Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:28 AM JST

PDB ID	:	5H2F / pdb_00005h2f
Title	:	Crystal structure of the PsbM-deletion mutant of photosystem II
Authors	:	Uto, S.; Kawakami, K.; Umena, Y.; Iwai, M.; Ikeuchi, M.; Shen, J.R.; Kamiya, N.
Deposited on	:	2016-10-15
Resolution	:	2.20 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:

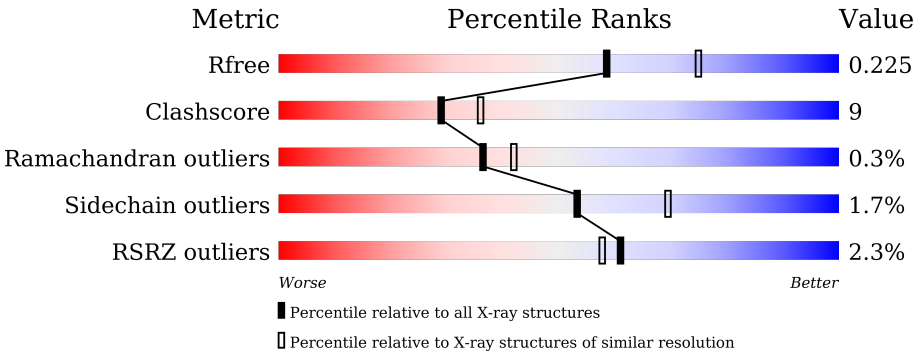
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	334	2% 87% 13%
1	a	334	10% 84% 16%
2	B	505	3% 86% 14%
2	b	505	% 82% 14%
3	C	455	% 85% 15%
3	c	455	84% 16%

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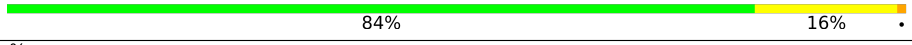
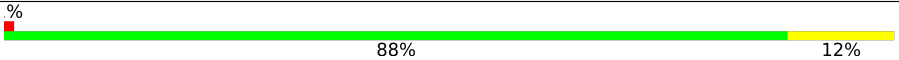
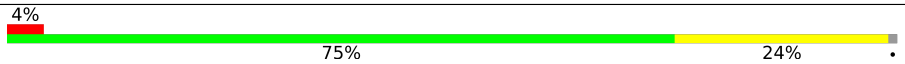
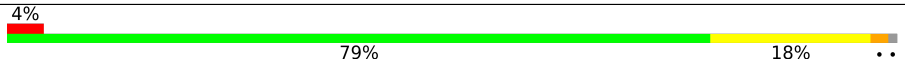
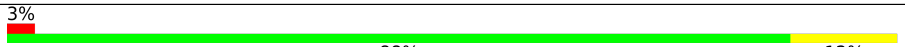
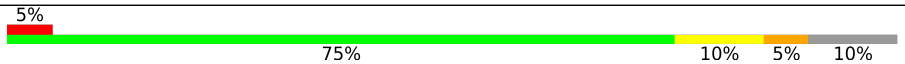
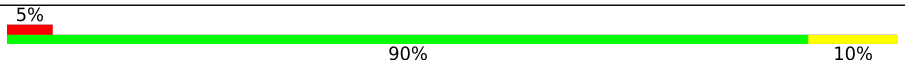
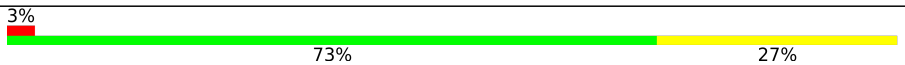
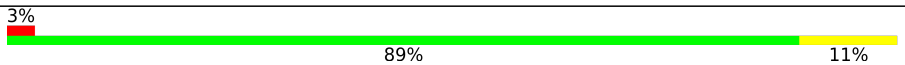
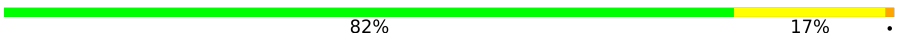
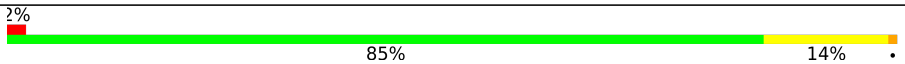
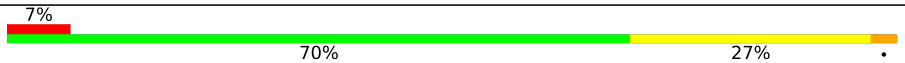
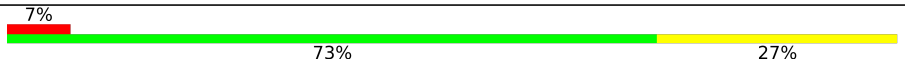
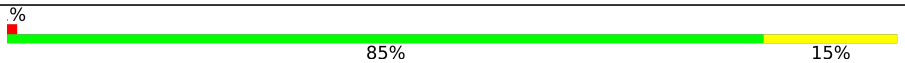
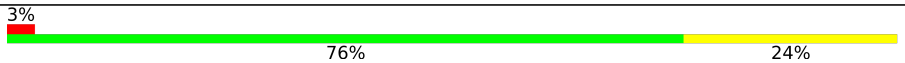
Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	80	
5	e	80	
6	F	33	
6	f	33	
7	H	63	
7	h	63	
8	I	36	
8	i	36	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	35	
11	l	35	
12	O	243	
12	o	243	
13	T	30	
13	t	30	
14	U	97	
14	u	97	
15	V	137	
15	v	137	
16	Y	29	

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Mol	Chain	Length	Quality of chain
16	y	29	3% 72% 28%
17	X	37	3% 81% 16%
17	x	37	3% 84% 11%
18	Z	62	10% 84% 16%
18	z	62	16% 84% 15%

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
31	DMS	B	631	-	-	X	-
31	DMS	B	638	-	-	X	-
31	DMS	O	303	-	-	X	-
31	DMS	O	304	-	-	X	-
31	DMS	O	312	-	-	X	-
31	DMS	V	212	-	-	X	-
31	DMS	a	425	-	-	X	-
31	DMS	b	638	-	-	X	-
31	DMS	c	924	-	-	X	-
31	DMS	d	415	-	-	X	-
31	DMS	f	103	-	-	X	-
31	DMS	o	304	-	-	X	-
31	DMS	o	308	-	-	X	-
31	DMS	u	205	-	-	X	-
34	HTG	D	415	-	-	X	-
39	HEC	V	202	X	-	-	-
39	HEC	v	202	X	-	-	-

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 51892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2598	1706	428	449	15			
1	a	334	Total	C	N	O	S	0	1	0
			2555	1675	427	438	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	3	0
			3950	2596	661	680	13			
2	b	483	Total	C	N	O	S	0	1	0
			3780	2484	631	652	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3470	2274	580	603	13			
3	c	455	Total	C	N	O	S	0	1	0
			3521	2305	589	614	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	3	0
			2732	1814	442	464	12			
4	d	341	Total	C	N	O	S	0	2	0
			2717	1805	441	459	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	79	Total 635	C 417	N 101	O 117	0	0	0
5	e	79	Total 636	C 418	N 101	O 117	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total 269	C 184	N 44	O 40	S 1	0	0	0
6	f	31	Total 250	C 170	N 42	O 37	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	63	Total 522	C 347	N 87	O 86	S 2	0	3	0
7	h	62	Total 501	C 335	N 82	O 82	S 2	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total 288	C 196	N 45	O 46	S 1	0	0	0
8	i	36	Total 293	C 199	N 46	O 47	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	36	Total 251	C 171	N 37	O 42	S 1	0	0	0
9	j	40	Total 277	C 186	N 41	O 49	S 1	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 286	C 198	N 42	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	35	Total 287	C 192	N 46	O 49	0	0	0
11	l	35	Total 287	C 192	N 46	O 49	0	0	0

- Molecule 12 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	O	243	Total 1853	C 1160	N 311	O 378	S 4	0	1	0
12	o	243	Total 1833	C 1149	N 305	O 375	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	T	30	Total 253	C 177	N 36	O 38	S 2	0	0	0
13	t	30	Total 253	C 177	N 36	O 38	S 2	0	0	0

- Molecule 14 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	U	97	Total 782	C 496	N 132	O 154	0	1	0
14	u	97	Total 766	C 487	N 129	O 150	0	0	0

- Molecule 15 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	V	137	Total 1066	C 677	N 177	O 208	S 4	0	1	0
15	v	137	Total 1058	C 671	N 175	O 208	S 4	0	1	0

- Molecule 16 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
16	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

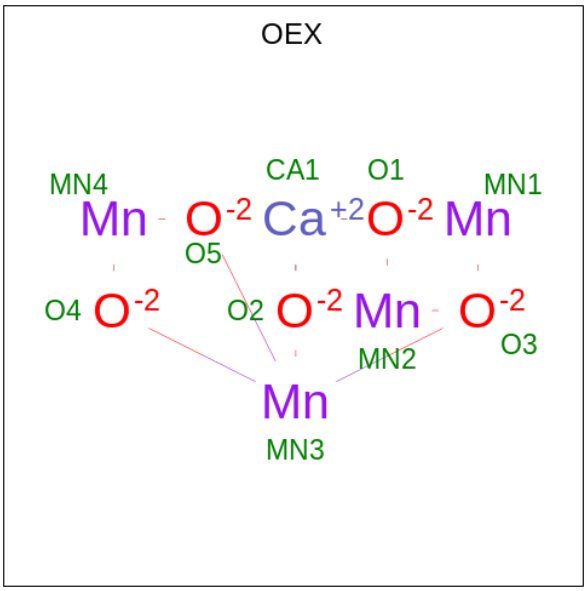
- Molecule 17 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	37	Total	C	N	O	0	1	0
			269	183	40	46			
17	x	36	Total	C	N	O	0	0	0
			253	172	37	44			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			453	311	68	72	2			
18	z	61	Total	C	N	O	S	0	0	0
			436	299	67	69	1			

- Molecule 19 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

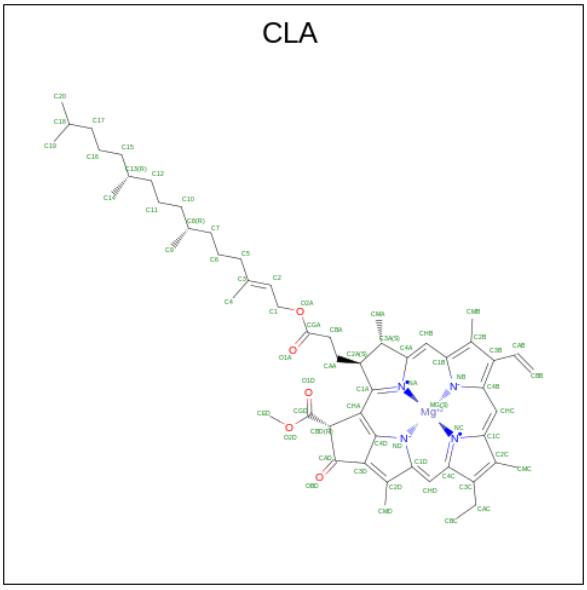
- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total Fe 1 1	0	0
20	a	1	Total Fe 1 1	0	0

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
22	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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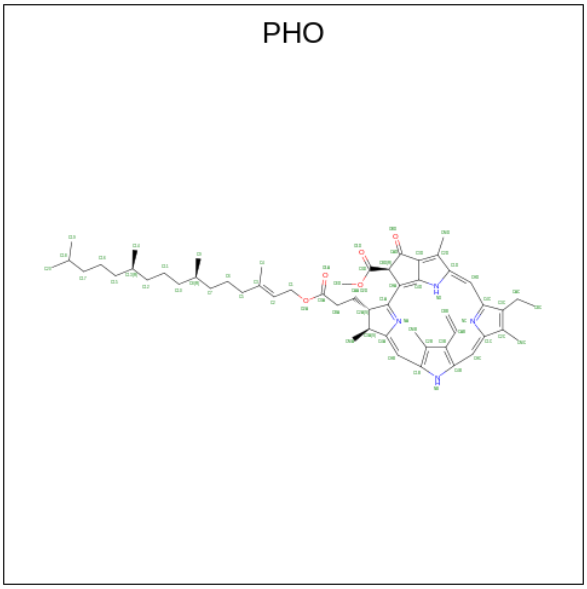
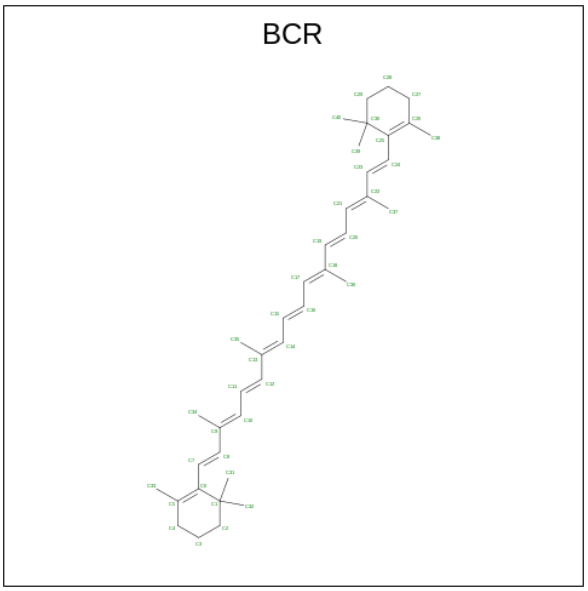
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 19 19	0	0
24	B	1	Total C 30 30	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	Y	1	Total C 39 39	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 20 20	0	0
24	b	1	Total C 31 31	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0

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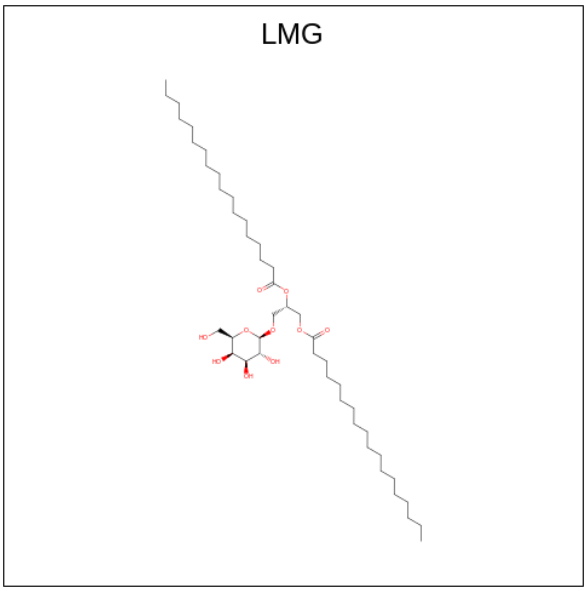
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 51 41 10	0	0
25	B	1	Total C O 40 30 10	0	0
25	C	1	Total C O 51 41 10	0	0
25	C	1	Total C O 40 30 10	0	0
25	D	1	Total C O 46 36 10	0	0
25	J	1	Total C O 45 35 10	0	0
25	b	1	Total C O 43 33 10	0	0

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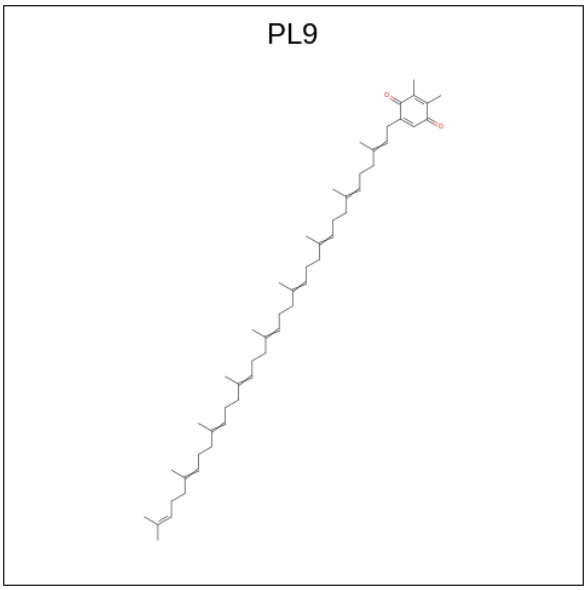
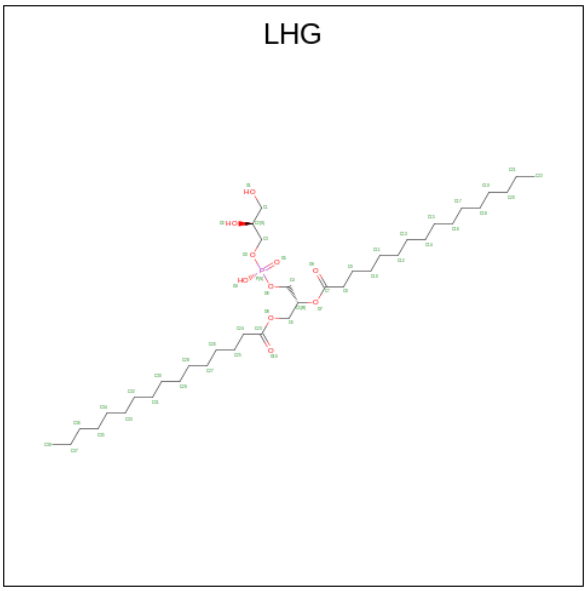
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	c	1	Total C O 51 41 10	0	0
25	c	1	Total C O 49 39 10	0	0
25	d	1	Total C O 47 37 10	0	0
25	i	1	Total C O 51 41 10	0	0
25	j	1	Total C O 47 37 10	0	0

- Molecule 26 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: $C_{53}H_{80}O_2$).



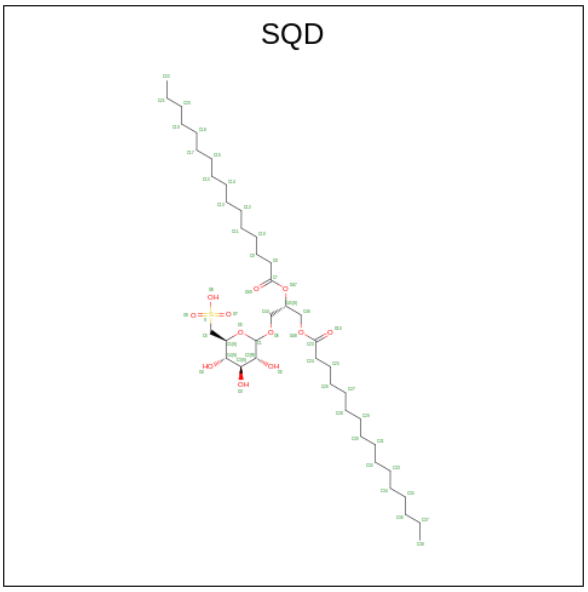
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 55 53 2	0	0
26	D	1	Total C O 55 53 2	0	0
26	a	1	Total C O 55 53 2	0	0
26	d	1	Total C O 55 53 2	0	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



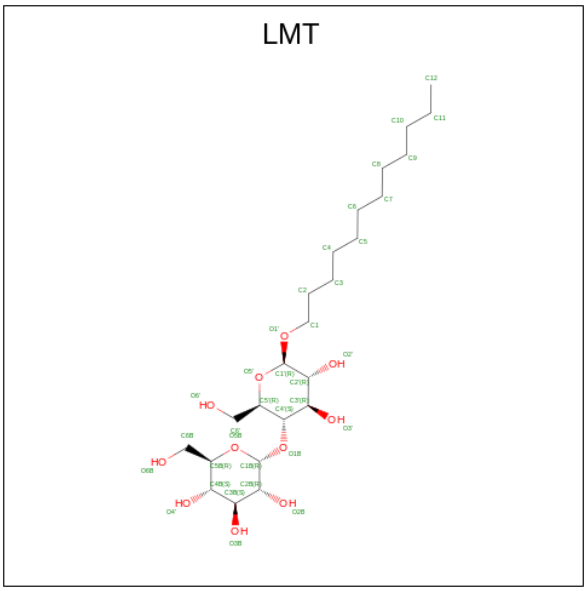
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			31	22	8	1		
27	C	1	Total	C	O	P	0	0
			30	21	8	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			45	34	10	1		
27	L	1	Total	C	O	P	0	0
			40	29	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			45	34	10	1		
27	d	1	Total	C	O	P	0	0
			33	24	8	1		
27	d	1	Total	C	O	P	0	0
			49	38	10	1		
27	d	1	Total	C	O	P	0	0
			46	35	10	1		
27	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 28 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
28	A	1	Total	C	O	S	0	0
			49	36	12	1		
28	C	1	Total	C	O	S	0	0
			54	41	12	1		
28	D	1	Total	C	O	S	0	0
			20	9	10	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			51	38	12	1		
28	b	1	Total	C	O	S	0	0
			38	26	11	1		
28	f	1	Total	C	O	S	0	0
			14	6	7	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

- 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 24 18 6	0	0
29	E	1	Total C O 24 18 6	0	0
29	I	1	Total C O 35 24 11	0	0
29	T	1	Total C O 24 18 6	0	0
29	Z	1	Total C O 35 24 11	0	0
29	a	1	Total C O 35 24 11	0	0
29	c	1	Total C O 35 24 11	0	0
29	c	1	Total C O 24 18 6	0	0
29	f	1	Total C O 25 19 6	0	0
29	t	1	Total C O 24 18 6	0	0

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C 5 5	0	0

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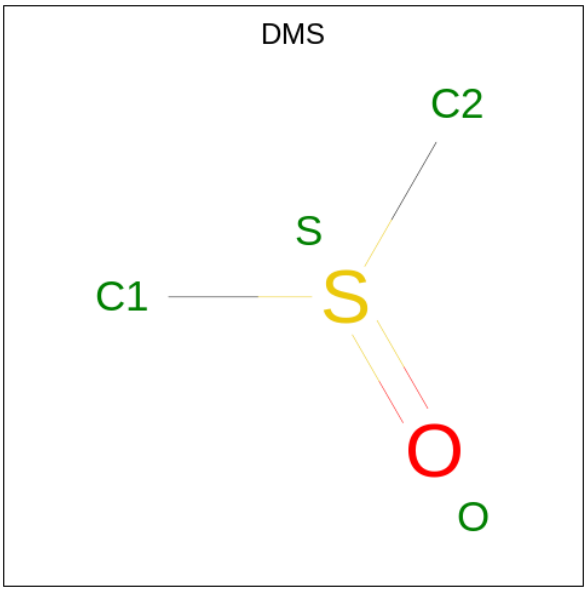
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	2	Total C 23 23	0	0
30	D	1	Total C 16 16	0	0
30	I	3	Total C 45 45	0	0
30	J	1	Total C 16 16	0	0
30	O	1	Total C 16 16	0	0
30	T	1	Total C 13 13	0	0
30	U	1	Total C 14 14	0	0
30	X	1	Total C 16 16	0	0
30	Z	1	Total C 9 9	0	0
30	a	2	Total C 16 16	0	0
30	b	2	Total C 27 27	0	0
30	c	1	Total C 10 10	0	0
30	d	1	Total C 16 16	0	0
30	i	4	Total C 58 58	0	0
30	j	1	Total C 16 16	0	0
30	t	1	Total C 16 16	0	0
30	u	1	Total C 11 11	0	0
30	x	1	Total C 15 15	0	0

- Molecule 31 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	O	S	0	0
			4	2	1	1		
31	D	1	Total	C	O	S	0	0
			4	2	1	1		
31	D	1	Total	C	O	S	0	0
			4	2	1	1		
31	F	1	Total	C	O	S	0	0
			4	2	1	1		
31	H	1	Total	C	O	S	0	0
			4	2	1	1		
31	I	1	Total	C	O	S	0	0
			4	2	1	1		
31	I	1	Total	C	O	S	0	0
			4	2	1	1		
31	L	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	O	1	Total	C	O	S	0	0
			4	2	1	1		
31	U	1	Total	C	O	S	0	0
			4	2	1	1		

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	c	1	Total	C	O	S	0	0
			4	2	1	1		
31	c	1	Total	C	O	S	0	0
			4	2	1	1		
31	d	1	Total	C	O	S	0	0
			4	2	1	1		
31	d	1	Total	C	O	S	0	0
			4	2	1	1		
31	d	1	Total	C	O	S	0	0
			4	2	1	1		
31	d	1	Total	C	O	S	0	0
			4	2	1	1		
31	d	1	Total	C	O	S	0	0
			4	2	1	1		
31	f	1	Total	C	O	S	0	0
			4	2	1	1		
31	i	1	Total	C	O	S	0	0
			4	2	1	1		
31	l	1	Total	C	O	S	0	0
			4	2	1	1		
31	l	1	Total	C	O	S	0	0
			4	2	1	1		
31	l	1	Total	C	O	S	0	0
			4	2	1	1		
31	o	1	Total	C	O	S	0	0
			4	2	1	1		
31	o	1	Total	C	O	S	0	0
			4	2	1	1		
31	o	1	Total	C	O	S	0	0
			4	2	1	1		
31	o	1	Total	C	O	S	0	0
			4	2	1	1		
31	o	1	Total	C	O	S	0	0
			4	2	1	1		
31	o	1	Total	C	O	S	0	0
			4	2	1	1		
31	o	1	Total	C	O	S	0	0
			4	2	1	1		
31	t	1	Total	C	O	S	0	0
			4	2	1	1		
31	t	1	Total	C	O	S	0	0
			4	2	1	1		

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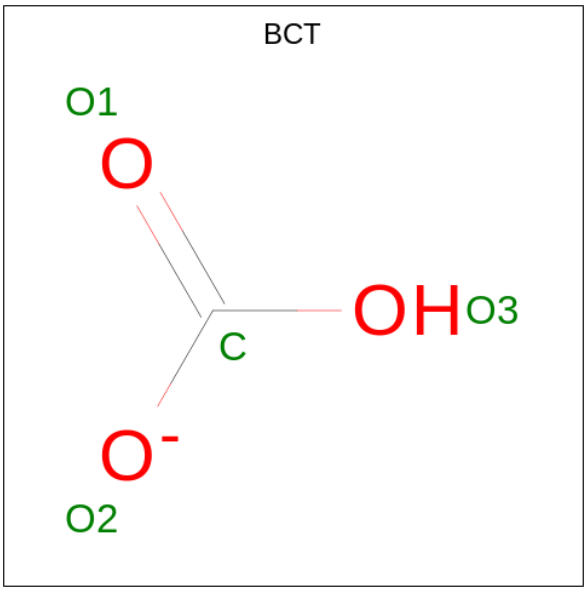
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	t	1	Total	C	O	S	0	0
			4	2	1	1		
31	u	1	Total	C	O	S	0	0
			4	2	1	1		
31	u	1	Total	C	O	S	0	0
			4	2	1	1		
31	u	1	Total	C	O	S	0	0
			4	2	1	1		
31	u	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v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

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).

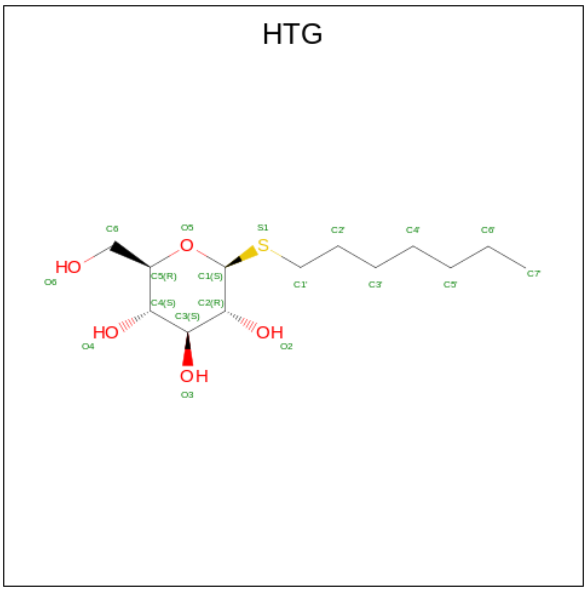


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 8 2 6	0	1
32	a	1	Total C O 4 1 3	0	0

- 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	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	o	1	Total Ca 1 1	0	0

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C S 9 8 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	D	1	Total C O S 19 13 5 1	0	0
34	D	1	Total C O S 19 13 5 1	0	0
34	V	1	Total C O S 14 8 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0

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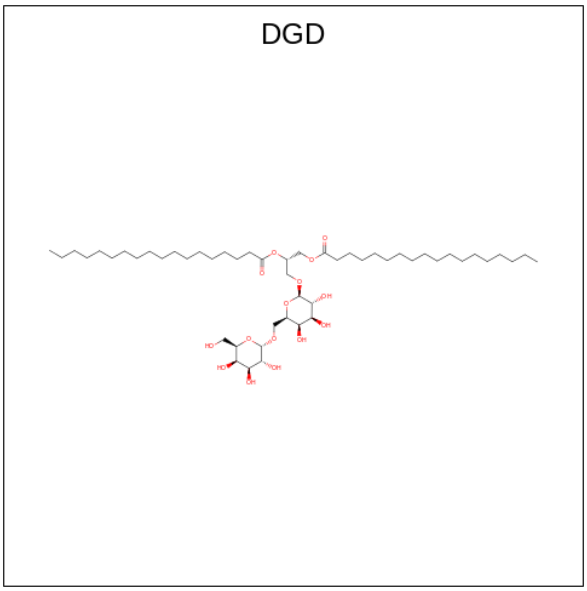
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	c	1	Total C O S 19 13 5 1	0	0
34	l	1	Total C O S 19 13 5 1	0	0
34	v	1	Total C O S 16 10 5 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 62 47 15	0	0
35	C	1	Total C O 62 47 15	0	0
35	C	1	Total C O 62 47 15	0	0
35	D	1	Total C O 50 41 9	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0

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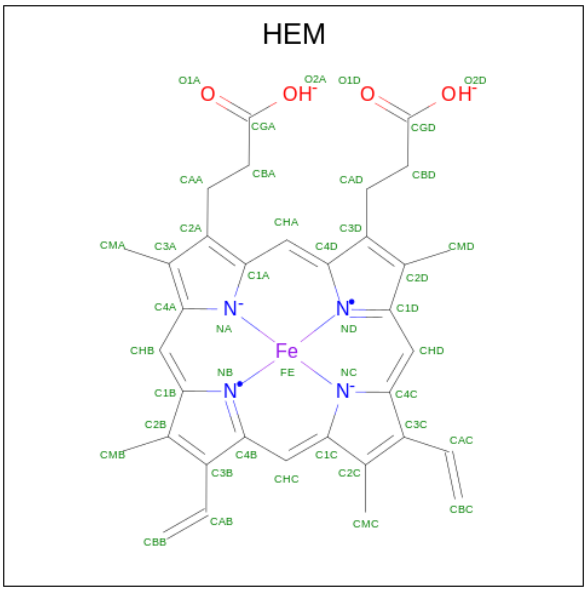
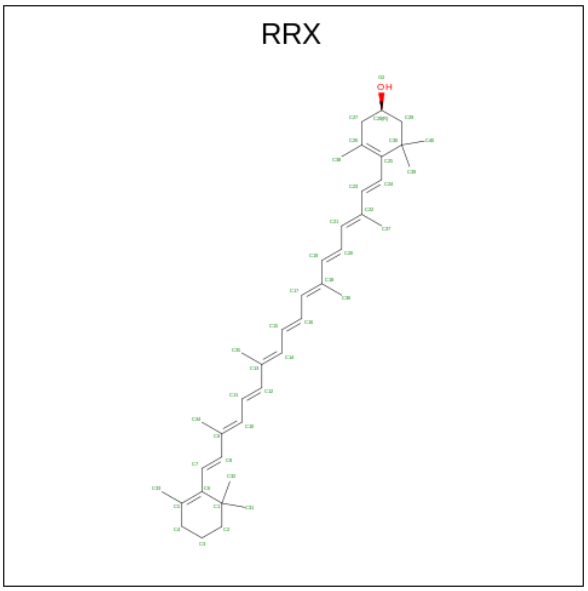
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	d	1	Total C O 43 37 6	0	0
35	h	1	Total C O 62 47 15	0	0

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).

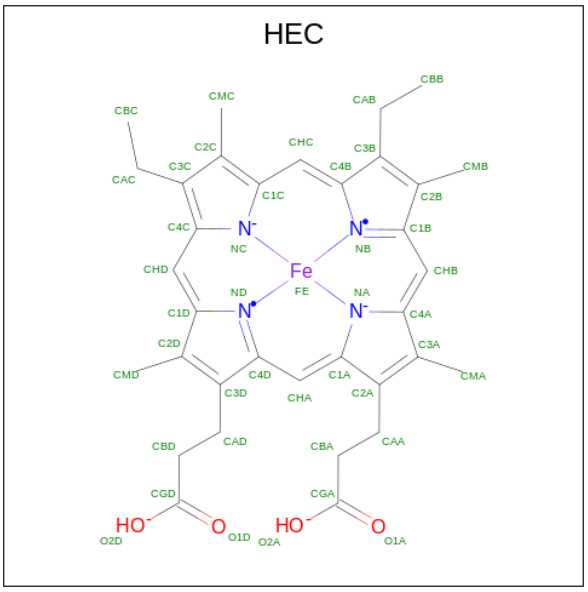


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	1	Total C O 41 40 1	0	0
37	h	1	Total C O 41 40 1	0	0

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	J	1	Total Mg 1 1	0	0
38	K	1	Total Mg 1 1	0	0
38	j	1	Total Mg 1 1	0	0
38	k	1	Total Mg 1 1	0	0

- Molecule 39 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	132	Total	O	0	0
			132	132		
40	B	256	Total	O	0	6
			262	262		
40	C	174	Total	O	0	4
			178	178		
40	D	130	Total	O	0	1
			131	131		
40	E	33	Total	O	0	2
			35	35		
40	F	4	Total	O	0	0
			4	4		
40	H	39	Total	O	0	0
			39	39		
40	I	5	Total	O	0	0
			5	5		
40	J	15	Total	O	0	1
			16	16		
40	K	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	L	18	Total O 19 19	0	1
40	O	161	Total O 166 166	0	5
40	T	12	Total O 12 12	0	0
40	U	72	Total O 74 74	0	2
40	V	110	Total O 113 113	0	3
40	Y	7	Total O 8 8	0	1
40	X	15	Total O 16 16	0	1
40	Z	5	Total O 5 5	0	0
40	a	122	Total O 123 123	0	1
40	b	251	Total O 261 261	0	10
40	c	216	Total O 220 220	0	4
40	d	115	Total O 115 115	0	0
40	e	16	Total O 17 17	0	1
40	f	4	Total O 4 4	0	0
40	h	31	Total O 31 31	0	0
40	i	5	Total O 5 5	0	0
40	j	10	Total O 10 10	0	0
40	k	9	Total O 10 10	0	1
40	l	14	Total O 15 15	0	1
40	o	153	Total O 156 156	0	3
40	t	10	Total O 10 10	0	0

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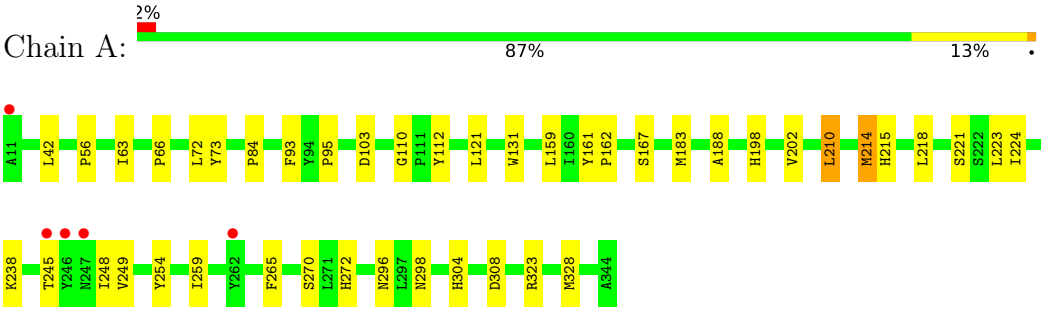
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	u	75	Total O 75 75	0	0
40	v	77	Total O 82 82	0	5
40	y	1	Total O 1 1	0	0
40	x	5	Total O 5 5	0	0
40	z	8	Total O 8 8	0	0

3 Residue-property plots (i)

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

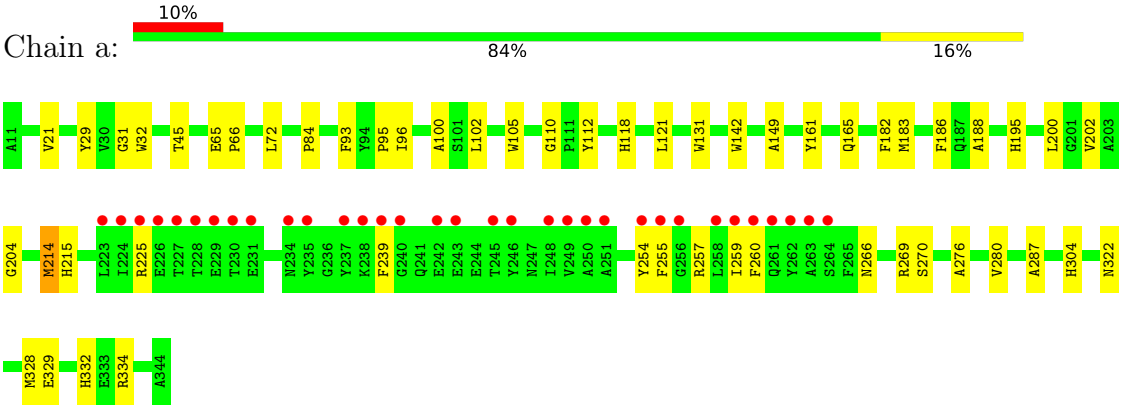
• Molecule 1: Photosystem II protein D1 1

Chain A:



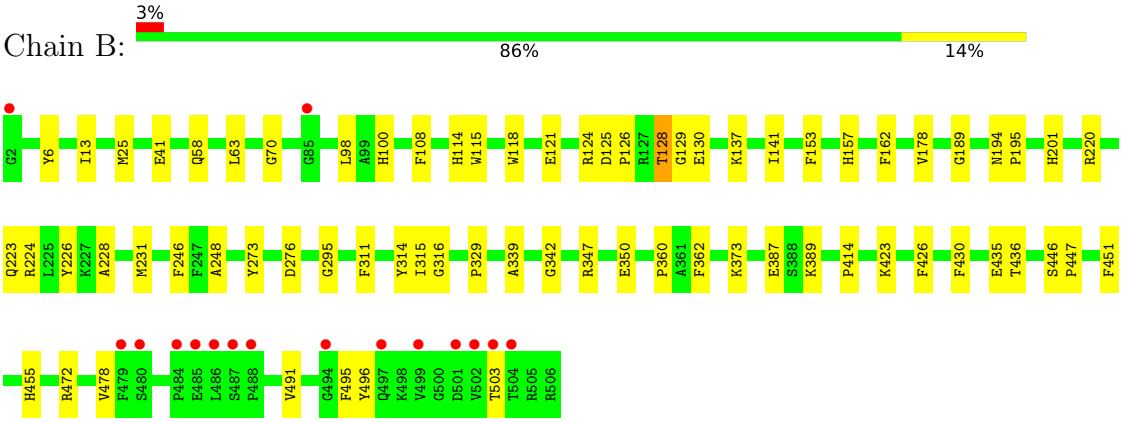
• Molecule 1: Photosystem II protein D1 1

Chain a:



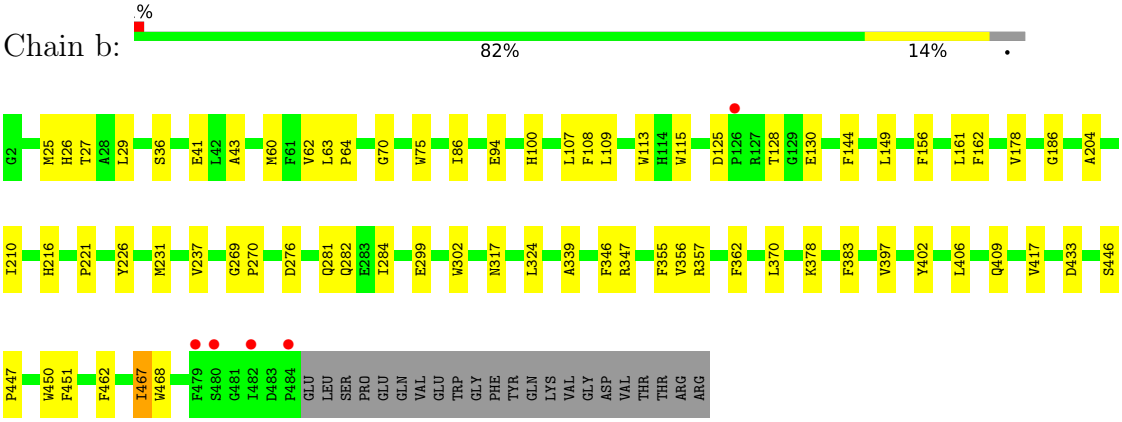
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



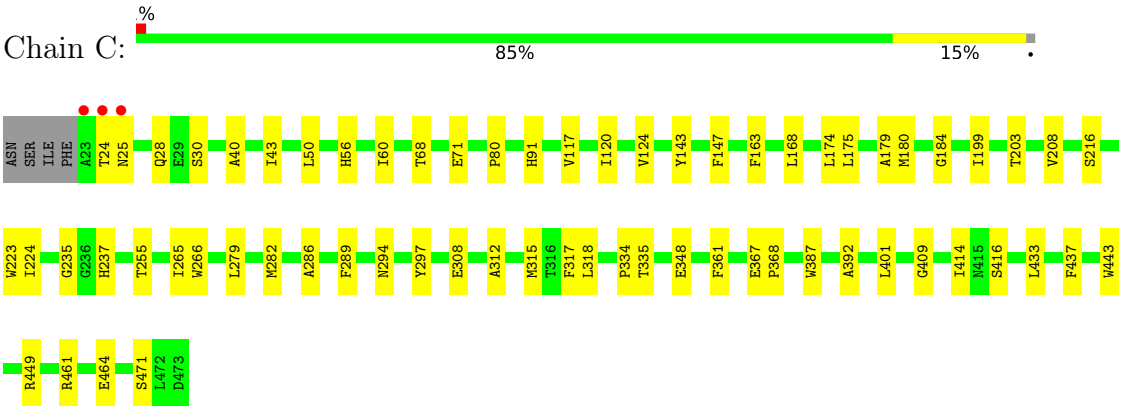
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



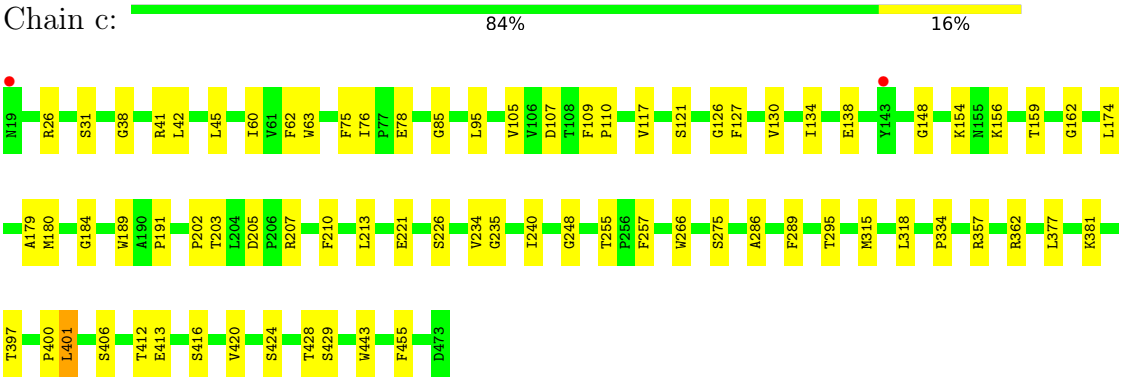
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



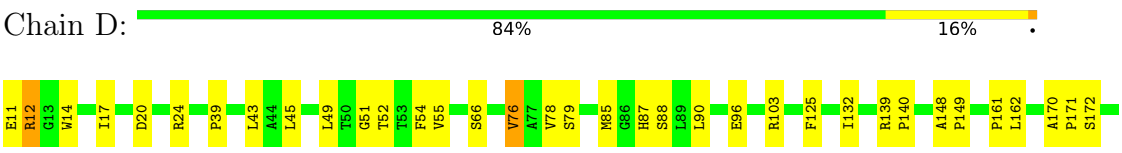
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



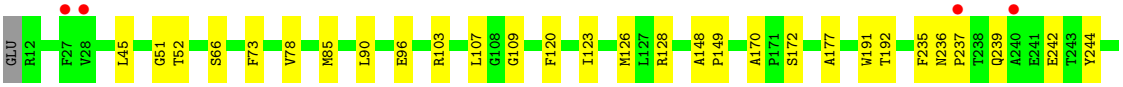
• Molecule 4: Photosystem II D2 protein

Chain D:



• Molecule 4: Photosystem II D2 protein

Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

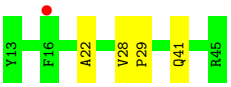
Chain E:

• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

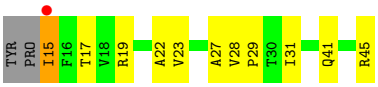
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



• Molecule 6: Cytochrome b559 subunit beta

Chain f:

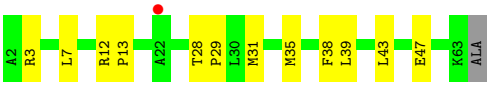


• Molecule 7: Photosystem II reaction center protein H

Chain H:

• Molecule 7: Photosystem II reaction center protein H

Chain h:

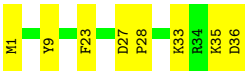


• Molecule 8: Photosystem II reaction center protein I

Chain I:

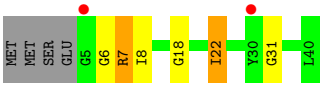
• Molecule 8: Photosystem II reaction center protein I

Chain i:



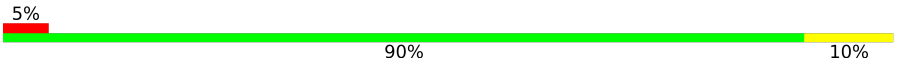
• Molecule 9: Photosystem II reaction center protein J

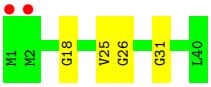
Chain J:



• Molecule 9: Photosystem II reaction center protein J

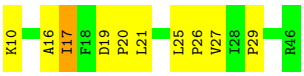
Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:



• Molecule 10: Photosystem II reaction center protein K

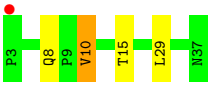
Chain k:

• Molecule 11: Photosystem II reaction center protein L

Chain L:

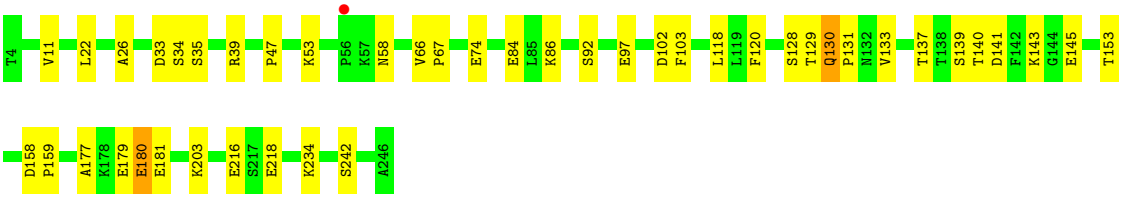
• Molecule 11: Photosystem II reaction center protein L

Chain l:



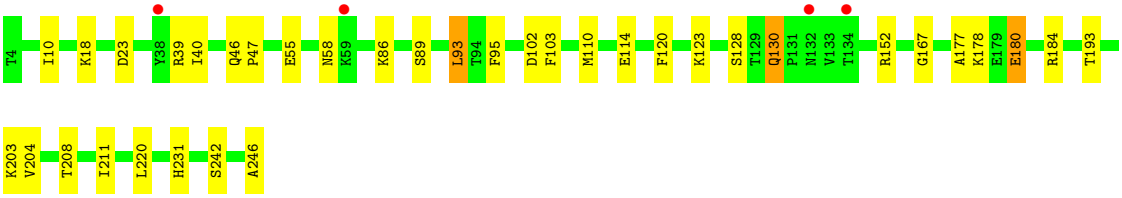
• Molecule 12: Photosystem II manganese-stabilizing polypeptide

Chain O:



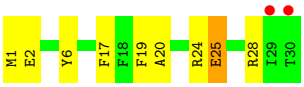
• Molecule 12: Photosystem II manganese-stabilizing polypeptide

Chain o:



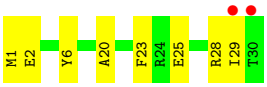
• Molecule 13: Photosystem II reaction center protein T

Chain T:



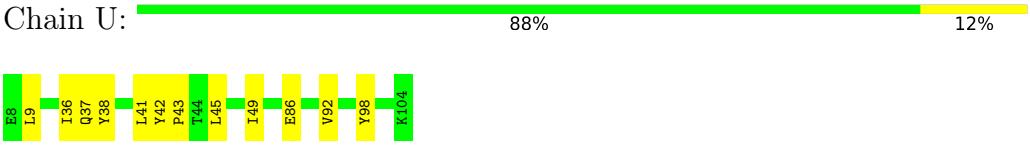
• Molecule 13: Photosystem II reaction center protein T

Chain t:



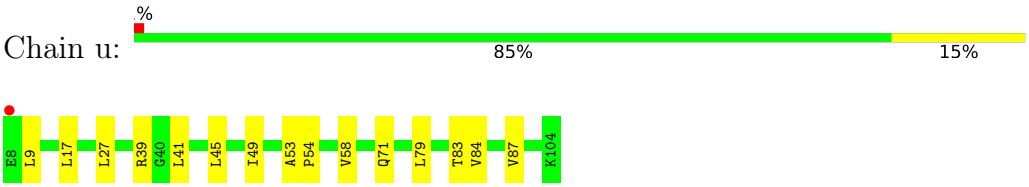
• Molecule 14: Photosystem II 12 kDa extrinsic protein

Chain U:



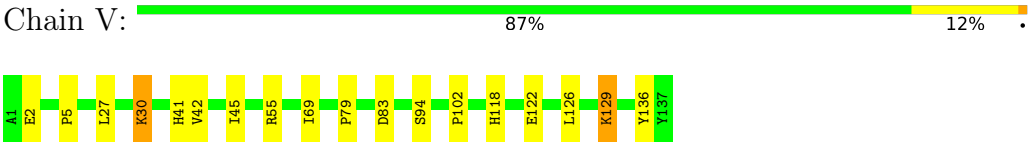
• Molecule 14: Photosystem II 12 kDa extrinsic protein

Chain u:



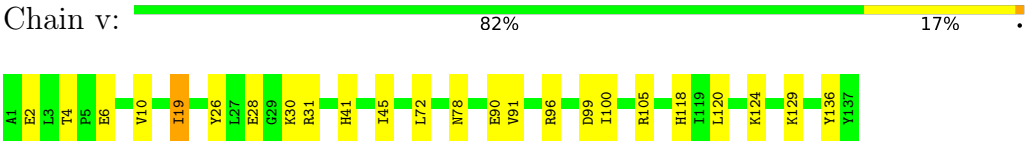
• Molecule 15: Cytochrome c-550

Chain V:



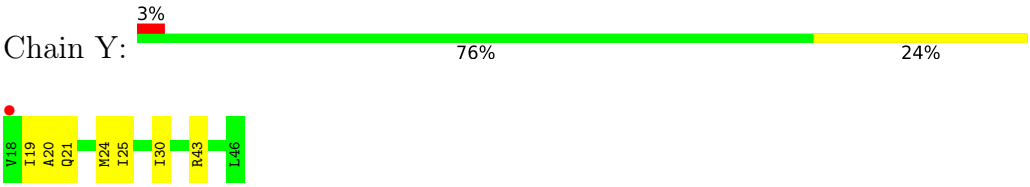
• Molecule 15: Cytochrome c-550

Chain v:



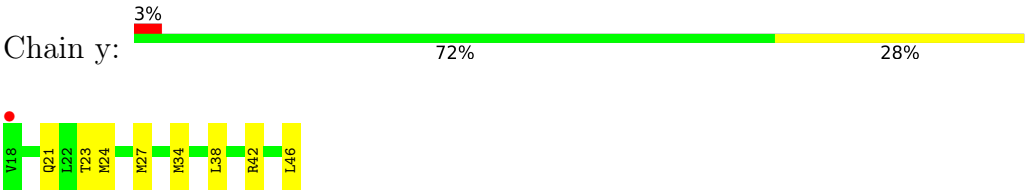
• Molecule 16: Photosystem II reaction center protein Ycf12

Chain Y:



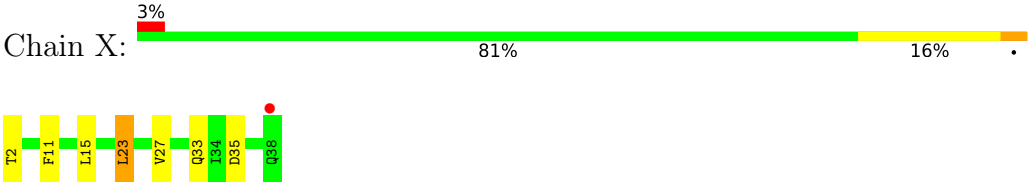
• Molecule 16: Photosystem II reaction center protein Ycf12

Chain y:



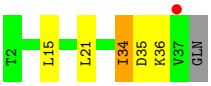
• Molecule 17: Photosystem II reaction center X protein

Chain X:



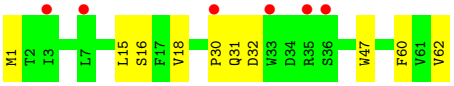
• Molecule 17: Photosystem II reaction center X protein

Chain x:



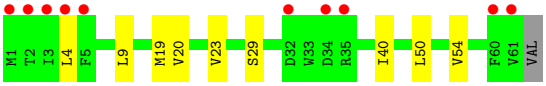
• Molecule 18: Photosystem II reaction center protein Z

Chain Z:



• Molecule 18: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.95Å 226.99Å 285.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.20) 96.3 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.174 , 0.226 0.174 , 0.225	Depositor DCC
R_{free} test set	19357 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	51892	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.09	3/2686 (0.1%)	1.03	6/3666 (0.2%)
1	a	1.13	8/2640 (0.3%)	1.05	3/3604 (0.1%)
2	B	1.07	3/4099 (0.1%)	1.03	4/5591 (0.1%)
2	b	1.06	2/3917 (0.1%)	1.02	3/5342 (0.1%)
3	C	1.03	5/3583 (0.1%)	1.00	2/4880 (0.0%)
3	c	1.01	2/3638 (0.1%)	1.04	3/4953 (0.1%)
4	D	1.10	2/2836 (0.1%)	0.99	1/3866 (0.0%)
4	d	1.04	0/2818	1.00	4/3842 (0.1%)
5	E	0.91	0/654	1.04	1/895 (0.1%)
5	e	0.89	0/655	1.05	3/896 (0.3%)
6	F	0.99	0/278	0.87	0/379
6	f	0.90	0/257	0.94	0/349
7	H	0.90	0/541	0.94	1/737 (0.1%)
7	h	0.90	0/517	0.93	0/704
8	I	0.89	0/285	1.00	0/385
8	i	0.82	0/290	0.93	0/392
9	J	0.94	0/257	1.08	1/349 (0.3%)
9	j	0.88	0/283	1.01	0/384
10	K	0.90	0/303	1.13	2/416 (0.5%)
10	k	0.85	0/296	1.05	0/408
11	L	0.97	0/294	1.03	1/399 (0.3%)
11	l	0.93	0/294	1.08	0/399
12	O	0.95	0/1887	1.02	1/2561 (0.0%)
12	o	0.86	0/1864	1.03	5/2535 (0.2%)
13	T	0.92	0/252	1.04	2/342 (0.6%)
13	t	0.89	0/252	1.02	1/342 (0.3%)
14	U	0.96	0/796	1.01	1/1078 (0.1%)
14	u	0.94	0/777	1.07	1/1054 (0.1%)
15	V	1.05	1/1090 (0.1%)	1.04	0/1480
15	v	0.95	0/1082	1.03	2/1472 (0.1%)
16	Y	0.80	0/216	1.04	0/289

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	y	0.69	0/208	1.05	0/278
17	X	0.73	0/275	1.10	0/373
17	x	0.77	0/256	1.05	0/349
18	Z	0.83	0/463	1.04	0/636
18	z	0.75	0/447	1.06	0/614
All	All	1.01	26/41286 (0.1%)	1.02	48/56239 (0.1%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	87	HIS	CG-CD2	8.02	1.44	1.35
1	A	56	PRO	CA-C	6.77	1.58	1.52
1	a	195	HIS	ND1-CE1	6.00	1.38	1.32
1	A	159	LEU	CA-C	5.80	1.58	1.52
1	a	195	HIS	CG-CD2	5.78	1.42	1.35
4	D	87	HIS	ND1-CE1	5.71	1.38	1.32
3	c	295	THR	CA-C	5.60	1.59	1.53
2	b	100	HIS	CG-ND1	-5.56	1.32	1.38
1	a	332	HIS	CG-CD2	5.51	1.42	1.35
15	V	69	ILE	C-O	5.51	1.30	1.24
3	C	317	PHE	N-CA	5.45	1.53	1.46
3	c	401	LEU	CA-C	-5.45	1.45	1.52
2	B	414	PRO	CA-C	5.41	1.57	1.52
3	C	56	HIS	CG-CD2	5.40	1.41	1.35
2	B	114	HIS	CG-CD2	5.27	1.41	1.35
2	b	26	HIS	CG-CD2	5.25	1.41	1.35
1	a	304	HIS	CG-CD2	5.21	1.41	1.35
1	a	332	HIS	ND1-CE1	5.20	1.37	1.32
1	a	118	HIS	CG-CD2	5.19	1.41	1.35
2	B	100	HIS	ND1-CE1	5.15	1.37	1.32
1	a	110	GLY	CA-C	5.14	1.55	1.51
3	C	387	TRP	CD2-CE2	5.12	1.50	1.41
1	A	198	HIS	ND1-CE1	5.11	1.37	1.32
3	C	56	HIS	CE1-NE2	5.08	1.37	1.32
3	C	91	HIS	CG-CD2	5.03	1.41	1.35
1	a	149	ALA	N-CA	-5.00	1.43	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	142	TRP	N-CA-C	7.31	121.91	112.92
2	B	342	GLY	N-CA-C	-7.27	104.63	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	269	GLY	CA-C-N	6.76	127.15	119.92
2	b	269	GLY	C-N-CA	6.76	127.15	119.92
5	E	76	VAL	N-CA-C	-6.39	104.11	110.62
1	A	167	SER	N-CA-C	6.36	118.06	108.46
12	o	130	GLN	CA-C-N	-6.29	114.30	120.52
12	o	130	GLN	C-N-CA	-6.29	114.30	120.52
1	A	110	GLY	CA-C-N	-6.07	112.31	119.05
1	A	110	GLY	C-N-CA	-6.07	112.31	119.05
2	B	295	GLY	N-CA-C	6.00	121.93	114.37
4	d	271	MET	N-CA-C	6.00	117.82	111.28
12	o	46	GLN	CA-C-N	5.89	125.65	119.76
12	o	46	GLN	C-N-CA	5.89	125.65	119.76
2	b	417	VAL	N-CA-C	-5.82	104.84	110.72
4	d	170	ALA	CA-C-N	-5.82	113.94	119.76
4	d	170	ALA	C-N-CA	-5.82	113.94	119.76
15	v	105	ARG	N-CA-C	5.72	118.25	111.33
3	c	377	LEU	N-CA-C	5.66	118.18	111.33
1	A	298	ASN	N-CA-C	5.64	118.69	110.17
3	c	357	ARG	N-CA-C	-5.53	106.03	112.89
13	T	25	GLU	CA-C-N	-5.50	114.72	120.38
13	T	25	GLU	C-N-CA	-5.50	114.72	120.38
2	B	478	VAL	N-CA-C	5.45	117.44	111.77
11	L	23	LEU	N-CA-C	-5.45	105.24	111.07
9	J	7	ARG	N-CA-C	5.45	117.66	111.02
5	e	38	VAL	N-CA-C	5.43	117.34	111.58
1	a	149	ALA	CA-C-N	-5.42	113.03	119.05
1	a	149	ALA	C-N-CA	-5.42	113.03	119.05
14	u	41	LEU	N-CA-C	5.41	118.34	111.69
3	C	71	GLU	N-CA-C	-5.40	105.47	111.36
5	e	34	GLY	N-CA-C	-5.38	105.98	112.49
13	t	20	ALA	N-CA-C	-5.37	106.23	112.89
15	v	10	VAL	N-CA-C	5.36	115.06	109.01
5	e	58	GLN	N-CA-C	5.31	117.07	111.28
2	B	189	GLY	N-CA-C	-5.29	108.39	115.32
1	A	131	TRP	CA-CB-CG	-5.18	103.75	113.60
12	O	128	SER	N-CA-C	5.17	118.01	109.85
10	K	25	LEU	CA-C-N	-5.15	114.31	119.56
10	K	25	LEU	C-N-CA	-5.15	114.31	119.56
4	d	262	SER	N-CA-C	-5.15	107.67	114.31
3	c	76	ILE	N-CA-C	-5.12	102.12	107.60
14	U	98	TYR	N-CA-C	5.10	117.96	111.69
3	C	120	ILE	N-CA-C	-5.07	105.76	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	o	86	LYS	N-CA-C	5.06	116.82	110.24
1	A	214	MET	N-CA-C	5.02	116.44	110.97
7	H	52	THR	N-CA-C	-5.02	106.32	112.90
4	D	76	VAL	CB-CA-C	-5.01	105.84	111.45

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	2598	0	2484	42	0
1	a	2555	0	2420	41	0
2	B	3950	0	3776	54	0
2	b	3780	0	3636	70	0
3	C	3470	0	3380	46	0
3	c	3521	0	3439	60	0
4	D	2732	0	2640	57	0
4	d	2717	0	2628	37	0
5	E	635	0	613	12	0
5	e	636	0	609	9	0
6	F	269	0	277	3	0
6	f	250	0	261	12	0
7	H	522	0	547	13	0
7	h	501	0	526	12	0
8	I	288	0	307	3	0
8	i	293	0	309	7	0
9	J	251	0	257	8	0
9	j	277	0	277	4	0
10	K	293	0	305	9	0
10	k	286	0	285	9	0
11	L	287	0	299	3	0
11	l	287	0	299	6	0
12	O	1853	0	1819	36	0
12	o	1833	0	1783	29	0
13	T	253	0	247	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	t	253	0	247	3	0
14	U	782	0	786	7	0
14	u	766	0	765	12	0
15	V	1066	0	1075	22	0
15	v	1058	0	1053	18	0
16	Y	215	0	246	3	0
16	y	207	0	221	9	0
17	X	269	0	297	6	0
17	x	253	0	274	4	0
18	Z	453	0	471	5	0
18	z	436	0	431	5	0
19	A	10	0	0	0	0
19	a	10	0	0	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	185	0	193	10	0
22	B	1014	0	1091	25	0
22	C	836	0	915	32	0
22	D	195	0	216	5	0
22	a	256	0	277	11	0
22	b	1016	0	1096	47	0
22	c	845	0	936	32	0
22	d	130	0	144	3	0
23	A	64	0	74	0	0
23	D	64	0	74	5	0
23	a	128	0	148	10	0
24	A	40	0	56	1	0
24	B	89	0	121	4	0
24	C	80	0	112	5	0
24	D	40	0	56	1	0
24	K	40	0	56	0	0
24	Y	39	0	53	2	0
24	a	40	0	56	1	0
24	b	91	0	123	11	0
24	c	80	0	112	8	0
24	d	40	0	56	2	0
24	k	40	0	56	2	0
24	y	40	0	56	3	0
25	A	51	0	72	2	0
25	B	40	0	50	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	91	0	122	3	0
25	D	46	0	62	5	0
25	J	45	0	60	1	0
25	b	43	0	56	1	0
25	c	100	0	140	4	0
25	d	47	0	64	4	0
25	i	51	0	72	3	0
25	j	47	0	64	2	0
26	A	55	0	80	10	0
26	D	55	0	80	5	0
26	a	55	0	80	10	0
26	d	55	0	80	5	0
27	A	31	0	36	1	0
27	C	30	0	33	1	0
27	D	143	0	211	18	0
27	L	40	0	53	7	0
27	a	94	0	137	7	0
27	d	128	0	178	6	0
27	l	49	0	74	3	0
28	A	49	0	64	2	0
28	C	54	0	78	6	0
28	D	20	0	16	0	0
28	a	105	0	147	6	0
28	b	38	0	47	2	0
28	f	14	0	8	1	0
28	l	54	0	78	1	0
29	A	35	0	46	6	0
29	B	24	0	35	3	0
29	E	24	0	35	1	0
29	I	35	0	46	0	0
29	T	24	0	35	1	0
29	Z	35	0	46	1	0
29	a	35	0	46	7	0
29	c	59	0	81	1	0
29	f	25	0	35	0	0
29	t	24	0	35	2	0
30	A	5	0	0	0	0
30	B	23	0	0	0	0
30	D	16	0	0	0	0
30	I	45	0	0	1	0
30	J	16	0	0	0	0
30	O	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	T	13	0	0	0	0
30	U	14	0	0	1	0
30	X	16	0	0	1	0
30	Z	9	0	0	0	0
30	a	16	0	0	0	0
30	b	27	0	0	0	0
30	c	10	0	0	0	0
30	d	16	0	0	0	0
30	i	58	0	0	0	0
30	j	16	0	0	1	0
30	t	16	0	0	0	0
30	u	11	0	0	0	0
30	x	15	0	0	0	0
31	A	20	0	30	4	0
31	B	60	0	90	20	0
31	C	60	0	90	6	0
31	D	12	0	18	3	0
31	F	4	0	6	0	0
31	H	4	0	6	1	0
31	I	8	0	12	0	0
31	L	4	0	6	0	0
31	O	48	0	72	22	0
31	U	8	0	12	1	0
31	V	40	0	60	20	0
31	a	20	0	30	8	0
31	b	36	0	54	14	0
31	c	76	0	114	23	0
31	d	20	0	30	8	0
31	f	4	0	6	4	0
31	i	4	0	6	1	0
31	l	12	0	18	1	0
31	o	28	0	42	15	0
31	t	12	0	18	0	0
31	u	16	0	24	6	0
31	v	36	0	54	8	0
32	A	8	0	0	1	0
32	a	4	0	0	0	0
33	B	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	o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	57	0	78	3	0
34	C	47	0	67	2	0
34	D	38	0	52	11	0
34	V	14	0	13	0	0
34	b	95	0	130	7	0
34	c	19	0	26	0	0
34	l	19	0	26	3	0
34	v	16	0	17	0	0
35	C	186	0	246	3	0
35	D	50	0	69	0	0
35	H	62	0	82	2	0
35	c	186	0	246	9	0
35	d	43	0	62	0	0
35	h	62	0	82	2	0
36	E	43	0	30	1	0
36	e	43	0	30	6	0
37	H	41	0	56	4	0
37	h	41	0	56	8	0
38	J	1	0	0	0	0
38	K	1	0	0	0	0
38	j	1	0	0	0	0
38	k	1	0	0	0	0
39	V	43	0	30	0	0
39	v	43	0	30	1	0
40	A	132	0	0	1	0
40	B	262	0	0	6	0
40	C	178	0	0	1	0
40	D	131	0	0	5	0
40	E	35	0	0	0	0
40	F	4	0	0	0	0
40	H	39	0	0	1	0
40	I	5	0	0	0	0
40	J	16	0	0	0	0
40	K	7	0	0	0	0
40	L	19	0	0	0	0
40	O	166	0	0	10	0
40	T	12	0	0	0	0
40	U	74	0	0	2	0
40	V	113	0	0	4	0
40	X	16	0	0	0	0
40	Y	8	0	0	0	0
40	Z	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	a	123	0	0	1	0
40	b	261	0	0	11	0
40	c	220	0	0	7	0
40	d	115	0	0	0	0
40	e	17	0	0	1	0
40	f	4	0	0	0	0
40	h	31	0	0	0	0
40	i	5	0	0	0	0
40	j	10	0	0	0	0
40	k	10	0	0	0	0
40	l	15	0	0	0	0
40	o	156	0	0	5	0
40	t	10	0	0	0	0
40	u	75	0	0	3	0
40	v	82	0	0	4	0
40	x	5	0	0	0	0
40	y	1	0	0	0	0
40	z	8	0	0	0	0
All	All	51892	0	50274	868	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 9.

All (868) 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)
3:c:362:ARG:HD3	31:c:924:DMS:H22	1.29	1.13
1:a:214:MET:HG2	26:a:415:PL9:H102	1.31	1.12
22:b:608:CLA:H92	22:b:608:CLA:H52	1.14	1.10
2:b:347[B]:ARG:NH2	40:b:845[B]:HOH:O	1.79	1.07
3:c:362:ARG:HH11	31:c:924:DMS:H23	1.19	1.07
22:b:608:CLA:H52	22:b:608:CLA:C9	1.85	1.05
12:O:66:VAL:HG13	12:O:67:PRO:HD2	1.37	1.05
2:b:125:ASP:HB3	2:b:128:THR:CG2	1.86	1.05
26:D:406:PL9:C33	27:L:101:LHG:H223	1.87	1.04
31:f:103:DMS:H12	31:v:206:DMS:H21	1.35	1.02
1:A:214:MET:HG2	26:A:411:PL9:H102	1.37	1.02
3:c:362:ARG:NH1	31:c:924:DMS:H23	1.74	1.02
4:d:85:MET:HE2	4:d:90[A]:LEU:HD21	1.43	1.00
16:y:23:THR:HG22	16:y:27:MET:HE2	1.42	0.99
31:O:310:DMS:H13	40:O:501:HOH:O	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:17:ILE:HD12	10:K:17:ILE:H	1.27	0.96
22:b:608:CLA:H92	22:b:608:CLA:C5	1.96	0.96
10:k:21:LEU:HD13	16:y:24:MET:HE3	1.49	0.94
12:o:208:THR:O	31:o:305:DMS:H13	1.66	0.94
2:b:355:PHE:HA	31:b:638:DMS:H21	1.51	0.93
25:d:409:LMG:O2	25:d:409:LMG:HC71	1.69	0.92
2:b:125:ASP:HB3	2:b:128:THR:HG22	1.50	0.92
27:D:411:LHG:H161	27:D:411:LHG:H322	1.52	0.91
31:f:103:DMS:C1	31:v:206:DMS:H21	2.00	0.91
12:O:133:VAL:HG22	31:O:304:DMS:C2	2.02	0.90
31:B:628:DMS:H12	40:D:502:HOH:O	1.70	0.90
1:A:103:ASP:OD1	31:A:419:DMS:H22	1.73	0.89
2:b:357:ARG:HE	31:d:415:DMS:H22	1.38	0.89
15:V:5:PRO:HD3	31:V:205:DMS:H13	1.54	0.88
3:c:362:ARG:HH11	31:c:924:DMS:C2	1.87	0.86
2:B:347[A]:ARG:NH2	40:B:701:HOH:O	2.09	0.86
31:B:638:DMS:H22	31:D:416:DMS:H11	1.57	0.86
12:O:66:VAL:CG1	12:O:67:PRO:HD2	2.04	0.86
10:K:17:ILE:H	10:K:17:ILE:CD1	1.88	0.85
24:b:618:BCR:HC31	28:b:621:SQD:C7	2.05	0.85
22:c:904:CLA:HBA1	22:c:904:CLA:HBD	1.59	0.85
24:b:620:BCR:H331	24:b:620:BCR:HC8	1.59	0.84
4:D:338:ASN:HB3	40:D:614:HOH:O	1.77	0.83
10:K:17:ILE:HD12	10:K:17:ILE:N	1.93	0.83
27:A:412:LHG:H352	30:I:105:UNL:C3	2.09	0.82
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.61	0.81
1:A:214:MET:HG2	26:A:411:PL9:C10	2.10	0.81
28:C:501:SQD:H381	9:J:22:ILE:HD11	1.63	0.81
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.61	0.80
1:A:304:HIS:HE1	31:V:212:DMS:C1	1.95	0.80
31:o:302:DMS:H11	40:o:473:HOH:O	1.81	0.79
3:c:148:GLY:O	3:c:156:LYS:NZ	2.14	0.79
34:B:623:HTG:H1'1	31:B:635:DMS:H22	1.62	0.79
2:B:360:PRO:HA	31:B:628:DMS:H11	1.65	0.79
31:o:308:DMS:H11	40:u:374:HOH:O	1.82	0.79
13:t:2:GLU:HG2	13:t:6:TYR:CE2	2.18	0.78
24:b:620:BCR:H331	24:b:620:BCR:C8	2.12	0.78
22:A:405:CLA:HMB3	22:A:405:CLA:HBB1	1.67	0.77
4:d:242:GLU:HG3	4:d:244:TYR:O	1.83	0.77
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.65	0.77
14:u:87:VAL:HG11	31:u:205:DMS:H12	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:o:208:THR:O	31:o:305:DMS:C1	2.33	0.77
10:K:19:ASP:HB3	10:K:20:PRO:HD3	1.67	0.76
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.67	0.76
3:C:40:ALA:O	3:C:43:ILE:HG13	1.86	0.76
31:c:925:DMS:H21	15:v:100:ILE:O	1.86	0.76
22:c:903:CLA:H61	22:c:913:CLA:H42	1.66	0.76
15:v:129[B]:LYS:HB3	31:v:210:DMS:S	2.26	0.76
12:O:133:VAL:HG22	31:O:304:DMS:H21	1.66	0.75
1:a:214:MET:CG	26:a:415:PL9:H102	2.13	0.75
14:u:9:LEU:HA	40:u:332:HOH:O	1.87	0.75
1:A:304:HIS:CE1	31:V:212:DMS:H13	2.22	0.75
12:o:208:THR:C	31:o:305:DMS:H13	2.11	0.75
14:u:87:VAL:HG21	31:u:205:DMS:H13	1.67	0.74
27:D:411:LHG:H142	27:D:411:LHG:H331	1.68	0.74
4:D:343[B]:GLU:OE2	34:D:415:HTG:H2	1.87	0.74
29:A:414:LMT:H2B	4:D:304:ARG:HH22	1.53	0.74
27:d:408:LHG:H332	27:d:408:LHG:H141	1.70	0.74
27:D:409:LHG:O9	27:L:101:LHG:HC81	1.88	0.73
2:b:125:ASP:CB	2:b:128:THR:HG22	2.19	0.73
31:B:638:DMS:C2	31:D:416:DMS:H11	2.19	0.73
31:c:933:DMS:H13	15:v:90:GLU:HB2	1.70	0.73
12:O:143:LYS:HE3	31:O:306:DMS:H22	1.71	0.72
2:b:125:ASP:HB3	2:b:128:THR:HG23	1.71	0.72
26:d:405:PL9:C33	27:l:102:LHG:H222	2.19	0.72
15:V:126:LEU:O	15:V:129[A]:LYS:HD2	1.89	0.72
22:B:608:CLA:H203	27:D:409:LHG:H122	1.71	0.72
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.25	0.71
15:V:27:LEU:HD21	31:V:206:DMS:C1	2.20	0.71
2:b:125:ASP:OD2	2:b:128:THR:HG22	1.89	0.71
2:b:299:GLU:HG3	40:b:879:HOH:O	1.89	0.71
22:b:608:CLA:H203	31:l:104:DMS:H21	1.73	0.71
31:O:310:DMS:H11	40:O:427:HOH:O	1.90	0.71
31:O:312:DMS:H22	40:O:467:HOH:O	1.89	0.71
31:B:642:DMS:H11	40:B:853:HOH:O	1.91	0.70
4:d:332:GLN:HG2	31:d:411:DMS:H22	1.72	0.70
1:a:65:GLU:HA	31:a:425:DMS:H12	1.71	0.70
2:b:282:GLN:NE2	40:b:701:HOH:O	2.24	0.70
2:b:383:PHE:CZ	12:o:167:GLY:HA2	2.27	0.70
3:c:362:ARG:HD3	31:c:924:DMS:C2	2.13	0.70
3:C:461:ARG:HG3	40:D:534:HOH:O	1.91	0.70
36:e:101:HEM:HBA2	36:e:101:HEM:HHA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:85:MET:HE2	4:D:90[A]:LEU:HD21	1.74	0.69
12:O:133:VAL:HG22	31:O:304:DMS:H22	1.72	0.69
3:c:138:GLU:HG3	31:c:935:DMS:H12	1.75	0.69
3:c:413:GLU:OE2	40:c:1001:HOH:O	2.11	0.69
31:B:632:DMS:H12	31:B:636:DMS:H22	1.75	0.69
4:D:14:TRP:CD1	34:D:414:HTG:H61	2.28	0.69
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.75	0.68
2:B:446:SER:HB2	2:B:447:PRO:CD	2.22	0.68
36:e:101:HEM:HMC2	6:f:31:ILE:HG13	1.74	0.68
1:A:121[A]:LEU:HD23	25:A:410:LMG:H202	1.74	0.68
2:b:36:SER:OG	24:b:619:BCR:H362	1.93	0.68
18:z:19:MET:HA	18:z:19:MET:HE2	1.74	0.68
4:D:343[A]:GLU:OE2	40:D:501:HOH:O	2.11	0.68
15:V:136:TYR:OH	40:V:301:HOH:O	2.10	0.68
3:C:279:LEU:HD22	22:C:510:CLA:HED2	1.76	0.67
1:A:304:HIS:HE1	31:V:212:DMS:H13	1.58	0.67
2:b:356:VAL:HG23	31:b:638:DMS:H22	1.76	0.67
4:d:338:ASN:O	31:d:415:DMS:H23	1.95	0.67
1:A:304:HIS:CE1	31:V:212:DMS:C1	2.76	0.67
1:a:215:HIS:HA	26:a:415:PL9:O1	1.95	0.67
10:K:16:ALA:O	10:K:19:ASP:HB2	1.94	0.67
7:H:2:ALA:N	40:H:201:HOH:O	2.28	0.67
31:B:640:DMS:H12	7:H:3[B]:ARG:NH2	2.10	0.66
2:b:467:ILE:HG13	4:d:126:MET:CE	2.25	0.66
15:V:27:LEU:HD21	31:V:206:DMS:H11	1.77	0.66
3:C:414:ILE:HD13	31:V:212:DMS:H12	1.77	0.66
11:L:14:ARG:HH22	28:b:621:SQD:H3	1.59	0.66
40:b:829:HOH:O	31:o:304:DMS:H12	1.96	0.66
12:o:178:LYS:HG2	31:o:304:DMS:C2	2.26	0.66
15:v:124:LYS:HE2	40:v:356:HOH:O	1.96	0.66
5:E:68:ASP:O	5:E:72:ALA:HB2	1.96	0.66
31:a:425:DMS:H11	40:o:513:HOH:O	1.95	0.66
27:D:409:LHG:HC12	27:L:101:LHG:O5	1.96	0.65
27:a:423:LHG:HC91	27:l:102:LHG:HC92	1.77	0.65
31:o:308:DMS:C1	40:u:374:HOH:O	2.40	0.65
25:B:621:LMG:H112	25:B:621:LMG:H312	1.79	0.65
31:c:924:DMS:H21	40:c:1006:HOH:O	1.96	0.65
27:D:411:LHG:H331	27:D:411:LHG:C14	2.25	0.65
12:o:178:LYS:HG2	31:o:304:DMS:H21	1.78	0.65
31:c:937:DMS:H21	31:c:942:DMS:H22	1.78	0.64
2:B:25:MET:HE1	2:B:108:PHE:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:177:ALA:O	31:O:312:DMS:H11	1.97	0.64
22:B:605:CLA:H43	22:B:606:CLA:H2	1.80	0.64
18:z:50:LEU:O	18:z:54:VAL:HG23	1.97	0.64
3:c:127:PHE:CE1	29:c:931:LMT:H51	2.32	0.64
22:a:409:CLA:HMB2	22:d:402:CLA:H122	1.80	0.64
3:C:279:LEU:HD12	3:C:282:MET:CE	2.27	0.64
3:C:367:GLU:HB2	31:C:530:DMS:H11	1.78	0.63
17:x:34:ILE:C	17:x:36:LYS:H	2.06	0.63
14:u:87:VAL:HG21	31:u:205:DMS:C1	2.29	0.63
1:a:214:MET:SD	23:a:411:PHO:HED3	2.39	0.63
37:h:101:RRX:H55	37:h:101:RRX:H46	1.81	0.63
14:U:9:LEU:HA	40:U:301:HOH:O	1.98	0.63
3:c:179:ALA:O	3:c:184:GLY:HA2	1.98	0.62
2:b:356:VAL:H	31:b:638:DMS:H22	1.64	0.62
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.80	0.62
1:A:304:HIS:HE1	31:V:212:DMS:H11	1.63	0.62
4:D:85:MET:CE	4:D:96:GLU:HG2	2.28	0.62
3:C:80:PRO:HA	31:C:527:DMS:H22	1.82	0.62
31:c:925:DMS:C2	15:v:100:ILE:O	2.48	0.62
2:B:350:GLU:HG3	31:B:631:DMS:C1	2.30	0.62
5:e:68:ASP:O	5:e:72:ALA:HB2	1.99	0.62
12:O:74[A]:GLU:OE2	40:O:401:HOH:O	2.16	0.62
24:Y:101:BCR:H321	24:Y:101:BCR:HC8	1.82	0.61
22:c:904:CLA:HBA1	22:c:904:CLA:CBD	2.29	0.61
1:a:183:MET:HA	22:a:407:CLA:HMD1	1.82	0.61
12:o:177:ALA:O	31:o:307:DMS:H11	2.00	0.61
26:A:411:PL9:H403	6:F:22:ALA:HB2	1.82	0.61
2:B:276:ASP:OD1	31:B:641:DMS:H23	2.00	0.61
5:e:22:ILE:O	5:e:25:ILE:HG22	2.01	0.61
12:o:102:ASP:OD1	12:o:123:LYS:NZ	2.32	0.61
1:A:265:PHE:HE2	26:A:411:PL9:H122	1.64	0.61
15:V:5:PRO:CD	31:V:205:DMS:H13	2.26	0.61
1:A:215:HIS:HA	26:A:411:PL9:O1	2.01	0.60
5:E:20:TRP:CD1	9:J:8:ILE:HD13	2.35	0.60
6:f:15:ILE:HG23	6:f:15:ILE:O	2.01	0.60
34:D:415:HTG:H3	15:V:55:ARG:HH12	1.66	0.60
37:h:101:RRX:H46	37:h:101:RRX:C33	2.32	0.60
2:b:25:MET:HE1	2:b:108:PHE:CD2	2.36	0.60
12:o:18:LYS:HE3	40:o:490:HOH:O	2.01	0.60
31:B:638:DMS:H22	31:D:416:DMS:C1	2.32	0.60
2:b:356:VAL:H	31:b:638:DMS:C2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:429:SER:HB3	35:c:918:DGD:HBT2	1.83	0.60
31:a:425:DMS:H21	40:o:500:HOH:O	2.01	0.59
2:b:378:LYS:HE3	31:b:636:DMS:H23	1.84	0.59
31:o:308:DMS:H12	14:u:9:LEU:HD21	1.83	0.59
25:D:412:LMG:H352	34:D:414:HTG:H6'2	1.84	0.59
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.85	0.59
12:O:216:GLU:CD	12:O:234:LYS:HD2	2.28	0.59
22:D:401:CLA:HMB1	22:D:401:CLA:HBB1	1.85	0.59
1:A:223:LEU:HD22	4:D:265:ARG:HG2	1.84	0.59
22:B:606:CLA:C14	22:B:611:CLA:HED2	2.33	0.58
26:D:406:PL9:C32	27:L:101:LHG:H223	2.32	0.58
12:O:47:PRO:HG3	12:O:120:PHE:CE1	2.38	0.58
1:a:270:SER:HB2	28:a:414:SQD:O49	2.03	0.58
22:b:615:CLA:HED3	11:l:8:GLN:O	2.04	0.58
7:h:3[A]:ARG:HH11	7:h:3[A]:ARG:HB2	1.69	0.58
24:c:916:BCR:C3	8:i:23:PHE:HB3	2.33	0.58
7:h:3[A]:ARG:HB2	7:h:3[A]:ARG:NH1	2.17	0.58
4:D:49:LEU:HD21	25:J:101:LMG:H341	1.84	0.58
14:U:92:VAL:HG21	31:U:203:DMS:H21	1.84	0.58
31:c:940:DMS:H11	40:c:1203:HOH:O	2.03	0.58
25:d:409:LMG:HC71	25:d:409:LMG:HO2	1.66	0.57
2:B:137:LYS:O	2:B:141:ILE:HG13	2.04	0.57
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.85	0.57
22:b:606:CLA:HHC	22:b:606:CLA:HBB1	1.86	0.57
2:B:223:GLN:NE2	40:B:703:HOH:O	2.37	0.57
3:c:38:GLY:HA3	22:c:912:CLA:HMD2	1.85	0.57
37:h:101:RRX:C23	37:h:101:RRX:H17	2.33	0.57
15:v:78:ASN:OD1	15:v:96:ARG:NH1	2.33	0.57
27:D:409:LHG:HC92	27:L:101:LHG:HC92	1.86	0.57
31:a:425:DMS:H11	12:o:152:ARG:HH21	1.70	0.57
24:b:620:BCR:HC8	24:b:620:BCR:C33	2.34	0.57
4:d:192:THR:HG23	22:d:402:CLA:HBC2	1.86	0.57
24:A:409:BCR:H401	31:A:419:DMS:H12	1.87	0.57
29:A:414:LMT:H2B	4:D:304:ARG:NH2	2.18	0.57
3:c:156:LYS:HE2	31:c:939:DMS:H12	1.87	0.57
12:O:39:ARG:HD3	40:O:413:HOH:O	2.04	0.56
31:O:310:DMS:C1	40:O:427:HOH:O	2.52	0.56
4:d:85:MET:CE	4:d:96:GLU:HG2	2.33	0.56
1:a:200:LEU:HD23	35:c:919:DGD:HAE1	1.87	0.56
2:b:29:LEU:HD11	24:b:618:BCR:H12C	1.87	0.56
26:A:411:PL9:H221	23:D:402:PHO:HMA2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:411:PHO:HHD	23:a:411:PHO:HBC2	1.87	0.56
31:b:638:DMS:C1	40:b:867[B]:HOH:O	2.53	0.56
1:a:322:ASN:OD1	3:c:412:THR:HA	2.06	0.56
1:a:200:LEU:CD2	35:c:919:DGD:HAE1	2.36	0.56
1:a:329:GLU:HG3	40:a:617:HOH:O	2.04	0.56
2:B:248:ALA:HB2	22:B:604:CLA:H51	1.87	0.56
34:D:415:HTG:C3	15:V:55:ARG:HH12	2.19	0.56
4:d:90[B]:LEU:HG	4:d:109:GLY:HA2	1.87	0.56
5:e:13:ILE:HG21	36:e:101:HEM:HAD2	1.88	0.56
12:O:39:ARG:NH1	40:O:404:HOH:O	2.39	0.56
2:b:125:ASP:CG	2:b:128:THR:HG22	2.30	0.56
22:c:911:CLA:H192	22:c:911:CLA:HBC3	1.87	0.56
22:b:609:CLA:H203	22:b:610:CLA:H191	1.87	0.56
12:O:145:GLU:CB	31:O:303:DMS:H21	2.36	0.56
29:B:622:LMT:H11	25:D:412:LMG:HC92	1.88	0.55
15:v:4:THR:HG22	31:v:205:DMS:H23	1.88	0.55
15:V:27:LEU:HD21	31:V:206:DMS:H12	1.87	0.55
29:a:419:LMT:H6'1	4:d:304:ARG:HH22	1.72	0.55
9:j:18:GLY:HA3	24:y:101:BCR:H371	1.87	0.55
12:O:58:ASN:HB3	2:b:339:ALA:HB2	1.89	0.55
10:k:21:LEU:HB2	16:y:24:MET:HE2	1.88	0.55
24:C:515:BCR:H331	24:C:515:BCR:C8	2.36	0.55
16:Y:20:ALA:O	16:Y:24:MET:HG2	2.07	0.55
2:b:125:ASP:CB	2:b:128:THR:CG2	2.73	0.55
40:b:704:HOH:O	31:o:304:DMS:H13	2.06	0.55
2:B:350:GLU:HG3	31:B:631:DMS:H11	1.88	0.55
40:b:910:HOH:O	31:d:415:DMS:H11	2.05	0.55
22:B:611:CLA:HHC	22:B:611:CLA:HBB1	1.87	0.55
2:b:281:GLN:NE2	40:b:702:HOH:O	2.39	0.55
22:b:608:CLA:H2	25:b:622:LMG:H151	1.89	0.55
3:c:126:GLY:O	3:c:130:VAL:HG23	2.07	0.55
8:I:13:THR:O	8:I:17:LEU:HG	2.07	0.55
15:V:129[B]:LYS:HB3	31:V:212:DMS:S	2.47	0.55
1:A:183:MET:HA	22:A:405:CLA:HMD1	1.88	0.55
31:A:420:DMS:H12	40:A:559:HOH:O	2.06	0.55
10:K:20:PRO:HB3	16:Y:21:GLN:HG3	1.88	0.55
2:b:63:LEU:N	2:b:64:PRO:HD2	2.21	0.55
36:e:101:HEM:CMC	6:f:31:ILE:HG13	2.37	0.55
10:k:19:ASP:HB3	10:k:20:PRO:HD3	1.88	0.55
2:B:389:LYS:NZ	34:D:415:HTG:H2'2	2.22	0.54
27:D:411:LHG:H161	27:D:411:LHG:C32	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:408:LHG:H132	27:d:408:LHG:H341	1.89	0.54
1:A:265:PHE:CE2	26:A:411:PL9:H122	2.42	0.54
35:c:918:DGD:HAT2	35:c:919:DGD:HBN2	1.88	0.54
2:b:324:LEU:HA	4:d:293[B]:LEU:HG	1.89	0.54
4:D:192:THR:HG23	22:D:403:CLA:HBC2	1.90	0.54
2:b:128:THR:HG23	2:b:130:GLU:H	1.72	0.54
25:d:409:LMG:H221	7:h:35:MET:HE2	1.89	0.54
28:A:413:SQD:H272	2:b:109:LEU:HD13	1.90	0.54
22:b:611:CLA:H152	22:b:611:CLA:OBD	2.07	0.54
28:C:501:SQD:H302	22:C:509:CLA:H71	1.90	0.54
25:D:412:LMG:O9	25:D:412:LMG:O2	2.19	0.54
12:O:66:VAL:CG1	12:O:67:PRO:CD	2.83	0.54
22:B:608:CLA:H191	26:D:406:PL9:H303	1.89	0.54
13:T:2:GLU:HG2	13:T:6:TYR:CE2	2.43	0.54
9:J:18:GLY:O	9:J:22:ILE:HD12	2.08	0.54
12:O:179:GLU:HG3	31:O:312:DMS:H12	1.90	0.54
3:c:191:PRO:O	40:c:1002:HOH:O	2.18	0.54
12:o:55:GLU:OE2	12:o:231:HIS:CD2	2.61	0.54
4:D:11:GLU:O	4:D:12:ARG:CB	2.56	0.53
1:a:334:ARG:HD3	4:d:320:LEU:HD13	1.89	0.53
24:c:916:BCR:HC32	8:i:23:PHE:HB3	1.88	0.53
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.89	0.53
25:d:409:LMG:O2	25:d:409:LMG:C7	2.51	0.53
2:B:314:TYR:CE1	2:B:316:GLY:HA3	2.43	0.53
22:C:505:CLA:H112	35:C:519:DGD:HBF1	1.89	0.53
24:C:516:BCR:H331	24:C:516:BCR:C8	2.39	0.53
27:a:423:LHG:C18	22:b:608:CLA:C14	2.87	0.53
4:d:272:LEU:C	4:d:272:LEU:HD23	2.32	0.53
31:f:103:DMS:H12	31:v:206:DMS:C2	2.25	0.53
15:v:129[A]:LYS:HB3	31:v:210:DMS:S	2.48	0.53
29:B:622:LMT:H11	25:D:412:LMG:C9	2.39	0.53
27:a:423:LHG:O9	27:l:102:LHG:HC81	2.07	0.53
2:b:467:ILE:HG13	4:d:126:MET:HE2	1.89	0.53
17:X:23:LEU:O	17:X:27:VAL:HG23	2.08	0.53
14:u:58:VAL:HG12	14:u:79:LEU:HD22	1.91	0.53
1:A:221:SER:HB2	4:D:139:ARG:O	2.09	0.53
18:z:9:LEU:HD13	18:z:54:VAL:HG11	1.90	0.53
27:D:410:LHG:H171	27:L:101:LHG:H201	1.91	0.53
15:V:126:LEU:O	15:V:129[A]:LYS:CD	2.56	0.53
4:D:272:LEU:C	4:D:272:LEU:HD23	2.34	0.53
30:U:201:UNL:C4	40:U:346:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.43	0.53
2:b:355:PHE:O	2:b:370:LEU:HA	2.08	0.53
22:b:603:CLA:H201	35:h:102:DGD:HBT1	1.91	0.53
35:c:917:DGD:HA82	25:i:101:LMG:H211	1.91	0.53
14:U:38:TYR:HB2	14:U:41:LEU:HD12	1.91	0.52
22:b:616:CLA:H161	7:h:7:LEU:HD21	1.90	0.52
4:D:85:MET:CE	4:D:90[A]:LEU:HD21	2.38	0.52
2:b:41:GLU:HB3	2:b:60:MET:SD	2.50	0.52
8:i:33:LYS:O	8:i:35:LYS:HG3	2.09	0.52
22:B:614:CLA:HBB1	22:B:614:CLA:HMB1	1.91	0.52
3:C:28:GLN:NE2	28:C:501:SQD:O7	2.36	0.52
22:C:505:CLA:H42	35:C:518:DGD:HB42	1.91	0.52
12:O:158:ASP:HB2	12:O:159:PRO:CD	2.39	0.52
1:a:266:ASN:HD22	4:d:237:PRO:HG3	1.74	0.52
22:b:605:CLA:H43	22:b:606:CLA:H2	1.91	0.52
22:b:609:CLA:HMB2	4:d:126:MET:HG2	1.91	0.52
36:e:101:HEM:HBA2	36:e:101:HEM:CHA	2.38	0.52
1:a:287:ALA:HA	22:a:407:CLA:CED	2.40	0.52
22:A:405:CLA:HBB1	22:A:405:CLA:CMB	2.38	0.52
22:c:904:CLA:HAB	22:c:913:CLA:H41	1.91	0.52
5:e:7:GLU:HG2	6:f:19:ARG:CZ	2.39	0.52
31:c:927:DMS:H11	15:v:99:ASP:O	2.10	0.52
34:D:415:HTG:H7'3	14:U:37:GLN:HE22	1.74	0.52
12:O:145:GLU:HB2	31:O:303:DMS:H21	1.91	0.52
4:d:123:ILE:HD11	35:h:102:DGD:HAW1	1.91	0.52
31:b:638:DMS:H13	40:b:867[B]:HOH:O	2.08	0.52
22:C:514:CLA:C4B	24:C:515:BCR:H383	2.40	0.52
22:a:408:CLA:HED1	26:d:405:PL9:H371	1.92	0.52
12:o:40:ILE:HD12	12:o:95:PHE:CD2	2.44	0.52
29:a:419:LMT:C6B	4:d:304:ARG:HH22	2.22	0.51
3:c:134:ILE:HD12	22:c:912:CLA:H43	1.92	0.51
6:f:45:ARG:HG2	31:f:103:DMS:O	2.09	0.51
27:d:407:LHG:HC62	11:l:15:THR:HG23	1.92	0.51
2:b:451:PHE:CD1	2:b:451:PHE:C	2.89	0.51
3:c:205:ASP:OD2	3:c:207:ARG:NH1	2.43	0.51
12:o:39:ARG:HG3	12:o:246:ALA:HB2	1.92	0.51
1:A:63:ILE:HB	3:C:335:THR:HG21	1.92	0.51
22:B:608:CLA:H193	4:D:281:MET:SD	2.50	0.51
4:D:343[B]:GLU:CD	34:D:415:HTG:H2	2.36	0.51
8:I:12:VAL:O	8:I:16:VAL:HG23	2.11	0.51
35:c:919:DGD:HA32	25:j:101:LMG:H111	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ARG:HG3	7:H:20:LYS:HG2	1.93	0.51
31:c:933:DMS:H12	15:v:91:VAL:HG22	1.93	0.51
22:b:602:CLA:C9	37:h:101:RRX:H25	2.40	0.51
34:D:415:HTG:H62	40:V:301:HOH:O	2.11	0.51
2:B:128:THR:HB	2:B:130:GLU:H	1.75	0.51
3:C:143:TYR:HE2	34:C:532:HTG:H61	1.76	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.51
3:c:159:THR:HG21	31:c:939:DMS:H21	1.92	0.51
22:c:910:CLA:HMB1	22:c:910:CLA:HBB1	1.93	0.51
4:d:332:GLN:HG2	31:d:411:DMS:C2	2.40	0.51
22:d:403:CLA:H192	17:x:15:LEU:HB2	1.93	0.51
24:k:101:BCR:H331	24:k:101:BCR:C8	2.40	0.51
3:C:147:PHE:CD2	22:C:514:CLA:H3A	2.46	0.51
15:v:2:GLU:HG3	31:v:205:DMS:H12	1.93	0.51
3:C:223:TRP:CG	3:C:224:ILE:H	2.29	0.50
14:u:45:LEU:HD21	14:u:71:GLN:HB3	1.94	0.50
16:y:34:MET:HA	16:y:34:MET:HE2	1.93	0.50
2:B:121:GLU:HA	7:H:2:ALA:HB1	1.93	0.50
2:b:299:GLU:HG2	2:b:402:TYR:HD1	1.75	0.50
3:C:334:PRO:HA	12:O:153:THR:OG1	2.11	0.50
31:b:630:DMS:H11	14:u:17:LEU:CD2	2.42	0.50
24:d:404:BCR:H331	24:d:404:BCR:C8	2.42	0.50
29:A:414:LMT:H12	34:b:623:HTG:H5	1.93	0.50
2:B:115:TRP:CD2	24:B:618:BCR:HC21	2.47	0.50
3:C:60:ILE:HG22	22:C:504:CLA:HHD	1.94	0.50
12:O:133:VAL:HG13	31:O:304:DMS:H21	1.93	0.50
1:A:223:LEU:CD2	4:D:265:ARG:HG2	2.42	0.50
2:b:357:ARG:NE	31:d:415:DMS:H22	2.18	0.50
22:b:614:CLA:HMB1	22:b:614:CLA:HBB1	1.94	0.50
10:k:25:LEU:N	10:k:26:PRO:CD	2.75	0.50
12:o:103:PHE:HA	12:o:120:PHE:O	2.12	0.50
29:A:414:LMT:H32	2:b:43:ALA:HA	1.93	0.49
22:b:609:CLA:H111	4:d:120:PHE:CE1	2.48	0.49
3:c:400:PRO:C	3:c:401:LEU:HD12	2.37	0.49
22:b:606:CLA:HHC	22:b:606:CLA:CBB	2.42	0.49
24:d:404:BCR:C40	9:j:25:VAL:HG21	2.42	0.49
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.47	0.49
18:Z:62:VAL:C	40:Z:203:HOH:O	2.55	0.49
27:a:423:LHG:H372	22:b:614:CLA:H43	1.94	0.49
2:B:495:PHE:C	2:B:496:TYR:HD1	2.21	0.49
2:b:446:SER:HB2	2:b:447:PRO:CD	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:u:202:DMS:H12	31:u:205:DMS:H22	1.95	0.49
3:C:180:MET:HG2	3:C:199:ILE:O	2.12	0.49
2:b:221:PRO:HA	22:b:610:CLA:HED3	1.93	0.49
16:y:38:LEU:O	16:y:42:ARG:HG2	2.13	0.49
3:C:203:THR:O	3:C:235:GLY:HA3	2.13	0.49
35:C:519:DGD:HBN1	27:D:411:LHG:H222	1.95	0.49
3:c:174:LEU:HB3	22:c:903:CLA:H161	1.94	0.49
22:c:904:CLA:HMB1	22:c:904:CLA:HBB1	1.93	0.49
22:B:606:CLA:HBB1	22:B:607:CLA:C5	2.43	0.49
3:C:308:GLU:HB2	3:C:361:PHE:CE2	2.47	0.49
12:O:129:THR:HA	12:O:141:ASP:O	2.13	0.49
2:b:62:VAL:HB	22:b:606:CLA:HED3	1.95	0.49
1:A:237:TYR:CB	4:D:265:ARG:HD2	2.43	0.49
22:B:608:CLA:HMB1	22:B:608:CLA:HBB1	1.94	0.49
26:a:415:PL9:H403	6:f:22:ALA:HB2	1.95	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.48
29:a:419:LMT:H6'1	4:d:304:ARG:NH2	2.28	0.48
22:b:615:CLA:OBD	11:l:10:VAL:CG2	2.61	0.48
1:A:121[B]:LEU:HD11	22:C:506:CLA:H152	1.94	0.48
26:A:411:PL9:H272	26:A:411:PL9:H251	1.66	0.48
34:B:623:HTG:H1	29:a:419:LMT:H21	1.95	0.48
31:B:638:DMS:H11	40:B:778:HOH:O	2.13	0.48
3:C:50:LEU:HD12	22:C:513:CLA:HMD2	1.94	0.48
26:D:406:PL9:H401	11:L:29:LEU:HD23	1.94	0.48
3:c:31:SER:CB	3:c:41:ARG:HG2	2.44	0.48
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.96	0.48
26:A:411:PL9:H301	4:D:45:LEU:HD22	1.96	0.48
29:a:419:LMT:C11	29:t:101:LMT:H122	2.43	0.48
27:a:423:LHG:C18	22:b:608:CLA:H141	2.43	0.48
4:d:267:LEU:C	4:d:267:LEU:HD23	2.38	0.48
37:H:101:RRX:H55	37:H:101:RRX:H46	1.95	0.48
35:c:917:DGD:HA71	25:i:101:LMG:H361	1.96	0.48
1:A:249:VAL:HG12	2:B:491:VAL:HG23	1.95	0.48
3:C:117:VAL:HG12	25:C:531:LMG:H222	1.95	0.48
23:a:410:PHO:HED2	4:d:257:PHE:CD2	2.49	0.48
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.95	0.48
12:o:193:THR:HG21	12:o:220:LEU:HD12	1.94	0.48
15:v:72:LEU:HD12	15:v:120:LEU:HD11	1.95	0.48
1:a:131:TRP:CH2	22:c:906:CLA:HAA2	2.49	0.48
12:o:114:GLU:OE1	31:o:303:DMS:H12	2.13	0.48
40:B:878:HOH:O	31:O:311:DMS:H13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:LEU:HB3	22:C:503:CLA:H161	1.95	0.48
27:D:410:LHG:H192	13:T:17:PHE:HZ	1.79	0.48
31:V:207:DMS:H23	40:V:380:HOH:O	2.14	0.48
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.95	0.48
4:d:73:PHE:CZ	25:j:101:LMG:H182	2.49	0.48
18:z:23:VAL:HG22	18:z:40:ILE:HG12	1.95	0.48
29:a:419:LMT:O2B	29:t:101:LMT:H6E	2.13	0.48
22:B:610:CLA:H42	25:D:412:LMG:H171	1.95	0.47
3:C:461:ARG:HD2	4:D:225:ASP:OD1	2.14	0.47
2:b:162:PHE:O	22:b:607:CLA:HHD	2.14	0.47
3:c:45:LEU:HD12	22:c:912:CLA:HED3	1.96	0.47
4:d:51:GLY:HA3	4:d:78:VAL:HG22	1.95	0.47
16:y:42:ARG:HD2	18:z:29:SER:OG	2.13	0.47
1:A:254:TYR:CD2	4:D:132:ILE:HG22	2.49	0.47
31:B:633:DMS:H22	4:D:140:PRO:HD2	1.96	0.47
27:a:416:LHG:H122	27:a:416:LHG:H242	1.97	0.47
2:b:462:PHE:CE1	22:b:614:CLA:HMB3	2.49	0.47
4:d:236:ASN:O	4:d:239:GLN:HG2	2.14	0.47
7:h:38:PHE:HB2	37:h:101:RRX:C10	2.43	0.47
12:o:55:GLU:OE2	12:o:231:HIS:HD2	1.96	0.47
1:A:304:HIS:CE1	31:V:212:DMS:H11	2.46	0.47
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.50	0.47
2:b:25:MET:HE3	24:b:618:BCR:C5	2.44	0.47
22:b:604:CLA:H18	22:b:610:CLA:H91	1.96	0.47
22:b:609:CLA:H142	7:h:39:LEU:HD21	1.97	0.47
3:c:202:PRO:HB3	3:c:234:VAL:HG12	1.96	0.47
24:c:916:BCR:HC31	8:i:23:PHE:HB3	1.96	0.47
14:u:27:LEU:HD22	14:u:49:ILE:HG21	1.96	0.47
3:C:414:ILE:HD13	31:V:212:DMS:C1	2.44	0.47
17:x:34:ILE:O	17:x:36:LYS:N	2.35	0.47
2:B:13:ILE:O	31:B:630:DMS:H11	2.14	0.47
2:B:228:ALA:HB2	29:B:622:LMT:H21	1.96	0.47
7:h:28:THR:HB	7:h:29:PRO:HD3	1.97	0.47
12:o:47:PRO:HG3	12:o:120:PHE:CE1	2.50	0.47
1:A:223:LEU:HD12	4:D:139:ARG:HH12	1.79	0.47
24:B:618:BCR:H331	24:B:618:BCR:C8	2.43	0.47
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.96	0.47
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.96	0.47
22:D:401:CLA:HBC2	22:D:401:CLA:CMC	2.45	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.47
24:Y:101:BCR:H312	18:Z:16:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.80	0.47
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.50	0.47
6:f:17:THR:HA	28:f:101:SQD:H62	1.97	0.47
31:B:638:DMS:C1	40:B:778:HOH:O	2.63	0.47
1:a:100:ALA:HB2	31:a:401:DMS:H12	1.97	0.47
18:Z:47:TRP:CD2	29:Z:101:LMT:H111	2.50	0.47
1:a:204:GLY:N	28:a:414:SQD:H221	2.30	0.47
1:A:270:SER:HB2	28:C:501:SQD:O49	2.16	0.47
1:a:257:ARG:O	4:d:128:ARG:NH2	2.48	0.47
24:k:101:BCR:H24C	24:k:101:BCR:H371	1.75	0.47
1:A:73:TYR:CD1	29:A:414:LMT:H3B	2.50	0.46
1:A:237:TYR:HD2	1:A:245:THR:HB	1.78	0.46
4:D:52:THR:HB	4:D:76:VAL:CG2	2.45	0.46
5:E:63:ILE:HG23	5:E:64:PRO:HD2	1.97	0.46
12:O:180:GLU:CD	12:O:180:GLU:H	2.24	0.46
31:b:630:DMS:H11	14:u:17:LEU:HD21	1.96	0.46
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.15	0.46
4:D:343[B]:GLU:HG3	40:V:301:HOH:O	2.14	0.46
27:D:411:LHG:H162	27:D:411:LHG:H111	1.96	0.46
1:a:29:TYR:CE1	1:a:31:GLY:HA3	2.50	0.46
22:c:908:CLA:H141	22:c:908:CLA:H161	1.70	0.46
3:C:265:ILE:HD11	3:C:449:ARG:HD3	1.98	0.46
22:C:507:CLA:HMC2	22:C:508:CLA:H102	1.96	0.46
4:D:178:ILE:O	4:D:181:PHE:HB3	2.15	0.46
2:b:276:ASP:O	31:b:629:DMS:H22	2.16	0.46
3:c:397:THR:HA	31:v:201:DMS:H13	1.97	0.46
3:C:368:PRO:HD3	31:C:530:DMS:H21	1.96	0.46
22:C:505:CLA:H201	27:D:411:LHG:C34	2.46	0.46
22:C:511:CLA:H192	22:C:511:CLA:HBC3	1.98	0.46
4:D:170:ALA:HB1	4:D:171:PRO:CD	2.45	0.46
2:b:357:ARG:HE	31:d:415:DMS:C2	2.18	0.46
2:b:450:TRP:CZ3	4:d:293[B]:LEU:HD21	2.51	0.46
22:C:509:CLA:C2B	22:C:511:CLA:HBA1	2.45	0.46
22:C:513:CLA:C11	22:C:514:CLA:H141	2.46	0.46
15:V:79:PRO:HD3	15:V:94:SER:HB3	1.97	0.46
28:a:414:SQD:H361	24:y:101:BCR:H392	1.98	0.46
2:b:216:HIS:HE1	22:b:610:CLA:C1A	2.29	0.46
2:B:25:MET:HE1	2:B:108:PHE:HD2	1.77	0.46
2:B:58:GLN:C	2:B:329:PRO:HB3	2.40	0.46
22:C:503:CLA:H61	22:C:513:CLA:H42	1.98	0.46
22:C:513:CLA:H92	22:C:514:CLA:H203	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:11:PHE:O	17:X:15[A]:LEU:HG	2.16	0.46
22:C:505:CLA:H191	27:D:411:LHG:C34	2.46	0.46
4:D:55:VAL:O	4:D:66:SER:HB3	2.15	0.46
4:D:162:LEU:HD21	35:H:102:DGD:HA21	1.97	0.46
31:a:425:DMS:C1	12:o:152:ARG:NH2	2.79	0.46
3:c:406:SER:HA	3:c:420:VAL:HG23	1.98	0.46
31:c:940:DMS:H13	40:c:1150:HOH:O	2.15	0.46
37:h:101:RRX:H47	37:h:101:RRX:H48	1.77	0.46
2:B:350:GLU:HG3	31:B:631:DMS:S	2.56	0.46
1:a:269:ARG:HD2	4:d:235:PHE:HB2	1.98	0.46
2:b:406:LEU:O	2:b:409:GLN:HG3	2.16	0.45
34:b:623:HTG:O4	31:b:633:DMS:H21	2.16	0.45
4:D:39:PRO:O	4:D:43:LEU:HG	2.17	0.45
18:Z:1:MET:HE3	18:Z:60:PHE:CD1	2.50	0.45
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.97	0.45
2:b:186:GLY:HA3	40:b:839:HOH:O	2.14	0.45
22:b:602:CLA:H151	22:b:602:CLA:H203	1.98	0.45
12:o:184:ARG:HD2	31:o:308:DMS:H22	1.99	0.45
10:K:21:LEU:HD13	16:Y:24:MET:HE2	1.99	0.45
28:a:414:SQD:H271	27:d:408:LHG:H151	1.98	0.45
3:c:95:LEU:HD21	22:c:902:CLA:OBD	2.15	0.45
3:c:154:LYS:HG2	3:c:266:TRP:CE3	2.52	0.45
3:c:257:PHE:CZ	31:c:934:DMS:H11	2.52	0.45
2:B:162:PHE:O	22:B:607:CLA:HHD	2.17	0.45
22:B:607:CLA:H102	22:B:607:CLA:H61	1.61	0.45
12:O:145:GLU:HB3	31:O:303:DMS:H21	1.99	0.45
26:a:415:PL9:H371	26:a:415:PL9:H351	1.60	0.45
22:b:602:CLA:H161	37:h:101:RRX:C16	2.47	0.45
3:c:203:THR:O	3:c:235:GLY:HA3	2.15	0.45
12:o:93:LEU:O	12:o:128:SER:HA	2.16	0.45
15:v:129[B]:LYS:HE3	15:v:136:TYR:O	2.16	0.45
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.51	0.45
3:C:443:TRP:CZ2	22:C:509:CLA:HMD1	2.52	0.45
22:C:514:CLA:NB	24:C:515:BCR:H383	2.31	0.45
15:V:30:LYS:HG3	15:V:118:HIS:CE1	2.52	0.45
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.46	0.45
12:O:92:SER:HB3	12:O:131:PRO:HA	1.99	0.45
9:j:26:GLY:HA2	30:j:103:UNL:C10	2.47	0.45
12:O:218:GLU:HG3	31:O:306:DMS:H13	1.98	0.45
23:a:410:PHO:ND	23:a:410:PHO:NC	2.64	0.45
4:d:332:GLN:HA	31:d:411:DMS:H23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.97	0.45
12:o:110:MET:HE2	31:o:303:DMS:H23	1.99	0.45
3:C:294:ASN:HA	3:C:297:TYR:O	2.17	0.45
4:D:79:SER:HA	4:D:172:SER:HB3	1.97	0.45
26:D:406:PL9:H322	27:L:101:LHG:H223	1.98	0.45
5:E:20:TRP:HD1	9:J:8:ILE:HD13	1.82	0.45
22:b:612:CLA:HBB1	22:b:612:CLA:HMB3	1.98	0.45
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.97	0.45
26:d:405:PL9:H411	11:l:29:LEU:CD2	2.47	0.45
10:k:20:PRO:HB3	16:y:21:GLN:HG3	1.99	0.45
2:B:360:PRO:CA	31:B:628:DMS:H11	2.43	0.45
22:B:606:CLA:HBB1	22:B:607:CLA:H51	1.99	0.45
4:D:52:THR:HB	4:D:76:VAL:HG21	1.97	0.45
12:O:86:LYS:HE3	40:O:549:HOH:O	2.15	0.45
2:b:346:PHE:HD2	31:b:638:DMS:H23	1.81	0.45
22:b:609:CLA:C14	7:h:39:LEU:HD21	2.46	0.45
3:c:443:TRP:CZ2	22:c:909:CLA:HMD1	2.52	0.45
24:c:915:BCR:C8	24:c:915:BCR:H331	2.44	0.45
14:u:53:ALA:HB1	14:u:54:PRO:HA	1.98	0.45
17:x:34:ILE:C	17:x:36:LYS:N	2.74	0.45
4:D:266:TRP:CG	27:D:410:LHG:HC2	2.51	0.45
24:c:916:BCR:H15C	24:c:916:BCR:H351	1.75	0.45
22:B:611:CLA:HHC	22:B:611:CLA:CBB	2.46	0.44
3:C:318:LEU:C	3:C:318:LEU:HD23	2.42	0.44
22:C:507:CLA:CMB	22:C:507:CLA:HBB1	2.47	0.44
15:V:41:HIS:HA	15:V:45:ILE:O	2.17	0.44
17:X:23:LEU:C	17:X:23:LEU:HD12	2.41	0.44
3:c:189:TRP:CE3	31:c:929:DMS:H21	2.52	0.44
12:o:180:GLU:CD	12:o:180:GLU:H	2.25	0.44
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.99	0.44
15:V:2:GLU:OE2	31:V:207:DMS:H12	2.16	0.44
3:c:154:LYS:NZ	40:c:1012:HOH:O	2.44	0.44
27:d:408:LHG:H342	27:d:408:LHG:H312	1.72	0.44
22:B:612:CLA:H112	22:B:612:CLA:H72	1.68	0.44
22:a:408:CLA:HBA1	22:a:408:CLA:C4A	2.47	0.44
23:a:411:PHO:CMB	23:a:411:PHO:HBB1	2.46	0.44
3:c:362:ARG:CD	31:c:924:DMS:H22	2.22	0.44
27:d:408:LHG:H111	27:d:408:LHG:H142	1.65	0.44
2:B:118:TRP:CZ2	11:L:4:ASN:HA	2.52	0.44
15:V:118:HIS:CE1	15:V:122:GLU:HG2	2.53	0.44
4:d:52:THR:O	4:d:66:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:620:BCR:H331	24:B:620:BCR:C8	2.48	0.44
3:C:68:THR:OG1	22:C:504:CLA:HED1	2.17	0.44
3:C:266:TRP:CZ3	22:C:508:CLA:HAC2	2.52	0.44
25:C:520:LMG:H241	9:J:22:ILE:HG12	1.99	0.44
25:C:531:LMG:HC1	25:C:531:LMG:HC8	1.77	0.44
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.99	0.44
5:E:39:SER:HB3	29:E:101:LMT:H6E	1.99	0.44
12:o:110:MET:HE3	12:o:110:MET:HB3	1.88	0.44
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.84	0.44
3:C:464:GLU:OE2	4:D:245:SER:OG	2.30	0.44
31:C:527:DMS:H11	15:V:102:PRO:HG2	2.00	0.44
4:D:24:ARG:NH2	17:X:35:ASP:OD2	2.51	0.44
5:E:60:GLN:NE2	5:E:62:SER:O	2.49	0.44
12:O:97:GLU:OE2	12:O:102:ASP:OD2	2.36	0.44
15:V:41:HIS:O	15:V:42:VAL:C	2.61	0.44
22:c:902:CLA:HBB2	22:c:908:CLA:H92	2.00	0.44
4:D:24:ARG:HH22	17:X:35:ASP:CG	2.26	0.44
12:O:133:VAL:CG2	31:O:304:DMS:H21	2.42	0.44
2:b:237:VAL:HG11	22:b:611:CLA:H201	1.98	0.44
22:b:602:CLA:H91	37:h:101:RRX:H25	1.99	0.44
22:A:408:CLA:H203	22:C:507:CLA:H101	2.00	0.44
2:B:226:TYR:HA	2:B:231:MET:HG3	1.99	0.44
2:B:339:ALA:HB2	12:o:58:ASN:HB3	2.00	0.44
2:B:423:LYS:HZ2	31:O:311:DMS:H22	1.83	0.44
22:B:606:CLA:H141	22:B:611:CLA:HED2	1.98	0.44
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.48	0.44
2:b:86:ILE:C	2:b:86:ILE:HD12	2.43	0.44
22:b:612:CLA:H72	22:b:612:CLA:H112	1.68	0.44
31:u:202:DMS:H23	31:u:203:DMS:H22	1.98	0.44
2:B:315:ILE:HG22	2:B:426:PHE:HB3	2.00	0.44
2:B:350:GLU:CG	31:B:631:DMS:H11	2.48	0.44
22:B:603:CLA:H41	7:H:46:LEU:HA	1.98	0.44
22:B:606:CLA:H122	22:B:611:CLA:HMA2	2.00	0.44
3:C:348:GLU:OE2	12:O:11:VAL:HA	2.17	0.44
28:C:501:SQD:H111	27:C:522:LHG:H261	2.00	0.44
37:H:101:RRX:H43	37:H:101:RRX:H47	1.77	0.44
15:V:2:GLU:OE2	31:V:207:DMS:C1	2.66	0.44
34:b:632:HTG:H1	40:v:315:HOH:O	2.18	0.44
22:c:904:CLA:H101	22:c:904:CLA:H62	1.80	0.44
7:h:43:LEU:O	7:h:47:GLU:HG3	2.18	0.44
1:A:308:ASP:OD1	1:A:308:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:433:ASP:OD1	2:b:433:ASP:C	2.60	0.43
35:c:917:DGD:HAH2	35:c:917:DGD:HAT2	1.87	0.43
7:h:3[A]:ARG:HH11	7:h:3[A]:ARG:CB	2.31	0.43
8:i:36:ASP:HB3	31:i:106:DMS:H13	2.00	0.43
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.99	0.43
22:A:406:CLA:HMB2	23:D:402:PHO:H152	2.01	0.43
22:B:606:CLA:CMA	22:B:607:CLA:HMA2	2.48	0.43
28:C:501:SQD:H132	28:C:501:SQD:H162	1.40	0.43
4:D:90[A]:LEU:HA	4:D:90[A]:LEU:HD23	1.41	0.43
40:D:630:HOH:O	30:X:101:UNL:C1	2.66	0.43
22:a:408:CLA:H203	22:a:408:CLA:H162	1.80	0.43
23:a:411:PHO:HBB1	23:a:411:PHO:HMB1	1.99	0.43
22:b:614:CLA:HBB1	22:b:614:CLA:CMB	2.49	0.43
3:c:63:TRP:HB2	22:c:911:CLA:HAC2	2.00	0.43
22:c:905:CLA:H62	22:c:905:CLA:H41	1.72	0.43
1:A:202:VAL:HG11	22:A:406:CLA:C3D	2.47	0.43
22:B:614:CLA:H121	25:B:621:LMG:H232	1.99	0.43
3:C:437:PHE:CE1	22:C:511:CLA:HMB2	2.53	0.43
5:E:17:VAL:HG23	9:J:7:ARG:CB	2.49	0.43
24:b:618:BCR:H353	34:l:106:HTG:H7'1	2.00	0.43
22:B:608:CLA:H112	22:B:608:CLA:H91	1.76	0.43
22:C:503:CLA:H193	34:C:521:HTG:H2'1	2.00	0.43
9:J:18:GLY:O	9:J:22:ILE:CD1	2.67	0.43
12:O:140:THR:HG23	31:O:304:DMS:H23	2.00	0.43
26:a:415:PL9:H303	4:d:45:LEU:HD22	2.00	0.43
2:B:224:ARG:HG3	7:H:25:TRP:CD2	2.53	0.43
2:B:423:LYS:NZ	31:O:311:DMS:H22	2.33	0.43
23:D:402:PHO:HBC2	23:D:402:PHO:HHD	2.01	0.43
2:b:27:THR:HG22	2:b:107:LEU:HD13	1.99	0.43
15:v:41:HIS:CD2	39:v:202:HEC:NB	2.85	0.43
1:A:210:LEU:C	1:A:210:LEU:HD23	2.44	0.43
32:A:421[B]:BCT:O3	4:D:214:HIS:CE1	2.71	0.43
10:K:26:PRO:O	10:K:29:PRO:HD2	2.18	0.43
23:a:411:PHO:H42	23:a:411:PHO:H11	1.84	0.43
24:c:915:BCR:H351	24:c:915:BCR:H15C	1.77	0.43
1:A:84:PRO:HA	1:A:112:TYR:CG	2.54	0.43
2:B:153:PHE:O	2:B:157:HIS:HB3	2.19	0.43
3:C:208:VAL:HG13	31:C:536:DMS:H21	2.00	0.43
1:a:102:LEU:HD23	1:a:102:LEU:HA	1.82	0.43
22:a:409:CLA:HBB1	23:a:411:PHO:H122	2.00	0.43
24:a:413:BCR:H24C	24:a:413:BCR:H371	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:62:PHE:CD1	3:c:62:PHE:C	2.96	0.43
3:c:121:SER:HB2	25:c:930:LMG:H241	1.99	0.43
12:o:204:VAL:HG13	12:o:211:ILE:HG22	2.00	0.43
4:D:170:ALA:HB1	4:D:171:PRO:HD2	2.01	0.43
1:a:161:TYR:CZ	1:a:165:GLN:HG3	2.54	0.43
22:b:611:CLA:CBB	22:b:611:CLA:HHC	2.49	0.43
31:b:638:DMS:H12	40:b:710:HOH:O	2.18	0.43
5:E:13:ILE:HG21	36:E:102:HEM:HAD2	2.00	0.43
31:O:303:DMS:H23	40:O:550:HOH:O	2.17	0.43
18:Z:15:LEU:O	18:Z:18:VAL:HG22	2.19	0.43
3:c:180:MET:HE2	3:c:180:MET:HB3	1.91	0.43
3:C:163:PHE:CD2	22:C:513:CLA:HAB	2.54	0.43
22:b:615:CLA:OBD	11:l:10:VAL:HG22	2.18	0.43
5:e:6:GLY:HA2	40:e:216:HOH:O	2.18	0.43
31:u:203:DMS:H22	31:u:205:DMS:H22	2.00	0.43
27:a:423:LHG:HC61	2:b:468:TRP:CH2	2.54	0.42
2:b:115:TRP:CD2	24:b:618:BCR:HC21	2.54	0.42
2:b:226:TYR:CD2	2:b:231:MET:HB2	2.54	0.42
22:b:602:CLA:H2	22:b:602:CLA:H72	2.01	0.42
5:e:53:ASP:OD2	5:e:53:ASP:C	2.61	0.42
25:A:410:LMG:H291	3:C:216:SER:HA	2.01	0.42
3:C:312:ALA:HB1	3:C:392:ALA:O	2.19	0.42
27:D:409:LHG:H361	27:D:409:LHG:HC82	2.00	0.42
7:H:39:LEU:C	7:H:39:LEU:HD23	2.45	0.42
1:a:239:PHE:O	13:t:29:ILE:HA	2.18	0.42
2:b:284:ILE:CG2	2:b:302:TRP:CZ3	3.02	0.42
3:c:424:SER:O	3:c:428:THR:HG23	2.19	0.42
3:C:124:VAL:HB	24:C:515:BCR:H362	2.00	0.42
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.55	0.42
1:a:72:LEU:HD11	29:a:419:LMT:H52	2.00	0.42
2:b:108:PHE:HE2	24:b:618:BCR:H333	1.84	0.42
22:c:914:CLA:H152	22:c:914:CLA:H111	1.57	0.42
4:D:291:LEU:HD21	35:H:102:DGD:CGB	2.50	0.42
23:a:411:PHO:ND	23:a:411:PHO:NC	2.67	0.42
3:c:138:GLU:HG3	31:c:935:DMS:C1	2.46	0.42
3:c:210:PHE:HA	3:c:213:LEU:HD12	2.02	0.42
26:d:405:PL9:H362	26:d:405:PL9:H402	2.01	0.42
5:e:63:ILE:HG23	5:e:64:PRO:HD2	2.02	0.42
15:v:31:ARG:HG2	15:v:31:ARG:HH11	1.85	0.42
31:C:540:DMS:H12	40:C:638:HOH:O	2.19	0.42
22:b:616:CLA:H152	22:b:616:CLA:H112	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:74:GLN:CD	5:e:74:GLN:H	2.27	0.42
10:k:11:LEU:HD11	10:k:22:VAL:HG21	2.02	0.42
16:y:34:MET:HE2	16:y:34:MET:CA	2.50	0.42
22:B:611:CLA:H152	22:B:611:CLA:OBD	2.18	0.42
27:D:409:LHG:H121	27:D:409:LHG:H332	2.00	0.42
7:H:25:TRP:HB2	31:H:103:DMS:H23	2.01	0.42
1:a:66:PRO:HD2	31:a:425:DMS:H13	2.02	0.42
23:a:411:PHO:HMA2	26:a:415:PL9:H221	2.00	0.42
28:a:414:SQD:H191	28:a:414:SQD:H222	1.69	0.42
2:b:144:PHE:CE2	2:b:210:ILE:HG23	2.54	0.42
3:c:117:VAL:HG12	25:c:930:LMG:H221	2.00	0.42
25:i:101:LMG:H151	25:i:101:LMG:H182	1.80	0.42
1:A:218:LEU:HD12	26:A:411:PL9:C3	2.49	0.42
10:K:19:ASP:HB3	10:K:20:PRO:CD	2.45	0.42
14:U:36:ILE:HG13	14:U:42:TYR:CG	2.55	0.42
2:b:94:GLU:HG2	34:b:623:HTG:H2'1	2.01	0.42
3:c:318:LEU:C	3:c:318:LEU:HD23	2.45	0.42
15:v:26:TYR:CE2	15:v:118:HIS:HD2	2.38	0.42
1:A:73:TYR:HD1	29:A:414:LMT:H3B	1.83	0.42
2:B:98:LEU:HB2	34:B:623:HTG:H7'3	2.02	0.42
2:B:201:HIS:CD2	2:B:201:HIS:C	2.94	0.42
31:B:629:DMS:H12	34:D:415:HTG:H7'2	2.02	0.42
22:D:401:CLA:H162	22:D:401:CLA:H203	1.75	0.42
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.20	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.56	0.42
1:a:121[A]:LEU:HD11	22:c:906:CLA:H203	2.01	0.42
1:a:202:VAL:HG11	22:a:409:CLA:C3D	2.50	0.42
2:b:113:TRP:CD1	22:b:617:CLA:HBA2	2.55	0.42
26:d:405:PL9:H411	11:l:29:LEU:HD23	2.01	0.42
12:o:23:ASP:O	12:o:203:LYS:HE3	2.20	0.42
22:A:408:CLA:C20	22:C:507:CLA:H101	2.49	0.42
2:B:387:GLU:HG2	34:D:415:HTG:H5'1	2.02	0.42
3:C:409:GLY:HA2	31:V:201:DMS:S	2.59	0.42
7:H:42:LEU:HD23	7:H:42:LEU:HA	1.93	0.42
12:O:22:LEU:O	12:O:203:LYS:NZ	2.45	0.42
1:a:45:THR:HG23	22:a:408:CLA:H201	2.02	0.42
22:b:606:CLA:H143	22:b:611:CLA:HED2	2.01	0.42
3:c:275:SER:HB3	22:c:910:CLA:HED3	2.02	0.42
35:c:918:DGD:HBF2	35:c:918:DGD:HBE2	1.85	0.42
3:c:121:SER:CB	25:c:930:LMG:H241	2.50	0.42
25:c:920:LMG:H142	10:k:24:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:e:101:HEM:CAC	6:f:27:ALA:HB1	2.50	0.42
6:f:19:ARG:O	6:f:23:VAL:HG23	2.20	0.42
1:A:323:ARG:HB3	4:D:329:MET:HA	2.02	0.41
4:D:52:THR:O	4:D:66:SER:HA	2.20	0.41
3:c:26:ARG:NH2	16:y:46:LEU:OXT	2.41	0.41
3:c:85:GLY:O	22:c:905:CLA:HED2	2.20	0.41
22:A:406:CLA:HAB	22:A:406:CLA:HHC	1.80	0.41
3:C:25:ASN:HA	3:C:30:SER:CB	2.50	0.41
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.41
12:O:33:ASP:C	12:O:35:SER:H	2.28	0.41
34:b:632:HTG:H3	40:v:315:HOH:O	2.20	0.41
3:c:60:ILE:HG22	22:c:904:CLA:HHD	2.02	0.41
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.56	0.41
3:c:189:TRP:HE3	31:c:929:DMS:H21	1.86	0.41
28:l:101:SQD:O6	13:t:23:PHE:HD1	2.03	0.41
1:a:255:PHE:CZ	26:a:415:PL9:H101	2.55	0.41
8:i:27:ASP:N	8:i:28:PRO:CD	2.84	0.41
24:y:101:BCR:HC8	24:y:101:BCR:H311	2.01	0.41
2:B:451:PHE:CD1	2:B:451:PHE:C	2.99	0.41
13:T:19:PHE:CZ	24:b:618:BCR:H332	2.56	0.41
13:T:28:ARG:HD3	13:T:28:ARG:HA	1.87	0.41
1:a:21:VAL:HG11	1:a:32:TRP:CE3	2.54	0.41
1:a:259:ILE:HG22	1:a:260:PHE:N	2.36	0.41
28:a:414:SQD:H322	22:c:909:CLA:H18	2.03	0.41
22:b:615:CLA:HBD	34:l:106:HTG:H1	2.02	0.41
34:b:626:HTG:O2	34:b:627:HTG:S1	2.78	0.41
3:c:42:LEU:HD21	22:c:912:CLA:H2A	2.01	0.41
3:c:455:PHE:HA	40:c:1070:HOH:O	2.19	0.41
22:A:405:CLA:H193	22:A:405:CLA:H161	1.70	0.41
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.55	0.41
37:H:101:RRX:H32	37:H:101:RRX:H28	1.89	0.41
2:b:75:TRP:CH2	34:b:626:HTG:H2'1	2.55	0.41
3:c:95:LEU:HD11	22:c:904:CLA:HAA1	2.01	0.41
22:c:902:CLA:H101	24:c:916:BCR:H17C	2.01	0.41
2:B:6:TYR:OH	27:D:409:LHG:HC11	2.21	0.41
2:B:124:ARG:HD2	2:B:129:GLY:O	2.20	0.41
3:C:168:LEU:HD21	22:C:510:CLA:H62	2.02	0.41
3:C:433:LEU:HD13	22:C:503:CLA:CHC	2.50	0.41
15:V:118:HIS:CE1	15:V:122:GLU:CG	3.04	0.41
1:a:93:PHE:HZ	22:a:412:CLA:HAA1	1.84	0.41
22:a:412:CLA:H11	8:i:9:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:255:THR:HG22	31:c:934:DMS:O	2.21	0.41
7:h:12:ARG:O	7:h:13:PRO:C	2.63	0.41
22:B:608:CLA:H2	25:B:621:LMG:H161	2.01	0.41
22:C:507:CLA:HBB1	22:C:507:CLA:HMB3	2.02	0.41
14:U:43:PRO:HD2	15:V:83:ASP:CG	2.46	0.41
2:b:156:PHE:HB3	2:b:162:PHE:HB3	2.03	0.41
24:c:916:BCR:H11C	24:c:916:BCR:H341	1.92	0.41
2:B:446:SER:CB	2:B:447:PRO:CD	2.91	0.41
4:D:54:PHE:O	5:E:49:THR:OG1	2.36	0.41
4:D:236:ASN:O	4:D:239:GLN:HG2	2.19	0.41
23:D:402:PHO:NC	23:D:402:PHO:ND	2.68	0.41
24:D:405:BCR:C8	24:D:405:BCR:H331	2.50	0.41
12:O:137:THR:C	12:O:139:SER:H	2.29	0.41
2:b:270:PRO:HG2	2:b:317:ASN:O	2.21	0.41
7:h:31:MET:O	7:h:35:MET:HG3	2.20	0.41
10:k:31:LEU:HD23	10:k:31:LEU:HA	1.86	0.41
15:v:41:HIS:HA	15:v:45:ILE:O	2.21	0.41
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.50	0.41
7:H:25:TRP:O	7:H:26:GLY:C	2.63	0.41
14:U:45:LEU:O	14:U:49:ILE:HG13	2.20	0.41
1:a:21:VAL:HG11	1:a:32:TRP:CZ3	2.56	0.41
1:a:182:PHE:O	1:a:186:PHE:HB2	2.21	0.41
22:b:615:CLA:HBA2	34:l:106:HTG:H2'1	2.02	0.41
22:b:617:CLA:H91	22:b:617:CLA:H112	1.82	0.41
3:C:286:ALA:HB2	22:C:503:CLA:HMD2	2.02	0.41
7:H:63:LYS:O	7:H:64:ALA:C	2.64	0.41
31:O:312:DMS:C2	40:O:467:HOH:O	2.59	0.41
26:a:415:PL9:HC2	26:a:415:PL9:H103	2.03	0.41
2:b:346:PHE:CD2	31:b:638:DMS:H23	2.55	0.41
22:c:902:CLA:C3D	22:c:904:CLA:H2	2.50	0.41
10:k:21:LEU:O	10:k:25:LEU:HG	2.21	0.41
1:A:42:LEU:HD23	28:A:413:SQD:H192	2.02	0.40
2:B:121:GLU:CA	7:H:2:ALA:HB1	2.50	0.40
2:B:224:ARG:HG2	7:H:24:GLY:O	2.22	0.40
2:B:273:TYR:HA	2:B:276:ASP:HB2	2.03	0.40
3:C:179:ALA:O	3:C:184:GLY:HA2	2.21	0.40
12:O:58:ASN:HB3	2:b:339:ALA:CB	2.51	0.40
3:c:109:PHE:N	3:c:110:PRO:CD	2.84	0.40
3:c:286:ALA:HB2	22:c:903:CLA:HMD2	2.04	0.40
22:c:910:CLA:HAB	22:c:910:CLA:HHC	1.86	0.40
1:A:72:LEU:HD21	29:T:102:LMT:H41	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:TRP:CZ3	24:B:618:BCR:H322	2.57	0.40
2:B:435:GLU:O	2:B:436:THR:C	2.64	0.40
22:B:613:CLA:HHC	22:B:613:CLA:HAB	1.91	0.40
12:O:130:GLN:NE2	12:O:141:ASP:H	2.20	0.40
1:a:259:ILE:HG13	26:a:415:PL9:H253	2.03	0.40
31:a:425:DMS:H11	12:o:152:ARG:NH2	2.33	0.40
4:d:103:ARG:O	4:d:107:LEU:HG	2.21	0.40
2:B:194:ASN:HA	2:B:195:PRO:HD2	1.90	0.40
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.09	0.40
13:T:20:ALA:O	13:T:24:ARG:HB3	2.21	0.40
15:V:129[A]:LYS:HB3	31:V:212:DMS:S	2.61	0.40
15:v:124:LYS:CE	40:v:356:HOH:O	2.63	0.40
2:B:41:GLU:OE1	2:B:63:LEU:HB2	2.21	0.40
37:H:101:RRX:H3	17:X:2:THR:N	2.20	0.40
12:O:103:PHE:HA	12:O:120:PHE:O	2.21	0.40
1:a:276:ALA:O	1:a:280:VAL:HG23	2.22	0.40
12:o:130:GLN:HG2	40:o:480:HOH:O	2.21	0.40
14:u:83:THR:OG1	14:u:84:VAL:N	2.54	0.40
1:A:66:PRO:O	31:A:420:DMS:H22	2.22	0.40
1:A:296:ASN:HB3	3:C:401:LEU:HA	2.03	0.40
22:A:408:CLA:H61	22:A:408:CLA:H41	1.70	0.40
4:D:17:ILE:O	4:D:20:ASP:HB2	2.22	0.40
4:D:125:PHE:CE1	23:D:402:PHO:HBD	2.57	0.40
22:D:401:CLA:HBB1	22:D:401:CLA:CMB	2.50	0.40
1:a:254:TYR:CD1	1:a:254:TYR:C	2.98	0.40
2:b:149:LEU:HB2	22:b:605:CLA:H171	2.04	0.40
2:b:204:ALA:CB	22:b:603:CLA:HAB	2.51	0.40
3:c:107:ASP:O	3:c:110:PRO:HD2	2.22	0.40
3:c:221:GLU:O	3:c:226:SER:HB3	2.22	0.40
22:c:913:CLA:H91	22:c:914:CLA:H141	2.03	0.40
6:f:15:ILE:O	6:f:15:ILE:CG2	2.68	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	333/334 (100%)	326 (98%)	6 (2%)	1 (0%)	36	42
1	a	333/334 (100%)	321 (96%)	11 (3%)	1 (0%)	36	42
2	B	506/505 (100%)	495 (98%)	11 (2%)	0	100	100
2	b	482/505 (95%)	465 (96%)	17 (4%)	0	100	100
3	C	449/455 (99%)	434 (97%)	13 (3%)	2 (0%)	30	34
3	c	454/455 (100%)	435 (96%)	18 (4%)	1 (0%)	43	51
4	D	343/342 (100%)	336 (98%)	6 (2%)	1 (0%)	36	42
4	d	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
5	E	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	9	8
5	e	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
6	F	31/33 (94%)	31 (100%)	0	0	100	100
6	f	29/33 (88%)	29 (100%)	0	0	100	100
7	H	64/63 (102%)	60 (94%)	4 (6%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	30 (88%)	4 (12%)	0	100	100
9	J	34/40 (85%)	33 (97%)	0	1 (3%)	3	2
9	j	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	0	100	100
11	l	33/35 (94%)	33 (100%)	0	0	100	100
12	O	242/243 (100%)	228 (94%)	12 (5%)	2 (1%)	16	16
12	o	241/243 (99%)	231 (96%)	10 (4%)	0	100	100
13	T	28/30 (93%)	28 (100%)	0	0	100	100
13	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	U	96/97 (99%)	92 (96%)	4 (4%)	0	100	100
14	u	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
15	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
15	v	136/137 (99%)	126 (93%)	9 (7%)	1 (1%)	18	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	Y	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
16	y	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
17	X	36/37 (97%)	35 (97%)	1 (3%)	0	100 100
17	x	34/37 (92%)	31 (91%)	1 (3%)	2 (6%)	1 0
18	Z	60/62 (97%)	56 (93%)	1 (2%)	3 (5%)	1 0
18	z	59/62 (95%)	55 (93%)	4 (7%)	0	100 100
All	All	5100/5190 (98%)	4921 (96%)	163 (3%)	16 (0%)	36 42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
3	C	24	THR
3	C	416	SER
5	E	6	GLY
18	Z	31	GLN
18	Z	32	ASP
3	c	416	SER
15	v	19	ILE
17	x	35	ASP
9	J	6	GLY
12	O	34	SER
18	Z	30	PRO
1	a	225	ARG
12	O	26	ALA
1	A	259	ILE
17	x	34	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	263/270 (97%)	259 (98%)	4 (2%)	57 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	252/270 (93%)	251 (100%)	1 (0%)	84 92
2	B	391/403 (97%)	385 (98%)	6 (2%)	57 73
2	b	378/403 (94%)	375 (99%)	3 (1%)	73 85
3	C	347/356 (98%)	343 (99%)	4 (1%)	63 78
3	c	356/356 (100%)	350 (98%)	6 (2%)	53 69
4	D	278/277 (100%)	278 (100%)	0	100 100
4	d	276/277 (100%)	275 (100%)	1 (0%)	84 92
5	E	68/71 (96%)	66 (97%)	2 (3%)	37 51
5	e	67/71 (94%)	65 (97%)	2 (3%)	36 49
6	F	27/27 (100%)	27 (100%)	0	100 100
6	f	25/27 (93%)	24 (96%)	1 (4%)	28 38
7	H	56/53 (106%)	56 (100%)	0	100 100
7	h	54/53 (102%)	54 (100%)	0	100 100
8	I	31/32 (97%)	30 (97%)	1 (3%)	34 47
8	i	31/32 (97%)	31 (100%)	0	100 100
9	J	23/28 (82%)	22 (96%)	1 (4%)	26 35
9	j	25/28 (89%)	25 (100%)	0	100 100
10	K	30/30 (100%)	27 (90%)	3 (10%)	7 7
10	k	28/30 (93%)	27 (96%)	1 (4%)	31 42
11	L	33/33 (100%)	33 (100%)	0	100 100
11	l	33/33 (100%)	32 (97%)	1 (3%)	36 49
12	O	203/206 (98%)	196 (97%)	7 (3%)	32 44
12	o	199/206 (97%)	194 (98%)	5 (2%)	42 56
13	T	24/26 (92%)	23 (96%)	1 (4%)	26 36
13	t	24/26 (92%)	22 (92%)	2 (8%)	10 11
14	U	85/84 (101%)	84 (99%)	1 (1%)	63 78
14	u	82/84 (98%)	81 (99%)	1 (1%)	63 78
15	V	117/117 (100%)	114 (97%)	3 (3%)	40 55
15	v	115/117 (98%)	111 (96%)	4 (4%)	32 43
16	Y	22/22 (100%)	18 (82%)	4 (18%)	2 1
16	y	19/22 (86%)	19 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	X	29/30 (97%)	27 (93%)	2 (7%)	14 16
17	x	27/30 (90%)	26 (96%)	1 (4%)	30 41
18	Z	45/52 (86%)	45 (100%)	0	100 100
18	z	40/52 (77%)	38 (95%)	2 (5%)	22 28
All	All	4103/4234 (97%)	4033 (98%)	70 (2%)	53 69

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	LEU
1	A	224	ILE
1	A	238	LYS
1	A	248	ILE
2	B	128	THR
2	B	246	PHE
2	B	362	PHE
2	B	373	LYS
2	B	472	ARG
2	B	503	THR
3	C	255	THR
3	C	289	PHE
3	C	315	MET
3	C	471	SER
5	E	65	LEU
5	E	82	GLN
8	I	33	LYS
9	J	22	ILE
10	K	10	LYS
10	K	17	ILE
10	K	27	VAL
12	O	53	LYS
12	O	84	GLU
12	O	118	LEU
12	O	130	GLN
12	O	180	GLU
12	O	181	GLU
12	O	242	SER
13	T	25	GLU
14	U	86	GLU
15	V	30	LYS
15	V	129[A]	LYS

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Mol	Chain	Res	Type
15	V	129[B]	LYS
16	Y	19	ILE
16	Y	25	ILE
16	Y	30	ILE
16	Y	43	ARG
17	X	23	LEU
17	X	33	GLN
1	a	214	MET
2	b	161	LEU
2	b	362	PHE
2	b	467	ILE
3	c	78	GLU
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	334	PRO
3	c	381	LYS
4	d	329	MET
5	e	7	GLU
5	e	25	ILE
6	f	15	ILE
10	k	27	VAL
11	l	10	VAL
12	o	10	ILE
12	o	89	SER
12	o	93	LEU
12	o	180	GLU
12	o	242	SER
13	t	25	GLU
13	t	28	ARG
14	u	39	ARG
15	v	6	GLU
15	v	19	ILE
15	v	28	GLU
15	v	30	LYS
17	x	21	LEU
18	z	4	LEU
18	z	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
1	A	304	HIS
2	B	53	ASN
2	B	223	GLN
2	B	331	ASN
2	B	394	GLN
3	C	44	ASN
3	C	418	ASN
4	D	186	GLN
4	D	255	GLN
4	D	332	GLN
6	F	44	GLN
12	O	58	ASN
12	O	88	ASN
12	O	104	GLN
12	O	155	ASN
14	U	37	GLN
14	U	71	GLN
14	U	78	ASN
14	U	81	HIS
15	V	34	GLN
18	Z	58	ASN
1	a	165	GLN
1	a	266	ASN
1	a	296	ASN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	281	GLN
2	b	331	ASN
3	c	201	ASN
4	d	186	GLN
4	d	332	GLN
10	k	40	GLN
11	l	6	ASN
12	o	82	GLN
12	o	104	GLN
12	o	124	ASN
12	o	147	ASN
12	o	231	HIS
14	u	37	GLN
14	u	73	GLN

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Mol	Chain	Res	Type
15	v	34	GLN
15	v	118	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	0.99	0	7,9,11	1.42	1 (14%)
13	FME	T	1	13	8,9,10	0.63	0	7,9,11	1.38	2 (28%)
13	FME	t	1	13	8,9,10	0.61	0	7,9,11	1.72	1 (14%)
8	FME	i	1	8	8,9,10	0.53	0	7,9,11	1.35	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	1/7/9/11	-
13	FME	T	1	13	-	2/7/9/11	-
13	FME	t	1	13	-	2/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	t	1	FME	CE-SD-CG	3.92	113.85	100.40
8	i	1	FME	O-C-CA	-2.32	118.69	124.78
8	I	1	FME	CE-SD-CG	2.26	108.15	100.40
13	T	1	FME	CE-SD-CG	2.24	108.08	100.40
13	T	1	FME	C-CA-N	2.05	113.42	109.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
13	T	1	FME	O1-CN-N-CA
13	T	1	FME	CA-CB-CG-SD
13	t	1	FME	O1-CN-N-CA
13	t	1	FME	CA-CB-CG-SD
8	i	1	FME	O1-CN-N-CA
8	i	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 352 ligands modelled in this entry, 15 are monoatomic and 27 are unknown - leaving 310 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	$\#\|Z\| > 2$
31	DMS	V	201	-	3,3,3	2.64	1 (33%)	3,3,3	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	DMS	v	201	-	3,3,3	2.59	1 (33%)	3,3,3	0.85	0
31	DMS	O	311	-	3,3,3	2.97	1 (33%)	3,3,3	0.91	0
36	HEM	E	102	6,5	50,50,50	2.00	8 (16%)	66,82,82	1.65	12 (18%)
31	DMS	t	103	-	3,3,3	2.70	1 (33%)	3,3,3	0.64	0
31	DMS	C	526	-	3,3,3	2.59	1 (33%)	3,3,3	0.56	0
34	HTG	V	203	-	14,14,19	0.69	0	18,19,24	3.11	7 (38%)
29	LMT	a	419	-	36,36,36	0.78	0	47,47,47	1.36	5 (10%)
31	DMS	c	928	-	3,3,3	2.70	1 (33%)	3,3,3	0.77	0
35	DGD	C	518	-	63,63,67	0.96	3 (4%)	77,77,81	1.28	10 (12%)
31	DMS	B	630	-	3,3,3	2.81	1 (33%)	3,3,3	0.91	0
22	CLA	c	910	3	69,73,73	2.18	19 (27%)	83,113,113	2.49	32 (38%)
31	DMS	c	923	-	3,3,3	2.50	1 (33%)	3,3,3	0.40	0
31	DMS	v	204	-	3,3,3	2.66	1 (33%)	3,3,3	0.69	0
22	CLA	B	603	2	69,73,73	2.59	23 (33%)	83,113,113	2.50	36 (43%)
32	BCT	A	421[B]	20	2,3,3	0.95	0	2,3,3	0.41	0
31	DMS	c	939	-	3,3,3	2.76	1 (33%)	3,3,3	0.65	0
31	DMS	l	105	-	3,3,3	2.74	1 (33%)	3,3,3	0.72	0
24	BCR	b	620	-	41,41,41	0.85	0	56,56,56	1.34	8 (14%)
22	CLA	B	602	40	69,73,73	2.79	23 (33%)	83,113,113	2.45	28 (33%)
22	CLA	C	504	3	69,73,73	2.68	23 (33%)	83,113,113	2.44	30 (36%)
25	LMG	J	101	38	45,45,55	0.99	2 (4%)	53,53,63	1.04	6 (11%)
29	LMT	A	414	-	36,36,36	0.80	0	47,47,47	1.14	4 (8%)
31	DMS	c	944	-	3,3,3	2.72	1 (33%)	3,3,3	0.78	0
22	CLA	B	617	2	59,63,73	2.21	17 (28%)	71,101,113	2.82	31 (43%)
31	DMS	I	106	-	3,3,3	2.68	1 (33%)	3,3,3	0.75	0
22	CLA	B	611	40	69,73,73	2.91	19 (27%)	83,113,113	2.44	24 (28%)
35	DGD	D	407	-	50,50,67	1.18	3 (6%)	58,58,81	1.31	6 (10%)
31	DMS	c	935	-	3,3,3	2.66	1 (33%)	3,3,3	0.89	0
24	BCR	D	405	-	41,41,41	1.00	1 (2%)	56,56,56	1.97	15 (26%)
31	DMS	A	419	-	3,3,3	2.66	1 (33%)	3,3,3	0.82	0
31	DMS	b	633	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	0
31	DMS	c	936	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
31	DMS	O	310	-	3,3,3	2.62	1 (33%)	3,3,3	0.86	0
36	HEM	e	101	6,5	50,50,50	2.03	9 (18%)	66,82,82	1.47	10 (15%)
34	HTG	B	626	-	19,19,19	0.73	0	23,24,24	1.83	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	c	904	3	69,73,73	2.61	21 (30%)	83,113,113	2.51	32 (38%)
22	CLA	b	614	2	63,67,73	2.36	19 (30%)	75,105,113	2.56	25 (33%)
24	BCR	Y	101	-	40,40,41	0.93	2 (5%)	52,54,56	1.70	15 (28%)
31	DMS	B	635	-	3,3,3	2.78	1 (33%)	3,3,3	0.69	0
22	CLA	c	905	40	69,73,73	2.65	21 (30%)	83,113,113	2.40	27 (32%)
34	HTG	v	203	-	16,16,19	1.05	1 (6%)	20,21,24	3.06	7 (35%)
22	CLA	C	510	3	69,73,73	2.17	21 (30%)	83,113,113	2.56	30 (36%)
31	DMS	c	927	-	3,3,3	2.64	1 (33%)	3,3,3	0.42	0
28	SQD	A	413	-	48,49,54	1.08	3 (6%)	57,60,65	1.74	9 (15%)
34	HTG	b	624	-	19,19,19	1.06	1 (5%)	23,24,24	2.19	6 (26%)
28	SQD	a	414	-	53,54,54	1.09	3 (5%)	62,65,65	2.00	12 (19%)
31	DMS	C	540	-	3,3,3	2.78	1 (33%)	3,3,3	0.89	0
31	DMS	B	642	-	3,3,3	2.66	1 (33%)	3,3,3	1.04	0
31	DMS	O	303	-	3,3,3	2.74	1 (33%)	3,3,3	0.77	0
25	LMG	d	409	-	47,47,55	1.09	3 (6%)	55,55,63	1.46	8 (14%)
31	DMS	v	209	-	3,3,3	2.63	1 (33%)	3,3,3	0.63	0
31	DMS	b	636	-	3,3,3	2.67	1 (33%)	3,3,3	0.70	0
35	DGD	c	917	-	63,63,67	0.97	3 (4%)	77,77,81	1.00	3 (3%)
31	DMS	F	101	-	3,3,3	2.66	1 (33%)	3,3,3	0.60	0
35	DGD	h	102	-	63,63,67	0.97	3 (4%)	77,77,81	1.14	5 (6%)
31	DMS	D	418	-	3,3,3	2.40	1 (33%)	3,3,3	0.67	0
22	CLA	b	612	2	69,73,73	2.18	20 (28%)	83,113,113	2.41	30 (36%)
31	DMS	D	416	-	3,3,3	2.50	1 (33%)	3,3,3	0.63	0
31	DMS	c	934	-	3,3,3	2.66	1 (33%)	3,3,3	0.67	0
24	BCR	C	516	-	41,41,41	0.91	0	56,56,56	1.36	7 (12%)
34	HTG	B	623	-	19,19,19	1.16	1 (5%)	23,24,24	1.78	3 (13%)
31	DMS	d	412	-	3,3,3	2.56	1 (33%)	3,3,3	0.83	0
31	DMS	A	416	-	3,3,3	2.66	1 (33%)	3,3,3	1.06	0
24	BCR	y	101	-	41,41,41	0.89	0	56,56,56	1.59	14 (25%)
25	LMG	A	410	-	51,51,55	0.95	2 (3%)	59,59,63	1.09	5 (8%)
31	DMS	C	524	-	3,3,3	2.48	1 (33%)	3,3,3	0.86	0
31	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.83	0
22	CLA	b	617	2	64,68,73	2.90	22 (34%)	77,107,113	2.64	30 (38%)
31	DMS	O	305	-	3,3,3	2.90	1 (33%)	3,3,3	0.84	0
22	CLA	B	604	2	69,73,73	2.25	18 (26%)	83,113,113	2.46	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMT	B	622	-	24,24,36	0.63	1 (4%)	29,29,47	0.84	1 (3%)
31	DMS	U	202	-	3,3,3	2.77	1 (33%)	3,3,3	1.29	0
31	DMS	C	537	-	3,3,3	2.75	1 (33%)	3,3,3	0.70	0
23	PHO	a	411	-	58,69,69	2.60	12 (20%)	56,99,99	3.03	14 (25%)
31	DMS	c	929	-	3,3,3	2.80	1 (33%)	3,3,3	0.84	0
22	CLA	B	605	2	69,73,73	2.08	19 (27%)	83,113,113	2.50	34 (40%)
23	PHO	A	407	-	58,69,69	2.45	14 (24%)	56,99,99	2.63	16 (28%)
25	LMG	c	920	-	51,51,55	0.99	2 (3%)	59,59,63	1.09	5 (8%)
31	DMS	O	308	-	3,3,3	2.79	1 (33%)	3,3,3	0.62	0
31	DMS	V	211	-	3,3,3	2.81	1 (33%)	3,3,3	0.77	0
22	CLA	B	613	2	69,73,73	2.64	22 (31%)	83,113,113	2.25	31 (37%)
31	DMS	t	105	-	3,3,3	2.71	1 (33%)	3,3,3	0.61	0
31	DMS	O	314	-	3,3,3	2.73	1 (33%)	3,3,3	0.76	0
31	DMS	o	305	-	3,3,3	2.60	1 (33%)	3,3,3	0.66	0
27	LHG	L	101	-	39,39,48	1.05	2 (5%)	42,45,54	1.19	4 (9%)
22	CLA	C	513	3	60,64,73	2.86	22 (36%)	72,102,113	2.51	26 (36%)
25	LMG	D	412	-	46,46,55	1.14	3 (6%)	54,54,63	1.12	2 (3%)
22	CLA	C	514	3	69,73,73	2.66	21 (30%)	83,113,113	2.39	28 (33%)
24	BCR	K	101	-	41,41,41	0.86	0	56,56,56	1.19	4 (7%)
31	DMS	C	528	-	3,3,3	2.63	1 (33%)	3,3,3	0.58	0
31	DMS	o	304	-	3,3,3	2.81	1 (33%)	3,3,3	1.15	0
24	BCR	c	916	-	41,41,41	0.86	0	56,56,56	1.55	10 (17%)
31	DMS	a	421	-	3,3,3	2.66	1 (33%)	3,3,3	0.60	0
22	CLA	C	508	40	69,73,73	2.29	21 (30%)	83,113,113	2.41	25 (30%)
31	DMS	a	402	-	3,3,3	2.38	1 (33%)	3,3,3	0.73	0
22	CLA	a	412	1	69,73,73	2.29	21 (30%)	83,113,113	2.35	30 (36%)
34	HTG	b	627	-	19,19,19	1.03	2 (10%)	23,24,24	1.84	3 (13%)
31	DMS	B	639	-	3,3,3	2.76	1 (33%)	3,3,3	0.71	0
31	DMS	c	937	-	3,3,3	2.88	1 (33%)	3,3,3	0.82	0
22	CLA	b	609	2	69,73,73	2.25	21 (30%)	83,113,113	2.23	27 (32%)
31	DMS	C	525	-	3,3,3	2.45	1 (33%)	3,3,3	0.62	0
27	LHG	d	407	-	48,48,48	0.75	2 (4%)	51,54,54	1.06	3 (5%)
22	CLA	C	505	40	69,73,73	3.02	22 (31%)	83,113,113	2.23	21 (25%)
28	SQD	a	418	-	50,51,54	1.16	3 (6%)	59,62,65	1.47	8 (13%)
25	LMG	C	520	-	51,51,55	1.08	2 (3%)	59,59,63	1.23	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	DGD	H	102	-	63,63,67	1.02	3 (4%)	77,77,81	1.16	6 (7%)
25	LMG	b	622	-	43,43,55	1.35	4 (9%)	51,51,63	1.90	12 (23%)
31	DMS	V	206	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
22	CLA	c	911	3	69,73,73	2.25	20 (28%)	83,113,113	2.36	27 (32%)
31	DMS	c	933	-	3,3,3	2.84	1 (33%)	3,3,3	0.92	0
31	DMS	u	203	-	3,3,3	2.72	1 (33%)	3,3,3	0.76	0
31	DMS	b	635	-	3,3,3	2.76	1 (33%)	3,3,3	0.55	0
31	DMS	V	208	-	3,3,3	2.60	1 (33%)	3,3,3	0.40	0
34	HTG	b	632	-	19,19,19	1.08	2 (10%)	23,24,24	2.54	7 (30%)
22	CLA	c	908	40	69,73,73	2.72	20 (28%)	83,113,113	2.50	23 (27%)
31	DMS	v	206	-	3,3,3	2.68	1 (33%)	3,3,3	0.73	0
31	DMS	o	302	-	3,3,3	2.68	1 (33%)	3,3,3	0.95	0
22	CLA	B	612	2	69,73,73	2.17	17 (24%)	83,113,113	2.42	30 (36%)
26	PL9	d	405	-	55,55,55	1.03	5 (9%)	68,69,69	1.48	9 (13%)
25	LMG	c	930	-	49,49,55	1.10	3 (6%)	57,57,63	1.06	4 (7%)
22	CLA	B	615	2	57,61,73	2.63	20 (35%)	68,98,113	3.03	30 (44%)
24	BCR	A	409	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	5 (8%)
31	DMS	t	104	-	3,3,3	2.71	1 (33%)	3,3,3	0.59	0
31	DMS	U	203	-	3,3,3	2.78	1 (33%)	3,3,3	1.24	0
31	DMS	b	638	-	3,3,3	2.98	1 (33%)	3,3,3	0.69	0
24	BCR	B	619	-	30,30,41	0.92	0	39,39,56	1.32	7 (17%)
27	LHG	a	416	-	48,48,48	1.13	2 (4%)	51,54,54	1.18	4 (7%)
31	DMS	C	529	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
22	CLA	B	616	2	69,73,73	2.66	21 (30%)	83,113,113	2.34	25 (30%)
28	SQD	D	408	-	19,20,54	0.97	2 (10%)	26,29,65	1.93	7 (26%)
34	HTG	b	623	-	19,19,19	1.10	1 (5%)	23,24,24	1.32	4 (17%)
31	DMS	V	212	-	3,3,3	2.78	1 (33%)	3,3,3	1.18	0
31	DMS	v	210	-	3,3,3	2.84	1 (33%)	3,3,3	0.78	0
31	DMS	u	205	-	3,3,3	3.07	1 (33%)	3,3,3	1.19	0
31	DMS	A	418	-	3,3,3	2.41	1 (33%)	3,3,3	1.25	0
22	CLA	b	610	2	69,73,73	2.60	21 (30%)	83,113,113	2.22	28 (33%)
31	DMS	V	210	-	3,3,3	2.77	1 (33%)	3,3,3	0.89	0
22	CLA	D	404	4	69,73,73	2.43	18 (26%)	83,113,113	2.22	24 (28%)
19	OEX	A	401	3,40,1	0,14,14	-	-	-		
22	CLA	d	402	4	69,73,73	2.08	22 (31%)	83,113,113	2.54	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	405	1	69,73,73	2.40	18 (26%)	83,113,113	2.27	26 (31%)
22	CLA	C	502	3	69,73,73	2.12	20 (28%)	83,113,113	2.41	25 (30%)
29	LMT	t	101	-	24,24,36	0.45	0	29,29,47	1.34	4 (13%)
22	CLA	b	608	40	69,73,73	2.44	22 (31%)	83,113,113	2.29	26 (31%)
31	DMS	C	538	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
27	LHG	d	401	-	32,32,48	1.24	2 (6%)	36,37,54	1.18	4 (11%)
34	HTG	D	415	-	19,19,19	1.16	1 (5%)	23,24,24	2.71	7 (30%)
25	LMG	j	101	38	47,47,55	1.01	2 (4%)	55,55,63	1.18	9 (16%)
28	SQD	C	501	-	53,54,54	1.04	3 (5%)	62,65,65	1.95	14 (22%)
22	CLA	b	603	2	69,73,73	2.83	20 (28%)	83,113,113	2.46	30 (36%)
28	SQD	l	101	-	53,54,54	1.12	4 (7%)	62,65,65	1.47	8 (12%)
31	DMS	A	417	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
31	DMS	I	101	-	3,3,3	2.71	1 (33%)	3,3,3	0.69	0
31	DMS	C	539	-	3,3,3	2.69	1 (33%)	3,3,3	0.61	0
22	CLA	c	907	3	69,73,73	2.37	20 (28%)	83,113,113	2.36	28 (33%)
25	LMG	i	101	-	51,51,55	0.99	2 (3%)	59,59,63	1.18	7 (11%)
31	DMS	C	536	-	3,3,3	2.68	1 (33%)	3,3,3	0.45	0
24	BCR	b	618	-	20,20,41	0.89	1 (5%)	27,27,56	1.73	5 (18%)
31	DMS	C	535	-	3,3,3	2.73	1 (33%)	3,3,3	0.78	0
24	BCR	d	404	-	41,41,41	1.05	3 (7%)	56,56,56	1.77	13 (23%)
31	DMS	b	634	-	3,3,3	2.71	1 (33%)	3,3,3	0.59	0
31	DMS	B	641	-	3,3,3	2.75	1 (33%)	3,3,3	0.84	0
27	LHG	d	408	-	45,45,48	1.04	2 (4%)	48,51,54	0.73	0
22	CLA	D	403	4	69,73,73	2.07	19 (27%)	83,113,113	2.55	27 (32%)
31	DMS	B	629	-	3,3,3	2.54	1 (33%)	3,3,3	1.19	0
22	CLA	B	607	2	69,73,73	2.37	20 (28%)	83,113,113	2.50	33 (39%)
22	CLA	a	408	40	69,73,73	2.57	23 (33%)	83,113,113	2.64	33 (39%)
29	LMT	I	102	-	36,36,36	0.68	1 (2%)	47,47,47	1.36	4 (8%)
22	CLA	b	606	2	69,73,73	2.25	19 (27%)	83,113,113	2.46	26 (31%)
28	SQD	b	621	-	37,38,54	1.04	2 (5%)	45,48,65	1.50	8 (17%)
22	CLA	b	604	2	69,73,73	2.61	20 (28%)	83,113,113	2.43	26 (31%)
34	HTG	C	523	-	8,8,19	0.38	0	7,7,24	1.42	1 (14%)
29	LMT	c	931	-	24,24,36	0.79	1 (4%)	29,29,47	0.86	2 (6%)
22	CLA	c	902	3	69,73,73	2.45	18 (26%)	83,113,113	2.54	23 (27%)
31	DMS	b	637	-	3,3,3	2.72	1 (33%)	3,3,3	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	DMS	b	631	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
24	BCR	c	915	-	41,41,41	0.84	1 (2%)	56,56,56	1.39	8 (14%)
31	DMS	u	202	-	3,3,3	2.62	1 (33%)	3,3,3	1.05	0
31	DMS	O	309	-	3,3,3	2.54	1 (33%)	3,3,3	0.59	0
27	LHG	a	423	-	44,44,48	1.02	2 (4%)	47,50,54	1.08	4 (8%)
31	DMS	O	306	-	3,3,3	2.70	1 (33%)	3,3,3	0.75	0
25	LMG	B	621	-	40,40,55	1.26	3 (7%)	48,48,63	1.39	8 (16%)
35	DGD	c	919	-	63,63,67	0.98	4 (6%)	77,77,81	1.15	6 (7%)
31	DMS	B	634	-	3,3,3	2.80	1 (33%)	3,3,3	0.65	0
31	DMS	O	313	-	3,3,3	2.63	1 (33%)	3,3,3	0.48	0
31	DMS	i	106	-	3,3,3	2.62	1 (33%)	3,3,3	0.55	0
22	CLA	D	401	40	69,73,73	1.92	17 (24%)	83,113,113	2.65	31 (37%)
31	DMS	f	103	-	3,3,3	2.70	1 (33%)	3,3,3	0.91	0
31	DMS	o	307	-	3,3,3	2.60	1 (33%)	3,3,3	0.58	0
22	CLA	A	408	1	69,73,73	2.16	19 (27%)	83,113,113	2.43	31 (37%)
22	CLA	a	409	40	65,69,73	2.15	20 (30%)	78,108,113	2.79	33 (42%)
31	DMS	v	211	-	3,3,3	2.76	1 (33%)	3,3,3	0.76	0
35	DGD	c	918	-	63,63,67	0.94	4 (6%)	77,77,81	1.03	4 (5%)
22	CLA	b	605	2	69,73,73	2.51	22 (31%)	83,113,113	2.35	22 (26%)
34	HTG	C	532	-	19,19,19	1.15	2 (10%)	23,24,24	1.90	1 (4%)
22	CLA	c	906	3	69,73,73	2.40	21 (30%)	83,113,113	2.23	23 (27%)
22	CLA	c	912	3	69,73,73	2.89	20 (28%)	83,113,113	2.25	29 (34%)
25	LMG	C	531	-	40,40,55	1.19	3 (7%)	48,48,63	1.13	3 (6%)
31	DMS	c	926	-	3,3,3	2.60	1 (33%)	3,3,3	0.78	0
31	DMS	A	420	-	3,3,3	2.74	1 (33%)	3,3,3	1.35	0
22	CLA	b	615	2	56,60,73	2.75	22 (39%)	67,97,113	2.53	31 (46%)
31	DMS	c	925	-	3,3,3	2.65	1 (33%)	3,3,3	1.11	0
31	DMS	B	638	-	3,3,3	2.64	1 (33%)	3,3,3	0.40	0
22	CLA	C	512	3	69,73,73	2.56	22 (31%)	83,113,113	2.46	29 (34%)
34	HTG	C	521	-	19,19,19	0.94	2 (10%)	23,24,24	1.64	2 (8%)
31	DMS	c	942	-	3,3,3	2.73	1 (33%)	3,3,3	0.72	0
31	DMS	o	306	-	3,3,3	2.65	1 (33%)	3,3,3	0.60	0
31	DMS	V	204	-	3,3,3	2.73	1 (33%)	3,3,3	0.82	0
22	CLA	b	616	2	69,73,73	2.38	20 (28%)	83,113,113	2.30	28 (33%)
22	CLA	d	403	4	69,73,73	2.92	22 (31%)	83,113,113	2.24	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	DMS	b	630	-	3,3,3	2.66	1 (33%)	3,3,3	0.29	0
29	LMT	Z	101	-	36,36,36	0.67	1 (2%)	47,47,47	1.15	3 (6%)
22	CLA	a	407	1	69,73,73	2.32	20 (28%)	83,113,113	2.25	29 (34%)
31	DMS	c	943	-	3,3,3	2.69	1 (33%)	3,3,3	0.81	0
27	LHG	D	409	-	48,48,48	1.02	2 (4%)	51,54,54	1.37	5 (9%)
34	HTG	l	106	-	19,19,19	1.01	2 (10%)	23,24,24	2.09	3 (13%)
31	DMS	c	924	-	3,3,3	2.82	1 (33%)	3,3,3	1.32	1 (33%)
27	LHG	D	411	-	44,44,48	0.98	2 (4%)	47,50,54	1.03	3 (6%)
22	CLA	b	602	40	69,73,73	3.34	20 (28%)	83,113,113	2.47	23 (27%)
37	RRX	H	101	-	42,42,42	0.82	0	57,58,58	1.47	8 (14%)
31	DMS	V	209	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
31	DMS	a	401	-	3,3,3	2.74	1 (33%)	3,3,3	0.81	0
31	DMS	O	307	-	3,3,3	2.79	1 (33%)	3,3,3	0.91	0
31	DMS	d	411	-	3,3,3	2.71	1 (33%)	3,3,3	0.94	0
24	BCR	b	619	-	31,31,41	1.10	2 (6%)	40,40,56	1.34	8 (20%)
31	DMS	B	633	-	3,3,3	2.66	1 (33%)	3,3,3	0.46	0
31	DMS	C	533	-	3,3,3	2.73	1 (33%)	3,3,3	0.75	0
27	LHG	l	102	-	48,48,48	0.93	2 (4%)	51,54,54	1.08	2 (3%)
24	BCR	a	413	-	41,41,41	1.14	2 (4%)	56,56,56	1.16	8 (14%)
31	DMS	V	205	-	3,3,3	2.62	1 (33%)	3,3,3	0.64	0
34	HTG	b	626	-	19,19,19	0.84	1 (5%)	23,24,24	1.61	5 (21%)
29	LMT	c	921	-	36,36,36	0.67	1 (2%)	47,47,47	1.03	4 (8%)
31	DMS	o	303	-	3,3,3	2.70	1 (33%)	3,3,3	0.81	0
26	PL9	D	406	-	55,55,55	0.94	3 (5%)	68,69,69	1.56	14 (20%)
31	DMS	a	424	-	3,3,3	2.71	1 (33%)	3,3,3	1.02	0
31	DMS	D	417	-	3,3,3	2.75	1 (33%)	3,3,3	0.60	0
29	LMT	T	102	-	24,24,36	0.73	1 (4%)	29,29,47	1.27	3 (10%)
31	DMS	C	534	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
23	PHO	D	402	-	58,69,69	2.79	11 (18%)	56,99,99	2.60	16 (28%)
31	DMS	v	208	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
31	DMS	B	637	-	3,3,3	2.78	1 (33%)	3,3,3	0.71	0
31	DMS	O	312	-	3,3,3	2.63	1 (33%)	3,3,3	0.96	0
31	DMS	V	207	-	3,3,3	2.75	1 (33%)	3,3,3	0.89	0
31	DMS	v	207	-	3,3,3	2.72	1 (33%)	3,3,3	0.65	0
22	CLA	C	511	3	69,73,73	2.36	20 (28%)	83,113,113	2.17	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	DMS	B	631	-	3,3,3	2.56	1 (33%)	3,3,3	0.62	0
35	DGD	C	517	-	63,63,67	0.85	3 (4%)	77,77,81	1.33	12 (15%)
22	CLA	C	509	3	69,73,73	2.43	20 (28%)	83,113,113	2.30	24 (28%)
24	BCR	B	620	-	41,41,41	0.97	2 (4%)	56,56,56	1.48	11 (19%)
32	BCT	a	422	20	2,3,3	0.87	0	2,3,3	1.11	0
35	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.20	9 (11%)
31	DMS	b	629	-	3,3,3	2.28	1 (33%)	3,3,3	1.10	0
27	LHG	A	412	-	30,30,48	1.38	2 (6%)	33,35,54	1.44	4 (12%)
31	DMS	B	628	-	3,3,3	2.80	1 (33%)	3,3,3	0.77	0
31	DMS	u	204	-	3,3,3	2.80	1 (33%)	3,3,3	0.81	0
31	DMS	c	938	-	3,3,3	2.76	1 (33%)	3,3,3	0.83	0
28	SQD	f	101	-	12,13,54	2.23	1 (8%)	15,16,65	1.26	2 (13%)
24	BCR	B	618	-	19,19,41	0.91	1 (5%)	26,26,56	1.42	5 (19%)
22	CLA	B	614	2	65,69,73	2.31	18 (27%)	78,108,113	2.25	28 (35%)
29	LMT	E	101	-	24,24,36	0.64	0	29,29,47	0.99	1 (3%)
31	DMS	O	304	-	3,3,3	2.57	1 (33%)	3,3,3	0.42	0
22	CLA	B	610	2	69,73,73	2.41	22 (31%)	83,113,113	2.22	23 (27%)
22	CLA	c	913	3	69,73,73	2.50	24 (34%)	83,113,113	2.31	27 (32%)
22	CLA	b	613	2	69,73,73	2.57	21 (30%)	83,113,113	2.34	28 (33%)
29	LMT	f	102	-	25,25,36	1.01	1 (4%)	30,30,47	1.22	5 (16%)
22	CLA	c	909	3	69,73,73	3.21	23 (33%)	83,113,113	2.36	26 (31%)
34	HTG	c	922	-	19,19,19	0.84	1 (5%)	23,24,24	1.70	2 (8%)
39	HEC	v	202	15	50,50,50	1.95	10 (20%)	68,82,82	1.66	10 (14%)
31	DMS	C	530	-	3,3,3	2.68	1 (33%)	3,3,3	0.85	0
31	DMS	l	103	-	3,3,3	2.71	1 (33%)	3,3,3	0.66	0
31	DMS	o	308	-	3,3,3	2.78	1 (33%)	3,3,3	0.83	0
22	CLA	c	914	3	69,73,73	2.36	20 (28%)	83,113,113	2.34	28 (33%)
22	CLA	b	611	40	69,73,73	2.55	21 (30%)	83,113,113	2.37	26 (31%)
22	CLA	B	609	2	69,73,73	2.58	22 (31%)	83,113,113	2.40	26 (31%)
31	DMS	B	636	-	3,3,3	2.60	1 (33%)	3,3,3	0.63	0
24	BCR	C	515	-	41,41,41	0.81	1 (2%)	56,56,56	1.48	9 (16%)
31	DMS	d	413	-	3,3,3	2.54	1 (33%)	3,3,3	0.39	0
31	DMS	c	940	-	3,3,3	2.72	1 (33%)	3,3,3	0.57	0
31	DMS	H	103	-	3,3,3	2.91	1 (33%)	3,3,3	1.19	0
31	DMS	B	632	-	3,3,3	2.65	1 (33%)	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	606	2	69,73,73	2.81	19 (27%)	83,113,113	2.49	30 (36%)
31	DMS	l	104	-	3,3,3	2.77	1 (33%)	3,3,3	0.57	0
22	CLA	C	503	3	69,73,73	2.41	20 (28%)	83,113,113	2.37	22 (26%)
22	CLA	C	507	3	69,73,73	2.28	21 (30%)	83,113,113	2.37	23 (27%)
22	CLA	A	406	40	59,63,73	2.34	21 (35%)	71,101,113	2.83	31 (43%)
27	LHG	D	410	-	48,48,48	0.79	2 (4%)	51,54,54	1.08	4 (7%)
23	PHO	a	410	-	58,69,69	2.60	13 (22%)	56,99,99	2.35	12 (21%)
31	DMS	B	640	-	3,3,3	2.63	1 (33%)	3,3,3	0.61	0
34	HTG	D	414	-	19,19,19	0.86	1 (5%)	23,24,24	1.84	1 (4%)
31	DMS	d	414	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
31	DMS	a	425	-	3,3,3	3.01	1 (33%)	3,3,3	0.88	0
24	BCR	k	101	-	41,41,41	0.91	0	56,56,56	1.23	6 (10%)
26	PL9	a	415	-	55,55,55	0.96	3 (5%)	68,69,69	1.49	12 (17%)
31	DMS	d	415	-	3,3,3	2.62	1 (33%)	3,3,3	0.61	0
32	BCT	A	421[A]	20	2,3,3	0.79	0	2,3,3	0.11	0
31	DMS	L	102	-	3,3,3	2.75	1 (33%)	3,3,3	0.95	0
39	HEC	V	202	15	50,50,50	1.90	10 (20%)	68,82,82	1.48	10 (14%)
22	CLA	c	903	3	69,73,73	2.03	18 (26%)	83,113,113	2.45	27 (32%)
34	HTG	B	627	-	19,19,19	1.01	1 (5%)	23,24,24	2.02	4 (17%)
27	LHG	C	522	-	29,29,48	1.31	2 (6%)	33,34,54	1.38	4 (12%)
37	RRX	h	101	-	42,42,42	0.97	0	57,58,58	1.19	5 (8%)
31	DMS	c	941	-	3,3,3	2.60	1 (33%)	3,3,3	0.52	0
22	CLA	C	506	3	69,73,73	2.59	19 (27%)	83,113,113	2.25	23 (27%)
31	DMS	C	527	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
22	CLA	b	607	2	69,73,73	2.25	22 (31%)	83,113,113	2.64	28 (33%)
35	DGD	d	406	-	42,42,67	1.24	3 (7%)	44,45,81	1.09	3 (6%)
19	OEX	a	403	3,40,1	0,14,14	-	-	-		
22	CLA	B	608	40	69,73,73	2.18	19 (27%)	83,113,113	2.40	33 (39%)
26	PL9	A	411	-	55,55,55	0.97	3 (5%)	68,69,69	1.72	14 (20%)

