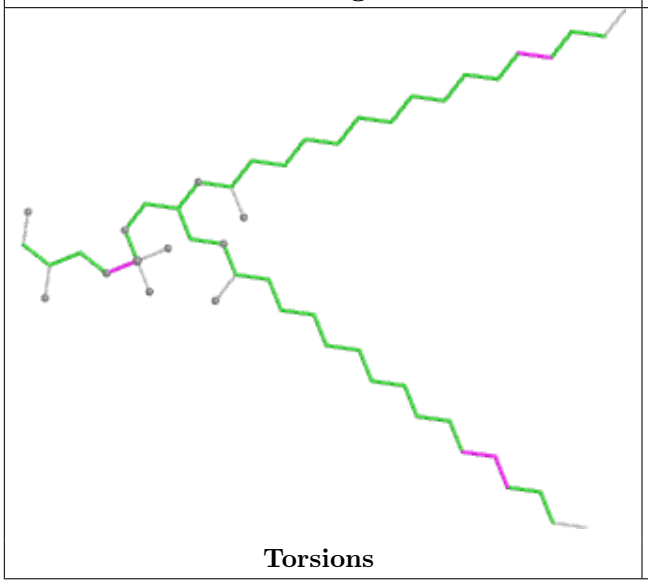
Ligand LHG D 407



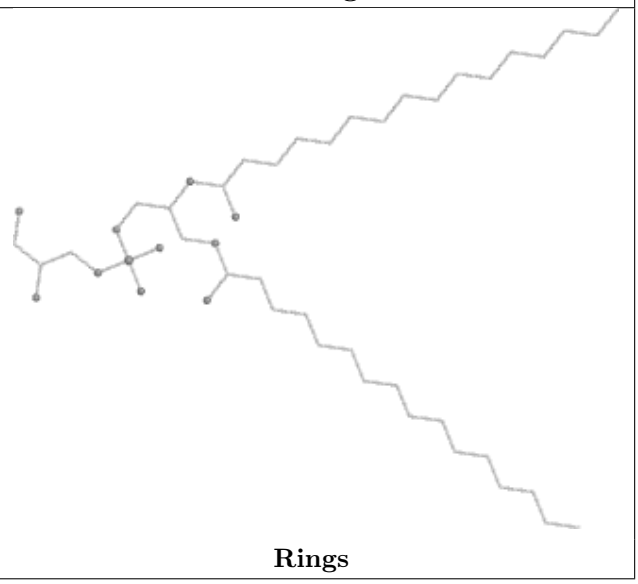
Bond lengths



Bond angles

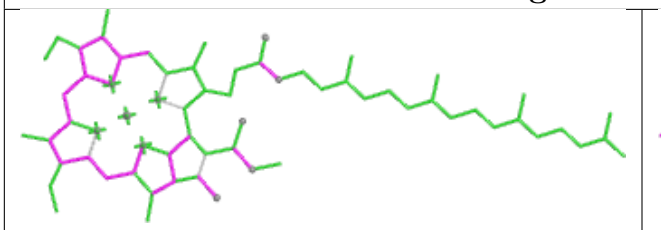


Torsions

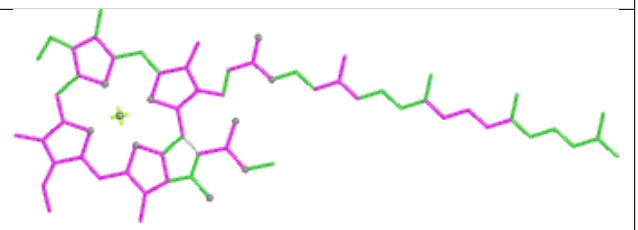


Rings

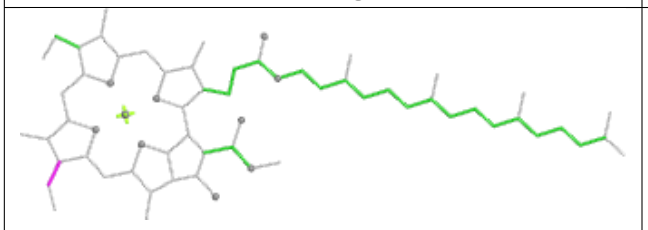
Ligand CLA a 406



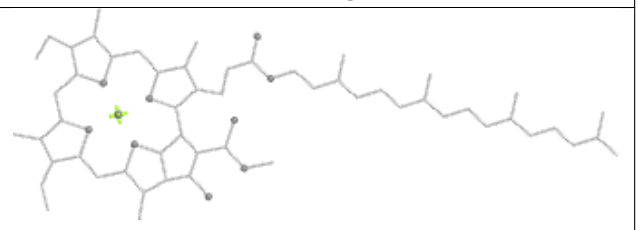
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.08	6 (1%) 67 75	13, 21, 37, 73	3 (0%)
1	a	334/344 (97%)	0.05	9 (2%) 56 62	15, 23, 47, 90	6 (1%)
2	B	504/505 (99%)	0.20	19 (3%) 44 50	14, 25, 48, 78	11 (2%)
2	b	504/505 (99%)	0.28	31 (6%) 26 31	16, 27, 58, 92	12 (2%)
3	C	451/455 (99%)	0.34	19 (4%) 40 47	17, 30, 46, 73	4 (0%)
3	c	455/455 (100%)	0.42	17 (3%) 45 52	16, 33, 49, 92	6 (1%)
4	D	342/342 (100%)	-0.09	5 (1%) 72 78	11, 22, 37, 97	1 (0%)
4	d	341/342 (99%)	-0.03	2 (0%) 85 89	12, 25, 39, 90	1 (0%)
5	E	81/84 (96%)	0.98	8 (9%) 13 14	20, 37, 66, 92	2 (2%)
5	e	81/84 (96%)	1.29	17 (20%) 2 2	23, 41, 71, 92	2 (2%)
6	F	34/44 (77%)	0.57	4 (11%) 9 10	23, 30, 50, 61	0
6	f	32/44 (72%)	0.84	3 (9%) 14 16	30, 34, 79, 84	0
7	H	65/65 (100%)	0.66	4 (6%) 26 31	18, 31, 46, 110	1 (1%)
7	h	65/65 (100%)	0.91	7 (10%) 11 12	27, 35, 52, 105	0
8	I	37/38 (97%)	1.13	6 (16%) 4 5	26, 33, 88, 108	0
8	i	37/38 (97%)	0.92	6 (16%) 4 5	27, 33, 73, 102	0
9	J	38/39 (97%)	1.07	6 (15%) 5 5	24, 35, 84, 98	0
9	j	39/39 (100%)	1.10	7 (17%) 3 3	29, 38, 84, 96	0
10	K	37/37 (100%)	0.79	3 (8%) 18 21	27, 35, 54, 65	0
10	k	37/37 (100%)	1.07	5 (13%) 7 7	30, 38, 55, 68	0
11	L	37/37 (100%)	0.04	3 (8%) 18 21	11, 19, 56, 82	1 (2%)
11	l	37/37 (100%)	0.18	2 (5%) 31 37	11, 20, 58, 83	1 (2%)
12	M	33/36 (91%)	0.27	3 (9%) 15 17	13, 21, 45, 89	1 (3%)
12	m	33/36 (91%)	0.16	2 (6%) 27 31	16, 21, 41, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.48	17 (6%) 22 26	16, 31, 66, 110	8 (3%)
13	o	243/244 (99%)	0.64	31 (12%) 7 9	15, 33, 71, 125	5 (2%)
14	T	29/32 (90%)	0.21	2 (6%) 23 26	16, 20, 43, 89	1 (3%)
14	t	29/32 (90%)	0.29	2 (6%) 23 26	16, 20, 46, 89	1 (3%)
15	U	97/104 (93%)	0.47	4 (4%) 41 48	21, 31, 54, 84	0
15	u	97/104 (93%)	0.33	2 (2%) 63 70	23, 33, 51, 84	0
16	V	137/137 (100%)	0.42	5 (3%) 46 53	16, 31, 51, 69	1 (0%)
16	v	137/137 (100%)	0.52	5 (3%) 46 53	24, 36, 57, 70	0
17	Y	29/30 (96%)	2.02	10 (34%) 1 0	35, 47, 82, 101	0
17	y	29/30 (96%)	2.00	14 (48%) 0 0	38, 50, 83, 100	0
18	X	39/40 (97%)	1.40	8 (20%) 2 2	31, 38, 75, 102	0
18	x	39/40 (97%)	1.20	7 (17%) 3 3	33, 41, 83, 102	0
19	Z	62/62 (100%)	1.84	21 (33%) 1 0	36, 47, 83, 96	0
19	z	62/62 (100%)	2.12	28 (45%) 0 0	42, 49, 82, 96	0
20	R	34/34 (100%)	3.20	27 (79%) 0 0	54, 75, 98, 106	0
All	All	5294/5384 (98%)	0.41	377 (7%) 22 25	11, 29, 61, 125	68 (1%)

All (377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	10.5
7	H	65	LEU	9.2
17	Y	18	VAL	8.2
7	h	65	LEU	7.4
20	R	24	LEU	7.3
19	Z	62	VAL	6.9
8	i	37	LEU	6.6
9	j	1	MET	6.4
19	Z	7	LEU	6.2
8	I	37	LEU	6.1
19	z	3	ILE	6.1
17	Y	19	ILE	6.0
1	a	11	ALA	5.9
20	R	28	VAL	5.9
14	T	30	THR	5.5
7	H	64	ALA	5.4
18	X	2	THR	5.4

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Mol	Chain	Res	Type	RSRZ
9	J	4	GLY	5.4
9	J	2	SER	5.4
19	Z	3	ILE	5.3
2	b	495	PHE	5.3
5	e	5	THR	5.3
7	h	64	ALA	5.1
17	y	18	VAL	5.0
19	Z	1	MET	4.9
13	o	58	ASN	4.9
13	O	56	PRO	4.8
20	R	31	VAL	4.8
18	x	2	THR	4.8
14	t	30	THR	4.7
7	h	66	GLY	4.7
13	O	58	ASN	4.7
2	b	86[A]	ILE	4.6
2	b	491	VAL	4.6
17	y	19	ILE	4.6
2	b	502	VAL	4.5
19	z	4	LEU	4.5
13	O	4	THR	4.5
2	B	479	PHE	4.5
2	b	486	LEU	4.5
20	R	23	ILE	4.5
8	I	38	GLU	4.5
2	b	493	TRP	4.4
18	X	40	SER	4.4
5	e	4	THR	4.4
13	o	63	ALA	4.4
11	l	1	MET	4.4
2	B	127	ARG	4.4
2	B	486	LEU	4.3
2	b	488	PRO	4.3
17	Y	22	LEU	4.3
20	R	10	LEU	4.3
2	b	84	THR	4.3
17	y	25	ILE	4.3
12	M	34	LYS	4.3
2	B	86	ILE	4.3
20	R	19	ALA	4.3
20	R	3	TRP	4.3
6	f	16	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
20	R	20	VAL	4.2
13	o	37	THR	4.2
20	R	6	LEU	4.2
19	Z	4	LEU	4.2
20	R	27	ALA	4.1
19	z	30	PRO	4.1
17	Y	25	ILE	4.1
19	Z	61	VAL	4.1
19	Z	60	PHE	4.0
19	z	41	PHE	4.0
18	X	31	ILE	4.0
20	R	18	TRP	4.0
3	c	19	ASN	4.0
2	b	293	ALA	3.9
3	C	23	ALA	3.9
13	o	4	THR	3.9
2	b	496	TYR	3.9
19	Z	41	PHE	3.8
19	z	60	PHE	3.8
5	E	84	LYS	3.8
5	E	61	ARG	3.8
7	H	66	GLY	3.8
19	Z	30	PRO	3.8
12	M	33	GLN	3.8
17	y	20	ALA	3.8
9	J	3	GLU	3.8
13	o	59	LYS	3.8
2	b	479	PHE	3.8
19	z	5	PHE	3.8
5	E	4	THR	3.7
13	O	246	ALA	3.7
6	f	15	ILE	3.7
14	t	29	ILE	3.7
17	Y	21	GLN	3.7
15	U	67	LEU	3.7
20	R	9	LEU	3.6
12	m	33	GLN	3.6
2	B	505	ARG	3.6
20	R	26	TYR	3.6
2	b	85	GLY	3.6
3	c	134	ILE	3.6
1	a	230	THR	3.6

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Mol	Chain	Res	Type	RSRZ
6	f	14	PRO	3.6
20	R	35	LEU	3.6
13	o	246	ALA	3.6
10	K	17	ILE	3.6
19	z	1	MET	3.6
18	x	40	SER	3.5
13	O	62	GLU	3.5
10	k	18	PHE	3.5
19	z	61	VAL	3.5
17	Y	20	ALA	3.5
16	V	106	ASN	3.4
16	v	106	ASN	3.4
11	L	1	MET	3.4
19	z	33	TRP	3.4
5	e	61	ARG	3.4
20	R	15	ALA	3.3
1	A	13	LEU	3.3
2	B	84	THR	3.3
12	m	34	LYS	3.3
13	O	61	GLN	3.3
9	j	3	GLU	3.3
20	R	13	LEU	3.3
18	x	38	GLN	3.3
9	J	5	GLY	3.3
9	j	4	GLY	3.3
16	V	14	SER	3.3
14	T	29	ILE	3.3
18	x	34	ILE	3.3
19	z	7	LEU	3.3
3	c	143	TYR	3.2
19	Z	10	ALA	3.2
4	D	238	THR	3.2
18	x	37	VAL	3.2
2	B	494	GLY	3.2
13	o	56	PRO	3.2
3	c	151	TRP	3.1
5	E	60	GLN	3.1
19	z	42	LEU	3.1
2	B	495	PHE	3.1
8	I	33	LYS	3.1
20	R	25	PRO	3.1
2	B	85	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
5	e	6	GLY	3.1
19	z	31	GLN	3.1
4	D	12	ARG	3.1
3	C	24	THR	3.1
1	A	11	ALA	3.1
3	C	246	ALA	3.1
9	j	5	GLY	3.1
19	Z	49	ALA	3.1
2	B	490	GLN	3.0
4	d	12	ARG	3.0
15	U	73	GLN	3.0
5	e	13	ILE	3.0
18	X	34	ILE	3.0
8	I	36	ASP	3.0
18	X	3	ILE	3.0
2	b	489	GLU	3.0
19	Z	31	GLN	3.0
3	C	260	ALA	3.0
1	A	235	TYR	2.9
1	a	262	TYR	2.9
19	Z	6	GLN	2.9
9	J	6	ARG	2.9
17	Y	23	THR	2.9
2	b	490	GLN	2.9
17	y	41	VAL	2.9
2	b	82	GLY	2.9
19	Z	53	VAL	2.9
5	e	14	ILE	2.9
20	R	5	VAL	2.8
13	O	60	ARG	2.8
2	b	487	SER	2.8
13	o	36	GLN	2.8
20	R	8	VAL	2.8
1	a	235	TYR	2.8
10	K	16	ALA	2.8
17	Y	27	MET	2.8
3	C	155	ASN	2.8
13	O	206	GLY	2.8
3	C	134	ILE	2.8
13	o	25	THR	2.8
2	B	485	GLU	2.8
2	B	492	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
17	y	43	ARG	2.8
19	Z	2	THR	2.8
7	h	6	TRP	2.8
13	O	23	ASP	2.8
3	c	20	SER	2.7
1	A	12	ASN	2.7
8	I	34	ARG	2.7
20	R	32	GLN	2.7
3	C	257	PHE	2.7
2	b	494	GLY	2.7
8	I	2	GLU	2.7
17	y	22	LEU	2.7
3	c	21	ILE	2.7
20	R	11	PRO	2.7
10	k	13	GLU	2.7
13	o	57	LYS	2.7
19	z	8	ALA	2.7
6	F	16	PHE	2.7
19	z	2	THR	2.7
19	z	9	LEU	2.7
20	R	14	LEU	2.7
2	b	484	PRO	2.7
16	v	14	SER	2.7
17	y	27	MET	2.7
11	l	3	PRO	2.7
13	O	5	LEU	2.7
4	D	11	GLU	2.7
10	k	17	ILE	2.7
15	u	8	GLU	2.7
2	b	373	LYS	2.6
8	i	33	LYS	2.6
13	o	32	ILE	2.6
2	B	491	VAL	2.6
2	b	499	VAL	2.6
13	o	23	ASP	2.6
13	o	24	ASP	2.6
19	z	35	ARG	2.6
16	V	86	GLN	2.6
1	a	260	PHE	2.6
5	e	79	PHE	2.6
2	B	488	PRO	2.6
5	E	83	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	b	295	GLY	2.6
13	o	55	GLU	2.6
10	K	10	LYS	2.6
13	O	59	LYS	2.6
3	C	255	THR	2.6
17	y	23	THR	2.6
2	b	223	GLN	2.6
1	a	248	ILE	2.6
8	i	36	ASP	2.6
13	O	55	GLU	2.6
19	Z	32	ASP	2.6
2	b	290	ALA	2.6
5	E	79	PHE	2.5
18	x	35	ASP	2.5
13	o	34	SER	2.5
20	R	7	VAL	2.5
2	b	505	ARG	2.5
13	o	60	ARG	2.5
2	b	126	PRO	2.5
3	C	462[A]	GLU	2.5
10	k	12	PRO	2.5
7	H	63	LYS	2.5
19	Z	33	TRP	2.5
9	j	2	SER	2.5
1	a	263	ALA	2.5
17	y	26	ALA	2.5
1	A	230	THR	2.5
4	D	136	VAL	2.5
13	o	61	GLN	2.5
16	v	17	LYS	2.5
15	U	8	GLU	2.5
2	b	127	ARG	2.4
5	e	10	PHE	2.4
5	e	83	LEU	2.4
20	R	33	LYS	2.4
5	e	20	TRP	2.4
5	e	18	ARG	2.4
2	B	500	GLY	2.4
3	c	183	GLY	2.4
16	v	16	GLY	2.4
3	C	142	GLU	2.4
13	o	62	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	75	PHE	2.4
5	e	84	LYS	2.4
3	C	245	ILE	2.4
5	e	25	ILE	2.4
19	z	10	ALA	2.4
4	d	24	ARG	2.4
2	b	492	GLU	2.4
19	Z	36	SER	2.4
19	z	50	LEU	2.4
9	j	7	ILE	2.4
13	o	135	SER	2.4
9	j	6	ARG	2.3
1	A	262	TYR	2.3
1	a	246	TYR	2.3
3	c	78	GLU	2.3
13	o	98	GLU	2.3
7	h	57	GLY	2.3
17	y	38	LEU	2.3
18	X	38	GLN	2.3
6	F	44	GLN	2.3
12	M	5	GLN	2.3
7	h	63	LYS	2.3
8	i	35	LYS	2.3
13	o	206	GLY	2.3
2	B	83	GLU	2.3
8	i	38	GLU	2.3
11	L	2	GLU	2.3
4	D	134	ARG	2.2
2	b	500	GLY	2.2
3	C	77	PRO	2.2
5	e	7	GLU	2.2
13	o	95	PHE	2.2
5	e	17	VAL	2.2
18	X	19	VAL	2.2
2	b	503	THR	2.2
13	o	137	THR	2.2
19	z	52	LEU	2.2
3	c	184	GLY	2.2
19	z	11	ALA	2.2
13	o	38	TYR	2.2
16	v	26	TYR	2.2
20	R	29	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	78	GLU	2.2
11	L	3	PRO	2.2
6	F	13	TYR	2.2
7	h	18	TYR	2.2
3	C	259	TRP	2.2
19	Z	35	ARG	2.2
19	z	18	VAL	2.2
13	O	25	THR	2.2
17	y	40	ALA	2.2
8	i	34	ARG	2.2
3	C	105	VAL	2.1
3	c	255	THR	2.1
9	J	15	VAL	2.1
13	O	87	VAL	2.1
16	V	18	THR	2.1
19	Z	56	VAL	2.1
13	O	89	SER	2.1
19	z	29	SER	2.1
16	V	6	GLU	2.1
13	O	63	ALA	2.1
6	F	17	THR	2.1
13	o	83	GLY	2.1
15	U	70	ARG	2.1
19	z	43	GLY	2.1
13	o	67	PRO	2.1
13	o	199	LEU	2.1
18	X	5	PRO	2.1
19	Z	42	LEU	2.1
17	Y	26	ALA	2.1
20	R	30	GLN	2.1
3	c	257	PHE	2.1
3	C	143	TYR	2.1
3	c	131	TYR	2.1
13	o	141	ASP	2.1
2	B	487	SER	2.1
3	c	145	SER	2.1
2	B	489	GLU	2.1
2	b	83	GLU	2.1
13	o	21	THR	2.1
3	c	155	ASN	2.1
19	z	23	VAL	2.1
5	E	82	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
18	x	15	LEU	2.1
2	B	290	ALA	2.1
19	z	28	ALA	2.1
20	R	16	ALA	2.1
13	O	141	ASP	2.1
2	b	485	GLU	2.0
3	c	146	PHE	2.0
1	a	264	SER	2.0
5	E	11	SER	2.0
5	e	32	ILE	2.0
13	o	181[A]	GLU	2.0
15	u	66	GLY	2.0
5	e	82	GLN	2.0
19	z	39	LEU	2.0
3	c	246	ALA	2.0
17	y	24	MET	2.0
13	o	243	ILE	2.0
3	C	192	GLY	2.0
3	C	254	THR	2.0
17	y	44	GLY	2.0
3	c	106	VAL	2.0
10	k	27	VAL	2.0
17	Y	41	VAL	2.0
19	z	54	VAL	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
12	FME	m	1	10/11	0.92	0.15	13,32,67,68	0
14	FME	t	1	10/11	0.93	0.09	12,22,31,68	0
14	FME	T	1	10/11	0.95	0.09	18,26,40,49	0
12	FME	M	1	10/11	0.95	0.14	23,36,70,74	0
8	FME	I	1	10/11	0.96	0.08	22,34,38,38	0
8	FME	i	1	10/11	0.97	0.08	21,31,39,42	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, 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
29	LMT	f	103	35/35	0.65	0.21	43,86,107,111	0
36	DGD	D	405	62/66	0.65	0.22	48,79,113,122	0
29	LMT	E	102	35/35	0.68	0.22	43,80,109,115	0
29	LMT	C	522	35/35	0.70	0.21	52,81,102,104	0
36	DGD	d	406	62/66	0.70	0.23	38,89,122,130	0
33	CA	b	604	1/1	0.71	0.19	117,117,117,117	0
28	GOL	v	203	6/6	0.72	0.22	39,74,86,87	0
34	LMG	z	101	39/55	0.72	0.24	45,82,99,107	0
29	LMT	b	625	25/35	0.72	0.20	44,67,109,119	0
28	GOL	V	203	6/6	0.72	0.23	50,64,71,72	0
37	LHG	e	101	42/49	0.72	0.22	52,89,118,129	0
28	GOL	B	637	6/6	0.73	0.23	51,72,83,86	0
32	UNL	B	635	33/-	0.74	0.23	33,58,102,102	0
29	LMT	m	102	35/35	0.74	0.19	33,61,79,95	0
28	GOL	O	302	6/6	0.75	0.14	49,55,57,61	0
35	HTG	B	626	19/19	0.75	0.18	48,81,94,95	0
32	UNL	b	634	33/-	0.75	0.23	29,62,111,117	0
32	UNL	m	101	10/-	0.75	0.22	35,50,55,61	0
32	UNL	A	420	28/-	0.75	0.22	50,71,78,86	0
35	HTG	d	412	16/19	0.76	0.19	38,78,97,98	0
35	HTG	B	634	19/19	0.76	0.17	32,76,109,127	0
35	HTG	c	923	19/19	0.77	0.16	45,80,94,97	0
32	UNL	I	101	40/-	0.77	0.22	27,62,110,120	0
32	UNL	K	101	34/-	0.77	0.19	37,61,83,88	0
35	HTG	D	411	16/19	0.77	0.20	38,102,111,112	0
35	HTG	b	627	19/19	0.77	0.17	49,86,110,116	0
32	UNL	M	102	10/-	0.78	0.19	28,38,57,58	0
34	LMG	C	521	51/55	0.78	0.18	32,69,88,108	0
32	UNL	c	926	32/-	0.78	0.23	39,79,98,105	0
32	UNL	a	418	30/-	0.78	0.22	42,66,98,106	0
32	UNL	i	101	40/-	0.79	0.21	28,62,105,117	0
29	LMT	m	104	35/35	0.79	0.18	29,59,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	HTG	c	922	19/19	0.80	0.17	43,67,84,95	0
28	GOL	C	525	6/6	0.80	0.16	32,41,61,69	0
32	UNL	j	102	10/-	0.80	0.21	47,57,63,63	0
29	LMT	c	921	35/35	0.80	0.18	46,76,97,104	0
32	UNL	J	102	10/-	0.80	0.23	39,51,64,67	0
27	SQD	a	402	54/54	0.80	0.16	29,55,76,90	0
35	HTG	b	603	19/19	0.81	0.18	46,84,110,111	0
29	LMT	a	401	35/35	0.81	0.18	21,53,74,80	0
29	LMT	A	417	35/35	0.81	0.17	22,57,79,97	0
34	LMG	Z	101	37/55	0.81	0.21	30,75,96,112	0
32	UNL	d	411	36/-	0.81	0.19	32,56,104,111	0
27	SQD	L	102	54/54	0.81	0.19	24,52,86,91	0
28	GOL	v	204	6/6	0.81	0.17	54,66,71,80	0
32	UNL	D	410	40/-	0.81	0.21	24,54,93,101	0
31	PL9	a	417	55/55	0.82	0.22	41,73,92,99	0
28	GOL	B	628	6/6	0.82	0.17	33,42,54,72	0
37	LHG	E	101	42/49	0.82	0.17	22,63,78,93	0
29	LMT	B	623	35/35	0.82	0.17	26,74,96,101	0
29	LMT	B	636	25/35	0.83	0.21	24,61,106,122	0
27	SQD	A	416	54/54	0.83	0.17	26,51,78,85	0
35	HTG	C	524	19/19	0.83	0.15	41,69,99,100	0
28	GOL	b	632	6/6	0.83	0.19	38,52,59,59	0
35	HTG	V	202	19/19	0.83	0.18	40,59,77,163	0
34	LMG	c	920	51/55	0.83	0.17	33,74,88,93	0
28	GOL	T	103	6/6	0.83	0.22	52,68,70,79	0
27	SQD	f	102	43/54	0.84	0.18	41,75,103,108	0
34	LMG	a	412	51/55	0.84	0.18	33,62,84,90	0
28	GOL	a	415	6/6	0.85	0.16	48,62,65,66	0
28	GOL	B	631	6/6	0.85	0.19	30,48,62,65	0
34	LMG	C	501	51/55	0.85	0.15	34,56,76,85	0
28	GOL	c	925	6/6	0.85	0.19	34,52,63,66	0
31	PL9	A	419	55/55	0.85	0.19	28,56,91,98	0
28	GOL	t	102	6/6	0.85	0.20	22,59,67,67	0
29	LMT	M	101	35/35	0.85	0.15	23,52,69,77	0
28	GOL	T	101	6/6	0.85	0.20	54,60,61,69	0
32	UNL	d	413	18/-	0.85	0.18	30,52,81,84	0
28	GOL	A	414	6/6	0.85	0.15	30,40,43,49	0
27	SQD	B	621	54/54	0.85	0.16	26,55,94,104	0
28	GOL	A	415	6/6	0.86	0.17	36,49,64,64	0
32	UNL	D	409	17/-	0.86	0.15	30,40,63,66	0
24	CLA	c	914	65/65	0.86	0.15	35,48,81,87	0
28	GOL	V	206	6/6	0.86	0.15	47,63,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMT	m	103	35/35	0.86	0.13	19,48,62,74	0
28	GOL	a	413	6/6	0.86	0.12	30,32,37,42	0
28	GOL	B	629	6/6	0.86	0.17	28,42,50,56	0
29	LMT	b	601	25/35	0.86	0.20	18,55,104,111	0
27	SQD	F	101	43/54	0.86	0.17	34,59,81,90	0
32	UNL	d	410	17/-	0.87	0.16	34,48,82,82	0
28	GOL	F	103	6/6	0.87	0.15	60,65,71,71	0
33	CA	B	601	1/1	0.87	0.09	83,83,83,83	0
35	HTG	C	523	19/19	0.87	0.16	54,62,86,88	0
35	HTG	b	626	19/19	0.88	0.19	30,50,86,86	0
32	UNL	X	101	18/-	0.88	0.16	29,44,62,79	0
34	LMG	C	520	51/55	0.88	0.16	22,52,72,90	0
24	CLA	b	605	65/65	0.89	0.14	29,48,89,102	0
34	LMG	c	919	51/55	0.89	0.16	29,57,78,81	0
28	GOL	f	101	6/6	0.89	0.14	44,50,62,64	0
26	BCR	k	101	40/40	0.89	0.13	34,45,63,75	0
35	HTG	B	633	19/19	0.90	0.12	28,54,70,76	0
35	HTG	b	602	19/19	0.90	0.13	29,45,65,68	0
27	SQD	a	411	54/54	0.90	0.15	32,52,73,81	0
28	GOL	B	632	6/6	0.90	0.14	24,40,53,57	0
35	HTG	B	625	19/19	0.90	0.17	28,43,74,86	0
28	GOL	B	627	6/6	0.90	0.17	23,36,45,72	0
33	CA	f	104	1/1	0.91	0.09	77,77,77,77	0
34	LMG	B	622	51/55	0.91	0.11	19,32,49,71	0
24	CLA	c	913	65/65	0.91	0.11	31,40,59,65	0
24	CLA	C	507	65/65	0.91	0.12	25,40,75,77	0
26	BCR	C	515	40/40	0.91	0.11	29,38,49,53	0
26	BCR	K	103	40/40	0.91	0.09	24,30,40,43	0
28	GOL	b	628	6/6	0.91	0.10	30,35,42,53	0
34	LMG	b	624	51/55	0.91	0.11	21,36,57,81	0
28	GOL	b	631	6/6	0.91	0.12	28,41,48,51	0
26	BCR	c	915	40/40	0.91	0.10	25,34,42,45	0
26	BCR	d	404	40/40	0.91	0.11	27,36,54,60	0
28	GOL	A	413	6/6	0.91	0.10	23,30,33,36	0
26	BCR	h	101	40/40	0.91	0.10	25,35,48,52	0
24	CLA	C	513	65/65	0.91	0.11	27,40,59,71	0
24	CLA	B	602	65/65	0.91	0.13	22,40,80,101	0
26	BCR	k	102	40/40	0.92	0.10	30,37,50,61	0
26	BCR	y	101	40/40	0.92	0.11	29,37,57,63	0
28	GOL	b	629	6/6	0.92	0.12	27,36,50,54	0
28	GOL	b	630	6/6	0.92	0.11	35,39,50,53	0
27	SQD	A	412	54/54	0.92	0.13	15,45,72,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	K	102	40/40	0.92	0.09	22,30,39,47	0
28	GOL	b	633	6/6	0.92	0.14	34,60,65,65	0
34	LMG	j	101	51/55	0.92	0.13	25,35,71,81	0
24	CLA	C	514	65/65	0.92	0.11	30,42,67,73	0
24	CLA	c	902	65/65	0.92	0.10	26,32,45,52	0
28	GOL	o	302	6/6	0.92	0.11	44,50,53,58	0
26	BCR	B	620	40/40	0.92	0.09	16,26,39,49	0
24	CLA	c	907	65/65	0.92	0.13	28,37,64,72	0
26	BCR	H	101	40/40	0.92	0.10	19,32,45,59	0
24	CLA	c	912	65/65	0.93	0.10	27,36,50,54	0
26	BCR	T	102	40/40	0.93	0.08	13,26,37,42	0
24	CLA	b	610	65/65	0.93	0.11	18,31,78,87	0
24	CLA	C	512	65/65	0.93	0.09	22,30,39,45	0
24	CLA	d	403	65/65	0.93	0.11	26,31,79,93	0
34	LMG	J	101	51/55	0.93	0.12	18,32,75,81	0
25	PHO	a	420	64/64	0.93	0.08	17,24,30,33	0
24	CLA	c	904	65/65	0.93	0.09	26,33,44,47	0
26	BCR	t	101	40/40	0.93	0.09	12,26,45,48	0
24	CLA	c	905	65/65	0.93	0.09	25,32,49,68	0
31	PL9	d	405	55/55	0.93	0.08	13,19,33,44	0
26	BCR	C	516	40/40	0.93	0.09	23,32,42,43	0
28	GOL	B	630	6/6	0.93	0.10	26,32,40,42	0
36	DGD	c	916	62/66	0.93	0.11	22,31,64,82	0
36	DGD	c	917	62/66	0.93	0.11	26,35,61,87	0
26	BCR	D	403	40/40	0.93	0.10	19,30,58,70	0
36	DGD	h	102	62/66	0.93	0.10	19,31,48,60	0
24	CLA	c	906	65/65	0.93	0.10	21,28,44,56	0
37	LHG	d	407	49/49	0.93	0.11	15,31,44,53	0
37	LHG	d	409	49/49	0.93	0.14	21,32,85,88	0
24	CLA	C	504	65/65	0.93	0.08	22,28,40,45	0
37	LHG	l	101	49/49	0.93	0.10	15,27,39,56	0
22	CL	U	201	1/1	0.94	0.09	50,50,50,50	0
28	GOL	V	204	6/6	0.94	0.11	19,26,30,37	0
28	GOL	V	205	6/6	0.94	0.08	34,41,45,52	0
31	PL9	D	404	55/55	0.94	0.08	11,18,31,41	0
24	CLA	C	508	65/65	0.94	0.09	23,35,47,54	0
24	CLA	C	510	65/65	0.94	0.09	23,30,45,62	0
28	GOL	a	414	6/6	0.94	0.12	25,34,43,53	0
24	CLA	C	511	65/65	0.94	0.09	21,29,38,45	0
24	CLA	c	908	65/65	0.94	0.09	26,33,49,60	0
24	CLA	c	910	65/65	0.94	0.09	27,34,47,53	0
24	CLA	c	911	65/65	0.94	0.09	24,31,43,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	615	65/65	0.94	0.10	12,21,66,79	0
24	CLA	B	617	65/65	0.94	0.12	16,28,79,88	0
24	CLA	C	502	65/65	0.94	0.09	22,30,42,54	0
24	CLA	a	407	65/65	0.94	0.11	18,23,72,84	0
23	BCT	a	419	4/4	0.94	0.12	21,32,41,50	0
26	BCR	A	411	40/40	0.94	0.08	15,22,29,31	0
26	BCR	B	619	40/40	0.94	0.08	15,23,46,49	0
24	CLA	b	606	65/65	0.94	0.08	22,28,38,48	0
24	CLA	C	505	65/65	0.94	0.09	18,27,47,61	0
24	CLA	b	613	65/65	0.94	0.08	23,29,42,48	0
24	CLA	b	614	65/65	0.94	0.08	20,29,39,42	0
36	DGD	C	517	62/66	0.94	0.10	19,28,60,72	0
36	DGD	C	518	62/66	0.94	0.11	19,29,78,90	0
24	CLA	b	615	65/65	0.94	0.08	17,22,38,46	0
36	DGD	H	102	62/66	0.94	0.09	16,28,46,59	0
24	CLA	b	618	65/65	0.94	0.11	14,24,78,80	0
24	CLA	b	619	65/65	0.94	0.09	20,30,49,51	0
36	DGD	c	918	62/66	0.94	0.10	25,31,52,70	0
24	CLA	b	620	65/65	0.94	0.12	19,33,77,78	0
26	BCR	a	410	40/40	0.94	0.07	15,23,28,32	0
37	LHG	D	406	49/49	0.94	0.10	14,26,38,52	0
37	LHG	D	408	49/49	0.94	0.15	17,29,88,100	0
26	BCR	b	621	40/40	0.94	0.07	14,24,33,38	0
26	BCR	b	622	40/40	0.94	0.08	14,24,43,51	0
26	BCR	b	623	40/40	0.94	0.09	18,31,42,48	0
24	CLA	C	506	65/65	0.94	0.09	18,27,47,54	0
24	CLA	c	903	65/65	0.94	0.09	24,30,41,51	0
28	GOL	C	526	6/6	0.95	0.07	17,21,26,26	0
24	CLA	b	609	65/65	0.95	0.08	16,24,37,44	0
24	CLA	B	608	65/65	0.95	0.07	11,19,28,40	0
24	CLA	b	611	65/65	0.95	0.07	13,20,31,34	0
35	HTG	O	303	19/19	0.95	0.11	23,32,46,55	0
24	CLA	b	612	65/65	0.95	0.07	21,28,40,43	0
24	CLA	d	402	65/65	0.95	0.08	16,20,36,46	0
24	CLA	B	609	65/65	0.95	0.07	15,24,30,36	0
25	PHO	A	408	64/64	0.95	0.07	12,16,23,24	0
25	PHO	a	408	64/64	0.95	0.07	15,18,27,30	0
33	CA	F	102	1/1	0.95	0.08	69,69,69,69	0
24	CLA	B	610	65/65	0.95	0.08	17,24,36,45	0
24	CLA	C	509	65/65	0.95	0.09	18,25,67,82	0
26	BCR	B	618	40/40	0.95	0.07	11,23,32,35	0
24	CLA	b	616	65/65	0.95	0.07	16,23,32,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	DGD	C	519	62/66	0.95	0.09	18,29,48,55	0
24	CLA	b	617	65/65	0.95	0.08	14,22,44,52	0
24	CLA	B	611	65/65	0.95	0.07	17,25,33,50	0
24	CLA	B	613	65/65	0.95	0.07	13,20,27,33	0
24	CLA	B	614	65/65	0.95	0.08	12,20,43,55	0
22	CL	v	201	1/1	0.95	0.07	62,62,62,62	0
23	BCT	A	404	4/4	0.95	0.13	21,24,36,47	0
24	CLA	D	402	65/65	0.95	0.10	18,27,68,84	0
24	CLA	B	603	65/65	0.95	0.07	17,24,36,47	0
24	CLA	a	409	65/65	0.95	0.12	18,26,79,83	0
24	CLA	B	606	65/65	0.95	0.07	13,20,31,41	0
35	HTG	B	624	19/19	0.95	0.09	20,32,43,46	0
24	CLA	B	607	65/65	0.95	0.10	16,25,70,76	0
24	CLA	c	909	65/65	0.95	0.10	23,28,67,91	0
24	CLA	b	607	65/65	0.95	0.08	21,28,38,50	0
38	HEM	e	102	43/43	0.95	0.13	37,46,76,95	0
24	CLA	B	604	65/65	0.96	0.07	16,25,32,38	0
24	CLA	b	608	65/65	0.96	0.08	15,23,51,62	0
24	CLA	C	503	65/65	0.96	0.07	20,25,39,63	0
24	CLA	d	401	65/65	0.96	0.07	14,18,27,47	0
24	CLA	B	605	65/65	0.96	0.08	13,19,44,57	0
28	GOL	v	205	6/6	0.96	0.12	23,35,46,50	0
24	CLA	B	612	65/65	0.96	0.06	12,18,30,37	0
24	CLA	D	401	65/65	0.96	0.06	12,16,32,36	0
25	PHO	A	409	64/64	0.96	0.06	13,20,29,35	0
37	LHG	D	407	49/49	0.96	0.08	13,22,44,57	0
24	CLA	A	407	65/65	0.96	0.09	13,20,71,73	0
24	CLA	a	406	65/65	0.96	0.07	15,17,32,38	0
37	LHG	L	101	49/49	0.96	0.08	12,26,38,46	0
24	CLA	A	410	65/65	0.96	0.10	17,26,80,89	0
37	LHG	d	408	49/49	0.96	0.08	15,23,41,54	0
24	CLA	A	405	65/65	0.96	0.07	13,17,27,52	0
24	CLA	B	616	65/65	0.96	0.08	16,23,42,45	0
33	CA	O	301	1/1	0.96	0.07	53,53,53,53	0
24	CLA	A	406	65/65	0.96	0.07	12,16,30,35	0
38	HEM	E	103	43/43	0.97	0.09	23,35,45,56	0
28	GOL	c	924	6/6	0.97	0.07	24,24,25,29	0
39	MG	j	103	1/1	0.97	0.09	33,33,33,33	0
40	HEC	V	201	43/43	0.97	0.08	22,25,32,39	0
40	HEC	v	202	43/43	0.97	0.08	28,31,40,46	0
33	CA	c	901	1/1	0.98	0.05	44,44,44,44	0
21	FE2	a	403	1/1	0.99	0.04	28,28,28,28	0

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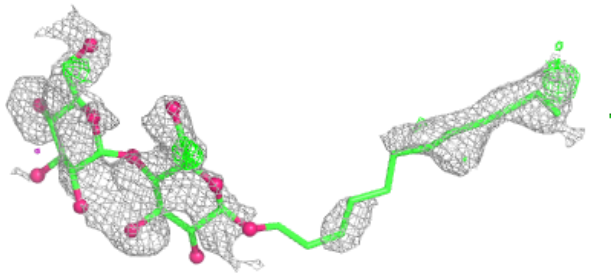
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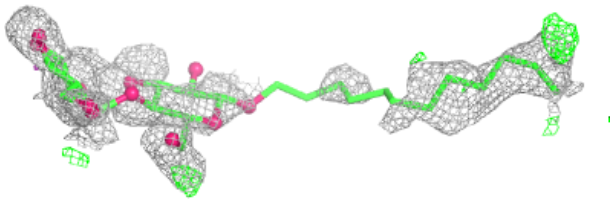
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	CA	o	301	1/1	0.99	0.04	54,54,54,54	0
30	OEX	A	418	10/10	0.99	0.04	15,20,24,28	0
30	OEX	a	416	10/10	0.99	0.04	18,21,24,34	0
39	MG	J	103	1/1	0.99	0.07	27,27,27,27	0
22	CL	a	404	1/1	0.99	0.04	20,20,20,20	0
22	CL	a	405	1/1	0.99	0.03	26,26,26,26	0
22	CL	A	402	1/1	0.99	0.03	18,18,18,18	0
22	CL	A	403	1/1	1.00	0.03	19,19,19,19	0
21	FE2	A	401	1/1	1.00	0.02	24,24,24,24	0

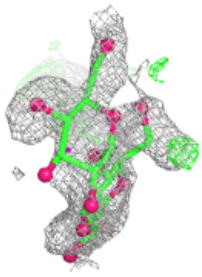
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT f 103:

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

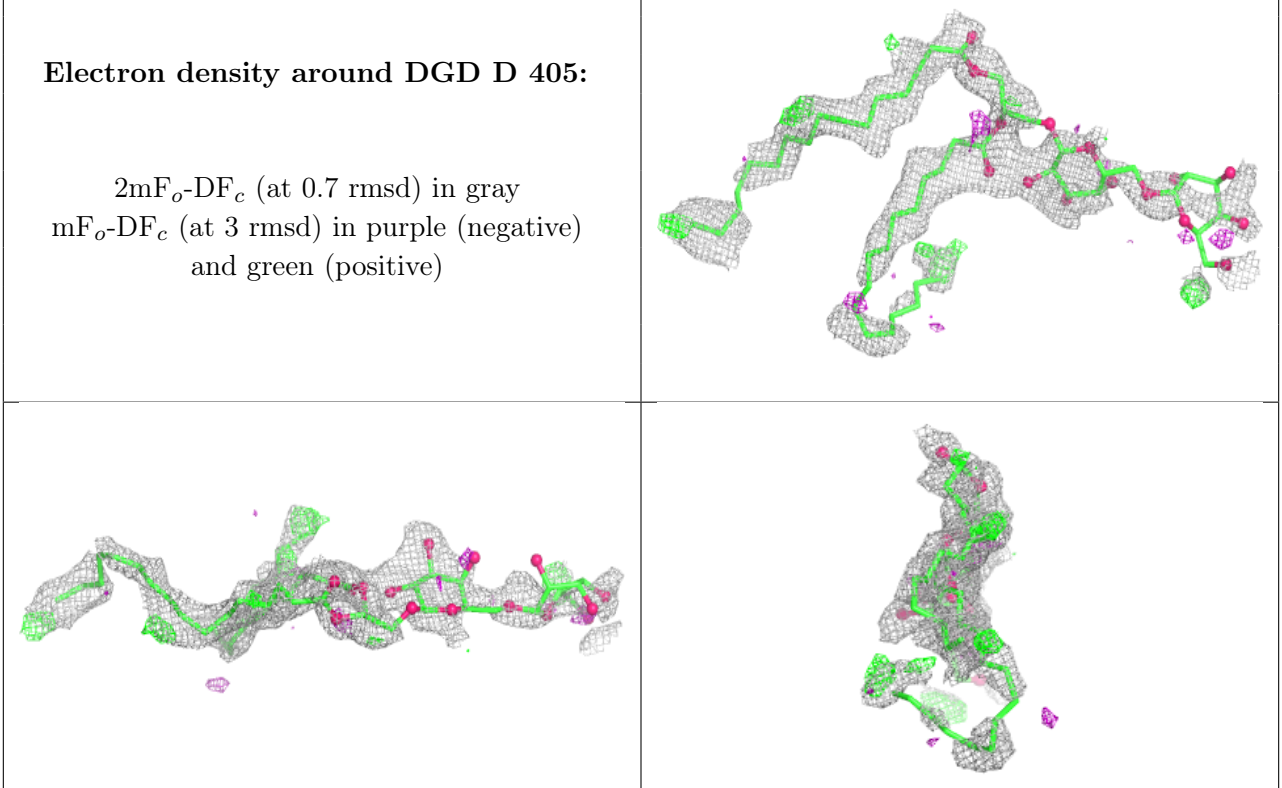






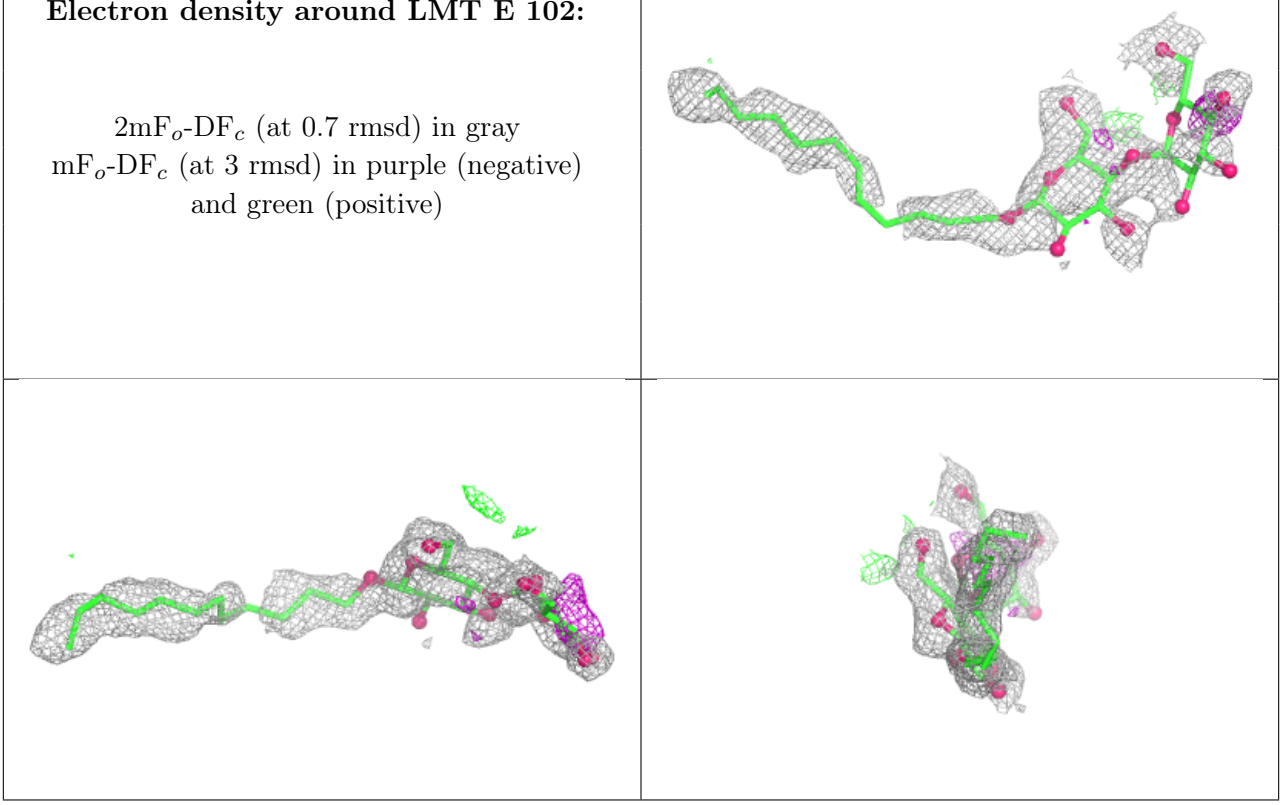
Electron density around DGD D 405:

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



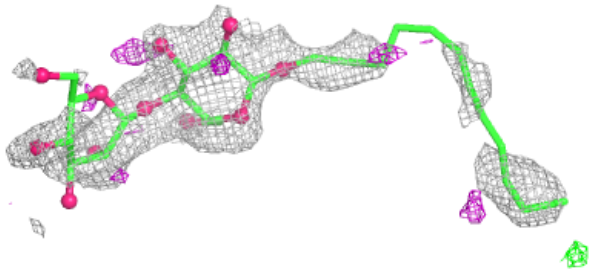
Electron density around LMT E 102:

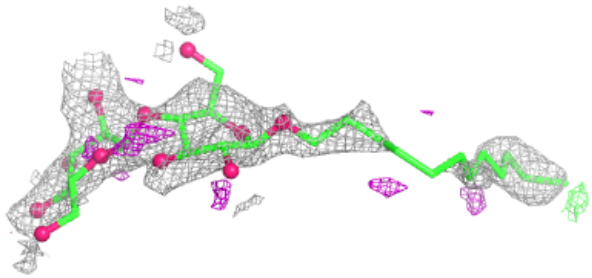
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

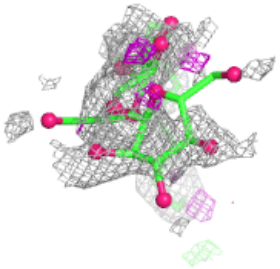


Electron density around LMT C 522:

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

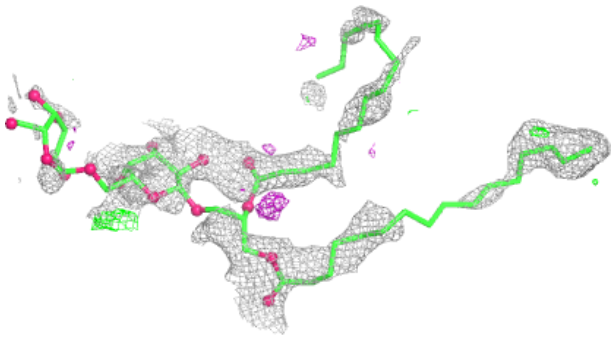


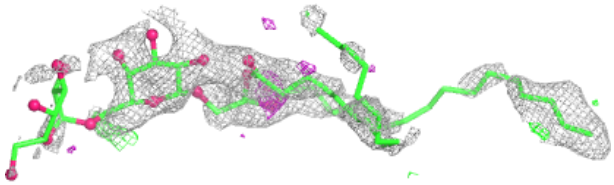


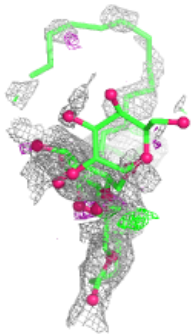


Electron density around DGD d 406:

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

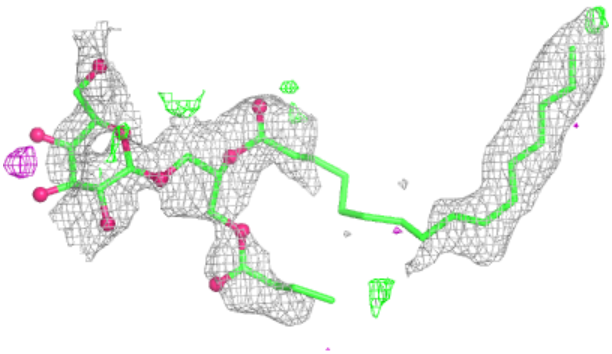


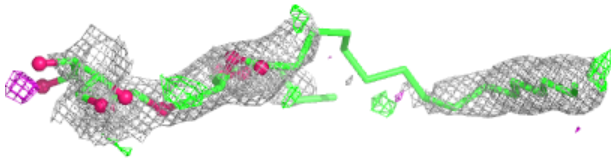


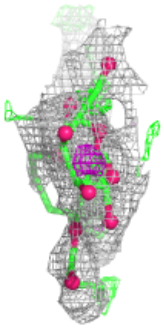


Electron density around LMG z 101:

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

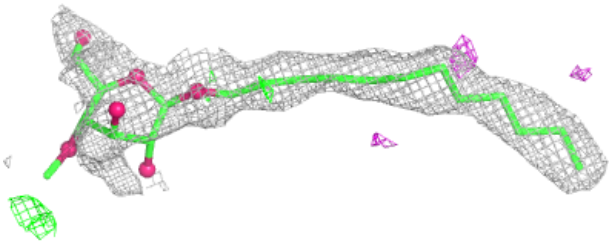


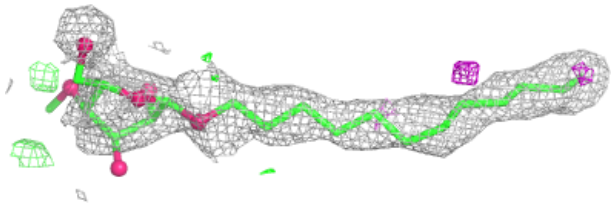


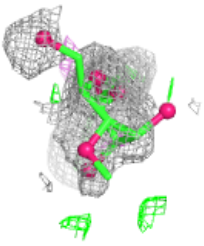


Electron density around LMT b 625:

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

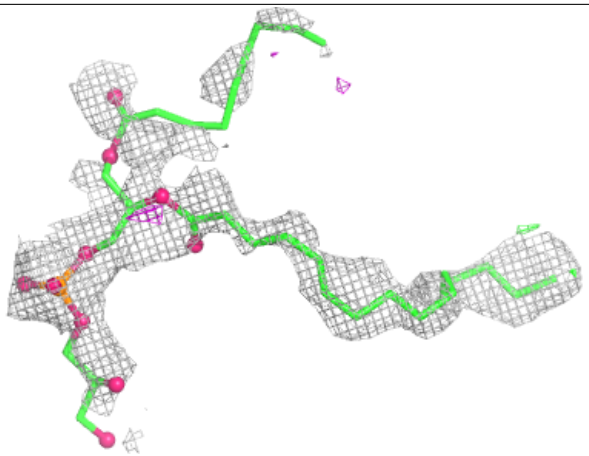


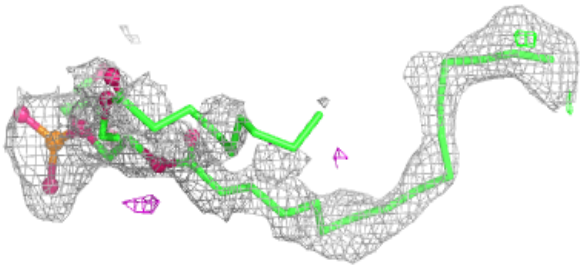




Electron density around LHG e 101:

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

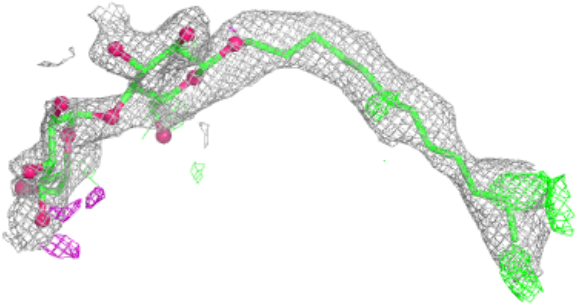


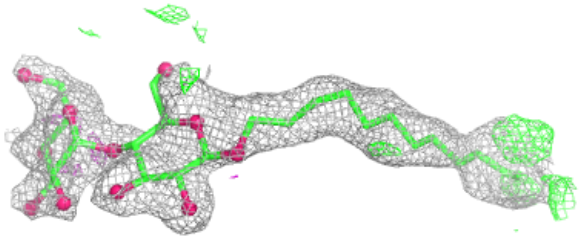


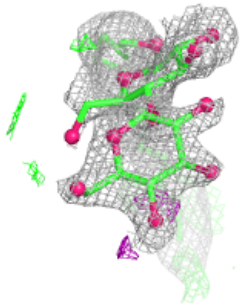


Electron density around LMT m 102:

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

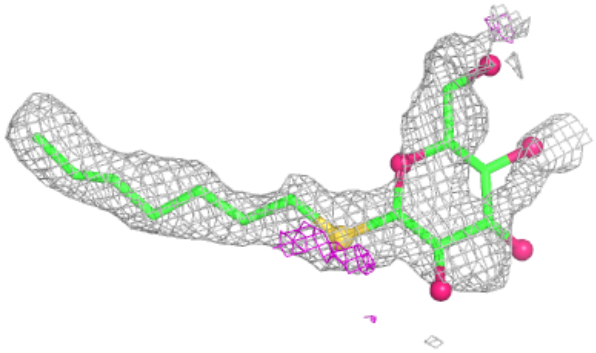


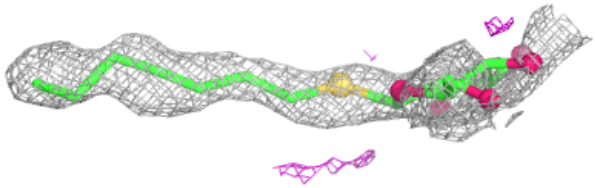


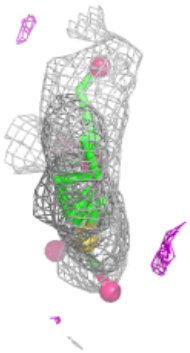


Electron density around HTG B 626:

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

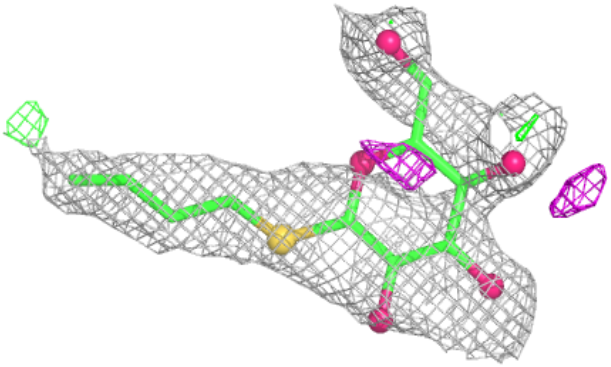


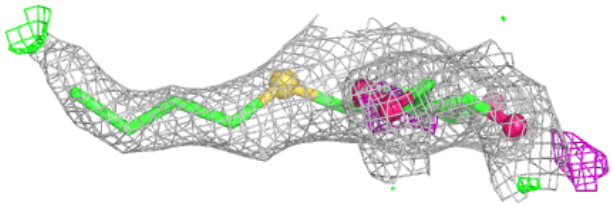


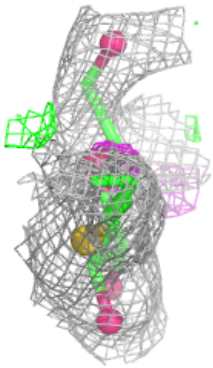


Electron density around HTG d 412:

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

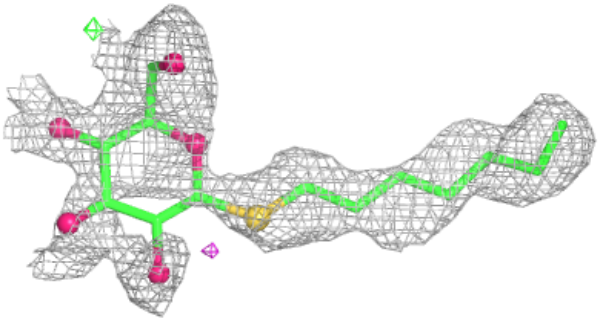


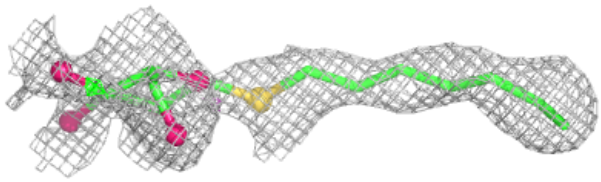


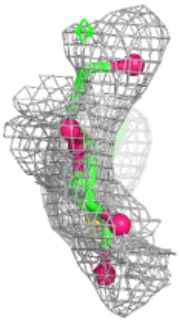


Electron density around HTG B 634:

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

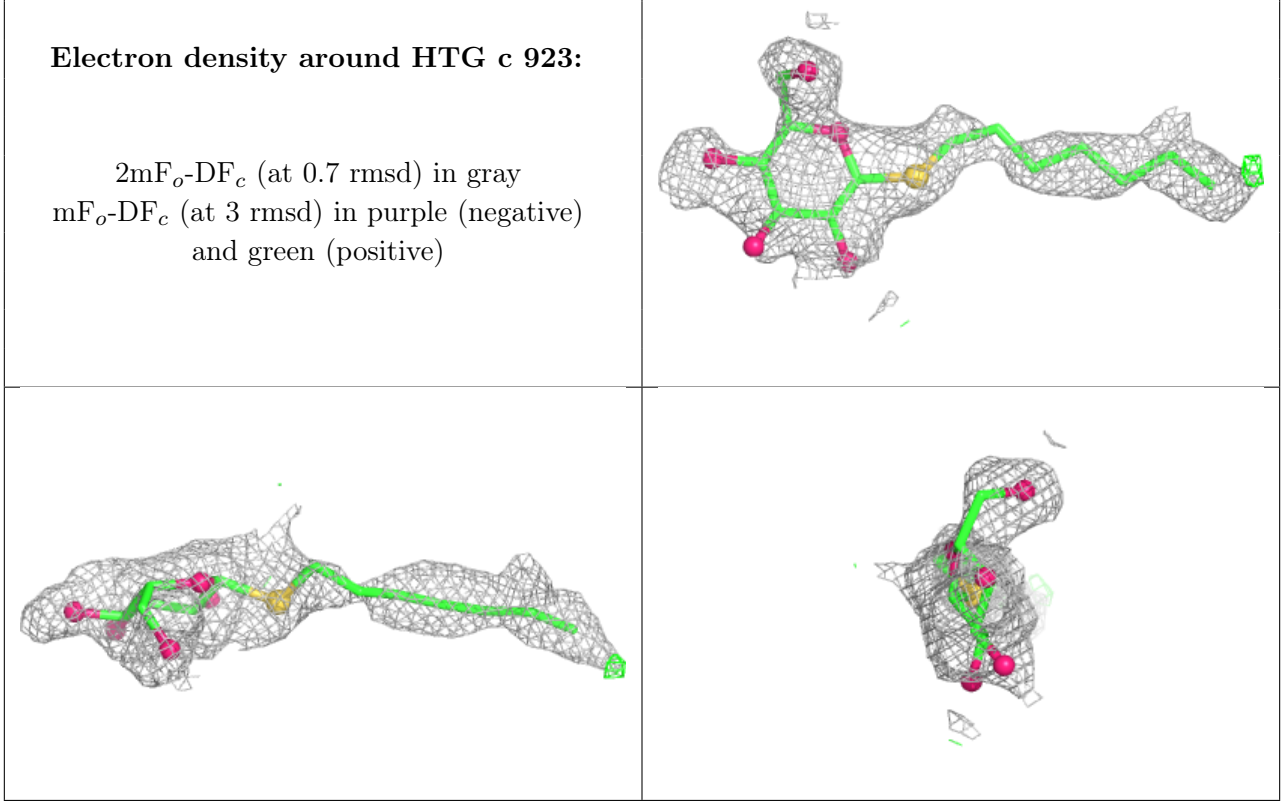






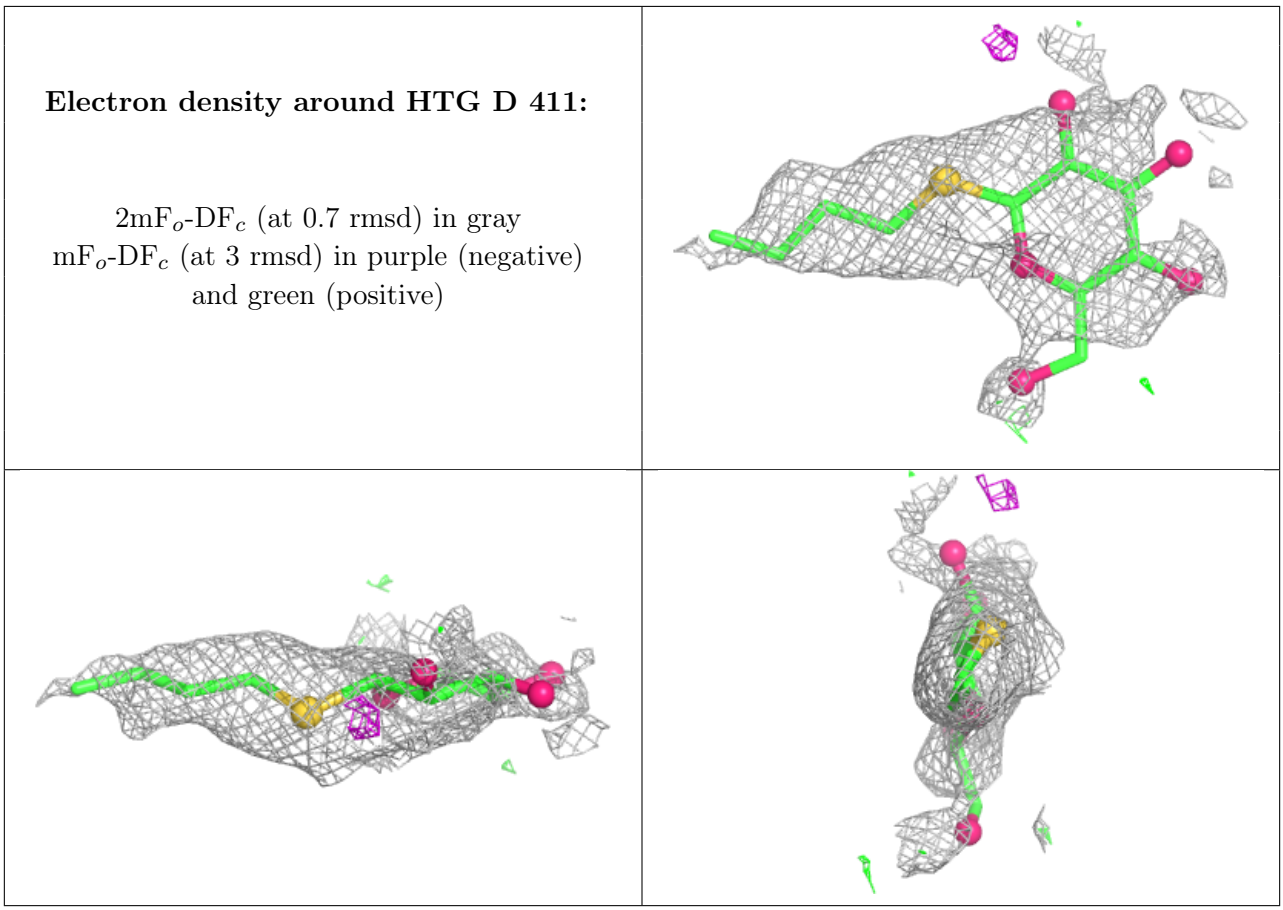
Electron density around HTG c 923:

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



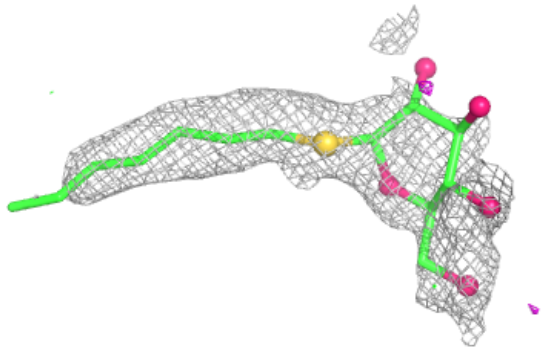
Electron density around HTG D 411:

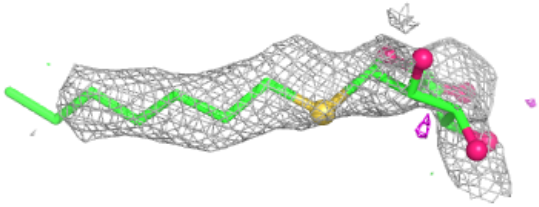
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

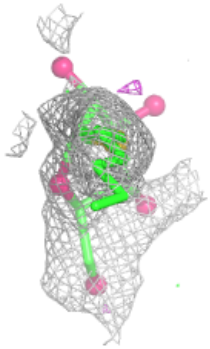


Electron density around HTG b 627:

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

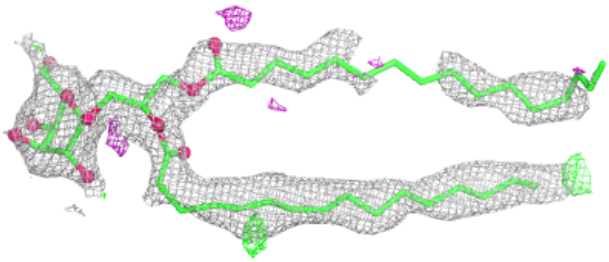


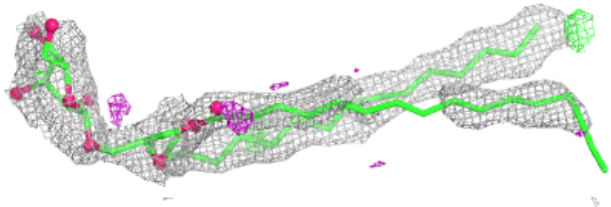


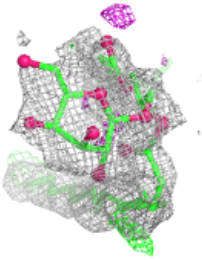


Electron density around LMG C 521:

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

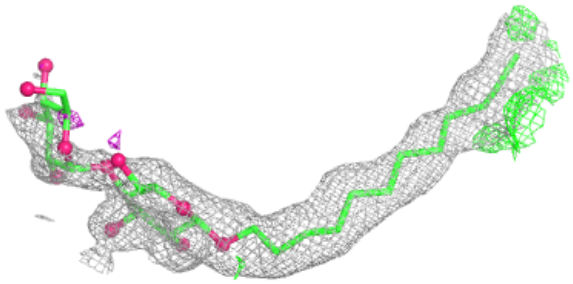


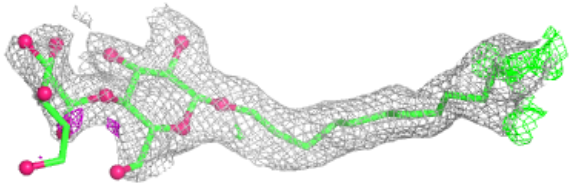


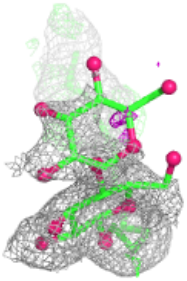


Electron density around LMT m 104:

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

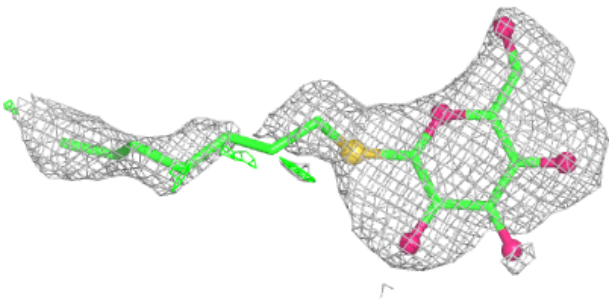


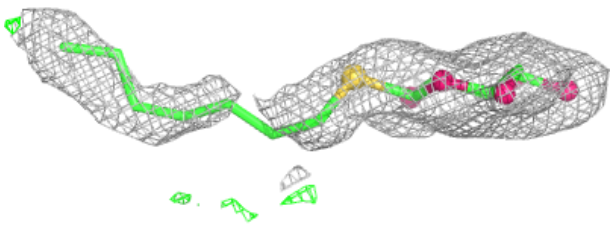


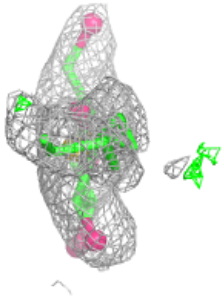


Electron density around HTG c 922:

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

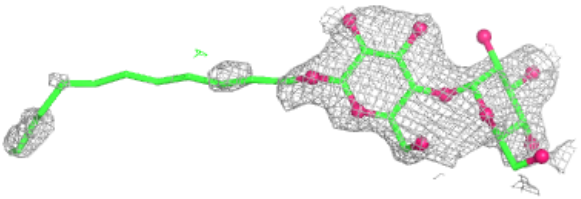


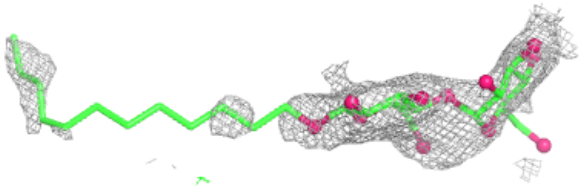


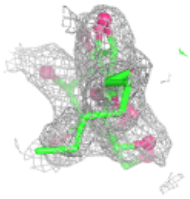


Electron density around LMT c 921:

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

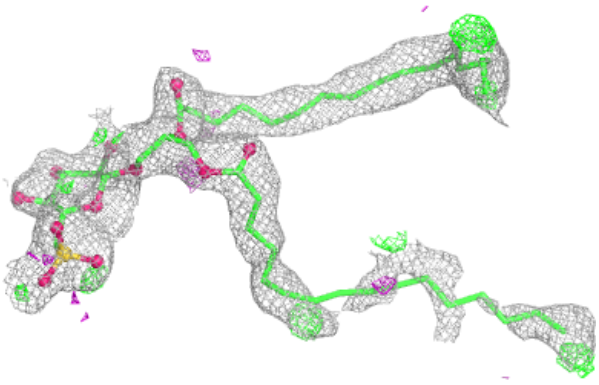


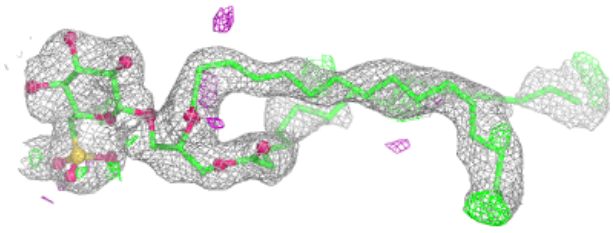


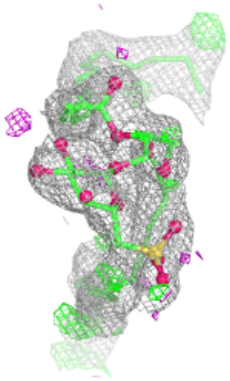


Electron density around SQD a 402:

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

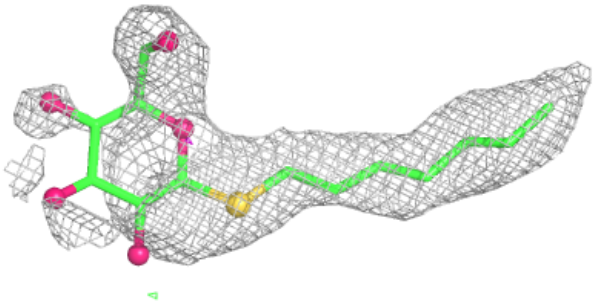


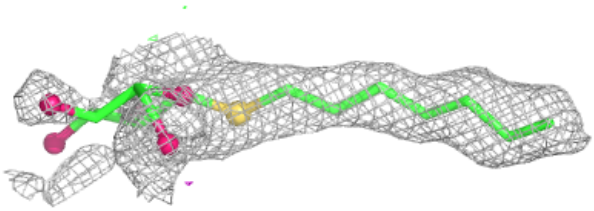


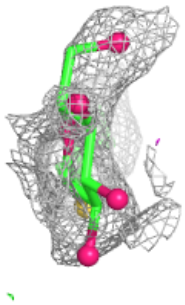


Electron density around HTG b 603:

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

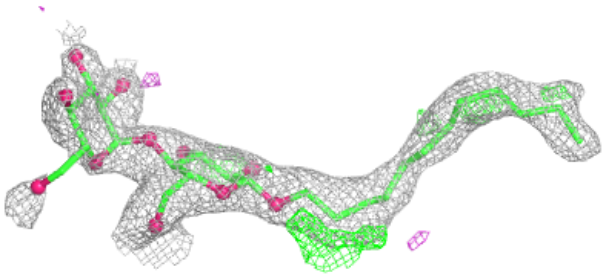


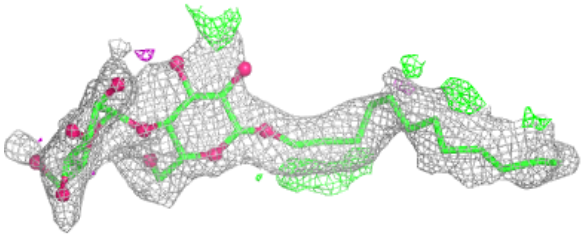


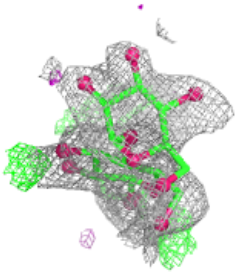


Electron density around LMT a 401:

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

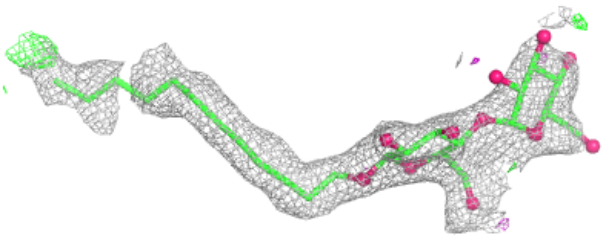


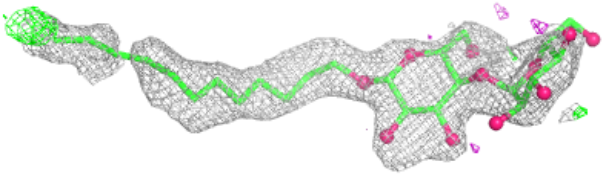


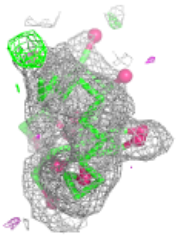


Electron density around LMT A 417:

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

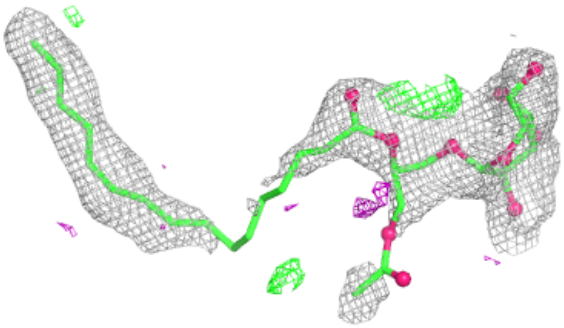


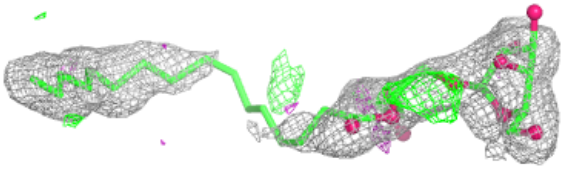


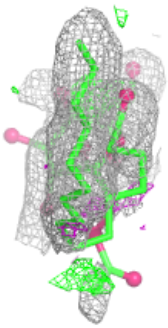


Electron density around LMG Z 101:

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

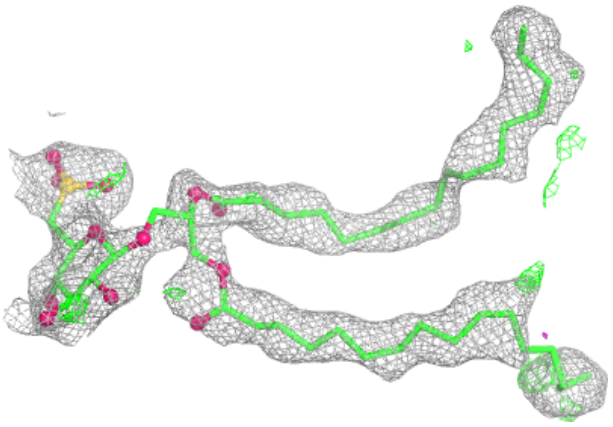


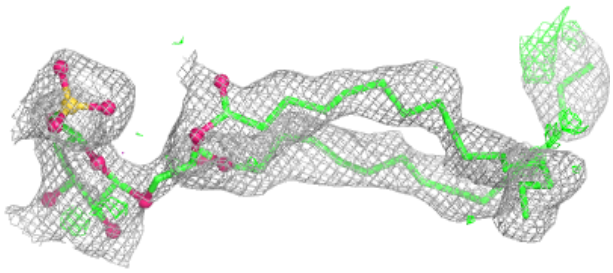




Electron density around SQD L 102:

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

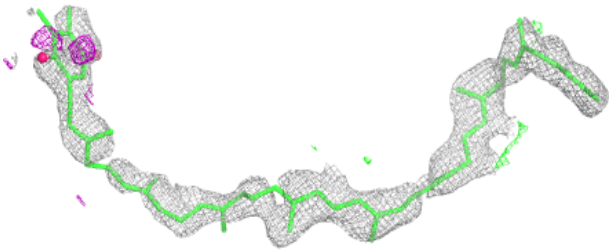


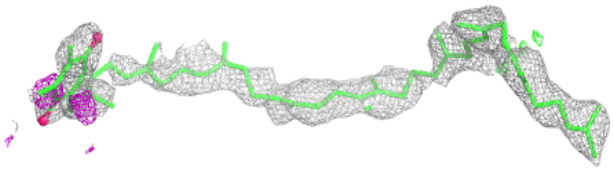


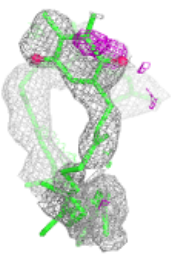


Electron density around PL9 a 417:

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

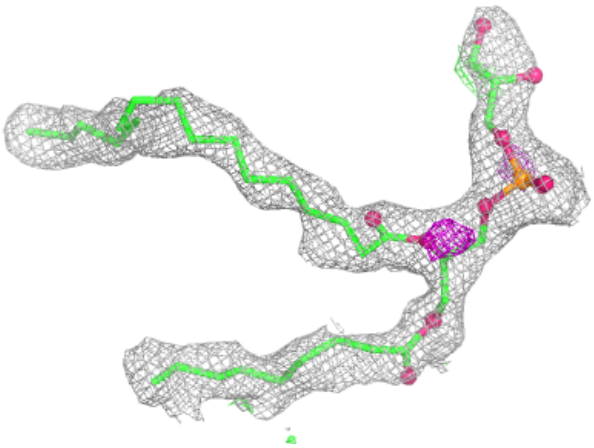


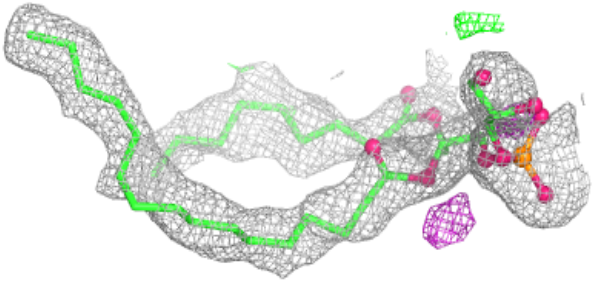


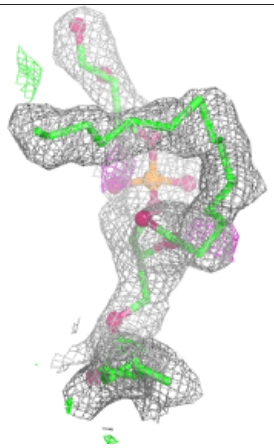


Electron density around LHG E 101:

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

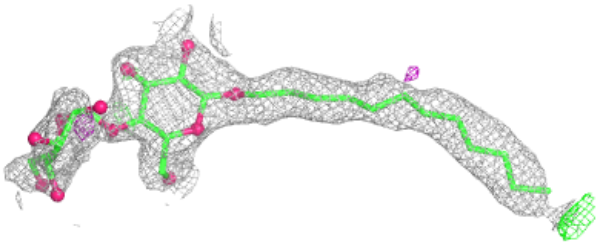


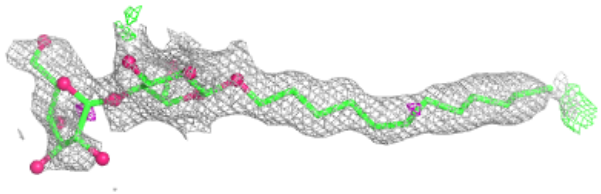


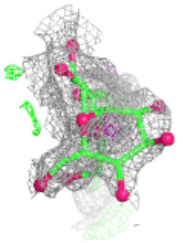


Electron density around LMT B 623:

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

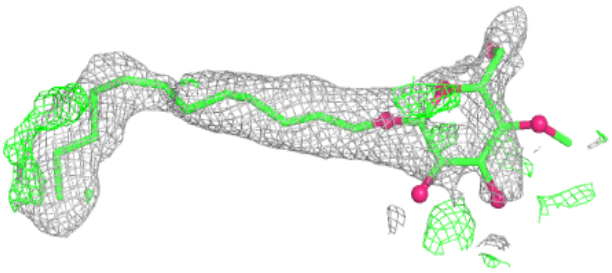


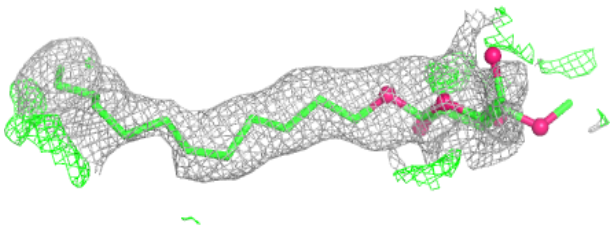


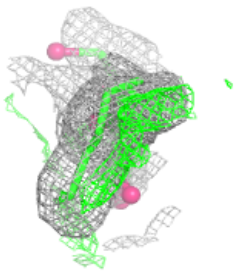


Electron density around LMT B 636:

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

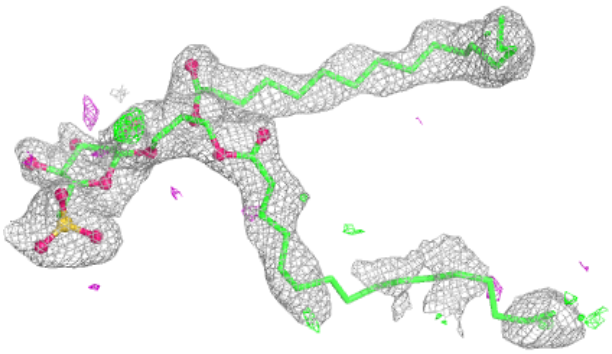


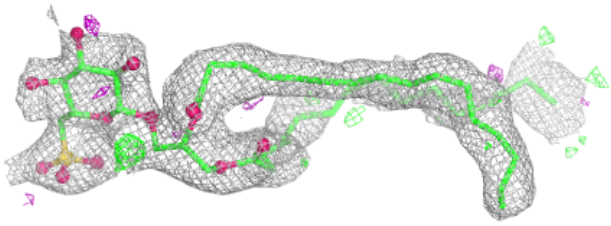


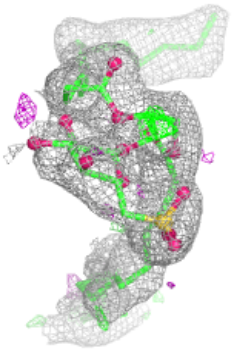


Electron density around SQD A 416:

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

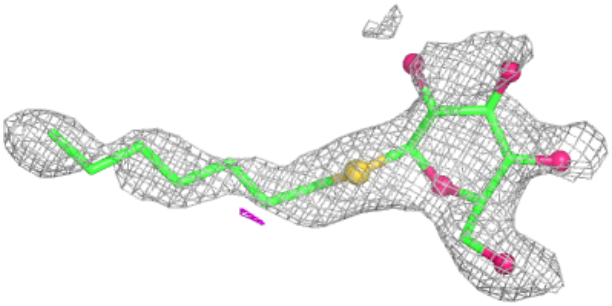


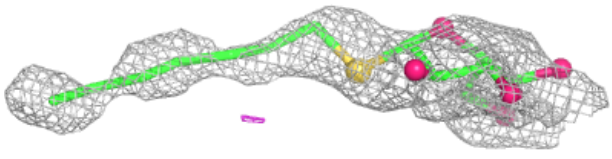


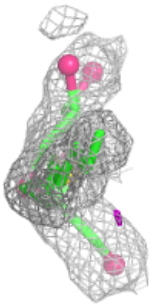


Electron density around HTG C 524:

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

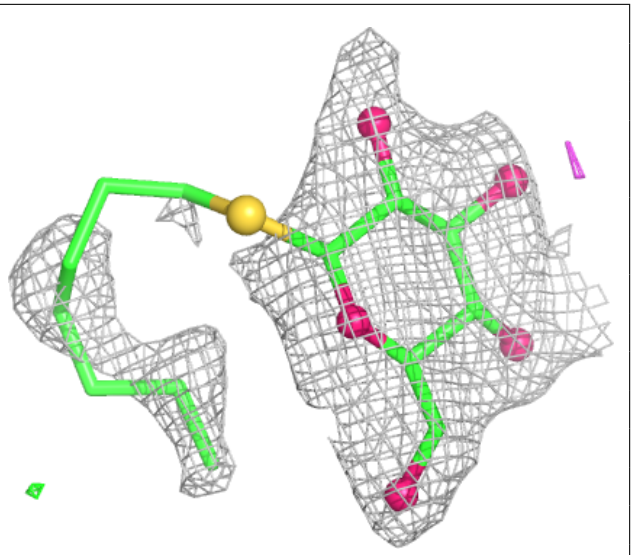


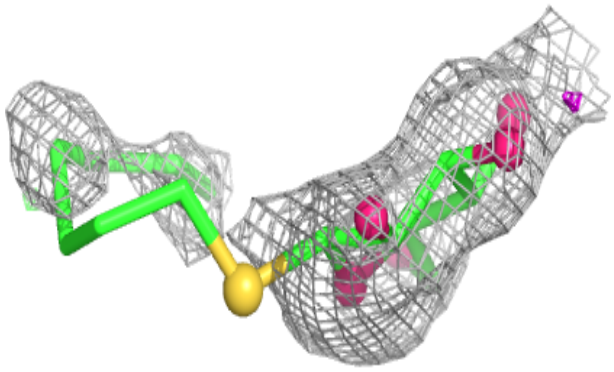


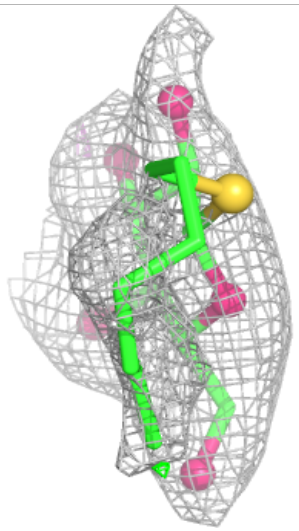


Electron density around HTG V 202:

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

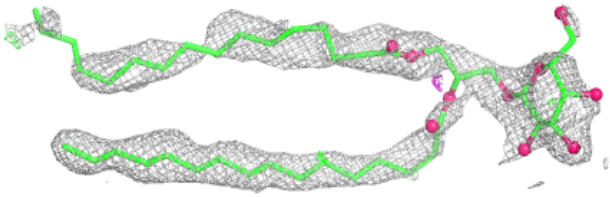


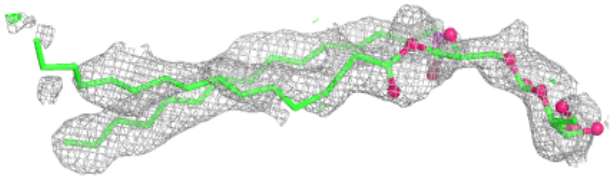


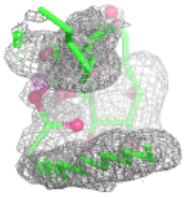


Electron density around LMG c 920:

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

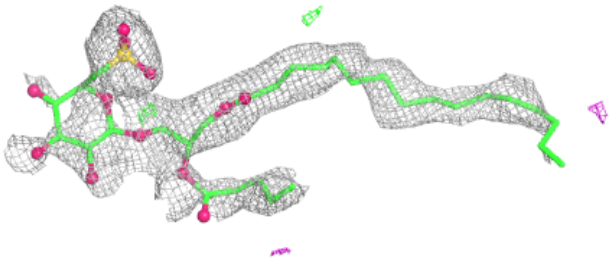


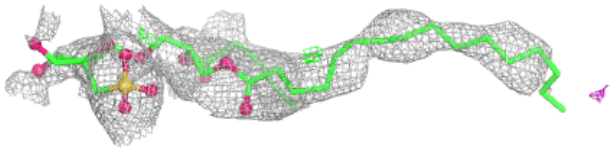


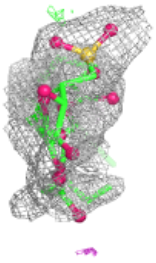


Electron density around SQD f 102:

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

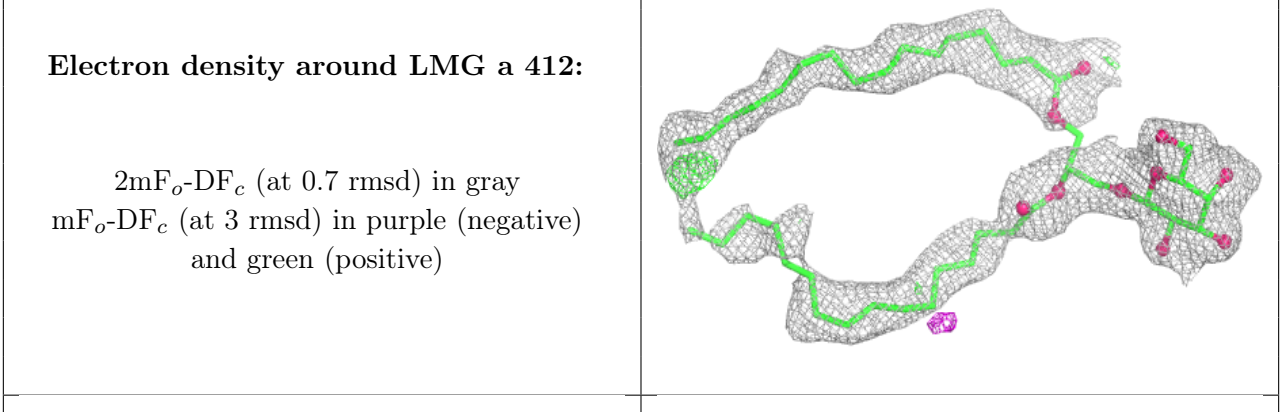






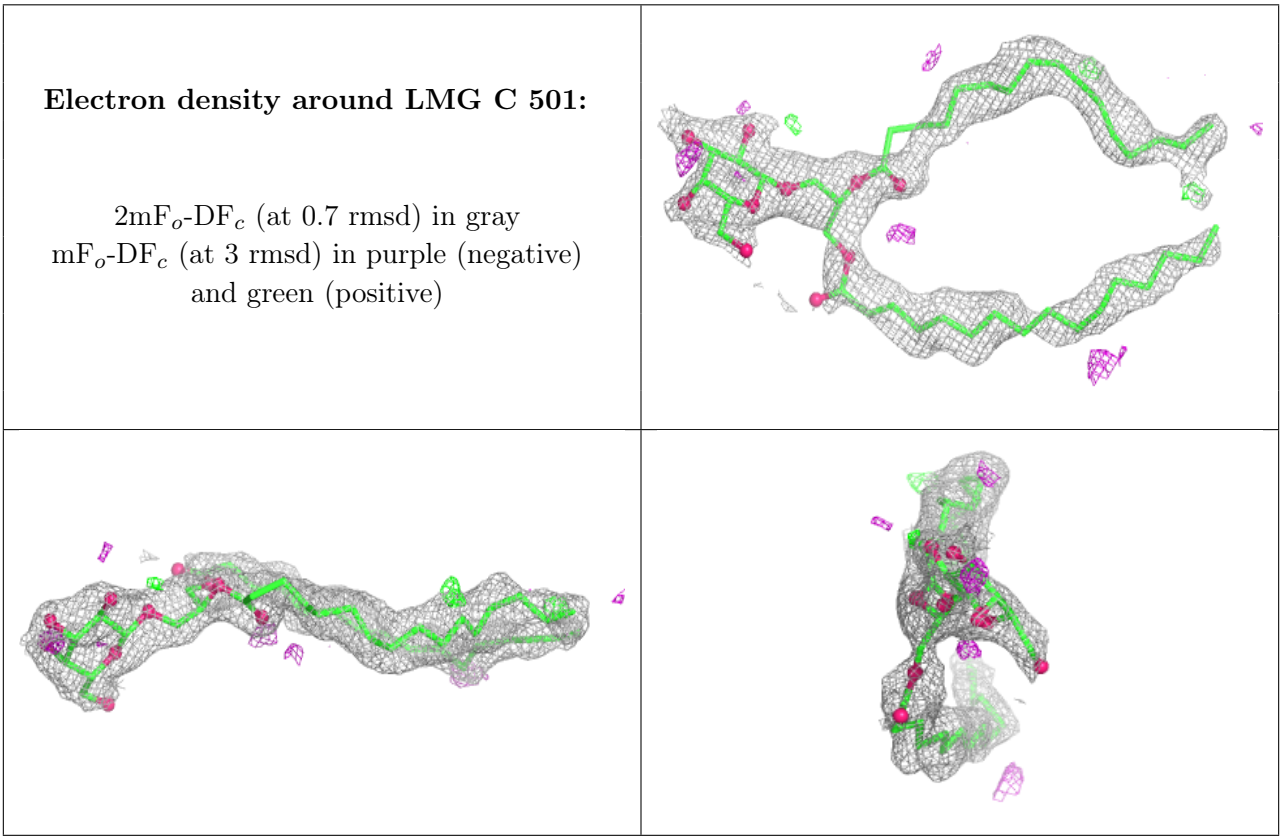
Electron density around LMG a 412:

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



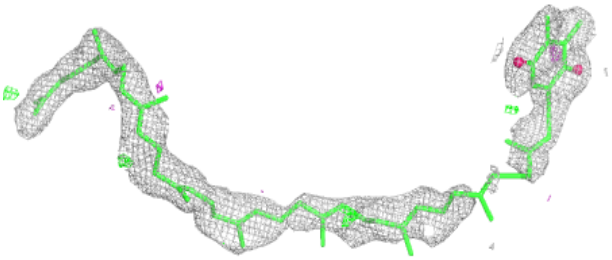
Electron density around LMG C 501:

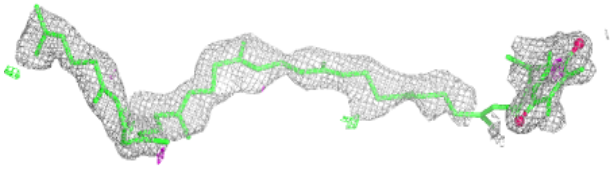
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

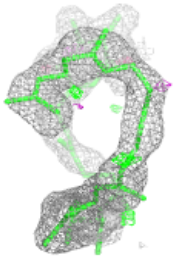


Electron density around PL9 A 419:

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

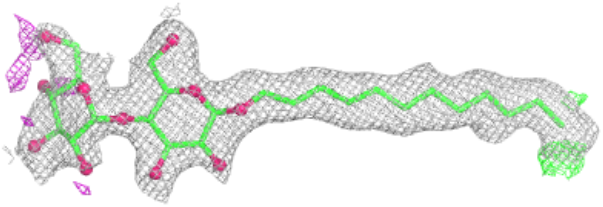


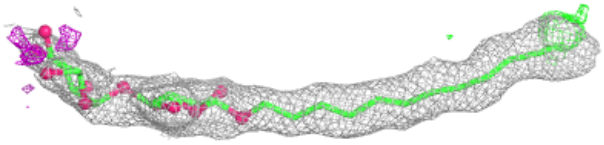




Electron density around LMT M 101:

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

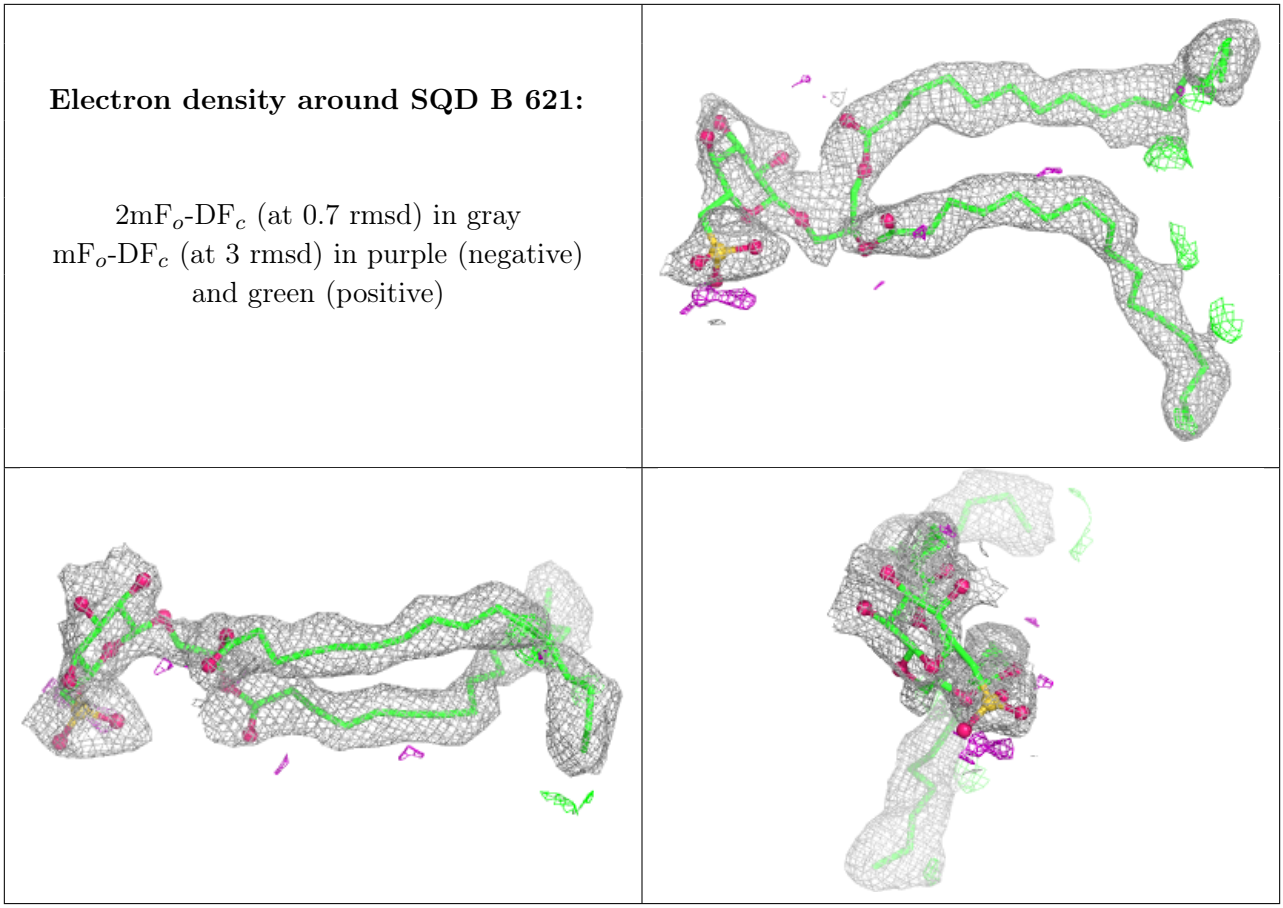






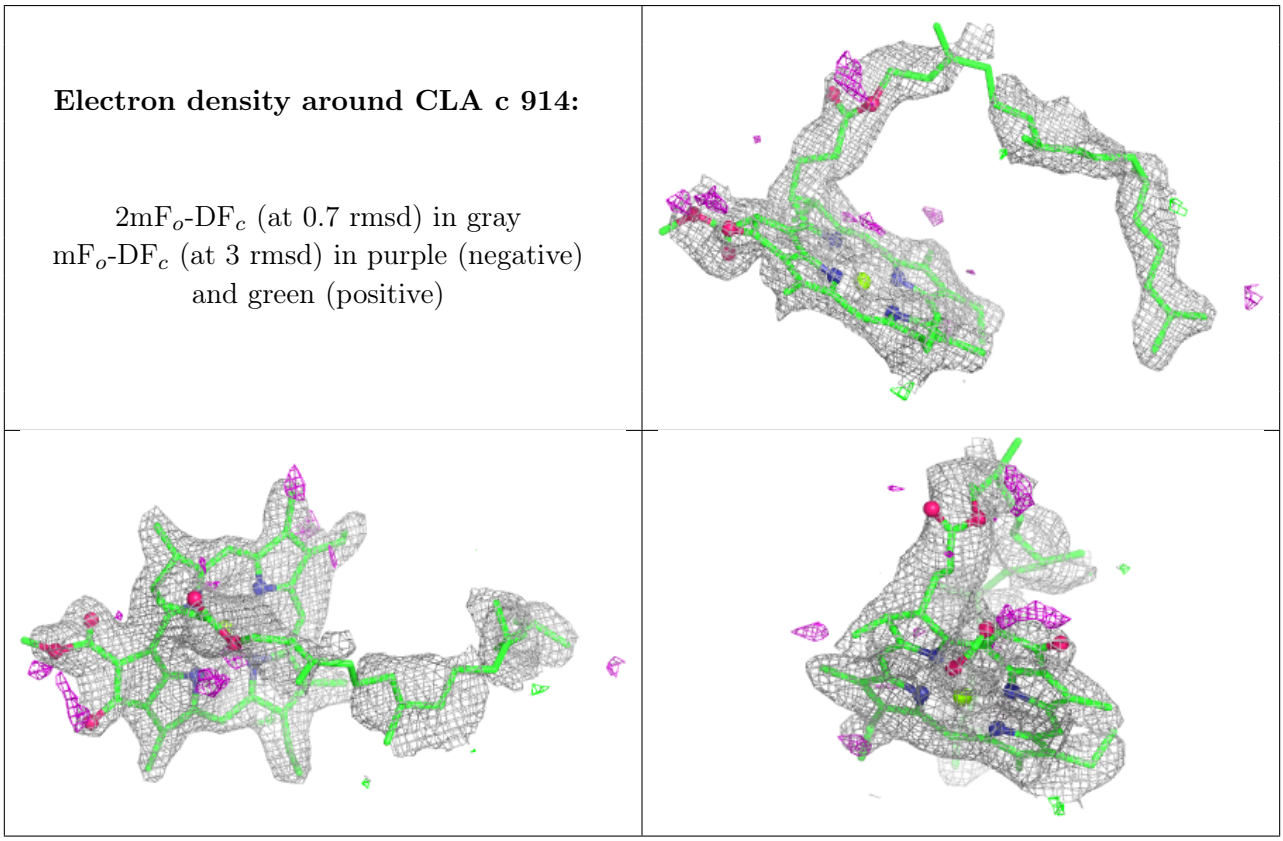
Electron density around SQD B 621:

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



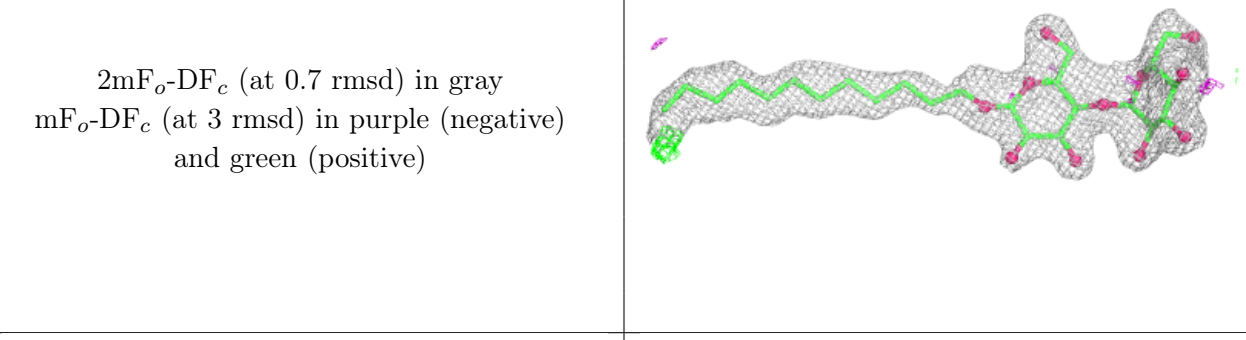
Electron density around CLA c 914:

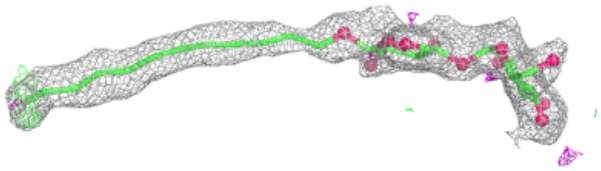
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

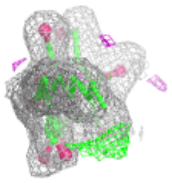


Electron density around LMT m 103:

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

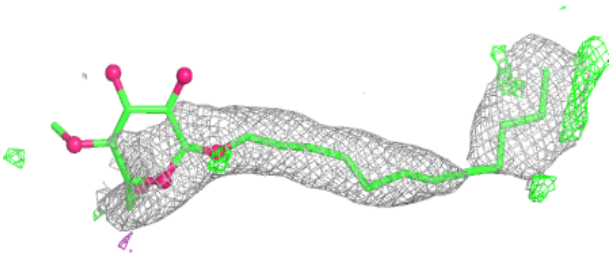


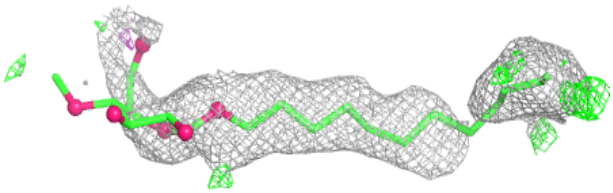


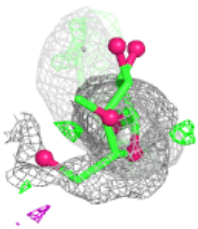


Electron density around LMT b 601:

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

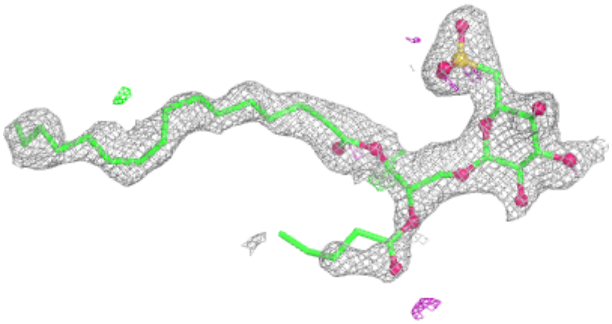


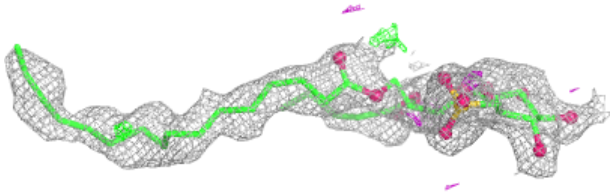


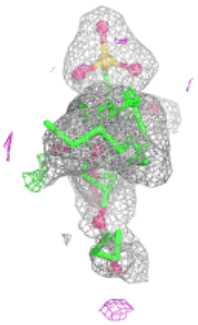


Electron density around SQD F 101:

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

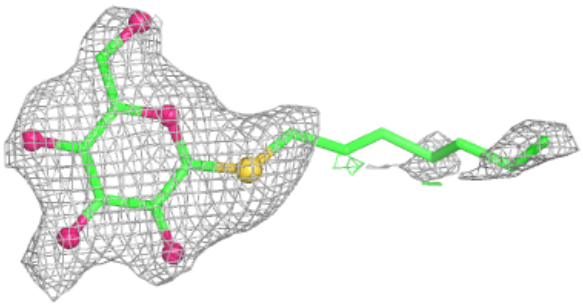


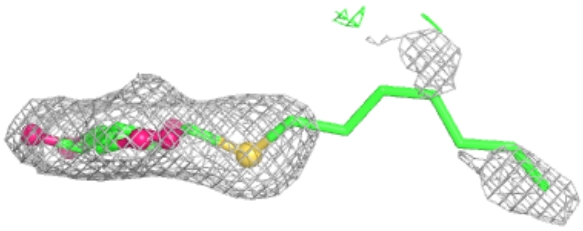


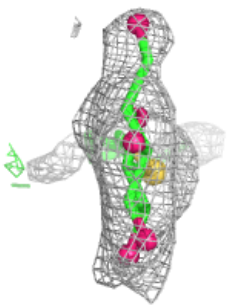


Electron density around HTG C 523:

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

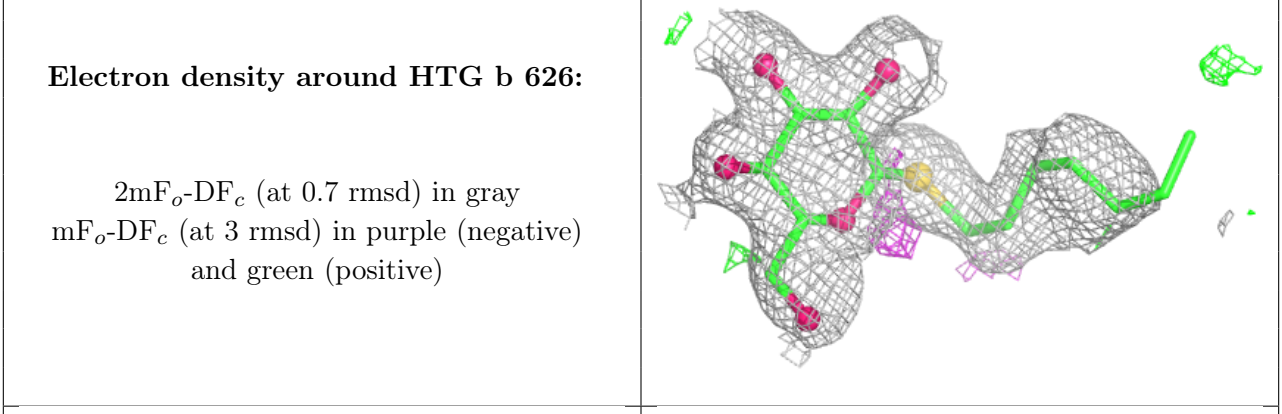






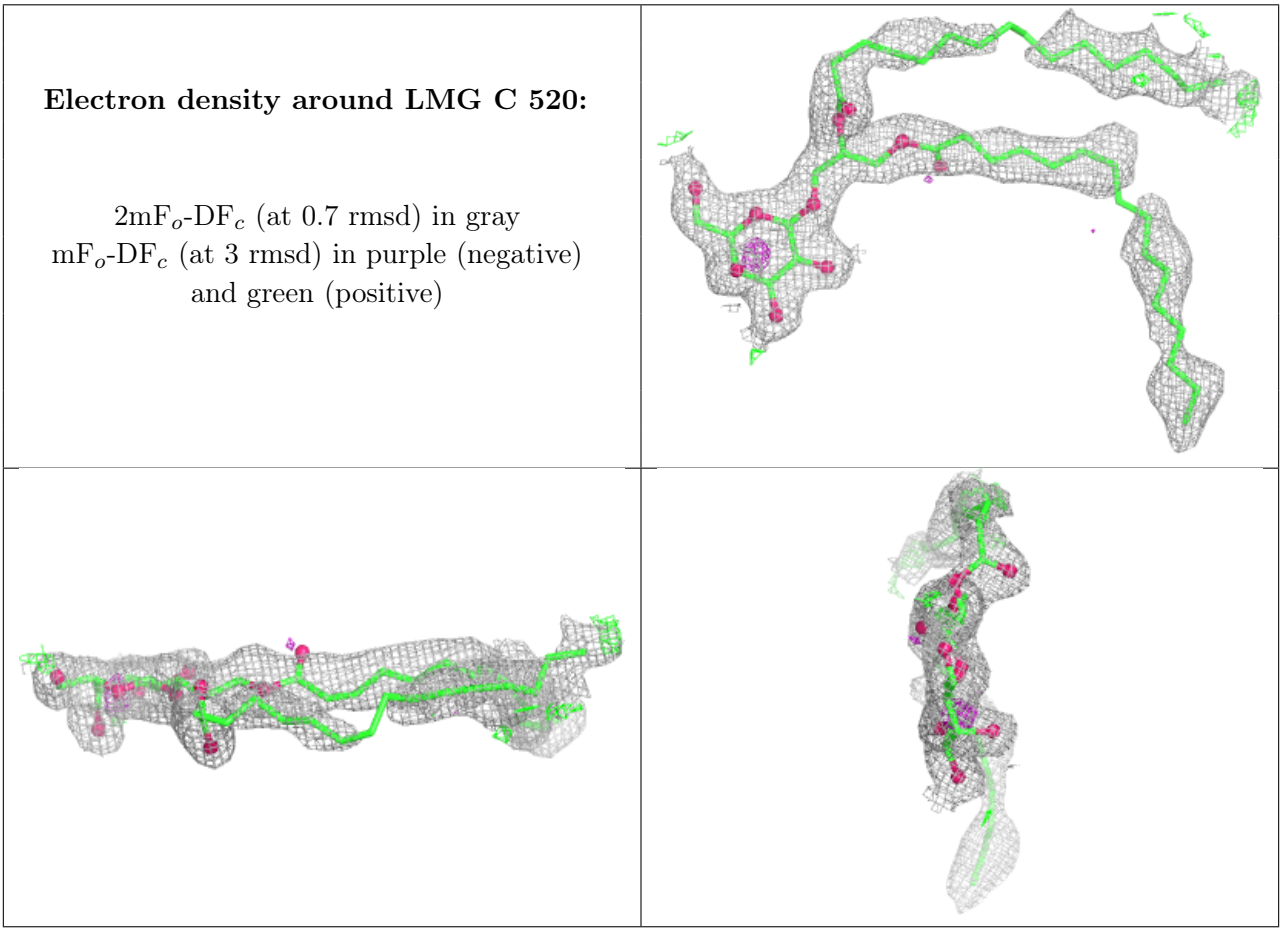
Electron density around HTG b 626:

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



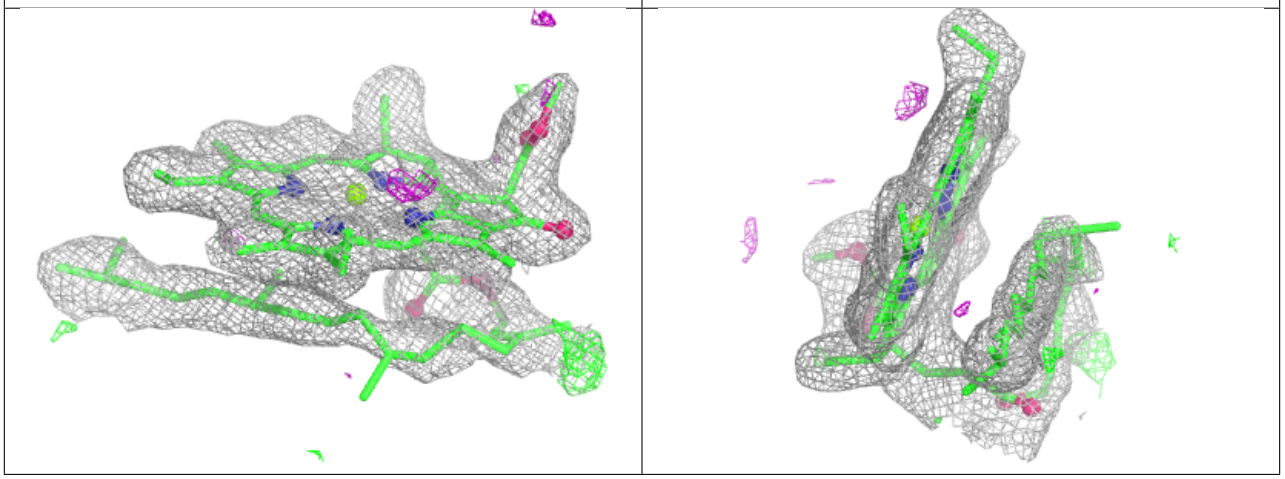
Electron density around LMG C 520:

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



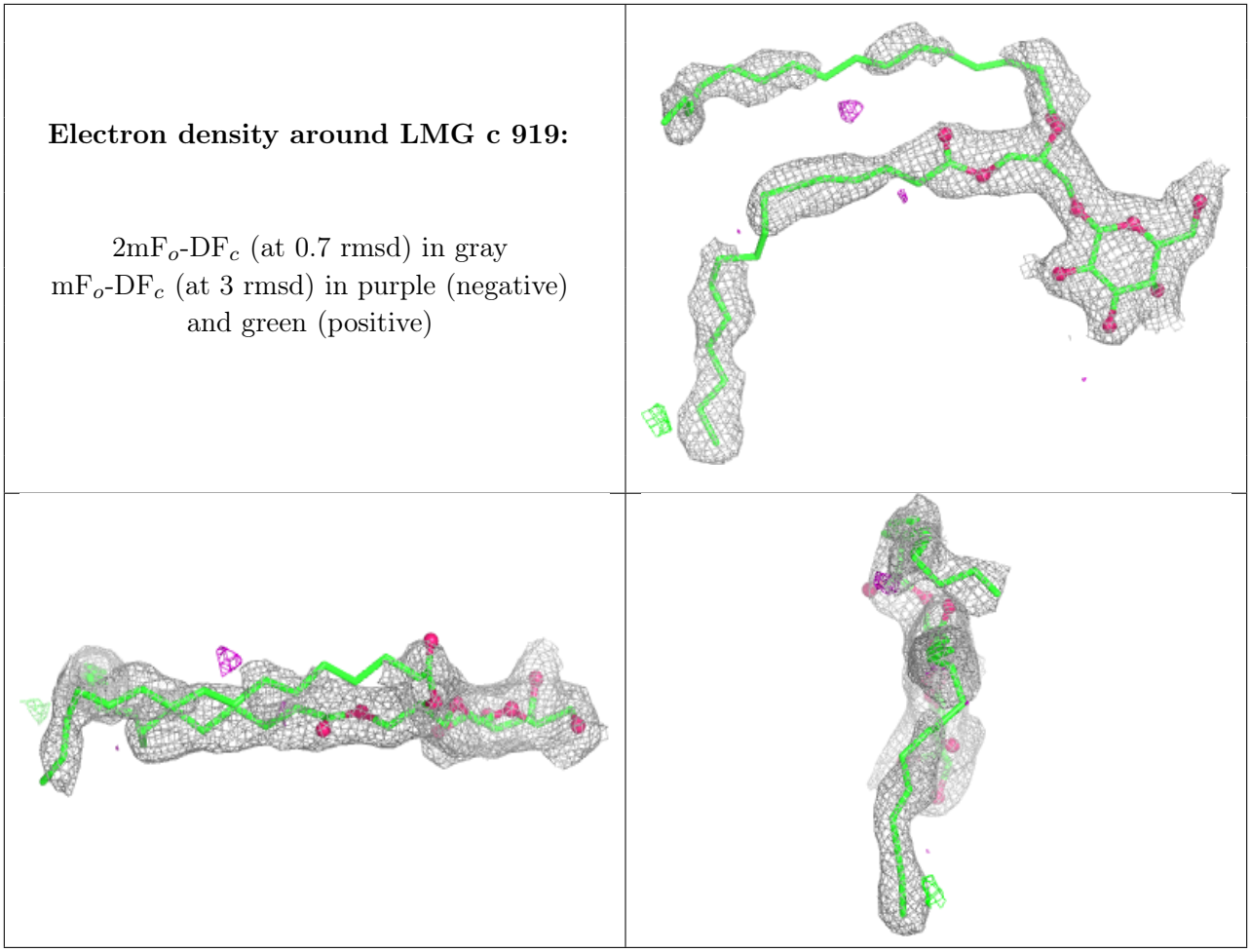
Electron density around CLA b 605:

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



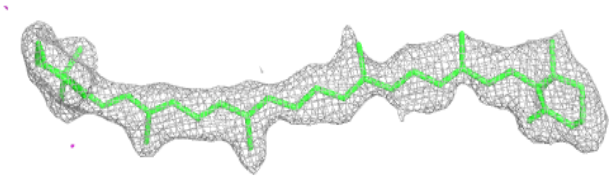
Electron density around LMG c 919:

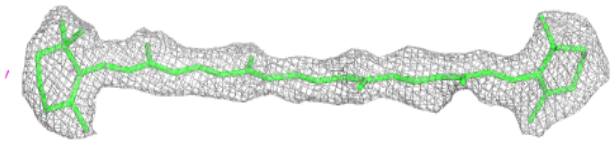
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

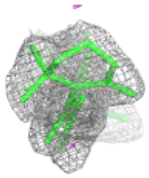


Electron density around BCR k 101:

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

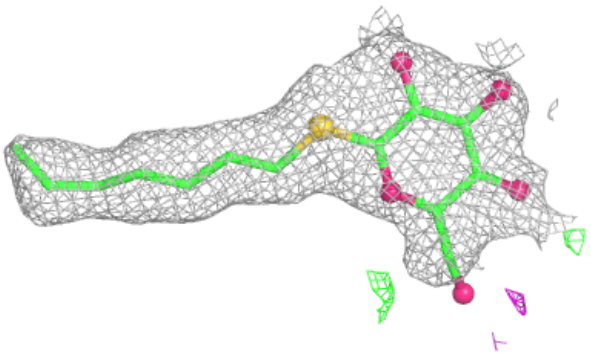


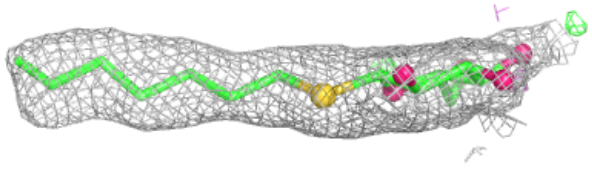


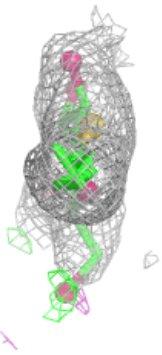


Electron density around HTG B 633:

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

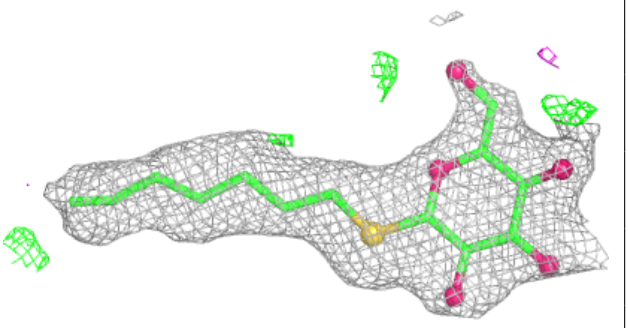


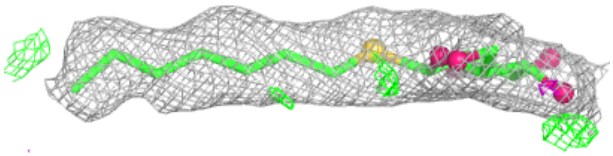


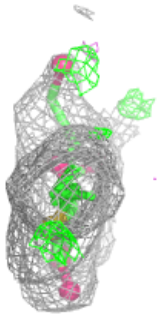


Electron density around HTG b 602:

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

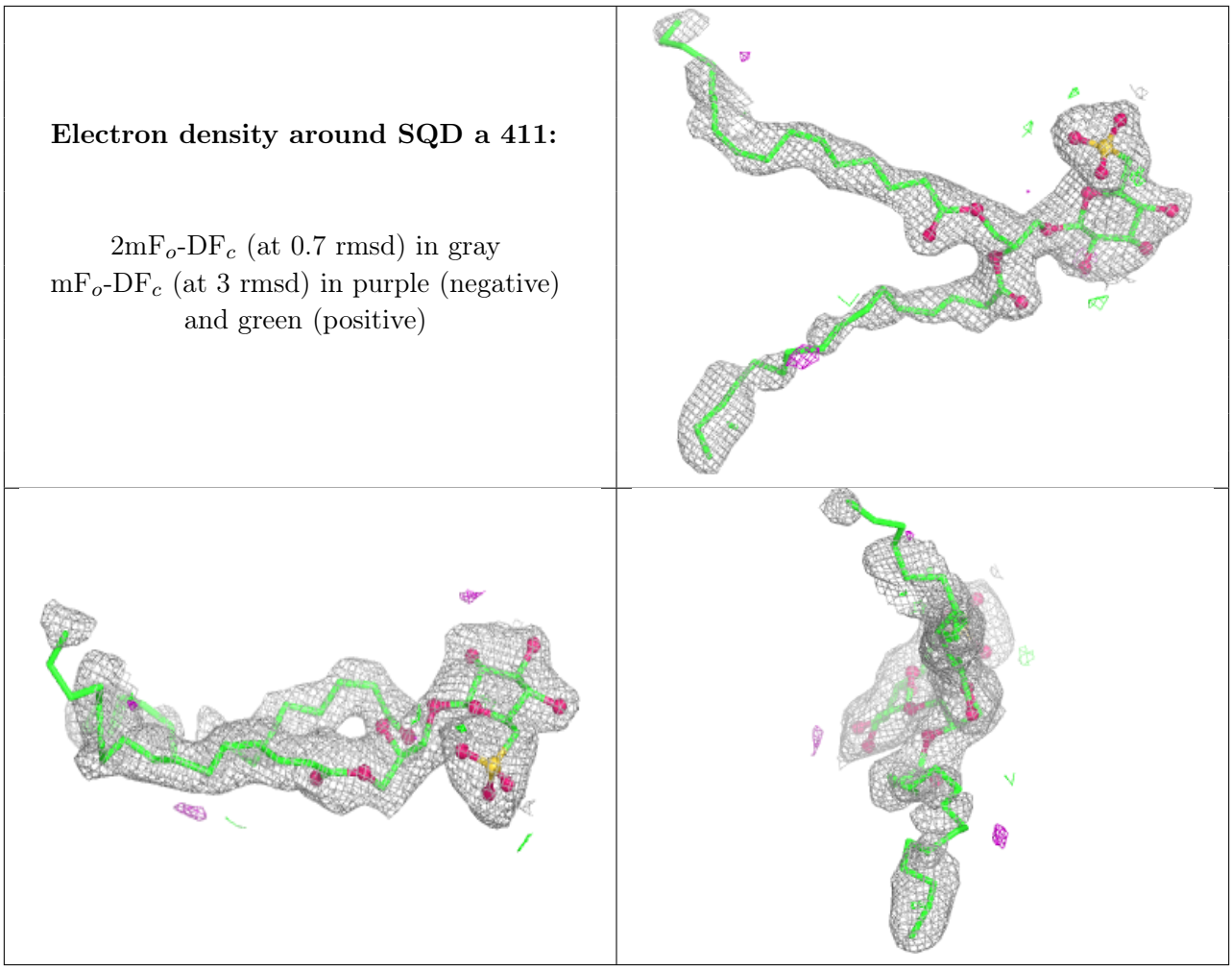






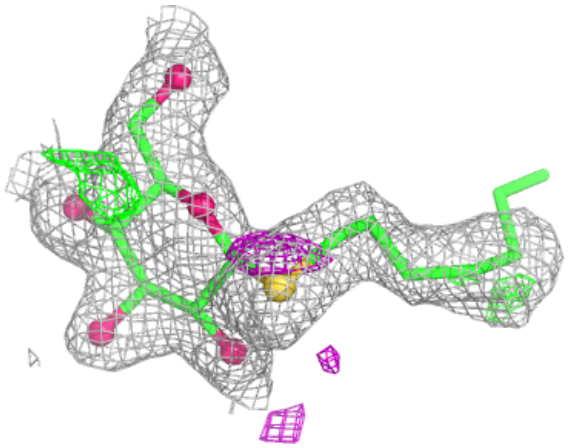
Electron density around SQD a 411:

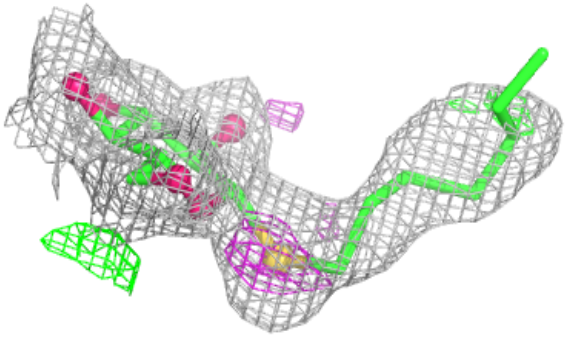
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

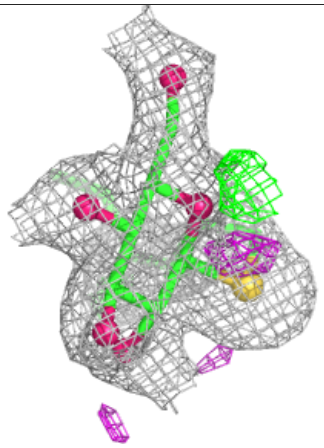


Electron density around HTG B 625:

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

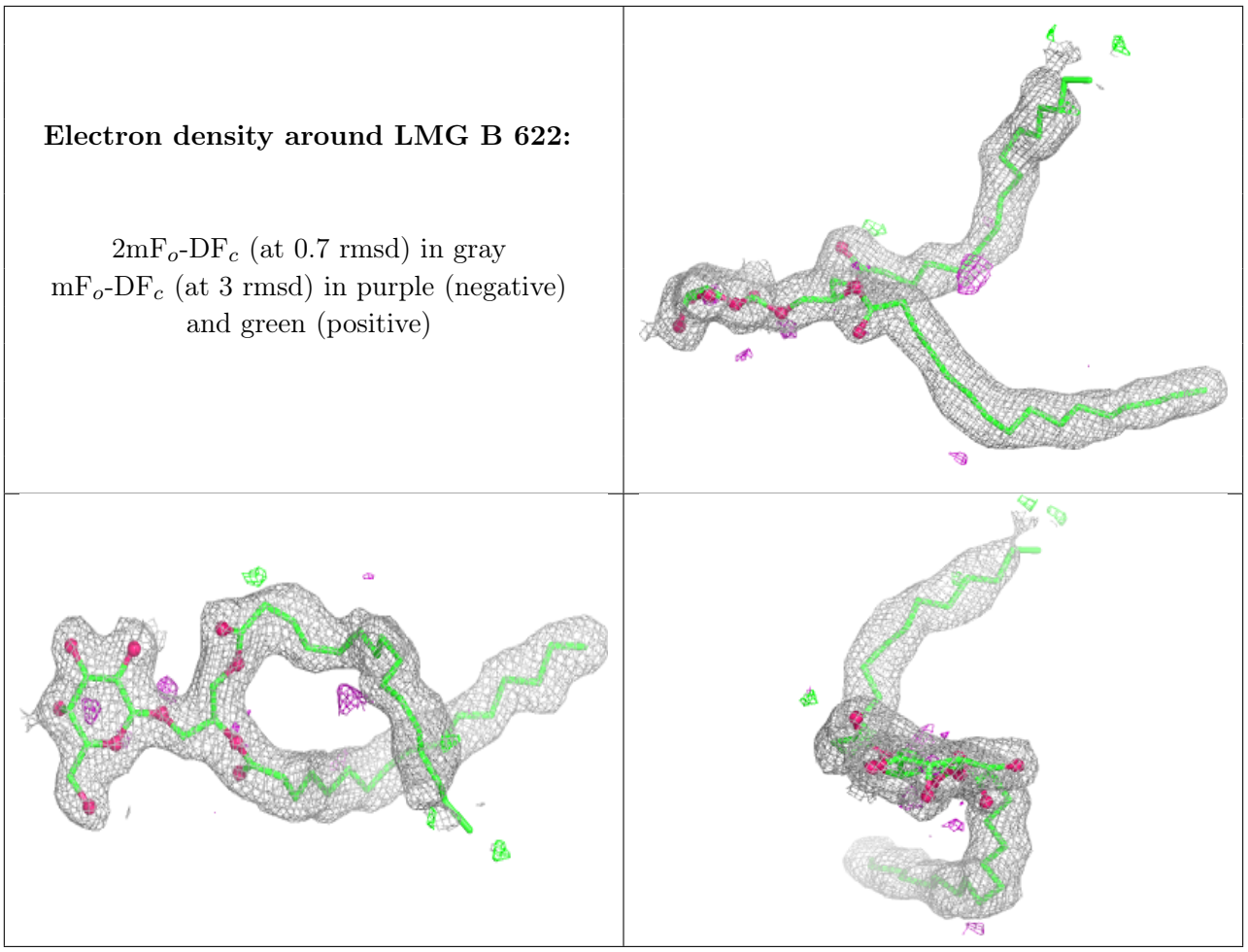






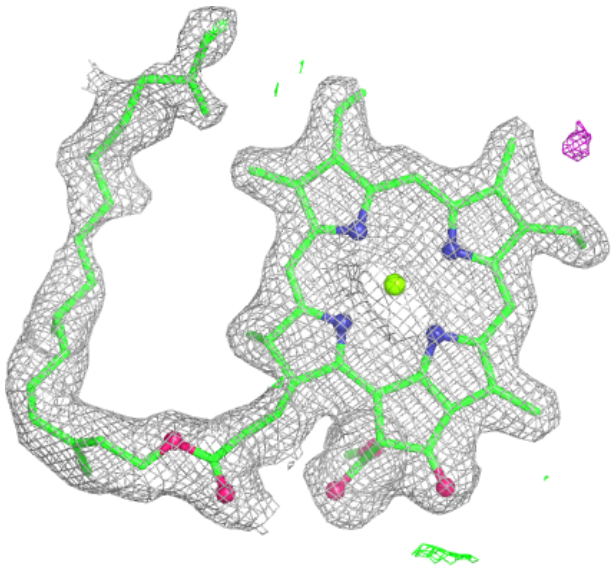
Electron density around LMG B 622:

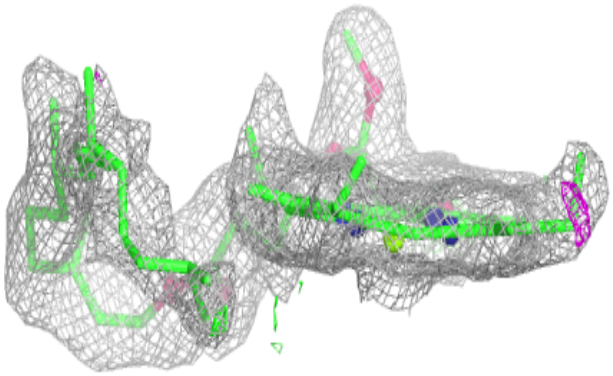
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

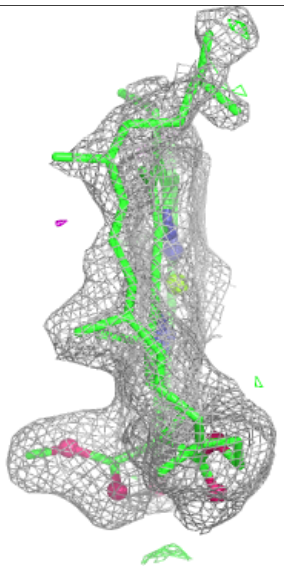


Electron density around CLA c 913:

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

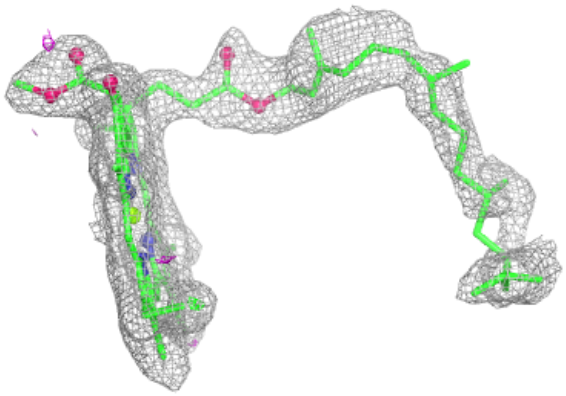


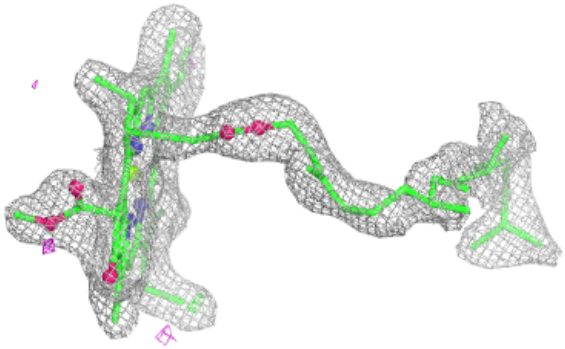


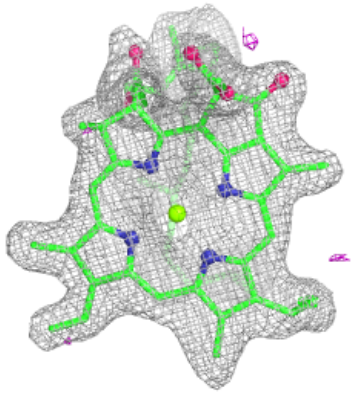


Electron density around CLA C 507:

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

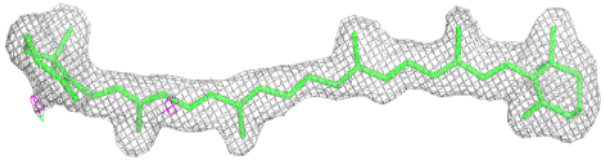


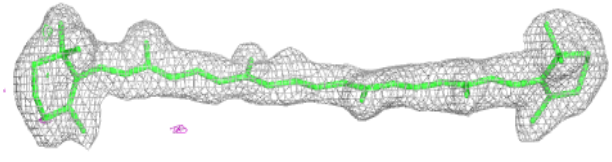


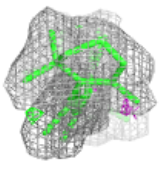


Electron density around BCR C 515:

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

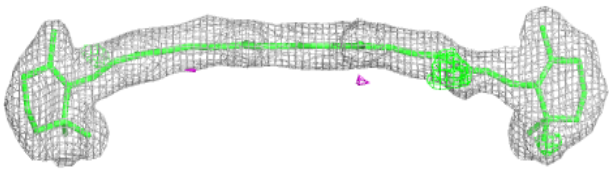


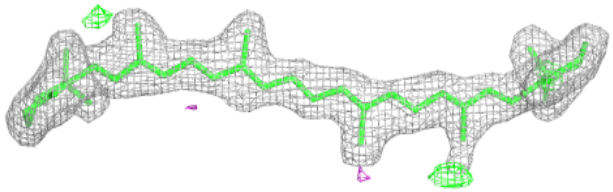


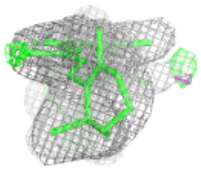


Electron density around BCR K 103:

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

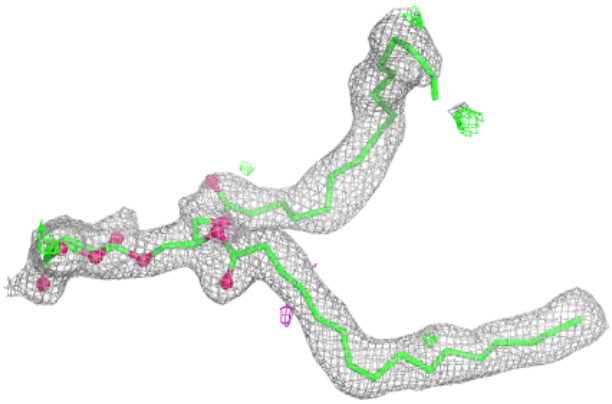


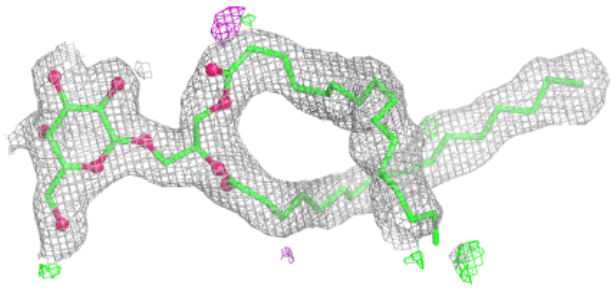


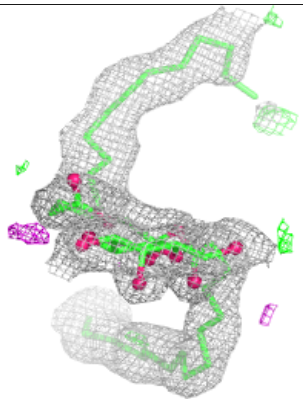


Electron density around LMG b 624:

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

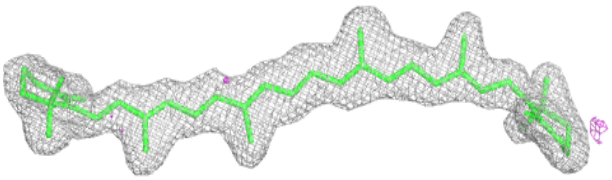


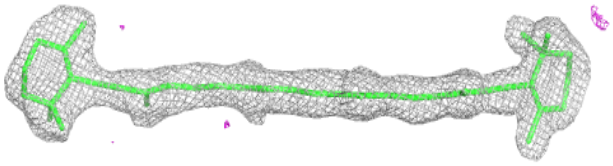


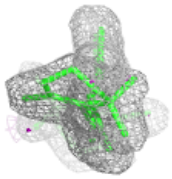


Electron density around BCR c 915:

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

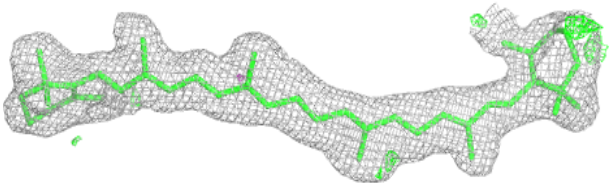


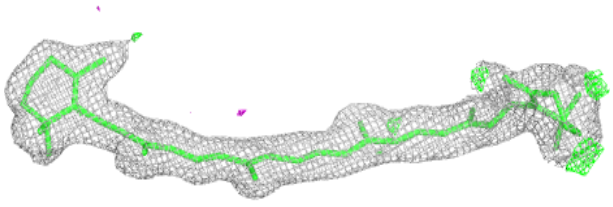


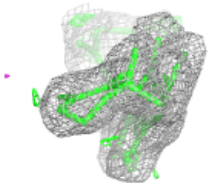


Electron density around BCR d 404:

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

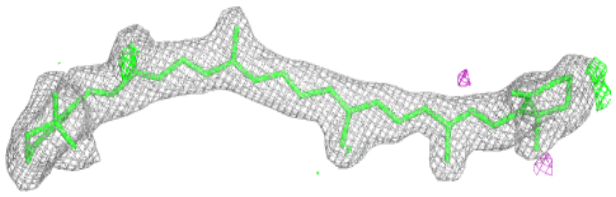


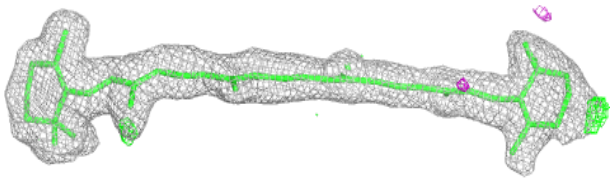


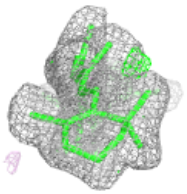


Electron density around BCR h 101:

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

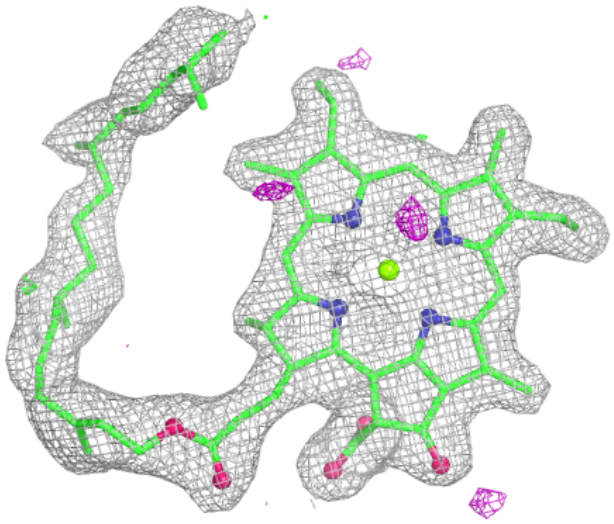


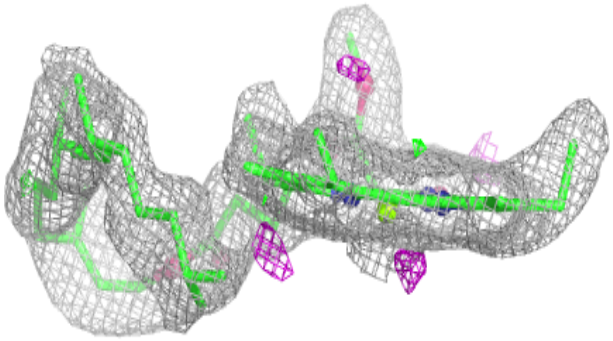


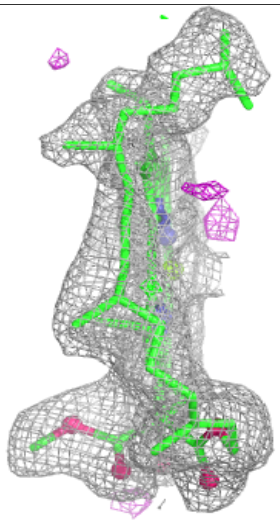


Electron density around CLA C 513:

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

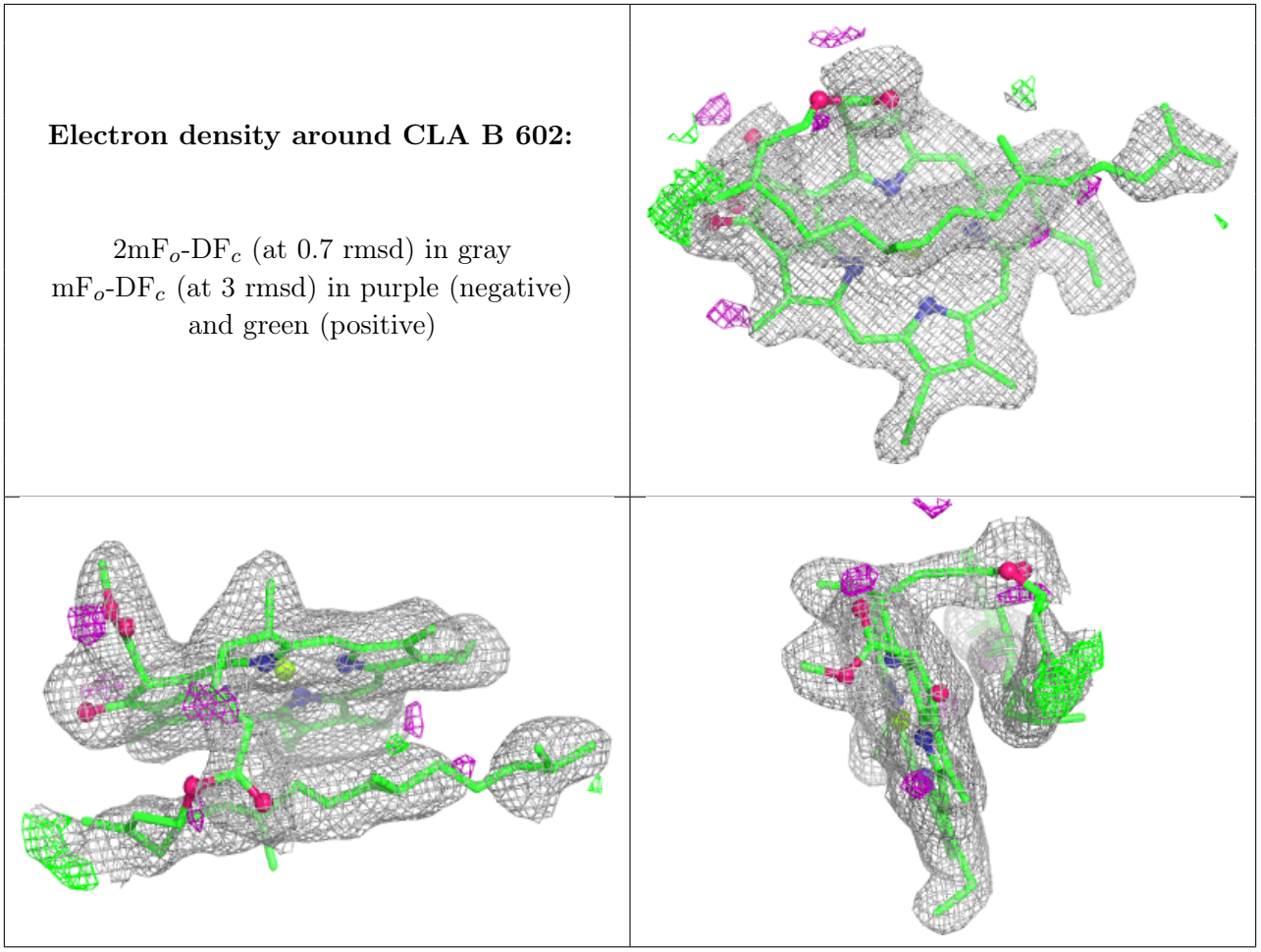






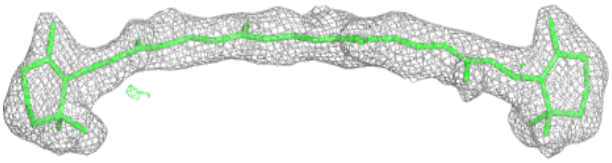
Electron density around CLA B 602:

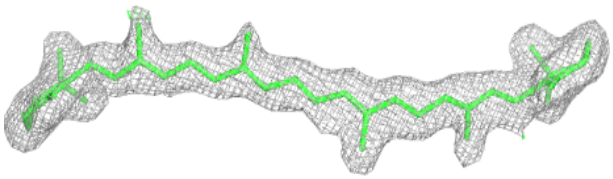
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

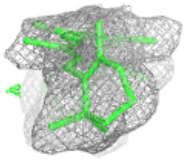


Electron density around BCR k 102:

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

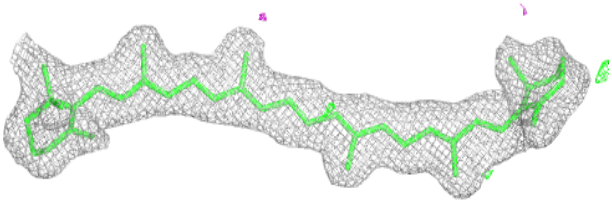


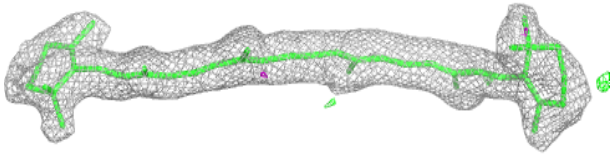


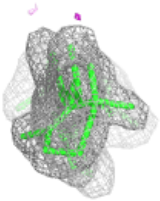


Electron density around BCR y 101:

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

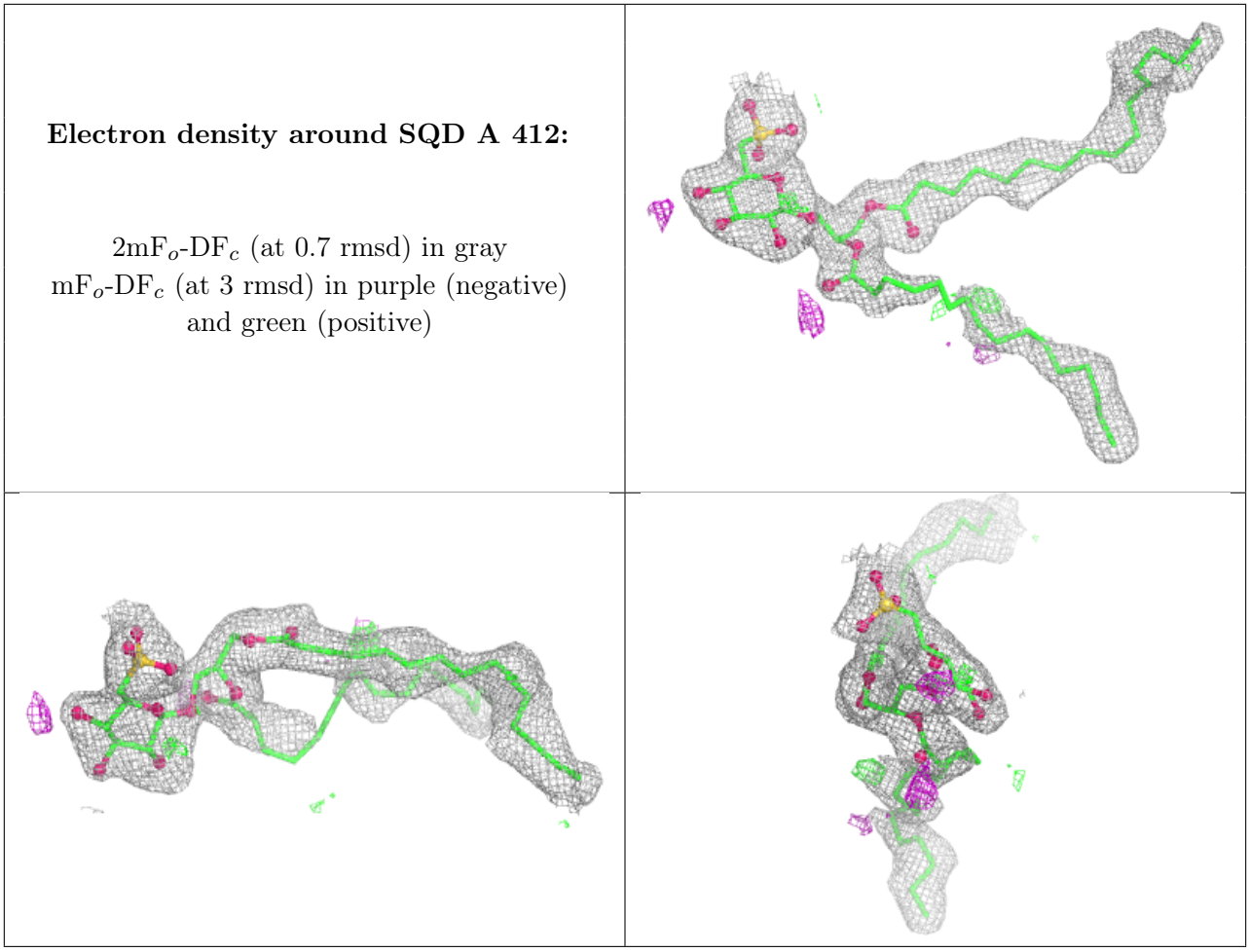






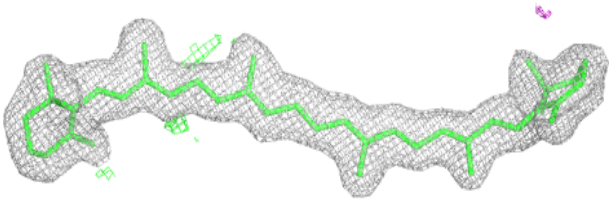
Electron density around SQD A 412:

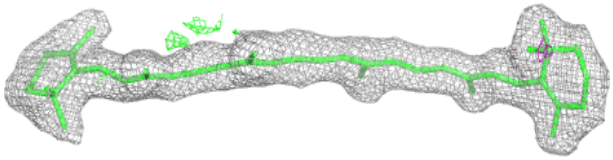
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

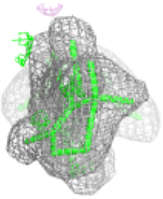


Electron density around BCR K 102:

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

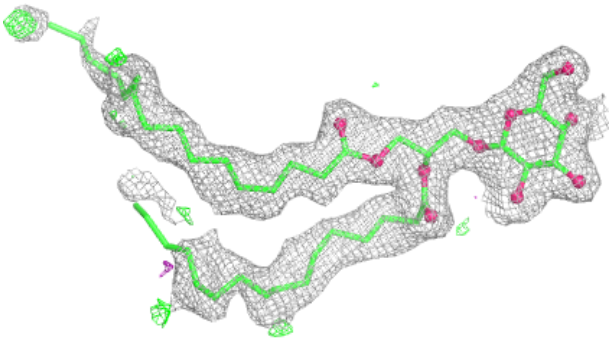


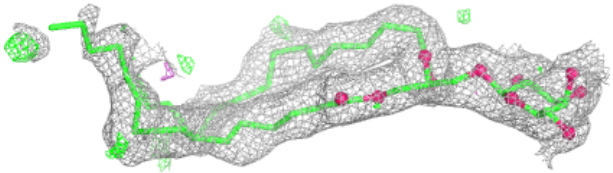


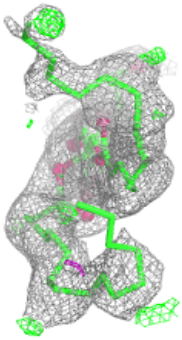


Electron density around LMG j 101:

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

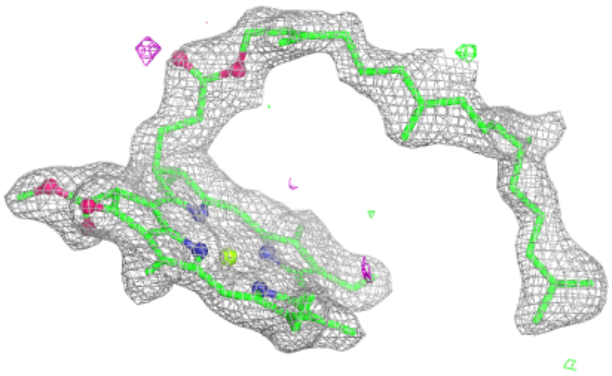


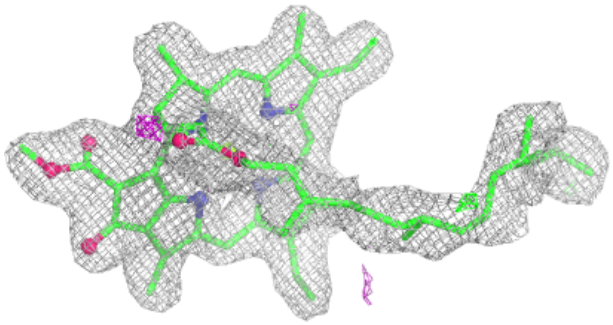


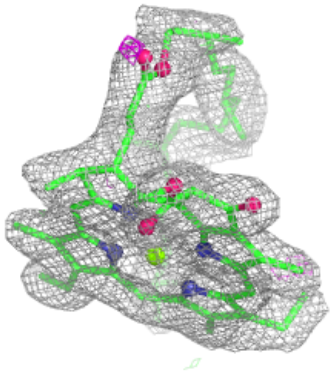


Electron density around CLA C 514:

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

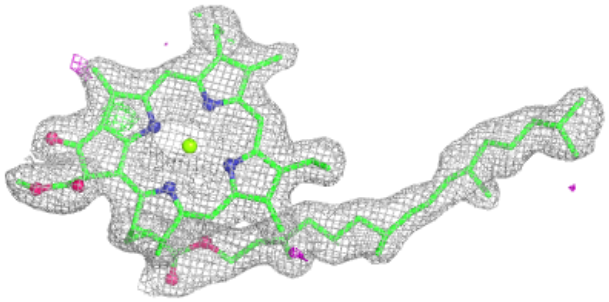


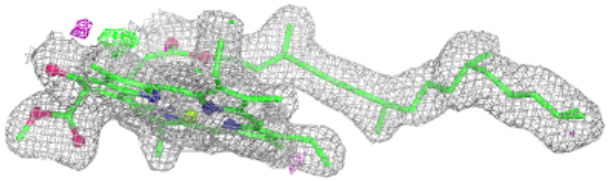


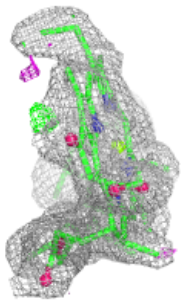


Electron density around CLA c 902:

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

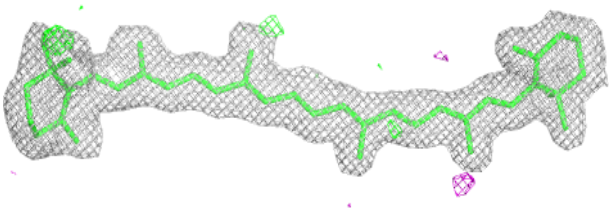


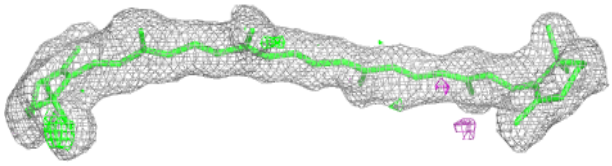


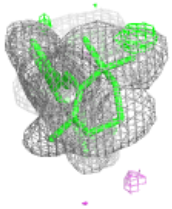


Electron density around BCR B 620:

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

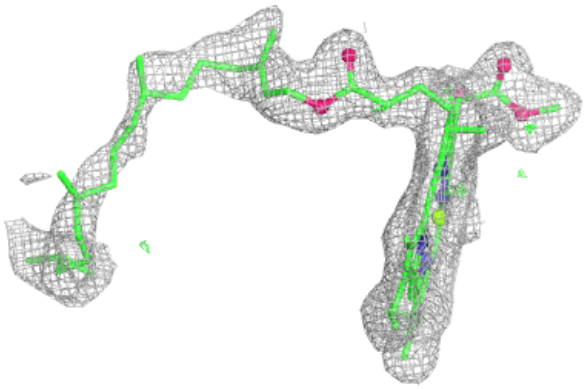


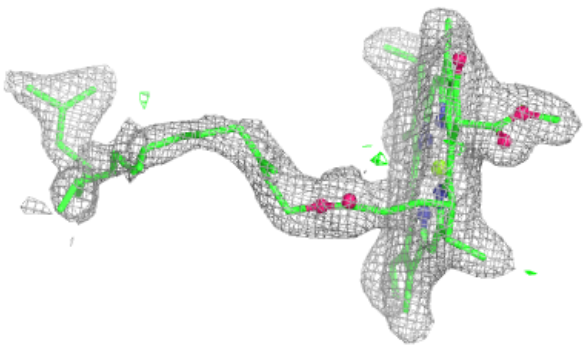


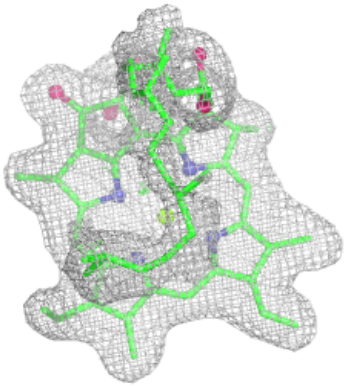


Electron density around CLA c 907:

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

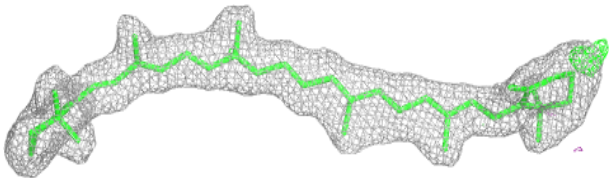


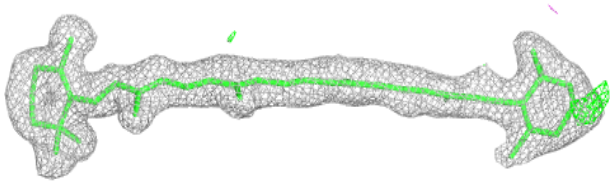


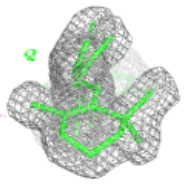


Electron density around BCR H 101:

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

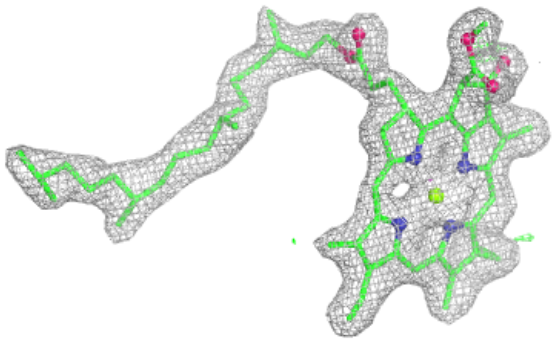


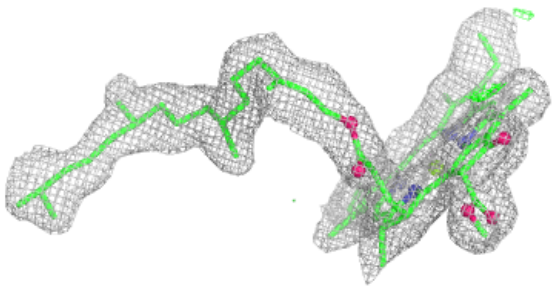


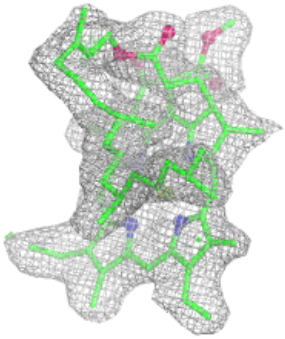


Electron density around CLA c 912:

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

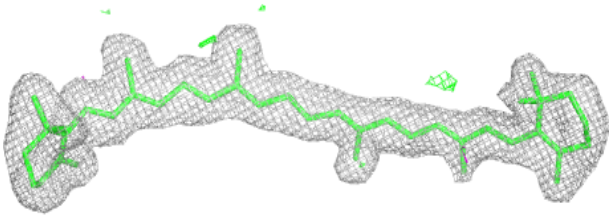


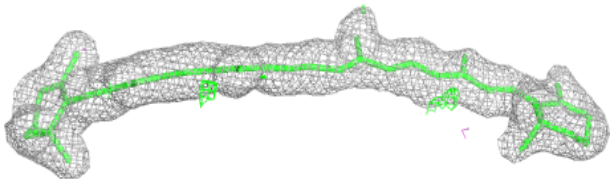


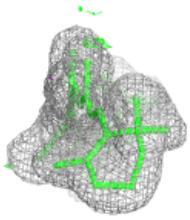


Electron density around BCR T 102:

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

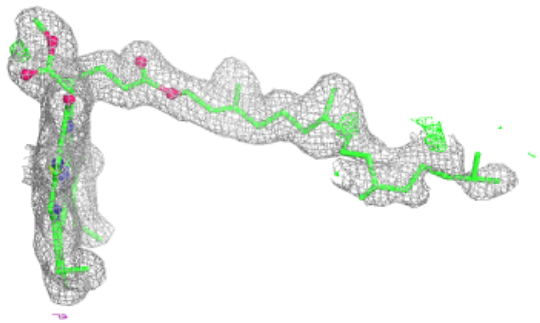


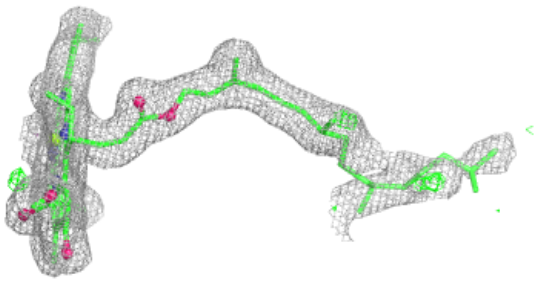


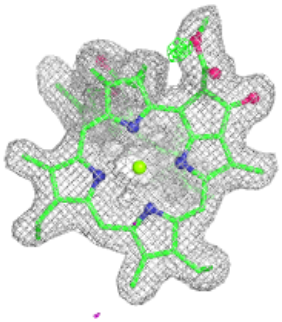


Electron density around CLA b 610:

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

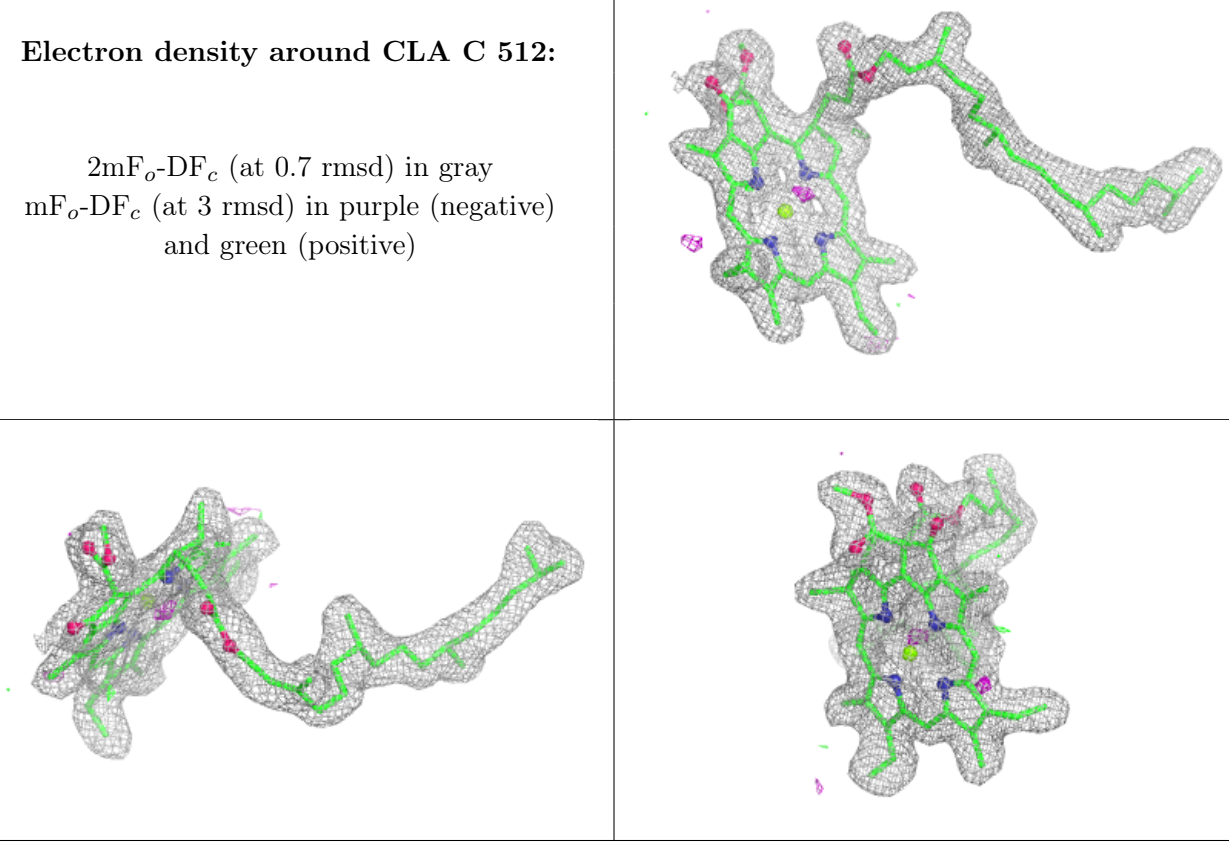






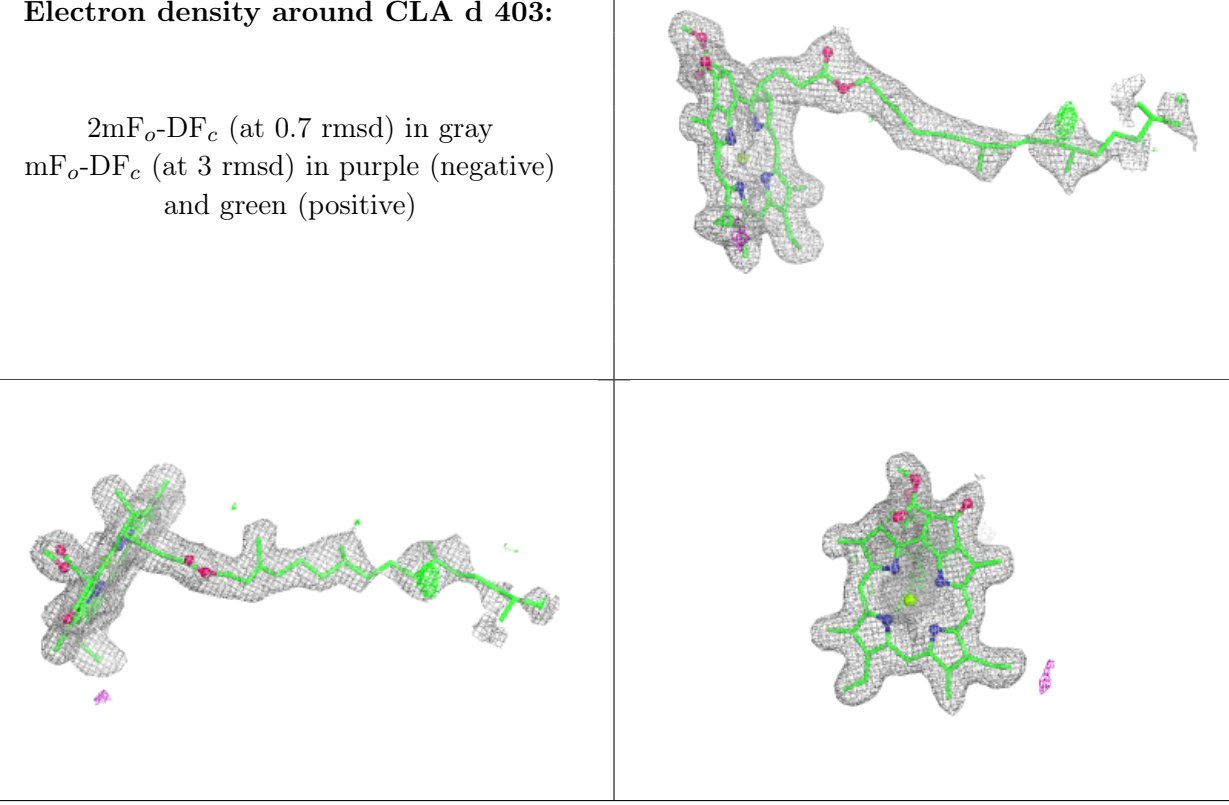
Electron density around CLA C 512:

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



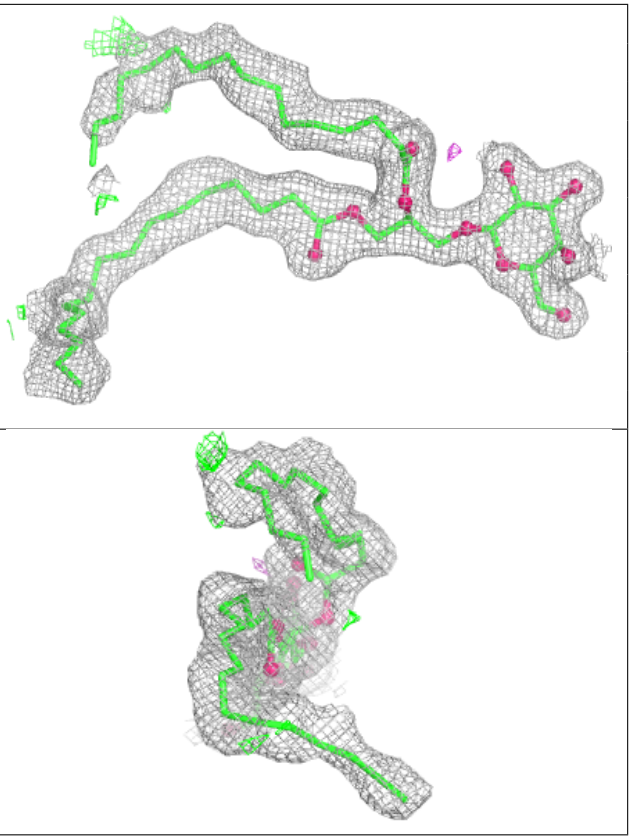
Electron density around CLA d 403:

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



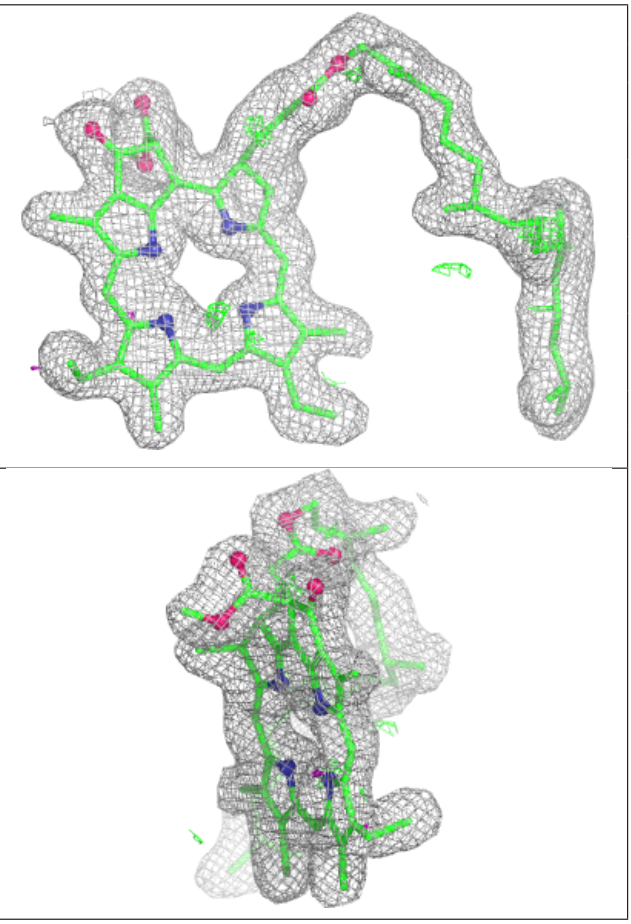
Electron density around LMG J 101:

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



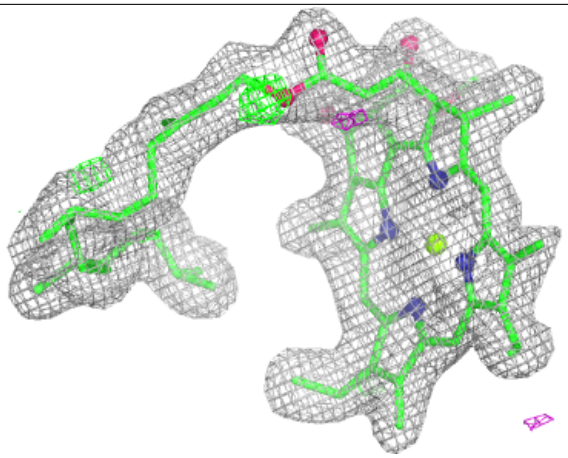
Electron density around PHO a 420:

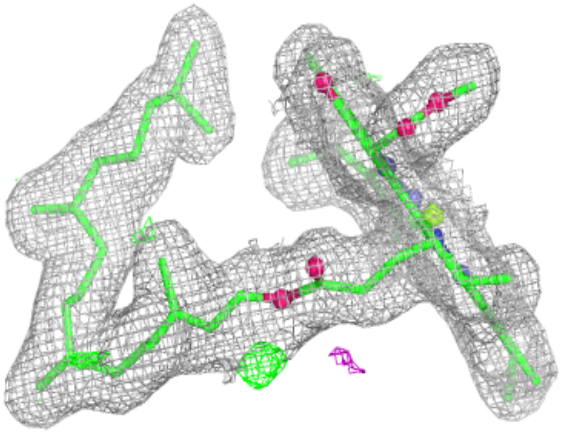
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

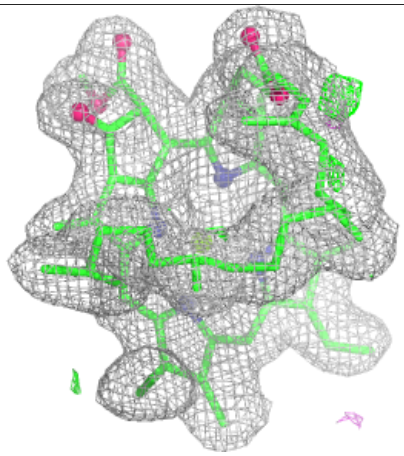


Electron density around CLA c 904:

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

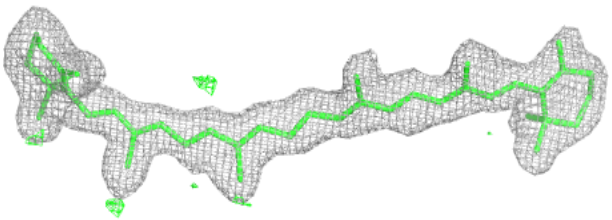


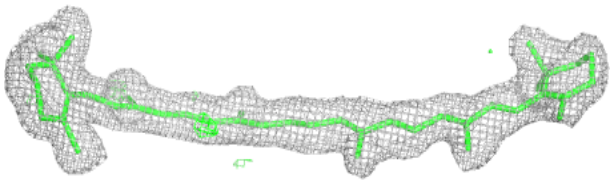


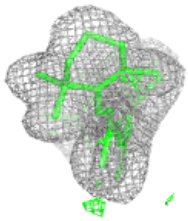


Electron density around BCR t 101:

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

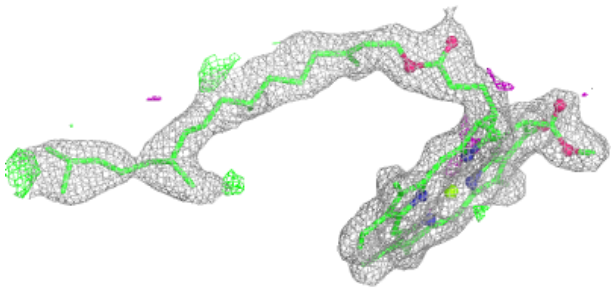


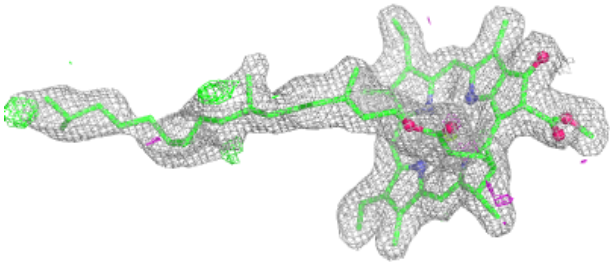


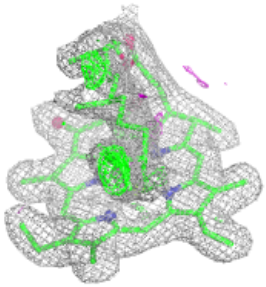


Electron density around CLA c 905:

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

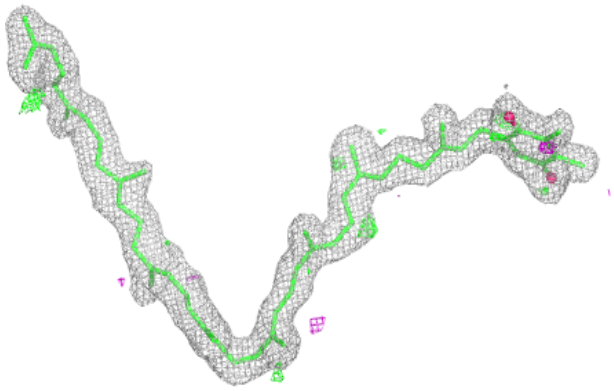


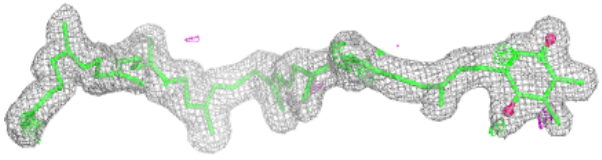


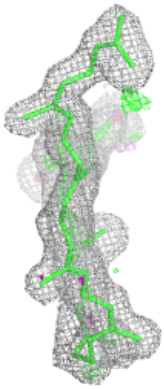


Electron density around PL9 d 405:

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

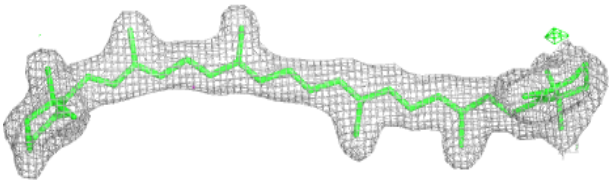


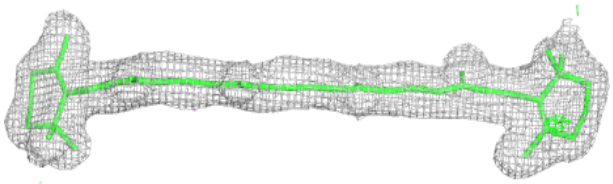


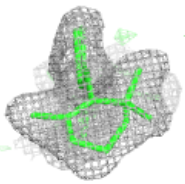


Electron density around BCR C 516:

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

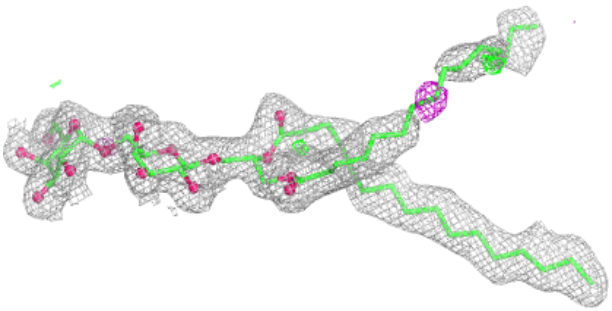


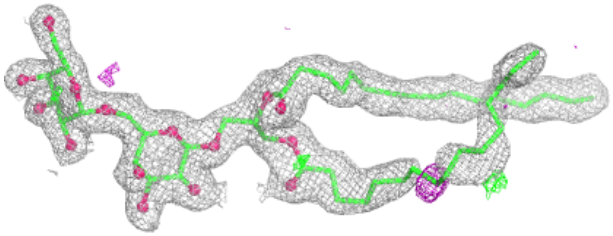


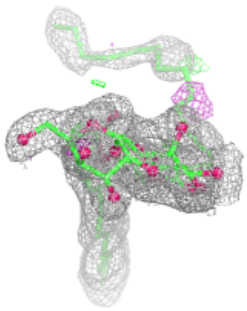


Electron density around DGD c 916:

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

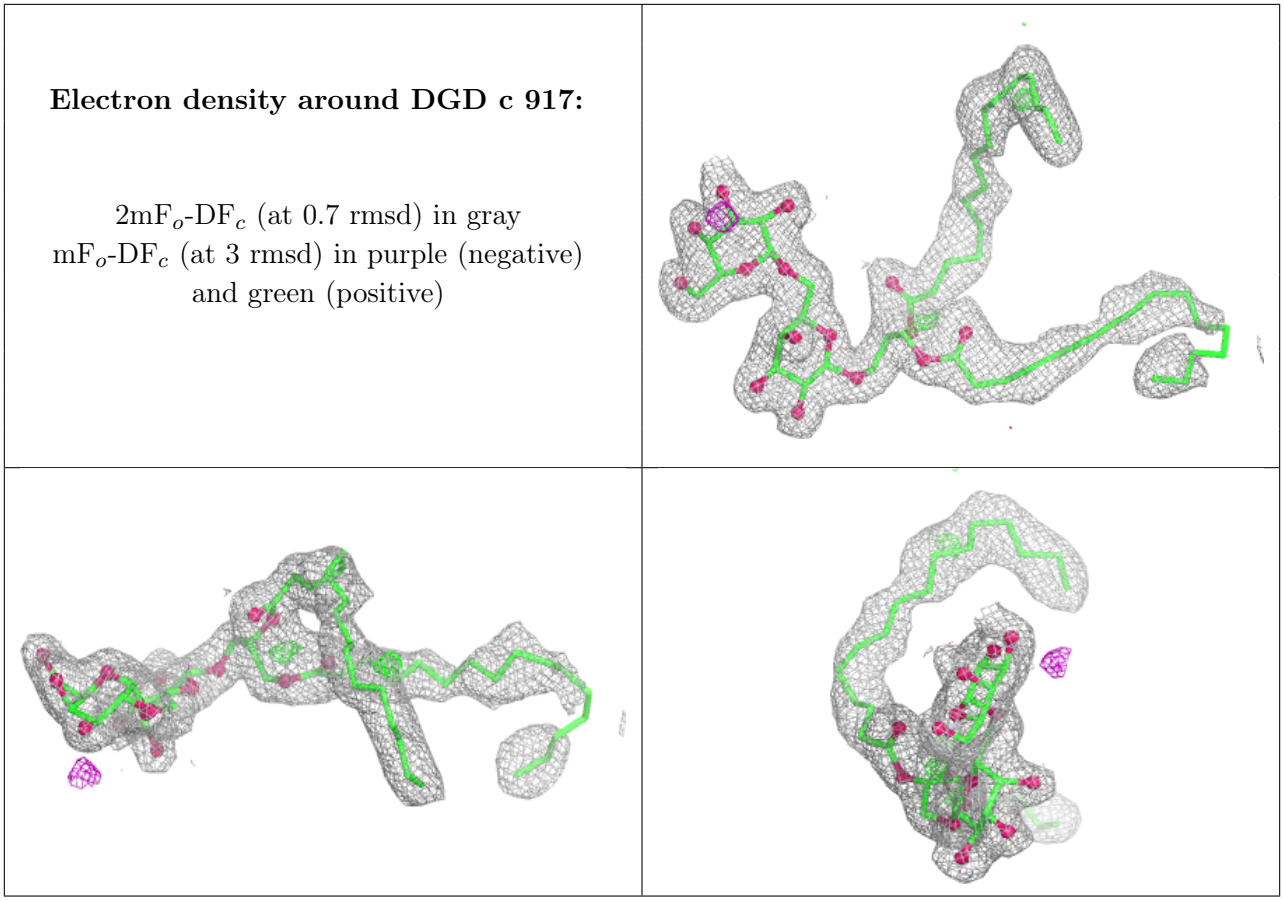






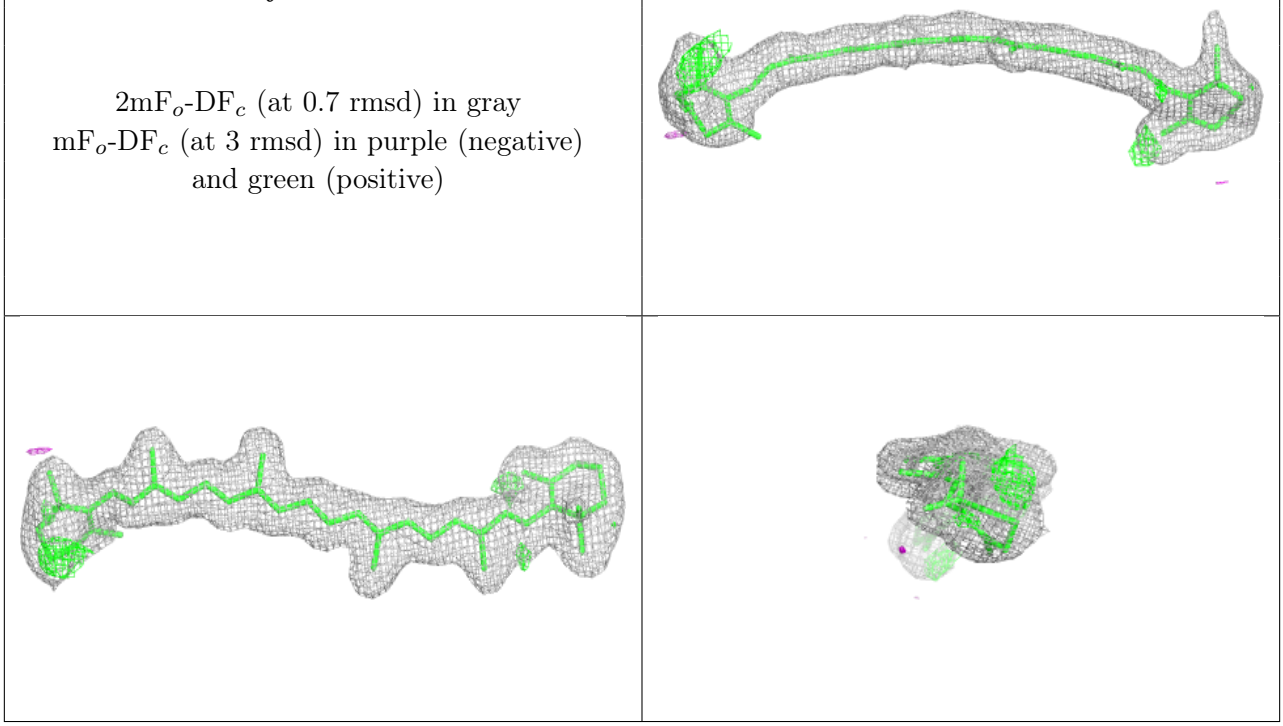
Electron density around DGD c 917:

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



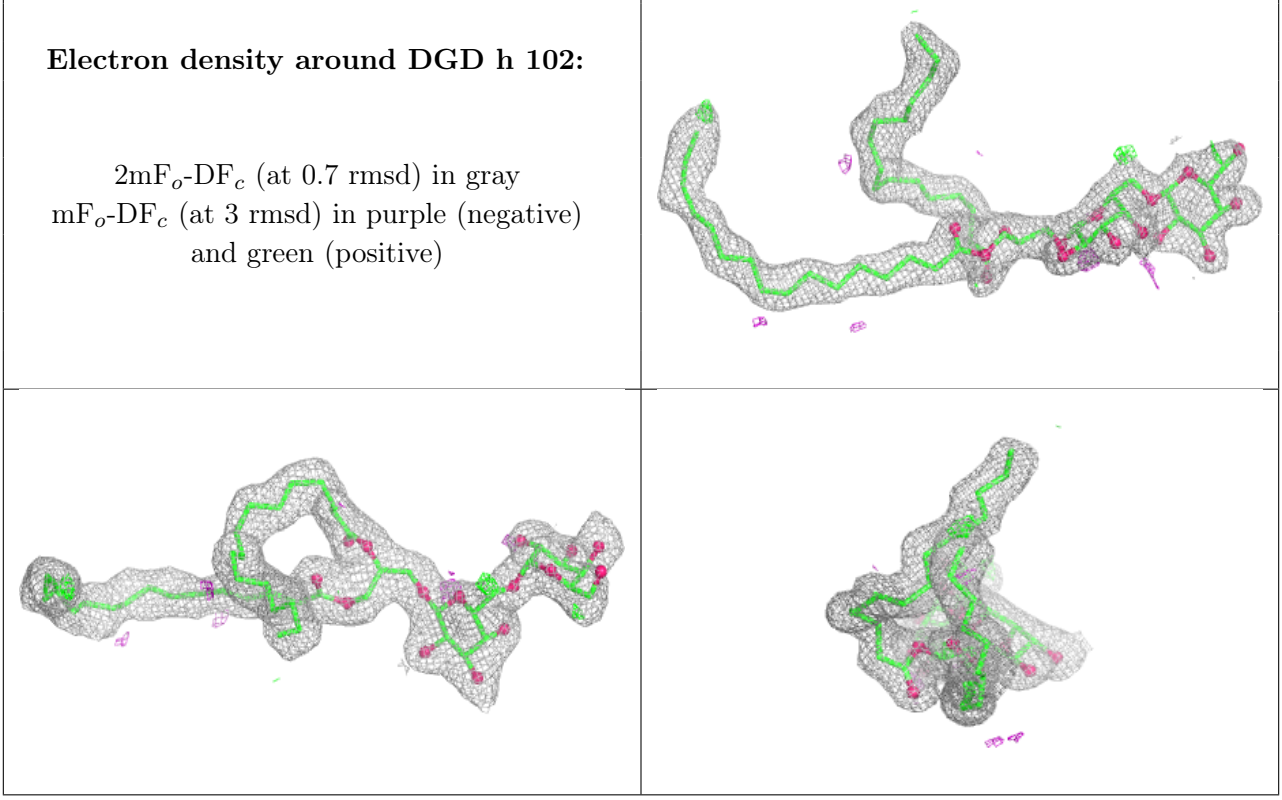
Electron density around BCR D 403:

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



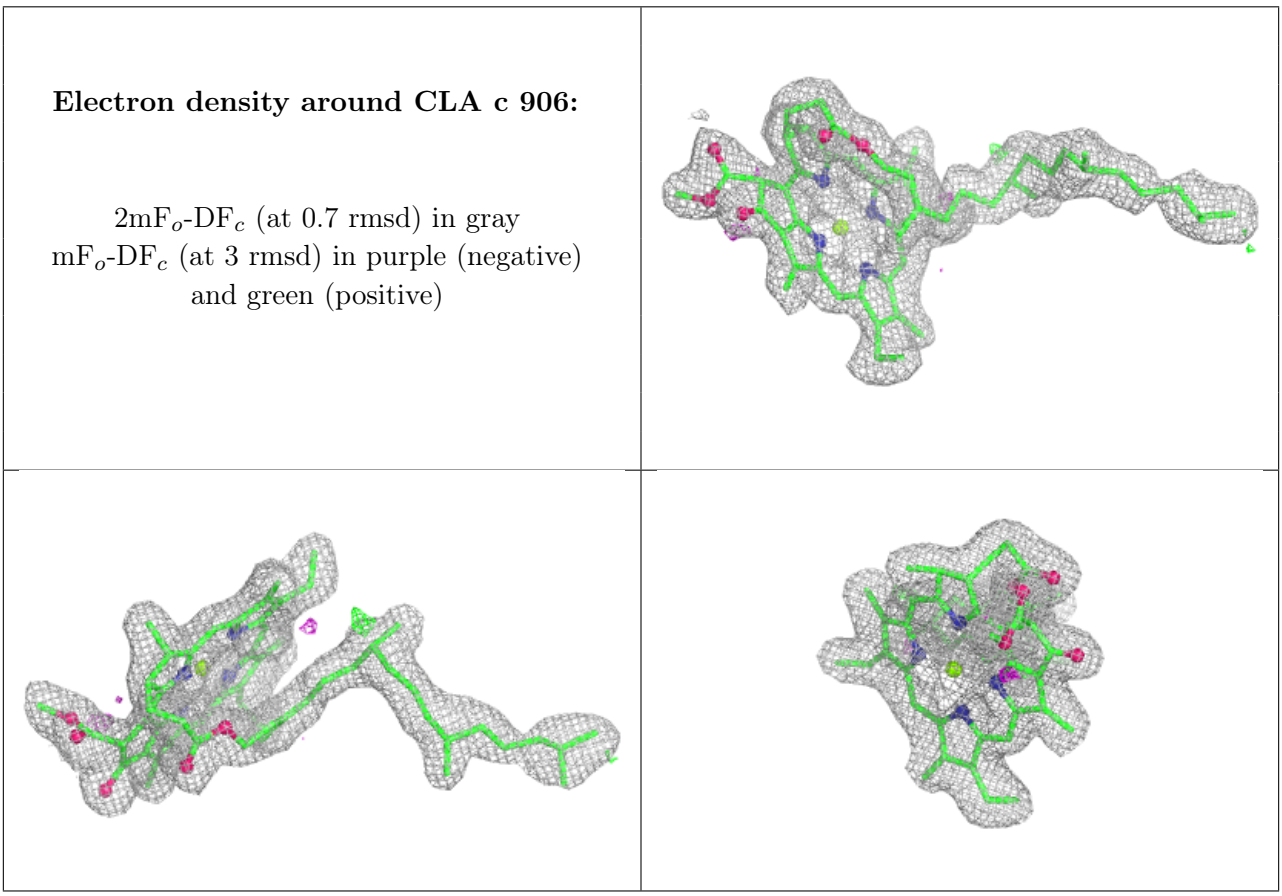
Electron density around DGD h 102:

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



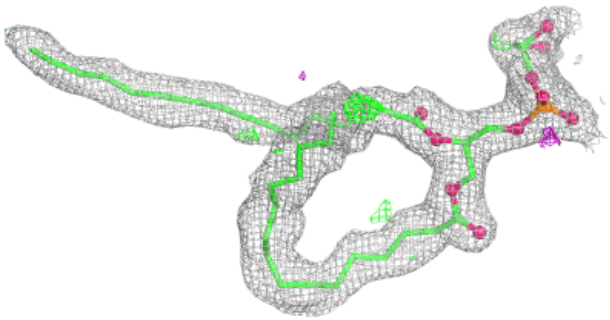
Electron density around CLA c 906:

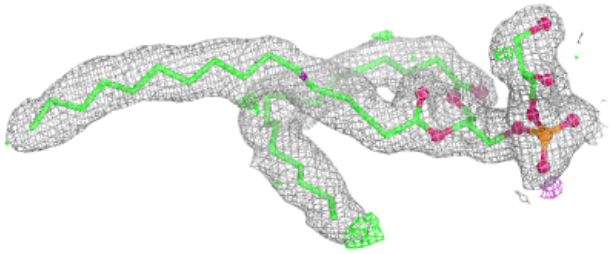
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

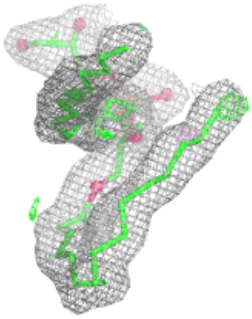


Electron density around LHG d 407:

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

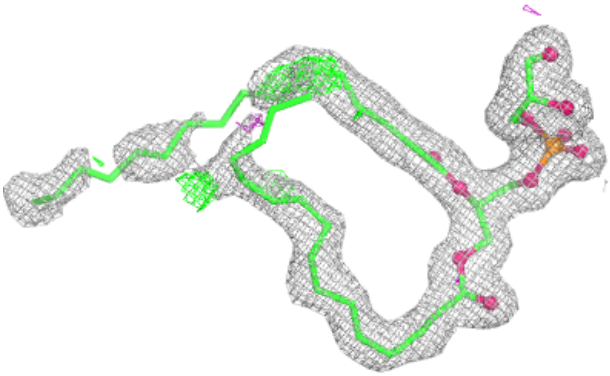


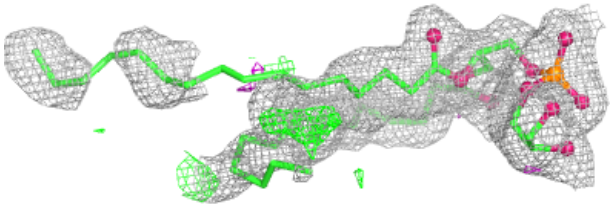


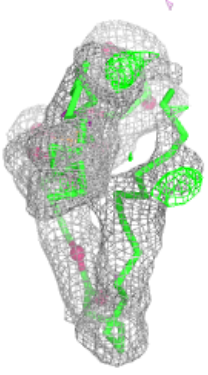


Electron density around LHG d 409:

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

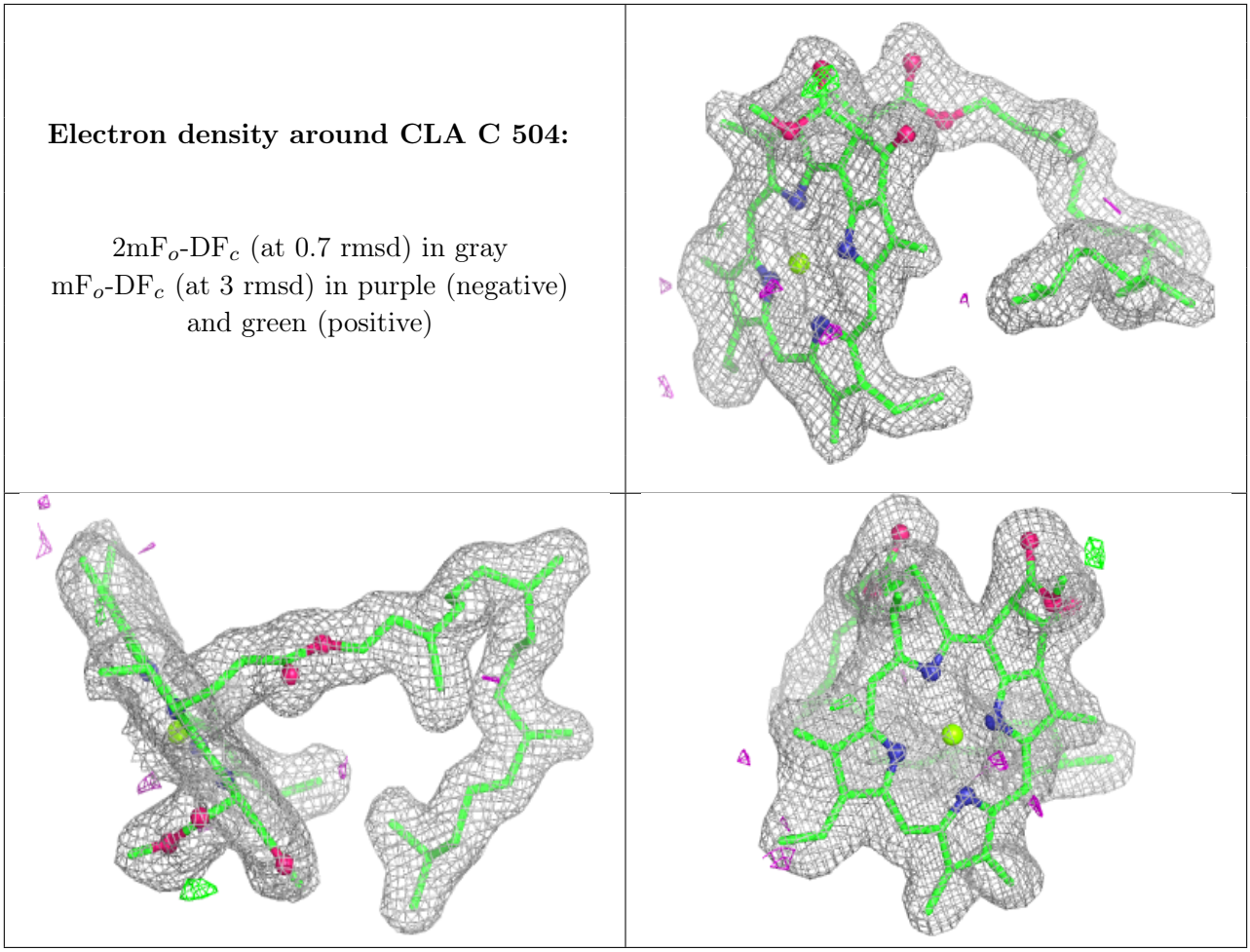






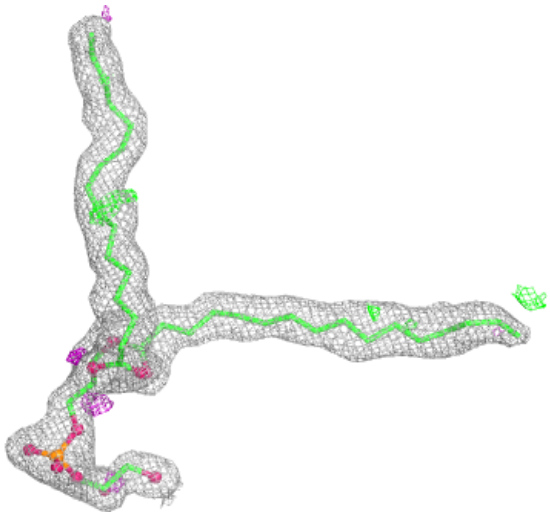
Electron density around CLA C 504:

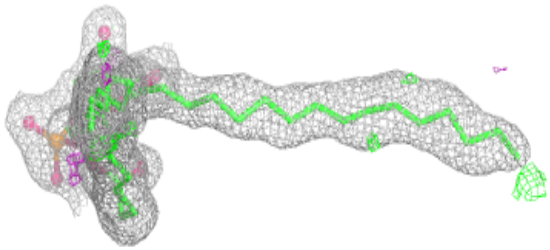
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

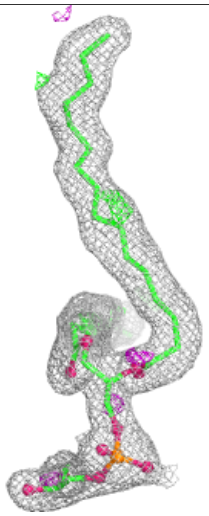


Electron density around LHG l 101:

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

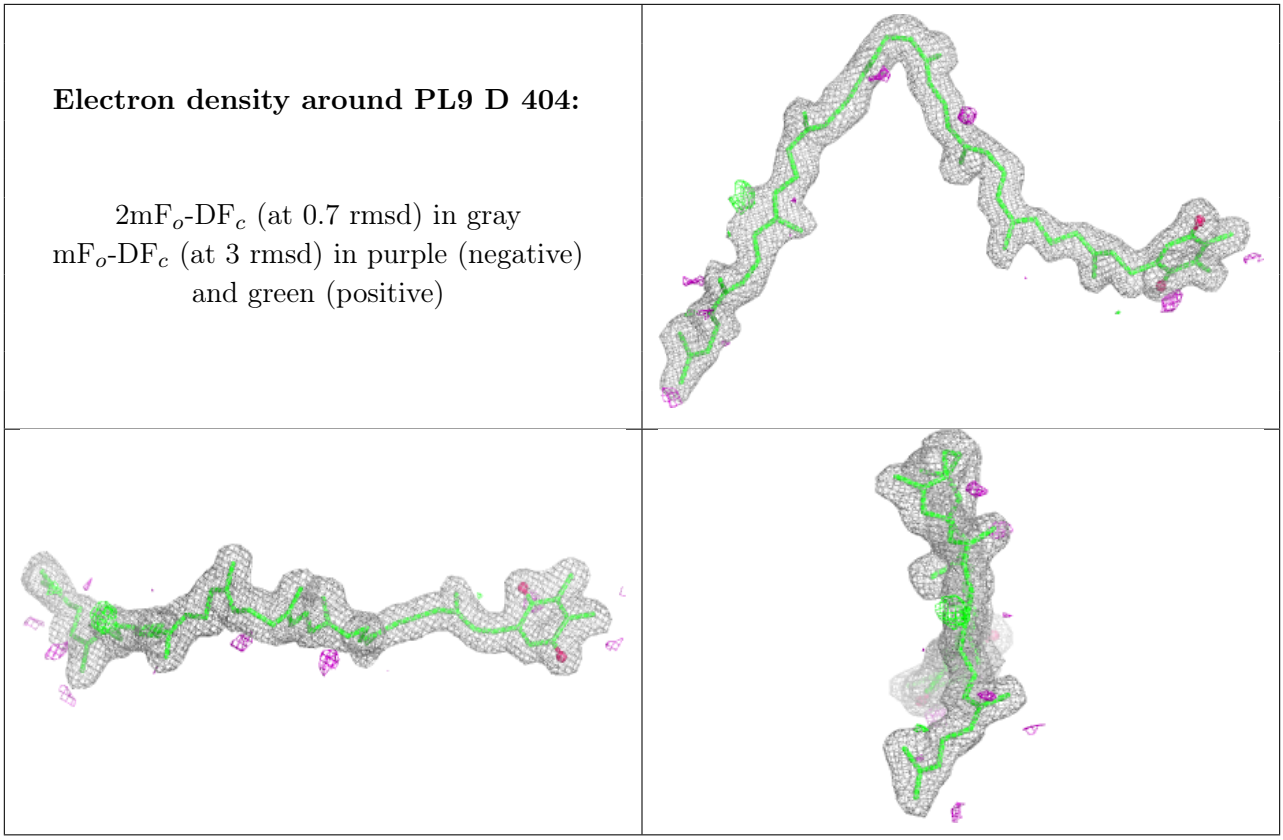






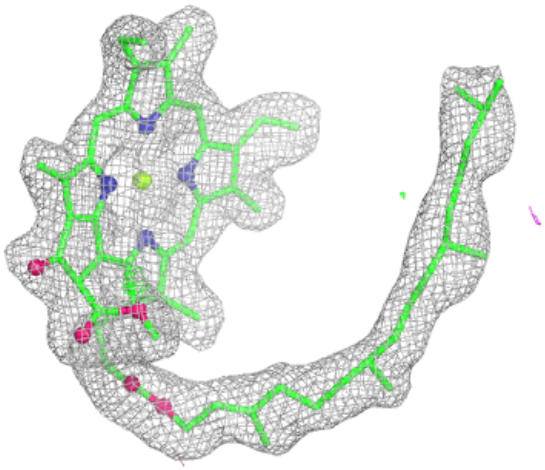
Electron density around PL9 D 404:

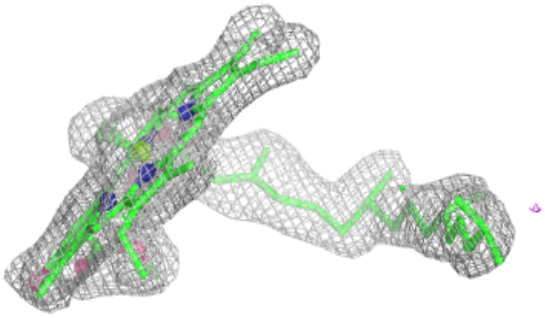
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

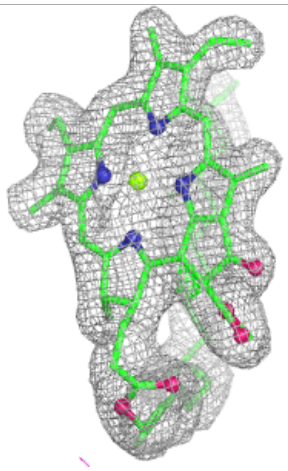


Electron density around CLA C 508:

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

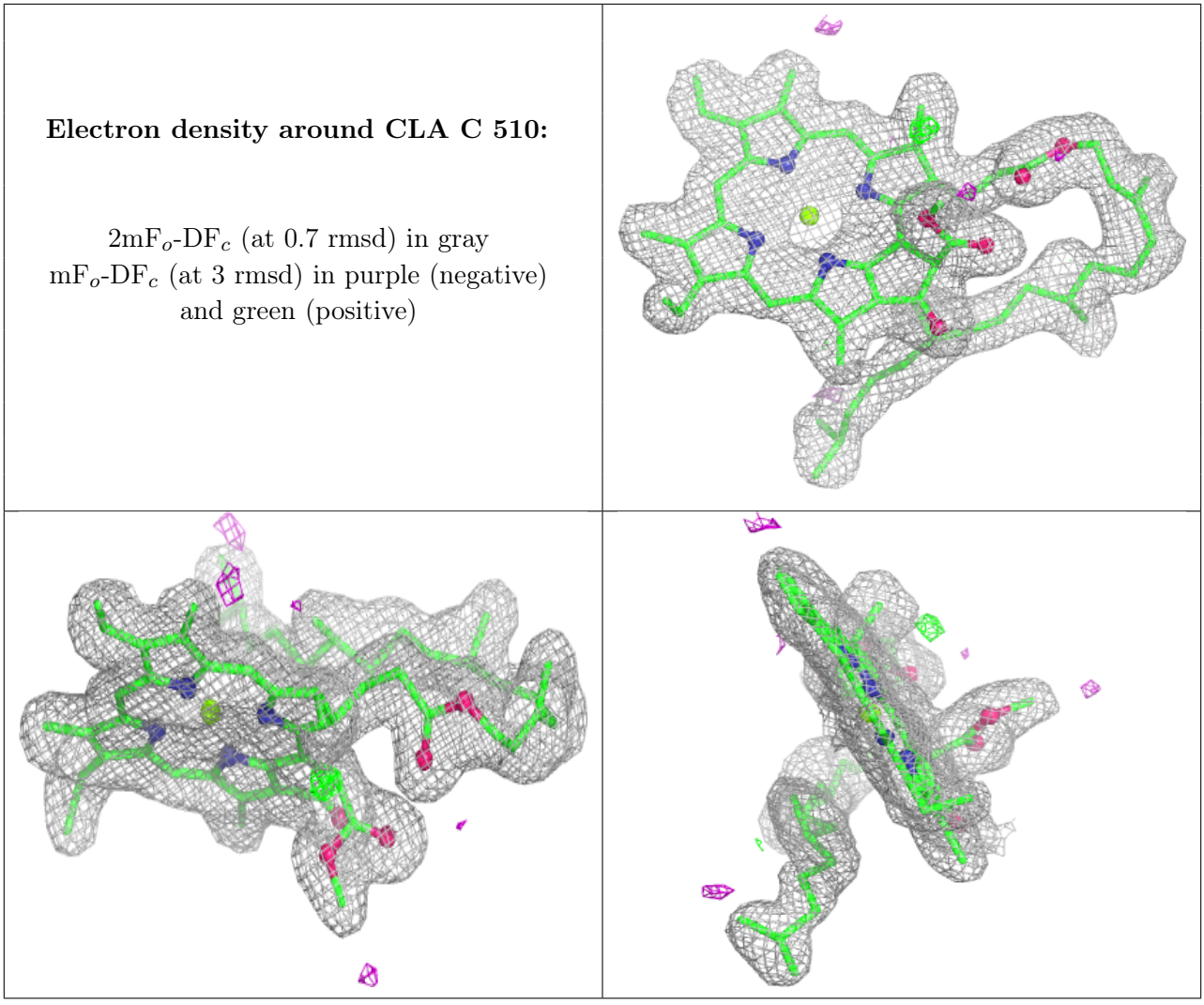






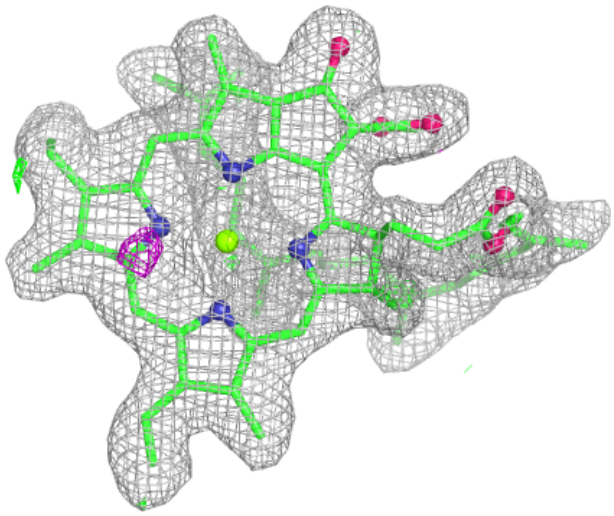
Electron density around CLA C 510:

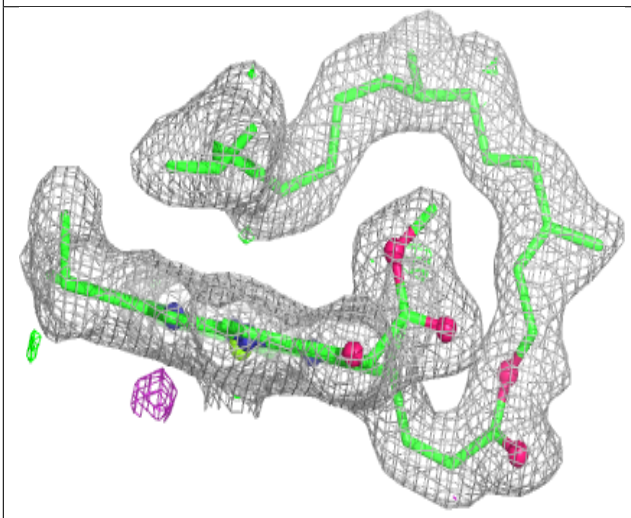
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

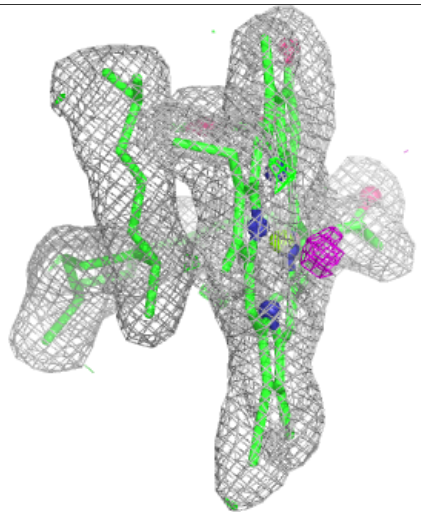


Electron density around CLA C 511:

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

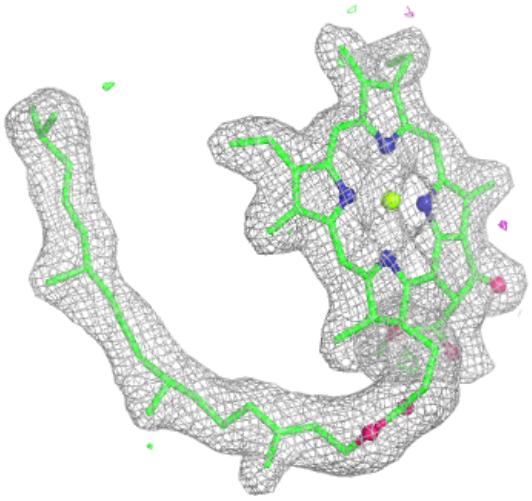


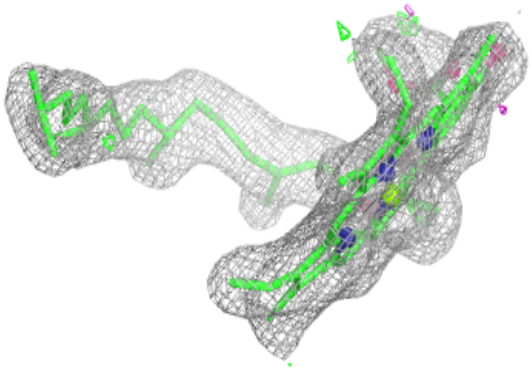


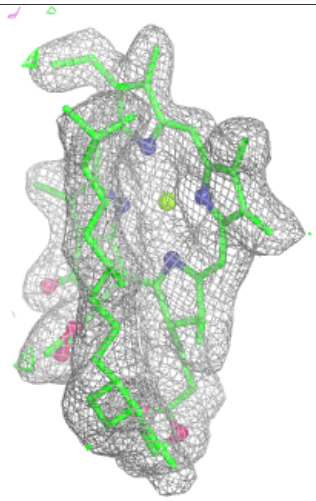


Electron density around CLA c 908:

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

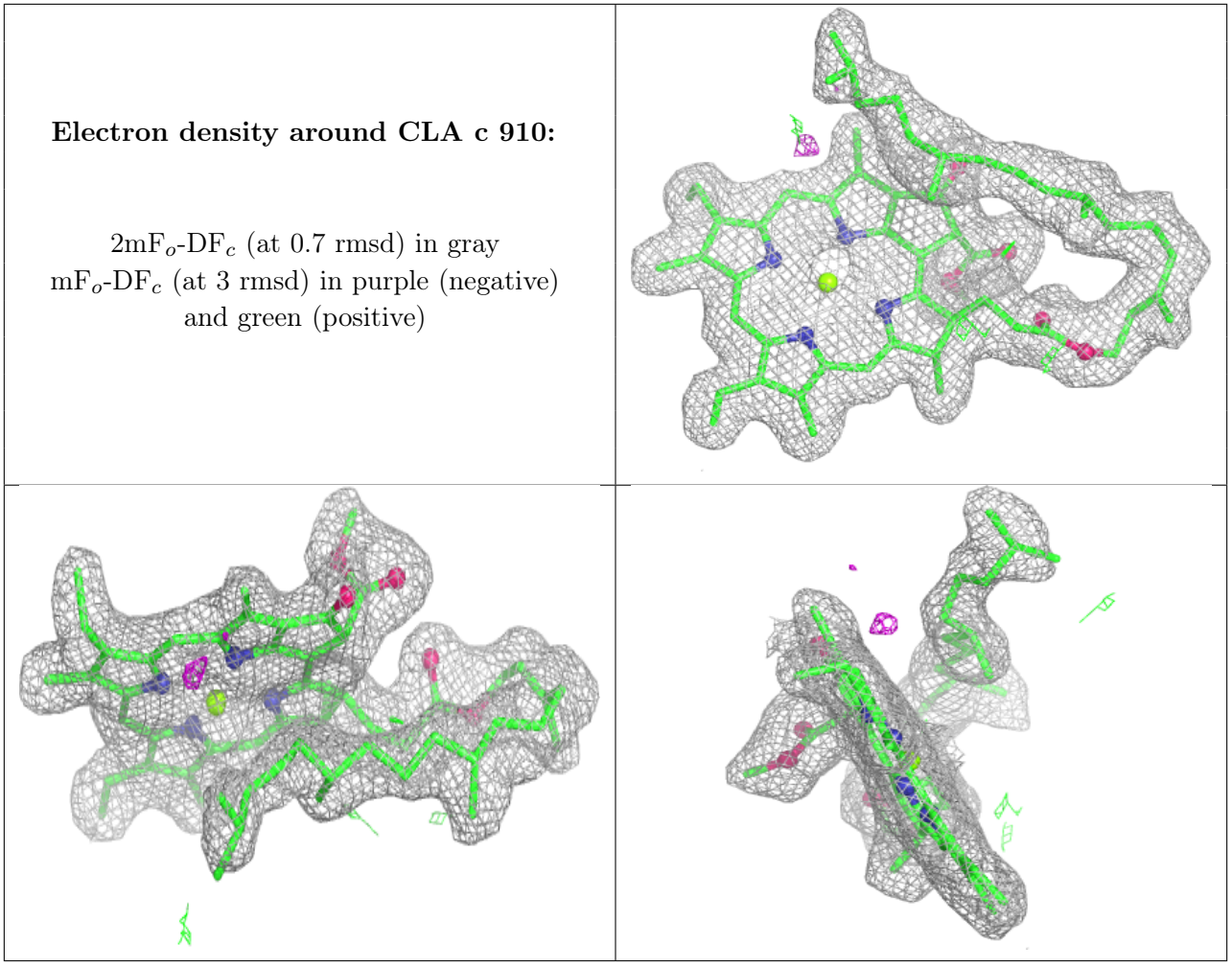






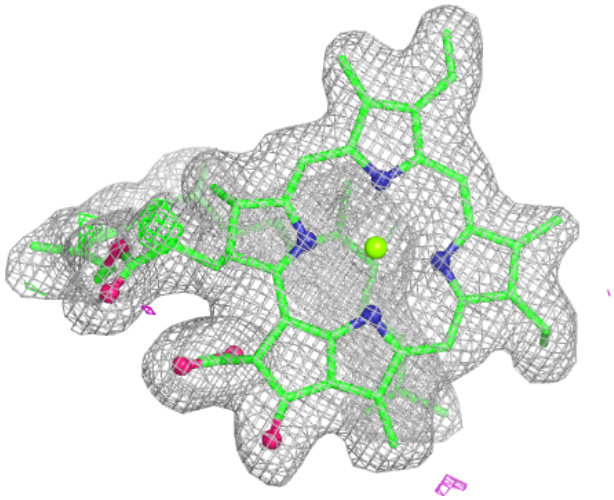
Electron density around CLA c 910:

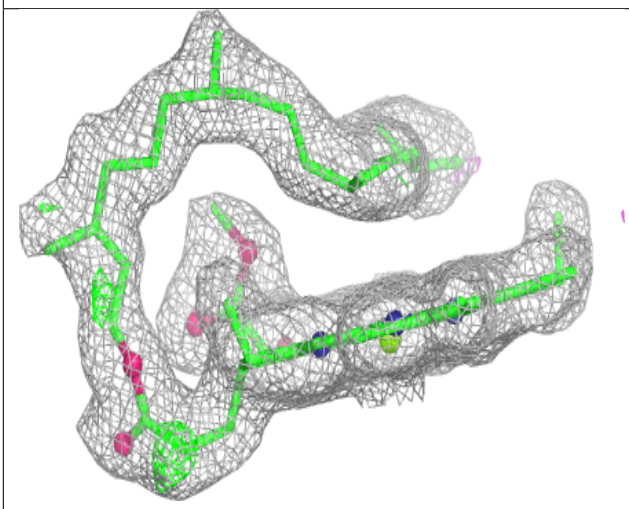
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

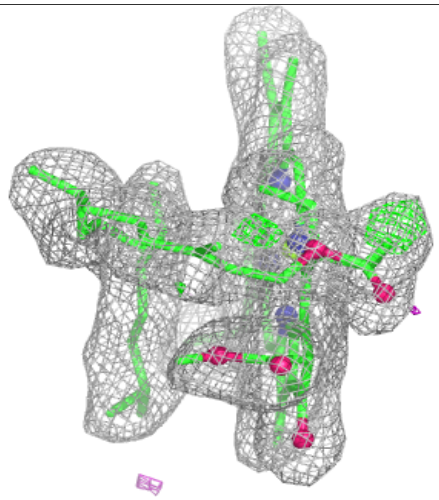


Electron density around CLA c 911:

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

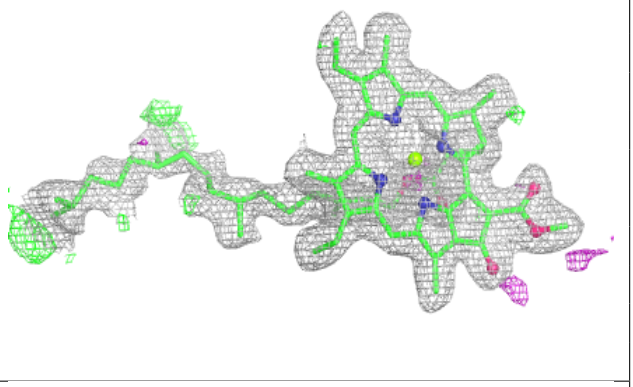


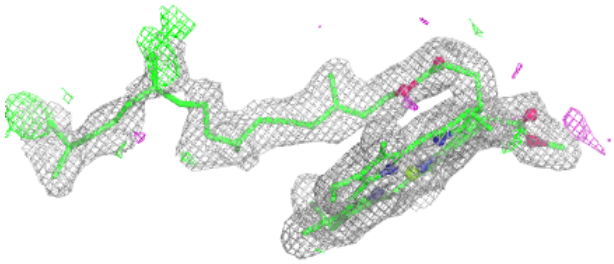


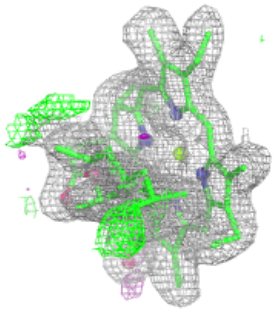


Electron density around CLA B 615:

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

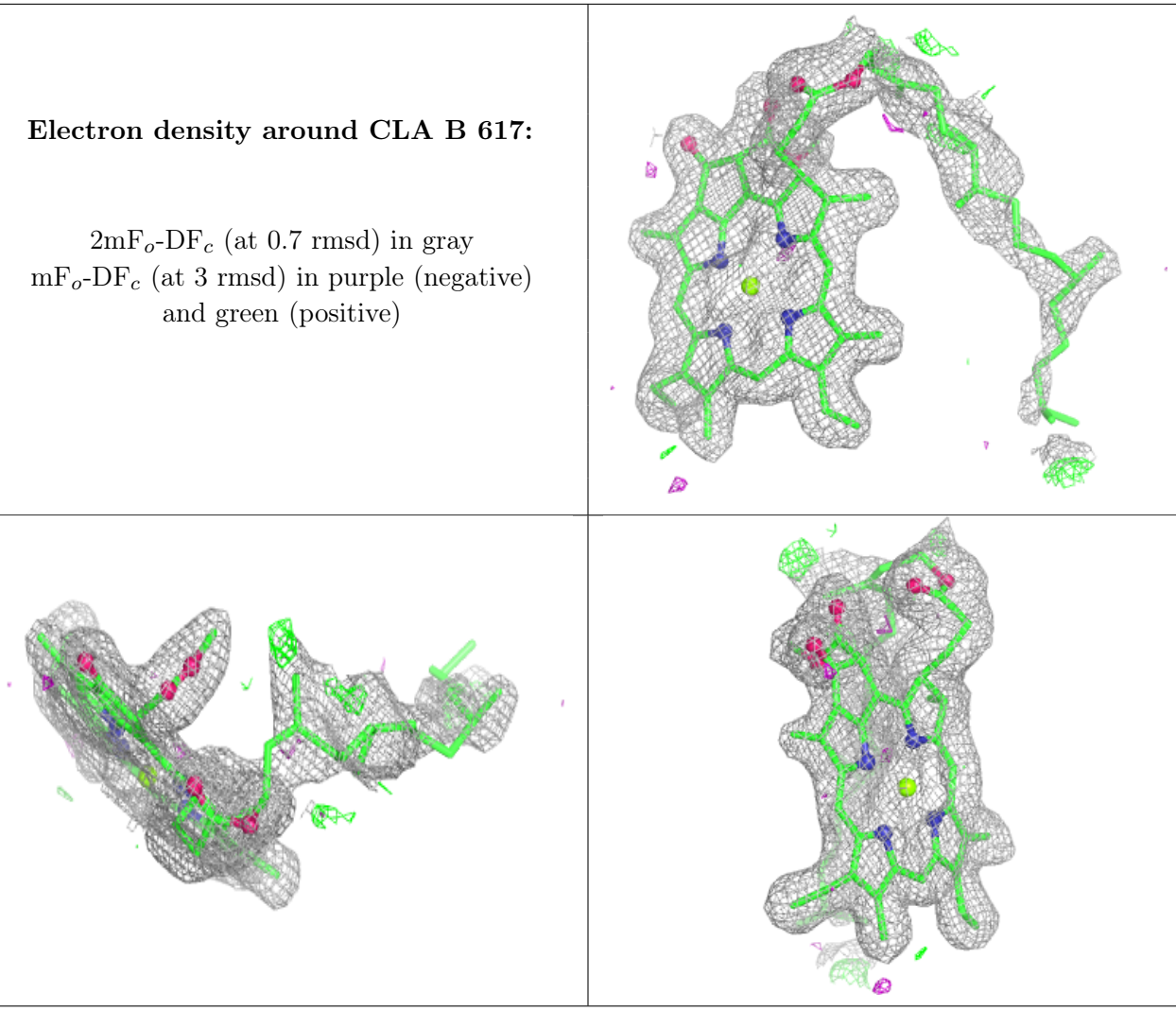






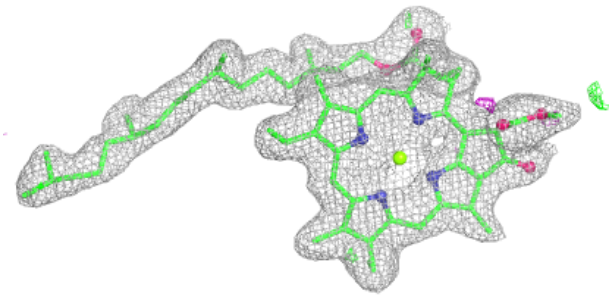
Electron density around CLA B 617:

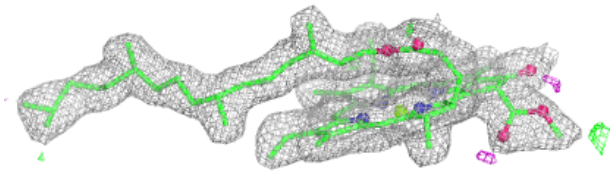
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

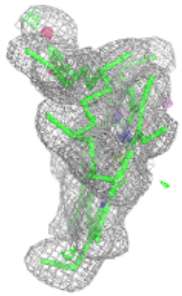


Electron density around CLA C 502:

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

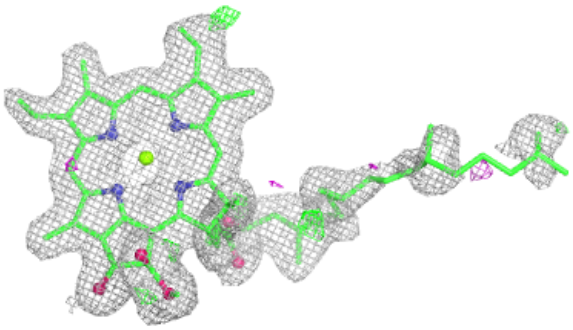


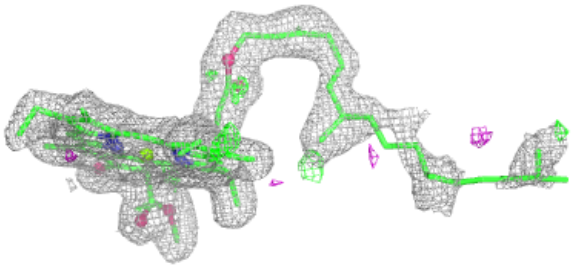


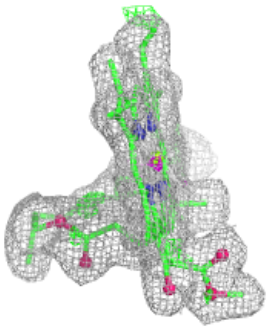


Electron density around CLA a 407:

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

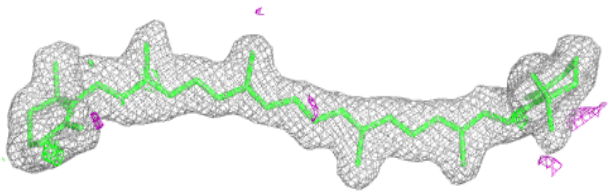


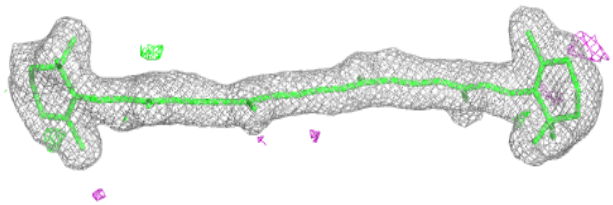


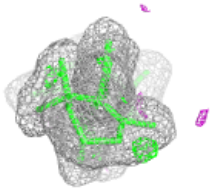


Electron density around BCR A 411:

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

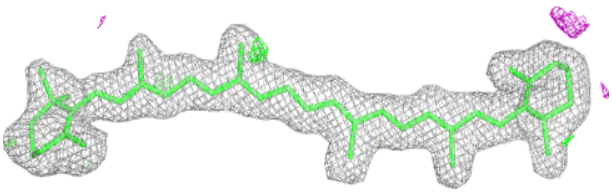


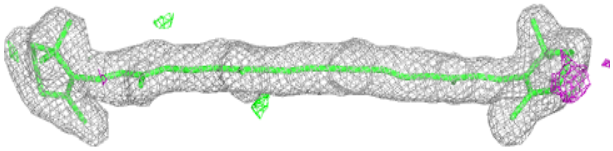


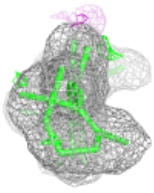


Electron density around BCR B 619:

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

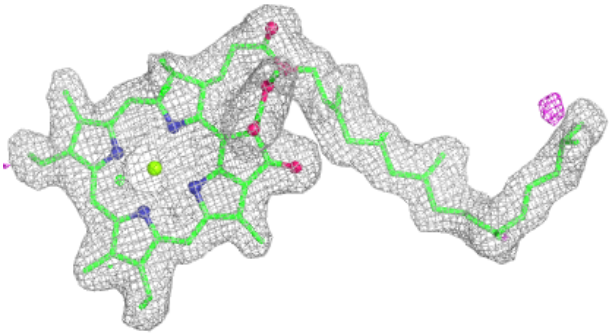


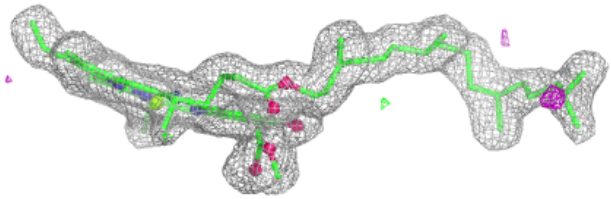


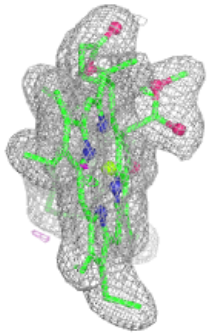


Electron density around CLA b 606:

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

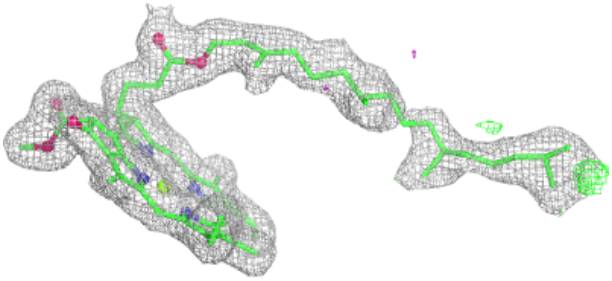


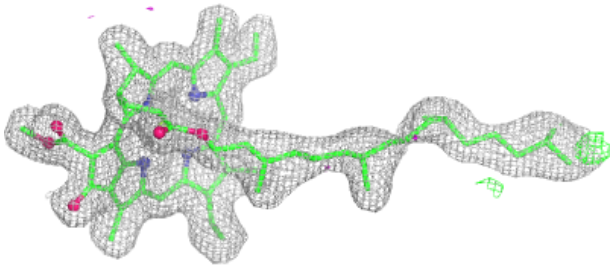


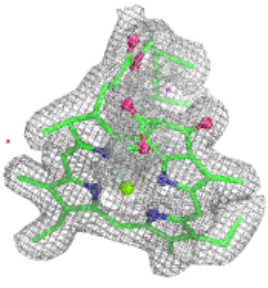


Electron density around CLA C 505:

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



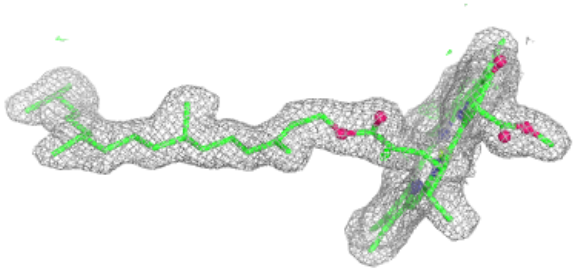


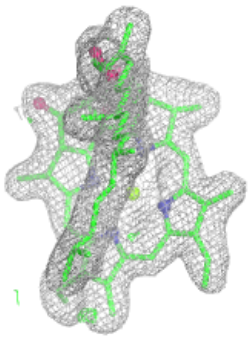


Electron density around CLA b 613:

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

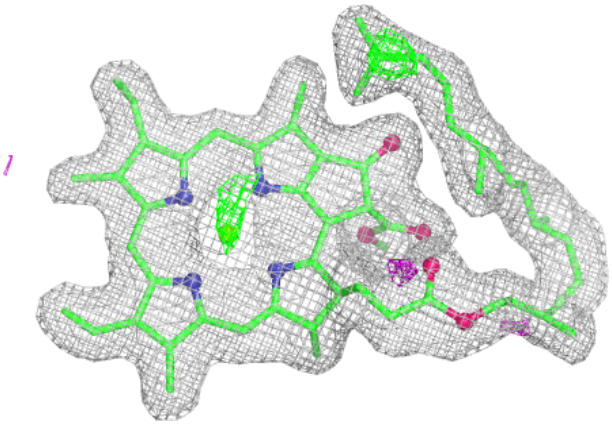


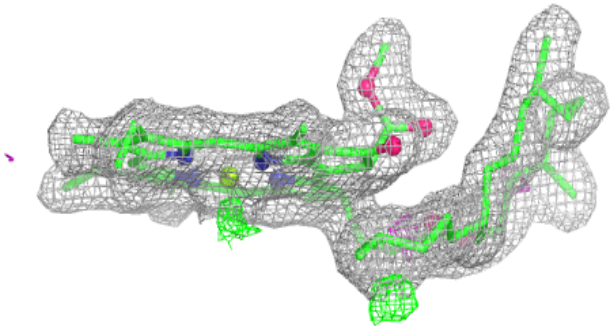


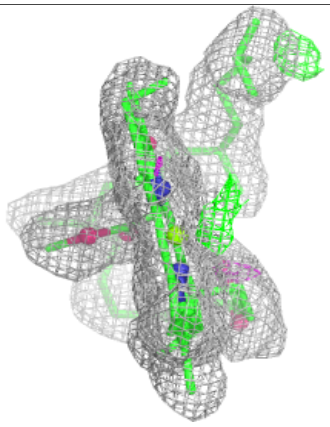


Electron density around CLA b 614:

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

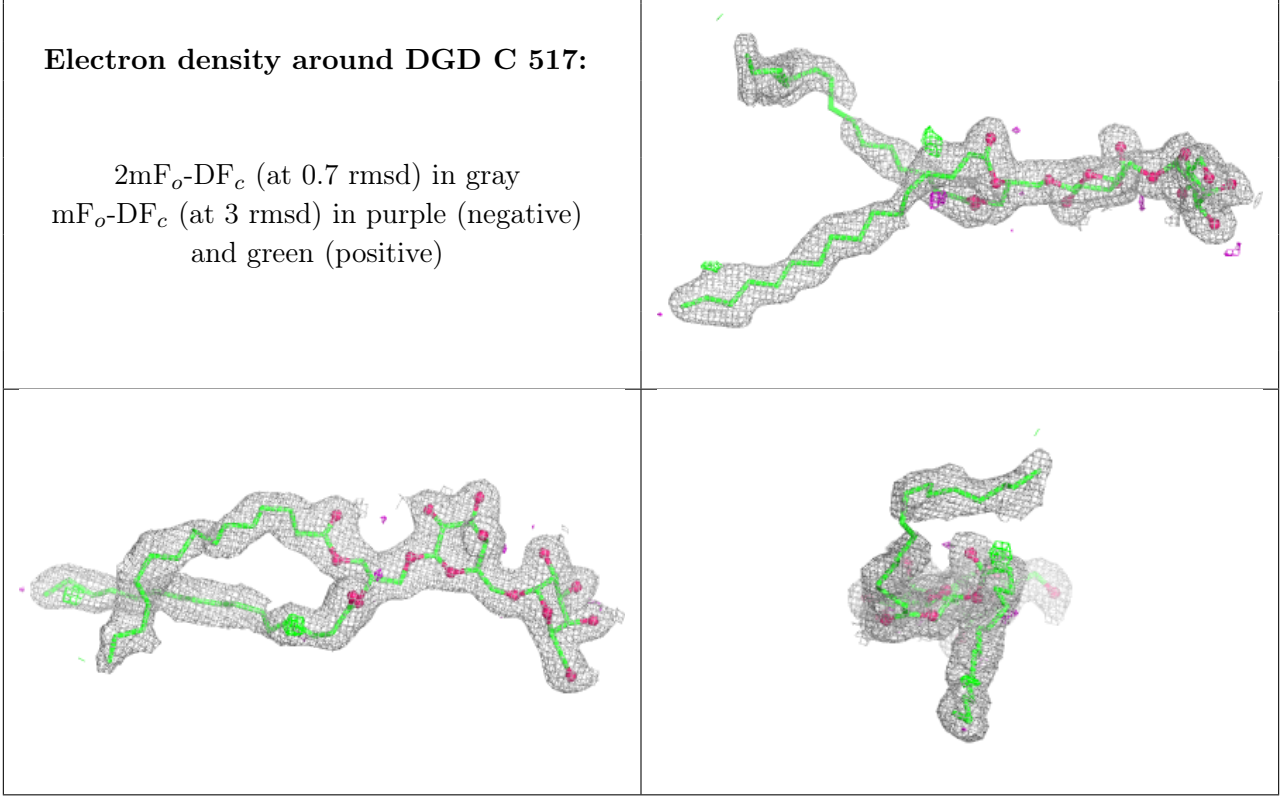






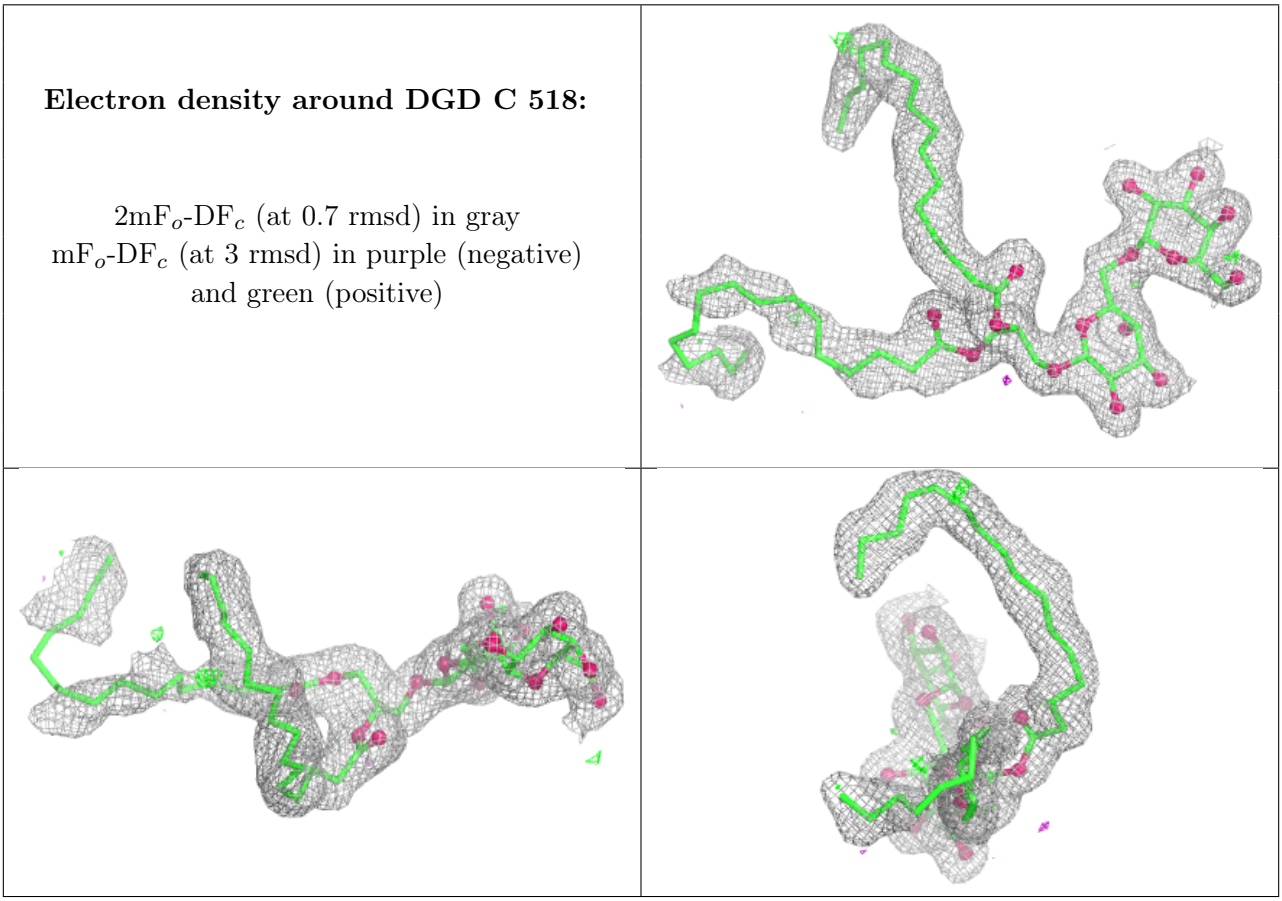
Electron density around DGD C 517:

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



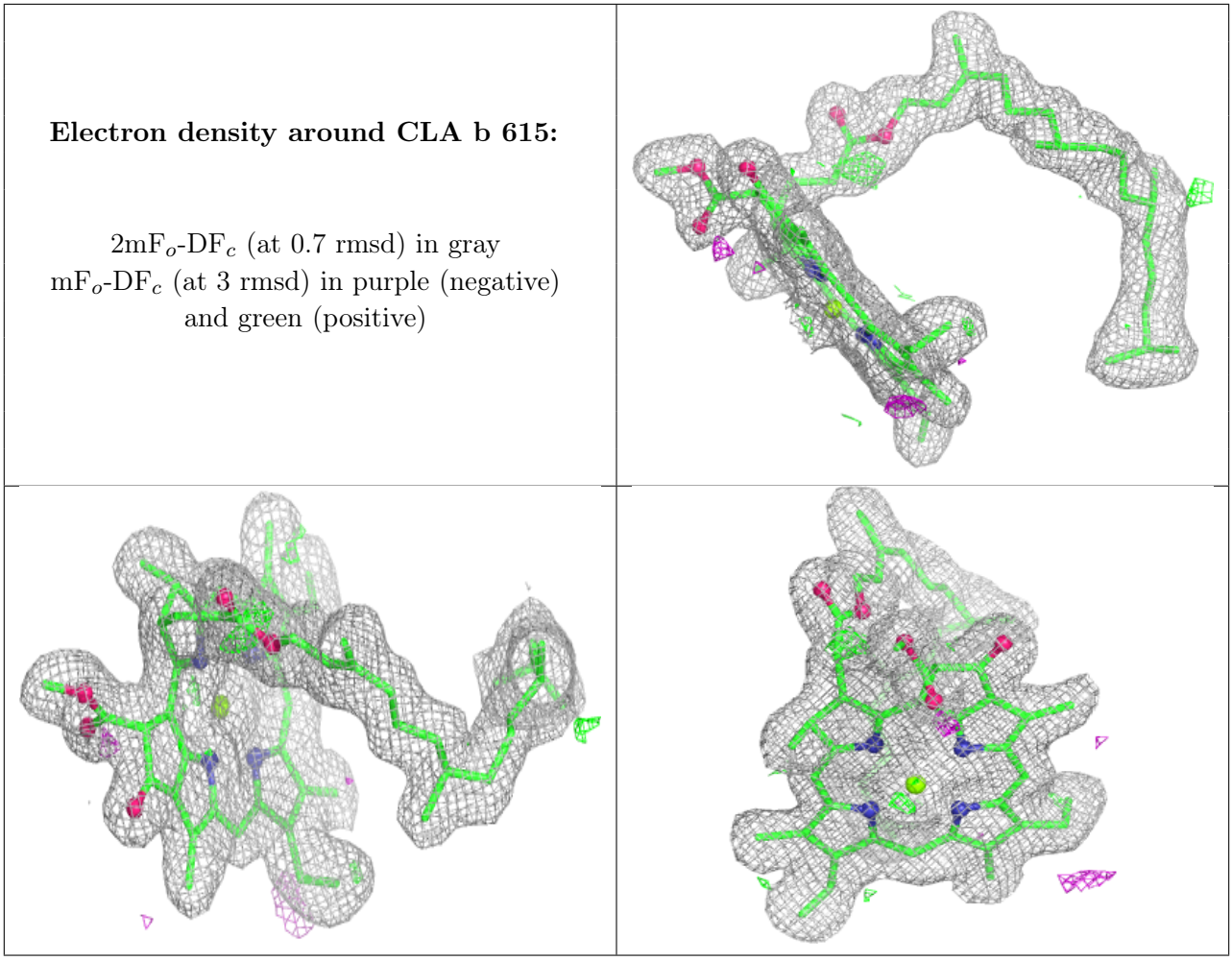
Electron density around DGD C 518:

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



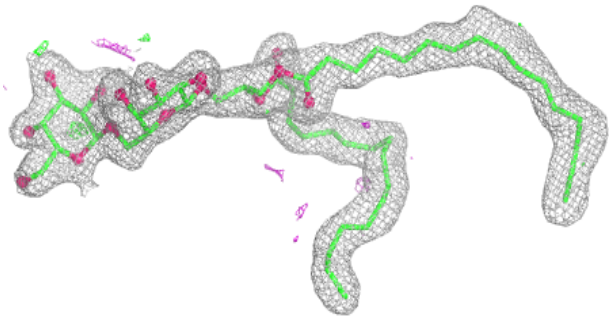
Electron density around CLA b 615:

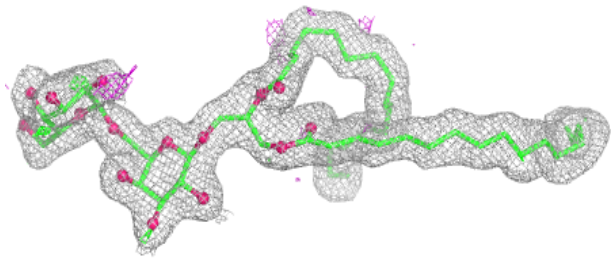
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

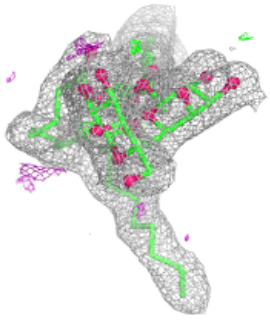


Electron density around DGD H 102:

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

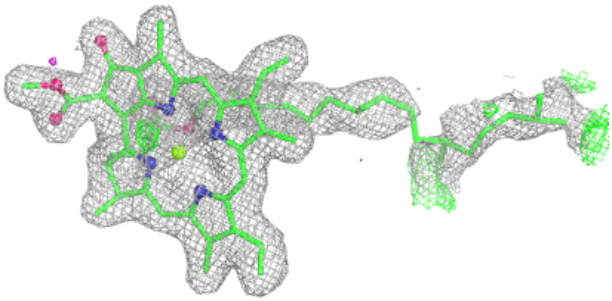


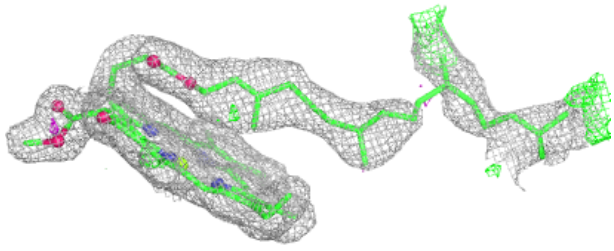


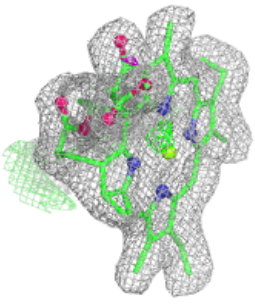


Electron density around CLA b 618:

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

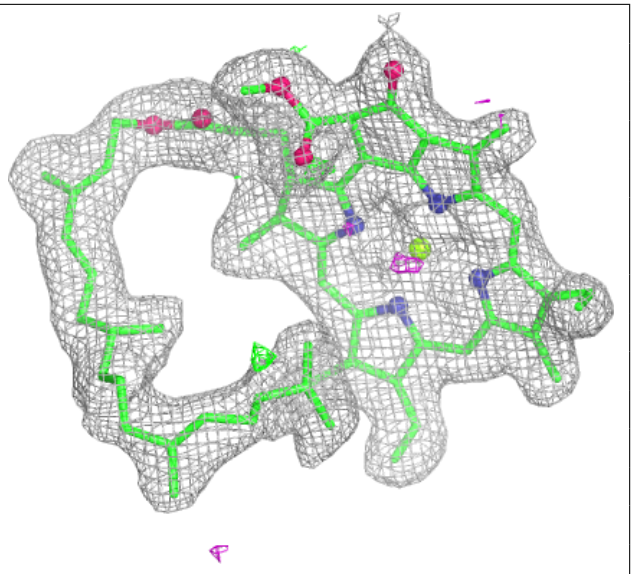


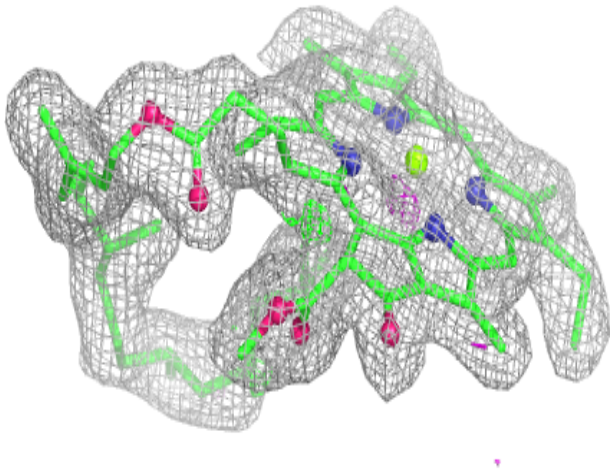




Electron density around CLA b 619:

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

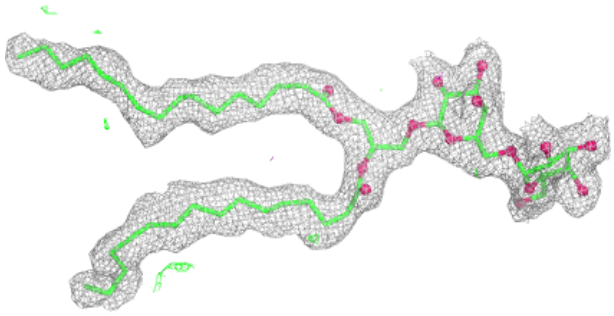


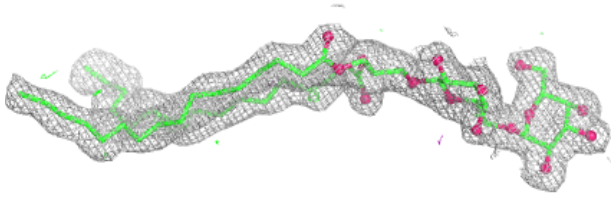


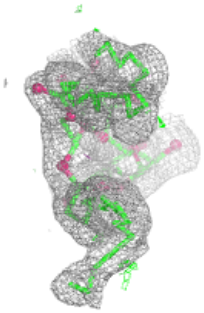


Electron density around DGD c 918:

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

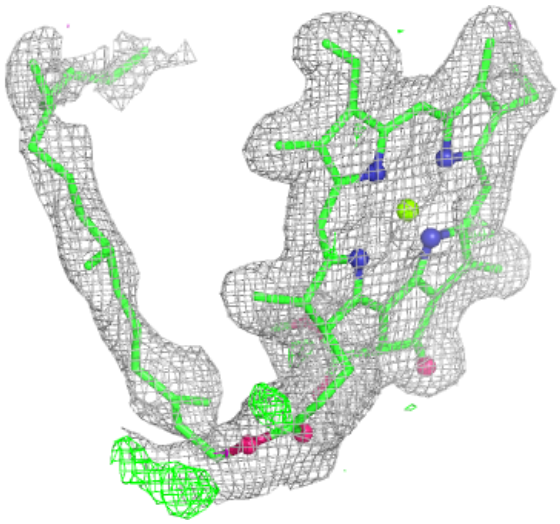


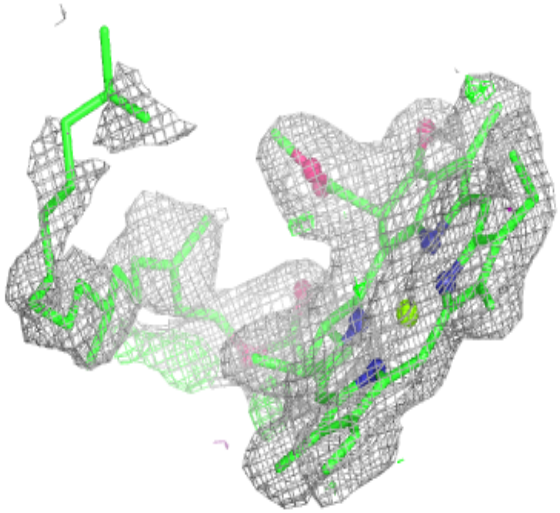


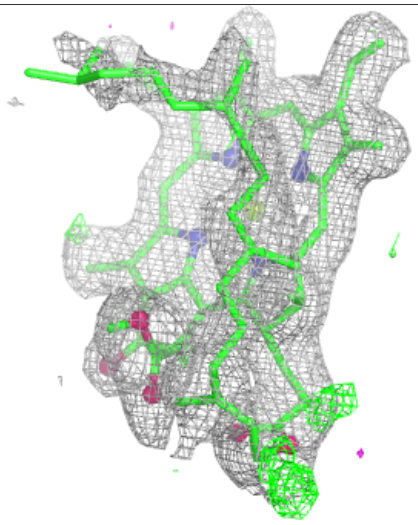


Electron density around CLA b 620:

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

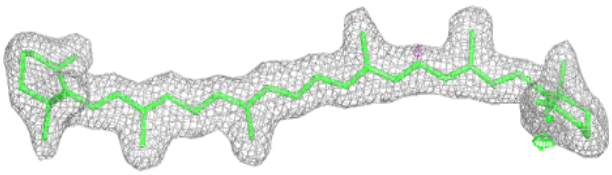


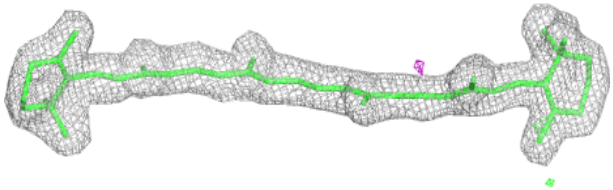


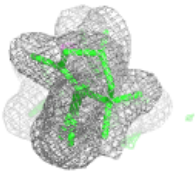


Electron density around BCR a 410:

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

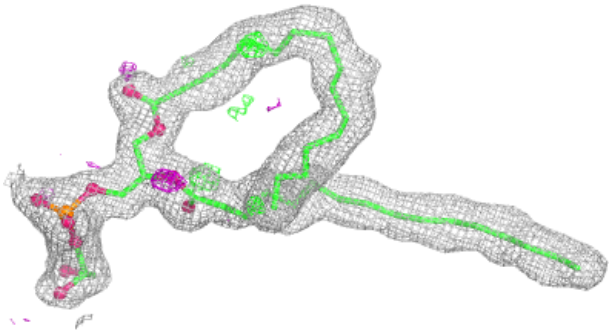


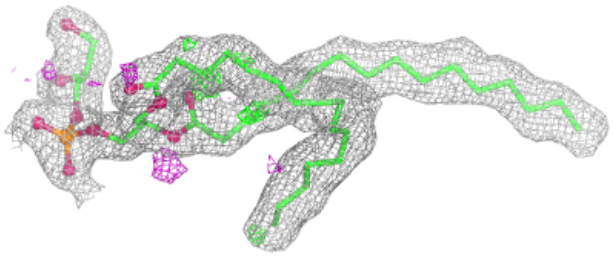




Electron density around LHG D 406:

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

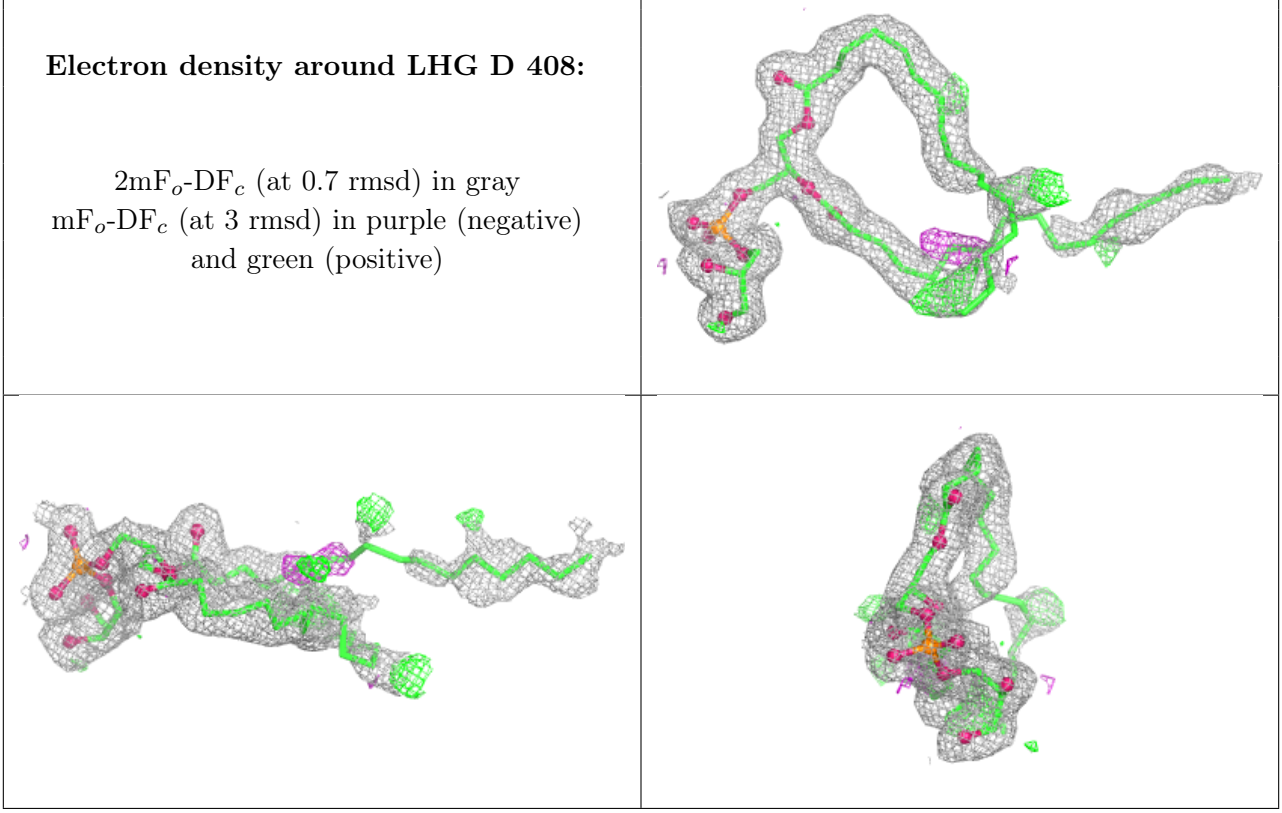






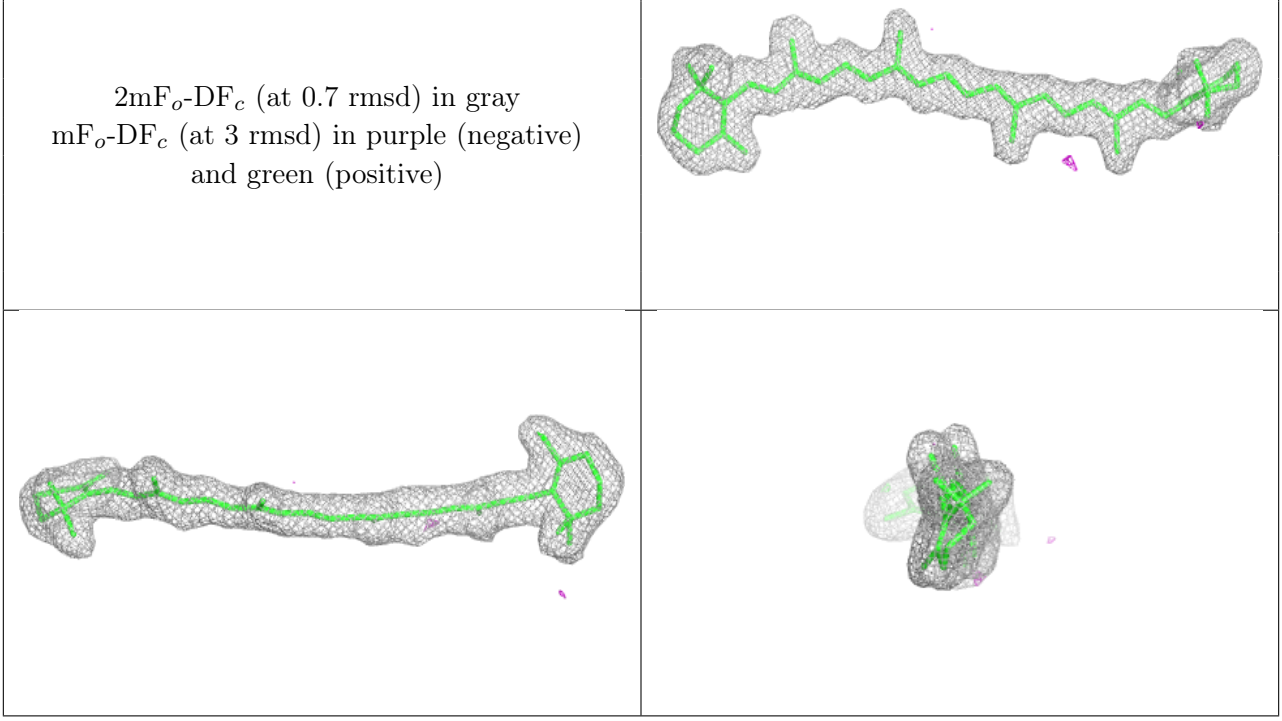
Electron density around LHG D 408:

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



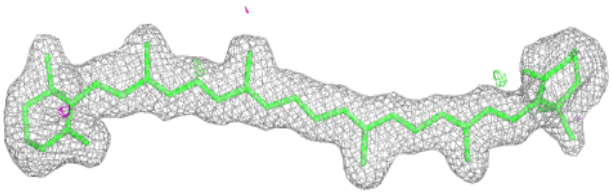
Electron density around BCR b 621:

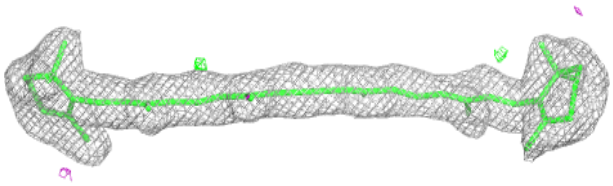
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

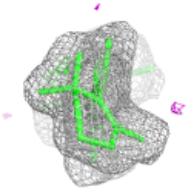


Electron density around BCR b 622:

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

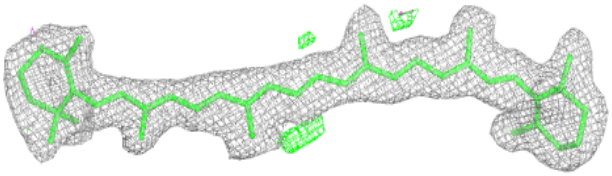


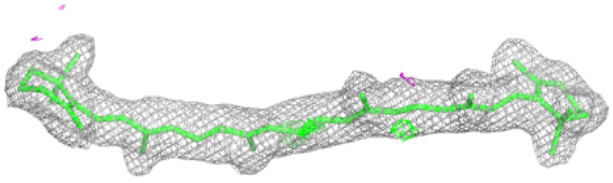


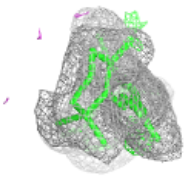


Electron density around BCR b 623:

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

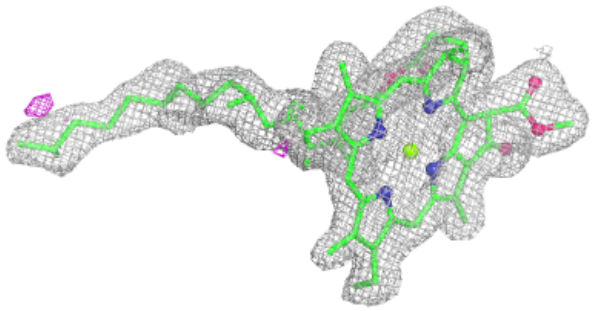


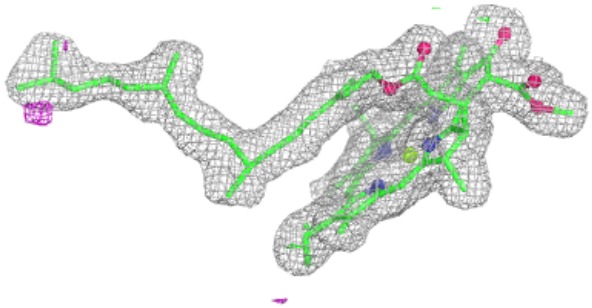


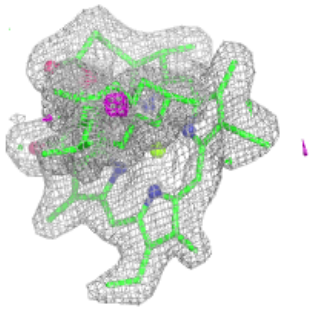


Electron density around CLA C 506:

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

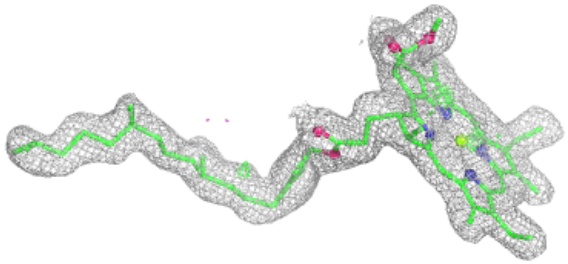


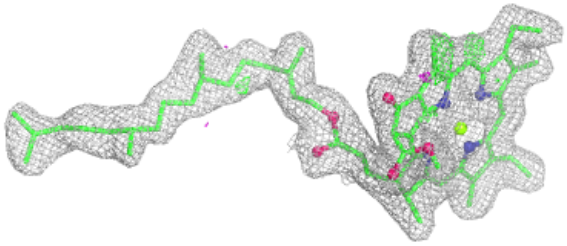


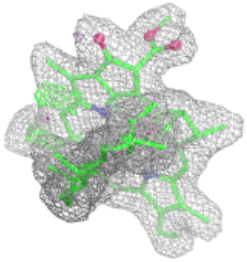


Electron density around CLA c 903:

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

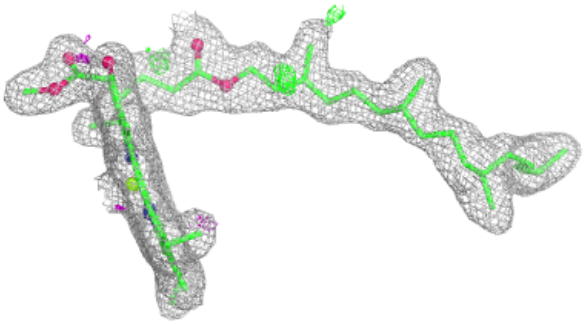


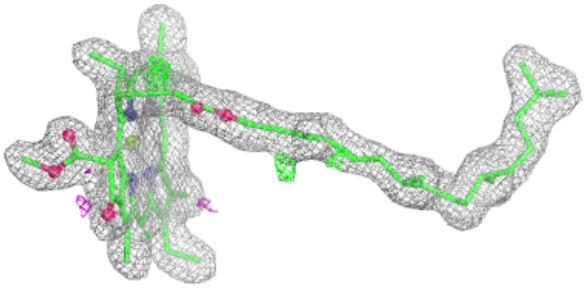


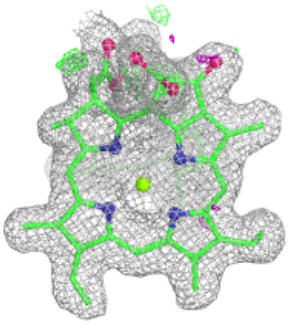


Electron density around CLA b 609:

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

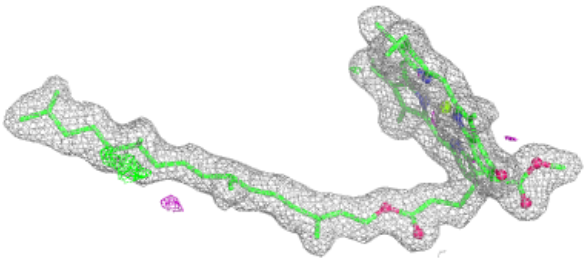


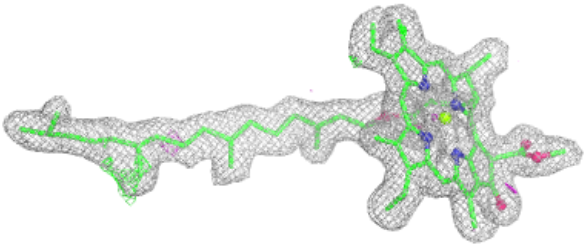


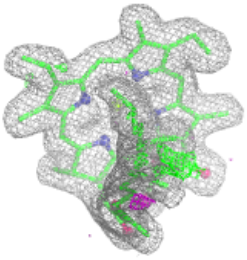


Electron density around CLA B 608:

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

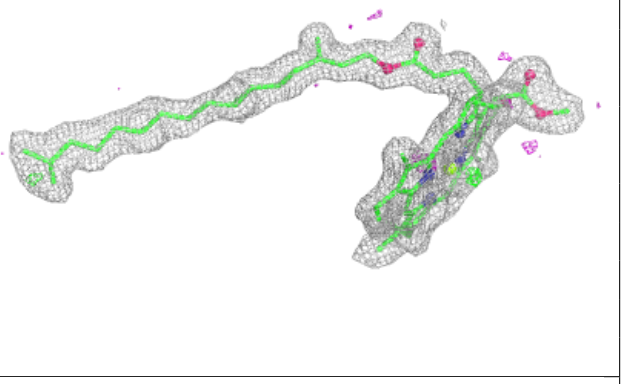


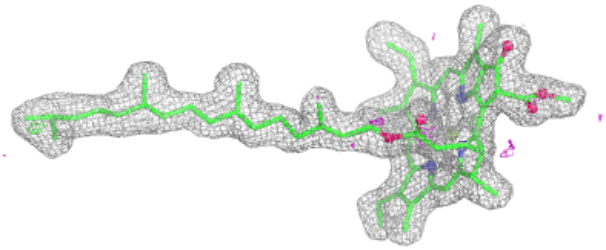


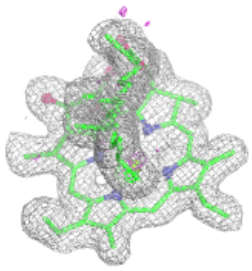


Electron density around CLA b 611:

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

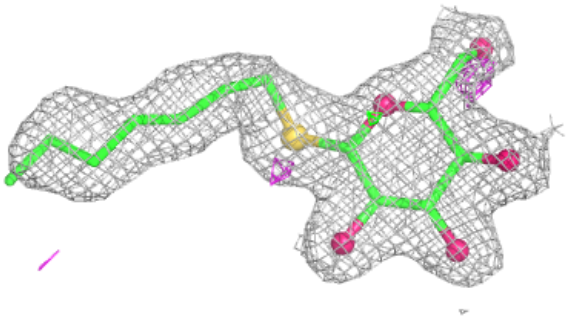


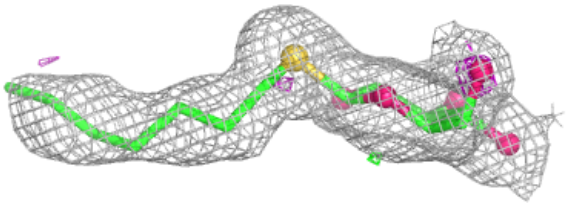


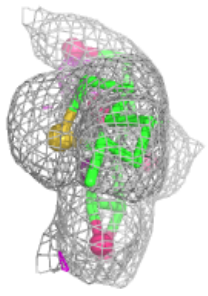


Electron density around HTG O 303:

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

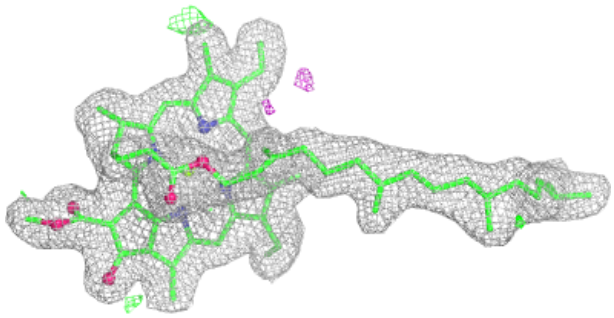


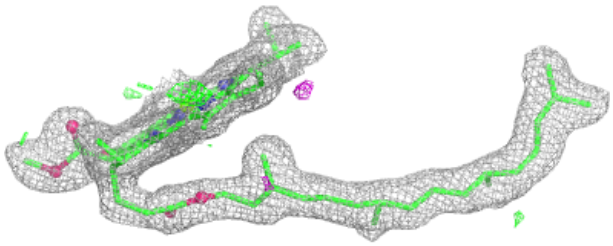


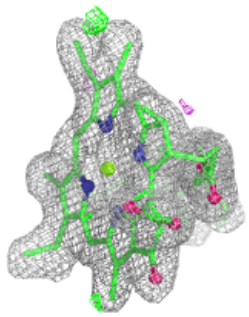


Electron density around CLA b 612:

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

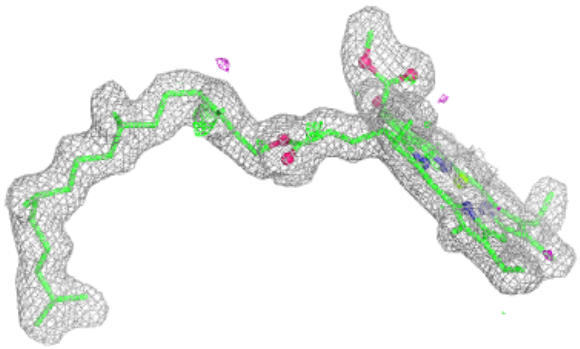


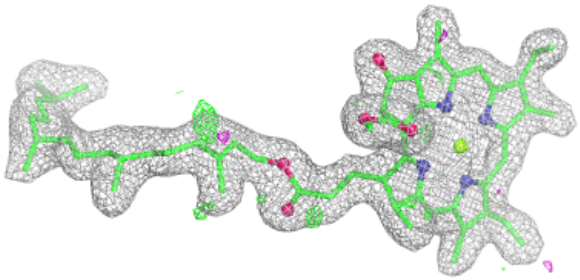


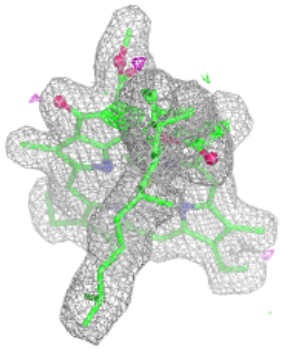


Electron density around CLA d 402:

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

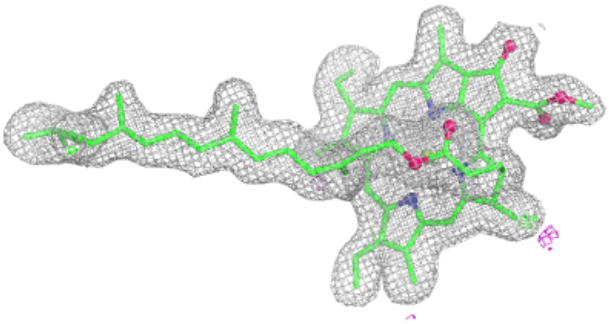


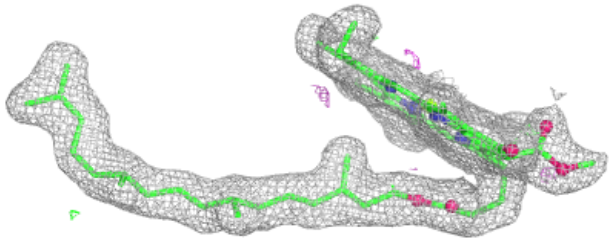


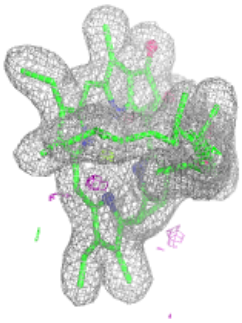


Electron density around CLA B 609:

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

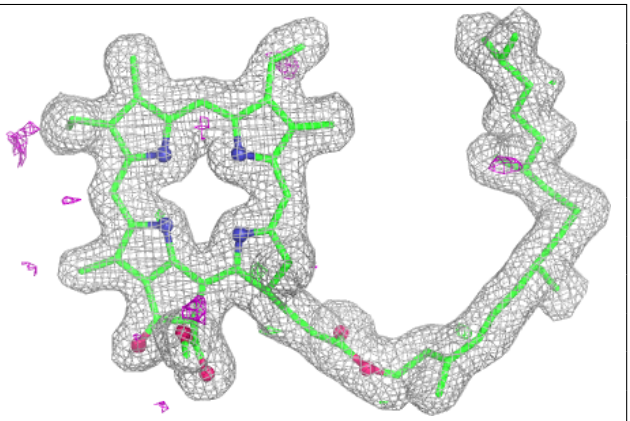


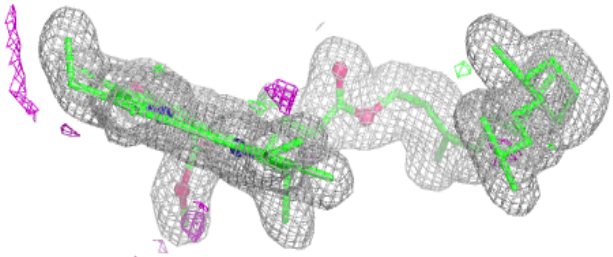




Electron density around PHO A 408:

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

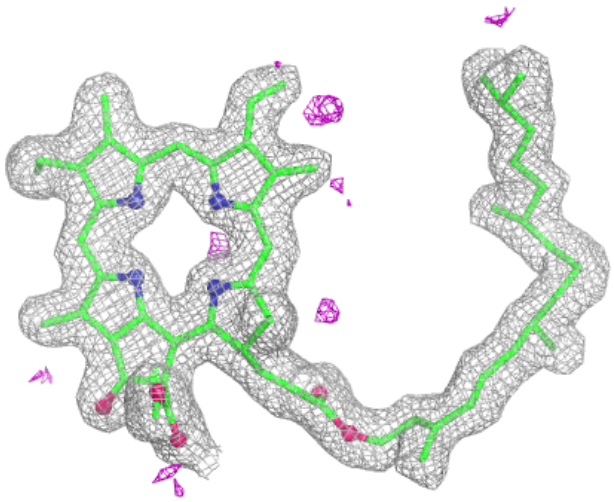


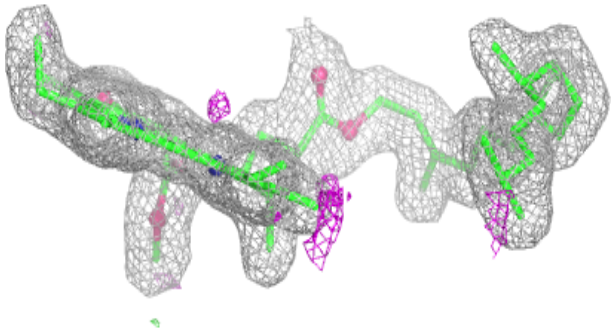


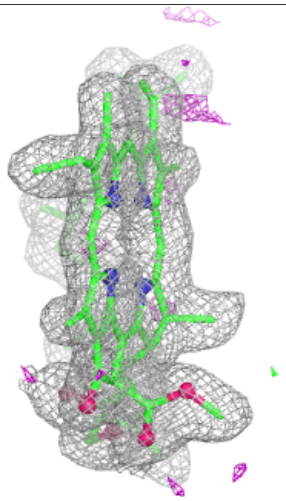


Electron density around PHO a 408:

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

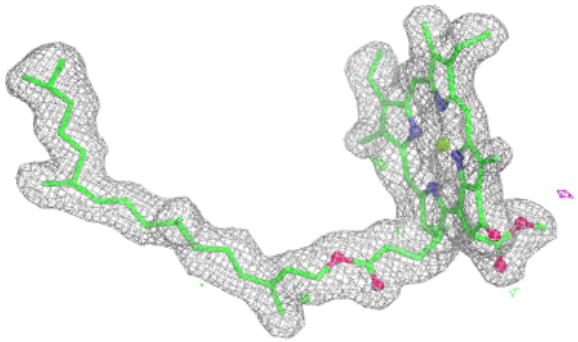


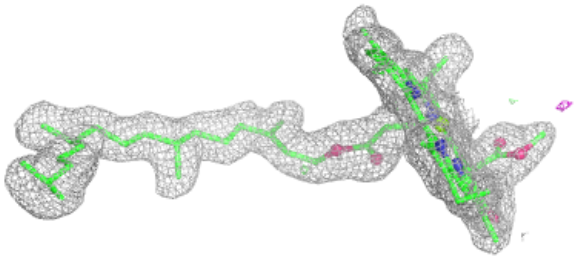


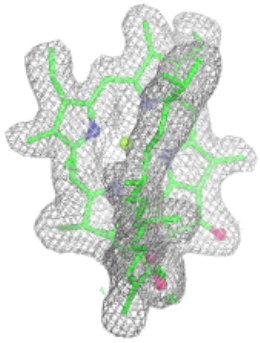


Electron density around CLA B 610:

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

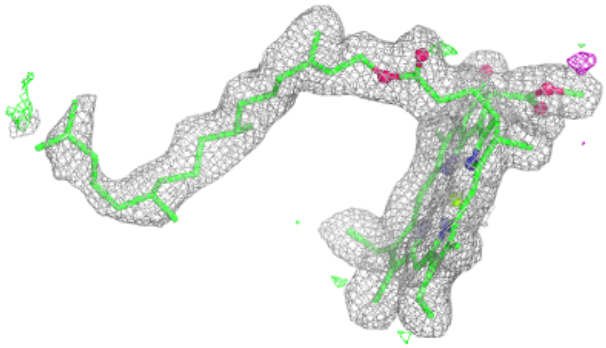


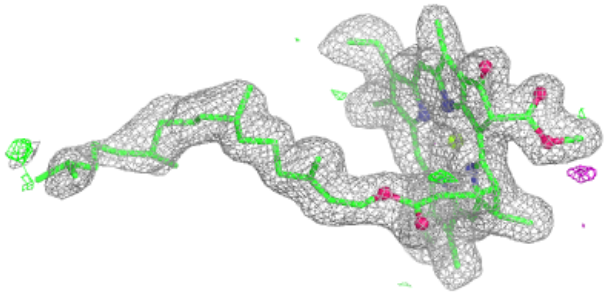


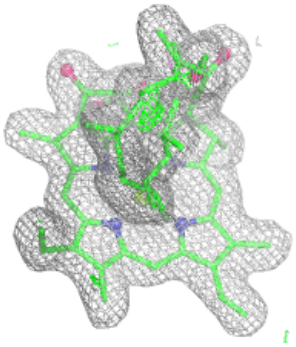


Electron density around CLA C 509:

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

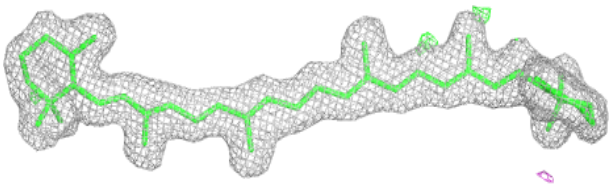


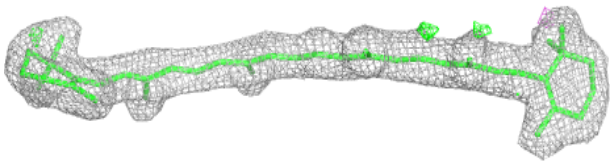


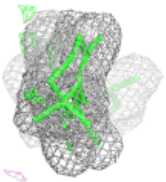


Electron density around BCR B 618:

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

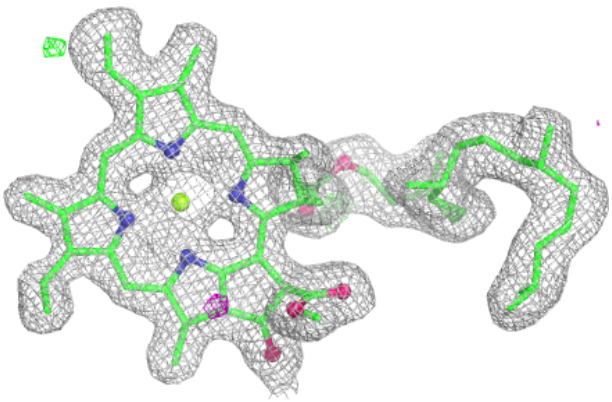


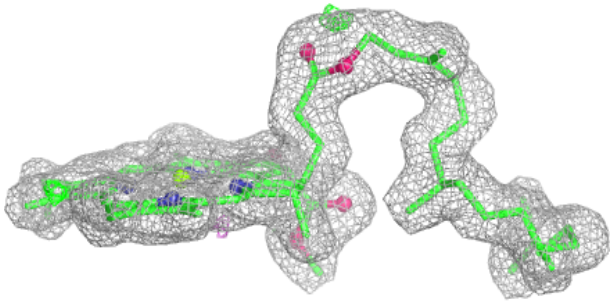


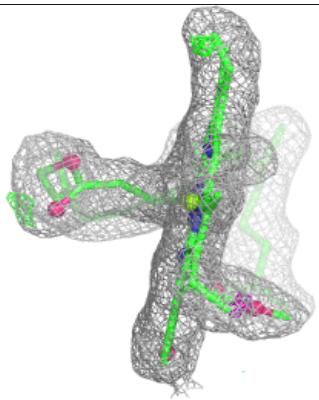


Electron density around CLA b 616:

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

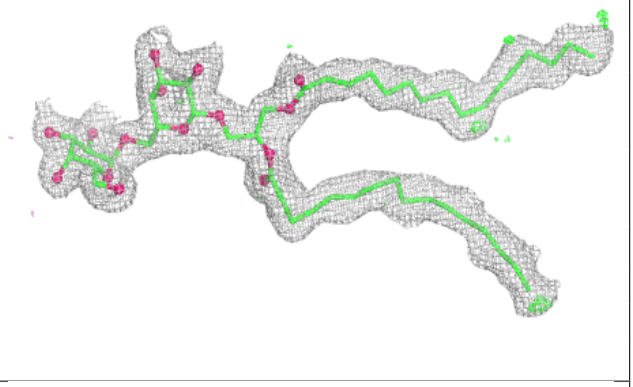


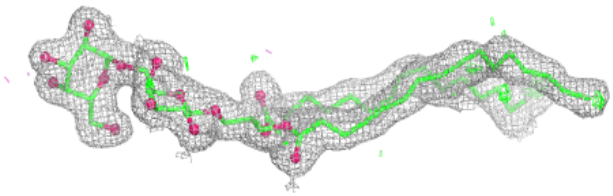


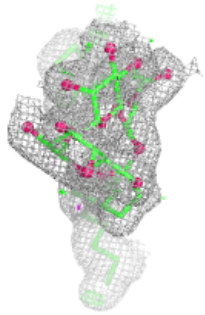


Electron density around DGD C 519:

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

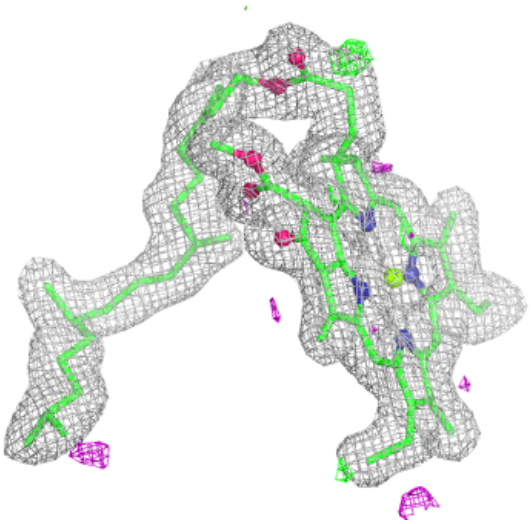


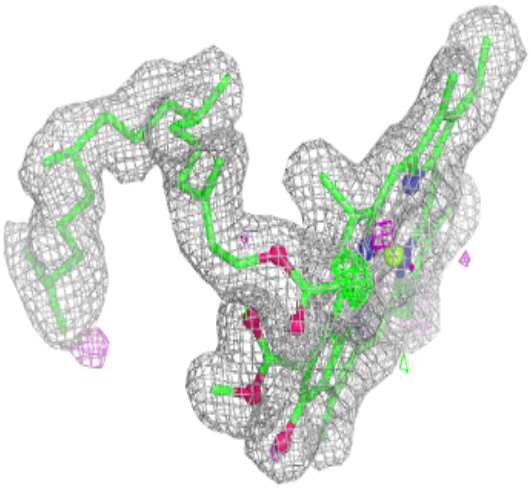


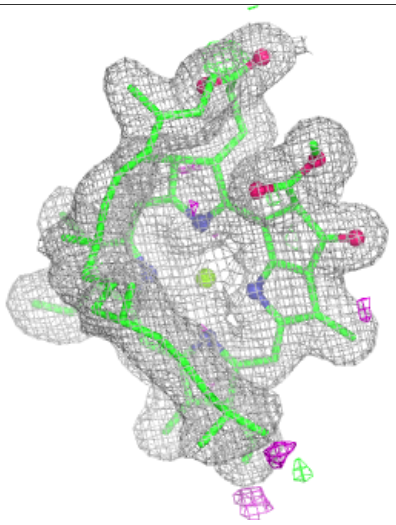


Electron density around CLA b 617:

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

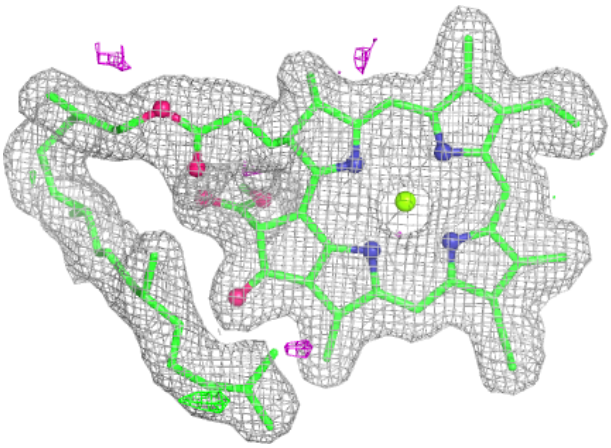


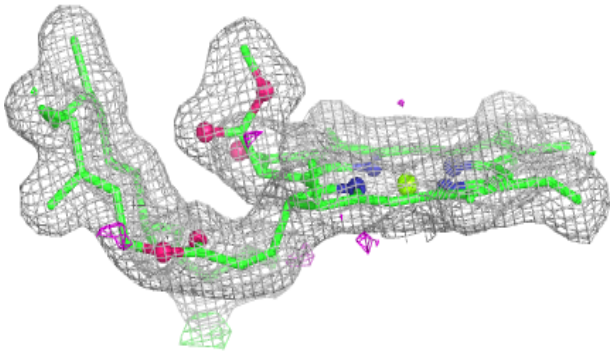




Electron density around CLA B 611:

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

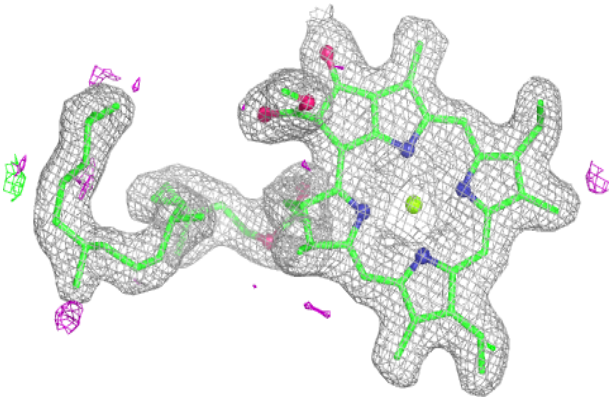


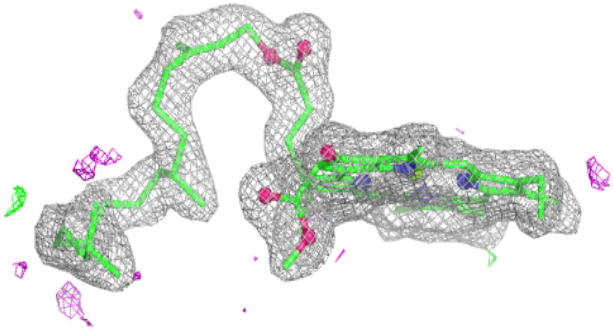




Electron density around CLA B 613:

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

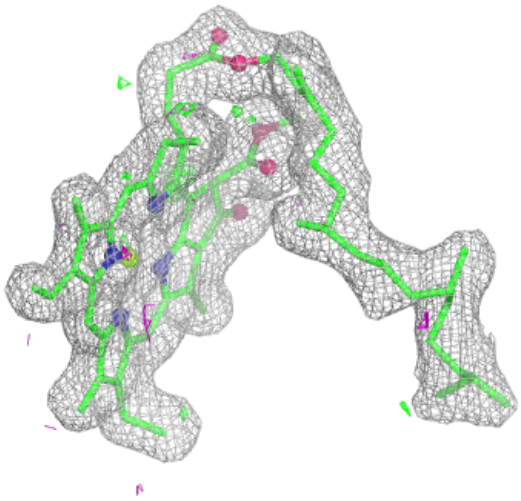


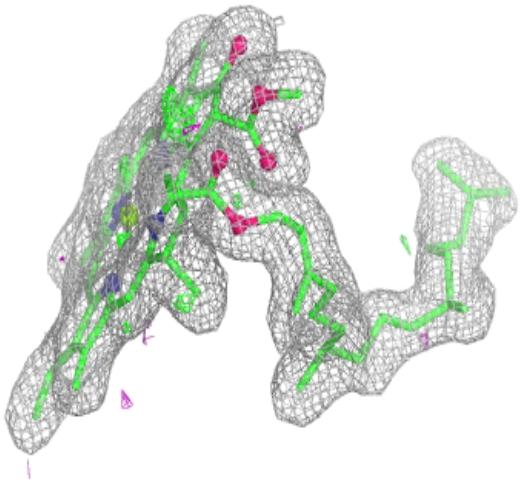


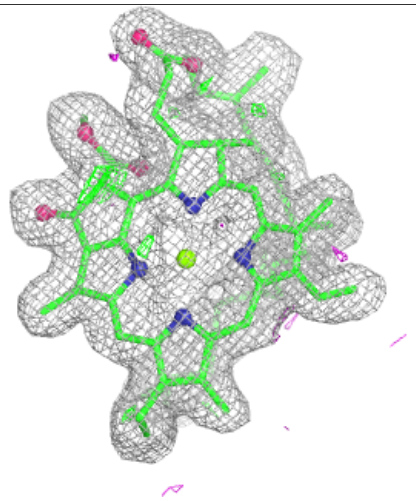


Electron density around CLA B 614:

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

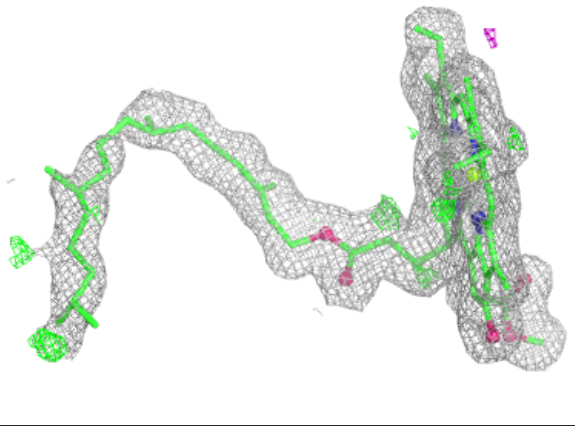


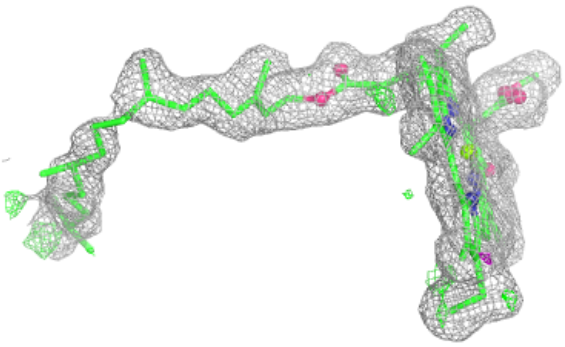


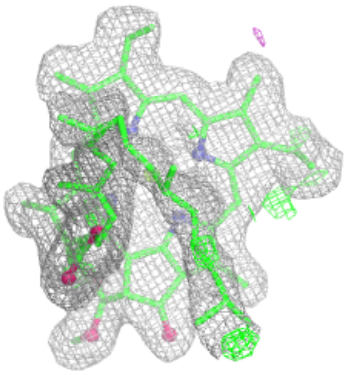


Electron density around CLA D 402:

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

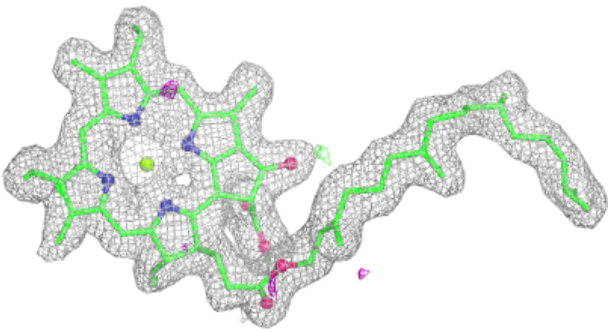


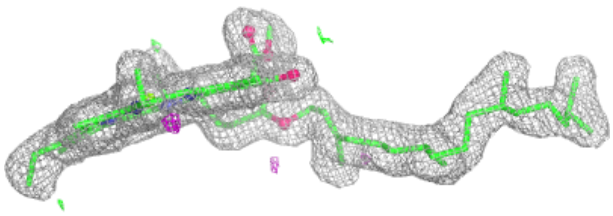


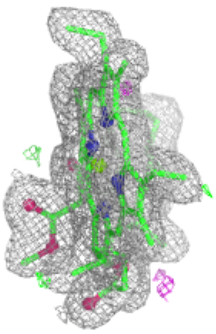


Electron density around CLA B 603:

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

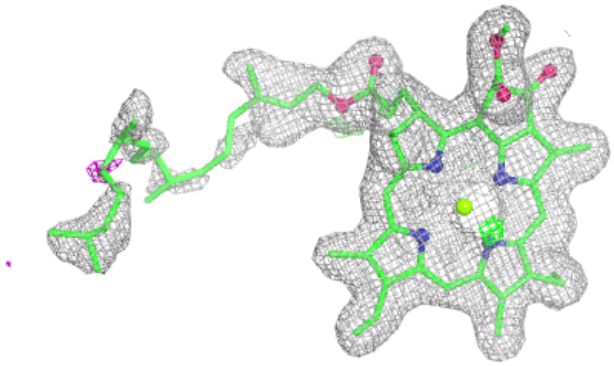


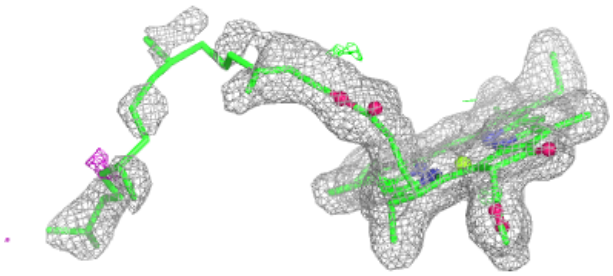


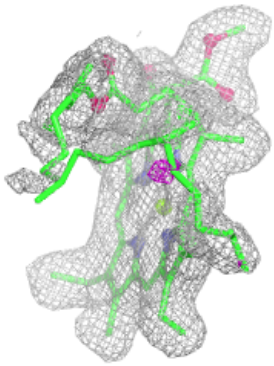


Electron density around CLA a 409:

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

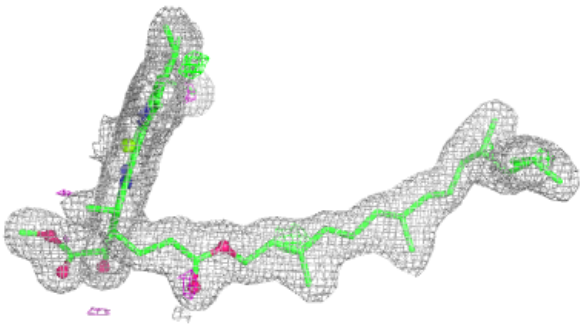


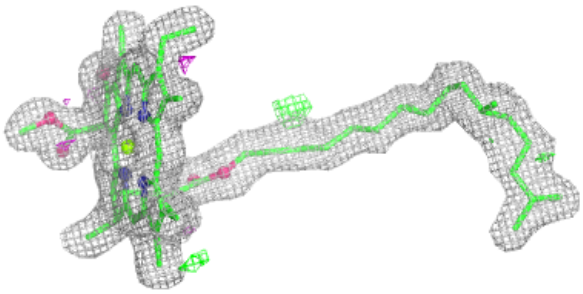


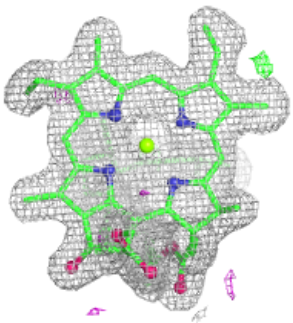


Electron density around CLA B 606:

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

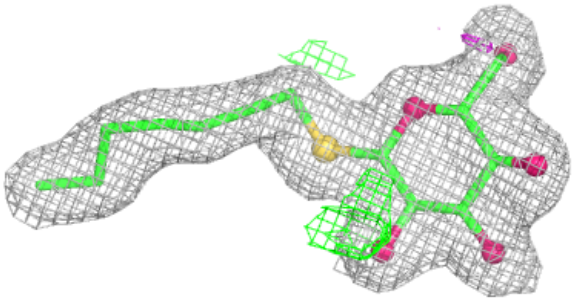


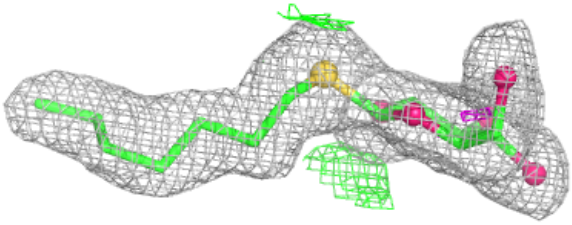


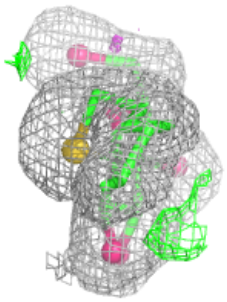


Electron density around HTG B 624:

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

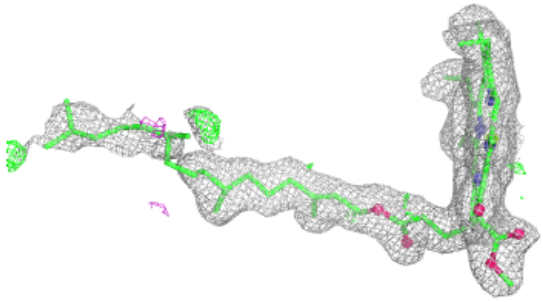


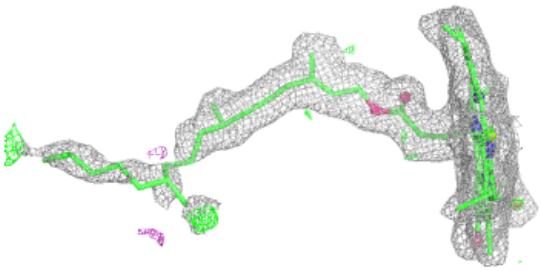


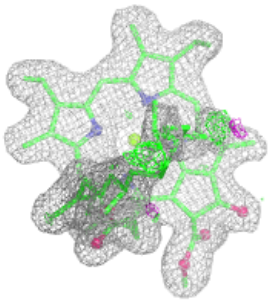


Electron density around CLA B 607:

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

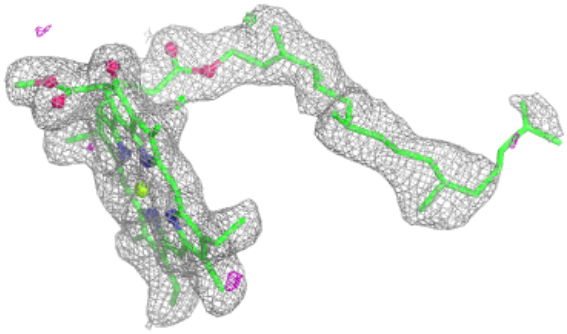


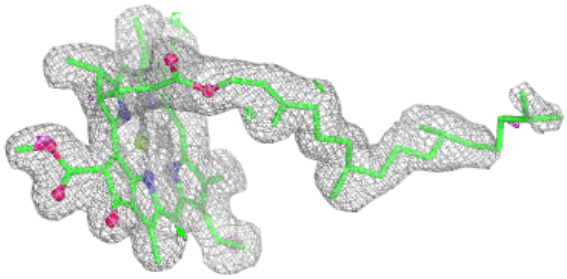


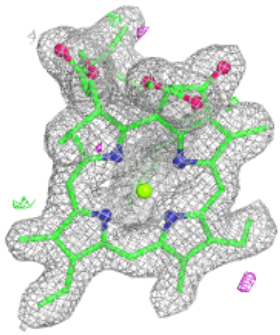


Electron density around CLA c 909:

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

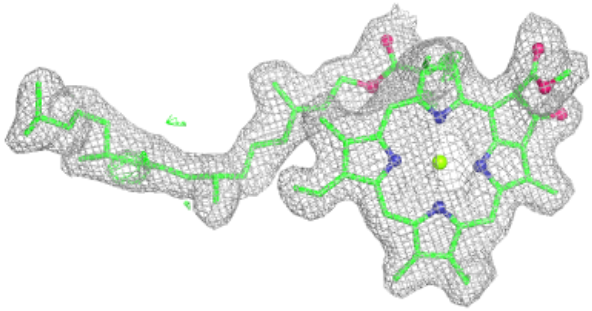


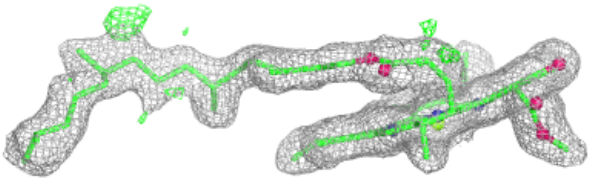


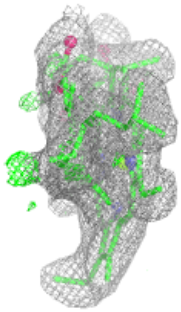


Electron density around CLA b 607:

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

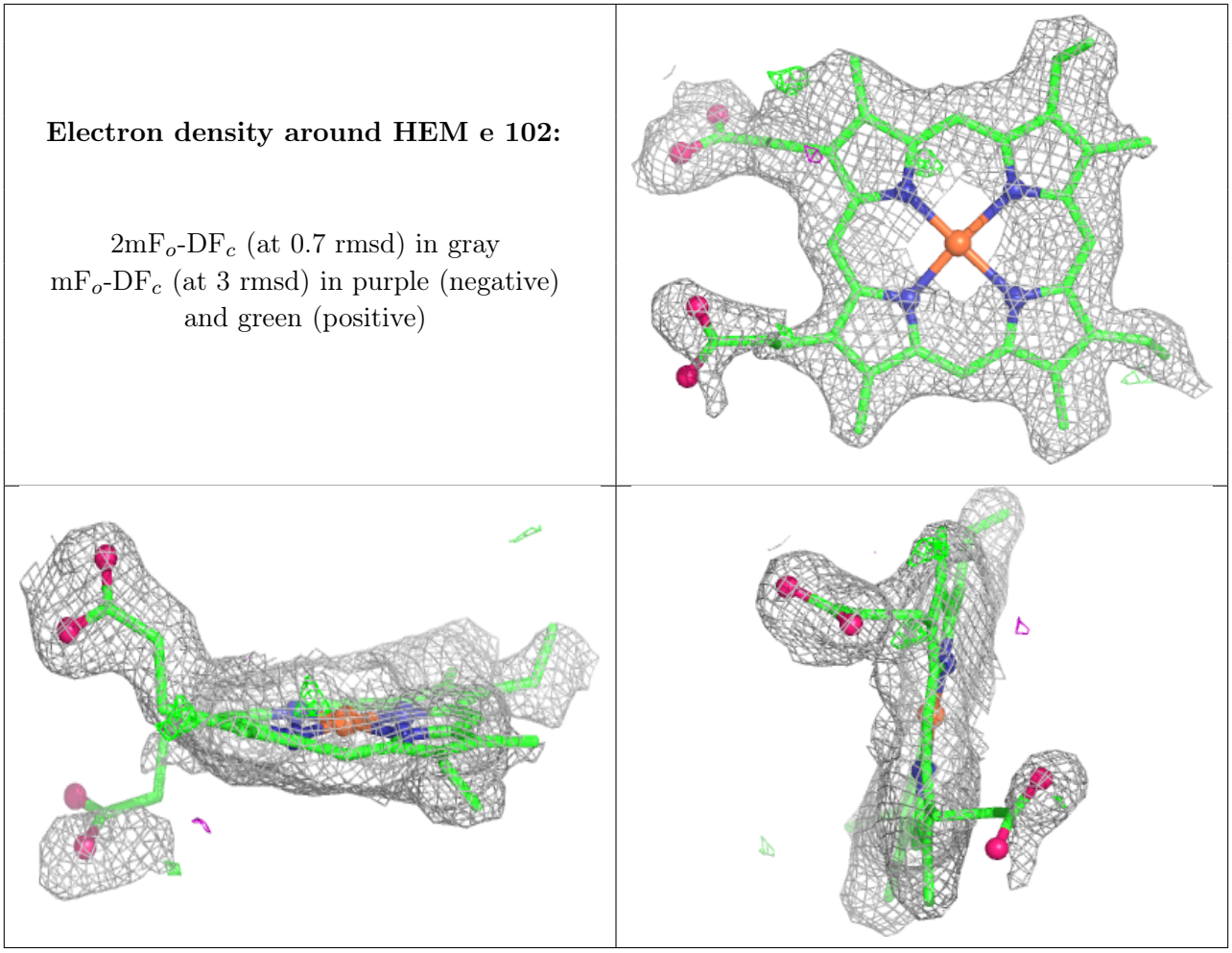






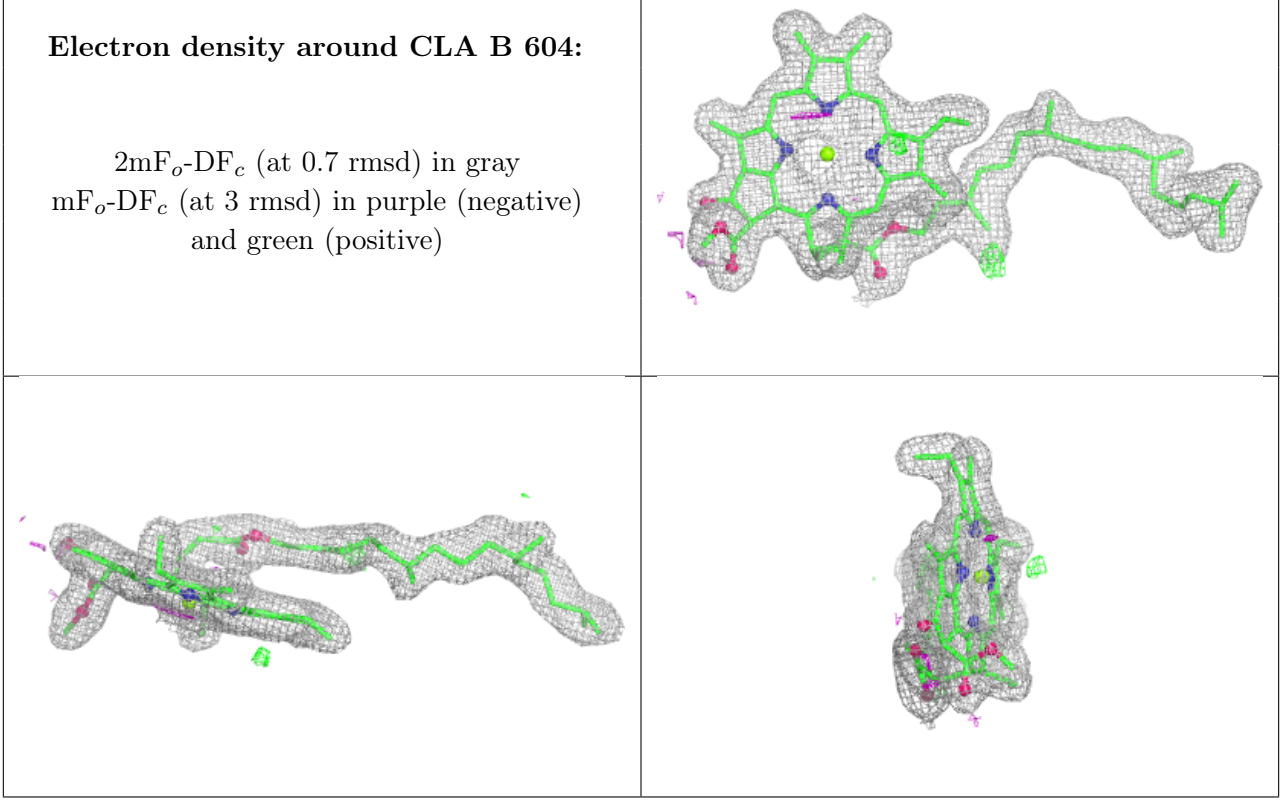
Electron density around HEM e 102:

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



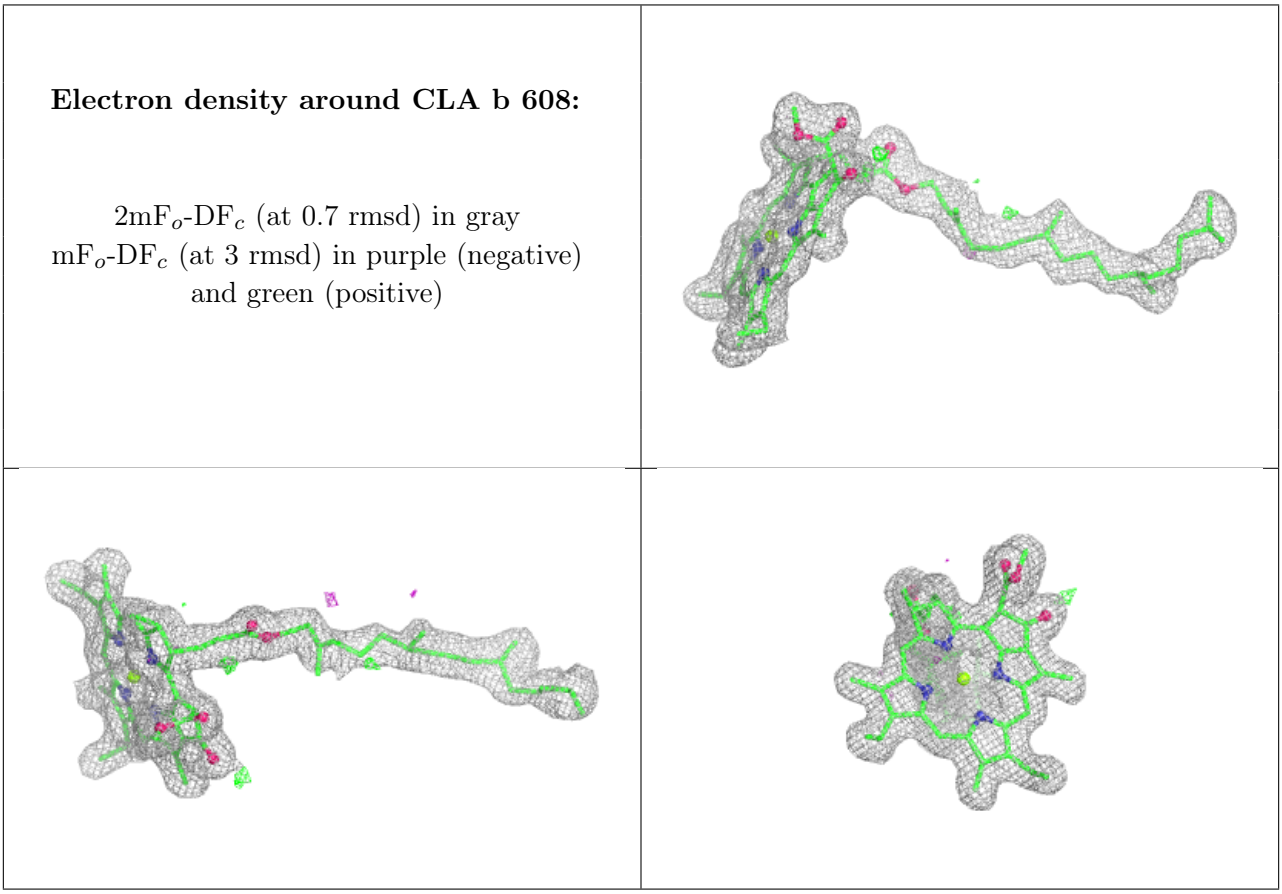
Electron density around CLA B 604:

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



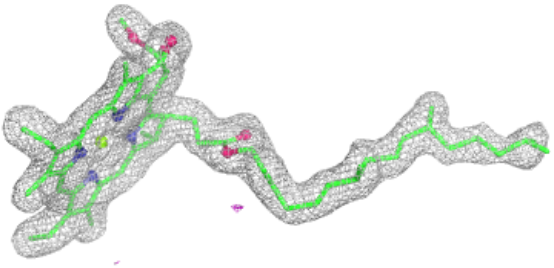
Electron density around CLA b 608:

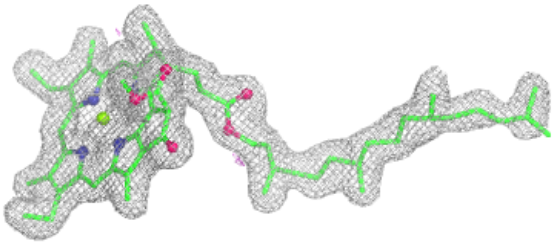
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

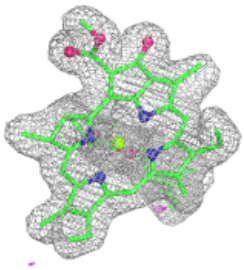


Electron density around CLA C 503:

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

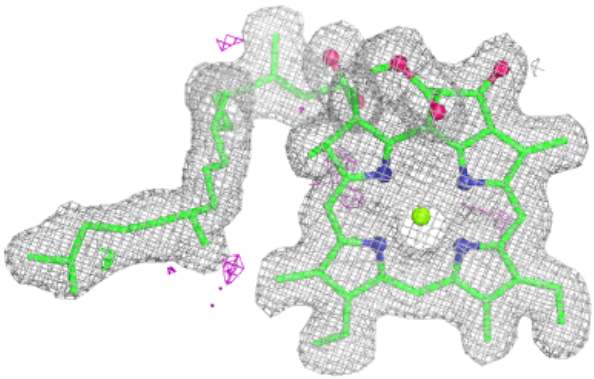


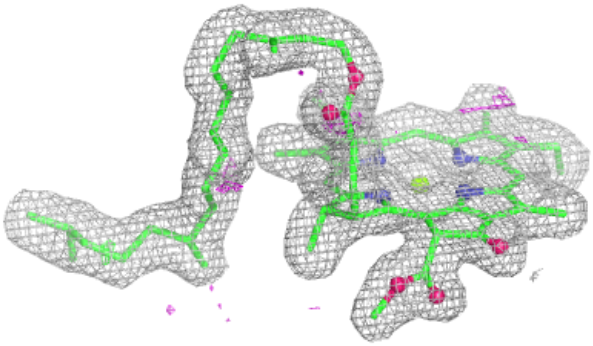


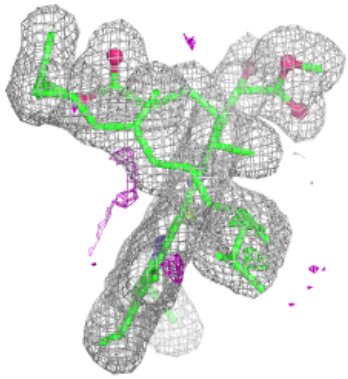


Electron density around CLA d 401:

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

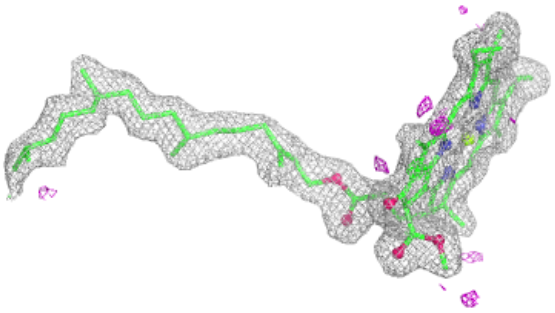


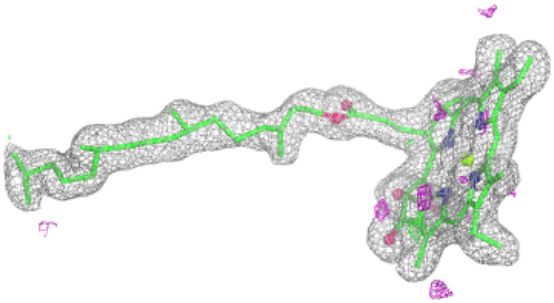


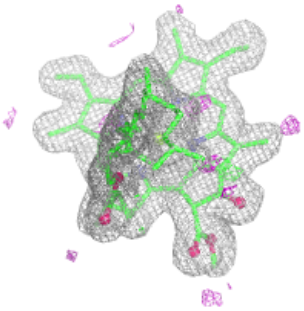


Electron density around CLA B 605:

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

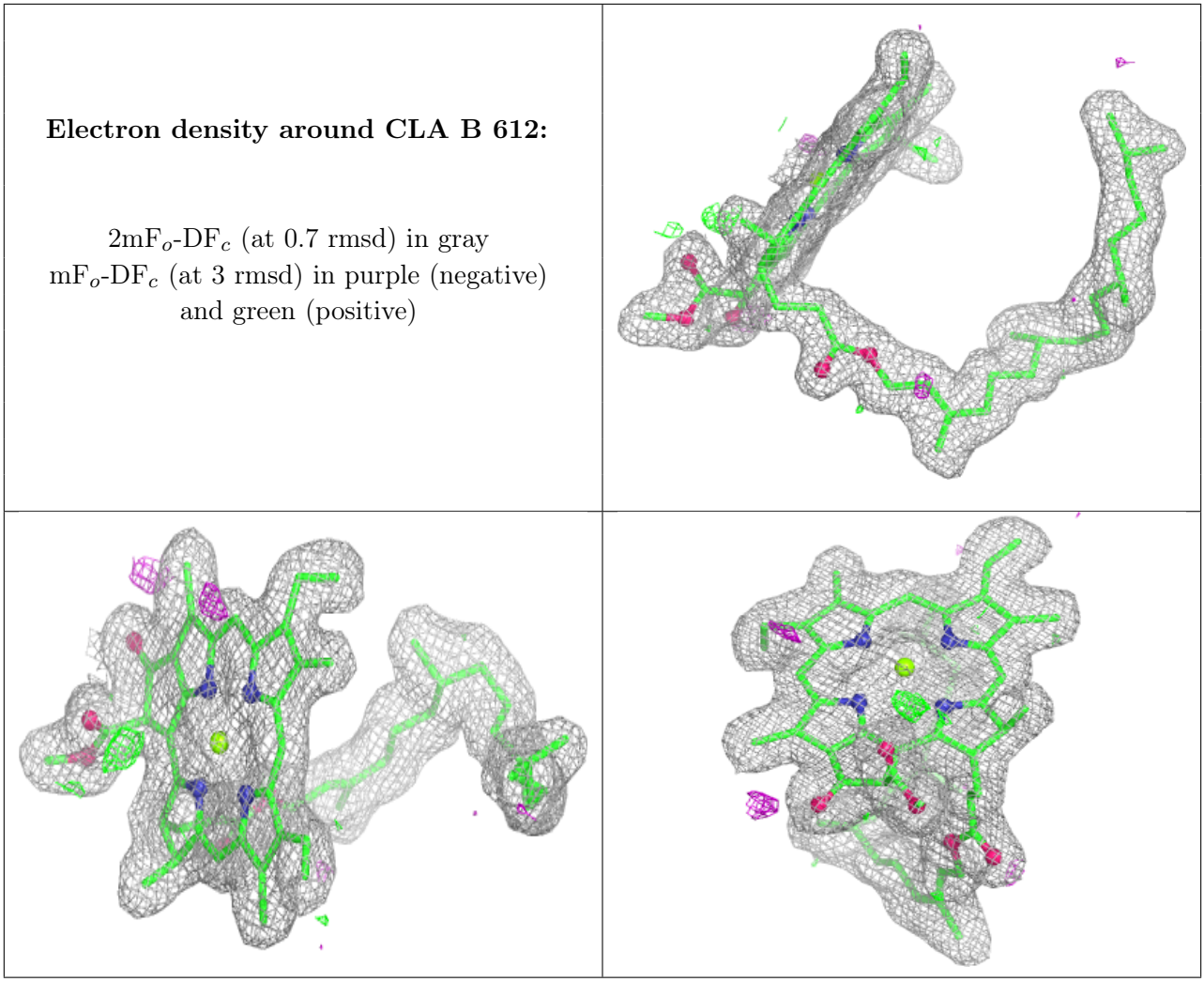






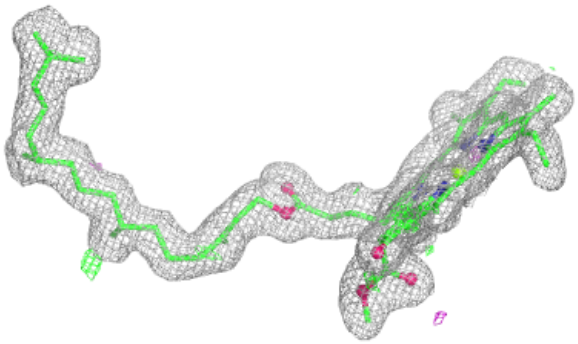
Electron density around CLA B 612:

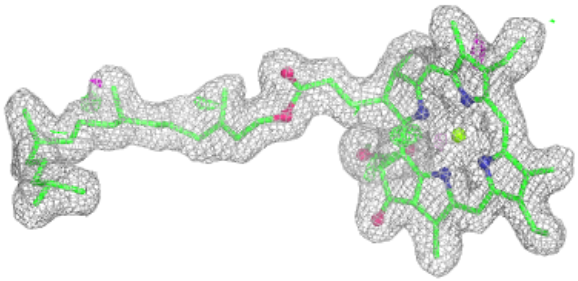
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

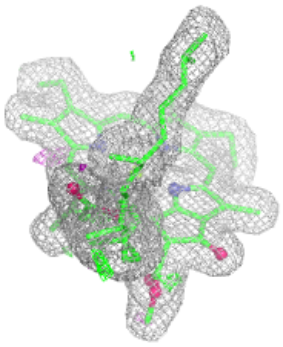


Electron density around CLA D 401:

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

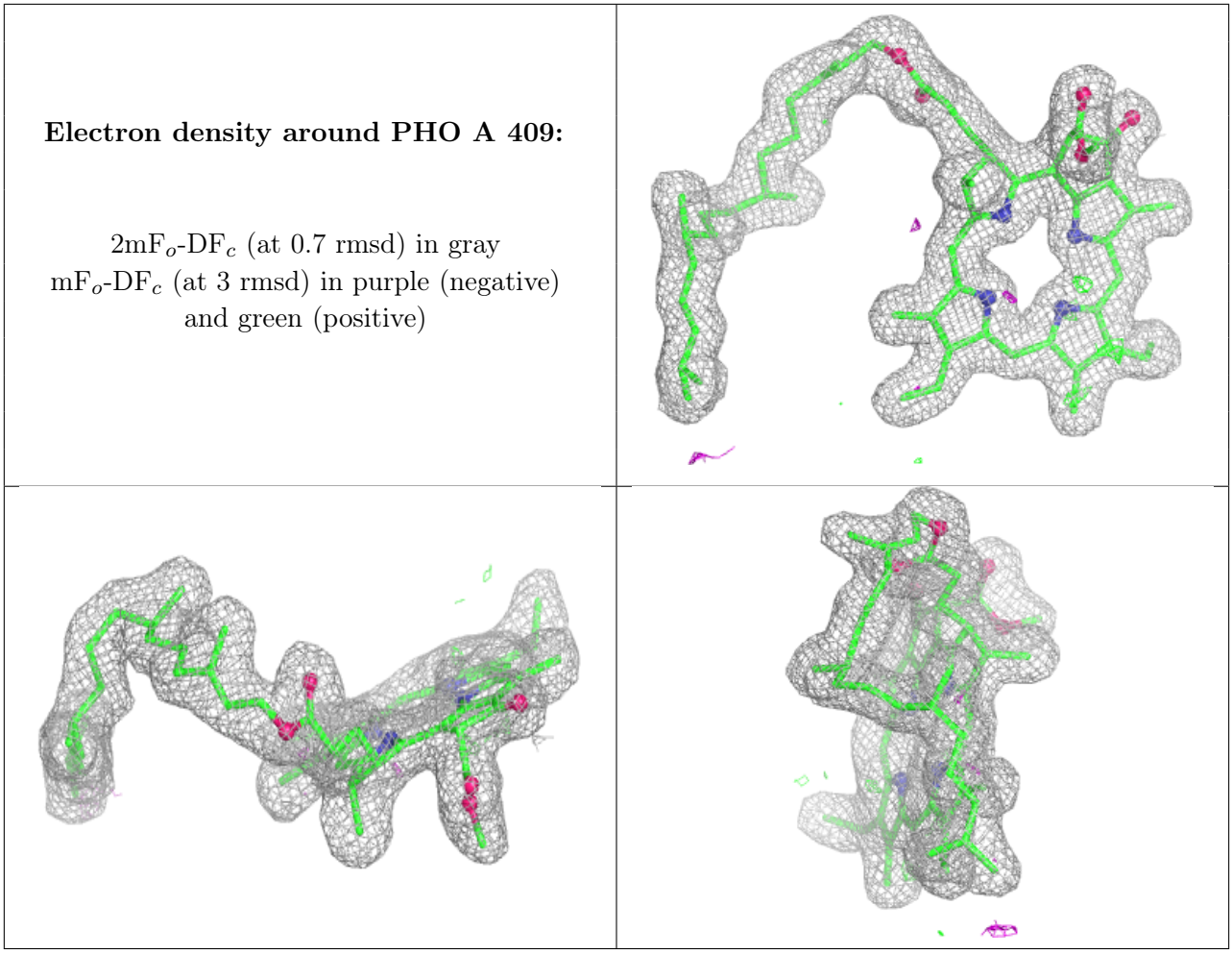






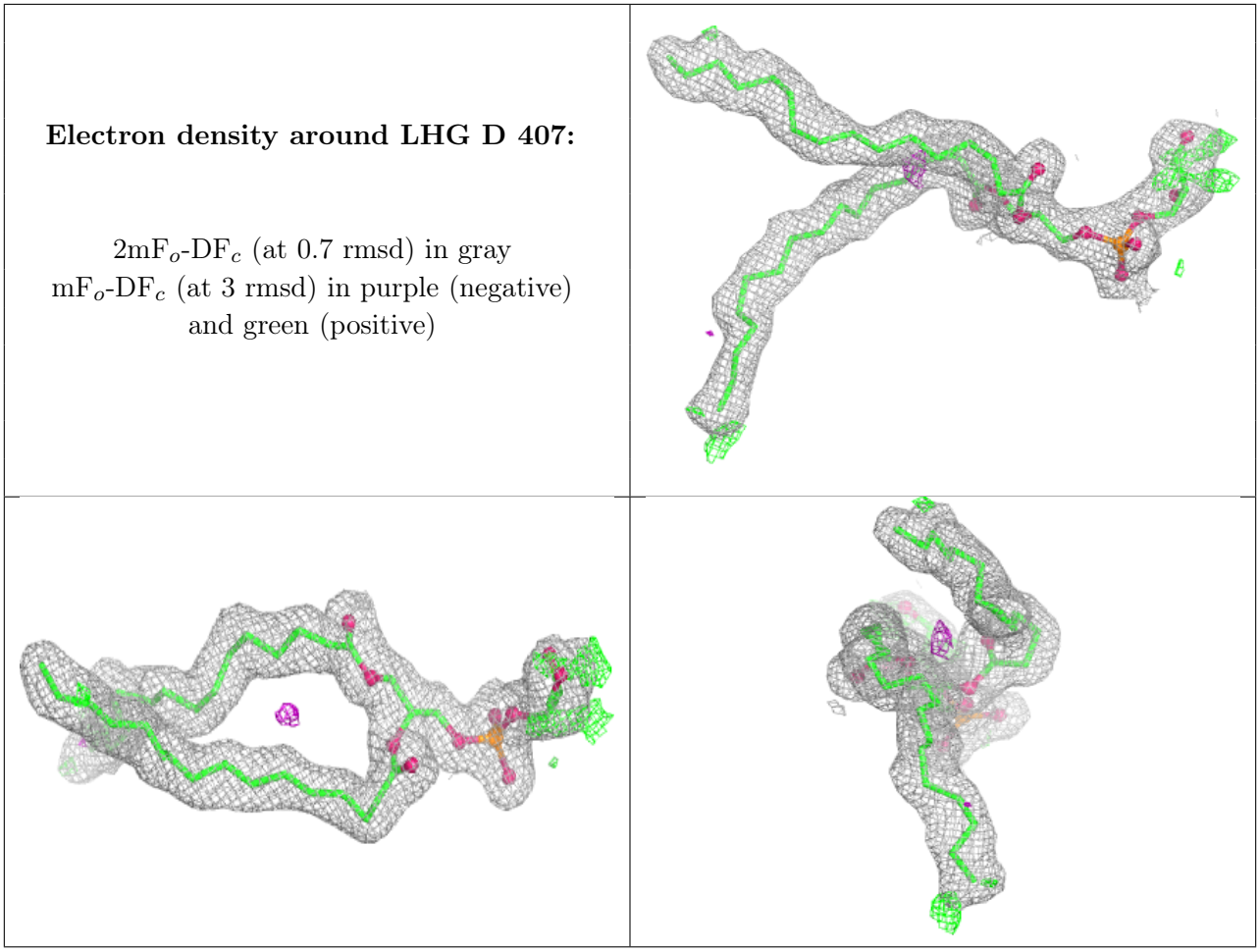
Electron density around PHO A 409:

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



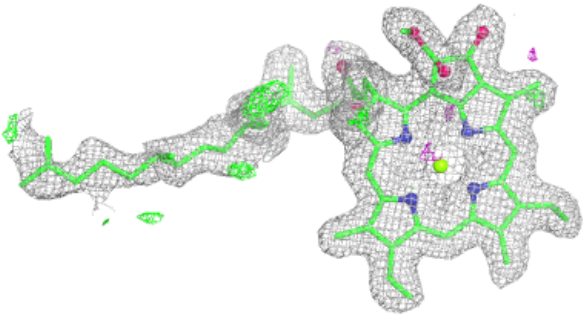
Electron density around LHG D 407:

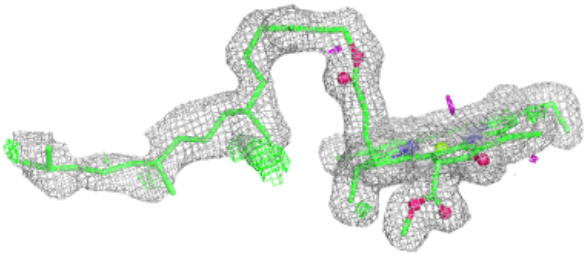
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

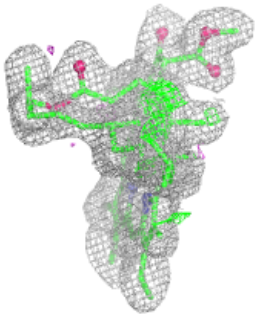


Electron density around CLA A 407:

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

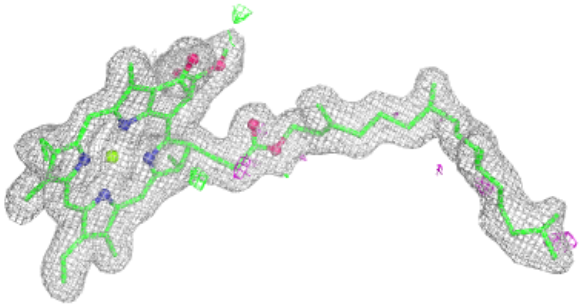


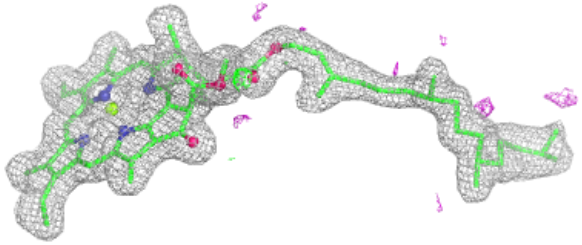


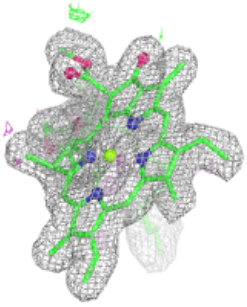


Electron density around CLA a 406:

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

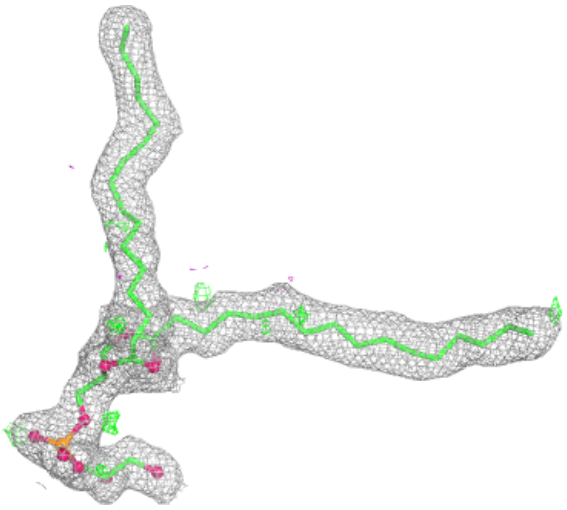


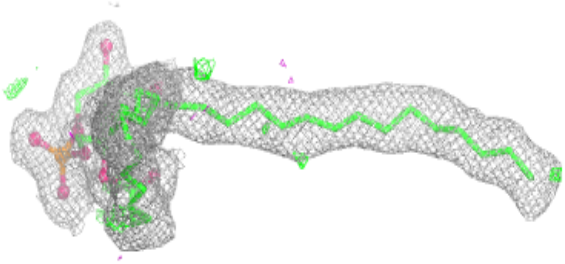


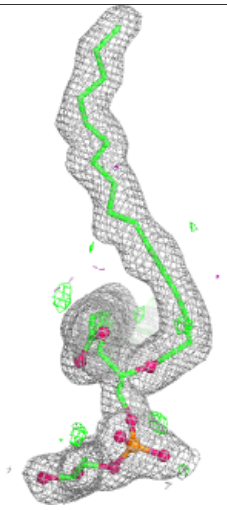


Electron density around LHG L 101:

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

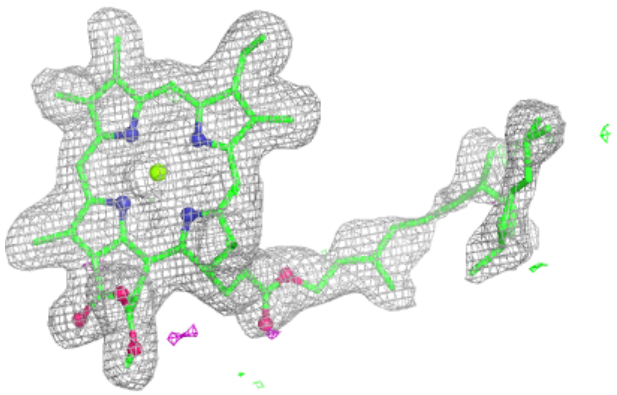


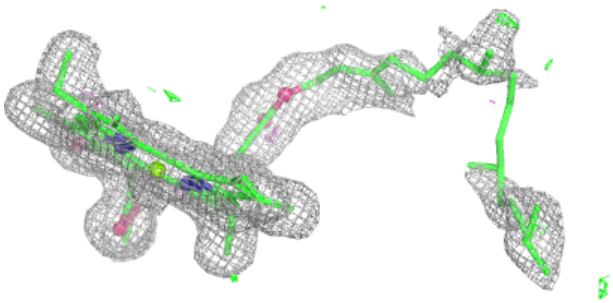


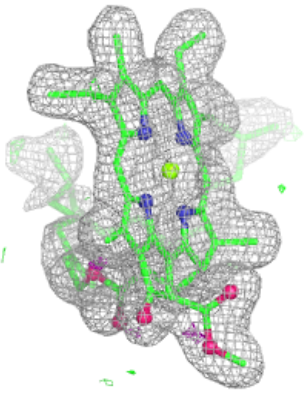


Electron density around CLA A 410:

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

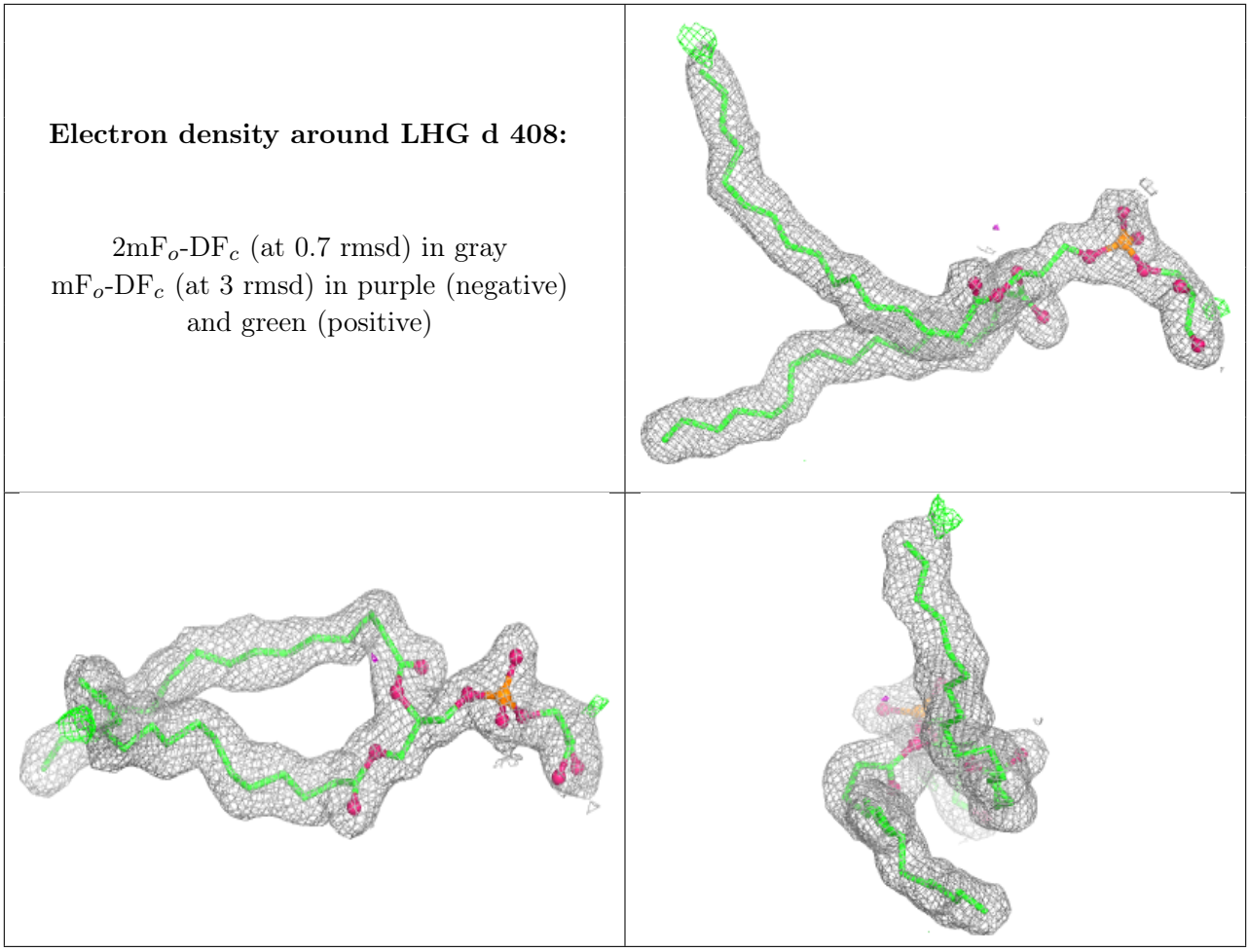






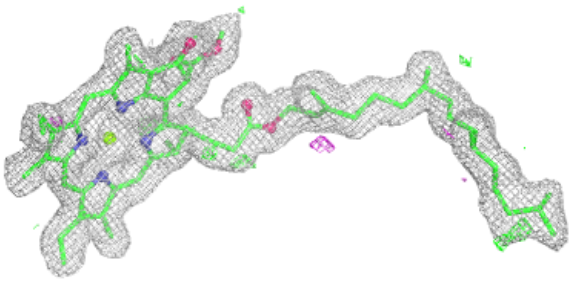
Electron density around LHG d 408:

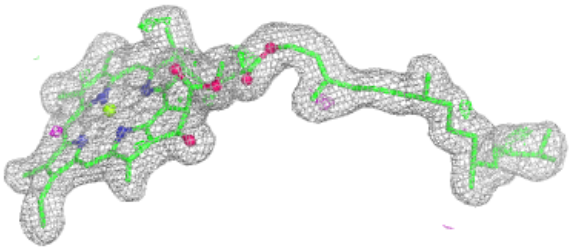
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

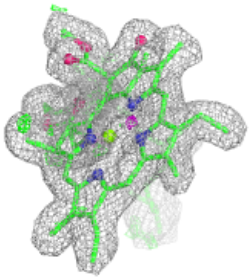


Electron density around CLA A 405:

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

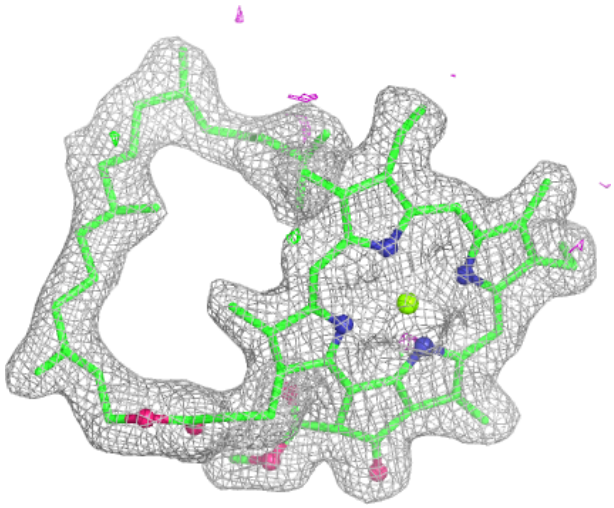


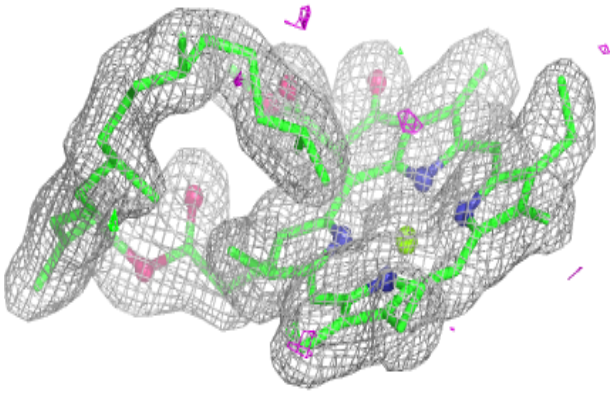


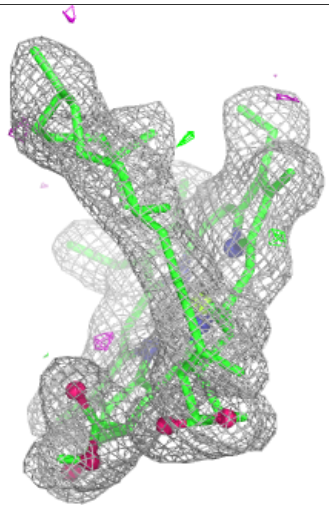


Electron density around CLA B 616:

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

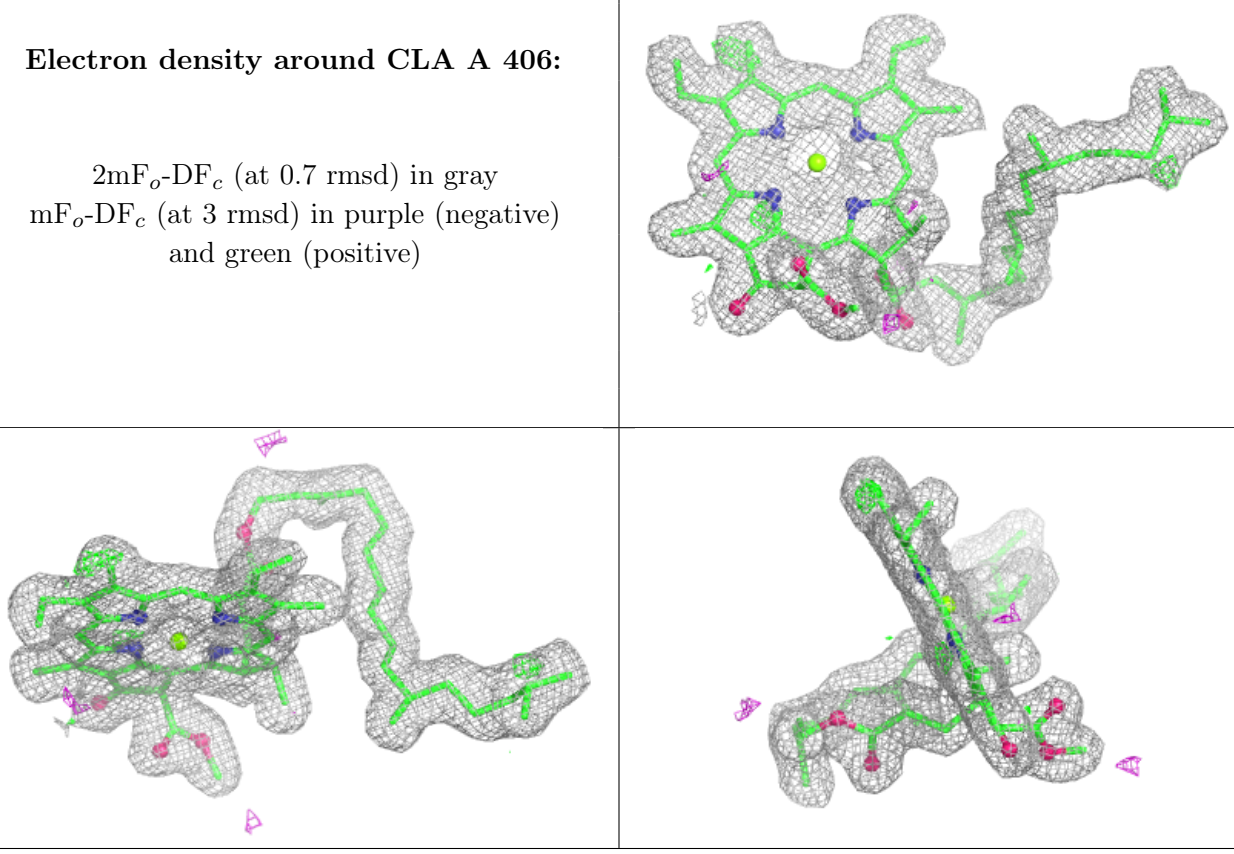






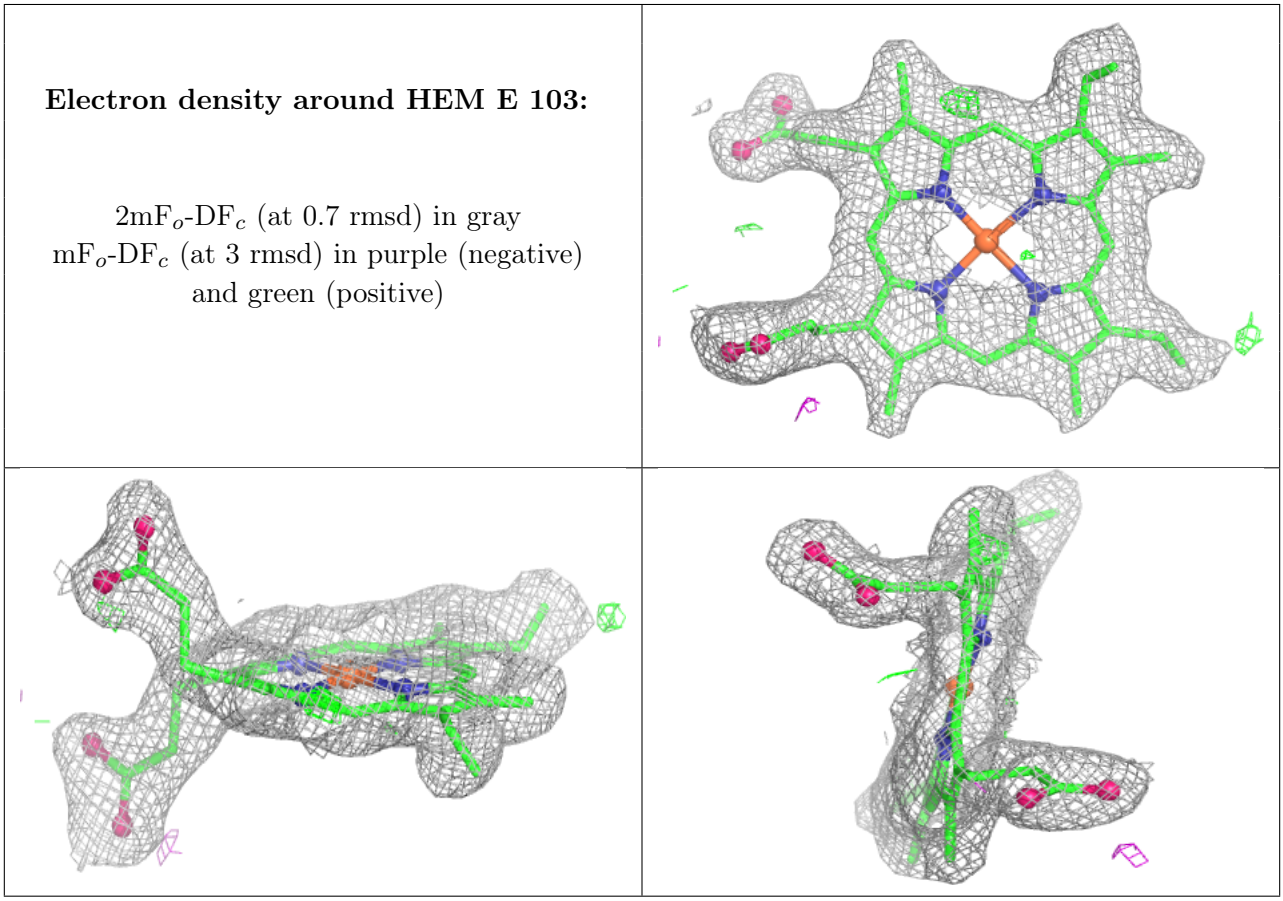
Electron density around CLA A 406:

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



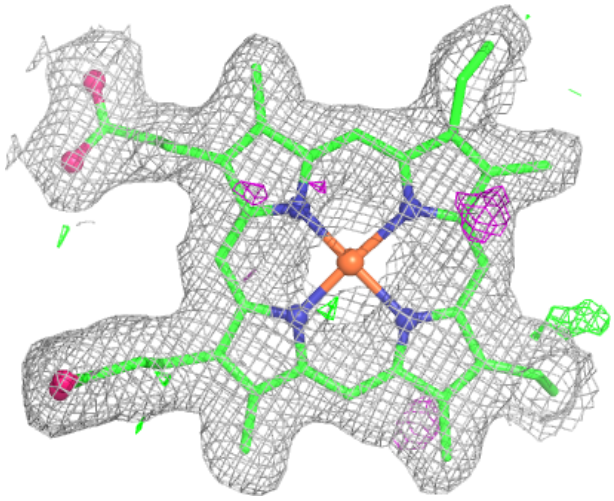
Electron density around HEM E 103:

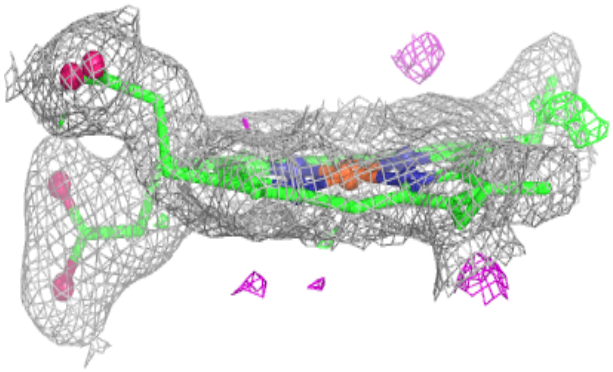
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC V 201:

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

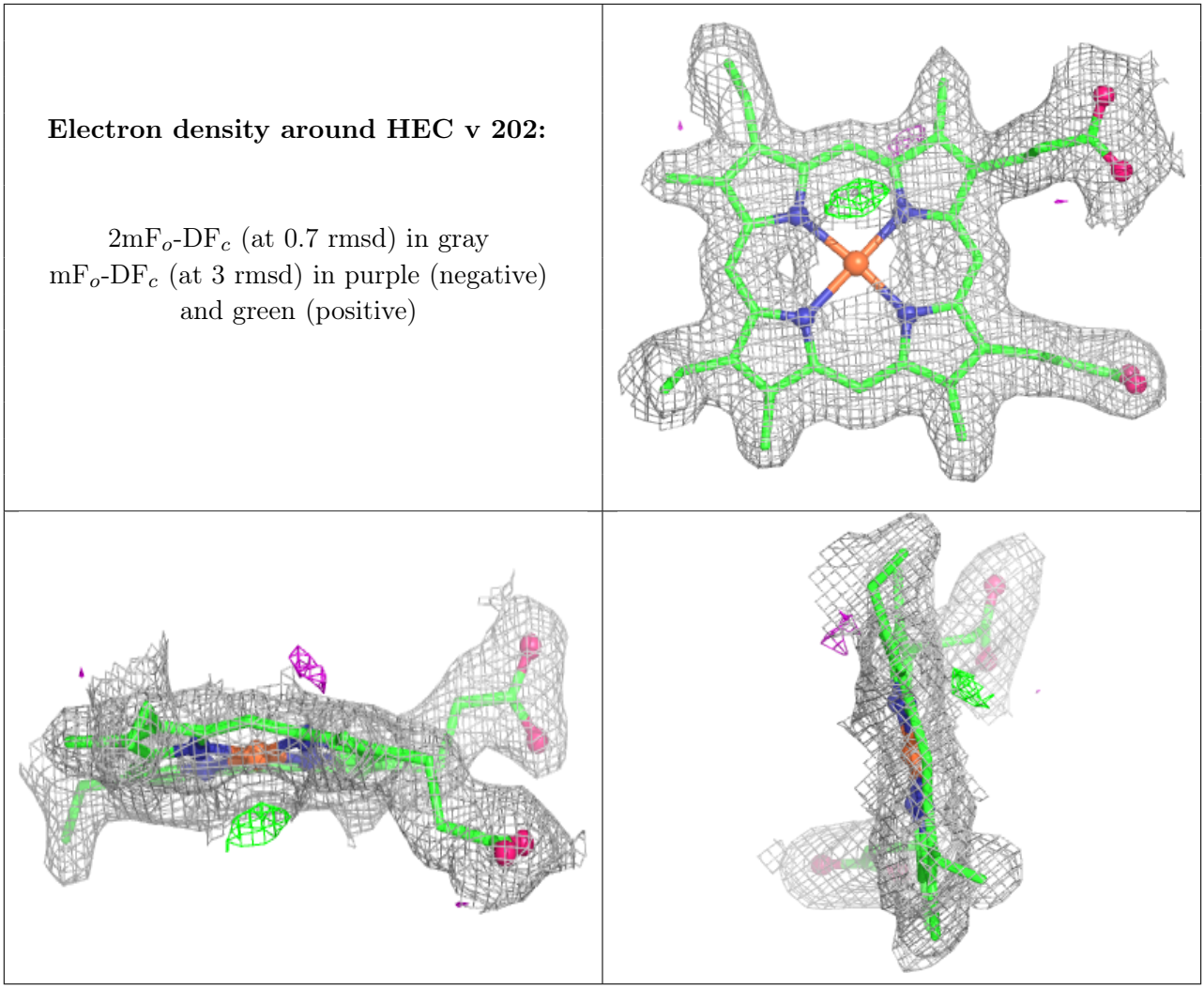






Electron density around HEC v 202:

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



6.5 Other polymers (i)

There are no such residues in this entry.