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	BCR	d	404	-	-	4/29/63/63	0/2/2/2
34	HTG	b	626	-	-	6/10/30/30	0/1/1/1
36	HEM	E	102	6,5	-	1/14/54/54	-
29	LMT	c	921	-	-	11/21/61/61	0/2/2/2
26	PL9	D	406	-	-	8/53/73/73	0/1/1/1
27	LHG	L	101	-	-	20/44/44/53	-
34	HTG	V	203	-	-	0/5/25/30	0/1/1/1
22	CLA	C	513	3	-	11/29/105/115	-
29	LMT	a	419	-	-	14/21/61/61	0/2/2/2
25	LMG	D	412	-	-	14/41/61/70	0/1/1/1
29	LMT	T	102	-	-	10/15/35/61	0/1/1/2
22	CLA	C	514	3	-	18/39/115/115	-
24	BCR	K	101	-	-	3/29/63/63	0/2/2/2
35	DGD	C	518	-	-	23/51/91/95	0/2/2/2
27	LHG	d	408	-	-	17/50/50/53	-
22	CLA	c	910	3	-	15/39/115/115	-
23	PHO	D	402	-	-	6/37/103/103	0/5/6/6
24	BCR	c	916	-	-	4/29/63/63	0/2/2/2
22	CLA	B	603	2	-	8/39/115/115	-
22	CLA	C	508	40	-	11/39/115/115	-
22	CLA	C	511	3	-	14/39/115/115	-
22	CLA	D	403	4	-	0/39/115/115	-
35	DGD	C	517	-	-	19/51/91/95	0/2/2/2
22	CLA	C	509	3	-	11/39/115/115	-
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
22	CLA	B	607	2	-	14/39/115/115	-
22	CLA	a	412	1	-	12/39/115/115	-
35	DGD	C	519	-	-	29/51/91/95	0/2/2/2
22	CLA	a	408	40	-	6/39/115/115	-
29	LMT	I	102	-	-	11/21/61/61	0/2/2/2
22	CLA	b	606	2	-	3/39/115/115	-
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
22	CLA	B	602	40	-	25/39/115/115	-
27	LHG	A	412	-	-	14/33/33/53	-
28	SQD	b	621	-	-	16/32/52/69	0/1/1/1
34	HTG	b	627	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	604	2	-	10/39/115/115	-
34	HTG	C	523	-	-	1/6/6/30	-
22	CLA	b	609	2	-	7/39/115/115	-
22	CLA	C	504	3	-	3/39/115/115	-
25	LMG	J	101	38	-	9/40/60/70	0/1/1/1
29	LMT	c	931	-	-	11/15/35/61	0/1/1/2
29	LMT	A	414	-	-	14/21/61/61	0/2/2/2
22	CLA	c	902	3	-	4/39/115/115	-
28	SQD	f	101	-	-	4/12/12/69	-
24	BCR	c	915	-	-	3/29/63/63	0/2/2/2
22	CLA	B	617	2	-	5/27/103/115	-
22	CLA	B	611	40	-	9/39/115/115	-
27	LHG	d	407	-	-	20/53/53/53	-
35	DGD	D	407	-	-	29/44/64/95	0/1/1/2
27	LHG	a	423	-	-	22/49/49/53	-
24	BCR	B	618	-	-	0/11/28/63	0/1/1/2
24	BCR	D	405	-	-	4/29/63/63	0/2/2/2
22	CLA	C	505	40	-	6/39/115/115	-
28	SQD	a	418	-	-	24/46/66/69	0/1/1/1
25	LMG	C	520	-	-	19/46/66/70	0/1/1/1
22	CLA	B	614	2	-	6/35/111/115	-
25	LMG	B	621	-	-	23/35/55/70	0/1/1/1
29	LMT	E	101	-	-	9/15/35/61	0/1/1/2
35	DGD	H	102	-	-	17/51/91/95	0/2/2/2
35	DGD	c	919	-	-	20/51/91/95	0/2/2/2
25	LMG	b	622	-	-	20/38/58/70	0/1/1/1
22	CLA	B	610	2	-	4/39/115/115	-
22	CLA	c	913	3	-	21/39/115/115	-
22	CLA	b	613	2	-	6/39/115/115	-
36	HEM	e	101	6,5	-	7/14/54/54	-
34	HTG	B	626	-	-	2/10/30/30	0/1/1/1
29	LMT	f	102	-	-	10/17/37/61	0/1/1/2
22	CLA	c	909	3	-	12/39/115/115	-
34	HTG	c	922	-	-	6/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	904	3	-	7/39/115/115	-
22	CLA	b	614	2	-	6/32/108/115	-
24	BCR	Y	101	-	-	6/29/60/63	0/2/2/2
22	CLA	c	911	3	-	7/39/115/115	-
22	CLA	c	905	40	-	15/39/115/115	-
34	HTG	v	203	-	-	5/7/27/30	0/1/1/1
39	HEC	v	202	15	1/1/3/7	5/14/54/54	-
22	CLA	C	510	3	-	13/39/115/115	-
22	CLA	D	401	40	-	6/39/115/115	-
28	SQD	A	413	-	-	26/44/64/69	0/1/1/1
34	HTG	b	624	-	-	4/10/30/30	0/1/1/1
22	CLA	c	914	3	-	16/39/115/115	-
28	SQD	a	414	-	-	27/49/69/69	0/1/1/1
34	HTG	b	632	-	-	6/10/30/30	0/1/1/1
22	CLA	A	408	1	-	13/39/115/115	-
22	CLA	b	611	40	-	7/39/115/115	-
22	CLA	c	908	40	-	11/39/115/115	-
22	CLA	a	409	40	-	10/35/111/115	-
22	CLA	B	609	2	-	2/39/115/115	-
25	LMG	d	409	-	-	28/42/62/70	0/1/1/1
24	BCR	C	515	-	-	4/29/63/63	0/2/2/2
22	CLA	B	612	2	-	11/39/115/115	-
26	PL9	d	405	-	-	6/53/73/73	0/1/1/1
25	LMG	c	930	-	-	12/44/64/70	0/1/1/1
22	CLA	B	606	2	-	11/39/115/115	-
22	CLA	C	503	3	-	9/39/115/115	-
22	CLA	C	507	3	-	11/39/115/115	-
35	DGD	c	917	-	-	21/51/91/95	0/2/2/2
35	DGD	c	918	-	-	22/51/91/95	0/2/2/2
22	CLA	B	615	2	-	11/25/101/115	-
24	BCR	A	409	-	-	2/29/63/63	0/2/2/2
22	CLA	A	406	40	-	5/27/103/115	-
22	CLA	b	605	2	-	11/39/115/115	-
27	LHG	D	410	-	-	12/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	906	3	-	10/39/115/115	-
34	HTG	C	532	-	-	7/10/30/30	0/1/1/1
35	DGD	h	102	-	-	18/51/91/95	0/2/2/2
22	CLA	c	912	3	-	4/39/115/115	-
22	CLA	b	612	2	-	10/39/115/115	-
25	LMG	C	531	-	-	14/35/55/70	0/1/1/1
24	BCR	C	516	-	-	0/29/63/63	0/2/2/2
34	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	BCR	B	619	-	-	1/24/41/63	0/1/1/2
22	CLA	b	615	2	-	6/24/100/115	-
27	LHG	a	416	-	-	28/53/53/53	-
23	PHO	a	410	-	-	1/37/103/103	0/5/6/6
22	CLA	B	616	2	-	12/39/115/115	-
22	CLA	C	512	3	-	1/39/115/115	-
28	SQD	D	408	-	-	3/12/32/69	0/1/1/1
34	HTG	b	623	-	-	6/10/30/30	0/1/1/1
34	HTG	C	521	-	-	4/10/30/30	0/1/1/1
24	BCR	y	101	-	-	5/29/63/63	0/2/2/2
25	LMG	A	410	-	-	28/46/66/70	0/1/1/1
34	HTG	D	414	-	-	3/10/30/30	0/1/1/1
22	CLA	b	610	2	-	3/39/115/115	-
22	CLA	D	404	4	-	13/39/115/115	-
22	CLA	b	616	2	-	9/39/115/115	-
22	CLA	d	403	4	-	10/39/115/115	-
22	CLA	b	617	2	-	8/33/109/115	-
29	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
22	CLA	a	407	1	-	7/39/115/115	-
22	CLA	d	402	4	-	10/39/115/115	-
22	CLA	B	604	2	-	7/39/115/115	-
22	CLA	A	405	1	-	7/39/115/115	-
24	BCR	k	101	-	-	4/29/63/63	0/2/2/2
26	PL9	a	415	-	-	15/53/73/73	0/1/1/1
29	LMT	B	622	-	-	8/15/35/61	0/1/1/2
39	HEC	V	202	15	1/1/3/7	4/14/54/54	-
22	CLA	C	502	3	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	903	3	-	10/39/115/115	-
27	LHG	D	409	-	-	15/53/53/53	-
22	CLA	b	608	40	-	16/39/115/115	-
29	LMT	t	101	-	-	10/15/35/61	0/1/1/2
34	HTG	l	106	-	-	6/10/30/30	0/1/1/1
34	HTG	B	627	-	-	7/10/30/30	0/1/1/1
27	LHG	d	401	-	-	15/34/34/53	-
27	LHG	C	522	-	-	15/31/31/53	-
25	LMG	j	101	38	-	13/42/62/70	0/1/1/1
34	HTG	D	415	-	-	8/10/30/30	0/1/1/1
28	SQD	C	501	-	-	27/49/69/69	0/1/1/1
23	PHO	a	411	-	-	6/37/103/103	0/5/6/6
27	LHG	D	411	-	-	12/49/49/53	-
22	CLA	b	603	2	-	3/39/115/115	-
27	LHG	l	102	-	-	26/53/53/53	-
28	SQD	l	101	-	-	32/49/69/69	0/1/1/1
22	CLA	b	602	40	-	23/39/115/115	-
37	RRX	H	101	-	-	1/29/65/65	0/2/2/2
37	RRX	h	101	-	-	8/29/65/65	0/2/2/2
22	CLA	B	605	2	-	9/39/115/115	-
23	PHO	A	407	-	-	2/37/103/103	0/5/6/6
22	CLA	C	506	3	-	5/39/115/115	-
22	CLA	b	607	2	-	7/39/115/115	-
25	LMG	c	920	-	-	21/46/66/70	0/1/1/1
35	DGD	d	406	-	-	30/44/44/95	-
22	CLA	B	613	2	-	4/39/115/115	-
22	CLA	c	907	3	-	11/39/115/115	-
24	BCR	b	619	-	-	4/26/43/63	0/1/1/2
25	LMG	i	101	-	-	26/46/66/70	0/1/1/1
24	BCR	b	618	-	-	7/13/30/63	0/1/1/2
22	CLA	B	608	40	-	7/39/115/115	-
24	BCR	a	413	-	-	2/29/63/63	0/2/2/2
26	PL9	A	411	-	-	12/53/73/73	0/1/1/1

All (1813) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	MG-NA	19.40	2.52	2.06
22	B	606	CLA	MG-NA	15.87	2.44	2.06
22	b	617	CLA	MG-NA	15.18	2.42	2.06
22	c	912	CLA	MG-NA	14.71	2.41	2.06
22	B	602	CLA	MG-NA	14.39	2.40	2.06
22	b	603	CLA	MG-NA	14.14	2.39	2.06
22	C	505	CLA	MG-NA	13.78	2.39	2.06
22	b	604	CLA	MG-NA	13.69	2.38	2.06
22	c	908	CLA	MG-NA	13.08	2.37	2.06
22	c	905	CLA	MG-NA	12.88	2.36	2.06
22	c	904	CLA	MG-NA	12.83	2.36	2.06
22	c	909	CLA	MG-NB	12.56	2.30	2.05
22	B	613	CLA	MG-NA	12.32	2.35	2.06
22	b	613	CLA	MG-NA	12.17	2.35	2.06
22	A	405	CLA	MG-NC	11.62	2.33	2.06
22	C	506	CLA	MG-NA	11.61	2.33	2.06
22	c	909	CLA	MG-NA	11.40	2.33	2.06
22	B	611	CLA	MG-NB	11.40	2.28	2.05
22	C	512	CLA	MG-NA	11.28	2.33	2.06
22	B	611	CLA	MG-NC	11.25	2.33	2.06
22	C	514	CLA	MG-NA	10.98	2.32	2.06
22	D	404	CLA	MG-NC	10.68	2.31	2.06
22	b	615	CLA	MG-NA	10.66	2.31	2.06
22	B	616	CLA	MG-NA	10.56	2.31	2.06
22	B	609	CLA	MG-ND	10.48	2.26	2.05
22	C	503	CLA	MG-NA	10.17	2.30	2.06
22	a	408	CLA	MG-NB	10.09	2.25	2.05
23	D	402	PHO	C1B-C2B	10.03	1.50	1.39
23	a	410	PHO	C1B-C2B	10.01	1.50	1.39
22	c	902	CLA	MG-NA	9.92	2.29	2.06
22	C	505	CLA	MG-ND	9.80	2.25	2.05
22	C	504	CLA	MG-NC	9.77	2.29	2.06
22	b	610	CLA	MG-NA	9.74	2.29	2.06
22	C	513	CLA	MG-NA	9.70	2.29	2.06
22	b	614	CLA	MG-NA	9.53	2.28	2.06
22	a	408	CLA	MG-ND	-9.49	1.87	2.05
22	b	608	CLA	MG-NA	9.39	2.28	2.06
22	B	615	CLA	MG-NC	9.39	2.28	2.06
22	b	616	CLA	MG-NA	9.38	2.28	2.06
22	B	603	CLA	MG-ND	-9.34	1.87	2.05
23	a	411	PHO	C1B-C2B	9.17	1.49	1.39
22	B	616	CLA	MG-NB	9.06	2.23	2.05
22	b	605	CLA	MG-NA	9.04	2.27	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	MG-NC	9.04	2.27	2.06
22	C	509	CLA	MG-NA	8.92	2.27	2.06
22	B	614	CLA	MG-NA	8.89	2.27	2.06
22	b	612	CLA	MG-NA	8.87	2.27	2.06
23	a	411	PHO	C1D-C2D	8.73	1.49	1.39
23	a	410	PHO	C1D-C2D	8.63	1.49	1.39
23	D	402	PHO	C1D-C2D	8.59	1.49	1.39
22	b	610	CLA	MG-ND	8.55	2.22	2.05
22	B	608	CLA	MG-NA	8.51	2.26	2.06
22	c	914	CLA	MG-NC	8.49	2.26	2.06
22	d	403	CLA	MG-NA	8.48	2.26	2.06
22	b	607	CLA	MG-NA	8.43	2.26	2.06
22	B	610	CLA	MG-NB	8.40	2.22	2.05
22	B	604	CLA	MG-NA	8.37	2.26	2.06
22	C	513	CLA	MG-NB	8.37	2.22	2.05
22	b	611	CLA	MG-NC	8.35	2.26	2.06
23	A	407	PHO	C1D-C2D	8.29	1.48	1.39
22	c	909	CLA	MG-ND	-8.26	1.89	2.05
22	c	906	CLA	MG-NA	8.26	2.25	2.06
22	C	504	CLA	MG-NA	8.13	2.25	2.06
22	B	612	CLA	MG-NA	8.10	2.25	2.06
22	C	508	CLA	MG-NA	8.09	2.25	2.06
22	c	912	CLA	MG-NC	8.05	2.25	2.06
22	B	607	CLA	MG-NA	8.00	2.25	2.06
36	e	101	HEM	C3D-C2D	7.97	1.53	1.36
36	E	102	HEM	C3D-C2D	7.96	1.53	1.36
22	d	403	CLA	MG-ND	-7.95	1.90	2.05
22	B	607	CLA	MG-NC	7.92	2.25	2.06
39	v	202	HEC	C3D-C2D	7.90	1.53	1.36
22	C	511	CLA	MG-NA	7.83	2.24	2.06
22	a	407	CLA	MG-NA	7.78	2.24	2.06
22	B	609	CLA	MG-NC	7.71	2.24	2.06
22	C	507	CLA	MG-NA	7.71	2.24	2.06
22	c	907	CLA	MG-NA	7.68	2.24	2.06
22	c	913	CLA	MG-NC	7.66	2.24	2.06
23	A	407	PHO	C1B-C2B	7.62	1.48	1.39
22	d	403	CLA	MG-NB	7.60	2.20	2.05
22	D	403	CLA	MG-NA	7.55	2.24	2.06
22	c	909	CLA	MG-NC	7.45	2.24	2.06
22	B	611	CLA	MG-ND	-7.40	1.91	2.05
22	C	509	CLA	MG-NC	7.29	2.23	2.06
28	f	101	SQD	C6-S	-7.16	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	907	CLA	MG-NB	7.15	2.20	2.05
22	C	514	CLA	MG-NC	7.15	2.23	2.06
22	b	609	CLA	MG-NA	7.07	2.23	2.06
22	A	406	CLA	MG-NA	7.05	2.23	2.06
22	b	611	CLA	MG-ND	-7.03	1.91	2.05
22	b	611	CLA	MG-NB	7.03	2.19	2.05
22	c	908	CLA	MG-ND	7.02	2.19	2.05
22	C	505	CLA	MG-NC	6.94	2.22	2.06
22	c	911	CLA	MG-NA	6.94	2.22	2.06
22	c	902	CLA	MG-ND	-6.94	1.92	2.05
22	c	905	CLA	MG-NC	6.93	2.22	2.06
22	B	605	CLA	MG-NA	6.88	2.22	2.06
22	b	606	CLA	MG-NB	6.81	2.19	2.05
39	V	202	HEC	C3D-C2D	6.71	1.51	1.36
22	B	603	CLA	MG-NA	6.71	2.22	2.06
22	b	602	CLA	MG-ND	6.69	2.19	2.05
22	B	617	CLA	MG-NA	6.58	2.21	2.06
23	D	402	PHO	C3B-C4B	6.57	1.49	1.41
22	c	913	CLA	MG-NB	6.56	2.18	2.05
22	C	510	CLA	MG-NA	6.53	2.21	2.06
22	c	913	CLA	MG-NA	6.53	2.21	2.06
22	b	605	CLA	MG-ND	-6.49	1.92	2.05
22	B	603	CLA	MG-NC	6.45	2.21	2.06
22	C	503	CLA	MG-ND	-6.44	1.93	2.05
22	C	511	CLA	MG-ND	-6.35	1.93	2.05
22	a	412	CLA	MG-ND	6.34	2.18	2.05
23	D	402	PHO	C3B-C2B	6.34	1.49	1.40
23	D	402	PHO	C4D-CHA	6.29	1.49	1.39
22	C	508	CLA	MG-NC	6.27	2.21	2.06
22	B	613	CLA	MG-NB	6.24	2.18	2.05
22	C	513	CLA	MG-NC	6.22	2.21	2.06
22	b	605	CLA	MG-NB	6.13	2.17	2.05
22	a	412	CLA	C3C-C2C	6.09	1.49	1.36
22	c	910	CLA	MG-NA	6.08	2.20	2.06
22	c	909	CLA	C3C-C2C	6.02	1.49	1.36
22	C	504	CLA	MG-ND	5.99	2.17	2.05
22	B	616	CLA	O2D-CGD	5.97	1.47	1.33
22	b	603	CLA	C3C-C2C	5.95	1.49	1.36
22	b	602	CLA	C3C-C2C	5.88	1.49	1.36
22	a	409	CLA	MG-NA	5.88	2.20	2.06
22	c	912	CLA	CHD-C1D	5.87	1.49	1.38
22	d	402	CLA	MG-NA	5.86	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	908	CLA	C3C-C2C	5.86	1.49	1.36
22	B	611	CLA	C3C-C2C	5.84	1.49	1.36
22	B	610	CLA	CHC-C1C	5.82	1.50	1.38
22	c	913	CLA	C3C-C2C	5.80	1.49	1.36
22	C	504	CLA	CHC-C1C	5.80	1.50	1.38
22	B	614	CLA	CHC-C1C	5.80	1.50	1.38
22	b	608	CLA	MG-NC	5.78	2.20	2.06
23	A	407	PHO	C4D-CHA	5.78	1.48	1.39
23	a	411	PHO	C3B-C4B	5.77	1.48	1.41
22	C	513	CLA	C3C-C2C	5.77	1.49	1.36
22	B	606	CLA	MG-NB	5.74	2.17	2.05
22	C	503	CLA	C3C-C2C	5.73	1.48	1.36
22	B	603	CLA	C3C-C2C	5.73	1.48	1.36
22	c	904	CLA	C3C-C2C	5.73	1.48	1.36
22	b	608	CLA	C3C-C2C	5.71	1.48	1.36
22	c	908	CLA	CHC-C1C	5.70	1.50	1.38
22	B	608	CLA	CHD-C1D	5.67	1.49	1.38
22	b	606	CLA	MG-NA	5.65	2.19	2.06
22	A	408	CLA	C3C-C2C	5.65	1.48	1.36
22	b	609	CLA	C3C-C2C	5.65	1.48	1.36
23	D	402	PHO	O2D-CGD	5.63	1.46	1.33
22	b	602	CLA	O2D-CGD	5.61	1.46	1.33
22	c	905	CLA	O2D-CGD	5.61	1.46	1.33
22	C	506	CLA	CHC-C1C	5.61	1.49	1.38
22	b	616	CLA	C3C-C2C	5.60	1.48	1.36
22	B	610	CLA	MG-NA	5.60	2.19	2.06
22	C	514	CLA	C3C-C2C	5.60	1.48	1.36
36	E	102	HEM	FE-NA	5.59	2.14	1.95
23	a	411	PHO	C3C-C2C	5.59	1.48	1.36
22	b	617	CLA	C3C-C2C	5.58	1.48	1.36
22	b	603	CLA	MG-ND	5.55	2.16	2.05
22	B	609	CLA	C3C-C2C	5.54	1.48	1.36
22	c	909	CLA	O2D-CGD	5.54	1.46	1.33
22	A	408	CLA	MG-NA	5.53	2.19	2.06
22	b	604	CLA	C3C-C2C	5.53	1.48	1.36
22	B	615	CLA	O2A-CGA	5.52	1.49	1.33
22	b	602	CLA	CHC-C1C	5.52	1.49	1.38
22	b	615	CLA	C3C-C2C	5.51	1.48	1.36
22	B	615	CLA	CHC-C1C	5.50	1.49	1.38
22	b	603	CLA	MG-NB	-5.49	1.94	2.05
22	c	905	CLA	C3C-C2C	5.49	1.48	1.36
22	b	608	CLA	CHD-C1D	5.49	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	410	PHO	C3B-C4B	5.48	1.47	1.41
22	b	602	CLA	O2A-CGA	5.48	1.49	1.33
22	a	409	CLA	MG-NB	5.48	2.16	2.05
22	c	910	CLA	CHD-C1D	5.48	1.49	1.38
22	c	914	CLA	O2D-CGD	5.47	1.46	1.33
23	a	411	PHO	C3B-C2B	5.46	1.47	1.40
22	C	511	CLA	OBD-CAD	5.46	1.31	1.22
22	C	509	CLA	C3C-C2C	5.45	1.48	1.36
22	C	505	CLA	CHD-C1D	5.45	1.49	1.38
22	C	505	CLA	C3C-C2C	5.45	1.48	1.36
22	B	612	CLA	C3C-C2C	5.44	1.48	1.36
22	c	912	CLA	CHC-C1C	5.42	1.49	1.38
22	c	903	CLA	MG-NC	5.41	2.19	2.06
23	A	407	PHO	C3B-C2B	5.41	1.47	1.40
22	c	912	CLA	O2D-CGD	5.41	1.46	1.33
22	b	603	CLA	O2D-CGD	5.41	1.46	1.33
22	b	606	CLA	MG-ND	-5.40	1.95	2.05
22	a	407	CLA	MG-ND	5.39	2.16	2.05
22	c	902	CLA	CHC-C1C	5.39	1.49	1.38
22	c	914	CLA	MG-NA	5.38	2.19	2.06
22	C	513	CLA	O2D-CGD	5.38	1.46	1.33
22	C	512	CLA	C3C-C2C	5.38	1.48	1.36
22	c	906	CLA	CHC-C1C	5.37	1.49	1.38
22	a	412	CLA	O2D-CGD	5.37	1.46	1.33
22	B	611	CLA	CHC-C1C	5.36	1.49	1.38
22	B	617	CLA	C3C-C2C	5.34	1.48	1.36
22	b	602	CLA	CHD-C1D	5.33	1.48	1.38
22	b	611	CLA	CHC-C1C	5.33	1.49	1.38
22	a	412	CLA	CHD-C1D	5.33	1.48	1.38
22	C	506	CLA	C3C-C2C	5.33	1.48	1.36
22	D	404	CLA	C3C-C2C	5.32	1.48	1.36
22	a	407	CLA	O2D-CGD	5.31	1.46	1.33
22	B	602	CLA	O2D-CGD	5.31	1.46	1.33
22	C	504	CLA	C3C-C2C	5.30	1.48	1.36
22	B	610	CLA	MG-NC	5.27	2.18	2.06
22	C	508	CLA	C3C-C2C	5.27	1.47	1.36
22	b	617	CLA	CHC-C1C	5.27	1.49	1.38
22	C	510	CLA	O2D-CGD	5.26	1.46	1.33
22	A	405	CLA	C3C-C2C	5.26	1.47	1.36
22	b	604	CLA	O2D-CGD	5.26	1.46	1.33
22	D	401	CLA	C3C-C2C	5.25	1.47	1.36
27	A	412	LHG	O7-C7	5.25	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	CHC-C1C	5.25	1.49	1.38
22	b	608	CLA	O2D-CGD	5.24	1.46	1.33
22	B	607	CLA	CHC-C4B	5.23	1.51	1.39
22	d	403	CLA	O2A-CGA	5.23	1.48	1.33
22	c	907	CLA	O2D-CGD	5.23	1.46	1.33
22	C	514	CLA	CHC-C1C	5.23	1.49	1.38
22	D	404	CLA	CHD-C1D	5.23	1.48	1.38
22	C	510	CLA	C3C-C2C	5.22	1.47	1.36
22	c	904	CLA	CHD-C1D	5.22	1.48	1.38
22	b	613	CLA	MG-ND	5.21	2.16	2.05
22	b	611	CLA	C3C-C2C	5.21	1.47	1.36
22	B	615	CLA	C3C-C2C	5.20	1.47	1.36
22	b	615	CLA	O2D-CGD	5.20	1.45	1.33
22	d	403	CLA	OBD-CAD	5.19	1.31	1.22
22	c	910	CLA	O2D-CGD	5.19	1.45	1.33
22	b	603	CLA	CHC-C1C	5.19	1.49	1.38
22	b	606	CLA	C3C-C2C	5.18	1.47	1.36
22	C	514	CLA	CHD-C1D	5.16	1.48	1.38
22	B	604	CLA	CHD-C1D	5.16	1.48	1.38
22	D	404	CLA	CHC-C1C	5.16	1.49	1.38
22	a	412	CLA	MG-NC	5.15	2.18	2.06
22	b	604	CLA	CHD-C1D	5.15	1.48	1.38
31	u	205	DMS	O-S	5.15	1.85	1.50
22	B	607	CLA	C3C-C2C	5.15	1.47	1.36
22	C	513	CLA	CHC-C1C	5.14	1.49	1.38
22	B	609	CLA	CHD-C1D	5.14	1.48	1.38
22	b	609	CLA	CHD-C1D	5.14	1.48	1.38
22	B	602	CLA	CHC-C1C	5.14	1.49	1.38
22	b	610	CLA	CHC-C1C	5.14	1.49	1.38
22	C	514	CLA	CHC-C4B	5.14	1.50	1.39
22	C	512	CLA	O2D-CGD	5.14	1.45	1.33
22	C	502	CLA	MG-NA	5.14	2.18	2.06
22	B	604	CLA	C3C-C2C	5.13	1.47	1.36
22	c	906	CLA	C3C-C2C	5.12	1.47	1.36
22	d	403	CLA	CHC-C1C	5.12	1.48	1.38
22	c	902	CLA	C3C-C2C	5.12	1.47	1.36
22	B	612	CLA	O2D-CGD	5.12	1.45	1.33
22	B	616	CLA	CHC-C1C	5.11	1.48	1.38
22	B	605	CLA	CHD-C1D	5.11	1.48	1.38
22	b	613	CLA	CHC-C1C	5.11	1.48	1.38
22	c	907	CLA	C3C-C2C	5.11	1.47	1.36
22	c	909	CLA	CHC-C1C	5.11	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	902	CLA	MG-NB	5.10	2.15	2.05
23	a	410	PHO	C4D-CHA	5.09	1.47	1.39
22	d	403	CLA	C3C-C2C	5.09	1.47	1.36
22	C	507	CLA	O2D-CGD	5.09	1.45	1.33
22	C	502	CLA	C3C-C2C	5.08	1.47	1.36
31	a	425	DMS	O-S	5.07	1.84	1.50
22	A	406	CLA	O2D-CGD	5.07	1.45	1.33
22	B	602	CLA	CHD-C1D	5.06	1.48	1.38
22	C	506	CLA	CHD-C1D	5.06	1.48	1.38
31	O	311	DMS	O-S	5.06	1.84	1.50
31	b	638	DMS	O-S	5.06	1.84	1.50
22	c	906	CLA	CHD-C1D	5.05	1.48	1.38
22	b	613	CLA	O2D-CGD	5.04	1.45	1.33
22	B	604	CLA	O2D-CGD	5.03	1.45	1.33
22	a	412	CLA	CHC-C1C	5.03	1.48	1.38
22	b	614	CLA	CHC-C1C	5.03	1.48	1.38
22	b	614	CLA	C3C-C2C	5.02	1.47	1.36
22	b	607	CLA	C3C-C2C	5.02	1.47	1.36
22	C	503	CLA	CHC-C1C	5.02	1.48	1.38
35	D	407	DGD	O2G-C1B	5.02	1.48	1.34
27	a	416	LHG	O8-C23	5.02	1.48	1.33
22	b	605	CLA	C4B-NB	-5.01	1.31	1.37
22	b	603	CLA	CHD-C4C	5.01	1.50	1.39
22	B	602	CLA	C3C-C2C	5.01	1.47	1.36
22	c	912	CLA	C3C-C2C	5.00	1.47	1.36
22	A	406	CLA	MG-NB	-5.00	1.95	2.05
39	V	202	HEC	FE-ND	5.00	2.10	1.94
22	b	609	CLA	CHC-C1C	5.00	1.48	1.38
22	C	508	CLA	CHC-C1C	5.00	1.48	1.38
22	C	507	CLA	CHD-C1D	4.99	1.48	1.38
22	B	615	CLA	O2D-CGD	4.99	1.45	1.33
22	C	512	CLA	MG-NB	4.99	2.15	2.05
22	b	611	CLA	O2D-CGD	4.98	1.45	1.33
22	b	615	CLA	CHD-C1D	4.98	1.48	1.38
22	b	614	CLA	O2D-CGD	4.97	1.45	1.33
25	b	622	LMG	O8-C28	4.97	1.47	1.33
22	d	402	CLA	CHC-C1C	4.96	1.48	1.38
22	a	407	CLA	CHC-C1C	4.95	1.48	1.38
22	b	616	CLA	O2D-CGD	4.95	1.45	1.33
39	V	202	HEC	FE-NB	4.95	2.10	1.94
22	c	914	CLA	C3C-C2C	4.95	1.47	1.36
22	C	505	CLA	CHD-C4C	4.94	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	CHB-C1B	4.94	1.50	1.39
22	C	507	CLA	CHC-C1C	4.94	1.48	1.38
22	B	616	CLA	C3C-C2C	4.94	1.47	1.36
22	A	408	CLA	O2D-CGD	4.94	1.45	1.33
22	c	910	CLA	OBD-CAD	4.94	1.31	1.22
22	C	502	CLA	CHC-C1C	4.94	1.48	1.38
22	C	514	CLA	O2D-CGD	4.93	1.45	1.33
23	A	407	PHO	C3D-C4D	-4.93	1.34	1.41
22	C	514	CLA	MG-NB	4.93	2.15	2.05
22	c	907	CLA	CHD-C1D	4.92	1.47	1.38
22	d	403	CLA	CHD-C1D	4.91	1.47	1.38
22	B	602	CLA	O2A-CGA	4.91	1.47	1.33
22	b	610	CLA	O2D-CGD	4.91	1.45	1.33
22	B	613	CLA	O2D-CGD	4.91	1.45	1.33
22	C	511	CLA	O2D-CGD	4.91	1.45	1.33
23	a	411	PHO	C4D-CHA	4.91	1.47	1.39
22	C	505	CLA	CHC-C1C	4.90	1.48	1.38
22	a	408	CLA	C3C-C2C	4.90	1.47	1.36
36	e	101	HEM	FE-NA	4.90	2.11	1.95
22	a	408	CLA	CHC-C1C	4.89	1.48	1.38
25	D	412	LMG	O8-C28	4.89	1.47	1.33
22	c	914	CLA	CHC-C1C	4.88	1.48	1.38
35	d	406	DGD	O2G-C1B	4.88	1.48	1.34
22	B	603	CLA	MG-NB	4.87	2.15	2.05
22	b	612	CLA	CHB-C1B	4.87	1.50	1.39
22	C	511	CLA	MG-NC	4.87	2.17	2.06
22	c	904	CLA	CHC-C1C	4.86	1.48	1.38
22	b	605	CLA	C3C-C2C	4.85	1.47	1.36
22	B	607	CLA	CHC-C1C	4.85	1.48	1.38
22	a	409	CLA	MG-ND	-4.85	1.96	2.05
31	H	103	DMS	O-S	4.84	1.82	1.50
35	d	406	DGD	O1G-C1A	4.83	1.47	1.33
22	B	613	CLA	C3C-C2C	4.83	1.47	1.36
22	C	504	CLA	CHC-C4B	4.83	1.50	1.39
22	B	606	CLA	CHC-C1C	4.82	1.48	1.38
22	A	408	CLA	CHD-C1D	4.82	1.47	1.38
31	O	305	DMS	O-S	4.82	1.82	1.50
31	c	937	DMS	O-S	4.82	1.82	1.50
22	b	614	CLA	CHD-C1D	4.81	1.47	1.38
22	c	911	CLA	CHC-C1C	4.81	1.48	1.38
22	C	509	CLA	CHC-C1C	4.81	1.48	1.38
31	B	628	DMS	O-S	4.81	1.82	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	402	CLA	C3C-C2C	4.80	1.46	1.36
25	B	621	LMG	O8-C28	4.80	1.47	1.33
22	b	617	CLA	O2D-CGD	4.80	1.44	1.33
23	a	411	PHO	OBD-CAD	4.79	1.29	1.22
22	B	609	CLA	CHC-C1C	4.79	1.48	1.38
22	c	903	CLA	C3C-C2C	4.79	1.46	1.36
25	D	412	LMG	O7-C10	4.78	1.47	1.34
31	c	933	DMS	O-S	4.78	1.82	1.50
31	v	210	DMS	O-S	4.78	1.82	1.50
22	b	610	CLA	C1D-ND	-4.78	1.31	1.37
31	c	924	DMS	O-S	4.77	1.82	1.50
22	B	604	CLA	MG-NC	4.77	2.17	2.06
22	b	610	CLA	C3C-C2C	4.77	1.46	1.36
22	c	906	CLA	CHD-C4C	4.77	1.50	1.39
36	e	101	HEM	FE-NC	4.76	2.11	1.95
36	e	101	HEM	FE-ND	4.76	2.09	1.94
31	B	630	DMS	O-S	4.76	1.82	1.50
25	C	531	LMG	O7-C10	4.75	1.47	1.34
23	D	402	PHO	C3D-C4D	-4.75	1.34	1.41
22	c	913	CLA	CHC-C1C	4.75	1.48	1.38
22	c	908	CLA	CHB-C1B	4.75	1.50	1.39
22	C	512	CLA	O2A-CGA	4.75	1.47	1.33
22	D	401	CLA	OBD-CAD	4.75	1.30	1.22
25	c	930	LMG	O7-C10	4.75	1.47	1.34
23	A	407	PHO	C3C-C2C	4.75	1.46	1.36
22	B	603	CLA	CHC-C1C	4.75	1.48	1.38
31	o	304	DMS	O-S	4.75	1.82	1.50
22	b	612	CLA	O2D-CGD	4.74	1.44	1.33
22	B	613	CLA	CHD-C1D	4.73	1.47	1.38
22	c	911	CLA	CHD-C1D	4.73	1.47	1.38
22	B	615	CLA	CHB-C1B	4.73	1.50	1.39
25	C	520	LMG	O8-C28	4.72	1.47	1.33
22	c	903	CLA	CHC-C1C	4.72	1.48	1.38
22	C	510	CLA	O2A-CGA	4.72	1.47	1.33
22	A	408	CLA	MG-NC	4.72	2.17	2.06
22	B	614	CLA	MG-ND	-4.72	1.96	2.05
22	C	502	CLA	MG-NC	4.72	2.17	2.06
35	D	407	DGD	O1G-C1A	4.72	1.47	1.33
27	a	416	LHG	O7-C7	4.71	1.47	1.34
22	C	508	CLA	CHD-C1D	4.71	1.47	1.38
22	B	603	CLA	CHD-C1D	4.71	1.47	1.38
22	b	616	CLA	CHB-C1B	4.71	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	914	CLA	CHB-C1B	4.70	1.50	1.39
22	c	914	CLA	CHD-C1D	4.70	1.47	1.38
22	B	612	CLA	CHD-C1D	4.70	1.47	1.38
31	B	634	DMS	O-S	4.70	1.82	1.50
31	V	211	DMS	O-S	4.70	1.82	1.50
31	c	929	DMS	O-S	4.69	1.82	1.50
22	C	507	CLA	C3C-C2C	4.69	1.46	1.36
22	B	607	CLA	O2D-CGD	4.69	1.44	1.33
25	i	101	LMG	O8-C28	4.68	1.47	1.33
31	B	635	DMS	O-S	4.68	1.81	1.50
27	C	522	LHG	O7-C7	4.68	1.47	1.34
22	b	607	CLA	O2D-CGD	4.68	1.44	1.33
36	E	102	HEM	FE-ND	4.68	2.09	1.94
22	B	608	CLA	O2D-CGD	4.67	1.44	1.33
22	c	908	CLA	CHC-C4B	4.67	1.49	1.39
22	c	905	CLA	CHC-C1C	4.67	1.48	1.38
25	c	920	LMG	O8-C28	4.67	1.47	1.33
31	o	308	DMS	O-S	4.66	1.81	1.50
22	b	607	CLA	CHC-C1C	4.66	1.48	1.38
31	B	637	DMS	O-S	4.66	1.81	1.50
22	C	514	CLA	CHB-C1B	4.66	1.49	1.39
22	C	503	CLA	CHD-C1D	4.66	1.47	1.38
22	D	404	CLA	O2D-CGD	4.65	1.44	1.33
22	C	509	CLA	CHD-C1D	4.65	1.47	1.38
22	c	913	CLA	O2D-CGD	4.65	1.44	1.33
22	a	407	CLA	CHD-C1D	4.65	1.47	1.38
31	O	308	DMS	O-S	4.64	1.81	1.50
22	B	614	CLA	C3C-C2C	4.64	1.46	1.36
22	C	510	CLA	CHD-C1D	4.64	1.47	1.38
23	a	410	PHO	C3C-C2C	4.64	1.46	1.36
31	O	307	DMS	O-S	4.64	1.81	1.50
31	B	641	DMS	O-S	4.64	1.81	1.50
31	c	939	DMS	O-S	4.64	1.81	1.50
27	d	401	LHG	O8-C23	4.64	1.46	1.33
31	V	212	DMS	O-S	4.64	1.81	1.50
31	V	210	DMS	O-S	4.64	1.81	1.50
22	b	607	CLA	CHD-C1D	4.63	1.47	1.38
31	b	635	DMS	O-S	4.63	1.81	1.50
31	C	540	DMS	O-S	4.63	1.81	1.50
31	u	204	DMS	O-S	4.63	1.81	1.50
31	v	211	DMS	O-S	4.63	1.81	1.50
28	a	414	SQD	O48-C23	4.63	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	l	104	DMS	O-S	4.62	1.81	1.50
22	b	615	CLA	O2A-CGA	4.62	1.46	1.33
22	B	610	CLA	C3C-C2C	4.62	1.46	1.36
31	c	938	DMS	O-S	4.61	1.81	1.50
22	c	903	CLA	CHD-C1D	4.61	1.47	1.38
22	B	607	CLA	MG-ND	-4.61	1.96	2.05
22	C	510	CLA	CHC-C1C	4.61	1.47	1.38
31	O	303	DMS	O-S	4.61	1.81	1.50
25	B	621	LMG	O7-C10	4.60	1.47	1.34
31	U	203	DMS	O-S	4.60	1.81	1.50
22	b	613	CLA	C3C-C2C	4.60	1.46	1.36
31	D	417	DMS	O-S	4.60	1.81	1.50
31	V	206	DMS	O-S	4.59	1.81	1.50
22	C	505	CLA	O2D-CGD	4.59	1.44	1.33
22	c	913	CLA	CHD-C1D	4.59	1.47	1.38
22	c	911	CLA	CHC-C4B	4.59	1.49	1.39
22	a	407	CLA	MG-NC	4.58	2.17	2.06
22	B	614	CLA	CHD-C1D	4.58	1.47	1.38
31	C	537	DMS	O-S	4.58	1.81	1.50
31	V	207	DMS	O-S	4.58	1.81	1.50
31	I	101	DMS	O-S	4.57	1.81	1.50
31	B	639	DMS	O-S	4.57	1.81	1.50
22	b	616	CLA	MG-NC	4.57	2.17	2.06
23	a	410	PHO	C3D-C2D	4.57	1.47	1.39
22	b	610	CLA	CHB-C1B	4.57	1.49	1.39
22	c	910	CLA	O2A-CGA	4.57	1.46	1.33
31	C	533	DMS	O-S	4.57	1.81	1.50
22	c	911	CLA	C3C-C2C	4.56	1.46	1.36
22	B	608	CLA	CHD-C4C	4.56	1.49	1.39
22	d	402	CLA	O2A-CGA	4.56	1.46	1.33
31	a	401	DMS	O-S	4.56	1.81	1.50
31	C	535	DMS	O-S	4.56	1.81	1.50
22	b	610	CLA	CHD-C1D	4.56	1.47	1.38
22	B	609	CLA	O2D-CGD	4.56	1.44	1.33
31	l	105	DMS	O-S	4.56	1.81	1.50
31	O	314	DMS	O-S	4.55	1.81	1.50
31	c	942	DMS	O-S	4.55	1.81	1.50
22	B	613	CLA	CHC-C4B	4.55	1.49	1.39
22	b	605	CLA	O2D-CGD	4.55	1.44	1.33
22	B	605	CLA	C3C-C2C	4.55	1.46	1.36
22	c	910	CLA	MG-NC	4.55	2.17	2.06
31	L	102	DMS	O-S	4.55	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	407	CLA	C3C-C2C	4.55	1.46	1.36
31	a	424	DMS	O-S	4.55	1.81	1.50
22	D	403	CLA	C3B-C4B	4.55	1.53	1.42
31	b	637	DMS	O-S	4.55	1.81	1.50
27	A	412	LHG	O8-C23	4.55	1.46	1.33
31	c	940	DMS	O-S	4.54	1.80	1.50
25	C	520	LMG	O7-C10	4.54	1.47	1.34
31	b	634	DMS	O-S	4.54	1.80	1.50
28	a	418	SQD	O48-C23	4.54	1.46	1.33
31	u	203	DMS	O-S	4.54	1.80	1.50
22	B	612	CLA	C3B-C4B	4.54	1.53	1.42
31	U	202	DMS	O-S	4.54	1.80	1.50
31	V	204	DMS	O-S	4.53	1.80	1.50
31	d	411	DMS	O-S	4.53	1.80	1.50
31	O	306	DMS	O-S	4.53	1.80	1.50
22	c	914	CLA	O2A-CGA	4.53	1.46	1.33
31	C	536	DMS	O-S	4.53	1.80	1.50
31	f	103	DMS	O-S	4.53	1.80	1.50
31	b	630	DMS	O-S	4.53	1.80	1.50
31	t	104	DMS	O-S	4.53	1.80	1.50
23	D	402	PHO	OBD-CAD	4.53	1.28	1.22
22	B	613	CLA	CHC-C1C	4.53	1.47	1.38
31	A	419	DMS	O-S	4.52	1.80	1.50
31	c	928	DMS	O-S	4.52	1.80	1.50
31	c	944	DMS	O-S	4.52	1.80	1.50
31	t	103	DMS	O-S	4.52	1.80	1.50
22	C	506	CLA	O2D-CGD	4.52	1.44	1.33
22	d	403	CLA	CHD-C4C	4.52	1.49	1.39
22	b	609	CLA	MG-ND	-4.52	1.96	2.05
31	B	633	DMS	O-S	4.52	1.80	1.50
22	B	616	CLA	CHD-C1D	4.52	1.47	1.38
31	t	105	DMS	O-S	4.52	1.80	1.50
31	l	103	DMS	O-S	4.52	1.80	1.50
31	o	302	DMS	O-S	4.51	1.80	1.50
22	b	606	CLA	O2D-CGD	4.51	1.44	1.33
31	c	943	DMS	O-S	4.51	1.80	1.50
22	B	616	CLA	C1B-NB	-4.51	1.32	1.37
31	v	207	DMS	O-S	4.51	1.80	1.50
22	b	616	CLA	CHC-C1C	4.51	1.47	1.38
22	d	403	CLA	O2D-CGD	4.51	1.44	1.33
22	B	615	CLA	MG-NA	4.51	2.17	2.06
31	A	420	DMS	O-S	4.50	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	o	303	DMS	O-S	4.50	1.80	1.50
31	C	534	DMS	O-S	4.50	1.80	1.50
23	A	407	PHO	O2D-CGD	4.50	1.44	1.33
22	C	504	CLA	O2D-CGD	4.50	1.44	1.33
22	C	505	CLA	CHB-C1B	4.50	1.49	1.39
31	b	631	DMS	O-S	4.49	1.80	1.50
31	d	414	DMS	O-S	4.49	1.80	1.50
22	c	906	CLA	O2D-CGD	4.49	1.44	1.33
31	c	936	DMS	O-S	4.49	1.80	1.50
22	A	408	CLA	MG-NB	-4.49	1.96	2.05
22	b	611	CLA	CHD-C1D	4.49	1.47	1.38
22	a	408	CLA	CHD-C4C	4.49	1.49	1.39
22	c	903	CLA	O2D-CGD	4.49	1.44	1.33
31	c	925	DMS	O-S	4.49	1.80	1.50
31	C	539	DMS	O-S	4.49	1.80	1.50
31	v	206	DMS	O-S	4.49	1.80	1.50
31	C	527	DMS	O-S	4.48	1.80	1.50
22	C	504	CLA	O2A-CGA	4.48	1.46	1.33
22	C	513	CLA	CHB-C1B	4.48	1.49	1.39
22	A	405	CLA	CHC-C1C	4.48	1.47	1.38
31	C	530	DMS	O-S	4.48	1.80	1.50
28	l	101	SQD	O47-C7	4.48	1.46	1.34
23	D	402	PHO	C3C-C2C	4.48	1.46	1.36
28	l	101	SQD	O48-C23	4.48	1.46	1.33
31	I	106	DMS	O-S	4.48	1.80	1.50
35	H	102	DGD	O1G-C1A	4.48	1.46	1.33
28	a	418	SQD	O47-C7	4.48	1.46	1.34
28	b	621	SQD	O48-C23	4.48	1.46	1.33
23	a	411	PHO	O2D-CGD	4.47	1.44	1.33
35	c	919	DGD	O1G-C1A	4.47	1.46	1.33
22	B	604	CLA	CHB-C1B	4.47	1.49	1.39
22	C	506	CLA	C1D-ND	-4.47	1.32	1.37
31	A	417	DMS	O-S	4.47	1.80	1.50
22	B	610	CLA	O2D-CGD	4.47	1.44	1.33
27	D	409	LHG	O8-C23	4.46	1.46	1.33
31	b	633	DMS	O-S	4.46	1.80	1.50
31	B	642	DMS	O-S	4.46	1.80	1.50
22	C	503	CLA	O2D-CGD	4.46	1.44	1.33
22	c	912	CLA	CHD-C4C	4.46	1.49	1.39
22	B	613	CLA	MG-ND	-4.46	1.97	2.05
31	C	529	DMS	O-S	4.46	1.80	1.50
22	C	504	CLA	CHD-C1D	4.45	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	CHC-C1C	4.45	1.47	1.38
31	A	416	DMS	O-S	4.45	1.80	1.50
31	b	636	DMS	O-S	4.45	1.80	1.50
31	V	209	DMS	O-S	4.45	1.80	1.50
31	v	204	DMS	O-S	4.44	1.80	1.50
22	B	611	CLA	O2D-CGD	4.44	1.44	1.33
31	c	927	DMS	O-S	4.44	1.80	1.50
31	C	538	DMS	O-S	4.44	1.80	1.50
31	F	101	DMS	O-S	4.44	1.80	1.50
31	c	934	DMS	O-S	4.44	1.80	1.50
25	j	101	LMG	O8-C28	4.44	1.46	1.33
22	c	909	CLA	CHC-C4B	4.44	1.49	1.39
22	C	506	CLA	MG-NC	4.44	2.16	2.06
22	b	615	CLA	CHB-C1B	4.44	1.49	1.39
31	B	638	DMS	O-S	4.44	1.80	1.50
31	c	935	DMS	O-S	4.43	1.80	1.50
22	b	613	CLA	CHD-C1D	4.43	1.47	1.38
22	b	615	CLA	MG-ND	-4.43	1.97	2.05
22	b	602	CLA	CHC-C4B	4.43	1.49	1.39
22	c	904	CLA	O2D-CGD	4.42	1.44	1.33
31	a	421	DMS	O-S	4.42	1.80	1.50
22	D	401	CLA	O2D-CGD	4.42	1.44	1.33
31	O	310	DMS	O-S	4.42	1.80	1.50
22	C	512	CLA	CHB-C1B	4.42	1.49	1.39
28	C	501	SQD	O47-C7	4.42	1.46	1.34
23	a	410	PHO	C3B-C2B	4.42	1.46	1.40
22	B	605	CLA	OBD-CAD	4.42	1.30	1.22
25	b	622	LMG	O7-C10	4.42	1.46	1.34
22	c	911	CLA	O2D-CGD	4.42	1.44	1.33
22	c	912	CLA	CHC-C4B	4.41	1.49	1.39
22	c	913	CLA	O2A-CGA	4.41	1.46	1.33
31	B	632	DMS	O-S	4.41	1.80	1.50
22	c	906	CLA	CHC-C4B	4.41	1.49	1.39
22	C	506	CLA	CHD-C4C	4.41	1.49	1.39
22	A	405	CLA	O2D-CGD	4.41	1.44	1.33
25	d	409	LMG	O8-C28	4.41	1.46	1.33
22	c	908	CLA	O2D-CGD	4.41	1.44	1.33
25	C	531	LMG	O8-C28	4.40	1.46	1.33
31	o	306	DMS	O-S	4.40	1.80	1.50
31	i	106	DMS	O-S	4.40	1.80	1.50
31	v	209	DMS	O-S	4.40	1.80	1.50
31	O	312	DMS	O-S	4.40	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	423	LHG	O8-C23	4.40	1.46	1.33
31	C	526	DMS	O-S	4.40	1.79	1.50
22	B	611	CLA	CHB-C1B	4.40	1.49	1.39
31	C	528	DMS	O-S	4.40	1.79	1.50
22	A	405	CLA	MG-ND	-4.39	1.97	2.05
31	v	205	DMS	O-S	4.39	1.79	1.50
31	O	313	DMS	O-S	4.39	1.79	1.50
31	c	926	DMS	O-S	4.39	1.79	1.50
23	a	410	PHO	O2D-CGD	4.39	1.43	1.33
22	C	514	CLA	O2A-CGA	4.39	1.46	1.33
25	A	410	LMG	O8-C28	4.39	1.46	1.33
22	c	909	CLA	CHD-C1D	4.39	1.46	1.38
31	v	208	DMS	O-S	4.38	1.79	1.50
22	b	617	CLA	MG-ND	4.38	2.14	2.05
22	B	606	CLA	C3C-C2C	4.38	1.46	1.36
22	D	403	CLA	C3C-C2C	4.38	1.46	1.36
22	a	407	CLA	CHB-C1B	4.38	1.49	1.39
22	B	606	CLA	CHD-C1D	4.38	1.46	1.38
31	V	205	DMS	O-S	4.38	1.79	1.50
22	C	512	CLA	CHC-C1C	4.38	1.47	1.38
31	o	307	DMS	O-S	4.38	1.79	1.50
22	b	605	CLA	MG-NC	4.37	2.16	2.06
22	a	409	CLA	O2D-CGD	4.37	1.43	1.33
25	c	930	LMG	O8-C28	4.36	1.46	1.33
22	B	606	CLA	CHC-C4B	4.36	1.49	1.39
34	B	623	HTG	C1'-S1	-4.36	1.75	1.81
31	o	305	DMS	O-S	4.36	1.79	1.50
22	C	513	CLA	CHD-C1D	4.36	1.46	1.38
22	C	511	CLA	CHD-C1D	4.35	1.46	1.38
27	C	522	LHG	O8-C23	4.35	1.46	1.33
31	B	640	DMS	O-S	4.35	1.79	1.50
22	A	405	CLA	CHD-C1D	4.34	1.46	1.38
31	V	201	DMS	O-S	4.34	1.79	1.50
31	V	208	DMS	O-S	4.34	1.79	1.50
22	C	508	CLA	CHC-C4B	4.33	1.49	1.39
22	B	611	CLA	CHD-C1D	4.33	1.46	1.38
31	d	415	DMS	O-S	4.33	1.79	1.50
35	C	518	DGD	O1G-C1A	4.33	1.46	1.33
31	c	941	DMS	O-S	4.33	1.79	1.50
22	C	502	CLA	CHD-C1D	4.33	1.46	1.38
22	c	908	CLA	O2A-CGA	4.33	1.46	1.33
22	c	912	CLA	CHB-C1B	4.33	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	CHB-C1B	4.32	1.49	1.39
31	u	202	DMS	O-S	4.32	1.79	1.50
22	c	911	CLA	MG-NC	4.32	2.16	2.06
22	c	902	CLA	CHD-C1D	4.32	1.46	1.38
22	b	613	CLA	O2A-CGA	4.32	1.46	1.33
35	h	102	DGD	O1G-C1A	4.32	1.46	1.33
22	c	910	CLA	C3C-C2C	4.31	1.45	1.36
31	O	304	DMS	O-S	4.31	1.79	1.50
22	b	603	CLA	O2A-CGA	4.31	1.45	1.33
22	b	602	CLA	CHD-C4C	4.31	1.49	1.39
22	C	507	CLA	MG-NC	4.31	2.16	2.06
22	C	508	CLA	O2D-CGD	4.31	1.43	1.33
22	B	607	CLA	O2A-CGA	4.31	1.45	1.33
31	B	636	DMS	O-S	4.30	1.79	1.50
22	A	408	CLA	CHC-C1C	4.30	1.47	1.38
31	B	629	DMS	O-S	4.29	1.79	1.50
22	D	403	CLA	CHD-C1D	4.29	1.46	1.38
22	a	409	CLA	CHD-C1D	4.29	1.46	1.38
22	B	604	CLA	CHC-C1C	4.29	1.47	1.38
22	D	404	CLA	OBD-CAD	4.29	1.29	1.22
22	b	616	CLA	CHD-C1D	4.29	1.46	1.38
22	b	610	CLA	O2A-CGA	4.29	1.45	1.33
23	D	402	PHO	O2A-CGA	4.29	1.45	1.33
22	B	602	CLA	CHB-C1B	4.29	1.49	1.39
22	D	404	CLA	CHB-C1B	4.29	1.49	1.39
22	C	509	CLA	O2D-CGD	4.28	1.43	1.33
22	c	904	CLA	O2A-CGA	4.28	1.45	1.33
22	B	616	CLA	CHB-C1B	4.28	1.49	1.39
22	c	906	CLA	MG-NC	4.28	2.16	2.06
22	C	507	CLA	O2A-CGA	4.27	1.45	1.33
31	v	201	DMS	O-S	4.27	1.79	1.50
31	d	413	DMS	O-S	4.27	1.79	1.50
22	b	611	CLA	CHB-C1B	4.27	1.49	1.39
22	C	511	CLA	C3C-C2C	4.27	1.45	1.36
22	b	612	CLA	C3C-C2C	4.27	1.45	1.36
22	c	904	CLA	OBD-CAD	4.27	1.29	1.22
22	A	405	CLA	OBD-CAD	4.27	1.29	1.22
22	A	406	CLA	CHC-C1C	4.27	1.47	1.38
22	b	615	CLA	CHC-C1C	4.27	1.47	1.38
22	C	511	CLA	CHB-C1B	4.27	1.49	1.39
22	B	610	CLA	CHD-C1D	4.26	1.46	1.38
22	d	403	CLA	CHC-C4B	4.26	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	401	LHG	O7-C7	4.26	1.46	1.34
22	B	608	CLA	CHC-C1C	4.25	1.47	1.38
22	c	909	CLA	CHB-C1B	4.25	1.48	1.39
25	i	101	LMG	O7-C10	4.25	1.46	1.34
31	B	631	DMS	O-S	4.25	1.78	1.50
22	B	606	CLA	C1B-NB	-4.25	1.32	1.37
22	B	611	CLA	CHC-C4B	4.24	1.48	1.39
22	B	614	CLA	MG-NC	4.24	2.16	2.06
22	B	606	CLA	CHB-C1B	4.24	1.48	1.39
31	d	412	DMS	O-S	4.24	1.78	1.50
22	c	904	CLA	C1B-NB	-4.24	1.32	1.37
22	B	609	CLA	O2A-CGA	4.24	1.45	1.33
22	d	402	CLA	CHD-C4C	4.24	1.48	1.39
35	h	102	DGD	O2G-C1B	4.23	1.46	1.34
22	A	406	CLA	MG-ND	4.23	2.14	2.05
22	B	617	CLA	O2D-CGD	4.22	1.43	1.33
22	b	608	CLA	CHC-C1C	4.22	1.47	1.38
22	b	613	CLA	CHC-C4B	4.22	1.48	1.39
28	a	414	SQD	O47-C7	4.22	1.46	1.34
22	D	404	CLA	C4C-C3C	4.22	1.52	1.45
31	O	309	DMS	O-S	4.22	1.78	1.50
31	c	923	DMS	O-S	4.21	1.78	1.50
22	D	401	CLA	CHC-C4B	4.21	1.48	1.39
22	B	617	CLA	O2A-CGA	4.21	1.45	1.33
31	D	416	DMS	O-S	4.21	1.78	1.50
22	a	409	CLA	CHC-C1C	4.21	1.47	1.38
22	B	608	CLA	CHB-C1B	4.21	1.48	1.39
22	C	506	CLA	CHC-C4B	4.20	1.48	1.39
22	c	905	CLA	CHB-C1B	4.19	1.48	1.39
22	d	402	CLA	O2D-CGD	4.19	1.43	1.33
22	c	907	CLA	CHD-C4C	4.19	1.48	1.39
22	B	605	CLA	CHC-C1C	4.19	1.47	1.38
22	c	907	CLA	CHC-C1C	4.19	1.47	1.38
39	v	202	HEC	FE-ND	4.19	2.07	1.94
22	B	602	CLA	CHD-C4C	4.18	1.48	1.39
27	l	102	LHG	O7-C7	4.18	1.46	1.34
22	B	604	CLA	O2A-CGA	4.18	1.45	1.33
22	D	401	CLA	MG-NA	4.17	2.16	2.06
22	d	402	CLA	CHD-C1D	4.16	1.46	1.38
22	b	614	CLA	CHB-C1B	4.16	1.48	1.39
22	c	907	CLA	O2A-CGA	4.16	1.45	1.33
25	c	920	LMG	O7-C10	4.16	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	CHD-C4C	4.16	1.48	1.39
22	b	617	CLA	O2A-CGA	4.16	1.45	1.33
22	C	507	CLA	CHB-C1B	4.16	1.48	1.39
22	C	504	CLA	CHD-C4C	4.15	1.48	1.39
27	d	408	LHG	O8-C23	4.14	1.45	1.33
22	b	612	CLA	CHC-C1C	4.14	1.46	1.38
22	b	611	CLA	C1D-ND	-4.14	1.32	1.37
22	C	508	CLA	CHB-C1B	4.14	1.48	1.39
22	C	507	CLA	CHD-C4C	4.14	1.48	1.39
22	c	902	CLA	O2D-CGD	4.14	1.43	1.33
22	c	909	CLA	CHD-C4C	4.14	1.48	1.39
22	b	604	CLA	CHC-C1C	4.13	1.46	1.38
22	b	605	CLA	CHD-C1D	4.13	1.46	1.38
22	c	906	CLA	O2A-CGA	4.13	1.45	1.33
22	B	617	CLA	CHC-C1C	4.13	1.46	1.38
22	B	606	CLA	MG-ND	-4.12	1.97	2.05
23	A	407	PHO	O2A-CGA	4.12	1.45	1.33
31	C	524	DMS	O-S	4.12	1.78	1.50
22	C	502	CLA	O2D-CGD	4.12	1.43	1.33
25	d	409	LMG	O7-C10	4.11	1.45	1.34
22	D	403	CLA	O2A-CGA	4.11	1.45	1.33
22	b	617	CLA	CHB-C1B	4.11	1.48	1.39
22	C	502	CLA	CHD-C4C	4.11	1.48	1.39
22	a	408	CLA	O2D-CGD	4.11	1.43	1.33
22	b	614	CLA	CHD-C4C	4.11	1.48	1.39
22	b	617	CLA	CHD-C1D	4.11	1.46	1.38
22	B	610	CLA	CHB-C1B	4.11	1.48	1.39
22	b	609	CLA	O2A-CGA	4.10	1.45	1.33
22	b	616	CLA	OBD-CAD	4.10	1.29	1.22
28	A	413	SQD	O48-C23	4.10	1.45	1.33
22	B	605	CLA	CHB-C1B	4.10	1.48	1.39
22	b	612	CLA	O2A-CGA	4.09	1.45	1.33
22	B	605	CLA	O2D-CGD	4.09	1.43	1.33
22	b	608	CLA	CHD-C4C	4.09	1.48	1.39
22	A	406	CLA	OBD-CAD	4.09	1.29	1.22
22	d	403	CLA	CHB-C1B	4.09	1.48	1.39
22	b	616	CLA	CHD-C4C	4.08	1.48	1.39
22	B	610	CLA	O2A-CGA	4.08	1.45	1.33
22	B	608	CLA	C3C-C2C	4.08	1.45	1.36
22	b	602	CLA	MG-NB	-4.08	1.97	2.05
25	A	410	LMG	O7-C10	4.07	1.45	1.34
22	B	615	CLA	OBD-CAD	4.07	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	CHB-C1B	4.06	1.48	1.39
22	C	510	CLA	OBD-CAD	4.06	1.29	1.22
22	C	513	CLA	CHC-C4B	4.06	1.48	1.39
22	b	605	CLA	CHC-C1C	4.05	1.46	1.38
22	C	502	CLA	MG-NB	4.05	2.13	2.05
22	b	610	CLA	CHC-C4B	4.05	1.48	1.39
22	B	602	CLA	MG-NB	4.04	2.13	2.05
22	c	911	CLA	CHD-C4C	4.04	1.48	1.39
22	c	913	CLA	CHB-C1B	4.04	1.48	1.39
22	C	506	CLA	O2A-CGA	4.04	1.45	1.33
22	c	905	CLA	CHC-C4B	4.03	1.48	1.39
22	c	906	CLA	CHB-C1B	4.03	1.48	1.39
22	b	606	CLA	O2A-CGA	4.03	1.45	1.33
35	C	519	DGD	O1G-C1A	4.03	1.45	1.33
22	C	512	CLA	CHD-C1D	4.03	1.46	1.38
22	C	511	CLA	CHC-C1C	4.02	1.46	1.38
22	b	616	CLA	O2A-CGA	4.02	1.45	1.33
22	b	603	CLA	CHD-C1D	4.02	1.46	1.38
22	D	403	CLA	C1B-C2B	4.01	1.52	1.43
22	c	911	CLA	MG-NB	4.01	2.13	2.05
22	B	614	CLA	CHB-C1B	4.01	1.48	1.39
31	a	402	DMS	O-S	4.00	1.77	1.50
22	c	906	CLA	C3B-C4B	4.00	1.52	1.42
22	a	412	CLA	CHB-C1B	4.00	1.48	1.39
22	b	610	CLA	OBD-CAD	4.00	1.29	1.22
22	a	407	CLA	CHD-C4C	4.00	1.48	1.39
35	H	102	DGD	O2G-C1B	4.00	1.45	1.34
22	a	412	CLA	O2A-CGA	3.99	1.45	1.33
31	A	418	DMS	O-S	3.99	1.77	1.50
22	C	502	CLA	CHB-C1B	3.99	1.48	1.39
25	J	101	LMG	O7-C10	3.99	1.45	1.34
22	b	606	CLA	CHC-C4B	3.98	1.48	1.39
22	b	605	CLA	C3B-C4B	3.98	1.52	1.42
22	b	605	CLA	CHC-C4B	3.98	1.48	1.39
22	C	509	CLA	CHC-C4B	3.98	1.48	1.39
22	b	613	CLA	OBD-CAD	3.98	1.29	1.22
22	C	507	CLA	CHC-C4B	3.98	1.48	1.39
22	C	503	CLA	CHC-C4B	3.98	1.48	1.39
22	c	909	CLA	OBD-CAD	3.97	1.29	1.22
31	C	525	DMS	O-S	3.97	1.77	1.50
22	C	513	CLA	O2A-CGA	3.97	1.44	1.33
22	B	616	CLA	CHD-C4C	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	CHC-C4B	3.97	1.48	1.39
31	D	418	DMS	O-S	3.97	1.77	1.50
22	C	510	CLA	C4B-NB	-3.97	1.32	1.37
22	B	612	CLA	OBD-CAD	3.97	1.29	1.22
22	B	603	CLA	CHB-C1B	3.96	1.48	1.39
22	b	604	CLA	C1B-NB	-3.96	1.32	1.37
22	D	403	CLA	CHB-C1B	3.95	1.48	1.39
22	c	911	CLA	OBD-CAD	3.95	1.29	1.22
22	a	412	CLA	CHD-C4C	3.95	1.48	1.39
22	B	604	CLA	CHD-C4C	3.95	1.48	1.39
23	D	402	PHO	C3D-C2D	3.94	1.46	1.39
22	B	614	CLA	OBD-CAD	3.94	1.29	1.22
22	b	610	CLA	MG-NC	3.94	2.15	2.06
22	B	608	CLA	OBD-CAD	3.94	1.29	1.22
22	B	603	CLA	O2D-CGD	3.94	1.42	1.33
25	J	101	LMG	O8-C28	3.93	1.44	1.33
23	a	411	PHO	C3D-C2D	3.93	1.46	1.39
22	B	602	CLA	CHC-C4B	3.93	1.48	1.39
22	C	502	CLA	O2A-CGA	3.93	1.44	1.33
28	A	413	SQD	O47-C7	3.92	1.45	1.34
22	B	614	CLA	O2A-CGA	3.92	1.44	1.33
22	b	604	CLA	C1D-ND	-3.91	1.33	1.37
27	L	101	LHG	O8-C23	3.91	1.44	1.33
22	B	614	CLA	O2D-CGD	3.91	1.42	1.33
22	C	509	CLA	CHD-C4C	3.91	1.48	1.39
22	c	904	CLA	CHB-C1B	3.91	1.48	1.39
39	v	202	HEC	FE-NB	3.91	2.07	1.94
35	c	918	DGD	O1G-C1A	3.91	1.44	1.33
22	B	610	CLA	CHC-C4B	3.90	1.48	1.39
22	c	903	CLA	MG-NA	3.90	2.15	2.06
27	l	102	LHG	O8-C23	3.90	1.44	1.33
22	B	605	CLA	CHD-C4C	3.90	1.48	1.39
22	B	615	CLA	CHC-C4B	3.89	1.48	1.39
22	B	609	CLA	MG-NB	-3.89	1.98	2.05
22	a	408	CLA	O2A-CGA	3.89	1.44	1.33
23	a	410	PHO	C3D-C4D	-3.89	1.35	1.41
22	C	502	CLA	CHC-C4B	3.89	1.48	1.39
22	a	409	CLA	O2A-CGA	3.88	1.44	1.33
27	D	411	LHG	O7-C7	3.88	1.45	1.34
22	c	907	CLA	C1D-ND	-3.88	1.33	1.37
22	c	908	CLA	OBD-CAD	3.88	1.29	1.22
35	c	917	DGD	O2G-C1B	3.88	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	903	CLA	CHB-C1B	3.88	1.48	1.39
22	b	615	CLA	CHD-C4C	3.88	1.48	1.39
27	a	423	LHG	O7-C7	3.87	1.45	1.34
22	C	505	CLA	C3B-C4B	3.87	1.51	1.42
22	D	404	CLA	O2A-CGA	3.87	1.44	1.33
22	c	902	CLA	CHC-C4B	3.86	1.48	1.39
22	D	404	CLA	CHD-C4C	3.86	1.48	1.39
22	A	406	CLA	CHC-C4B	3.86	1.48	1.39
22	a	407	CLA	C4B-NB	-3.86	1.33	1.37
22	B	613	CLA	C1B-NB	-3.86	1.33	1.37
28	C	501	SQD	O48-C23	3.85	1.44	1.33
22	b	612	CLA	CHD-C1D	3.85	1.45	1.38
22	c	911	CLA	C3D-C2D	3.85	1.49	1.39
22	B	611	CLA	CHD-C4C	3.85	1.48	1.39
27	L	101	LHG	O7-C7	3.85	1.45	1.34
22	b	611	CLA	CHC-C4B	3.85	1.48	1.39
22	C	509	CLA	CHB-C1B	3.84	1.48	1.39
22	C	512	CLA	CHD-C4C	3.84	1.48	1.39
22	c	914	CLA	MG-ND	3.84	2.13	2.05
22	B	603	CLA	O2A-CGA	3.84	1.44	1.33
22	C	511	CLA	CHD-C4C	3.84	1.48	1.39
22	b	607	CLA	CHC-C4B	3.83	1.48	1.39
22	b	617	CLA	C1D-ND	-3.83	1.33	1.37
27	D	409	LHG	O7-C7	3.83	1.45	1.34
22	B	606	CLA	O2D-CGD	3.83	1.42	1.33
23	a	411	PHO	C3D-C4D	-3.83	1.35	1.41
22	c	914	CLA	CHD-C4C	3.83	1.48	1.39
22	b	608	CLA	CHC-C4B	3.83	1.48	1.39
22	a	408	CLA	OBD-CAD	3.82	1.29	1.22
22	b	609	CLA	OBD-CAD	3.82	1.29	1.22
22	C	504	CLA	CHB-C1B	3.82	1.48	1.39
22	B	602	CLA	C4C-C3C	3.82	1.51	1.45
22	C	505	CLA	CHC-C4B	3.82	1.48	1.39
22	b	609	CLA	C4B-NB	-3.81	1.33	1.37
22	C	503	CLA	C3B-C4B	3.81	1.51	1.42
22	B	616	CLA	O2A-CGA	3.80	1.44	1.33
22	D	403	CLA	C1D-ND	-3.80	1.33	1.37
22	c	914	CLA	CHC-C4B	3.80	1.47	1.39
22	c	909	CLA	O2A-CGA	3.80	1.44	1.33
22	b	609	CLA	O2D-CGD	3.80	1.42	1.33
22	A	408	CLA	CHD-C4C	3.80	1.47	1.39
22	C	512	CLA	OBD-CAD	3.80	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	O2A-CGA	3.79	1.44	1.33
22	c	913	CLA	MG-ND	-3.79	1.98	2.05
22	b	606	CLA	CHD-C1D	3.79	1.45	1.38
22	a	412	CLA	C4B-NB	-3.79	1.33	1.37
22	c	909	CLA	C3B-C4B	3.79	1.51	1.42
22	C	503	CLA	O2A-CGA	3.79	1.44	1.33
34	C	532	HTG	C1'-S1	-3.78	1.76	1.81
22	C	513	CLA	CHD-C4C	3.78	1.47	1.39
22	b	613	CLA	CHB-C1B	3.78	1.47	1.39
22	b	608	CLA	C3D-C2D	3.77	1.49	1.39
22	c	910	CLA	CHD-C4C	3.77	1.47	1.39
22	a	412	CLA	C1D-ND	-3.77	1.33	1.37
22	d	403	CLA	C3D-C2D	3.76	1.49	1.39
31	b	629	DMS	O-S	3.76	1.75	1.50
25	j	101	LMG	O7-C10	3.76	1.44	1.34
22	A	405	CLA	CHC-C4B	3.76	1.47	1.39
22	c	908	CLA	CHD-C1D	3.75	1.45	1.38
22	C	504	CLA	OBD-CAD	3.75	1.28	1.22
22	B	609	CLA	C1D-ND	-3.75	1.33	1.37
22	C	506	CLA	OBD-CAD	3.75	1.28	1.22
22	D	404	CLA	CHC-C4B	3.75	1.47	1.39
22	b	609	CLA	CHC-C4B	3.75	1.47	1.39
22	B	612	CLA	O2A-CGA	3.74	1.44	1.33
36	E	102	HEM	FE-NC	3.74	2.07	1.95
22	D	401	CLA	CHD-C4C	3.74	1.47	1.39
22	C	506	CLA	C3B-C4B	3.73	1.51	1.42
39	v	202	HEC	FE-NC	3.73	2.07	1.95
22	b	602	CLA	OBD-CAD	3.73	1.28	1.22
22	B	617	CLA	CHC-C4B	3.73	1.47	1.39
22	b	602	CLA	C3D-C2D	3.72	1.49	1.39
22	C	514	CLA	CHD-C4C	3.72	1.47	1.39
35	c	919	DGD	O2G-C1B	3.72	1.44	1.34
22	C	510	CLA	C3D-C2D	3.71	1.49	1.39
22	b	604	CLA	MG-ND	3.71	2.13	2.05
22	b	609	CLA	CHB-C1B	3.71	1.47	1.39
22	a	408	CLA	CHD-C1D	3.71	1.45	1.38
22	C	506	CLA	C4C-C3C	3.71	1.51	1.45
34	b	623	HTG	C1'-S1	-3.71	1.76	1.81
22	B	612	CLA	CHD-C4C	3.70	1.47	1.39
22	C	509	CLA	C3D-C2D	3.70	1.49	1.39
22	B	617	CLA	CHD-C1D	3.70	1.45	1.38
22	b	603	CLA	C4D-ND	3.70	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	409	CLA	CHD-C4C	3.70	1.47	1.39
22	c	903	CLA	CHD-C4C	3.69	1.47	1.39
22	b	614	CLA	O2A-CGA	3.68	1.44	1.33
22	a	408	CLA	C1D-ND	-3.68	1.33	1.37
22	B	612	CLA	CHC-C4B	3.68	1.47	1.39
22	b	607	CLA	CHB-C1B	3.68	1.47	1.39
35	c	917	DGD	O1G-C1A	3.68	1.44	1.33
22	D	403	CLA	O2D-CGD	3.67	1.42	1.33
22	B	617	CLA	CHB-C1B	3.67	1.47	1.39
22	b	605	CLA	CHB-C1B	3.67	1.47	1.39
22	c	904	CLA	CHD-C4C	3.67	1.47	1.39
22	B	607	CLA	CHD-C1D	3.67	1.45	1.38
22	c	908	CLA	CHD-C4C	3.66	1.47	1.39
27	D	411	LHG	O8-C23	3.66	1.44	1.33
22	D	401	CLA	C3B-C4B	3.66	1.51	1.42
22	A	406	CLA	CHD-C4C	3.65	1.47	1.39
22	C	508	CLA	CHD-C4C	3.65	1.47	1.39
22	B	606	CLA	C1D-ND	-3.65	1.33	1.37
22	b	606	CLA	CHD-C4C	3.65	1.47	1.39
22	a	409	CLA	C3C-C2C	3.65	1.44	1.36
23	a	411	PHO	O2A-CGA	3.64	1.44	1.33
22	c	913	CLA	CHD-C4C	3.64	1.47	1.39
22	d	403	CLA	C4C-C3C	3.64	1.51	1.45
22	B	613	CLA	O2A-CGA	3.64	1.44	1.33
22	A	408	CLA	OBD-CAD	3.64	1.28	1.22
22	B	613	CLA	CHB-C1B	3.64	1.47	1.39
22	a	409	CLA	CHB-C1B	3.64	1.47	1.39
22	c	902	CLA	CHB-C1B	3.63	1.47	1.39
22	c	911	CLA	O2A-CGA	3.63	1.43	1.33
22	B	617	CLA	MG-ND	3.63	2.13	2.05
22	b	611	CLA	O2A-CGA	3.63	1.43	1.33
22	b	611	CLA	CHD-C4C	3.62	1.47	1.39
22	C	511	CLA	O2A-CGA	3.62	1.43	1.33
22	C	512	CLA	CHC-C4B	3.62	1.47	1.39
22	c	911	CLA	CHB-C1B	3.62	1.47	1.39
22	b	604	CLA	CHC-C4B	3.62	1.47	1.39
22	b	603	CLA	CHC-C4B	3.62	1.47	1.39
22	b	615	CLA	C3D-C2D	3.61	1.49	1.39
22	b	613	CLA	C3B-C4B	3.61	1.51	1.42
22	c	910	CLA	CHB-C1B	3.61	1.47	1.39
22	c	913	CLA	CHC-C4B	3.61	1.47	1.39
22	b	615	CLA	CHC-C4B	3.61	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	905	CLA	MG-NB	3.60	2.12	2.05
22	C	503	CLA	CHB-C1B	3.60	1.47	1.39
22	c	902	CLA	O2A-CGA	3.60	1.43	1.33
22	B	617	CLA	CHD-C4C	3.60	1.47	1.39
22	B	615	CLA	CHD-C4C	3.60	1.47	1.39
22	b	604	CLA	CHD-C4C	3.60	1.47	1.39
22	b	607	CLA	C1D-ND	-3.60	1.33	1.37
22	c	903	CLA	CHC-C4B	3.59	1.47	1.39
22	b	607	CLA	C3B-C4B	3.59	1.51	1.42
22	a	407	CLA	O2A-CGA	3.59	1.43	1.33
22	c	907	CLA	OBD-CAD	3.59	1.28	1.22
23	a	410	PHO	O2A-CGA	3.58	1.43	1.33
22	d	402	CLA	MG-NC	3.58	2.14	2.06
22	B	617	CLA	C3D-C2D	3.58	1.48	1.39
22	b	616	CLA	CHC-C4B	3.58	1.47	1.39
35	c	918	DGD	O2G-C1B	3.58	1.44	1.34
22	A	408	CLA	O2A-CGA	3.57	1.43	1.33
22	B	611	CLA	C3B-C4B	3.57	1.51	1.42
22	B	605	CLA	MG-ND	3.56	2.12	2.05
22	c	902	CLA	OBD-CAD	3.55	1.28	1.22
22	c	913	CLA	OBD-CAD	3.55	1.28	1.22
22	c	905	CLA	CHD-C1D	3.55	1.45	1.38
22	B	610	CLA	C1B-NB	-3.54	1.33	1.37
22	B	611	CLA	C3D-C2D	3.54	1.48	1.39
22	a	407	CLA	CHC-C4B	3.54	1.47	1.39
22	c	905	CLA	C3D-C2D	3.54	1.48	1.39
22	A	406	CLA	C3B-C4B	3.54	1.51	1.42
22	b	602	CLA	C3B-C4B	3.54	1.51	1.42
22	B	613	CLA	CHD-C4C	3.53	1.47	1.39
22	A	406	CLA	C1D-ND	-3.53	1.33	1.37
39	v	202	HEC	CBC-CAC	-3.53	1.35	1.51
22	b	605	CLA	O2A-CGA	3.53	1.43	1.33
22	a	408	CLA	MG-NA	3.53	2.14	2.06
27	d	408	LHG	O7-C7	3.53	1.44	1.34
22	C	514	CLA	C3B-C4B	3.53	1.51	1.42
22	B	610	CLA	C1D-ND	-3.53	1.33	1.37
22	A	406	CLA	O2A-CGA	3.53	1.43	1.33
22	c	903	CLA	O2A-CGA	3.53	1.43	1.33
22	b	608	CLA	MG-NB	3.52	2.12	2.05
22	b	607	CLA	O2A-CGA	3.52	1.43	1.33
22	B	609	CLA	CHD-C4C	3.52	1.47	1.39
22	b	603	CLA	C3B-C4B	3.52	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	C3D-C2D	3.51	1.48	1.39
22	C	511	CLA	CHC-C4B	3.51	1.47	1.39
22	B	603	CLA	CHC-C4B	3.51	1.47	1.39
22	A	408	CLA	CHC-C4B	3.51	1.47	1.39
22	B	611	CLA	O2A-CGA	3.50	1.43	1.33
22	C	512	CLA	C3B-C4B	3.50	1.50	1.42
22	B	605	CLA	O2A-CGA	3.50	1.43	1.33
22	d	402	CLA	CHB-C1B	3.50	1.47	1.39
22	c	910	CLA	CHC-C1C	3.49	1.45	1.38
22	c	905	CLA	O2A-CGA	3.49	1.43	1.33
22	A	405	CLA	C1D-ND	-3.49	1.33	1.37
22	b	606	CLA	C3B-C4B	3.49	1.50	1.42
22	b	617	CLA	C4D-CHA	3.48	1.50	1.38
22	B	606	CLA	O2A-CGA	3.48	1.43	1.33
22	C	509	CLA	MG-NB	3.48	2.12	2.05
34	v	203	HTG	C1'-S1	-3.48	1.77	1.81
22	c	907	CLA	C1B-NB	-3.47	1.33	1.37
25	b	622	LMG	O1-C1	3.47	1.46	1.40
22	B	609	CLA	CHC-C4B	3.47	1.47	1.39
22	A	406	CLA	C1B-NB	-3.46	1.33	1.37
22	D	404	CLA	C3B-C4B	3.46	1.50	1.42
22	b	606	CLA	C1B-C2B	3.46	1.51	1.43
22	b	612	CLA	CHC-C4B	3.45	1.47	1.39
22	B	617	CLA	C1B-NB	-3.45	1.33	1.37
22	b	617	CLA	CHC-C4B	3.45	1.47	1.39
22	c	910	CLA	C4C-C3C	3.44	1.51	1.45
22	b	609	CLA	MG-NC	3.44	2.14	2.06
22	b	607	CLA	C1B-NB	-3.44	1.33	1.37
22	D	403	CLA	CHD-C4C	3.44	1.47	1.39
22	C	513	CLA	OBD-CAD	3.43	1.28	1.22
22	B	609	CLA	C1B-NB	-3.43	1.33	1.37
22	c	907	CLA	CHC-C4B	3.42	1.47	1.39
23	A	407	PHO	C3A-C2A	-3.42	1.51	1.54
26	A	411	PL9	C7-C3	3.42	1.54	1.51
22	B	609	CLA	CHB-C1B	3.42	1.47	1.39
22	c	912	CLA	C3B-C4B	3.42	1.50	1.42
22	B	603	CLA	OBD-CAD	3.42	1.28	1.22
22	b	605	CLA	C4D-CHA	3.42	1.50	1.38
22	b	617	CLA	OBD-CAD	3.41	1.28	1.22
22	a	408	CLA	CHC-C4B	3.41	1.47	1.39
22	c	903	CLA	C3D-C2D	3.41	1.48	1.39
22	C	505	CLA	MG-NB	3.41	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	C3D-C2D	3.41	1.48	1.39
22	c	912	CLA	OBD-CAD	3.41	1.28	1.22
22	C	508	CLA	O2A-CGA	3.41	1.43	1.33
35	C	517	DGD	O1G-C1A	3.41	1.43	1.33
22	d	402	CLA	C3B-C4B	3.41	1.50	1.42
22	c	910	CLA	C3D-C2D	3.41	1.48	1.39
22	c	910	CLA	C3B-C4B	3.40	1.50	1.42
22	b	602	CLA	C4D-CHA	3.40	1.50	1.38
22	c	903	CLA	C3B-C4B	3.40	1.50	1.42
22	C	503	CLA	OBD-CAD	3.40	1.28	1.22
22	b	611	CLA	C4C-C3C	3.40	1.50	1.45
22	b	615	CLA	C4C-C3C	3.40	1.50	1.45
22	c	905	CLA	MG-ND	-3.40	1.99	2.05
22	B	602	CLA	OBD-CAD	3.39	1.28	1.22
22	c	912	CLA	O2A-CGA	3.39	1.43	1.33
22	C	506	CLA	C1B-NB	-3.39	1.33	1.37
22	b	613	CLA	C3D-C2D	3.39	1.48	1.39
22	B	609	CLA	C3D-C2D	3.39	1.48	1.39
22	c	907	CLA	CHB-C1B	3.38	1.47	1.39
22	b	610	CLA	CHD-C4C	3.38	1.47	1.39
22	C	509	CLA	C3B-C4B	3.37	1.50	1.42
22	c	908	CLA	C3D-C2D	3.37	1.48	1.39
34	l	106	HTG	C1'-S1	-3.37	1.77	1.81
22	b	608	CLA	O2A-CGA	3.37	1.43	1.33
22	D	401	CLA	CHD-C1D	3.36	1.44	1.38
22	b	617	CLA	C1C-NC	-3.35	1.32	1.37
22	b	606	CLA	C1B-NB	-3.35	1.33	1.37
22	C	504	CLA	C4D-CHA	3.35	1.50	1.38
22	D	404	CLA	C1D-ND	-3.35	1.33	1.37
22	B	616	CLA	CHC-C4B	3.35	1.46	1.39
22	D	403	CLA	C4C-C3C	3.35	1.50	1.45
22	A	405	CLA	CHB-C1B	3.35	1.46	1.39
22	C	502	CLA	C3D-C2D	3.34	1.48	1.39
22	c	902	CLA	CHD-C4C	3.34	1.46	1.39
22	b	605	CLA	C1B-NB	-3.34	1.33	1.37
22	C	510	CLA	CHD-C4C	3.34	1.46	1.39
22	B	613	CLA	C1D-ND	-3.34	1.33	1.37
22	C	504	CLA	C3B-C4B	3.33	1.50	1.42
22	B	610	CLA	C3D-C2D	3.33	1.48	1.39
22	B	610	CLA	C4D-CHA	3.32	1.50	1.38
22	c	902	CLA	C3B-C4B	3.32	1.50	1.42
22	B	611	CLA	C4C-C3C	3.31	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	913	CLA	C3D-C2D	3.31	1.48	1.39
22	C	513	CLA	C3B-C4B	3.30	1.50	1.42
27	D	410	LHG	O7-C7	3.30	1.43	1.34
22	B	602	CLA	C1D-ND	-3.30	1.33	1.37
22	C	509	CLA	C1C-NC	-3.30	1.32	1.37
22	c	908	CLA	C4D-CHA	3.30	1.50	1.38
22	C	510	CLA	C1B-NB	-3.30	1.33	1.37
22	C	514	CLA	C4D-CHA	3.30	1.50	1.38
22	C	505	CLA	O2A-CGA	3.29	1.43	1.33
22	B	603	CLA	C1B-C2B	3.29	1.51	1.43
22	C	505	CLA	C4D-CHA	3.29	1.50	1.38
22	c	905	CLA	CHD-C4C	3.28	1.46	1.39
22	c	909	CLA	C4C-C3C	3.28	1.50	1.45
22	C	508	CLA	OBD-CAD	3.28	1.28	1.22
22	C	512	CLA	C4D-CHA	3.28	1.50	1.38
22	B	603	CLA	C3B-C4B	3.28	1.50	1.42
22	a	408	CLA	CHB-C1B	3.28	1.46	1.39
22	b	606	CLA	C1D-ND	-3.28	1.33	1.37
39	V	202	HEC	CBB-CAB	-3.27	1.36	1.51
22	b	610	CLA	C3D-C2D	3.27	1.48	1.39
22	b	613	CLA	CHD-C4C	3.27	1.46	1.39
27	D	410	LHG	O8-C23	3.26	1.42	1.33
22	c	906	CLA	C3D-C2D	3.26	1.48	1.39
22	B	606	CLA	C3B-C4B	3.25	1.50	1.42
22	c	904	CLA	C4B-NB	-3.25	1.33	1.37
22	B	616	CLA	C1D-ND	-3.25	1.33	1.37
22	C	511	CLA	C4C-C3C	3.25	1.50	1.45
39	v	202	HEC	CBB-CAB	-3.25	1.37	1.51
22	C	512	CLA	C1D-ND	-3.24	1.33	1.37
22	c	913	CLA	C1D-ND	-3.24	1.33	1.37
22	B	607	CLA	CHB-C1B	3.24	1.46	1.39
22	c	914	CLA	OBD-CAD	3.24	1.28	1.22
22	B	610	CLA	CHD-C4C	3.24	1.46	1.39
22	C	512	CLA	C1B-C2B	3.23	1.50	1.43
22	B	612	CLA	C1B-C2B	3.23	1.50	1.43
22	A	406	CLA	CHD-C1D	3.22	1.44	1.38
22	b	604	CLA	C3D-C2D	3.22	1.47	1.39
22	B	610	CLA	C3B-C4B	3.22	1.50	1.42
22	b	617	CLA	C3D-C2D	3.22	1.47	1.39
22	C	512	CLA	C4C-C3C	3.22	1.50	1.45
22	B	606	CLA	C1C-C2C	3.22	1.50	1.44
22	c	912	CLA	C4D-CHA	3.22	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	415	HTG	C1'-S1	-3.21	1.77	1.81
22	b	605	CLA	C3D-C2D	3.21	1.47	1.39
22	D	401	CLA	C3D-C2D	3.21	1.47	1.39
22	c	911	CLA	C3B-C4B	3.21	1.50	1.42
23	A	407	PHO	C4B-NB	-3.20	1.32	1.38
22	D	403	CLA	CHC-C4B	3.20	1.46	1.39
39	V	202	HEC	CBC-CAC	-3.20	1.37	1.51
23	A	407	PHO	C3D-C2D	3.19	1.45	1.39
34	b	624	HTG	C1'-S1	-3.19	1.77	1.81
36	E	102	HEM	CAC-C3C	3.19	1.56	1.47
22	c	904	CLA	CHC-C4B	3.19	1.46	1.39
22	B	616	CLA	C1C-NC	-3.19	1.33	1.37
22	b	607	CLA	CHD-C4C	3.19	1.46	1.39
22	c	914	CLA	C3D-C2D	3.19	1.47	1.39
22	B	604	CLA	CHC-C4B	3.19	1.46	1.39
22	A	405	CLA	CHD-C4C	3.18	1.46	1.39
22	B	616	CLA	C4D-CHA	3.18	1.49	1.38
22	c	905	CLA	C4C-C3C	3.18	1.50	1.45
22	b	616	CLA	C4C-C3C	3.18	1.50	1.45
22	C	512	CLA	C3D-C2D	3.17	1.47	1.39
22	a	409	CLA	C1B-C2B	3.17	1.50	1.43
22	b	612	CLA	C1B-NB	-3.17	1.33	1.37
22	C	507	CLA	C3B-C4B	3.17	1.50	1.42
22	A	405	CLA	C3D-C2D	3.17	1.47	1.39
22	B	616	CLA	C3D-C2D	3.17	1.47	1.39
22	C	514	CLA	C3D-C2D	3.17	1.47	1.39
23	A	407	PHO	OBD-CAD	3.16	1.26	1.22
22	B	605	CLA	C3B-C4B	3.16	1.50	1.42
22	D	404	CLA	C3D-C2D	3.16	1.47	1.39
22	c	906	CLA	MG-NB	3.16	2.12	2.05
22	d	402	CLA	C4C-C3C	3.15	1.50	1.45
22	b	615	CLA	MG-NC	3.15	2.13	2.06
22	b	610	CLA	C3B-C4B	3.15	1.50	1.42
22	B	612	CLA	CHB-C1B	3.15	1.46	1.39
22	C	503	CLA	C4D-CHA	3.15	1.49	1.38
22	b	604	CLA	C3B-C4B	3.15	1.50	1.42
22	B	614	CLA	C3D-C2D	3.15	1.47	1.39
22	D	403	CLA	MG-NC	3.15	2.13	2.06
22	B	610	CLA	C4B-NB	-3.14	1.33	1.37
28	A	413	SQD	C6-S	-3.14	1.65	1.77
22	B	602	CLA	C4D-CHA	3.14	1.49	1.38
22	b	608	CLA	OBD-CAD	3.14	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	C3B-C4B	3.14	1.50	1.42
22	a	407	CLA	OBD-CAD	3.13	1.27	1.22
22	a	407	CLA	C3D-C2D	3.13	1.47	1.39
22	B	604	CLA	MG-NB	-3.13	1.99	2.05
22	b	604	CLA	C4D-CHA	3.13	1.49	1.38
22	b	612	CLA	C3D-C2D	3.13	1.47	1.39
22	C	507	CLA	C1D-ND	-3.13	1.33	1.37
22	b	611	CLA	C4D-CHA	3.13	1.49	1.38
22	A	405	CLA	O2A-CGA	3.12	1.42	1.33
22	B	602	CLA	C3D-C2D	3.12	1.47	1.39
22	C	510	CLA	CHC-C4B	3.12	1.46	1.39
22	B	607	CLA	C4D-CHA	3.11	1.49	1.38
22	B	605	CLA	C4C-C3C	3.11	1.50	1.45
23	a	410	PHO	OBD-CAD	3.11	1.26	1.22
22	A	406	CLA	CHB-C1B	3.11	1.46	1.39
22	C	514	CLA	C1C-C2C	3.10	1.50	1.44
22	B	606	CLA	CHD-C4C	3.10	1.46	1.39
22	C	510	CLA	CHB-C1B	3.09	1.46	1.39
22	B	608	CLA	CHC-C4B	3.09	1.46	1.39
22	c	903	CLA	C4D-CHA	3.09	1.49	1.38
22	B	615	CLA	CHD-C1D	3.08	1.44	1.38
22	C	511	CLA	C3D-C2D	3.08	1.47	1.39
22	d	403	CLA	C3B-C4B	3.08	1.50	1.42
22	d	402	CLA	OBD-CAD	3.08	1.27	1.22
36	E	102	HEM	CAB-C3B	3.08	1.55	1.47
22	B	615	CLA	C3D-C2D	3.08	1.47	1.39
22	B	609	CLA	C4D-CHA	3.08	1.49	1.38
22	B	611	CLA	OBD-CAD	3.07	1.27	1.22
22	B	613	CLA	OBD-CAD	3.07	1.27	1.22
22	d	403	CLA	C4D-ND	3.07	1.41	1.37
22	B	605	CLA	CHC-C4B	3.07	1.46	1.39
22	B	602	CLA	C1C-NC	-3.07	1.33	1.37
22	D	401	CLA	CHB-C1B	3.06	1.46	1.39
22	b	608	CLA	C4D-CHA	3.06	1.49	1.38
22	b	607	CLA	MG-NC	3.06	2.13	2.06
22	a	412	CLA	OBD-CAD	3.06	1.27	1.22
22	C	510	CLA	C4C-C3C	3.06	1.50	1.45
22	b	612	CLA	CHD-C4C	3.06	1.46	1.39
22	A	408	CLA	C3B-C4B	3.06	1.49	1.42
22	a	408	CLA	C3D-C2D	3.05	1.47	1.39
36	e	101	HEM	CAB-C3B	3.05	1.55	1.47
22	c	904	CLA	C4D-CHA	3.05	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	OBD-CAD	3.05	1.27	1.22
22	C	506	CLA	C3D-C2D	3.05	1.47	1.39
27	d	407	LHG	O7-C7	3.05	1.42	1.34
22	B	616	CLA	MG-NC	3.04	2.13	2.06
22	b	611	CLA	C3D-C2D	3.04	1.47	1.39
22	C	505	CLA	C1C-NC	-3.04	1.33	1.37
22	C	507	CLA	C3D-C2D	3.04	1.47	1.39
22	b	612	CLA	C1B-C2B	3.04	1.50	1.43
22	c	906	CLA	C4D-CHA	3.03	1.49	1.38
22	D	401	CLA	C1B-C2B	3.03	1.50	1.43
22	C	504	CLA	C1C-C2C	3.03	1.50	1.44
22	c	907	CLA	C4C-C3C	3.03	1.50	1.45
22	a	408	CLA	MG-NC	3.03	2.13	2.06
22	a	412	CLA	C1B-NB	-3.03	1.34	1.37
22	b	617	CLA	C4B-NB	-3.03	1.34	1.37
22	B	617	CLA	C3B-C4B	3.02	1.49	1.42
22	b	617	CLA	C1B-C2B	3.02	1.50	1.43
35	C	517	DGD	O2G-C1B	3.02	1.42	1.34
22	B	603	CLA	C1C-NC	-3.02	1.33	1.37
22	C	506	CLA	C4D-CHA	3.02	1.49	1.38
22	c	913	CLA	C4B-NB	-3.02	1.34	1.37
35	C	518	DGD	O3G-C1D	3.02	1.45	1.40
22	c	907	CLA	C3B-C4B	3.02	1.49	1.42
22	c	902	CLA	C1C-C2C	3.01	1.50	1.44
22	A	405	CLA	C4C-C3C	3.01	1.50	1.45
22	B	608	CLA	O2A-CGA	3.01	1.42	1.33
22	b	616	CLA	MG-ND	3.01	2.11	2.05
22	B	602	CLA	C1B-NB	-3.01	1.34	1.37
22	A	408	CLA	C4C-C3C	3.01	1.50	1.45
22	B	614	CLA	CHD-C4C	3.01	1.46	1.39
22	c	911	CLA	C1C-NC	-3.01	1.33	1.37
22	c	907	CLA	C4D-CHA	3.01	1.49	1.38
22	D	401	CLA	CHC-C1C	3.00	1.44	1.38
22	B	615	CLA	C4D-CHA	3.00	1.49	1.38
22	a	409	CLA	CHC-C4B	3.00	1.46	1.39
22	b	613	CLA	C4D-CHA	2.99	1.49	1.38
22	C	505	CLA	C3D-C2D	2.99	1.47	1.39
22	B	613	CLA	MG-NC	-2.99	1.99	2.06
29	f	102	LMT	O1'-C1'	2.99	1.45	1.40
22	B	610	CLA	C1B-C2B	2.99	1.50	1.43
22	b	616	CLA	C1D-ND	-2.99	1.34	1.37
22	B	605	CLA	C1B-C2B	2.98	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	C1D-ND	-2.98	1.34	1.37
22	C	513	CLA	C4D-CHA	2.98	1.49	1.38
22	b	615	CLA	C4D-CHA	2.98	1.49	1.38
22	C	513	CLA	C3D-C2D	2.98	1.47	1.39
22	b	604	CLA	CHB-C1B	2.98	1.46	1.39
22	C	508	CLA	C4D-CHA	2.98	1.49	1.38
22	c	906	CLA	C1C-NC	-2.98	1.33	1.37
22	b	609	CLA	C4D-CHA	2.98	1.49	1.38
22	c	908	CLA	MG-NB	-2.97	1.99	2.05
22	b	614	CLA	OBD-CAD	2.97	1.27	1.22
22	b	616	CLA	C3D-C2D	2.97	1.47	1.39
22	b	607	CLA	C1C-C2C	2.97	1.50	1.44
22	C	509	CLA	OBD-CAD	2.96	1.27	1.22
22	B	615	CLA	MG-ND	-2.96	1.99	2.05
22	B	613	CLA	C3D-C2D	2.96	1.47	1.39
22	B	615	CLA	C1D-ND	-2.96	1.34	1.37
22	C	506	CLA	CHB-C1B	2.96	1.46	1.39
22	C	507	CLA	C4D-CHA	2.96	1.48	1.38
22	A	408	CLA	CHB-C1B	2.96	1.46	1.39
22	B	605	CLA	C4D-CHA	2.96	1.48	1.38
22	a	409	CLA	C3B-C4B	2.96	1.49	1.42
34	C	521	HTG	C1'-S1	-2.95	1.77	1.81
22	B	605	CLA	MG-NC	2.95	2.13	2.06
22	d	403	CLA	C1C-NC	-2.95	1.33	1.37
22	B	615	CLA	C1C-C2C	2.95	1.50	1.44
22	a	407	CLA	C3B-C4B	2.95	1.49	1.42
22	B	612	CLA	C3D-C2D	2.95	1.47	1.39
22	c	902	CLA	C4C-C3C	2.95	1.50	1.45
22	C	507	CLA	MG-NB	2.95	2.11	2.05
22	B	611	CLA	C1C-C2C	2.95	1.50	1.44
22	b	615	CLA	C1C-NC	-2.94	1.33	1.37
22	c	911	CLA	C1B-NB	-2.94	1.34	1.37
22	b	616	CLA	MG-NB	2.94	2.11	2.05
22	C	502	CLA	C4D-CHA	2.94	1.48	1.38
22	c	912	CLA	C3D-C2D	2.93	1.47	1.39
22	A	408	CLA	C4D-CHA	2.93	1.48	1.38
22	b	608	CLA	C1B-NB	-2.93	1.34	1.37
22	a	412	CLA	C4D-CHA	2.93	1.48	1.38
22	B	605	CLA	C1B-NB	-2.93	1.34	1.37
22	C	502	CLA	OBD-CAD	2.93	1.27	1.22
22	C	508	CLA	C3D-C2D	2.92	1.47	1.39
22	a	409	CLA	OBD-CAD	2.92	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	407	CLA	C4D-CHA	2.92	1.48	1.38
35	H	102	DGD	O5D-C1E	2.92	1.45	1.40
22	b	606	CLA	C4D-CHA	2.92	1.48	1.38
22	b	609	CLA	C3D-C2D	2.92	1.47	1.39
28	a	414	SQD	C6-S	-2.92	1.66	1.77
22	b	602	CLA	C1C-C2C	2.92	1.50	1.44
22	b	613	CLA	C4B-NB	-2.91	1.34	1.37
22	C	512	CLA	C4D-ND	2.91	1.41	1.37
22	b	615	CLA	C3B-C4B	2.91	1.49	1.42
22	C	513	CLA	C1B-C2B	2.91	1.50	1.43
22	C	514	CLA	OBD-CAD	2.91	1.27	1.22
22	D	401	CLA	O2A-CGA	2.91	1.41	1.33
22	b	611	CLA	C1B-NB	-2.91	1.34	1.37
22	c	911	CLA	C4D-CHA	2.91	1.48	1.38
34	b	627	HTG	C1'-S1	-2.90	1.77	1.81
22	b	613	CLA	C1D-ND	-2.90	1.34	1.37
22	b	617	CLA	C3B-C4B	2.90	1.49	1.42
22	c	909	CLA	C4D-CHA	2.90	1.48	1.38
22	B	608	CLA	C3B-C4B	2.90	1.49	1.42
22	c	909	CLA	C3D-C2D	2.90	1.47	1.39
22	B	608	CLA	C3D-C2D	2.90	1.47	1.39
22	b	616	CLA	C4D-CHA	2.89	1.48	1.38
22	C	505	CLA	C1D-ND	-2.89	1.34	1.37
22	b	614	CLA	C4D-CHA	2.89	1.48	1.38
34	B	627	HTG	C1'-S1	-2.89	1.77	1.81
22	B	614	CLA	CHC-C4B	2.89	1.45	1.39
22	b	606	CLA	C3D-C2D	2.89	1.47	1.39
22	B	613	CLA	C1B-C2B	2.88	1.50	1.43
22	c	906	CLA	OBD-CAD	2.88	1.27	1.22
22	c	914	CLA	C1C-C2C	2.87	1.50	1.44
22	B	617	CLA	C4D-CHA	2.87	1.48	1.38
39	V	202	HEC	FE-NC	2.87	2.04	1.95
35	C	519	DGD	O2G-C1B	2.87	1.42	1.34
22	c	913	CLA	C3B-C4B	2.87	1.49	1.42
22	b	603	CLA	C3D-C2D	2.86	1.46	1.39
22	c	910	CLA	C1B-C2B	2.86	1.50	1.43
28	a	418	SQD	C6-S	-2.86	1.66	1.77
22	c	906	CLA	C1B-C2B	2.86	1.50	1.43
34	b	632	HTG	O5-C1	2.86	1.46	1.42
27	d	407	LHG	O8-C23	2.86	1.41	1.33
22	b	612	CLA	OBD-CAD	2.86	1.27	1.22
22	b	616	CLA	C1B-C2B	2.86	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	C1B-C2B	2.86	1.50	1.43
22	B	609	CLA	C4D-ND	2.86	1.41	1.37
22	C	512	CLA	C1C-C2C	2.86	1.50	1.44
22	b	614	CLA	C4C-C3C	2.85	1.50	1.45
26	a	415	PL9	C6-C5	2.85	1.50	1.35
22	d	402	CLA	CHC-C4B	2.85	1.45	1.39
22	b	602	CLA	C4D-ND	2.84	1.41	1.37
26	A	411	PL9	C2-C3	2.84	1.42	1.34
22	c	904	CLA	C1D-ND	-2.83	1.34	1.37
23	a	411	PHO	C3A-C2A	-2.83	1.52	1.54
22	b	608	CLA	C1B-C2B	2.83	1.49	1.43
22	C	511	CLA	C4D-CHA	2.83	1.48	1.38
22	A	406	CLA	C3C-C2C	2.83	1.42	1.36
22	D	401	CLA	C1D-ND	-2.82	1.34	1.37
22	B	615	CLA	C1C-NC	-2.82	1.33	1.37
22	C	506	CLA	C1B-C2B	2.82	1.49	1.43
22	b	614	CLA	MG-NC	2.82	2.13	2.06
22	a	407	CLA	C1D-ND	-2.82	1.34	1.37
22	C	509	CLA	C4D-CHA	2.82	1.48	1.38
22	d	402	CLA	MG-NB	-2.82	2.00	2.05
22	c	913	CLA	C4D-CHA	2.81	1.48	1.38
22	b	604	CLA	C1C-C2C	2.81	1.50	1.44
22	b	611	CLA	C3B-C4B	2.81	1.49	1.42
22	c	905	CLA	C1B-NB	-2.81	1.34	1.37
22	b	615	CLA	C1C-C2C	2.80	1.50	1.44
22	b	616	CLA	C3B-C4B	2.80	1.49	1.42
22	b	609	CLA	CHD-C4C	2.80	1.45	1.39
22	b	611	CLA	OBD-CAD	2.80	1.27	1.22
24	A	409	BCR	C19-C18	2.80	1.52	1.45
22	b	608	CLA	C1D-ND	-2.80	1.34	1.37
22	c	904	CLA	C1C-NC	-2.80	1.33	1.37
22	A	406	CLA	C4B-NB	-2.80	1.34	1.37
22	B	615	CLA	C4C-C3C	2.79	1.49	1.45
22	C	505	CLA	C1B-C2B	2.79	1.49	1.43
22	A	405	CLA	C4D-CHA	2.79	1.48	1.38
22	b	605	CLA	CHD-C4C	2.79	1.45	1.39
22	C	513	CLA	MG-ND	-2.79	2.00	2.05
22	c	902	CLA	C4D-CHA	2.79	1.48	1.38
22	a	412	CLA	CHC-C4B	2.79	1.45	1.39
22	B	616	CLA	C3B-C4B	2.79	1.49	1.42
22	c	913	CLA	C4C-C3C	2.79	1.49	1.45
39	V	202	HEC	CMC-C2C	2.78	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	409	CLA	C3D-C2D	2.78	1.46	1.39
22	b	604	CLA	C4C-C3C	2.78	1.49	1.45
22	a	412	CLA	C3B-C4B	2.78	1.49	1.42
22	d	403	CLA	C4D-CHA	2.77	1.48	1.38
22	b	612	CLA	MG-NC	2.77	2.12	2.06
22	a	409	CLA	C4D-CHA	2.77	1.48	1.38
22	c	904	CLA	C3D-C2D	2.77	1.46	1.39
22	b	606	CLA	CHB-C1B	2.77	1.45	1.39
22	b	603	CLA	C4D-CHA	2.77	1.48	1.38
22	c	910	CLA	MG-NB	-2.77	2.00	2.05
22	C	510	CLA	C4D-CHA	2.77	1.48	1.38
36	e	101	HEM	CAC-C3C	2.77	1.55	1.47
22	B	608	CLA	C4C-C3C	2.77	1.49	1.45
22	b	614	CLA	C3D-C2D	2.77	1.46	1.39
22	c	905	CLA	C4D-CHA	2.76	1.48	1.38
22	b	609	CLA	MG-NB	2.76	2.11	2.05
22	B	613	CLA	C4C-C3C	2.76	1.49	1.45
22	B	608	CLA	C4D-CHA	2.76	1.48	1.38
26	D	406	PL9	C7-C3	2.75	1.54	1.51
22	b	615	CLA	OBD-CAD	2.75	1.27	1.22
22	b	614	CLA	C1B-C2B	2.74	1.49	1.43
22	B	607	CLA	C3D-C2D	2.74	1.46	1.39
22	a	412	CLA	C1B-C2B	2.74	1.49	1.43
22	c	903	CLA	C1B-C2B	2.74	1.49	1.43
22	B	604	CLA	C3B-C4B	2.73	1.49	1.42
22	C	502	CLA	C3B-C4B	2.72	1.49	1.42
22	C	502	CLA	C1B-NB	-2.72	1.34	1.37
22	c	914	CLA	C3B-C4B	2.71	1.49	1.42
22	B	604	CLA	C3D-C2D	2.71	1.46	1.39
22	a	412	CLA	MG-NA	2.71	2.12	2.06
22	B	617	CLA	C1D-ND	-2.71	1.34	1.37
22	a	412	CLA	C3D-C2D	2.71	1.46	1.39
22	c	910	CLA	CHC-C4B	2.71	1.45	1.39
22	b	609	CLA	C1D-ND	-2.71	1.34	1.37
22	B	614	CLA	C4D-CHA	2.71	1.48	1.38
22	b	610	CLA	C4D-CHA	2.71	1.48	1.38
39	v	202	HEC	CMD-C2D	2.70	1.56	1.50
22	A	406	CLA	C4D-CHA	2.70	1.48	1.38
22	D	403	CLA	C4D-CHA	2.70	1.48	1.38
22	c	904	CLA	MG-NC	2.69	2.12	2.06
29	I	102	LMT	O1'-C1'	2.69	1.44	1.40
22	C	505	CLA	C4B-NB	-2.69	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	v	202	HEC	CAC-C3C	2.68	1.58	1.51
22	b	605	CLA	C1B-C2B	2.68	1.49	1.43
22	c	907	CLA	C3D-C2D	2.68	1.46	1.39
35	C	517	DGD	O5D-C1E	2.68	1.44	1.40
22	D	404	CLA	C4D-CHA	2.68	1.47	1.38
24	d	404	BCR	C12-C13	2.68	1.51	1.45
22	b	617	CLA	C1C-C2C	2.68	1.49	1.44
22	B	604	CLA	C4D-CHA	2.68	1.47	1.38
34	b	626	HTG	C1'-S1	-2.68	1.78	1.81
28	C	501	SQD	C6-S	-2.68	1.67	1.77
22	B	608	CLA	MG-NB	-2.68	2.00	2.05
22	B	607	CLA	C1D-ND	-2.67	1.34	1.37
22	b	609	CLA	C1C-NC	-2.67	1.33	1.37
22	b	607	CLA	C1B-C2B	2.67	1.49	1.43
24	D	405	BCR	C8-C9	2.67	1.51	1.45
22	b	607	CLA	MG-NB	2.67	2.11	2.05
22	b	608	CLA	C3B-C4B	2.67	1.49	1.42
22	B	603	CLA	C1D-ND	-2.67	1.34	1.37
22	D	401	CLA	C4D-CHA	2.67	1.47	1.38
22	d	403	CLA	C1C-C2C	2.66	1.49	1.44
26	a	415	PL9	C7-C3	2.66	1.54	1.51
22	b	614	CLA	C3B-C4B	2.66	1.49	1.42
22	c	908	CLA	MG-NC	2.66	2.12	2.06
22	C	507	CLA	C4C-C3C	2.66	1.49	1.45
22	c	909	CLA	C1C-C2C	2.65	1.49	1.44
22	b	612	CLA	MG-NB	2.65	2.11	2.05
22	B	604	CLA	OBD-CAD	2.65	1.27	1.22
22	c	904	CLA	C4C-C3C	2.65	1.49	1.45
26	d	405	PL9	C6-C5	2.65	1.49	1.35
22	c	909	CLA	C1B-C2B	2.64	1.49	1.43
22	D	403	CLA	MG-ND	-2.64	2.00	2.05
22	c	909	CLA	C1D-ND	-2.64	1.34	1.37
39	V	202	HEC	CAC-C3C	2.64	1.57	1.51
22	B	616	CLA	OBD-CAD	2.64	1.27	1.22
22	b	603	CLA	OBD-CAD	2.64	1.27	1.22
22	a	408	CLA	C4D-CHA	2.63	1.47	1.38
29	c	921	LMT	O1'-C1'	2.63	1.44	1.40
26	a	415	PL9	C2-C3	2.63	1.41	1.34
25	d	409	LMG	O1-C1	2.63	1.44	1.40
39	V	202	HEC	CMA-C3A	2.63	1.56	1.50
22	A	405	CLA	C3B-C4B	2.63	1.48	1.42
22	B	611	CLA	C4D-CHA	2.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	931	LMT	O1'-C1'	2.62	1.44	1.40
22	a	407	CLA	C1B-NB	-2.62	1.34	1.37
22	b	612	CLA	C1D-ND	-2.62	1.34	1.37
22	B	607	CLA	C1C-C2C	2.62	1.49	1.44
22	b	602	CLA	C1B-C2B	2.62	1.49	1.43
22	b	609	CLA	C4D-ND	2.62	1.41	1.37
35	c	917	DGD	O5D-C1E	2.62	1.44	1.40
22	b	603	CLA	MG-NC	2.61	2.12	2.06
22	b	612	CLA	C4D-CHA	2.61	1.47	1.38
22	b	602	CLA	C4C-C3C	2.61	1.49	1.45
26	A	411	PL9	C6-C5	2.61	1.48	1.35
22	A	406	CLA	C4D-ND	2.61	1.41	1.37
36	E	102	HEM	CMA-C3A	2.61	1.56	1.50
22	b	609	CLA	C3B-C4B	2.61	1.48	1.42
34	D	414	HTG	C1'-S1	-2.61	1.78	1.81
22	C	511	CLA	C3B-C4B	2.60	1.48	1.42
22	c	906	CLA	C4B-NB	-2.60	1.34	1.37
22	c	910	CLA	MG-ND	-2.60	2.00	2.05
22	c	912	CLA	C1C-NC	-2.59	1.33	1.37
22	c	904	CLA	C1B-C2B	2.59	1.49	1.43
39	v	202	HEC	CMC-C2C	2.59	1.56	1.50
22	b	604	CLA	OBD-CAD	2.59	1.26	1.22
35	C	518	DGD	O2G-C1B	2.59	1.41	1.34
22	b	607	CLA	C4D-CHA	2.59	1.47	1.38
22	c	914	CLA	C4D-CHA	2.59	1.47	1.38
22	c	911	CLA	C1D-ND	-2.59	1.34	1.37
34	c	922	HTG	C1'-S1	-2.59	1.78	1.81
22	a	409	CLA	C3D-C4D	-2.58	1.38	1.44
22	B	605	CLA	C3D-C2D	2.58	1.46	1.39
26	d	405	PL9	C18-C19	2.58	1.39	1.33
22	b	613	CLA	C1B-C2B	2.58	1.49	1.43
22	b	614	CLA	C1C-NC	-2.57	1.34	1.37
22	b	617	CLA	C1B-NB	-2.57	1.34	1.37
22	c	910	CLA	C4D-CHA	2.57	1.47	1.38
36	e	101	HEM	CMD-C2D	2.56	1.56	1.50
22	c	911	CLA	C4D-ND	2.56	1.41	1.37
22	C	503	CLA	C4B-NB	-2.55	1.34	1.37
22	b	604	CLA	O2A-CGA	2.55	1.40	1.33
22	b	610	CLA	C1B-C2B	2.55	1.49	1.43
22	a	409	CLA	C1D-ND	-2.55	1.34	1.37
22	B	607	CLA	C3D-C4D	-2.55	1.38	1.44
22	B	602	CLA	C3B-C4B	2.55	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	C1D-ND	-2.54	1.34	1.37
24	a	413	BCR	C5-C6	2.54	1.38	1.34
22	B	603	CLA	C3D-C4D	-2.54	1.38	1.44
22	C	509	CLA	C4C-C3C	2.54	1.49	1.45
22	b	607	CLA	C3D-C2D	2.54	1.46	1.39
22	c	912	CLA	C4C-C3C	2.54	1.49	1.45
22	b	613	CLA	C1A-CHA	2.54	1.53	1.43
22	c	909	CLA	C1C-NC	-2.53	1.34	1.37
22	c	906	CLA	C1D-ND	-2.53	1.34	1.37
29	Z	101	LMT	O1'-C1'	2.53	1.44	1.40
24	b	618	BCR	C14-C13	2.53	1.35	1.33
22	a	409	CLA	C4B-NB	-2.52	1.34	1.37
22	C	507	CLA	C1C-C2C	2.52	1.49	1.44
22	B	613	CLA	C3B-C4B	2.52	1.48	1.42
22	B	606	CLA	C1B-C2B	2.52	1.49	1.43
22	c	908	CLA	C3B-C2B	2.52	1.49	1.41
22	c	903	CLA	OBD-CAD	2.51	1.26	1.22
22	A	406	CLA	C3D-C2D	2.51	1.46	1.39
22	c	905	CLA	C3B-C4B	2.50	1.48	1.42
36	e	101	HEM	CMB-C2B	2.50	1.56	1.50
22	A	408	CLA	C3D-C2D	2.49	1.45	1.39
22	C	508	CLA	C1D-ND	-2.49	1.34	1.37
22	C	514	CLA	C1D-ND	-2.49	1.34	1.37
22	B	612	CLA	C4D-CHA	2.49	1.47	1.38
22	D	401	CLA	C4B-NB	-2.49	1.34	1.37
22	a	412	CLA	MG-NB	2.49	2.10	2.05
28	b	621	SQD	C6-S	-2.49	1.68	1.77
22	b	610	CLA	C1B-NB	-2.49	1.34	1.37
22	C	508	CLA	C4D-ND	2.49	1.41	1.37
22	C	511	CLA	C1B-NB	-2.48	1.34	1.37
22	C	510	CLA	MG-NC	2.48	2.12	2.06
23	A	407	PHO	C3B-C4B	2.48	1.44	1.41
22	c	912	CLA	C1B-NB	-2.48	1.34	1.37
22	B	602	CLA	C1C-C2C	2.48	1.49	1.44
22	C	509	CLA	C4D-ND	2.48	1.41	1.37
22	d	402	CLA	C4D-CHA	2.48	1.47	1.38
23	a	410	PHO	CBD-CGD	-2.48	1.49	1.52
22	b	605	CLA	C1C-NC	-2.48	1.34	1.37
22	B	603	CLA	C3D-C2D	2.48	1.45	1.39
22	D	404	CLA	C1B-C2B	2.47	1.49	1.43
22	C	502	CLA	C1D-ND	-2.47	1.34	1.37
22	b	607	CLA	MG-ND	2.47	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	408	CLA	C1B-NB	-2.47	1.34	1.37
22	B	606	CLA	C1C-NC	-2.47	1.34	1.37
22	c	908	CLA	C3B-C4B	2.47	1.48	1.42
22	C	508	CLA	C1B-NB	-2.47	1.34	1.37
24	A	409	BCR	C12-C13	2.47	1.51	1.45
22	b	606	CLA	MG-NC	2.47	2.12	2.06
22	C	502	CLA	C4C-C3C	2.46	1.49	1.45
22	c	912	CLA	C4D-ND	2.46	1.41	1.37
22	b	613	CLA	C1C-NC	-2.46	1.34	1.37
22	d	402	CLA	C1B-NB	-2.45	1.34	1.37
22	b	611	CLA	C1C-C2C	2.45	1.49	1.44
22	B	603	CLA	C4D-CHA	2.45	1.47	1.38
22	b	603	CLA	C1D-ND	-2.45	1.34	1.37
22	b	614	CLA	C1C-C2C	2.45	1.49	1.44
35	c	919	DGD	O5D-C1E	2.44	1.44	1.40
22	B	616	CLA	C1B-C2B	2.44	1.49	1.43
22	C	513	CLA	C1D-ND	-2.44	1.34	1.37
22	B	603	CLA	C1C-C2C	2.44	1.49	1.44
22	C	509	CLA	MG-ND	-2.44	2.01	2.05
22	C	504	CLA	C1B-NB	-2.44	1.34	1.37
22	b	605	CLA	C4C-C3C	2.43	1.49	1.45
22	C	513	CLA	C1C-C2C	2.43	1.49	1.44
22	C	504	CLA	C1B-C2B	2.43	1.49	1.43
28	l	101	SQD	C6-S	-2.43	1.68	1.77
22	d	402	CLA	C3D-C2D	2.42	1.45	1.39
22	b	603	CLA	C1B-NB	-2.42	1.34	1.37
22	C	503	CLA	CHD-C4C	2.42	1.44	1.39
24	d	404	BCR	C23-C22	2.42	1.51	1.45
22	b	607	CLA	C4C-C3C	2.41	1.49	1.45
22	b	608	CLA	C4D-ND	2.41	1.41	1.37
22	A	405	CLA	C1B-C2B	2.41	1.48	1.43
34	C	532	HTG	C1-S1	-2.40	1.77	1.80
22	b	612	CLA	C3B-C4B	2.40	1.48	1.42
23	a	410	PHO	C1B-NB	-2.39	1.34	1.38
22	b	604	CLA	C1B-C2B	2.39	1.48	1.43
22	c	905	CLA	C1B-C2B	2.39	1.48	1.43
22	C	507	CLA	C1C-NC	-2.39	1.34	1.37
22	B	608	CLA	C1B-NB	-2.38	1.34	1.37
22	C	508	CLA	C1C-C2C	2.38	1.49	1.44
22	B	609	CLA	C1C-C2C	2.38	1.49	1.44
22	B	609	CLA	C4C-C3C	2.38	1.49	1.45
22	C	502	CLA	C4B-NB	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	611	CLA	C1B-NB	-2.37	1.34	1.37
22	A	406	CLA	MG-NC	-2.37	2.00	2.06
22	B	612	CLA	MG-NB	2.37	2.10	2.05
22	D	403	CLA	CHC-C1C	2.37	1.43	1.38
23	A	407	PHO	CBD-CGD	-2.37	1.49	1.52
22	B	614	CLA	C1B-C2B	2.37	1.48	1.43
22	b	612	CLA	C4B-NB	-2.36	1.34	1.37
22	b	605	CLA	C1D-ND	-2.36	1.34	1.37
22	C	514	CLA	C1B-C2B	2.36	1.48	1.43
22	c	905	CLA	C1C-NC	-2.35	1.34	1.37
22	c	914	CLA	C1D-ND	-2.35	1.34	1.37
22	B	607	CLA	C4C-C3C	2.35	1.49	1.45
22	B	614	CLA	C4C-C3C	2.35	1.49	1.45
22	B	602	CLA	C1B-C2B	2.35	1.48	1.43
22	B	609	CLA	C3B-C4B	2.35	1.48	1.42
35	D	407	DGD	O3G-C1D	2.35	1.44	1.40
22	b	617	CLA	C3B-C2B	2.35	1.49	1.41
22	c	908	CLA	C4C-C3C	2.34	1.49	1.45
35	d	406	DGD	O3G-C1D	2.34	1.44	1.40
22	b	616	CLA	C3B-C2B	2.34	1.49	1.41
22	B	606	CLA	OBD-CAD	2.34	1.26	1.22
22	c	909	CLA	C4B-NB	-2.34	1.34	1.37
22	c	913	CLA	C1B-NB	-2.34	1.34	1.37
26	D	406	PL9	C6-C5	2.33	1.47	1.35
28	D	408	SQD	O6-C1	2.33	1.44	1.40
34	l	106	HTG	C1-S1	-2.32	1.77	1.80
22	d	402	CLA	MG-ND	-2.32	2.01	2.05
22	c	912	CLA	C1B-C2B	2.32	1.48	1.43
22	C	504	CLA	C1C-NC	-2.32	1.34	1.37
22	B	607	CLA	CHD-C4C	2.32	1.44	1.39
22	C	510	CLA	C3B-C4B	2.32	1.48	1.42
24	b	619	BCR	C8-C9	2.32	1.50	1.46
22	C	510	CLA	C4D-ND	2.32	1.40	1.37
22	B	613	CLA	C4B-NB	-2.32	1.34	1.37
24	b	619	BCR	C12-C13	2.32	1.50	1.45
22	C	505	CLA	C3D-C4D	-2.32	1.38	1.44
22	d	402	CLA	C4D-ND	2.31	1.40	1.37
22	a	408	CLA	C4D-ND	2.31	1.40	1.37
22	B	608	CLA	C1B-C2B	2.31	1.48	1.43
22	c	902	CLA	C1D-ND	-2.31	1.34	1.37
25	B	621	LMG	O1-C1	2.31	1.44	1.40
22	a	408	CLA	C3B-C4B	2.30	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	MG-ND	2.30	2.10	2.05
39	V	202	HEC	CAB-C3B	2.30	1.57	1.51
22	C	512	CLA	C1B-NB	-2.30	1.35	1.37
29	B	622	LMT	O1'-C1'	2.30	1.44	1.40
28	l	101	SQD	O6-C1	2.30	1.44	1.40
39	v	202	HEC	CAB-C3B	2.30	1.57	1.51
22	d	403	CLA	C1B-C2B	2.29	1.48	1.43
22	C	513	CLA	C1B-NB	-2.29	1.35	1.37
22	c	903	CLA	C1D-ND	-2.29	1.35	1.37
22	B	604	CLA	C1C-NC	-2.29	1.34	1.37
22	D	403	CLA	OBD-CAD	2.29	1.26	1.22
22	a	409	CLA	C4C-C3C	2.29	1.49	1.45
22	b	610	CLA	C1C-NC	-2.29	1.34	1.37
22	b	611	CLA	C1B-C2B	2.29	1.48	1.43
22	B	607	CLA	OBD-CAD	2.28	1.26	1.22
22	C	511	CLA	C3D-C4D	-2.28	1.39	1.44
22	b	604	CLA	C4B-NB	-2.28	1.35	1.37
22	b	608	CLA	C4C-C3C	2.28	1.49	1.45
22	C	514	CLA	C3B-C2B	2.28	1.48	1.41
22	c	904	CLA	C3B-C4B	2.28	1.48	1.42
22	c	914	CLA	C1B-C2B	2.27	1.48	1.43
22	C	508	CLA	C3B-C2B	2.27	1.48	1.41
22	A	408	CLA	CHB-C4A	-2.27	1.32	1.37
28	D	408	SQD	C6-S	-2.27	1.69	1.77
24	d	404	BCR	C30-C25	-2.27	1.50	1.53
22	a	408	CLA	C1D-C2D	2.27	1.49	1.45
22	B	607	CLA	C3B-C2B	2.27	1.48	1.41
22	c	908	CLA	C4D-ND	2.27	1.40	1.37
22	C	514	CLA	C4D-ND	2.26	1.40	1.37
22	c	903	CLA	C4C-C3C	2.26	1.48	1.45
25	C	531	LMG	O1-C1	2.25	1.44	1.40
22	c	911	CLA	C1B-C2B	2.25	1.48	1.43
22	B	609	CLA	OBD-CAD	2.25	1.26	1.22
22	C	508	CLA	C1B-C2B	2.25	1.48	1.43
22	B	610	CLA	C1C-C2C	2.25	1.48	1.44
22	c	907	CLA	C3D-C4D	-2.25	1.39	1.44
22	C	503	CLA	C1B-C2B	2.25	1.48	1.43
24	a	413	BCR	C12-C13	2.24	1.50	1.45
22	C	503	CLA	C4C-C3C	2.24	1.48	1.45
22	B	614	CLA	C3B-C4B	2.24	1.48	1.42
22	b	602	CLA	C3B-C2B	2.24	1.48	1.41
22	b	611	CLA	C3D-C4D	-2.24	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	MG-NB	-2.24	2.01	2.05
22	c	905	CLA	C1D-ND	-2.24	1.35	1.37
24	C	515	BCR	C19-C18	2.24	1.50	1.45
36	e	101	HEM	CMA-C3A	2.24	1.55	1.50
22	B	606	CLA	C4D-CHA	2.24	1.46	1.38
22	b	610	CLA	C1C-C2C	2.23	1.48	1.44
22	B	613	CLA	C3D-C4D	-2.23	1.39	1.44
22	b	606	CLA	C1C-NC	-2.23	1.34	1.37
22	b	607	CLA	O2A-C1	-2.22	1.39	1.46
22	C	510	CLA	C1B-C2B	2.22	1.48	1.43
34	C	521	HTG	C1-S1	-2.22	1.77	1.80
22	B	609	CLA	C3D-C4D	-2.22	1.39	1.44
22	A	405	CLA	C3A-C2A	-2.22	1.48	1.54
22	C	507	CLA	C4B-NB	-2.22	1.35	1.37
22	C	511	CLA	C1C-C2C	2.22	1.48	1.44
24	Y	101	BCR	C5-C6	2.22	1.36	1.33
22	c	914	CLA	C4C-C3C	2.22	1.48	1.45
22	C	503	CLA	C1C-C2C	2.21	1.48	1.44
26	D	406	PL9	C2-C3	2.21	1.40	1.34
34	b	632	HTG	C1'-S1	-2.21	1.78	1.81
22	B	612	CLA	C4B-NB	-2.21	1.35	1.37
26	d	405	PL9	C7-C3	2.21	1.53	1.51
22	c	907	CLA	C1B-C2B	2.20	1.48	1.43
22	B	604	CLA	C4D-ND	2.20	1.40	1.37
22	c	913	CLA	C3B-C2B	2.20	1.48	1.41
22	a	407	CLA	C1C-NC	-2.20	1.34	1.37
22	C	503	CLA	C1D-ND	-2.20	1.35	1.37
22	D	404	CLA	C1C-C2C	2.19	1.48	1.44
22	B	617	CLA	C4B-NB	-2.19	1.35	1.37
22	A	408	CLA	C3D-C4D	-2.19	1.39	1.44
22	D	403	CLA	C3D-C2D	2.18	1.45	1.39
22	d	402	CLA	C4B-NB	-2.18	1.35	1.37
22	A	406	CLA	C3D-C4D	-2.18	1.39	1.44
22	b	617	CLA	CHD-C4C	2.17	1.44	1.39
22	B	608	CLA	C1C-NC	-2.17	1.34	1.37
22	c	906	CLA	C4C-C3C	2.17	1.48	1.45
22	c	913	CLA	C1B-C2B	2.16	1.48	1.43
22	c	909	CLA	C3D-C4D	-2.16	1.39	1.44
22	C	509	CLA	C4B-NB	-2.16	1.35	1.37
22	c	905	CLA	C4D-ND	2.16	1.40	1.37
22	c	902	CLA	C3D-C2D	2.16	1.45	1.39
24	c	915	BCR	C23-C22	2.15	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	513	CLA	C4C-C3C	2.15	1.48	1.45
22	b	605	CLA	OBD-CAD	2.15	1.26	1.22
22	D	401	CLA	C1B-NB	-2.15	1.35	1.37
26	d	405	PL9	C23-C24	2.15	1.38	1.33
22	C	502	CLA	C1C-C2C	2.14	1.48	1.44
22	b	615	CLA	C1B-C2B	2.14	1.48	1.43
22	c	913	CLA	C1C-C2C	2.14	1.48	1.44
24	Y	101	BCR	C7-C6	2.14	1.48	1.46
22	C	514	CLA	C4C-C3C	2.13	1.48	1.45
22	b	608	CLA	C4B-NB	-2.13	1.35	1.37
22	C	505	CLA	C4D-ND	2.13	1.40	1.37
22	B	615	CLA	C3B-C4B	2.13	1.47	1.42
22	B	607	CLA	C3B-C4B	2.12	1.47	1.42
22	B	612	CLA	C1D-ND	-2.12	1.35	1.37
24	B	620	BCR	C26-C25	2.12	1.38	1.34
22	C	510	CLA	MG-NB	-2.12	2.01	2.05
22	B	615	CLA	C1B-C2B	2.12	1.48	1.43
22	c	904	CLA	C3D-C4D	-2.12	1.39	1.44
22	C	511	CLA	C4D-ND	2.12	1.40	1.37
22	B	602	CLA	C4D-ND	2.12	1.40	1.37
22	a	412	CLA	C3D-C4D	-2.11	1.39	1.44
22	c	907	CLA	MG-ND	-2.11	2.01	2.05
22	C	508	CLA	C4C-C3C	2.11	1.48	1.45
22	c	903	CLA	C4D-ND	2.11	1.40	1.37
29	T	102	LMT	O1'-C1'	2.11	1.43	1.40
22	b	615	CLA	C4D-ND	2.10	1.40	1.37
22	C	504	CLA	C3B-C2B	2.10	1.48	1.41
22	B	609	CLA	C1B-C2B	2.10	1.48	1.43
22	d	402	CLA	C1B-C2B	2.10	1.48	1.43
22	b	608	CLA	C3D-C4D	-2.10	1.39	1.44
22	c	910	CLA	C4D-ND	2.10	1.40	1.37
22	b	617	CLA	C4D-ND	2.10	1.40	1.37
22	B	603	CLA	C1B-NB	-2.10	1.35	1.37
22	B	616	CLA	C4B-NB	-2.09	1.35	1.37
22	b	615	CLA	C3D-C4D	-2.09	1.39	1.44
34	b	627	HTG	O5-C1	2.09	1.45	1.42
35	c	918	DGD	O3G-C1D	2.09	1.43	1.40
22	D	403	CLA	C1C-C2C	2.09	1.48	1.44
22	C	504	CLA	C4D-ND	2.08	1.40	1.37
22	b	613	CLA	C4C-C3C	2.08	1.48	1.45
22	D	404	CLA	C4B-NB	-2.08	1.35	1.37
22	B	614	CLA	C1C-C2C	2.08	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	610	CLA	C4C-C3C	2.08	1.48	1.45
35	c	918	DGD	O5D-C1E	2.07	1.43	1.40
22	C	503	CLA	C1C-NC	-2.07	1.34	1.37
22	c	914	CLA	C1B-NB	-2.07	1.35	1.37
22	B	602	CLA	C3B-C2B	2.07	1.48	1.41
22	b	612	CLA	C3D-C4D	-2.06	1.39	1.44
22	a	408	CLA	C3B-C2B	2.06	1.48	1.41
22	d	402	CLA	C3D-C4D	-2.06	1.39	1.44
22	B	613	CLA	C4D-CHA	2.06	1.45	1.38
24	B	620	BCR	C19-C18	2.06	1.50	1.45
22	C	512	CLA	MG-NC	2.06	2.11	2.06
25	D	412	LMG	O1-C1	2.06	1.43	1.40
22	b	613	CLA	C1B-NB	-2.06	1.35	1.37
25	b	622	LMG	C4-C5	2.06	1.57	1.53
25	c	930	LMG	O1-C1	2.06	1.43	1.40
35	c	919	DGD	O2G-C2G	-2.05	1.41	1.46
22	C	513	CLA	C4D-ND	2.05	1.40	1.37
22	a	408	CLA	C1B-NB	-2.05	1.35	1.37
22	C	504	CLA	C4C-C3C	2.05	1.48	1.45
22	a	408	CLA	C4C-C3C	2.05	1.48	1.45
22	B	617	CLA	C1C-C2C	2.04	1.48	1.44
22	c	913	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	611	CLA	C1B-C2B	2.04	1.48	1.43
22	a	408	CLA	C1B-C2B	2.04	1.48	1.43
22	C	510	CLA	CHB-C4A	-2.04	1.32	1.37
22	a	407	CLA	C4C-C3C	2.04	1.48	1.45
22	B	604	CLA	C4C-C3C	2.04	1.48	1.45
22	C	505	CLA	C3B-C2B	2.03	1.48	1.41
22	d	403	CLA	C1D-C2D	2.03	1.49	1.45
22	b	607	CLA	OBD-CAD	2.03	1.26	1.22
22	b	609	CLA	C1B-NB	-2.03	1.35	1.37
22	c	908	CLA	C1D-ND	-2.03	1.35	1.37
22	C	512	CLA	C1C-NC	-2.02	1.34	1.37
22	c	906	CLA	C3B-C2B	2.02	1.48	1.41
22	B	608	CLA	C3D-C4D	-2.02	1.39	1.44
36	E	102	HEM	CMD-C2D	2.02	1.55	1.50
22	B	602	CLA	C3D-C4D	-2.02	1.39	1.44
22	b	610	CLA	C4C-C3C	2.02	1.48	1.45
22	C	506	CLA	C1A-CHA	2.01	1.51	1.43
26	d	405	PL9	C28-C29	2.01	1.37	1.33
22	B	610	CLA	OBD-CAD	2.01	1.25	1.22
22	c	912	CLA	C1D-ND	-2.01	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	618	BCR	C5-C6	2.01	1.37	1.34
22	B	616	CLA	C4C-C3C	2.01	1.48	1.45
22	B	610	CLA	C4D-ND	2.01	1.40	1.37
35	h	102	DGD	O5D-C1E	2.01	1.43	1.40
22	B	603	CLA	C4C-C3C	2.00	1.48	1.45
22	C	507	CLA	C1B-NB	-2.00	1.35	1.37

All (2614) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	602	CLA	C4A-NA-C1A	11.72	111.97	106.71
22	C	506	CLA	C4A-NA-C1A	11.20	111.74	106.71
22	B	602	CLA	C4A-NA-C1A	10.95	111.63	106.71
22	c	912	CLA	C4A-NA-C1A	10.35	111.36	106.71
22	D	401	CLA	C2B-C1B-NB	10.01	116.94	110.23
22	c	909	CLA	C4A-NA-C1A	9.96	111.19	106.71
22	c	904	CLA	C4A-NA-C1A	9.82	111.12	106.71
22	b	608	CLA	C4A-NA-C1A	9.79	111.11	106.71
22	c	908	CLA	C4A-NA-C1A	9.69	111.06	106.71
22	C	514	CLA	C4A-NA-C1A	9.68	111.06	106.71
22	B	615	CLA	C2D-C1D-ND	9.54	117.14	110.10
22	c	905	CLA	C4A-NA-C1A	9.23	110.85	106.71
34	V	203	HTG	O5-C1-C2	-9.01	98.98	110.31
23	D	402	PHO	C2D-C1D-ND	8.99	115.73	109.53
22	B	606	CLA	C4A-NA-C1A	8.85	110.68	106.71
23	a	411	PHO	C2B-C1B-NB	8.82	115.62	109.53
22	C	507	CLA	C4A-NA-C1A	8.72	110.63	106.71
22	B	615	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	d	402	CLA	C2B-C1B-NB	8.71	116.07	110.23
23	A	407	PHO	C1C-C2C-C3C	-8.59	101.47	108.61
34	l	106	HTG	C1'-S1-C1	8.58	116.14	100.09
22	C	510	CLA	C2B-C1B-NB	8.58	115.98	110.23
23	a	411	PHO	C2D-C1D-ND	8.58	115.45	109.53
22	b	617	CLA	C4A-NA-C1A	8.54	110.54	106.71
22	B	616	CLA	C4A-NA-C1A	8.53	110.54	106.71
28	a	414	SQD	O6-C1-C2	8.49	121.56	108.30
22	C	505	CLA	C4A-NA-C1A	8.46	110.51	106.71
22	C	504	CLA	C4A-NA-C1A	8.43	110.50	106.71
34	C	532	HTG	C1'-S1-C1	8.39	115.79	100.09
22	C	513	CLA	C4A-NA-C1A	8.39	110.48	106.71
22	C	503	CLA	C2B-C1B-NB	8.30	115.80	110.23
23	A	407	PHO	C2B-C1B-NB	8.19	115.18	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	D	414	HTG	C1'-S1-C1	8.16	115.35	100.09
23	a	411	PHO	O2D-CGD-CBD	8.14	121.31	111.00
22	A	406	CLA	C2B-C1B-NB	8.09	115.66	110.23
22	c	911	CLA	C2B-C1B-NB	8.08	115.65	110.23
22	C	512	CLA	C4A-NA-C1A	8.08	110.34	106.71
22	c	910	CLA	C2B-C1B-NB	8.00	115.60	110.23
22	b	614	CLA	C4A-NA-C1A	7.98	110.29	106.71
22	C	512	CLA	C2B-C1B-NB	7.98	115.58	110.23
34	b	632	HTG	C1'-S1-C1	7.96	114.97	100.09
22	B	611	CLA	O2D-CGD-CBD	7.92	125.33	111.27
22	C	508	CLA	C4A-NA-C1A	7.91	110.26	106.71
22	D	403	CLA	C4A-NA-C1A	7.88	110.25	106.71
22	D	403	CLA	C2C-C1C-NC	7.75	117.24	109.97
22	a	409	CLA	C2B-C1B-NB	7.74	115.42	110.23
34	v	203	HTG	O5-C1-C2	-7.74	100.58	110.31
34	b	624	HTG	C1'-S1-C1	7.69	114.47	100.09
22	b	605	CLA	C4A-NA-C1A	7.62	110.13	106.71
22	a	409	CLA	C2C-C1C-NC	7.61	117.10	109.97
22	B	617	CLA	C2B-C1B-NB	7.60	115.33	110.23
34	D	415	HTG	C1'-S1-C1	7.58	114.27	100.09
22	d	403	CLA	C4A-NA-C1A	7.56	110.11	106.71
22	A	408	CLA	C2B-C1B-NB	7.56	115.30	110.23
22	b	606	CLA	CHD-C4C-C3C	-7.54	113.75	124.84
22	b	607	CLA	C2B-C1B-NB	7.54	115.29	110.23
22	c	902	CLA	CHD-C1D-ND	-7.52	117.55	124.45
22	A	405	CLA	C2B-C1B-NB	7.52	115.27	110.23
22	b	615	CLA	C4A-NA-C1A	7.49	110.07	106.71
22	B	605	CLA	C4A-NA-C1A	7.48	110.07	106.71
22	B	608	CLA	C2B-C1B-NB	7.46	115.23	110.23
22	c	902	CLA	C2D-C1D-ND	7.44	115.59	110.10
22	B	612	CLA	C2B-C1B-NB	7.43	115.21	110.23
23	a	411	PHO	C4D-ND-C1D	-7.43	101.27	108.83
22	a	408	CLA	C2B-C1B-NB	7.41	115.20	110.23
23	D	402	PHO	C4D-ND-C1D	-7.40	101.30	108.83
34	v	203	HTG	C1'-S1-C1	7.39	113.91	100.09
22	c	907	CLA	C2B-C1B-NB	7.38	115.18	110.23
22	D	404	CLA	C2B-C1B-NB	7.36	115.16	110.23
22	b	616	CLA	C4A-NA-C1A	7.33	110.00	106.71
22	b	617	CLA	C2D-C1D-ND	7.31	115.49	110.10
22	B	604	CLA	O2D-CGD-CBD	7.29	124.23	111.27
23	a	411	PHO	C1-C2-C3	-7.29	113.43	126.04
22	A	406	CLA	CHC-C4B-NB	7.24	131.92	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	612	CLA	C4A-NA-C1A	7.24	109.96	106.71
22	b	603	CLA	O2D-CGD-CBD	7.22	124.10	111.27
22	C	509	CLA	C4A-NA-C1A	7.17	109.93	106.71
34	B	627	HTG	C1'-S1-C1	7.17	113.50	100.09
22	b	611	CLA	C2D-C1D-ND	7.12	115.35	110.10
22	b	605	CLA	C2B-C1B-NB	7.10	114.99	110.23
34	b	627	HTG	C1'-S1-C1	7.09	113.35	100.09
23	a	410	PHO	C2D-C1D-ND	7.08	114.41	109.53
22	c	908	CLA	CHD-C1D-ND	-7.07	117.95	124.45
22	c	903	CLA	C2B-C1B-NB	7.06	114.97	110.23
22	b	612	CLA	C4A-NA-C1A	7.01	109.86	106.71
23	D	402	PHO	C2B-C1B-NB	6.99	114.35	109.53
22	c	905	CLA	C2B-C1B-NB	6.98	114.91	110.23
22	C	502	CLA	O2D-CGD-O1D	-6.96	110.22	123.84
22	B	611	CLA	C4A-NA-C1A	6.96	109.84	106.71
22	B	610	CLA	C4A-NA-C1A	6.93	109.82	106.71
22	b	604	CLA	C2B-C1B-NB	6.91	114.86	110.23
22	a	408	CLA	CHD-C1D-ND	-6.89	118.12	124.45
28	a	414	SQD	O9-S-C6	6.88	115.12	106.94
22	d	402	CLA	C2D-C1D-ND	6.86	115.16	110.10
22	c	906	CLA	C2B-C1B-NB	6.86	114.83	110.23
22	b	603	CLA	CHD-C1D-ND	-6.85	118.16	124.45
22	c	907	CLA	CHD-C1D-ND	-6.82	118.18	124.45
22	c	902	CLA	C4A-NA-C1A	6.81	109.77	106.71
22	B	603	CLA	C2B-C1B-NB	6.80	114.79	110.23
22	A	405	CLA	C2D-C1D-ND	6.80	115.12	110.10
22	C	507	CLA	C2B-C1B-NB	6.79	114.78	110.23
28	C	501	SQD	O6-C1-C2	6.79	118.90	108.30
22	b	603	CLA	C2B-C1B-NB	6.77	114.77	110.23
22	b	609	CLA	C2B-C1B-NB	6.76	114.77	110.23
22	B	604	CLA	C2B-C1B-NB	6.73	114.75	110.23
22	C	510	CLA	C2C-C1C-NC	6.73	116.28	109.97
22	b	602	CLA	O2D-CGD-CBD	6.73	123.22	111.27
22	A	406	CLA	C2C-C1C-NC	6.72	116.27	109.97
22	c	910	CLA	CHC-C4B-NB	6.70	131.35	124.26
34	D	415	HTG	O5-C1-C2	-6.70	101.88	110.31
22	D	401	CLA	C2C-C1C-NC	6.69	116.24	109.97
34	B	623	HTG	C1'-S1-C1	6.69	112.61	100.09
23	a	410	PHO	O2D-CGD-CBD	6.68	119.45	111.00
22	B	609	CLA	CHD-C1D-ND	-6.66	118.33	124.45
22	b	606	CLA	CHD-C1D-ND	-6.66	118.33	124.45
22	C	503	CLA	C2D-C1D-ND	6.66	115.01	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	403	CLA	C1C-C2C-C3C	-6.64	99.97	106.96
22	b	607	CLA	CHD-C1D-ND	-6.64	118.35	124.45
22	c	913	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	a	409	CLA	C2D-C1D-ND	6.59	114.96	110.10
22	b	612	CLA	C2D-C1D-ND	6.58	114.96	110.10
22	C	508	CLA	O2D-CGD-CBD	6.57	122.94	111.27
22	B	608	CLA	C4D-CHA-C1A	-6.54	113.28	121.25
23	A	407	PHO	O2D-CGD-CBD	6.53	119.27	111.00
22	C	502	CLA	C4A-NA-C1A	6.51	109.63	106.71
34	c	922	HTG	C1'-S1-C1	6.50	112.25	100.09
34	C	521	HTG	C1'-S1-C1	6.49	112.23	100.09
22	C	502	CLA	O2D-CGD-CBD	6.49	122.79	111.27
22	A	408	CLA	C2D-C1D-ND	6.46	114.87	110.10
22	C	509	CLA	C2B-C1B-NB	6.46	114.56	110.23
39	v	202	HEC	C1D-ND-C4D	6.46	111.75	105.07
22	c	909	CLA	C2B-C1B-NB	6.45	114.56	110.23
22	a	409	CLA	C1C-C2C-C3C	-6.43	100.19	106.96
22	C	505	CLA	CHD-C1D-ND	-6.42	118.55	124.45
22	B	604	CLA	CHC-C4B-NB	6.42	131.05	124.26
22	B	614	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	B	605	CLA	C2D-C1D-ND	6.39	114.81	110.10
22	D	401	CLA	C1C-C2C-C3C	-6.38	100.25	106.96
22	B	607	CLA	CHC-C4B-NB	6.37	131.00	124.26
22	b	614	CLA	CHD-C1D-ND	-6.35	118.61	124.45
22	b	613	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
22	a	409	CLA	CHD-C1D-ND	-6.32	118.64	124.45
22	d	403	CLA	C2B-C1B-NB	6.32	114.47	110.23
22	B	603	CLA	CHC-C4B-NB	6.32	130.95	124.26
22	b	616	CLA	C2D-C1D-ND	6.31	114.76	110.10
22	B	615	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
22	c	902	CLA	C2B-C1B-NB	6.30	114.46	110.23
22	a	412	CLA	C2B-C1B-NB	6.28	114.44	110.23
22	b	604	CLA	C2C-C1C-NC	6.27	115.84	109.97
23	a	410	PHO	C1C-C2C-C3C	-6.26	103.40	108.61
22	B	610	CLA	CHD-C4C-C3C	-6.25	115.65	124.84
22	b	605	CLA	C2D-C1D-ND	6.25	114.71	110.10
22	b	607	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
22	B	614	CLA	CHC-C4B-NB	6.25	130.87	124.26
22	A	406	CLA	C1C-C2C-C3C	-6.24	100.39	106.96
23	A	407	PHO	C2D-C1D-ND	6.24	113.83	109.53
22	B	605	CLA	C2C-C1C-NC	6.23	115.81	109.97
22	B	609	CLA	C2D-C1D-ND	6.22	114.69	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	626	HTG	C1'-S1-C1	6.22	111.73	100.09
22	B	609	CLA	O2D-CGD-CBD	6.22	122.32	111.27
22	a	408	CLA	CHC-C4B-NB	6.21	130.83	124.26
23	a	410	PHO	C2B-C1B-NB	6.20	113.81	109.53
22	b	606	CLA	C2D-C1D-ND	6.17	114.65	110.10
22	a	408	CLA	CHD-C4C-C3C	-6.15	115.81	124.84
22	c	914	CLA	C4A-NA-C1A	6.14	109.47	106.71
24	D	405	BCR	C24-C23-C22	-6.14	116.96	126.23
22	b	610	CLA	CHD-C1D-ND	-6.14	118.81	124.45
22	c	908	CLA	C2D-C1D-ND	6.14	114.63	110.10
22	C	514	CLA	CHC-C4B-NB	6.14	130.75	124.26
22	B	617	CLA	O2D-CGD-CBD	6.13	122.17	111.27
22	B	617	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
22	B	611	CLA	C2D-C1D-ND	6.10	114.60	110.10
22	b	616	CLA	CHC-C4B-NB	6.07	130.69	124.26
22	b	607	CLA	O2D-CGD-CBD	6.07	122.06	111.27
22	b	610	CLA	CHC-C4B-NB	6.07	130.68	124.26
22	c	910	CLA	C2C-C1C-NC	6.06	115.65	109.97
22	c	913	CLA	C2B-C1B-NB	6.06	114.29	110.23
22	b	611	CLA	C2B-C1B-NB	6.05	114.29	110.23
22	B	611	CLA	CHD-C1D-ND	-6.05	118.89	124.45
22	a	407	CLA	C2D-C1D-ND	6.04	114.56	110.10
22	B	607	CLA	O2D-CGD-O1D	-6.04	112.03	123.84
22	a	412	CLA	O2D-CGD-CBD	6.03	121.99	111.27
22	B	614	CLA	C2D-C1D-ND	6.02	114.54	110.10
22	C	504	CLA	C2B-C1B-NB	6.02	114.27	110.23
22	a	408	CLA	C2D-C1D-ND	6.02	114.54	110.10
28	C	501	SQD	O9-S-C6	6.02	114.09	106.94
22	b	607	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	C	502	CLA	C2D-C1D-ND	6.00	114.53	110.10
22	B	613	CLA	C2B-C1B-NB	6.00	114.25	110.23
25	b	622	LMG	O1-C1-C2	5.99	117.66	108.30
22	c	914	CLA	C4D-CHA-C1A	-5.99	113.96	121.25
22	B	617	CLA	CHD-C1D-ND	-5.99	118.95	124.45
22	B	612	CLA	C2D-C1D-ND	5.97	114.50	110.10
22	b	614	CLA	CHC-C4B-NB	5.95	130.56	124.26
22	B	615	CLA	C2B-C1B-NB	5.95	114.22	110.23
22	b	607	CLA	C2D-C1D-ND	5.93	114.47	110.10
22	c	907	CLA	C2C-C1C-NC	5.93	115.53	109.97
22	b	606	CLA	C2B-C1B-NB	5.93	114.21	110.23
22	B	606	CLA	C2D-C1D-ND	5.93	114.47	110.10
22	C	509	CLA	C2D-C1D-ND	5.92	114.46	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	612	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
22	c	912	CLA	C2B-C1B-NB	5.90	114.19	110.23
22	b	617	CLA	O2D-CGD-CBD	5.90	121.75	111.27
22	B	602	CLA	O2D-CGD-CBD	5.89	121.74	111.27
22	D	403	CLA	C2B-C1B-NB	5.89	114.18	110.23
23	a	411	PHO	C1C-C2C-C3C	-5.88	103.72	108.61
22	b	605	CLA	C4D-CHA-C1A	-5.88	114.10	121.25
27	A	412	LHG	O7-C7-C8	5.87	121.88	111.09
22	B	606	CLA	C2B-C1B-NB	5.86	114.16	110.23
22	C	506	CLA	C2B-C1B-NB	5.85	114.16	110.23
22	C	504	CLA	C2D-C1D-ND	5.84	114.41	110.10
22	B	616	CLA	CHD-C1D-ND	-5.83	119.09	124.45
22	B	614	CLA	C2B-C1B-NB	5.83	114.14	110.23
22	C	513	CLA	C2D-C1D-ND	5.83	114.40	110.10
22	C	511	CLA	C2C-C1C-NC	5.82	115.43	109.97
22	C	511	CLA	C2B-C1B-NB	5.80	114.12	110.23
23	A	407	PHO	C4D-ND-C1D	-5.79	102.94	108.83
22	B	607	CLA	O2D-CGD-CBD	5.79	121.55	111.27
22	B	617	CLA	C2D-C1D-ND	5.79	114.37	110.10
22	b	613	CLA	C4A-NA-C1A	5.76	109.29	106.71
22	B	611	CLA	C2B-C1B-NB	5.75	114.09	110.23
23	D	402	PHO	C3D-C4D-ND	5.74	115.55	107.72
22	b	614	CLA	CMB-C2B-C1B	5.74	134.11	125.37
22	B	616	CLA	C2D-C1D-ND	5.74	114.33	110.10
22	b	604	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
22	b	611	CLA	C2C-C1C-NC	5.73	115.34	109.97
22	D	401	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
22	c	910	CLA	C4A-NA-C1A	5.73	109.28	106.71
22	D	404	CLA	CHD-C1D-ND	-5.73	119.19	124.45
22	D	403	CLA	C2D-C1D-ND	5.72	114.32	110.10
22	B	607	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
27	D	409	LHG	O7-C7-C8	5.71	123.81	111.50
22	b	611	CLA	O2D-CGD-CBD	5.69	121.38	111.27
22	d	402	CLA	C4D-CHA-C1A	-5.68	114.34	121.25
22	A	405	CLA	C2C-C1C-NC	5.68	115.29	109.97
22	b	607	CLA	O2D-CGD-O1D	-5.68	112.74	123.84
22	c	912	CLA	CHC-C4B-NB	5.67	130.26	124.26
22	C	507	CLA	CHD-C1D-ND	-5.66	119.25	124.45
22	C	510	CLA	C3B-C2B-C1B	-5.66	100.33	107.16
22	c	904	CLA	C2B-C1B-NB	5.66	114.03	110.23
22	a	408	CLA	C4D-CHA-C1A	-5.66	114.36	121.25
22	C	508	CLA	C2D-C1D-ND	5.65	114.27	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	C2D-C1D-ND	5.64	114.26	110.10
22	c	903	CLA	C2D-C1D-ND	5.63	114.25	110.10
22	b	608	CLA	C4D-CHA-C1A	-5.63	114.40	121.25
22	C	507	CLA	C2D-C1D-ND	5.62	114.25	110.10
22	D	401	CLA	C2D-C1D-ND	5.62	114.25	110.10
22	B	616	CLA	C2B-C1B-NB	5.62	114.00	110.23
22	C	508	CLA	C2B-C1B-NB	5.61	113.99	110.23
22	A	408	CLA	C2C-C1C-NC	5.61	115.22	109.97
22	B	608	CLA	C2C-C1C-NC	5.60	115.22	109.97
22	c	904	CLA	C4D-CHA-C1A	-5.60	114.44	121.25
22	c	914	CLA	C2D-C1D-ND	5.59	114.22	110.10
22	B	617	CLA	C2C-C1C-NC	5.58	115.20	109.97
25	d	409	LMG	O1-C1-C2	5.58	117.01	108.30
22	B	602	CLA	CHC-C4B-NB	5.56	130.14	124.26
36	E	102	HEM	C4D-ND-C1D	5.56	110.81	105.07
22	D	401	CLA	C3B-C2B-C1B	-5.55	100.46	107.16
22	B	607	CLA	C2C-C1C-NC	5.55	115.17	109.97
22	B	615	CLA	CHC-C4B-NB	5.55	130.13	124.26
22	b	617	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
22	C	502	CLA	CHD-C1D-ND	-5.55	119.36	124.45
39	V	202	HEC	C1D-ND-C4D	5.54	110.79	105.07
22	c	905	CLA	C2D-C1D-ND	5.52	114.17	110.10
22	b	610	CLA	C1C-C2C-C3C	-5.52	101.16	106.96
34	V	203	HTG	C1'-S1-C1	5.51	110.71	100.16
25	b	622	LMG	O7-C10-C11	5.51	123.37	111.50
23	a	411	PHO	C3D-C4D-ND	5.51	115.23	107.72
22	B	604	CLA	C2C-C1C-NC	5.50	115.12	109.97
22	B	609	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
22	c	904	CLA	CHB-C1B-NB	-5.49	118.44	124.26
27	a	416	LHG	O7-C7-C8	5.49	123.33	111.50
34	b	626	HTG	C1'-S1-C1	5.49	110.35	100.09
22	A	406	CLA	CHD-C1D-ND	-5.48	119.42	124.45
22	a	412	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
23	a	410	PHO	C4D-ND-C1D	-5.46	103.28	108.83
22	c	911	CLA	CHC-C4B-NB	5.45	130.03	124.26
22	B	615	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
22	D	404	CLA	CHC-C4B-NB	5.44	130.02	124.26
22	c	908	CLA	O2D-CGD-CBD	5.44	120.93	111.27
22	B	606	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
22	d	402	CLA	O2D-CGD-CBD	5.42	120.91	111.27
22	a	412	CLA	C4D-CHA-C1A	-5.41	114.66	121.25
22	B	609	CLA	C2C-C1C-NC	5.41	115.04	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	512	CLA	C2D-C1D-ND	5.41	114.09	110.10
22	c	914	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
22	C	509	CLA	CHC-C4B-NB	5.41	129.98	124.26
22	C	510	CLA	C4D-CHA-C1A	-5.40	114.67	121.25
22	a	408	CLA	C2C-C1C-NC	5.40	115.03	109.97
22	A	406	CLA	C2D-C1D-ND	5.40	114.08	110.10
22	B	613	CLA	C4A-NA-C1A	5.40	109.13	106.71
22	B	603	CLA	C2C-C1C-NC	5.39	115.02	109.97
22	b	615	CLA	CHC-C4B-NB	5.37	129.94	124.26
22	c	903	CLA	C4A-NA-C1A	5.36	109.12	106.71
22	c	903	CLA	C1-C2-C3	-5.36	116.77	126.04
22	c	911	CLA	CHD-C1D-ND	-5.36	119.53	124.45
22	c	908	CLA	CHC-C4B-NB	5.36	129.93	124.26
22	D	403	CLA	CHC-C4B-NB	5.35	129.92	124.26
22	B	607	CLA	C2B-C1B-NB	5.35	113.82	110.23
22	b	611	CLA	C4A-NA-C1A	5.35	109.11	106.71
22	C	504	CLA	CHC-C4B-NB	5.35	129.92	124.26
22	b	613	CLA	C2D-C1D-ND	5.35	114.04	110.10
22	A	408	CLA	CHD-C1D-ND	-5.35	119.54	124.45
22	c	902	CLA	CMD-C2D-C1D	5.31	134.08	124.71
24	D	405	BCR	C7-C8-C9	-5.31	118.21	126.23
22	a	408	CLA	CHD-C4C-NC	5.31	132.56	124.20
28	A	413	SQD	O9-S-C6	5.30	113.24	106.94
22	b	610	CLA	C2C-C1C-NC	5.30	114.94	109.97
36	E	102	HEM	CBD-CAD-C3D	-5.30	97.91	112.63
23	A	407	PHO	C3D-C4D-ND	5.29	114.93	107.72
22	a	412	CLA	C2C-C1C-NC	5.27	114.91	109.97
23	D	402	PHO	O2D-CGD-CBD	5.27	117.67	111.00
22	b	617	CLA	C2B-C1B-NB	5.27	113.76	110.23
22	a	408	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
22	c	903	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
22	D	403	CLA	C1-C2-C3	-5.26	116.95	126.04
36	e	101	HEM	C4D-ND-C1D	5.25	110.50	105.07
22	c	906	CLA	C4A-NA-C1A	5.25	109.06	106.71
22	B	615	CLA	CHD-C1D-ND	-5.25	119.63	124.45
22	b	611	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
22	b	609	CLA	CHC-C4B-NB	5.24	129.80	124.26
22	B	603	CLA	C2D-C1D-ND	5.24	113.96	110.10
22	B	613	CLA	CHD-C1D-ND	-5.24	119.64	124.45
22	c	906	CLA	C3B-C2B-C1B	-5.23	100.84	107.16
22	C	505	CLA	C2B-C1B-NB	5.23	113.74	110.23
22	C	510	CLA	C1C-C2C-C3C	-5.22	101.47	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	616	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
22	D	404	CLA	C4A-NA-C1A	5.22	109.05	106.71
23	D	402	PHO	C1-C2-C3	-5.22	117.02	126.04
22	C	510	CLA	C4A-NA-C1A	5.21	109.05	106.71
22	b	614	CLA	C2D-C1D-ND	5.21	113.94	110.10
22	B	605	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
22	A	408	CLA	CHC-C4B-NB	5.21	129.77	124.26
34	b	632	HTG	O5-C5-C4	5.21	119.15	109.69
22	C	508	CLA	CHD-C1D-ND	-5.20	119.67	124.45
22	c	913	CLA	CHC-C4B-NB	5.19	129.75	124.26
22	C	510	CLA	CHC-C4B-NB	5.19	129.75	124.26
22	b	610	CLA	C2B-C1B-NB	5.19	113.71	110.23
28	l	101	SQD	O6-C1-C2	5.19	116.40	108.30
22	b	605	CLA	C2C-C1C-NC	5.17	114.82	109.97
22	b	608	CLA	CHC-C4B-NB	5.17	129.73	124.26
22	d	402	CLA	C2C-C1C-NC	5.17	114.82	109.97
22	A	405	CLA	C3B-C2B-C1B	-5.17	100.92	107.16
22	c	913	CLA	C1-C2-C3	-5.17	117.10	126.04
22	d	403	CLA	CHC-C4B-NB	5.17	129.73	124.26
22	B	610	CLA	C2D-C1D-ND	5.16	113.91	110.10
35	d	406	DGD	O2G-C1B-C2B	5.16	122.63	111.50
22	c	902	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
22	c	902	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
22	a	407	CLA	C4A-NA-C1A	5.16	109.02	106.71
22	c	914	CLA	CHC-C4B-NB	5.15	129.71	124.26
22	C	504	CLA	C3B-C2B-C1B	-5.14	100.95	107.16
22	b	615	CLA	C4D-CHA-C1A	-5.14	114.99	121.25
24	d	404	BCR	C7-C8-C9	-5.14	118.47	126.23
22	b	603	CLA	C2D-C1D-ND	5.14	113.89	110.10
28	a	414	SQD	O47-C7-C8	5.13	122.56	111.50
22	C	505	CLA	C2C-C1C-NC	5.13	114.78	109.97
22	B	606	CLA	CHC-C4B-NB	5.13	129.69	124.26
22	B	602	CLA	CHD-C1D-ND	-5.13	119.74	124.45
22	a	409	CLA	CHC-C4B-NB	5.11	129.67	124.26
22	C	507	CLA	C2C-C1C-NC	5.10	114.75	109.97
22	C	514	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
22	c	905	CLA	CHC-C4B-NB	5.10	129.65	124.26
22	c	906	CLA	C2D-C1D-ND	5.09	113.86	110.10
22	b	615	CLA	C2B-C1B-NB	5.09	113.64	110.23
22	c	913	CLA	O2D-CGD-CBD	5.08	120.30	111.27
22	C	507	CLA	CHC-C4B-NB	5.08	129.63	124.26
22	c	910	CLA	C4D-CHA-C1A	-5.07	115.07	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	604	CLA	O2D-CGD-CBD	5.07	120.28	111.27
22	a	407	CLA	CHD-C1D-ND	-5.07	119.80	124.45
22	c	913	CLA	C2D-C1D-ND	5.06	113.83	110.10
22	c	911	CLA	C4A-NA-C1A	5.05	108.98	106.71
22	b	608	CLA	C2C-C1C-NC	5.05	114.70	109.97
22	B	605	CLA	C2B-C1B-NB	5.05	113.62	110.23
22	b	613	CLA	CAC-C3C-C4C	5.04	131.35	124.81
22	C	504	CLA	CHD-C4C-C3C	-5.04	117.44	124.84
22	B	617	CLA	O2D-CGD-O1D	-5.03	114.00	123.84
22	c	911	CLA	CHD-C4C-C3C	-5.03	117.45	124.84
22	B	610	CLA	CHD-C1D-ND	-5.02	119.84	124.45
22	c	911	CLA	C2D-C1D-ND	5.02	113.80	110.10
22	c	903	CLA	O2D-CGD-O1D	-5.01	114.04	123.84
22	C	502	CLA	C2C-C1C-NC	5.00	114.66	109.97
22	c	906	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	b	604	CLA	C2D-C1D-ND	5.00	113.79	110.10
22	a	409	CLA	C4D-CHA-C1A	-5.00	115.16	121.25
22	B	609	CLA	C4D-CHA-C1A	-5.00	115.16	121.25
22	B	617	CLA	CHC-C4B-NB	4.99	129.54	124.26
22	c	908	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
22	b	606	CLA	CHD-C4C-NC	4.98	132.05	124.20
22	b	615	CLA	C2D-C1D-ND	4.98	113.77	110.10
22	b	617	CLA	CHC-C4B-NB	4.97	129.52	124.26
22	B	603	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
22	C	503	CLA	C3B-C2B-C1B	-4.96	101.17	107.16
22	C	503	CLA	O2D-CGD-CBD	4.96	120.08	111.27
22	c	907	CLA	O2D-CGD-CBD	4.95	120.06	111.27
24	b	618	BCR	C3-C4-C5	-4.94	105.25	114.08
22	b	607	CLA	C1-C2-C3	-4.94	117.50	126.04
22	B	607	CLA	C2D-C1D-ND	4.94	113.74	110.10
22	D	401	CLA	CHC-C4B-NB	4.93	129.48	124.26
22	c	904	CLA	C2C-C1C-NC	4.93	114.59	109.97
22	B	611	CLA	CHD-C4C-C3C	-4.93	117.60	124.84
22	A	405	CLA	C1C-C2C-C3C	-4.93	101.78	106.96
22	b	609	CLA	C3B-C2B-C1B	-4.93	101.22	107.16
22	b	612	CLA	C2C-C1C-NC	4.92	114.58	109.97
22	A	406	CLA	CHD-C4C-C3C	-4.91	117.62	124.84
22	b	604	CLA	C4-C3-C5	4.91	123.53	115.27
28	a	418	SQD	C1-O5-C5	-4.91	104.05	113.69
22	C	503	CLA	O2D-CGD-O1D	-4.91	114.24	123.84
22	C	503	CLA	C4A-NA-C1A	4.91	108.91	106.71
22	b	613	CLA	C4D-CHA-C1A	-4.90	115.28	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	609	CLA	CHD-C4C-C3C	-4.90	117.63	124.84
22	c	913	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
22	C	513	CLA	CHD-C4C-C3C	-4.90	117.64	124.84
22	b	612	CLA	CHD-C1D-ND	-4.89	119.96	124.45
22	c	903	CLA	CHC-C4B-NB	4.89	129.43	124.26
27	C	522	LHG	O7-C7-C8	4.89	122.04	111.50
22	B	605	CLA	CHD-C1D-ND	-4.87	119.97	124.45
22	b	604	CLA	C1C-C2C-C3C	-4.87	101.83	106.96
23	a	411	PHO	O2D-CGD-O1D	-4.87	114.32	123.84
22	b	602	CLA	C2D-C1D-ND	4.86	113.69	110.10
28	D	408	SQD	O6-C1-C2	4.86	115.89	108.30
22	c	910	CLA	C2D-C1D-ND	4.85	113.68	110.10
22	b	604	CLA	CHD-C1D-ND	-4.84	120.00	124.45
22	B	604	CLA	CHD-C1D-ND	-4.84	120.00	124.45
22	b	613	CLA	C2B-C1B-NB	4.84	113.48	110.23
22	b	606	CLA	O2D-CGD-CBD	4.84	119.87	111.27
22	B	611	CLA	O2D-CGD-O1D	-4.84	114.38	123.84
22	C	512	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
22	b	612	CLA	C4D-CHA-C1A	-4.84	115.36	121.25
22	B	603	CLA	C4D-CHA-C1A	-4.83	115.37	121.25
22	C	503	CLA	C4D-CHA-C1A	-4.82	115.38	121.25
22	b	602	CLA	C2B-C1B-NB	4.82	113.46	110.23
34	v	203	HTG	C1-C2-C3	-4.81	101.08	110.59
22	C	512	CLA	CHD-C1D-ND	-4.80	120.05	124.45
22	c	903	CLA	C2C-C1C-NC	4.79	114.46	109.97
26	A	411	PL9	C7-C3-C4	4.79	120.77	116.88
22	B	612	CLA	CHD-C1D-ND	-4.79	120.05	124.45
22	b	605	CLA	C3B-C2B-C1B	-4.79	101.39	107.16
22	b	612	CLA	C2B-C1B-NB	4.78	113.44	110.23
22	B	613	CLA	C2D-C1D-ND	4.78	113.63	110.10
22	C	513	CLA	C2B-C1B-NB	4.78	113.44	110.23
29	I	102	LMT	O1B-C4'-C3'	4.78	119.99	107.28
28	l	101	SQD	O47-C7-C8	4.78	121.80	111.50
22	b	616	CLA	C2B-C1B-NB	4.78	113.43	110.23
22	b	614	CLA	C2C-C1C-NC	4.77	114.44	109.97
24	C	515	BCR	C33-C5-C6	-4.77	119.17	124.53
22	C	507	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
22	b	606	CLA	C4D-CHA-C1A	-4.76	115.45	121.25
22	B	612	CLA	C4D-CHA-C1A	-4.76	115.45	121.25
22	b	603	CLA	CHA-C4D-ND	4.76	142.46	132.50
22	B	605	CLA	CHC-C4B-NB	4.76	129.29	124.26
22	C	508	CLA	CHD-C4C-C3C	-4.75	117.85	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	510	CLA	O2D-CGD-CBD	4.75	119.71	111.27
35	c	919	DGD	O2G-C1B-C2B	4.75	121.74	111.50
22	d	402	CLA	C1D-ND-C4D	-4.75	102.96	106.33
22	d	403	CLA	C2C-C1C-NC	4.75	114.42	109.97
22	c	902	CLA	C2C-C1C-NC	4.75	114.42	109.97
22	c	907	CLA	C4A-NA-C1A	4.74	108.84	106.71
22	c	908	CLA	O2D-CGD-O1D	-4.74	114.57	123.84
22	a	409	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
22	c	911	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
22	C	506	CLA	CHC-C4B-NB	4.72	129.26	124.26
22	A	405	CLA	CHC-C4B-NB	4.72	129.26	124.26
22	a	412	CLA	C4-C3-C5	4.72	123.21	115.27
22	B	609	CLA	C2B-C1B-NB	4.72	113.40	110.23
28	A	413	SQD	O48-C23-C24	4.72	126.72	111.91
22	a	409	CLA	O2D-CGD-CBD	4.71	119.64	111.27
22	a	408	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
22	B	607	CLA	C1C-C2C-C3C	-4.70	102.01	106.96
22	C	505	CLA	C1C-C2C-C3C	-4.70	102.02	106.96
22	A	408	CLA	C1C-C2C-C3C	-4.68	102.03	106.96
22	b	606	CLA	C2C-C1C-NC	4.68	114.36	109.97
22	B	613	CLA	C4D-CHA-C1A	-4.68	115.56	121.25
22	b	607	CLA	C2C-C1C-NC	4.66	114.34	109.97
22	c	910	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
22	c	904	CLA	C2D-C1D-ND	4.66	113.54	110.10
22	D	404	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
22	C	507	CLA	C3B-C2B-C1B	-4.65	101.54	107.16
22	b	617	CLA	C3B-C2B-C1B	-4.65	101.54	107.16
22	a	407	CLA	O2D-CGD-CBD	4.65	119.54	111.27
22	B	604	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
22	b	610	CLA	CHD-C4C-C3C	-4.65	118.00	124.84
22	A	406	CLA	C4-C3-C5	4.65	123.09	115.27
22	C	504	CLA	CHA-C4D-ND	4.65	142.23	132.50
22	B	603	CLA	C4A-NA-C1A	4.65	108.80	106.71
22	b	603	CLA	CHC-C4B-NB	4.64	129.17	124.26
22	b	612	CLA	CHC-C4B-NB	4.64	129.17	124.26
22	C	511	CLA	C1C-C2C-C3C	-4.64	102.08	106.96
22	B	608	CLA	CHC-C4B-NB	4.64	129.17	124.26
22	b	607	CLA	C4D-CHA-C1A	-4.64	115.60	121.25
22	B	611	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
22	b	616	CLA	CHD-C1D-ND	-4.63	120.19	124.45
22	C	512	CLA	CHD-C4C-C3C	-4.63	118.03	124.84
22	C	513	CLA	O2D-CGD-CBD	4.63	119.49	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	509	CLA	O2D-CGD-CBD	4.62	119.48	111.27
22	B	607	CLA	C4D-CHA-C1A	-4.62	115.63	121.25
22	B	612	CLA	CHD-C4C-C3C	-4.62	118.06	124.84
22	a	409	CLA	CHD-C4C-C3C	-4.61	118.06	124.84
22	D	401	CLA	CMB-C2B-C1B	4.61	132.39	125.37
22	C	502	CLA	C2B-C1B-NB	4.60	113.32	110.23
22	C	505	CLA	O2D-CGD-CBD	4.60	119.44	111.27
28	C	501	SQD	O8-S-C6	4.60	113.06	105.74
22	B	615	CLA	O2D-CGD-CBD	4.59	119.43	111.27
22	d	403	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
28	a	418	SQD	O6-C1-C2	4.59	115.47	108.30
22	d	402	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
22	b	609	CLA	C2C-C1C-NC	4.58	114.26	109.97
22	B	613	CLA	C2C-C1C-NC	4.58	114.26	109.97
28	l	101	SQD	O7-S-C6	4.58	112.38	106.94
24	Y	101	BCR	C38-C26-C25	-4.58	119.39	124.53
22	C	512	CLA	C2C-C1C-NC	4.58	114.26	109.97
24	y	101	BCR	C33-C5-C6	-4.57	119.39	124.53
22	B	611	CLA	C2C-C1C-NC	4.57	114.25	109.97
22	D	401	CLA	CHD-C4C-NC	4.57	131.40	124.20
22	B	607	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
22	b	615	CLA	C2C-C1C-NC	4.57	114.25	109.97
22	A	405	CLA	CHD-C1D-ND	-4.56	120.26	124.45
29	I	102	LMT	C1'-O5'-C5'	4.56	122.64	113.69
24	d	404	BCR	C38-C26-C25	-4.56	119.41	124.53
22	B	605	CLA	O2D-CGD-CBD	4.55	119.36	111.27
22	C	510	CLA	C2D-C1D-ND	4.54	113.45	110.10
22	A	408	CLA	C4A-NA-C1A	4.54	108.75	106.71
22	b	609	CLA	C4A-NA-C1A	4.53	108.74	106.71
22	a	412	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
22	c	909	CLA	C2D-C1D-ND	4.52	113.43	110.10
22	c	904	CLA	C3B-C2B-C1B	-4.52	101.71	107.16
22	c	905	CLA	C2C-C1C-NC	4.52	114.20	109.97
22	B	613	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
22	C	502	CLA	CHD-C4C-C3C	-4.51	118.22	124.84
22	c	903	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
22	b	602	CLA	CHC-C4B-NB	4.50	129.02	124.26
22	c	909	CLA	C1C-C2C-C3C	-4.50	102.23	106.96
22	c	914	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
34	V	203	HTG	O2-C2-C1	4.49	118.51	110.27
22	b	614	CLA	CHD-C4C-C3C	-4.49	118.24	124.84
22	B	608	CLA	C1C-C2C-C3C	-4.49	102.24	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	614	CLA	CAC-C3C-C4C	4.49	130.63	124.81
22	B	610	CLA	C2C-C1C-NC	4.48	114.17	109.97
22	B	612	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
22	a	407	CLA	CHC-C4B-NB	4.47	128.99	124.26
22	C	503	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
28	A	413	SQD	O6-C1-C2	4.45	115.25	108.30
23	D	402	PHO	C4-C3-C5	4.45	122.76	115.27
22	B	604	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
22	a	407	CLA	CAC-C3C-C4C	4.44	130.57	124.81
22	C	512	CLA	C1-O2A-CGA	4.43	128.08	116.44
22	c	910	CLA	CAC-C3C-C4C	4.43	130.56	124.81
22	B	606	CLA	C4D-CHA-C1A	-4.43	115.86	121.25
22	B	603	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
22	c	907	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
22	B	612	CLA	C2C-C1C-NC	4.42	114.12	109.97
28	C	501	SQD	C1-O5-C5	-4.42	105.01	113.69
22	c	902	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
22	C	513	CLA	CHC-C4B-NB	4.42	128.93	124.26
22	c	909	CLA	O2D-CGD-CBD	4.42	119.11	111.27
22	c	913	CLA	CHD-C1D-ND	-4.41	120.40	124.45
22	c	910	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
22	b	603	CLA	C4A-NA-C1A	4.41	108.69	106.71
22	D	404	CLA	O2D-CGD-CBD	4.41	119.10	111.27
28	C	501	SQD	C1-C2-C3	-4.40	100.83	110.00
22	c	908	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
22	d	402	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
22	C	511	CLA	C2D-C1D-ND	4.40	113.35	110.10
22	b	604	CLA	CHC-C4B-NB	4.40	128.91	124.26
22	B	617	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
22	b	616	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
24	c	916	BCR	C15-C14-C13	-4.39	121.04	127.31
22	B	617	CLA	C4D-CHA-C1A	-4.39	115.91	121.25
22	d	403	CLA	C1-O2A-CGA	4.39	127.95	116.44
22	a	412	CLA	CHB-C1B-NB	-4.38	119.62	124.26
22	B	614	CLA	C4D-CHA-C1A	-4.38	115.92	121.25
22	c	909	CLA	C3B-C2B-C1B	-4.37	101.88	107.16
22	B	609	CLA	C1C-C2C-C3C	-4.37	102.37	106.96
35	D	407	DGD	C4D-C3D-C2D	4.37	118.44	110.82
22	B	615	CLA	C2C-C1C-NC	4.36	114.06	109.97
22	C	511	CLA	CHD-C4C-C3C	-4.36	118.44	124.84
35	H	102	DGD	O1G-C1A-O1A	-4.35	112.61	123.59
22	c	902	CLA	O2D-CGD-CBD	4.35	119.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	610	CLA	CHD-C4C-NC	4.35	131.05	124.20
22	b	614	CLA	CMD-C2D-C1D	4.35	132.37	124.71
22	B	611	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
22	B	613	CLA	CHB-C1B-NB	-4.34	119.66	124.26
23	a	410	PHO	C3D-C4D-ND	4.33	113.63	107.72
22	b	613	CLA	O2D-CGD-CBD	4.33	118.97	111.27
22	B	605	CLA	CHD-C4C-C3C	-4.33	118.47	124.84
22	B	602	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
22	b	617	CLA	CBC-CAC-C3C	-4.33	100.49	112.43
22	C	503	CLA	CMB-C2B-C1B	4.33	131.96	125.37
35	D	407	DGD	O2G-C1B-C2B	4.33	120.82	111.50
22	b	615	CLA	O2D-CGD-CBD	4.32	118.94	111.27
22	c	908	CLA	CHD-C4C-NC	4.32	131.00	124.20
22	b	603	CLA	CMD-C2D-C1D	4.31	132.32	124.71
22	c	914	CLA	C2B-C1B-NB	4.31	113.12	110.23
22	A	408	CLA	C4-C3-C5	4.31	122.52	115.27
27	l	102	LHG	O7-C7-C8	4.31	120.78	111.50
22	b	605	CLA	O2D-CGD-CBD	4.31	118.92	111.27
25	D	412	LMG	O7-C10-C11	4.30	120.76	111.50
22	b	602	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
22	a	407	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
22	C	514	CLA	C3B-C2B-C1B	-4.30	101.98	107.16
25	d	409	LMG	O7-C10-C11	4.29	120.75	111.50
22	c	914	CLA	C2C-C1C-NC	4.29	113.99	109.97
22	c	911	CLA	CHD-C4C-NC	4.28	130.95	124.20
22	A	406	CLA	C3B-C2B-C1B	-4.28	102.00	107.16
22	C	502	CLA	CHC-C4B-NB	4.28	128.79	124.26
25	C	520	LMG	O8-C28-C29	4.28	125.33	111.91
22	c	905	CLA	CHD-C1D-ND	-4.28	120.52	124.45
28	a	414	SQD	C1-C2-C3	-4.27	101.10	110.00
36	e	101	HEM	CBD-CAD-C3D	-4.27	100.77	112.63
24	c	915	BCR	C33-C5-C6	-4.27	119.74	124.53
22	B	606	CLA	CMC-C2C-C1C	4.26	131.53	125.04
22	b	602	CLA	C1-O2A-CGA	4.26	127.61	116.44
22	c	905	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
22	B	610	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
22	B	617	CLA	C1-O2A-CGA	4.25	127.59	116.44
22	C	514	CLA	C2B-C1B-NB	4.25	113.08	110.23
22	C	504	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
25	B	621	LMG	O7-C10-C11	4.25	120.65	111.50
22	b	608	CLA	C2B-C1B-NB	4.25	113.08	110.23
22	B	617	CLA	CHD-C4C-NC	4.24	130.89	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	913	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
34	D	415	HTG	O5-C5-C4	4.24	117.40	109.69
22	b	609	CLA	O2D-CGD-CBD	4.24	118.80	111.27
22	C	508	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
22	b	602	CLA	C4D-CHA-C1A	-4.23	116.10	121.25
22	C	506	CLA	C2C-C1C-NC	4.23	113.94	109.97
22	b	617	CLA	CHD-C1D-ND	-4.23	120.57	124.45
22	b	612	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
35	C	517	DGD	O3G-C3G-C2G	-4.22	100.71	110.90
28	C	501	SQD	O47-C7-C8	4.22	120.60	111.50
37	H	101	RRX	C24-C23-C22	-4.22	119.86	126.23
22	c	907	CLA	CHC-C4B-NB	4.22	128.72	124.26
22	B	603	CLA	O2D-CGD-CBD	4.22	118.76	111.27
22	b	611	CLA	CHD-C1D-ND	-4.21	120.58	124.45
22	b	617	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
26	A	411	PL9	C53-C6-C1	4.21	123.60	114.99
22	B	617	CLA	O2A-CGA-CBA	4.21	125.11	111.91
22	c	911	CLA	CMC-C2C-C1C	4.21	131.44	125.04
28	A	413	SQD	O47-C7-C8	4.21	120.57	111.50
22	a	407	CLA	C2B-C1B-NB	4.21	113.05	110.23
22	C	503	CLA	CHC-C4B-NB	4.20	128.71	124.26
22	a	407	CLA	C2C-C1C-NC	4.20	113.91	109.97
22	b	611	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
22	C	511	CLA	O2D-CGD-O1D	-4.20	115.63	123.84
22	b	608	CLA	CHA-C4D-ND	4.20	141.29	132.50
22	D	401	CLA	CHB-C1B-NB	-4.20	119.81	124.26
22	b	611	CLA	C4D-CHA-C1A	-4.20	116.14	121.25
22	b	617	CLA	C2C-C1C-NC	4.20	113.90	109.97
22	c	913	CLA	C2C-C1C-NC	4.20	113.90	109.97
22	a	407	CLA	C1C-C2C-C3C	-4.20	102.55	106.96
22	C	506	CLA	CAC-C3C-C4C	4.19	130.25	124.81
22	c	907	CLA	CHD-C4C-C3C	-4.19	118.68	124.84
22	B	614	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
22	C	514	CLA	C2D-C1D-ND	4.19	113.19	110.10
22	b	608	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
22	C	507	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
22	c	906	CLA	CHD-C4C-C3C	-4.18	118.69	124.84
22	a	408	CLA	O2D-CGD-CBD	4.18	118.70	111.27
22	B	606	CLA	CHC-C1C-NC	-4.18	117.86	124.20
22	b	602	CLA	CHD-C4C-C3C	-4.18	118.70	124.84
22	c	904	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
22	c	902	CLA	C1D-ND-C4D	-4.17	103.37	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	602	CLA	CAC-C3C-C4C	4.17	130.22	124.81
35	c	917	DGD	O2G-C1B-C2B	4.17	120.49	111.50
22	c	903	CLA	CHA-C4D-ND	4.17	141.22	132.50
22	B	608	CLA	C2D-C1D-ND	4.17	113.17	110.10
22	C	513	CLA	C1-O2A-CGA	4.16	127.36	116.44
22	C	514	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
22	C	508	CLA	CHC-C4B-NB	4.16	128.66	124.26
22	C	508	CLA	C2C-C1C-NC	4.16	113.87	109.97
22	d	403	CLA	CHD-C1D-ND	-4.15	120.64	124.45
22	B	613	CLA	CHD-C4C-C3C	-4.15	118.73	124.84
22	b	606	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
22	a	409	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
26	D	406	PL9	C40-C39-C41	4.14	122.24	115.27
22	a	409	CLA	C3B-C4B-NB	4.13	114.35	110.52
22	C	502	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
25	C	520	LMG	O7-C10-C11	4.13	120.41	111.50
26	d	405	PL9	C35-C34-C36	4.13	122.22	115.27
22	b	607	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
22	C	513	CLA	CHD-C1D-ND	-4.13	120.66	124.45
23	a	410	PHO	O2D-CGD-O1D	-4.12	115.78	123.84
22	a	412	CLA	O2D-CGD-O1D	-4.12	115.78	123.84
22	c	907	CLA	CHB-C1B-NB	-4.12	119.90	124.26
34	b	632	HTG	C1-O5-C5	4.12	120.17	112.58
22	D	403	CLA	C4D-CHA-C1A	-4.11	116.24	121.25
22	b	610	CLA	C2D-C1D-ND	4.11	113.14	110.10
22	a	409	CLA	C4A-NA-C1A	4.11	108.56	106.71
22	D	404	CLA	CAC-C3C-C4C	4.11	130.14	124.81
27	d	407	LHG	O8-C23-O10	-4.11	113.22	123.59
22	c	905	CLA	CHD-C4C-C3C	-4.10	118.81	124.84
22	B	609	CLA	O2D-CGD-O1D	-4.10	115.81	123.84
22	D	404	CLA	C2D-C1D-ND	4.10	113.13	110.10
22	b	613	CLA	C2C-C1C-NC	4.10	113.81	109.97
22	C	514	CLA	CHA-C4D-ND	4.09	141.06	132.50
22	c	909	CLA	CHC-C4B-NB	4.09	128.59	124.26
22	D	404	CLA	C2C-C1C-NC	4.09	113.81	109.97
22	b	616	CLA	CHD-C4C-C3C	-4.09	118.83	124.84
36	E	102	HEM	C4C-NC-C1C	4.09	109.35	105.35
24	b	618	BCR	C33-C5-C6	-4.09	119.94	124.53
23	a	411	PHO	C4-C3-C5	4.09	122.15	115.27
22	b	603	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
22	B	606	CLA	O2D-CGD-O1D	-4.09	115.85	123.84
22	c	912	CLA	CHA-C4D-ND	4.08	141.04	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	609	CLA	CHC-C4B-NB	4.08	128.58	124.26
22	B	608	CLA	C3B-C2B-C1B	-4.08	102.24	107.16
22	A	408	CLA	C1D-ND-C4D	-4.07	103.44	106.33
22	B	616	CLA	C2C-C1C-NC	4.07	113.78	109.97
22	B	615	CLA	CHD-C4C-NC	4.06	130.60	124.20
22	B	615	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
22	c	906	CLA	CHD-C1D-ND	-4.05	120.73	124.45
22	c	909	CLA	CHD-C1D-ND	-4.05	120.73	124.45
22	B	613	CLA	CAC-C3C-C4C	4.05	130.07	124.81
22	B	604	CLA	O2D-CGD-O1D	-4.05	115.92	123.84
22	B	610	CLA	C4D-CHA-C1A	-4.05	116.32	121.25
22	B	616	CLA	CHD-C4C-NC	4.05	130.58	124.20
22	B	607	CLA	C4-C3-C5	4.04	122.08	115.27
22	d	403	CLA	O2D-CGD-CBD	4.04	118.45	111.27
22	c	906	CLA	C2C-C1C-NC	4.04	113.76	109.97
22	B	605	CLA	C4D-CHA-C1A	-4.04	116.33	121.25
22	b	615	CLA	CHD-C4C-C3C	-4.04	118.90	124.84
27	D	409	LHG	O7-C7-O9	-4.04	113.94	123.70
22	B	604	CLA	CHD-C4C-C3C	-4.04	118.91	124.84
22	B	602	CLA	O1D-CGD-CBD	-4.03	116.23	124.48
22	B	609	CLA	CHA-C4D-ND	4.03	140.94	132.50
22	C	513	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
22	c	914	CLA	CHD-C1D-ND	-4.02	120.76	124.45
22	b	605	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
22	c	913	CLA	CHD-C4C-C3C	-4.02	118.93	124.84
28	b	621	SQD	O7-S-C6	4.02	111.72	106.94
22	c	903	CLA	C1D-CHD-C4C	-4.02	117.39	126.06
22	c	911	CLA	O2D-CGD-CBD	4.02	118.41	111.27
22	C	506	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
22	C	511	CLA	C4A-NA-C1A	4.02	108.51	106.71
22	c	913	CLA	O2D-CGD-O1D	-4.02	115.99	123.84
22	C	510	CLA	CHB-C1B-NB	-4.01	120.01	124.26
22	c	903	CLA	O2D-CGD-CBD	4.01	118.39	111.27
22	d	402	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
22	c	914	CLA	CMC-C2C-C1C	4.00	131.14	125.04
22	b	613	CLA	CHC-C4B-NB	4.00	128.49	124.26
22	c	907	CLA	C2D-C1D-ND	3.99	113.05	110.10
22	b	609	CLA	CHA-C4D-ND	3.99	140.85	132.50
22	A	406	CLA	C4D-CHA-C1A	-3.99	116.39	121.25
22	C	503	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
25	b	622	LMG	C7-O1-C1	3.99	121.53	113.74
22	b	614	CLA	C2B-C1B-NB	3.99	112.90	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	616	CLA	O2D-CGD-CBD	3.98	118.33	111.27
39	v	202	HEC	CBC-CAC-C3C	3.98	123.39	112.43
25	C	531	LMG	O7-C10-C11	3.98	120.07	111.50
22	b	610	CLA	CMC-C2C-C1C	3.97	131.09	125.04
22	C	509	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
28	A	413	SQD	O48-C23-O10	-3.97	113.57	123.59
22	D	401	CLA	C1D-CHD-C4C	-3.97	117.49	126.06
22	B	602	CLA	C2C-C1C-NC	3.97	113.69	109.97
22	b	612	CLA	CHD-C4C-NC	3.97	130.46	124.20
22	b	603	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
22	A	406	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
22	b	604	CLA	C3B-C2B-C1B	-3.97	102.38	107.16
22	a	412	CLA	CHD-C4C-C3C	-3.96	119.01	124.84
22	b	617	CLA	C3C-C4C-NC	3.96	115.02	110.57
22	B	612	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
22	b	605	CLA	CHD-C4C-C3C	-3.96	119.02	124.84
22	b	616	CLA	C2C-C1C-NC	3.96	113.68	109.97
26	d	405	PL9	O1-C4-C3	-3.96	116.36	120.72
22	d	403	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
22	a	409	CLA	C4-C3-C5	3.95	121.91	115.27
22	b	607	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
22	b	611	CLA	C3B-C2B-C1B	-3.94	102.40	107.16
34	V	203	HTG	C1-C2-C3	-3.94	102.81	110.59
34	B	627	HTG	C1-O5-C5	3.94	119.84	112.58
22	c	904	CLA	CMD-C2D-C1D	3.93	131.65	124.71
22	c	909	CLA	C2C-C1C-NC	3.93	113.66	109.97
37	H	101	RRX	C31-C1-C6	-3.93	103.93	110.30
34	b	624	HTG	O5-C1-C2	3.93	115.25	110.31
22	c	908	CLA	C2B-C1B-NB	3.93	112.86	110.23
22	D	403	CLA	CHD-C1D-ND	-3.92	120.85	124.45
22	C	514	CLA	O2D-CGD-CBD	3.92	118.23	111.27
22	c	903	CLA	CHD-C1D-ND	-3.92	120.85	124.45
22	C	504	CLA	CHD-C1D-ND	-3.92	120.86	124.45
22	C	510	CLA	CMB-C2B-C1B	3.91	131.32	125.37
22	C	513	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
22	B	615	CLA	C3B-C2B-C1B	-3.90	102.45	107.16
35	C	517	DGD	C3G-C2G-C1G	-3.90	102.56	111.79
22	b	603	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
26	a	415	PL9	C53-C6-C1	3.90	122.96	114.99
22	d	402	CLA	O2A-CGA-CBA	3.90	124.14	111.91
22	B	603	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
22	A	408	CLA	O2D-CGD-CBD	3.90	118.19	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	930	LMG	O7-C10-C11	3.90	119.90	111.50
29	a	419	LMT	C4B-C3B-C2B	-3.90	104.02	110.82
22	b	608	CLA	CGD-CBD-CAD	-3.89	98.13	110.73
22	B	605	CLA	CMC-C2C-C1C	3.89	130.97	125.04
22	b	612	CLA	C3D-C2D-C1D	-3.89	100.52	105.83
34	B	627	HTG	O5-C1-C2	3.89	115.21	110.31
22	c	904	CLA	CHA-C4D-ND	3.89	140.64	132.50
27	a	423	LHG	O7-C7-C8	3.89	119.88	111.50
22	c	914	CLA	O2D-CGD-O1D	-3.89	116.24	123.84
22	b	607	CLA	CMD-C2D-C1D	3.89	131.56	124.71
22	c	903	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
22	b	611	CLA	C3D-C2D-C1D	-3.88	100.53	105.83
22	C	511	CLA	CHA-C4D-ND	3.88	140.62	132.50
22	B	607	CLA	CHA-C4D-ND	3.88	140.62	132.50
22	C	514	CLA	C4D-CHA-C1A	-3.88	116.53	121.25
22	C	508	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
22	c	912	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
24	Y	101	BCR	C16-C15-C14	-3.87	115.54	123.47
29	T	102	LMT	C1'-C2'-C3'	3.87	118.06	110.00
22	a	408	CLA	CED-O2D-CGD	3.87	124.69	115.94
22	b	611	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
22	C	509	CLA	C4D-CHA-C1A	-3.87	116.54	121.25
22	c	909	CLA	C4D-CHA-C1A	-3.87	116.54	121.25
22	b	616	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
22	a	408	CLA	C4A-NA-C1A	3.86	108.44	106.71
22	b	610	CLA	C4A-NA-C1A	3.86	108.44	106.71
22	c	910	CLA	O2D-CGD-CBD	3.85	118.11	111.27
22	b	607	CLA	C1-O2A-CGA	3.85	126.55	116.44
22	a	407	CLA	C4-C3-C5	3.85	121.75	115.27
22	B	608	CLA	CGD-CBD-CAD	-3.85	98.27	110.73
22	A	406	CLA	CMC-C2C-C1C	3.85	130.90	125.04
22	C	512	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
22	C	512	CLA	CMB-C2B-C1B	3.85	131.23	125.37
22	c	914	CLA	C3B-C2B-C1B	-3.85	102.52	107.16
22	C	514	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
22	B	608	CLA	O2D-CGD-CBD	3.84	118.09	111.27
22	c	909	CLA	CHD-C4C-C3C	-3.84	119.20	124.84
22	C	512	CLA	CHC-C4B-NB	3.84	128.32	124.26
22	b	614	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
24	B	620	BCR	C2-C1-C6	3.83	116.37	110.48
22	c	906	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
22	B	613	CLA	CHC-C4B-NB	3.82	128.31	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	612	CLA	O2D-CGD-O1D	-3.82	116.36	123.84
22	c	905	CLA	C3B-C4B-NB	3.82	114.06	110.52
22	C	511	CLA	O2D-CGD-CBD	3.82	118.05	111.27
22	B	602	CLA	CHA-C4D-ND	3.81	140.48	132.50
22	b	607	CLA	C3D-C2D-C1D	-3.81	100.63	105.83
22	b	613	CLA	CHD-C4C-NC	3.81	130.20	124.20
22	C	512	CLA	CHB-C1B-NB	-3.81	120.23	124.26
22	B	606	CLA	CAC-C3C-C4C	3.81	129.75	124.81
22	C	509	CLA	CHD-C4C-C3C	-3.80	119.25	124.84
22	B	610	CLA	O2D-CGD-CBD	3.80	118.03	111.27
35	h	102	DGD	O1G-C1A-C2A	3.80	123.84	111.91
25	b	622	LMG	C3-C4-C5	3.80	117.02	110.24
22	C	511	CLA	CHC-C4B-NB	3.80	128.28	124.26
26	D	406	PL9	C7-C8-C9	-3.80	120.47	126.79
22	C	514	CLA	CHD-C1D-ND	-3.80	120.97	124.45
22	B	604	CLA	C4A-NA-C1A	3.79	108.41	106.71
22	B	609	CLA	CAC-C3C-C4C	3.79	129.73	124.81
22	c	906	CLA	C4D-CHA-C1A	-3.79	116.64	121.25
22	a	412	CLA	C2D-C1D-ND	3.79	112.90	110.10
24	d	404	BCR	C30-C25-C26	-3.79	117.28	122.61
22	A	408	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
22	B	612	CLA	C3D-C2D-C1D	-3.78	100.67	105.83
22	b	604	CLA	CMC-C2C-C1C	3.78	130.80	125.04
22	c	904	CLA	C1-C2-C3	-3.78	119.50	126.04
22	c	912	CLA	C3B-C2B-C1B	-3.78	102.60	107.16
35	H	102	DGD	O1G-C1A-C2A	3.78	123.76	111.91
24	c	915	BCR	C15-C14-C13	-3.78	121.92	127.31
22	B	616	CLA	C3D-C2D-C1D	-3.78	100.68	105.83
22	C	507	CLA	C3D-C2D-C1D	-3.78	100.68	105.83
22	C	510	CLA	CHA-C4D-ND	3.77	140.40	132.50
22	c	903	CLA	C4D-CHA-C1A	-3.77	116.66	121.25
22	B	611	CLA	CMD-C2D-C1D	3.77	131.36	124.71
22	B	608	CLA	CBC-CAC-C3C	-3.77	102.04	112.43
22	b	607	CLA	CHD-C4C-NC	3.77	130.14	124.20
22	C	504	CLA	O2D-CGD-CBD	3.77	117.96	111.27
22	c	905	CLA	C3D-C2D-C1D	-3.77	100.69	105.83
25	c	920	LMG	O8-C28-C29	3.76	123.72	111.91
22	b	613	CLA	CHD-C1D-ND	-3.76	121.00	124.45
22	B	606	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
22	b	610	CLA	C3B-C2B-C1B	-3.76	102.63	107.16
22	b	614	CLA	O2D-CGD-CBD	3.76	117.94	111.27
22	c	910	CLA	CHB-C1B-NB	-3.75	120.28	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	605	CLA	CHA-C4D-ND	3.75	140.34	132.50
26	a	415	PL9	C7-C3-C4	3.74	119.92	116.88
22	C	509	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
22	B	608	CLA	CHD-C1D-ND	-3.74	121.02	124.45
22	B	609	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
22	B	617	CLA	C3B-C2B-C1B	-3.73	102.66	107.16
22	D	404	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
22	c	914	CLA	CHD-C4C-NC	3.73	130.08	124.20
22	D	401	CLA	CBC-CAC-C3C	-3.73	102.16	112.43
22	A	408	CLA	CHD-C4C-C3C	-3.73	119.36	124.84
22	c	911	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
22	c	902	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
22	C	505	CLA	CHD-C4C-C3C	-3.72	119.37	124.84
22	C	513	CLA	C3D-C2D-C1D	-3.72	100.75	105.83
22	C	504	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
22	c	908	CLA	C2C-C1C-NC	3.72	113.45	109.97
22	B	617	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
22	b	606	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
22	B	603	CLA	C3D-C2D-C1D	-3.71	100.76	105.83
22	B	611	CLA	O2A-CGA-CBA	3.71	123.56	111.91
22	B	615	CLA	C1-O2A-CGA	3.71	126.19	116.44
22	c	904	CLA	CHD-C1D-ND	-3.71	121.04	124.45
22	B	614	CLA	C2C-C1C-NC	3.71	113.45	109.97
22	B	608	CLA	C4-C3-C5	3.71	121.51	115.27
22	b	602	CLA	C2C-C1C-NC	3.71	113.45	109.97
22	b	615	CLA	CHA-C4D-ND	3.71	140.26	132.50
24	d	404	BCR	C16-C15-C14	-3.71	115.88	123.47
24	A	409	BCR	C15-C16-C17	-3.70	115.90	123.47
22	B	605	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
22	b	616	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
22	C	505	CLA	C3B-C2B-C1B	-3.69	102.70	107.16
24	B	618	BCR	C3-C4-C5	-3.69	107.48	114.08
22	c	911	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
22	b	604	CLA	C4A-NA-C1A	3.69	108.36	106.71
22	C	503	CLA	C2C-C1C-NC	3.69	113.43	109.97
22	b	615	CLA	C3D-C2D-C1D	-3.69	100.80	105.83
22	C	503	CLA	C3D-C2D-C1D	-3.68	100.80	105.83
22	c	907	CLA	C3B-C2B-C1B	-3.68	102.72	107.16
22	B	612	CLA	CMD-C2D-C1D	3.68	131.20	124.71
22	C	513	CLA	CHA-C4D-ND	3.68	140.20	132.50
22	b	612	CLA	CHA-C4D-ND	3.68	140.20	132.50
22	B	603	CLA	C3B-C2B-C1B	-3.68	102.72	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	906	CLA	C3D-C2D-C1D	-3.67	100.82	105.83
22	B	614	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
22	B	614	CLA	CHD-C4C-C3C	-3.67	119.44	124.84
22	b	606	CLA	C4-C3-C5	3.67	121.45	115.27
22	C	509	CLA	C2C-C1C-NC	3.67	113.41	109.97
22	D	403	CLA	C3B-C4B-NB	3.67	113.92	110.52
22	D	401	CLA	C4D-CHA-C1A	-3.67	116.78	121.25
22	B	605	CLA	CAC-C3C-C4C	3.67	129.57	124.81
22	A	408	CLA	C4D-CHA-C1A	-3.67	116.78	121.25
22	c	902	CLA	CHD-C4C-NC	3.67	129.98	124.20
22	b	602	CLA	O2D-CGD-O1D	-3.66	116.67	123.84
22	a	407	CLA	C3D-C2D-C1D	-3.66	100.83	105.83
22	B	608	CLA	C4A-NA-C1A	3.66	108.35	106.71
24	k	101	BCR	C24-C23-C22	-3.66	120.70	126.23
22	C	508	CLA	CMD-C2D-C1D	3.66	131.16	124.71
28	a	418	SQD	O47-C7-C8	3.66	119.39	111.50
22	b	608	CLA	C3B-C2B-C1B	-3.66	102.75	107.16
22	b	617	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
22	b	612	CLA	C3B-C2B-C1B	-3.66	102.75	107.16
22	b	617	CLA	CHA-C4D-ND	3.65	140.14	132.50
22	C	509	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
22	B	616	CLA	CHB-C1B-NB	-3.65	120.39	124.26
22	b	604	CLA	CHD-C4C-NC	3.65	129.96	124.20
22	c	909	CLA	CHA-C4D-ND	3.65	140.13	132.50
22	d	402	CLA	C4-C3-C5	3.64	121.40	115.27
22	b	604	CLA	C3D-C2D-C1D	-3.64	100.86	105.83
22	B	615	CLA	C4-C3-C5	3.64	121.40	115.27
22	B	607	CLA	C4A-NA-C1A	3.64	108.34	106.71
22	d	403	CLA	CMD-C2D-C1D	3.64	131.13	124.71
22	B	613	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
36	e	101	HEM	C4C-NC-C1C	3.64	108.91	105.35
22	b	606	CLA	C4A-NA-C1A	3.64	108.34	106.71
22	b	613	CLA	C3D-C2D-C1D	-3.64	100.87	105.83
27	D	411	LHG	O8-C23-O10	-3.63	114.42	123.59
24	C	515	BCR	C38-C26-C25	-3.63	120.45	124.53
24	b	620	BCR	C7-C8-C9	-3.63	120.74	126.23
22	A	408	CLA	C3B-C2B-C1B	-3.63	102.78	107.16
22	B	616	CLA	CHA-C4D-ND	3.63	140.09	132.50
22	C	509	CLA	CHD-C1D-ND	-3.63	121.12	124.45
22	C	508	CLA	C3B-C2B-C1B	-3.63	102.78	107.16
22	b	612	CLA	CMB-C2B-C1B	3.62	130.89	125.37
22	B	606	CLA	C2C-C1C-NC	3.62	113.37	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	V	202	HEC	CBB-CAB-C3B	3.62	122.42	112.43
22	b	613	CLA	C3B-C2B-C1B	-3.62	102.79	107.16
22	b	613	CLA	C4-C3-C5	3.62	121.36	115.27
22	B	608	CLA	CHA-C4D-ND	3.62	140.06	132.50
22	c	906	CLA	C1-O2A-CGA	3.61	125.92	116.44
22	B	603	CLA	C7-C6-C5	-3.61	103.55	113.36
35	C	518	DGD	O5D-C6D-C5D	3.61	115.73	109.05
34	b	624	HTG	C1-C2-C3	3.61	117.72	110.59
22	b	608	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
22	b	612	CLA	CMD-C2D-C1D	3.61	131.08	124.71
22	B	616	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
22	c	904	CLA	O2A-CGA-CBA	3.60	123.22	111.91
22	b	614	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
22	A	406	CLA	CHB-C1B-NB	-3.60	120.44	124.26
22	B	604	CLA	C3D-C2D-C1D	-3.60	100.92	105.83
22	c	908	CLA	C4-C3-C5	3.60	121.33	115.27
22	A	406	CLA	CHD-C4C-NC	3.60	129.87	124.20
22	D	403	CLA	C2A-C1A-CHA	-3.60	117.57	123.86
24	D	405	BCR	C28-C27-C26	-3.60	107.65	114.08
22	B	614	CLA	O2D-CGD-O1D	-3.60	116.81	123.84
22	A	406	CLA	CHA-C4D-ND	3.60	140.02	132.50
22	B	602	CLA	C2B-C1B-NB	3.60	112.64	110.23
22	B	602	CLA	CMD-C2D-C1D	3.60	131.05	124.71
22	B	617	CLA	C4A-NA-C1A	3.59	108.32	106.71
22	c	914	CLA	C3D-C2D-C1D	-3.59	100.94	105.83
22	b	616	CLA	O2D-CGD-CBD	3.59	117.64	111.27
26	d	405	PL9	C7-C8-C9	-3.59	120.82	126.79
22	C	505	CLA	CMD-C2D-C1D	3.58	131.03	124.71
35	c	918	DGD	O2G-C1B-C2B	3.58	119.22	111.50
22	d	402	CLA	CHD-C4C-C3C	-3.57	119.59	124.84
27	d	401	LHG	O7-C7-C8	3.57	119.19	111.50
22	C	514	CLA	CHD-C4C-NC	3.56	129.82	124.20
25	b	622	LMG	O6-C1-O1	3.56	118.41	109.97
22	c	903	CLA	CHD-C4C-NC	3.56	129.81	124.20
22	c	910	CLA	CHA-C4D-ND	3.56	139.94	132.50
22	C	507	CLA	O2D-CGD-CBD	3.56	117.59	111.27
35	h	102	DGD	O2G-C1B-C2B	3.55	119.16	111.50
22	C	504	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
22	b	605	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
22	C	510	CLA	CHD-C4C-C3C	-3.55	119.63	124.84
22	a	409	CLA	C1-C2-C3	-3.55	119.91	126.04
22	c	905	CLA	CHA-C4D-ND	3.54	139.91	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	L	101	LHG	O7-C7-C8	3.54	119.14	111.50
22	b	605	CLA	C3D-C2D-C1D	-3.54	101.00	105.83
22	B	616	CLA	C3B-C2B-C1B	-3.54	102.89	107.16
35	h	102	DGD	O1G-C1A-O1A	-3.54	114.66	123.59
35	C	519	DGD	O6D-C1D-O3G	-3.54	101.59	109.97
22	D	401	CLA	O2D-CGD-CBD	3.54	117.55	111.27
22	C	512	CLA	CHA-C4D-ND	3.53	139.89	132.50
22	B	610	CLA	C2B-C1B-NB	3.53	112.60	110.23
22	b	609	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
34	C	523	HTG	C1-S1-C1'	3.52	112.50	100.40
22	C	505	CLA	CHA-C4D-ND	3.52	139.86	132.50
22	C	507	CLA	CAC-C3C-C4C	3.52	129.37	124.81
22	b	608	CLA	O2D-CGD-CBD	3.52	117.52	111.27
22	b	603	CLA	C2C-C1C-NC	3.52	113.27	109.97
22	b	604	CLA	CHA-C4D-ND	3.51	139.85	132.50
22	B	606	CLA	CHA-C4D-ND	3.51	139.85	132.50
22	B	612	CLA	CMB-C2B-C1B	3.51	130.72	125.37
22	b	602	CLA	CHA-C4D-ND	3.51	139.84	132.50
22	D	403	CLA	CHD-C4C-C3C	-3.51	119.68	124.84
22	B	611	CLA	CHA-C4D-ND	3.51	139.84	132.50
28	a	414	SQD	C1-O5-C5	-3.51	106.80	113.69
22	c	903	CLA	C3D-C2D-C1D	-3.50	101.05	105.83
22	b	615	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
22	C	508	CLA	C3D-C2D-C1D	-3.50	101.05	105.83
22	c	904	CLA	C3D-C2D-C1D	-3.50	101.05	105.83
22	B	607	CLA	CMD-C2D-C1D	3.50	130.89	124.71
22	c	912	CLA	C2D-C1D-ND	3.50	112.69	110.10
22	c	904	CLA	CHD-C4C-C3C	-3.50	119.69	124.84
29	a	419	LMT	C2'-C3'-C4'	3.50	117.68	109.68
22	b	608	CLA	CHD-C4C-C3C	-3.50	119.70	124.84
22	C	514	CLA	O2A-CGA-CBA	3.50	122.88	111.91
24	c	916	BCR	C33-C5-C6	-3.50	120.60	124.53
22	B	602	CLA	C1-O2A-CGA	3.49	125.61	116.44
22	C	506	CLA	CHD-C1D-ND	-3.49	121.24	124.45
22	c	910	CLA	C2A-C1A-CHA	-3.49	117.75	123.86
22	B	611	CLA	O2A-CGA-O1A	-3.49	114.78	123.59
26	D	406	PL9	C53-C6-C1	3.49	122.13	114.99
22	C	514	CLA	CMC-C2C-C1C	3.49	130.36	125.04
24	K	101	BCR	C24-C23-C22	-3.49	120.96	126.23
22	b	614	CLA	C3B-C2B-C1B	-3.49	102.95	107.16
22	b	607	CLA	CHA-C4D-ND	3.48	139.78	132.50
34	v	203	HTG	O4-C4-C3	-3.48	102.30	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	409	CLA	CMC-C2C-C1C	3.48	130.34	125.04
22	d	402	CLA	CHB-C1B-NB	-3.48	120.57	124.26
22	b	617	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
26	D	406	PL9	C20-C19-C21	3.48	121.12	115.27
22	c	905	CLA	C4D-CHA-C1A	-3.47	117.02	121.25
22	b	602	CLA	C3B-C2B-C1B	-3.47	102.97	107.16
25	b	622	LMG	C4-C3-C2	3.47	116.88	110.82
22	C	508	CLA	CHA-C4D-ND	3.47	139.76	132.50
22	b	606	CLA	C3B-C2B-C1B	-3.47	102.98	107.16
22	c	908	CLA	C3B-C2B-C1B	-3.46	102.98	107.16
22	C	505	CLA	CHD-C4C-NC	3.46	129.66	124.20
22	b	610	CLA	CHD-C4C-NC	3.46	129.65	124.20
22	c	904	CLA	CMB-C2B-C1B	3.46	130.63	125.37
22	B	607	CLA	C3D-C2D-C1D	-3.45	101.12	105.83
22	C	504	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
22	B	602	CLA	C2D-C1D-ND	3.45	112.64	110.10
25	A	410	LMG	O7-C10-C11	3.45	118.93	111.50
22	B	604	CLA	CHA-C4D-ND	3.45	139.71	132.50
22	C	513	CLA	O1D-CGD-CBD	-3.44	117.44	124.48
22	a	407	CLA	CHA-C4D-ND	3.44	139.69	132.50
29	E	101	LMT	O5'-C5'-C6'	3.44	114.98	106.44
22	B	613	CLA	C2A-C1A-CHA	-3.44	117.85	123.86
22	D	403	CLA	O2D-CGD-CBD	3.44	117.38	111.27
22	B	614	CLA	CHA-C4D-ND	3.43	139.68	132.50
22	b	604	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
27	D	411	LHG	O8-C23-C24	3.43	122.67	111.91
22	d	403	CLA	CHA-C4D-ND	3.43	139.67	132.50
22	C	513	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
22	B	607	CLA	C1-C2-C3	-3.43	120.11	126.04
22	b	602	CLA	O2A-CGA-CBA	3.43	122.66	111.91
22	b	614	CLA	C4-C3-C5	3.42	121.03	115.27
22	B	606	CLA	C3C-C4C-NC	3.42	114.41	110.57
34	D	415	HTG	O5-C1-S1	3.42	118.01	109.82
22	d	402	CLA	CHC-C4B-NB	3.42	127.88	124.26
35	C	518	DGD	O2G-C1B-C2B	3.42	118.87	111.50
22	C	513	CLA	C2C-C1C-NC	3.42	113.17	109.97
22	B	602	CLA	C3B-C2B-C1B	-3.41	103.04	107.16
22	b	615	CLA	CAC-C3C-C4C	3.41	129.24	124.81
22	c	912	CLA	O2D-CGD-CBD	3.41	117.32	111.27
27	D	409	LHG	O8-C23-C24	3.41	122.60	111.91
22	b	617	CLA	CHB-C1B-NB	-3.41	120.65	124.26
22	b	606	CLA	CHA-C4D-ND	3.40	139.62	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	502	CLA	CAC-C3C-C4C	3.40	129.22	124.81
22	b	616	CLA	CHD-C4C-NC	3.39	129.55	124.20
22	d	402	CLA	CHD-C1D-ND	-3.39	121.33	124.45
22	c	902	CLA	CMB-C2B-C1B	3.39	130.54	125.37
22	C	506	CLA	C3B-C2B-C1B	-3.39	103.07	107.16
22	d	402	CLA	C3D-C2D-C1D	-3.39	101.21	105.83
22	c	908	CLA	CBC-CAC-C3C	-3.39	103.09	112.43
22	b	605	CLA	C3C-C4C-NC	3.38	114.36	110.57
22	A	406	CLA	C4A-NA-C1A	3.38	108.22	106.71
22	c	912	CLA	O2A-CGA-O1A	-3.37	115.08	123.59
22	B	609	CLA	C3B-C2B-C1B	-3.37	103.09	107.16
25	b	622	LMG	O6-C5-C6	3.37	114.82	106.44
22	c	906	CLA	CHB-C1B-NB	-3.37	120.69	124.26
22	B	605	CLA	CHA-C4D-ND	3.37	139.55	132.50
22	b	609	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
22	B	615	CLA	CED-O2D-CGD	3.37	123.56	115.94
22	b	613	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
22	C	504	CLA	C2C-C1C-NC	3.37	113.12	109.97
35	C	519	DGD	O1G-C1A-C2A	3.37	122.47	111.91
35	C	519	DGD	O2G-C1B-C2B	3.36	118.75	111.50
22	B	608	CLA	CAC-C3C-C4C	3.36	129.17	124.81
39	V	202	HEC	CBD-CAD-C3D	-3.36	103.28	112.63
22	A	408	CLA	CMD-C2D-C1D	3.36	130.64	124.71
22	a	412	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
29	f	102	LMT	O1'-C1'-C2'	3.36	113.55	108.30
23	D	402	PHO	C1C-C2C-C3C	-3.36	105.82	108.61
22	b	602	CLA	CHD-C1D-ND	-3.36	121.37	124.45
22	d	403	CLA	C2D-C1D-ND	3.36	112.58	110.10
22	b	609	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
22	C	507	CLA	CHA-C4D-ND	3.36	139.52	132.50
24	D	405	BCR	C29-C30-C25	3.36	115.65	110.48
22	b	604	CLA	O2A-CGA-O1A	-3.36	115.12	123.59
22	a	409	CLA	CHD-C4C-NC	3.36	129.49	124.20
22	B	612	CLA	CHB-C1B-NB	-3.36	120.70	124.26
29	Z	101	LMT	C3B-C4B-C5B	3.35	116.22	110.24
28	a	418	SQD	O48-C23-C24	3.35	122.43	111.91
22	b	614	CLA	CAA-CBA-CGA	-3.35	103.45	113.25
22	C	508	CLA	C4D-CHA-C1A	-3.35	117.17	121.25
22	b	609	CLA	C3C-C4C-NC	3.35	114.33	110.57
22	B	603	CLA	CHA-C4D-ND	3.35	139.50	132.50
22	B	607	CLA	CHC-C1C-NC	-3.35	119.13	124.20
22	d	403	CLA	C4D-CHA-C1A	-3.34	117.18	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	511	CLA	C3B-C2B-C1B	-3.34	103.13	107.16
22	b	617	CLA	O1D-CGD-CBD	-3.34	117.65	124.48
22	B	603	CLA	CHC-C1C-NC	-3.34	119.14	124.20
22	D	401	CLA	CMC-C2C-C1C	3.34	130.12	125.04
22	D	401	CLA	C3D-C2D-C1D	-3.34	101.28	105.83
22	B	605	CLA	CMD-C2D-C1D	3.34	130.59	124.71
34	V	203	HTG	O5-C1-S1	3.34	117.80	109.82
22	c	907	CLA	CMD-C2D-C1D	3.34	130.59	124.71
22	b	617	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
22	B	613	CLA	CMD-C2D-C1D	3.33	130.59	124.71
22	a	408	CLA	CBC-CAC-C3C	-3.33	103.25	112.43
22	B	606	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
22	C	511	CLA	C4D-CHA-C1A	-3.33	117.20	121.25
22	C	506	CLA	O2D-CGD-CBD	3.32	117.17	111.27
22	c	914	CLA	CHA-C4D-ND	3.32	139.45	132.50
22	d	402	CLA	O2A-CGA-O1A	-3.32	115.20	123.59
37	H	101	RRX	C7-C8-C9	-3.32	121.21	126.23
22	d	402	CLA	CHA-C4D-ND	3.32	139.44	132.50
22	c	911	CLA	C4D-CHA-C1A	-3.32	117.21	121.25
22	c	912	CLA	C2C-C1C-NC	3.32	113.08	109.97
24	y	101	BCR	C24-C23-C22	-3.31	121.23	126.23
22	b	603	CLA	CHD-C4C-C3C	-3.31	119.98	124.84
22	B	616	CLA	C4D-CHA-C1A	-3.31	117.22	121.25
22	B	615	CLA	C1D-ND-C4D	-3.31	103.99	106.33
22	C	510	CLA	CHB-C4A-NA	3.30	129.08	124.51
22	c	902	CLA	C4-C3-C5	3.30	120.82	115.27
22	B	606	CLA	O2D-CGD-CBD	3.30	117.13	111.27
22	b	616	CLA	CED-O2D-CGD	3.30	123.40	115.94
22	a	408	CLA	C3D-C2D-C1D	-3.30	101.33	105.83
22	C	513	CLA	CHD-C4C-NC	3.30	129.40	124.20
22	B	611	CLA	C3B-C2B-C1B	-3.29	103.19	107.16
22	C	508	CLA	CHD-C4C-NC	3.29	129.39	124.20
22	C	511	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
22	B	607	CLA	C3C-C4C-NC	3.29	114.26	110.57
28	D	408	SQD	O7-S-C6	3.29	110.85	106.94
22	d	402	CLA	CMB-C2B-C1B	3.29	130.38	125.37
22	b	603	CLA	C4-C3-C5	3.29	120.80	115.27
22	b	609	CLA	C2D-C1D-ND	3.29	112.53	110.10
24	y	101	BCR	C21-C20-C19	-3.29	112.96	123.22
22	b	613	CLA	C3C-C4C-NC	3.28	114.25	110.57
22	b	611	CLA	CHA-C4D-ND	3.28	139.37	132.50
22	b	609	CLA	C4D-CHA-C1A	-3.28	117.26	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	D	407	DGD	C3D-C4D-C5D	3.28	114.88	109.77
22	A	405	CLA	C3D-C2D-C1D	-3.28	101.36	105.83
22	C	507	CLA	CMC-C2C-C1C	3.28	130.03	125.04
39	V	202	HEC	CBC-CAC-C3C	3.28	121.47	112.43
22	B	612	CLA	C2A-C1A-CHA	-3.28	118.13	123.86
22	c	908	CLA	C3D-C2D-C1D	-3.27	101.36	105.83
22	A	408	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
22	c	907	CLA	C3B-C4B-NB	3.27	113.55	110.52
22	B	615	CLA	CMD-C2D-C1D	3.27	130.48	124.71
22	B	605	CLA	CHD-C4C-NC	3.27	129.36	124.20
22	B	615	CLA	O2A-CGA-CBA	3.27	122.18	111.91
22	b	611	CLA	C3C-C4C-NC	3.27	114.24	110.57
22	d	403	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
22	B	614	CLA	C3D-C2D-C1D	-3.27	101.37	105.83
22	b	606	CLA	C1-C2-C3	-3.27	120.39	126.04
22	C	506	CLA	C2D-C1D-ND	3.26	112.51	110.10
22	b	612	CLA	C7-C6-C5	-3.26	104.51	113.36
22	C	509	CLA	O2A-CGA-O1A	-3.26	115.37	123.59
22	B	610	CLA	CHA-C4D-ND	3.26	139.31	132.50
22	C	514	CLA	CHC-C1C-NC	-3.26	119.26	124.20
22	b	603	CLA	C3D-C2D-C1D	-3.25	101.39	105.83
22	c	912	CLA	C4-C3-C5	3.25	120.75	115.27
22	c	914	CLA	O2D-CGD-CBD	3.25	117.05	111.27
22	B	605	CLA	C3B-C2B-C1B	-3.25	103.24	107.16
22	c	905	CLA	O2D-CGD-CBD	3.25	117.04	111.27
22	c	906	CLA	CHC-C4B-NB	3.25	127.69	124.26
22	B	610	CLA	C3B-C2B-C1B	-3.24	103.25	107.16
22	B	617	CLA	CHA-C4D-ND	3.24	139.28	132.50
22	C	509	CLA	CMB-C2B-C1B	3.24	130.31	125.37
26	a	415	PL9	C35-C34-C36	3.24	120.73	115.27
22	c	907	CLA	CHD-C4C-NC	3.24	129.31	124.20
22	c	910	CLA	C1-O2A-CGA	3.24	124.94	116.44
22	c	912	CLA	CHD-C1D-ND	-3.24	121.48	124.45
22	c	902	CLA	C4D-CHA-C1A	-3.24	117.31	121.25
24	b	619	BCR	C29-C30-C25	3.24	115.46	110.48
28	D	408	SQD	O6-C44-C45	3.24	114.96	108.76
22	A	406	CLA	O2D-CGD-CBD	3.24	117.02	111.27
22	a	407	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
28	D	408	SQD	O8-S-C6	3.23	110.89	105.74
22	C	512	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
22	B	608	CLA	CHB-C1B-NB	-3.23	120.84	124.26
22	a	408	CLA	CHA-C4D-ND	3.23	139.25	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	606	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
22	A	408	CLA	CHA-C4D-ND	3.23	139.25	132.50
22	c	907	CLA	C3D-C2D-C1D	-3.22	101.44	105.83
22	a	407	CLA	C4D-CHA-C1A	-3.22	117.33	121.25
28	f	101	SQD	O8-S-C6	3.22	110.97	105.77
22	B	602	CLA	CHD-C4C-C3C	-3.22	120.11	124.84
22	d	403	CLA	CHD-C4C-C3C	-3.22	120.11	124.84
27	a	423	LHG	O8-C23-C24	3.21	122.00	111.91
22	D	403	CLA	CMC-C2C-C1C	3.21	129.93	125.04
24	y	101	BCR	C38-C26-C25	-3.21	120.92	124.53
34	v	203	HTG	O5-C1-S1	3.21	117.50	109.82
22	C	512	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
22	C	502	CLA	C3B-C2B-C1B	-3.21	103.29	107.16
22	B	604	CLA	C4D-CHA-C1A	-3.20	117.35	121.25
22	a	412	CLA	CHA-C4D-ND	3.20	139.19	132.50
22	C	505	CLA	CHC-C4B-NB	3.20	127.64	124.26
22	b	607	CLA	C3C-C4C-NC	3.20	114.16	110.57
22	D	404	CLA	CHA-C4D-ND	3.20	139.19	132.50
22	C	504	CLA	C3C-C4C-NC	3.20	114.16	110.57
22	C	504	CLA	C4-C3-C5	3.20	120.65	115.27
22	b	610	CLA	CBC-CAC-C3C	-3.19	103.62	112.43
22	C	513	CLA	CMB-C2B-C1B	3.19	130.23	125.37
22	C	503	CLA	CAC-C3C-C4C	3.19	128.95	124.81
22	D	403	CLA	C3D-C2D-C1D	-3.19	101.48	105.83
22	b	616	CLA	CHA-C4D-ND	3.19	139.17	132.50
22	c	907	CLA	C4D-CHA-C1A	-3.19	117.37	121.25
22	B	615	CLA	CHA-C4D-ND	3.19	139.16	132.50
22	D	404	CLA	CMD-C2D-C1D	3.18	130.32	124.71
22	b	606	CLA	C3C-C4C-NC	3.18	114.14	110.57
22	b	616	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
35	c	919	DGD	O1G-C1A-C2A	3.18	121.90	111.91
28	b	621	SQD	O5-C1-C2	-3.18	103.61	110.35
22	c	905	CLA	C5-C3-C2	-3.18	114.68	121.12
22	b	605	CLA	CAC-C3C-C4C	3.18	128.93	124.81
22	B	607	CLA	CHD-C4C-NC	3.18	129.21	124.20
22	c	910	CLA	O2A-CGA-CBA	3.18	121.88	111.91
22	B	606	CLA	CHD-C1D-ND	-3.17	121.54	124.45
37	h	101	RRX	C7-C8-C9	-3.17	121.44	126.23
36	E	102	HEM	C4A-NA-C1A	3.17	108.45	105.35
22	b	603	CLA	C1-C2-C3	-3.17	120.56	126.04
22	C	509	CLA	C3D-C2D-C1D	-3.17	101.51	105.83
22	B	611	CLA	CHD-C4C-NC	3.17	129.19	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	905	CLA	C4-C3-C5	3.17	120.60	115.27
22	B	603	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	c	905	CLA	C3B-C2B-C1B	-3.17	103.34	107.16
23	D	402	PHO	C4D-CHA-CBD	3.17	109.95	108.52
22	B	609	CLA	CHD-C4C-NC	3.16	129.19	124.20
22	B	615	CLA	O1D-CGD-CBD	-3.16	118.02	124.48
22	b	606	CLA	CMB-C2B-C1B	3.16	130.18	125.37
25	C	520	LMG	O8-C28-O10	-3.16	115.62	123.59
22	b	611	CLA	CHC-C4B-NB	3.16	127.60	124.26
34	v	203	HTG	O3-C3-C2	3.15	117.64	110.35
25	c	920	LMG	O7-C10-C11	3.15	118.29	111.50
22	B	603	CLA	C3B-C4B-NB	3.15	113.44	110.52
22	c	902	CLA	CHA-C4D-ND	3.15	139.08	132.50
22	B	603	CLA	O2A-CGA-CBA	3.15	121.78	111.91
22	B	612	CLA	CHC-C4B-NB	3.15	127.59	124.26
35	c	919	DGD	O2G-C1B-O1B	-3.14	116.10	123.70
22	c	905	CLA	CHD-C4C-NC	3.14	129.15	124.20
22	a	412	CLA	C1-C2-C3	-3.14	120.61	126.04
27	d	407	LHG	O8-C23-C24	3.14	121.76	111.91
22	b	602	CLA	C3D-C2D-C1D	-3.14	101.55	105.83
22	C	509	CLA	C4-C3-C5	3.13	120.54	115.27
22	a	409	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
22	C	512	CLA	C3D-C2D-C1D	-3.13	101.56	105.83
29	t	101	LMT	C1'-C2'-C3'	-3.13	103.48	110.00
28	b	621	SQD	O6-C1-C2	3.13	113.19	108.30
22	c	911	CLA	CHB-C1B-NB	-3.13	120.95	124.26
22	B	606	CLA	C3D-C2D-C1D	-3.13	101.56	105.83
22	b	612	CLA	CAC-C3C-C4C	3.12	128.86	124.81
22	b	609	CLA	C4-C3-C5	3.12	120.52	115.27
34	b	632	HTG	O5-C1-S1	3.12	117.29	109.82
22	a	412	CLA	CHC-C4B-NB	3.12	127.56	124.26
22	D	403	CLA	CHC-C1C-NC	-3.12	119.47	124.20
22	B	603	CLA	C1-C2-C3	-3.12	120.65	126.04
22	B	617	CLA	O2A-CGA-O1A	-3.12	115.72	123.59
39	v	202	HEC	CBB-CAB-C3B	3.12	121.02	112.43
22	B	612	CLA	O2D-CGD-CBD	3.12	116.81	111.27
22	C	513	CLA	C4-C3-C5	3.11	120.51	115.27
22	b	615	CLA	C4-C3-C5	3.11	120.51	115.27
22	B	605	CLA	CHB-C1B-NB	-3.11	120.96	124.26
22	c	910	CLA	CMC-C2C-C1C	3.11	129.78	125.04
24	B	618	BCR	C2-C3-C4	-3.11	104.43	111.38
22	c	909	CLA	C3D-C2D-C1D	-3.11	101.59	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	609	CLA	C3C-C4C-NC	3.11	114.06	110.57
22	C	511	CLA	O2A-CGA-O1A	-3.11	115.75	123.59
22	c	904	CLA	CAC-C3C-C4C	3.11	128.84	124.81
22	c	913	CLA	CHA-C4D-ND	3.11	139.00	132.50
22	b	604	CLA	C2A-C3A-C4A	-3.10	96.86	101.87
22	C	506	CLA	CHA-C4D-ND	3.10	138.99	132.50
22	B	608	CLA	CMB-C2B-C1B	3.10	130.09	125.37
22	c	908	CLA	CHA-C4D-ND	3.10	138.99	132.50
24	d	404	BCR	C37-C22-C21	-3.10	118.58	122.92
22	d	402	CLA	C3B-C4B-NB	3.10	113.39	110.52
22	b	613	CLA	O2A-CGA-CBA	3.09	121.62	111.91
39	v	202	HEC	C2A-C1A-NA	-3.09	107.31	110.32
24	B	620	BCR	C38-C26-C25	-3.09	121.06	124.53
22	b	613	CLA	C11-C12-C13	-3.09	105.92	115.92
22	B	602	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
22	C	510	CLA	O2A-CGA-CBA	3.09	121.61	111.91
22	A	405	CLA	CHD-C4C-C3C	-3.09	120.30	124.84
29	t	101	LMT	O5'-C5'-C4'	3.09	115.30	109.69
22	a	408	CLA	C4B-CHC-C1C	-3.09	119.01	126.34
37	h	101	RRX	C11-C10-C9	-3.09	122.91	127.31
25	B	621	LMG	O8-C28-C29	3.09	121.59	111.91
22	b	604	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
22	C	513	CLA	C4D-CHA-C1A	-3.08	117.50	121.25
22	c	904	CLA	C7-C6-C5	-3.08	105.00	113.36
26	A	411	PL9	C22-C23-C24	-3.08	120.25	127.66
22	b	602	CLA	CHD-C4C-NC	3.08	129.05	124.20
22	A	405	CLA	O2A-CGA-O1A	-3.08	115.83	123.59
22	a	412	CLA	CHD-C1D-ND	-3.07	121.63	124.45
26	A	411	PL9	C32-C33-C34	-3.07	120.27	127.66
22	a	409	CLA	C2A-C1A-CHA	-3.07	118.49	123.86
22	D	403	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
22	C	506	CLA	C1-O2A-CGA	3.07	124.49	116.44
22	B	617	CLA	C3B-C4B-NB	3.06	113.36	110.52
26	A	411	PL9	C45-C44-C46	3.06	120.42	115.27
22	C	505	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	C	516	BCR	C7-C8-C9	-3.06	121.61	126.23
22	a	408	CLA	CHB-C4A-NA	3.06	128.74	124.51
24	y	101	BCR	C16-C15-C14	-3.06	117.21	123.47
22	B	605	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	c	911	CLA	CAC-C3C-C4C	3.05	128.77	124.81
22	b	608	CLA	C4-C3-C5	3.05	120.41	115.27
39	v	202	HEC	C3D-C4D-ND	-3.05	107.40	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	609	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
22	c	908	CLA	CMD-C2D-C1D	3.04	130.08	124.71
22	c	914	CLA	C1-O2A-CGA	3.04	124.43	116.44
22	C	506	CLA	C4D-CHA-C1A	-3.04	117.54	121.25
22	c	910	CLA	C1D-CHD-C4C	-3.04	119.49	126.06
22	c	911	CLA	CHA-C4D-ND	3.04	138.86	132.50
22	C	505	CLA	C3D-C2D-C1D	-3.04	101.68	105.83
22	C	504	CLA	CHB-C1B-NB	-3.04	121.04	124.26
22	C	502	CLA	C3D-C2D-C1D	-3.03	101.69	105.83
22	C	511	CLA	CAC-C3C-C4C	3.03	128.75	124.81
22	a	409	CLA	CMD-C2D-C1D	3.03	130.06	124.71
22	C	502	CLA	CHA-C4D-ND	3.03	138.84	132.50
22	B	610	CLA	CMC-C2C-C1C	3.03	129.65	125.04
22	D	403	CLA	C3B-C2B-C1B	-3.03	103.51	107.16
22	B	603	CLA	CMD-C2D-C1D	3.03	130.05	124.71
22	b	610	CLA	CHC-C1C-NC	-3.03	119.61	124.20
35	C	518	DGD	O6E-C1E-C2E	3.02	116.75	110.35
22	D	404	CLA	C1-O2A-CGA	3.02	124.38	116.44
24	B	620	BCR	C7-C8-C9	-3.02	121.67	126.23
22	A	405	CLA	C7-C6-C5	-3.02	105.15	113.36
24	C	515	BCR	C7-C8-C9	-3.02	121.67	126.23
28	l	101	SQD	O48-C23-C24	3.02	121.39	111.91
22	D	404	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
22	c	911	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	C	514	CLA	CHB-C1B-NB	-3.02	121.06	124.26
22	B	608	CLA	C3D-C2D-C1D	-3.02	101.72	105.83
22	B	610	CLA	CBC-CAC-C3C	-3.01	104.12	112.43
37	H	101	RRX	C16-C17-C18	-3.01	123.01	127.31
22	b	615	CLA	C3B-C2B-C1B	-3.01	103.52	107.16
22	c	909	CLA	CMB-C2B-C1B	3.01	129.96	125.37
28	b	621	SQD	O48-C23-C24	3.01	121.36	111.91
24	B	620	BCR	C32-C1-C6	-3.01	105.42	110.30
22	c	909	CLA	CHD-C4C-NC	3.01	128.95	124.20
34	c	922	HTG	C1-O5-C5	3.01	118.13	112.58
22	B	610	CLA	C3D-C2D-C1D	-3.01	101.73	105.83
35	H	102	DGD	O2G-C1B-C2B	3.01	117.98	111.50
24	D	405	BCR	C33-C5-C6	-3.00	121.16	124.53
22	B	608	CLA	C3B-C4B-NB	3.00	113.30	110.52
27	a	416	LHG	O8-C23-C24	3.00	121.32	111.91
24	Y	101	BCR	C37-C22-C23	3.00	122.80	118.08
34	b	632	HTG	C3-C4-C5	3.00	115.59	110.24
22	b	610	CLA	C1-C2-C3	-3.00	120.86	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	509	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	b	615	CLA	C1-O2A-CGA	3.00	124.30	116.44
24	C	516	BCR	C11-C10-C9	-2.99	123.04	127.31
22	c	913	CLA	C3D-C2D-C1D	-2.99	101.75	105.83
22	A	405	CLA	C4-C3-C5	2.99	120.30	115.27
22	c	904	CLA	CHC-C4B-NB	2.99	127.42	124.26
22	c	909	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
26	D	406	PL9	C10-C9-C11	2.99	120.29	115.27
24	d	404	BCR	C21-C20-C19	-2.99	113.90	123.22
22	a	409	CLA	C1-O2A-CGA	2.98	124.27	116.44
22	C	505	CLA	C2D-C1D-ND	2.98	112.30	110.10
22	B	605	CLA	CMB-C2B-C1B	2.98	129.91	125.37
22	C	502	CLA	CMB-C2B-C1B	2.98	129.91	125.37
22	d	403	CLA	CMB-C2B-C1B	2.98	129.90	125.37
22	c	905	CLA	CMD-C2D-C1D	2.98	129.96	124.71
24	D	405	BCR	C38-C26-C25	-2.98	121.19	124.53
28	C	501	SQD	O48-C23-O10	-2.97	116.08	123.59
22	c	907	CLA	CHA-C4D-ND	2.97	138.72	132.50
28	A	413	SQD	O3-C3-C2	2.97	117.22	110.35
22	b	614	CLA	CHA-C4D-ND	2.97	138.71	132.50
28	A	413	SQD	C1-O5-C5	-2.97	107.86	113.69
28	a	414	SQD	O48-C23-C24	2.97	121.23	111.91
22	a	409	CLA	C1D-ND-C4D	-2.97	104.23	106.33
22	B	612	CLA	C1D-ND-C4D	-2.97	104.23	106.33
24	B	619	BCR	C28-C27-C26	-2.97	108.78	114.08
22	B	602	CLA	C3D-C2D-C1D	-2.97	101.78	105.83
22	c	906	CLA	CHA-C4D-ND	2.96	138.70	132.50
22	C	505	CLA	C4D-CHA-C1A	-2.96	117.64	121.25
22	B	606	CLA	C4-C3-C5	2.96	120.25	115.27
22	B	604	CLA	C1D-CHD-C4C	-2.96	119.67	126.06
22	b	606	CLA	CMC-C2C-C1C	2.96	129.55	125.04
25	C	531	LMG	O8-C28-C29	2.96	121.19	111.91
22	b	607	CLA	CHB-C1B-NB	-2.96	121.12	124.26
22	C	514	CLA	C3D-C2D-C1D	-2.96	101.79	105.83
22	B	617	CLA	CBC-CAC-C3C	-2.96	104.28	112.43
22	C	514	CLA	CMB-C2B-C1B	2.96	129.87	125.37
22	b	610	CLA	C3D-C2D-C1D	-2.96	101.80	105.83
22	C	510	CLA	C1-C2-C3	-2.96	120.93	126.04
24	c	915	BCR	C7-C8-C9	-2.96	121.77	126.23
25	j	101	LMG	C7-O1-C1	-2.96	107.96	113.74
27	D	409	LHG	C5-O7-C7	-2.95	110.52	117.79
22	C	511	CLA	CHD-C4C-NC	2.95	128.86	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	b	623	HTG	C2'-C1'-S1	-2.95	102.86	112.40
22	C	503	CLA	CHA-C4D-ND	2.95	138.67	132.50
24	c	916	BCR	C11-C10-C9	-2.95	123.10	127.31
22	B	616	CLA	CHC-C4B-NB	2.95	127.38	124.26
23	a	411	PHO	CMB-C2B-C3B	2.95	130.19	124.68
25	A	410	LMG	O8-C28-C29	2.95	121.15	111.91
22	B	610	CLA	C1-C2-C3	-2.94	120.95	126.04
22	C	510	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	B	615	CLA	C4D-CHA-C1A	-2.94	117.67	121.25
22	c	905	CLA	CAC-C3C-C4C	2.93	128.62	124.81
22	C	509	CLA	CHD-C4C-NC	2.93	128.82	124.20
22	a	412	CLA	CBC-CAC-C3C	-2.93	104.35	112.43
25	J	101	LMG	O8-C28-O10	-2.93	116.20	123.59
22	a	407	CLA	CMD-C2D-C1D	2.93	129.87	124.71
22	b	613	CLA	CED-O2D-CGD	2.93	122.56	115.94
24	c	916	BCR	C38-C26-C25	-2.93	121.24	124.53
22	c	914	CLA	CHC-C1C-NC	-2.92	119.77	124.20
22	B	610	CLA	CHC-C4B-NB	2.92	127.35	124.26
22	D	401	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
22	D	403	CLA	C4-C3-C5	2.92	120.19	115.27
22	a	412	CLA	CHD-C4C-NC	2.92	128.81	124.20
26	A	411	PL9	C20-C19-C21	2.92	120.19	115.27
22	b	617	CLA	CAC-C3C-C4C	2.92	128.60	124.81
22	b	609	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
22	b	609	CLA	CHD-C1D-ND	-2.92	121.77	124.45
29	A	414	LMT	C1'-C2'-C3'	-2.92	103.92	110.00
22	C	502	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
37	h	101	RRX	C16-C17-C18	-2.91	123.15	127.31
22	B	615	CLA	C3C-C4C-NC	2.91	113.84	110.57
24	d	404	BCR	C37-C22-C23	2.90	122.65	118.08
22	b	603	CLA	C4D-CHA-C1A	-2.90	117.72	121.25
29	t	101	LMT	O1'-C1'-C2'	2.90	112.83	108.30
35	C	518	DGD	O3G-C1D-C2D	2.90	112.83	108.30
22	c	902	CLA	C3B-C2B-C1B	-2.90	103.66	107.16
22	A	408	CLA	O2A-CGA-O1A	-2.90	116.27	123.59
22	b	608	CLA	C3D-C2D-C1D	-2.90	101.87	105.83
27	A	412	LHG	O8-C23-C24	2.90	121.00	111.91
24	d	404	BCR	C35-C13-C14	-2.90	118.87	122.92
22	b	615	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
22	A	406	CLA	CAC-C3C-C4C	2.89	128.56	124.81
22	b	610	CLA	CHA-C4D-ND	2.89	138.54	132.50
25	J	101	LMG	C7-O1-C1	-2.89	108.10	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	609	CLA	CAC-C3C-C4C	2.89	128.56	124.81
22	B	613	CLA	C3D-C2D-C1D	-2.88	101.89	105.83
27	D	410	LHG	O8-C6-C5	-2.88	100.04	108.43
37	H	101	RRX	C10-C11-C12	-2.88	114.22	123.22
22	B	603	CLA	CHD-C4C-NC	2.88	128.74	124.20
22	d	402	CLA	C2A-C1A-CHA	-2.88	118.82	123.86
22	B	614	CLA	O2D-CGD-CBD	2.88	116.39	111.27
24	K	101	BCR	C33-C5-C6	-2.88	121.30	124.53
22	c	908	CLA	CED-O2D-CGD	-2.88	109.43	115.94
22	b	605	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
22	b	603	CLA	O2A-CGA-CBA	2.87	120.93	111.91
22	B	605	CLA	C6-C5-C3	-2.87	105.92	113.45
36	e	101	HEM	C4A-NA-C1A	2.87	108.16	105.35
22	C	503	CLA	CHD-C4C-NC	2.87	128.73	124.20
26	a	415	PL9	C20-C19-C21	2.87	120.10	115.27
22	B	606	CLA	C1D-ND-C4D	-2.87	104.30	106.33
22	B	606	CLA	CHD-C4C-NC	2.87	128.72	124.20
22	D	401	CLA	C3B-C4B-NB	2.87	113.17	110.52
22	C	509	CLA	CHA-C4D-ND	2.87	138.50	132.50
26	d	405	PL9	C53-C6-C1	2.86	120.85	114.99
39	v	202	HEC	CBD-CAD-C3D	-2.86	104.67	112.63
22	C	514	CLA	C2C-C1C-NC	2.86	112.65	109.97
22	B	617	CLA	CAC-C3C-C4C	2.86	128.52	124.81
26	A	411	PL9	C37-C36-C34	-2.86	103.56	112.98
22	C	511	CLA	CMD-C2D-C1D	2.86	129.75	124.71
26	a	415	PL9	C42-C43-C44	-2.86	120.78	127.66
22	c	913	CLA	CHD-C4C-NC	2.86	128.71	124.20
22	B	609	CLA	CHB-C4A-NA	2.86	128.46	124.51
22	C	507	CLA	C3C-C4C-NC	2.86	113.77	110.57
22	c	906	CLA	CHD-C4C-NC	2.85	128.70	124.20
22	c	911	CLA	O2A-CGA-O1A	-2.85	116.39	123.59
25	b	622	LMG	O8-C28-C29	2.85	120.86	111.91
22	C	509	CLA	C5-C3-C2	-2.85	115.35	121.12
22	B	602	CLA	CMC-C2C-C1C	2.85	129.38	125.04
22	c	910	CLA	C3B-C4B-NB	2.85	113.16	110.52
22	b	615	CLA	CED-O2D-CGD	2.85	122.38	115.94
24	B	620	BCR	C23-C24-C25	-2.85	119.20	127.20
22	C	511	CLA	C4D-C3D-CAD	2.85	111.45	108.10
24	Y	101	BCR	C24-C23-C22	-2.85	121.93	126.23
24	k	101	BCR	C32-C1-C6	-2.84	105.69	110.30
34	C	521	HTG	C1-O5-C5	2.84	117.82	112.58
26	A	411	PL9	C25-C24-C26	2.84	120.05	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	626	HTG	O5-C1-C2	-2.84	106.75	110.31
35	D	407	DGD	O1G-C1A-C2A	2.84	120.81	111.91
22	B	613	CLA	C1-O2A-CGA	2.84	123.89	116.44
24	b	618	BCR	C11-C10-C9	-2.83	123.26	127.31
22	C	510	CLA	CAC-C3C-C4C	2.83	128.49	124.81
22	a	407	CLA	CHD-C4C-C3C	-2.83	120.68	124.84
24	D	405	BCR	C16-C17-C18	-2.83	123.27	127.31
22	B	608	CLA	CED-O2D-CGD	2.83	122.33	115.94
24	A	409	BCR	C38-C26-C25	-2.82	121.36	124.53
22	B	612	CLA	C7-C6-C5	-2.82	105.69	113.36
22	c	910	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
22	C	502	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
22	B	605	CLA	CGD-CBD-CAD	-2.82	101.60	110.73
23	A	407	PHO	CMB-C2B-C3B	2.82	129.95	124.68
22	B	609	CLA	C1D-CHD-C4C	-2.82	119.98	126.06
34	D	415	HTG	C3-C4-C5	2.81	115.25	110.24
29	Z	101	LMT	O5B-C5B-C4B	2.81	114.80	109.69
22	B	608	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	a	410	PHO	C7-C6-C5	-2.81	105.73	113.36
22	c	909	CLA	C1-O2A-CGA	2.81	123.81	116.44
25	B	621	LMG	C3-C4-C5	2.81	115.24	110.24
22	B	616	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
27	d	401	LHG	O8-C23-C24	2.80	120.70	111.91
22	b	611	CLA	CHD-C4C-NC	2.80	128.62	124.20
22	B	617	CLA	O2A-C1-C2	2.80	115.99	108.64
25	i	101	LMG	O8-C28-C29	2.80	120.69	111.91
22	C	512	CLA	CMD-C2D-C1D	2.80	129.64	124.71
22	C	510	CLA	C3D-C2D-C1D	-2.80	102.01	105.83
28	b	621	SQD	O48-C23-O10	-2.80	116.54	123.59
22	c	912	CLA	C4D-CHA-C1A	-2.79	117.85	121.25
22	B	603	CLA	C3C-C4C-NC	2.79	113.70	110.57
24	c	916	BCR	C35-C13-C14	-2.79	119.01	122.92
22	b	612	CLA	CMC-C2C-C1C	2.79	129.29	125.04
22	a	412	CLA	C3B-C4B-NB	2.79	113.10	110.52
22	a	409	CLA	CAC-C3C-C4C	2.79	128.43	124.81
22	B	610	CLA	C1-O2A-CGA	2.79	123.75	116.44
22	C	510	CLA	C1D-CHD-C4C	-2.79	120.05	126.06
22	c	902	CLA	C1-O2A-CGA	2.78	123.75	116.44
22	B	604	CLA	C2A-C3A-C4A	-2.78	97.37	101.87
22	B	612	CLA	CHD-C4C-NC	2.78	128.59	124.20
28	C	501	SQD	O5-C1-C2	-2.78	104.46	110.35
22	D	401	CLA	C1-C2-C3	-2.78	121.24	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	603	CLA	C3D-C4D-CHA	-2.77	106.38	112.72
22	c	914	CLA	CMD-C2D-C1D	2.77	129.60	124.71
22	b	617	CLA	C1D-CHD-C4C	-2.77	120.08	126.06
22	c	913	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
22	C	511	CLA	CHD-C1D-ND	-2.77	121.91	124.45
25	i	101	LMG	O6-C1-C2	-2.77	104.49	110.35
22	a	412	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
22	b	612	CLA	C3B-C4B-NB	2.77	113.08	110.52
24	b	620	BCR	C24-C23-C22	-2.77	122.05	126.23
22	C	513	CLA	CHB-C1B-NB	-2.77	121.33	124.26
22	C	508	CLA	C4-C3-C5	2.77	119.92	115.27
22	a	407	CLA	O2A-CGA-O1A	-2.76	116.61	123.59
27	L	101	LHG	C6-C5-C4	-2.76	105.25	111.79
22	b	607	CLA	C14-C13-C12	-2.76	101.29	111.29
22	c	910	CLA	CHD-C4C-C3C	-2.76	120.78	124.84
36	E	102	HEM	CBA-CAA-C2A	-2.76	104.95	112.63
22	C	514	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
22	C	505	CLA	C7-C6-C5	-2.76	105.86	113.36
22	A	405	CLA	C4D-CHA-C1A	-2.76	117.89	121.25
22	b	616	CLA	O2A-CGA-O1A	-2.76	116.63	123.59
22	b	606	CLA	CAC-C3C-C4C	2.76	128.39	124.81
34	b	627	HTG	C3-C4-C5	2.76	115.16	110.24
27	D	411	LHG	O7-C7-C8	2.76	117.44	111.50
22	c	906	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	c	907	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	A	406	CLA	O2A-CGA-O1A	-2.75	116.64	123.59
22	b	615	CLA	C6-C5-C3	2.75	119.12	114.62
34	B	626	HTG	C3-C4-C5	2.75	115.15	110.24
22	C	504	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
22	b	611	CLA	O2A-CGA-CBA	2.75	120.55	111.91
22	b	606	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
22	B	607	CLA	CBC-CAC-C3C	-2.75	104.85	112.43
22	c	910	CLA	CHC-C4B-C3B	-2.75	115.49	127.71
22	c	912	CLA	O2A-CGA-CBA	2.75	120.53	111.91
24	C	516	BCR	C37-C22-C23	2.75	122.40	118.08
22	B	608	CLA	CHD-C4C-C3C	-2.75	120.80	124.84
22	C	502	CLA	CHD-C4C-NC	2.75	128.53	124.20
22	b	609	CLA	CMD-C2D-C1D	2.74	129.55	124.71
29	c	931	LMT	O5'-C5'-C6'	2.74	113.26	106.44
22	b	607	CLA	C3B-C4B-NB	2.74	113.06	110.52
22	c	912	CLA	CHD-C4C-C3C	-2.74	120.81	124.84
39	V	202	HEC	C4C-NC-C1C	2.74	108.03	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	608	CLA	C1D-ND-C4D	2.74	108.28	106.33
22	c	909	CLA	C1-C2-C3	-2.74	121.30	126.04
22	B	607	CLA	CHD-C1D-ND	-2.74	121.94	124.45
22	c	911	CLA	CBC-CAC-C3C	-2.74	104.88	112.43
25	i	101	LMG	O7-C10-C11	2.74	117.40	111.50
22	A	406	CLA	C4D-C3D-CAD	2.74	111.32	108.10
22	c	903	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
24	D	405	BCR	C29-C28-C27	-2.73	105.27	111.38
23	D	402	PHO	C1A-C2A-C3A	-2.73	100.24	102.84
24	Y	101	BCR	C1-C6-C7	2.73	123.51	115.78
22	c	911	CLA	C3D-C2D-C1D	-2.73	102.10	105.83
22	b	602	CLA	CED-O2D-CGD	2.73	122.12	115.94
22	b	604	CLA	C3C-C4C-NC	2.73	113.63	110.57
24	d	404	BCR	C30-C25-C24	2.73	123.50	115.78
22	b	616	CLA	CMC-C2C-C1C	2.73	129.20	125.04
34	D	415	HTG	C1-C2-C3	-2.73	105.20	110.59
28	l	101	SQD	O5-C1-C2	-2.73	104.58	110.35
22	B	615	CLA	CHC-C1C-NC	-2.73	120.07	124.20
25	d	409	LMG	C8-O7-C10	-2.73	111.08	117.79
22	B	604	CLA	CHC-C1C-NC	-2.72	120.07	124.20
22	C	507	CLA	C4-C3-C5	2.72	119.85	115.27
26	D	406	PL9	C50-C49-C48	-2.72	114.78	122.65
22	B	603	CLA	CHC-C4B-C3B	-2.72	115.61	127.71
22	B	604	CLA	O2A-CGA-CBA	2.72	120.44	111.91
36	E	102	HEM	C3B-C2B-C1B	2.72	108.50	106.49
35	C	517	DGD	O2G-C1B-O1B	-2.72	117.14	123.70
22	A	405	CLA	CHC-C1C-NC	-2.71	120.08	124.20
22	B	612	CLA	CHA-C4D-ND	2.71	138.17	132.50
22	C	513	CLA	C1-C2-C3	-2.71	121.35	126.04
22	C	510	CLA	C3B-C4B-NB	2.71	113.03	110.52
22	B	616	CLA	O1D-CGD-CBD	-2.71	118.94	124.48
28	a	414	SQD	O9-S-O7	-2.71	104.57	113.95
22	c	908	CLA	O2A-CGA-CBA	2.71	120.41	111.91
22	C	508	CLA	CHB-C1B-NB	-2.71	121.39	124.26
22	b	606	CLA	CHC-C4B-NB	2.71	127.12	124.26
39	V	202	HEC	C4B-NB-C1B	2.71	107.87	105.07
22	A	406	CLA	O1D-CGD-CBD	-2.71	118.95	124.48
29	c	921	LMT	O2'-C2'-C3'	-2.70	104.10	110.35
22	C	502	CLA	C1-O2A-CGA	2.70	123.53	116.44
24	b	620	BCR	C3-C4-C5	-2.70	109.26	114.08
22	B	613	CLA	CMC-C2C-C1C	2.70	129.15	125.04
22	B	602	CLA	O2A-CGA-CBA	2.70	120.38	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	CMD-C2D-C1D	2.70	129.47	124.71
24	D	405	BCR	C10-C11-C12	-2.70	114.80	123.22
28	b	621	SQD	O9-S-C6	2.70	110.14	106.94
22	b	610	CLA	C7-C6-C5	-2.70	106.04	113.36
22	b	616	CLA	O1D-CGD-CBD	-2.70	118.97	124.48
22	c	907	CLA	O2A-CGA-CBA	2.69	120.36	111.91
22	B	609	CLA	C11-C12-C13	-2.69	107.21	115.92
24	C	515	BCR	C29-C30-C25	2.69	114.63	110.48
27	a	423	LHG	O8-C23-O10	-2.69	116.79	123.59
22	D	404	CLA	C4-C3-C5	2.69	119.80	115.27
29	c	921	LMT	O1'-C1'-C2'	2.69	112.51	108.30
22	b	613	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
22	B	606	CLA	C7-C6-C5	-2.69	106.05	113.36
28	a	414	SQD	C44-O6-C1	-2.69	108.48	113.74
35	C	517	DGD	O5D-C6D-C5D	-2.69	104.07	109.05
35	c	918	DGD	O1G-C1A-C2A	2.69	120.34	111.91
22	a	408	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
26	d	405	PL9	C22-C23-C24	-2.69	121.19	127.66
22	C	512	CLA	CHD-C4C-NC	2.69	128.44	124.20
22	c	903	CLA	C6-C5-C3	-2.69	106.41	113.45
22	b	613	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	c	903	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
22	A	408	CLA	C5-C3-C2	-2.68	115.69	121.12
22	b	616	CLA	C1D-CHD-C4C	-2.68	120.27	126.06
22	B	615	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
22	C	511	CLA	C3D-C4D-CHA	-2.68	106.59	112.72
24	k	101	BCR	C2-C1-C6	2.68	114.61	110.48
27	D	409	LHG	O8-C23-O10	-2.68	116.83	123.59
23	A	407	PHO	CBC-CAC-C3C	-2.68	108.96	112.88
22	d	402	CLA	CMA-C3A-C2A	-2.68	103.02	113.83
22	b	613	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
22	b	616	CLA	CHB-C1B-NB	-2.68	121.42	124.26
22	C	504	CLA	O2A-CGA-CBA	2.68	120.31	111.91
22	D	401	CLA	CHA-C4D-ND	2.67	138.09	132.50
22	b	616	CLA	O2A-CGA-CBA	2.67	120.30	111.91
22	A	408	CLA	CHD-C4C-NC	2.67	128.41	124.20
22	C	513	CLA	C1D-CHD-C4C	-2.67	120.30	126.06
35	C	518	DGD	O1G-C1A-O1A	-2.67	116.85	123.59
34	B	623	HTG	O4-C4-C3	-2.67	104.17	110.35
22	C	512	CLA	C3B-C4B-NB	2.67	112.99	110.52
28	a	414	SQD	O2-C2-C1	2.67	116.53	110.05
34	b	626	HTG	C3-C4-C5	2.67	115.00	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	407	PHO	CMA-C3A-C4A	-2.67	108.53	114.38
22	D	404	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
22	B	616	CLA	C6-C7-C8	-2.67	107.30	115.92
22	C	504	CLA	CHD-C4C-NC	2.67	128.40	124.20
22	B	613	CLA	O2D-CGD-CBD	2.66	116.00	111.27
22	c	909	CLA	CMD-C2D-C1D	2.66	129.40	124.71
22	b	602	CLA	C4-C3-C5	2.66	119.75	115.27
22	C	511	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
22	b	611	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
24	C	516	BCR	C33-C5-C6	-2.66	121.54	124.53
22	B	602	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
22	C	508	CLA	O2A-CGA-CBA	2.66	120.24	111.91
22	b	603	CLA	C1-O2A-CGA	2.66	123.41	116.44
25	b	622	LMG	O7-C10-O9	-2.66	117.28	123.70
24	d	404	BCR	C24-C23-C22	-2.66	122.22	126.23
22	C	507	CLA	CHD-C4C-NC	2.65	128.39	124.20
22	C	512	CLA	C4D-CHA-C1A	-2.65	118.02	121.25
26	a	415	PL9	C10-C9-C11	2.65	119.74	115.27
35	C	517	DGD	O6E-C1E-C2E	-2.65	104.73	110.35
24	a	413	BCR	C28-C27-C26	-2.65	109.34	114.08
22	B	607	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
23	A	407	PHO	CED-O2D-CGD	2.65	121.94	115.94
35	c	919	DGD	O1G-C1A-O1A	-2.65	116.90	123.59
22	c	908	CLA	C1-C2-C3	-2.65	121.46	126.04
26	D	406	PL9	C37-C38-C39	-2.65	121.28	127.66
24	y	101	BCR	C1-C6-C7	2.65	123.28	115.78
22	c	906	CLA	O2A-CGA-CBA	2.64	120.21	111.91
22	b	609	CLA	C11-C12-C13	-2.64	107.37	115.92
22	C	510	CLA	C1-O2A-CGA	2.64	123.38	116.44
25	j	101	LMG	C9-C8-C7	-2.64	105.54	111.79
22	c	911	CLA	O2A-CGA-CBA	2.64	120.19	111.91
22	A	406	CLA	CHC-C4B-C3B	-2.64	115.97	127.71
22	c	902	CLA	CMC-C2C-C1C	2.64	129.06	125.04
22	c	907	CLA	C4-C3-C5	2.64	119.71	115.27
22	a	409	CLA	CHC-C4B-C3B	-2.64	115.97	127.71
39	v	202	HEC	C4C-NC-C1C	2.64	107.93	105.35
22	A	406	CLA	C1-C2-C3	-2.64	121.48	126.04
26	D	406	PL9	C25-C24-C26	2.64	119.70	115.27
22	C	512	CLA	C3C-C4C-NC	2.63	113.53	110.57
22	b	615	CLA	CHD-C1D-ND	-2.63	122.03	124.45
22	c	914	CLA	O1D-CGD-CBD	-2.63	119.09	124.48
22	b	614	CLA	CED-O2D-CGD	2.63	121.89	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	602	CLA	C4D-CHA-C1A	-2.63	118.05	121.25
26	D	406	PL9	C12-C13-C14	-2.63	121.32	127.66
23	a	410	PHO	OBD-CAD-C3D	-2.63	123.61	127.98
22	b	614	CLA	CHD-C4C-NC	2.63	128.35	124.20
22	A	405	CLA	C1D-ND-C4D	-2.63	104.47	106.33
22	B	614	CLA	O2A-CGA-CBA	2.63	120.16	111.91
22	d	403	CLA	CHD-C4C-NC	2.63	128.34	124.20
22	b	604	CLA	O1D-CGD-CBD	-2.63	119.11	124.48
22	C	514	CLA	C1D-CHD-C4C	-2.63	120.39	126.06
22	B	608	CLA	C1-O2A-CGA	2.63	123.33	116.44
22	A	405	CLA	CHA-C4D-ND	2.62	137.99	132.50
22	B	613	CLA	O2A-CGA-CBA	2.62	120.14	111.91
22	a	407	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
22	b	615	CLA	CMD-C2D-C1D	2.62	129.34	124.71
22	C	510	CLA	CHD-C1D-ND	-2.62	122.04	124.45
22	C	506	CLA	C4-C3-C5	2.62	119.68	115.27
25	d	409	LMG	O2-C2-C1	2.62	116.41	110.05
26	a	415	PL9	C40-C39-C41	2.62	119.68	115.27
22	b	609	CLA	C1-C2-C3	-2.62	121.52	126.04
24	D	405	BCR	C38-C26-C27	2.62	118.64	113.62
22	b	613	CLA	C1-C2-C3	-2.62	121.52	126.04
35	C	519	DGD	O3G-C3G-C2G	-2.62	104.59	110.90
25	j	101	LMG	O7-C10-C11	2.61	117.14	111.50
22	C	502	CLA	CMC-C2C-C1C	2.61	129.02	125.04
22	C	511	CLA	C3D-C2D-C1D	-2.61	102.27	105.83
22	C	508	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
22	c	910	CLA	CMB-C2B-C1B	2.61	129.34	125.37
25	j	101	LMG	O8-C28-C29	2.61	120.10	111.91
28	D	408	SQD	C3-C4-C5	2.61	114.89	110.24
22	B	606	CLA	CMD-C2D-C1D	2.61	129.31	124.71
22	b	608	CLA	CHD-C4C-NC	2.61	128.31	124.20
22	c	906	CLA	CAC-C3C-C4C	2.61	128.19	124.81
22	B	613	CLA	CHD-C4C-NC	2.61	128.31	124.20
22	D	403	CLA	CHC-C4B-C3B	-2.61	116.11	127.71
22	A	406	CLA	C3D-C2D-C1D	-2.61	102.27	105.83
22	C	507	CLA	CMB-C2B-C1B	2.60	129.33	125.37
22	c	907	CLA	CMB-C2B-C1B	2.60	129.33	125.37
22	C	504	CLA	CMC-C2C-C1C	2.60	129.00	125.04
24	b	618	BCR	C7-C8-C9	-2.60	122.30	126.23
24	C	515	BCR	C8-C7-C6	-2.60	119.90	127.20
22	d	402	CLA	CMD-C2D-C1D	2.60	129.29	124.71
22	b	605	CLA	C1D-CHD-C4C	-2.60	120.45	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	408	CLA	C1D-CHD-C4C	-2.60	120.45	126.06
22	c	903	CLA	CMC-C2C-C1C	2.60	128.99	125.04
22	d	403	CLA	C4D-C3D-CAD	2.60	111.16	108.10
22	C	509	CLA	O2A-CGA-CBA	2.59	120.05	111.91
22	b	608	CLA	CHD-C1D-ND	-2.59	122.07	124.45
22	c	910	CLA	CHD-C1D-ND	-2.59	122.07	124.45
22	B	610	CLA	CMB-C2B-C1B	2.59	129.32	125.37
22	b	617	CLA	CHD-C4C-NC	2.59	128.29	124.20
22	a	412	CLA	CMC-C2C-C1C	2.59	128.99	125.04
26	A	411	PL9	C3-C4-C5	2.59	121.97	118.60
28	f	101	SQD	O7-S-C6	2.59	110.03	106.92
22	D	401	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	b	610	CLA	O2D-CGD-CBD	2.59	115.86	111.27
35	C	518	DGD	O2G-C1B-O1B	-2.59	117.45	123.70
22	a	412	CLA	O2A-CGA-CBA	2.59	120.02	111.91
22	b	614	CLA	C4C-C3C-C2C	-2.59	103.13	106.90
24	K	101	BCR	C20-C21-C22	-2.58	123.62	127.31
29	a	419	LMT	O5B-C5B-C6B	2.58	112.86	106.44
24	D	405	BCR	C36-C18-C19	2.58	122.14	118.08
25	d	409	LMG	O7-C10-O9	-2.58	117.46	123.70
22	B	610	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
26	A	411	PL9	C30-C29-C31	2.58	119.61	115.27
22	A	406	CLA	CMD-C2D-C1D	2.58	129.26	124.71
24	D	405	BCR	C15-C14-C13	-2.58	123.63	127.31
22	B	612	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	B	613	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
22	b	611	CLA	O2A-CGA-O1A	-2.57	117.09	123.59
22	c	914	CLA	CED-O2D-CGD	2.57	121.76	115.94
22	d	403	CLA	CED-O2D-CGD	2.57	121.75	115.94
22	c	912	CLA	O2A-C1-C2	-2.57	101.88	108.64
26	a	415	PL9	C32-C33-C34	-2.57	121.47	127.66
22	c	905	CLA	CHC-C4B-C3B	-2.57	116.28	127.71
29	f	102	LMT	C3'-C4'-C5'	-2.57	105.03	110.93
28	C	501	SQD	O48-C23-C24	2.57	119.97	111.91
22	B	606	CLA	C4C-C3C-C2C	-2.57	103.16	106.90
34	D	415	HTG	O2-C2-C3	2.57	116.28	110.35
22	b	617	CLA	C1-O2A-CGA	2.57	123.18	116.44
22	C	513	CLA	CMD-C2D-C1D	2.57	129.23	124.71
24	A	409	BCR	C36-C18-C17	-2.56	119.33	122.92
22	C	502	CLA	O2A-CGA-CBA	2.56	119.96	111.91
22	D	403	CLA	O2A-CGA-CBA	2.56	119.96	111.91
22	b	614	CLA	CHB-C1B-NB	-2.56	121.54	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	406	PL9	C51-C49-C50	2.56	120.27	114.60
22	b	610	CLA	CAC-C3C-C4C	2.56	128.13	124.81
22	B	603	CLA	C5-C3-C2	-2.56	115.93	121.12
26	A	411	PL9	C37-C38-C39	-2.56	121.49	127.66
22	A	408	CLA	CMC-C2C-C1C	2.56	128.94	125.04
23	A	407	PHO	O1D-CGD-CBD	-2.56	120.48	124.74
28	a	414	SQD	O47-C7-O49	-2.56	117.52	123.70
22	a	412	CLA	CED-O2D-CGD	2.56	121.72	115.94
22	B	609	CLA	C6-C5-C3	-2.56	106.75	113.45
22	c	914	CLA	O2A-CGA-CBA	2.56	119.93	111.91
22	B	613	CLA	CHA-C4D-ND	2.55	137.84	132.50
22	b	602	CLA	CHC-C1C-NC	-2.55	120.33	124.20
22	C	510	CLA	C3C-C4C-NC	2.55	113.44	110.57
25	d	409	LMG	C3-C4-C5	2.55	114.79	110.24
22	b	603	CLA	CAA-CBA-CGA	-2.55	105.80	113.25
22	c	904	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
22	c	903	CLA	C3D-C4D-CHA	-2.55	106.89	112.72
22	b	610	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
22	D	403	CLA	CHA-C4D-ND	2.55	137.83	132.50
22	A	405	CLA	CAA-CBA-CGA	-2.55	105.81	113.25
22	C	512	CLA	C4C-C3C-C2C	-2.54	103.19	106.90
28	l	101	SQD	O9-S-C6	2.54	109.96	106.94
22	c	914	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	i	101	LMG	C31-C30-C29	-2.54	104.06	113.19
22	c	904	CLA	C4D-C3D-CAD	2.54	111.09	108.10
22	C	504	CLA	C4D-CHA-C1A	-2.54	118.16	121.25
25	D	412	LMG	O8-C28-C29	2.54	119.87	111.91
22	B	616	CLA	O2A-CGA-CBA	2.54	119.87	111.91
22	c	913	CLA	C4D-CHA-C1A	-2.54	118.16	121.25
22	D	404	CLA	C3D-C2D-C1D	-2.54	102.37	105.83
27	D	410	LHG	C14-C13-C12	-2.54	101.55	114.42
22	b	604	CLA	CHC-C1C-NC	-2.54	120.36	124.20
25	i	101	LMG	C1-O6-C5	-2.53	108.71	113.69
22	b	612	CLA	CBC-CAC-C3C	-2.53	105.44	112.43
22	D	401	CLA	CHD-C1D-ND	-2.53	122.13	124.45
22	B	614	CLA	C1-C2-C3	-2.53	121.66	126.04
24	c	916	BCR	C16-C17-C18	-2.53	123.70	127.31
22	b	614	CLA	C3C-C4C-NC	2.53	113.41	110.57
22	B	604	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
22	D	401	CLA	C4-C3-C5	2.53	119.53	115.27
28	l	101	SQD	O47-C7-O49	-2.53	117.59	123.70
24	Y	101	BCR	C8-C9-C10	-2.53	115.06	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	509	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
22	c	912	CLA	CMC-C2C-C1C	2.53	128.89	125.04
22	a	408	CLA	CBB-CAB-C3B	-2.53	115.05	127.62
22	B	603	CLA	C1-O2A-CGA	2.53	123.07	116.44
35	D	407	DGD	O1G-C1G-C2G	2.53	115.78	108.43
28	D	408	SQD	C4-C3-C2	2.52	115.23	110.82
22	c	903	CLA	O2A-CGA-CBA	2.52	119.82	111.91
24	B	619	BCR	C15-C16-C17	-2.52	118.31	123.47
24	K	101	BCR	C16-C17-C18	-2.52	123.71	127.31
35	C	518	DGD	C3B-C2B-C1B	-2.52	104.45	113.62
27	a	423	LHG	O7-C7-O9	-2.52	117.61	123.70
22	B	616	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
22	d	402	CLA	CAC-C3C-C4C	2.52	128.08	124.81
22	B	617	CLA	C4-C3-C5	2.52	119.51	115.27
22	B	610	CLA	CAC-C3C-C4C	2.52	128.08	124.81
27	L	101	LHG	O7-C7-O9	-2.52	117.61	123.70
22	b	616	CLA	C4D-CHA-C1A	-2.52	118.18	121.25
22	C	502	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
23	A	407	PHO	C4D-CHA-CBD	2.52	109.66	108.52
29	f	102	LMT	O5'-C5'-C6'	2.52	112.69	106.44
22	b	611	CLA	C1D-CHD-C4C	-2.51	120.63	126.06
22	b	607	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
22	B	607	CLA	OBD-CAD-C3D	-2.51	122.47	128.52
22	B	604	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
22	B	605	CLA	C1D-CHD-C4C	-2.51	120.64	126.06
35	h	102	DGD	C3D-C4D-C5D	-2.51	105.76	110.24
22	B	611	CLA	CHC-C4B-NB	2.51	126.92	124.26
22	c	907	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	a	407	CLA	O2A-CGA-CBA	2.51	119.78	111.91
22	C	503	CLA	CMC-C2C-C1C	2.51	128.86	125.04
22	b	612	CLA	C1D-CHD-C4C	-2.51	120.65	126.06
22	A	405	CLA	C1D-CHD-C4C	-2.51	120.65	126.06
22	D	404	CLA	C4D-CHA-C1A	-2.50	118.20	121.25
22	B	603	CLA	OBD-CAD-C3D	-2.50	122.50	128.52
24	k	101	BCR	C11-C10-C9	-2.50	123.74	127.31
22	b	612	CLA	C3C-C4C-NC	2.50	113.37	110.57
25	j	101	LMG	O2-C2-C1	-2.50	103.98	110.05
35	C	518	DGD	C6D-C5D-C4D	2.50	117.31	112.09
22	A	405	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
24	Y	101	BCR	C7-C8-C9	-2.50	122.46	126.23
22	B	616	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	a	407	CLA	CMC-C2C-C1C	2.49	128.84	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	906	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
22	a	409	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
22	C	508	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
25	c	930	LMG	O8-C28-C29	2.49	119.73	111.91
22	B	605	CLA	C4-C3-C5	2.49	119.46	115.27
22	D	403	CLA	C4-C3-C2	-2.49	117.29	123.68
22	B	611	CLA	O1D-CGD-CBD	-2.49	119.40	124.48
24	Y	101	BCR	C34-C9-C8	2.49	121.99	118.08
22	c	904	CLA	CAA-CBA-CGA	-2.48	105.99	113.25
22	b	613	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
22	c	911	CLA	C1D-CHD-C4C	-2.48	120.71	126.06
22	a	408	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
22	C	502	CLA	C4D-CHA-C1A	-2.48	118.23	121.25
22	A	408	CLA	C3B-C4B-NB	2.48	112.81	110.52
24	C	516	BCR	C38-C26-C25	-2.48	121.75	124.53
35	c	919	DGD	C2G-O2G-C1B	-2.48	111.70	117.79
22	b	615	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
22	a	408	CLA	CHC-C4B-C3B	-2.47	116.71	127.71
22	A	408	CLA	CAC-C3C-C4C	2.47	128.02	124.81
28	C	501	SQD	O9-S-O7	-2.47	105.39	113.95
22	C	508	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
28	C	501	SQD	O2-C2-C1	2.47	116.05	110.05
22	B	617	CLA	CHB-C1B-NB	-2.47	121.64	124.26
24	y	101	BCR	C7-C6-C5	-2.47	115.48	121.46
22	B	614	CLA	CHC-C4B-C3B	-2.47	116.73	127.71
22	B	610	CLA	C1D-CHD-C4C	-2.47	120.73	126.06
22	B	603	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
23	a	410	PHO	O2A-CGA-CBA	2.47	119.65	111.91
22	C	510	CLA	C4-C3-C5	2.47	119.42	115.27
26	A	411	PL9	C26-C27-C28	2.47	119.98	111.88
22	c	914	CLA	CAC-C3C-C4C	2.47	128.01	124.81
22	d	402	CLA	C1D-CHD-C4C	-2.46	120.74	126.06
35	D	407	DGD	C1D-C2D-C3D	2.46	115.13	110.00
27	d	401	LHG	O4-P-O5	2.46	120.33	110.68
22	b	617	CLA	C4-C3-C5	2.46	119.41	115.27
22	a	409	CLA	CHB-C1B-NB	-2.46	121.65	124.26
22	b	612	CLA	C1D-ND-C4D	-2.46	104.59	106.33
22	b	611	CLA	CHC-C1C-NC	-2.46	120.47	124.20
22	B	609	CLA	O2A-CGA-CBA	2.46	119.62	111.91
22	C	510	CLA	C11-C10-C8	-2.46	107.98	115.92
22	D	404	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
22	b	610	CLA	CHB-C1B-NB	-2.46	121.66	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	C1D-ND-C4D	-2.45	104.59	106.33
22	C	514	CLA	CMD-C2D-C1D	2.45	129.03	124.71
22	B	605	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	B	604	CLA	CMC-C2C-C1C	2.45	128.77	125.04
22	A	405	CLA	C3C-C4C-NC	2.45	113.31	110.57
23	A	407	PHO	C4B-NB-C1B	-2.45	105.04	108.83
22	B	612	CLA	C3C-C4C-NC	2.45	113.31	110.57
28	b	621	SQD	C3-C4-C5	2.44	114.60	110.24
22	C	504	CLA	CHC-C1C-NC	-2.44	120.50	124.20
35	c	917	DGD	O2G-C1B-O1B	-2.44	117.80	123.70
34	l	106	HTG	O5-C1-C2	-2.44	107.24	110.31
24	D	405	BCR	C32-C1-C6	2.44	114.26	110.30
22	B	615	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
39	v	202	HEC	CHA-C1A-NA	2.44	127.08	124.44
22	B	617	CLA	CHB-C4A-NA	2.44	127.88	124.51
25	A	410	LMG	C8-O7-C10	-2.44	111.79	117.79
22	C	504	CLA	C5-C3-C2	-2.44	116.19	121.12
22	c	911	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
22	b	617	CLA	O2A-CGA-CBA	2.43	119.55	111.91
25	B	621	LMG	O7-C10-O9	-2.43	117.82	123.70
37	H	101	RRX	C38-C26-C25	-2.43	121.80	124.53
22	B	610	CLA	C3C-C4C-NC	2.43	113.30	110.57
22	b	609	CLA	CHD-C4C-NC	2.43	128.03	124.20
22	B	606	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
22	B	602	CLA	CHB-C1B-NB	-2.43	121.69	124.26
22	C	504	CLA	CMD-C2D-C1D	2.43	128.99	124.71
22	b	604	CLA	C4D-CHA-C1A	-2.43	118.30	121.25
22	b	610	CLA	CMB-C2B-C1B	2.43	129.06	125.37
22	a	408	CLA	C1D-ND-C4D	-2.43	104.61	106.33
27	d	401	LHG	O8-C23-O10	-2.42	117.47	123.59
22	c	904	CLA	OBD-CAD-C3D	-2.42	122.69	128.52
22	B	612	CLA	CAC-C3C-C4C	2.42	127.95	124.81
26	D	406	PL9	C40-C39-C38	-2.42	117.47	123.68
35	c	918	DGD	O1G-C1A-O1A	-2.42	117.49	123.59
22	C	512	CLA	O2D-CGD-CBD	2.42	115.57	111.27
23	a	411	PHO	C4B-NB-C1B	-2.42	105.08	108.83
22	b	615	CLA	C3C-C4C-NC	2.42	113.28	110.57
22	b	612	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	C	505	CLA	C1-O2A-CGA	2.42	122.79	116.44
22	a	407	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
34	v	203	HTG	O2-C2-C1	2.42	114.71	110.27
28	C	501	SQD	C45-O47-C7	-2.42	111.84	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	620	BCR	C10-C11-C12	-2.42	115.68	123.22
22	a	412	CLA	OBD-CAD-C3D	-2.41	122.71	128.52
24	B	620	BCR	C33-C5-C6	-2.41	121.82	124.53
22	b	603	CLA	CMB-C2B-C3B	2.41	132.44	126.59
22	c	912	CLA	CAC-C3C-C4C	2.41	127.94	124.81
22	C	506	CLA	C3D-C2D-C1D	-2.41	102.54	105.83
22	a	408	CLA	O2A-CGA-CBA	2.41	119.48	111.91
22	C	505	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
22	c	912	CLA	CMD-C2D-C1D	2.41	128.96	124.71
22	B	604	CLA	C3C-C4C-NC	2.41	113.27	110.57
22	c	912	CLA	CHC-C1C-NC	-2.41	120.55	124.20
22	c	913	CLA	C1-O2A-CGA	2.41	122.75	116.44
35	C	519	DGD	O2G-C1B-O1B	-2.41	117.89	123.70
24	D	405	BCR	C30-C25-C24	2.41	122.58	115.78
35	c	919	DGD	O2E-C2E-C3E	-2.40	104.79	110.35
34	b	623	HTG	C1-O5-C5	2.40	117.01	112.58
36	E	102	HEM	CHB-C1B-NB	2.40	127.33	124.37
22	b	610	CLA	C16-C15-C13	-2.40	108.16	115.92
35	C	517	DGD	O2G-C1B-C2B	2.40	116.67	111.50
24	a	413	BCR	C40-C30-C25	-2.40	106.41	110.30
25	d	409	LMG	O8-C28-C29	2.40	119.43	111.91
22	a	412	CLA	CMB-C2B-C1B	2.40	129.02	125.37
24	c	915	BCR	C38-C26-C25	-2.40	121.84	124.53
22	b	607	CLA	O2A-CGA-O1A	-2.40	117.55	123.59
24	Y	101	BCR	C15-C14-C13	-2.40	123.89	127.31
25	c	930	LMG	O7-C10-O9	-2.39	117.92	123.70
22	C	507	CLA	C1D-CHD-C4C	-2.39	120.90	126.06
22	B	617	CLA	CHC-C4B-C3B	-2.39	117.08	127.71
35	d	406	DGD	O2G-C1B-O1B	-2.39	117.93	123.70
24	A	409	BCR	C33-C5-C6	-2.39	121.85	124.53
22	b	616	CLA	CAC-C3C-C4C	2.39	127.91	124.81
22	B	617	CLA	C3C-C4C-NC	2.39	113.25	110.57
25	J	101	LMG	O3-C3-C2	-2.39	104.83	110.35
22	C	502	CLA	C3C-C4C-NC	2.39	113.25	110.57
22	B	604	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
22	B	609	CLA	CMC-C2C-C1C	2.38	128.67	125.04
29	c	931	LMT	O1'-C1'-C2'	2.38	112.02	108.30
22	b	615	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
22	b	610	CLA	CMD-C2D-C1D	2.38	128.91	124.71
22	B	605	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
22	b	614	CLA	C4D-CHA-C1A	-2.38	118.35	121.25
36	E	102	HEM	CAD-CBD-CGD	2.38	118.73	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	404	BCR	C15-C14-C13	-2.38	123.91	127.31
22	b	616	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
22	a	412	CLA	CMD-C2D-C3D	2.38	133.09	127.61
22	c	912	CLA	CMB-C2B-C1B	2.38	128.99	125.37
34	l	106	HTG	C1-C2-C3	-2.38	105.89	110.59
22	B	602	CLA	CED-O2D-CGD	2.38	121.31	115.94
22	C	507	CLA	C1-O2A-CGA	2.38	122.68	116.44
22	A	405	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
22	b	611	CLA	CMC-C2C-C1C	2.38	128.66	125.04
22	B	602	CLA	CHC-C1C-NC	-2.37	120.60	124.20
22	b	615	CLA	O2A-CGA-CBA	2.37	119.36	111.91
22	B	602	CLA	CMB-C2B-C1B	2.37	128.98	125.37
22	c	908	CLA	C4D-CHA-C1A	-2.37	118.36	121.25
22	c	905	CLA	CED-O2D-CGD	2.37	121.30	115.94
22	C	506	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
22	b	603	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
22	B	613	CLA	CMB-C2B-C1B	2.37	128.98	125.37
22	B	609	CLA	C3D-C4D-CHA	-2.37	107.30	112.72
24	a	413	BCR	C23-C24-C25	-2.37	120.56	127.20
22	b	605	CLA	CHC-C4B-NB	2.37	126.76	124.26
29	c	921	LMT	C1B-O1B-C4'	-2.37	112.11	117.96
22	b	608	CLA	CMB-C2B-C1B	2.36	128.97	125.37
22	c	910	CLA	C3D-C4D-CHA	-2.36	107.31	112.72
22	B	608	CLA	C1-C2-C3	-2.36	121.95	126.04
22	C	510	CLA	CMD-C2D-C1D	2.36	128.88	124.71
22	D	404	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
22	b	617	CLA	C4-C3-C2	-2.36	117.62	123.68
22	C	510	CLA	CHC-C4B-C3B	-2.36	117.22	127.71
25	C	531	LMG	O6-C5-C6	2.36	112.30	106.44
22	b	605	CLA	CGD-CBD-CAD	-2.36	103.10	110.73
22	b	612	CLA	C4B-CHC-C1C	-2.36	120.75	126.34
22	c	904	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	a	407	CLA	C5-C3-C2	-2.35	116.35	121.12
24	a	413	BCR	C8-C7-C6	-2.35	120.60	127.20
22	d	402	CLA	CMC-C2C-C1C	2.35	128.62	125.04
22	d	403	CLA	C3D-C2D-C1D	-2.35	102.62	105.83
22	C	514	CLA	C1-O2A-CGA	2.35	122.61	116.44
25	J	101	LMG	O8-C28-C29	2.35	119.28	111.91
22	D	401	CLA	CHC-C4B-C3B	-2.35	117.26	127.71
22	A	408	CLA	O2A-CGA-CBA	2.35	119.28	111.91
28	a	418	SQD	C44-O6-C1	-2.35	109.15	113.74
22	b	614	CLA	CHC-C4B-C3B	-2.35	117.27	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	T	102	LMT	O5'-C1'-C2'	2.35	115.32	110.35
36	e	101	HEM	C1B-NB-C4B	2.34	107.50	105.07
22	c	906	CLA	C4C-C3C-C2C	-2.34	103.48	106.90
39	v	202	HEC	C1D-C2D-C3D	-2.34	104.49	106.96
22	b	613	CLA	CMC-C2C-C1C	2.34	128.60	125.04
27	a	416	LHG	O7-C7-O9	-2.34	118.05	123.70
22	B	611	CLA	C3C-C4C-NC	2.34	113.19	110.57
25	c	930	LMG	C1-O6-C5	2.34	118.28	113.69
28	D	408	SQD	C1-O5-C5	-2.34	109.10	113.69
22	a	407	CLA	C7-C6-C5	-2.34	107.01	113.36
22	a	407	CLA	C1D-CHD-C4C	-2.34	121.02	126.06
22	b	607	CLA	CHC-C4B-NB	2.34	126.73	124.26
24	B	619	BCR	C24-C23-C22	-2.33	122.71	126.23
22	C	512	CLA	C3A-C2A-C1A	2.33	104.83	101.34
22	B	613	CLA	C3D-C4D-ND	2.33	114.01	110.24
24	c	916	BCR	C36-C18-C19	2.33	121.75	118.08
34	V	203	HTG	C1-O5-C5	-2.33	108.28	112.58
22	c	910	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	B	617	CLA	C1D-CHD-C4C	-2.33	121.03	126.06
22	b	604	CLA	C5-C3-C2	-2.33	116.40	121.12
22	C	507	CLA	C4C-C3C-C2C	-2.33	103.50	106.90
22	C	507	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
22	b	612	CLA	O2A-CGA-CBA	2.33	119.21	111.91
22	c	910	CLA	C3C-C4C-NC	2.33	113.18	110.57
22	b	615	CLA	CHC-C1C-NC	-2.33	120.67	124.20
22	a	412	CLA	C5-C3-C2	-2.33	116.41	121.12
22	D	403	CLA	C1D-ND-C4D	-2.33	104.68	106.33
22	B	608	CLA	C4-C3-C2	-2.33	117.71	123.68
22	d	402	CLA	C3D-C4D-CHA	-2.32	107.41	112.72
22	c	914	CLA	CMB-C2B-C1B	2.32	128.91	125.37
26	A	411	PL9	C10-C9-C11	2.32	119.18	115.27
22	A	406	CLA	C5-C3-C2	-2.32	116.42	121.12
22	c	909	CLA	CMC-C2C-C3C	2.32	132.42	126.12
22	B	603	CLA	C1D-CHD-C4C	-2.32	121.05	126.06
22	A	406	CLA	CED-O2D-CGD	2.32	121.19	115.94
22	B	605	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
22	A	408	CLA	CHC-C4B-C3B	-2.32	117.39	127.71
22	c	907	CLA	CAC-C3C-C4C	2.32	127.82	124.81
26	d	405	PL9	C42-C43-C44	-2.32	122.08	127.66
22	B	605	CLA	O2A-CGA-CBA	2.32	119.18	111.91
22	b	605	CLA	CMB-C2B-C1B	2.32	128.90	125.37
22	C	506	CLA	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	101	BCR	C24-C25-C26	-2.31	115.86	121.46
25	B	621	LMG	O6-C5-C4	2.31	113.90	109.69
27	a	416	LHG	C6-O8-C23	2.31	125.69	117.12
25	B	621	LMG	C4-C3-C2	2.31	114.86	110.82
22	D	401	CLA	CAC-C3C-C4C	2.31	127.81	124.81
22	c	912	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
22	B	608	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
24	B	620	BCR	C15-C14-C13	-2.31	124.01	127.31
22	b	617	CLA	C4D-CHA-C1A	-2.31	118.44	121.25
22	B	604	CLA	CHC-C4B-C3B	-2.31	117.43	127.71
34	b	623	HTG	O5-C1-C2	2.31	113.22	110.31
22	A	408	CLA	CMB-C2B-C1B	2.31	128.89	125.37
22	D	403	CLA	CAC-C3C-C4C	2.31	127.81	124.81
22	a	408	CLA	CMD-C2D-C1D	2.31	128.78	124.71
22	A	405	CLA	O2A-CGA-CBA	2.31	119.15	111.91
22	B	614	CLA	CMB-C2B-C1B	2.31	128.88	125.37
22	C	503	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
24	y	101	BCR	C15-C14-C13	-2.31	124.02	127.31
25	i	101	LMG	O1-C1-C2	2.31	111.90	108.30
23	a	410	PHO	C4B-NB-C1B	-2.31	105.26	108.83
24	B	620	BCR	C40-C30-C25	-2.30	106.56	110.30
24	B	619	BCR	C23-C24-C25	-2.30	120.73	127.20
22	c	904	CLA	C4-C3-C5	2.30	119.15	115.27
22	D	401	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
22	B	607	CLA	CMC-C2C-C1C	2.30	128.55	125.04
22	B	613	CLA	C1D-ND-C4D	-2.30	104.70	106.33
26	a	415	PL9	C51-C49-C50	2.30	119.69	114.60
22	b	615	CLA	CHC-C4B-C3B	-2.30	117.47	127.71
22	a	409	CLA	CHA-C4D-ND	2.30	137.31	132.50
22	D	403	CLA	C3C-C4C-NC	2.30	113.15	110.57
22	B	614	CLA	C1D-CHD-C4C	-2.30	121.10	126.06
22	b	614	CLA	O2A-CGA-CBA	2.30	119.12	111.91
22	B	609	CLA	C1-O2A-CGA	2.30	122.47	116.44
22	c	909	CLA	CAC-C3C-C2C	2.30	131.46	127.53
24	B	619	BCR	C20-C21-C22	-2.30	124.03	127.31
24	B	620	BCR	C15-C16-C17	-2.30	118.77	123.47
22	b	617	CLA	CMD-C2D-C1D	2.29	128.76	124.71
22	c	907	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
22	b	603	CLA	C4D-C3D-CAD	2.29	110.80	108.10
22	C	508	CLA	CHC-C1C-NC	-2.29	120.72	124.20
24	b	620	BCR	C33-C5-C6	-2.29	121.95	124.53
22	b	608	CLA	C2D-C1D-ND	2.29	111.79	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	905	CLA	C7-C6-C5	-2.29	107.14	113.36
22	B	608	CLA	CHC-C4B-C3B	-2.29	117.52	127.71
22	a	407	CLA	C3C-C4C-NC	2.29	113.14	110.57
22	c	904	CLA	C3D-C4D-CHA	-2.29	107.48	112.72
28	C	501	SQD	O7-S-C6	-2.29	104.22	106.94
22	B	615	CLA	CHC-C4B-C3B	-2.29	117.52	127.71
22	c	912	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
22	B	608	CLA	CMC-C2C-C1C	2.29	128.53	125.04
28	a	414	SQD	O5-C1-C2	-2.29	105.50	110.35
22	b	613	CLA	CMD-C2D-C3D	2.29	132.88	127.61
23	a	411	PHO	C11-C12-C13	-2.29	108.52	115.92
22	C	502	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
22	B	604	CLA	CHD-C4C-NC	2.29	127.81	124.20
22	B	606	CLA	C3D-C4D-CHA	-2.29	107.49	112.72
22	C	511	CLA	O2A-CGA-CBA	2.29	119.08	111.91
22	B	612	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
39	V	202	HEC	C3B-C4B-NB	-2.28	107.62	110.17
22	C	503	CLA	C6-C5-C3	-2.28	107.47	113.45
35	C	517	DGD	O3D-C3D-C2D	-2.28	105.07	110.35
35	H	102	DGD	C3B-C2B-C1B	-2.28	105.32	113.62
22	B	603	CLA	C6-C7-C8	-2.28	108.54	115.92
22	B	602	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
22	c	905	CLA	CMB-C2B-C1B	2.28	128.84	125.37
22	C	510	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
22	B	613	CLA	CHC-C1C-NC	-2.28	120.75	124.20
22	B	611	CLA	C1D-CHD-C4C	-2.28	121.14	126.06
22	c	907	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
22	B	606	CLA	CMB-C2B-C1B	2.28	128.84	125.37
22	B	608	CLA	CHB-C4A-NA	2.28	127.66	124.51
22	b	607	CLA	C4C-C3C-C2C	-2.28	103.58	106.90
22	a	412	CLA	CHC-C1C-C2C	-2.27	120.41	126.73
22	C	511	CLA	CBC-CAC-C3C	-2.27	106.16	112.43
22	b	617	CLA	CHC-C1C-NC	-2.27	120.76	124.20
22	b	612	CLA	C1-C2-C3	-2.27	122.11	126.04
22	B	613	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
22	C	508	CLA	C1D-CHD-C4C	-2.27	121.16	126.06
39	V	202	HEC	CMD-C2D-C1D	2.27	128.49	125.04
31	c	924	DMS	O-S-C2	2.27	118.11	106.54
22	d	402	CLA	CHD-C4C-NC	2.27	127.78	124.20
22	b	606	CLA	C3B-C4B-NB	2.27	112.62	110.52
34	b	627	HTG	C1-O5-C5	2.27	116.76	112.58
22	B	604	CLA	C2A-C1A-CHA	-2.27	119.90	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	102	LMT	C2'-C3'-C4'	-2.27	104.51	109.68
22	c	907	CLA	C1D-CHD-C4C	-2.26	121.17	126.06
22	b	612	CLA	C3D-C4D-CHA	-2.26	107.54	112.72
22	c	913	CLA	CMD-C2D-C1D	2.26	128.70	124.71
22	b	615	CLA	CHD-C4C-NC	2.26	127.77	124.20
22	b	605	CLA	O2A-CGA-CBA	2.26	119.01	111.91
22	b	604	CLA	CAC-C3C-C4C	2.26	127.75	124.81
36	E	102	HEM	CMD-C2D-C1D	2.26	128.48	125.04
27	C	522	LHG	O8-C23-C24	2.26	119.00	111.91
25	B	621	LMG	O1-C1-C2	2.26	111.83	108.30
22	b	603	CLA	OBD-CAD-C3D	-2.26	123.08	128.52
22	B	607	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
22	c	912	CLA	C3D-C4D-CHA	-2.26	107.56	112.72
27	D	410	LHG	O8-C23-O10	-2.26	117.89	123.59
22	b	609	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
23	D	402	PHO	OBD-CAD-C3D	-2.26	124.23	127.98
22	a	408	CLA	C4-C3-C5	2.26	119.07	115.27
22	B	603	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
22	c	913	CLA	C6-C5-C3	-2.26	107.54	113.45
34	b	624	HTG	C1-O5-C5	2.25	116.74	112.58
22	d	403	CLA	CAC-C3C-C4C	2.25	127.73	124.81
24	a	413	BCR	C24-C23-C22	-2.25	122.83	126.23
35	C	519	DGD	O4D-C4D-C3D	-2.25	105.14	110.35
22	a	408	CLA	C3D-C4D-CHA	-2.25	107.57	112.72
22	C	506	CLA	CHD-C4C-C3C	-2.25	121.53	124.84
22	C	512	CLA	C6-C7-C8	-2.25	108.65	115.92
22	C	506	CLA	CMC-C2C-C1C	2.25	128.46	125.04
23	a	411	PHO	CMA-C3A-C4A	-2.25	109.45	114.38
22	b	612	CLA	CHC-C4B-C3B	-2.25	117.71	127.71
23	D	402	PHO	O2D-CGD-O1D	-2.25	119.44	123.84
22	a	412	CLA	C3D-C2D-C1D	-2.25	102.77	105.83
22	B	602	CLA	CHD-C4C-NC	2.25	127.74	124.20
22	c	907	CLA	CHC-C4B-C3B	-2.24	117.72	127.71
23	A	407	PHO	C1A-C2A-C3A	-2.24	100.70	102.84
22	B	603	CLA	C1D-ND-C4D	-2.24	104.74	106.33
22	D	404	CLA	CMB-C2B-C1B	2.24	128.78	125.37
22	b	609	CLA	C4D-C3D-CAD	2.24	110.74	108.10
22	c	910	CLA	C4D-C3D-CAD	2.24	110.74	108.10
22	c	913	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
22	B	605	CLA	C4D-C3D-CAD	2.24	110.73	108.10
22	B	606	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
22	b	610	CLA	O2A-CGA-O1A	-2.24	117.94	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	b	632	HTG	C4-C3-C2	-2.24	106.92	110.82
22	b	606	CLA	CHC-C1C-NC	-2.24	120.81	124.20
22	C	512	CLA	CED-O2D-CGD	2.24	121.00	115.94
22	B	615	CLA	CMC-C2C-C1C	2.24	128.44	125.04
22	B	616	CLA	C4C-C3C-C2C	-2.24	103.64	106.90
22	C	506	CLA	C3A-C2A-C1A	2.23	104.68	101.34
22	B	607	CLA	C4C-C3C-C2C	-2.23	103.64	106.90
22	b	616	CLA	CHB-C4A-NA	2.23	127.60	124.51
22	B	616	CLA	CMD-C2D-C1D	2.23	128.65	124.71
22	b	611	CLA	C1D-ND-C4D	-2.23	104.75	106.33
22	c	910	CLA	CED-O2D-CGD	2.23	120.98	115.94
22	b	615	CLA	C3B-C4B-NB	2.23	112.58	110.52
22	b	604	CLA	O2A-CGA-CBA	2.23	118.90	111.91
22	B	615	CLA	CMB-C2B-C1B	2.23	128.76	125.37
22	C	504	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
24	c	916	BCR	C7-C8-C9	-2.23	122.87	126.23
22	D	401	CLA	CMD-C2D-C3D	2.23	132.74	127.61
22	A	408	CLA	C3D-C4D-CHA	-2.23	107.63	112.72
22	C	508	CLA	CMC-C2C-C1C	2.23	128.43	125.04
22	a	409	CLA	CHB-C4A-NA	2.23	127.59	124.51
22	B	609	CLA	CMD-C2D-C1D	2.22	128.63	124.71
22	a	408	CLA	C6-C5-C3	-2.22	107.63	113.45
22	a	407	CLA	C11-C10-C8	-2.22	108.74	115.92
22	b	606	CLA	OBD-CAD-C3D	-2.22	123.17	128.52
22	a	409	CLA	CHC-C1C-C2C	-2.22	120.56	126.73
22	B	617	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
22	C	513	CLA	CED-O2D-CGD	2.22	120.96	115.94
22	B	614	CLA	C7-C6-C5	-2.22	107.33	113.36
22	D	404	CLA	CHB-C1B-NB	-2.22	121.91	124.26
24	b	618	BCR	C1-C6-C7	2.22	122.06	115.78
24	B	618	BCR	C35-C13-C12	2.22	120.65	118.51
22	C	504	CLA	CED-O2D-CGD	2.22	120.95	115.94
22	b	616	CLA	C6-C7-C8	-2.22	108.76	115.92
22	c	911	CLA	C16-C15-C13	-2.22	108.76	115.92
26	d	405	PL9	C10-C9-C11	2.21	119.00	115.27
37	h	101	RRX	C10-C11-C12	-2.21	116.31	123.22
35	H	102	DGD	C2G-O2G-C1B	-2.21	112.34	117.79
22	D	401	CLA	C6-C5-C3	-2.21	107.65	113.45
35	C	519	DGD	O1G-C1A-O1A	-2.21	118.01	123.59
22	c	913	CLA	O2A-CGA-CBA	2.21	118.85	111.91
22	C	511	CLA	CMC-C2C-C1C	2.21	128.41	125.04
37	h	101	RRX	C2-C1-C6	2.21	113.89	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	611	CLA	C9-C8-C10	-2.21	103.28	111.29
34	b	632	HTG	O2-C2-C3	2.21	115.46	110.35
22	B	615	CLA	CAA-CBA-CGA	-2.21	106.79	113.25
24	B	619	BCR	C11-C12-C13	-2.21	120.21	126.42
22	c	906	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
24	C	516	BCR	C37-C22-C21	-2.21	119.83	122.92
22	B	614	CLA	CHD-C4C-NC	2.21	127.69	124.20
25	C	520	LMG	O8-C9-C8	2.21	114.86	108.43
22	c	903	CLA	C3C-C4C-NC	2.21	113.05	110.57
25	d	409	LMG	O6-C5-C6	2.21	111.92	106.44
24	d	404	BCR	C10-C11-C12	-2.21	116.33	123.22
34	b	626	HTG	C2'-C1'-S1	-2.21	105.27	112.40
24	Y	101	BCR	C36-C18-C19	2.21	121.55	118.08
24	k	101	BCR	C38-C26-C25	-2.20	122.05	124.53
35	C	517	DGD	C4E-C3E-C2E	-2.20	106.97	110.82
26	D	406	PL9	C22-C23-C24	-2.20	122.35	127.66
22	B	605	CLA	C5-C3-C2	-2.20	116.66	121.12
25	B	621	LMG	O6-C1-O1	2.20	115.19	109.97
22	A	405	CLA	CMB-C2B-C1B	2.20	128.72	125.37
22	C	509	CLA	C1D-ND-C4D	-2.20	104.77	106.33
22	c	903	CLA	CMD-C2D-C1D	2.20	128.59	124.71
22	b	610	CLA	CHC-C4B-C3B	-2.20	117.92	127.71
22	B	607	CLA	C1-O2A-CGA	2.20	122.22	116.44
22	B	613	CLA	CBA-CAA-C2A	-2.20	107.37	113.86
29	f	102	LMT	C1-O1'-C1'	2.20	117.49	113.84
22	a	409	CLA	O2A-CGA-CBA	2.20	118.81	111.91
22	b	609	CLA	C3D-C4D-CHA	-2.20	107.70	112.72
22	a	412	CLA	CAC-C3C-C4C	2.20	127.66	124.81
22	c	906	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
25	c	920	LMG	O8-C9-C8	2.19	114.82	108.43
22	c	910	CLA	CMD-C2D-C1D	2.19	128.58	124.71
25	j	101	LMG	O4-C4-C5	-2.19	103.85	109.30
24	c	915	BCR	C8-C7-C6	-2.19	121.04	127.20
22	a	408	CLA	CMC-C2C-C3C	2.19	132.07	126.12
22	c	914	CLA	C3C-C4C-NC	2.19	113.03	110.57
39	V	202	HEC	CHD-C4C-NC	2.19	127.88	123.85
22	a	408	CLA	CHB-C1B-NB	-2.19	121.94	124.26
24	b	620	BCR	C16-C17-C18	-2.19	124.19	127.31
22	B	607	CLA	C4B-CHC-C1C	-2.19	121.15	126.34
22	B	605	CLA	C3B-C4B-NB	2.19	112.54	110.52
34	b	624	HTG	O5-C5-C6	2.19	111.87	106.44
22	B	617	CLA	C1-C2-C3	-2.18	122.27	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	616	CLA	CHC-C4B-C3B	-2.18	118.00	127.71
22	d	403	CLA	C3D-C4D-CHA	-2.18	107.73	112.72
28	a	418	SQD	O5-C1-O6	2.18	115.14	109.97
22	b	613	CLA	CMB-C2B-C1B	2.18	128.69	125.37
22	C	503	CLA	CHB-C1B-C2B	-2.18	121.08	127.24
35	C	519	DGD	O6E-C5E-C6E	2.18	111.85	106.44
23	a	410	PHO	CAC-C3C-C2C	2.18	131.25	127.53
25	j	101	LMG	O8-C28-O10	-2.18	118.09	123.59
22	B	607	CLA	C1D-CHD-C4C	-2.18	121.36	126.06
22	A	406	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
22	b	607	CLA	C3D-C4D-CHA	-2.18	107.74	112.72
22	B	609	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
23	D	402	PHO	CMB-C2B-C3B	2.17	128.74	124.68
23	A	407	PHO	C7-C6-C5	-2.17	107.46	113.36
22	B	616	CLA	C3B-C4B-NB	2.17	112.53	110.52
34	b	623	HTG	C4'-C3'-C2'	-2.17	103.41	114.42
22	b	615	CLA	C1D-CHD-C4C	-2.17	121.38	126.06
22	c	912	CLA	CHD-C4C-NC	2.17	127.62	124.20
24	y	101	BCR	C8-C9-C10	-2.17	115.61	118.94
22	B	608	CLA	CHD-C4C-NC	2.17	127.62	124.20
22	c	913	CLA	CBB-CAB-C3B	-2.17	116.84	127.62
22	d	403	CLA	CHC-C4B-C3B	-2.17	118.08	127.71
22	c	908	CLA	C1D-CHD-C4C	-2.17	121.39	126.06
24	y	101	BCR	C34-C9-C8	2.16	121.49	118.08
22	b	608	CLA	CBC-CAC-C3C	-2.16	106.46	112.43
22	A	408	CLA	CHC-C1C-NC	-2.16	120.92	124.20
22	b	608	CLA	CMD-C2D-C1D	2.16	128.52	124.71
22	b	603	CLA	CAC-C3C-C4C	2.16	127.61	124.81
26	D	406	PL9	C42-C43-C44	-2.16	122.46	127.66
22	b	605	CLA	C1-O2A-CGA	2.16	122.11	116.44
22	b	606	CLA	CMD-C2D-C1D	2.16	128.52	124.71
22	c	911	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	B	603	CLA	CHB-C1B-NB	-2.16	121.97	124.26
25	i	101	LMG	C6-C5-C4	2.16	118.06	113.00
22	D	403	CLA	CED-O2D-CGD	2.16	120.82	115.94
22	c	904	CLA	C3C-C4C-NC	2.16	112.99	110.57
22	c	912	CLA	CHB-C1B-NB	-2.16	121.97	124.26
35	d	406	DGD	O1G-C1A-C2A	2.16	118.68	111.91
22	c	913	CLA	C1D-CHD-C4C	-2.16	121.40	126.06
22	c	903	CLA	C16-C15-C13	-2.16	108.95	115.92
24	C	515	BCR	C24-C23-C22	-2.16	122.98	126.23
22	D	404	CLA	CHC-C4B-C3B	-2.16	118.12	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	515	BCR	C36-C18-C19	2.15	121.47	118.08
25	c	920	LMG	O3-C3-C4	-2.15	105.37	110.35
22	A	408	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
24	b	620	BCR	C15-C14-C13	-2.15	124.24	127.31
39	v	202	HEC	CMD-C2D-C1D	2.15	128.31	125.04
34	B	626	HTG	O5-C5-C4	2.15	113.60	109.69
22	b	603	CLA	C4C-C3C-C2C	-2.15	103.76	106.90
26	D	406	PL9	C36-C37-C38	-2.15	104.82	111.88
23	D	402	PHO	CED-O2D-CGD	2.15	120.80	115.94
22	b	602	CLA	CMC-C2C-C1C	2.15	128.31	125.04
22	D	401	CLA	O2A-CGA-CBA	2.15	118.65	111.91
28	a	418	SQD	O48-C23-O10	-2.15	118.17	123.59
22	C	514	CLA	C2A-C1A-CHA	-2.15	120.11	123.86
22	B	605	CLA	C1D-ND-C4D	-2.15	104.81	106.33
22	B	605	CLA	CHC-C4B-C3B	-2.15	118.17	127.71
24	Y	101	BCR	C21-C20-C19	-2.14	116.53	123.22
22	c	910	CLA	C4C-C3C-C2C	-2.14	103.77	106.90
22	b	602	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
22	c	905	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
22	B	614	CLA	CMD-C2D-C1D	2.14	128.49	124.71
22	C	504	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
22	C	512	CLA	C4D-C3D-CAD	2.14	110.62	108.10
22	B	604	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
28	A	413	SQD	C45-O47-C7	-2.14	112.52	117.79
24	b	620	BCR	C32-C1-C6	-2.14	106.83	110.30
24	y	101	BCR	C10-C11-C12	-2.14	116.54	123.22
34	B	626	HTG	O5-C5-C6	2.14	111.75	106.44
22	C	513	CLA	C4C-C3C-C2C	-2.14	103.78	106.90
24	y	101	BCR	C35-C13-C14	-2.14	119.93	122.92
25	b	622	LMG	C9-O8-C28	2.14	125.04	117.12
24	Y	101	BCR	C10-C11-C12	-2.14	116.55	123.22
22	b	608	CLA	CHC-C4B-C3B	-2.14	118.21	127.71
24	b	619	BCR	C35-C13-C14	-2.14	119.93	122.92
29	A	414	LMT	O3B-C3B-C2B	2.14	115.29	110.35
22	C	503	CLA	C3C-C4C-NC	2.13	112.97	110.57
22	b	608	CLA	C1-O2A-CGA	2.13	122.04	116.44
22	B	608	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
22	A	406	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
35	C	517	DGD	O6D-C1D-O3G	-2.13	104.92	109.97
22	a	408	CLA	C1D-CHD-C4C	-2.13	121.46	126.06
24	c	916	BCR	C21-C20-C19	-2.13	116.57	123.22
22	b	617	CLA	CHC-C4B-C3B	-2.13	118.23	127.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	410	LMG	O8-C28-O10	-2.13	118.22	123.59
35	h	102	DGD	C3G-O3G-C1D	-2.13	109.58	113.74
26	d	405	PL9	C22-C21-C19	2.13	119.97	112.98
22	C	504	CLA	C3D-C4D-CHA	-2.13	107.86	112.72
22	C	510	CLA	C3D-C4D-CHA	-2.13	107.86	112.72
22	B	612	CLA	O1D-CGD-CBD	-2.13	120.14	124.48
24	b	619	BCR	C30-C25-C24	2.13	121.79	115.78
22	c	909	CLA	CHC-C1C-NC	-2.13	120.98	124.20
27	A	412	LHG	C6-O8-C23	2.12	124.99	117.12
22	B	614	CLA	C2A-C1A-CHA	-2.12	120.14	123.86
29	A	414	LMT	O1'-C1'-C2'	2.12	111.62	108.30
22	b	603	CLA	C1D-CHD-C4C	-2.12	121.48	126.06
22	D	404	CLA	CMC-C2C-C1C	2.12	128.27	125.04
22	b	608	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
22	b	615	CLA	C3D-C4D-CHA	-2.12	107.87	112.72
22	B	613	CLA	C3C-C4C-NC	2.12	112.95	110.57
22	B	612	CLA	C3B-C4B-NB	2.12	112.48	110.52
24	y	101	BCR	C23-C24-C25	-2.12	121.25	127.20
36	e	101	HEM	CHA-C4D-ND	2.12	126.99	124.37
27	D	410	LHG	C34-C33-C32	-2.12	103.67	114.42
22	B	615	CLA	CHB-C1B-C2B	-2.12	121.25	127.24
22	c	904	CLA	C6-C5-C3	-2.12	107.90	113.45
27	d	407	LHG	O7-C7-C8	2.12	116.06	111.50
36	e	101	HEM	CAA-C2A-C1A	2.12	129.05	124.89
22	B	614	CLA	CHD-C1D-ND	-2.12	122.51	124.45
22	C	513	CLA	C3C-C4C-NC	2.12	112.94	110.57
24	k	101	BCR	C15-C16-C17	-2.11	119.14	123.47
22	a	407	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
24	a	413	BCR	C32-C1-C31	-2.11	102.04	108.53
22	b	611	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
22	c	909	CLA	O2A-CGA-CBA	2.11	118.53	111.91
22	d	403	CLA	O2A-CGA-CBA	2.11	118.53	111.91
24	Y	101	BCR	C11-C12-C13	-2.11	120.49	126.42
22	c	904	CLA	CBB-CAB-C3B	-2.11	117.12	127.62
22	a	408	CLA	CBA-CAA-C2A	-2.11	107.64	113.86
22	c	910	CLA	C1D-ND-C4D	-2.11	104.84	106.33
22	B	607	CLA	C3D-C4D-CHA	-2.11	107.90	112.72
22	C	509	CLA	CHC-C4B-C3B	-2.11	118.33	127.71
37	H	101	RRX	C20-C21-C22	-2.11	124.30	127.31
22	b	602	CLA	C5-C3-C2	-2.11	116.85	121.12
22	b	617	CLA	CMB-C2B-C1B	2.11	128.58	125.37
34	V	203	HTG	O5-C5-C6	2.11	111.67	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	607	CLA	C1D-ND-C4D	-2.11	104.84	106.33
24	C	515	BCR	C11-C12-C13	-2.10	120.50	126.42
22	c	913	CLA	CMB-C2B-C1B	2.10	128.57	125.37
22	B	605	CLA	C6-C7-C8	-2.10	109.12	115.92
24	d	404	BCR	C12-C13-C14	2.10	122.17	118.94
27	C	522	LHG	P-O6-C4	2.10	124.08	118.30
22	B	612	CLA	C3D-C4D-ND	2.10	113.64	110.24
29	Z	101	LMT	O3B-C3B-C2B	-2.10	105.49	110.35
28	A	413	SQD	C1-C2-C3	-2.10	105.62	110.00
27	l	102	LHG	C6-O8-C23	2.10	124.90	117.12
22	C	512	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	c	912	CLA	C4D-C3D-CAD	2.10	110.57	108.10
24	b	619	BCR	C24-C25-C26	-2.10	116.38	121.46
25	A	410	LMG	O6-C1-C2	-2.09	105.92	110.35
22	a	409	CLA	C1D-CHD-C4C	-2.09	121.54	126.06
24	A	409	BCR	C35-C13-C12	2.09	121.38	118.08
22	c	909	CLA	OBD-CAD-C3D	-2.09	123.48	128.52
22	c	908	CLA	CHB-C1B-NB	-2.09	122.04	124.26
22	C	507	CLA	CMD-C2D-C1D	2.09	128.40	124.71
22	C	504	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
25	c	920	LMG	O4-C4-C3	-2.09	105.51	110.35
22	b	612	CLA	CHB-C1B-NB	-2.09	122.04	124.26
34	B	627	HTG	O5-C1-S1	-2.09	104.83	109.82
22	a	407	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
22	a	408	CLA	C3B-C4B-NB	2.09	112.45	110.52
22	B	612	CLA	C1-C2-C3	-2.09	122.43	126.04
22	B	611	CLA	CMC-C2C-C1C	2.09	128.22	125.04
27	C	522	LHG	O4-P-O5	2.09	118.86	110.68
28	b	621	SQD	C1-C2-C3	-2.09	105.65	110.00
24	a	413	BCR	C16-C15-C14	-2.09	119.20	123.47
29	a	419	LMT	O4'-C4B-C5B	2.09	114.48	109.30
29	T	102	LMT	O1'-C1-C2	2.08	116.87	109.56
22	c	904	CLA	O2A-C1-C2	2.08	114.11	108.64
22	B	606	CLA	C16-C15-C13	-2.08	109.19	115.92
22	b	603	CLA	CED-O2D-CGD	2.08	120.65	115.94
22	c	913	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
24	D	405	BCR	C2-C1-C6	2.08	113.69	110.48
35	C	518	DGD	O1G-C1A-C2A	2.08	118.44	111.91
34	b	626	HTG	C4'-C3'-C2'	-2.08	103.86	114.42
22	d	403	CLA	CHC-C1C-NC	-2.08	121.05	124.20
22	c	902	CLA	C3D-C4D-CHA	-2.08	107.97	112.72
29	c	921	LMT	C1B-O5B-C5B	2.08	117.77	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	608	CLA	CBB-CAB-C3B	-2.08	117.28	127.62
24	a	413	BCR	C15-C16-C17	-2.08	119.22	123.47
22	A	405	CLA	C4C-C3C-C2C	-2.08	103.87	106.90
22	c	911	CLA	C1-O2A-CGA	2.08	121.89	116.44
22	B	611	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
24	c	915	BCR	C15-C16-C17	-2.08	119.22	123.47
28	C	501	SQD	C44-O6-C1	-2.08	109.69	113.74
22	B	611	CLA	CAA-CBA-CGA	-2.07	107.19	113.25
24	B	620	BCR	C33-C5-C4	2.07	117.60	113.62
24	b	619	BCR	C23-C24-C25	-2.07	121.38	127.20
24	b	619	BCR	C37-C22-C21	-2.07	120.02	122.92
24	c	915	BCR	C35-C13-C14	-2.07	120.02	122.92
22	b	615	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
22	c	907	CLA	CHC-C1C-C2C	-2.07	120.98	126.73
22	A	406	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
23	D	402	PHO	C4-C3-C2	-2.07	118.37	123.68
22	a	409	CLA	CED-O2D-CGD	2.07	120.62	115.94
24	c	916	BCR	C37-C22-C21	-2.07	120.02	122.92
22	B	613	CLA	C4-C3-C5	2.07	118.75	115.27
22	c	910	CLA	C4-C3-C5	2.07	118.75	115.27
22	B	614	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
22	B	604	CLA	CAC-C3C-C4C	2.07	127.49	124.81
22	B	608	CLA	C3D-C4D-CHA	-2.07	108.00	112.72
34	b	624	HTG	C4-C3-C2	2.07	114.43	110.82
22	A	405	CLA	CHB-C4A-NA	2.07	127.37	124.51
35	c	917	DGD	O4D-C4D-C5D	-2.06	104.17	109.30
24	Y	101	BCR	C30-C25-C24	2.06	121.62	115.78
26	A	411	PL9	C35-C34-C36	2.06	118.74	115.27
36	E	102	HEM	C2A-C1A-NA	-2.06	107.84	110.15
27	A	412	LHG	O7-C7-O9	-2.06	118.87	122.96
22	B	606	CLA	CHB-C1B-NB	-2.06	122.08	124.26
29	B	622	LMT	O5'-C5'-C4'	2.06	113.44	109.69
26	d	405	PL9	C31-C32-C33	-2.06	105.11	111.88
28	a	414	SQD	O48-C23-O10	-2.06	118.39	123.59
22	B	604	CLA	CED-O2D-CGD	2.06	120.59	115.94
24	B	618	BCR	C32-C1-C6	-2.06	106.96	110.30
22	c	913	CLA	C4C-C3C-C2C	-2.06	103.90	106.90
22	b	610	CLA	C4D-CHA-C1A	-2.06	118.75	121.25
22	c	902	CLA	C3B-C4B-NB	2.06	112.42	110.52
22	C	505	CLA	CMC-C2C-C3C	2.06	131.70	126.12
37	H	101	RRX	C33-C5-C6	-2.05	122.22	124.53
24	B	618	BCR	C1-C6-C5	-2.05	119.72	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	918	DGD	C3A-C2A-C1A	-2.05	106.16	113.62
22	C	503	CLA	C16-C15-C13	-2.05	109.29	115.92
22	c	911	CLA	CHC-C4B-C3B	-2.05	118.59	127.71
35	C	517	DGD	O1G-C1A-O1A	-2.05	118.42	123.59
24	b	619	BCR	C20-C21-C22	-2.05	124.38	127.31
35	C	517	DGD	O6E-C5E-C6E	2.05	111.53	106.44
22	b	603	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	b	608	CLA	CMC-C2C-C3C	2.05	131.68	126.12
29	I	102	LMT	C3'-C4'-C5'	-2.05	106.23	110.93
26	a	415	PL9	C46-C47-C48	-2.05	105.15	111.88
35	H	102	DGD	C1D-O6D-C5D	-2.05	109.67	113.69
22	b	609	CLA	CBB-CAB-C3B	-2.05	117.44	127.62
35	C	517	DGD	C6D-C5D-C4D	2.04	116.36	112.09
24	B	619	BCR	C15-C14-C13	-2.04	124.39	127.31
22	B	614	CLA	C4C-C3C-C2C	-2.04	103.92	106.90
25	C	520	LMG	O6-C5-C6	2.04	111.52	106.44
22	B	604	CLA	C6-C5-C3	2.04	118.81	113.45
25	b	622	LMG	O8-C9-C8	2.04	114.38	108.43
22	b	616	CLA	CMD-C2D-C3D	2.04	132.31	127.61
23	A	407	PHO	O2A-CGA-CBA	2.04	118.31	111.91
22	B	614	CLA	C3C-C4C-NC	2.04	112.86	110.57
22	c	902	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
23	D	402	PHO	CAC-C3C-C4C	2.04	129.44	124.27
22	a	409	CLA	CMB-C2B-C3B	2.04	131.53	126.59
34	B	623	HTG	C2'-C1'-S1	-2.04	105.81	112.40
22	A	408	CLA	CHB-C1B-C2B	-2.04	121.48	127.24
22	b	605	CLA	CHB-C1B-NB	-2.04	122.10	124.26
25	j	101	LMG	O3-C3-C4	2.04	115.06	110.35
29	f	102	LMT	O1B-C4'-C5'	2.04	116.04	108.87
22	c	903	CLA	CHC-C4B-C3B	-2.04	118.65	127.71
22	B	603	CLA	CAC-C3C-C2C	2.04	131.01	127.53
35	C	518	DGD	O3D-C3D-C2D	-2.04	105.64	110.35
24	y	101	BCR	C35-C13-C12	2.04	121.29	118.08
22	A	405	CLA	CHB-C1B-NB	-2.04	122.10	124.26
22	C	506	CLA	CHC-C4B-C3B	-2.04	118.65	127.71
29	A	414	LMT	O2B-C2B-C3B	2.04	115.05	110.35
22	c	905	CLA	C1D-CHD-C4C	-2.03	121.67	126.06
28	a	418	SQD	C4-C3-C2	2.03	114.38	110.82
22	c	909	CLA	C4C-C3C-C2C	-2.03	103.93	106.90
22	B	614	CLA	CAC-C3C-C4C	2.03	127.45	124.81
22	B	607	CLA	O2A-CGA-CBA	2.03	118.29	111.91
29	t	101	LMT	C1-O1'-C1'	-2.03	110.47	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	607	CLA	CHC-C4B-C3B	-2.03	118.67	127.71
34	b	626	HTG	O5-C1-C2	-2.03	107.76	110.31
22	C	506	CLA	C7-C6-C5	-2.03	107.84	113.36
22	B	613	CLA	C3D-C4D-CHA	-2.03	108.07	112.72
22	c	914	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	c	905	CLA	C4C-C3C-C2C	-2.03	103.94	106.90
22	C	514	CLA	C3D-C4D-CHA	-2.03	108.08	112.72
36	E	102	HEM	C1B-NB-C4B	2.03	107.17	105.07
22	B	602	CLA	CHC-C4B-C3B	-2.03	118.68	127.71
28	l	101	SQD	O48-C23-O10	-2.03	118.47	123.59
22	C	512	CLA	CHC-C4B-C3B	-2.03	118.69	127.71
22	B	614	CLA	C3B-C4B-NB	2.03	112.40	110.52
27	L	101	LHG	O8-C23-O10	-2.03	118.47	123.59
22	c	904	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
25	b	622	LMG	O6-C5-C4	2.03	113.38	109.69
22	d	402	CLA	CHC-C4B-C3B	-2.03	118.70	127.71
22	c	912	CLA	C1-O2A-CGA	2.03	121.76	116.44
22	b	613	CLA	CHB-C1B-NB	-2.03	122.11	124.26
35	C	519	DGD	C6D-C5D-C4D	2.03	116.32	112.09
22	B	603	CLA	CAA-CBA-CGA	-2.03	107.33	113.25
22	C	514	CLA	C4C-C3C-C2C	-2.03	103.94	106.90
36	e	101	HEM	CAD-CBD-CGD	2.03	117.96	113.60
22	c	914	CLA	C3D-C4D-CHA	-2.02	108.09	112.72
22	D	401	CLA	C16-C15-C13	-2.02	109.38	115.92
22	b	607	CLA	C1D-CHD-C4C	-2.02	121.69	126.06
22	B	612	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
36	e	101	HEM	C1D-C2D-C3D	-2.02	104.83	106.96
39	V	202	HEC	O2D-CGD-CBD	2.02	120.53	114.03
22	B	603	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
22	B	608	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
22	b	611	CLA	CHB-C1B-NB	-2.02	122.12	124.26
22	A	406	CLA	CHB-C4A-NA	2.02	127.30	124.51
36	E	102	HEM	O1D-CGD-CBD	-2.02	116.60	123.08
22	c	912	CLA	CHC-C4B-C3B	-2.02	118.73	127.71
25	J	101	LMG	C9-C8-C7	-2.02	107.02	111.79
29	a	419	LMT	O3B-C3B-C2B	2.02	115.01	110.35
22	D	401	CLA	C4A-NA-C1A	2.02	107.61	106.71
22	C	514	CLA	C3C-C4C-NC	2.02	112.83	110.57
36	e	101	HEM	CMD-C2D-C1D	2.01	128.11	125.04
22	c	905	CLA	CMC-C2C-C1C	2.01	128.11	125.04
22	C	506	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
24	C	515	BCR	C36-C18-C17	-2.01	120.10	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	616	CLA	CMB-C2B-C1B	2.01	128.43	125.37
22	c	909	CLA	C4-C3-C5	2.01	118.65	115.27
22	c	904	CLA	C1D-CHD-C4C	-2.01	121.72	126.06
22	B	611	CLA	C4-C3-C5	2.01	118.65	115.27
25	j	101	LMG	C31-C30-C29	-2.01	105.97	113.19
22	d	403	CLA	CBB-CAB-C3B	-2.01	117.63	127.62
24	c	915	BCR	C24-C23-C22	-2.01	123.20	126.23
25	J	101	LMG	O7-C10-C11	2.01	115.83	111.50
22	B	607	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
24	b	619	BCR	C38-C26-C25	-2.01	122.28	124.53
22	C	511	CLA	C4-C3-C5	2.01	118.65	115.27
22	C	505	CLA	C6-C5-C3	2.00	118.71	113.45
24	C	516	BCR	C8-C7-C6	-2.00	121.57	127.20
26	a	415	PL9	C30-C29-C31	2.00	118.64	115.27
22	B	617	CLA	CMC-C2C-C1C	2.00	128.09	125.04
26	a	415	PL9	C7-C8-C9	-2.00	123.46	126.79
23	a	411	PHO	C16-C15-C13	-2.00	109.45	115.92
22	b	610	CLA	O2A-CGA-CBA	2.00	118.19	111.91
24	b	620	BCR	C23-C24-C25	-2.00	121.58	127.20
22	B	603	CLA	C3D-C4D-CHA	-2.00	108.15	112.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
39	V	202	HEC	NA
39	v	202	HEC	NA

All (1800) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	408	CLA	C4-C3-C5-C6
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	602	CLA	O2A-C1-C2-C3
22	B	602	CLA	C11-C10-C8-C9
22	B	606	CLA	C4B-C3B-CAB-CBB
22	B	606	CLA	C2-C3-C5-C6
22	B	606	CLA	C4-C3-C5-C6
22	B	610	CLA	C2B-C3B-CAB-CBB
22	B	610	CLA	C4B-C3B-CAB-CBB
22	B	612	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	C2-C1-O2A-CGA
22	B	615	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	D	401	CLA	CHA-CBD-CGD-O1D
22	a	408	CLA	CHA-CBD-CGD-O2D
22	a	409	CLA	CHA-CBD-CGD-O1D
22	b	602	CLA	C2-C1-O2A-CGA
22	b	602	CLA	CHA-CBD-CGD-O1D
22	b	602	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	C4-C3-C5-C6
22	b	607	CLA	CHA-CBD-CGD-O1D
22	b	615	CLA	CHA-CBD-CGD-O1D
22	b	615	CLA	CHA-CBD-CGD-O2D
22	c	903	CLA	CHA-CBD-CGD-O1D
22	c	903	CLA	CAD-CBD-CGD-O1D
22	c	904	CLA	C1A-C2A-CAA-CBA
22	c	909	CLA	CHA-CBD-CGD-O1D
22	c	909	CLA	CHA-CBD-CGD-O2D
22	c	914	CLA	C11-C12-C13-C15
23	a	411	PHO	C4C-C3C-CAC-CBC
24	D	405	BCR	C21-C22-C23-C24
24	D	405	BCR	C37-C22-C23-C24
24	D	405	BCR	C23-C24-C25-C30
24	Y	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C21-C22-C23-C24
24	Y	101	BCR	C37-C22-C23-C24
24	b	618	BCR	C7-C8-C9-C10
24	b	618	BCR	C7-C8-C9-C34
24	b	619	BCR	C7-C8-C9-C10
24	b	619	BCR	C7-C8-C9-C34
24	d	404	BCR	C21-C22-C23-C24
24	d	404	BCR	C37-C22-C23-C24
24	d	404	BCR	C23-C24-C25-C26
24	k	101	BCR	C11-C12-C13-C35
24	y	101	BCR	C7-C8-C9-C10
24	y	101	BCR	C7-C8-C9-C34
24	y	101	BCR	C37-C22-C23-C24
25	B	621	LMG	C2-C1-O1-C7
25	C	531	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
25	D	412	LMG	C11-C10-O7-C8
25	d	409	LMG	C2-C1-O1-C7
25	d	409	LMG	O6-C1-O1-C7
26	A	411	PL9	C9-C11-C12-C13
26	A	411	PL9	C25-C24-C26-C27
26	A	411	PL9	C26-C27-C28-C29
26	a	415	PL9	C14-C16-C17-C18
26	a	415	PL9	C35-C34-C36-C37
27	A	412	LHG	C4-O6-P-O3
27	A	412	LHG	C4-O6-P-O4
27	A	412	LHG	C4-O6-P-O5
27	a	416	LHG	C3-O3-P-O5
27	a	416	LHG	C3-O3-P-O6
27	a	416	LHG	C4-O6-P-O5
27	a	423	LHG	O1-C1-C2-C3
27	a	423	LHG	C4-O6-P-O5
27	d	401	LHG	C4-O6-P-O3
27	d	401	LHG	C4-O6-P-O4
27	d	401	LHG	C5-C4-O6-P
27	d	401	LHG	O10-C23-O8-C6
27	d	401	LHG	C24-C23-O8-C6
27	d	407	LHG	C3-O3-P-O5
27	d	407	LHG	C3-O3-P-O6
27	d	407	LHG	C4-O6-P-O4
27	l	102	LHG	O1-C1-C2-C3
27	l	102	LHG	C3-O3-P-O4
28	A	413	SQD	C2-C1-O6-C44
28	A	413	SQD	C5-C6-S-O7
28	A	413	SQD	C5-C6-S-O8
28	A	413	SQD	C5-C6-S-O9
28	C	501	SQD	C5-C6-S-O8
28	D	408	SQD	O6-C44-C45-C46
28	D	408	SQD	O6-C44-C45-O47
28	a	414	SQD	C5-C6-S-O7
28	a	414	SQD	C5-C6-S-O8
28	a	414	SQD	C5-C6-S-O9
28	a	418	SQD	C2-C1-O6-C44
28	a	418	SQD	O6-C44-C45-O47
28	l	101	SQD	O5-C5-C6-S
29	B	622	LMT	C2-C1-O1'-C1'
29	E	101	LMT	C2'-C1'-O1'-C1
29	I	102	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
29	a	419	LMT	O5'-C1'-O1'-C1
29	c	931	LMT	C2'-C1'-O1'-C1
29	c	931	LMT	O5'-C1'-O1'-C1
29	f	102	LMT	C2'-C1'-O1'-C1
29	f	102	LMT	O5'-C1'-O1'-C1
29	t	101	LMT	C2-C1-O1'-C1'
34	B	627	HTG	C2-C1-S1-C1'
34	B	627	HTG	O5-C1-S1-C1'
34	C	521	HTG	O5-C1-S1-C1'
34	C	532	HTG	O5-C1-S1-C1'
34	D	415	HTG	C2-C1-S1-C1'
34	D	415	HTG	O5-C1-S1-C1'
34	D	415	HTG	C2'-C1'-S1-C1
34	b	632	HTG	O5-C1-S1-C1'
34	c	922	HTG	C2-C1-S1-C1'
34	c	922	HTG	O5-C1-S1-C1'
34	l	106	HTG	C2-C1-S1-C1'
34	l	106	HTG	O5-C1-S1-C1'
34	v	203	HTG	C2'-C1'-S1-C1
35	D	407	DGD	O1G-C1G-C2G-O2G
35	D	407	DGD	C2D-C1D-O3G-C3G
35	D	407	DGD	O6D-C1D-O3G-C3G
35	d	406	DGD	C2B-C1B-O2G-C2G
37	h	101	RRX	C7-C8-C9-C10
37	h	101	RRX	C7-C8-C9-C34
27	A	412	LHG	C8-C7-O7-C5
29	I	102	LMT	C3'-C4'-O1B-C1B
27	A	412	LHG	O9-C7-O7-C5
23	a	411	PHO	O1D-CGD-O2D-CED
22	C	514	CLA	O1D-CGD-O2D-CED
22	C	514	CLA	CBD-CGD-O2D-CED
22	c	912	CLA	CBD-CGD-O2D-CED
22	c	913	CLA	CBD-CGD-O2D-CED
23	a	411	PHO	CBD-CGD-O2D-CED
22	B	617	CLA	O1A-CGA-O2A-C1
22	b	602	CLA	O1A-CGA-O2A-C1
25	A	410	LMG	O10-C28-O8-C9
25	B	621	LMG	O10-C28-O8-C9
28	l	101	SQD	O10-C23-O48-C46
22	b	608	CLA	C5-C6-C7-C8
22	b	617	CLA	O1D-CGD-O2D-CED
22	c	914	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	D	412	LMG	O9-C10-O7-C8
22	C	510	CLA	C3-C5-C6-C7
22	C	513	CLA	C3-C5-C6-C7
22	b	617	CLA	C3-C5-C6-C7
22	c	913	CLA	C3-C5-C6-C7
22	b	602	CLA	CBA-CGA-O2A-C1
28	l	101	SQD	C24-C23-O48-C46
35	d	406	DGD	C2A-C1A-O1G-C1G
29	c	921	LMT	C4'-C5'-C6'-O6'
22	c	910	CLA	CBD-CGD-O2D-CED
34	c	922	HTG	O5-C5-C6-O6
22	B	615	CLA	C4-C3-C5-C6
22	A	408	CLA	C2-C3-C5-C6
22	B	615	CLA	C2-C3-C5-C6
22	b	606	CLA	C2-C3-C5-C6
26	A	411	PL9	C23-C24-C26-C27
26	a	415	PL9	C33-C34-C36-C37
22	A	408	CLA	C3-C5-C6-C7
22	B	602	CLA	C3-C5-C6-C7
22	b	605	CLA	C3-C5-C6-C7
22	B	617	CLA	CBA-CGA-O2A-C1
25	A	410	LMG	C29-C28-O8-C9
25	B	621	LMG	C29-C28-O8-C9
28	b	621	SQD	C24-C23-O48-C46
29	A	414	LMT	O5B-C5B-C6B-O6B
29	c	921	LMT	O5'-C5'-C6'-O6'
34	b	624	HTG	S1-C1'-C2'-C3'
25	b	622	LMG	O9-C10-O7-C8
35	d	406	DGD	O1B-C1B-O2G-C2G
29	a	419	LMT	C4'-C5'-C6'-O6'
29	c	931	LMT	C4'-C5'-C6'-O6'
34	b	626	HTG	C4-C5-C6-O6
22	B	615	CLA	O1A-CGA-O2A-C1
25	D	412	LMG	O10-C28-O8-C9
28	b	621	SQD	O10-C23-O48-C46
23	a	411	PHO	C2C-C3C-CAC-CBC
25	d	409	LMG	C8-C9-O8-C28
25	D	412	LMG	O6-C5-C6-O5
29	t	101	LMT	O5'-C5'-C6'-O6'
34	b	627	HTG	O5-C5-C6-O6
22	a	407	CLA	C2C-C3C-CAC-CBC
22	b	617	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	a	412	CLA	C3-C5-C6-C7
35	d	406	DGD	O1A-C1A-O1G-C1G
29	a	419	LMT	O5'-C5'-C6'-O6'
29	c	931	LMT	O5'-C5'-C6'-O6'
25	b	622	LMG	C11-C10-O7-C8
25	d	409	LMG	C11-C10-O7-C8
27	C	522	LHG	C8-C7-O7-C5
22	C	513	CLA	O1D-CGD-O2D-CED
22	c	902	CLA	CBD-CGD-O2D-CED
34	D	415	HTG	O5-C5-C6-O6
29	f	102	LMT	C4'-C5'-C6'-O6'
27	d	408	LHG	C11-C12-C13-C14
35	c	918	DGD	C8B-C9B-CAB-CBB
28	C	501	SQD	C13-C14-C15-C16
28	a	414	SQD	C17-C18-C19-C20
35	D	407	DGD	CCB-CDB-CEB-CFB
25	D	412	LMG	C4-C5-C6-O5
22	B	615	CLA	CBA-CGA-O2A-C1
25	D	412	LMG	C29-C28-O8-C9
34	C	532	HTG	S1-C1'-C2'-C3'
34	l	106	HTG	S1-C1'-C2'-C3'
36	e	101	HEM	C1A-C2A-CAA-CBA
29	I	102	LMT	O5B-C5B-C6B-O6B
34	b	626	HTG	O5-C5-C6-O6
34	b	627	HTG	C4-C5-C6-O6
34	c	922	HTG	C4-C5-C6-O6
36	e	101	HEM	C3A-C2A-CAA-CBA
39	V	202	HEC	C2C-C3C-CAC-CBC
29	T	102	LMT	C4'-C5'-C6'-O6'
34	l	106	HTG	C4-C5-C6-O6
28	A	413	SQD	O5-C1-O6-C44
28	b	621	SQD	O5-C1-O6-C44
26	D	406	PL9	C39-C41-C42-C43
26	a	415	PL9	C9-C11-C12-C13
26	a	415	PL9	C34-C36-C37-C38
29	A	414	LMT	C4B-C5B-C6B-O6B
29	t	101	LMT	C4'-C5'-C6'-O6'
22	b	616	CLA	O1D-CGD-O2D-CED
27	a	423	LHG	C1-C2-C3-O3
34	C	532	HTG	C4-C5-C6-O6
22	B	602	CLA	CBA-CGA-O2A-C1
22	c	913	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	C	531	LMG	C29-C28-O8-C9
25	b	622	LMG	C29-C28-O8-C9
25	i	101	LMG	C29-C28-O8-C9
35	D	407	DGD	C2A-C1A-O1G-C1G
34	v	203	HTG	C1'-C2'-C3'-C4'
35	c	917	DGD	C1B-C2B-C3B-C4B
22	c	907	CLA	C5-C6-C7-C8
22	c	911	CLA	O1D-CGD-O2D-CED
39	v	202	HEC	C2B-C3B-CAB-CBB
22	b	612	CLA	C13-C15-C16-C17
28	l	101	SQD	C23-C24-C25-C26
25	D	412	LMG	C2-C1-O1-C7
35	H	102	DGD	C6B-C7B-C8B-C9B
22	c	913	CLA	O1A-CGA-O2A-C1
29	T	102	LMT	O5'-C5'-C6'-O6'
29	f	102	LMT	O5'-C5'-C6'-O6'
22	c	905	CLA	C4-C3-C5-C6
22	B	602	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C9
22	C	510	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9
22	b	608	CLA	C6-C7-C8-C9
22	c	905	CLA	C14-C13-C15-C16
22	c	910	CLA	C11-C10-C8-C9
22	c	912	CLA	C11-C10-C8-C9
22	c	913	CLA	C6-C7-C8-C9
22	B	607	CLA	O1D-CGD-O2D-CED
24	A	409	BCR	C36-C18-C19-C20
24	K	101	BCR	C11-C12-C13-C35
24	Y	101	BCR	C36-C18-C19-C20
24	c	916	BCR	C37-C22-C23-C24
37	h	101	RRX	C37-C22-C23-C24
24	b	618	BCR	C11-C12-C13-C14
29	A	414	LMT	C4'-C5'-C6'-O6'
27	a	416	LHG	C7-C8-C9-C10
28	C	501	SQD	C7-C8-C9-C10
25	C	531	LMG	O10-C28-O8-C9
22	C	502	CLA	C13-C15-C16-C17
22	b	617	CLA	C5-C6-C7-C8
22	B	616	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
27	D	411	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	D	401	CLA	C2C-C3C-CAC-CBC
27	a	423	LHG	C24-C23-O8-C6
22	A	408	CLA	C13-C15-C16-C17
22	B	606	CLA	C13-C15-C16-C17
22	B	607	CLA	C13-C15-C16-C17
22	C	505	CLA	C8-C10-C11-C12
22	C	510	CLA	C10-C11-C12-C13
22	b	604	CLA	C5-C6-C7-C8
22	c	910	CLA	C13-C15-C16-C17
25	A	410	LMG	C28-C29-C30-C31
25	c	920	LMG	C28-C29-C30-C31
35	C	518	DGD	C1A-C2A-C3A-C4A
35	c	918	DGD	C1A-C2A-C3A-C4A
35	c	918	DGD	C1B-C2B-C3B-C4B
34	b	624	HTG	C1'-C2'-C3'-C4'
34	l	106	HTG	C1'-C2'-C3'-C4'
35	C	517	DGD	O6E-C5E-C6E-O5E
22	A	405	CLA	C15-C16-C17-C18
22	B	605	CLA	C13-C15-C16-C17
22	B	607	CLA	C15-C16-C17-C18
22	B	616	CLA	C8-C10-C11-C12
22	C	507	CLA	C10-C11-C12-C13
22	C	510	CLA	C15-C16-C17-C18
22	D	404	CLA	C15-C16-C17-C18
22	b	609	CLA	C13-C15-C16-C17
27	a	423	LHG	O1-C1-C2-O2
28	f	101	SQD	O6-C1-O5-C5
25	b	622	LMG	O10-C28-O8-C9
25	C	520	LMG	C10-C11-C12-C13
25	d	409	LMG	C10-C11-C12-C13
27	a	423	LHG	C23-C24-C25-C26
28	A	413	SQD	C23-C24-C25-C26
28	b	621	SQD	C23-C24-C25-C26
35	C	518	DGD	C1B-C2B-C3B-C4B
35	d	406	DGD	C1B-C2B-C3B-C4B
25	c	930	LMG	O6-C5-C6-O5
34	l	106	HTG	O5-C5-C6-O6
22	B	616	CLA	C5-C6-C7-C8
22	b	602	CLA	C10-C11-C12-C13
22	b	612	CLA	C10-C11-C12-C13
22	d	403	CLA	C8-C10-C11-C12
29	t	101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	C2B-C3B-C4B-C5B
22	C	504	CLA	O1D-CGD-O2D-CED
25	j	101	LMG	O6-C5-C6-O5
25	d	409	LMG	O9-C10-O7-C8
27	C	522	LHG	O9-C7-O7-C5
22	c	910	CLA	C2-C1-O2A-CGA
25	c	930	LMG	C10-C11-C12-C13
27	A	412	LHG	C23-C24-C25-C26
27	C	522	LHG	C7-C8-C9-C10
39	V	202	HEC	C4C-C3C-CAC-CBC
22	B	602	CLA	C13-C15-C16-C17
22	B	614	CLA	C11-C10-C8-C7
22	c	909	CLA	C11-C10-C8-C7
25	i	101	LMG	O10-C28-O8-C9
24	k	101	BCR	C9-C10-C11-C12
22	C	503	CLA	O1D-CGD-O2D-CED
22	C	512	CLA	O1D-CGD-O2D-CED
22	A	408	CLA	C10-C11-C12-C13
25	b	622	LMG	C4-C5-C6-O5
25	B	621	LMG	O6-C1-O1-C7
28	a	418	SQD	O5-C1-O6-C44
29	E	101	LMT	O5'-C1'-O1'-C1
22	B	609	CLA	C13-C15-C16-C17
22	b	608	CLA	C10-C11-C12-C13
22	b	616	CLA	C5-C6-C7-C8
26	a	415	PL9	C19-C21-C22-C23
26	a	415	PL9	C24-C26-C27-C28
26	a	415	PL9	C39-C41-C42-C43
26	a	415	PL9	C44-C46-C47-C48
29	f	102	LMT	O1'-C1-C2-C3
25	B	621	LMG	C28-C29-C30-C31
34	b	623	HTG	S1-C1'-C2'-C3'
28	a	418	SQD	C32-C33-C34-C35
22	B	612	CLA	C15-C16-C17-C18
22	C	514	CLA	C15-C16-C17-C18
22	c	910	CLA	C15-C16-C17-C18
22	B	602	CLA	O1A-CGA-O2A-C1
35	D	407	DGD	O1A-C1A-O1G-C1G
35	C	519	DGD	O6E-C5E-C6E-O5E
22	c	912	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	C5-C6-C7-C8
22	b	608	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	c	908	CLA	C5-C6-C7-C8
22	c	903	CLA	O1D-CGD-O2D-CED
22	c	909	CLA	CBD-CGD-O2D-CED
27	d	401	LHG	C8-C7-O7-C5
22	A	408	CLA	C8-C10-C11-C12
22	B	611	CLA	C15-C16-C17-C18
22	C	509	CLA	C13-C15-C16-C17
22	b	605	CLA	C13-C15-C16-C17
22	b	616	CLA	C10-C11-C12-C13
22	d	403	CLA	C15-C16-C17-C18
27	L	101	LHG	C4-O6-P-O3
27	l	102	LHG	C3-O3-P-O6
25	C	531	LMG	C28-C29-C30-C31
34	B	623	HTG	C4-C5-C6-O6
27	d	408	LHG	C31-C32-C33-C34
34	B	627	HTG	S1-C1'-C2'-C3'
27	D	409	LHG	C23-C24-C25-C26
27	d	401	LHG	O9-C7-O7-C5
22	B	608	CLA	C8-C10-C11-C12
22	c	905	CLA	C10-C11-C12-C13
22	c	909	CLA	C10-C11-C12-C13
22	B	607	CLA	C2A-CAA-CBA-CGA
24	b	618	BCR	C9-C10-C11-C12
25	b	622	LMG	C10-C11-C12-C13
25	c	920	LMG	C15-C16-C17-C18
25	c	930	LMG	C35-C36-C37-C38
25	d	409	LMG	C20-C21-C22-C23
27	a	423	LHG	C26-C27-C28-C29
35	c	918	DGD	C3A-C4A-C5A-C6A
35	D	407	DGD	C2B-C1B-O2G-C2G
34	C	532	HTG	O5-C5-C6-O6
34	C	521	HTG	C1'-C2'-C3'-C4'
25	C	531	LMG	C13-C14-C15-C16
25	J	101	LMG	C30-C31-C32-C33
25	b	622	LMG	C19-C20-C21-C22
25	j	101	LMG	C30-C31-C32-C33
27	d	407	LHG	C14-C15-C16-C17
27	l	102	LHG	C26-C27-C28-C29
28	l	101	SQD	C17-C18-C19-C20
29	B	622	LMT	C6-C7-C8-C9
35	C	517	DGD	C2B-C3B-C4B-C5B
35	C	517	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
35	C	519	DGD	C5B-C6B-C7B-C8B
35	d	406	DGD	CAA-CBA-CCA-CDA
22	C	507	CLA	C16-C17-C18-C20
22	C	508	CLA	C16-C17-C18-C20
22	a	407	CLA	C16-C17-C18-C19
22	c	906	CLA	C16-C17-C18-C19
22	c	907	CLA	C16-C17-C18-C19
22	c	913	CLA	C16-C17-C18-C19
22	c	914	CLA	C16-C17-C18-C19
25	d	409	LMG	C19-C20-C21-C22
25	i	101	LMG	C11-C12-C13-C14
28	C	501	SQD	C17-C18-C19-C20
28	a	418	SQD	C13-C14-C15-C16
28	l	101	SQD	C34-C35-C36-C37
35	C	519	DGD	CAB-CBB-CCB-CDB
35	D	407	DGD	C8B-C9B-CAB-CBB
35	d	406	DGD	CBB-CCB-CDB-CEB
35	h	102	DGD	C8A-C9A-CAA-CBA
35	D	407	DGD	O1B-C1B-O2G-C2G
27	l	102	LHG	C7-C8-C9-C10
22	C	509	CLA	CBD-CGD-O2D-CED
27	l	102	LHG	C10-C11-C12-C13
28	A	413	SQD	C9-C10-C11-C12
28	l	101	SQD	C24-C25-C26-C27
22	B	608	CLA	O1D-CGD-O2D-CED
27	a	423	LHG	O10-C23-O8-C6
25	A	410	LMG	C16-C17-C18-C19
25	A	410	LMG	C29-C30-C31-C32
25	B	621	LMG	C14-C15-C16-C17
27	d	408	LHG	C10-C11-C12-C13
28	a	418	SQD	C12-C13-C14-C15
28	a	418	SQD	C15-C16-C17-C18
34	b	632	HTG	C2'-C3'-C4'-C5'
35	C	519	DGD	C7B-C8B-C9B-CAB
35	H	102	DGD	CCB-CDB-CEB-CFB
35	c	917	DGD	C7B-C8B-C9B-CAB
35	d	406	DGD	C5B-C6B-C7B-C8B
35	h	102	DGD	C5B-C6B-C7B-C8B
27	d	407	LHG	O2-C2-C3-O3
25	c	930	LMG	C37-C38-C39-C40
25	d	409	LMG	C29-C30-C31-C32
27	l	102	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
28	a	414	SQD	C15-C16-C17-C18
28	a	418	SQD	C24-C25-C26-C27
28	a	418	SQD	C27-C28-C29-C30
29	I	102	LMT	C5-C6-C7-C8
35	C	518	DGD	CBB-CCB-CDB-CEB
35	c	918	DGD	C3B-C4B-C5B-C6B
35	d	406	DGD	C6A-C7A-C8A-C9A
25	d	409	LMG	C29-C28-O8-C9
25	C	520	LMG	C31-C32-C33-C34
25	d	409	LMG	C12-C13-C14-C15
27	a	416	LHG	C15-C16-C17-C18
27	d	401	LHG	C27-C28-C29-C30
28	C	501	SQD	C15-C16-C17-C18
28	b	621	SQD	C31-C32-C33-C34
28	l	101	SQD	C14-C15-C16-C17
29	T	102	LMT	O1'-C1-C2-C3
22	C	503	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C20
22	c	914	CLA	C4-C3-C5-C6
25	A	410	LMG	C38-C39-C40-C41
25	A	410	LMG	C39-C40-C41-C42
25	b	622	LMG	C31-C32-C33-C34
25	c	920	LMG	C35-C36-C37-C38
25	c	930	LMG	C32-C33-C34-C35
25	j	101	LMG	C37-C38-C39-C40
27	a	416	LHG	C34-C35-C36-C37
28	A	413	SQD	C26-C27-C28-C29
29	B	622	LMT	O1'-C1-C2-C3
34	C	523	HTG	C2'-C3'-C4'-C5'
22	A	405	CLA	C14-C13-C15-C16
22	B	611	CLA	C14-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C9
22	b	603	CLA	C11-C12-C13-C14
22	b	604	CLA	C6-C7-C8-C9
22	c	907	CLA	C14-C13-C15-C16
22	c	908	CLA	C11-C10-C8-C9
35	C	519	DGD	C1A-C2A-C3A-C4A
25	C	520	LMG	C34-C35-C36-C37
25	j	101	LMG	C36-C37-C38-C39
27	C	522	LHG	C24-C25-C26-C27
27	a	416	LHG	C11-C12-C13-C14
27	d	407	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
28	a	414	SQD	C29-C30-C31-C32
28	l	101	SQD	C12-C13-C14-C15
34	b	624	HTG	C3'-C4'-C5'-C6'
35	C	519	DGD	C5A-C6A-C7A-C8A
35	C	519	DGD	CBB-CCB-CDB-CEB
35	D	407	DGD	C4A-C5A-C6A-C7A
35	c	919	DGD	C4A-C5A-C6A-C7A
22	c	905	CLA	C15-C16-C17-C18
24	b	618	BCR	C11-C12-C13-C35
25	b	622	LMG	C21-C22-C23-C24
25	c	920	LMG	C20-C21-C22-C23
25	d	409	LMG	C34-C35-C36-C37
27	D	411	LHG	C13-C14-C15-C16
27	D	411	LHG	C18-C19-C20-C21
28	C	501	SQD	C9-C10-C11-C12
29	Z	101	LMT	C4-C5-C6-C7
35	C	517	DGD	C4A-C5A-C6A-C7A
27	D	409	LHG	O1-C1-C2-C3
27	D	410	LHG	O1-C1-C2-C3
27	d	407	LHG	O1-C1-C2-C3
34	b	626	HTG	S1-C1'-C2'-C3'
25	B	621	LMG	C11-C10-O7-C8
25	b	622	LMG	C17-C18-C19-C20
27	D	411	LHG	C29-C30-C31-C32
27	d	408	LHG	C15-C16-C17-C18
27	l	102	LHG	C27-C28-C29-C30
28	a	418	SQD	C28-C29-C30-C31
29	a	419	LMT	C11-C10-C9-C8
29	c	921	LMT	C2-C3-C4-C5
35	c	917	DGD	C7A-C8A-C9A-CAA
35	d	406	DGD	C3B-C4B-C5B-C6B
35	d	406	DGD	C8B-C9B-CAB-CBB
35	h	102	DGD	C2B-C3B-C4B-C5B
35	h	102	DGD	CBB-CCB-CDB-CEB
27	a	423	LHG	C7-C8-C9-C10
28	a	418	SQD	C7-C8-C9-C10
25	C	520	LMG	C20-C21-C22-C23
25	J	101	LMG	C12-C13-C14-C15
25	d	409	LMG	C32-C33-C34-C35
25	i	101	LMG	C14-C15-C16-C17
27	l	102	LHG	C13-C14-C15-C16
28	C	501	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	a	414	SQD	C16-C17-C18-C19
29	A	414	LMT	C6-C7-C8-C9
29	I	102	LMT	C6-C7-C8-C9
29	f	102	LMT	C2-C3-C4-C5
35	C	518	DGD	C2A-C3A-C4A-C5A
35	C	519	DGD	C2A-C3A-C4A-C5A
35	H	102	DGD	C7A-C8A-C9A-CAA
35	d	406	DGD	C4B-C5B-C6B-C7B
35	h	102	DGD	C3B-C4B-C5B-C6B
22	C	513	CLA	C4B-C3B-CAB-CBB
22	A	408	CLA	C16-C17-C18-C20
22	B	611	CLA	C16-C17-C18-C20
22	C	508	CLA	C16-C17-C18-C19
22	C	514	CLA	C16-C17-C18-C19
22	b	608	CLA	C16-C17-C18-C19
22	b	608	CLA	C16-C17-C18-C20
22	b	616	CLA	C16-C17-C18-C19
22	c	906	CLA	C16-C17-C18-C20
22	c	908	CLA	C16-C17-C18-C20
22	c	914	CLA	C16-C17-C18-C20
25	A	410	LMG	C20-C21-C22-C23
25	A	410	LMG	C21-C22-C23-C24
25	b	622	LMG	C14-C15-C16-C17
25	d	409	LMG	C11-C12-C13-C14
27	a	416	LHG	C25-C26-C27-C28
28	a	418	SQD	C29-C30-C31-C32
29	a	419	LMT	C2-C3-C4-C5
35	c	919	DGD	C9A-CAA-CBA-CCA
27	d	401	LHG	C11-C12-C13-C14
27	d	407	LHG	C26-C27-C28-C29
28	A	413	SQD	C28-C29-C30-C31
28	a	414	SQD	C13-C14-C15-C16
28	a	414	SQD	C32-C33-C34-C35
29	I	102	LMT	C7-C8-C9-C10
29	c	931	LMT	C7-C8-C9-C10
29	t	101	LMT	C7-C8-C9-C10
35	C	518	DGD	C7A-C8A-C9A-CAA
35	D	407	DGD	CAA-CBA-CCA-CDA
35	c	918	DGD	CAB-CBB-CCB-CDB
35	c	919	DGD	C6A-C7A-C8A-C9A
35	c	919	DGD	CCB-CDB-CEB-CFB
22	A	405	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	C	520	LMG	C15-C16-C17-C18
27	C	522	LHG	C26-C27-C28-C29
27	d	401	LHG	C26-C27-C28-C29
28	C	501	SQD	C18-C19-C20-C21
28	a	414	SQD	C18-C19-C20-C21
28	a	418	SQD	C18-C19-C20-C21
29	Z	101	LMT	C3-C4-C5-C6
35	C	518	DGD	CCA-CDA-CEA-CFA
35	d	406	DGD	CCA-CDA-CEA-CFA
25	A	410	LMG	C17-C18-C19-C20
25	C	520	LMG	C18-C19-C20-C21
27	l	102	LHG	C16-C17-C18-C19
28	a	414	SQD	C31-C32-C33-C34
22	c	910	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	C10-C11-C12-C13
22	c	907	CLA	C15-C16-C17-C18
29	I	102	LMT	C1-C2-C3-C4
29	t	101	LMT	C1-C2-C3-C4
29	A	414	LMT	C2-C1-O1'-C1'
29	c	931	LMT	C2-C1-O1'-C1'
29	f	102	LMT	C2-C1-O1'-C1'
25	B	621	LMG	C15-C16-C17-C18
27	l	102	LHG	C28-C29-C30-C31
28	C	501	SQD	C30-C31-C32-C33
28	a	414	SQD	C27-C28-C29-C30
28	a	418	SQD	C17-C18-C19-C20
29	c	931	LMT	C2-C3-C4-C5
35	C	518	DGD	C6A-C7A-C8A-C9A
35	D	407	DGD	C2B-C3B-C4B-C5B
22	A	408	CLA	C16-C17-C18-C19
22	B	606	CLA	C16-C17-C18-C20
22	a	407	CLA	C16-C17-C18-C20
22	c	909	CLA	C16-C17-C18-C19
25	C	520	LMG	C16-C17-C18-C19
25	c	920	LMG	C30-C31-C32-C33
27	A	412	LHG	C26-C27-C28-C29
27	a	416	LHG	C12-C13-C14-C15
27	a	416	LHG	C32-C33-C34-C35
35	D	407	DGD	C3B-C4B-C5B-C6B
35	c	919	DGD	C4B-C5B-C6B-C7B
28	C	501	SQD	O6-C44-C45-C46
34	D	415	HTG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
25	J	101	LMG	C34-C35-C36-C37
27	l	102	LHG	C29-C30-C31-C32
35	c	918	DGD	CAA-CBA-CCA-CDA
23	a	410	PHO	O2A-C1-C2-C3
22	B	605	CLA	C3-C5-C6-C7
22	b	602	CLA	C3-C5-C6-C7
29	B	622	LMT	C1-C2-C3-C4
22	B	605	CLA	C10-C11-C12-C13
22	B	612	CLA	C4-C3-C5-C6
26	d	405	PL9	C40-C39-C41-C42
26	a	415	PL9	C13-C14-C16-C17
28	l	101	SQD	C8-C7-O47-C45
25	i	101	LMG	C12-C13-C14-C15
27	C	522	LHG	C9-C10-C11-C12
28	a	414	SQD	C24-C25-C26-C27
35	c	919	DGD	C2A-C3A-C4A-C5A
27	D	410	LHG	O1-C1-C2-O2
28	f	101	SQD	O5-C1-O6-C44
25	b	622	LMG	C18-C19-C20-C21
27	a	416	LHG	C9-C10-C11-C12
27	d	408	LHG	C13-C14-C15-C16
35	H	102	DGD	CAB-CBB-CCB-CDB
22	B	614	CLA	O1D-CGD-O2D-CED
22	A	406	CLA	C6-C7-C8-C9
22	C	507	CLA	C16-C17-C18-C19
22	a	407	CLA	C4C-C3C-CAC-CBC
25	c	920	LMG	C18-C19-C20-C21
28	l	101	SQD	C27-C28-C29-C30
22	B	606	CLA	C2B-C3B-CAB-CBB
28	b	621	SQD	C28-C29-C30-C31
28	l	101	SQD	C28-C29-C30-C31
35	c	918	DGD	CBA-CCA-CDA-CEA
35	d	406	DGD	C9A-CAA-CBA-CCA
28	A	413	SQD	C11-C12-C13-C14
28	A	413	SQD	C27-C28-C29-C30
29	f	102	LMT	C11-C10-C9-C8
35	D	407	DGD	C2A-C3A-C4A-C5A
25	d	409	LMG	C28-C29-C30-C31
22	a	408	CLA	C15-C16-C17-C18
22	c	913	CLA	C15-C16-C17-C18
25	J	101	LMG	O6-C5-C6-O5
27	d	407	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
34	b	632	HTG	O5-C5-C6-O6
25	c	930	LMG	C34-C35-C36-C37
28	C	501	SQD	C12-C13-C14-C15
28	a	418	SQD	C31-C32-C33-C34
28	l	101	SQD	C26-C27-C28-C29
35	C	517	DGD	C4B-C5B-C6B-C7B
35	D	407	DGD	C5A-C6A-C7A-C8A
25	B	621	LMG	O9-C10-O7-C8
28	l	101	SQD	O49-C7-O47-C45
29	Z	101	LMT	C1-C2-C3-C4
22	C	510	CLA	C2-C1-O2A-CGA
25	j	101	LMG	C31-C32-C33-C34
27	D	410	LHG	C14-C15-C16-C17
27	a	416	LHG	C29-C30-C31-C32
35	C	518	DGD	C5A-C6A-C7A-C8A
24	Y	101	BCR	C1-C6-C7-C8
25	d	409	LMG	O10-C28-O8-C9
25	B	621	LMG	C12-C13-C14-C15
27	D	409	LHG	C10-C11-C12-C13
27	L	101	LHG	C13-C14-C15-C16
28	b	621	SQD	C29-C30-C31-C32
22	C	514	CLA	C16-C17-C18-C20
25	C	520	LMG	C28-C29-C30-C31
25	i	101	LMG	C10-C11-C12-C13
22	B	603	CLA	C3-C5-C6-C7
22	b	610	CLA	C3-C5-C6-C7
24	D	405	BCR	C23-C24-C25-C26
24	b	618	BCR	C1-C6-C7-C8
24	b	618	BCR	C5-C6-C7-C8
24	d	404	BCR	C23-C24-C25-C30
37	h	101	RRX	C1-C6-C7-C8
37	h	101	RRX	C5-C6-C7-C8
25	i	101	LMG	C34-C35-C36-C37
35	c	917	DGD	C8A-C9A-CAA-CBA
22	c	904	CLA	CBA-CGA-O2A-C1
25	c	920	LMG	C19-C20-C21-C22
27	D	409	LHG	C31-C32-C33-C34
27	a	416	LHG	C10-C11-C12-C13
35	C	518	DGD	CAA-CBA-CCA-CDA
35	D	407	DGD	C7B-C8B-C9B-CAB
27	a	423	LHG	C29-C30-C31-C32
28	a	418	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	C15-C16-C17-C18
27	l	102	LHG	C34-C35-C36-C37
35	C	518	DGD	C3B-C4B-C5B-C6B
22	A	408	CLA	C11-C12-C13-C15
22	B	611	CLA	C12-C13-C15-C16
22	B	612	CLA	C2-C3-C5-C6
22	C	506	CLA	C11-C12-C13-C15
22	C	509	CLA	C12-C13-C15-C16
22	D	404	CLA	C6-C7-C8-C10
22	a	409	CLA	C6-C7-C8-C10
22	a	412	CLA	C6-C7-C8-C10
22	b	603	CLA	C11-C12-C13-C15
22	b	604	CLA	C6-C7-C8-C10
22	b	607	CLA	C6-C7-C8-C10
22	b	608	CLA	C12-C13-C15-C16
22	b	612	CLA	C12-C13-C15-C16
22	c	905	CLA	C2-C3-C5-C6
22	c	907	CLA	C12-C13-C15-C16
22	c	908	CLA	C11-C10-C8-C7
22	c	913	CLA	C12-C13-C15-C16
22	c	914	CLA	C2-C3-C5-C6
22	d	403	CLA	C6-C7-C8-C10
26	d	405	PL9	C38-C39-C41-C42
28	A	413	SQD	C17-C18-C19-C20
28	A	413	SQD	C25-C26-C27-C28
22	C	502	CLA	C15-C16-C17-C18
22	B	606	CLA	C16-C17-C18-C19
22	B	602	CLA	O1D-CGD-O2D-CED
22	a	412	CLA	O1D-CGD-O2D-CED
29	Z	101	LMT	O5B-C5B-C6B-O6B
25	c	920	LMG	C11-C12-C13-C14
27	D	409	LHG	C15-C16-C17-C18
27	d	408	LHG	C28-C29-C30-C31
28	A	413	SQD	C18-C19-C20-C21
29	a	419	LMT	C6-C7-C8-C9
22	b	607	CLA	C2A-CAA-CBA-CGA
22	a	409	CLA	C8-C10-C11-C12
22	c	904	CLA	C8-C10-C11-C12
27	D	409	LHG	C29-C30-C31-C32
28	A	413	SQD	C15-C16-C17-C18
25	A	410	LMG	C18-C19-C20-C21
25	C	520	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	C6A-C7A-C8A-C9A
22	c	906	CLA	C13-C15-C16-C17
22	c	908	CLA	C13-C15-C16-C17
25	i	101	LMG	C30-C31-C32-C33
28	b	621	SQD	C24-C25-C26-C27
28	l	101	SQD	C33-C34-C35-C36
34	b	626	HTG	C3'-C4'-C5'-C6'
29	a	419	LMT	C1-C2-C3-C4
29	c	921	LMT	C6-C7-C8-C9
22	c	904	CLA	O1A-CGA-O2A-C1
22	B	607	CLA	C10-C11-C12-C13
22	A	406	CLA	O1D-CGD-O2D-CED
25	i	101	LMG	C35-C36-C37-C38
27	D	409	LHG	C28-C29-C30-C31
27	D	410	LHG	C32-C33-C34-C35
27	L	101	LHG	C24-C25-C26-C27
28	a	414	SQD	C30-C31-C32-C33
25	A	410	LMG	C11-C10-O7-C8
25	i	101	LMG	C11-C10-O7-C8
27	a	416	LHG	C8-C7-O7-C5
27	a	423	LHG	O6-C4-C5-O7
25	J	101	LMG	C16-C17-C18-C19
27	C	522	LHG	C12-C13-C14-C15
29	E	101	LMT	C11-C10-C9-C8
29	c	921	LMT	C4-C5-C6-C7
35	d	406	DGD	C2A-C3A-C4A-C5A
22	c	910	CLA	C8-C10-C11-C12
29	I	102	LMT	C4-C5-C6-C7
35	D	407	DGD	C3A-C4A-C5A-C6A
27	a	416	LHG	O9-C7-O7-C5
35	D	407	DGD	C6B-C7B-C8B-C9B
22	B	612	CLA	C13-C15-C16-C17
22	a	412	CLA	C15-C16-C17-C18
28	A	413	SQD	O6-C44-C45-O47
28	C	501	SQD	O6-C44-C45-O47
28	a	414	SQD	O6-C44-C45-O47
35	d	406	DGD	O2G-C2G-C3G-O3G
25	C	520	LMG	C12-C13-C14-C15
35	c	919	DGD	C8A-C9A-CAA-CBA
22	B	611	CLA	C16-C17-C18-C19
25	C	531	LMG	C12-C13-C14-C15
25	c	920	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
28	l	101	SQD	C9-C10-C11-C12
28	l	101	SQD	C11-C12-C13-C14
35	c	917	DGD	O6E-C5E-C6E-O5E
22	D	404	CLA	C8-C10-C11-C12
26	a	415	PL9	C15-C14-C16-C17
28	a	414	SQD	C7-C8-C9-C10
26	A	411	PL9	C4-C3-C7-C8
25	i	101	LMG	C16-C17-C18-C19
28	A	413	SQD	C16-C17-C18-C19
29	c	921	LMT	C1-C2-C3-C4
22	A	408	CLA	C11-C12-C13-C14
22	B	607	CLA	C11-C12-C13-C14
22	B	616	CLA	C11-C12-C13-C14
22	C	506	CLA	C11-C12-C13-C14
22	C	509	CLA	C14-C13-C15-C16
22	D	404	CLA	C6-C7-C8-C9
22	a	409	CLA	C6-C7-C8-C9
22	a	412	CLA	C6-C7-C8-C9
22	b	608	CLA	C14-C13-C15-C16
22	b	612	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
22	c	909	CLA	C11-C10-C8-C9
22	c	913	CLA	C14-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C9
35	d	406	DGD	CAB-CBB-CCB-CDB
25	A	410	LMG	C33-C34-C35-C36
25	B	621	LMG	C13-C14-C15-C16
28	C	501	SQD	C28-C29-C30-C31
28	C	501	SQD	C34-C35-C36-C37
34	D	414	HTG	C2'-C3'-C4'-C5'
35	D	407	DGD	CCA-CDA-CEA-CFA
22	B	602	CLA	C10-C11-C12-C13
22	c	910	CLA	C10-C11-C12-C13
22	d	403	CLA	CBD-CGD-O2D-CED
27	A	412	LHG	C27-C28-C29-C30
27	D	409	LHG	C16-C17-C18-C19
22	C	507	CLA	C1A-C2A-CAA-CBA
22	c	909	CLA	C1A-C2A-CAA-CBA
22	c	907	CLA	C16-C17-C18-C20
22	c	908	CLA	C16-C17-C18-C19
22	c	913	CLA	C16-C17-C18-C20
25	i	101	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
25	i	101	LMG	C33-C34-C35-C36
29	T	102	LMT	C11-C10-C9-C8
35	C	519	DGD	C9A-CAA-CBA-CCA
35	C	519	DGD	C2B-C3B-C4B-C5B
35	c	917	DGD	C9A-CAA-CBA-CCA
22	b	602	CLA	C13-C15-C16-C17
22	b	608	CLA	C8-C10-C11-C12
27	a	416	LHG	C4-O6-P-O3
27	L	101	LHG	C16-C17-C18-C19
29	c	921	LMT	O1'-C1-C2-C3
29	t	101	LMT	C11-C10-C9-C8
35	c	919	DGD	C3B-C4B-C5B-C6B
35	c	919	DGD	C5B-C6B-C7B-C8B
29	a	419	LMT	O5B-C5B-C6B-O6B
35	C	519	DGD	O6D-C5D-C6D-O5D
25	A	410	LMG	C31-C32-C33-C34
27	d	408	LHG	C25-C26-C27-C28
22	C	507	CLA	C5-C6-C7-C8
29	a	419	LMT	C2B-C1B-O1B-C4'
27	d	408	LHG	C16-C17-C18-C19
22	D	401	CLA	O1D-CGD-O2D-CED
25	c	920	LMG	C32-C33-C34-C35
25	d	409	LMG	C21-C22-C23-C24
35	C	517	DGD	CAA-CBA-CCA-CDA
35	C	519	DGD	C4A-C5A-C6A-C7A
29	a	419	LMT	O5B-C1B-O1B-C4'
23	D	402	PHO	C2C-C3C-CAC-CBC
22	A	406	CLA	C6-C7-C8-C10
28	l	101	SQD	C31-C32-C33-C34
35	C	519	DGD	C9B-CAB-CBB-CCB
35	c	918	DGD	C8A-C9A-CAA-CBA
27	d	407	LHG	C12-C13-C14-C15
25	A	410	LMG	O9-C10-O7-C8
25	J	101	LMG	C17-C18-C19-C20
22	B	612	CLA	C10-C11-C12-C13
34	B	623	HTG	O5-C5-C6-O6
25	c	920	LMG	C12-C13-C14-C15
27	l	102	LHG	C30-C31-C32-C33
28	a	414	SQD	C14-C15-C16-C17
34	b	623	HTG	C2'-C3'-C4'-C5'
27	C	522	LHG	C23-C24-C25-C26
25	C	520	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	L	101	LHG	C14-C15-C16-C17
35	c	917	DGD	C2A-C3A-C4A-C5A
22	b	605	CLA	C16-C17-C18-C19
25	A	410	LMG	C35-C36-C37-C38
25	B	621	LMG	C7-C8-C9-O8
25	C	520	LMG	C33-C34-C35-C36
25	D	412	LMG	O1-C7-C8-C9
25	d	409	LMG	C7-C8-C9-O8
27	d	408	LHG	C4-C5-C6-O8
28	A	413	SQD	O6-C44-C45-C46
28	C	501	SQD	C33-C34-C35-C36
28	a	414	SQD	O6-C44-C45-C46
35	D	407	DGD	C1G-C2G-C3G-O3G
35	c	919	DGD	C6B-C7B-C8B-C9B
29	E	101	LMT	O5'-C5'-C6'-O6'
25	A	410	LMG	C22-C23-C24-C25
25	b	622	LMG	C15-C16-C17-C18
35	C	518	DGD	O6D-C5D-C6D-O5D
35	C	518	DGD	C2G-C3G-O3G-C1D
35	c	918	DGD	C2G-C3G-O3G-C1D
35	c	918	DGD	C5D-C6D-O5D-C1E
25	i	101	LMG	C18-C19-C20-C21
27	a	423	LHG	C14-C15-C16-C17
29	I	102	LMT	C9-C10-C11-C12
35	H	102	DGD	CDB-CEB-CFB-CGB
39	v	202	HEC	C4B-C3B-CAB-CBB
22	c	911	CLA	C8-C10-C11-C12
25	C	520	LMG	C22-C23-C24-C25
28	A	413	SQD	C19-C20-C21-C22
29	Z	101	LMT	C9-C10-C11-C12
34	B	626	HTG	C2'-C3'-C4'-C5'
35	c	917	DGD	C8B-C9B-CAB-CBB
25	C	531	LMG	C14-C15-C16-C17
27	L	101	LHG	C10-C11-C12-C13
28	l	101	SQD	C19-C20-C21-C22
29	I	102	LMT	C11-C10-C9-C8
28	l	101	SQD	C25-C26-C27-C28
35	h	102	DGD	CDB-CEB-CFB-CGB
25	b	622	LMG	C13-C14-C15-C16
23	D	402	PHO	C8-C10-C11-C12
25	A	410	LMG	C11-C12-C13-C14
25	b	622	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	Z	101	LMT	C11-C10-C9-C8
35	C	517	DGD	C3B-C4B-C5B-C6B
28	C	501	SQD	C8-C7-O47-C45
25	B	621	LMG	C17-C18-C19-C20
27	d	408	LHG	C19-C20-C21-C22
34	B	626	HTG	C3'-C4'-C5'-C6'
34	D	415	HTG	C4'-C5'-C6'-C7'
22	b	614	CLA	C8-C10-C11-C12
26	A	411	PL9	C30-C29-C31-C32
27	A	412	LHG	C25-C26-C27-C28
27	l	102	LHG	C9-C10-C11-C12
28	l	101	SQD	C10-C11-C12-C13
22	C	503	CLA	C16-C17-C18-C20
22	C	509	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C19
28	a	414	SQD	C35-C36-C37-C38
27	l	102	LHG	C35-C36-C37-C38
28	A	413	SQD	C30-C31-C32-C33
29	A	414	LMT	C9-C10-C11-C12
22	B	612	CLA	C8-C10-C11-C12
22	B	614	CLA	C10-C11-C12-C13
28	b	621	SQD	C35-C36-C37-C38
35	C	517	DGD	C6B-C7B-C8B-C9B
25	C	531	LMG	O6-C5-C6-O5
29	c	921	LMT	O5B-C5B-C6B-O6B
35	h	102	DGD	C6B-C7B-C8B-C9B
22	B	615	CLA	O1D-CGD-O2D-CED
22	c	909	CLA	C13-C15-C16-C17
27	A	412	LHG	C32-C33-C34-C35
28	l	101	SQD	C13-C14-C15-C16
29	a	419	LMT	O1'-C1-C2-C3
35	c	918	DGD	C2B-C3B-C4B-C5B
22	C	513	CLA	CBA-CGA-O2A-C1
27	L	101	LHG	O6-C4-C5-O7
35	H	102	DGD	O2G-C1B-C2B-C3B
22	c	909	CLA	C16-C17-C18-C20
25	c	920	LMG	C39-C40-C41-C42
35	C	518	DGD	C3A-C4A-C5A-C6A
35	c	919	DGD	C8B-C9B-CAB-CBB
27	d	408	LHG	C12-C13-C14-C15
29	T	102	LMT	C1-C2-C3-C4
22	c	908	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	L	101	LHG	C19-C20-C21-C22
29	A	414	LMT	C11-C10-C9-C8
34	D	414	HTG	C1'-C2'-C3'-C4'
22	C	504	CLA	C8-C10-C11-C12
25	b	622	LMG	C2-C1-O1-C7
25	i	101	LMG	C15-C16-C17-C18
27	d	407	LHG	C29-C30-C31-C32
27	a	423	LHG	O7-C5-C6-O8
27	A	412	LHG	C3-O3-P-O5
35	C	518	DGD	CDB-CEB-CFB-CGB
22	b	603	CLA	C13-C15-C16-C17
22	b	613	CLA	C8-C10-C11-C12
23	a	411	PHO	CHA-CBD-CGD-O2D
25	c	930	LMG	C38-C39-C40-C41
25	i	101	LMG	C13-C14-C15-C16
27	d	407	LHG	C35-C36-C37-C38
34	D	414	HTG	C4'-C5'-C6'-C7'
35	c	919	DGD	CBB-CCB-CDB-CEB
35	d	406	DGD	C7B-C8B-C9B-CAB
27	D	410	LHG	C26-C27-C28-C29
29	A	414	LMT	C4-C5-C6-C7
35	d	406	DGD	C2B-C3B-C4B-C5B
22	A	405	CLA	C12-C13-C15-C16
22	B	602	CLA	C11-C10-C8-C7
22	B	602	CLA	C12-C13-C15-C16
22	B	605	CLA	C11-C12-C13-C15
22	B	607	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	B	607	CLA	C12-C13-C15-C16
22	B	612	CLA	C12-C13-C15-C16
22	B	616	CLA	C11-C12-C13-C15
22	B	616	CLA	C12-C13-C15-C16
22	a	407	CLA	C12-C13-C15-C16
22	a	409	CLA	C11-C10-C8-C7
22	a	412	CLA	C11-C12-C13-C15
22	b	604	CLA	C2-C3-C5-C6
22	b	605	CLA	C6-C7-C8-C10
22	b	614	CLA	C11-C10-C8-C7
22	c	903	CLA	C11-C12-C13-C15
22	c	905	CLA	C11-C10-C8-C7
22	c	905	CLA	C11-C12-C13-C15
22	c	908	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	c	910	CLA	C11-C10-C8-C7
22	d	402	CLA	C11-C12-C13-C15
26	A	411	PL9	C28-C29-C31-C32
25	j	101	LMG	C16-C17-C18-C19
34	C	521	HTG	C2'-C3'-C4'-C5'
34	D	415	HTG	C3'-C4'-C5'-C6'
22	A	408	CLA	C11-C10-C8-C9
22	B	607	CLA	C14-C13-C15-C16
22	B	612	CLA	C14-C13-C15-C16
22	C	514	CLA	C11-C10-C8-C9
22	D	404	CLA	C14-C13-C15-C16
22	a	407	CLA	C14-C13-C15-C16
22	a	409	CLA	C11-C10-C8-C9
22	a	412	CLA	C11-C12-C13-C14
22	b	605	CLA	C6-C7-C8-C9
22	c	903	CLA	C11-C12-C13-C14
25	B	621	LMG	C29-C30-C31-C32
28	C	501	SQD	C11-C12-C13-C14
27	a	416	LHG	C33-C34-C35-C36
29	T	102	LMT	C9-C10-C11-C12
34	b	627	HTG	C3'-C4'-C5'-C6'
35	h	102	DGD	CDA-CEA-CFA-CGA
22	B	605	CLA	O1D-CGD-O2D-CED
35	C	519	DGD	C4D-C5D-C6D-O5D
25	c	920	LMG	C33-C34-C35-C36
29	A	414	LMT	C3-C4-C5-C6
29	c	931	LMT	C4-C5-C6-C7
25	c	930	LMG	C11-C12-C13-C14
25	d	409	LMG	C22-C23-C24-C25
29	A	414	LMT	C5-C6-C7-C8
34	b	624	HTG	C2'-C3'-C4'-C5'
22	c	914	CLA	CBA-CGA-O2A-C1
25	i	101	LMG	C40-C41-C42-C43
27	a	416	LHG	C13-C14-C15-C16
29	A	414	LMT	C2-C3-C4-C5
22	a	409	CLA	C10-C11-C12-C13
22	d	403	CLA	C13-C15-C16-C17
35	C	517	DGD	CAB-CBB-CCB-CDB
22	b	611	CLA	CBD-CGD-O2D-CED
25	b	622	LMG	C16-C17-C18-C19
27	l	102	LHG	C11-C10-C9-C8
22	B	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	C	502	CLA	C4B-C3B-CAB-CBB
22	c	904	CLA	C5-C6-C7-C8
27	L	101	LHG	O6-C4-C5-C6
25	A	410	LMG	C19-C20-C21-C22
25	c	920	LMG	C31-C32-C33-C34
25	B	621	LMG	C10-C11-C12-C13
28	a	418	SQD	C24-C23-O48-C46
22	a	408	CLA	C2C-C3C-CAC-CBC
29	E	101	LMT	C3-C4-C5-C6
22	a	409	CLA	C14-C13-C15-C16
22	C	513	CLA	O1A-CGA-O2A-C1
25	b	622	LMG	C32-C33-C34-C35
35	c	918	DGD	CDA-CEA-CFA-CGA
22	B	609	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
22	c	914	CLA	C5-C6-C7-C8
22	c	914	CLA	C13-C15-C16-C17
25	i	101	LMG	O8-C28-C29-C30
35	c	917	DGD	O6D-C5D-C6D-O5D
27	a	416	LHG	C31-C32-C33-C34
35	c	918	DGD	C5B-C6B-C7B-C8B
27	d	408	LHG	C2-C3-O3-P
35	C	519	DGD	CCB-CDB-CEB-CFB
24	k	101	BCR	C19-C20-C21-C22
35	c	917	DGD	C4D-C5D-C6D-O5D
29	T	102	LMT	C2-C1-O1'-C1'
25	C	520	LMG	C38-C39-C40-C41
25	i	101	LMG	C22-C23-C24-C25
25	j	101	LMG	C13-C14-C15-C16
29	I	102	LMT	C4B-C5B-C6B-O6B
35	c	919	DGD	CDB-CEB-CFB-CGB
27	L	101	LHG	C15-C16-C17-C18
28	A	413	SQD	C11-C10-C9-C8
22	c	903	CLA	C15-C16-C17-C18
25	B	621	LMG	O1-C7-C8-C9
25	i	101	LMG	C7-C8-C9-O8
27	a	423	LHG	C4-C5-C6-O8
28	a	418	SQD	O6-C44-C45-C46
28	l	101	SQD	C44-C45-C46-O48
35	H	102	DGD	O1G-C1G-C2G-C3G
35	d	406	DGD	O1G-C1G-C2G-C3G
35	d	406	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
25	i	101	LMG	C29-C30-C31-C32
29	t	101	LMT	C9-C10-C11-C12
34	b	626	HTG	C2'-C3'-C4'-C5'
25	A	410	LMG	C36-C37-C38-C39
25	J	101	LMG	C35-C36-C37-C38
35	C	517	DGD	C5A-C6A-C7A-C8A
35	C	519	DGD	CDB-CEB-CFB-CGB
35	c	917	DGD	CDA-CEA-CFA-CGA
22	C	514	CLA	O2A-C1-C2-C3
23	A	407	PHO	O2A-C1-C2-C3
25	i	101	LMG	C31-C32-C33-C34
28	C	501	SQD	C27-C28-C29-C30
34	C	532	HTG	C2'-C3'-C4'-C5'
22	D	404	CLA	C3-C5-C6-C7
25	c	920	LMG	C21-C22-C23-C24
35	C	519	DGD	CBA-CCA-CDA-CEA
22	b	615	CLA	C4-C3-C5-C6
22	D	404	CLA	C16-C17-C18-C19
25	d	409	LMG	C36-C37-C38-C39
28	a	418	SQD	C9-C10-C11-C12
22	c	914	CLA	C10-C11-C12-C13
25	D	412	LMG	C12-C13-C14-C15
28	C	501	SQD	C35-C36-C37-C38
35	c	917	DGD	C3B-C4B-C5B-C6B
35	d	406	DGD	CDB-CEB-CFB-CGB
22	C	502	CLA	O1D-CGD-O2D-CED
27	d	407	LHG	O1-C1-C2-O2
22	c	905	CLA	C8-C10-C11-C12
25	B	621	LMG	C18-C19-C20-C21
27	A	412	LHG	C33-C34-C35-C36
27	D	411	LHG	C16-C17-C18-C19
35	d	406	DGD	C4A-C5A-C6A-C7A
35	C	519	DGD	C2A-C1A-O1G-C1G
27	A	412	LHG	C24-C25-C26-C27
22	b	602	CLA	C16-C17-C18-C20
22	b	612	CLA	C16-C17-C18-C20
22	c	911	CLA	C16-C17-C18-C20
27	a	423	LHG	C28-C29-C30-C31
29	f	102	LMT	C1-C2-C3-C4
22	C	502	CLA	C2B-C3B-CAB-CBB
22	C	513	CLA	C2B-C3B-CAB-CBB
27	L	101	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
29	f	102	LMT	C9-C10-C11-C12
27	L	101	LHG	C11-C10-C9-C8
35	C	518	DGD	CDA-CEA-CFA-CGA
35	c	918	DGD	C6A-C7A-C8A-C9A
35	D	407	DGD	C5B-C6B-C7B-C8B
25	B	621	LMG	O7-C8-C9-O8
28	l	101	SQD	O47-C45-C46-O48
35	D	407	DGD	O2G-C2G-C3G-O3G
35	d	406	DGD	O1G-C1G-C2G-O2G
22	D	401	CLA	C4C-C3C-CAC-CBC
29	t	101	LMT	C3-C4-C5-C6
25	C	520	LMG	C37-C38-C39-C40
27	d	408	LHG	C32-C33-C34-C35
29	t	101	LMT	C2-C3-C4-C5
26	a	415	PL9	C45-C44-C46-C47
22	C	507	CLA	C2-C1-O2A-CGA
22	B	603	CLA	C11-C12-C13-C14
22	B	611	CLA	C11-C12-C13-C14
22	B	612	CLA	C11-C12-C13-C14
22	B	614	CLA	C11-C12-C13-C14
22	C	507	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C12-C13-C14
22	c	908	CLA	C14-C13-C15-C16
22	c	914	CLA	C11-C12-C13-C14
27	L	101	LHG	C25-C26-C27-C28
28	C	501	SQD	C10-C11-C12-C13
35	C	518	DGD	C9A-CAA-CBA-CCA
22	C	508	CLA	C5-C6-C7-C8
27	D	411	LHG	C2-C3-O3-P
27	a	416	LHG	C14-C15-C16-C17
35	C	518	DGD	CBA-CCA-CDA-CEA
35	c	917	DGD	C3A-C4A-C5A-C6A
22	B	615	CLA	C2A-CAA-CBA-CGA
22	B	602	CLA	C16-C17-C18-C19
22	b	605	CLA	C16-C17-C18-C20
22	b	612	CLA	C16-C17-C18-C19
24	C	515	BCR	C23-C24-C25-C26
24	C	515	BCR	C23-C24-C25-C30
24	b	619	BCR	C23-C24-C25-C26
24	b	619	BCR	C23-C24-C25-C30
24	c	916	BCR	C5-C6-C7-C8
22	C	511	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	C	514	CLA	CBA-CGA-O2A-C1
24	y	101	BCR	C21-C22-C23-C24
37	h	101	RRX	C21-C22-C23-C24
22	d	403	CLA	C10-C11-C12-C13
28	C	501	SQD	O49-C7-O47-C45
28	C	501	SQD	C31-C32-C33-C34
34	b	632	HTG	C3'-C4'-C5'-C6'
28	C	501	SQD	C24-C25-C26-C27
35	c	918	DGD	C4A-C5A-C6A-C7A
35	H	102	DGD	C9B-CAB-CBB-CCB
22	b	613	CLA	O1D-CGD-O2D-CED
27	d	401	LHG	C31-C32-C33-C34
29	Z	101	LMT	C5-C6-C7-C8
27	a	423	LHG	O2-C2-C3-O3
22	A	408	CLA	C11-C10-C8-C7
22	B	602	CLA	C11-C12-C13-C15
22	B	603	CLA	C11-C12-C13-C15
22	B	605	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C12-C13-C15
22	C	509	CLA	C11-C10-C8-C7
22	C	514	CLA	C11-C10-C8-C7
22	D	404	CLA	C12-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C15
22	b	604	CLA	C11-C10-C8-C7
22	c	907	CLA	C6-C7-C8-C10
22	c	913	CLA	C6-C7-C8-C10
22	c	913	CLA	C11-C12-C13-C15
22	c	914	CLA	C12-C13-C15-C16
22	d	403	CLA	C11-C10-C8-C7
23	D	402	PHO	C11-C12-C13-C15
24	c	915	BCR	C9-C10-C11-C12
25	j	101	LMG	C35-C36-C37-C38
28	A	413	SQD	C13-C14-C15-C16
35	C	519	DGD	CAA-CBA-CCA-CDA
29	T	102	LMT	C5-C6-C7-C8
22	B	603	CLA	C13-C15-C16-C17
22	C	507	CLA	C13-C15-C16-C17
22	c	913	CLA	C8-C10-C11-C12
25	D	412	LMG	C35-C36-C37-C38
35	d	406	DGD	C9B-CAB-CBB-CCB
25	d	409	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
27	a	416	LHG	C30-C31-C32-C33
34	B	627	HTG	C2'-C1'-S1-C1
34	b	623	HTG	C2'-C1'-S1-C1
34	c	922	HTG	C2'-C1'-S1-C1
22	C	509	CLA	C16-C17-C18-C20
22	a	409	CLA	C12-C13-C15-C16
35	C	518	DGD	C4D-C5D-C6D-O5D
35	c	919	DGD	CAA-CBA-CCA-CDA
25	c	930	LMG	C14-C15-C16-C17
22	B	617	CLA	CAD-CBD-CGD-O2D
22	C	513	CLA	CAD-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	c	904	CLA	CAD-CBD-CGD-O2D
22	c	913	CLA	CAD-CBD-CGD-O2D
22	d	403	CLA	CAD-CBD-CGD-O2D
23	D	402	PHO	CAD-CBD-CGD-O2D
36	e	101	HEM	C2C-C3C-CAC-CBC
22	B	612	CLA	O1D-CGD-O2D-CED
29	A	414	LMT	O5'-C5'-C6'-O6'
29	T	102	LMT	C2-C3-C4-C5
25	C	520	LMG	C21-C22-C23-C24
35	c	917	DGD	O6E-C1E-O5D-C6D
35	c	918	DGD	O6E-C1E-O5D-C6D
26	a	415	PL9	C43-C44-C46-C47
29	A	414	LMT	C1-C2-C3-C4
34	b	623	HTG	C4'-C5'-C6'-C7'
35	d	406	DGD	C3A-C4A-C5A-C6A
27	C	522	LHG	C4-C5-C6-O8
35	D	407	DGD	O1G-C1G-C2G-C3G
22	c	914	CLA	O1A-CGA-O2A-C1
22	C	508	CLA	C10-C11-C12-C13
22	B	617	CLA	O1D-CGD-O2D-CED
25	c	920	LMG	C34-C35-C36-C37
25	c	930	LMG	C33-C34-C35-C36
27	a	416	LHG	C27-C28-C29-C30
25	d	409	LMG	C15-C16-C17-C18
35	C	518	DGD	C4B-C5B-C6B-C7B
27	l	102	LHG	C14-C15-C16-C17
35	D	407	DGD	C8A-C9A-CAA-CBA
27	L	101	LHG	C1-C2-C3-O3
22	B	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	513	CLA	CHA-CBD-CGD-O1D
22	b	608	CLA	CHA-CBD-CGD-O1D
22	c	905	CLA	CHA-CBD-CGD-O1D
22	c	908	CLA	CHA-CBD-CGD-O1D
28	a	418	SQD	O10-C23-O48-C46
25	i	101	LMG	C36-C37-C38-C39
35	C	517	DGD	C8B-C9B-CAB-CBB
35	H	102	DGD	C7B-C8B-C9B-CAB
29	B	622	LMT	C4-C5-C6-C7
25	B	621	LMG	O1-C7-C8-O7
25	d	409	LMG	O7-C8-C9-O8
25	i	101	LMG	O7-C8-C9-O8
27	C	522	LHG	O7-C5-C6-O8
28	b	621	SQD	O47-C45-C46-O48
35	H	102	DGD	O1G-C1G-C2G-O2G
34	b	626	HTG	C4'-C5'-C6'-C7'
22	C	514	CLA	O1A-CGA-O2A-C1
34	B	623	HTG	C1'-C2'-C3'-C4'
27	D	409	LHG	O1-C1-C2-O2
34	c	922	HTG	S1-C1'-C2'-C3'
25	C	520	LMG	C14-C15-C16-C17
26	a	415	PL9	C4-C3-C7-C8
28	a	414	SQD	C11-C10-C9-C8
29	c	921	LMT	C9-C10-C11-C12
22	B	605	CLA	C11-C10-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C9
22	c	906	CLA	C14-C13-C15-C16
22	c	913	CLA	C11-C12-C13-C14
23	D	402	PHO	C11-C12-C13-C14
27	D	410	LHG	C13-C14-C15-C16
22	b	617	CLA	C8-C10-C11-C12
27	A	412	LHG	C28-C29-C30-C31
28	a	414	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	A	409	BCR	C17-C18-C19-C20
24	c	916	BCR	C21-C22-C23-C24
24	k	101	BCR	C11-C12-C13-C14
25	j	101	LMG	C34-C35-C36-C37
22	c	903	CLA	C16-C17-C18-C19
22	c	906	CLA	C8-C10-C11-C12
22	B	617	CLA	C2-C1-O2A-CGA
25	C	531	LMG	C29-C30-C31-C32
29	E	101	LMT	C5-C6-C7-C8
27	D	410	LHG	C3-O3-P-O6
25	b	622	LMG	C29-C30-C31-C32
25	d	409	LMG	C30-C31-C32-C33
27	d	401	LHG	C9-C10-C11-C12
28	a	414	SQD	C25-C26-C27-C28
22	b	604	CLA	C4-C3-C5-C6
22	b	602	CLA	C4B-C3B-CAB-CBB
22	c	902	CLA	C4B-C3B-CAB-CBB
27	L	101	LHG	C4-O6-P-O5
27	a	416	LHG	C4-O6-P-O4
27	l	102	LHG	C3-O3-P-O5
28	f	101	SQD	O5-C5-C6-S
22	b	609	CLA	C16-C17-C18-C20
25	c	930	LMG	C28-C29-C30-C31
29	c	921	LMT	C3-C4-C5-C6
35	C	519	DGD	O6D-C1D-O3G-C3G
22	b	612	CLA	C8-C10-C11-C12
27	a	416	LHG	O6-C4-C5-C6
27	a	423	LHG	O6-C4-C5-C6
35	D	407	DGD	CDA-CEA-CFA-CGA
35	h	102	DGD	O2G-C1B-C2B-C3B
27	d	407	LHG	C34-C35-C36-C37
27	D	410	LHG	C30-C31-C32-C33
22	B	602	CLA	C16-C17-C18-C20
22	c	911	CLA	C16-C17-C18-C19
27	d	407	LHG	C16-C17-C18-C19
22	B	602	CLA	CAD-CBD-CGD-O1D
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	608	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CAD-CBD-CGD-O1D
22	C	513	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	b	602	CLA	CAD-CBD-CGD-O1D
22	b	608	CLA	CAD-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O1D
22	c	905	CLA	CAD-CBD-CGD-O1D
28	b	621	SQD	O5-C5-C6-S
35	C	519	DGD	O1A-C1A-O1G-C1G
22	b	611	CLA	C8-C10-C11-C12
27	L	101	LHG	C26-C27-C28-C29
35	h	102	DGD	CCB-CDB-CEB-CFB
35	c	919	DGD	C2A-C1A-O1G-C1G
25	j	101	LMG	C39-C40-C41-C42
34	b	623	HTG	C3'-C4'-C5'-C6'
22	B	602	CLA	C6-C7-C8-C10
22	B	603	CLA	C6-C7-C8-C10
22	B	604	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C10-C8-C7
22	B	616	CLA	C11-C10-C8-C7
22	C	505	CLA	C12-C13-C15-C16
22	C	510	CLA	C12-C13-C15-C16
22	C	514	CLA	C6-C7-C8-C10
22	C	514	CLA	C11-C12-C13-C15
22	b	602	CLA	C11-C10-C8-C7
22	b	608	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C10-C8-C7
22	b	609	CLA	C11-C10-C8-C7
22	b	609	CLA	C11-C12-C13-C15
22	c	905	CLA	C12-C13-C15-C16
22	c	906	CLA	C12-C13-C15-C16
22	c	907	CLA	C11-C12-C13-C15
22	c	909	CLA	C11-C12-C13-C15
22	c	910	CLA	C6-C7-C8-C10
22	c	912	CLA	C11-C10-C8-C7
25	d	409	LMG	C14-C15-C16-C17
27	a	416	LHG	C16-C17-C18-C19
29	B	622	LMT	C11-C10-C9-C8
28	a	414	SQD	C33-C34-C35-C36
35	C	517	DGD	CBB-CCB-CDB-CEB
35	C	519	DGD	C4E-C5E-C6E-O5E
29	B	622	LMT	C9-C10-C11-C12
25	J	101	LMG	C18-C19-C20-C21
25	A	410	LMG	O1-C7-C8-C9
25	A	410	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	A	410	LMG	O1-C7-C8-O7
25	A	410	LMG	O7-C8-C9-O8
25	D	412	LMG	O1-C7-C8-O7
25	c	930	LMG	O1-C7-C8-O7
28	b	621	SQD	O6-C44-C45-O47
28	l	101	SQD	O6-C44-C45-O47
35	H	102	DGD	C5B-C6B-C7B-C8B
27	D	411	LHG	C15-C16-C17-C18
35	C	518	DGD	C5D-C6D-O5D-C1E
25	c	920	LMG	C37-C38-C39-C40
27	d	401	LHG	C11-C10-C9-C8
22	c	906	CLA	C2-C3-C5-C6
28	l	101	SQD	C15-C16-C17-C18
22	B	602	CLA	C11-C12-C13-C14
22	B	607	CLA	C11-C10-C8-C9
22	B	616	CLA	C14-C13-C15-C16
22	C	514	CLA	C6-C7-C8-C9
22	b	604	CLA	C11-C10-C8-C9
22	c	905	CLA	C11-C10-C8-C9
22	d	403	CLA	C11-C10-C8-C9
22	C	514	CLA	C3-C5-C6-C7
22	c	905	CLA	C3-C5-C6-C7
22	D	404	CLA	C16-C17-C18-C20
26	A	411	PL9	C39-C41-C42-C43
27	l	102	LHG	O1-C1-C2-O2
35	c	917	DGD	C5B-C6B-C7B-C8B
29	A	414	LMT	C7-C8-C9-C10
22	c	914	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	C2B-C3B-CAB-CBB
22	C	503	CLA	C2B-C3B-CAB-CBB
22	b	602	CLA	C2B-C3B-CAB-CBB
22	b	610	CLA	C2B-C3B-CAB-CBB
22	d	402	CLA	C2B-C3B-CAB-CBB
25	J	101	LMG	C14-C15-C16-C17
25	c	920	LMG	C36-C37-C38-C39
35	h	102	DGD	C7A-C8A-C9A-CAA
34	b	632	HTG	C4'-C5'-C6'-C7'
35	c	918	DGD	CCA-CDA-CEA-CFA
27	C	522	LHG	O7-C7-C8-C9
27	d	401	LHG	C4-C5-O7-C7
22	C	508	CLA	C2A-CAA-CBA-CGA
22	c	910	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
35	h	102	DGD	C9A-CAA-CBA-CCA
22	B	613	CLA	O1A-CGA-O2A-C1
22	d	402	CLA	C2-C1-O2A-CGA
27	d	408	LHG	C29-C30-C31-C32
34	C	532	HTG	C1'-C2'-C3'-C4'
25	j	101	LMG	C18-C19-C20-C21
27	C	522	LHG	C13-C14-C15-C16
35	D	407	DGD	C4B-C5B-C6B-C7B
27	L	101	LHG	C5-C6-O8-C23
25	b	622	LMG	C20-C21-C22-C23
25	d	409	LMG	C18-C19-C20-C21
22	C	510	CLA	O1D-CGD-O2D-CED
24	a	413	BCR	C1-C6-C7-C8
24	c	916	BCR	C1-C6-C7-C8
22	b	615	CLA	C2-C3-C5-C6
22	b	605	CLA	C2C-C3C-CAC-CBC
35	d	406	DGD	C7A-C8A-C9A-CAA
34	B	627	HTG	C1'-C2'-C3'-C4'
22	C	506	CLA	O1D-CGD-O2D-CED
35	c	917	DGD	C2E-C1E-O5D-C6D
35	c	918	DGD	C2E-C1E-O5D-C6D
35	c	918	DGD	C4B-C5B-C6B-C7B
27	d	408	LHG	O7-C5-C6-O8
35	h	102	DGD	O1G-C1G-C2G-O2G
27	a	423	LHG	C4-O6-P-O3
27	d	407	LHG	C4-O6-P-O3
28	l	101	SQD	C7-C8-C9-C10
25	C	531	LMG	C21-C22-C23-C24
35	C	517	DGD	O6D-C5D-C6D-O5D
25	A	410	LMG	C7-C8-C9-O8
25	C	531	LMG	O1-C7-C8-C9
28	b	621	SQD	C44-C45-C46-O48
22	b	602	CLA	C4-C3-C5-C6
27	a	423	LHG	C10-C11-C12-C13
22	C	511	CLA	C2-C3-C5-C6
22	C	511	CLA	C6-C7-C8-C10
22	b	602	CLA	C6-C7-C8-C10
29	a	419	LMT	C7-C8-C9-C10
35	C	517	DGD	CDA-CEA-CFA-CGA
22	C	510	CLA	C11-C12-C13-C14
22	b	602	CLA	C11-C12-C13-C14
22	c	905	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	c	907	CLA	C6-C7-C8-C9
22	c	908	CLA	C11-C12-C13-C14
22	c	914	CLA	C14-C13-C15-C16
22	d	402	CLA	C11-C12-C13-C14
24	C	515	BCR	C13-C14-C15-C16
22	a	408	CLA	C4C-C3C-CAC-CBC
27	D	409	LHG	C25-C26-C27-C28
27	a	416	LHG	C17-C18-C19-C20
35	h	102	DGD	CAA-CBA-CCA-CDA
27	l	102	LHG	C31-C32-C33-C34
29	B	622	LMT	C3-C4-C5-C6
35	c	918	DGD	C9A-CAA-CBA-CCA
29	E	101	LMT	C1-C2-C3-C4
22	b	616	CLA	C4-C3-C5-C6
27	a	416	LHG	C35-C36-C37-C38
22	B	606	CLA	C8-C10-C11-C12
25	C	531	LMG	C10-C11-C12-C13
35	C	517	DGD	C4D-C5D-C6D-O5D
22	C	503	CLA	C4B-C3B-CAB-CBB
22	b	610	CLA	C4B-C3B-CAB-CBB
22	c	913	CLA	C4B-C3B-CAB-CBB
22	d	402	CLA	C4B-C3B-CAB-CBB
34	b	623	HTG	C4-C5-C6-O6
37	H	101	RRX	C9-C10-C11-C12
37	h	101	RRX	C9-C10-C11-C12
29	c	921	LMT	C5-C6-C7-C8
27	D	410	LHG	C29-C30-C31-C32
28	a	414	SQD	C28-C29-C30-C31
22	b	611	CLA	C16-C17-C18-C20
36	e	101	HEM	C4C-C3C-CAC-CBC
22	b	606	CLA	O1D-CGD-O2D-CED
27	d	407	LHG	C31-C32-C33-C34
36	e	101	HEM	CAA-CBA-CGA-O1A
25	B	621	LMG	C4-C5-C6-O5
27	a	416	LHG	O2-C2-C3-O3
22	B	616	CLA	C13-C15-C16-C17
35	C	518	DGD	C2E-C1E-O5D-C6D
22	c	902	CLA	C2A-CAA-CBA-CGA
25	C	520	LMG	O1-C7-C8-O7
28	A	413	SQD	O47-C45-C46-O48
27	D	409	LHG	C11-C10-C9-C8
22	B	613	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	A	413	SQD	C24-C23-O48-C46
22	c	906	CLA	C4-C3-C5-C6
27	d	401	LHG	C25-C26-C27-C28
26	A	411	PL9	C13-C14-C16-C17
26	D	406	PL9	C43-C44-C46-C47
22	b	611	CLA	C11-C12-C13-C14
23	D	402	PHO	C6-C7-C8-C9
25	j	101	LMG	C32-C33-C34-C35
27	l	102	LHG	C1-C2-C3-O3
35	h	102	DGD	O1G-C1G-C2G-C3G
27	d	407	LHG	C28-C29-C30-C31
25	D	412	LMG	C21-C22-C23-C24
35	C	519	DGD	CDA-CEA-CFA-CGA
22	B	605	CLA	O2A-C1-C2-C3
25	C	531	LMG	C17-C18-C19-C20
36	e	101	HEM	CAA-CBA-CGA-O2A
34	v	203	HTG	S1-C1'-C2'-C3'
22	B	616	CLA	C4-C3-C5-C6
22	A	408	CLA	C12-C13-C15-C16
22	C	506	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	508	CLA	C11-C12-C13-C15
22	C	510	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C12-C13-C15
22	c	903	CLA	C12-C13-C15-C16
22	c	904	CLA	C6-C7-C8-C10
34	B	627	HTG	C4'-C5'-C6'-C7'
28	a	418	SQD	C10-C11-C12-C13
29	E	101	LMT	O1'-C1-C2-C3
35	H	102	DGD	C5A-C6A-C7A-C8A
24	K	101	BCR	C9-C10-C11-C12
27	l	102	LHG	C23-C24-C25-C26
22	d	402	CLA	C15-C16-C17-C18
35	c	917	DGD	CAA-CBA-CCA-CDA
27	l	102	LHG	C17-C18-C19-C20
26	a	415	PL9	C3-C7-C8-C9
35	C	517	DGD	C8A-C9A-CAA-CBA
26	d	405	PL9	C35-C34-C36-C37
28	l	101	SQD	C11-C10-C9-C8
22	b	602	CLA	C2-C3-C5-C6
22	c	913	CLA	C2B-C3B-CAB-CBB
22	c	911	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	a	412	CLA	C10-C11-C12-C13
37	h	101	RRX	C19-C20-C21-C22
34	v	203	HTG	C4-C5-C6-O6
27	d	407	LHG	C11-C12-C13-C14
28	b	621	SQD	C34-C35-C36-C37
29	a	419	LMT	C4-C5-C6-C7
35	C	519	DGD	C4B-C5B-C6B-C7B
35	C	519	DGD	C6B-C7B-C8B-C9B
26	D	406	PL9	C34-C36-C37-C38
35	c	917	DGD	C6A-C7A-C8A-C9A
26	A	411	PL9	C15-C14-C16-C17
35	H	102	DGD	CCA-CDA-CEA-CFA
35	c	919	DGD	O1A-C1A-O1G-C1G
35	D	407	DGD	C6A-C7A-C8A-C9A
22	B	613	CLA	C10-C11-C12-C13
25	c	920	LMG	C22-C23-C24-C25
22	C	510	CLA	C2A-CAA-CBA-CGA
34	C	521	HTG	O5-C5-C6-O6
35	H	102	DGD	O1B-C1B-C2B-C3B
24	a	413	BCR	C5-C6-C7-C8
24	y	101	BCR	C23-C24-C25-C30
22	b	616	CLA	C8-C10-C11-C12
27	D	411	LHG	C26-C27-C28-C29
35	C	519	DGD	C8A-C9A-CAA-CBA
28	a	414	SQD	C10-C11-C12-C13
22	C	511	CLA	C4-C3-C5-C6
28	f	101	SQD	C45-C44-O6-C1
22	B	610	CLA	C2-C3-C5-C6
36	e	101	HEM	C2A-CAA-CBA-CGA
35	c	917	DGD	C5D-C6D-O5D-C1E
27	D	409	LHG	C19-C20-C21-C22
35	D	407	DGD	C9B-CAB-CBB-CCB
25	A	410	LMG	C15-C16-C17-C18
35	C	518	DGD	C8A-C9A-CAA-CBA
39	V	202	HEC	CAD-CBD-CGD-O2D
28	b	621	SQD	C44-C45-O47-C7
22	b	608	CLA	C4B-C3B-CAB-CBB
28	A	413	SQD	O10-C23-O48-C46
22	C	511	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C15
25	i	101	LMG	O10-C28-C29-C30
28	D	408	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
29	c	931	LMT	O1'-C1-C2-C3
27	D	410	LHG	C35-C36-C37-C38
22	b	607	CLA	C16-C17-C18-C20
22	b	609	CLA	C16-C17-C18-C19
22	d	402	CLA	C16-C17-C18-C19
26	A	411	PL9	C2-C3-C7-C8
34	C	532	HTG	C2'-C1'-S1-C1
34	b	632	HTG	C2'-C1'-S1-C1
22	c	913	CLA	CAA-CBA-CGA-O2A
35	c	917	DGD	O2G-C1B-C2B-C3B
22	B	604	CLA	C4-C3-C5-C6
22	a	412	CLA	C4-C3-C5-C6
39	v	202	HEC	CAD-CBD-CGD-O2D
22	b	616	CLA	C2-C3-C5-C6
26	d	405	PL9	C33-C34-C36-C37
22	B	604	CLA	C11-C10-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	C	511	CLA	C11-C10-C8-C9
22	C	514	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	b	609	CLA	C11-C12-C13-C14
22	c	907	CLA	C11-C12-C13-C14
22	c	909	CLA	C11-C12-C13-C14
22	c	910	CLA	C11-C12-C13-C14
29	c	931	LMT	C9-C10-C11-C12
22	b	616	CLA	C3A-C2A-CAA-CBA
27	d	408	LHG	C27-C28-C29-C30
22	C	511	CLA	O1A-CGA-O2A-C1
25	j	101	LMG	C40-C41-C42-C43
22	A	405	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	B	608	CLA	CAD-CBD-CGD-O2D
22	B	611	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	C	511	CLA	CAD-CBD-CGD-O2D
22	D	404	CLA	CAD-CBD-CGD-O2D
22	a	407	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	b	611	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	c	906	CLA	CAD-CBD-CGD-O2D
22	c	914	CLA	CAD-CBD-CGD-O2D
22	c	911	CLA	CBA-CGA-O2A-C1
22	c	903	CLA	C16-C17-C18-C20
27	D	411	LHG	C31-C32-C33-C34
22	C	514	CLA	C10-C11-C12-C13
22	c	913	CLA	C10-C11-C12-C13
35	D	407	DGD	CBB-CCB-CDB-CEB
22	B	602	CLA	CAA-CBA-CGA-O2A
25	d	409	LMG	O8-C28-C29-C30
28	a	414	SQD	O47-C7-C8-C9
29	T	102	LMT	C7-C8-C9-C10
25	D	412	LMG	C34-C35-C36-C37
22	a	408	CLA	C16-C17-C18-C20
39	V	202	HEC	CAD-CBD-CGD-O1D
39	v	202	HEC	CAD-CBD-CGD-O1D
22	C	509	CLA	C5-C6-C7-C8
22	B	616	CLA	C2-C3-C5-C6
24	Y	101	BCR	C17-C18-C19-C20
27	d	408	LHG	C17-C18-C19-C20
25	C	520	LMG	O1-C7-C8-C9
28	A	413	SQD	C44-C45-C46-O48
28	l	101	SQD	O6-C44-C45-C46
35	c	919	DGD	O6D-C5D-C6D-O5D
27	C	522	LHG	O6-C4-C5-O7
27	l	102	LHG	O6-C4-C5-O7
28	l	101	SQD	O47-C7-C8-C9
34	D	415	HTG	C4-C5-C6-O6
25	A	410	LMG	C40-C41-C42-C43
23	a	411	PHO	C5-C6-C7-C8
22	D	404	CLA	O2A-C1-C2-C3
22	d	402	CLA	O2A-C1-C2-C3
35	C	518	DGD	C2B-C3B-C4B-C5B
22	C	513	CLA	CAA-CBA-CGA-O2A
35	d	406	DGD	C2D-C1D-O3G-C3G
25	B	621	LMG	C20-C21-C22-C23
22	b	604	CLA	CBD-CGD-O2D-CED
27	D	409	LHG	C30-C31-C32-C33
22	A	406	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O2D
22	C	503	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	C	511	CLA	CHA-CBD-CGD-O1D
22	D	401	CLA	CHA-CBD-CGD-O2D
22	a	408	CLA	CHA-CBD-CGD-O1D
22	a	409	CLA	CHA-CBD-CGD-O2D
22	b	607	CLA	CHA-CBD-CGD-O2D
22	b	612	CLA	CHA-CBD-CGD-O2D
22	b	617	CLA	CHA-CBD-CGD-O2D
22	c	913	CLA	CHA-CBD-CGD-O1D
26	d	405	PL9	C36-C37-C38-C39
35	d	406	DGD	C8A-C9A-CAA-CBA
25	B	621	LMG	C16-C17-C18-C19
25	D	412	LMG	O7-C8-C9-O8
35	h	102	DGD	C7B-C8B-C9B-CAB
22	c	902	CLA	C13-C15-C16-C17
27	a	423	LHG	C12-C13-C14-C15
22	A	405	CLA	C2C-C3C-CAC-CBC
28	C	501	SQD	O47-C7-C8-C9
22	d	402	CLA	C16-C17-C18-C20
23	A	407	PHO	CHA-CBD-CGD-O1D
22	b	613	CLA	CBA-CGA-O2A-C1
34	B	627	HTG	C4-C5-C6-O6
35	C	519	DGD	C6A-C7A-C8A-C9A
22	c	910	CLA	C11-C12-C13-C15
26	D	406	PL9	C28-C29-C31-C32
22	b	611	CLA	C16-C17-C18-C19
26	d	405	PL9	C4-C3-C7-C8
35	H	102	DGD	C8A-C9A-CAA-CBA
22	B	602	CLA	C6-C7-C8-C9
22	B	603	CLA	C6-C7-C8-C9
22	B	604	CLA	C6-C7-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	a	412	CLA	C14-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C10-C8-C9
22	b	609	CLA	C11-C10-C8-C9
22	c	903	CLA	C14-C13-C15-C16
22	c	910	CLA	C6-C7-C8-C9
22	D	401	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	b	617	CLA	C2B-C3B-CAB-CBB
25	c	920	LMG	C40-C41-C42-C43
29	E	101	LMT	C4-C5-C6-C7
22	C	511	CLA	CAA-CBA-CGA-O2A
22	b	604	CLA	C2A-CAA-CBA-CGA
26	D	406	PL9	C11-C12-C13-C14
22	b	614	CLA	CAA-CBA-CGA-O2A
22	a	412	CLA	C8-C10-C11-C12
35	h	102	DGD	CAB-CBB-CCB-CDB
22	C	513	CLA	CAA-CBA-CGA-O1A
35	c	917	DGD	O1B-C1B-C2B-C3B
22	C	514	CLA	C4-C3-C5-C6
25	c	920	LMG	C13-C14-C15-C16
22	C	503	CLA	C15-C16-C17-C18
29	a	419	LMT	C5-C6-C7-C8
22	c	913	CLA	CAA-CBA-CGA-O1A
24	K	101	BCR	C11-C12-C13-C14
22	B	613	CLA	CBA-CGA-O2A-C1
22	C	511	CLA	CBA-CGA-O2A-C1
22	b	602	CLA	C1A-C2A-CAA-CBA
22	A	405	CLA	C4C-C3C-CAC-CBC
27	D	410	LHG	C25-C26-C27-C28
22	b	614	CLA	C2-C1-O2A-CGA
28	l	101	SQD	C16-C17-C18-C19
25	d	409	LMG	O10-C28-C29-C30
28	b	621	SQD	O6-C44-C45-C46
35	h	102	DGD	C1G-C2G-C3G-O3G
27	D	411	LHG	C30-C31-C32-C33
29	Z	101	LMT	C7-C8-C9-C10
26	D	406	PL9	C45-C44-C46-C47
22	C	502	CLA	CAA-CBA-CGA-O2A
29	c	931	LMT	C5-C6-C7-C8
35	d	406	DGD	CDA-CEA-CFA-CGA
22	b	611	CLA	C4B-C3B-CAB-CBB
27	D	410	LHG	C4-O6-P-O5
27	L	101	LHG	C4-O6-P-O4
27	d	407	LHG	C4-O6-P-O5
28	a	414	SQD	C19-C20-C21-C22
22	B	602	CLA	CAA-CBA-CGA-O1A
24	c	915	BCR	C23-C24-C25-C30
27	C	522	LHG	C27-C28-C29-C30
22	b	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	CAA-CBA-CGA-O1A
22	B	611	CLA	C4C-C3C-CAC-CBC
22	c	911	CLA	CAA-CBA-CGA-O2A
22	B	607	CLA	C16-C17-C18-C19
25	B	621	LMG	O8-C28-C29-C30
28	l	101	SQD	O49-C7-C8-C9
26	A	411	PL9	C20-C19-C21-C22
26	D	406	PL9	C35-C34-C36-C37
22	A	406	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	CAD-CBD-CGD-O1D
22	c	907	CLA	CAD-CBD-CGD-O1D
28	C	501	SQD	C5-C6-S-O7
28	a	418	SQD	C5-C6-S-O9
22	C	511	CLA	CAA-CBA-CGA-O1A
22	C	514	CLA	C8-C10-C11-C12
22	C	508	CLA	C11-C12-C13-C14
22	D	404	CLA	C11-C10-C8-C9
22	c	905	CLA	C6-C7-C8-C9
22	c	910	CLA	C14-C13-C15-C16
28	C	501	SQD	C32-C33-C34-C35
25	C	531	LMG	O8-C28-C29-C30
27	D	411	LHG	O8-C23-C24-C25
35	C	519	DGD	O1G-C1A-C2A-C3A
27	a	423	LHG	C30-C31-C32-C33
27	l	102	LHG	C11-C12-C13-C14
22	B	608	CLA	C13-C15-C16-C17
35	c	919	DGD	CCA-CDA-CEA-CFA
22	b	602	CLA	CAA-CBA-CGA-O2A
27	D	409	LHG	O7-C7-C8-C9
27	L	101	LHG	O7-C7-C8-C9
28	a	418	SQD	O48-C23-C24-C25
22	B	606	CLA	C10-C11-C12-C13
28	C	501	SQD	O49-C7-C8-C9
27	D	411	LHG	C11-C12-C13-C14
22	B	610	CLA	C4-C3-C5-C6
26	D	406	PL9	C30-C29-C31-C32
22	C	511	CLA	C11-C10-C8-C7
22	D	404	CLA	C11-C10-C8-C7
22	a	412	CLA	C12-C13-C15-C16
22	b	612	CLA	C6-C7-C8-C10
34	v	203	HTG	C2-C1-S1-C1'
35	C	519	DGD	O1A-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
22	d	402	CLA	CAA-CBA-CGA-O2A
27	C	522	LHG	O8-C23-C24-C25
27	a	423	LHG	O8-C23-C24-C25
35	c	918	DGD	O2G-C1B-C2B-C3B
35	c	919	DGD	O1G-C1A-C2A-C3A
24	B	619	BCR	C11-C12-C13-C14
24	C	515	BCR	C21-C22-C23-C24
24	c	915	BCR	C11-C12-C13-C14
22	C	502	CLA	CAA-CBA-CGA-O1A
27	L	101	LHG	O9-C7-C8-C9
28	a	418	SQD	O10-C23-C24-C25
36	E	102	HEM	CAD-CBD-CGD-O1D
22	c	906	CLA	CAA-CBA-CGA-O2A
25	A	410	LMG	O6-C1-O1-C7
35	C	517	DGD	O6E-C1E-O5D-C6D
22	b	613	CLA	O1A-CGA-O2A-C1
25	i	101	LMG	C21-C22-C23-C24
39	v	202	HEC	C4C-C3C-CAC-CBC
35	C	517	DGD	O2G-C1B-C2B-C3B
22	B	611	CLA	C5-C6-C7-C8
27	D	409	LHG	O9-C7-C8-C9
35	c	919	DGD	O1A-C1A-C2A-C3A
22	b	607	CLA	C16-C17-C18-C19
35	H	102	DGD	C3B-C4B-C5B-C6B

There are no ring outliers.

211 monomers are involved in 519 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	V	201	DMS	1	0
31	v	201	DMS	1	0
31	O	311	DMS	3	0
36	E	102	HEM	1	0
29	a	419	LMT	7	0
35	C	518	DGD	1	0
31	B	630	DMS	1	0
22	c	910	CLA	3	0
22	B	603	CLA	1	0
32	A	421[B]	BCT	1	0
31	c	939	DMS	2	0
24	b	620	BCR	3	0
22	C	504	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	J	101	LMG	1	0
29	A	414	LMT	6	0
22	B	611	CLA	6	0
31	c	935	DMS	2	0
24	D	405	BCR	1	0
31	A	419	DMS	2	0
31	b	633	DMS	1	0
31	O	310	DMS	3	0
36	e	101	HEM	6	0
22	c	904	CLA	8	0
22	b	614	CLA	4	0
24	Y	101	BCR	2	0
31	B	635	DMS	1	0
22	c	905	CLA	2	0
22	C	510	CLA	2	0
31	c	927	DMS	1	0
28	A	413	SQD	2	0
28	a	414	SQD	6	0
31	C	540	DMS	1	0
31	B	642	DMS	1	0
31	O	303	DMS	4	0
25	d	409	LMG	4	0
31	b	636	DMS	1	0
35	c	917	DGD	3	0
35	h	102	DGD	2	0
22	b	612	CLA	2	0
31	D	416	DMS	3	0
31	c	934	DMS	2	0
24	C	516	BCR	1	0
34	B	623	HTG	3	0
24	y	101	BCR	3	0
25	A	410	LMG	2	0
31	v	205	DMS	2	0
22	b	617	CLA	2	0
22	B	604	CLA	1	0
29	B	622	LMT	3	0
23	a	411	PHO	8	0
31	c	929	DMS	2	0
22	B	605	CLA	1	0
25	c	920	LMG	1	0
22	B	613	CLA	1	0
31	o	305	DMS	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	L	101	LHG	7	0
22	C	513	CLA	5	0
25	D	412	LMG	5	0
22	C	514	CLA	5	0
31	o	304	DMS	4	0
24	c	916	BCR	6	0
22	C	508	CLA	2	0
22	a	412	CLA	2	0
34	b	627	HTG	1	0
31	c	937	DMS	1	0
22	b	609	CLA	5	0
27	d	407	LHG	1	0
22	C	505	CLA	4	0
25	C	520	LMG	1	0
35	H	102	DGD	2	0
25	b	622	LMG	1	0
31	V	206	DMS	3	0
22	c	911	CLA	2	0
31	c	933	DMS	2	0
31	u	203	DMS	2	0
34	b	632	HTG	2	0
22	c	908	CLA	2	0
31	v	206	DMS	3	0
31	o	302	DMS	1	0
22	B	612	CLA	1	0
26	d	405	PL9	5	0
25	c	930	LMG	3	0
24	A	409	BCR	1	0
31	U	203	DMS	1	0
31	b	638	DMS	9	0
27	a	416	LHG	1	0
34	b	623	HTG	3	0
31	V	212	DMS	11	0
31	v	210	DMS	2	0
31	u	205	DMS	5	0
22	b	610	CLA	4	0
22	d	402	CLA	2	0
22	A	405	CLA	4	0
29	t	101	LMT	2	0
22	b	608	CLA	7	0
34	D	415	HTG	9	0
25	j	101	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	501	SQD	6	0
22	b	603	CLA	2	0
28	l	101	SQD	1	0
25	i	101	LMG	3	0
31	C	536	DMS	1	0
24	b	618	BCR	7	0
24	d	404	BCR	2	0
31	B	641	DMS	1	0
27	d	408	LHG	5	0
22	D	403	CLA	1	0
31	B	629	DMS	1	0
22	B	607	CLA	5	0
22	a	408	CLA	4	0
22	b	606	CLA	5	0
28	b	621	SQD	2	0
22	b	604	CLA	1	0
29	c	931	LMT	1	0
22	c	902	CLA	4	0
24	c	915	BCR	2	0
31	u	202	DMS	2	0
27	a	423	LHG	6	0
31	O	306	DMS	2	0
25	B	621	LMG	3	0
35	c	919	DGD	4	0
31	i	106	DMS	1	0
22	D	401	CLA	4	0
31	f	103	DMS	4	0
31	o	307	DMS	1	0
22	A	408	CLA	3	0
22	a	409	CLA	3	0
35	c	918	DGD	3	0
22	b	605	CLA	2	0
34	C	532	HTG	1	0
22	c	906	CLA	2	0
22	c	912	CLA	4	0
25	C	531	LMG	2	0
31	A	420	DMS	2	0
22	b	615	CLA	5	0
31	c	925	DMS	2	0
31	B	638	DMS	5	0
34	C	521	HTG	1	0
31	c	942	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	616	CLA	2	0
22	d	403	CLA	1	0
31	b	630	DMS	2	0
29	Z	101	LMT	1	0
22	a	407	CLA	2	0
27	D	409	LHG	7	0
34	l	106	HTG	3	0
31	c	924	DMS	7	0
27	D	411	LHG	8	0
22	b	602	CLA	5	0
37	H	101	RRX	4	0
31	a	401	DMS	1	0
31	d	411	DMS	3	0
24	b	619	BCR	1	0
31	B	633	DMS	1	0
27	l	102	LHG	3	0
24	a	413	BCR	1	0
31	V	205	DMS	2	0
34	b	626	HTG	2	0
31	o	303	DMS	2	0
26	D	406	PL9	5	0
29	T	102	LMT	1	0
23	D	402	PHO	5	0
31	O	312	DMS	4	0
31	V	207	DMS	3	0
22	C	511	CLA	3	0
31	B	631	DMS	4	0
22	C	509	CLA	3	0
24	B	620	BCR	1	0
35	C	519	DGD	2	0
31	b	629	DMS	1	0
27	A	412	LHG	1	0
31	B	628	DMS	3	0
28	f	101	SQD	1	0
24	B	618	BCR	3	0
22	B	614	CLA	2	0
29	E	101	LMT	1	0
31	O	304	DMS	6	0
22	B	610	CLA	1	0
22	c	913	CLA	3	0
22	c	909	CLA	2	0
39	v	202	HEC	1	0

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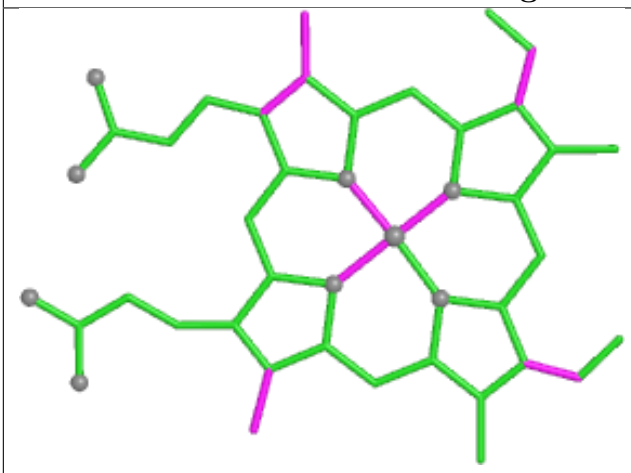
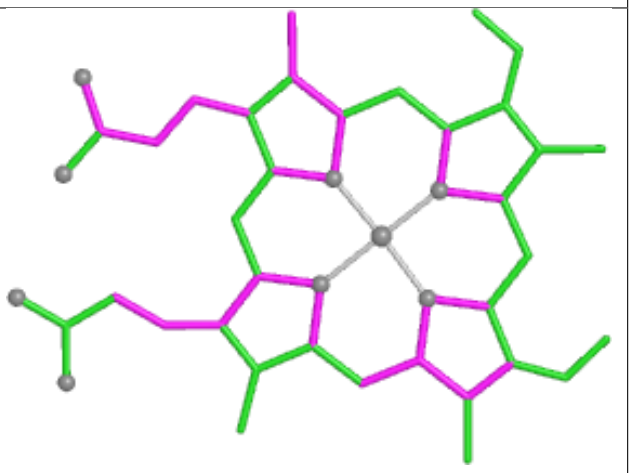
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	C	530	DMS	2	0
31	o	308	DMS	4	0
22	c	914	CLA	2	0
22	b	611	CLA	4	0
31	B	636	DMS	1	0
24	C	515	BCR	4	0
31	c	940	DMS	2	0
31	H	103	DMS	1	0
31	B	632	DMS	1	0
22	B	606	CLA	7	0
31	l	104	DMS	1	0
22	C	503	CLA	5	0
22	C	507	CLA	5	0
22	A	406	CLA	3	0
27	D	410	LHG	3	0
23	a	410	PHO	2	0
31	B	640	DMS	1	0
34	D	414	HTG	2	0
31	a	425	DMS	7	0
24	k	101	BCR	2	0
26	a	415	PL9	10	0
31	d	415	DMS	5	0
22	c	903	CLA	3	0
27	C	522	LHG	1	0
37	h	101	RRX	8	0
22	C	506	CLA	1	0
31	C	527	DMS	2	0
22	b	607	CLA	1	0
22	B	608	CLA	6	0
26	A	411	PL9	10	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.

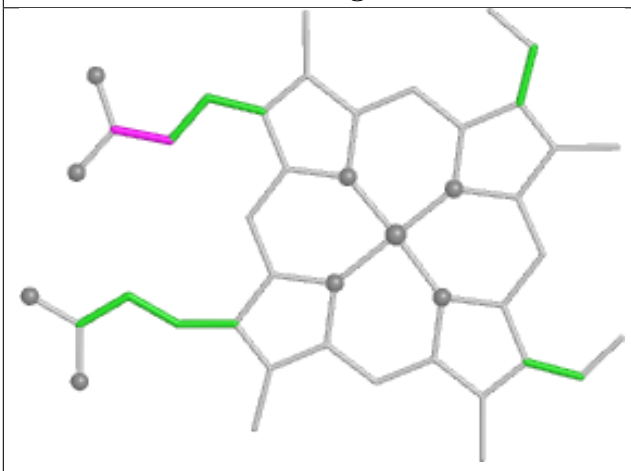
Ligand HEM E 102



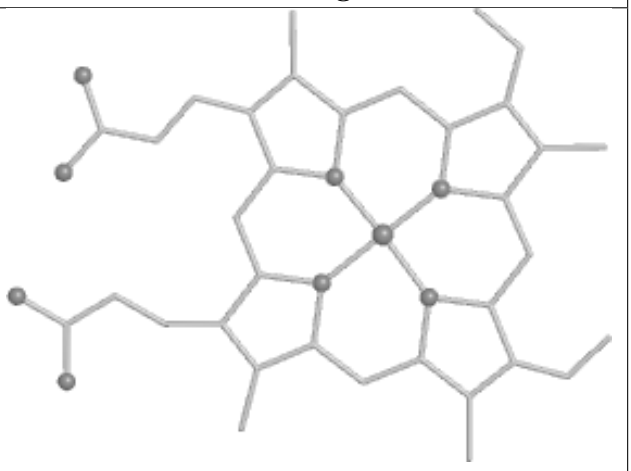
Bond lengths



Bond angles

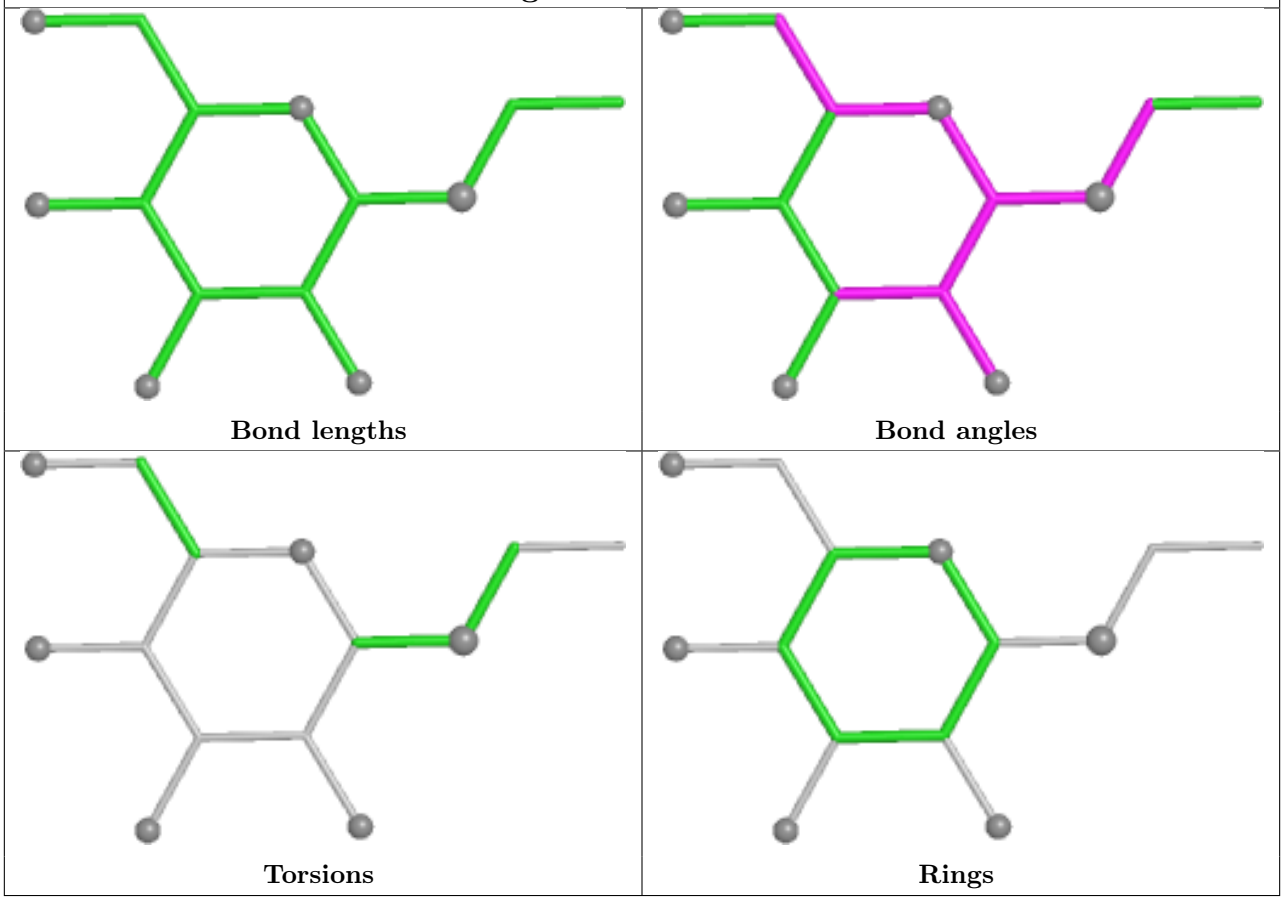


Torsions

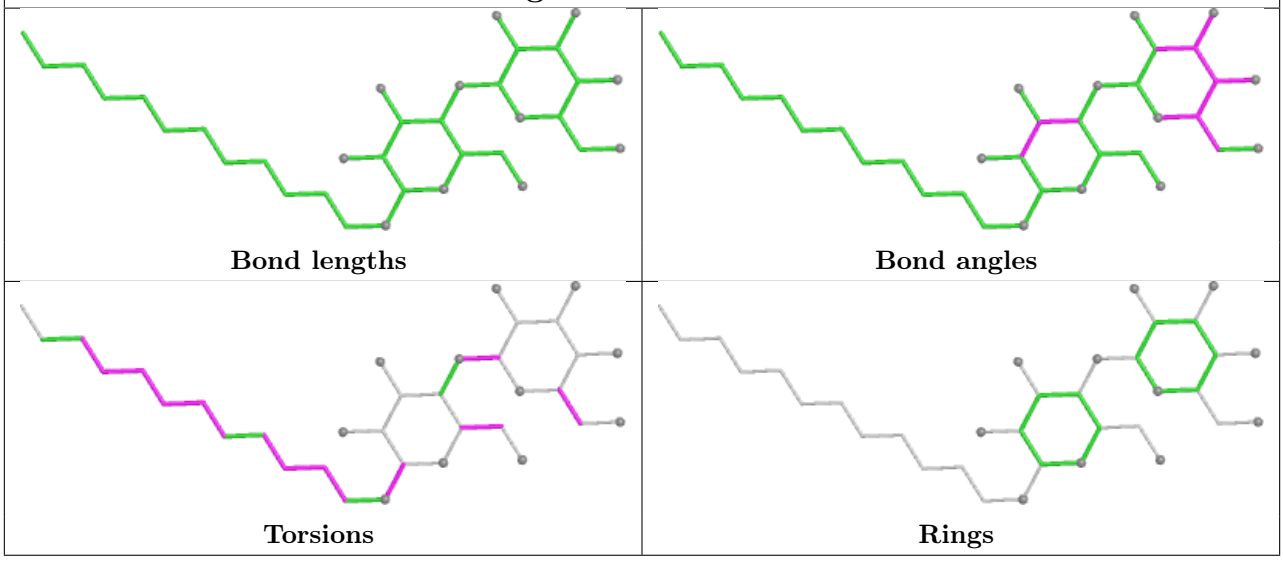


Rings

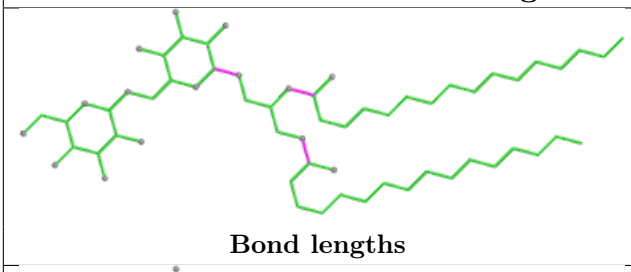
Ligand HTG V 203



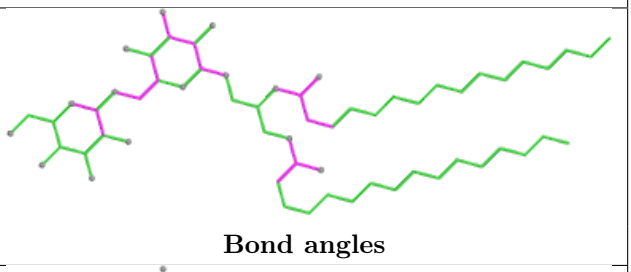
Ligand LMT a 419



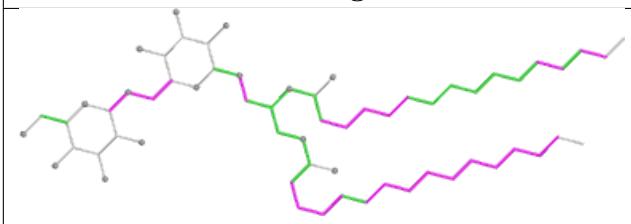
Ligand DGD C 518



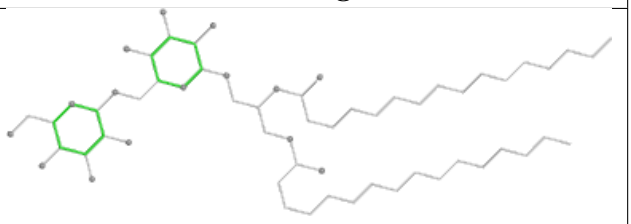
Bond lengths



Bond angles

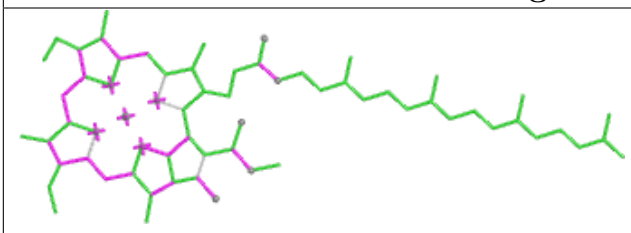


Torsions



Rings

Ligand CLA c 910



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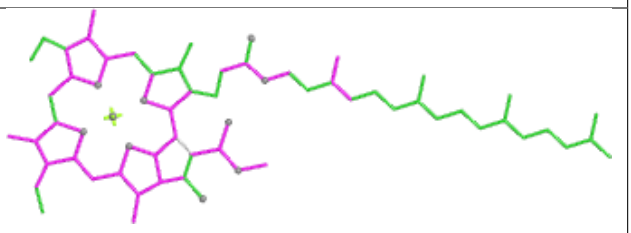
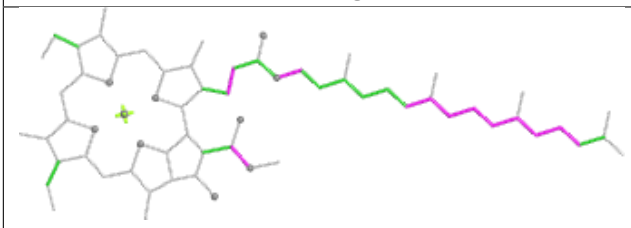


Bond angles



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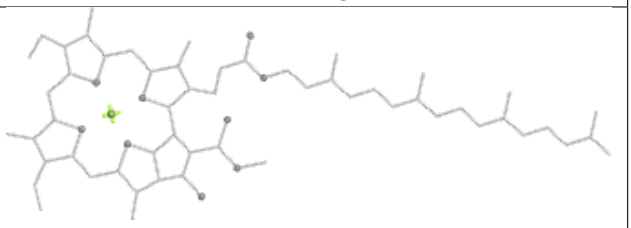
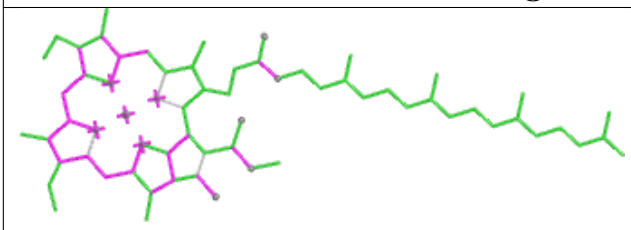


Rings

Ligand CLA B 603



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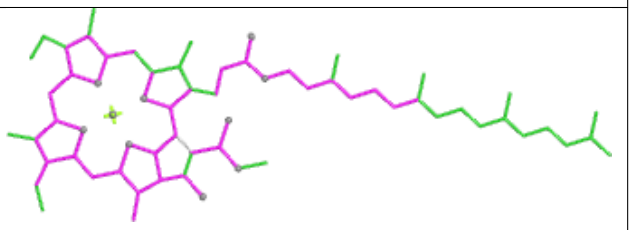
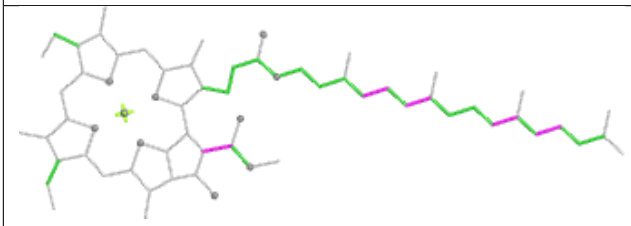
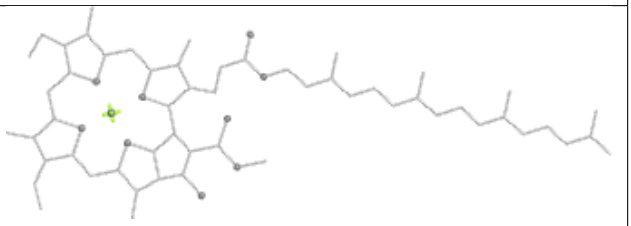


Bond angles

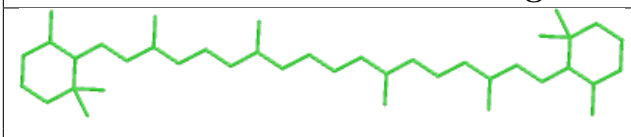


Torsions



Rings

Ligand BCR b 620



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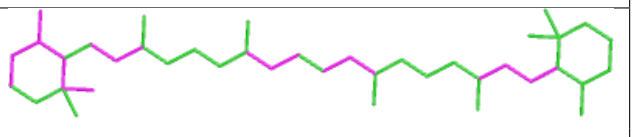
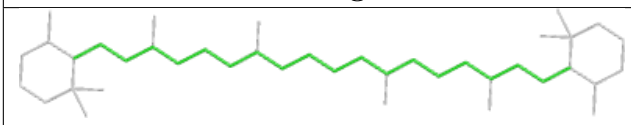


Bond angles



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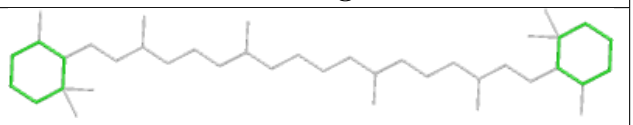
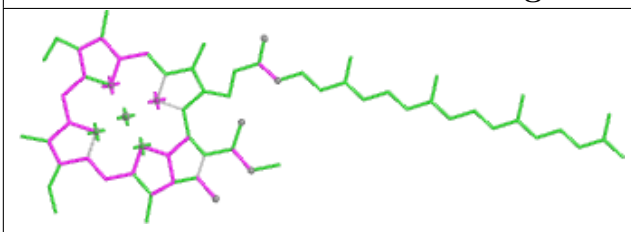


Rings

Ligand CLA B 602



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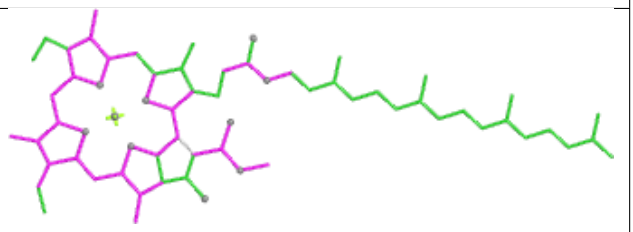
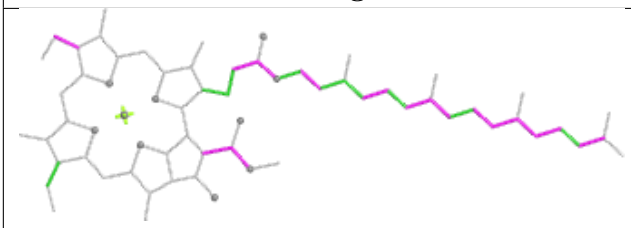


Bond angles



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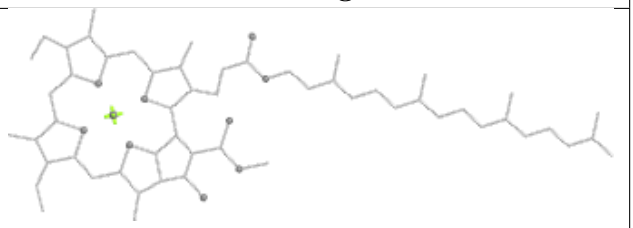
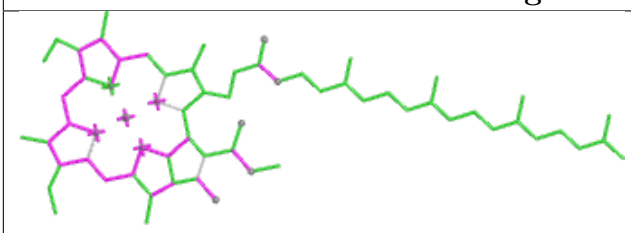


Rings

Ligand CLA C 504



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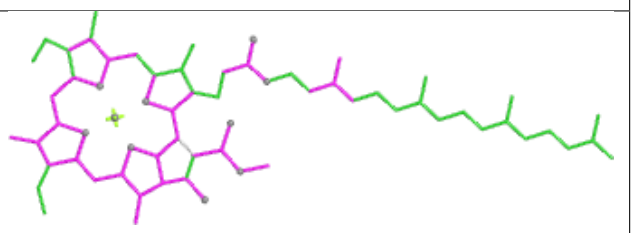
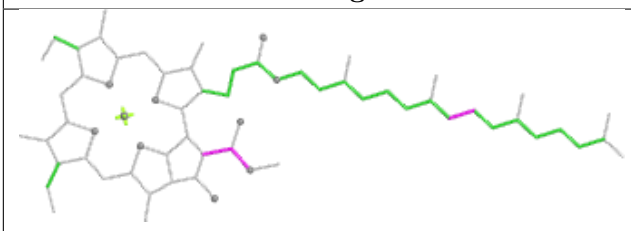


Bond angles



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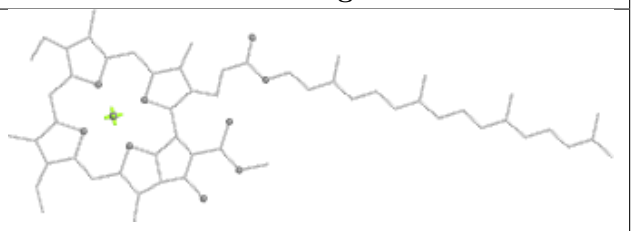
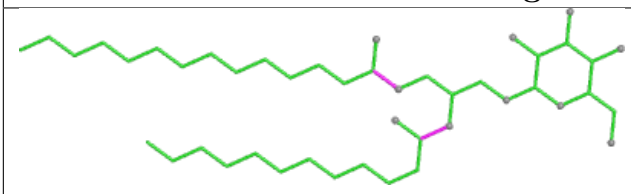


Rings

Ligand LMG J 101



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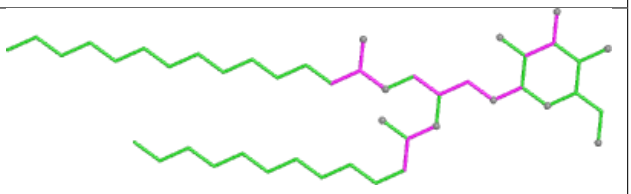
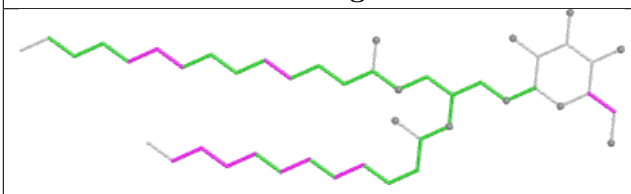


Bond angles



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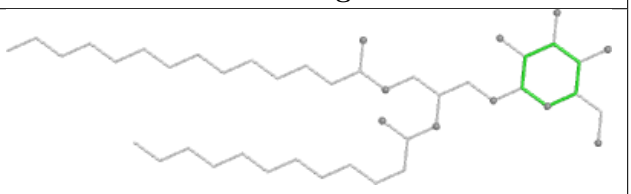
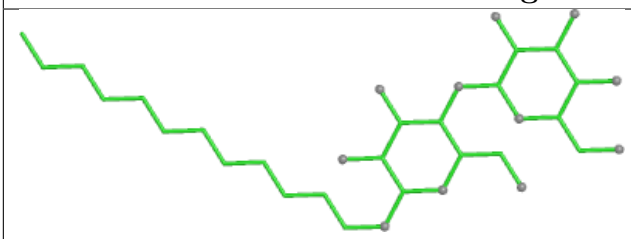


Rings

Ligand LMT A 414



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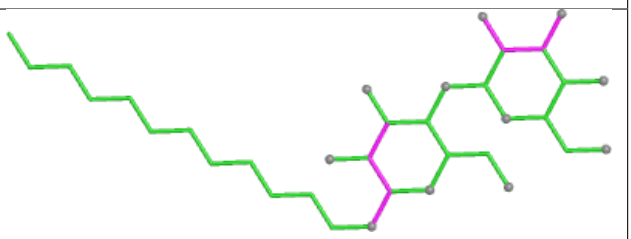
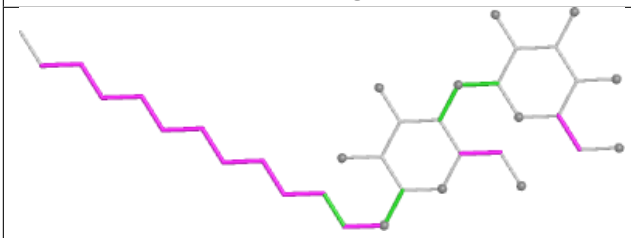


Bond angles



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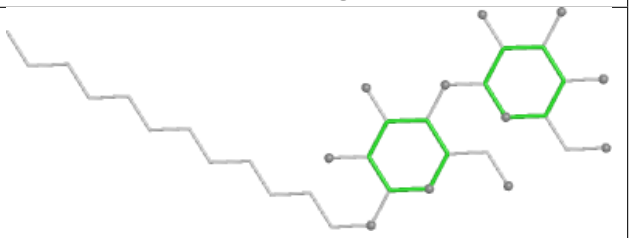
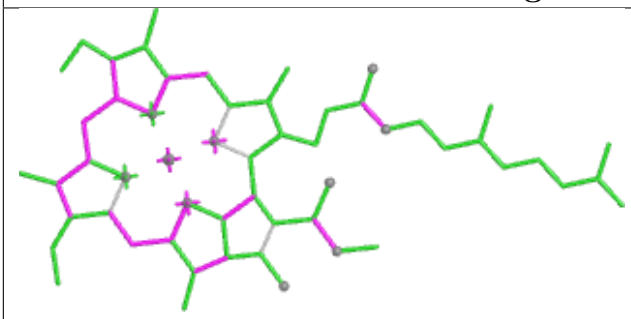
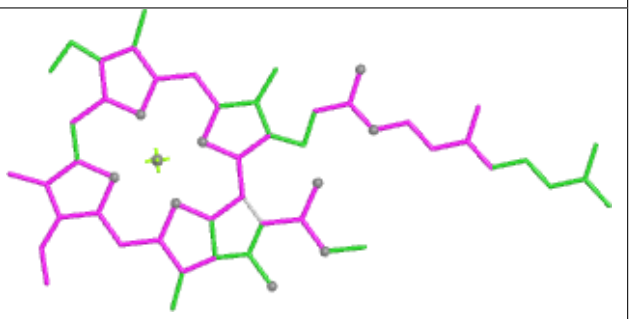
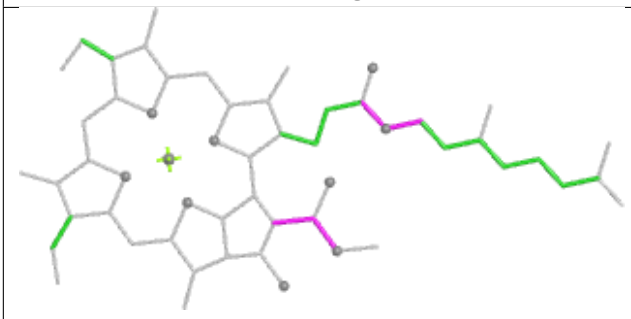
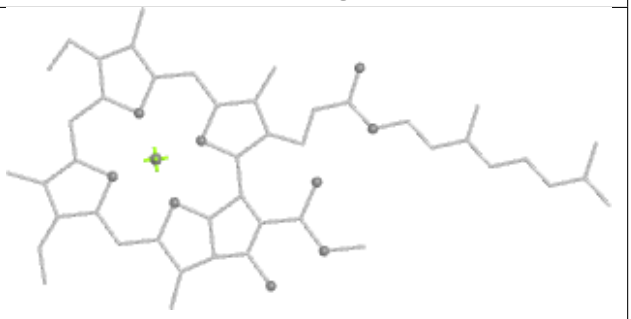
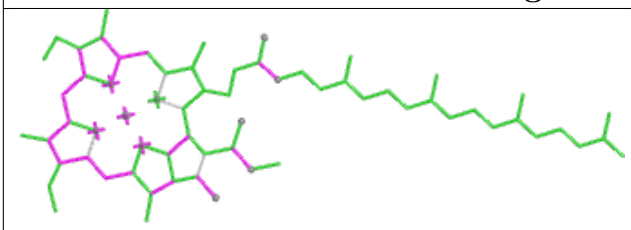
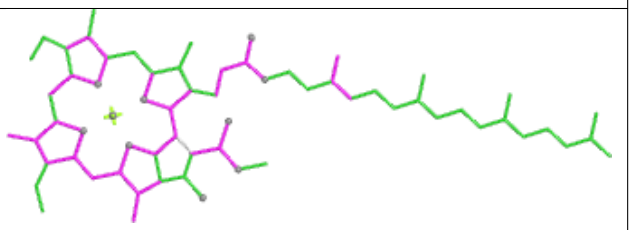
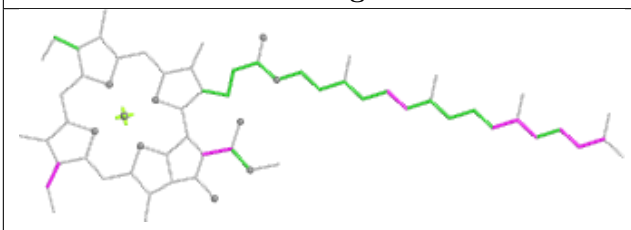
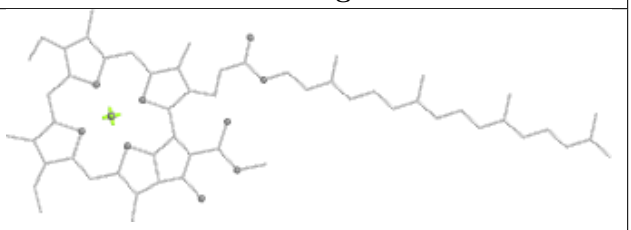
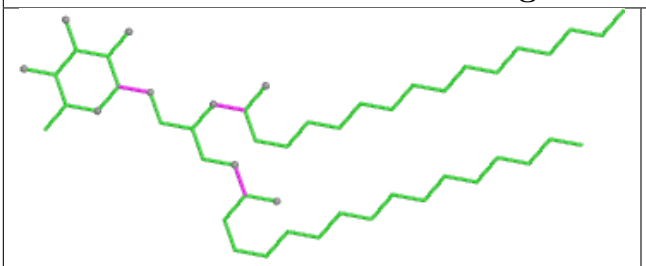


Rings

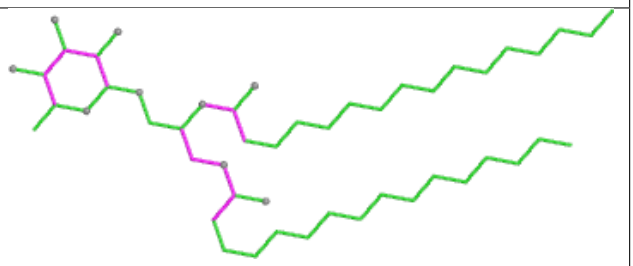
Ligand CLA B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

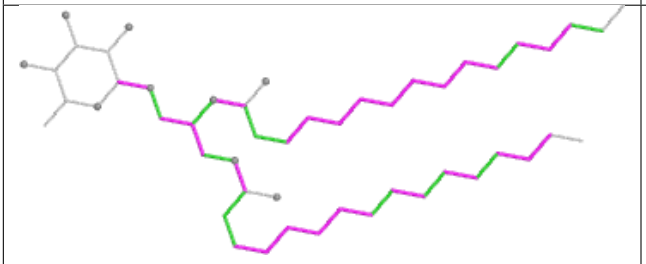
Ligand DGD D 407



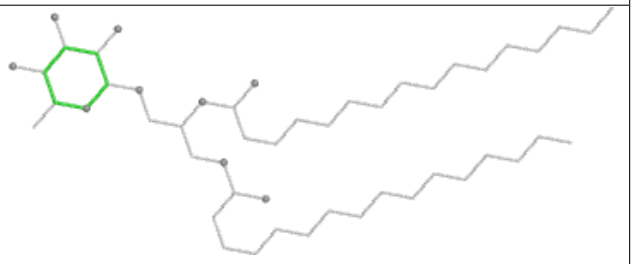
Bond lengths



Bond angles



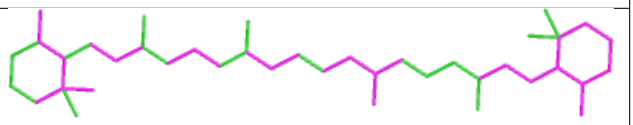
Torsions



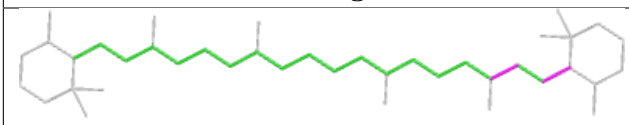
Rings

Ligand BCR D 405

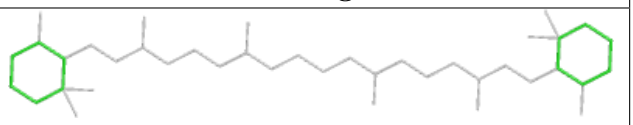
Bond lengths



Bond angles

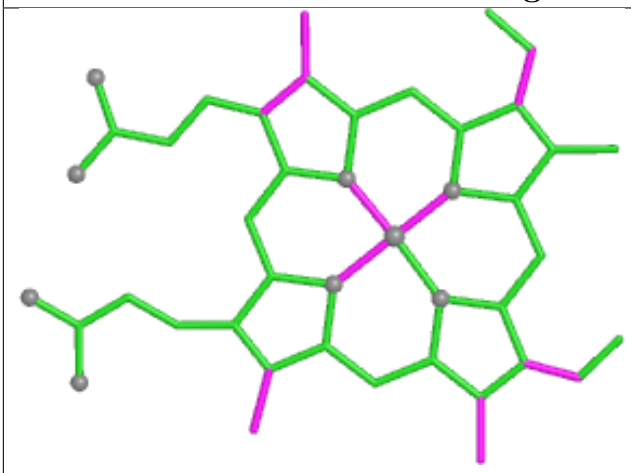


Torsions

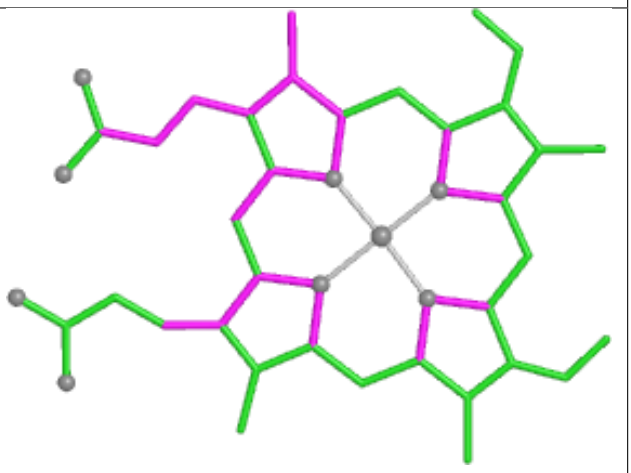


Rings

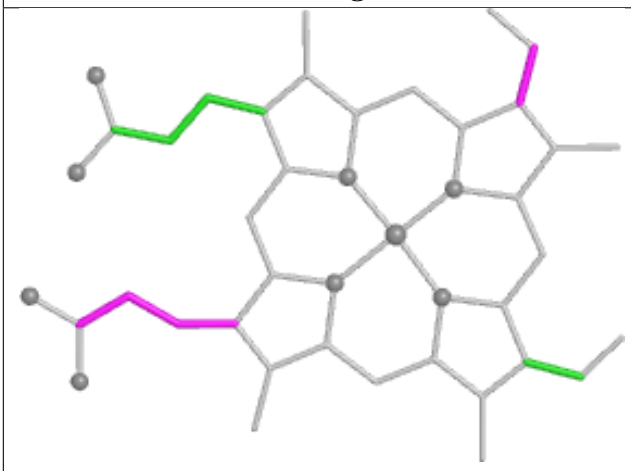
Ligand HEM e 101



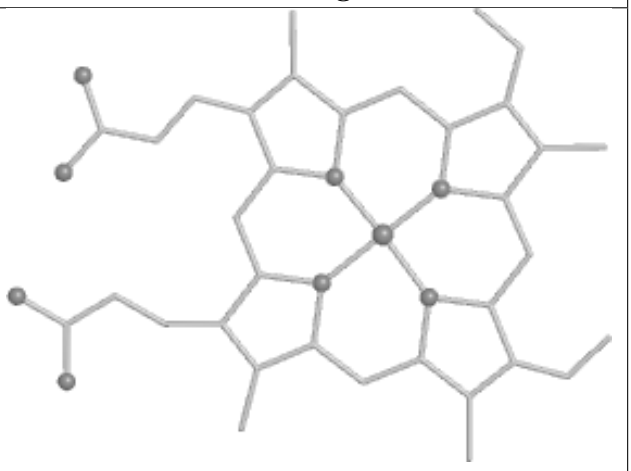
Bond lengths



Bond angles

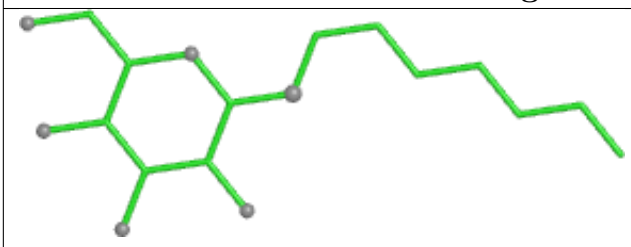


Torsions

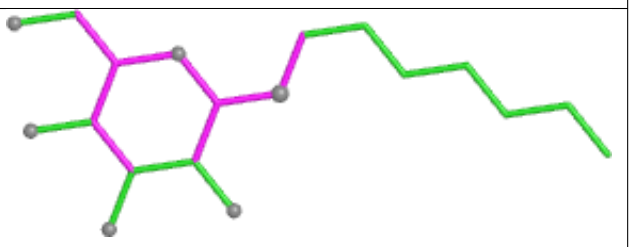


Rings

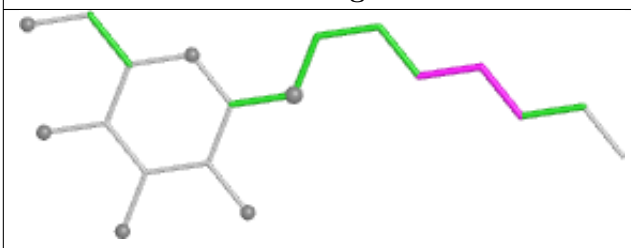
Ligand HTG B 626



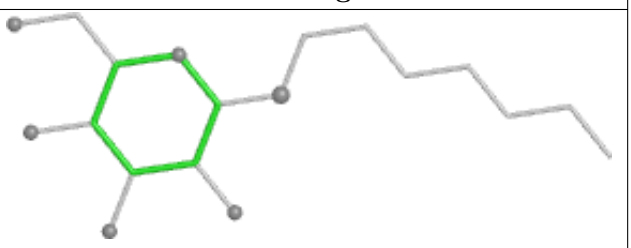
Bond lengths



Bond angles

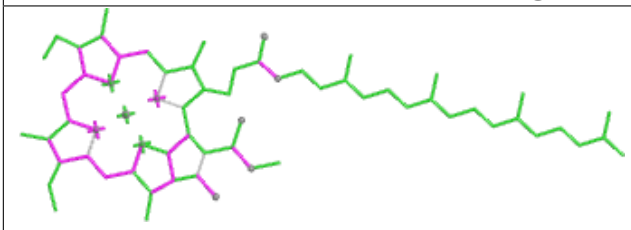


Torsions

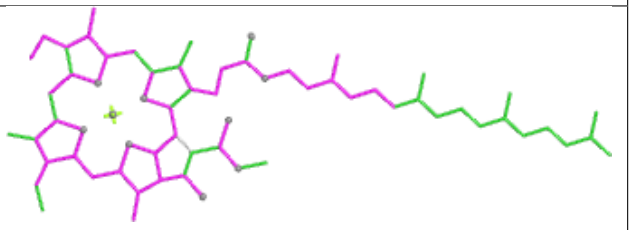


Rings

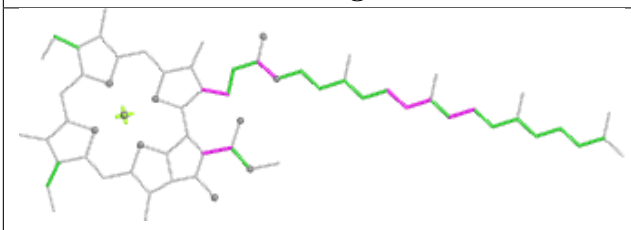
Ligand CLA c 904



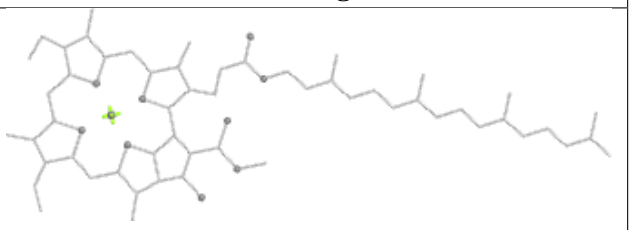
Bond lengths



Bond angles

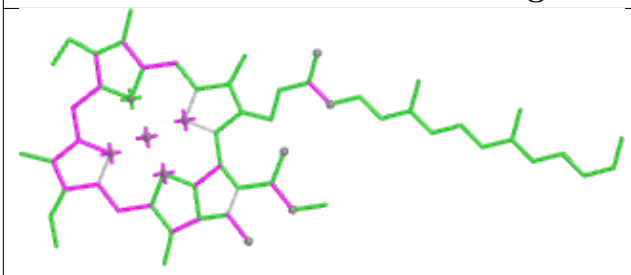


Torsions

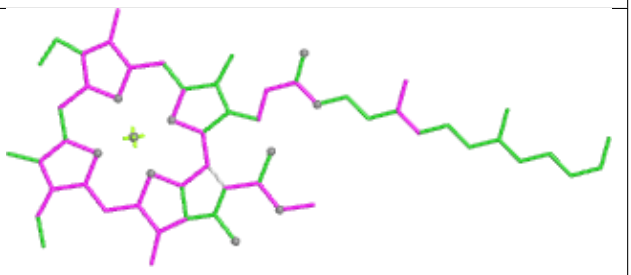


Rings

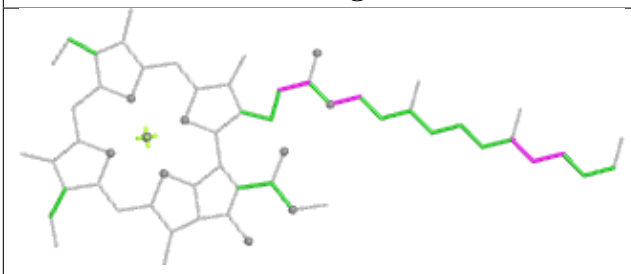
Ligand CLA b 614



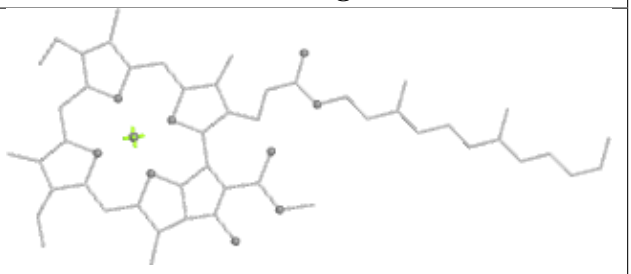
Bond lengths



Bond angles



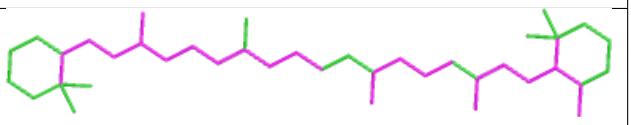
Torsions



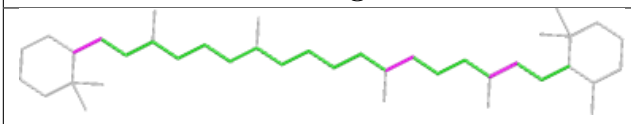
Rings

Ligand BCR Y 101

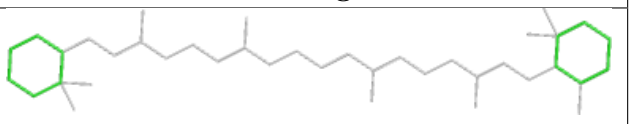
Bond lengths



Bond angles

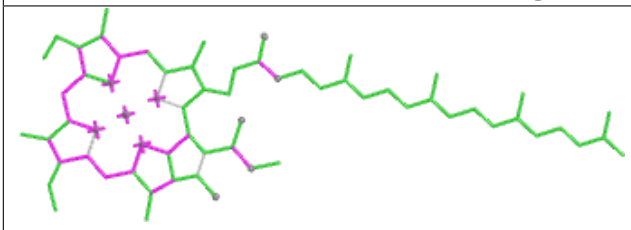


Torsions

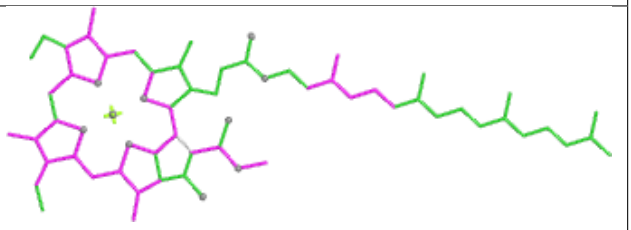


Rings

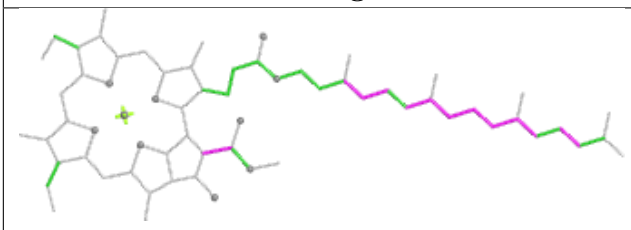
Ligand CLA c 905



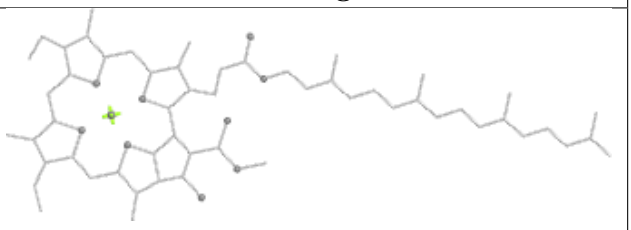
Bond lengths



Bond angles

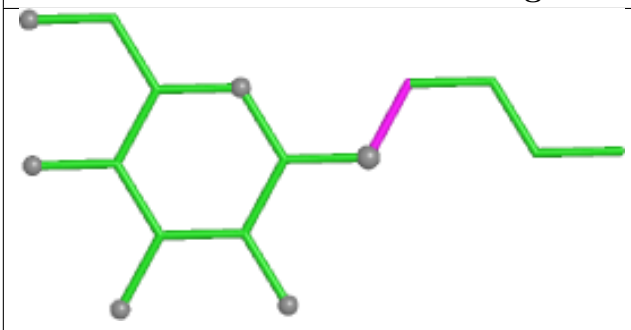


Torsions



Rings

Ligand HTG v 203



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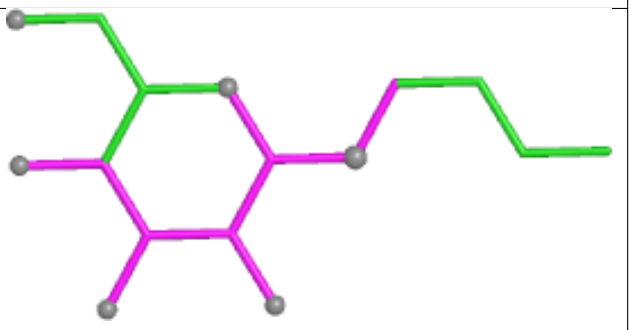
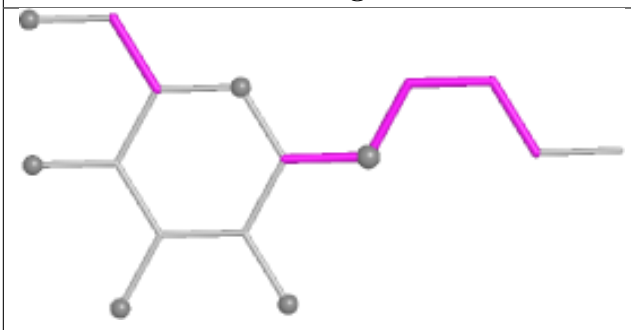
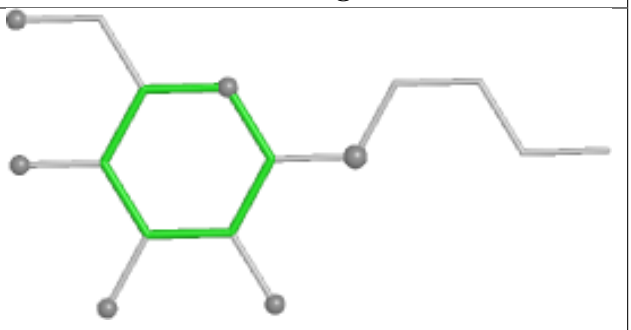


Bond angles

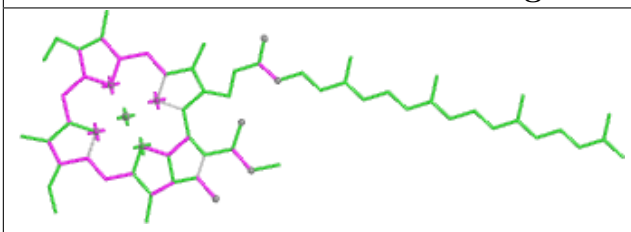


Torsions



Rings

Ligand CLA C 510



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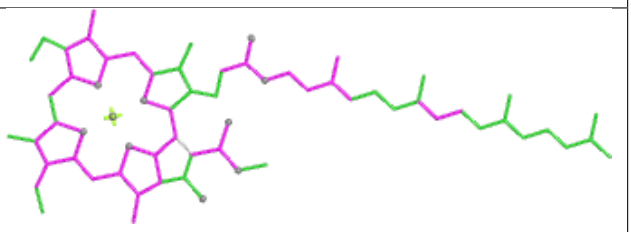
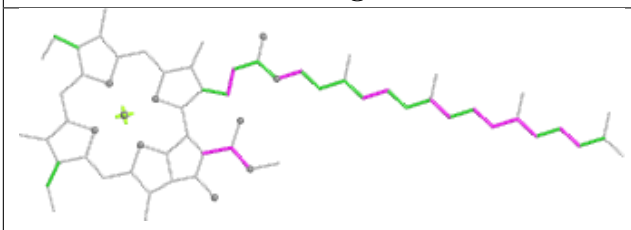


Bond angles



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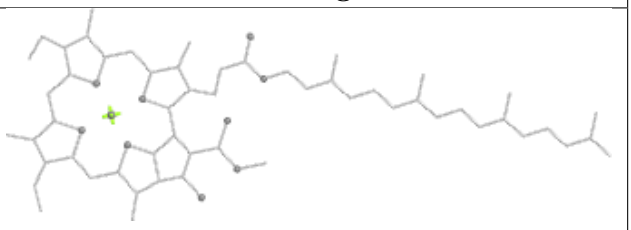
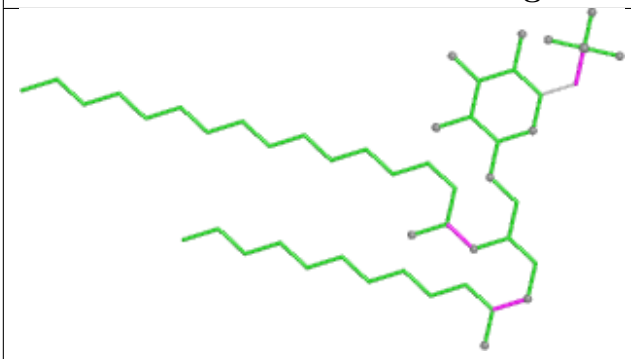


Rings

Ligand SQD A 413



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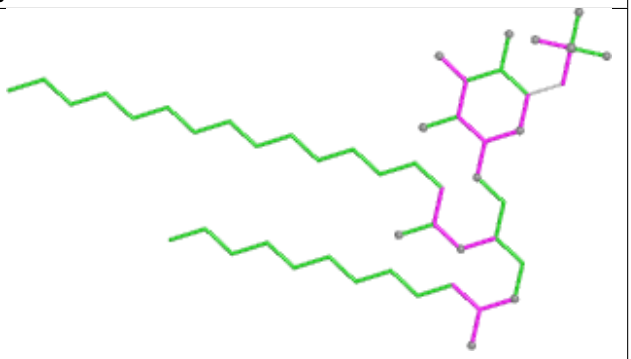
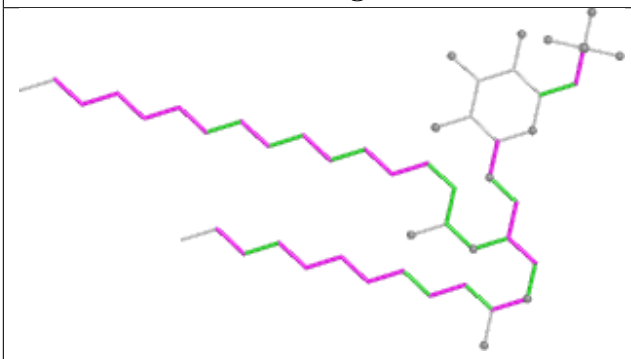


Bond angles



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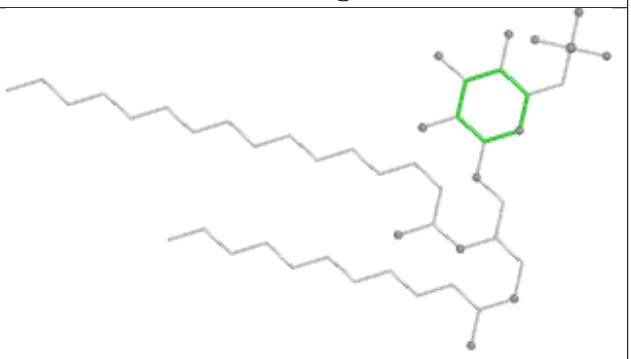
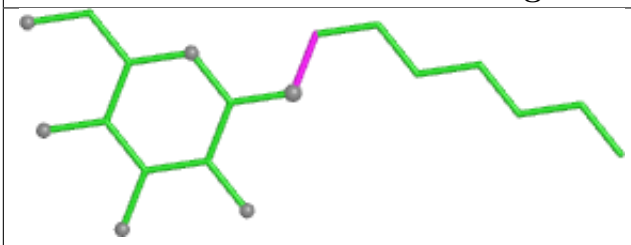


Rings

Ligand HTG b 624



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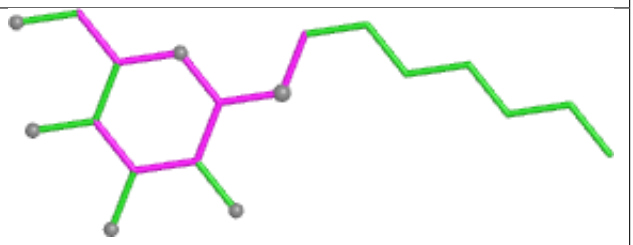
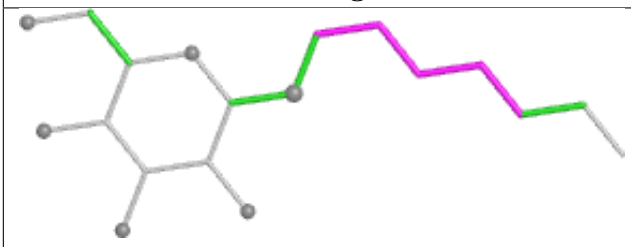
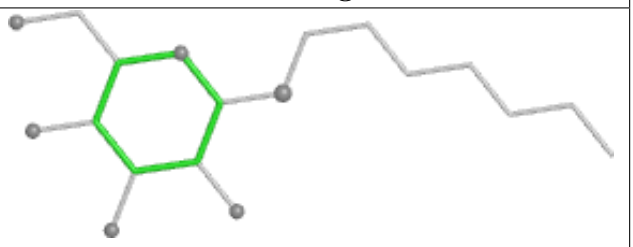


Bond angles

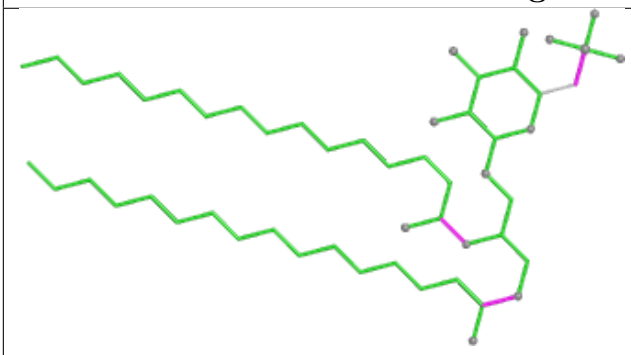


Torsions

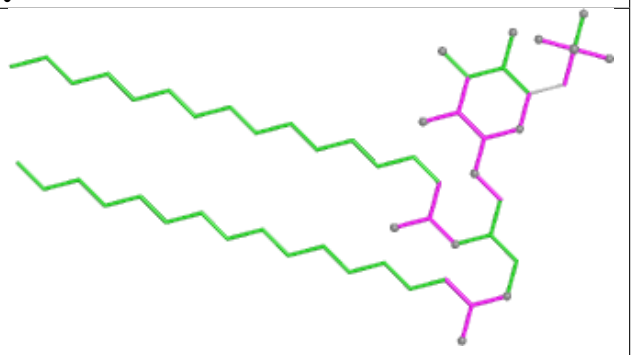


Rings

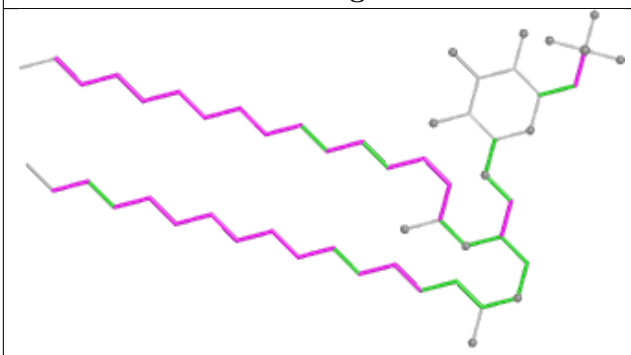
Ligand SQD a 414



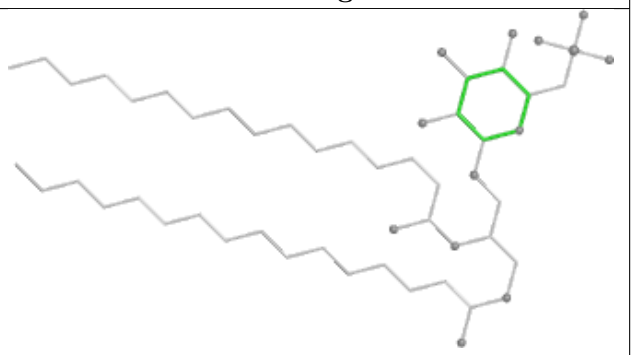
Bond lengths



Bond angles

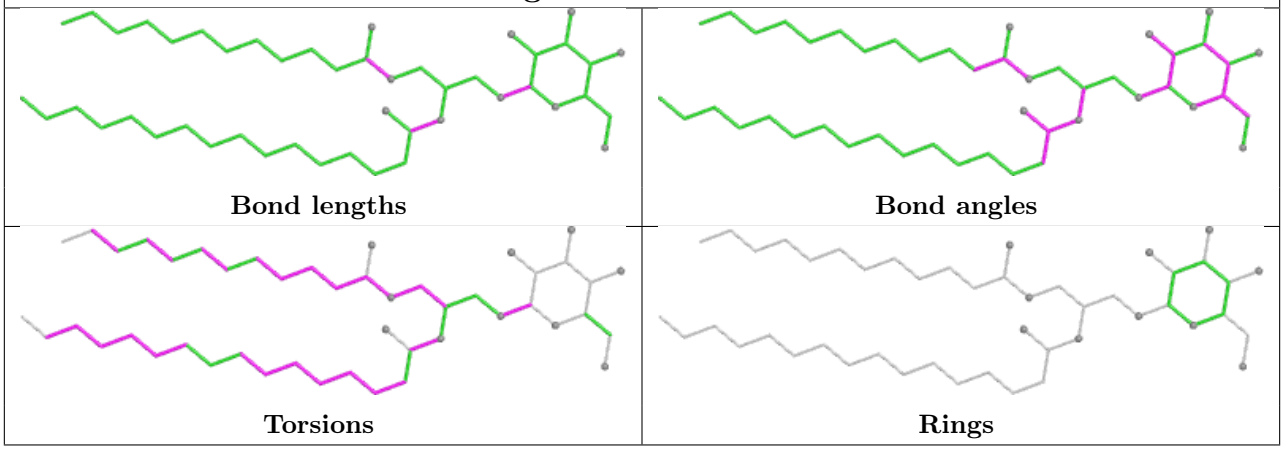


Torsions

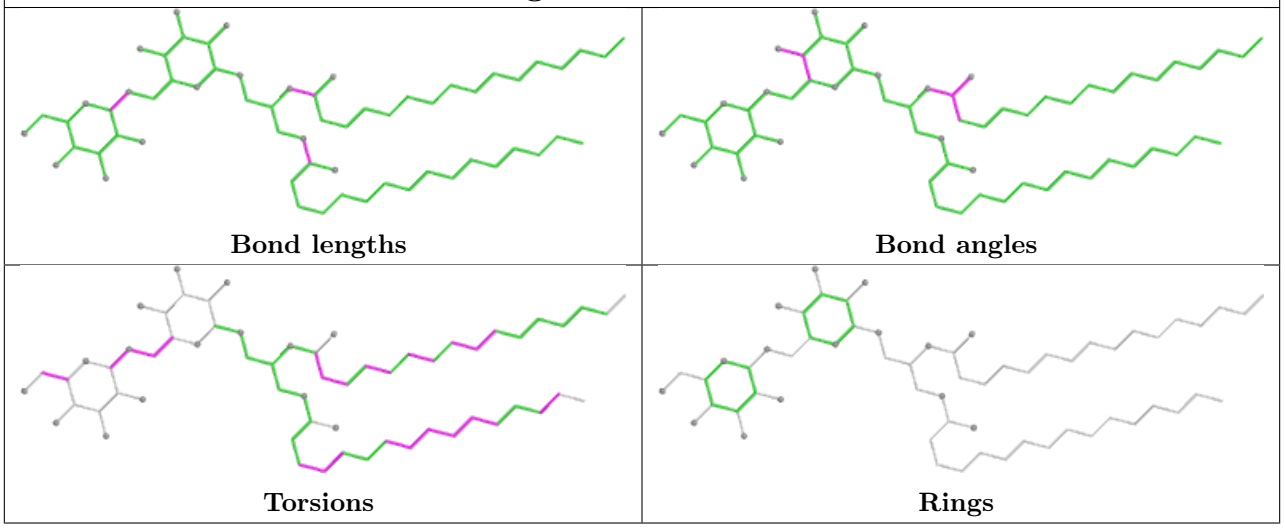


Rings

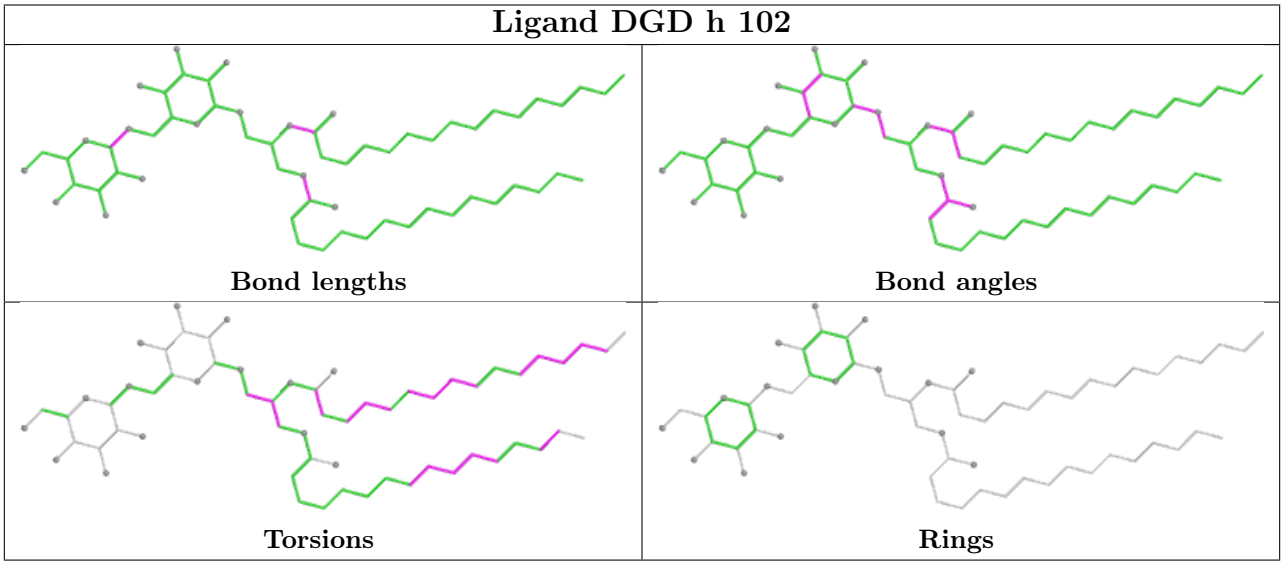
Ligand LMG d 409



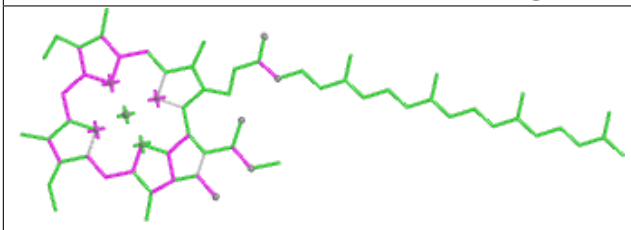
Ligand DGD c 917



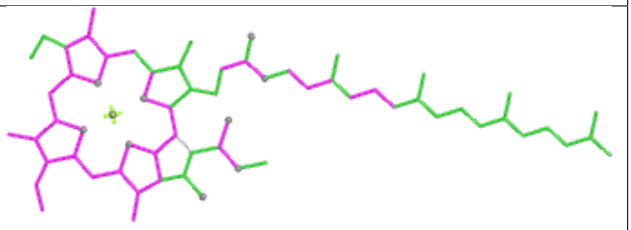
Ligand DGD h 102



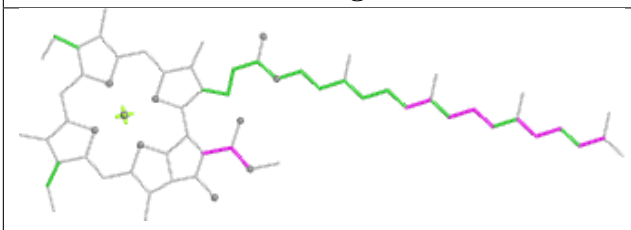
Ligand CLA b 612



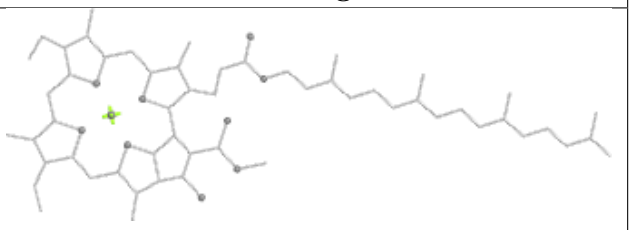
Bond lengths



Bond angles



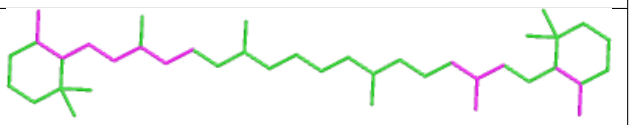
Torsions



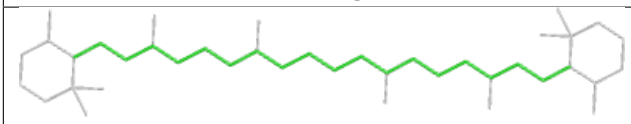
Rings

Ligand BCR C 516

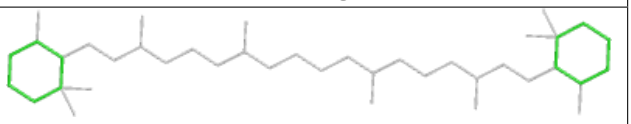
Bond lengths



Bond angles

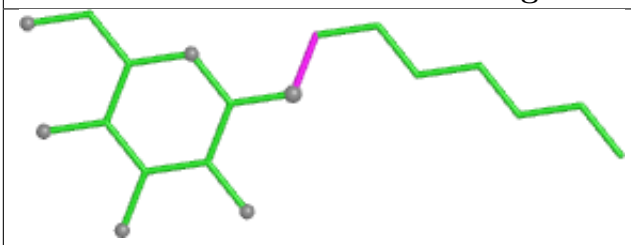


Torsions

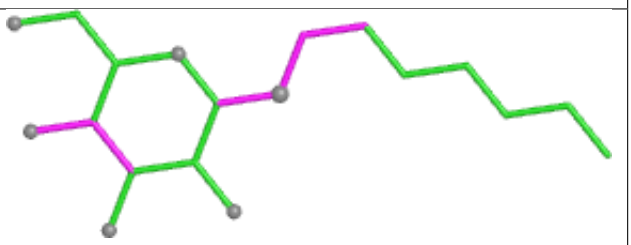


Rings

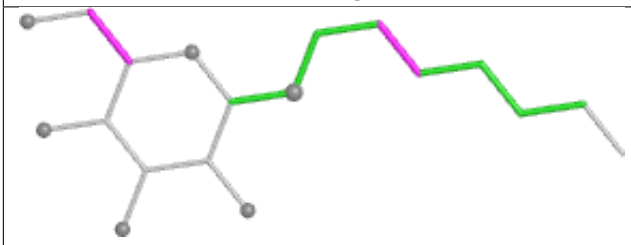
Ligand HTG B 623



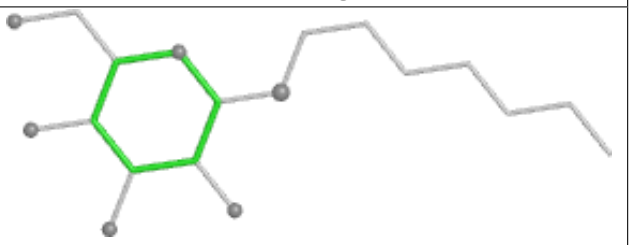
Bond lengths



Bond angles

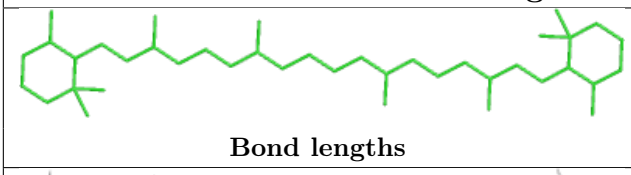


Torsions

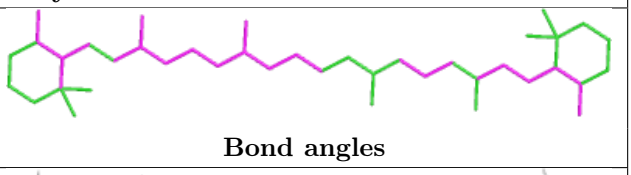


Rings

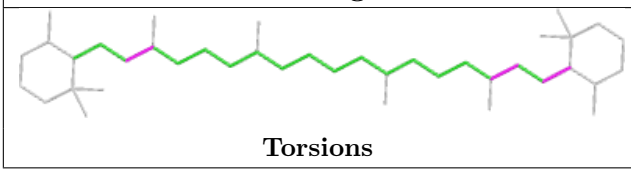
Ligand BCR y 101



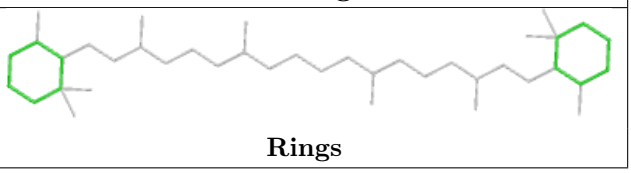
Bond lengths



Bond angles

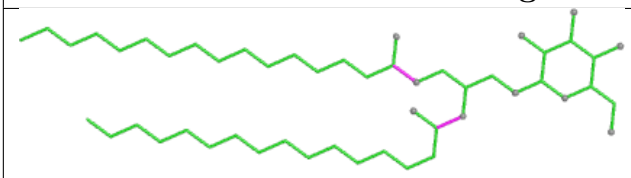


Torsions

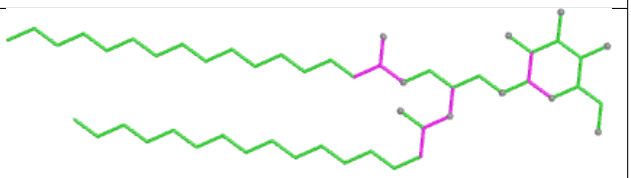


Rings

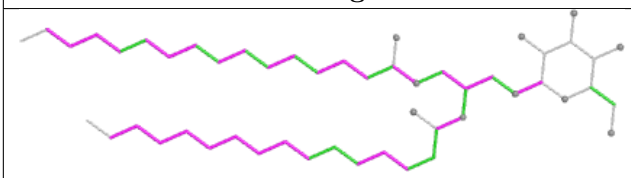
Ligand LMG A 410



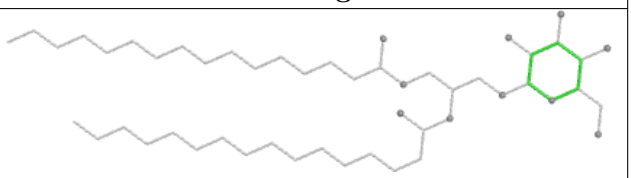
Bond lengths



Bond angles

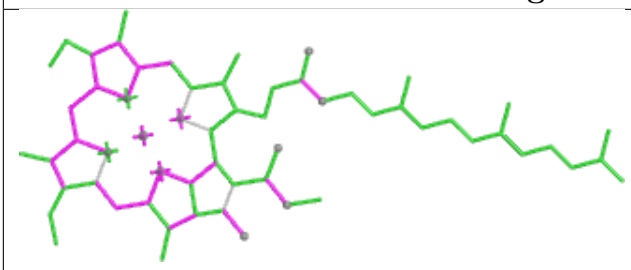


Torsions



Rings

Ligand CLA b 617



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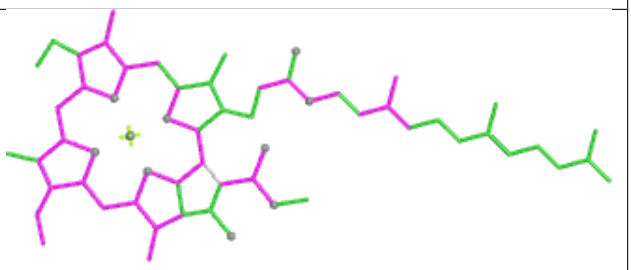
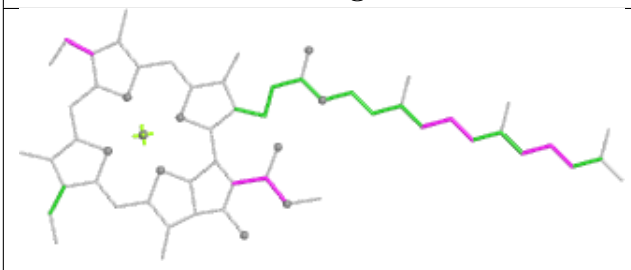
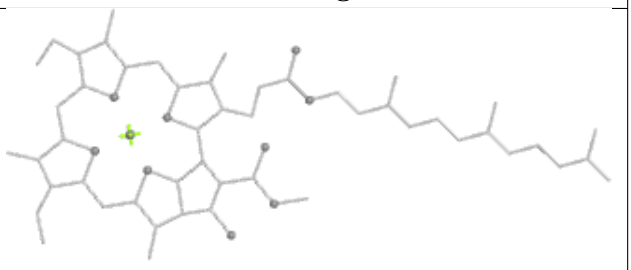


Bond angles

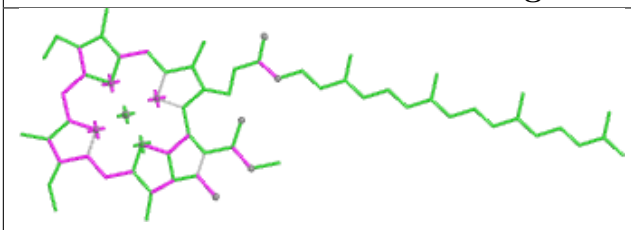


Torsions



Rings

Ligand CLA B 604



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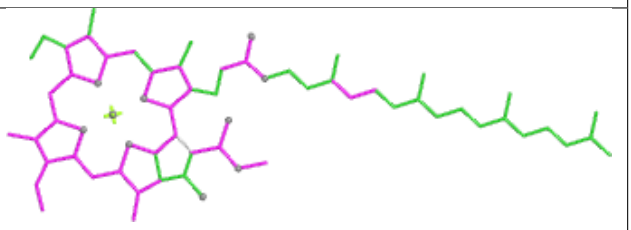
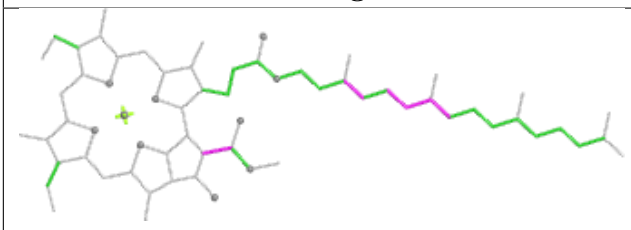
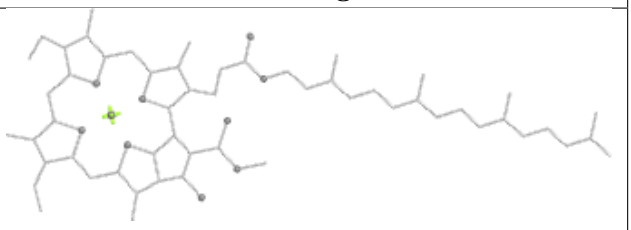


Bond angles

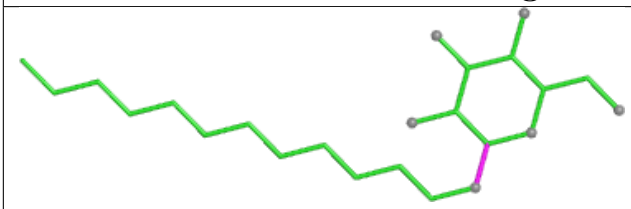


Torsions



Rings

Ligand LMT B 622



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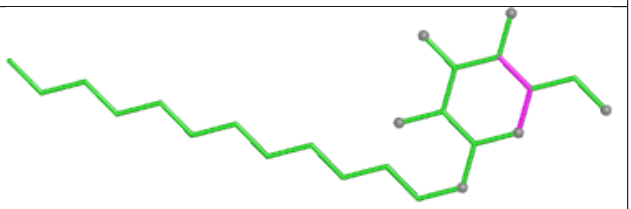
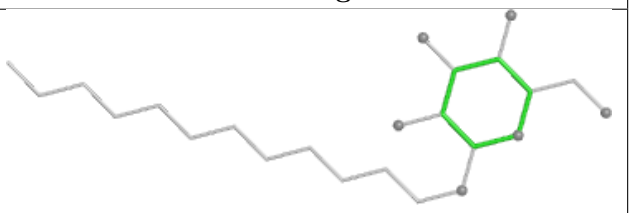


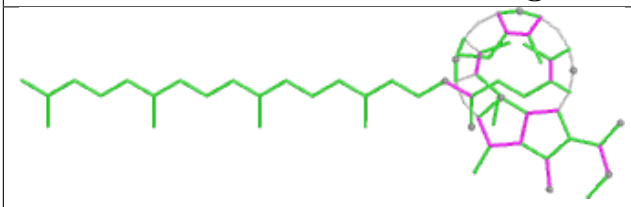
Bond angles

Torsions



Rings

Ligand PHO a 411



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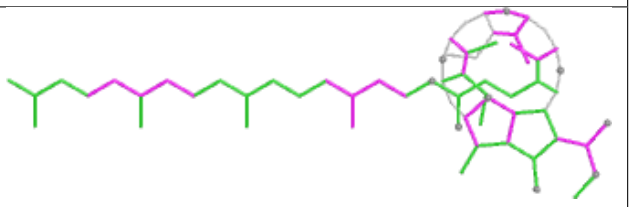
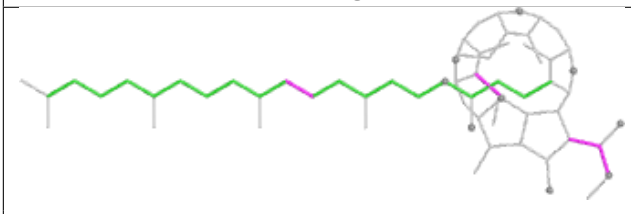


Bond angles



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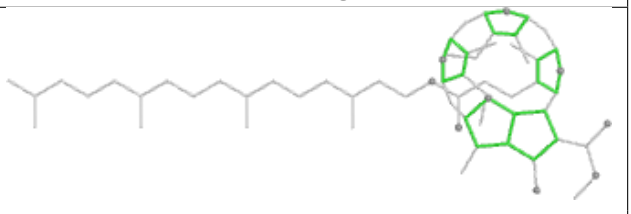
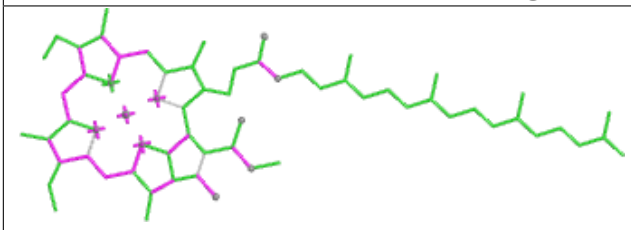


Rings

Ligand CLA B 605



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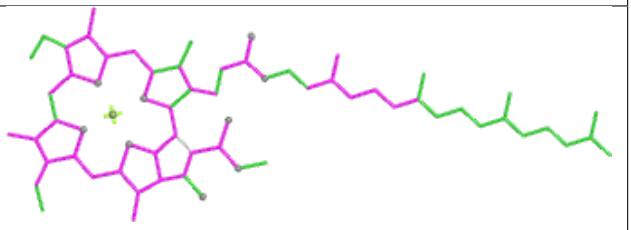
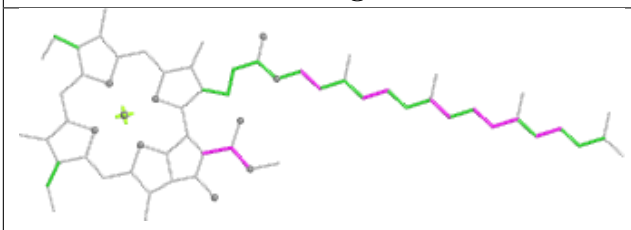


Bond angles



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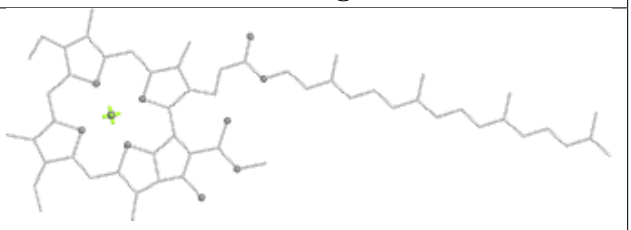
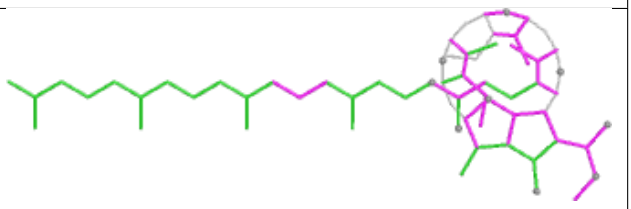


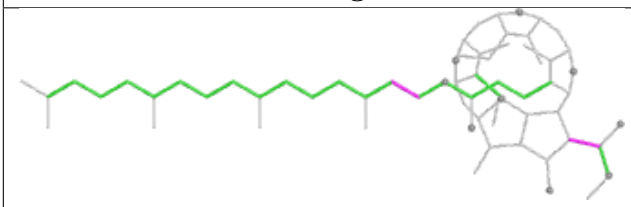
Rings

Ligand PHO A 407

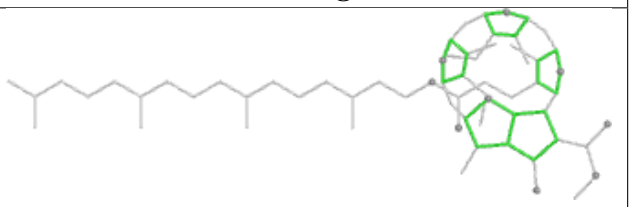
Bond lengths



Bond angles

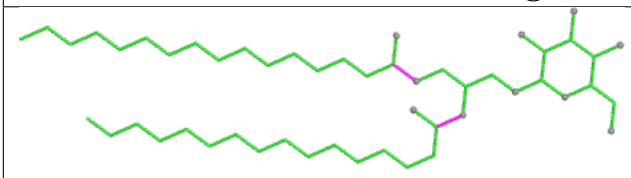


Torsions

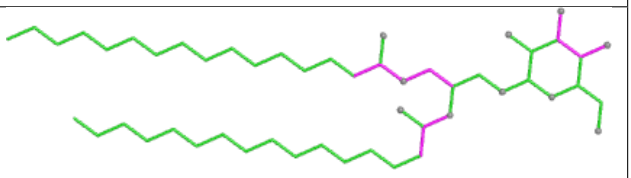


Rings

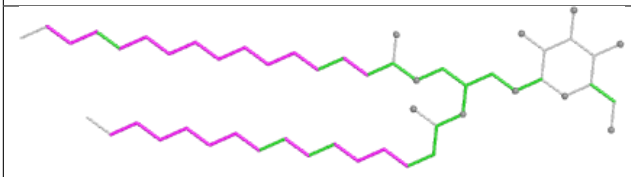
Ligand LMG c 920



Bond lengths



Bond angles



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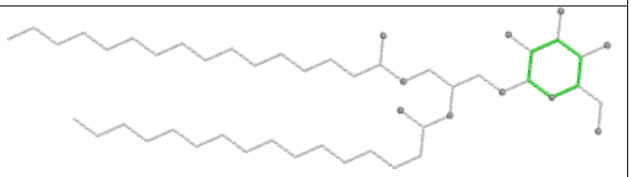
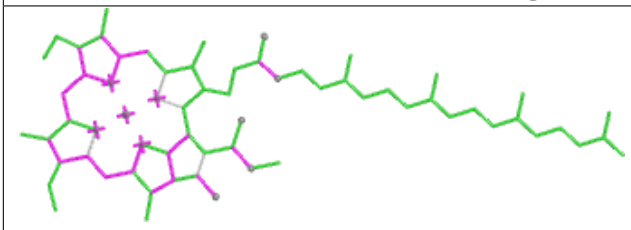


Rings

Ligand CLA B 613



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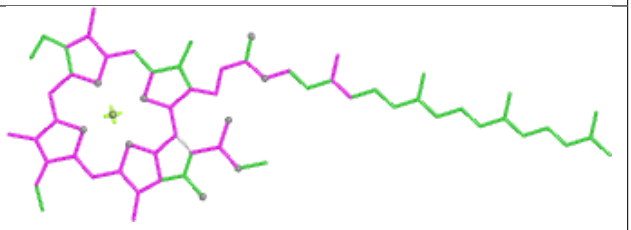
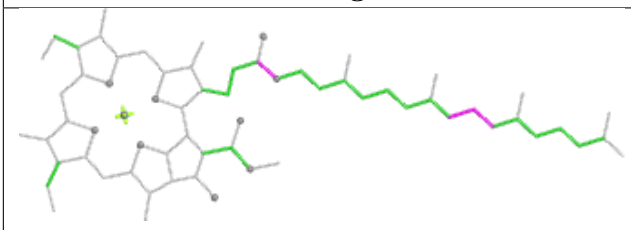
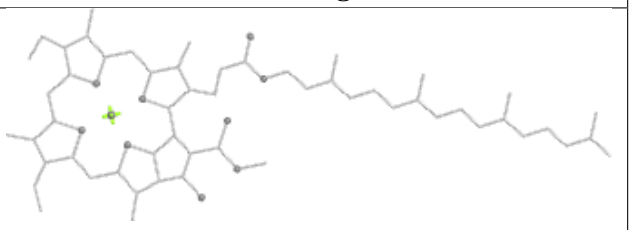


Bond angles

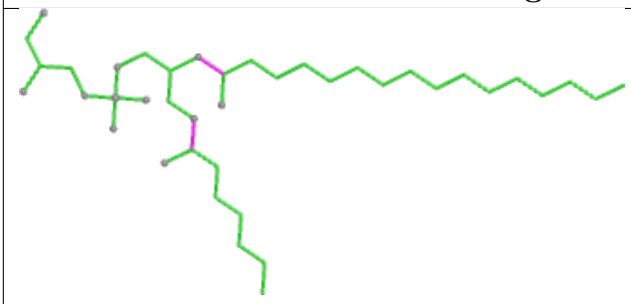


Torsions



Rings

Ligand LHG L 101



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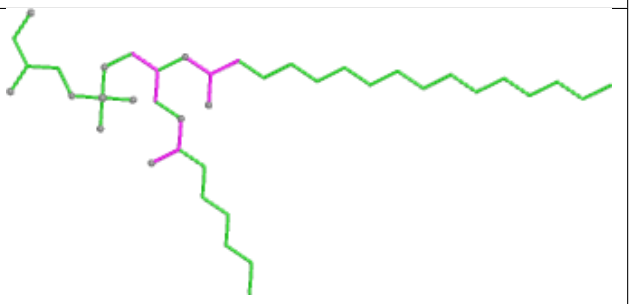
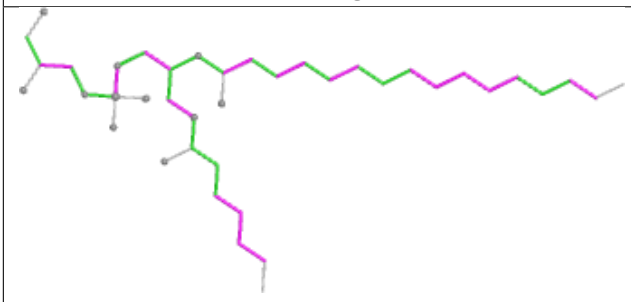


Bond angles



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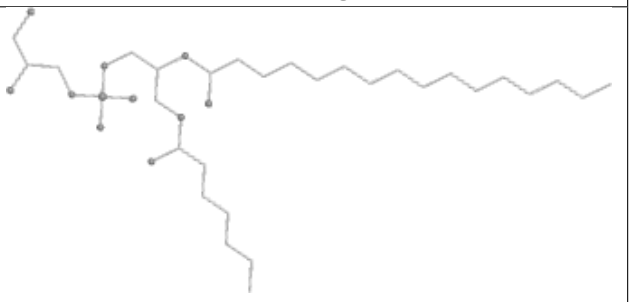
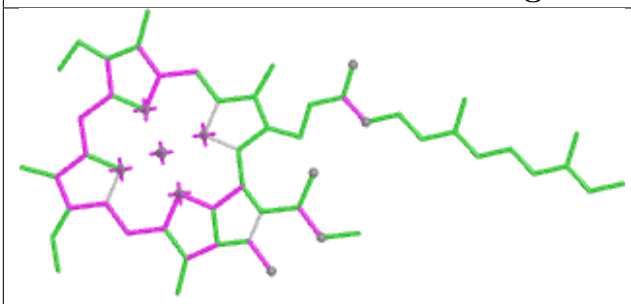


Rings

Ligand CLA C 513



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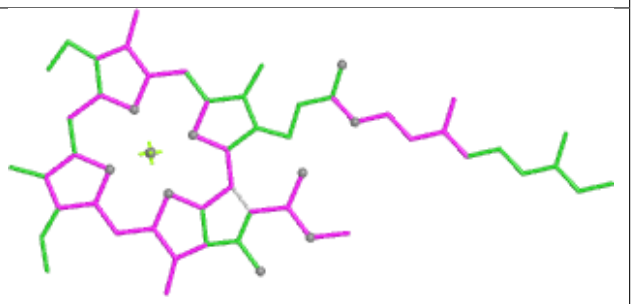
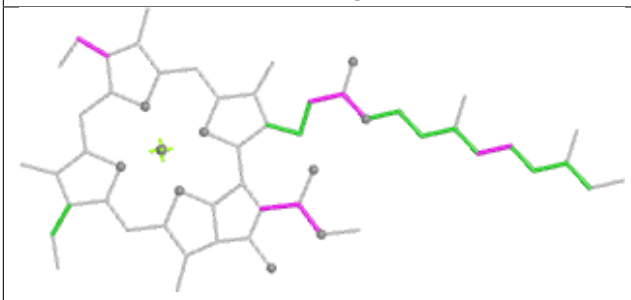


Bond angles



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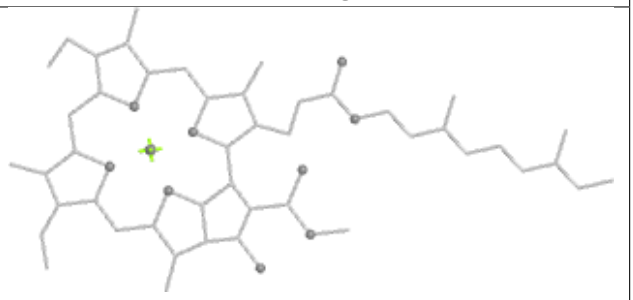
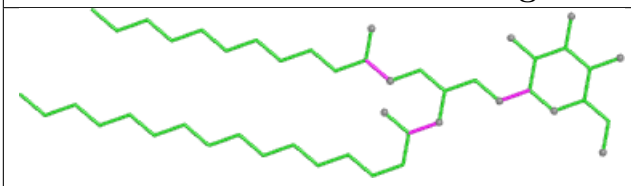


Rings

Ligand LMG D 412



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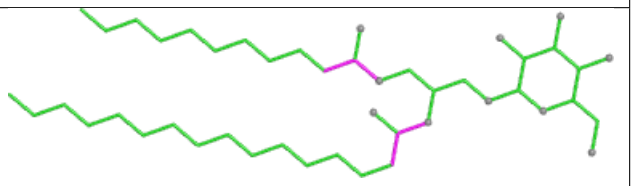
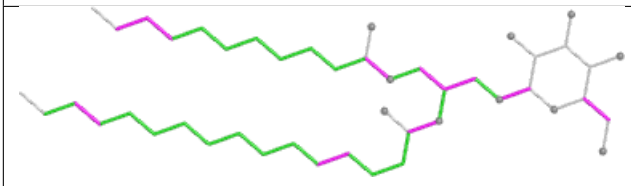
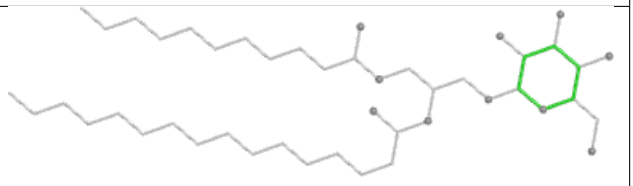


Bond angles

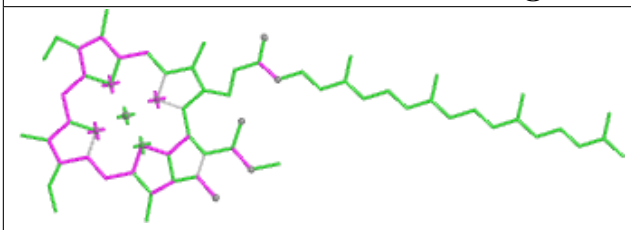


Torsions

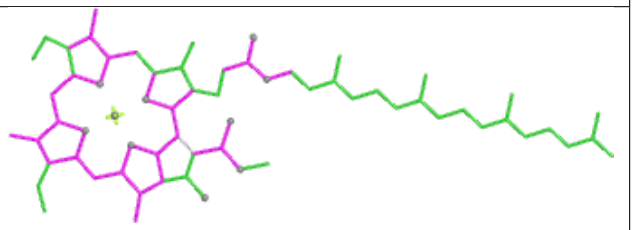


Rings

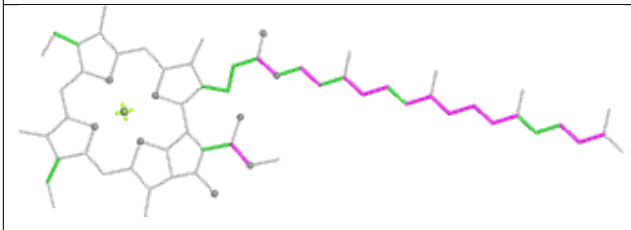
Ligand CLA C 514



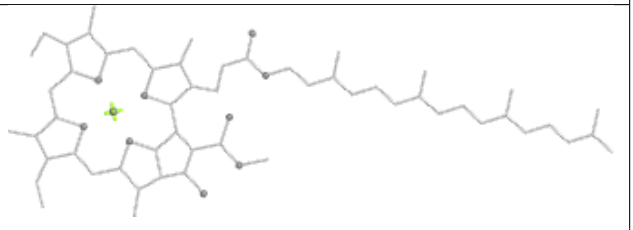
Bond lengths



Bond angles

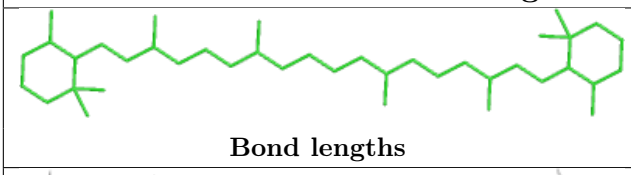


Torsions

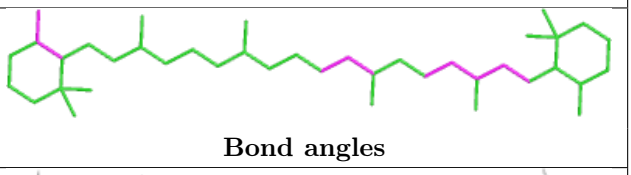


Rings

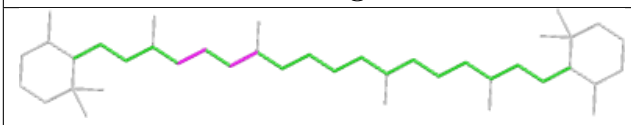
Ligand BCR K 101



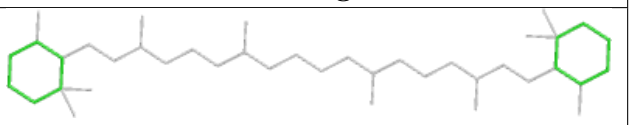
Bond lengths



Bond angles



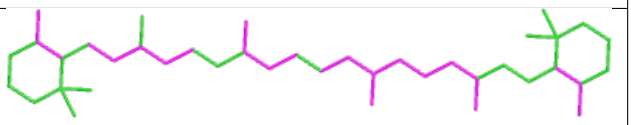
Torsions



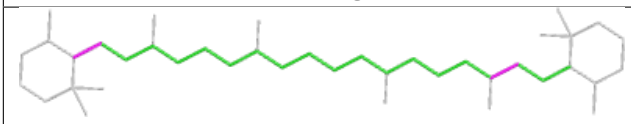
Rings

Ligand BCR c 916

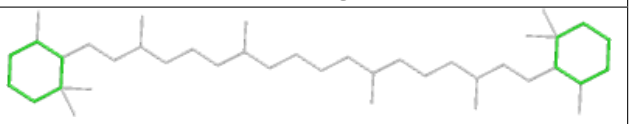
Bond lengths



Bond angles

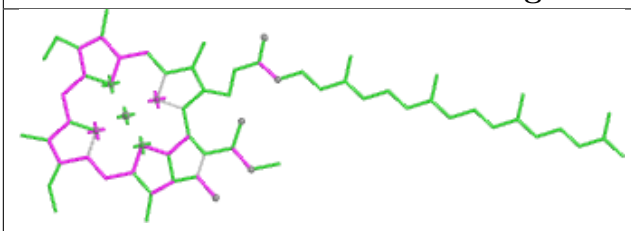


Torsions

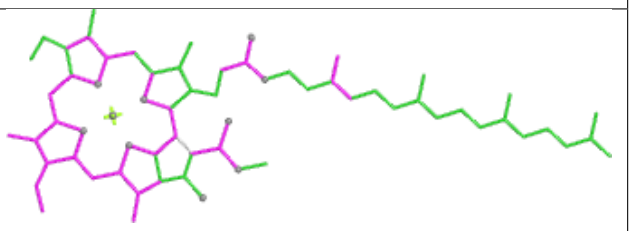


Rings

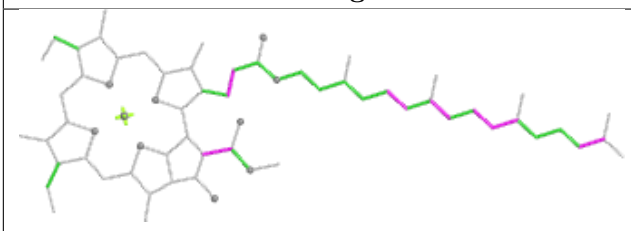
Ligand CLA C 508



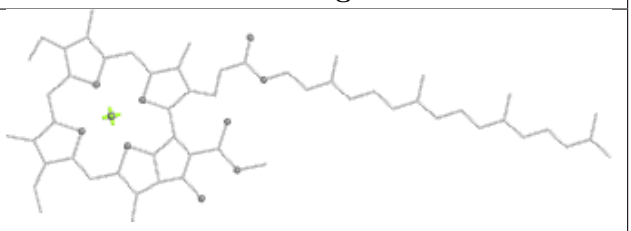
Bond lengths



Bond angles

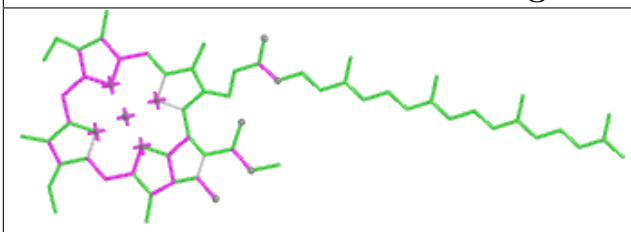


Torsions

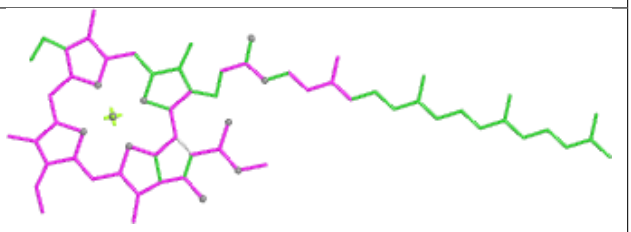


Rings

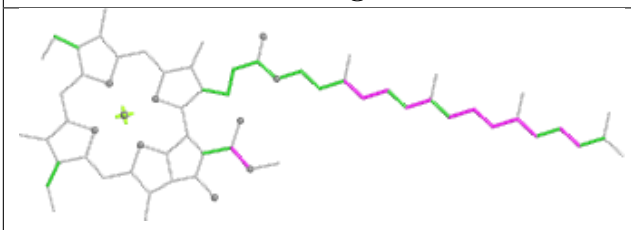
Ligand CLA a 412



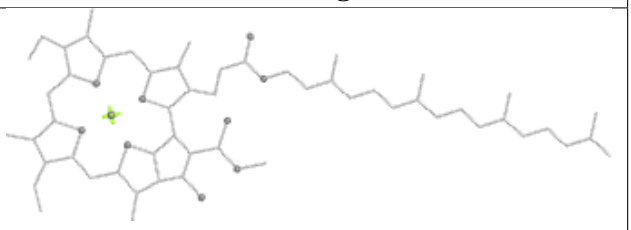
Bond lengths



Bond angles

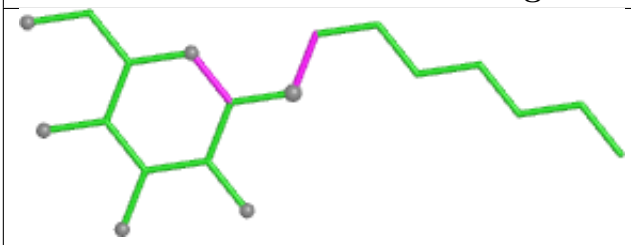


Torsions



Rings

Ligand HTG b 627



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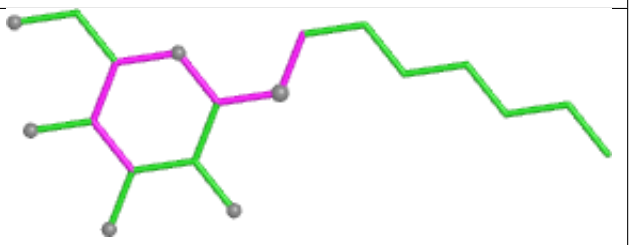
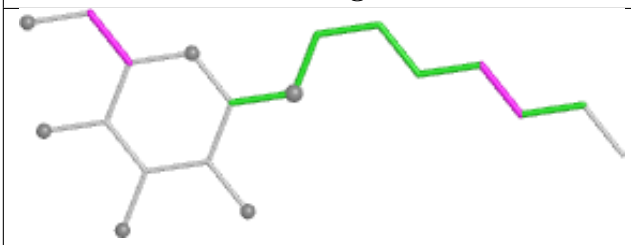
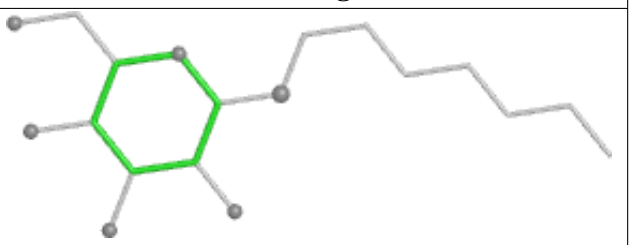


Bond angles

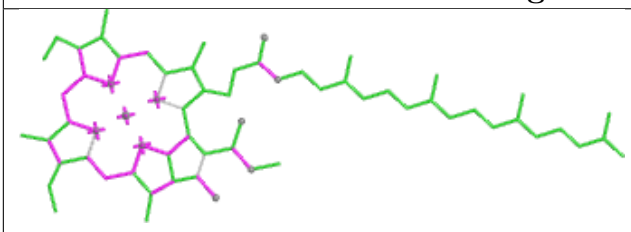


Torsions

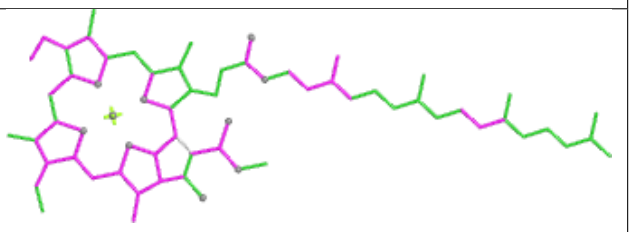


Rings

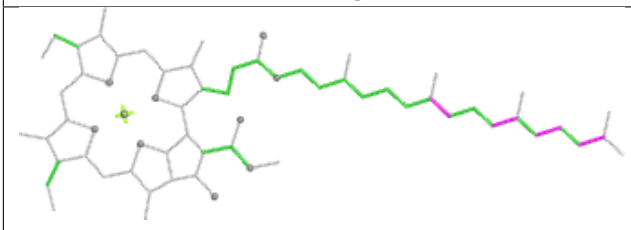
Ligand CLA b 609



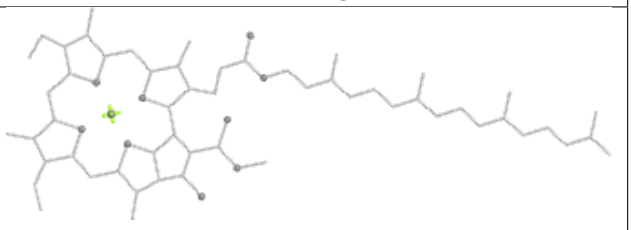
Bond lengths



Bond angles

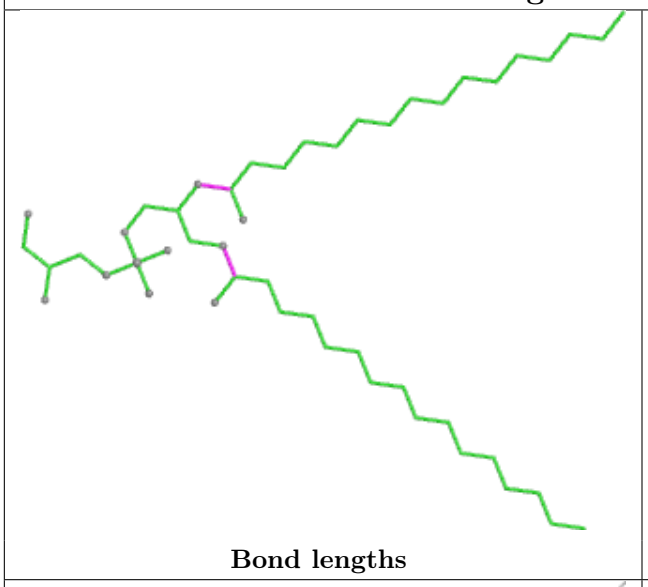


Torsions



Rings

Ligand LHG d 407



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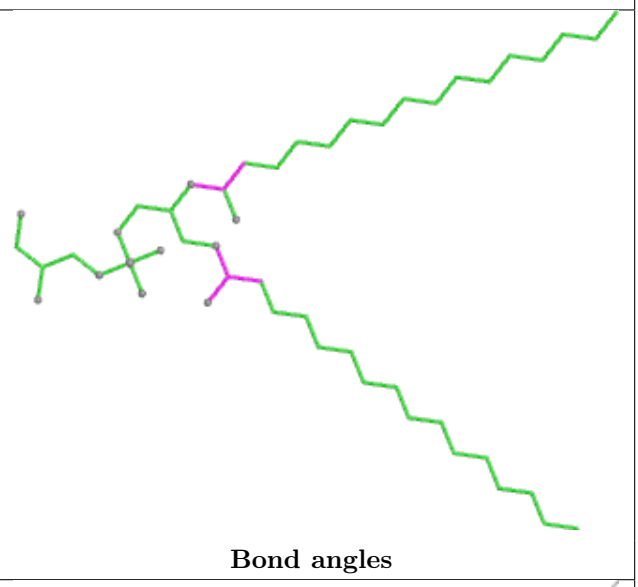
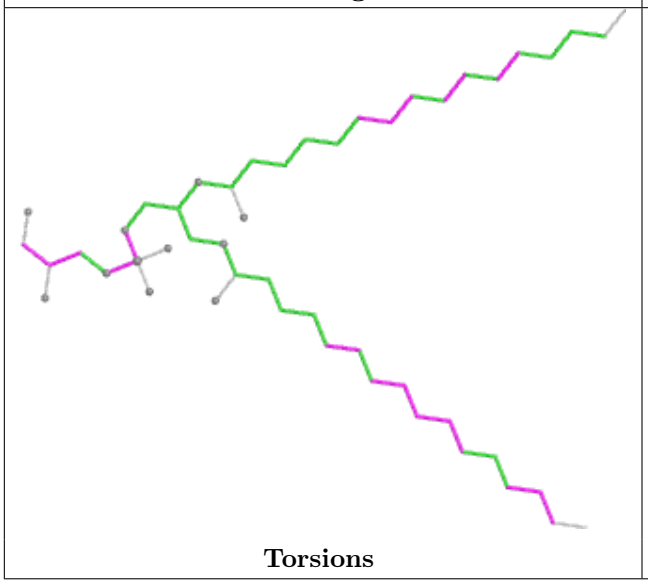


Bond angles



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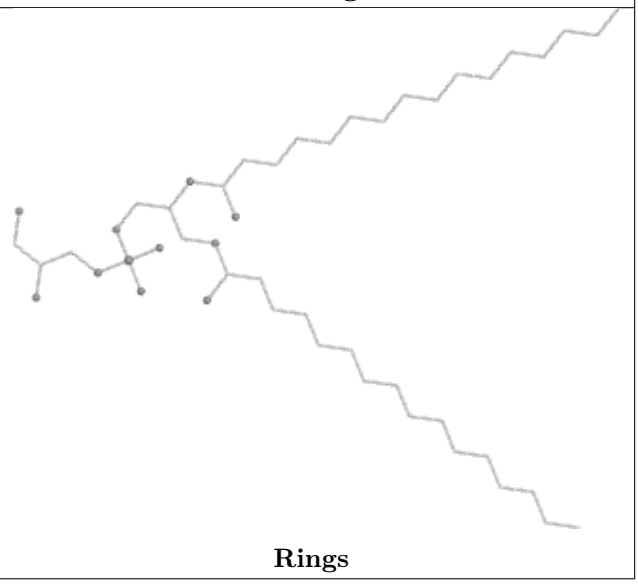
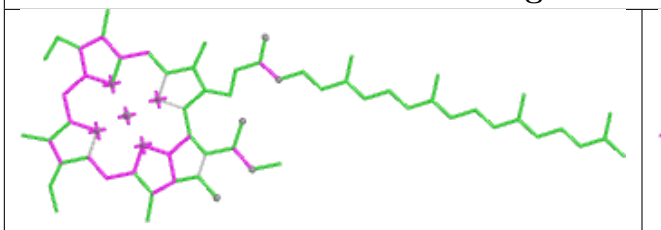


Rings

Ligand CLA C 505



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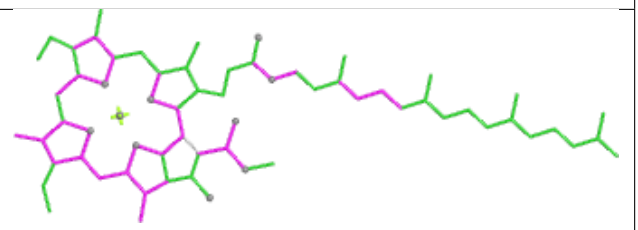
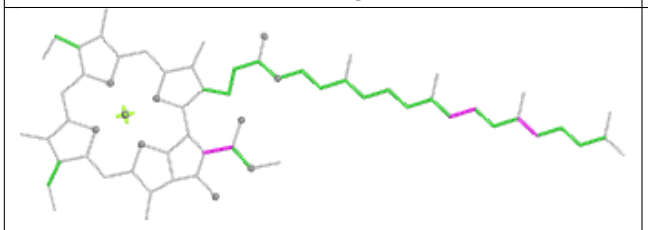


Bond angles



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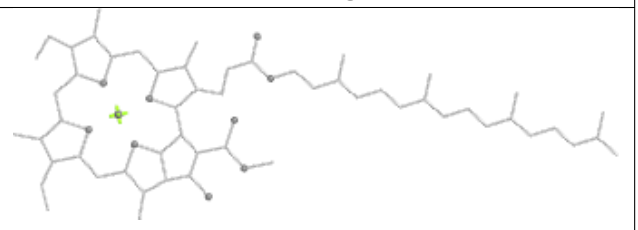
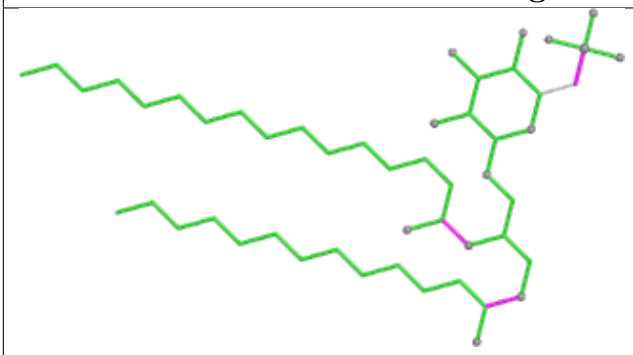
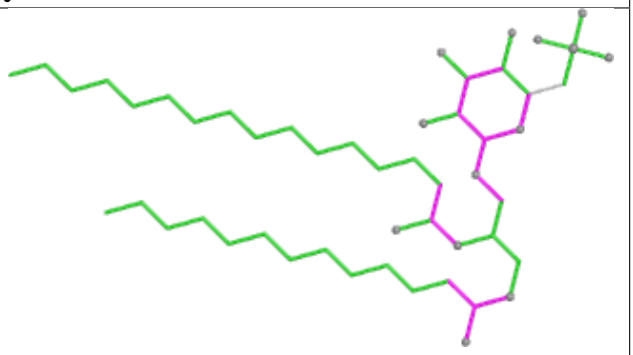


Rings

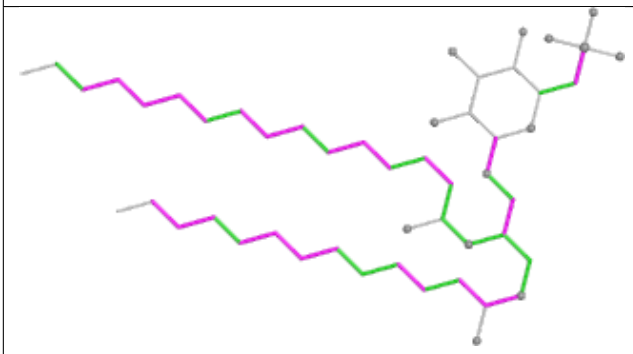
Ligand SQD a 418



Bond lengths



Bond angles



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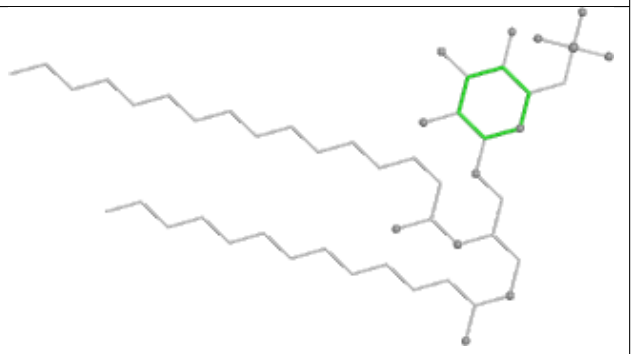
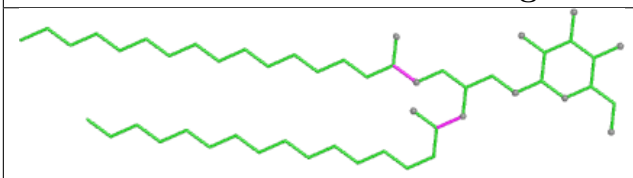
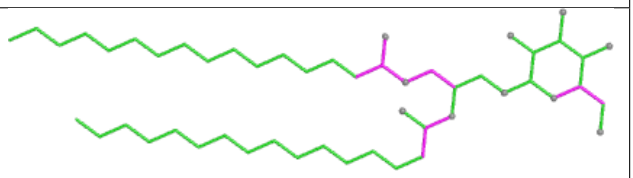


Rings

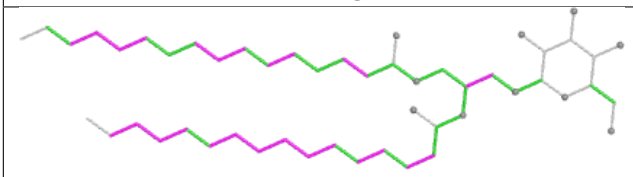
Ligand LMG C 520



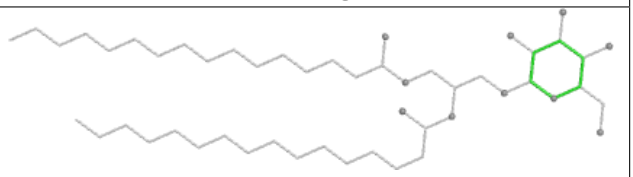
Bond lengths



Bond angles

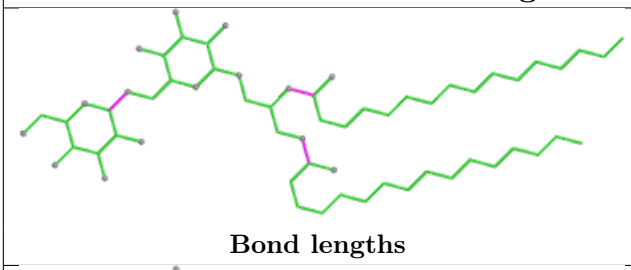


Torsions



Rings

Ligand DGD H 102



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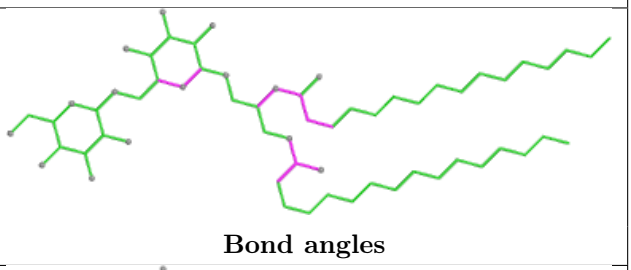
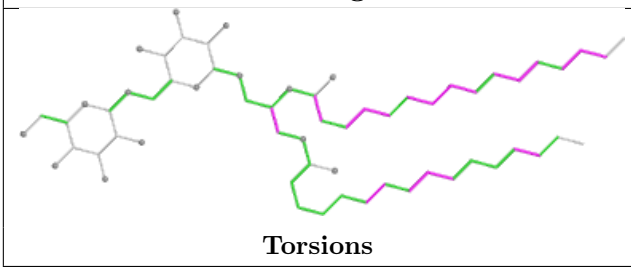
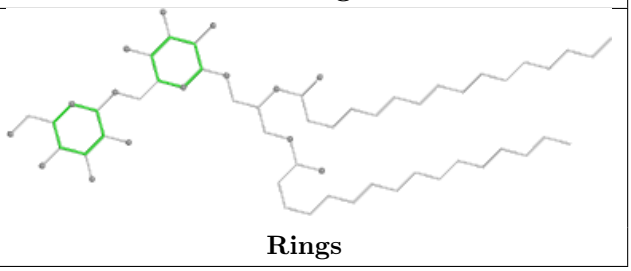


Bond angles

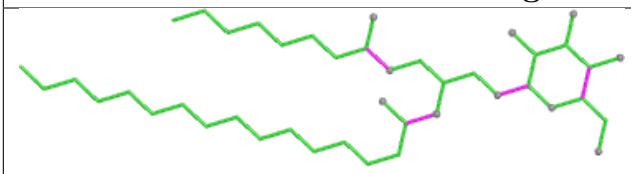


Torsions



Rings

Ligand LMG b 622



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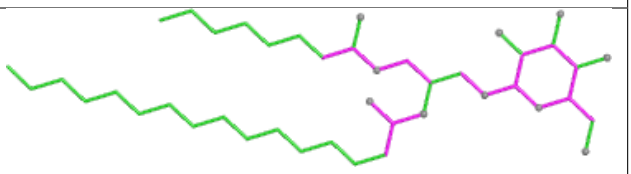
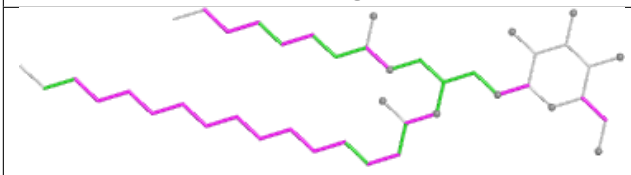


Bond angles



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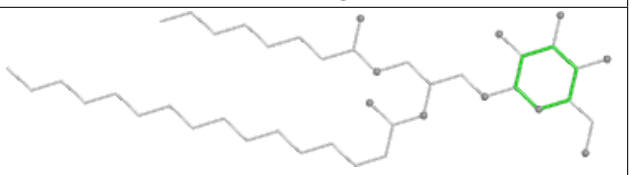
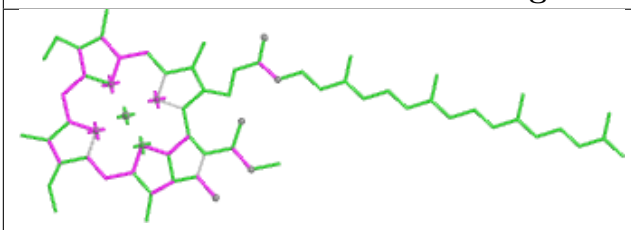


Rings

Ligand CLA c 911



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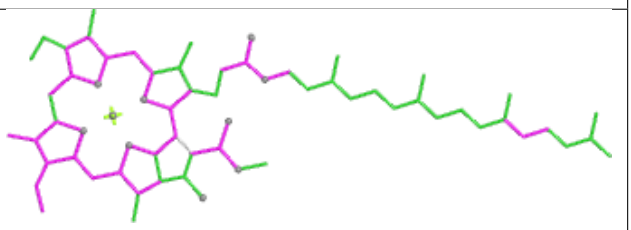
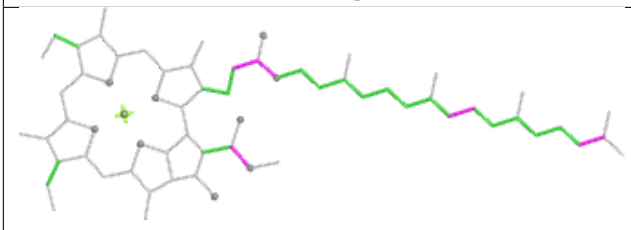


Bond angles



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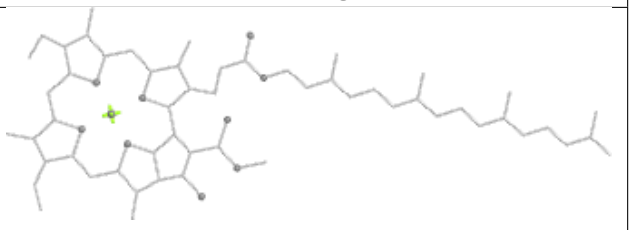
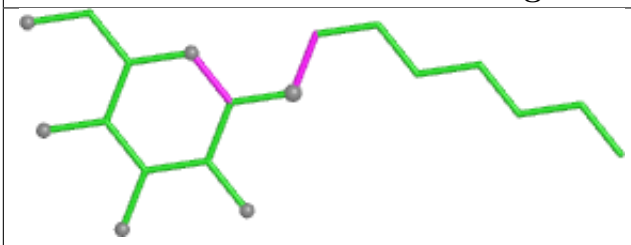
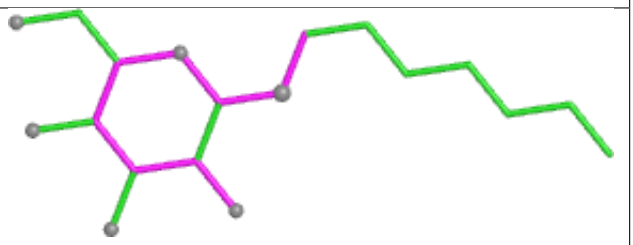


Rings

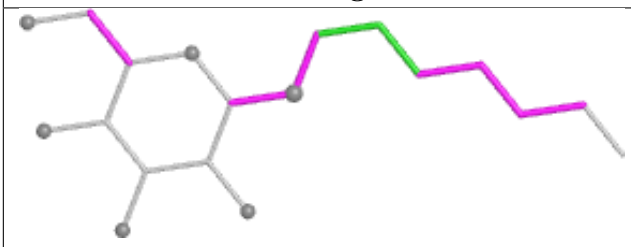
Ligand HTG b 632



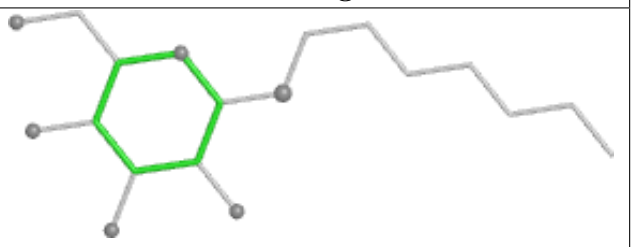
Bond lengths



Bond angles

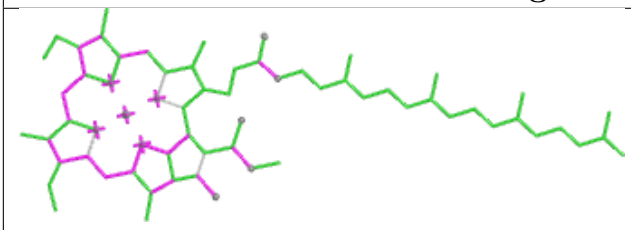


Torsions

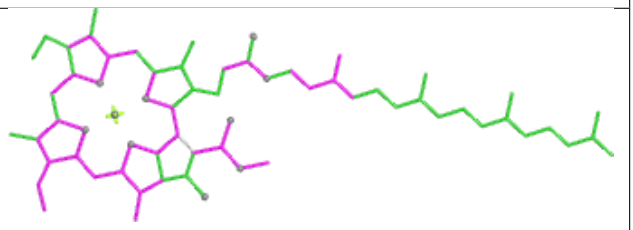


Rings

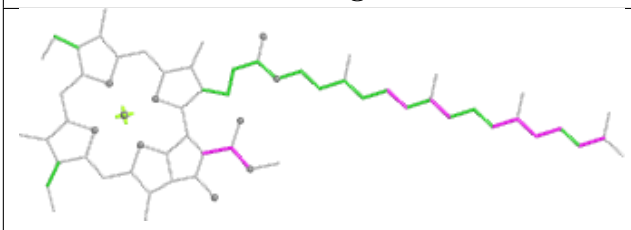
Ligand CLA c 908



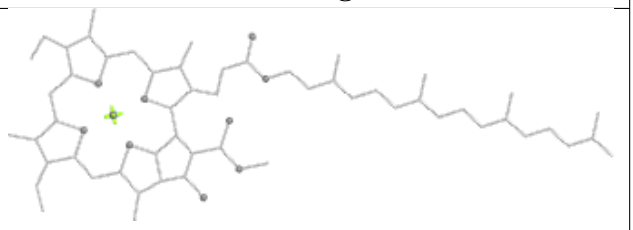
Bond lengths



Bond angles

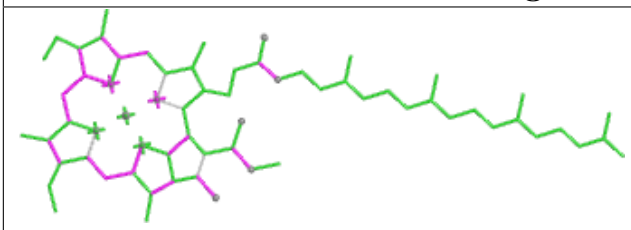


Torsions

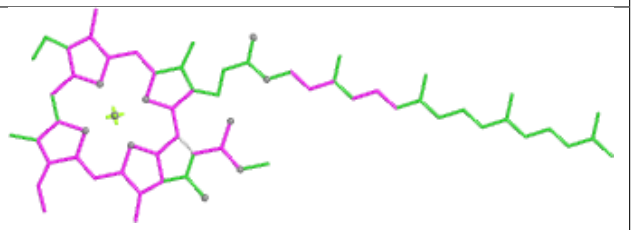


Rings

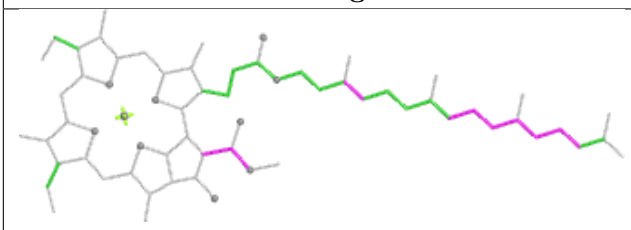
Ligand CLA B 612



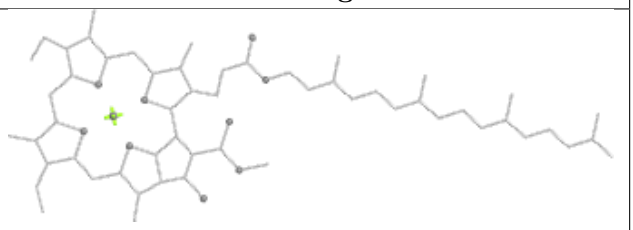
Bond lengths



Bond angles

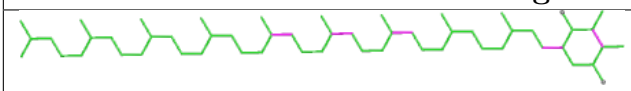


Torsions



Rings

Ligand PL9 d 405



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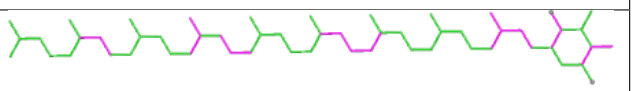

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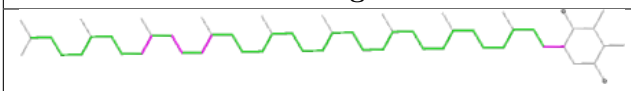
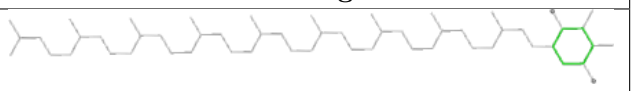
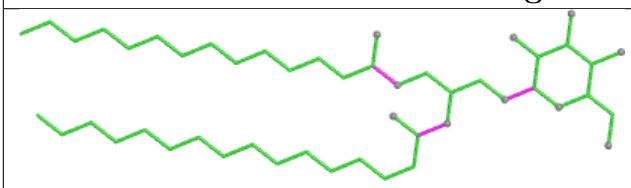


Torsions



Rings

Ligand LMG c 930



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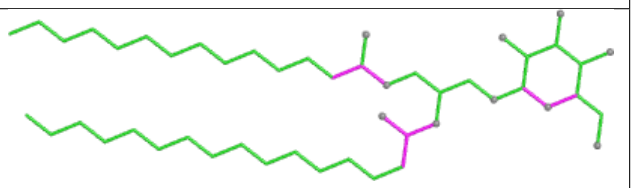
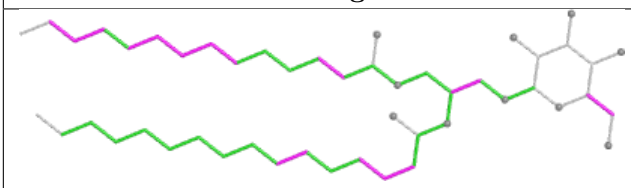


Bond angles



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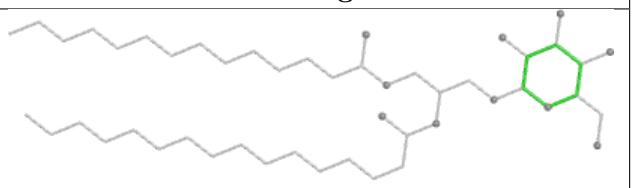
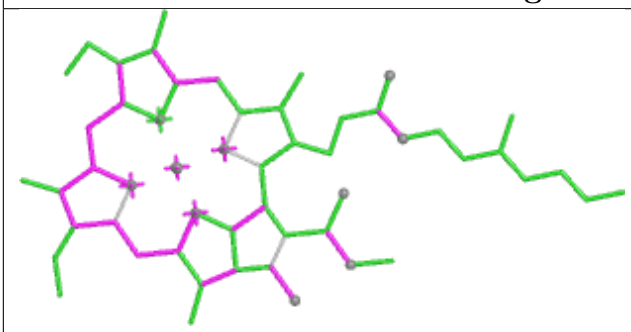


Rings

Ligand CLA B 615



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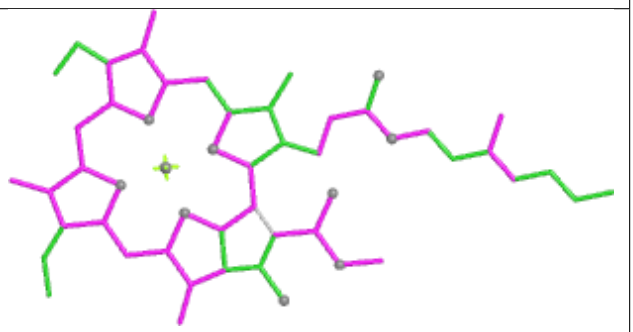
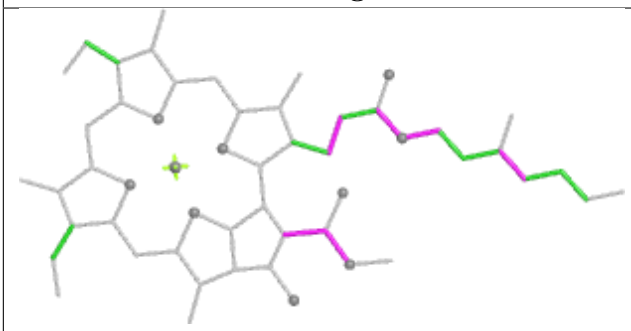
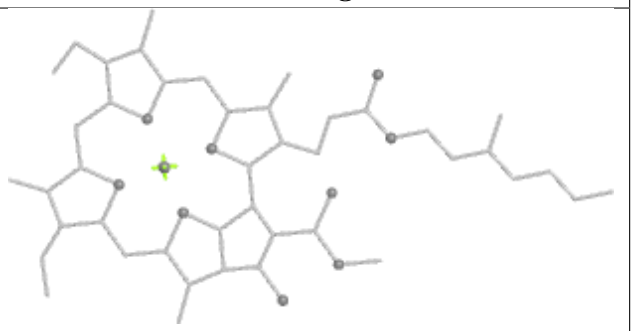


Bond angles

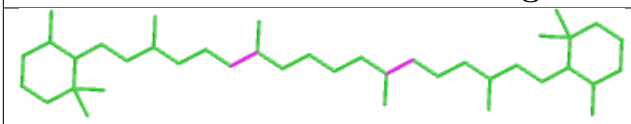


Torsions



Rings

Ligand BCR A 409



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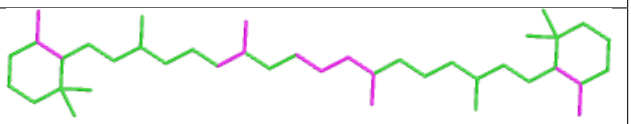

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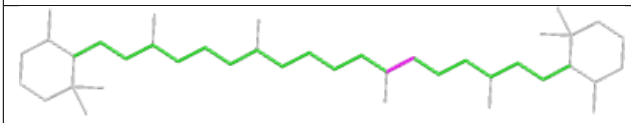

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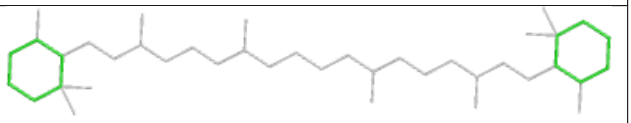
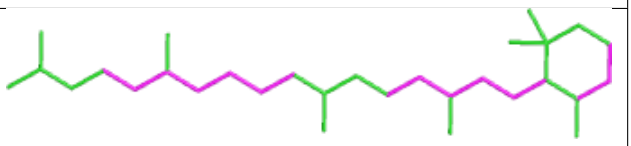


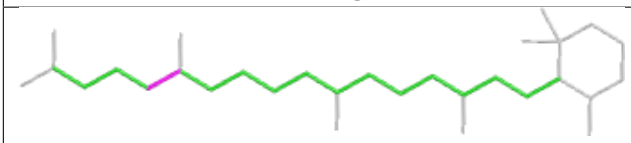
Rings

Ligand BCR B 619

Bond lengths



Bond angles



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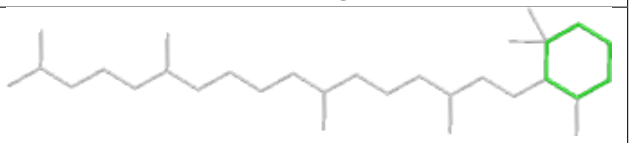
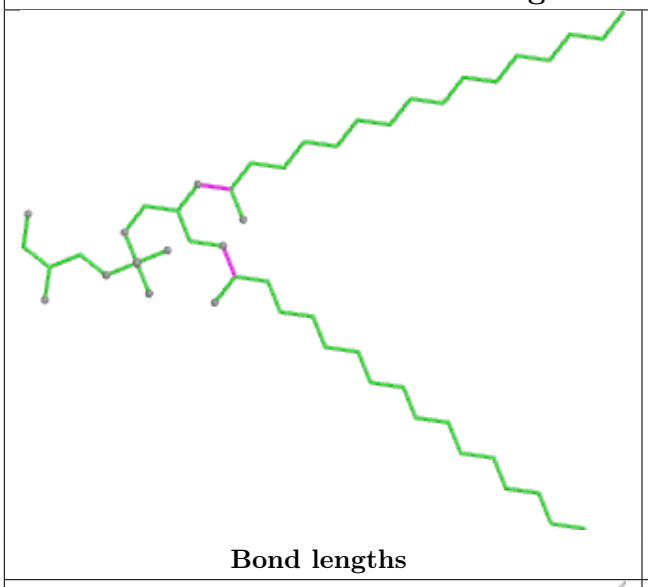


Rings

Ligand LHG a 416



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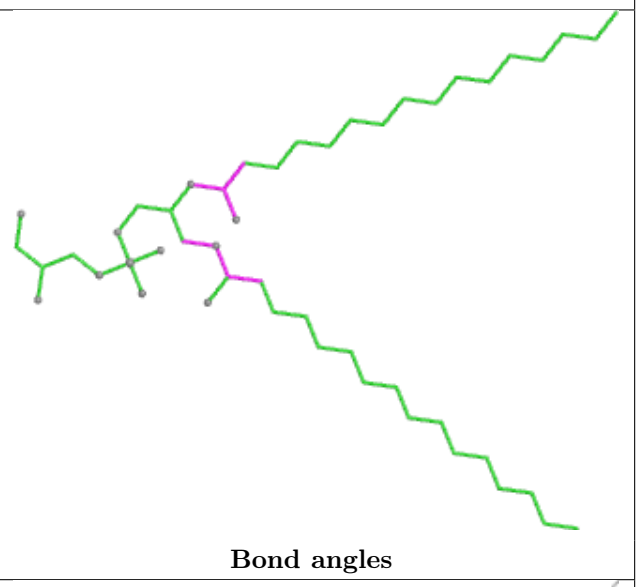
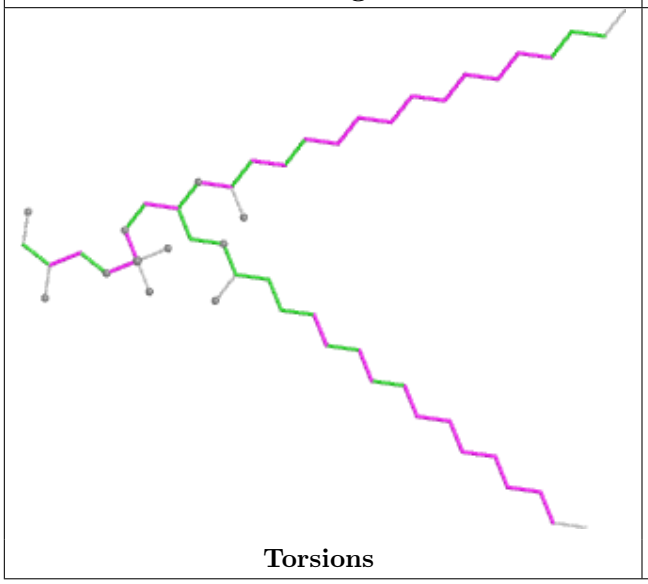


Bond angles



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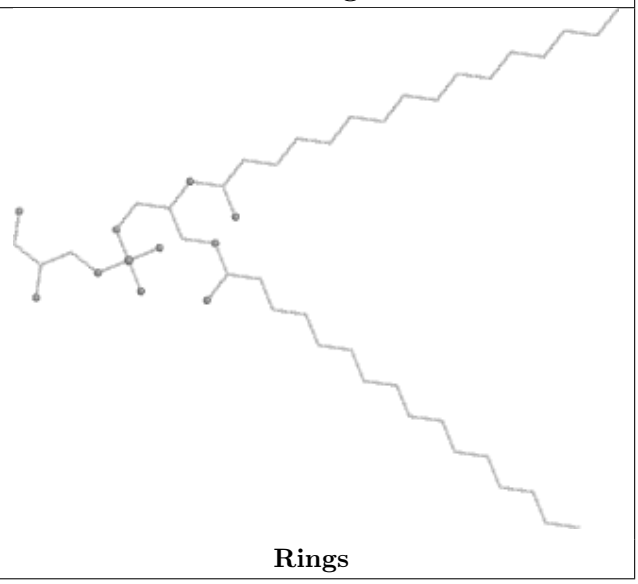
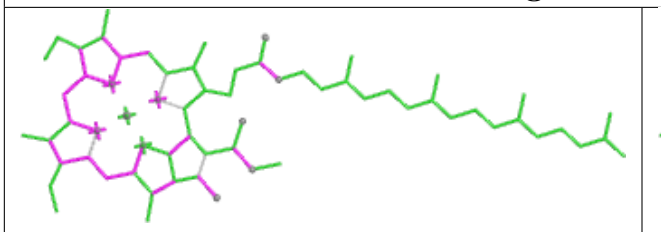


Rings

Ligand CLA B 616



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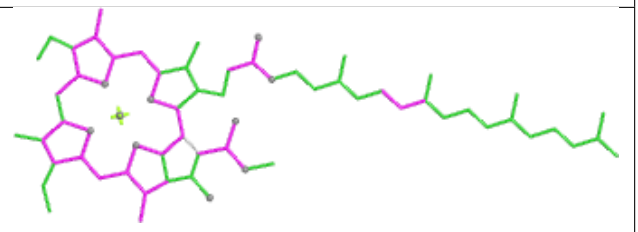

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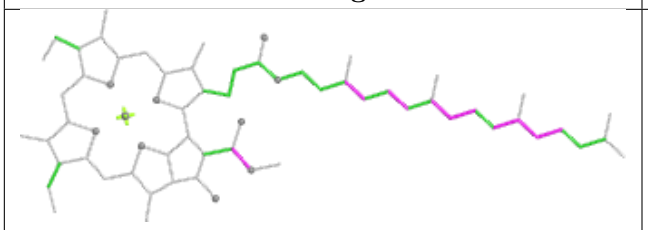

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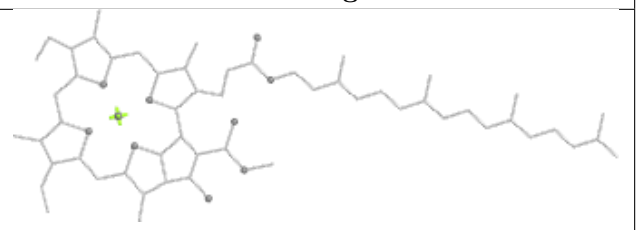
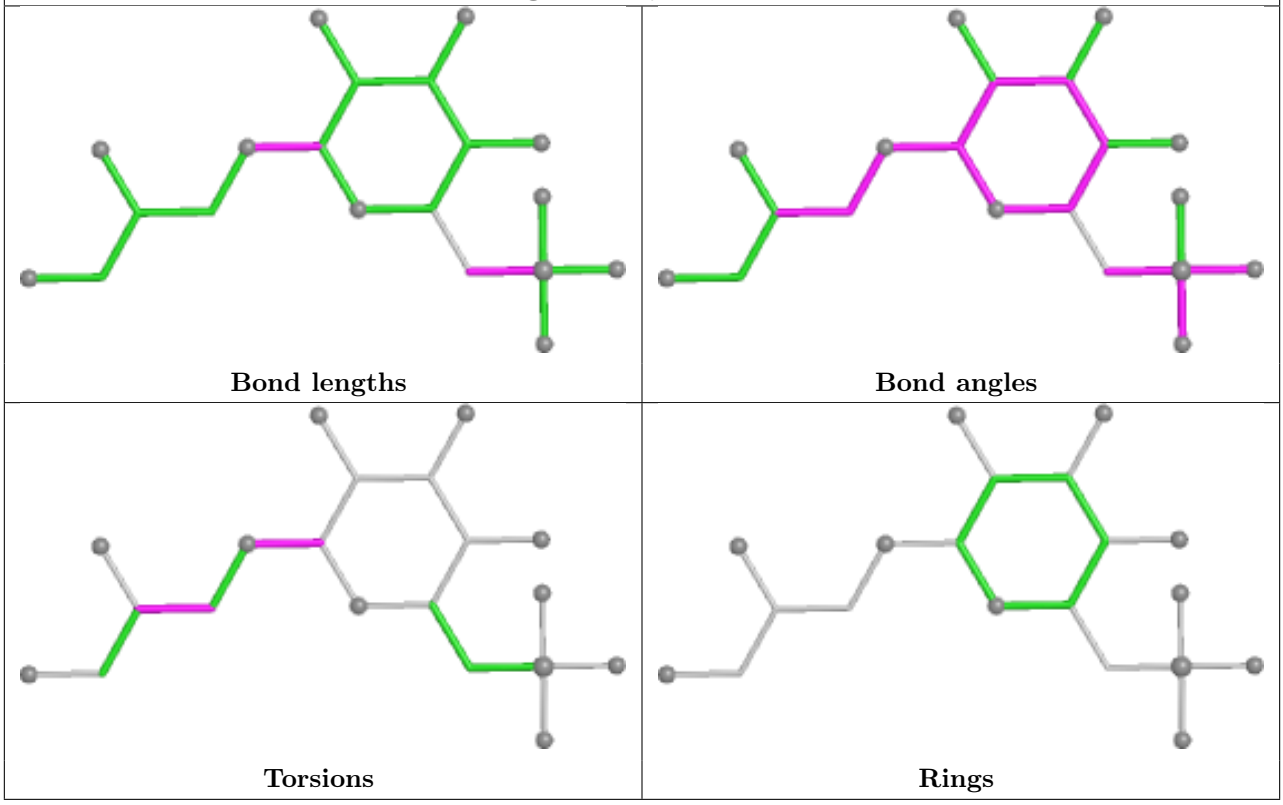
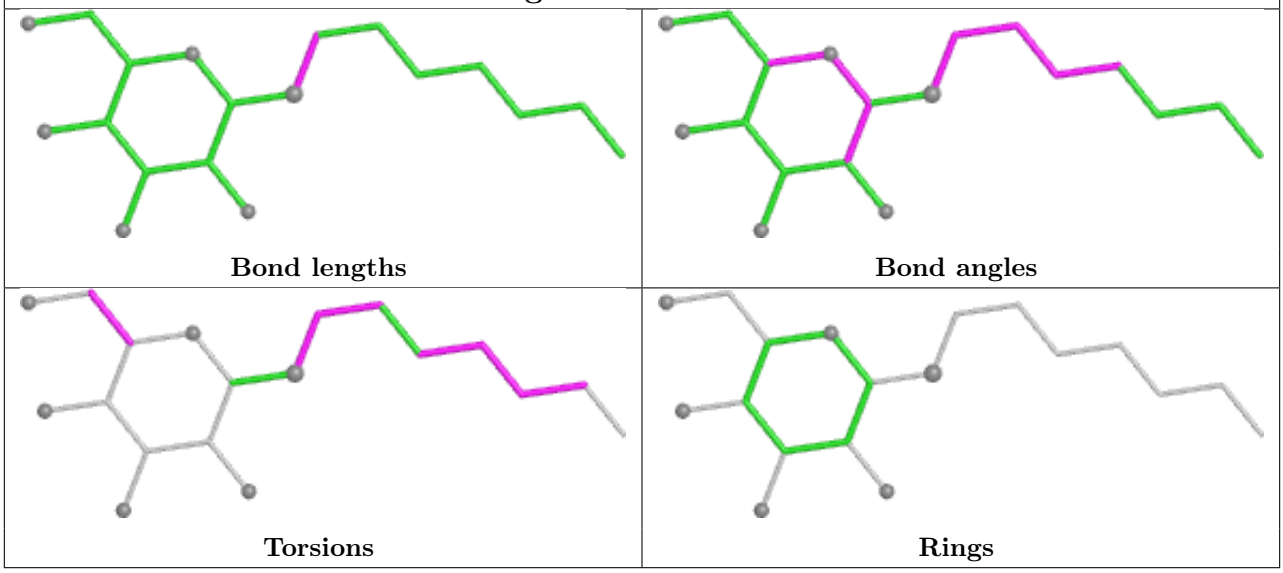


Rings

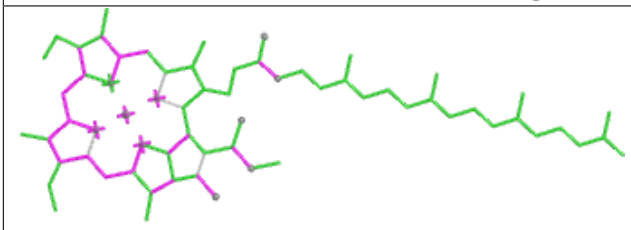
Ligand SQD D 408



Ligand HTG b 623



Ligand CLA b 610



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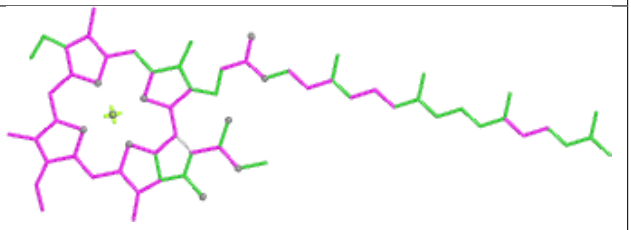
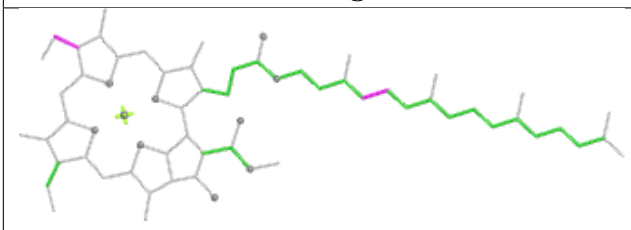


Bond angles



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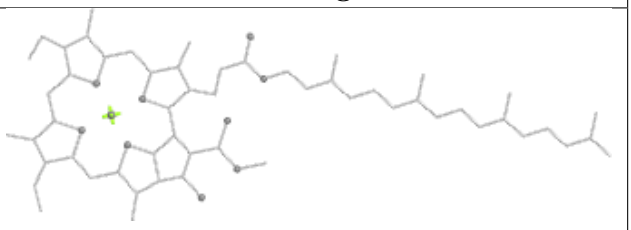
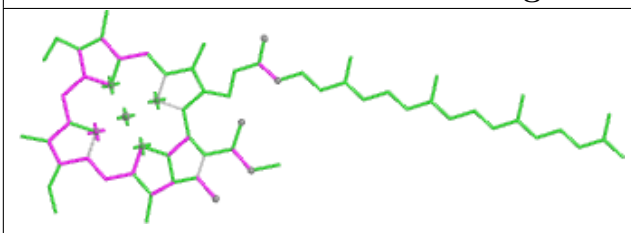


Rings

Ligand CLA D 404



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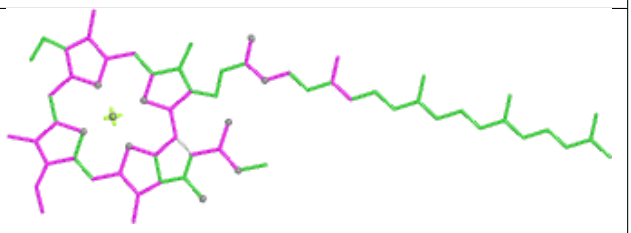
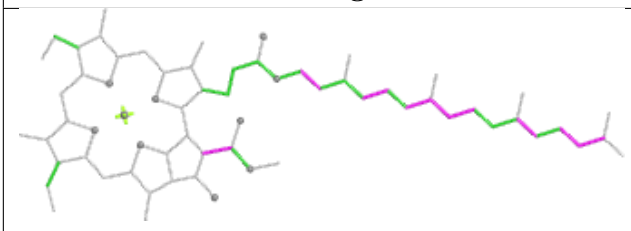


Bond angles



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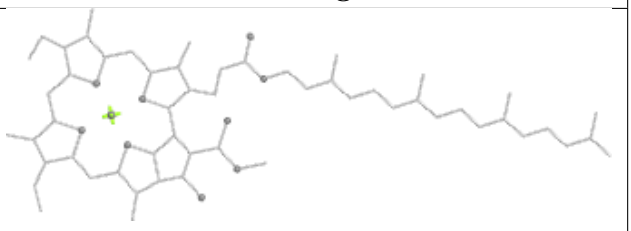
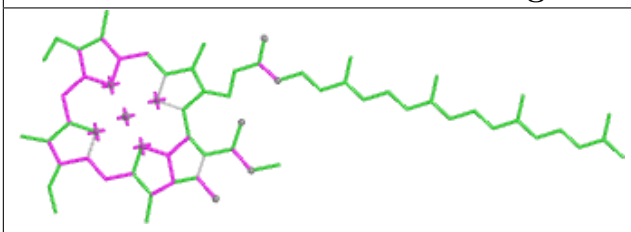


Rings

Ligand CLA d 402



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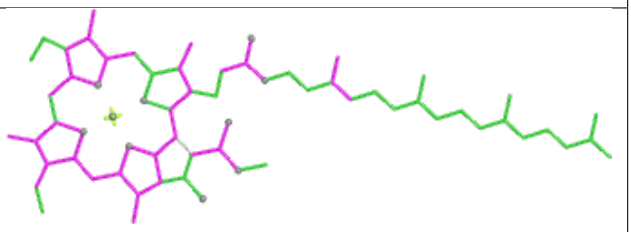
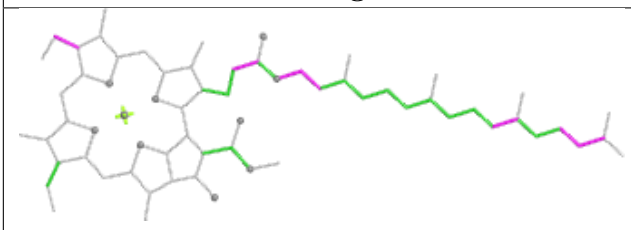


Bond angles



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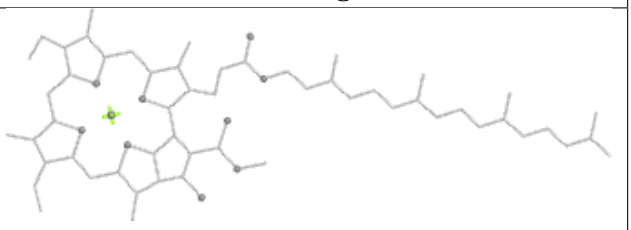
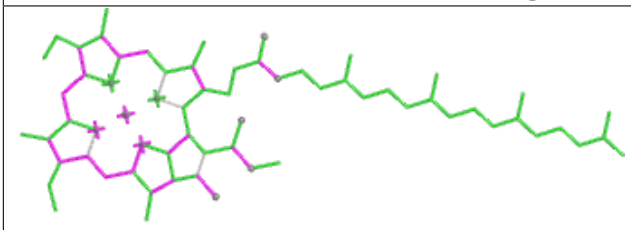


Rings

Ligand CLA A 405



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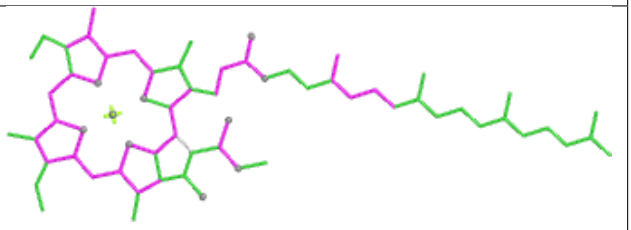
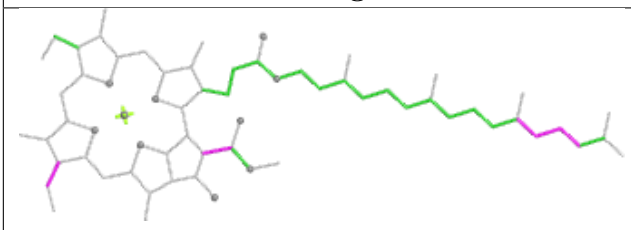


Bond angles



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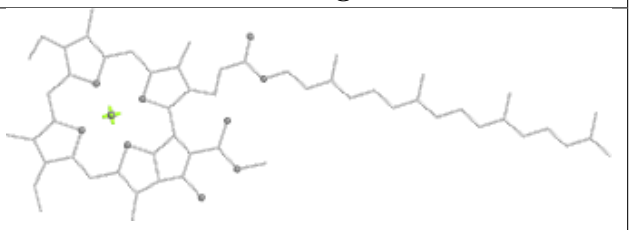
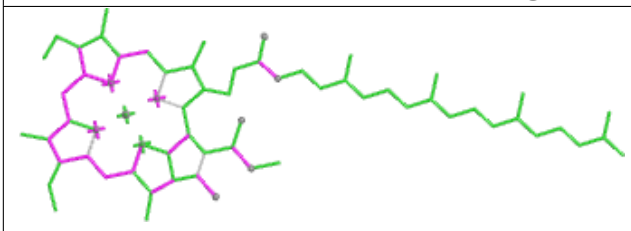
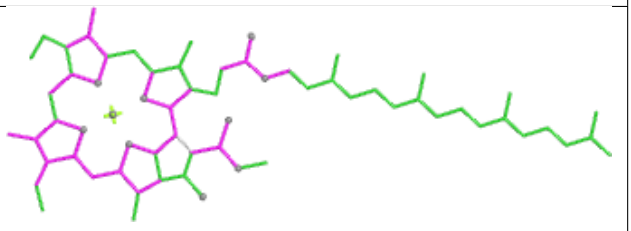


Rings

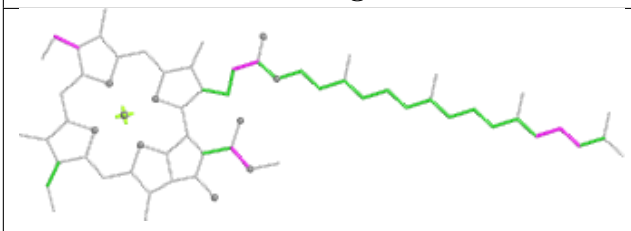
Ligand CLA C 502



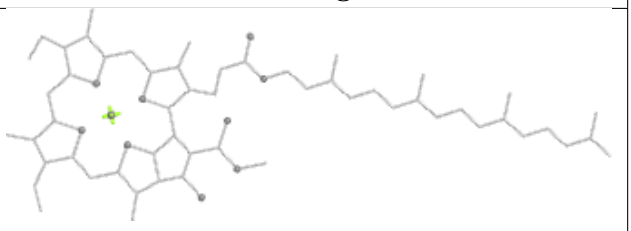
Bond lengths



Bond angles

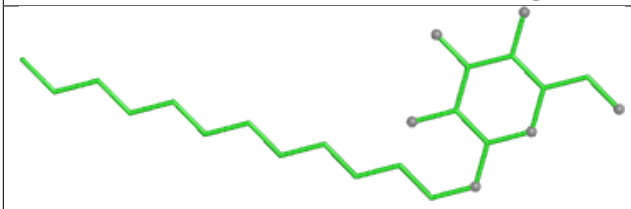


Torsions

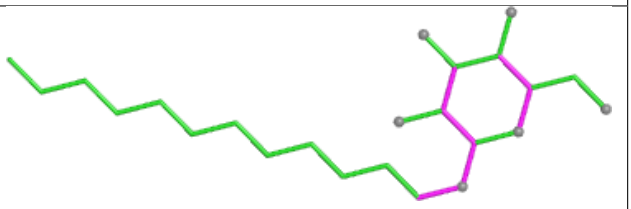


Rings

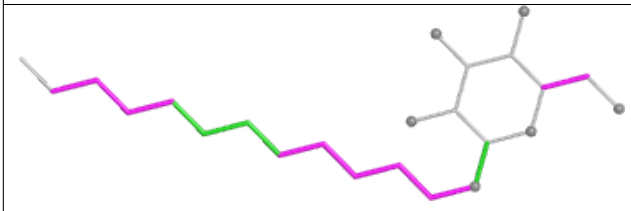
Ligand LMT t 101



Bond lengths



Bond angles



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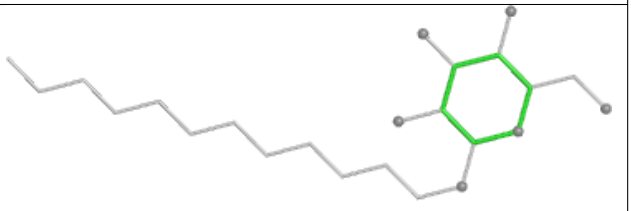
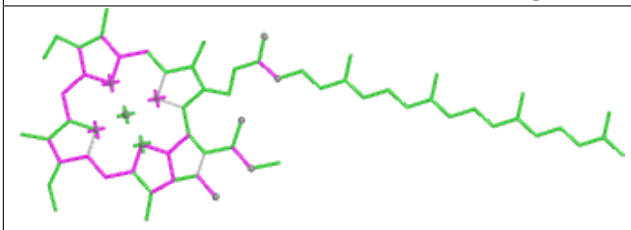
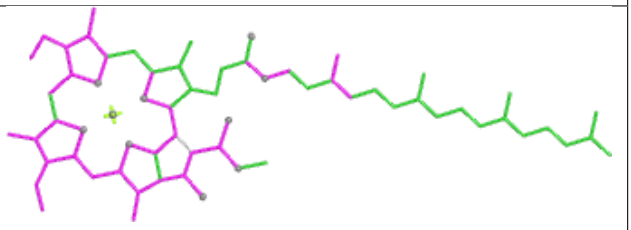


Rings

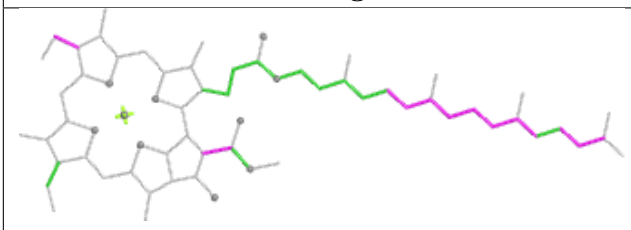
Ligand CLA b 608



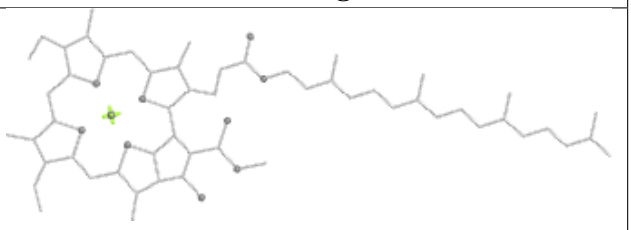
Bond lengths



Bond angles

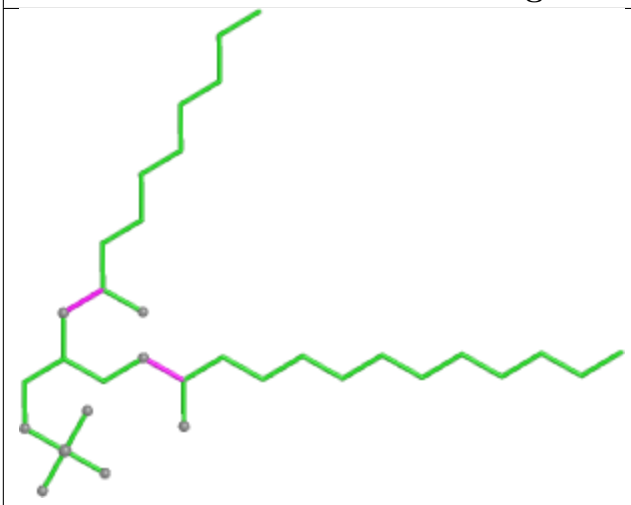


Torsions



Rings

Ligand LHG d 401



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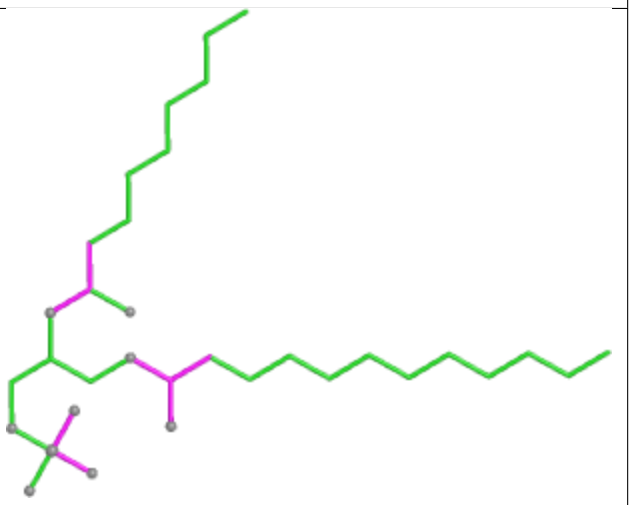
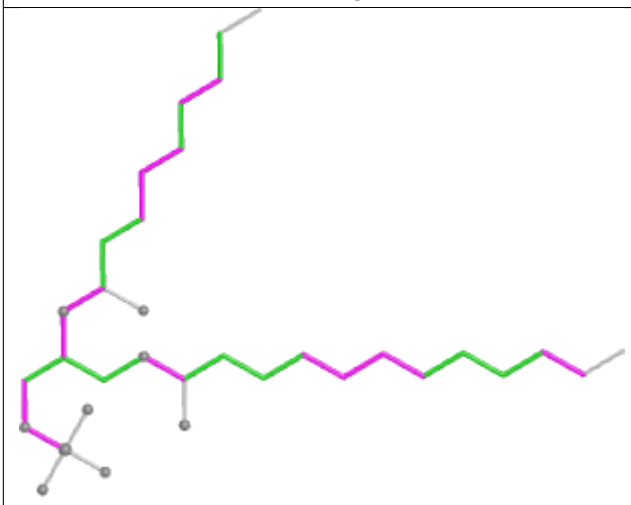
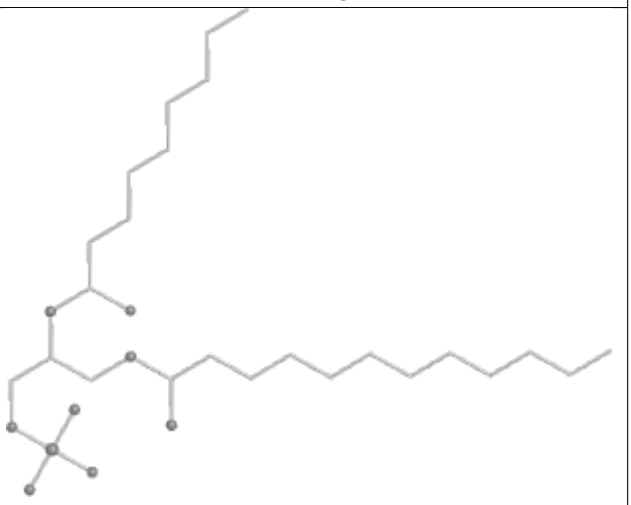


Bond angles

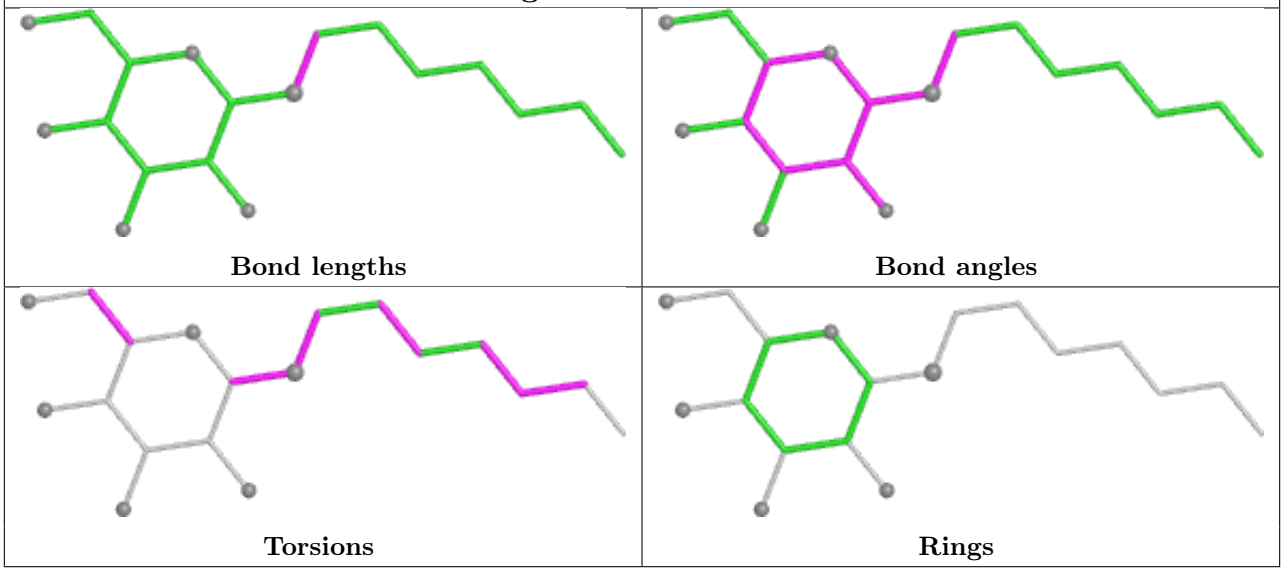


Torsions

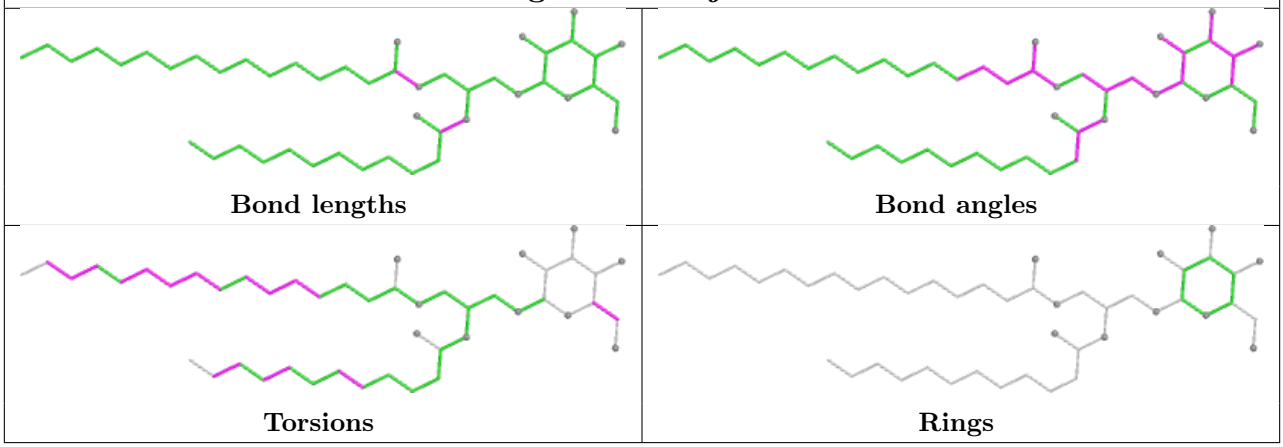


Rings

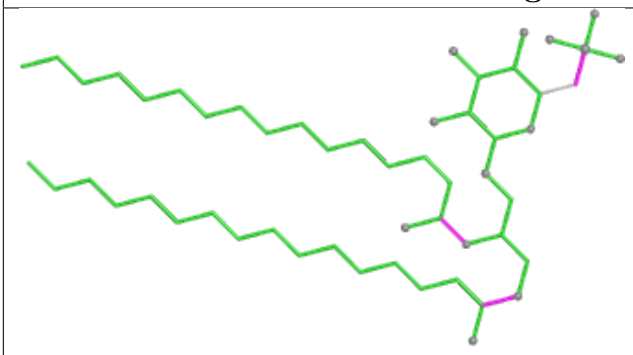
Ligand HTG D 415



Ligand LMG j 101



Ligand SQD C 501



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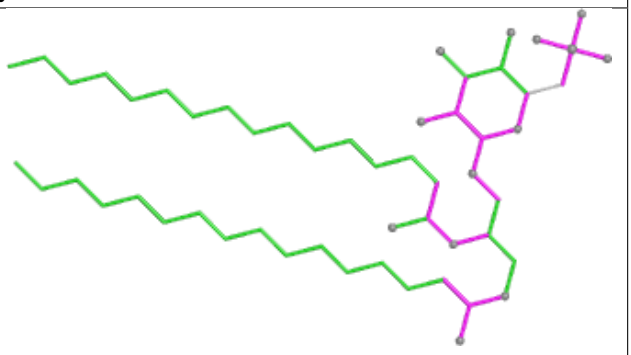
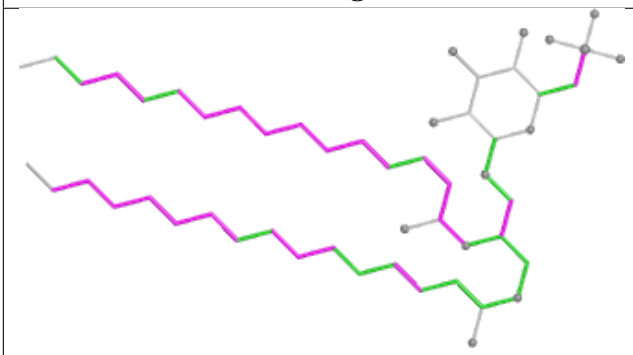
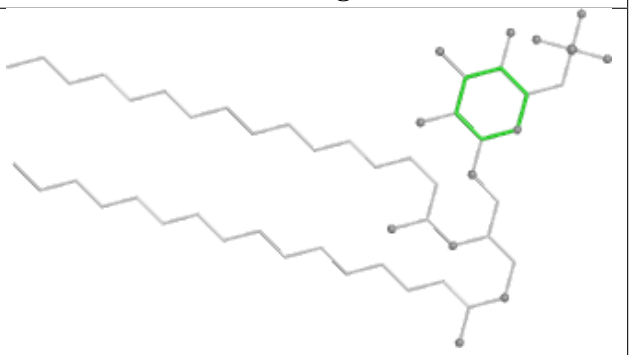


Bond angles

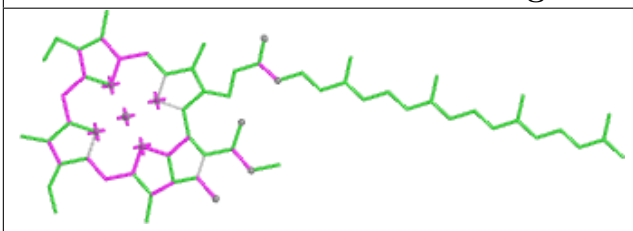


Torsions



Rings

Ligand CLA b 603



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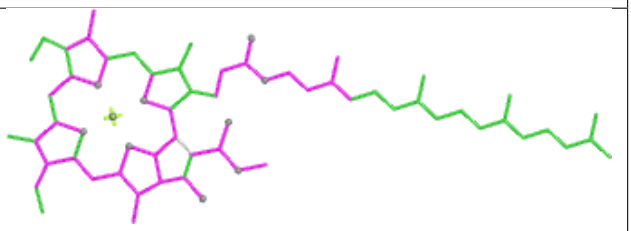
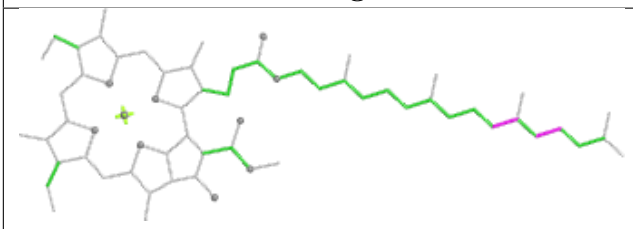


Bond angles



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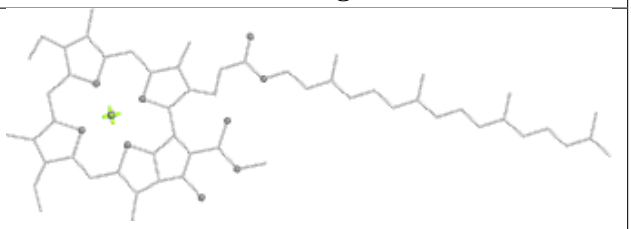
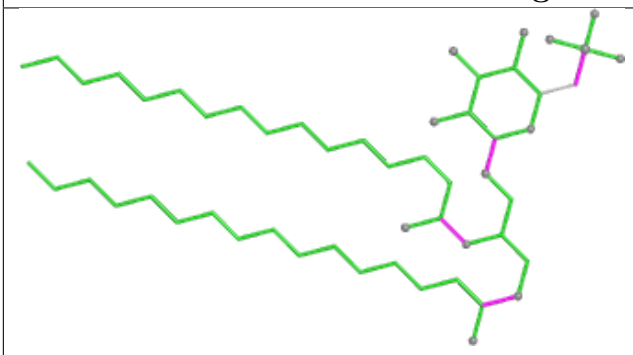


Rings

Ligand SQD l 101



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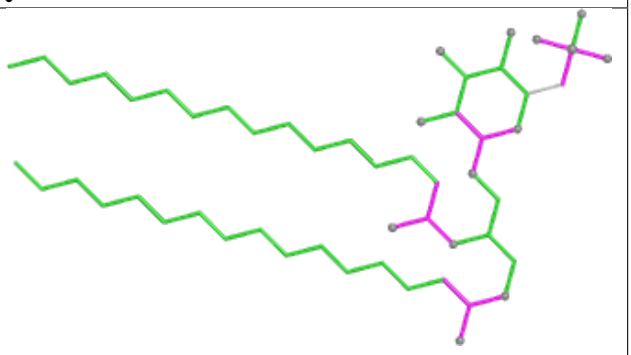
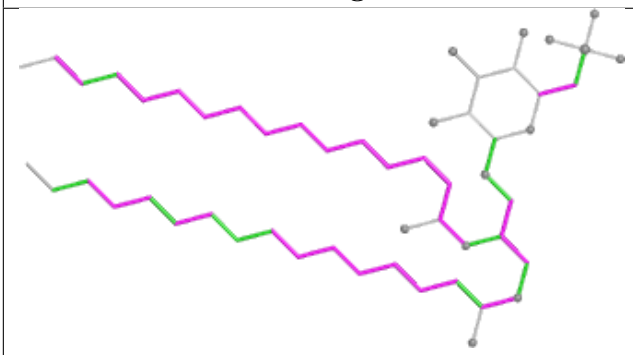


Bond angles



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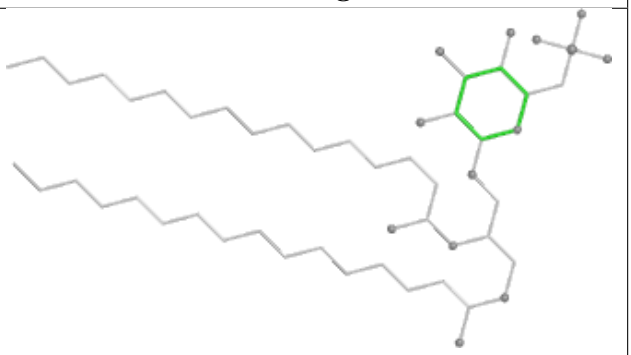
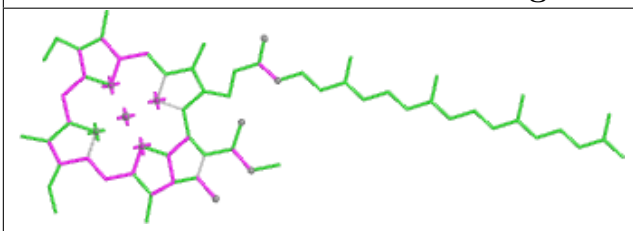


Rings

Ligand CLA c 907



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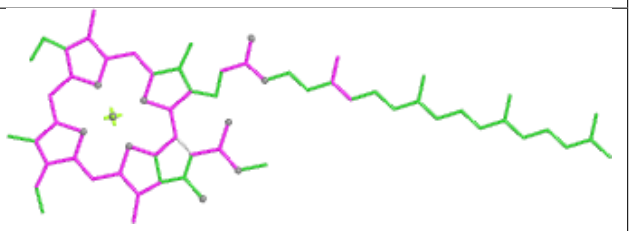
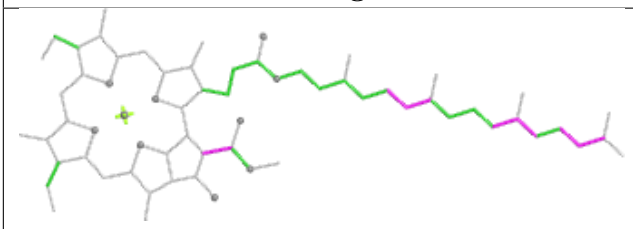


Bond angles



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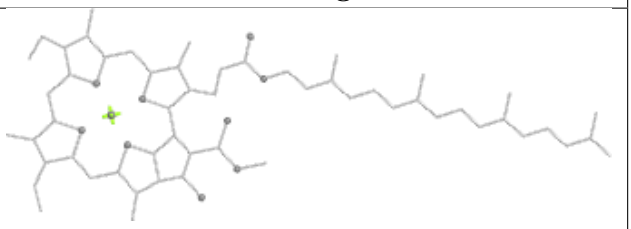
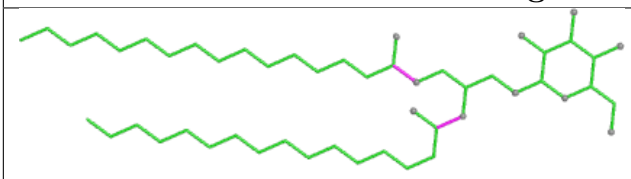


Rings

Ligand LMG i 101



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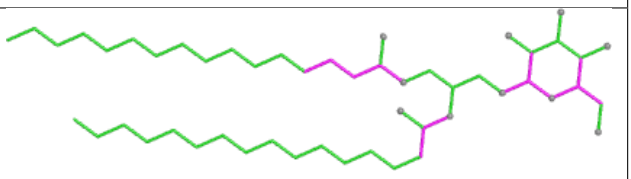
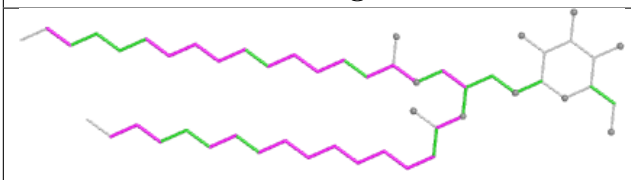


Bond angles



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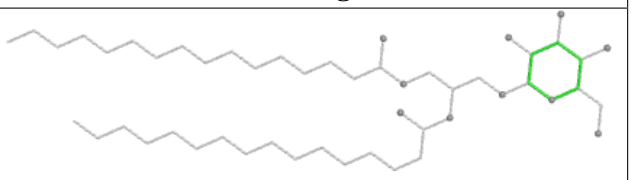
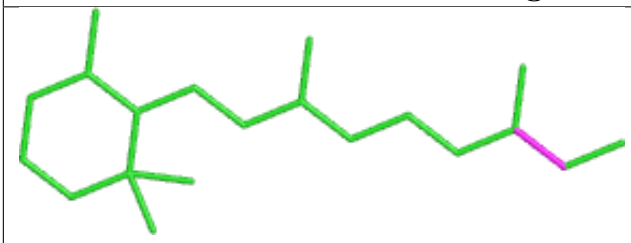


Rings

Ligand BCR b 618



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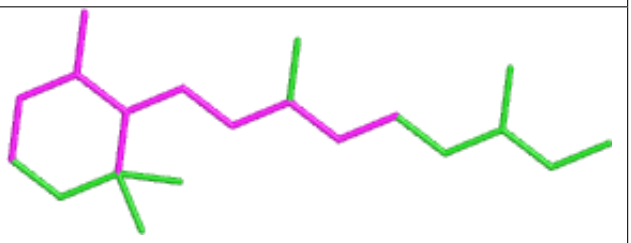
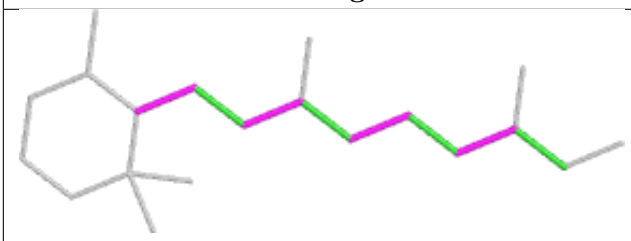
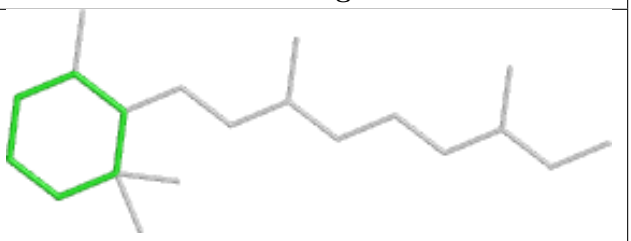


Bond angles

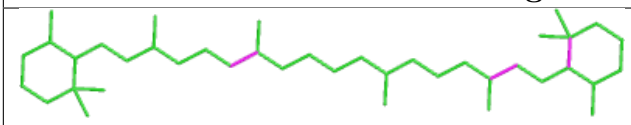


Torsions



Rings

Ligand BCR d 404



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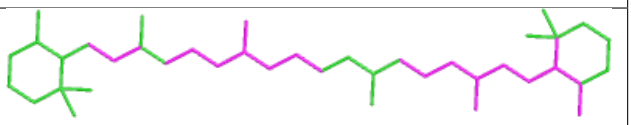
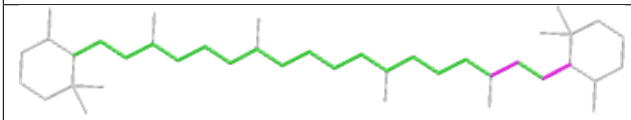


Bond angles



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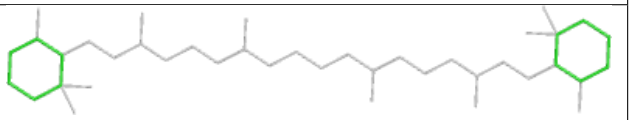
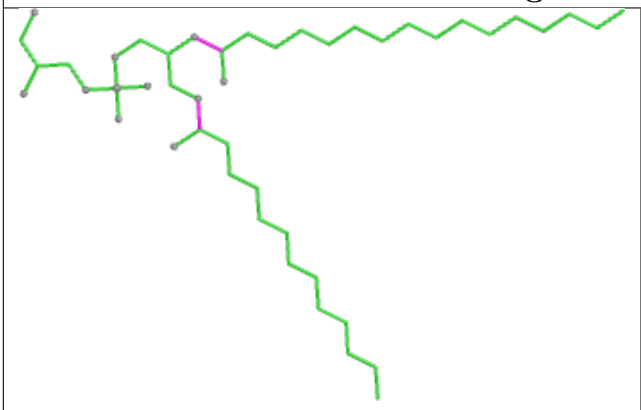


Rings

Ligand LHG d 408



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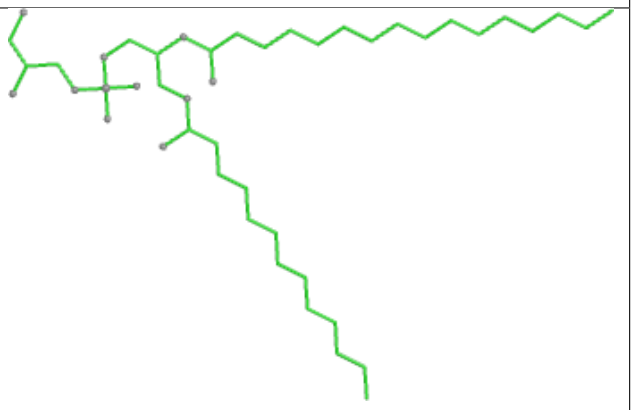

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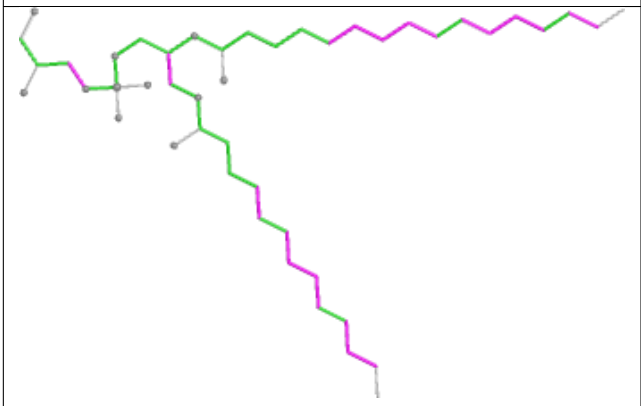

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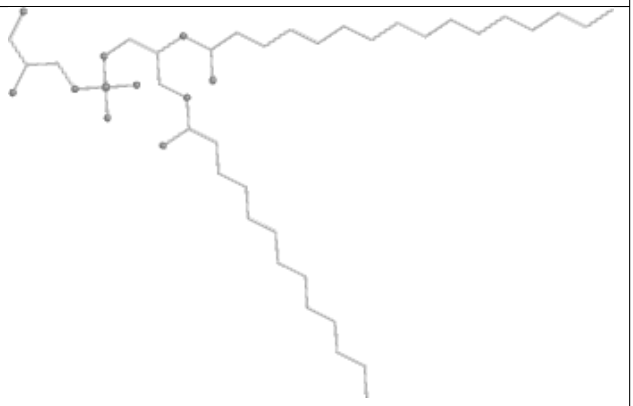
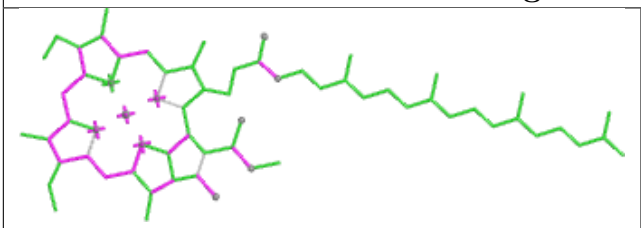


Rings

Ligand CLA D 403



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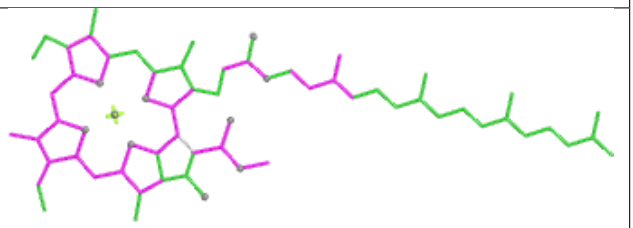
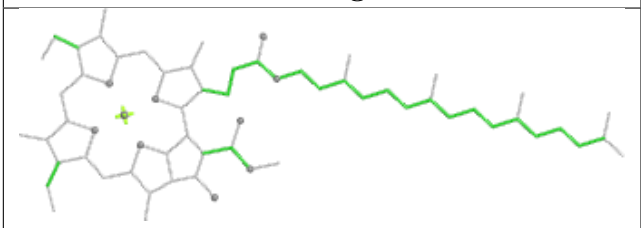
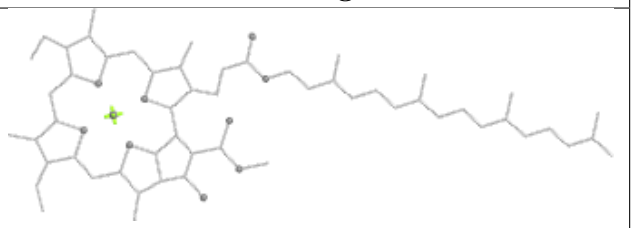


Bond angles

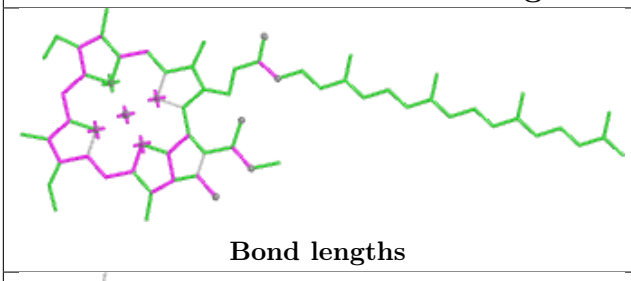


Torsions



Rings

Ligand CLA B 607



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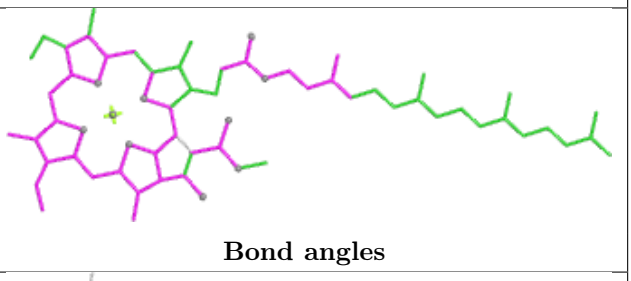
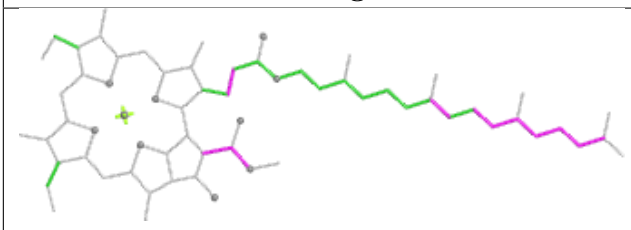


Bond angles



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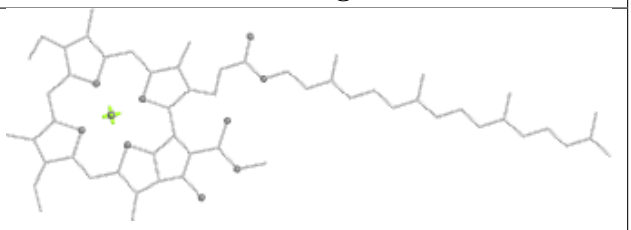
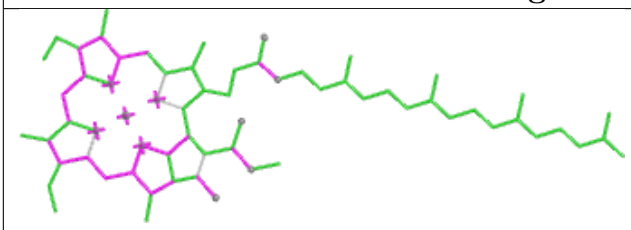


Rings

Ligand CLA a 408



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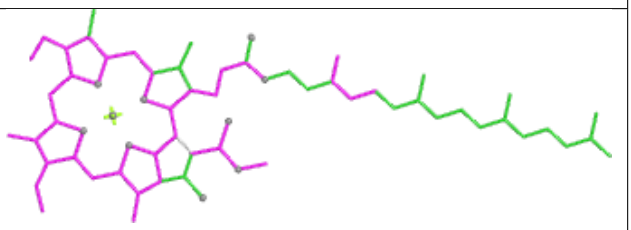
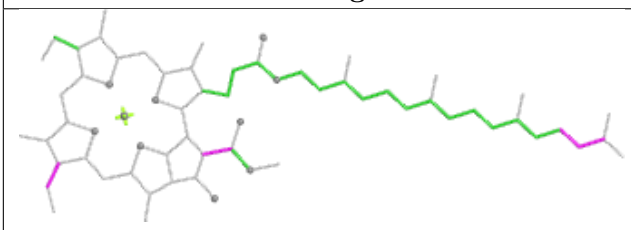


Bond angles



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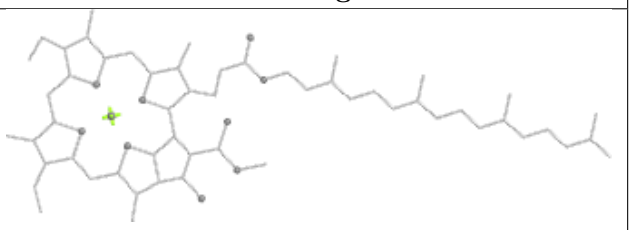
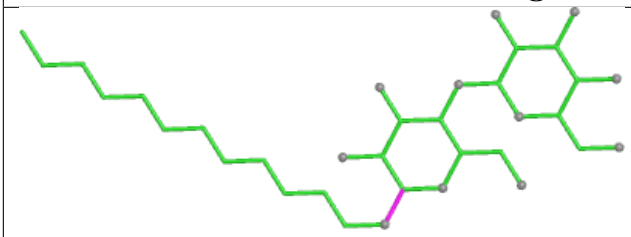
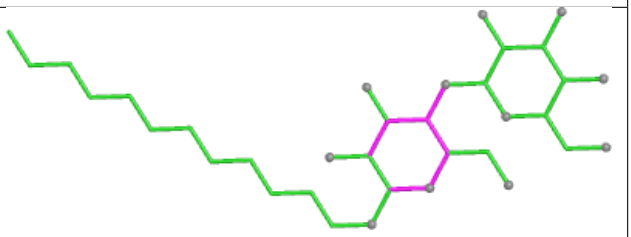


Rings

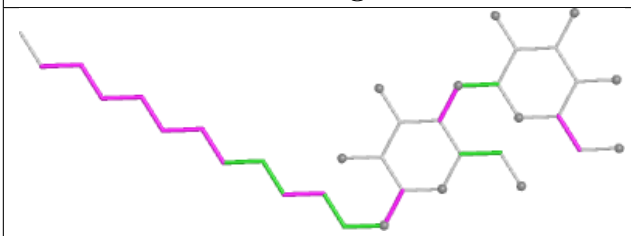
Ligand LMT I 102



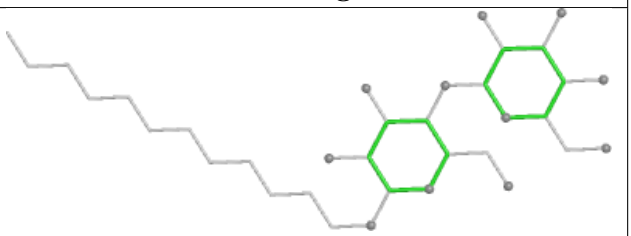
Bond lengths



Bond angles

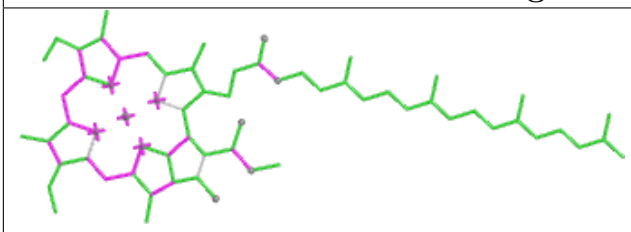


Torsions

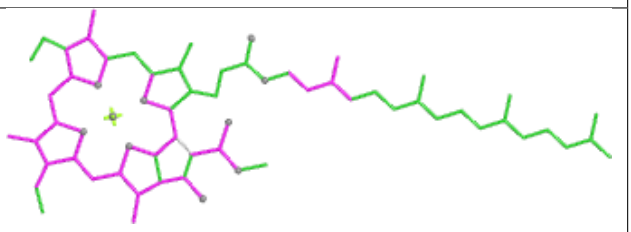


Rings

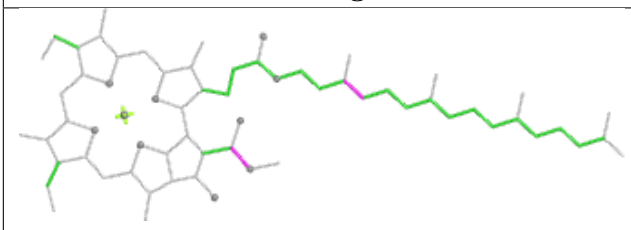
Ligand CLA b 606



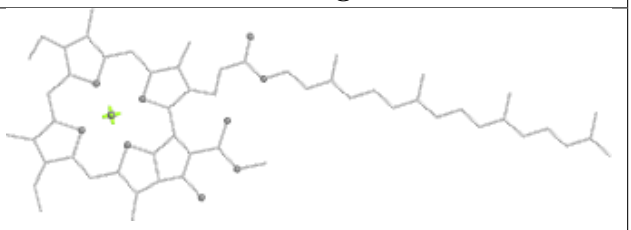
Bond lengths



Bond angles

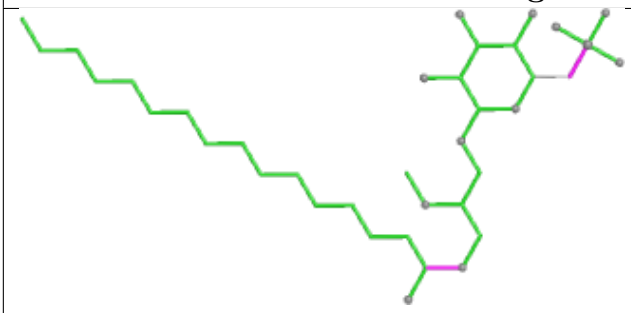


Torsions

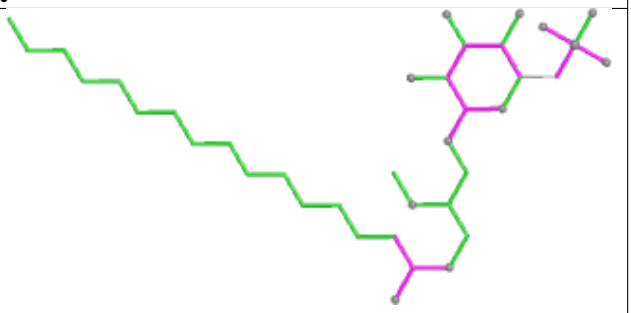


Rings

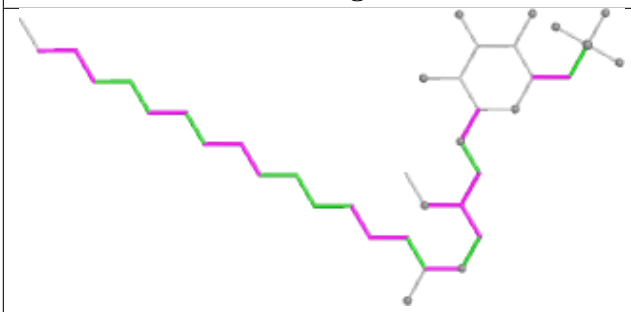
Ligand SQD b 621



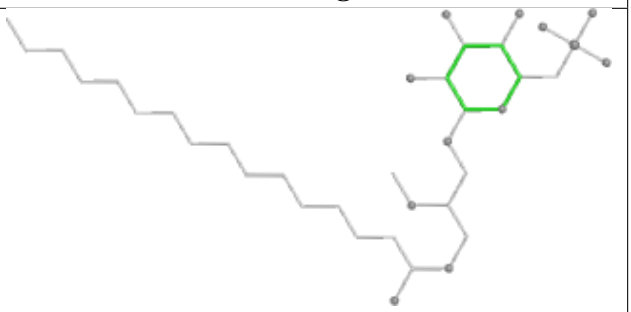
Bond lengths



Bond angles

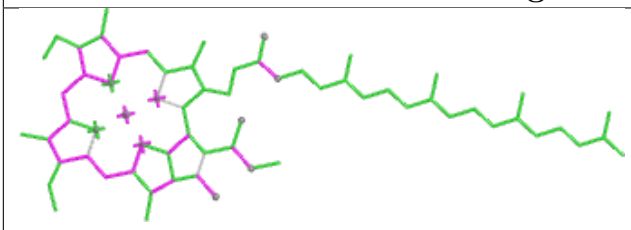


Torsions

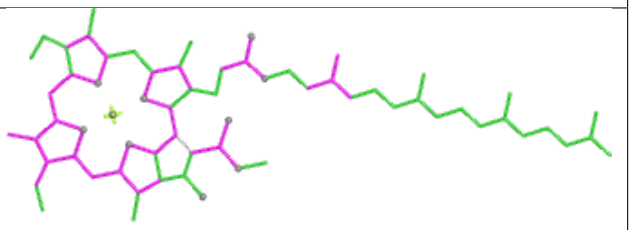


Rings

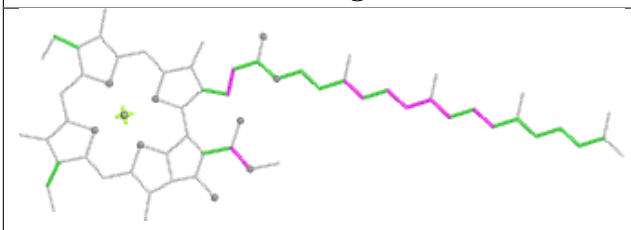
Ligand CLA b 604



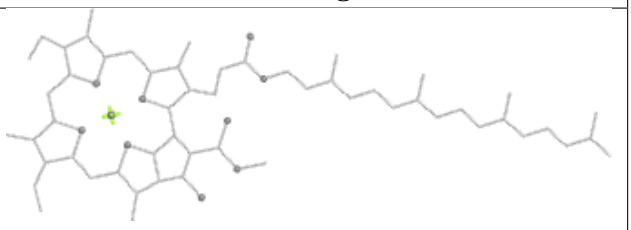
Bond lengths



Bond angles

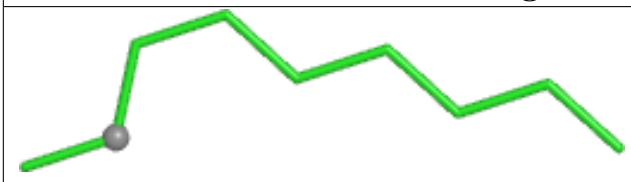


Torsions

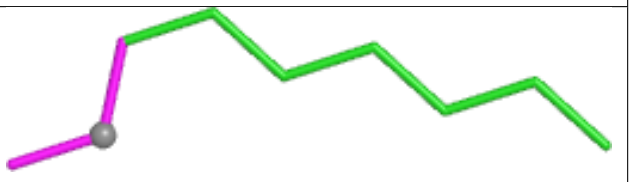


Rings

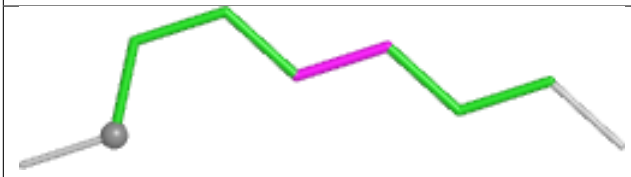
Ligand HTG C 523



Bond lengths



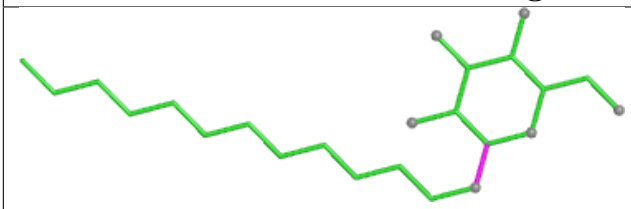
Bond angles



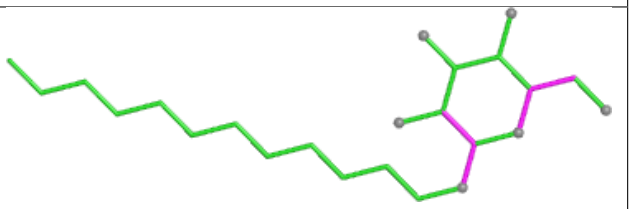
Torsions

Rings

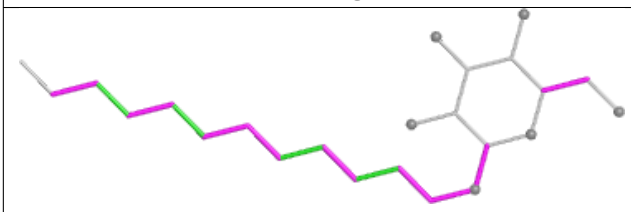
Ligand LMT c 931



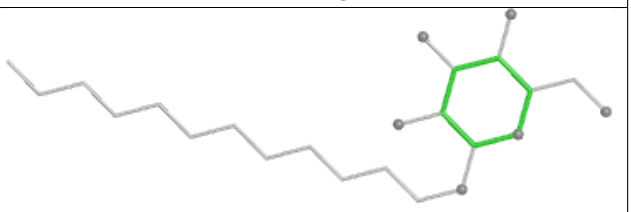
Bond lengths



Bond angles

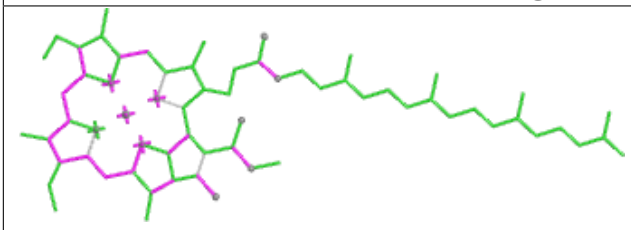


Torsions

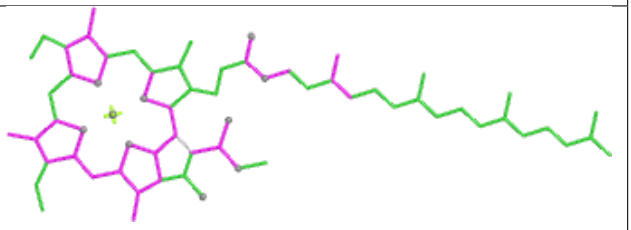


Rings

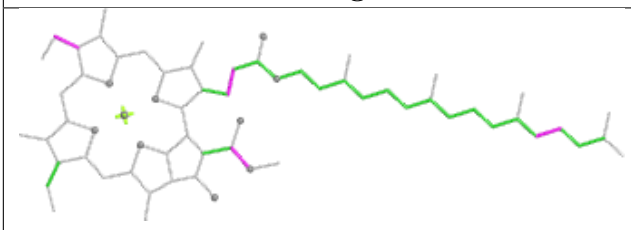
Ligand CLA c 902



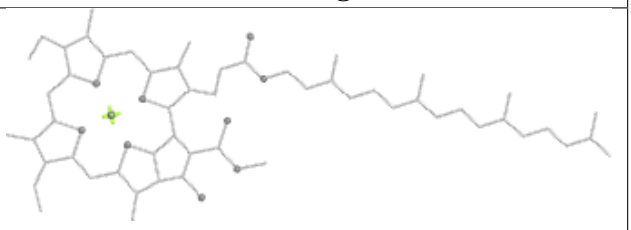
Bond lengths



Bond angles



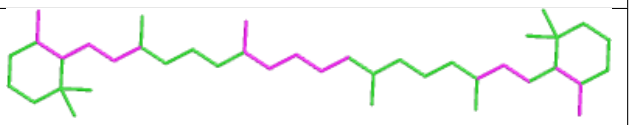
Torsions



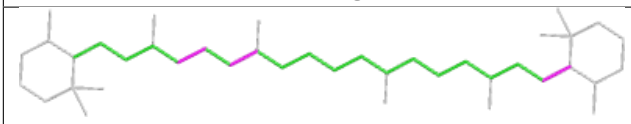
Rings

Ligand BCR c 915

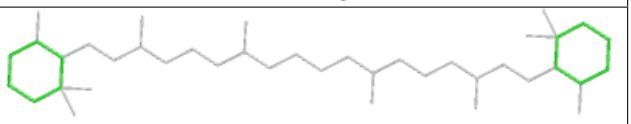
Bond lengths



Bond angles

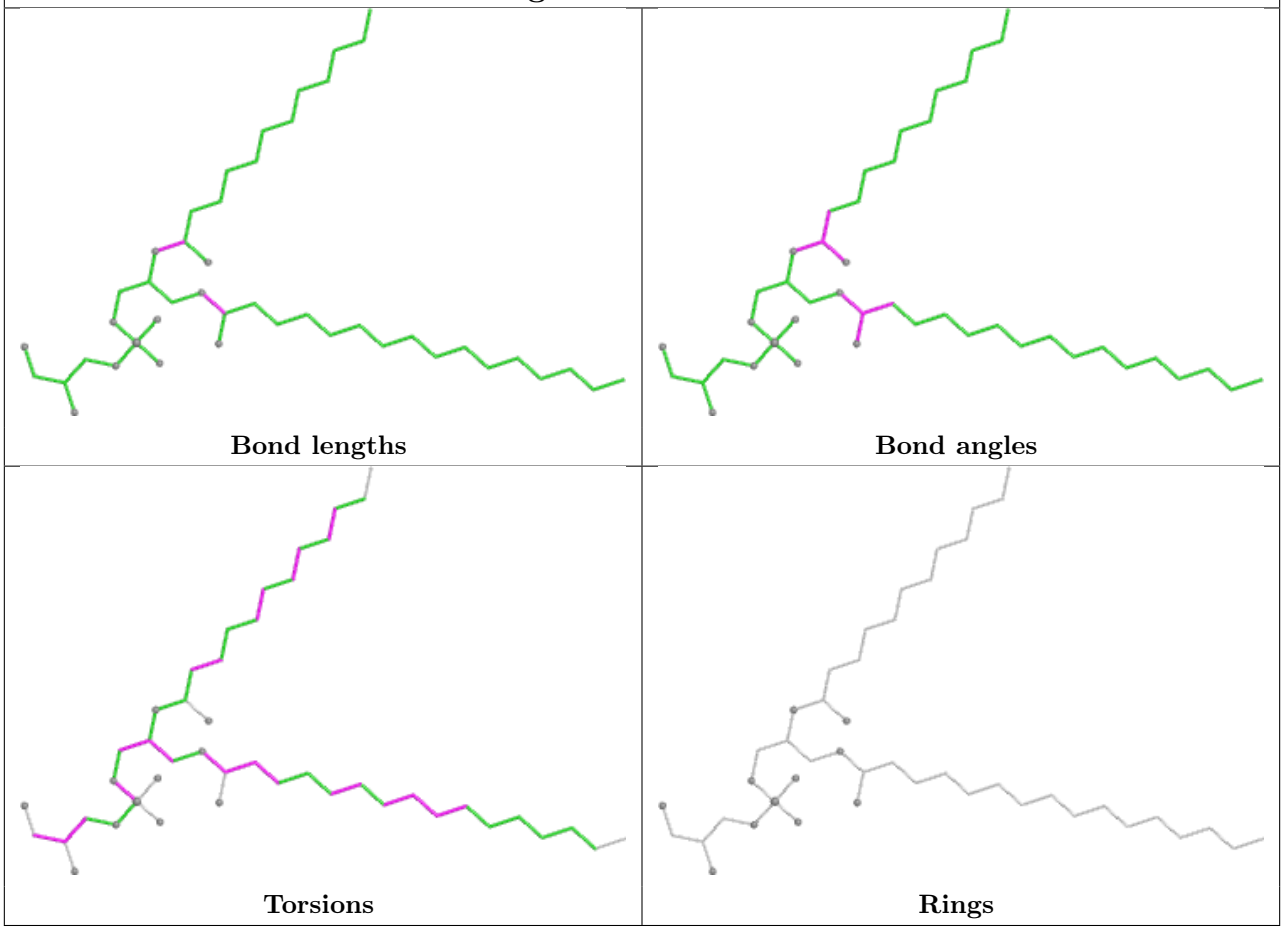


Torsions

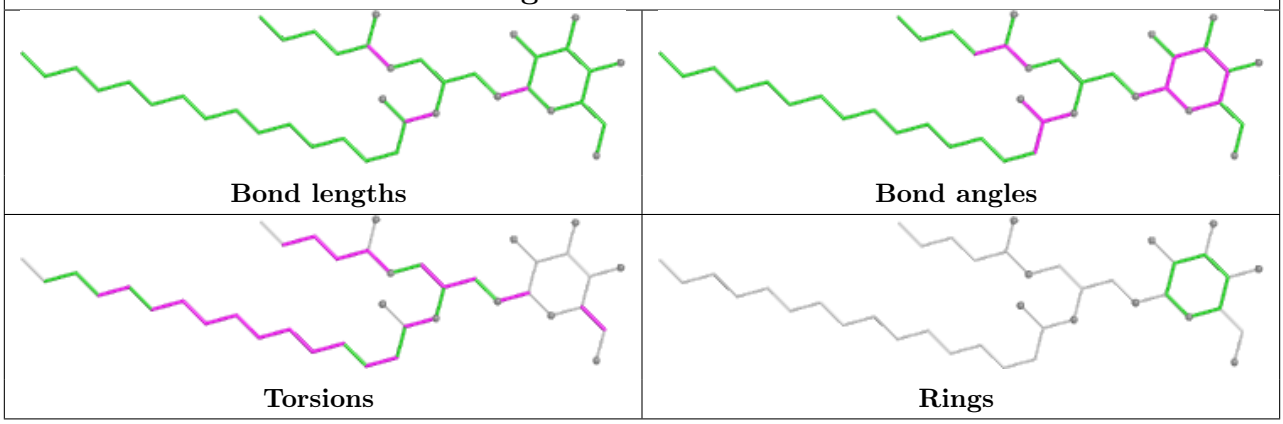


Rings

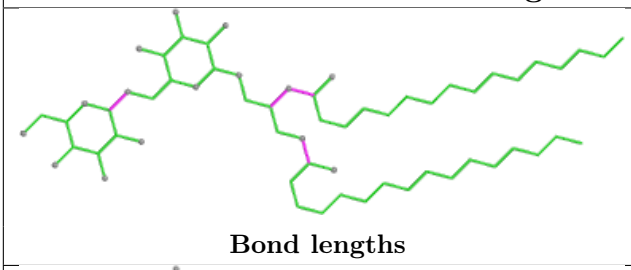
Ligand LHG a 423



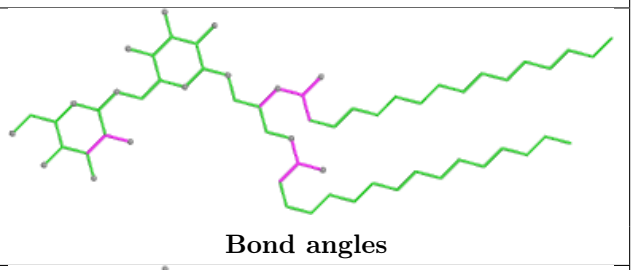
Ligand LMG B 621



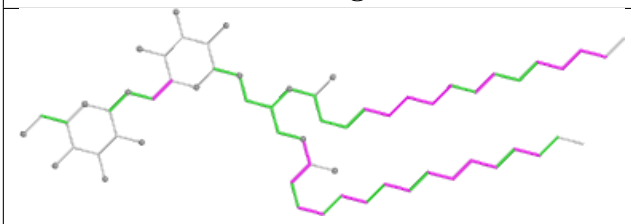
Ligand DGD c 919



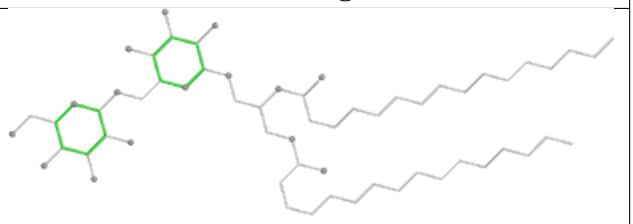
Bond lengths



Bond angles

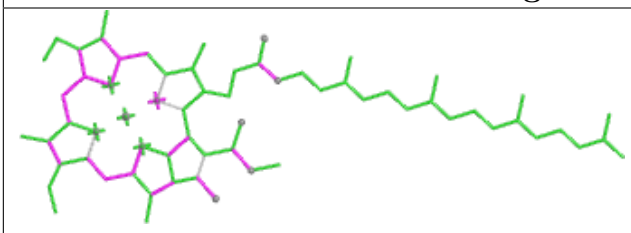


Torsions



Rings

Ligand CLA D 401



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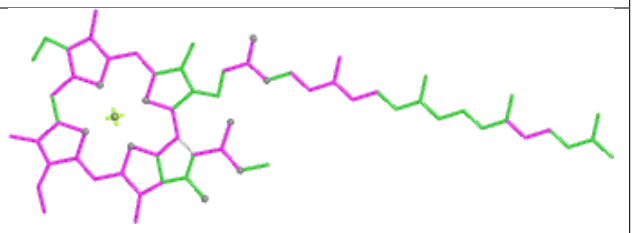
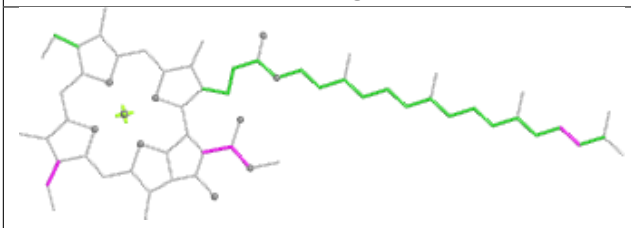


Bond angles



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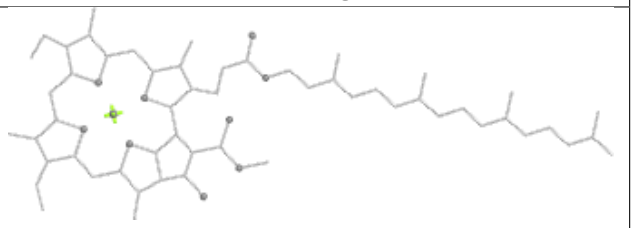
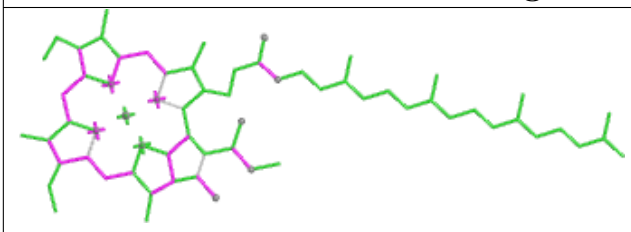


Rings

Ligand CLA A 408



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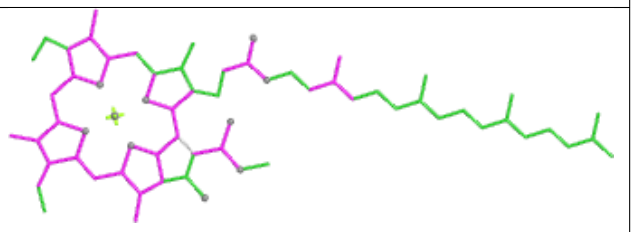
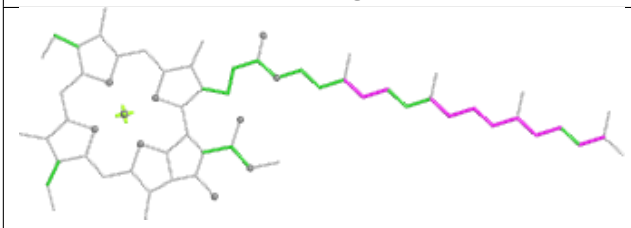


Bond angles



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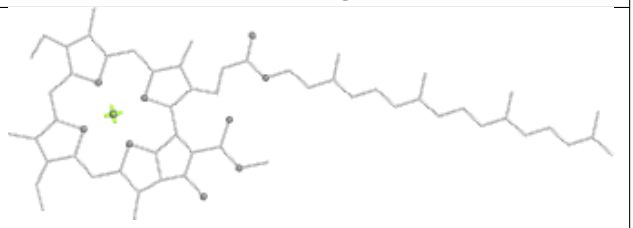
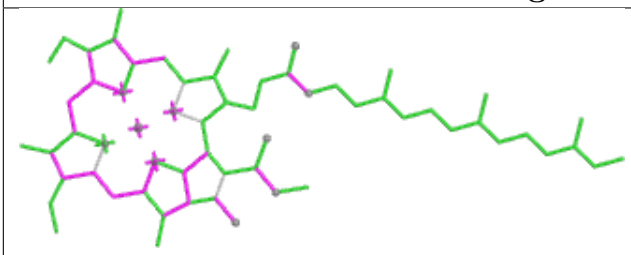
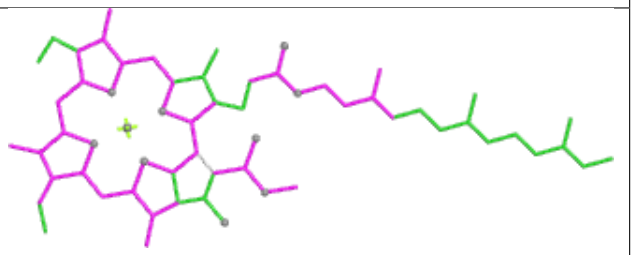


Rings

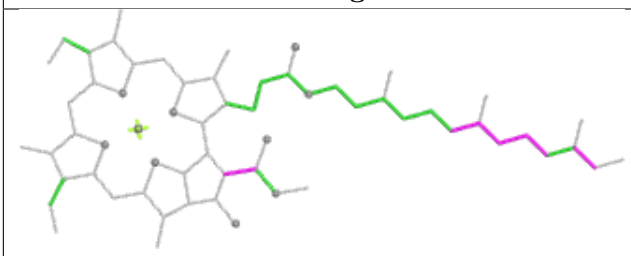
Ligand CLA a 409



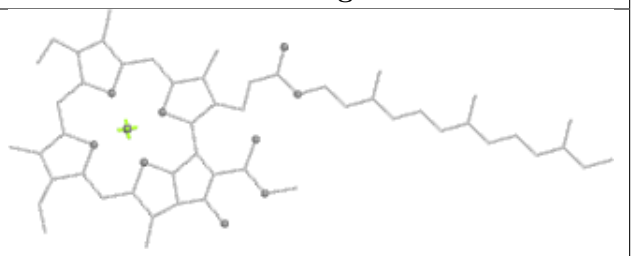
Bond lengths



Bond angles

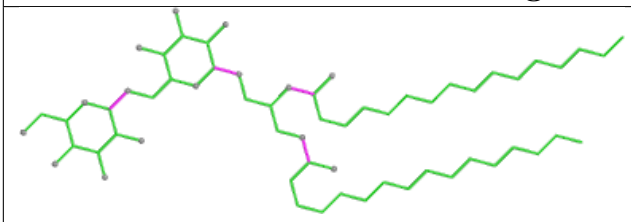


Torsions

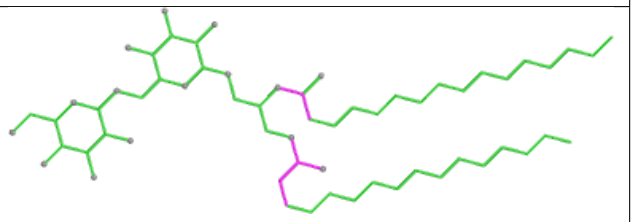


Rings

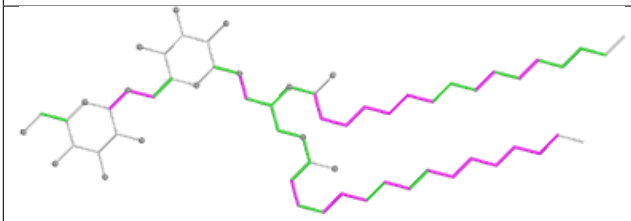
Ligand DGD c 918



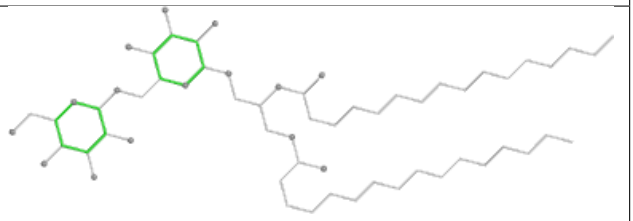
Bond lengths



Bond angles

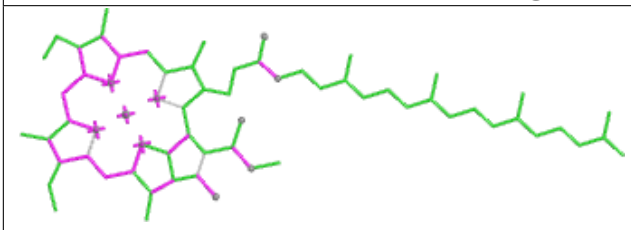


Torsions

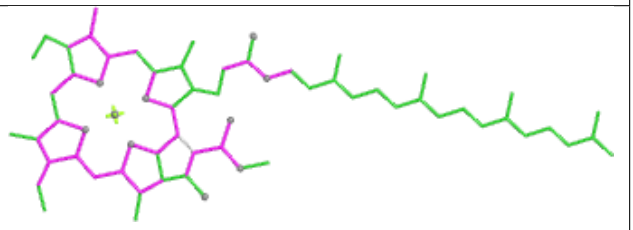


Rings

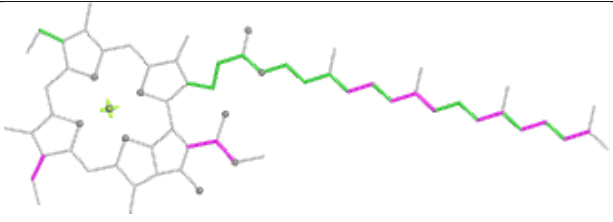
Ligand CLA b 605



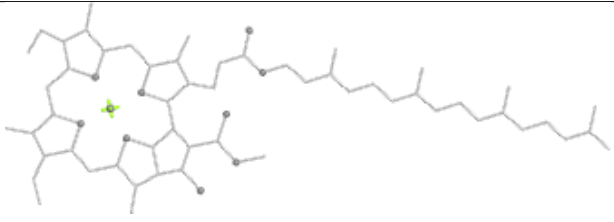
Bond lengths



Bond angles

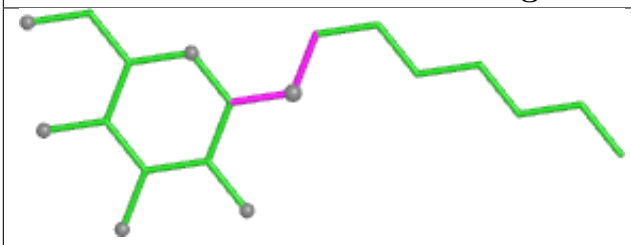


Torsions

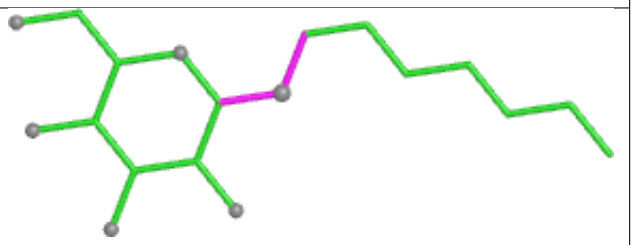


Rings

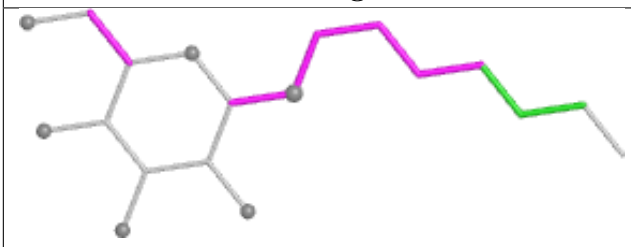
Ligand HTG C 532



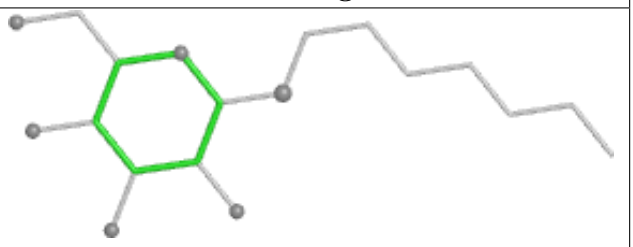
Bond lengths



Bond angles

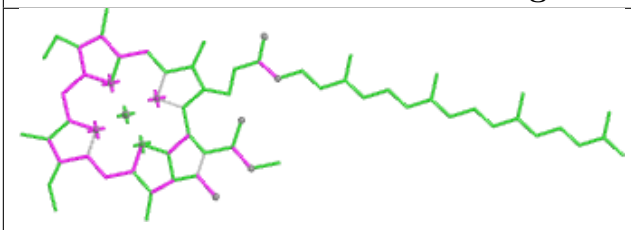


Torsions



Rings

Ligand CLA c 906



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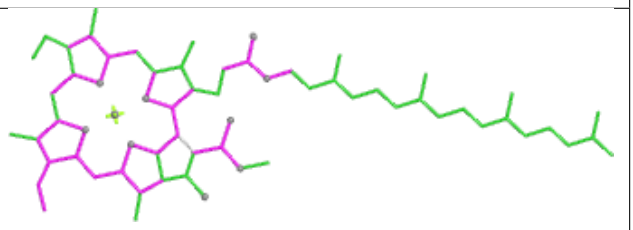
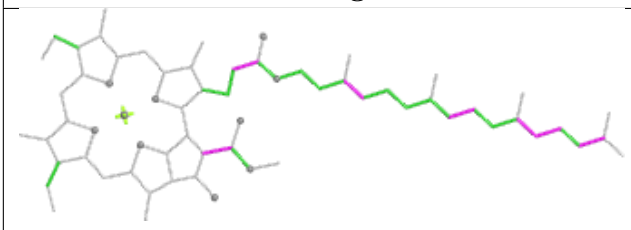
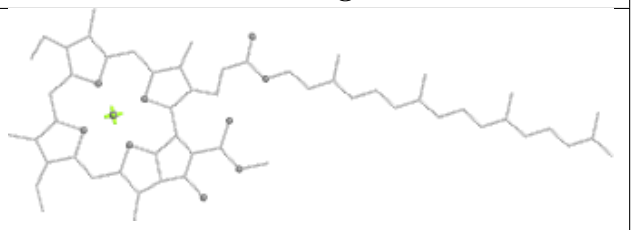


Bond angles

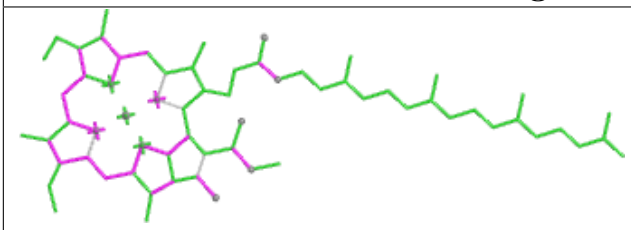


Torsions

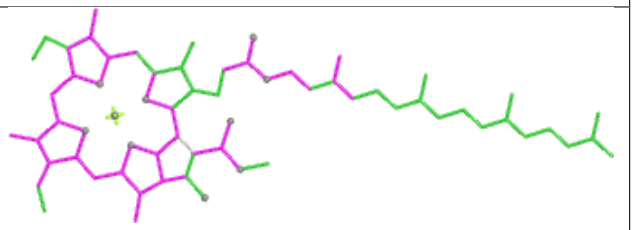


Rings

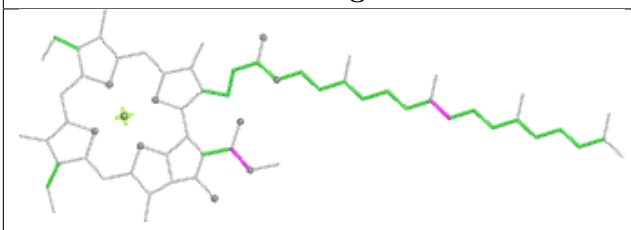
Ligand CLA c 912



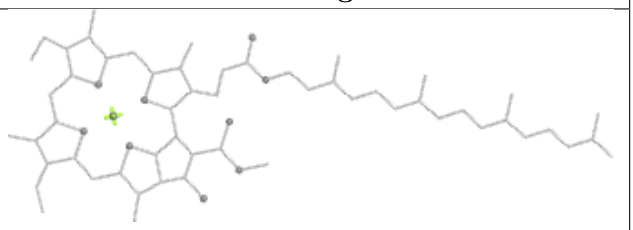
Bond lengths



Bond angles

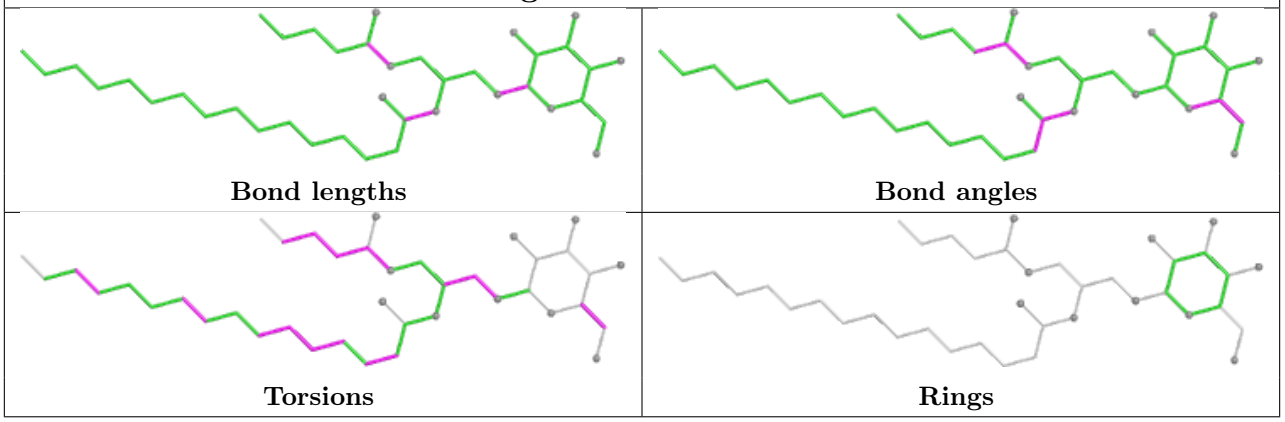


Torsions

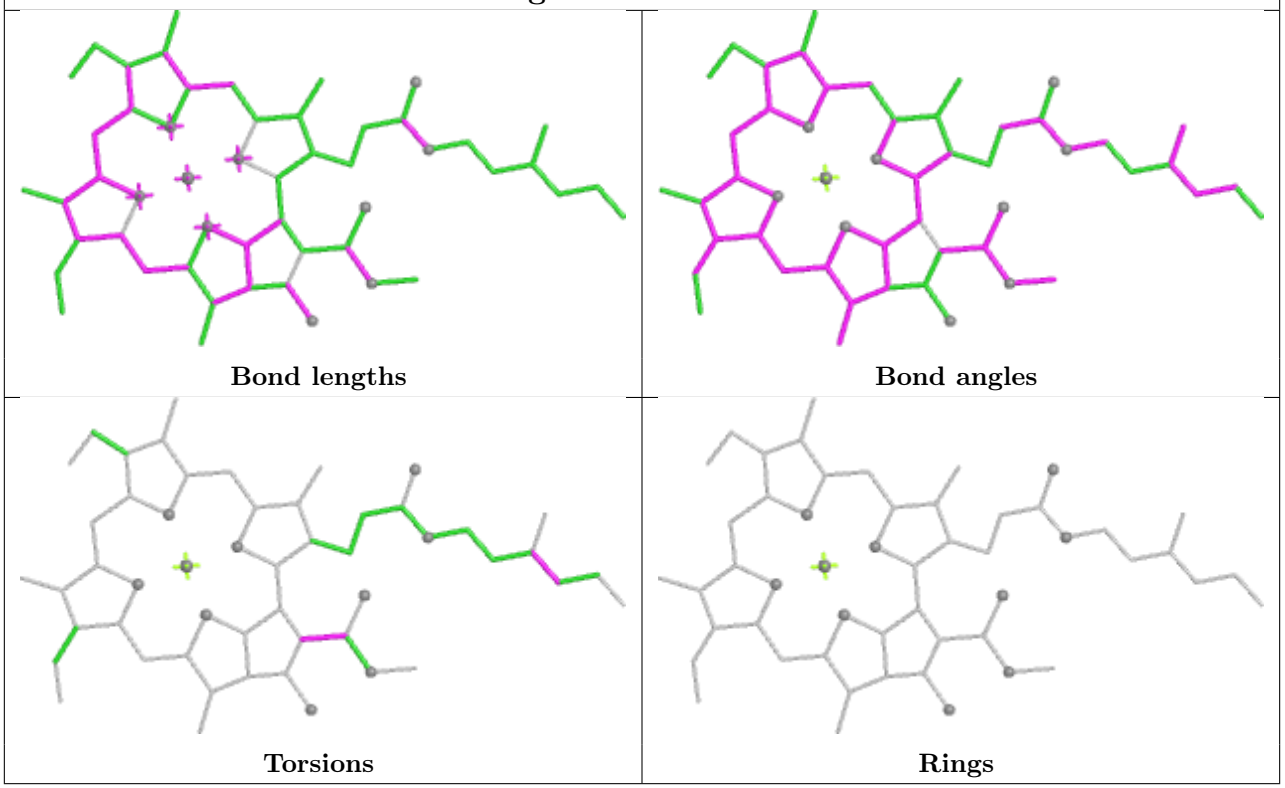


Rings

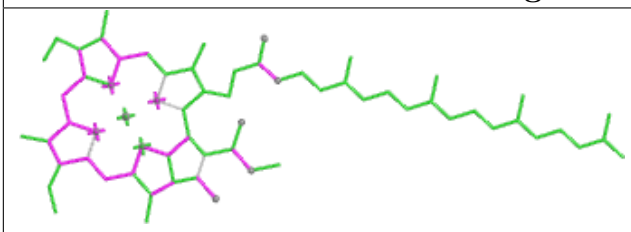
Ligand LMG C 531



Ligand CLA b 615



Ligand CLA C 512



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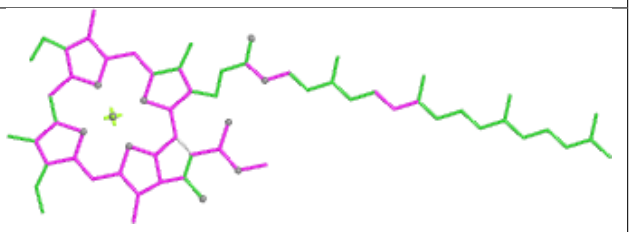
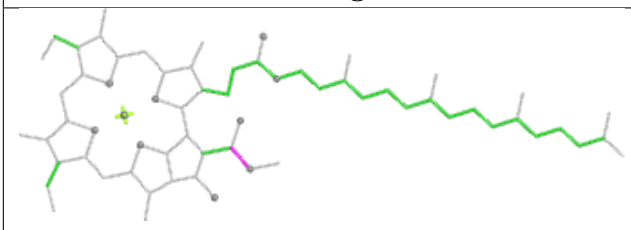
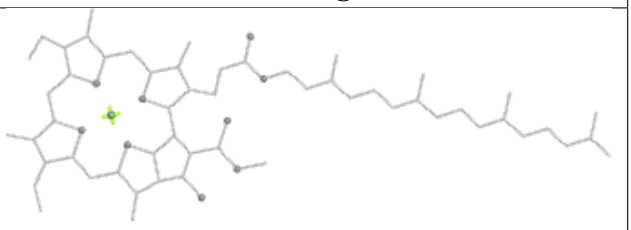


Bond angles

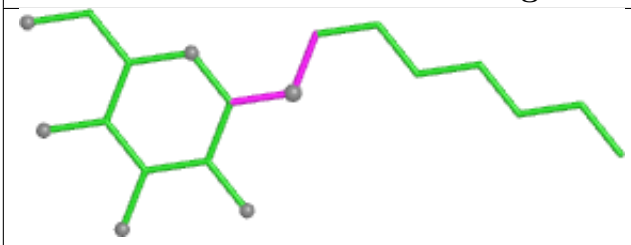


Torsions

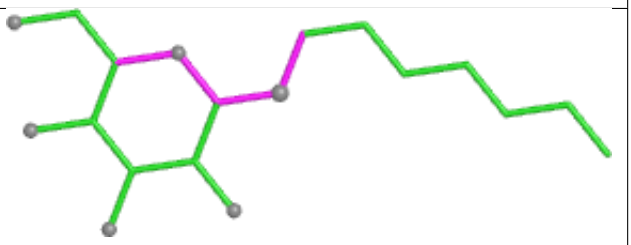


Rings

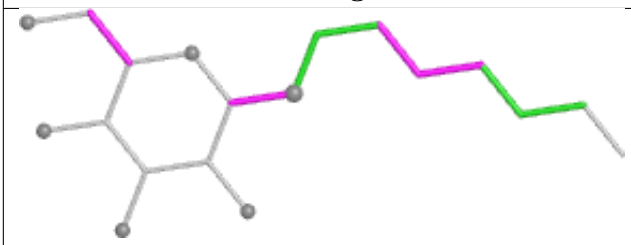
Ligand HTG C 521



Bond lengths



Bond angles



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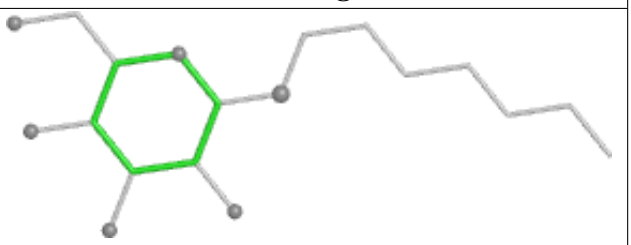
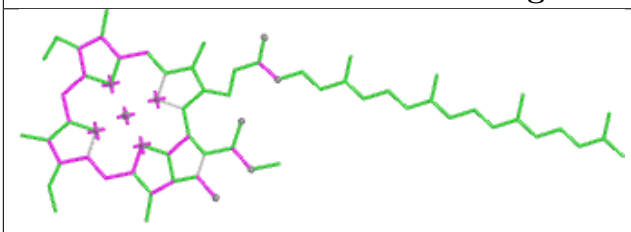


Rings

Ligand CLA b 616



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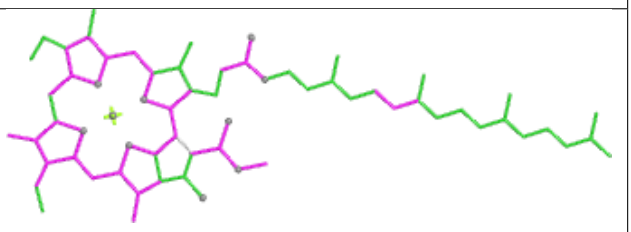
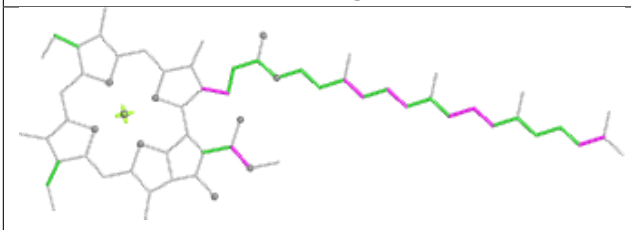
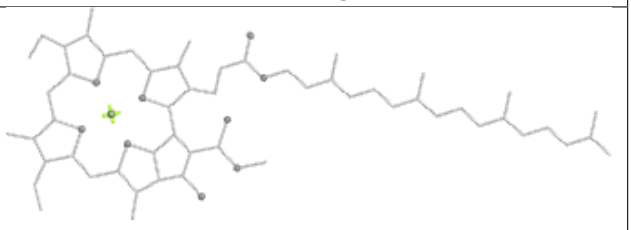


Bond angles

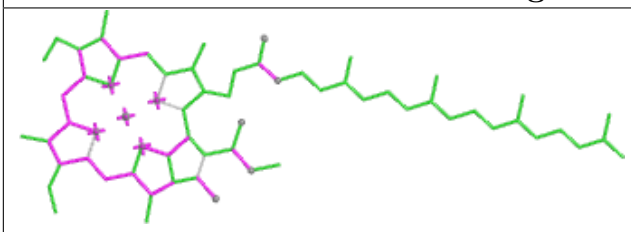


Torsions

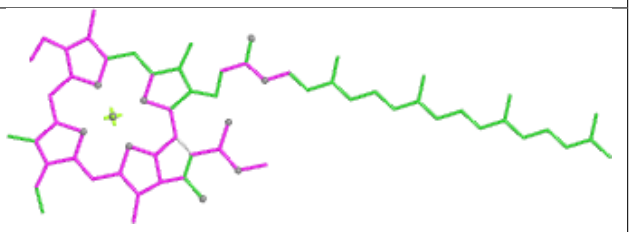


Rings

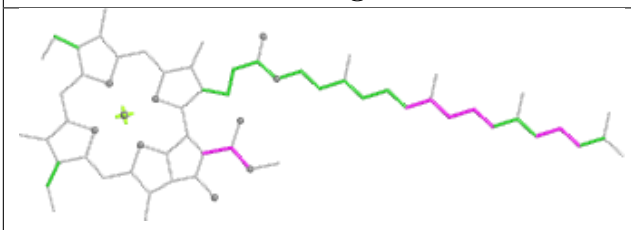
Ligand CLA d 403



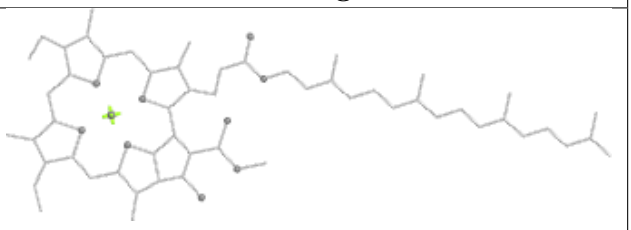
Bond lengths



Bond angles

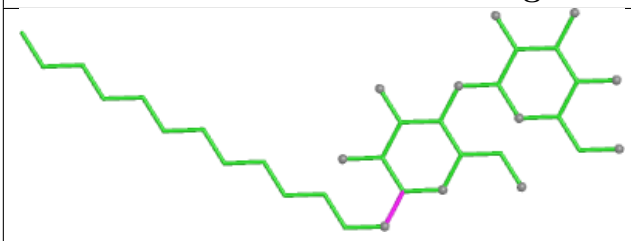


Torsions

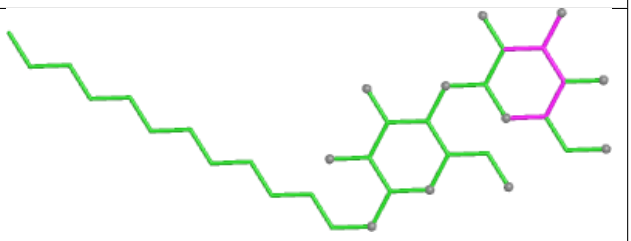


Rings

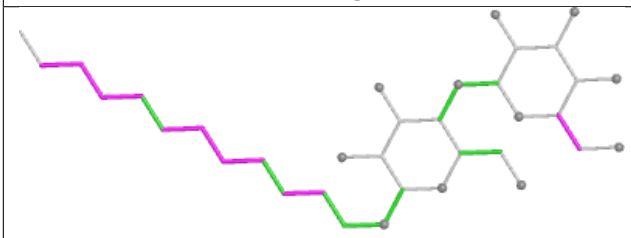
Ligand LMT Z 101



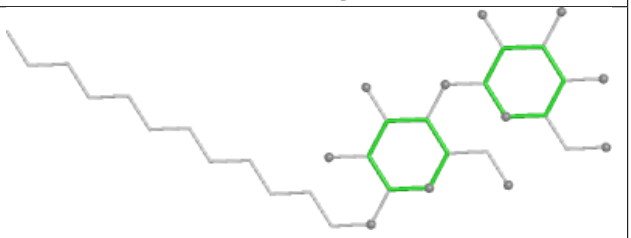
Bond lengths



Bond angles

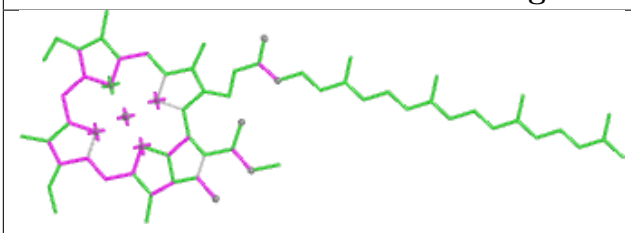


Torsions

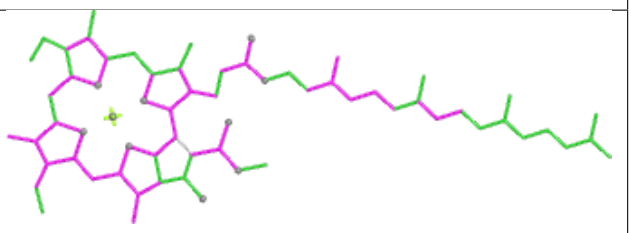


Rings

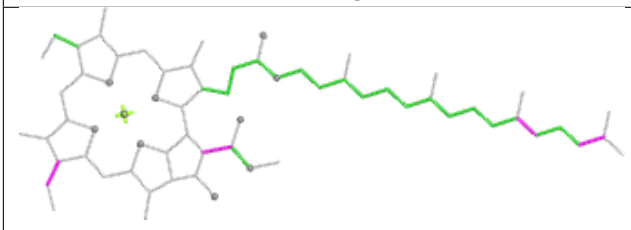
Ligand CLA a 407



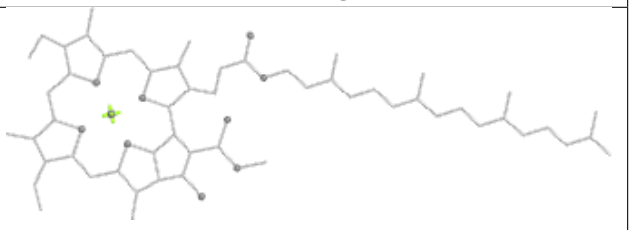
Bond lengths



Bond angles

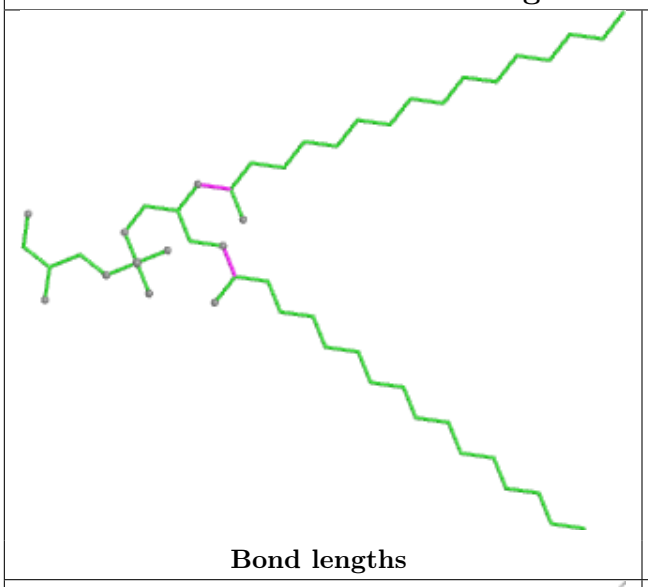


Torsions



Rings

Ligand LHG D 409



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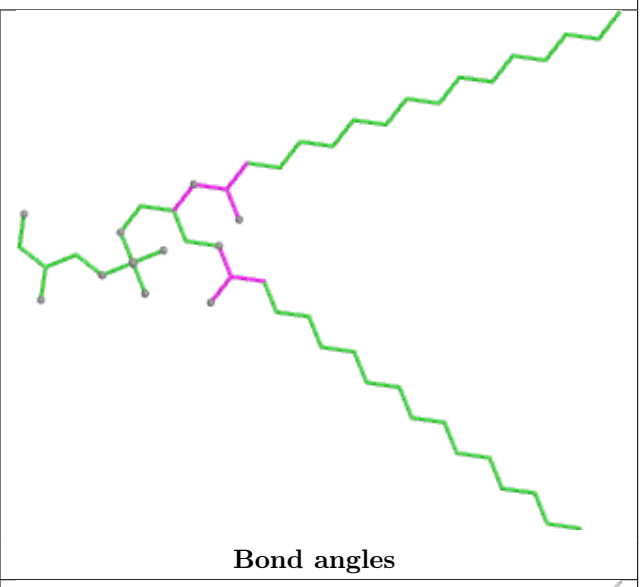
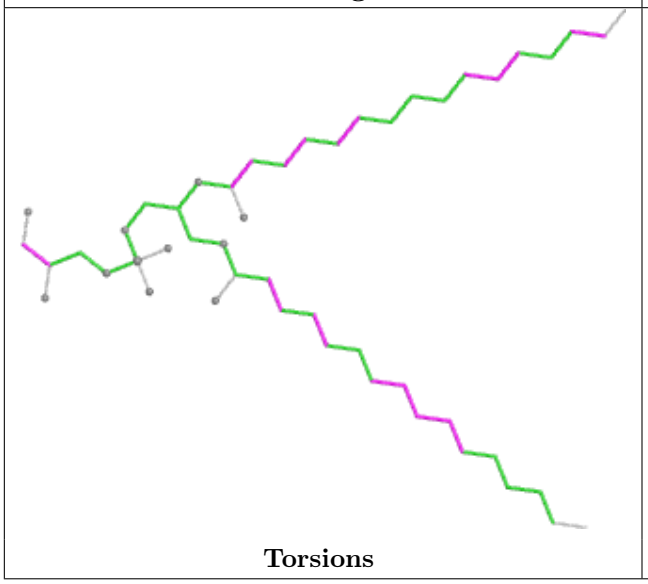
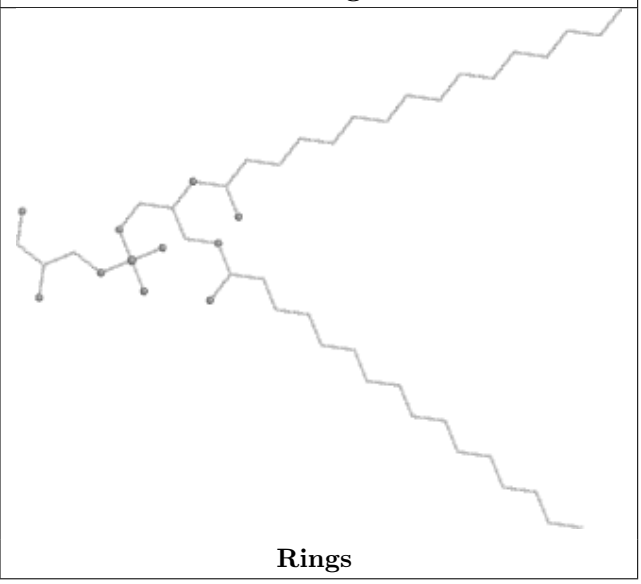


Bond angles

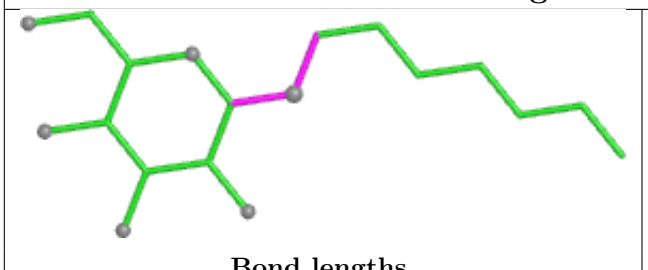


Torsions



Rings

Ligand HTG l 106



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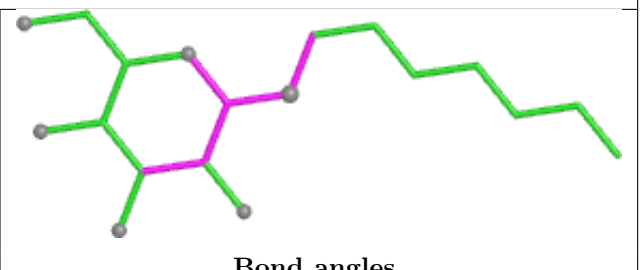
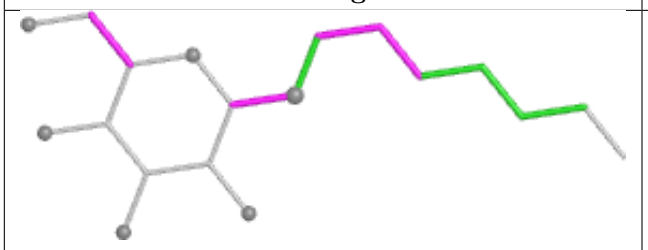
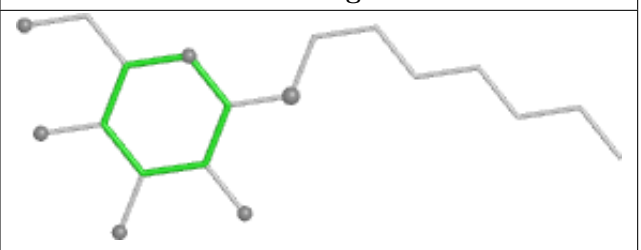


Bond angles

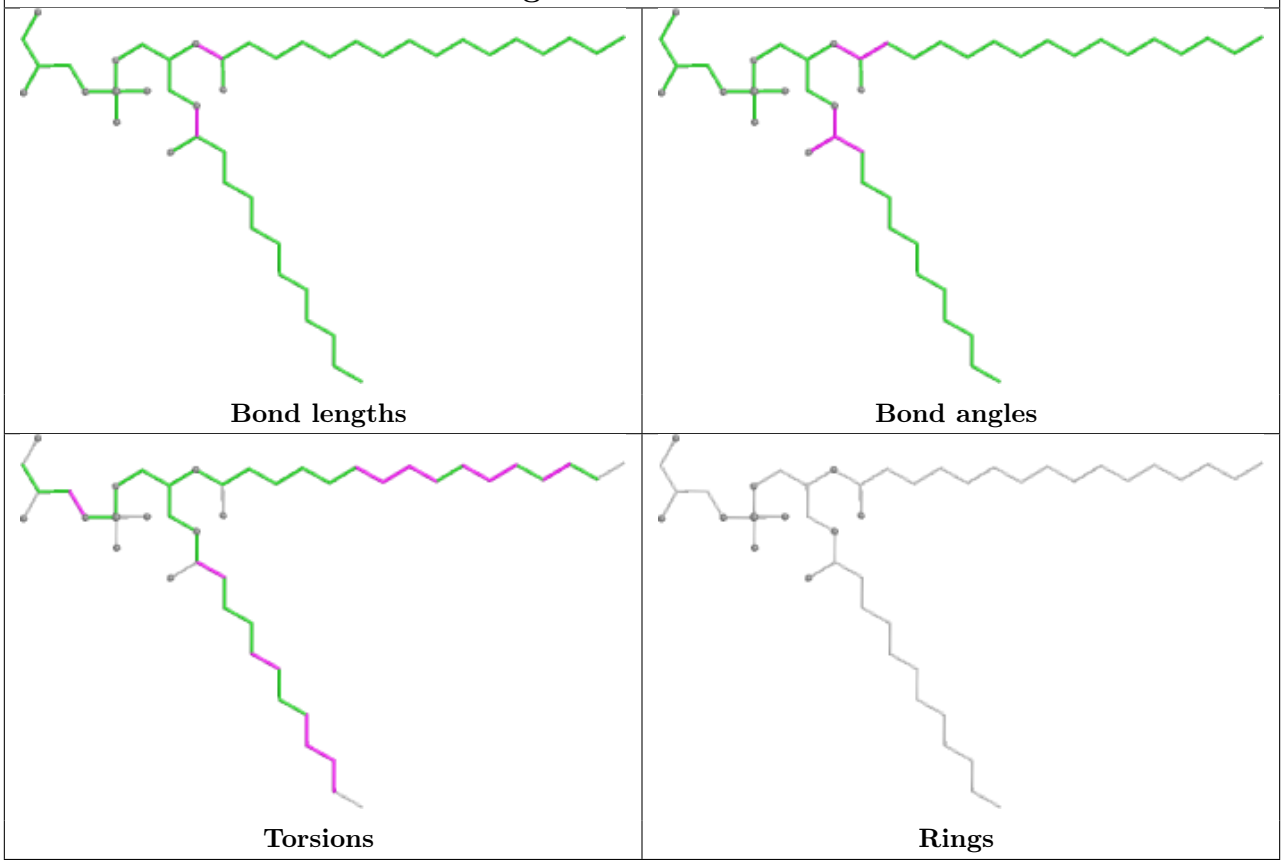


Torsions

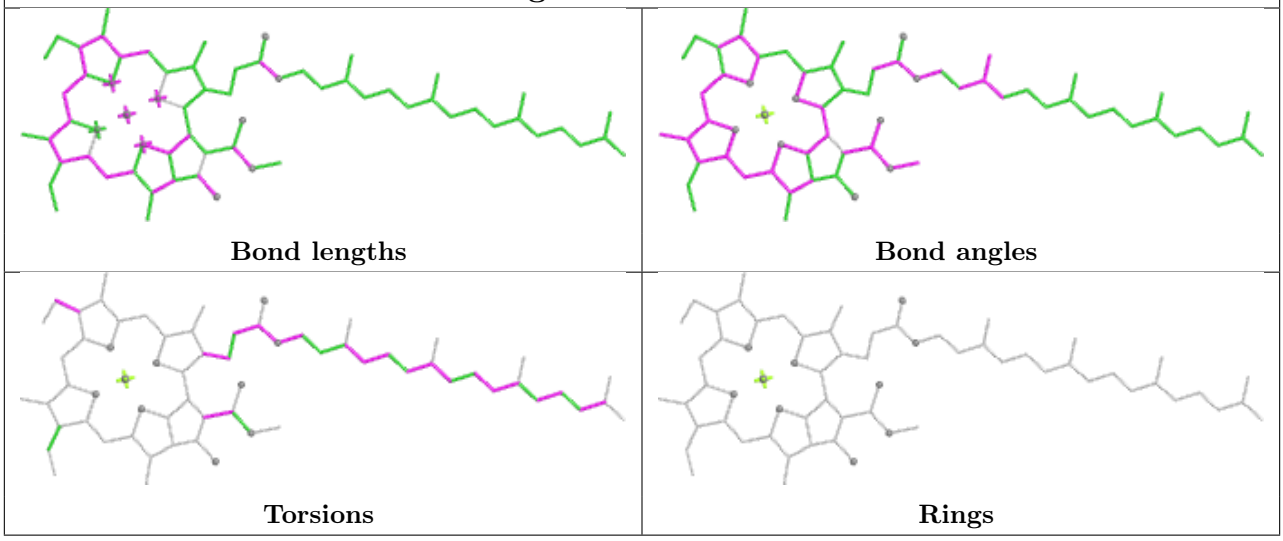


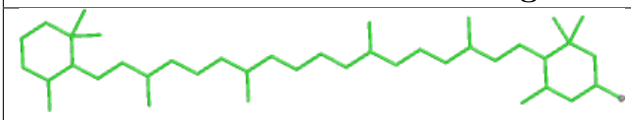
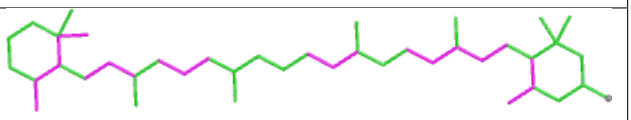
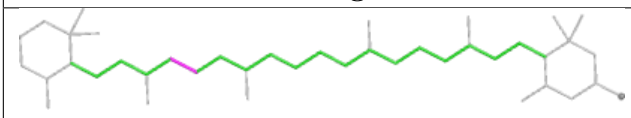
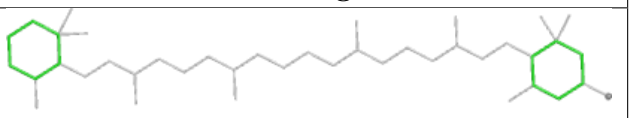
Rings

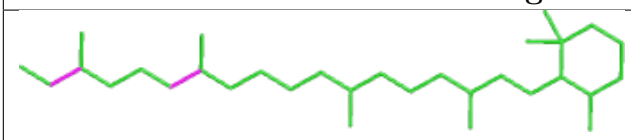
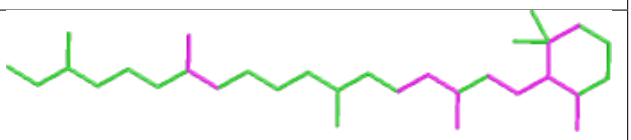
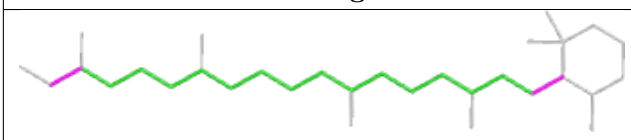
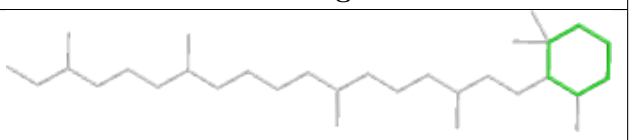
Ligand LHG D 411



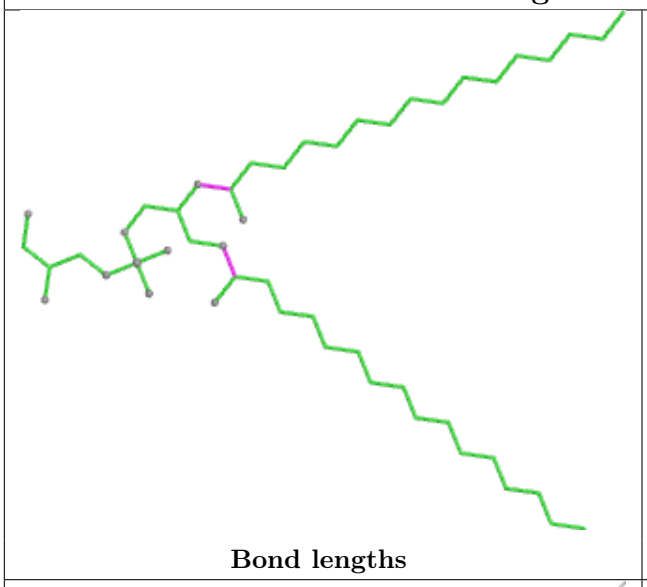
Ligand CLA b 602



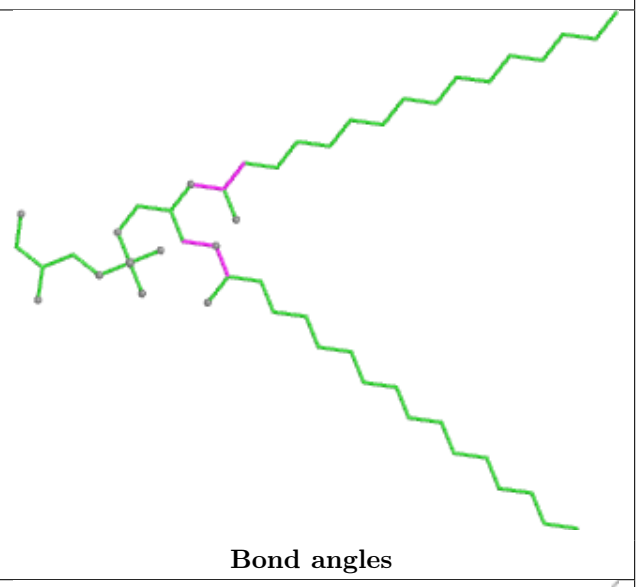
Ligand RRX H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

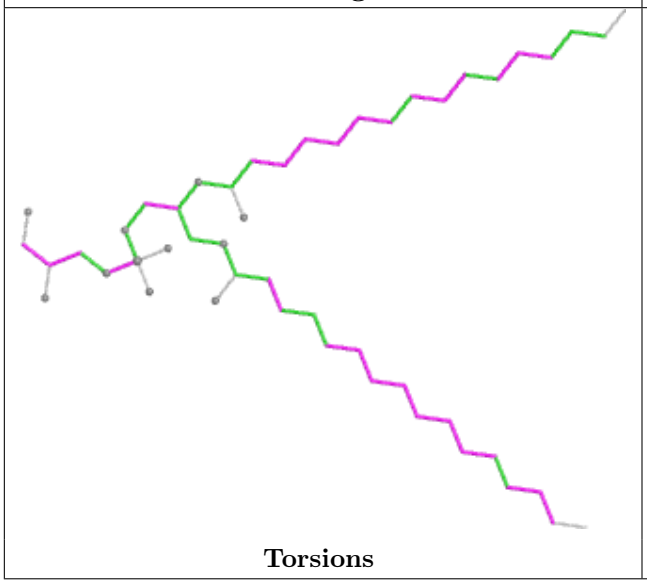
Ligand LHG l 102



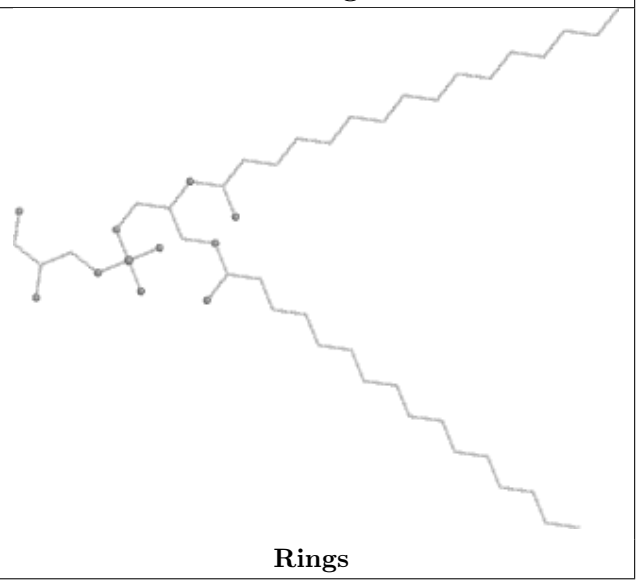
Bond lengths



Bond angles



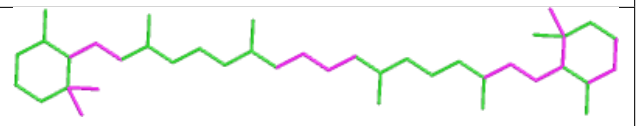
Torsions



Rings

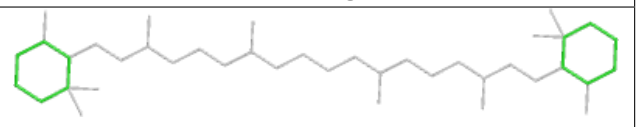
Ligand BCR a 413

Bond lengths



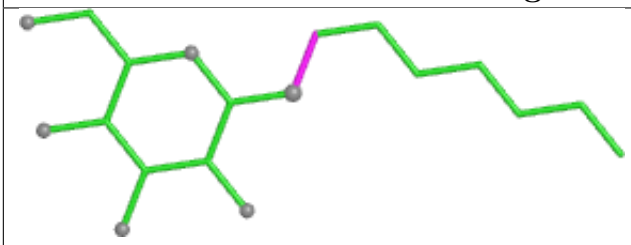
Bond angles

Torsions



Rings

Ligand HTG b 626



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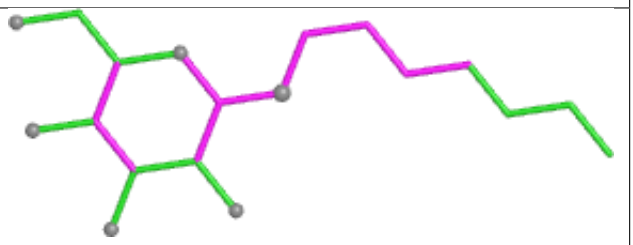
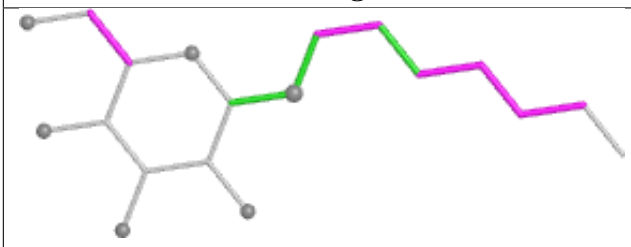


Bond angles



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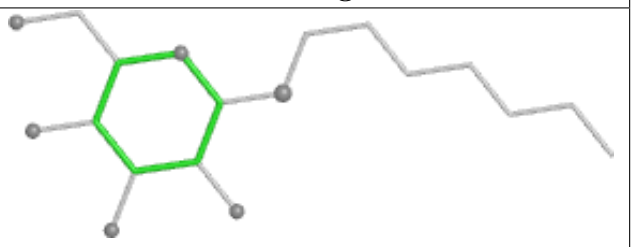
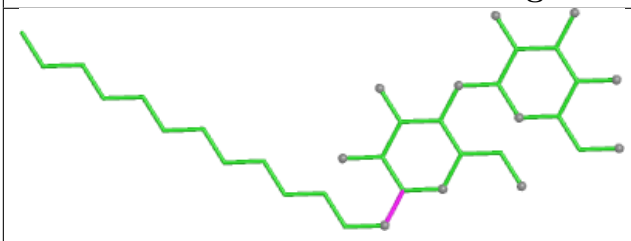


Rings

Ligand LMT c 921



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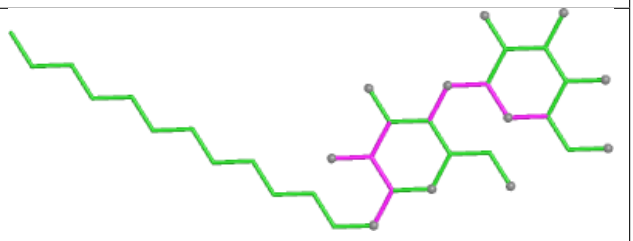
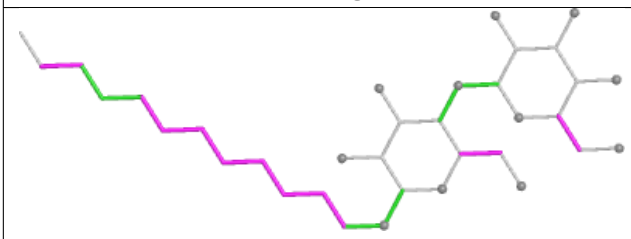


Bond angles



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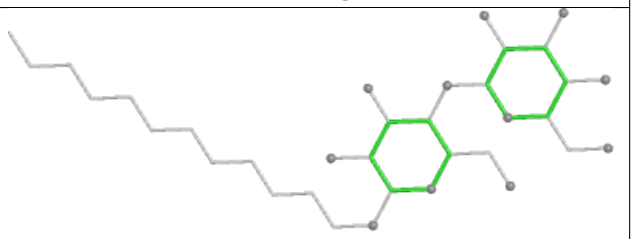
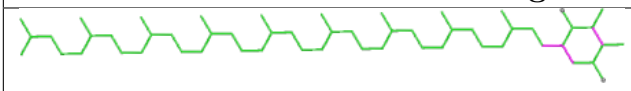


Rings

Ligand PL9 D 406



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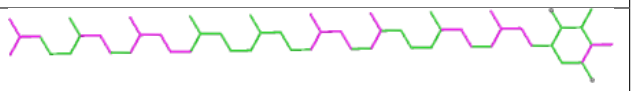
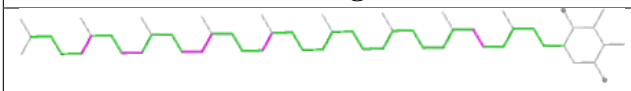


Bond angles



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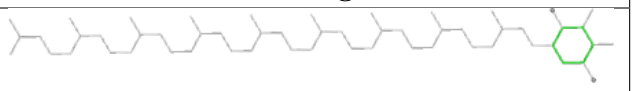
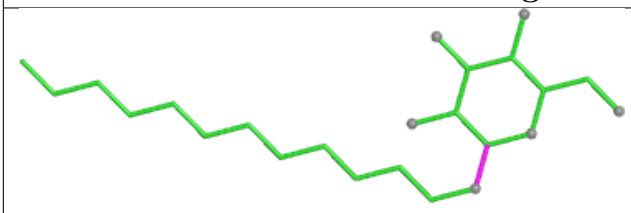


Rings

Ligand LMT T 102



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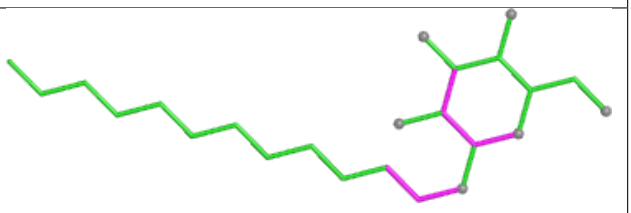
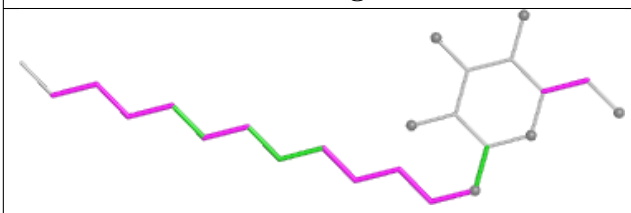
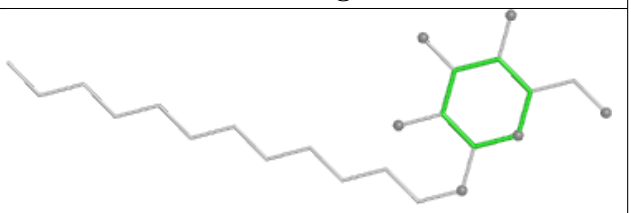


Bond angles

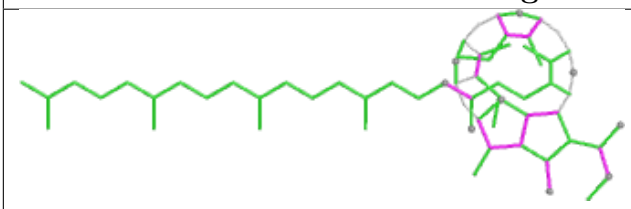


Torsions



Rings

Ligand PHO D 402



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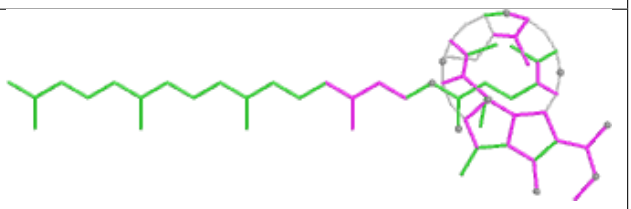
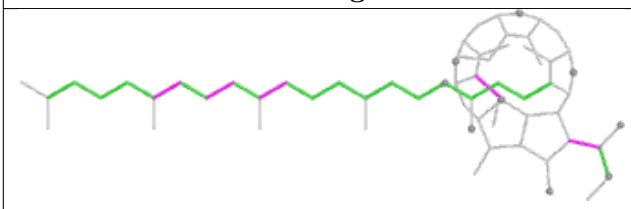


Bond angles



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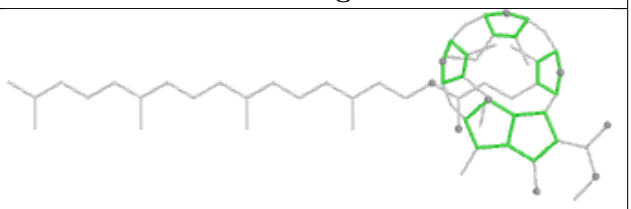
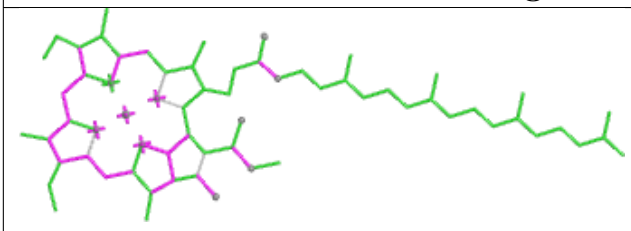


Rings

Ligand CLA C 511



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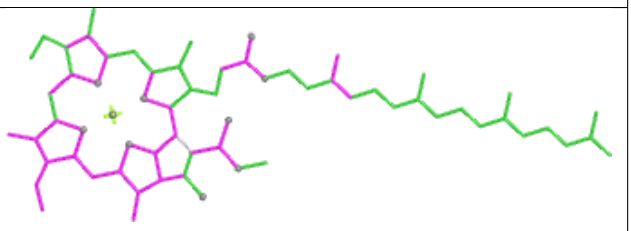
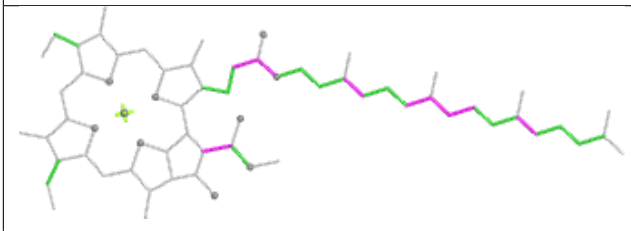


Bond angles



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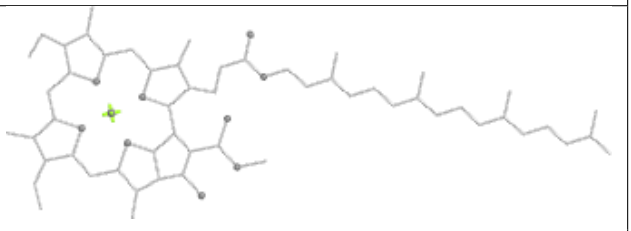
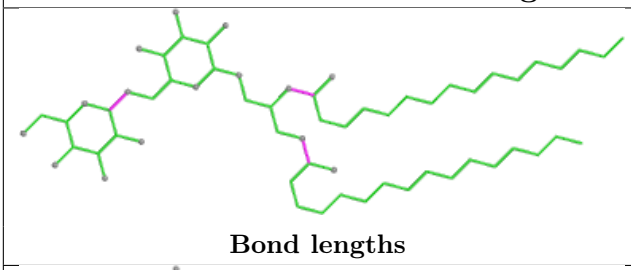


Rings

Ligand DGD C 517



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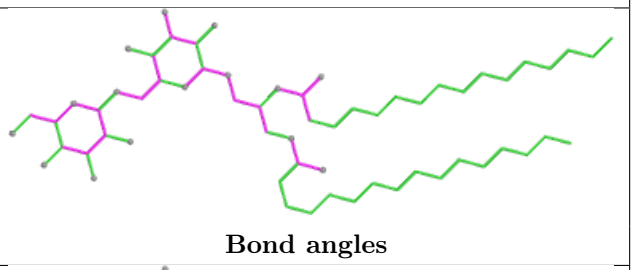
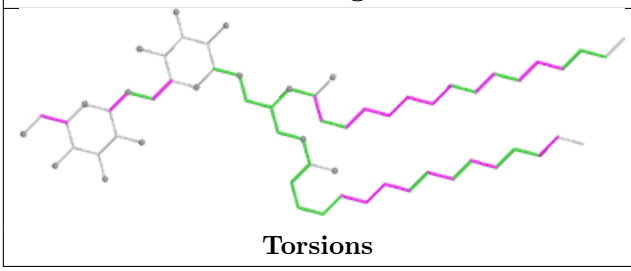


Bond angles



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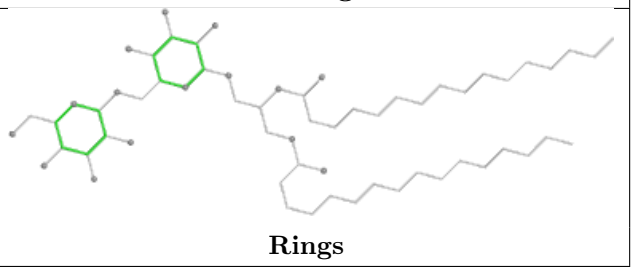
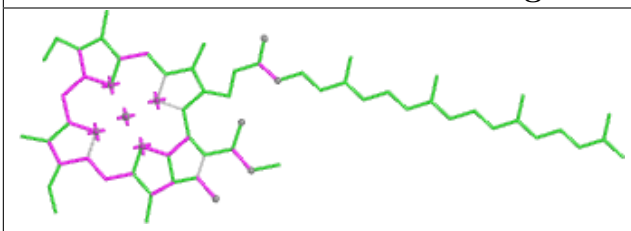


Rings

Ligand CLA C 509



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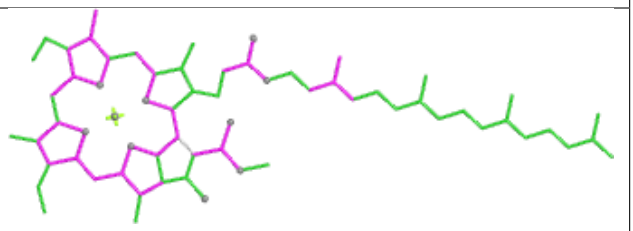
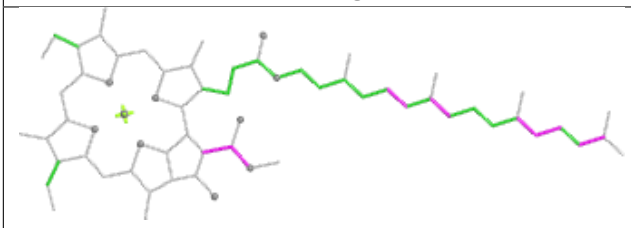


Bond angles



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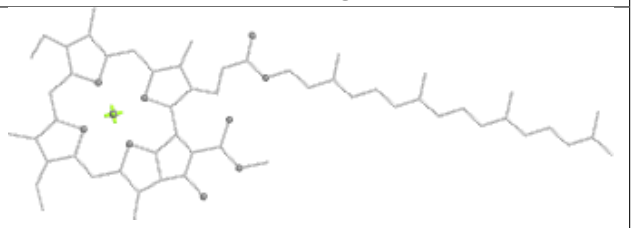
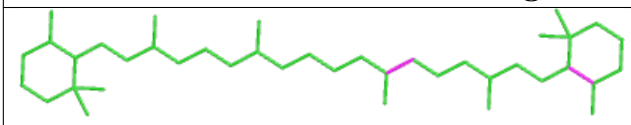


Rings

Ligand BCR B 620



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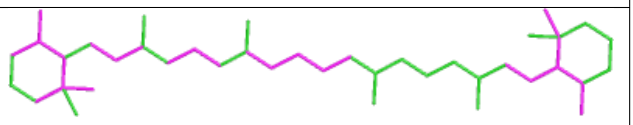

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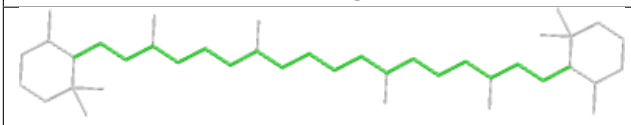

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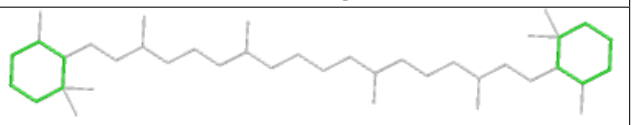
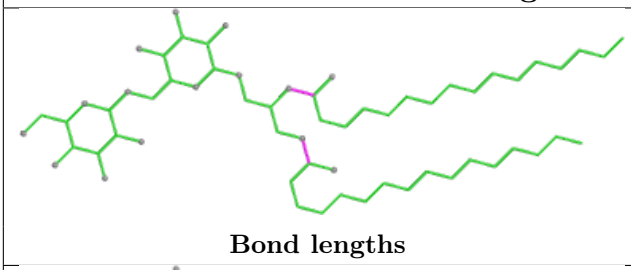


Rings

Ligand DGD C 519



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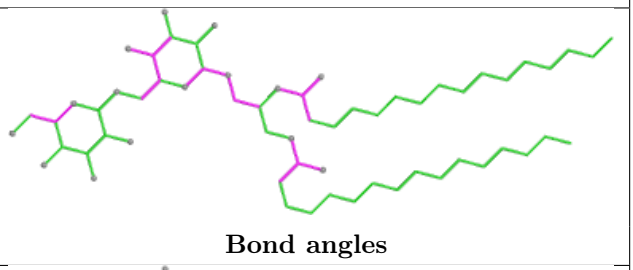
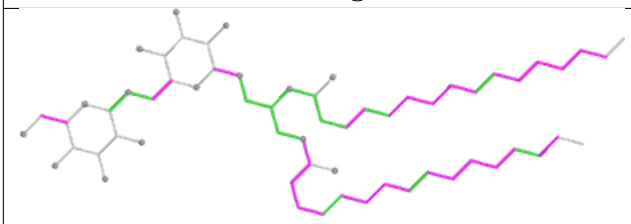
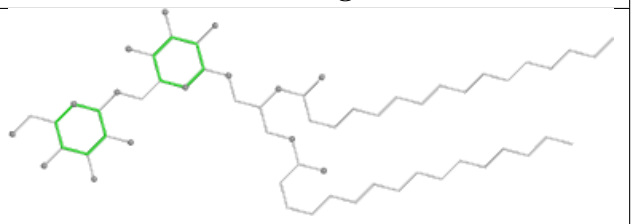


Bond angles

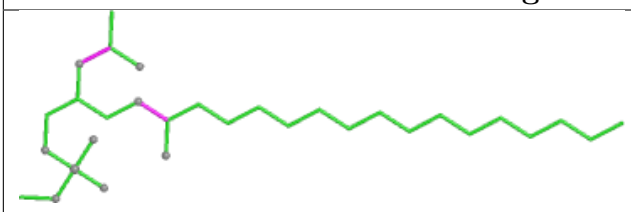


Torsions



Rings

Ligand LHG A 412



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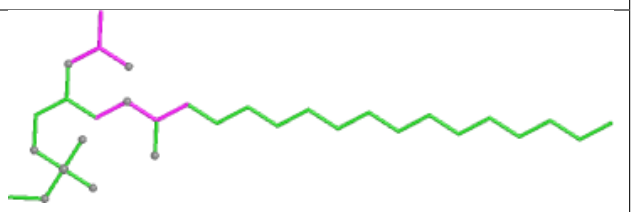
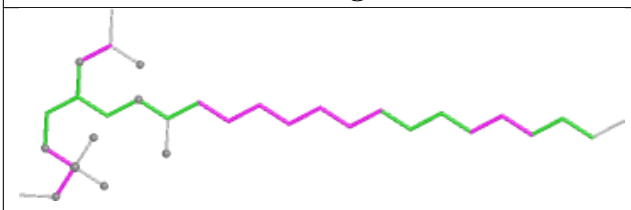
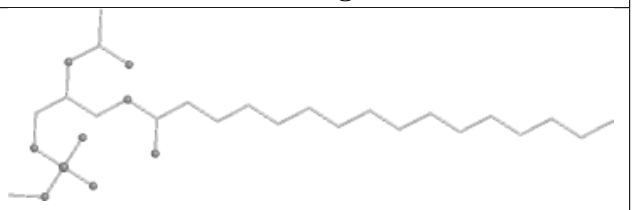


Bond angles

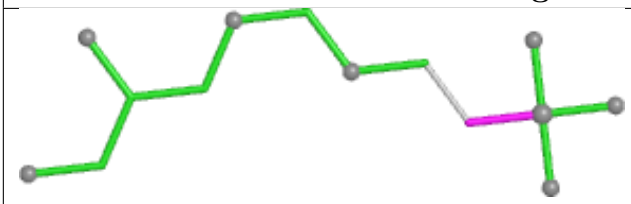


Torsions

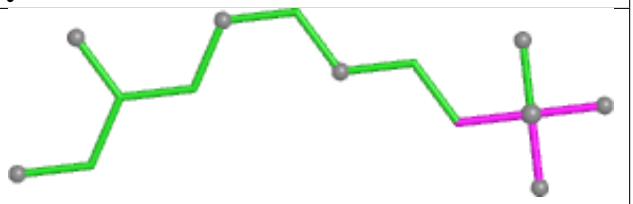


Rings

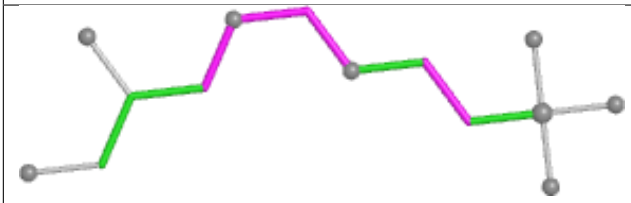
Ligand SQD f 101



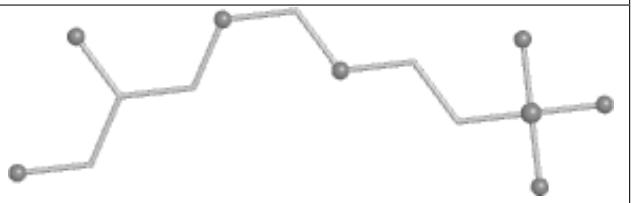
Bond lengths



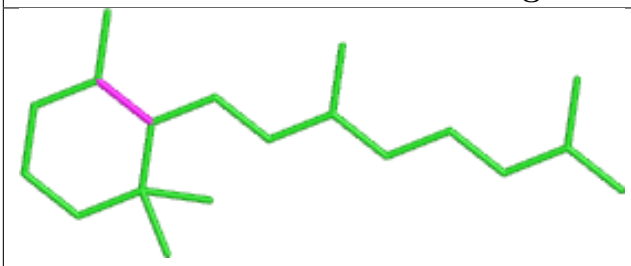
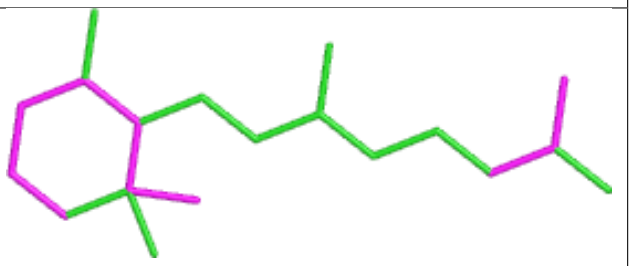
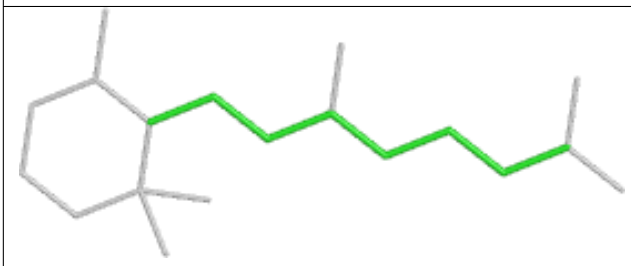
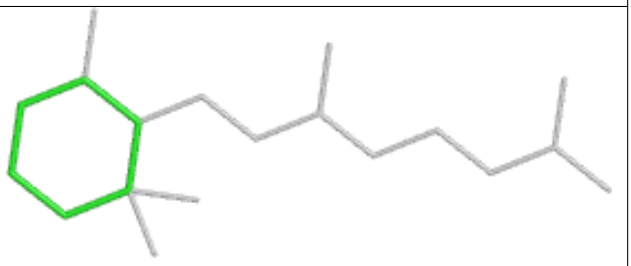
Bond angles

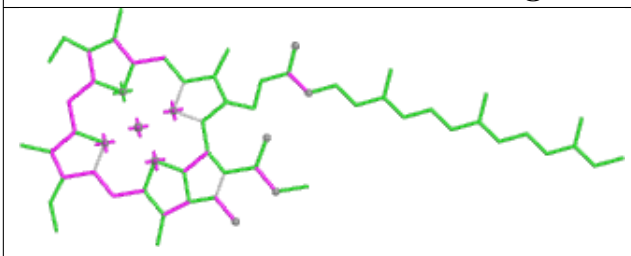
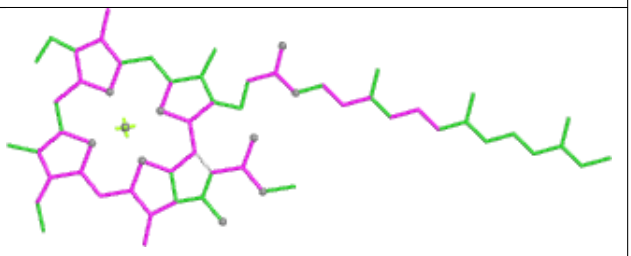
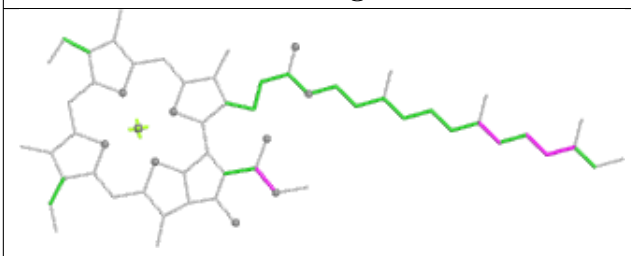
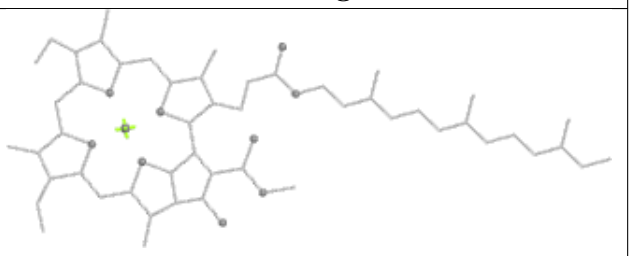


Torsions

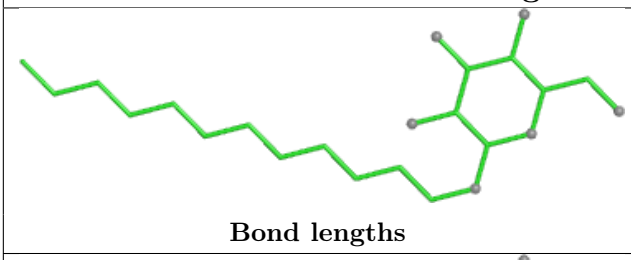


Rings

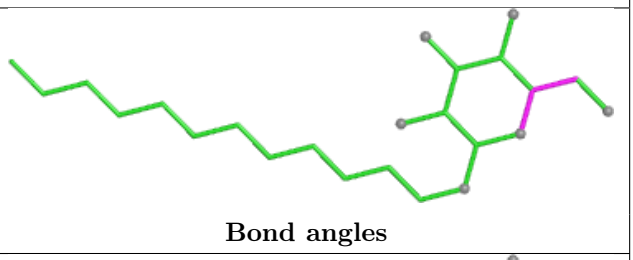
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

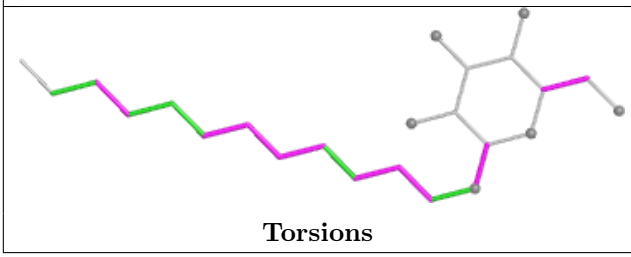
Ligand LMT E 101



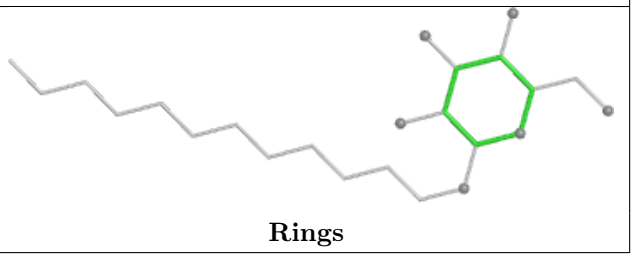
Bond lengths



Bond angles

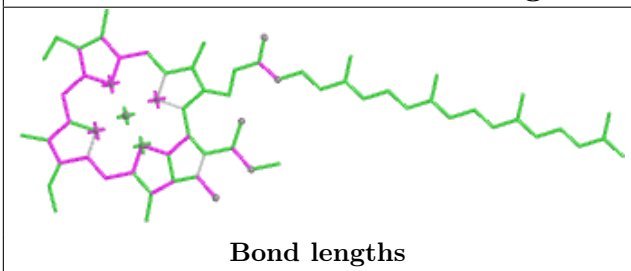


Torsions

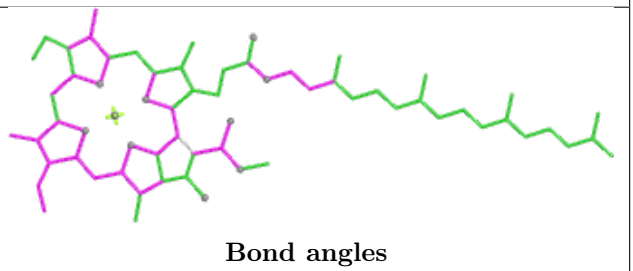


Rings

Ligand CLA B 610



Bond lengths



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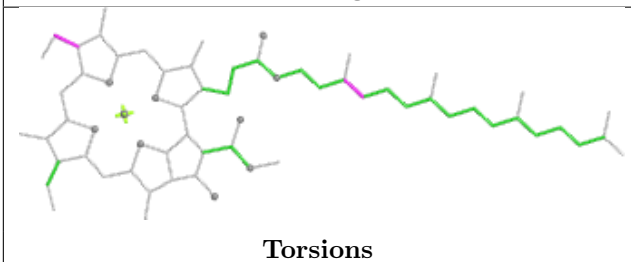
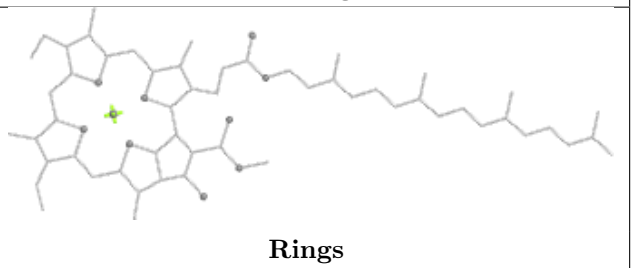
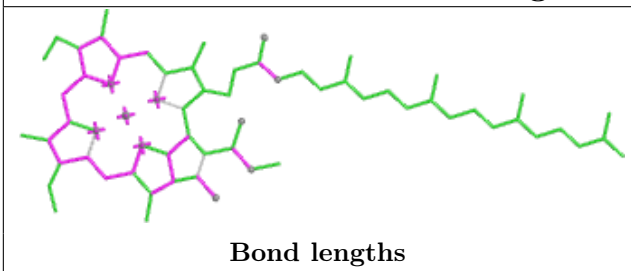


Torsions

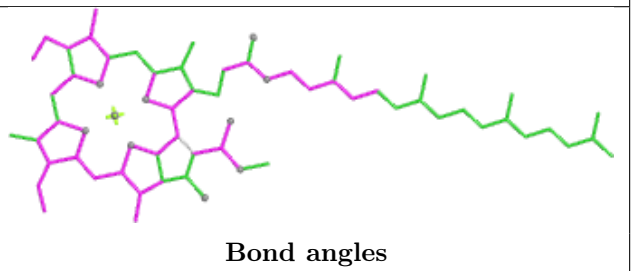


Rings

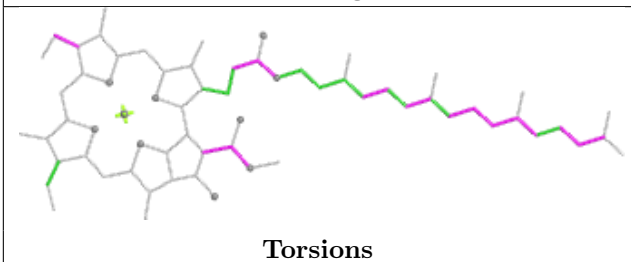
Ligand CLA c 913



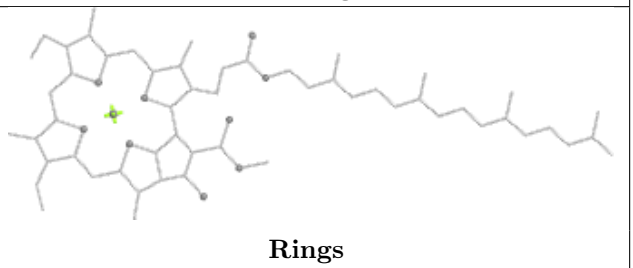
Bond lengths



Bond angles

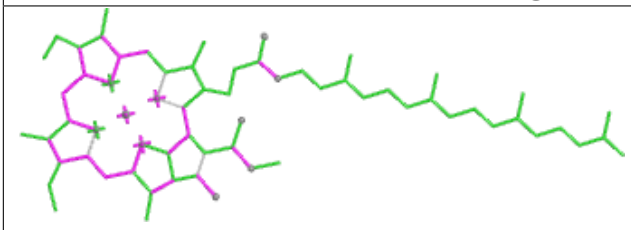


Torsions

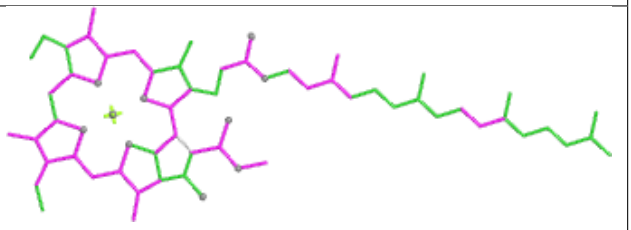


Rings

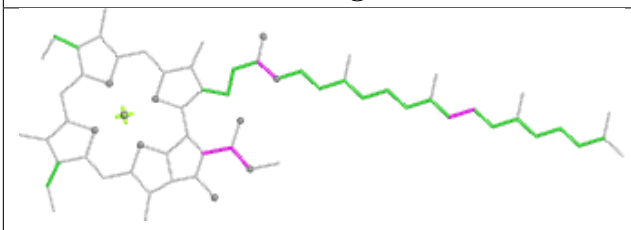
Ligand CLA b 613



Bond lengths



Bond angles



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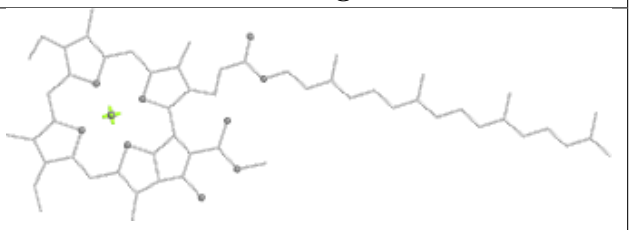
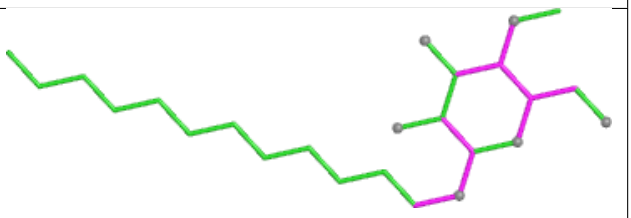


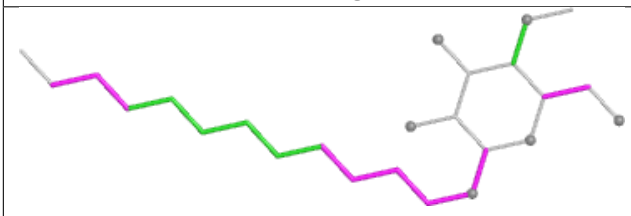
Rings

Ligand LMT f 102

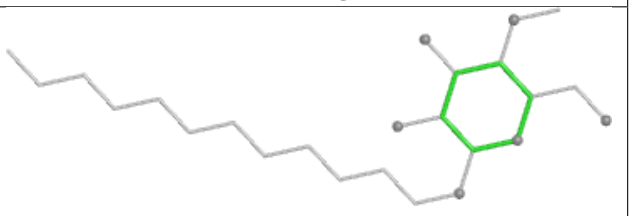
Bond lengths



Bond angles

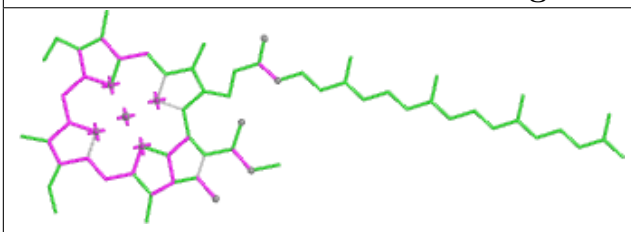


Torsions

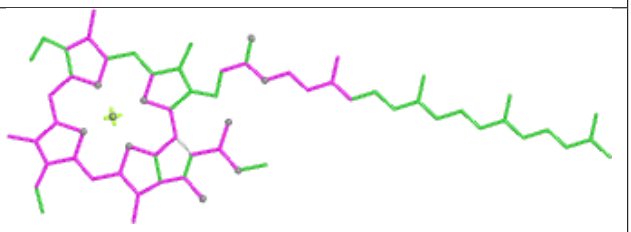


Rings

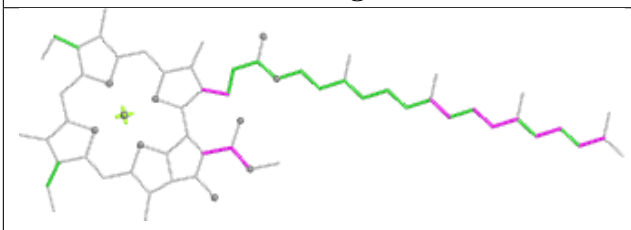
Ligand CLA c 909



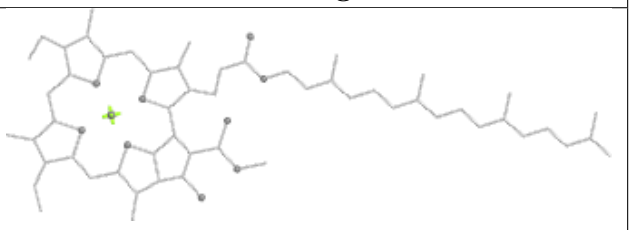
Bond lengths



Bond angles

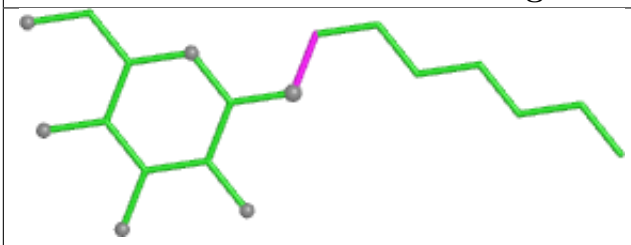


Torsions

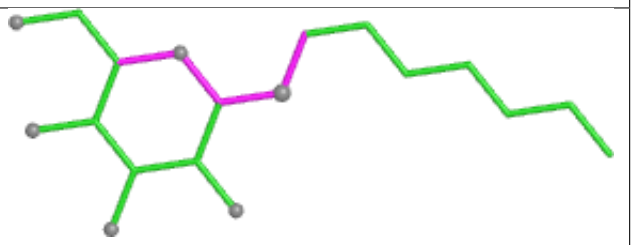


Rings

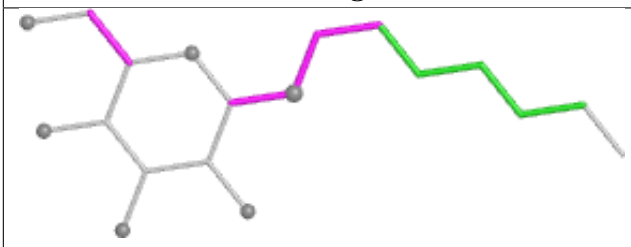
Ligand HTG c 922



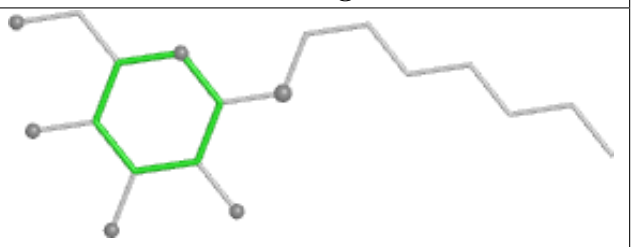
Bond lengths



Bond angles

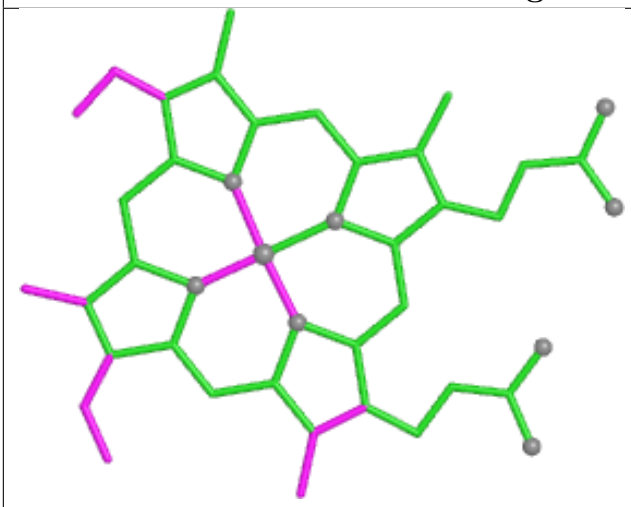


Torsions



Rings

Ligand HEC v 202



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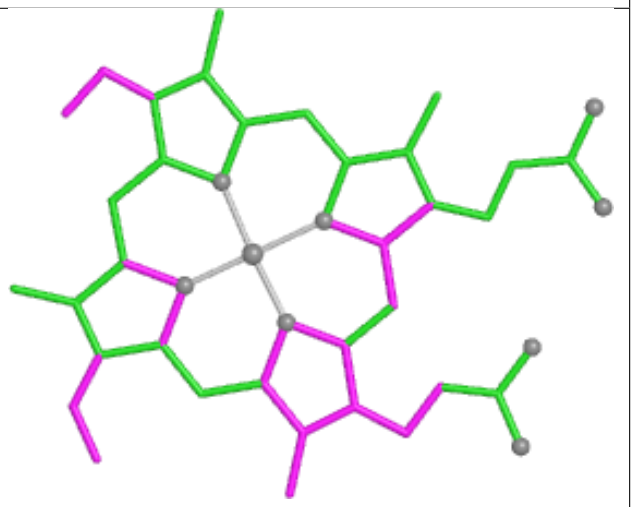
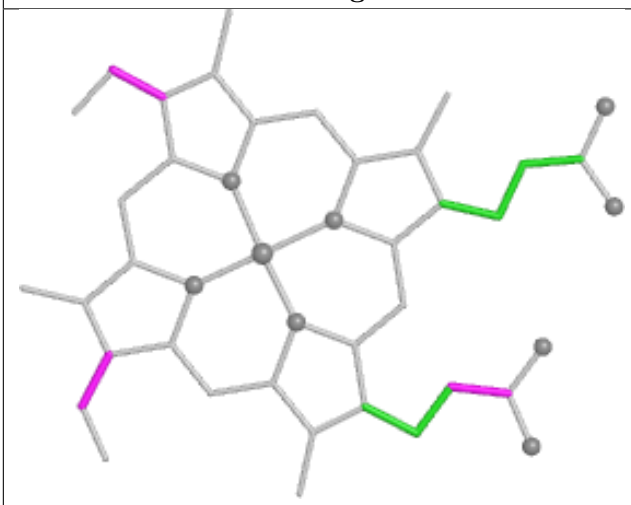
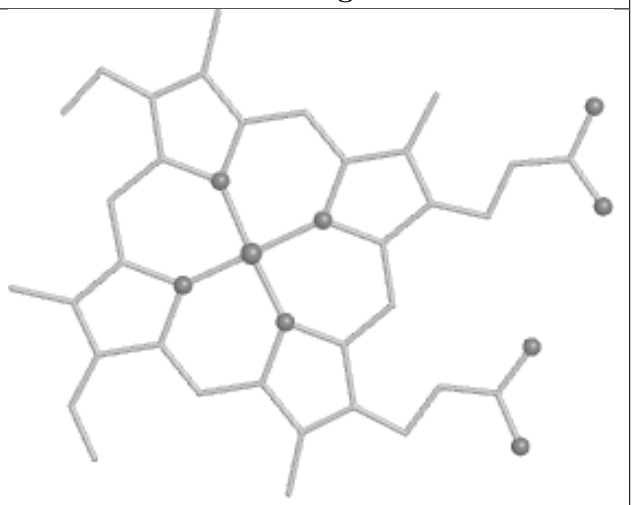


Bond angles

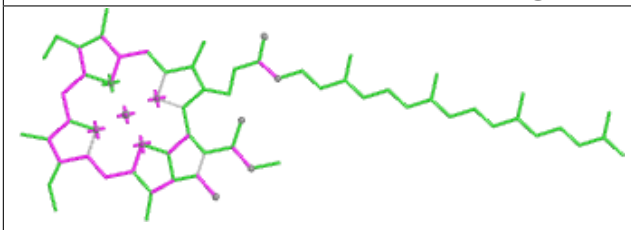


Torsions

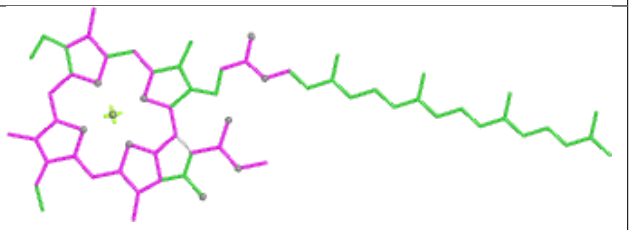


Rings

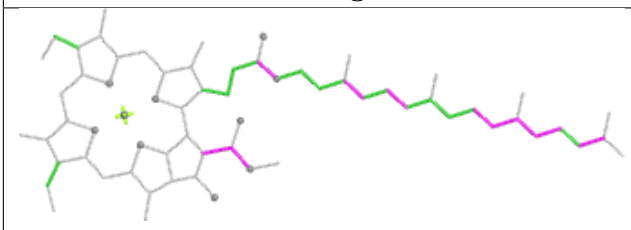
Ligand CLA c 914



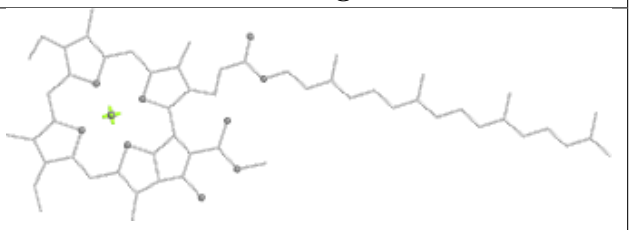
Bond lengths



Bond angles

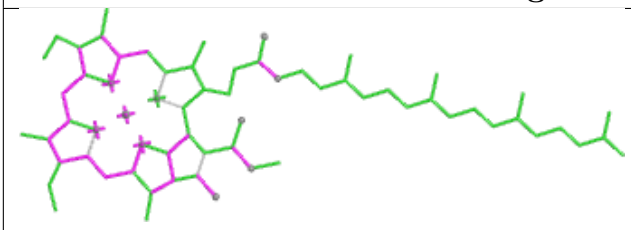


Torsions



Rings

Ligand CLA b 611



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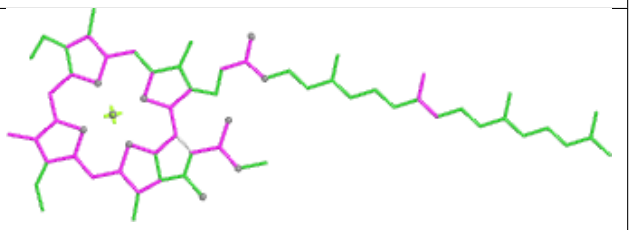
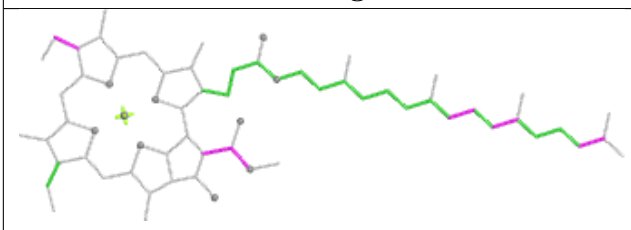
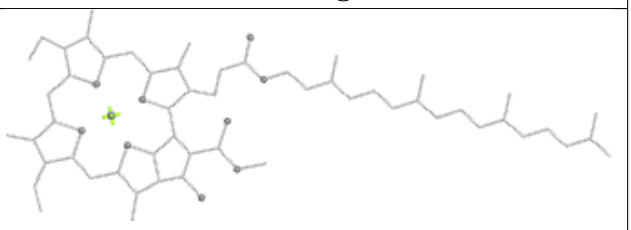


Bond angles

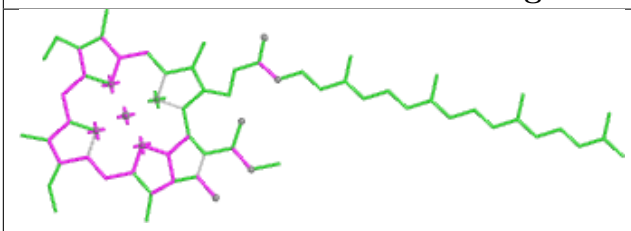


Torsions

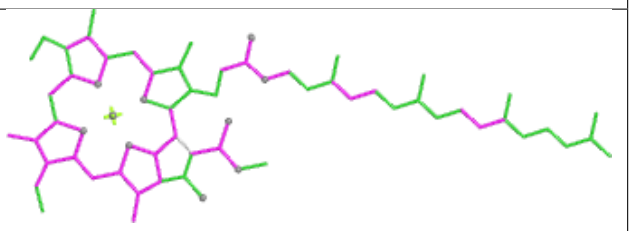


Rings

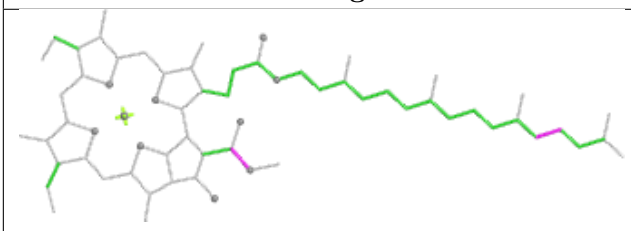
Ligand CLA B 609



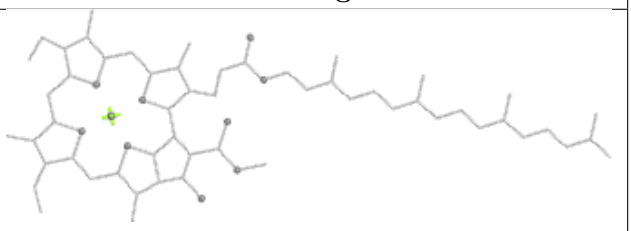
Bond lengths



Bond angles



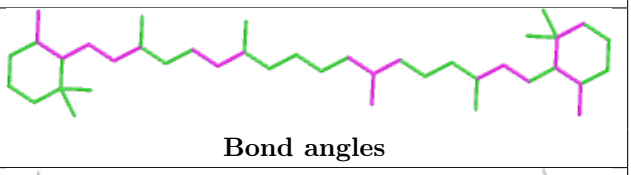
Torsions



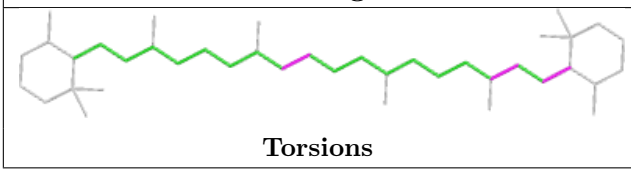
Rings

Ligand BCR C 515

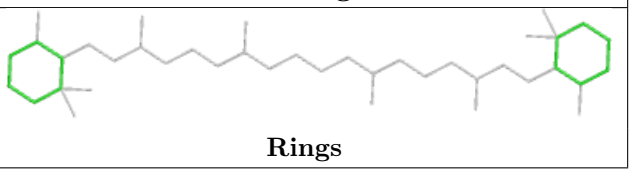
Bond lengths



Bond angles

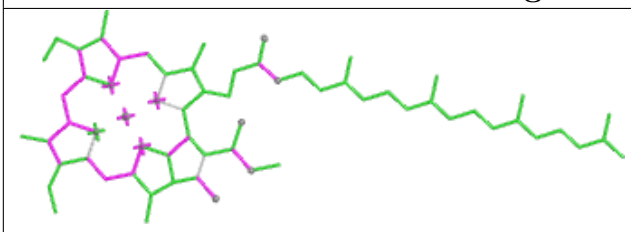


Torsions

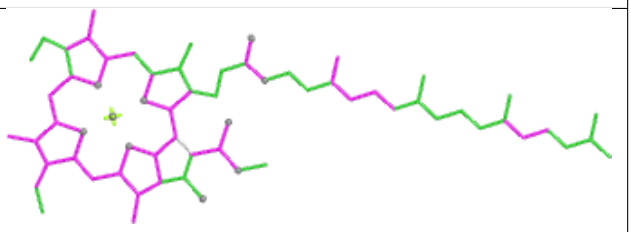


Rings

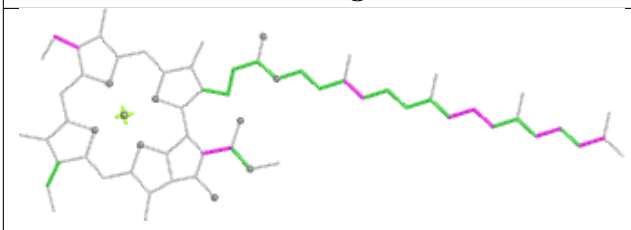
Ligand CLA B 606



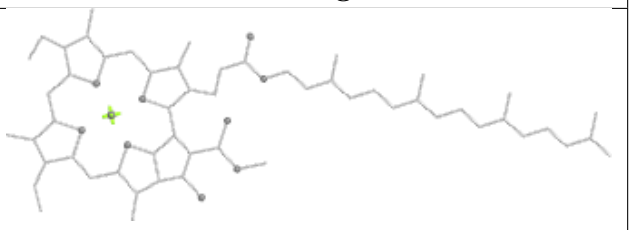
Bond lengths



Bond angles

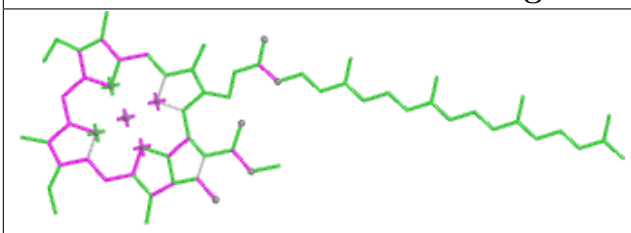


Torsions

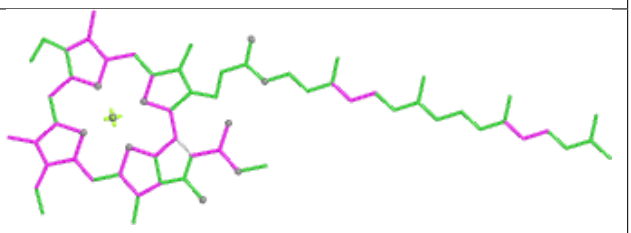


Rings

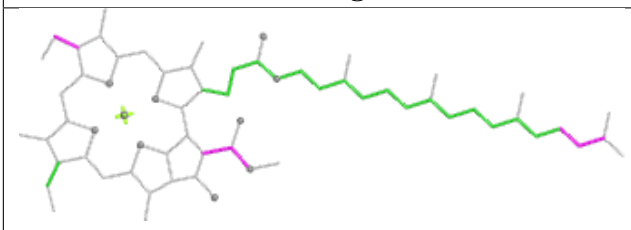
Ligand CLA C 503



Bond lengths



Bond angles



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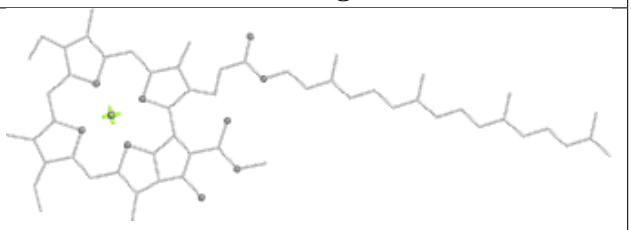
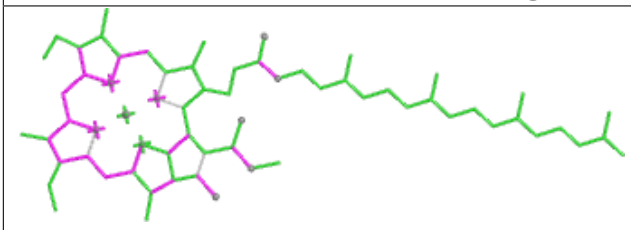


Rings

Ligand CLA C 507



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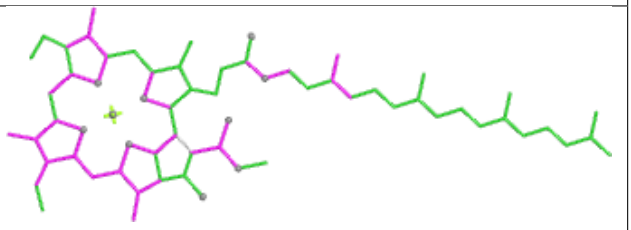
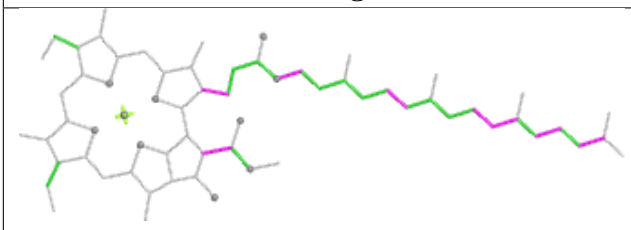
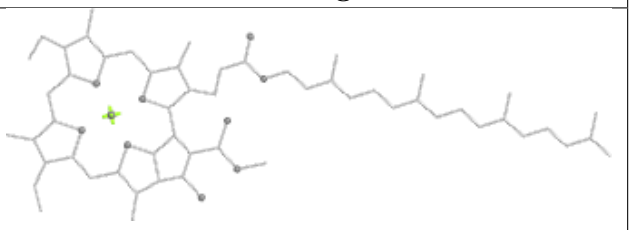


Bond angles

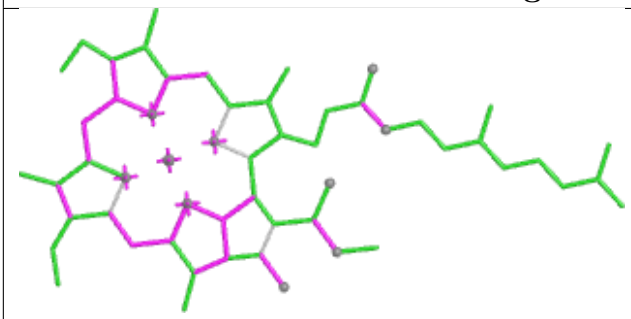


Torsions



Rings

Ligand CLA A 406



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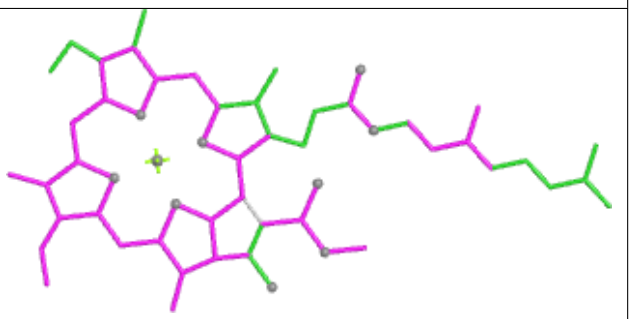
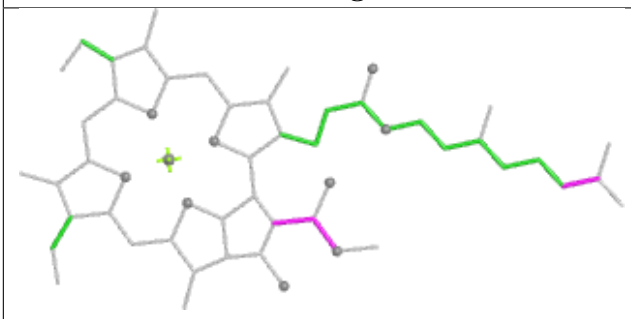
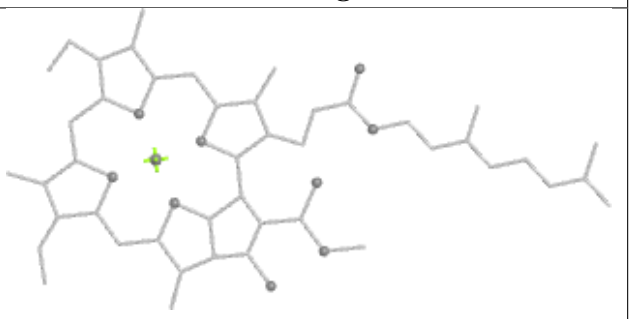


Bond angles

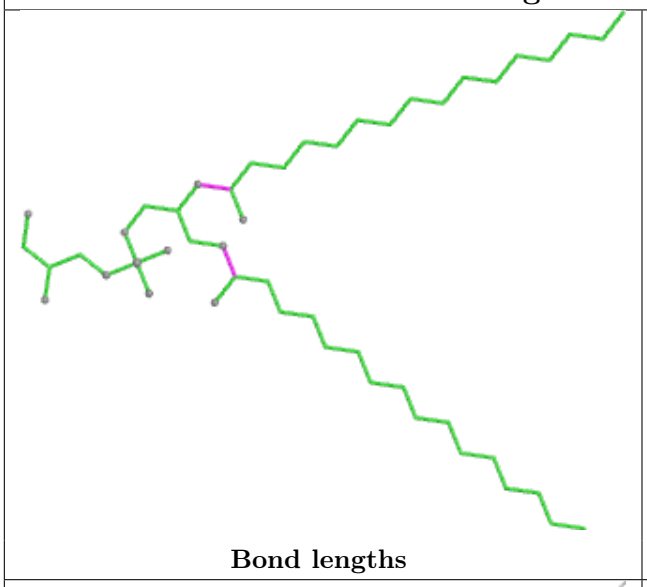


Torsions

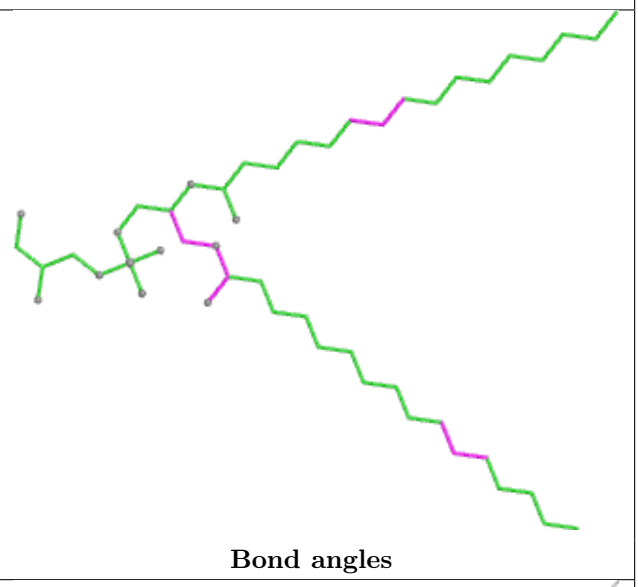


Rings

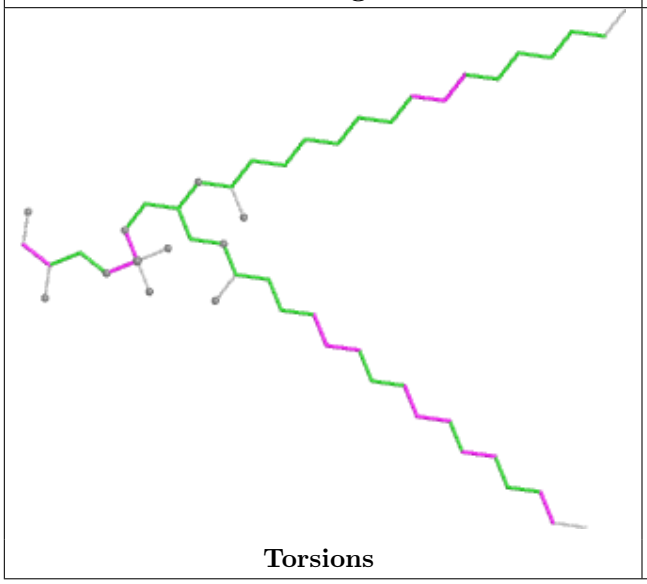
Ligand LHG D 410



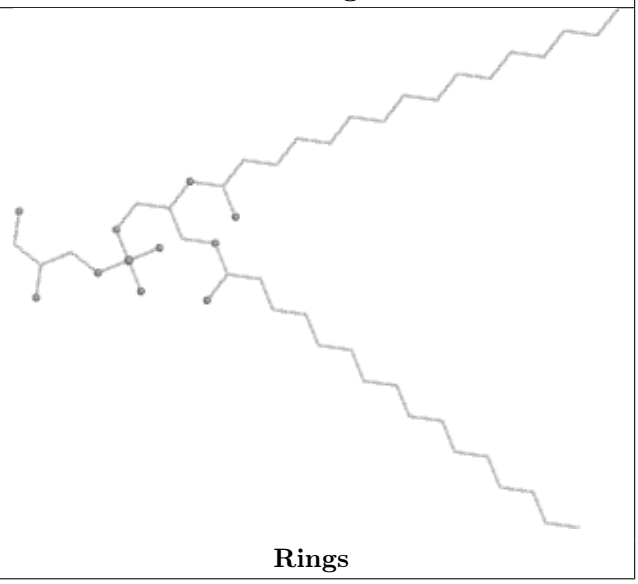
Bond lengths



Bond angles

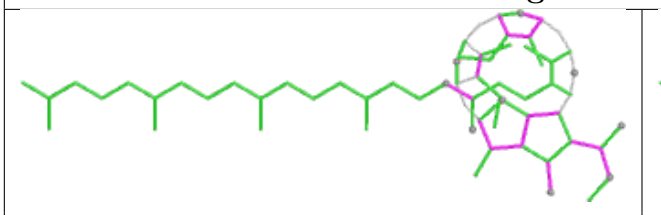


Torsions

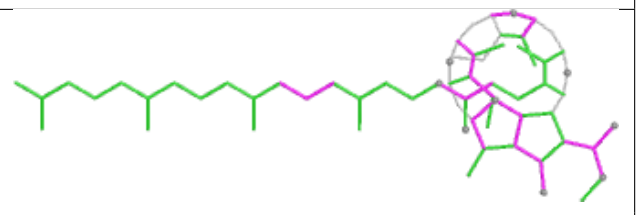


Rings

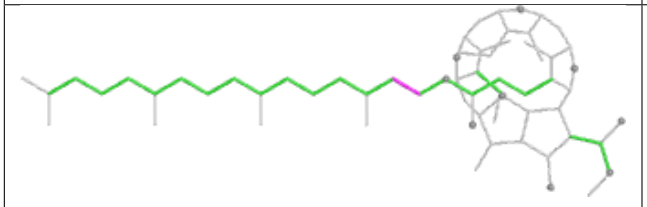
Ligand PHO a 410



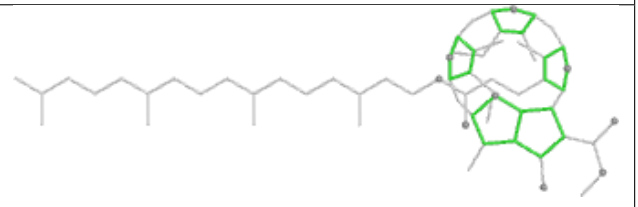
Bond lengths



Bond angles

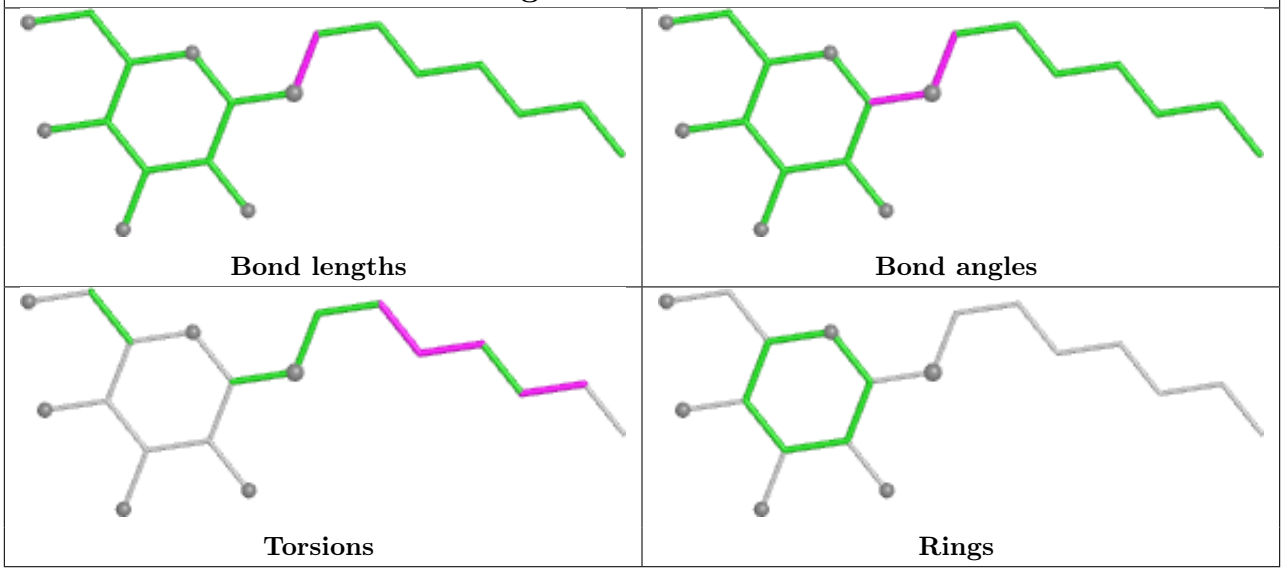


Torsions

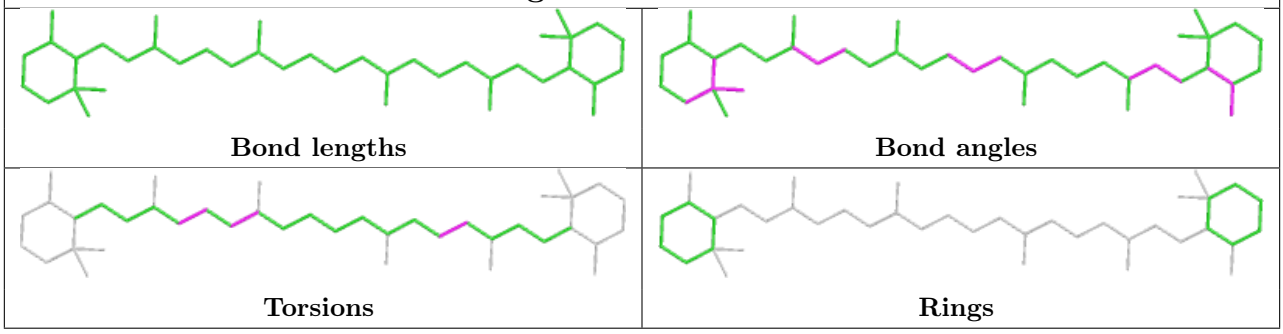


Rings

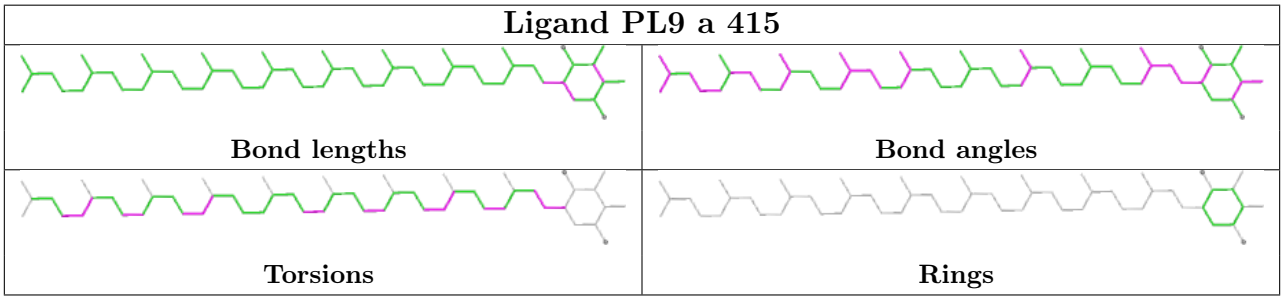
Ligand HTG D 414



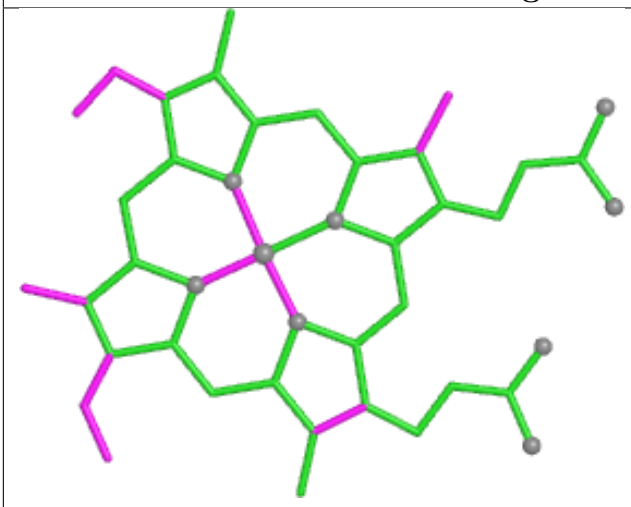
Ligand BCR k 101



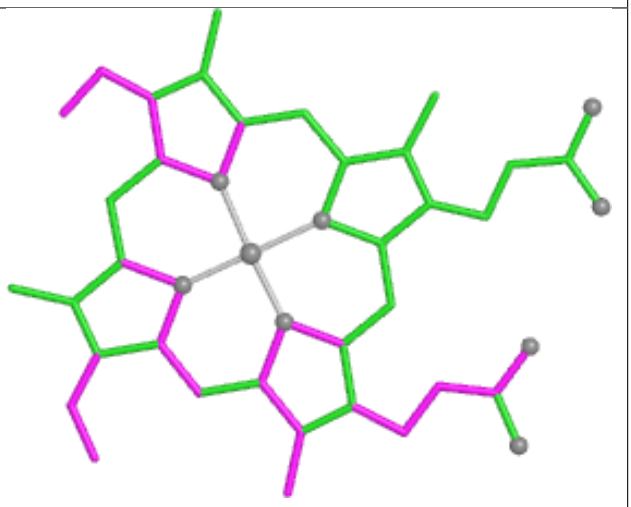
Ligand PL9 a 415



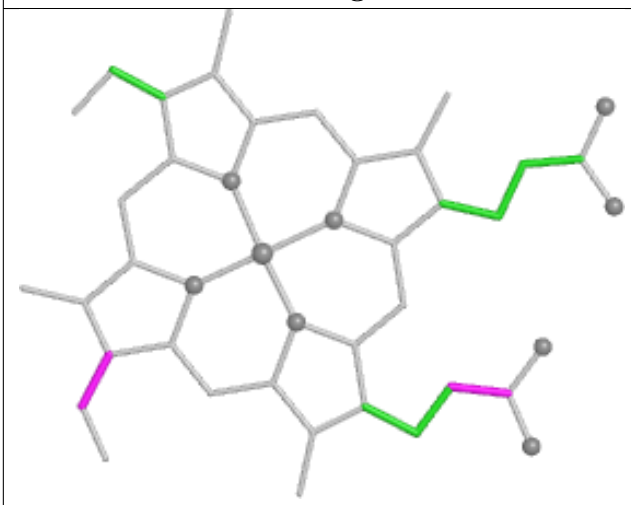
Ligand HEC V 202



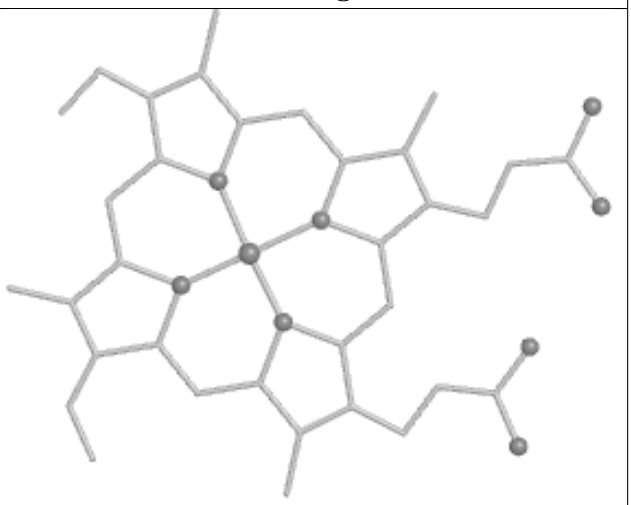
Bond lengths



Bond angles

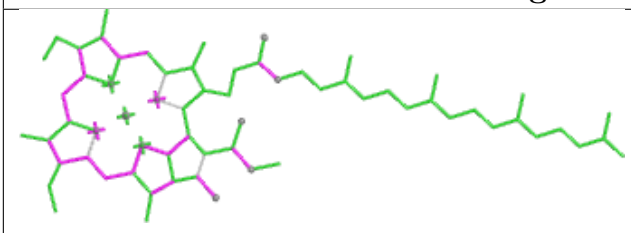


Torsions

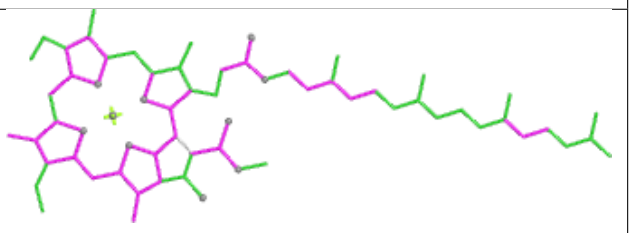


Rings

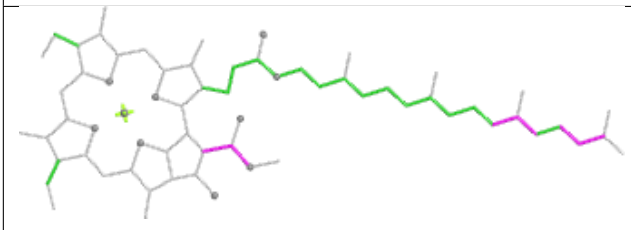
Ligand CLA c 903



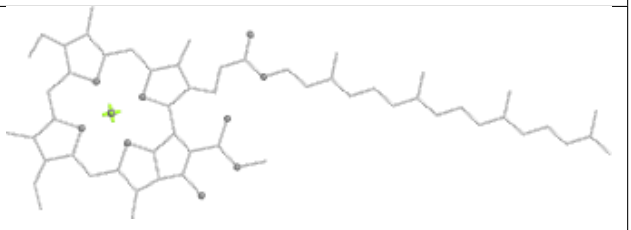
Bond lengths



Bond angles

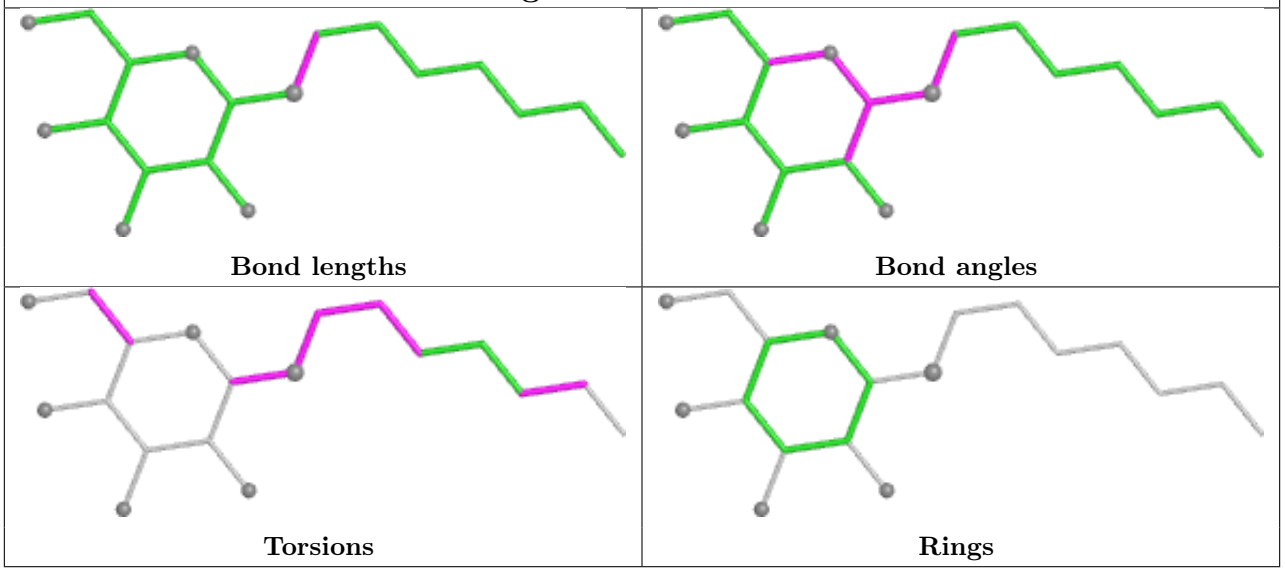


Torsions

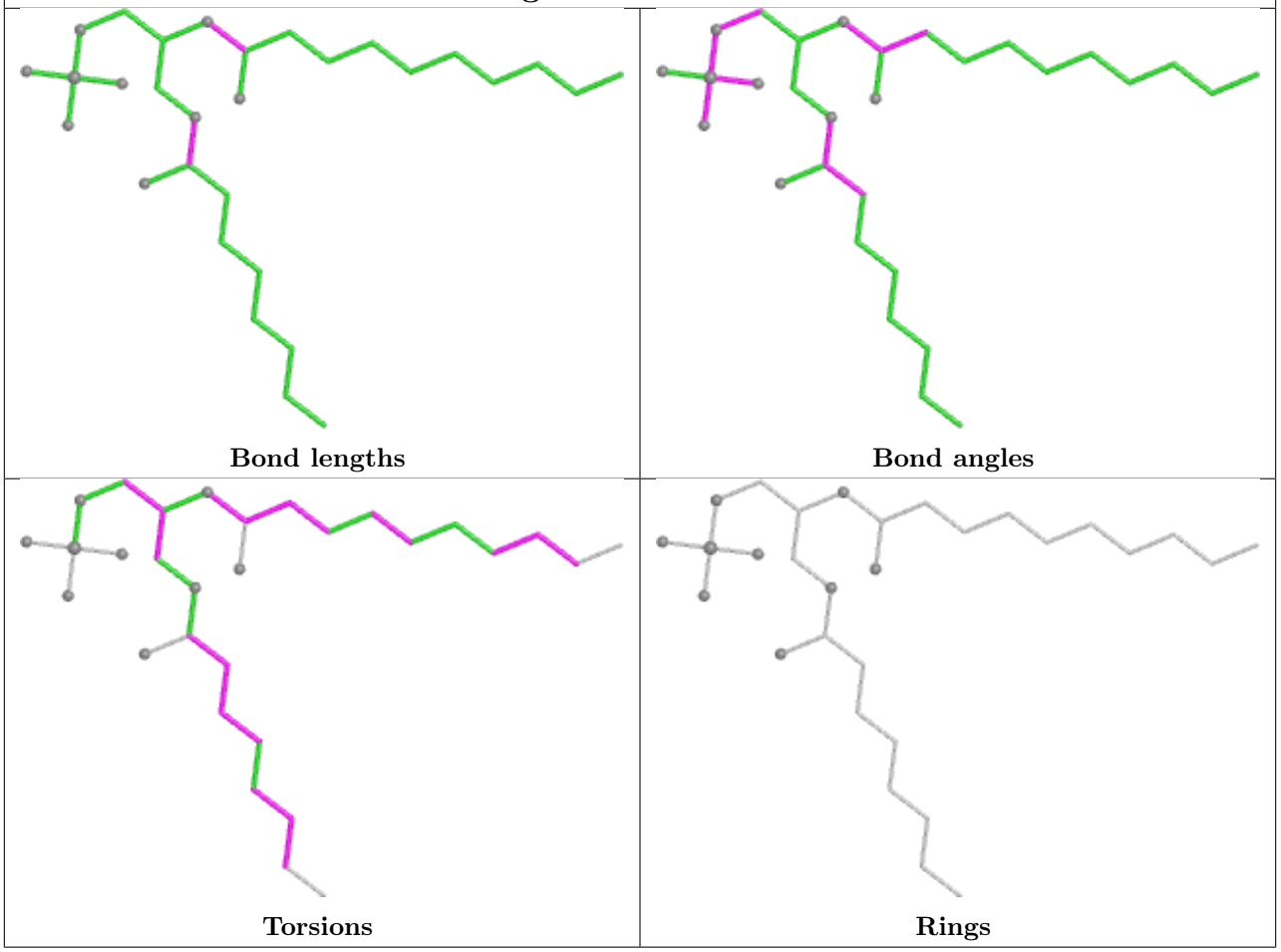


Rings

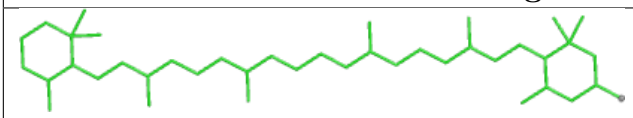
Ligand HTG B 627



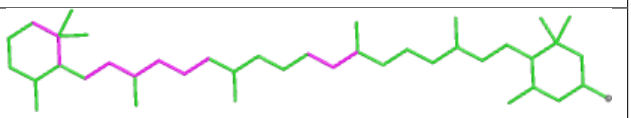
Ligand LHG C 522



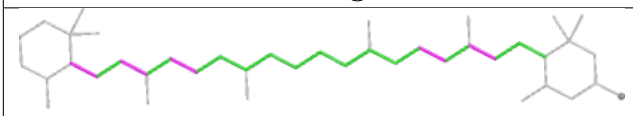
Ligand RRX h 101



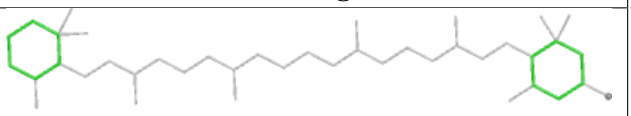
Bond lengths



Bond angles

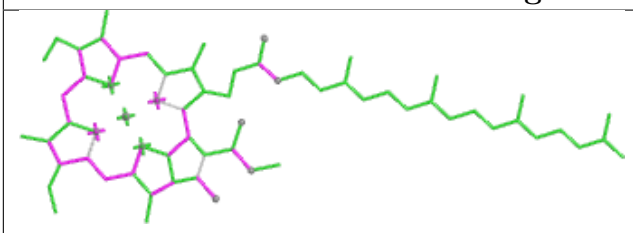


Torsions

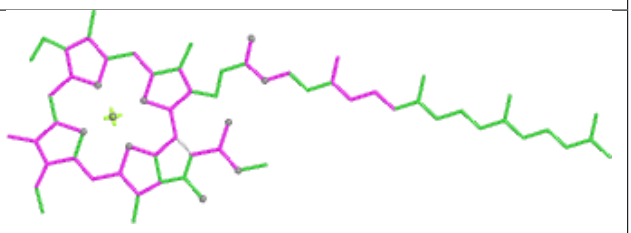


Rings

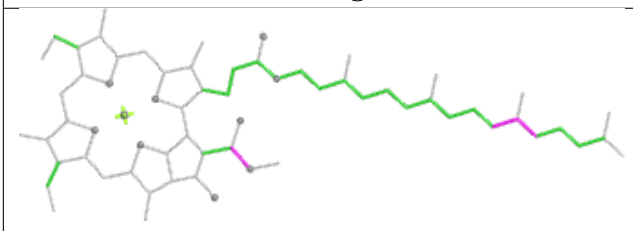
Ligand CLA C 506



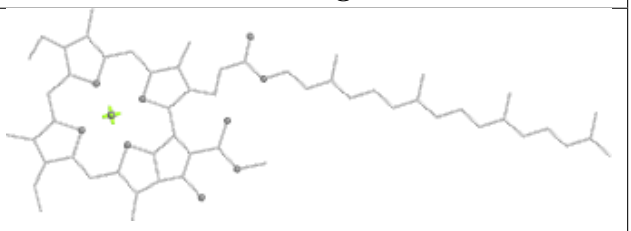
Bond lengths



Bond angles

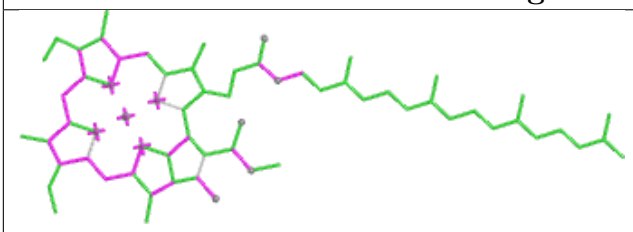


Torsions

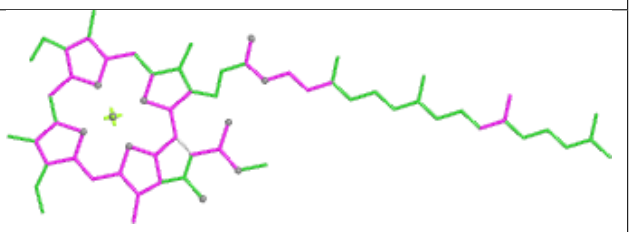


Rings

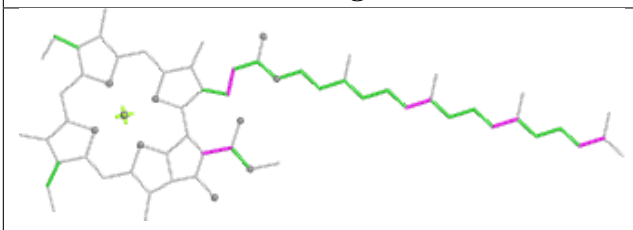
Ligand CLA b 607



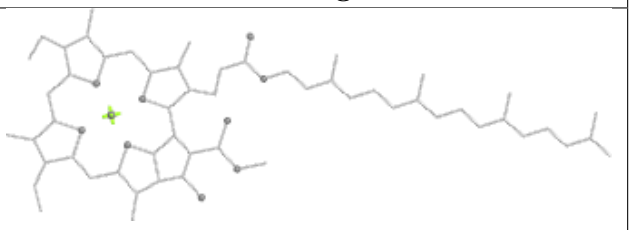
Bond lengths



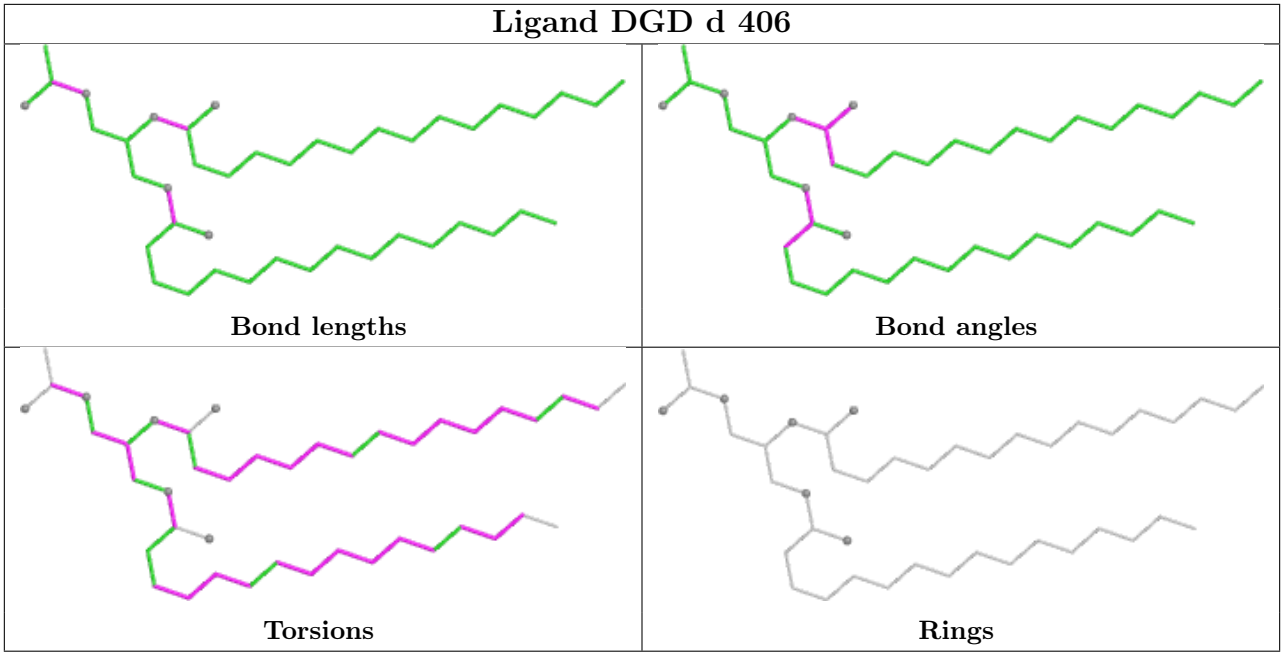
Bond angles

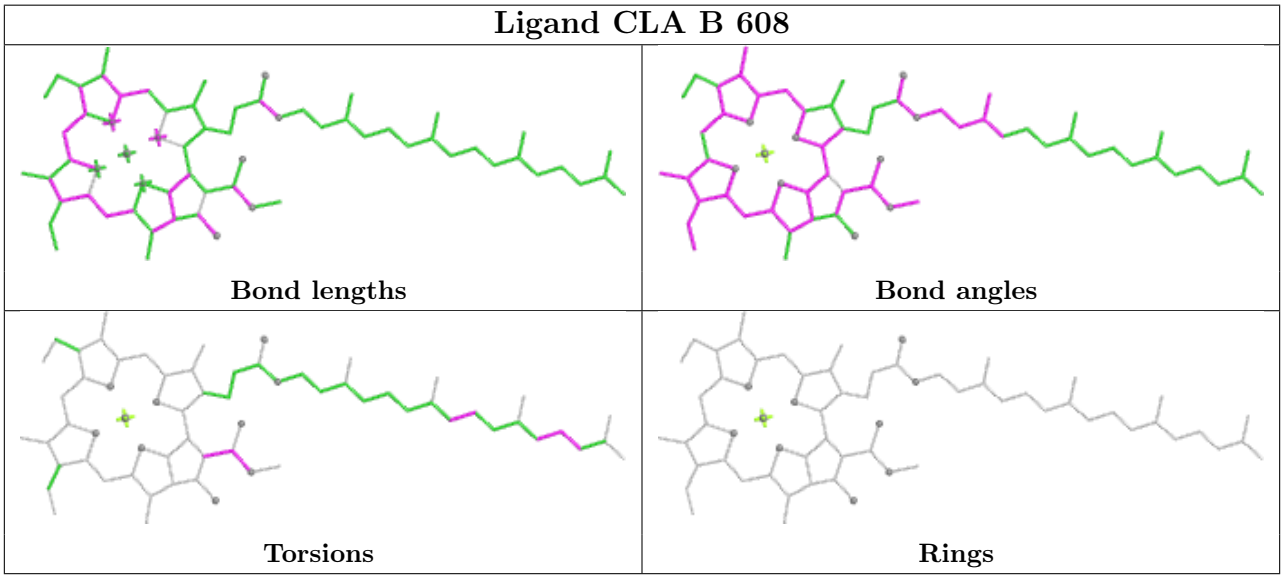


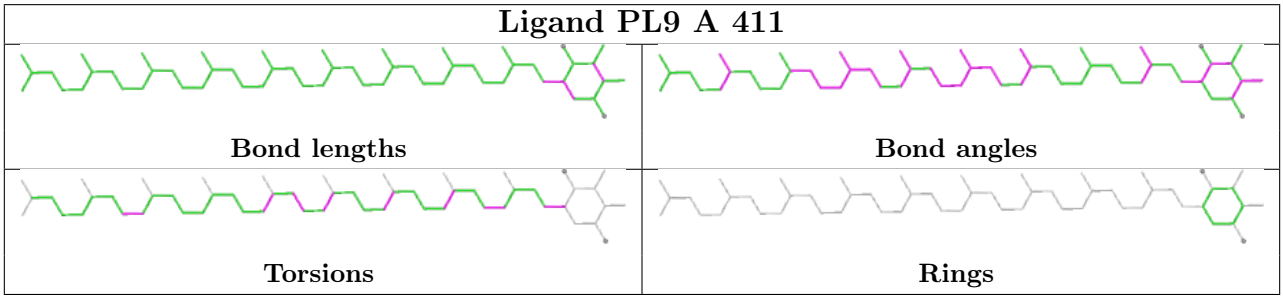
Torsions



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	334/334 (100%)	-0.48	7 (2%) 63 60	17, 28, 66, 87	1 (0%)
1	a	334/334 (100%)	-0.18	33 (9%) 13 10	17, 30, 96, 135	1 (0%)
2	B	505/505 (100%)	-0.32	16 (3%) 50 47	21, 33, 67, 109	3 (0%)
2	b	483/505 (95%)	-0.32	5 (1%) 79 77	19, 35, 57, 124	1 (0%)
3	C	451/455 (99%)	-0.29	3 (0%) 84 82	24, 37, 55, 106	0
3	c	455/455 (100%)	-0.14	2 (0%) 88 87	27, 41, 57, 89	1 (0%)
4	D	342/342 (100%)	-0.55	0 100 100	14, 29, 51, 86	3 (0%)
4	d	341/342 (99%)	-0.41	4 (1%) 76 74	16, 32, 59, 85	2 (0%)
5	E	79/80 (98%)	0.19	3 (3%) 44 41	30, 53, 77, 89	0
5	e	79/80 (98%)	0.43	3 (3%) 44 41	35, 54, 91, 96	0
6	F	33/33 (100%)	0.03	1 (3%) 52 49	32, 38, 68, 87	0
6	f	31/33 (93%)	0.18	1 (3%) 50 47	34, 42, 62, 95	0
7	H	63/63 (100%)	0.11	1 (1%) 70 67	22, 41, 51, 104	3 (4%)
7	h	62/63 (98%)	0.31	1 (1%) 70 67	26, 48, 62, 74	1 (1%)
8	I	34/36 (94%)	-0.08	0 100 100	33, 42, 60, 78	0
8	i	35/36 (97%)	-0.19	0 100 100	34, 43, 71, 95	0
9	J	36/40 (90%)	0.02	2 (5%) 30 27	29, 46, 73, 82	0
9	j	40/40 (100%)	0.25	2 (5%) 34 31	34, 47, 81, 92	0
10	K	37/37 (100%)	-0.11	0 100 100	36, 44, 55, 70	0
10	k	37/37 (100%)	0.18	1 (2%) 56 53	39, 47, 68, 81	0
11	L	35/35 (100%)	-0.25	1 (2%) 53 50	23, 32, 66, 78	0
11	l	35/35 (100%)	-0.04	1 (2%) 53 50	25, 35, 75, 92	0
12	O	243/243 (100%)	-0.20	1 (0%) 88 87	20, 39, 69, 104	1 (0%)
12	o	243/243 (100%)	-0.19	4 (1%) 70 67	24, 42, 71, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	T	29/30 (96%)	-0.24	2 (6%) 23 20	26, 32, 59, 89	0
13	t	29/30 (96%)	-0.16	2 (6%) 23 20	27, 34, 66, 98	0
14	U	97/97 (100%)	-0.32	0 100 100	26, 36, 58, 89	1 (1%)
14	u	97/97 (100%)	-0.31	1 (1%) 79 77	28, 37, 51, 76	0
15	V	137/137 (100%)	-0.53	0 100 100	22, 34, 50, 70	1 (0%)
15	v	137/137 (100%)	-0.11	0 100 100	24, 44, 61, 84	1 (0%)
16	Y	29/29 (100%)	0.28	1 (3%) 48 45	40, 54, 69, 81	0
16	y	29/29 (100%)	0.53	1 (3%) 48 45	51, 62, 70, 74	0
17	X	37/37 (100%)	0.31	1 (2%) 56 53	27, 50, 72, 83	1 (2%)
17	x	36/37 (97%)	0.63	1 (2%) 55 52	41, 54, 88, 89	0
18	Z	62/62 (100%)	0.70	6 (9%) 13 10	42, 54, 88, 106	0
18	z	61/62 (98%)	1.04	10 (16%) 4 3	49, 64, 98, 102	0
All	All	5147/5190 (99%)	-0.21	117 (2%) 61 58	14, 37, 70, 135	21 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	486	LEU	5.6
1	a	230	THR	5.5
17	x	37	VAL	5.2
7	H	64	ALA	4.8
1	A	246	TYR	4.6
13	t	30	THR	4.4
1	a	242	GLU	4.4
2	B	479	PHE	4.4
3	c	19	ASN	4.1
11	L	3	PRO	4.1
1	a	262	TYR	3.9
18	Z	33	TRP	3.9
1	a	235	TYR	3.7
18	z	3	ILE	3.6
1	a	240	GLY	3.6
9	j	2	MET	3.6
2	B	485	GLU	3.6
2	b	479	PHE	3.6
1	A	230	THR	3.5
13	t	29	ILE	3.5
1	a	256	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
4	d	27	PHE	3.4
13	T	29	ILE	3.4
16	y	18	VAL	3.4
1	A	245	THR	3.3
1	a	254	TYR	3.3
1	a	231	GLU	3.3
1	a	263	ALA	3.2
1	a	245	THR	3.2
11	l	3	PRO	3.2
5	E	5	THR	3.2
1	a	261	GLN	3.2
12	o	132	ASN	3.2
18	z	2	THR	3.2
1	a	228	THR	3.1
18	z	61	VAL	3.1
1	a	224	ILE	3.1
2	b	482	ILE	3.0
2	B	504	THR	3.0
1	a	229	GLU	3.0
1	a	255	PHE	3.0
1	A	231	GLU	3.0
6	F	16	PHE	2.9
2	B	487	SER	2.9
18	Z	35	ARG	2.9
2	B	499	VAL	2.9
2	b	480	SER	2.9
2	B	2	GLY	2.8
4	d	237	PRO	2.8
1	a	258	LEU	2.8
9	J	30	TYR	2.8
18	z	5	PHE	2.8
1	a	249	VAL	2.8
2	B	494	GLY	2.7
3	C	23	ALA	2.7
3	c	143	TYR	2.7
2	B	484	PRO	2.7
18	z	32	ASP	2.6
1	a	248	ILE	2.6
6	f	15	ILE	2.6
18	z	4	LEU	2.6
5	e	72	ALA	2.6
18	z	60	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
17	X	38	GLN	2.6
2	b	126	PRO	2.6
1	a	259	ILE	2.6
12	o	59	LYS	2.6
18	Z	3	ILE	2.5
1	a	246	TYR	2.5
1	a	223	LEU	2.5
18	z	34	ASP	2.5
18	z	35	ARG	2.5
2	B	501	ASP	2.5
1	a	238	LYS	2.4
2	b	484	PRO	2.4
1	a	226	GLU	2.4
1	A	11	ALA	2.3
5	e	84	LYS	2.3
1	a	264	SER	2.3
1	a	260	PHE	2.3
5	E	80	LEU	2.3
4	d	240	ALA	2.3
1	a	227	THR	2.3
16	Y	18	VAL	2.3
2	B	488	PRO	2.3
1	A	262	TYR	2.3
2	B	85	GLY	2.3
1	a	250	ALA	2.3
2	B	503	THR	2.3
1	a	243	GLU	2.3
4	d	28	VAL	2.3
5	E	83	LEU	2.3
3	C	25	ASN	2.3
18	z	1	MET	2.3
5	e	61	ARG	2.3
7	h	22	ALA	2.3
1	a	234	ASN	2.2
3	C	24	THR	2.2
14	u	8	GLU	2.2
18	Z	36	SER	2.2
10	k	18	PHE	2.2
1	a	237	TYR	2.2
18	Z	7	LEU	2.2
18	Z	30	PRO	2.2
9	J	5	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	480	SER	2.2
2	B	497	GLN	2.1
1	a	251	ALA	2.1
1	a	239	PHE	2.1
1	a	225	ARG	2.1
13	T	30	THR	2.1
1	A	247	ASN	2.1
12	O	56	PRO	2.1
2	B	502	VAL	2.1
9	j	1	MET	2.0
12	o	38	TYR	2.0
12	o	134	THR	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
13	FME	T	1	10/11	0.88	0.14	38,42,72,75	0
13	FME	t	1	10/11	0.92	0.10	33,38,80,91	0
8	FME	I	1	10/11	0.96	0.09	33,37,40,41	0
8	FME	i	1	10/11	0.97	0.09	36,41,45,48	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
31	DMS	c	942	4/4	0.60	0.24	101,103,111,117	0
31	DMS	c	936	4/4	0.64	0.22	106,116,116,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	DMS	C	537	4/4	0.67	0.29	88,103,104,113	0
30	UNL	c	932	10/-	0.70	0.23	56,74,80,83	0
31	DMS	O	307	4/4	0.70	0.24	84,97,98,104	0
30	UNL	i	104	16/-	0.70	0.23	67,76,87,89	0
31	DMS	c	937	4/4	0.70	0.25	80,90,91,100	0
31	DMS	B	639	4/4	0.70	0.20	72,87,90,102	0
34	HTG	b	624	19/19	0.70	0.18	69,97,109,110	0
31	DMS	O	305	4/4	0.71	0.20	68,70,79,99	0
29	LMT	f	102	25/35	0.71	0.21	61,93,105,108	0
34	HTG	c	922	19/19	0.71	0.16	70,93,109,112	0
30	UNL	t	102	16/-	0.72	0.16	59,71,78,80	0
30	UNL	i	105	10/-	0.72	0.22	67,78,86,87	0
31	DMS	u	205	4/4	0.73	0.26	64,67,73,83	0
31	DMS	b	637	4/4	0.73	0.20	90,97,101,112	0
30	UNL	a	417	10/-	0.73	0.24	75,80,84,87	0
30	UNL	Z	102	9/-	0.74	0.17	57,71,79,81	0
34	HTG	b	627	19/19	0.74	0.16	50,92,108,109	0
34	HTG	D	415	19/19	0.74	0.19	39,69,80,87	0
35	DGD	d	406	43/66	0.74	0.22	58,85,139,146	0
34	HTG	D	414	19/19	0.75	0.18	63,103,114,115	0
34	HTG	b	632	19/19	0.75	0.20	56,74,91,92	0
31	DMS	b	636	4/4	0.75	0.23	88,95,109,113	0
31	DMS	c	938	4/4	0.75	0.20	86,91,98,103	0
34	HTG	B	627	19/19	0.76	0.16	51,104,113,116	0
31	DMS	v	207	4/4	0.76	0.31	84,93,97,117	0
29	LMT	I	102	35/35	0.77	0.15	76,88,100,102	0
31	DMS	d	414	4/4	0.77	0.28	102,112,113,120	0
30	UNL	I	105	16/-	0.77	0.20	70,82,88,90	0
30	UNL	a	420	6/-	0.77	0.20	56,59,60,60	0
30	UNL	b	628	11/-	0.77	0.16	58,63,78,79	0
31	DMS	V	211	4/4	0.77	0.23	77,84,85,85	0
31	DMS	u	204	4/4	0.78	0.20	50,68,69,75	0
27	LHG	A	412	31/49	0.78	0.19	66,83,107,117	0
31	DMS	v	204	4/4	0.78	0.19	87,88,90,91	0
31	DMS	a	401	4/4	0.78	0.28	75,84,85,104	0
30	UNL	u	201	11/-	0.78	0.20	47,53,69,69	0
34	HTG	v	203	16/19	0.78	0.15	52,69,81,97	0
35	DGD	D	407	50/66	0.78	0.20	60,87,120,123	0
31	DMS	l	105	4/4	0.78	0.26	100,103,110,115	0
31	DMS	c	943	4/4	0.79	0.21	77,82,87,92	0
22	CLA	b	602	65/65	0.79	0.16	49,67,89,98	0
31	DMS	l	103	4/4	0.79	0.24	91,95,97,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	DMS	c	935	4/4	0.79	0.16	71,78,81,84	0
31	DMS	u	203	4/4	0.79	0.21	56,68,72,84	0
29	LMT	A	414	35/35	0.79	0.17	59,86,109,114	0
31	DMS	C	540	4/4	0.79	0.22	82,83,91,97	0
31	DMS	H	103	4/4	0.79	0.21	63,67,69,74	0
31	DMS	v	205	4/4	0.79	0.19	70,72,78,80	0
31	DMS	L	102	4/4	0.79	0.23	79,80,91,100	0
29	LMT	T	102	24/35	0.80	0.17	42,80,98,101	0
31	DMS	f	103	4/4	0.80	0.24	87,89,90,100	0
31	DMS	O	313	4/4	0.80	0.26	89,100,100,107	0
27	LHG	a	416	49/49	0.80	0.17	60,84,100,108	0
34	HTG	V	203	14/19	0.81	0.15	48,52,79,84	0
31	DMS	c	944	4/4	0.81	0.20	79,82,89,92	0
29	LMT	Z	101	35/35	0.81	0.16	40,105,123,128	0
31	DMS	C	539	4/4	0.81	0.23	88,90,93,95	0
25	LMG	D	412	46/55	0.81	0.19	41,68,138,142	0
31	DMS	B	634	4/4	0.81	0.23	57,68,73,95	0
30	UNL	j	103	16/-	0.81	0.16	59,67,71,74	0
31	DMS	C	534	4/4	0.81	0.17	105,111,112,121	0
31	DMS	B	631	4/4	0.82	0.19	78,80,84,87	0
28	SQD	D	408	20/54	0.82	0.15	65,97,105,108	0
31	DMS	B	637	4/4	0.82	0.20	69,76,80,88	0
34	HTG	l	106	19/19	0.82	0.17	63,97,108,109	0
31	DMS	U	203	4/4	0.82	0.23	62,73,74,76	0
30	UNL	T	101	13/-	0.82	0.16	63,71,77,79	0
24	BCR	B	618	19/40	0.82	0.15	50,59,74,77	0
30	UNL	I	104	16/-	0.83	0.18	60,71,84,86	0
34	HTG	C	532	19/19	0.83	0.14	69,98,111,112	0
26	PL9	A	411	55/55	0.83	0.20	61,73,87,92	0
28	SQD	l	101	54/54	0.83	0.16	53,82,119,123	0
30	UNL	U	201	14/-	0.83	0.17	44,57,65,66	0
27	LHG	d	401	33/49	0.83	0.14	62,94,138,142	0
31	DMS	t	105	4/4	0.83	0.23	89,93,101,108	0
29	LMT	a	419	35/35	0.83	0.18	46,69,93,100	0
29	LMT	E	101	24/35	0.83	0.17	61,82,97,113	0
29	LMT	t	101	24/35	0.83	0.13	50,71,109,119	0
31	DMS	c	940	4/4	0.83	0.19	74,74,75,80	0
30	UNL	I	103	13/-	0.83	0.17	53,57,77,82	0
31	DMS	C	533	4/4	0.83	0.19	79,84,85,89	0
29	LMT	c	931	24/35	0.84	0.18	50,84,95,98	0
28	SQD	b	621	38/54	0.84	0.16	58,90,110,112	0
31	DMS	C	536	4/4	0.84	0.20	77,80,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	LMG	b	622	43/55	0.84	0.17	48,78,88,98	0
31	DMS	d	415	4/4	0.84	0.17	60,63,67,79	0
31	DMS	C	538	4/4	0.84	0.14	79,86,86,87	0
30	UNL	b	625	16/-	0.84	0.15	43,52,64,67	0
34	HTG	C	523	9/19	0.84	0.17	63,69,81,86	0
31	DMS	V	207	4/4	0.84	0.18	64,71,71,76	0
29	LMT	c	921	35/35	0.84	0.15	74,90,99,103	0
31	DMS	o	308	4/4	0.85	0.16	76,77,82,91	0
31	DMS	V	210	4/4	0.85	0.19	70,73,78,88	0
26	PL9	a	415	55/55	0.85	0.22	64,84,106,111	0
25	LMG	c	930	49/55	0.85	0.13	44,78,96,106	0
31	DMS	b	634	4/4	0.85	0.15	68,76,79,86	0
28	SQD	f	101	14/54	0.85	0.12	77,89,96,96	0
27	LHG	C	522	30/49	0.85	0.14	55,79,127,134	0
31	DMS	c	929	4/4	0.85	0.25	69,73,76,78	0
31	DMS	O	314	4/4	0.85	0.19	78,80,86,91	0
25	LMG	d	409	47/55	0.85	0.15	49,76,113,114	0
25	LMG	C	531	40/55	0.85	0.14	37,81,103,107	0
31	DMS	V	209	4/4	0.86	0.21	76,87,89,93	0
30	UNL	x	101	15/-	0.86	0.11	43,50,56,58	0
31	DMS	o	305	4/4	0.86	0.17	78,82,86,87	0
30	UNL	B	624	7/-	0.86	0.18	30,45,51,56	0
31	DMS	t	103	4/4	0.86	0.17	89,102,103,103	0
28	SQD	a	418	51/54	0.86	0.14	47,70,91,97	0
31	DMS	c	941	4/4	0.86	0.15	73,79,87,88	0
31	DMS	O	308	4/4	0.86	0.17	64,72,73,80	0
31	DMS	B	636	4/4	0.86	0.14	60,62,67,69	0
25	LMG	B	621	40/55	0.86	0.16	47,82,108,112	0
31	DMS	c	927	4/4	0.86	0.21	87,89,91,97	0
30	UNL	A	415	5/-	0.86	0.18	68,72,73,75	0
30	UNL	i	103	16/-	0.86	0.14	53,64,79,82	0
31	DMS	a	421	4/4	0.87	0.19	85,87,87,94	0
31	DMS	o	302	4/4	0.87	0.17	59,64,71,75	0
31	DMS	o	303	4/4	0.87	0.21	60,77,80,83	0
31	DMS	D	417	4/4	0.87	0.16	72,72,77,86	0
31	DMS	b	635	4/4	0.87	0.16	62,69,76,86	0
31	DMS	U	202	4/4	0.87	0.21	42,49,58,67	0
24	BCR	b	618	20/40	0.87	0.18	57,65,70,71	0
27	LHG	l	102	49/49	0.87	0.14	38,61,91,95	0
30	UNL	J	103	16/-	0.87	0.13	44,57,77,77	0
31	DMS	B	642	4/4	0.87	0.16	65,66,75,82	0
31	DMS	C	529	4/4	0.87	0.16	72,78,78,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMT	B	622	24/35	0.87	0.12	57,67,73,78	0
31	DMS	l	104	4/4	0.87	0.20	79,80,86,87	0
31	DMS	v	210	4/4	0.87	0.25	63,71,80,91	0
31	DMS	t	104	4/4	0.88	0.15	101,101,104,111	0
30	UNL	i	102	16/-	0.88	0.15	41,51,80,81	0
24	BCR	b	619	31/40	0.88	0.11	47,54,63,67	0
31	DMS	A	416	4/4	0.88	0.19	60,67,69,72	0
31	DMS	C	535	4/4	0.88	0.16	70,79,83,86	0
31	DMS	A	417	4/4	0.88	0.15	76,82,83,85	0
31	DMS	V	204	4/4	0.88	0.16	66,73,76,76	0
31	DMS	O	303	4/4	0.88	0.15	68,71,78,79	0
31	DMS	b	638	4/4	0.88	0.20	49,52,54,70	0
28	SQD	A	413	49/54	0.88	0.15	46,65,91,95	0
34	HTG	C	521	19/19	0.88	0.12	55,80,93,96	0
31	DMS	C	528	4/4	0.88	0.21	88,89,90,90	0
31	DMS	V	212	4/4	0.89	0.17	51,54,55,72	0
27	LHG	D	409	49/49	0.89	0.15	38,56,85,97	0
31	DMS	v	206	4/4	0.89	0.17	69,72,72,77	0
31	DMS	C	530	4/4	0.89	0.17	71,79,82,83	0
31	DMS	b	631	4/4	0.89	0.16	68,72,79,80	0
31	DMS	V	205	4/4	0.89	0.13	64,66,67,71	0
31	DMS	O	311	4/4	0.89	0.15	48,56,59,61	0
31	DMS	B	632	4/4	0.89	0.14	49,57,67,69	0
30	UNL	D	413	16/-	0.89	0.12	38,46,52,58	0
30	UNL	O	301	16/-	0.89	0.16	39,47,73,74	0
37	RRX	h	101	41/41	0.89	0.12	40,49,75,82	0
31	DMS	c	928	4/4	0.90	0.15	73,74,74,80	0
30	UNL	B	625	16/-	0.90	0.12	40,47,59,59	0
22	CLA	B	602	65/65	0.90	0.11	39,56,101,107	0
24	BCR	B	619	30/40	0.90	0.10	44,51,61,63	0
31	DMS	i	106	4/4	0.90	0.19	72,76,79,89	0
28	SQD	a	414	54/54	0.90	0.13	36,69,81,87	0
31	DMS	V	208	4/4	0.90	0.15	73,74,77,78	0
31	DMS	c	939	4/4	0.90	0.15	88,92,95,102	0
30	UNL	X	101	16/-	0.90	0.12	35,53,62,64	0
31	DMS	I	101	4/4	0.90	0.19	64,69,74,76	0
31	DMS	o	304	4/4	0.90	0.18	70,70,70,74	0
34	HTG	B	626	19/19	0.90	0.12	42,69,81,87	0
31	DMS	I	106	4/4	0.90	0.18	64,74,78,80	0
22	CLA	c	914	65/65	0.90	0.12	47,60,95,108	0
25	LMG	i	101	51/55	0.91	0.12	45,57,80,81	0
25	LMG	c	920	51/55	0.91	0.13	37,61,87,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	DMS	d	412	4/4	0.91	0.13	58,59,66,66	0
31	DMS	F	101	4/4	0.91	0.16	69,70,74,77	0
31	DMS	B	638	4/4	0.91	0.16	81,82,86,93	0
31	DMS	u	202	4/4	0.91	0.15	47,53,55,68	0
31	DMS	A	420	4/4	0.91	0.16	37,39,39,57	0
31	DMS	B	641	4/4	0.91	0.14	46,49,61,66	0
31	DMS	a	425	4/4	0.91	0.17	39,47,51,62	0
25	LMG	C	520	51/55	0.91	0.12	34,60,90,92	0
27	LHG	a	423	45/49	0.91	0.11	39,58,72,74	0
31	DMS	O	304	4/4	0.91	0.15	74,80,84,88	0
24	BCR	c	915	40/40	0.91	0.11	43,59,68,69	0
31	DMS	v	208	4/4	0.91	0.17	88,90,91,94	0
31	DMS	v	209	4/4	0.91	0.14	72,74,76,81	0
31	DMS	O	306	4/4	0.91	0.15	69,69,70,81	0
31	DMS	v	211	4/4	0.91	0.14	65,77,82,90	0
30	UNL	d	410	16/-	0.92	0.10	40,49,57,60	0
25	LMG	A	410	51/55	0.92	0.11	47,62,83,91	0
27	LHG	L	101	40/49	0.92	0.11	37,53,63,66	0
27	LHG	d	408	46/49	0.92	0.13	29,41,93,97	0
31	DMS	O	309	4/4	0.92	0.16	61,70,70,74	0
34	HTG	b	626	19/19	0.92	0.11	47,69,86,90	0
22	CLA	c	913	65/65	0.92	0.11	42,54,96,98	0
24	BCR	d	404	40/40	0.93	0.09	27,38,63,66	0
31	DMS	d	413	4/4	0.93	0.24	67,69,73,80	0
31	DMS	o	306	4/4	0.93	0.15	66,71,74,83	0
24	BCR	k	101	40/40	0.93	0.09	36,45,51,52	0
24	BCR	y	101	40/40	0.93	0.09	32,41,51,53	0
24	BCR	Y	101	39/40	0.93	0.08	34,40,48,50	0
31	DMS	C	527	4/4	0.93	0.16	74,80,80,81	0
32	BCT	a	422	4/4	0.93	0.10	51,52,56,57	0
22	CLA	C	507	65/65	0.93	0.11	37,45,85,88	0
31	DMS	c	926	4/4	0.93	0.14	63,64,67,68	0
31	DMS	B	635	4/4	0.93	0.15	61,63,66,73	0
35	DGD	c	918	62/66	0.93	0.10	34,42,98,113	0
22	CLA	b	617	60/65	0.93	0.10	32,41,75,80	0
37	RRX	H	101	41/41	0.93	0.10	32,42,58,62	0
22	CLA	C	514	65/65	0.93	0.10	44,55,83,86	0
22	CLA	B	615	53/65	0.94	0.09	31,36,71,84	0
22	CLA	b	607	65/65	0.94	0.08	29,37,58,65	0
31	DMS	a	424	4/4	0.94	0.12	38,47,50,65	0
24	BCR	C	515	40/40	0.94	0.09	37,50,58,59	0
31	DMS	B	633	4/4	0.94	0.17	65,71,71,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	b	615	52/65	0.94	0.09	36,42,71,76	0
22	CLA	B	617	55/65	0.94	0.09	28,35,72,76	0
34	HTG	b	623	19/19	0.94	0.09	42,46,54,63	0
22	CLA	c	904	65/65	0.94	0.08	32,44,50,54	0
22	CLA	c	907	65/65	0.94	0.11	39,47,102,108	0
24	BCR	c	916	40/40	0.94	0.08	33,42,48,49	0
22	CLA	c	908	65/65	0.94	0.09	34,39,53,61	0
31	DMS	B	640	4/4	0.94	0.17	47,53,57,63	0
28	SQD	C	501	54/54	0.94	0.11	32,64,83,89	0
25	LMG	j	101	47/55	0.94	0.10	33,43,69,74	0
35	DGD	C	518	62/66	0.94	0.10	29,40,89,109	0
31	DMS	c	934	4/4	0.94	0.11	64,73,74,77	0
22	CLA	B	607	65/65	0.94	0.08	28,34,56,65	0
22	CLA	B	608	65/65	0.94	0.09	24,29,64,79	0
35	DGD	h	102	62/66	0.94	0.09	28,42,53,58	0
22	CLA	d	403	65/65	0.94	0.10	35,40,85,90	0
31	DMS	A	419	4/4	0.94	0.17	58,60,70,72	0
31	DMS	c	933	4/4	0.95	0.12	57,64,66,70	0
22	CLA	b	614	59/65	0.95	0.08	26,32,76,82	0
31	DMS	O	310	4/4	0.95	0.14	66,68,68,73	0
24	BCR	B	620	40/40	0.95	0.07	30,37,49,50	0
22	CLA	C	509	65/65	0.95	0.09	29,35,81,102	0
24	BCR	C	516	40/40	0.95	0.08	32,39,47,54	0
24	BCR	D	405	40/40	0.95	0.08	26,35,62,66	0
24	BCR	K	101	40/40	0.95	0.08	31,39,43,43	0
31	DMS	V	201	4/4	0.95	0.10	46,48,54,58	0
32	BCT	A	421[A]	4/4	0.95	0.10	34,36,39,39	4
32	BCT	A	421[B]	4/4	0.95	0.10	27,29,30,34	4
26	PL9	D	406	55/55	0.95	0.07	21,30,37,51	0
33	CA	B	601	1/1	0.95	0.05	64,64,64,64	0
33	CA	O	302	1/1	0.95	0.06	59,59,59,59	0
34	HTG	B	623	19/19	0.95	0.09	41,47,64,66	0
22	CLA	C	512	65/65	0.95	0.08	31,39,48,51	0
26	PL9	d	405	55/55	0.95	0.07	23,32,39,43	0
24	BCR	a	413	40/40	0.95	0.07	26,31,38,39	0
22	CLA	c	902	65/65	0.95	0.08	34,39,50,51	0
22	CLA	C	513	56/65	0.95	0.08	37,48,62,65	0
27	LHG	D	411	45/49	0.95	0.10	31,39,90,94	0
24	BCR	b	620	40/40	0.95	0.07	33,39,48,49	0
22	CLA	c	906	65/65	0.95	0.08	30,40,50,54	0
31	DMS	D	416	4/4	0.95	0.12	55,59,60,69	0
22	CLA	B	611	65/65	0.95	0.08	26,33,41,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	D	404	65/65	0.95	0.09	30,37,94,104	0
31	DMS	b	630	4/4	0.95	0.15	56,63,63,64	0
31	DMS	B	629	4/4	0.95	0.14	48,52,58,65	0
31	DMS	b	633	4/4	0.95	0.14	68,68,70,78	0
22	CLA	c	909	65/65	0.95	0.08	31,37,80,97	0
22	CLA	c	910	65/65	0.95	0.09	28,38,58,64	0
22	CLA	c	912	65/65	0.95	0.08	35,45,50,53	0
35	DGD	C	519	62/66	0.95	0.09	23,36,76,85	0
22	CLA	a	412	65/65	0.95	0.11	27,32,102,116	0
35	DGD	H	102	62/66	0.95	0.08	28,37,46,50	0
22	CLA	B	604	65/65	0.95	0.08	26,30,40,47	0
35	DGD	c	919	62/66	0.95	0.09	29,40,73,79	0
22	CLA	C	508	65/65	0.95	0.08	32,42,55,59	0
23	PHO	a	411	64/64	0.95	0.06	26,33,40,48	0
25	LMG	J	101	45/55	0.95	0.09	28,36,71,79	0
22	CLA	b	610	65/65	0.95	0.08	32,41,45,54	0
22	CLA	A	408	65/65	0.96	0.09	19,29,99,110	0
27	LHG	d	407	49/49	0.96	0.07	28,36,56,63	0
31	DMS	d	411	4/4	0.96	0.12	60,62,64,64	0
22	CLA	b	608	65/65	0.96	0.08	27,31,73,74	0
31	DMS	B	630	4/4	0.96	0.13	63,67,68,75	0
22	CLA	b	609	65/65	0.96	0.06	27,34,42,45	0
23	PHO	A	407	64/64	0.96	0.06	20,25,30,32	0
23	PHO	D	402	64/64	0.96	0.06	25,29,35,39	0
23	PHO	a	410	64/64	0.96	0.06	21,28,32,36	0
22	CLA	B	614	61/65	0.96	0.07	25,31,70,83	0
24	BCR	A	409	40/40	0.96	0.06	25,30,37,38	0
22	CLA	b	611	65/65	0.96	0.07	28,35,40,43	0
22	CLA	b	612	65/65	0.96	0.08	27,31,72,83	0
22	CLA	B	606	65/65	0.96	0.07	24,30,42,46	0
22	CLA	C	510	65/65	0.96	0.09	31,36,59,64	0
22	CLA	b	616	65/65	0.96	0.07	30,37,53,57	0
31	DMS	c	924	4/4	0.96	0.14	37,42,47,49	0
31	DMS	c	925	4/4	0.96	0.11	51,58,60,61	0
22	CLA	C	511	65/65	0.96	0.06	31,36,41,46	0
22	CLA	B	610	65/65	0.96	0.06	30,37,42,46	0
31	DMS	O	312	4/4	0.96	0.14	37,51,56,59	0
22	CLA	C	502	65/65	0.96	0.07	33,39,52,62	0
22	CLA	c	905	65/65	0.96	0.08	30,35,62,66	0
35	DGD	C	517	62/66	0.96	0.09	24,35,80,88	0
22	CLA	C	503	65/65	0.96	0.07	28,32,47,56	0
22	CLA	C	504	65/65	0.96	0.06	29,37,42,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	DMS	v	201	4/4	0.96	0.16	42,48,50,51	0
22	CLA	C	505	65/65	0.96	0.07	28,34,58,60	0
35	DGD	c	917	62/66	0.96	0.08	26,42,81,94	0
27	LHG	D	410	49/49	0.96	0.07	29,36,51,61	0
22	CLA	C	506	65/65	0.96	0.07	30,37,50,54	0
31	DMS	V	206	4/4	0.96	0.09	45,48,51,62	0
22	CLA	b	603	65/65	0.96	0.07	29,36,46,49	0
36	HEM	E	102	43/43	0.96	0.09	48,56,62,65	0
22	CLA	c	911	65/65	0.96	0.06	29,38,46,52	0
22	CLA	b	604	65/65	0.96	0.07	26,32,45,50	0
38	MG	J	102	1/1	0.96	0.06	30,30,30,30	0
22	CLA	B	609	65/65	0.97	0.06	25,30,38,39	0
31	DMS	C	526	4/4	0.97	0.09	48,48,50,51	0
22	CLA	B	616	65/65	0.97	0.06	30,36,50,57	0
22	CLA	A	406	55/65	0.97	0.06	21,27,49,60	0
31	DMS	b	629	4/4	0.97	0.09	29,31,36,45	0
22	CLA	a	408	65/65	0.97	0.05	20,26,35,41	0
22	CLA	a	409	61/65	0.97	0.07	25,29,80,87	0
22	CLA	B	603	65/65	0.97	0.06	27,36,43,47	0
22	CLA	b	613	65/65	0.97	0.06	26,32,37,40	0
22	CLA	B	612	65/65	0.97	0.06	23,29,55,60	0
22	CLA	B	613	65/65	0.97	0.06	24,30,37,40	0
22	CLA	A	405	65/65	0.97	0.06	18,23,36,54	0
22	CLA	b	605	65/65	0.97	0.07	23,29,63,65	0
22	CLA	d	402	65/65	0.97	0.05	21,27,42,50	0
36	HEM	e	101	43/43	0.97	0.09	43,55,85,93	0
31	DMS	o	307	4/4	0.97	0.19	48,56,62,64	0
22	CLA	b	606	65/65	0.97	0.06	24,28,40,40	0
22	CLA	c	903	65/65	0.97	0.07	27,34,54,65	0
38	MG	k	102	1/1	0.97	0.07	48,48,48,48	0
31	DMS	c	923	4/4	0.98	0.09	37,40,42,43	0
22	CLA	B	605	65/65	0.98	0.06	24,28,60,66	0
31	DMS	B	628	4/4	0.98	0.07	27,29,32,38	0
31	DMS	D	418	4/4	0.98	0.06	35,39,42,43	0
31	DMS	C	525	4/4	0.98	0.08	34,35,38,40	0
22	CLA	a	407	65/65	0.98	0.05	23,26,45,61	0
21	CL	A	404	1/1	0.98	0.04	28,28,28,28	0
22	CLA	D	401	65/65	0.98	0.05	19,23,31,36	0
31	DMS	A	418	4/4	0.98	0.05	29,30,31,31	0
38	MG	K	102	1/1	0.98	0.05	51,51,51,51	0
22	CLA	D	403	65/65	0.98	0.05	18,24,45,52	0
39	HEC	V	202	43/43	0.98	0.06	23,29,36,40	0

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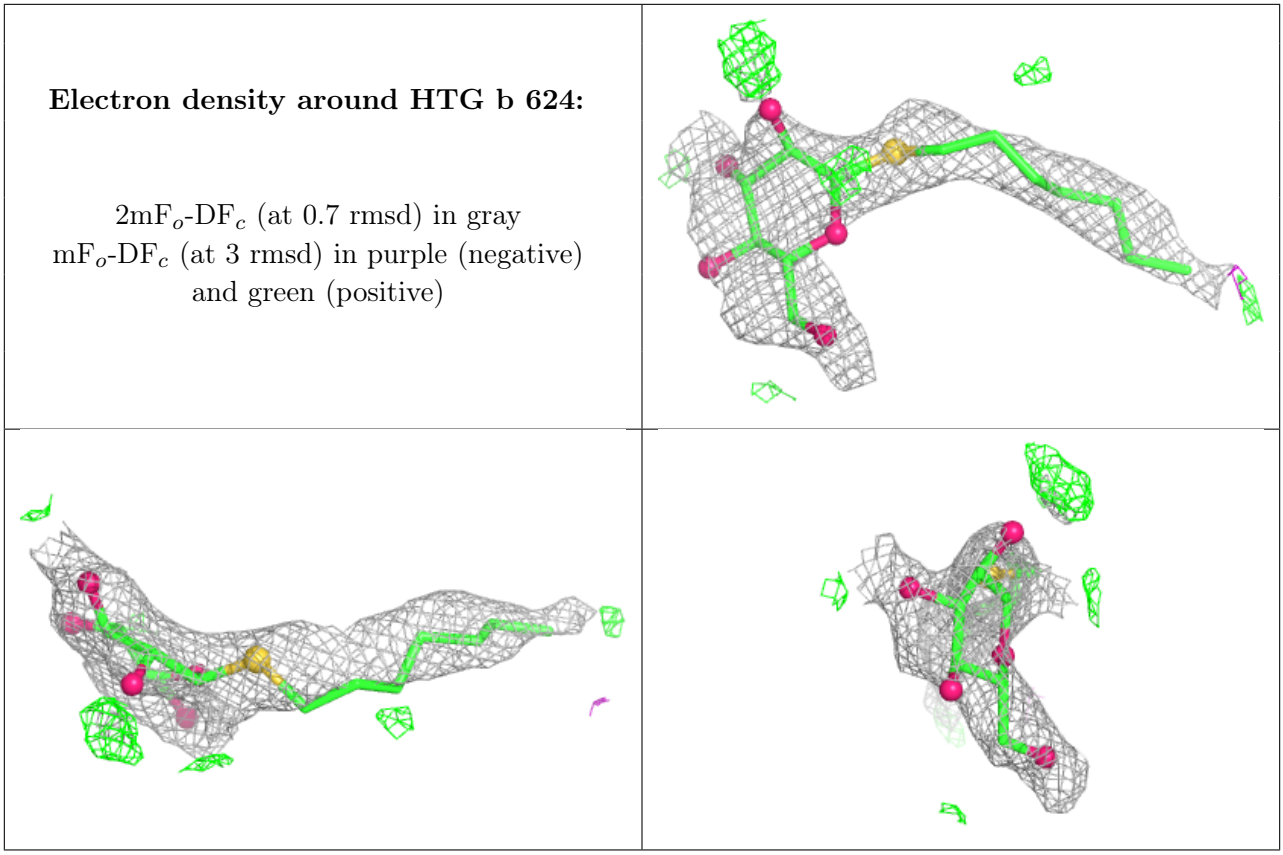
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
39	HEC	v	202	43/43	0.98	0.06	33,37,42,46	0
21	CL	a	406	1/1	0.99	0.03	32,32,32,32	0
33	CA	b	601	1/1	0.99	0.03	59,59,59,59	0
33	CA	c	901	1/1	0.99	0.05	48,48,48,48	0
33	CA	o	301	1/1	0.99	0.04	55,55,55,55	0
31	DMS	a	402	4/4	0.99	0.07	30,32,34,34	0
38	MG	j	102	1/1	0.99	0.08	40,40,40,40	0
31	DMS	C	524	4/4	0.99	0.06	38,42,43,43	0
21	CL	A	403	1/1	0.99	0.04	29,29,29,29	0
21	CL	a	405	1/1	0.99	0.04	31,31,31,31	0
19	OEX	A	401	10/10	1.00	0.05	25,27,31,32	0
19	OEX	a	403	10/10	1.00	0.03	29,31,32,33	0
20	FE2	A	402	1/1	1.00	0.01	39,39,39,39	0
20	FE2	a	404	1/1	1.00	0.01	42,42,42,42	0

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

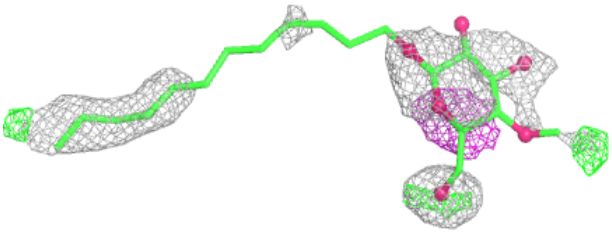
Electron density around HTG b 624:

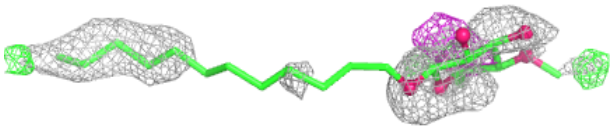
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

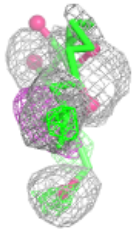


Electron density around LMT f 102:

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

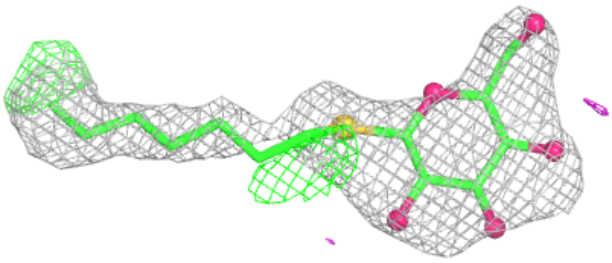


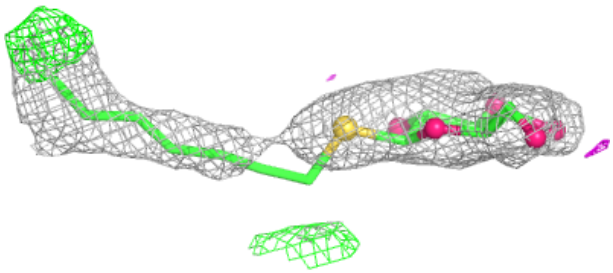


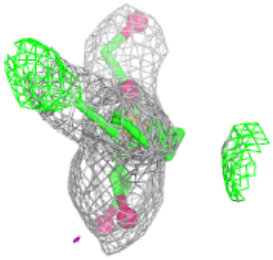


Electron density around HTG c 922:

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

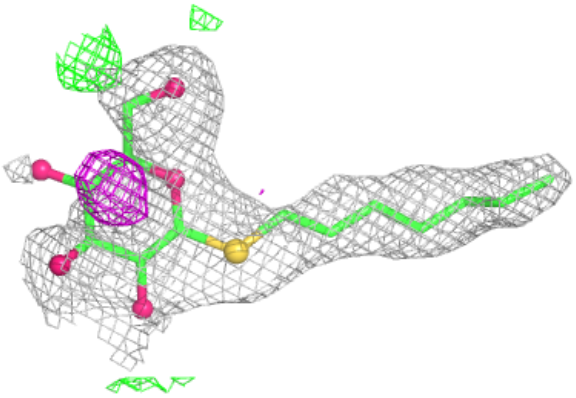


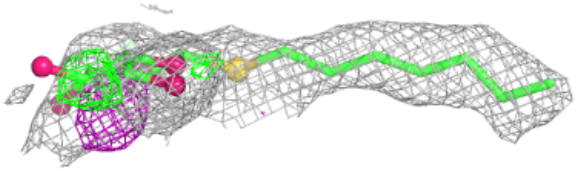


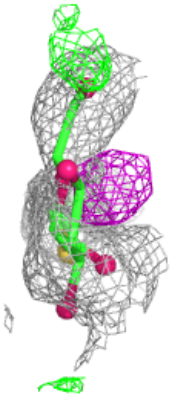


Electron density around HTG b 627:

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

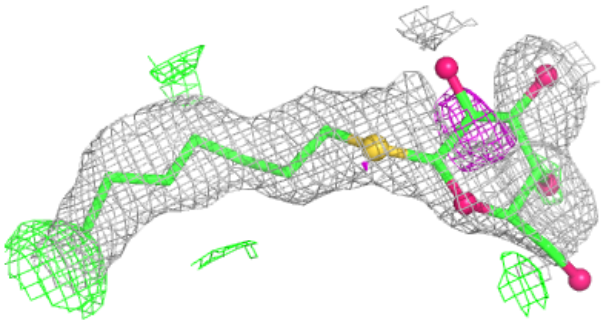


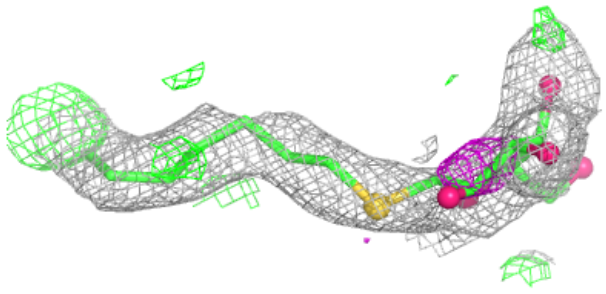


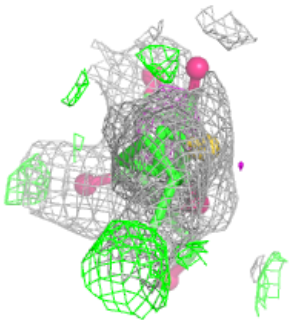


Electron density around HTG D 415:

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

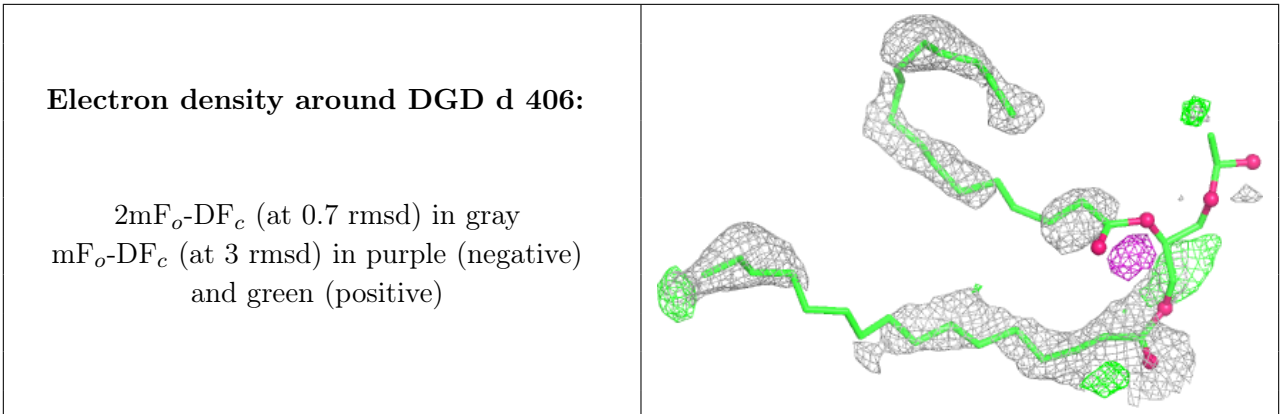


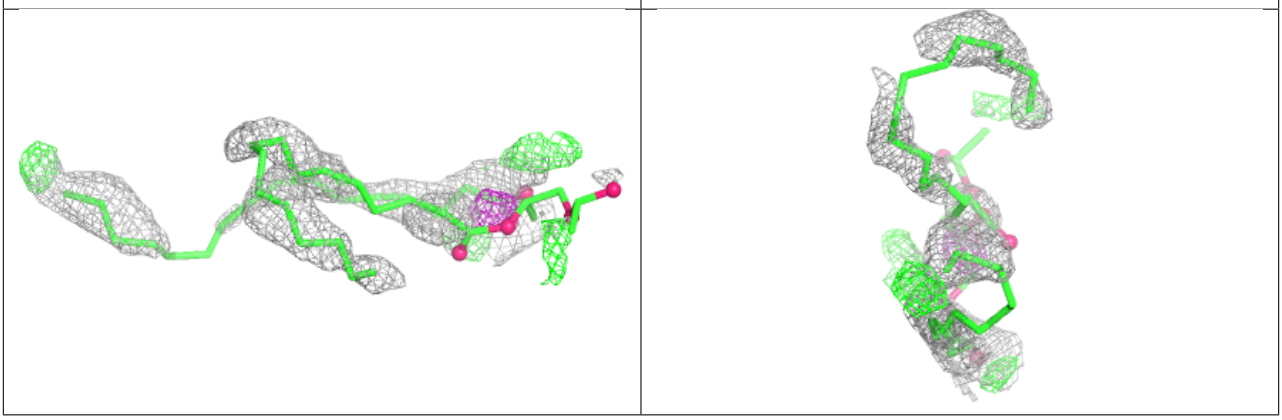




Electron density around DGD d 406:

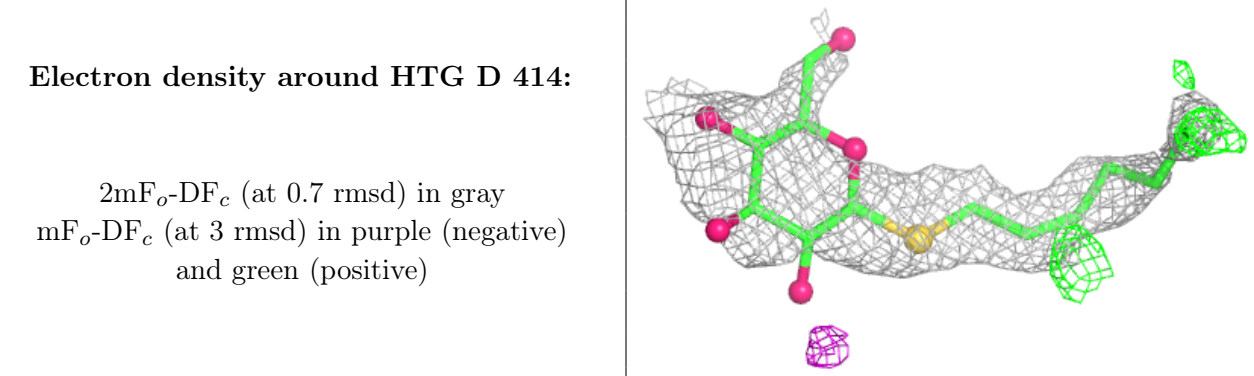
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

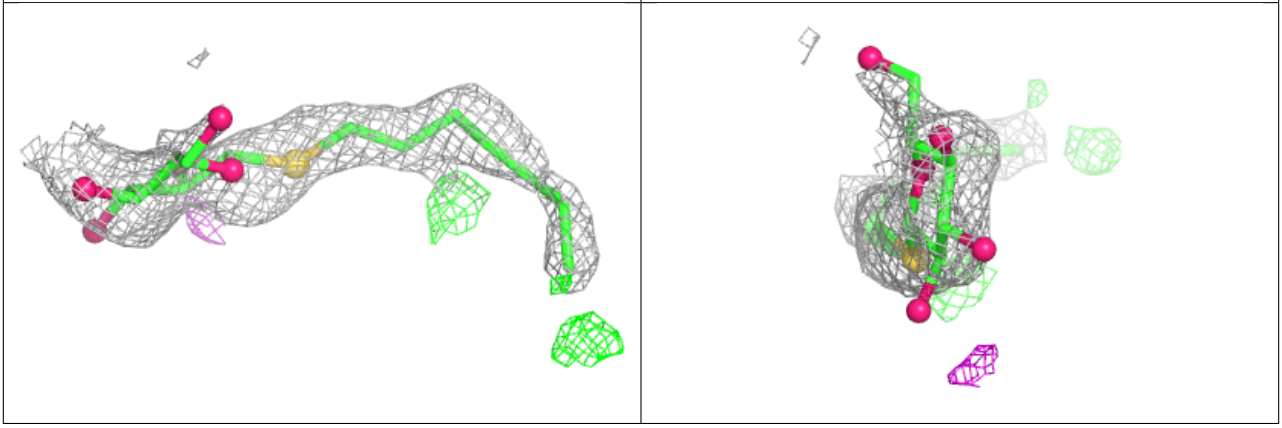




Electron density around HTG D 414:

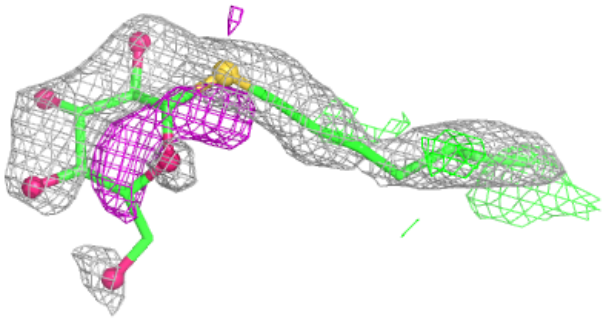
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

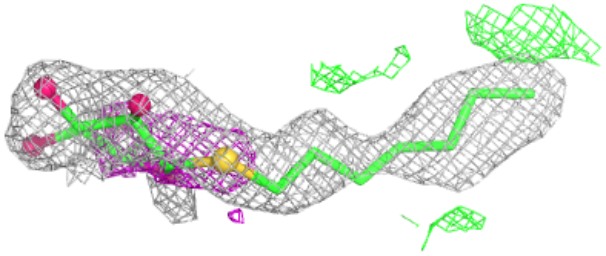


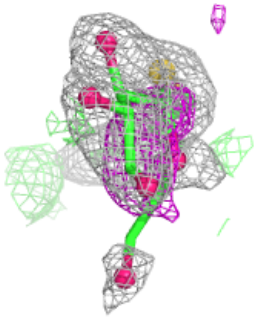


Electron density around HTG b 632:

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

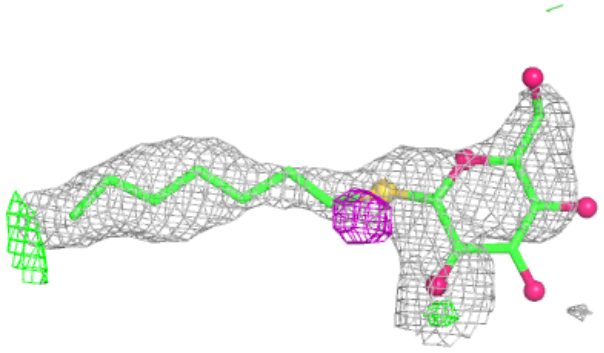


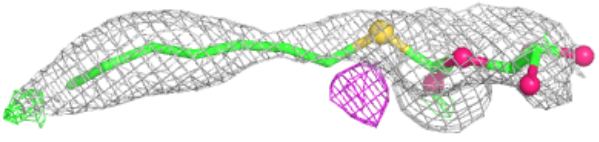


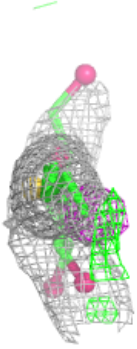


Electron density around HTG B 627:

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

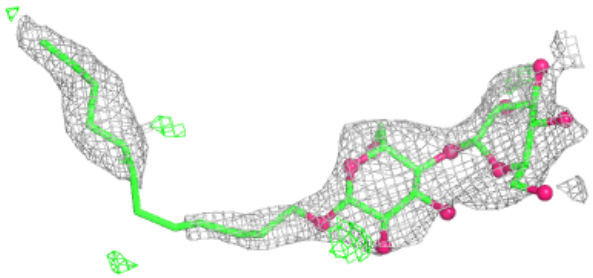


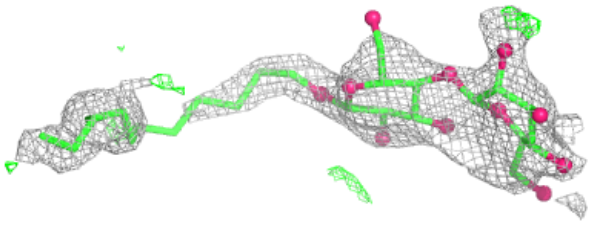


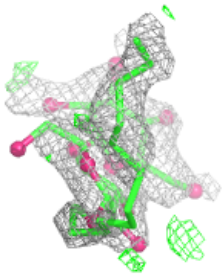


Electron density around LMT I 102:

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

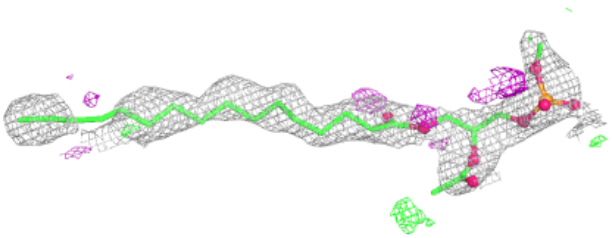


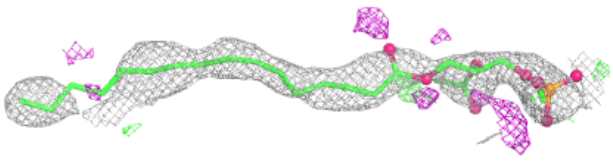


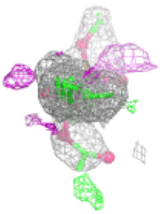


Electron density around LHG A 412:

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

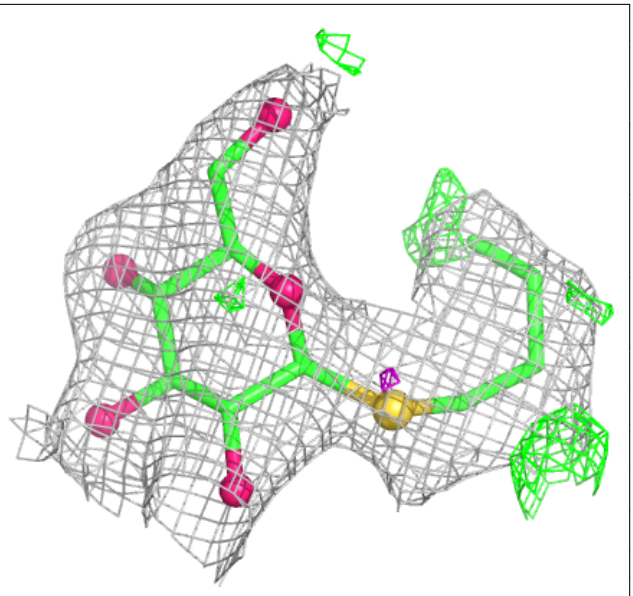


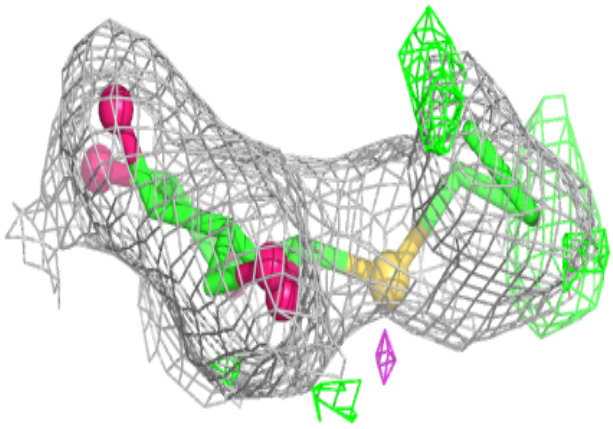


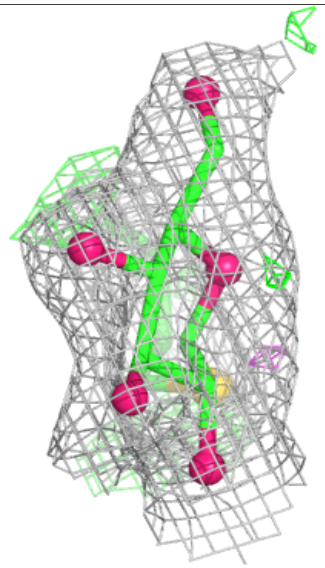


Electron density around HTG v 203:

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

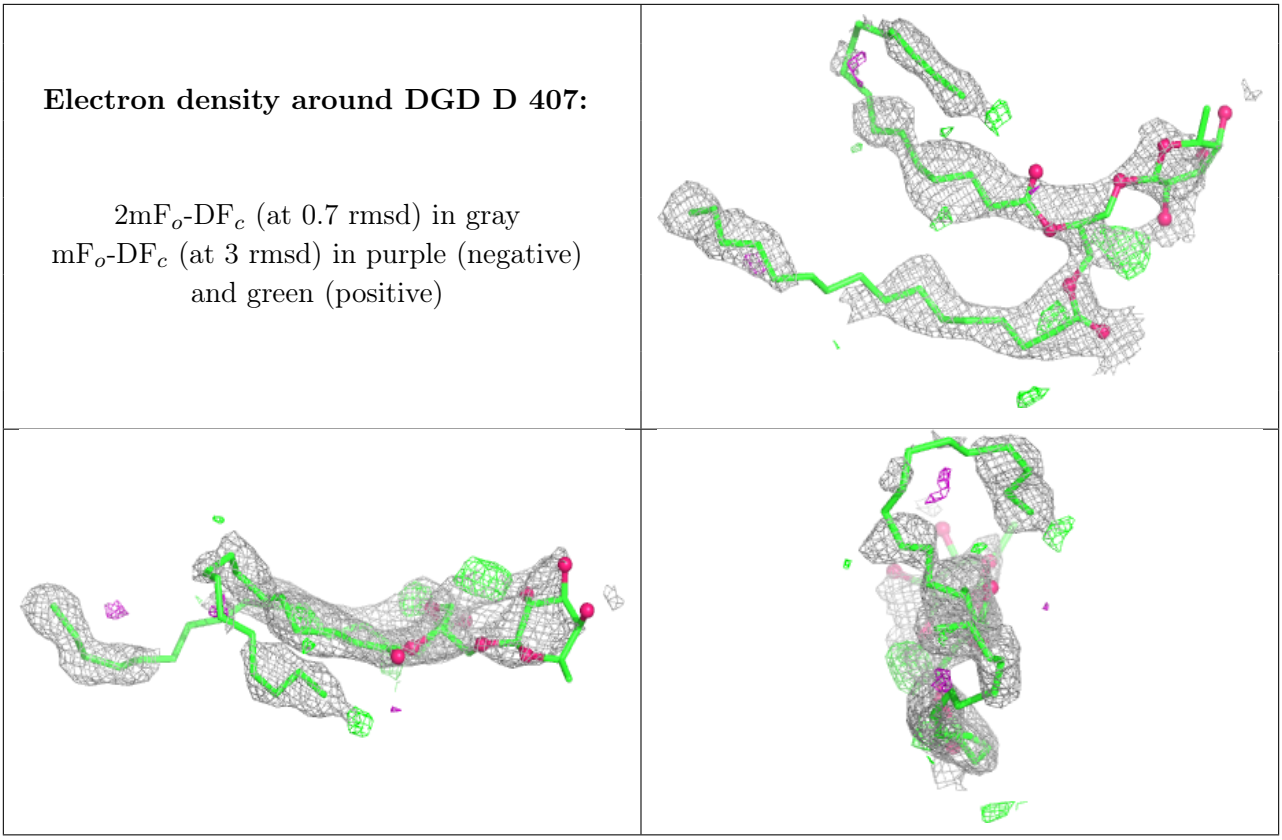






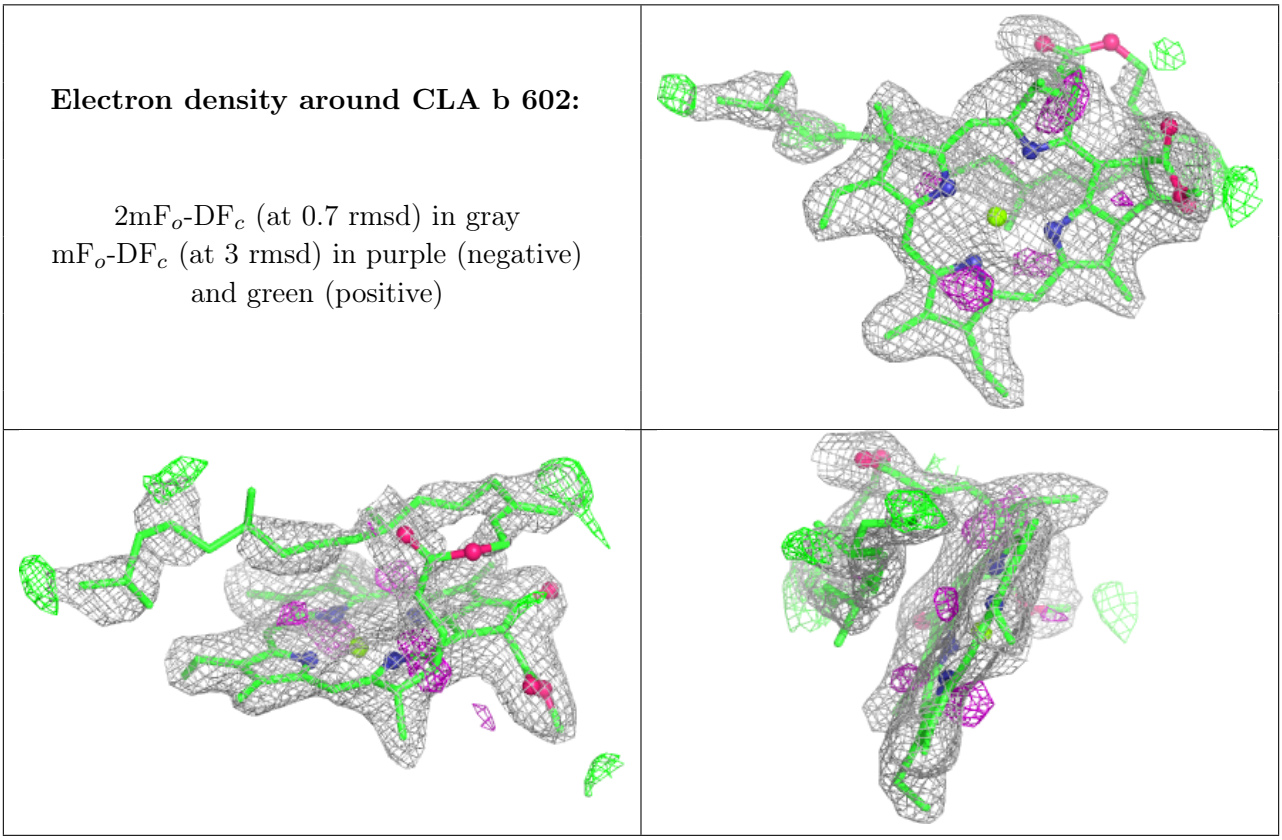
Electron density around DGD D 407:

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



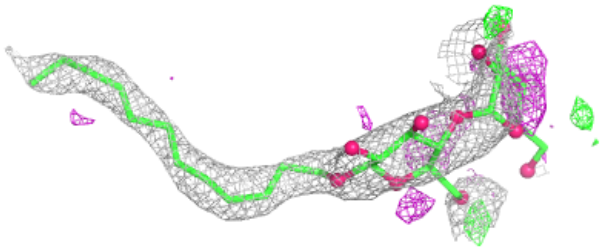
Electron density around CLA b 602:

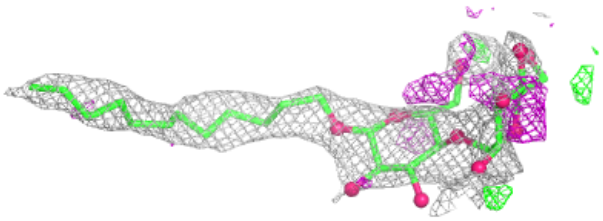
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

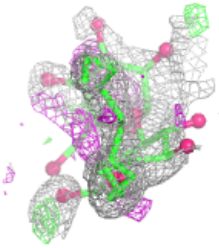


Electron density around LMT A 414:

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

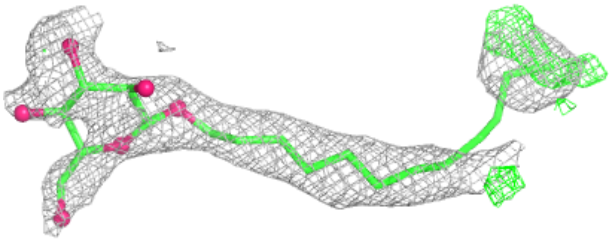


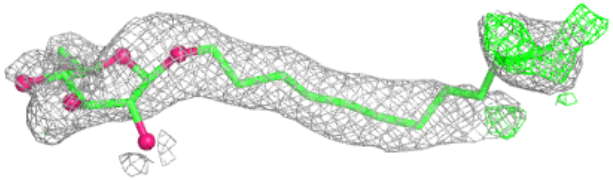


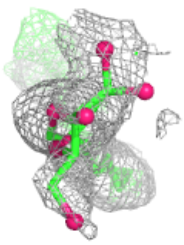


Electron density around LMT T 102:

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

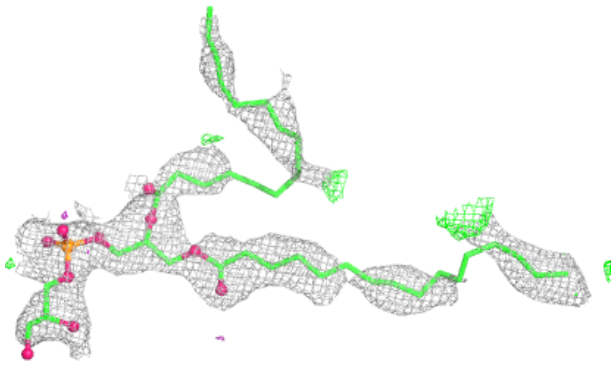


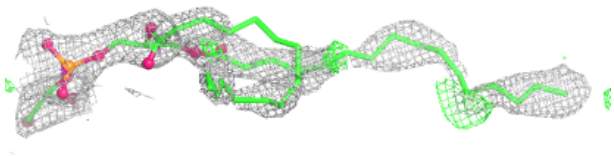


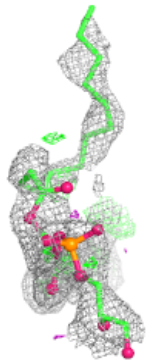


Electron density around LHG a 416:

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

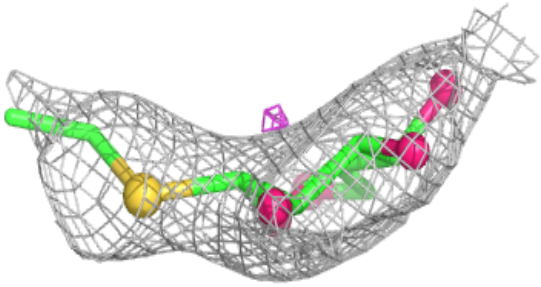


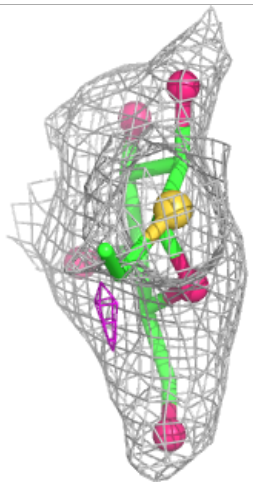




Electron density around HTG V 203:

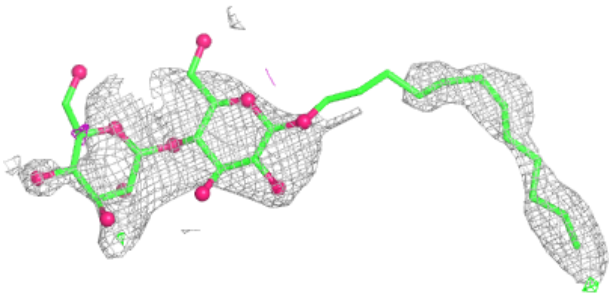
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

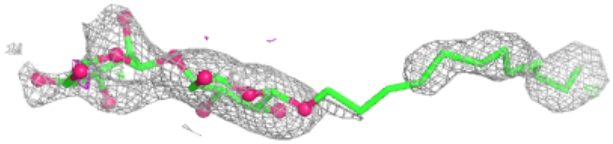


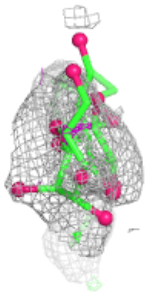


Electron density around LMT Z 101:

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

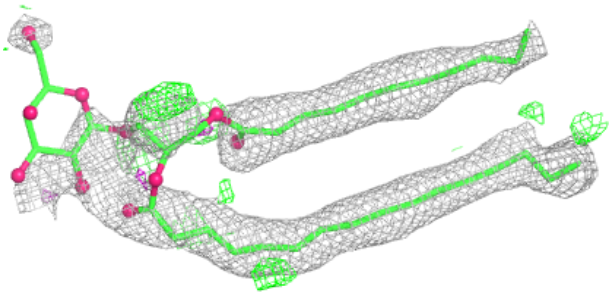


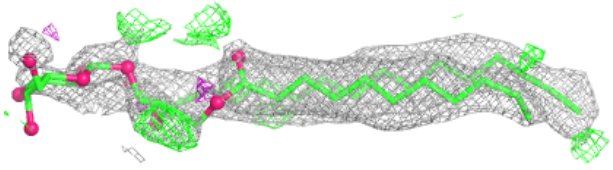




Electron density around LMG D 412:

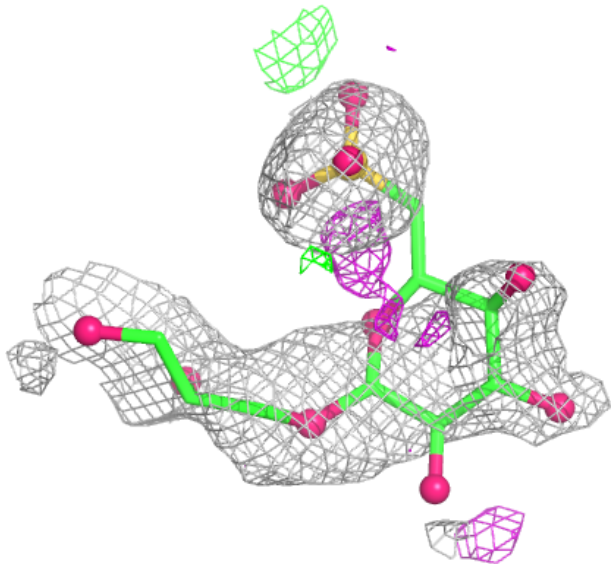
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

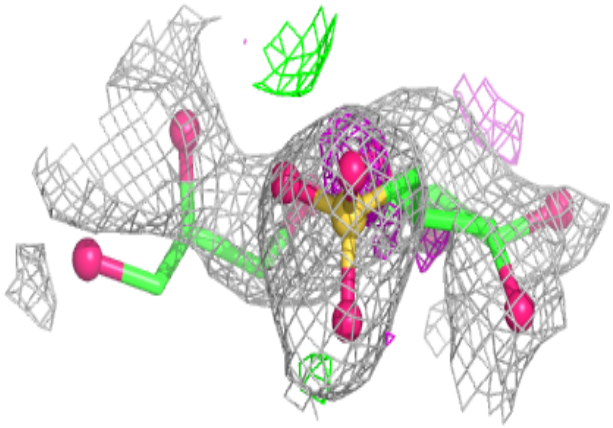


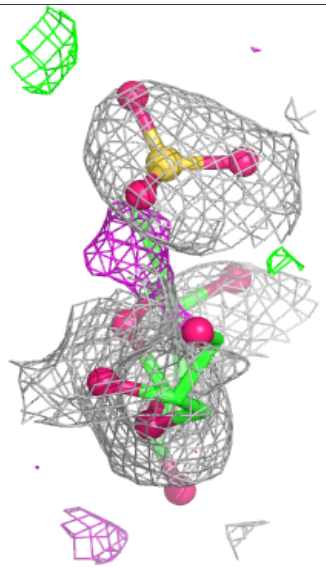


Electron density around SQD D 408:

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

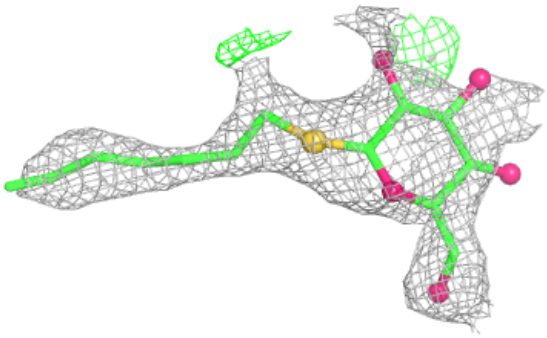


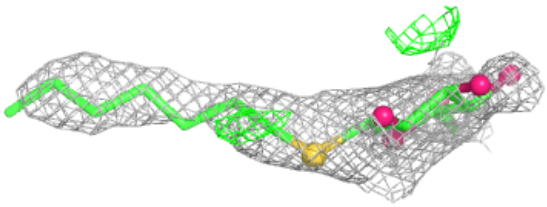


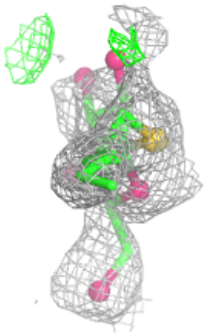


Electron density around HTG l 106:

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

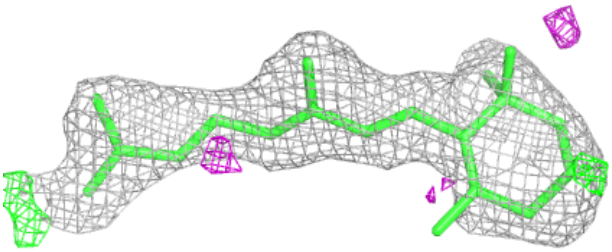


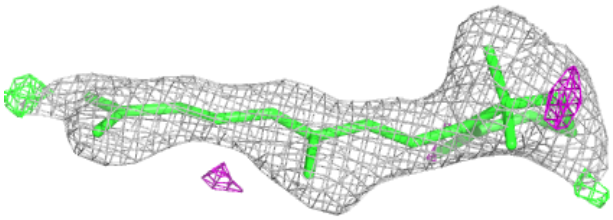


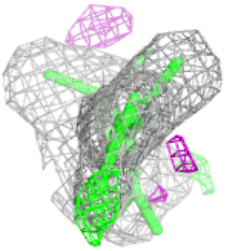


Electron density around BCR B 618:

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

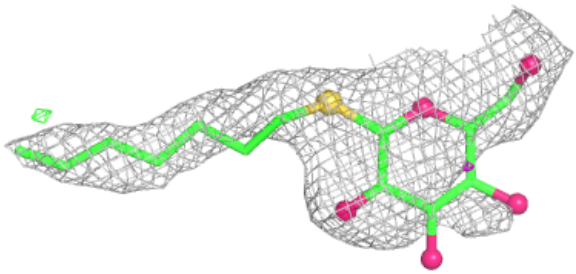


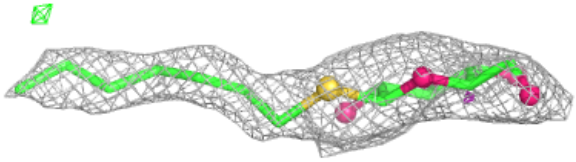


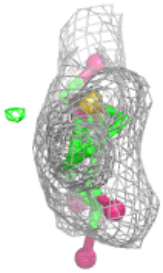


Electron density around HTG C 532:

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

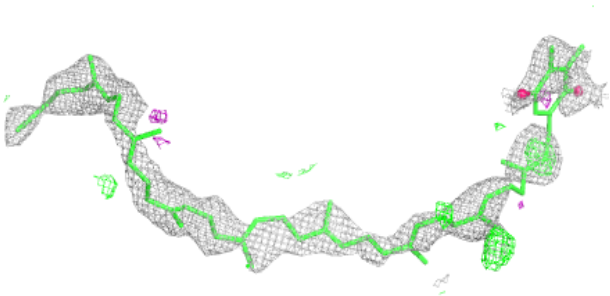


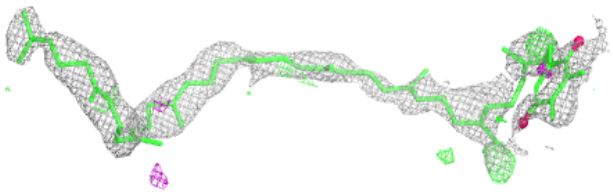


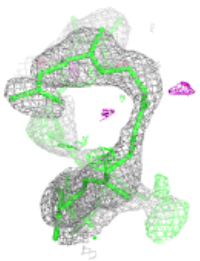


Electron density around PL9 A 411:

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

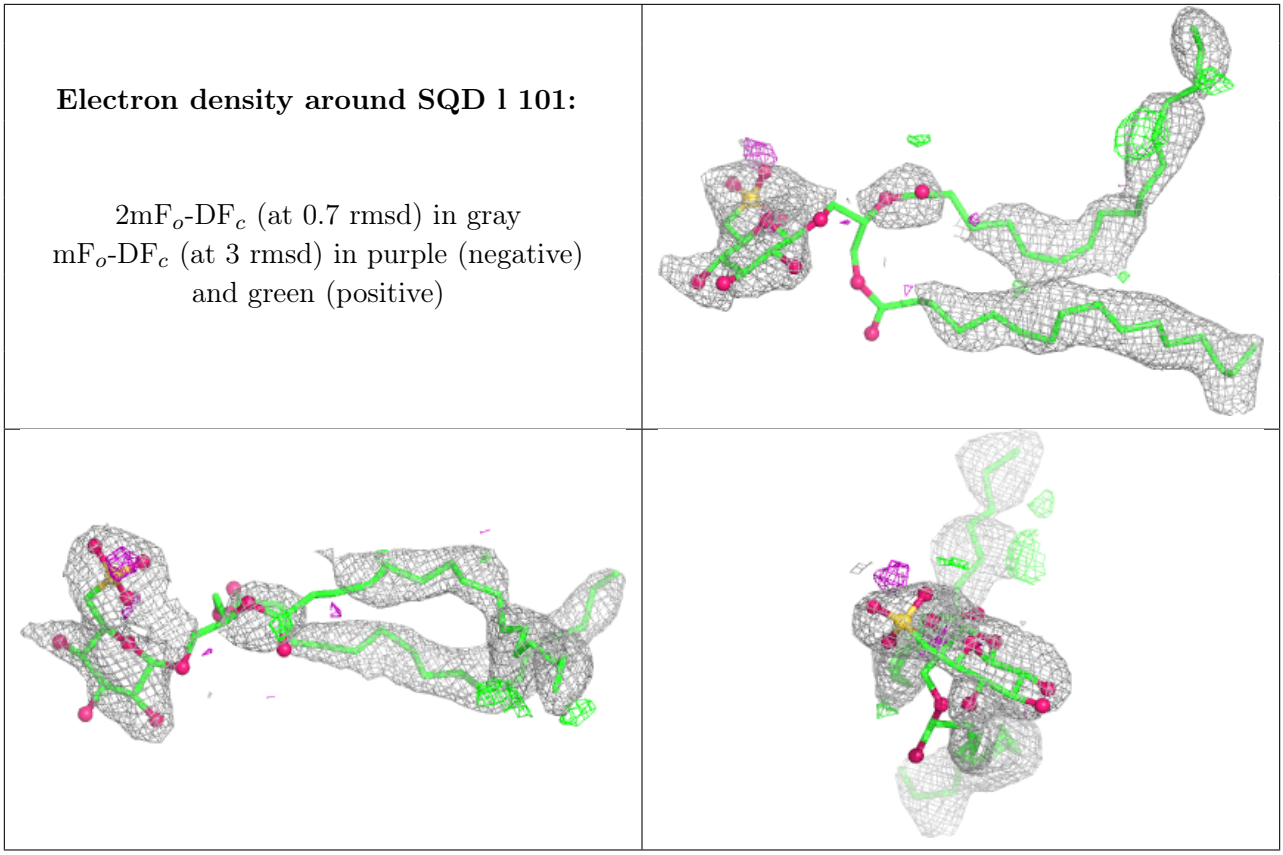






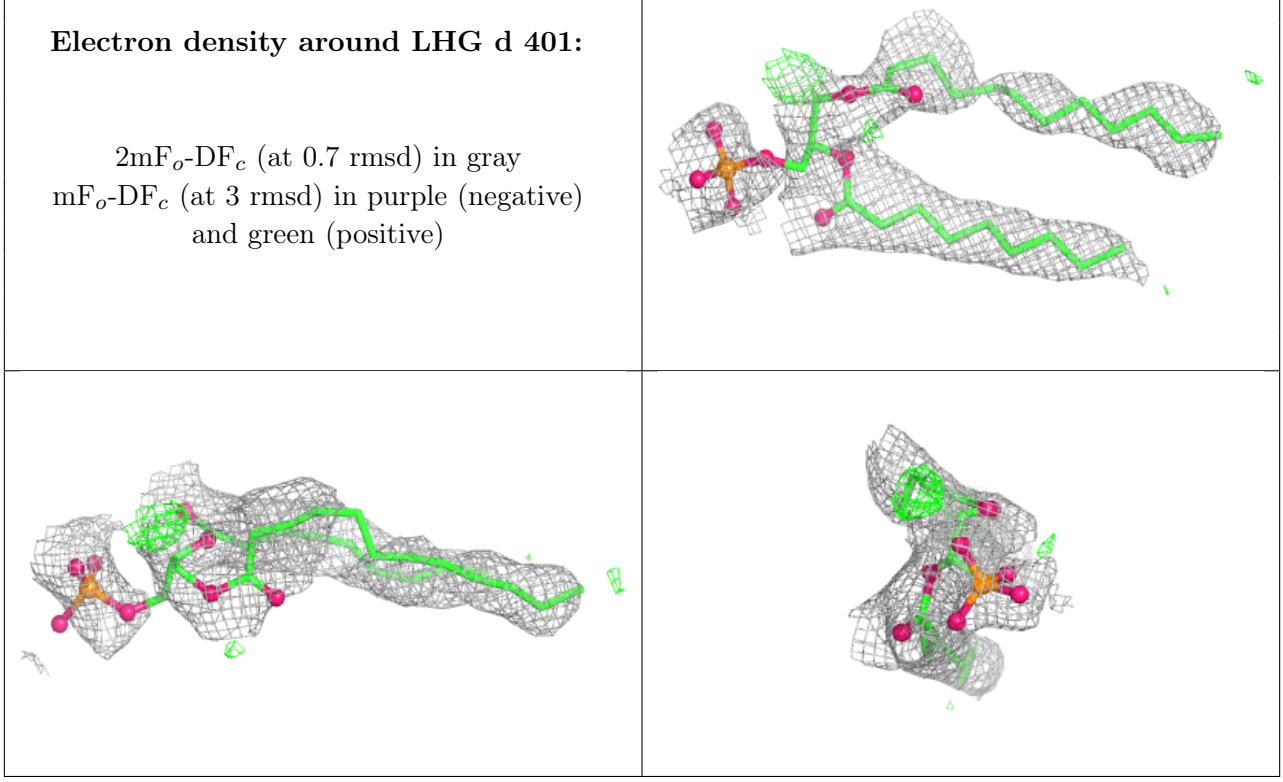
Electron density around SQD l 101:

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



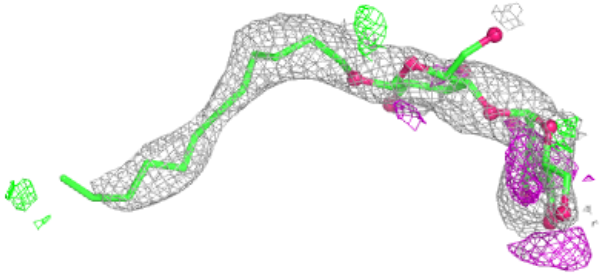
Electron density around LHG d 401:

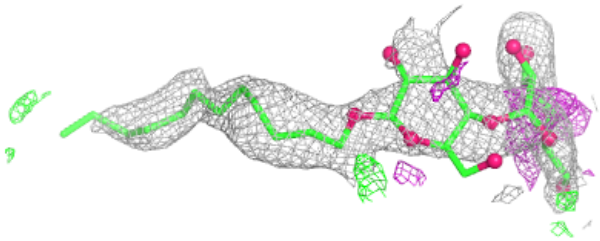
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

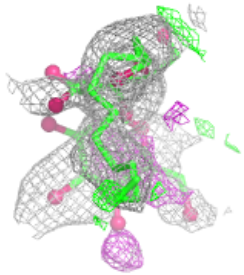


Electron density around LMT a 419:

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

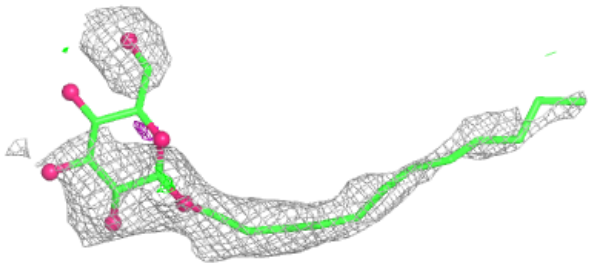


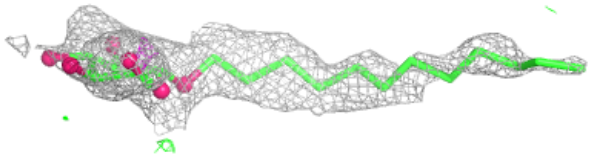


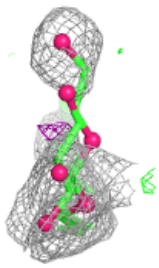


Electron density around LMT E 101:

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

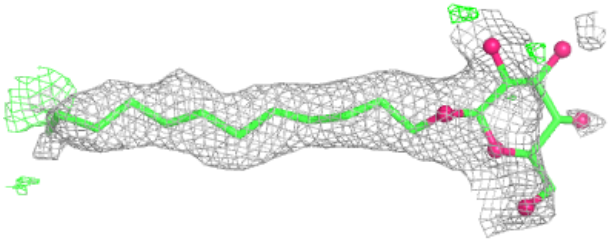


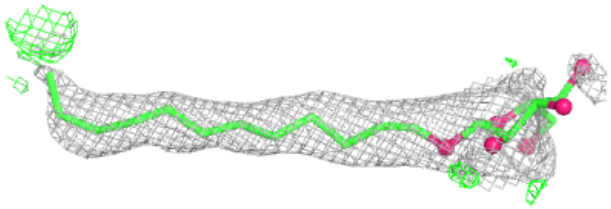


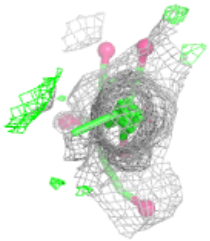


Electron density around LMT t 101:

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

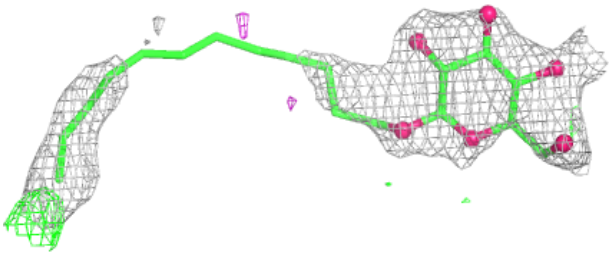


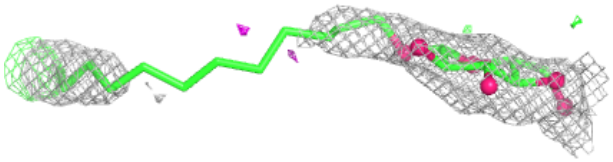


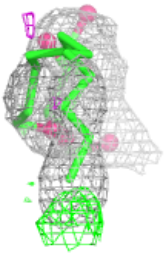


Electron density around LMT c 931:

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

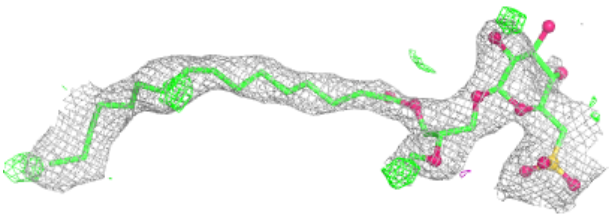


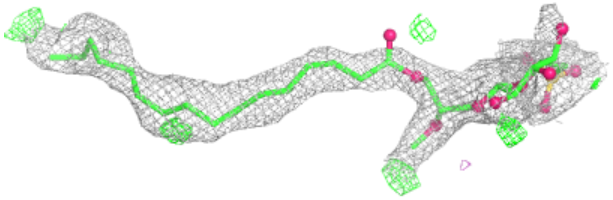


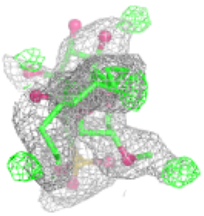


Electron density around SQD b 621:

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

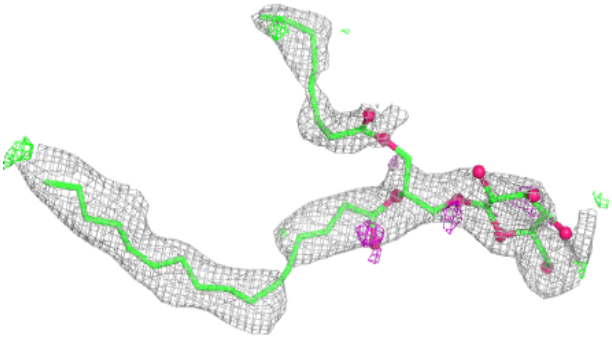


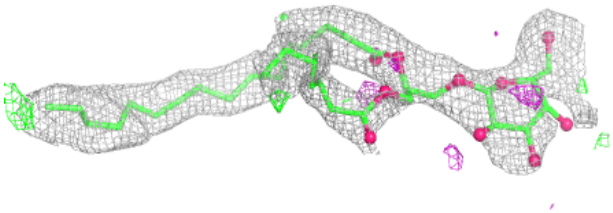


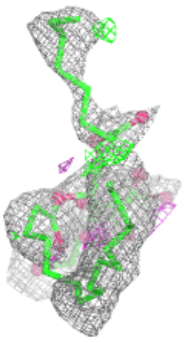


Electron density around LMG b 622:

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

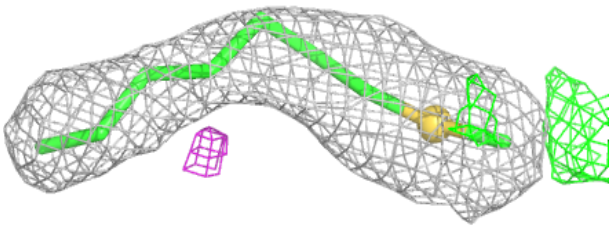


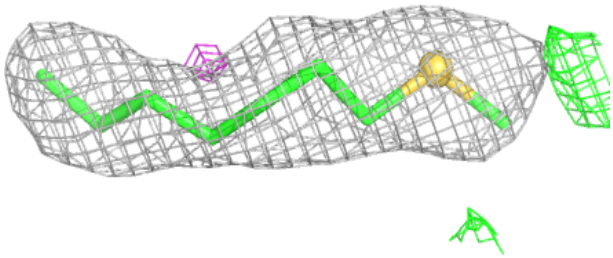


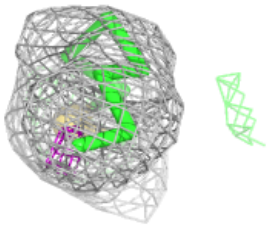


Electron density around HTG C 523:

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

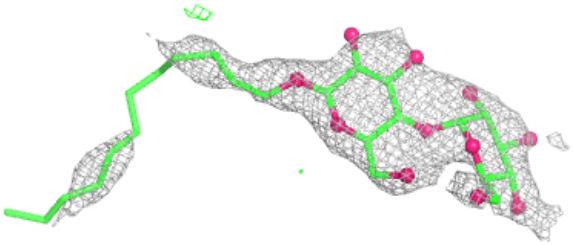


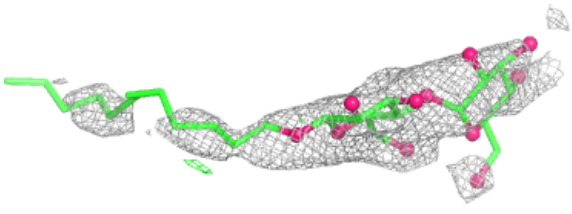


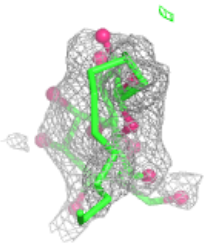


Electron density around LMT c 921:

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

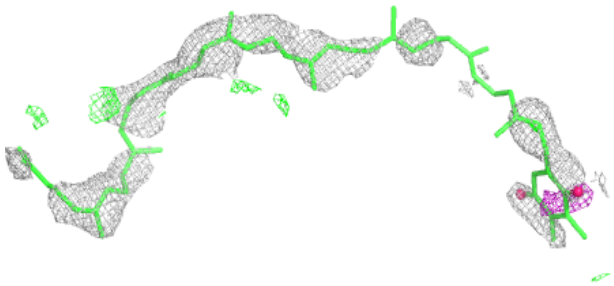


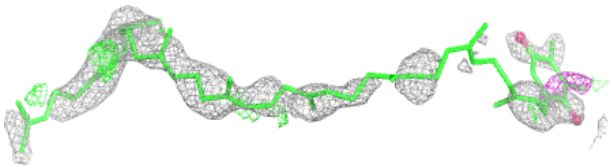


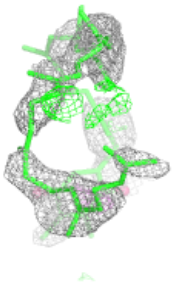


Electron density around PL9 a 415:

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

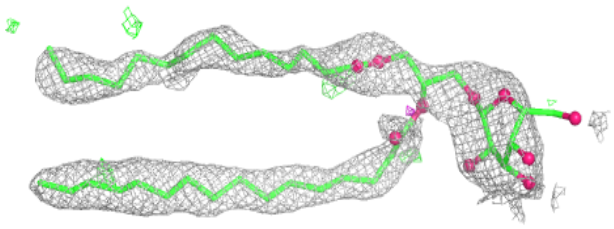


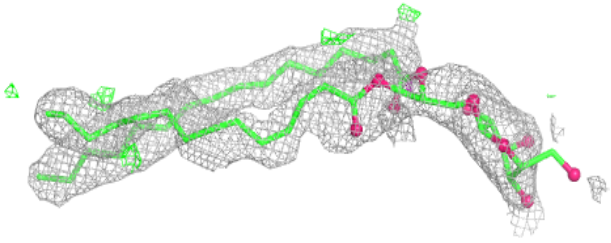


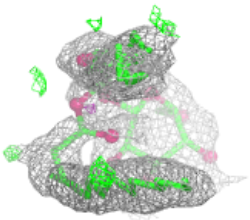


Electron density around LMG c 930:

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

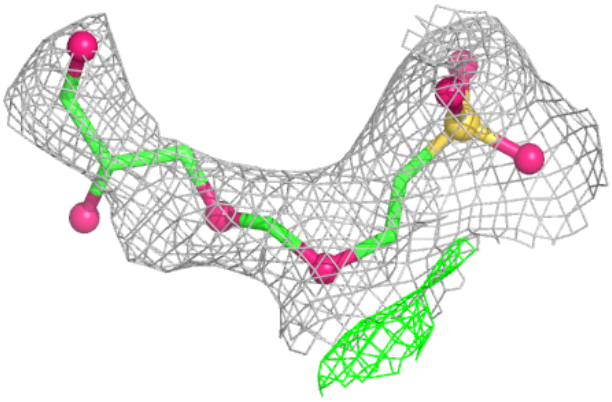


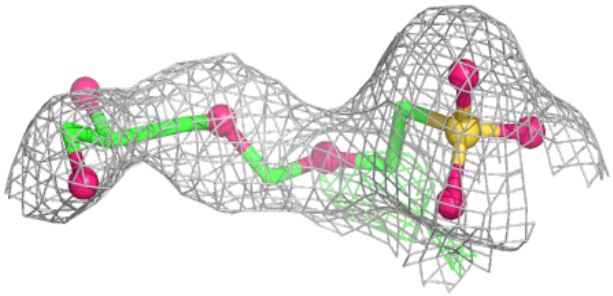


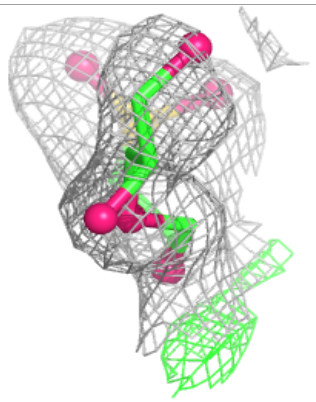


Electron density around SQD f 101:

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

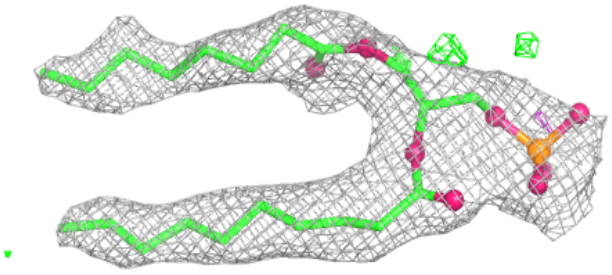


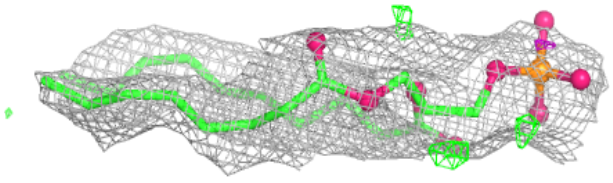


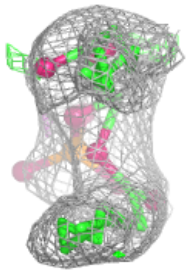


Electron density around LHG C 522:

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

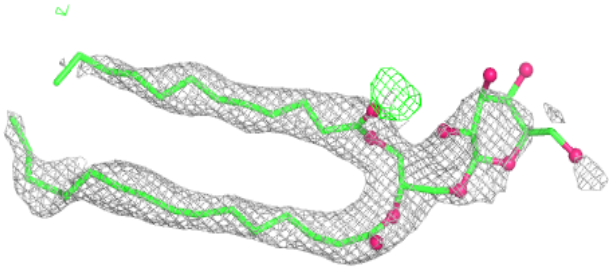


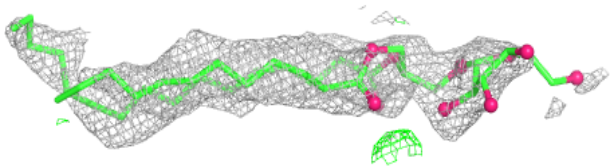


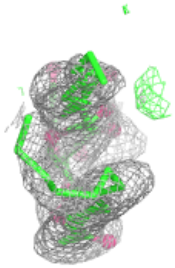


Electron density around LMG d 409:

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

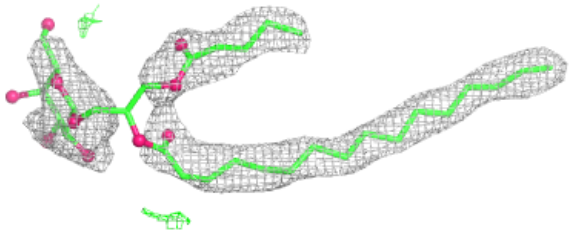


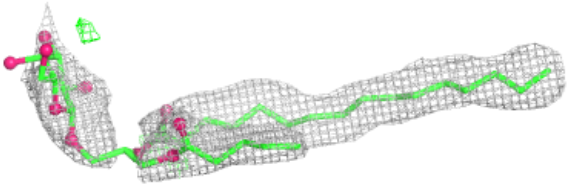


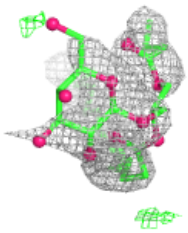


Electron density around LMG C 531:

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

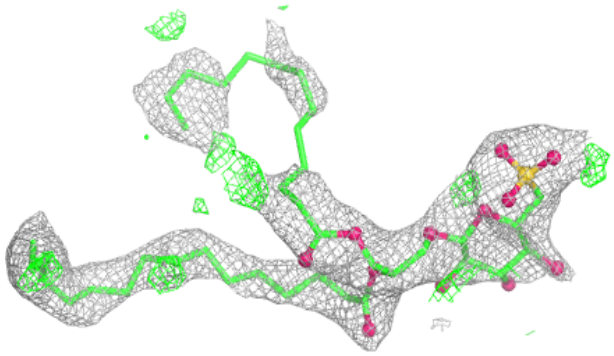


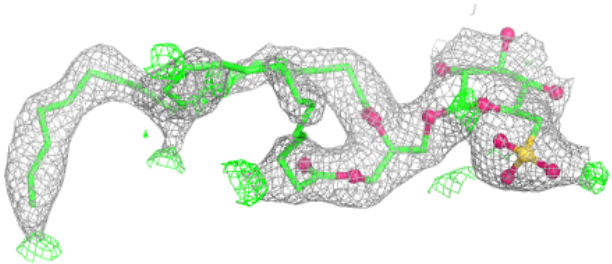


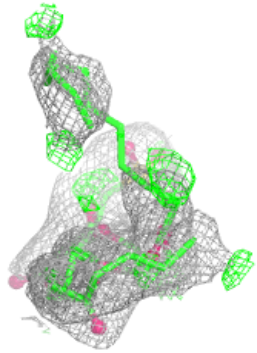


Electron density around SQD a 418:

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

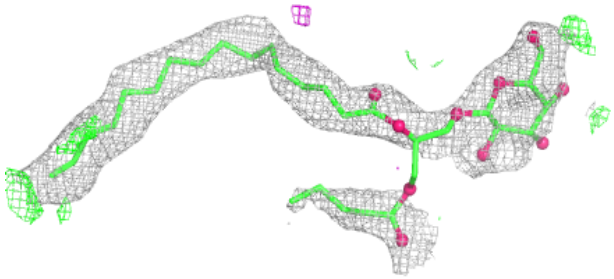


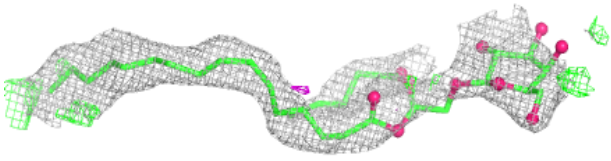


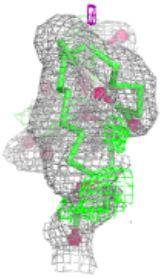


Electron density around LMG B 621:

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

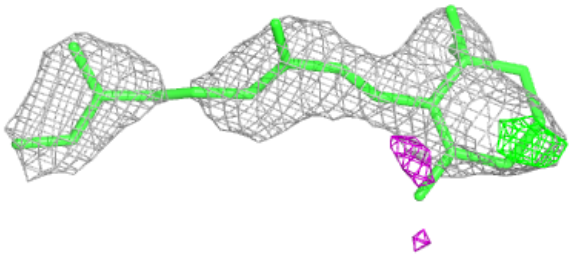


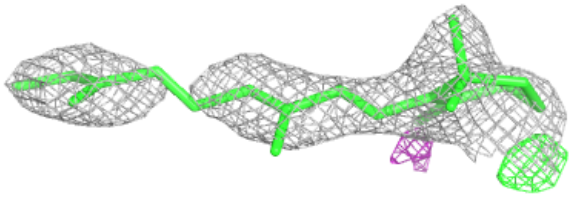


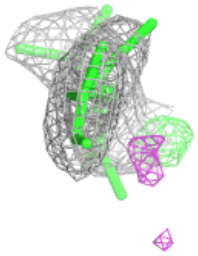


Electron density around BCR b 618:

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

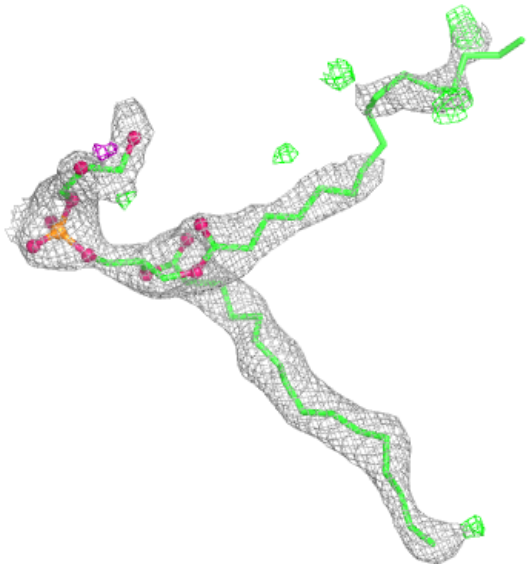


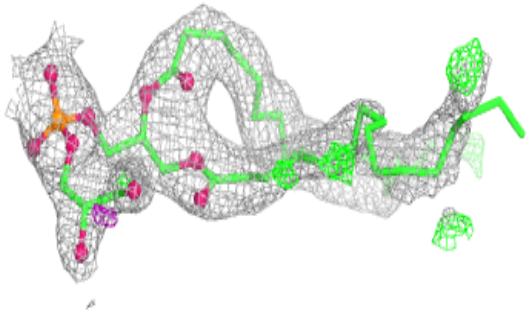


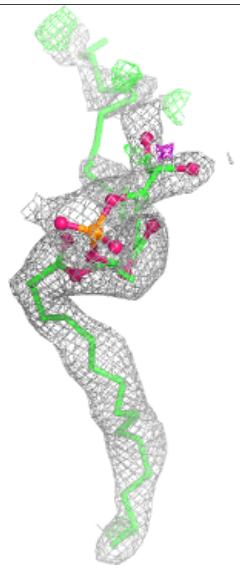


Electron density around LHG l 102:

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

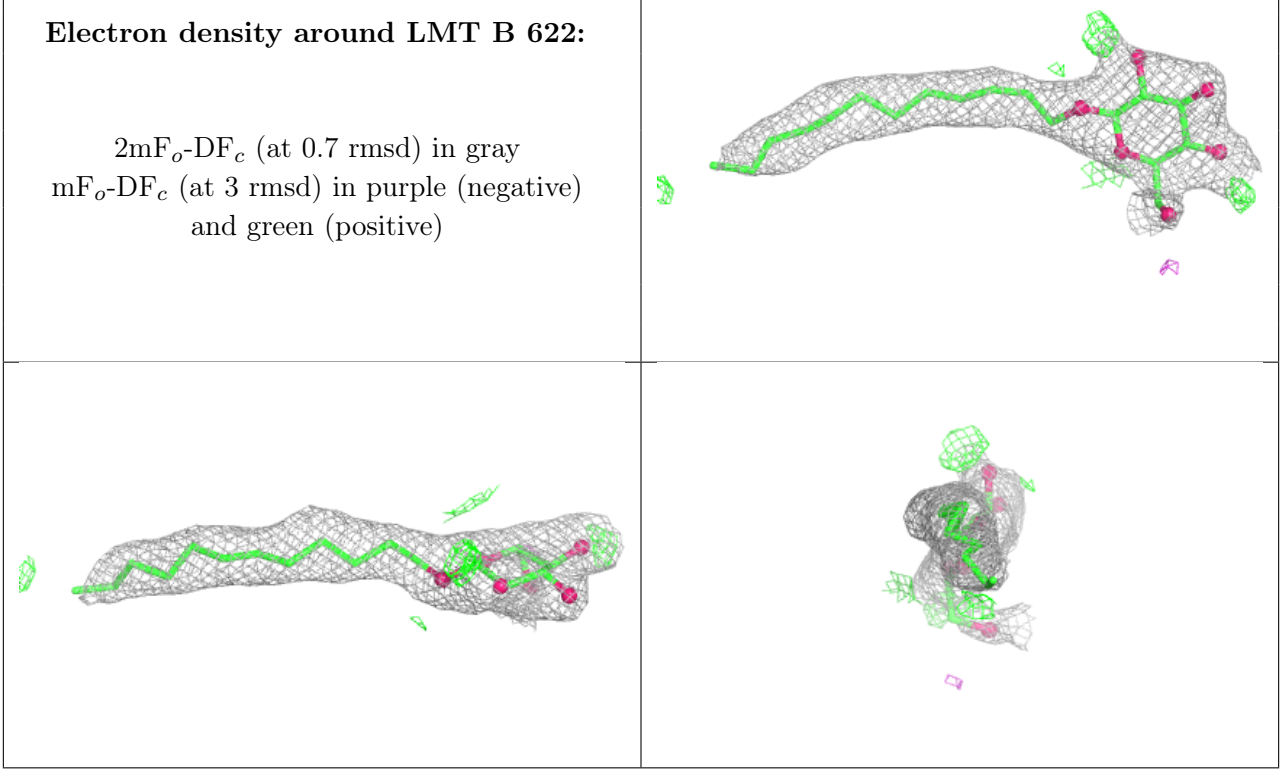






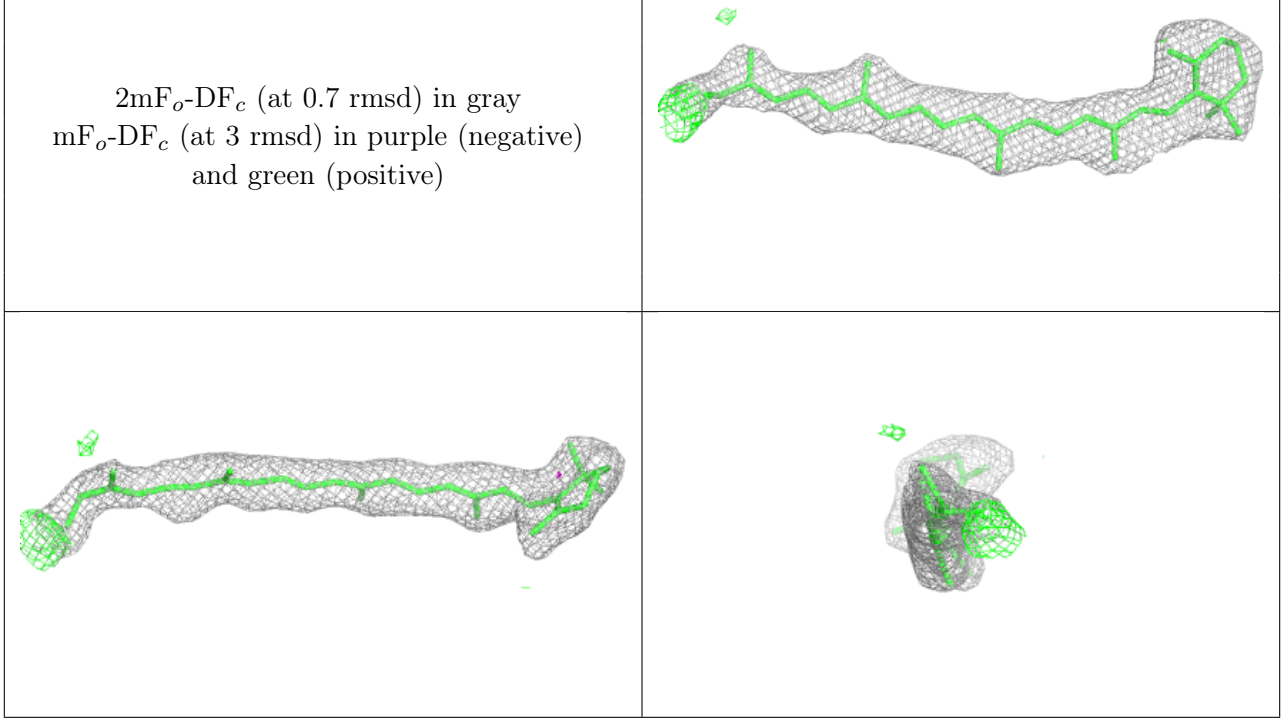
Electron density around LMT B 622:

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



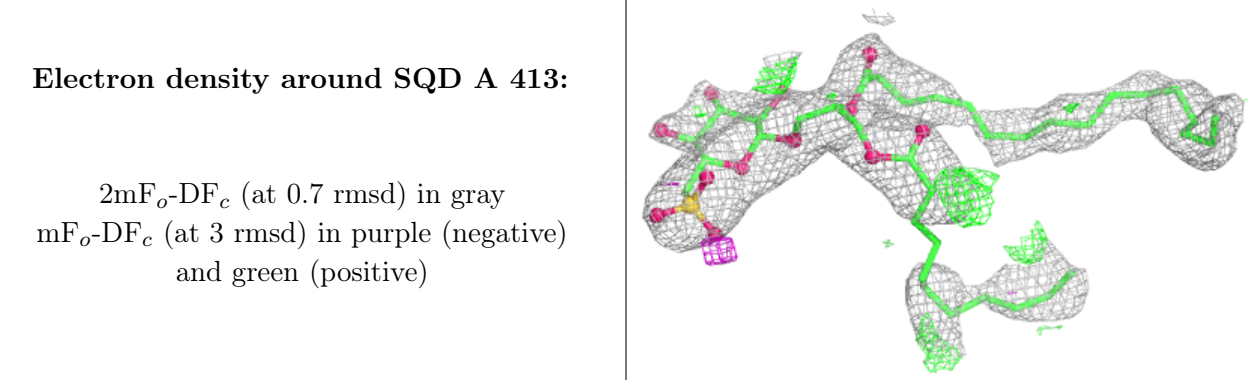
Electron density around BCR b 619:

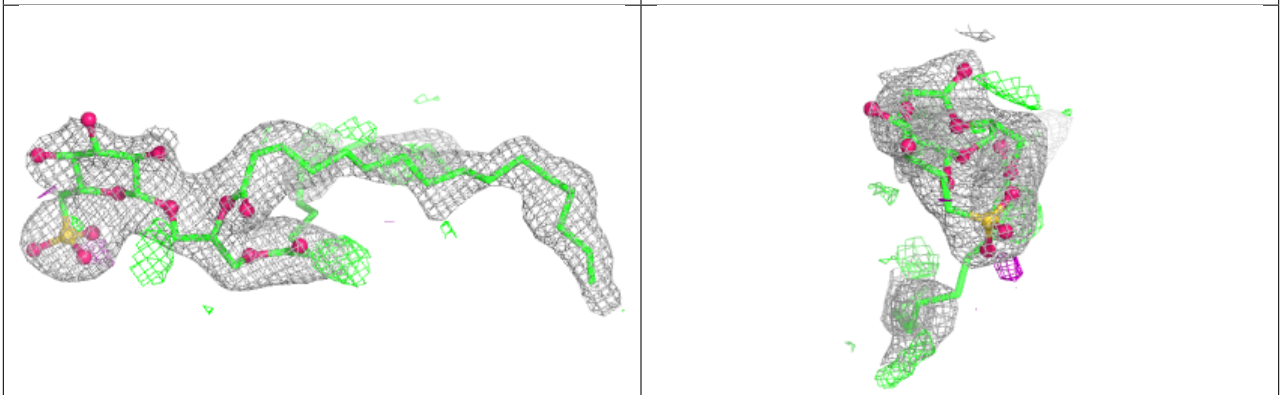
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD A 413:

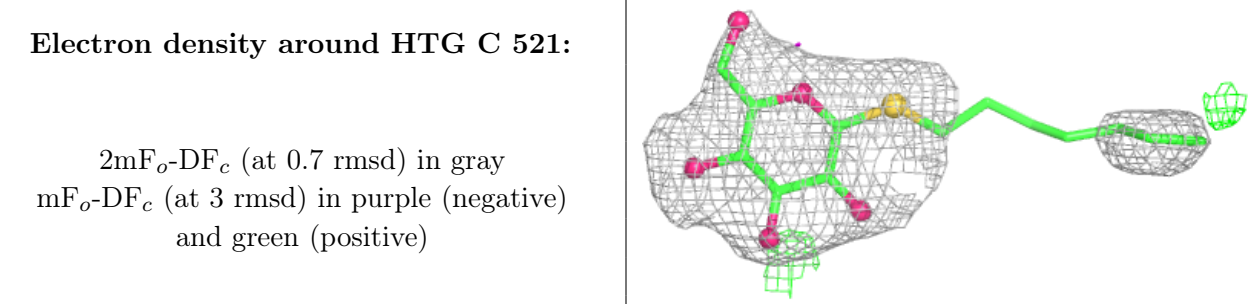
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

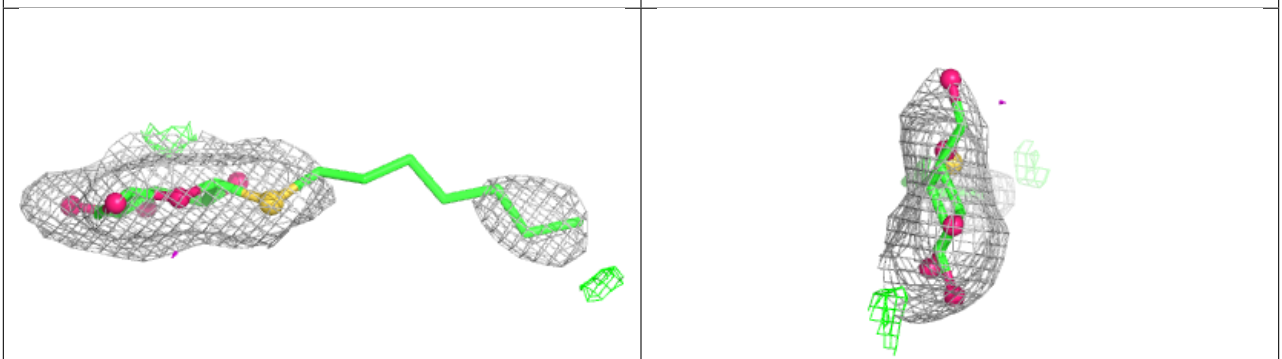




Electron density around HTG C 521:

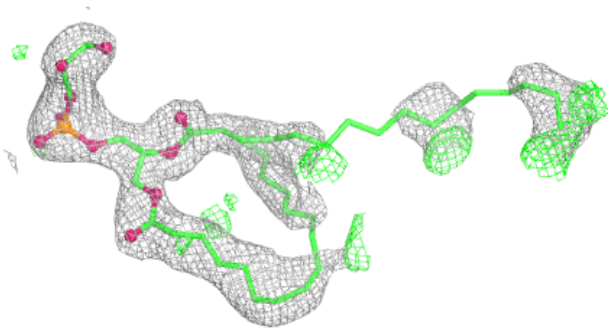
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

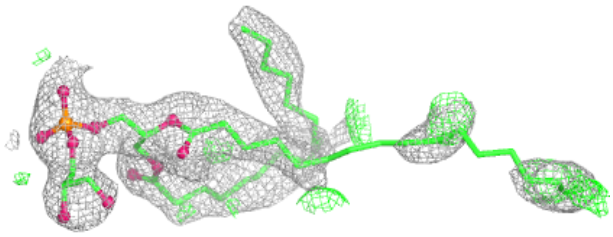




Electron density around LHG D 409:

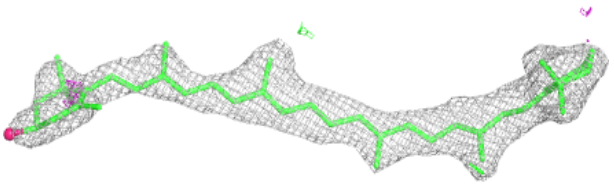
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

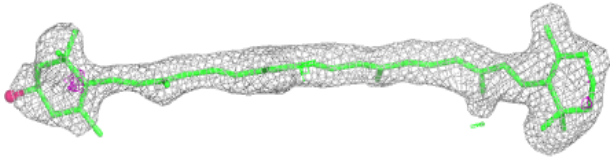


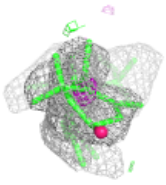


Electron density around RRX h 101:

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

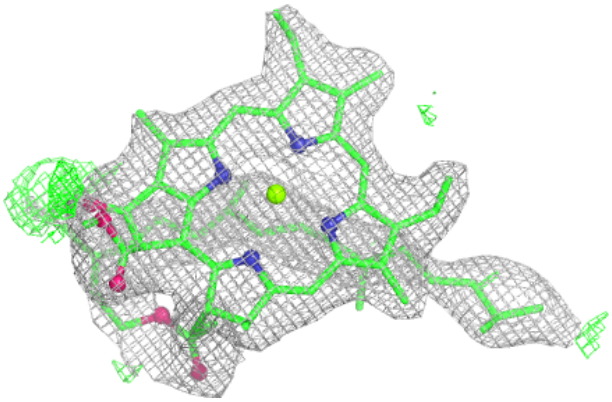


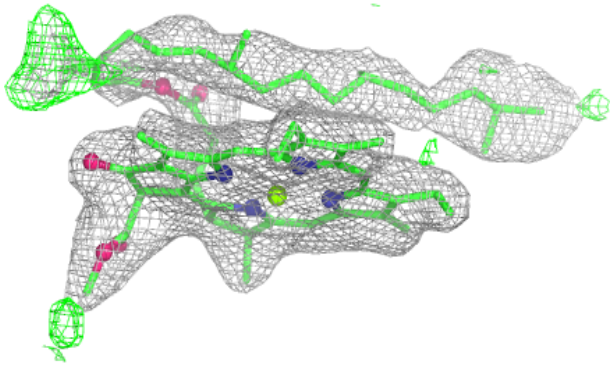


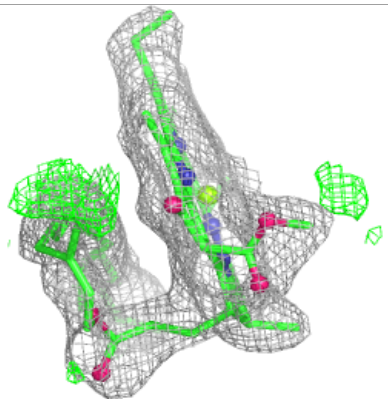


Electron density around CLA B 602:

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

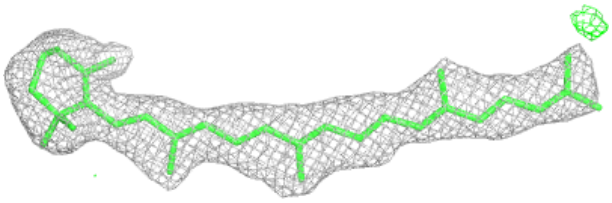


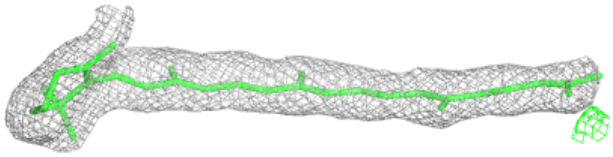


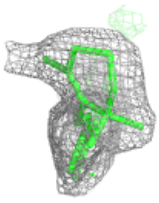


Electron density around BCR B 619:

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

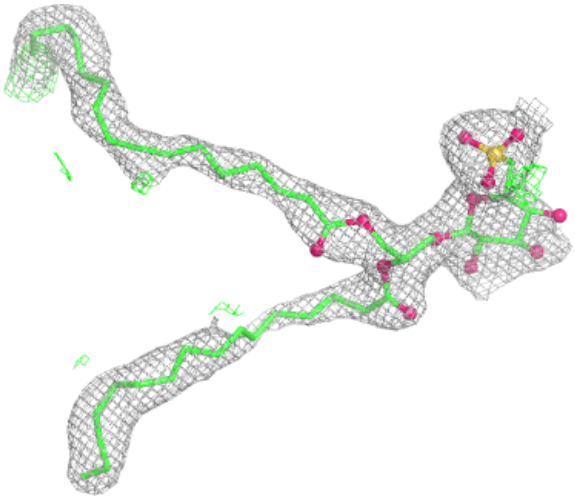


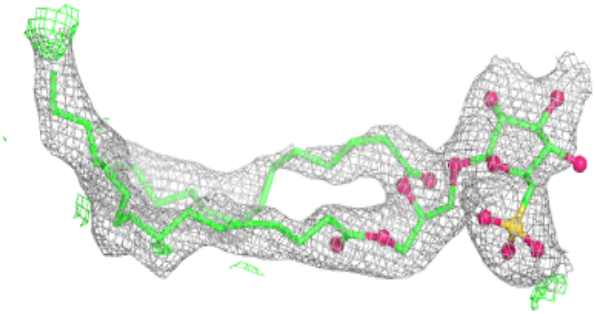


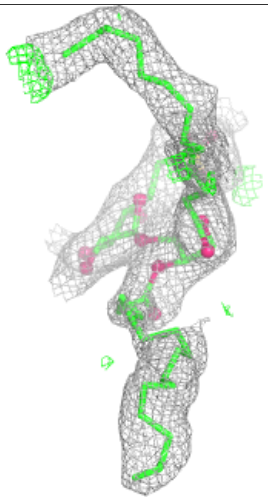


Electron density around SQD a 414:

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

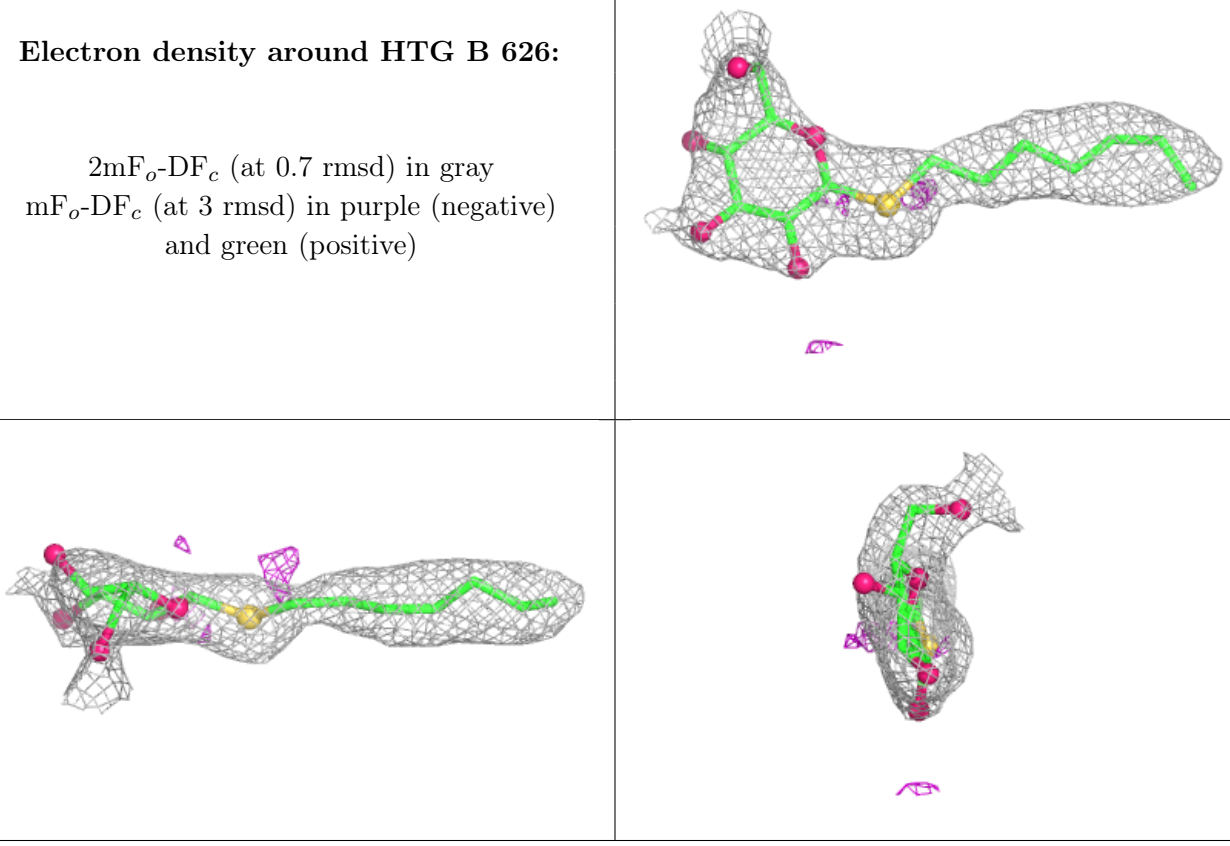






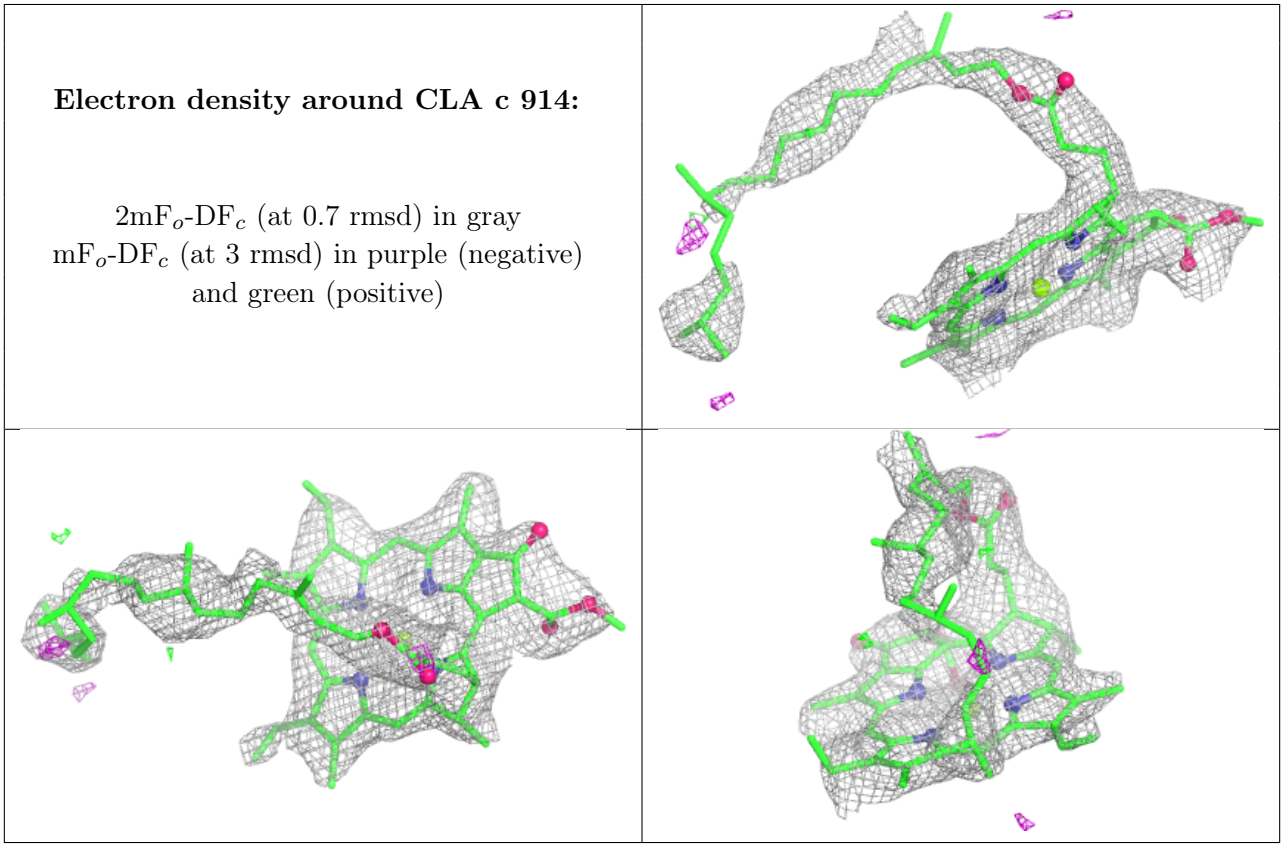
Electron density around HTG B 626:

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



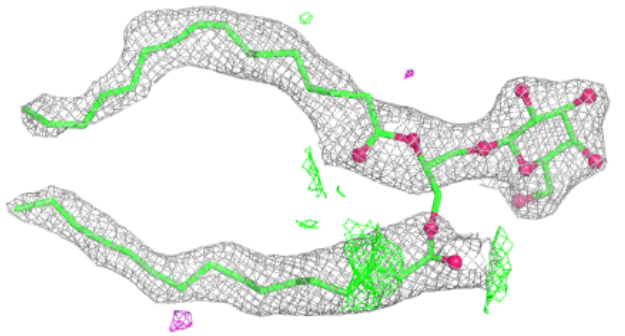
Electron density around CLA c 914:

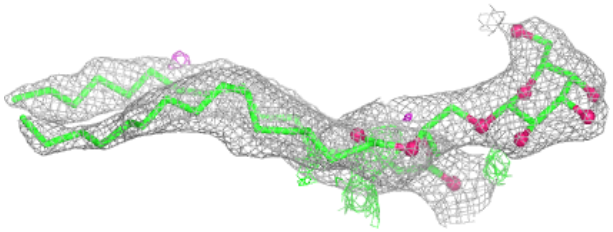
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

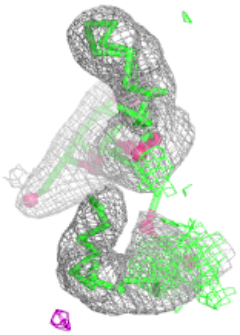


Electron density around LMG i 101:

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

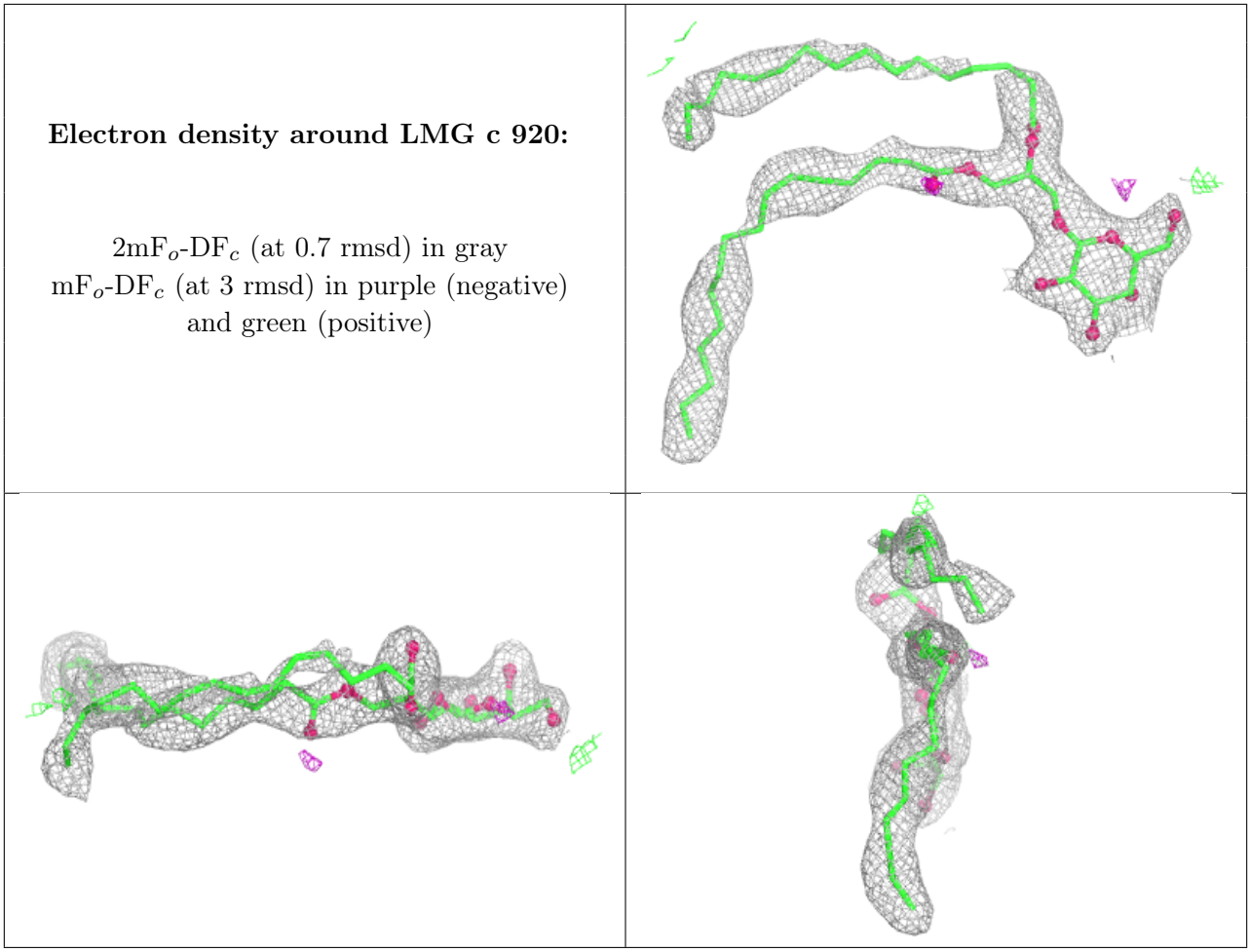






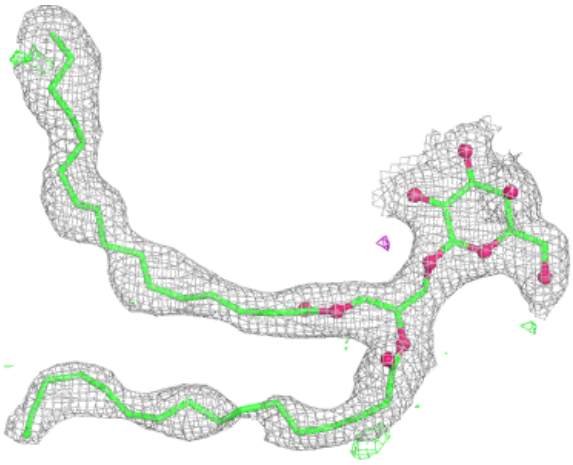
Electron density around LMG c 920:

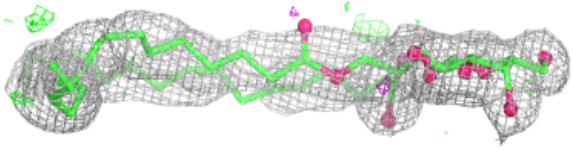
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

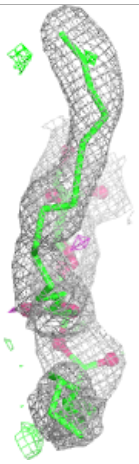


Electron density around LMG C 520:

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

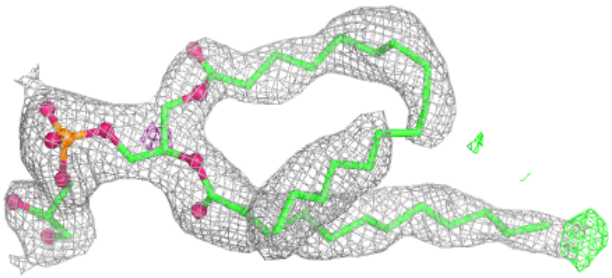


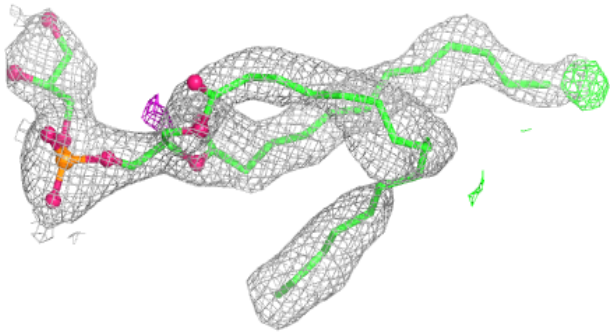


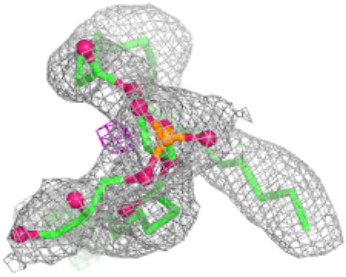


Electron density around LHG a 423:

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

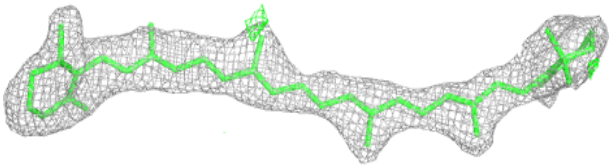


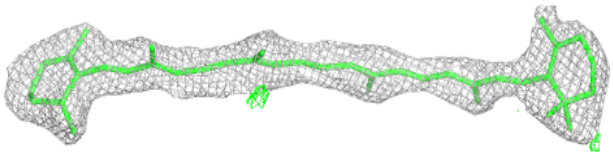


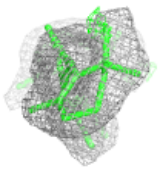


Electron density around BCR c 915:

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

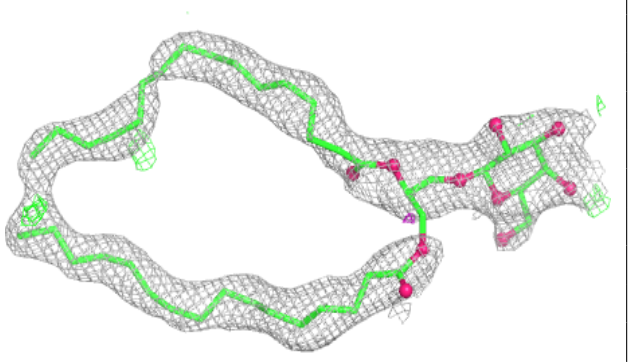


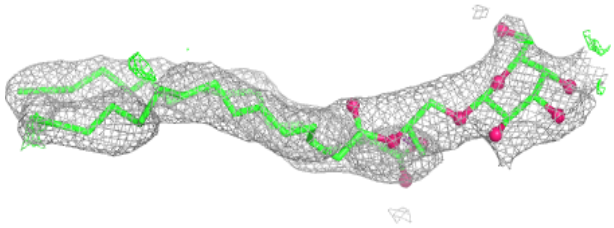


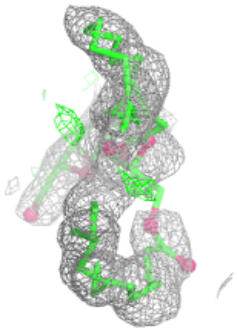


Electron density around LMG A 410:

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

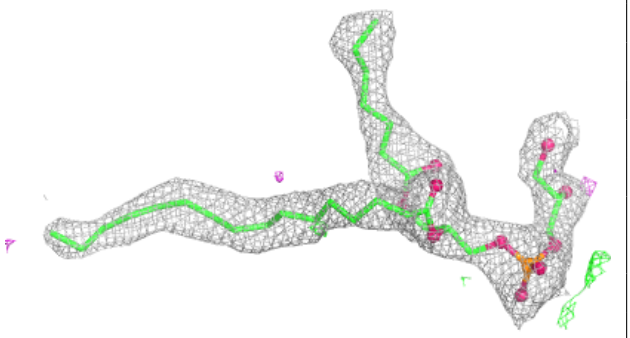


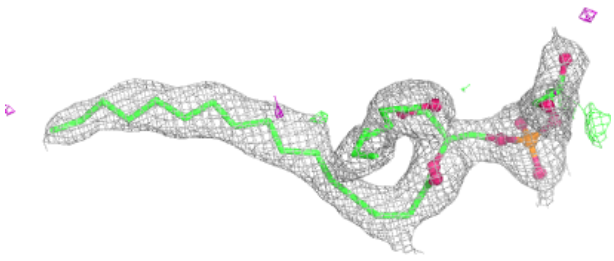


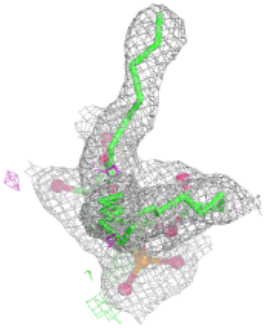


Electron density around LHG L 101:

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

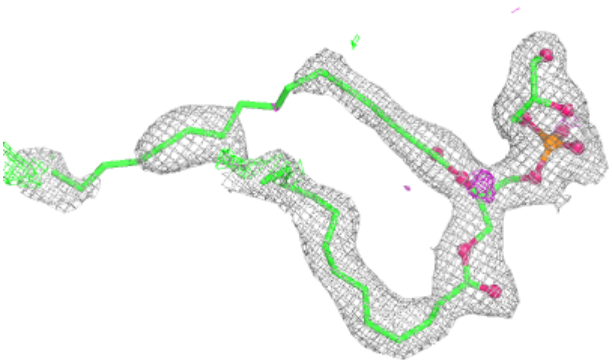


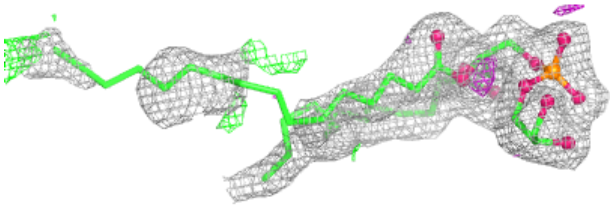


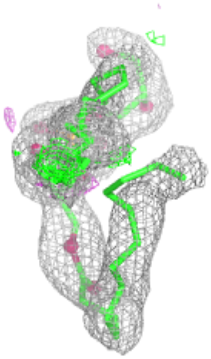


Electron density around LHG d 408:

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

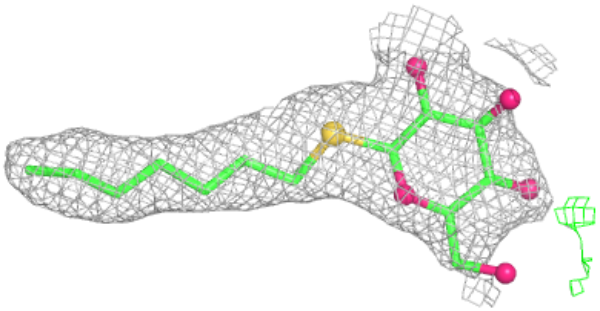


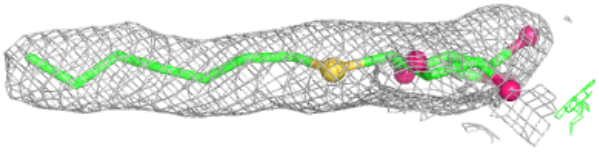


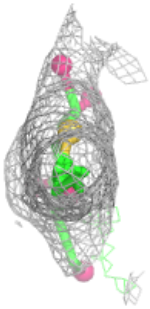


Electron density around HTG b 626:

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

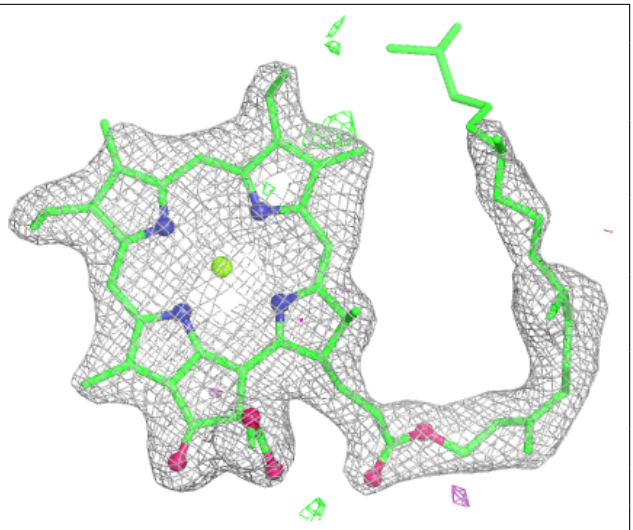


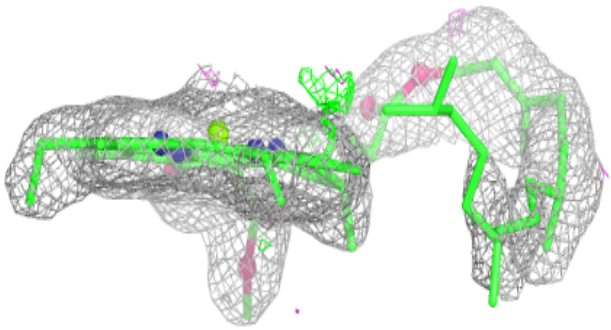


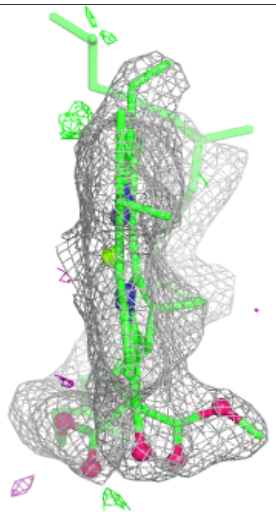


Electron density around CLA c 913:

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

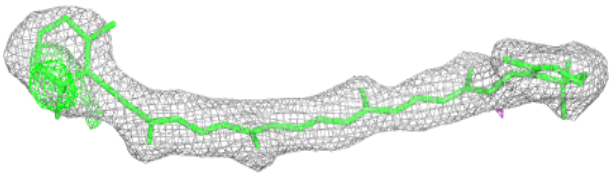


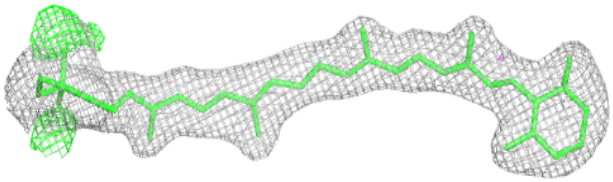


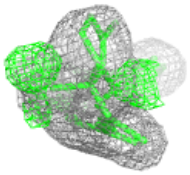


Electron density around BCR d 404:

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

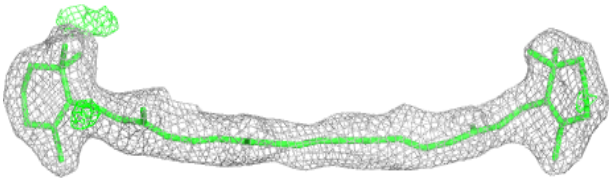


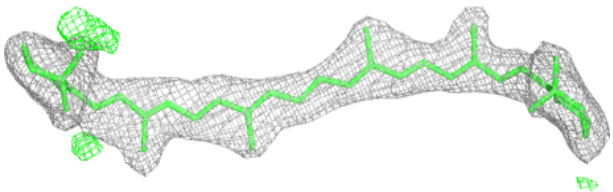


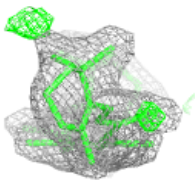


Electron density around BCR k 101:

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

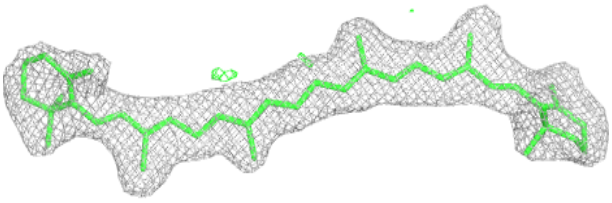


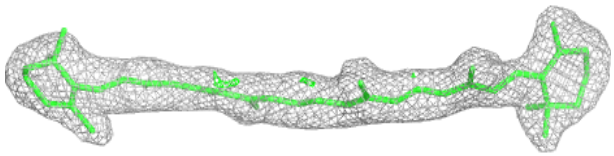


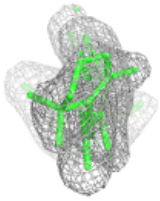


Electron density around BCR y 101:

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

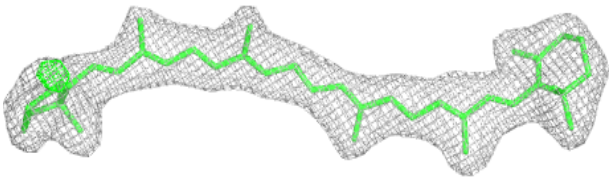


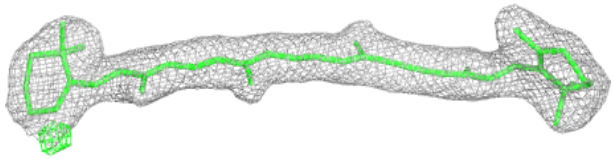


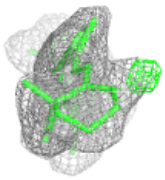


Electron density around BCR Y 101:

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

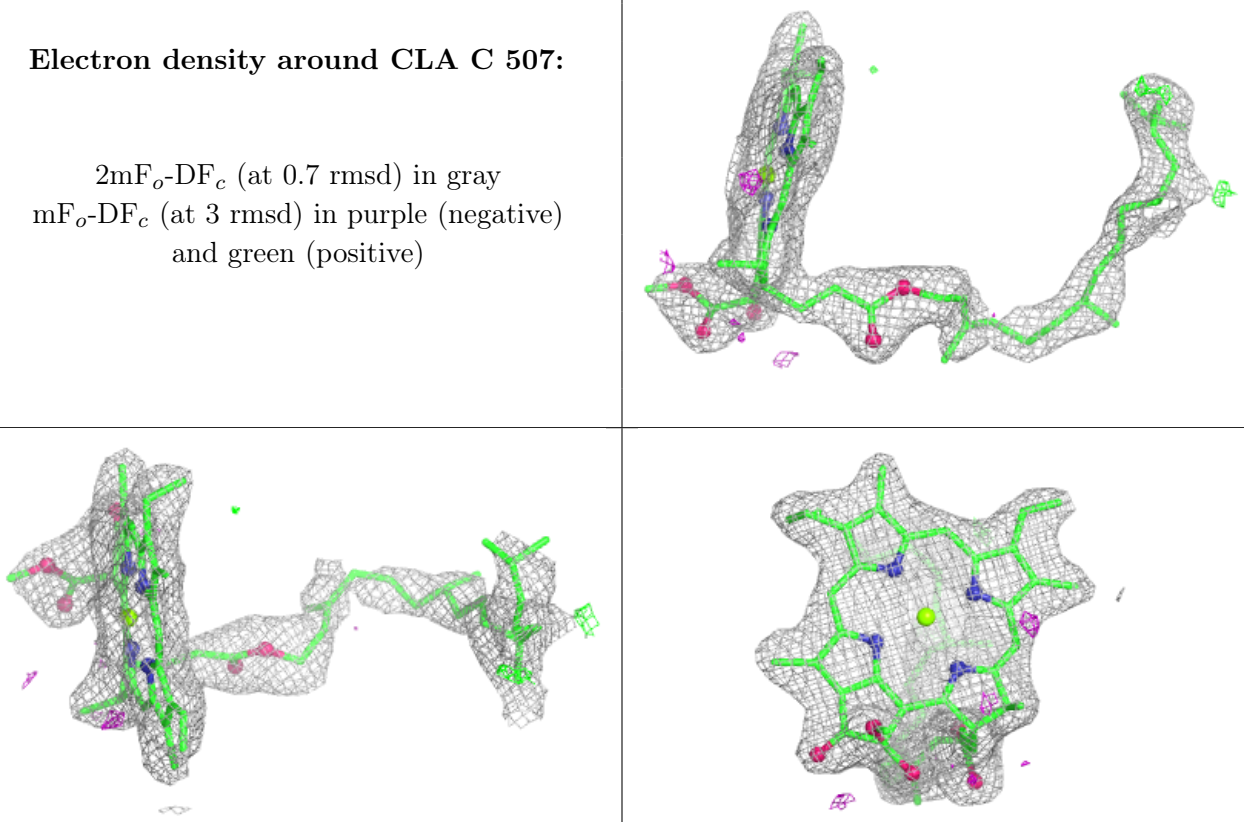






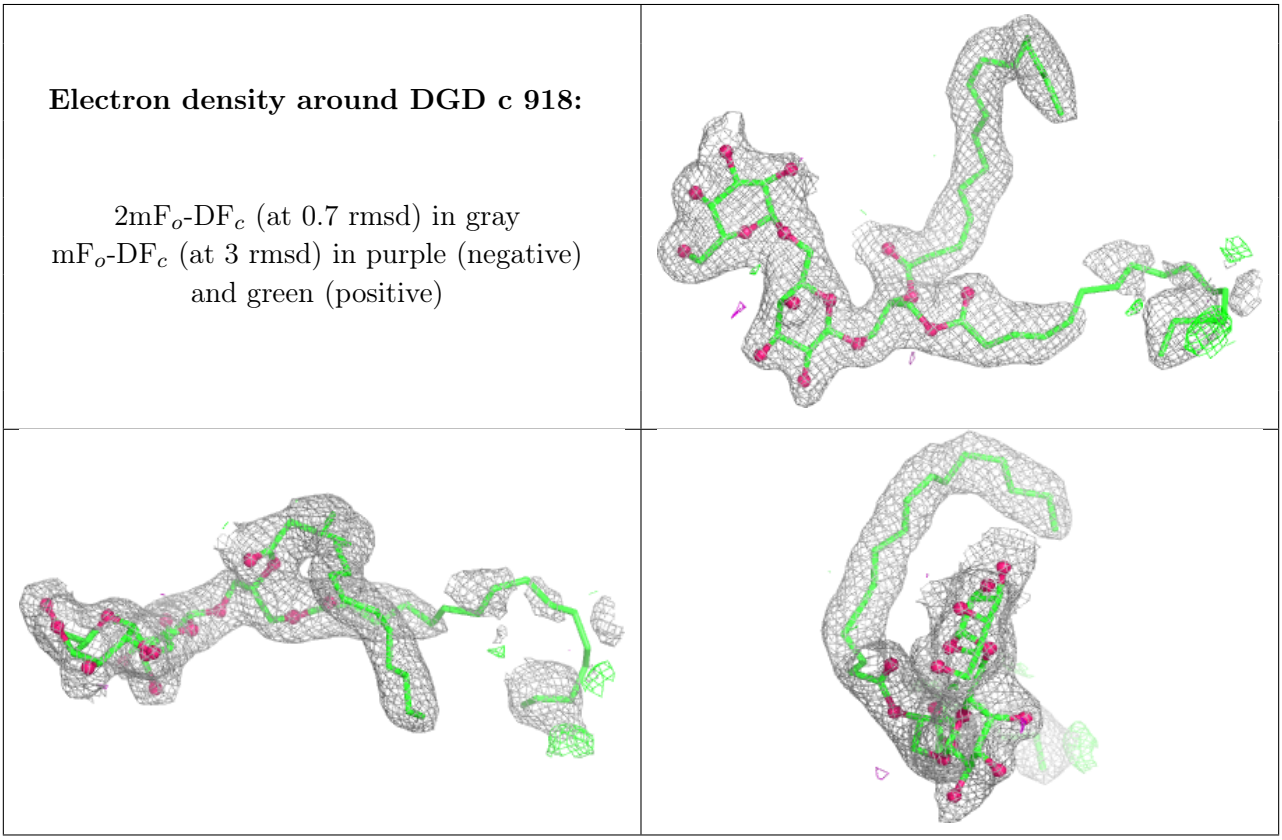
Electron density around CLA C 507:

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



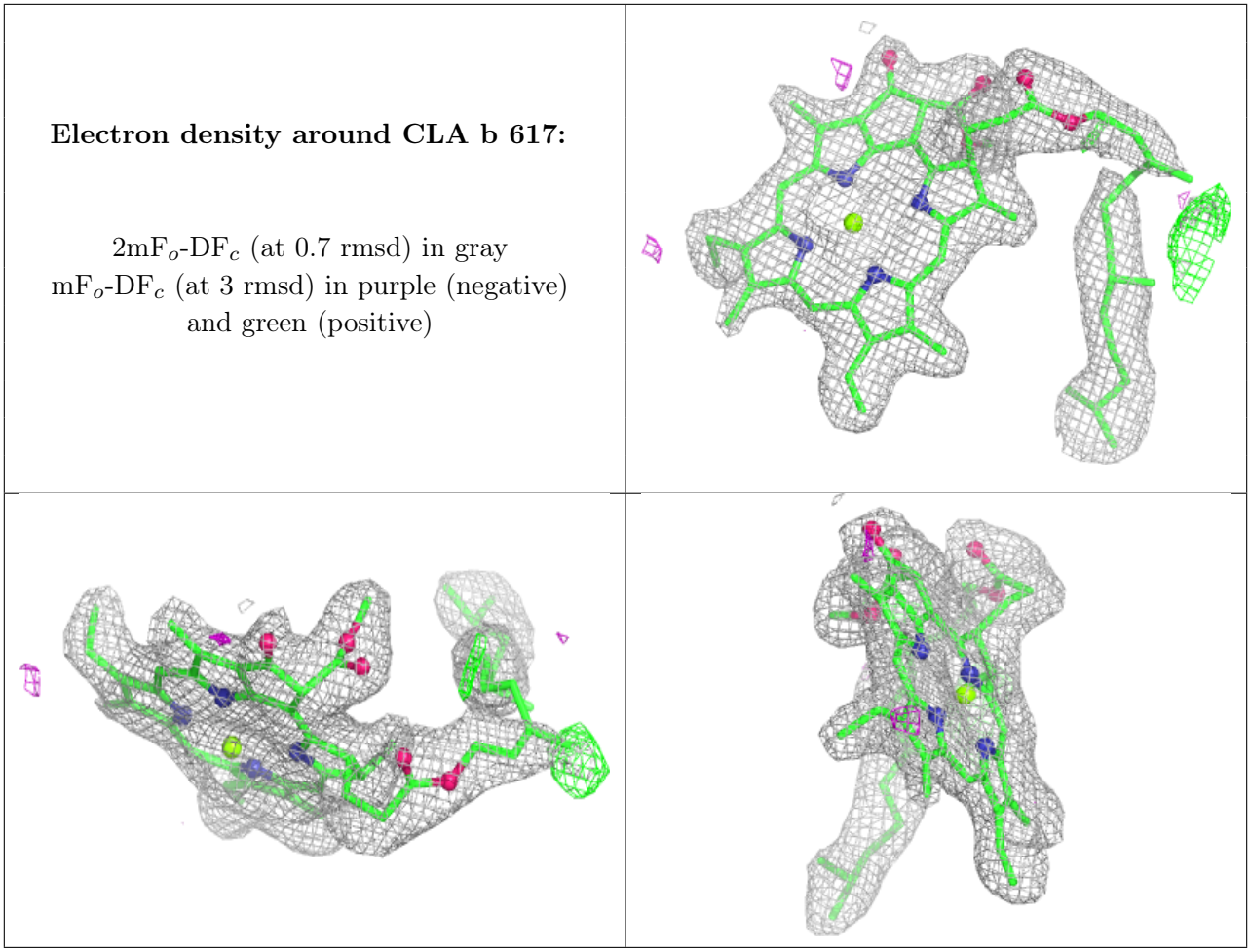
Electron density around DGD c 918:

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



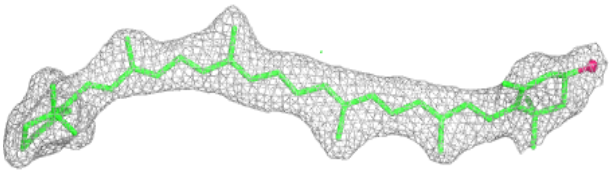
Electron density around CLA b 617:

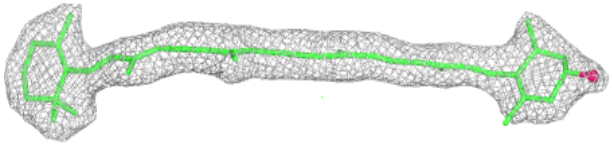
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

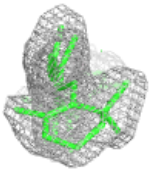


Electron density around RRX H 101:

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

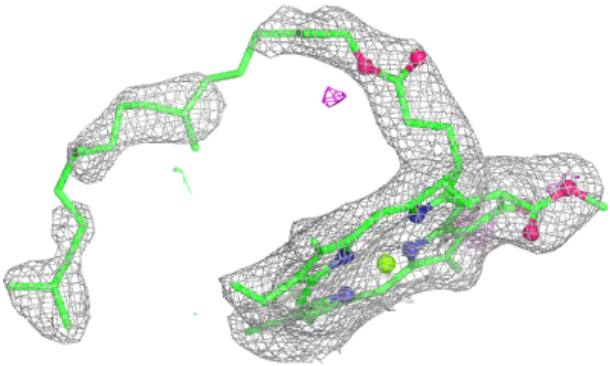


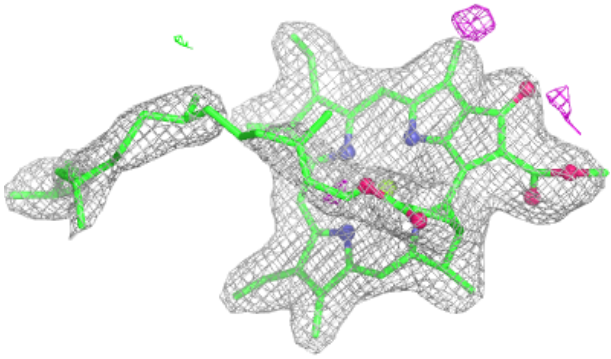


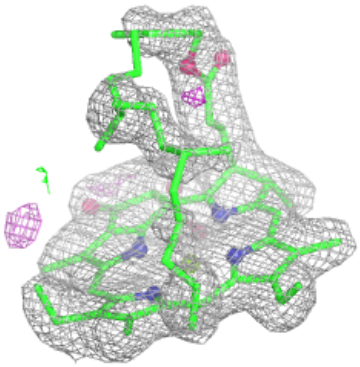


Electron density around CLA C 514:

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

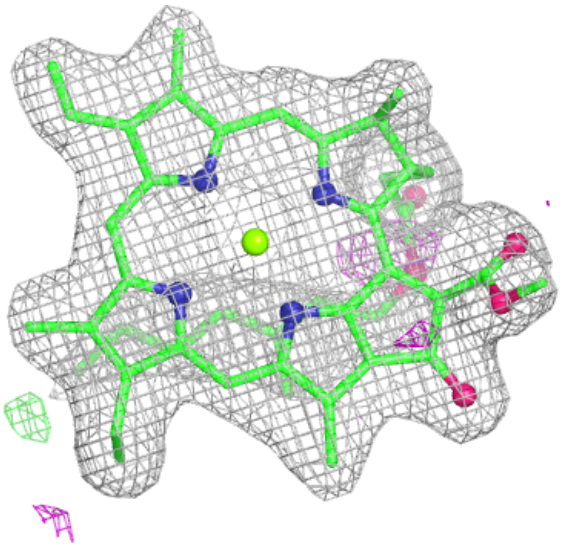


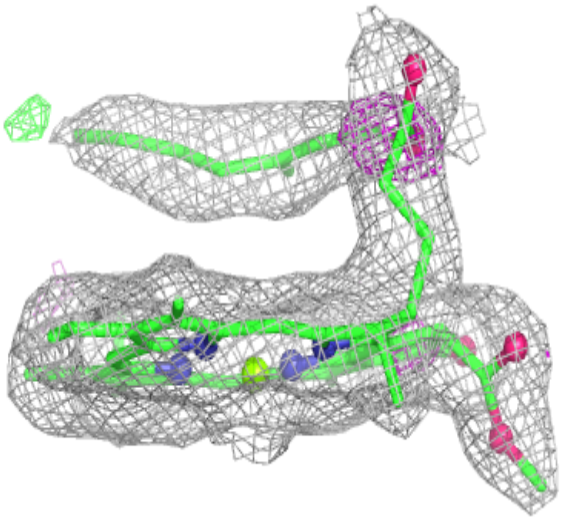


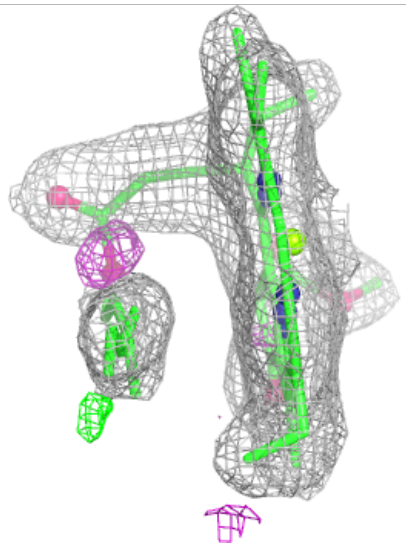


Electron density around CLA B 615:

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

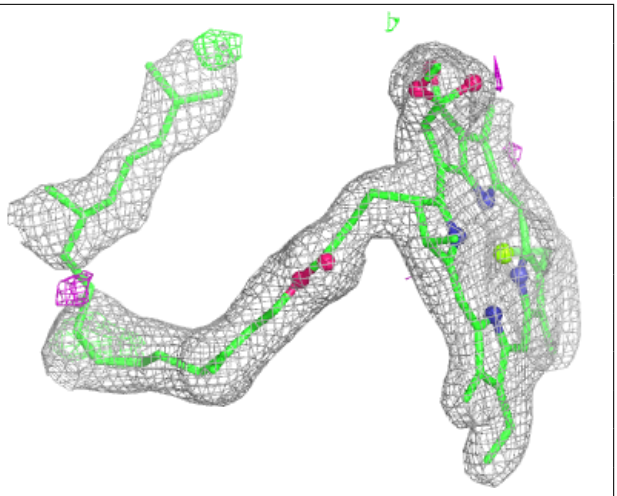


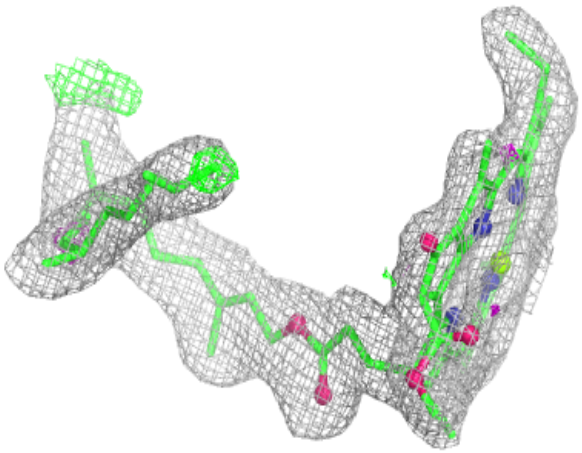


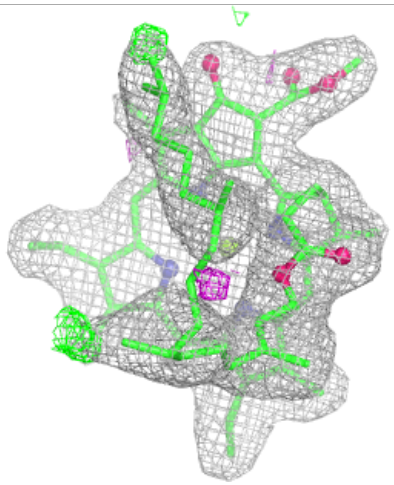


Electron density around CLA b 607:

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

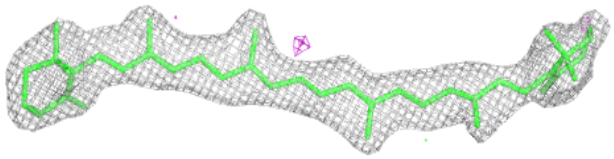


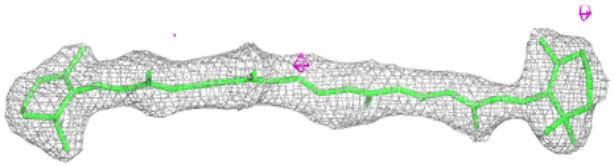


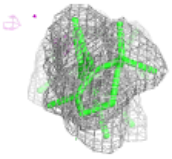


Electron density around BCR C 515:

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

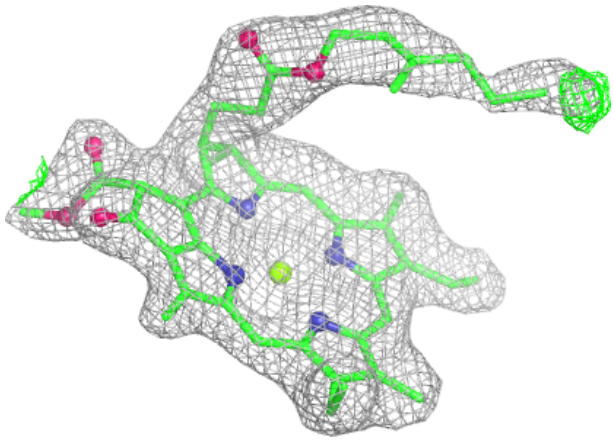


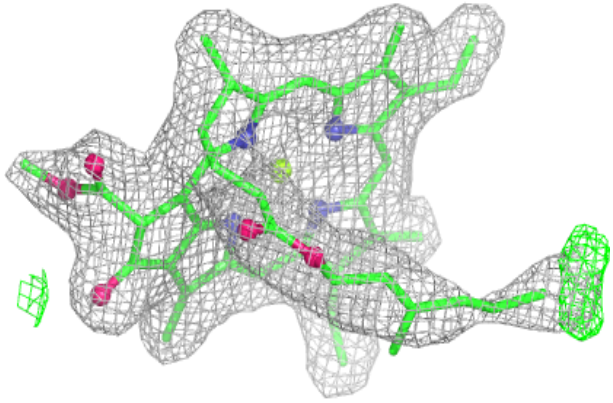


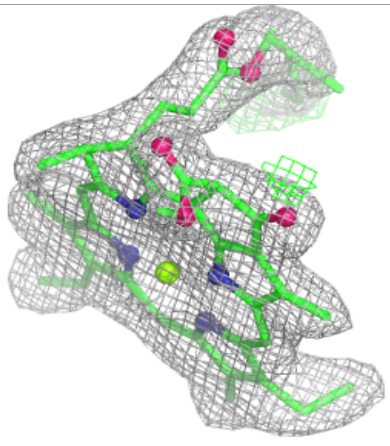


Electron density around CLA b 615:

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

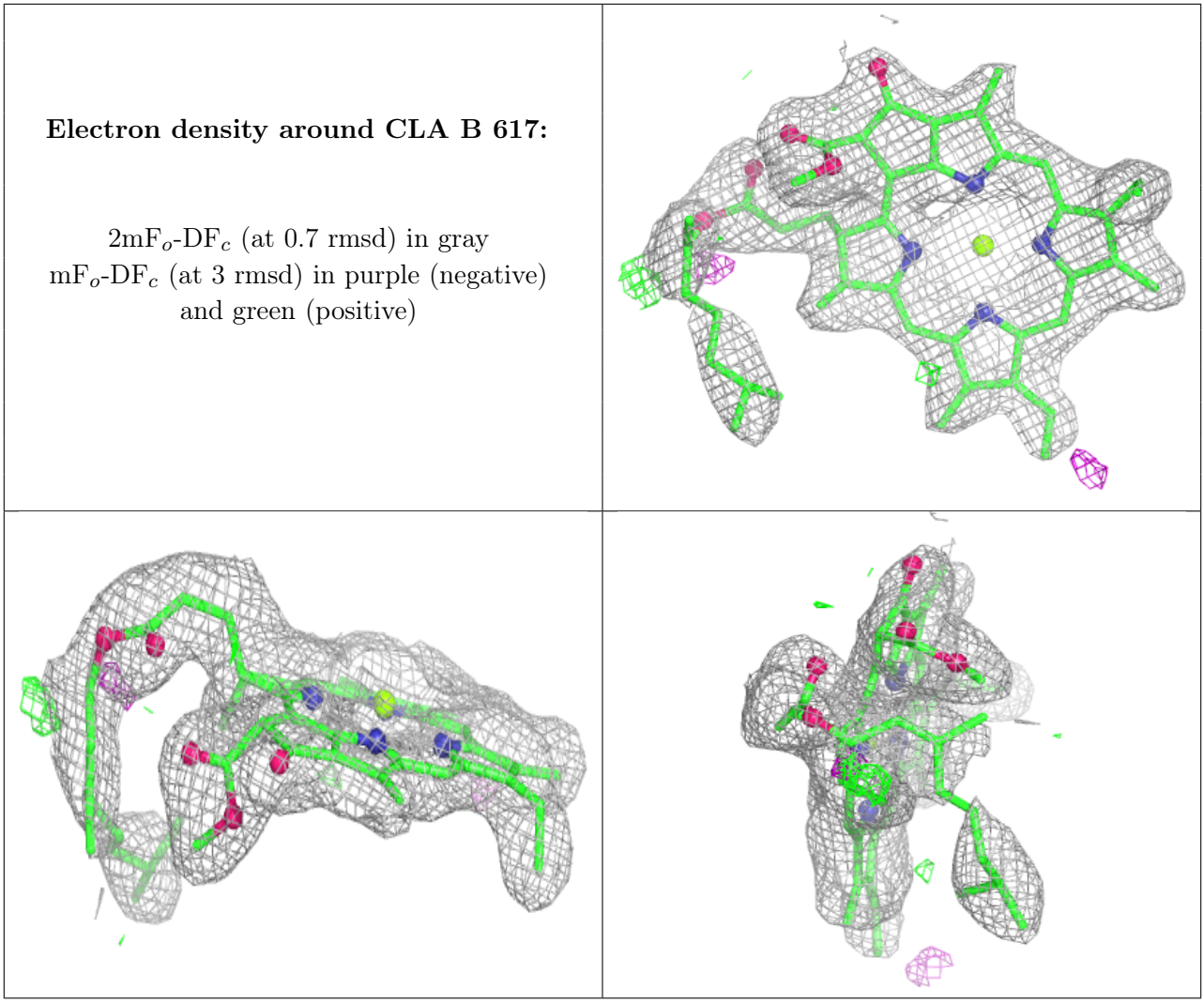






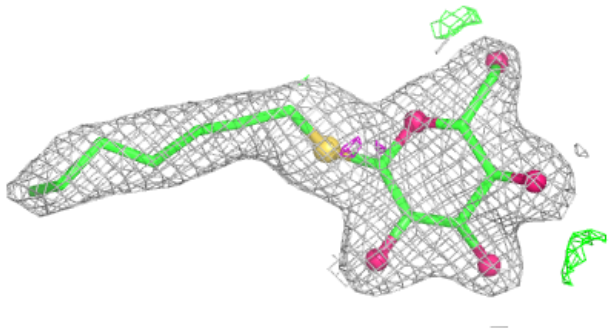
Electron density around CLA B 617:

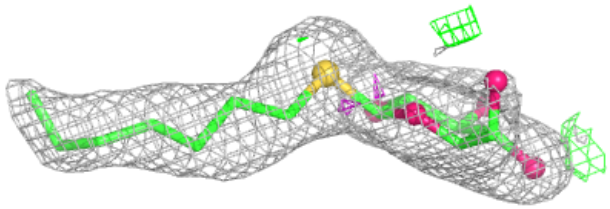
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

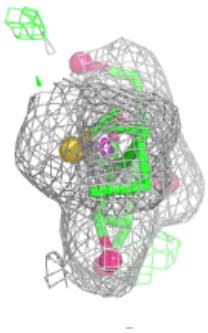


Electron density around HTG b 623:

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

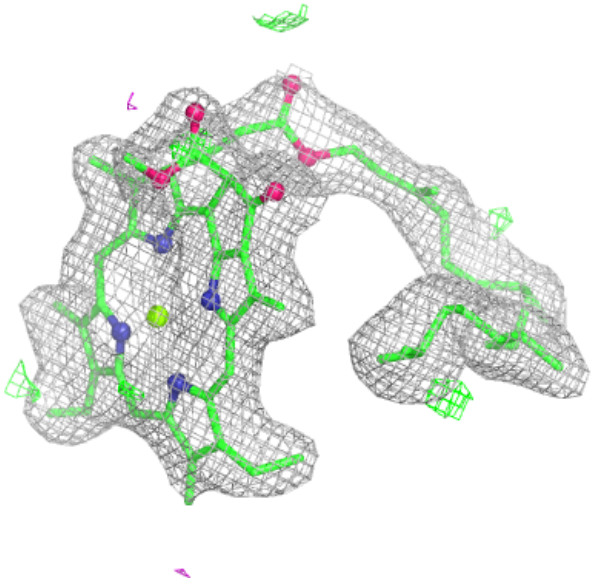


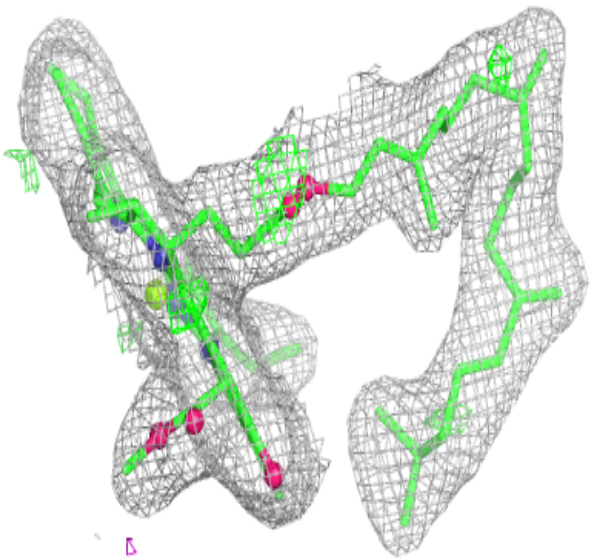


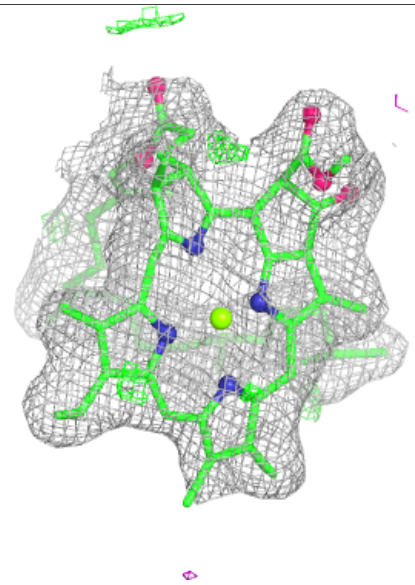


Electron density around CLA c 904:

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

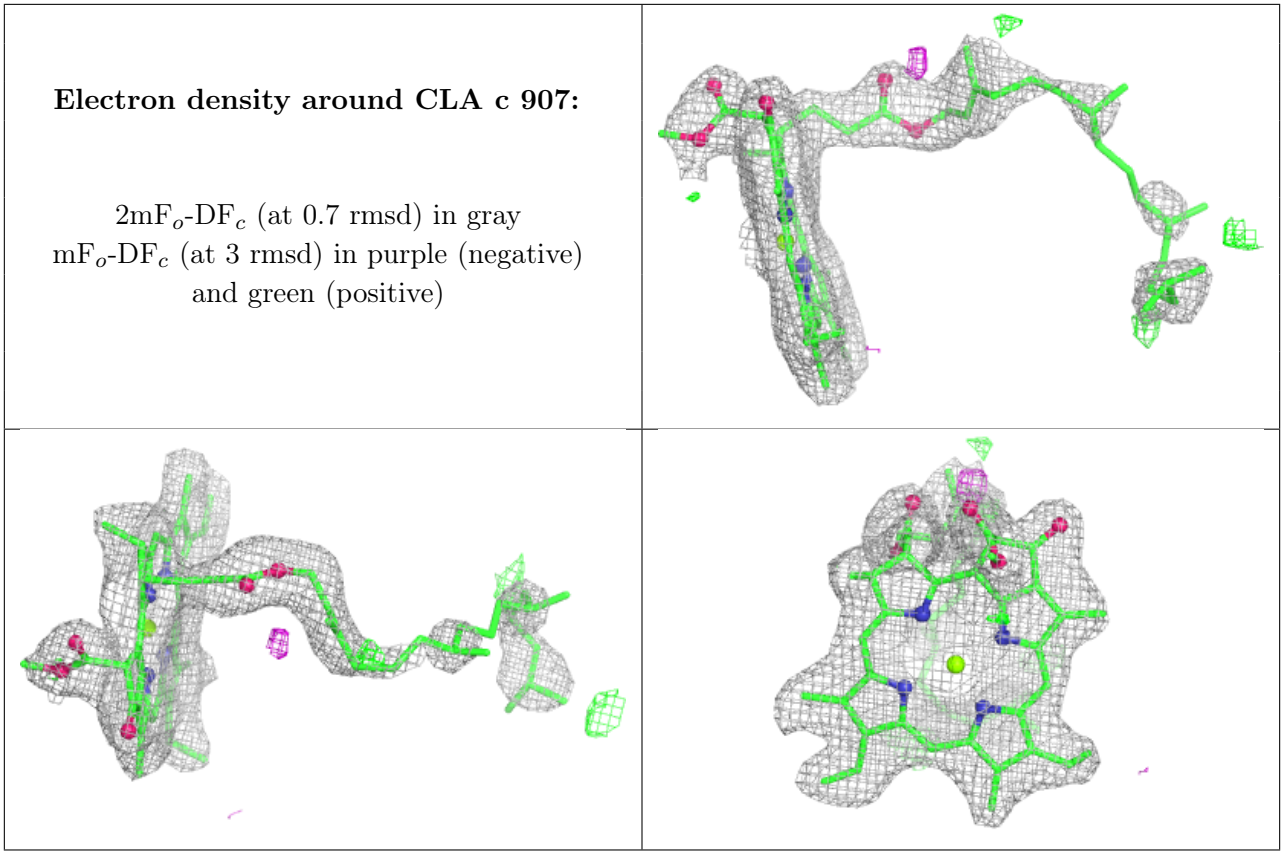






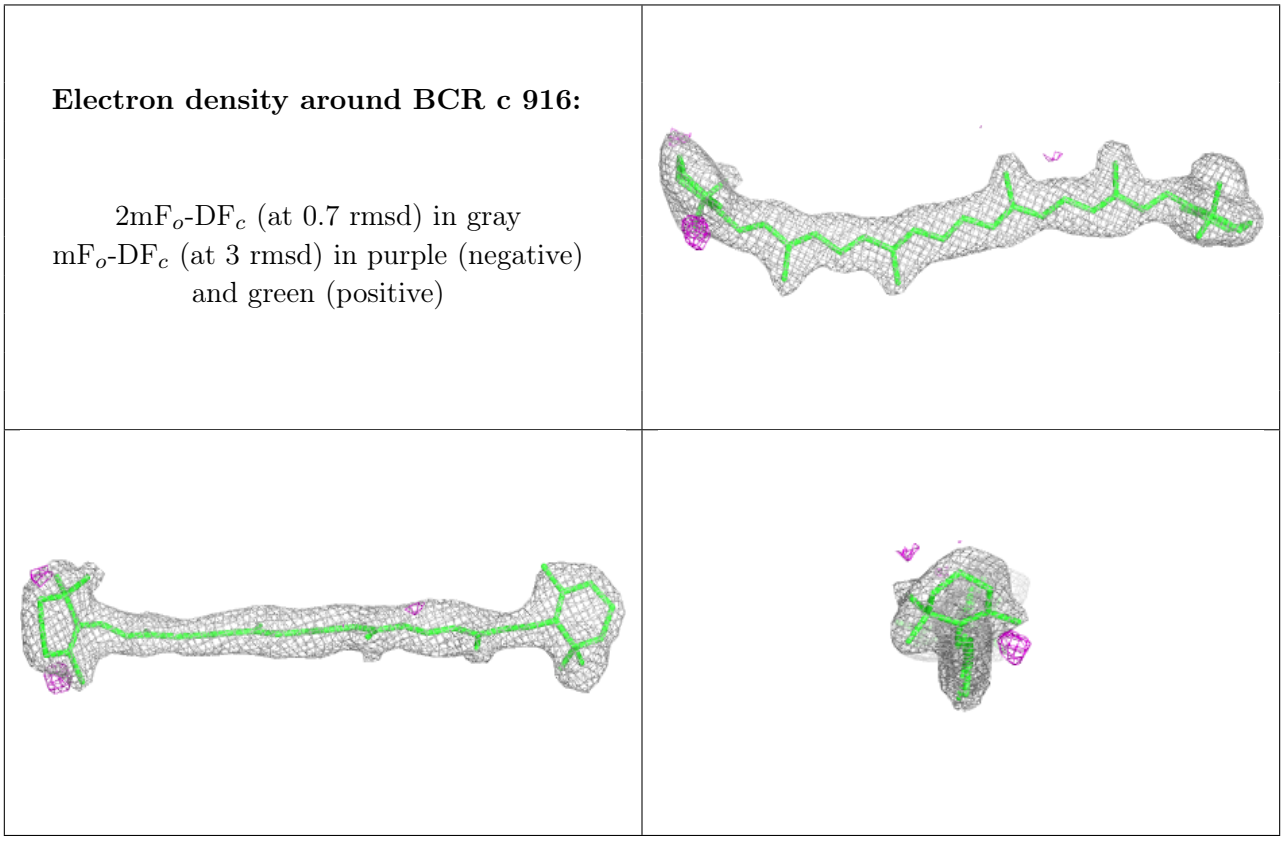
Electron density around CLA c 907:

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



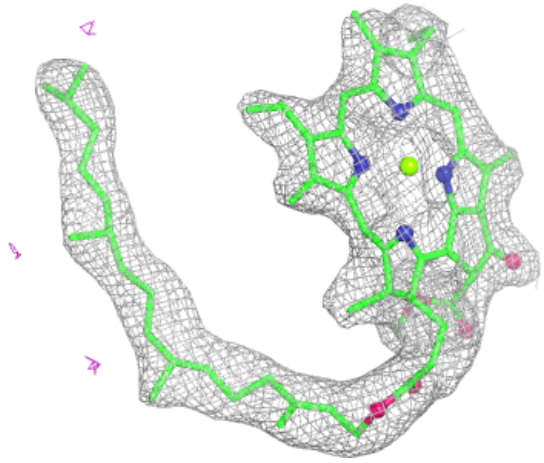
Electron density around BCR c 916:

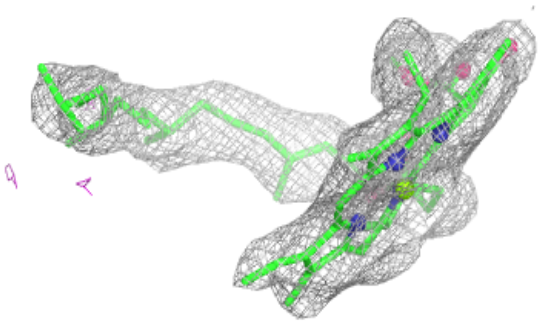
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

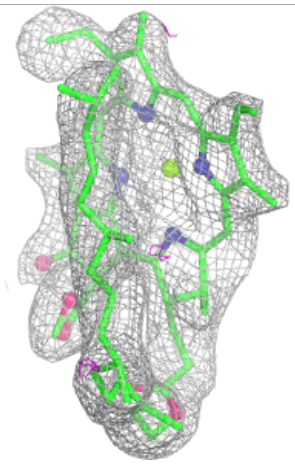


Electron density around CLA c 908:

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

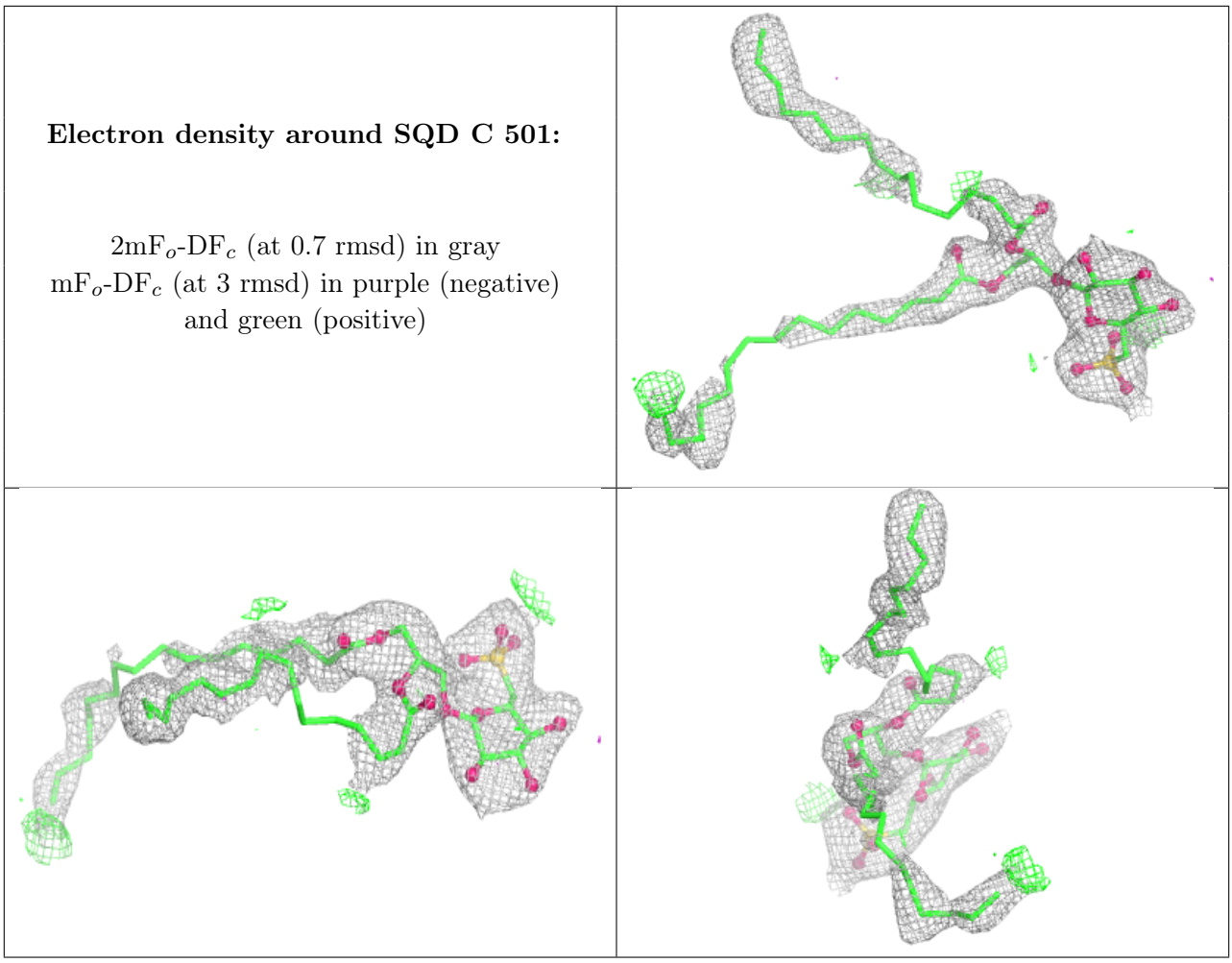






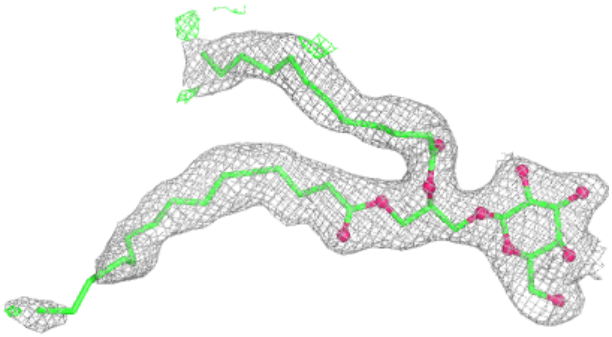
Electron density around SQD C 501:

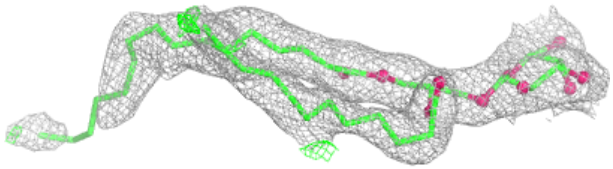
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

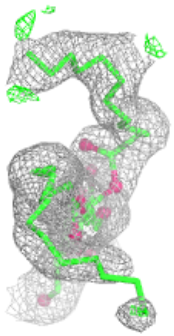


Electron density around LMG j 101:

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

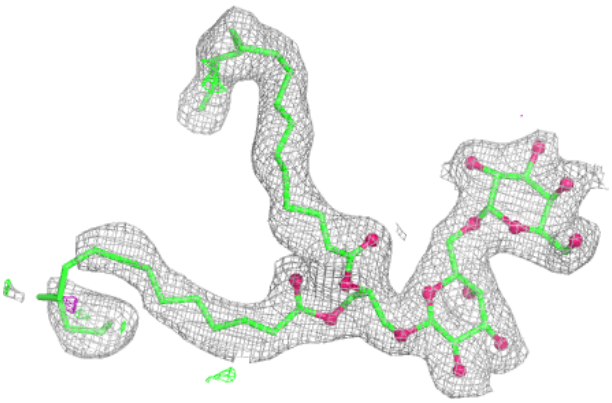


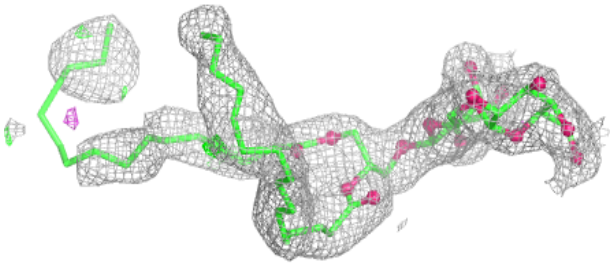


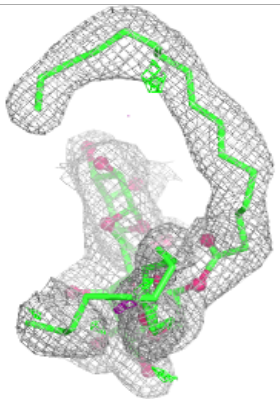


Electron density around DGD C 518:

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

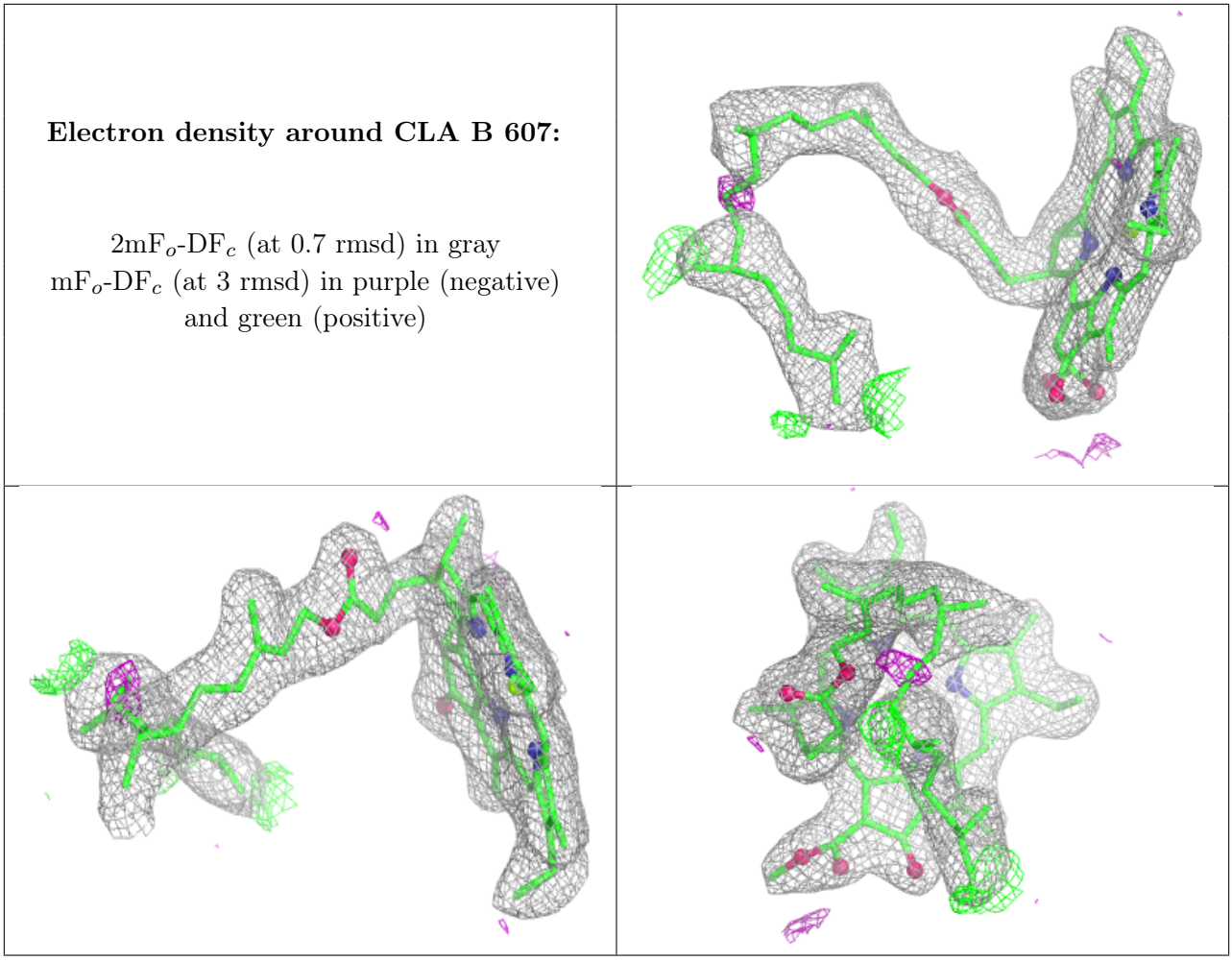






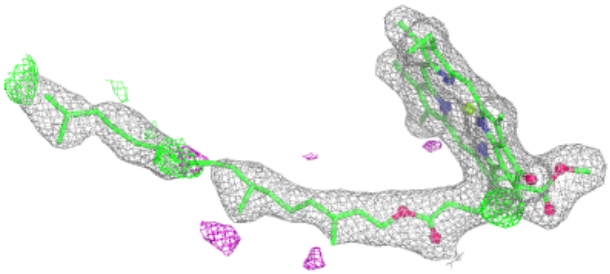
Electron density around CLA B 607:

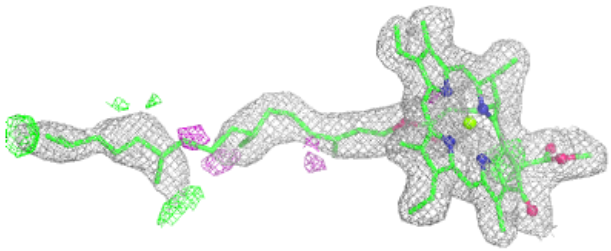
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

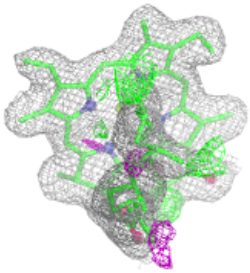


Electron density around CLA B 608:

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

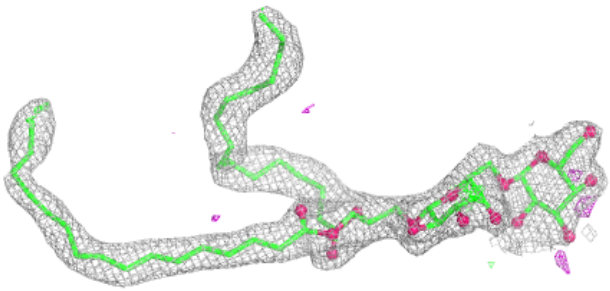


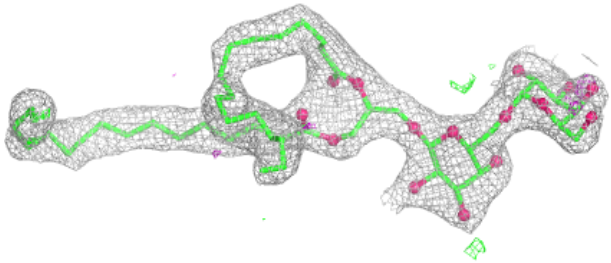


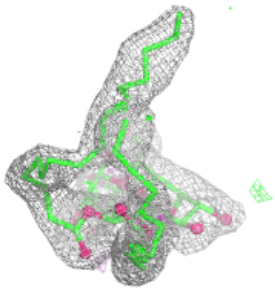


Electron density around DGD h 102:

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

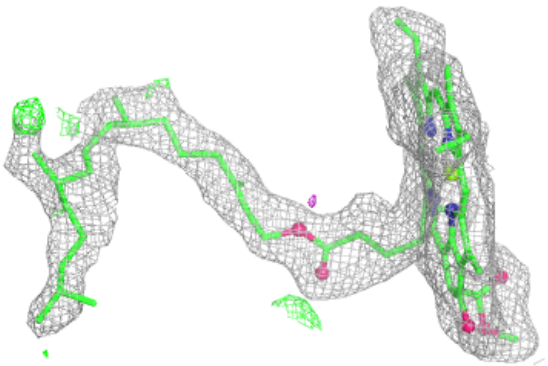


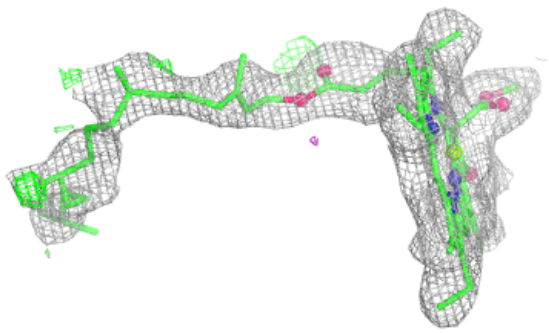


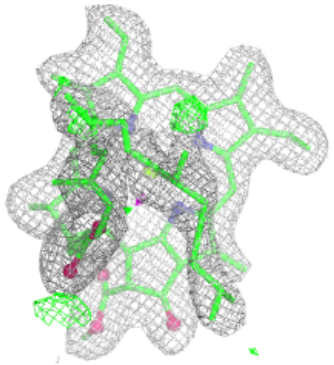


Electron density around CLA d 403:

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

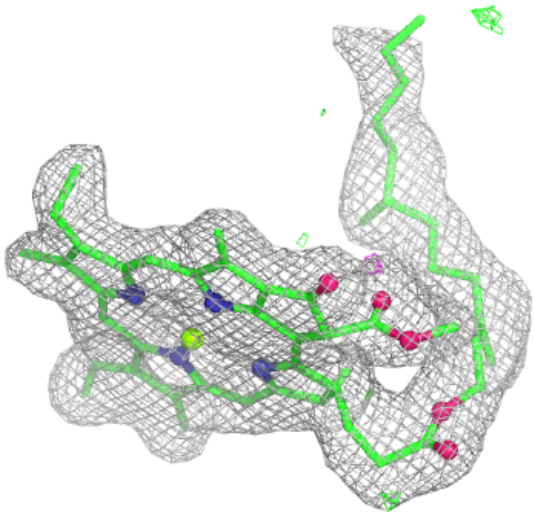


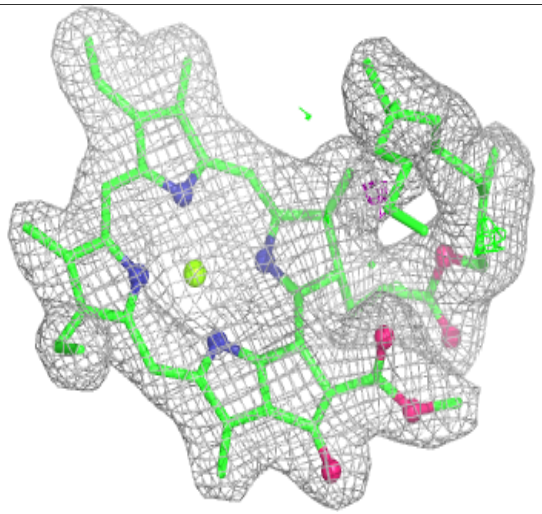


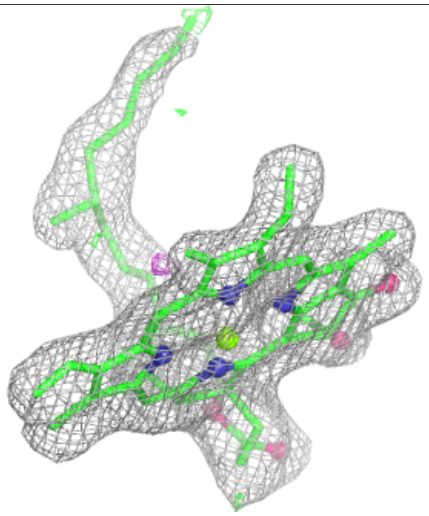


Electron density around CLA b 614:

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

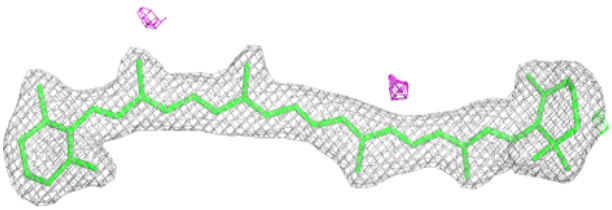


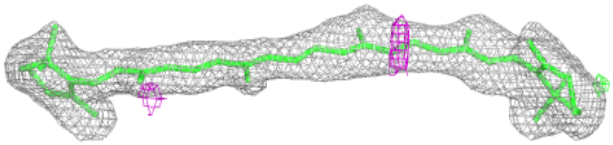


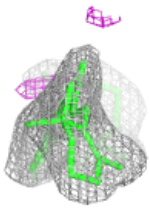


Electron density around BCR B 620:

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

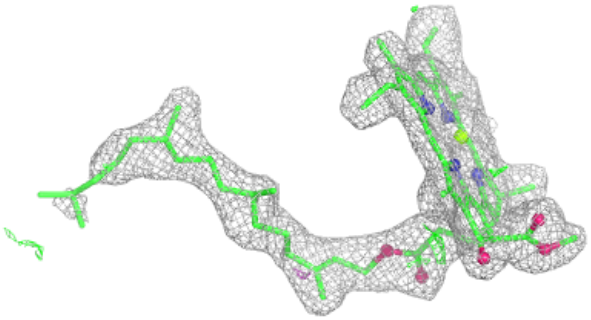


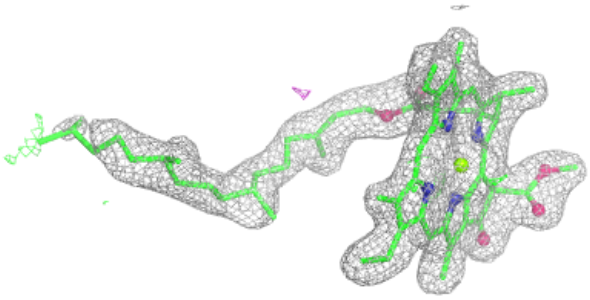


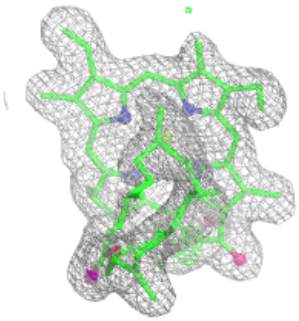


Electron density around CLA C 509:

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

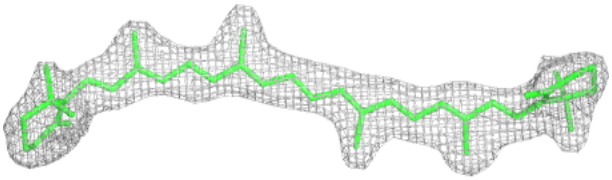


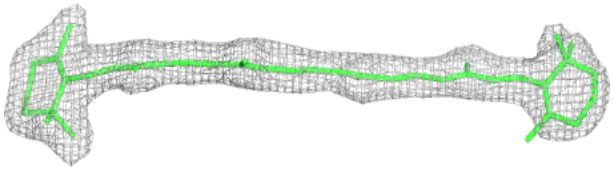


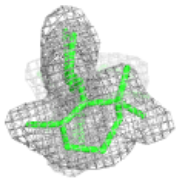


Electron density around BCR C 516:

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

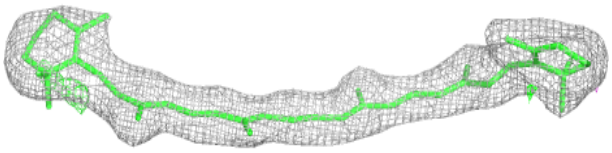


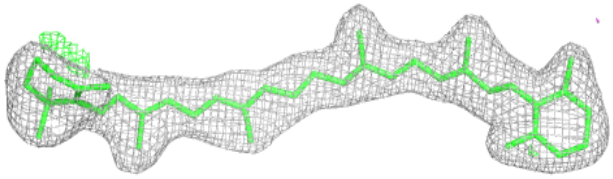


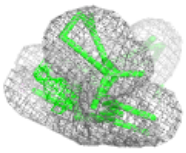


Electron density around BCR D 405:

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

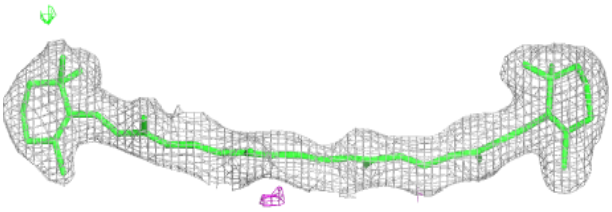


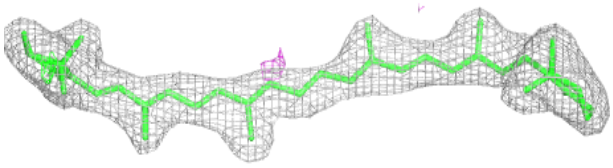


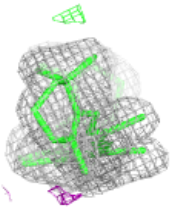


Electron density around BCR K 101:

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

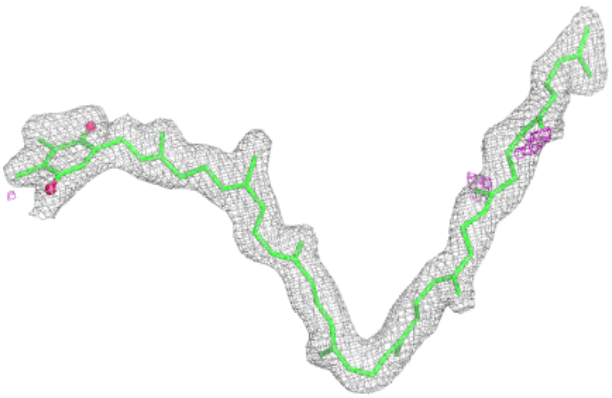


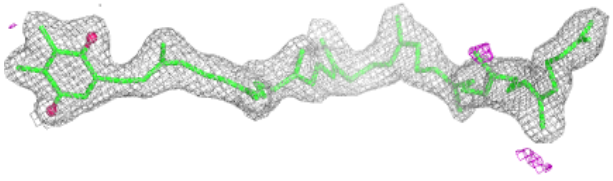


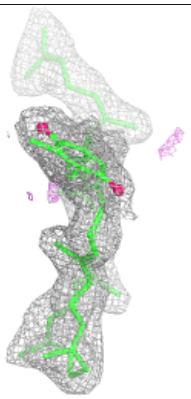


Electron density around PL9 D 406:

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

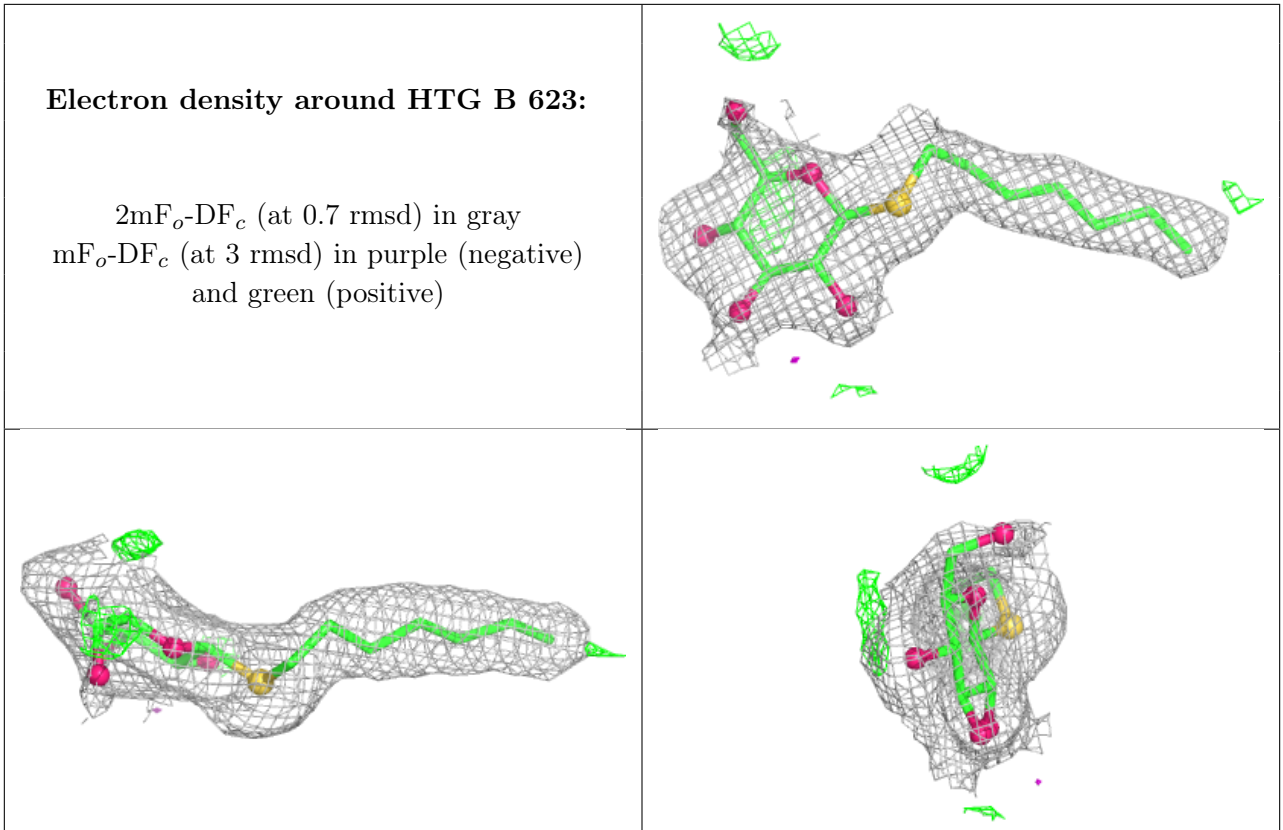






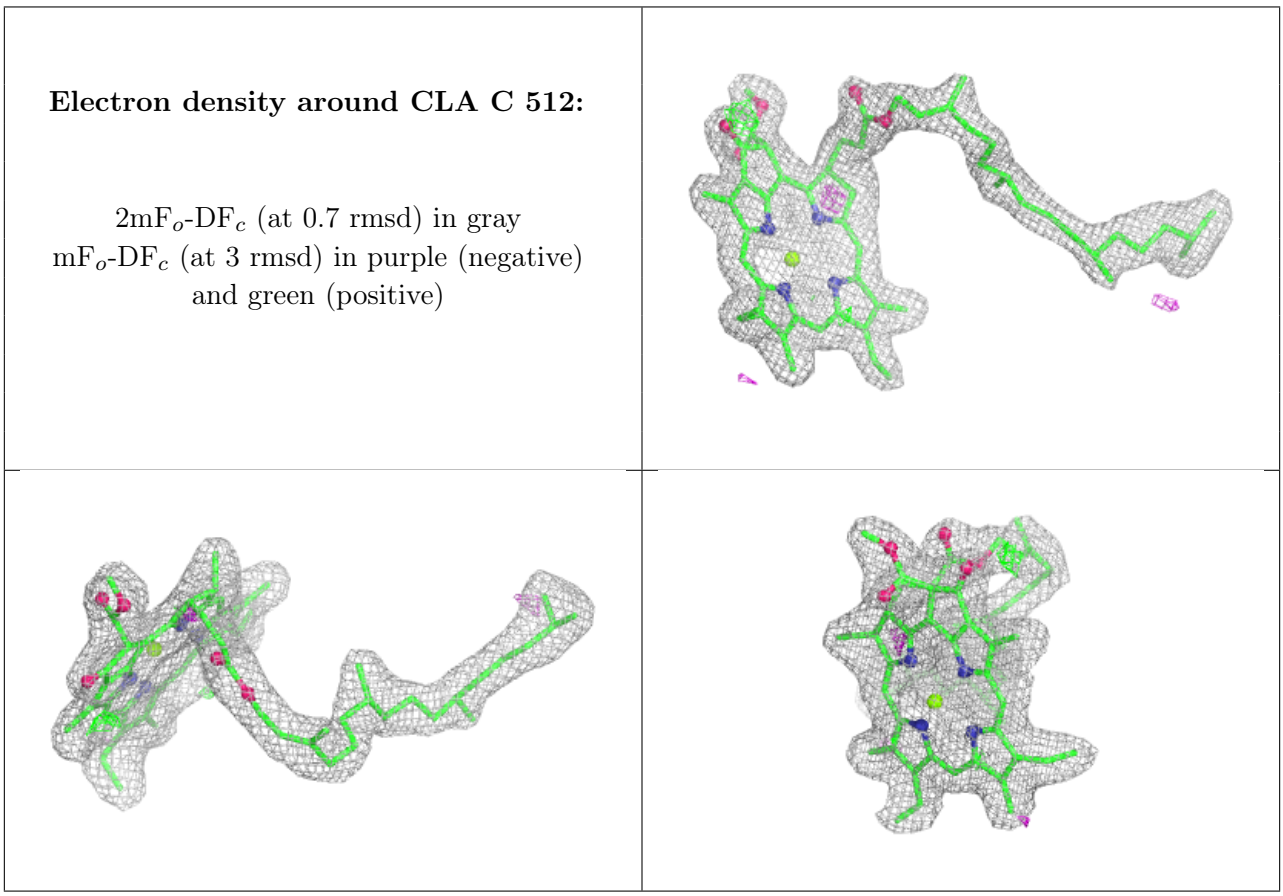
Electron density around HTG B 623:

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



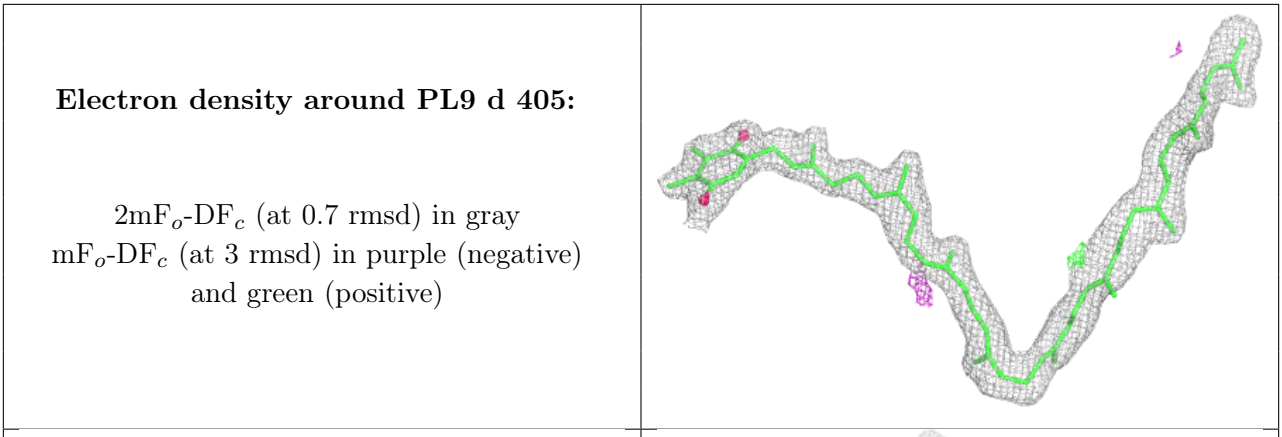
Electron density around CLA C 512:

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



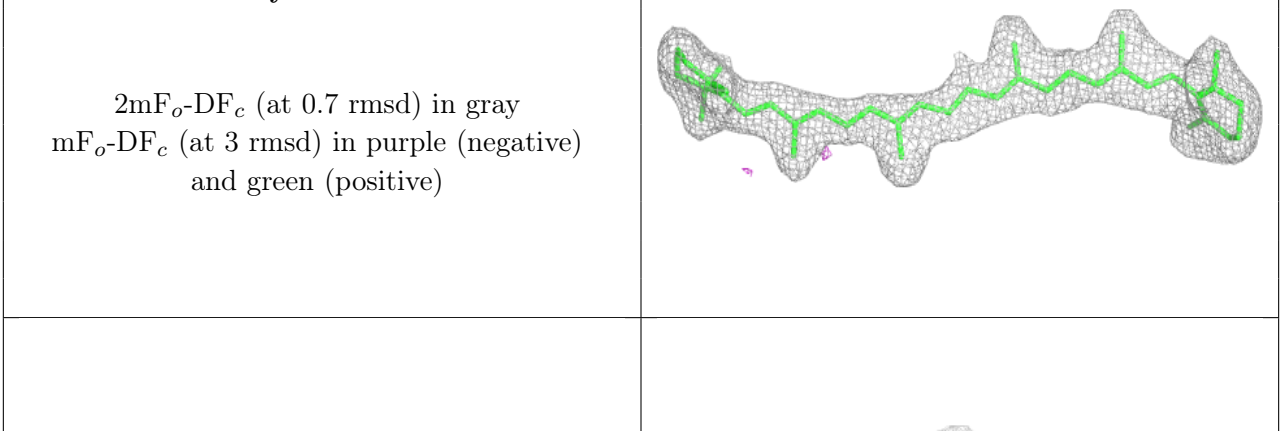
Electron density around PL9 d 405:

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



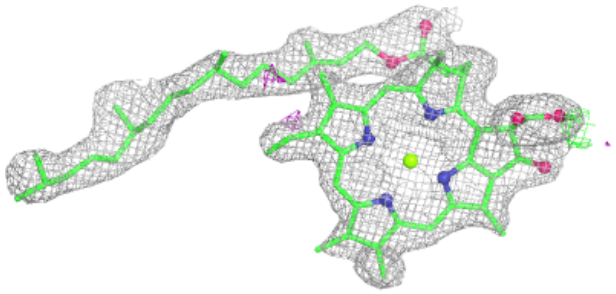
Electron density around BCR a 413:

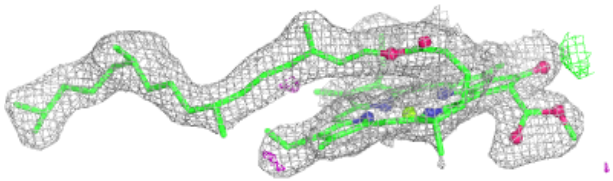
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

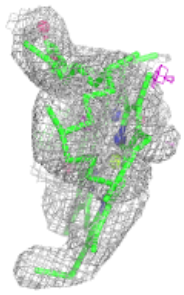


Electron density around CLA c 902:

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

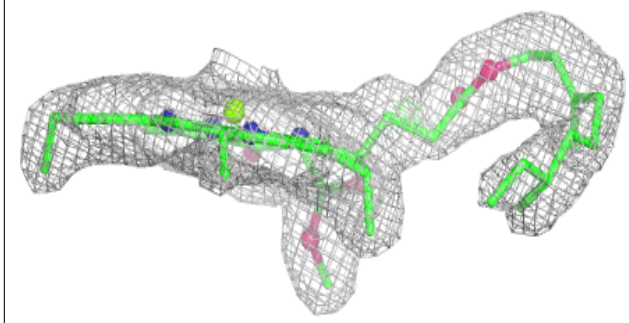


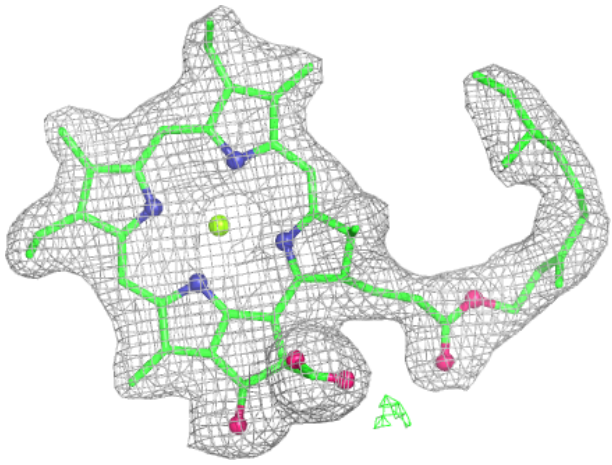


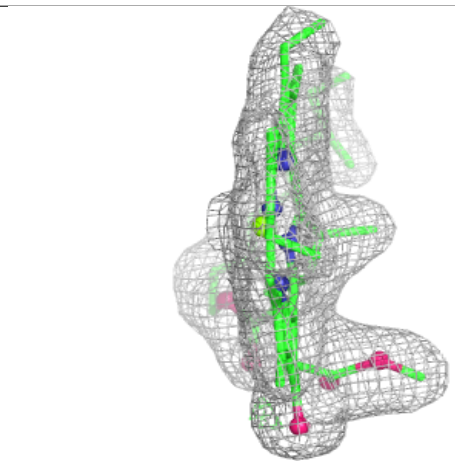


Electron density around CLA C 513:

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

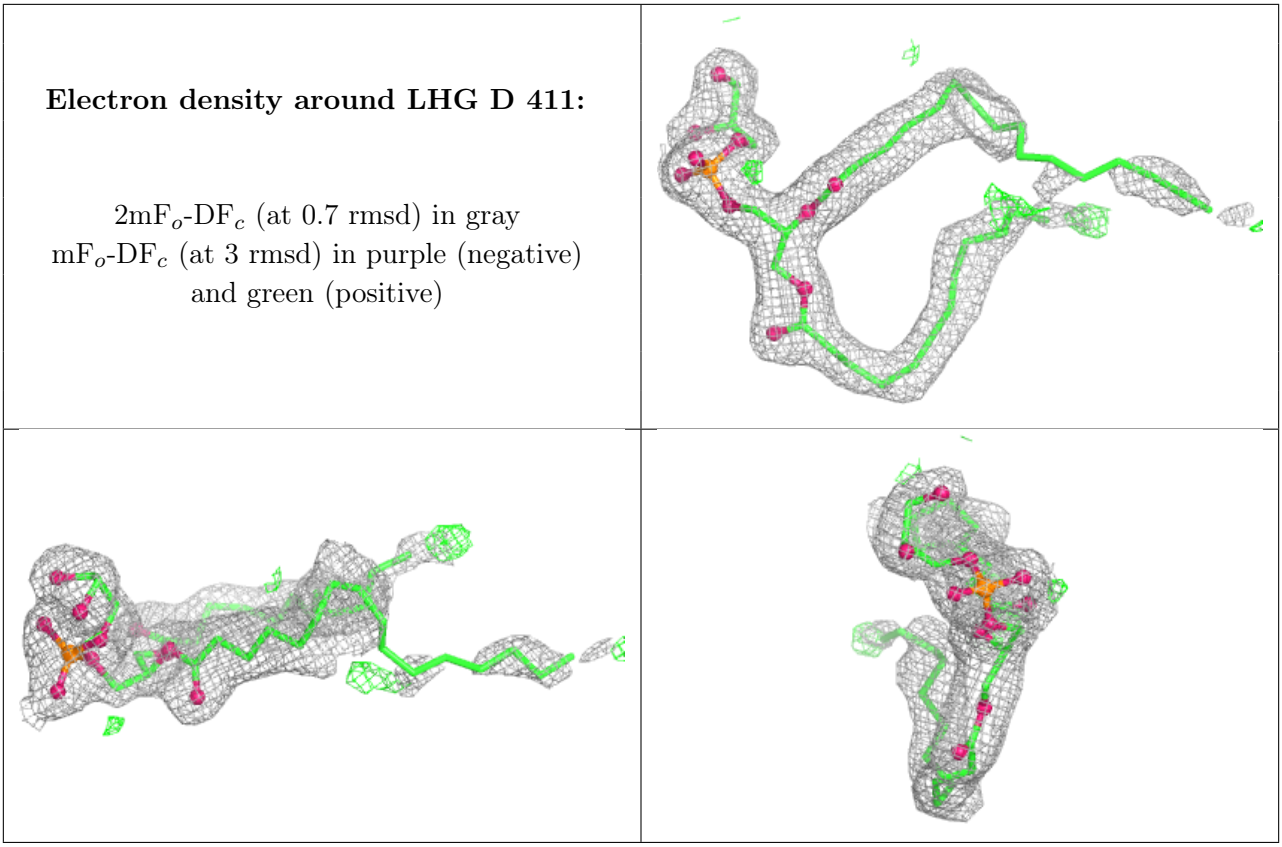






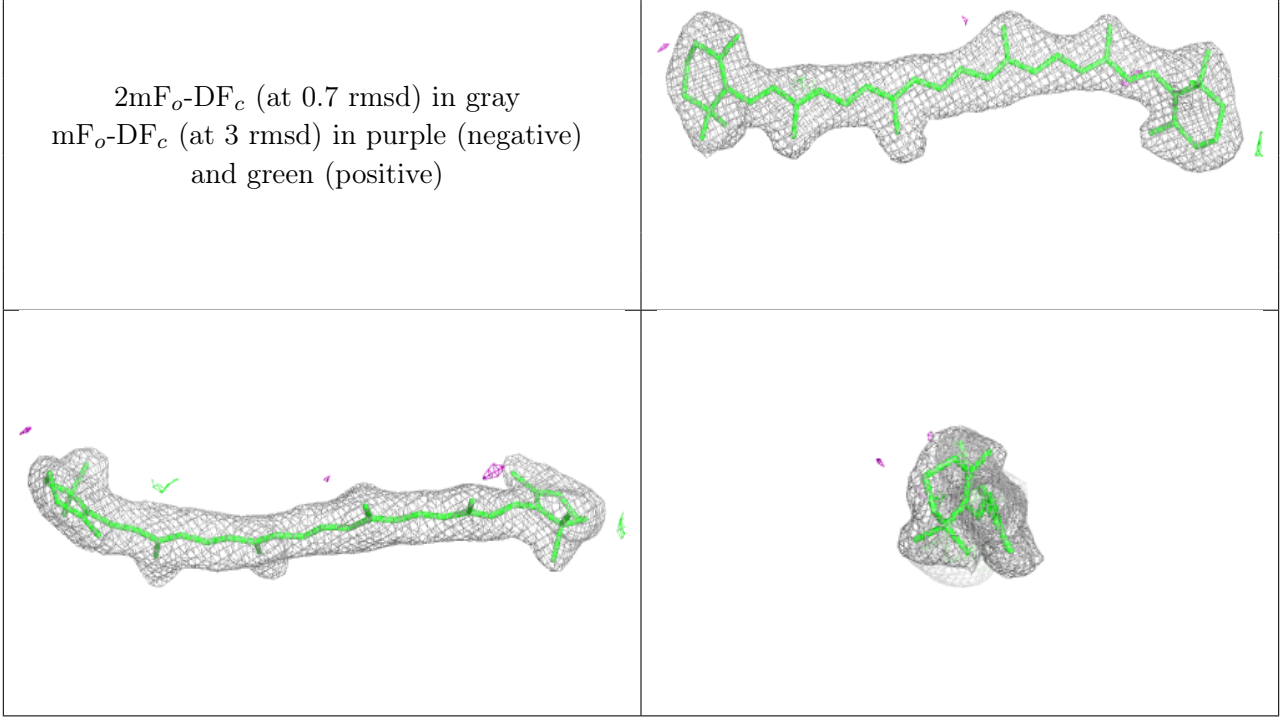
Electron density around LHG D 411:

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



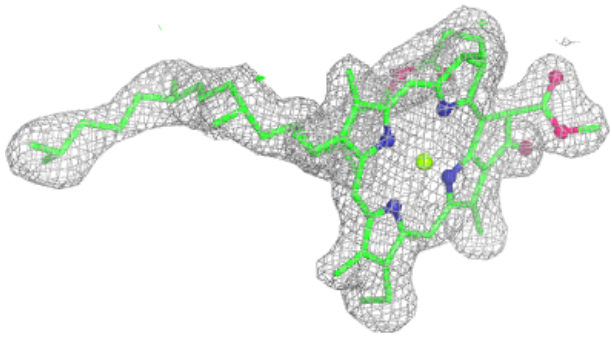
Electron density around BCR b 620:

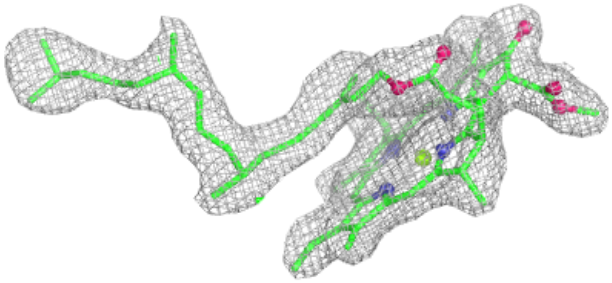
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

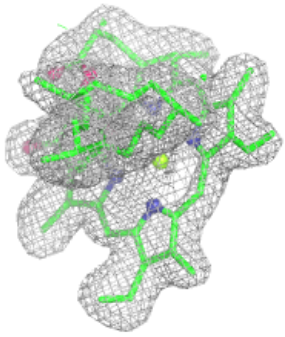


Electron density around CLA c 906:

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

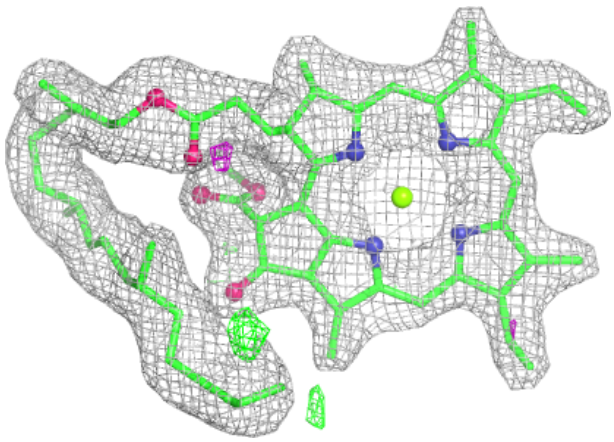


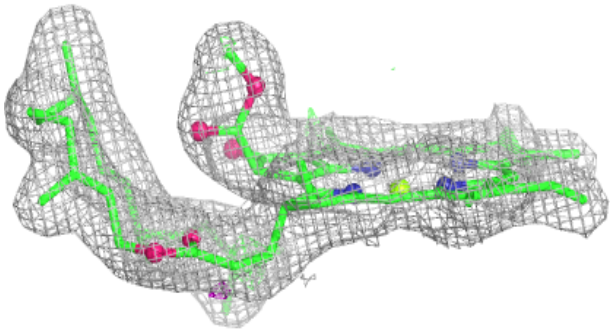


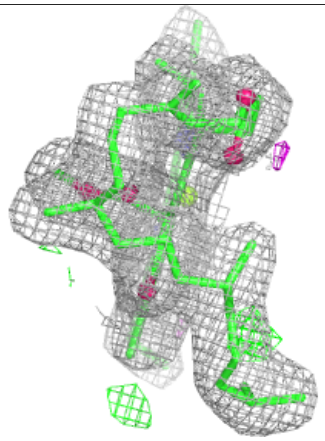


Electron density around CLA B 611:

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

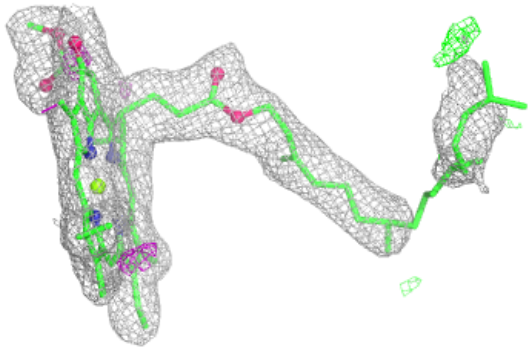


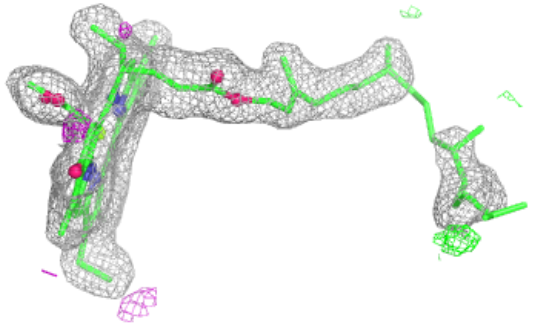


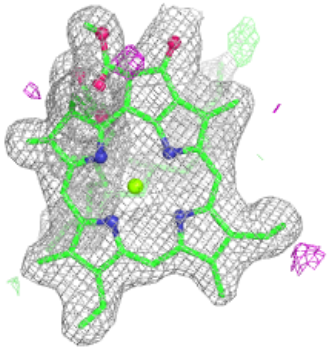


Electron density around CLA D 404:

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

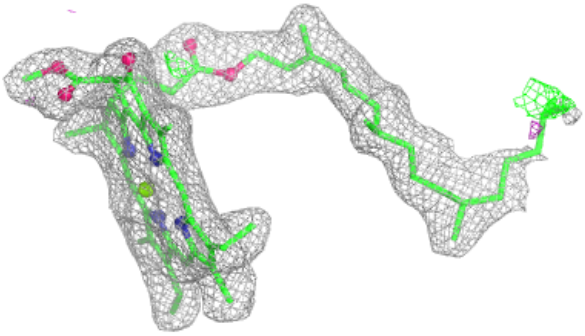


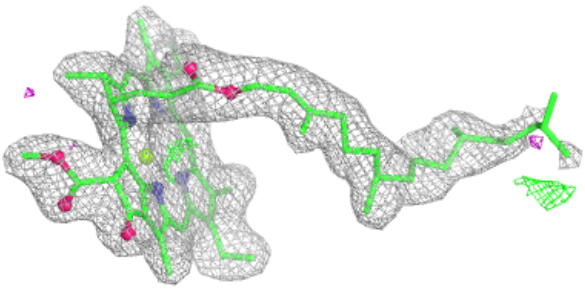


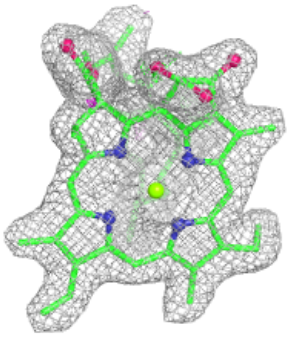


Electron density around CLA c 909:

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

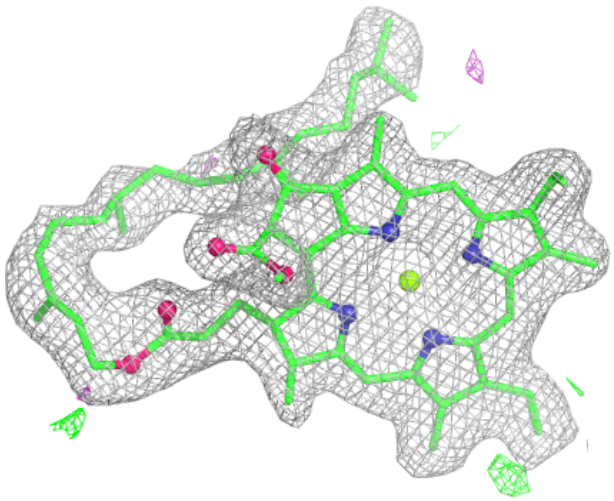


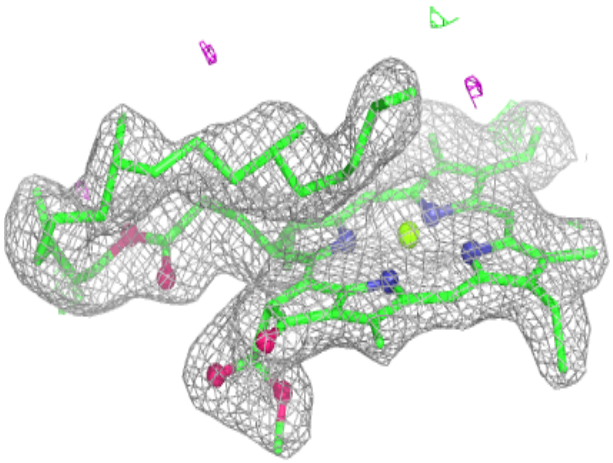


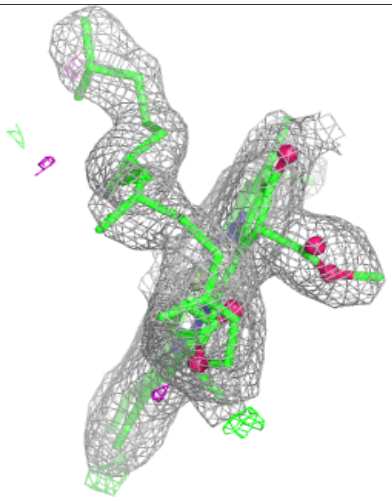


Electron density around CLA c 910:

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

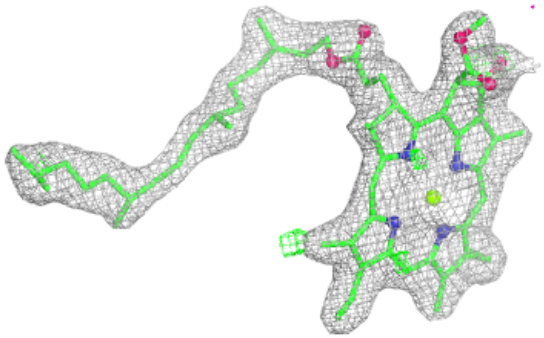


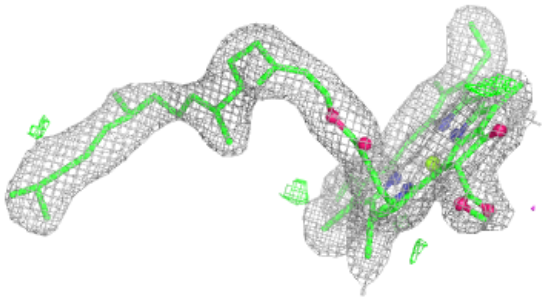


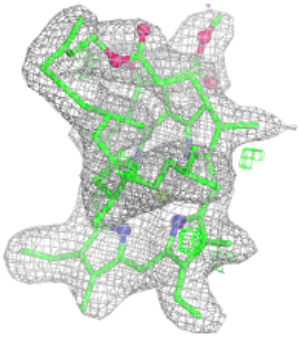


Electron density around CLA c 912:

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

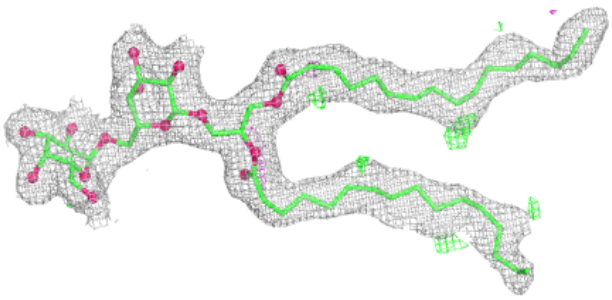


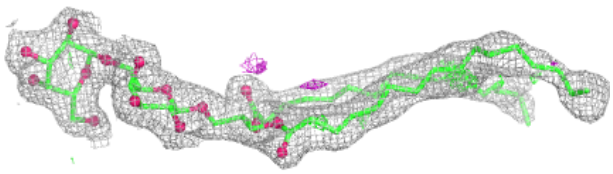


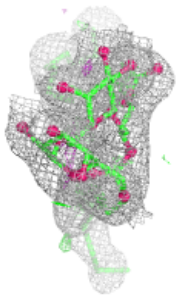


Electron density around DGD C 519:

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

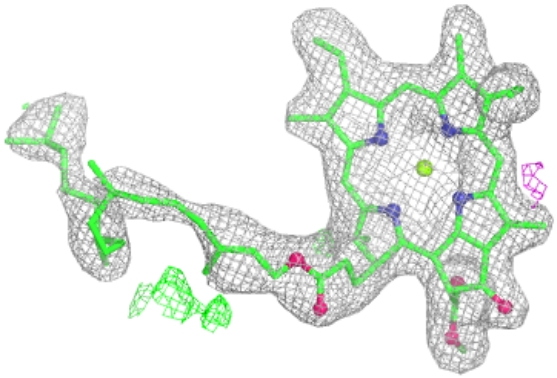


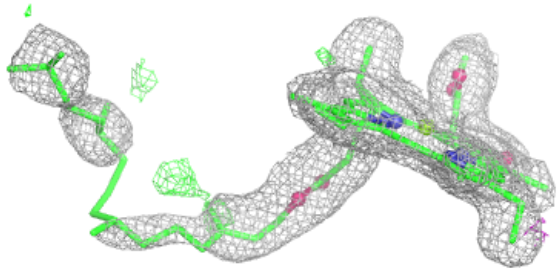


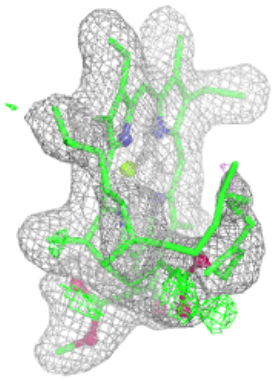


Electron density around CLA a 412:

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

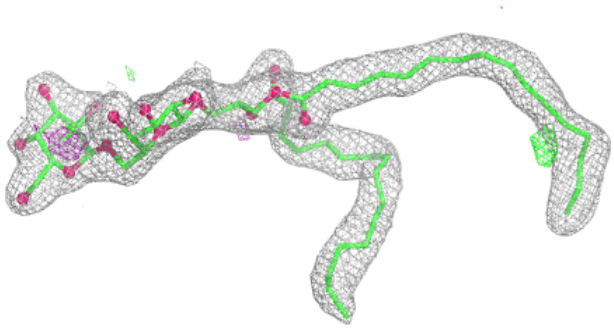


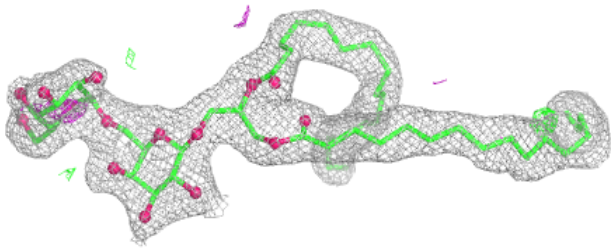


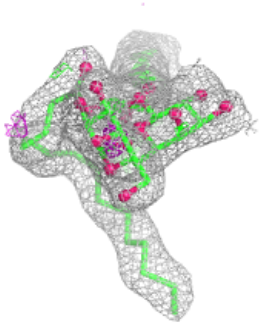


Electron density around DGD H 102:

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

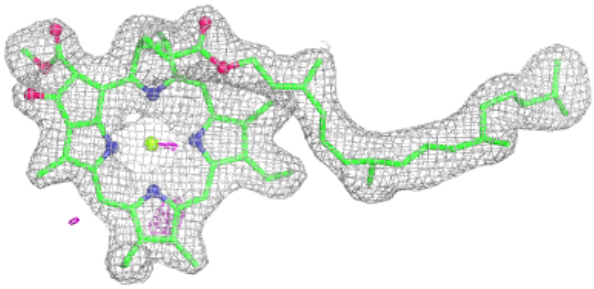


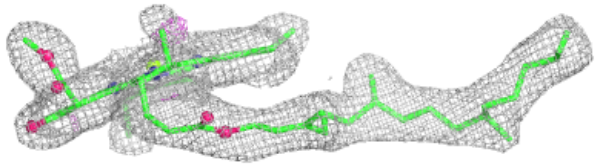


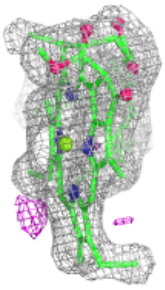


Electron density around CLA B 604:

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

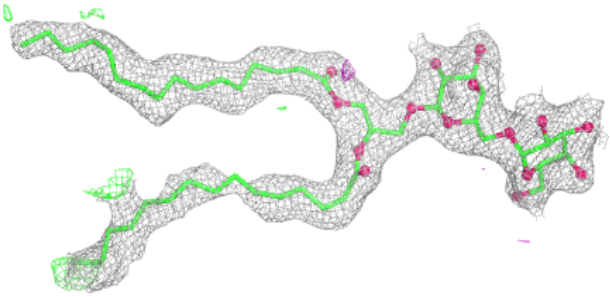


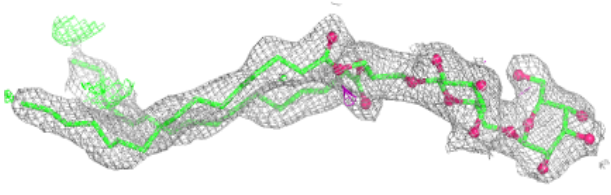


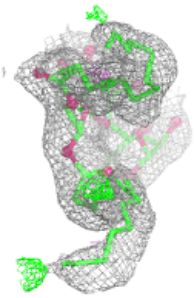


Electron density around DGD c 919:

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

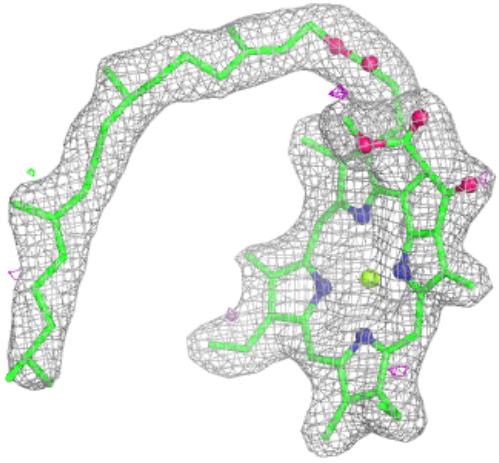


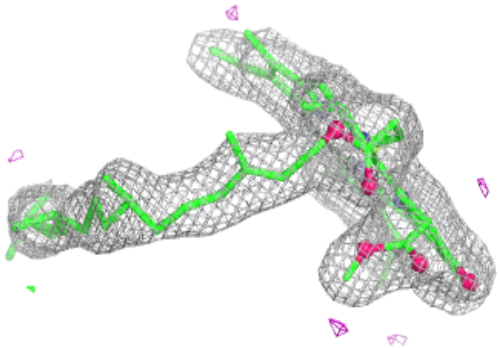


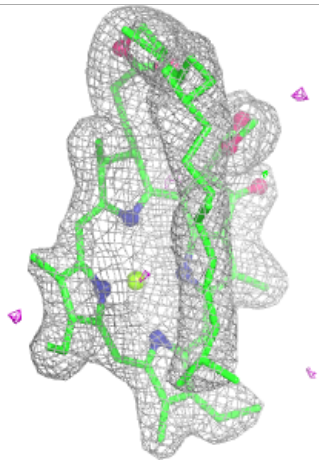


Electron density around CLA C 508:

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

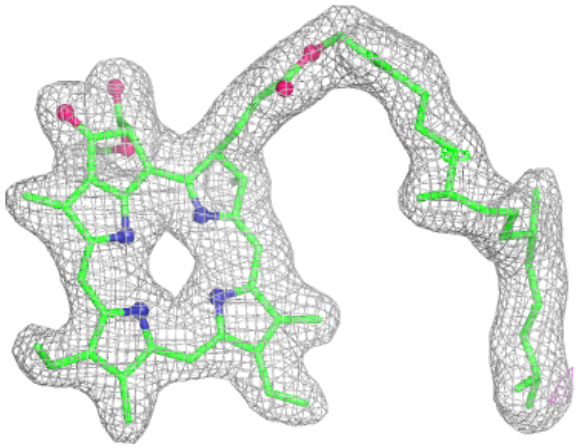


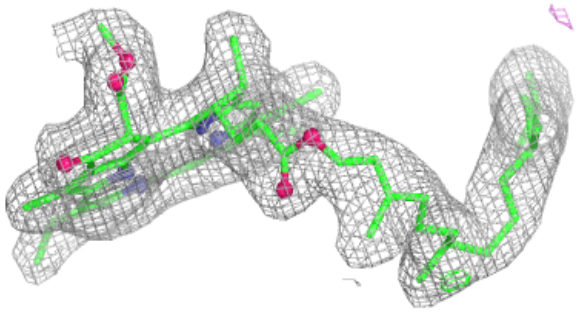




Electron density around PHO a 411:

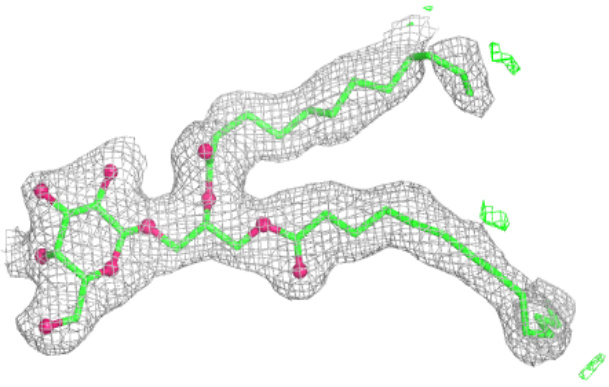
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

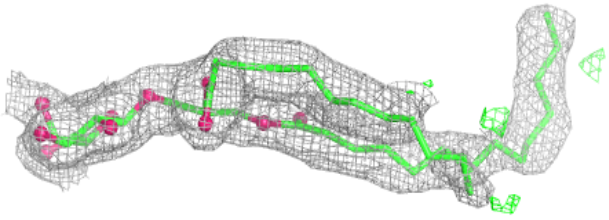


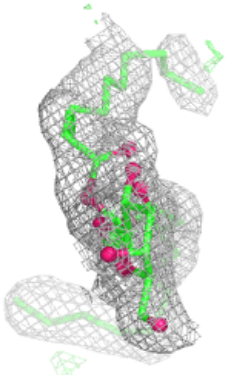


Electron density around LMG J 101:

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

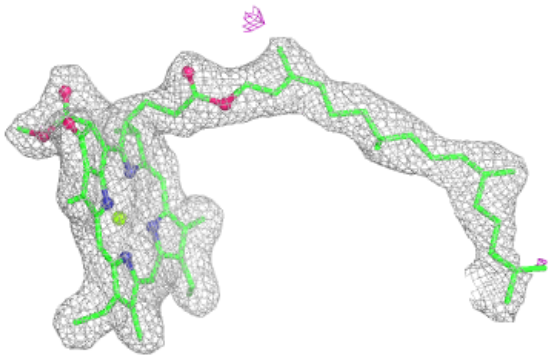


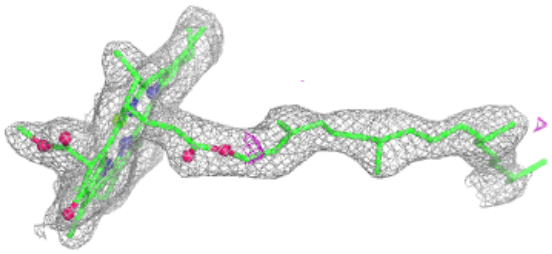


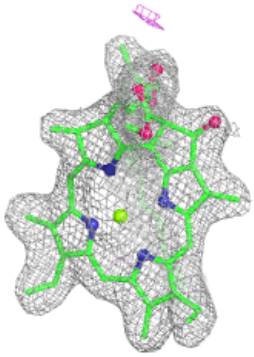


Electron density around CLA b 610:

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

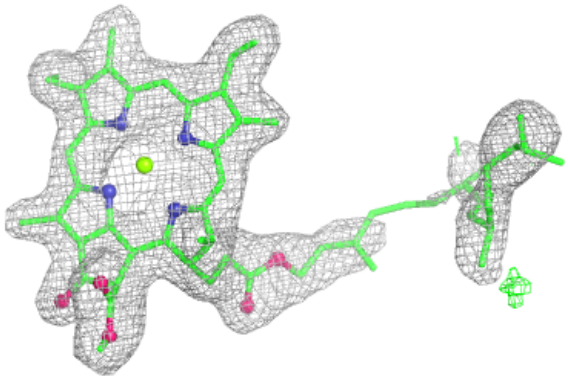


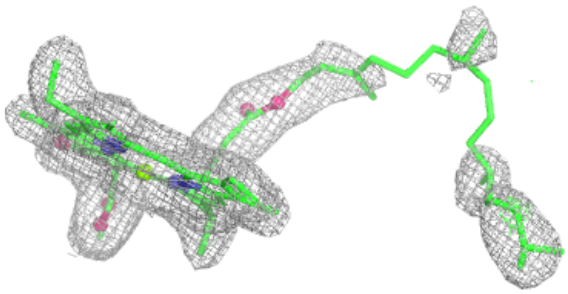


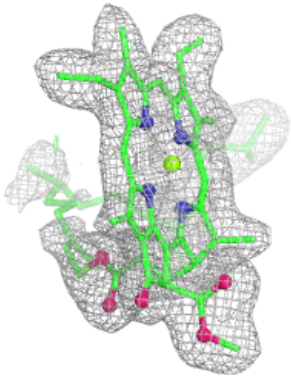


Electron density around CLA A 408:

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

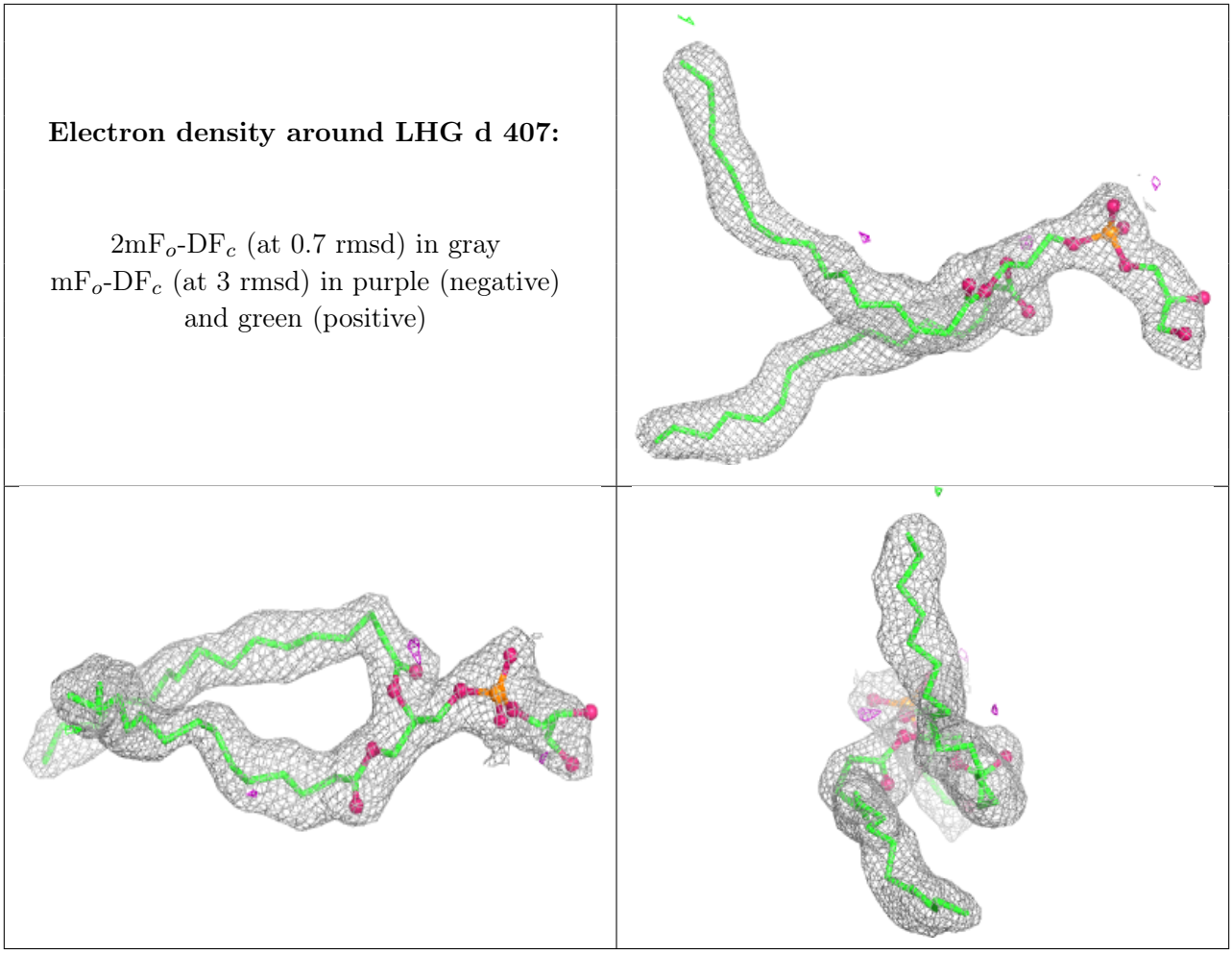






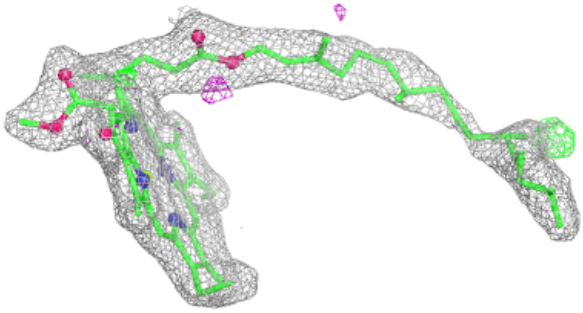
Electron density around LHG d 407:

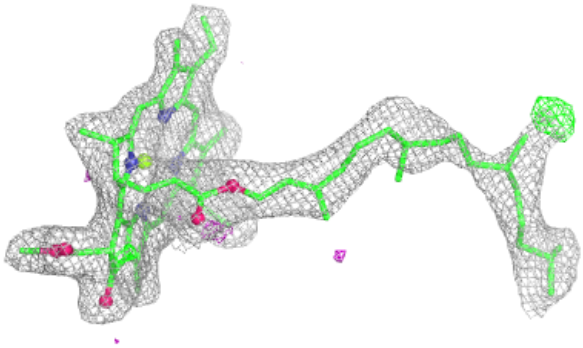
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

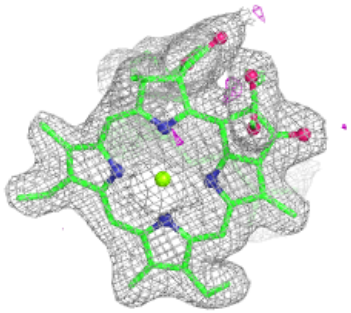


Electron density around CLA b 608:

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

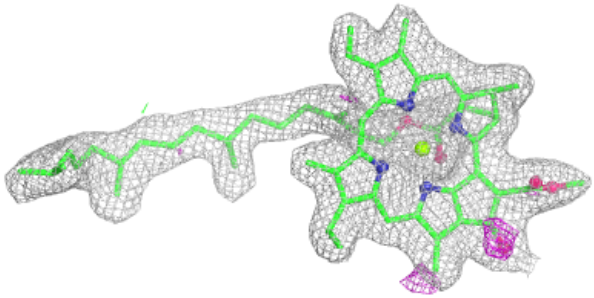


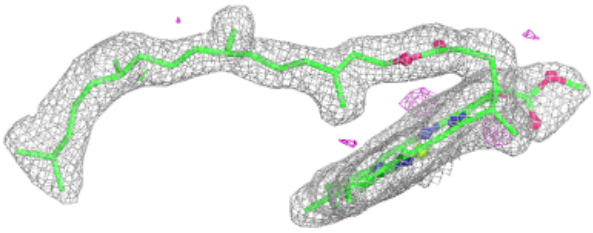


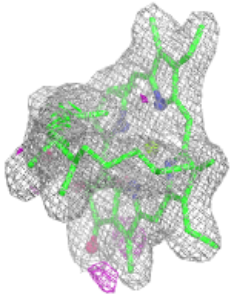


Electron density around CLA b 609:

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

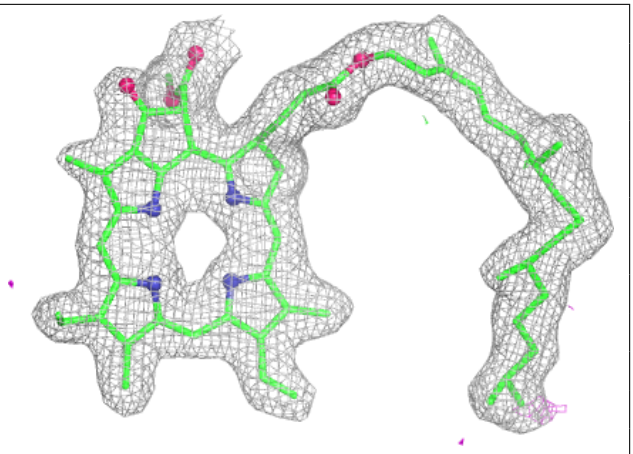


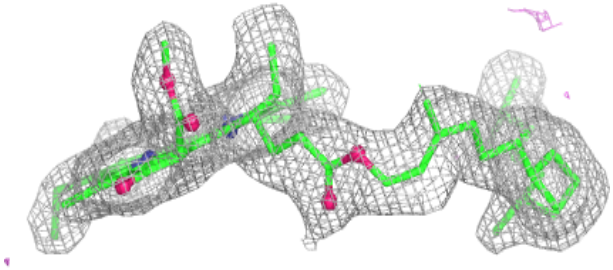




Electron density around PHO A 407:

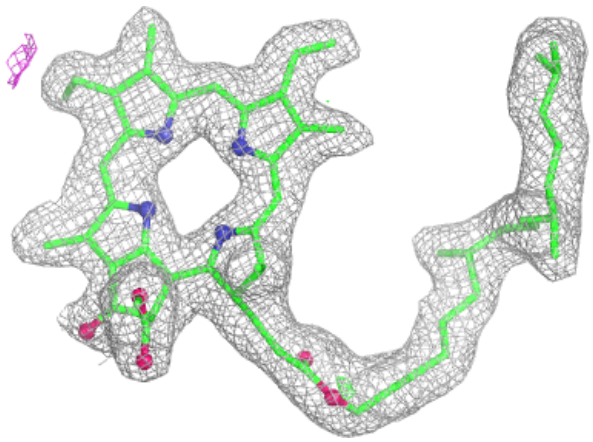
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

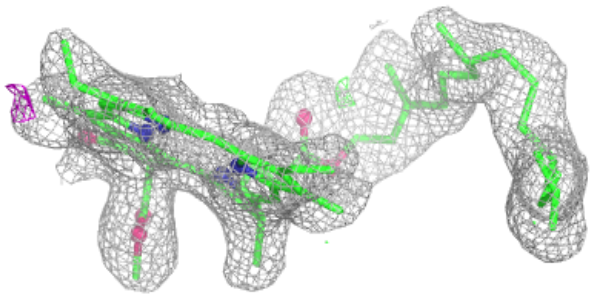


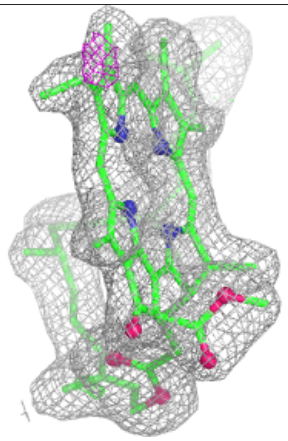


Electron density around PHO D 402:

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

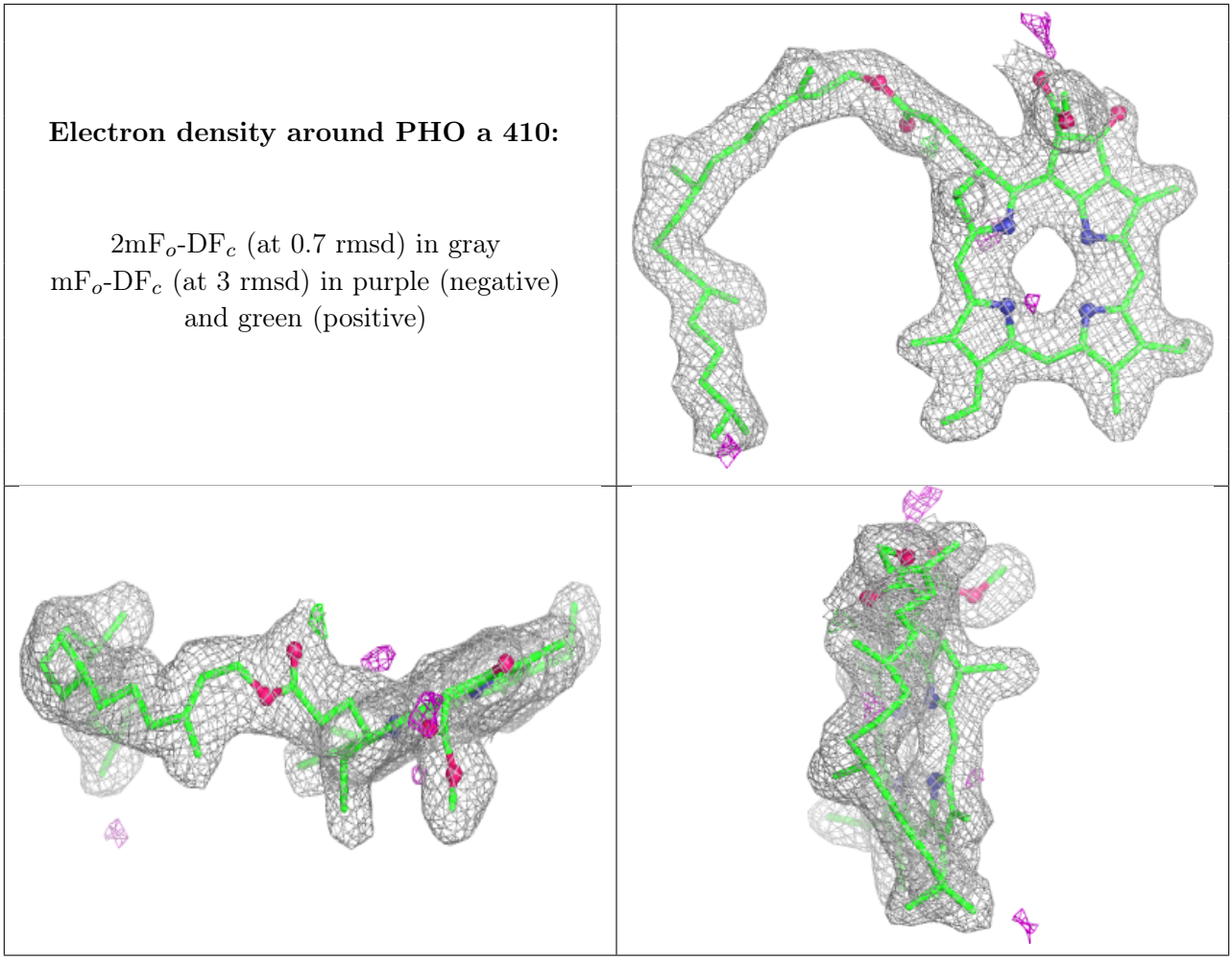






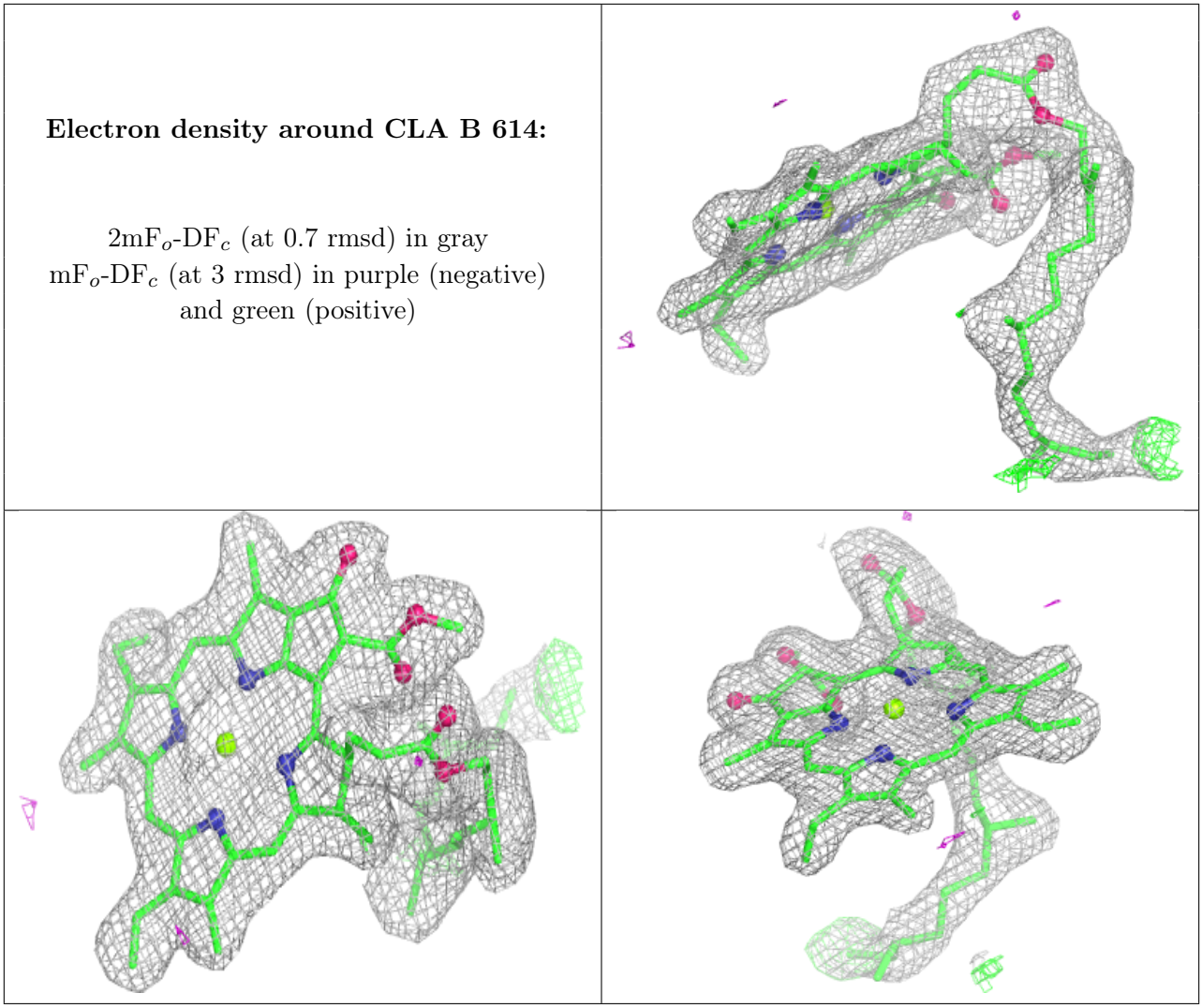
Electron density around PHO a 410:

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



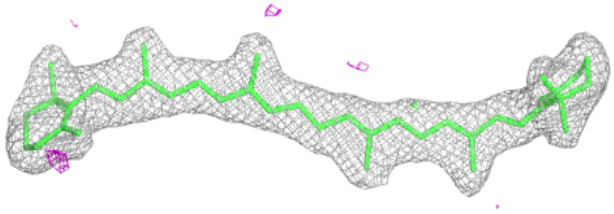
Electron density around CLA B 614:

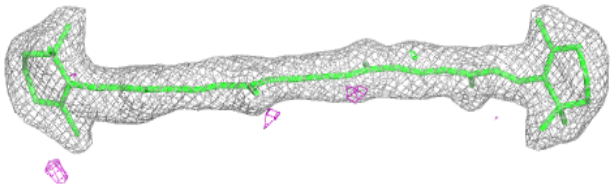
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

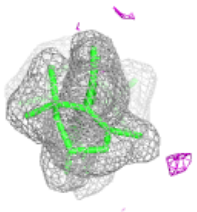


Electron density around BCR A 409:

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

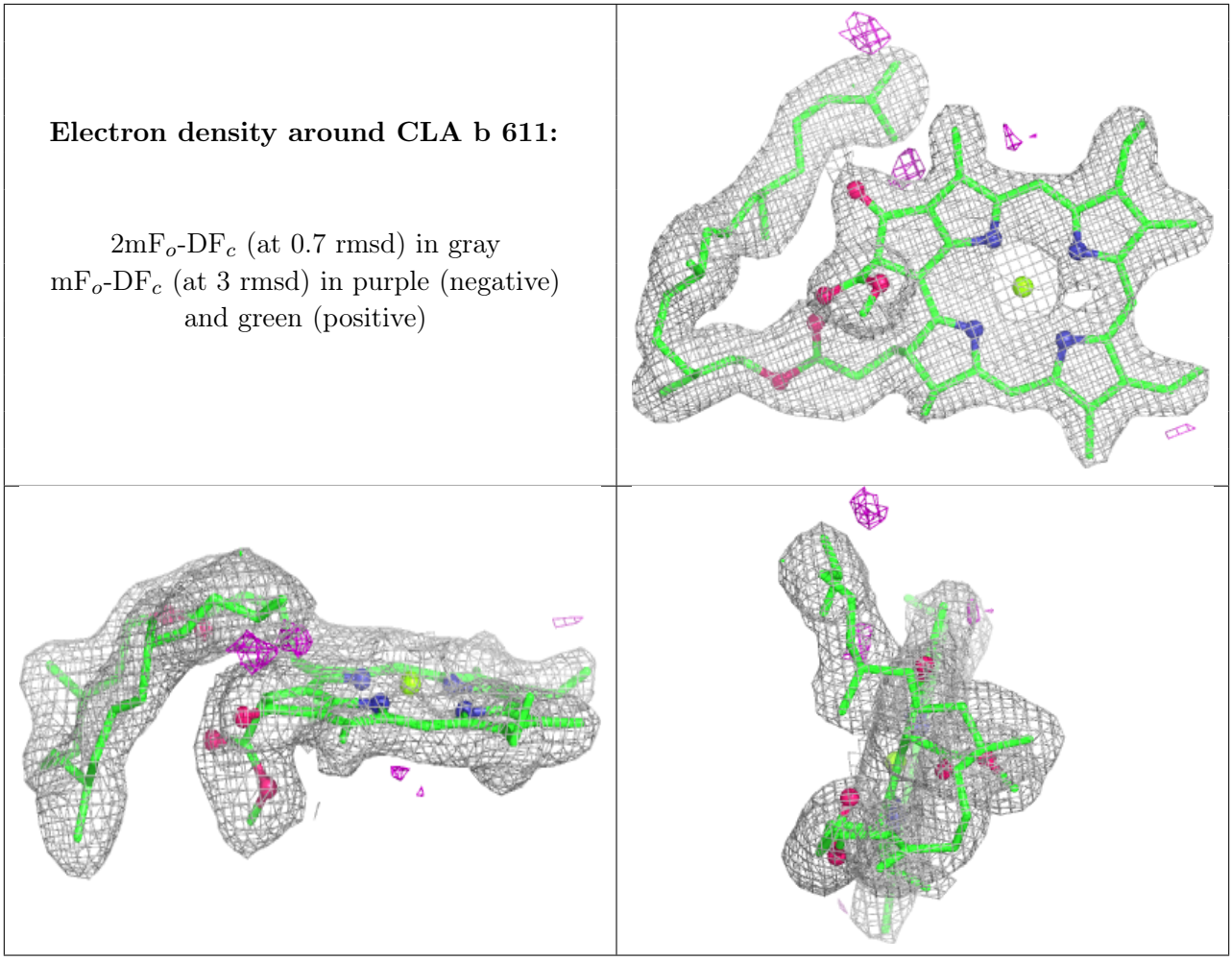






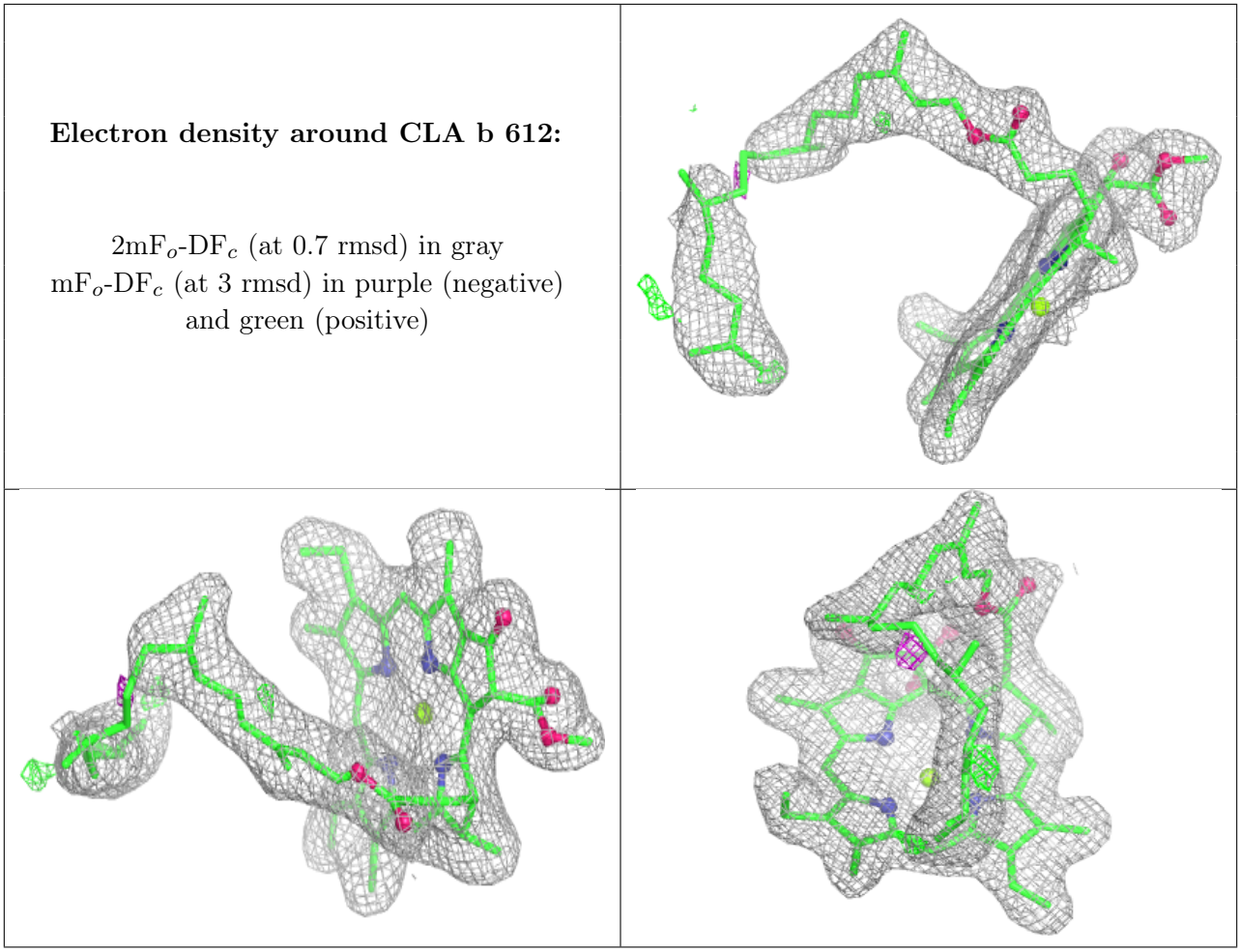
Electron density around CLA b 611:

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



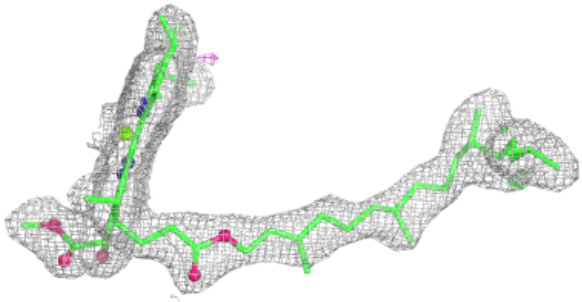
Electron density around CLA b 612:

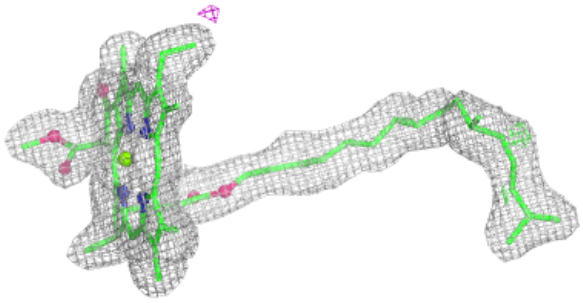
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

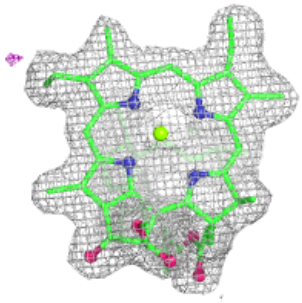


Electron density around CLA B 606:

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

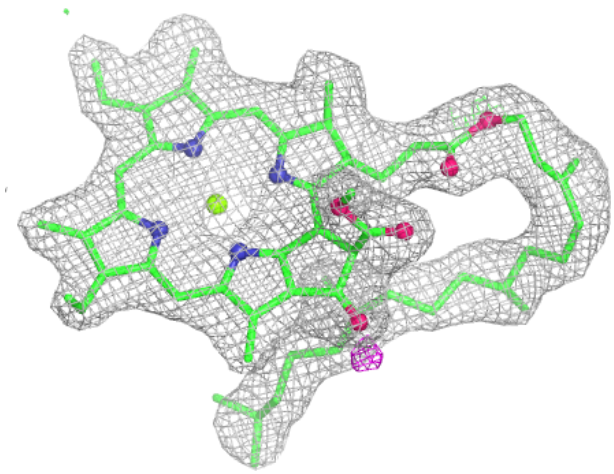


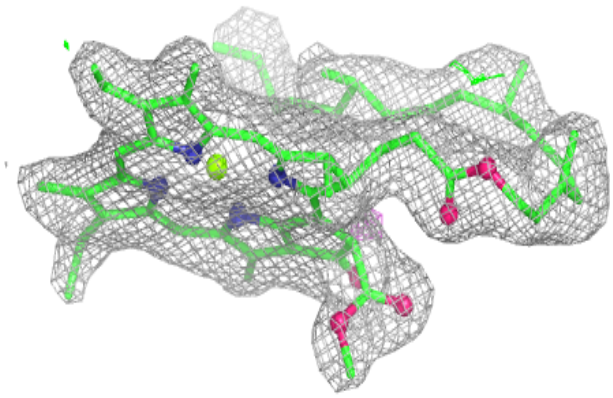


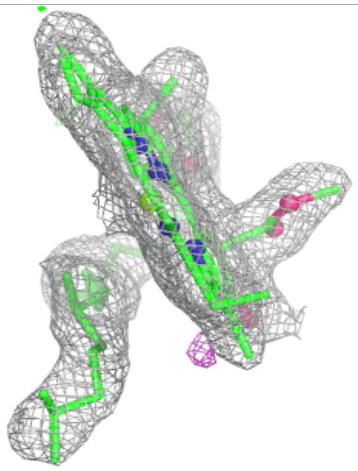


Electron density around CLA C 510:

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

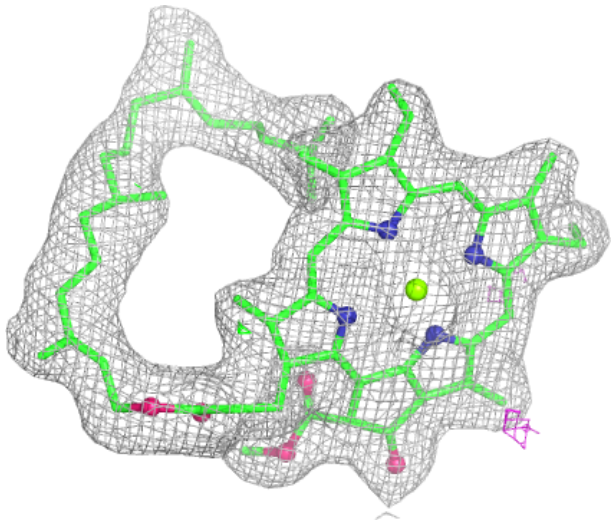


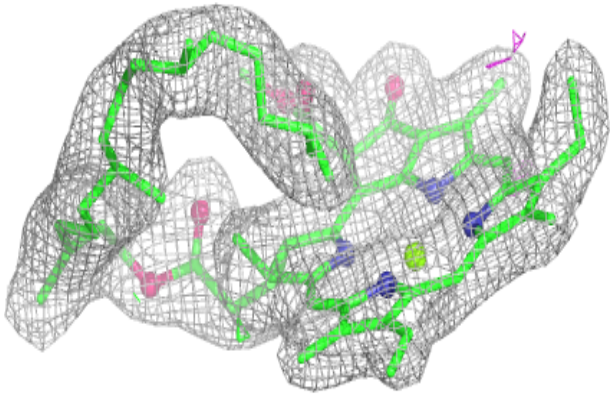


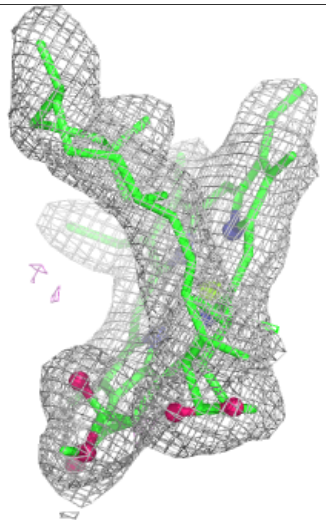


Electron density around CLA b 616:

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

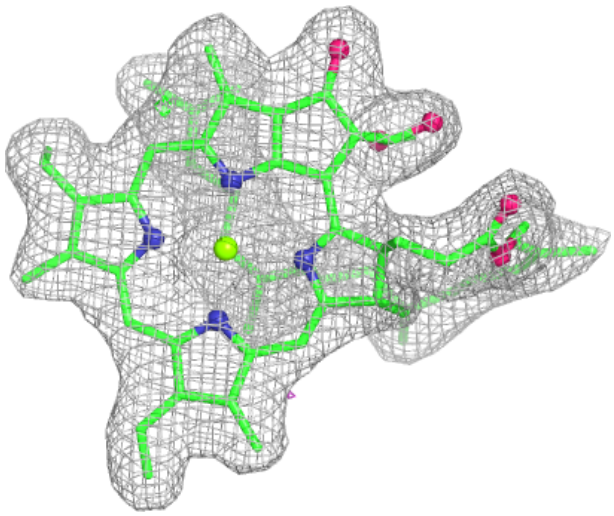


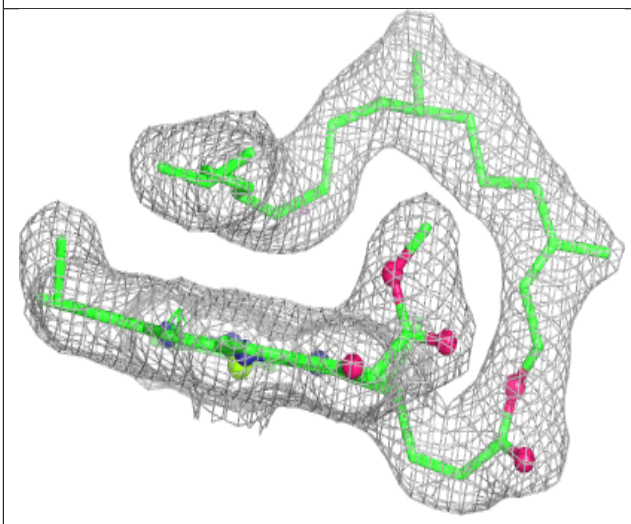


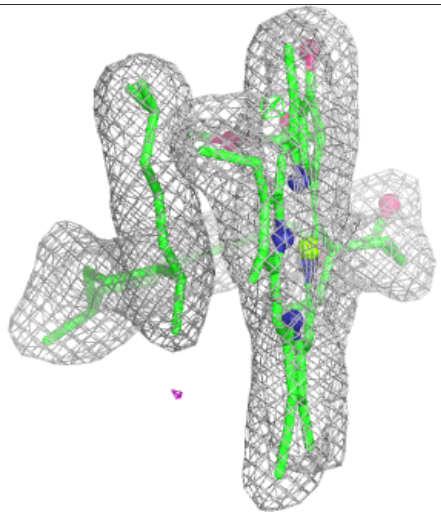


Electron density around CLA C 511:

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

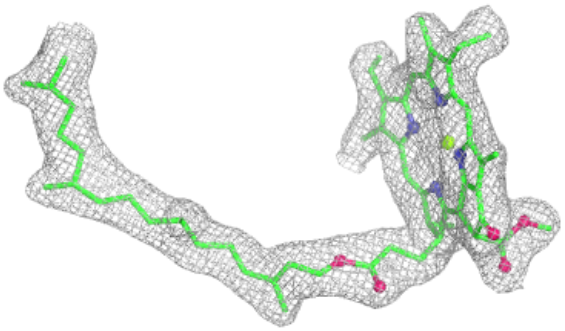


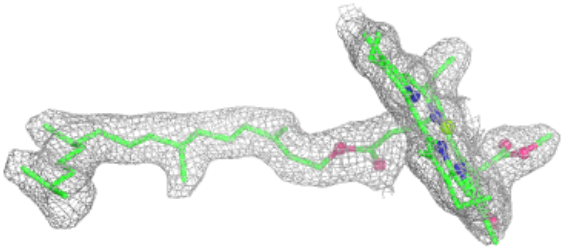


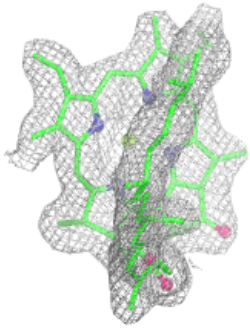


Electron density around CLA B 610:

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

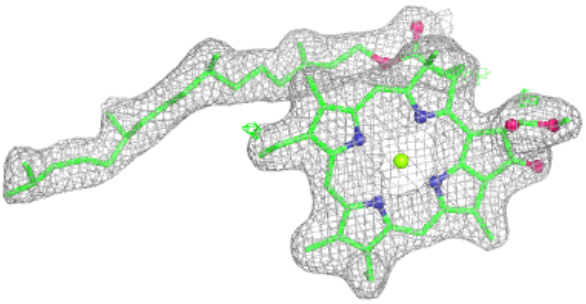


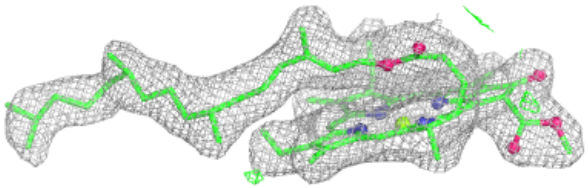


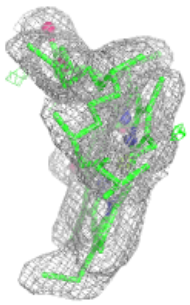


Electron density around CLA C 502:

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

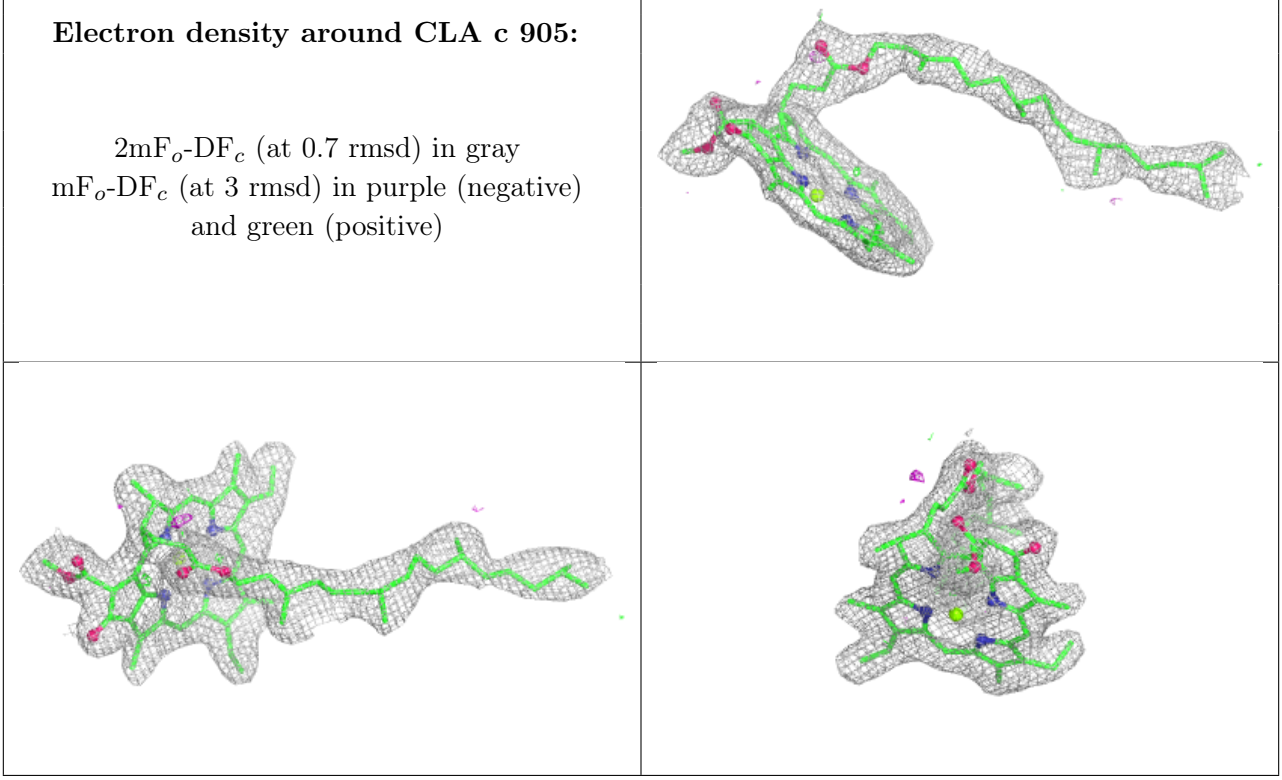






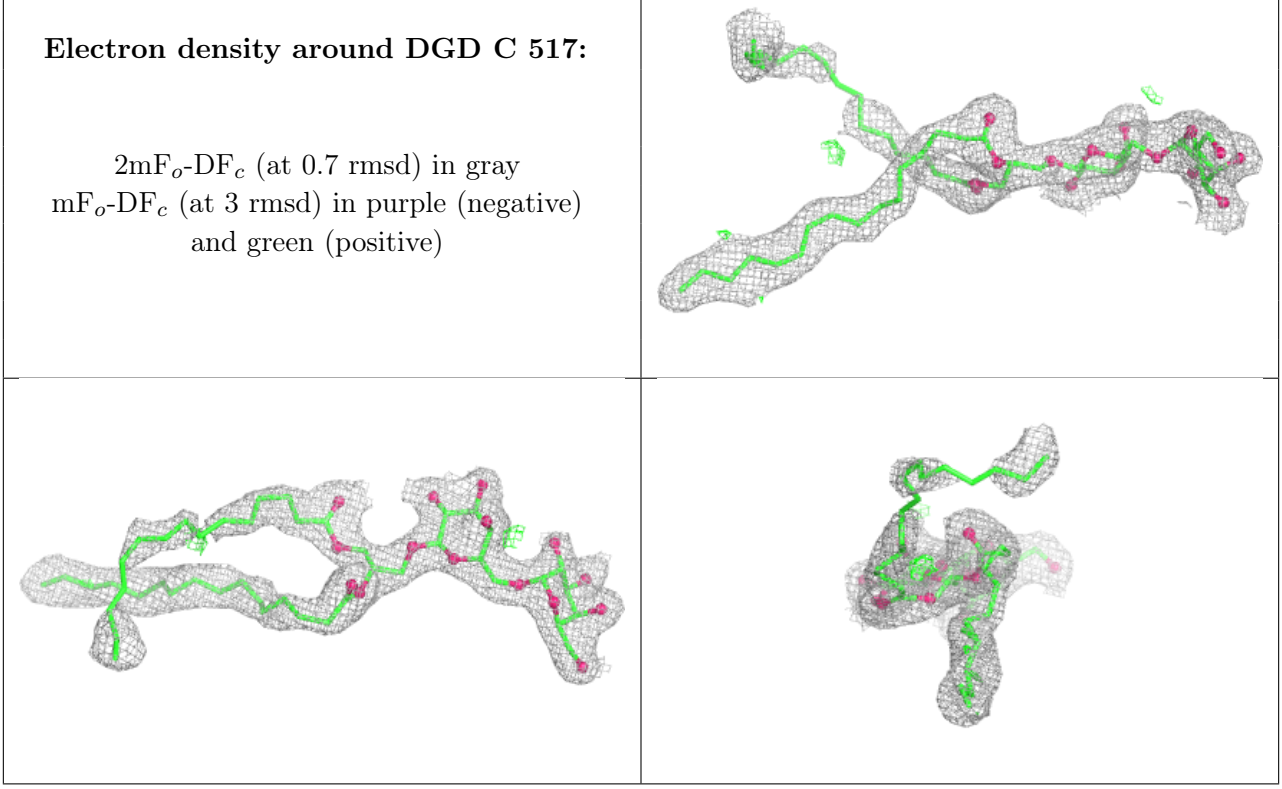
Electron density around CLA c 905:

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



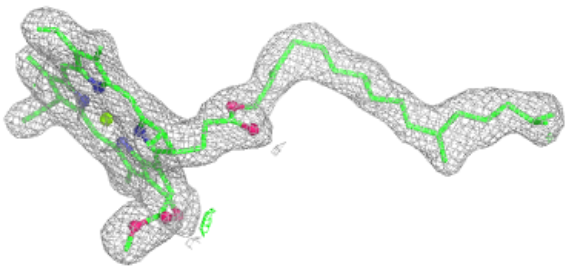
Electron density around DGD C 517:

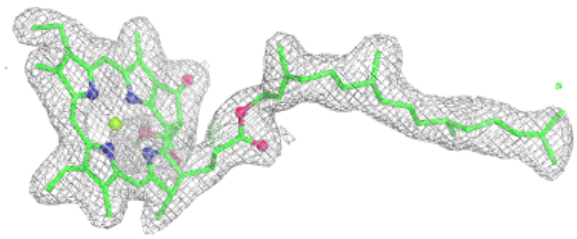
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

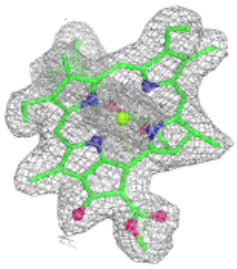


Electron density around CLA C 503:

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

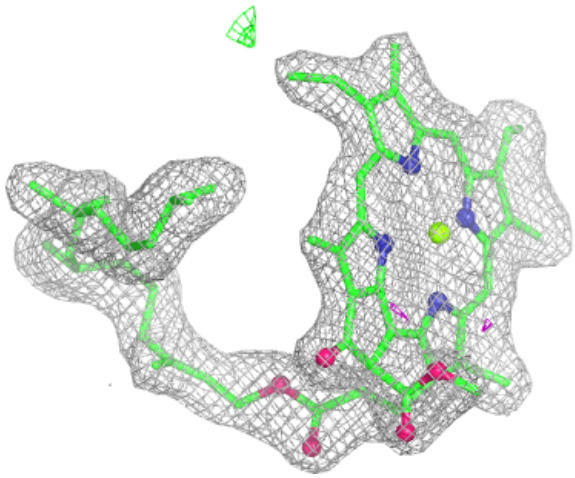


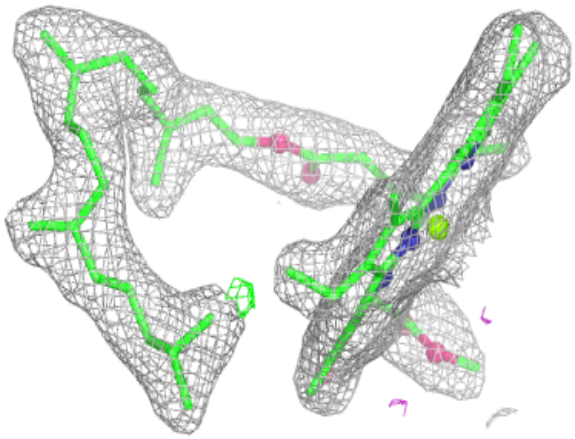


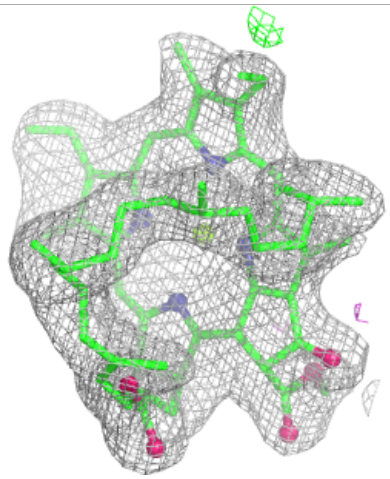


Electron density around CLA C 504:

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

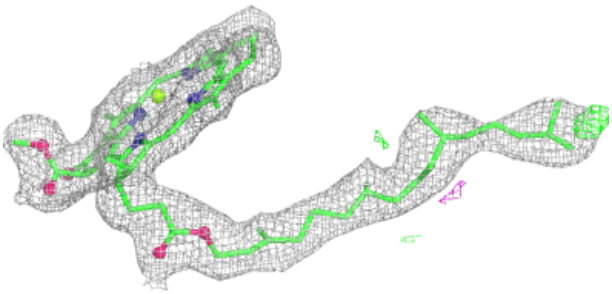


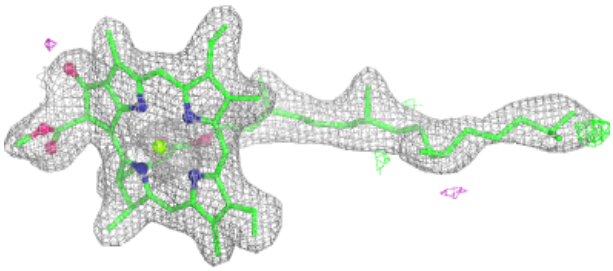


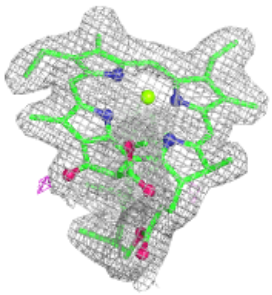


Electron density around CLA C 505:

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

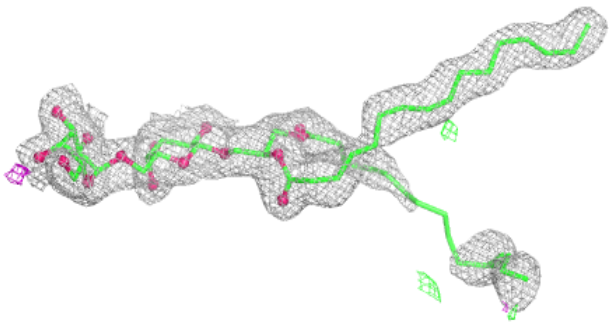


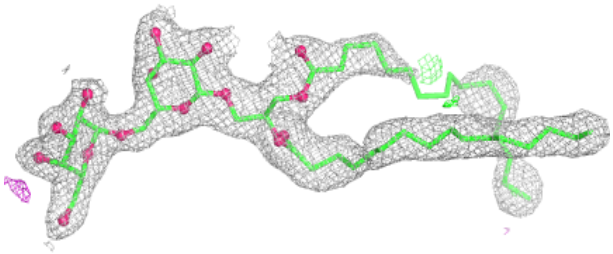




Electron density around DGD c 917:

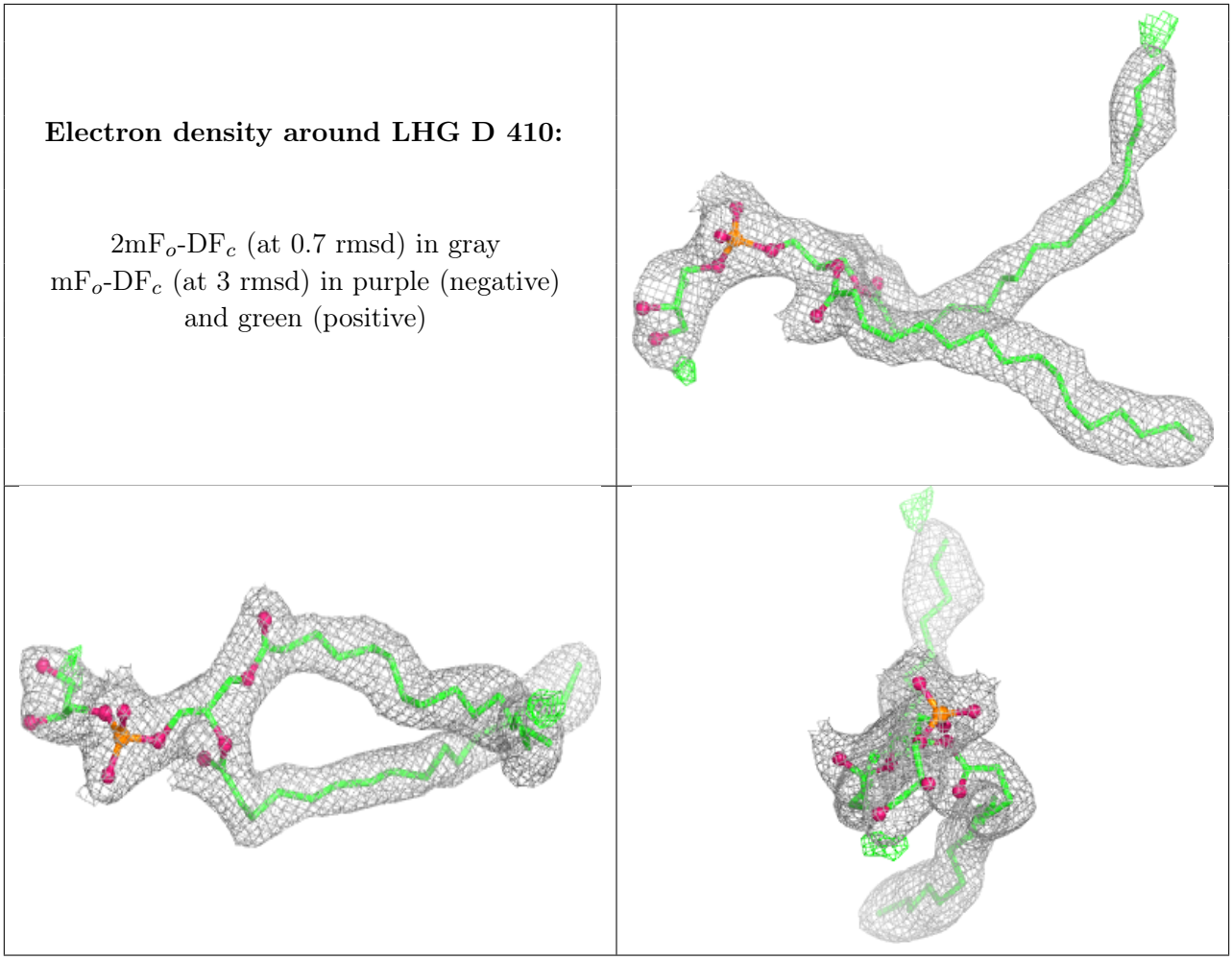
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





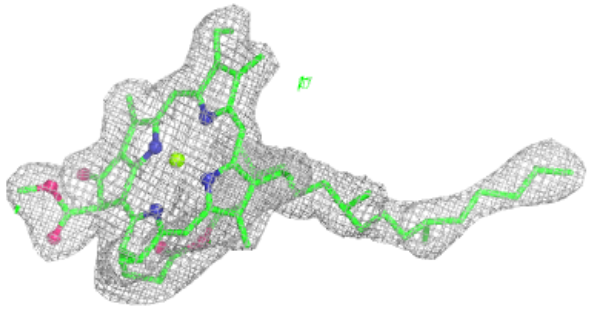
Electron density around LHG D 410:

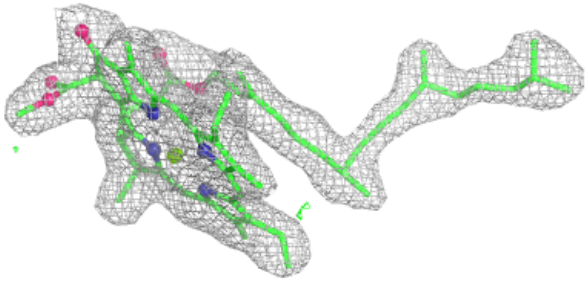
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

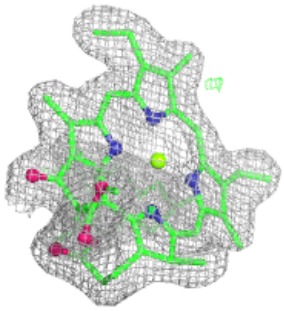


Electron density around CLA C 506:

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

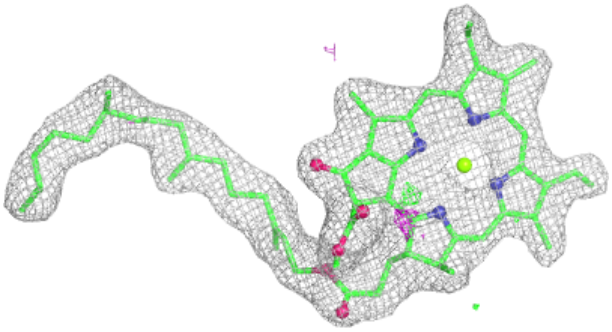


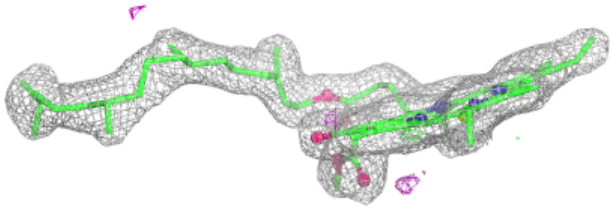


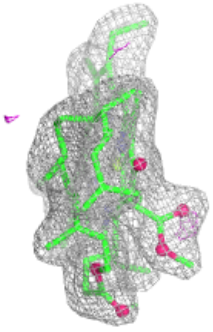


Electron density around CLA b 603:

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

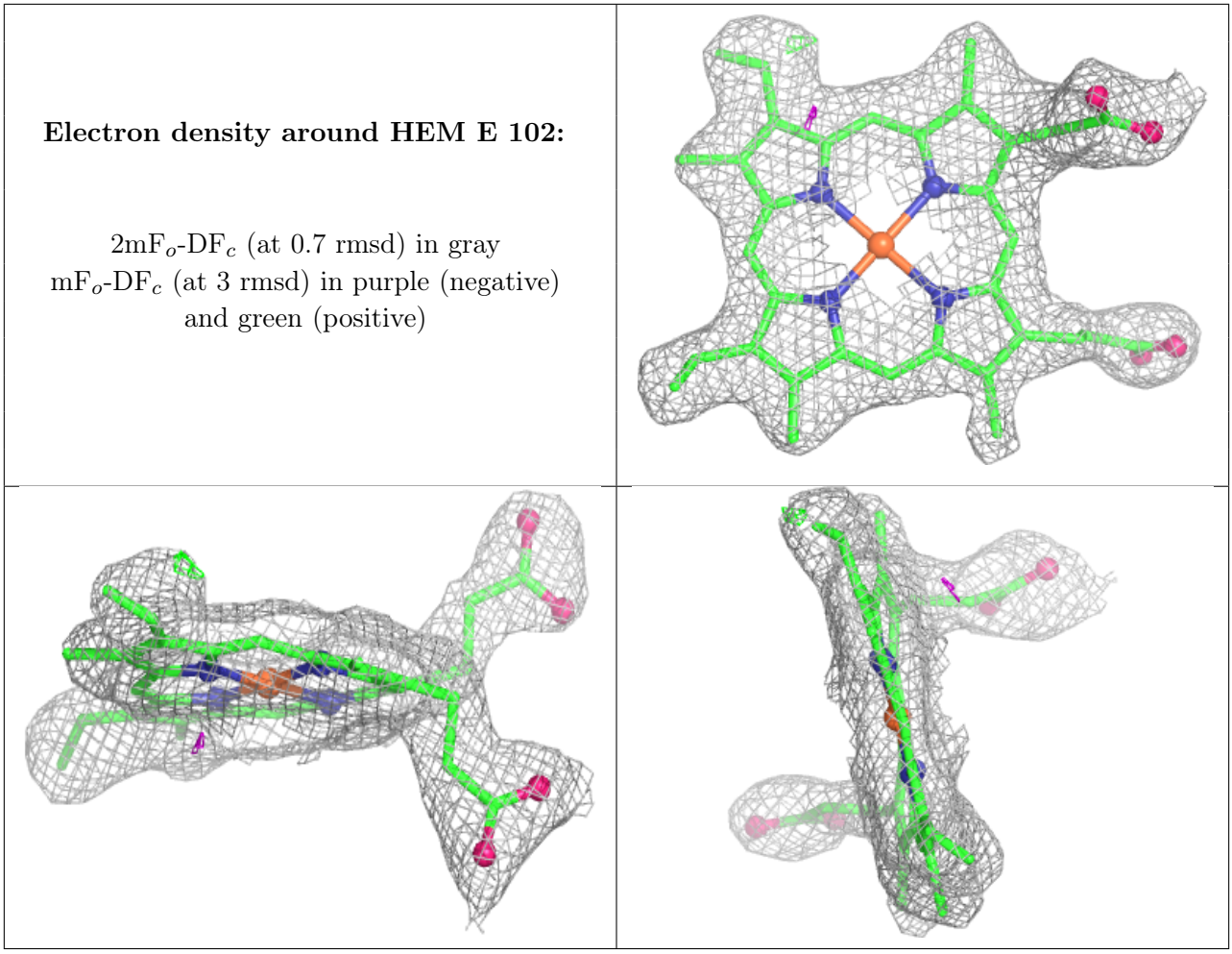






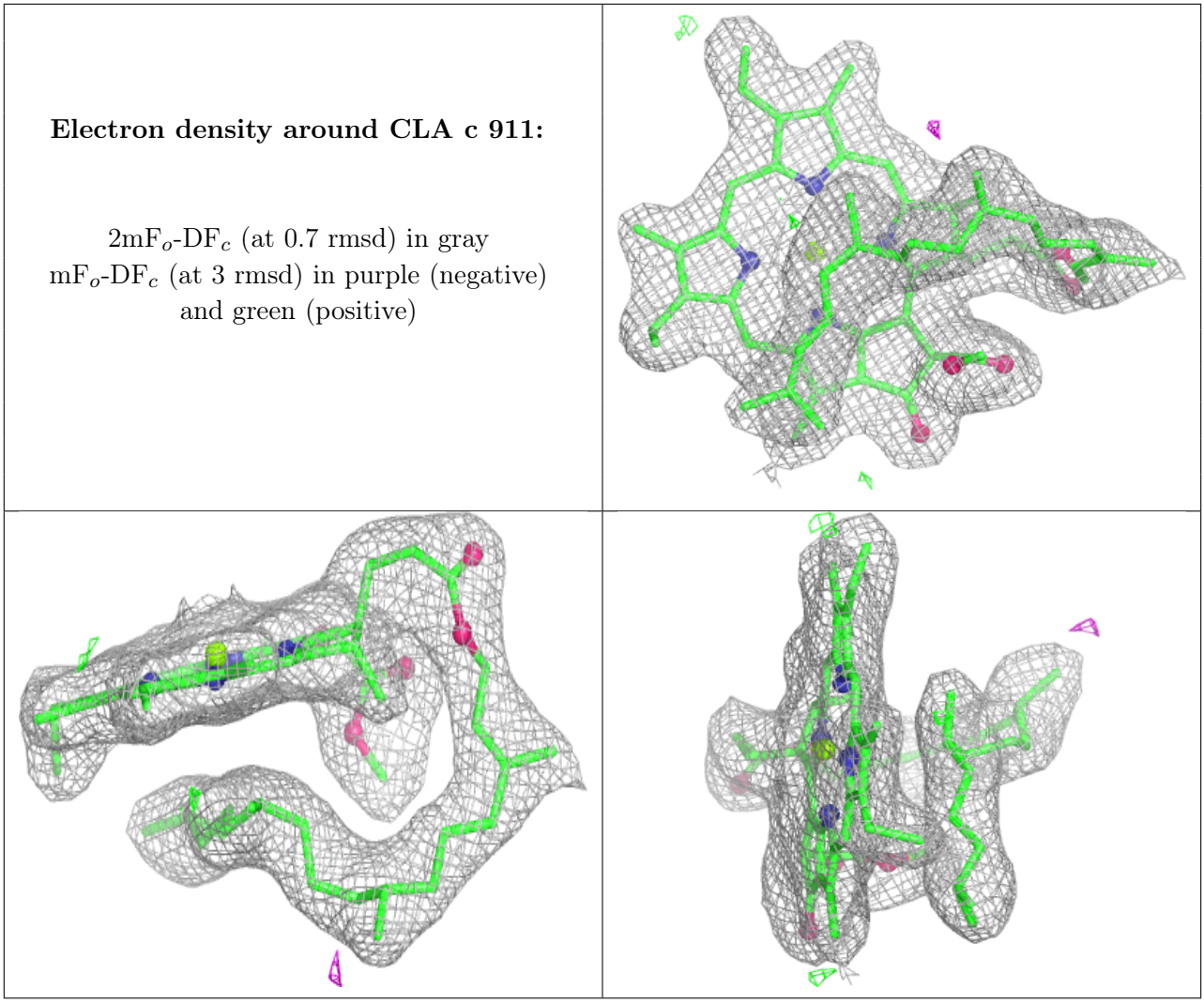
Electron density around HEM E 102:

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



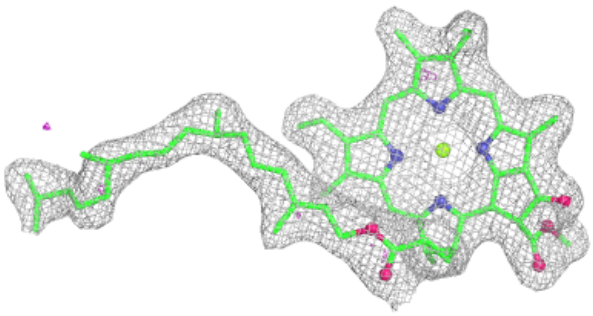
Electron density around CLA c 911:

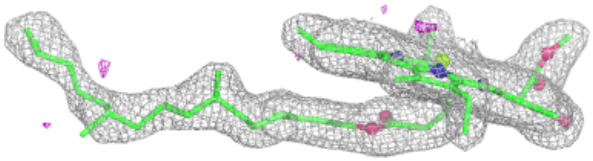
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

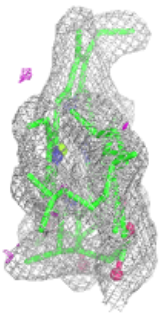


Electron density around CLA b 604:

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

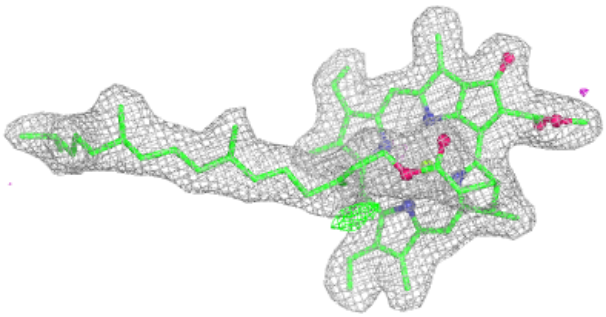


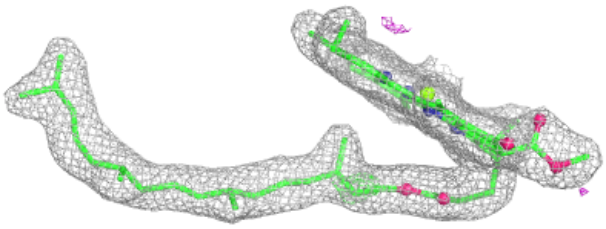




Electron density around CLA B 609:

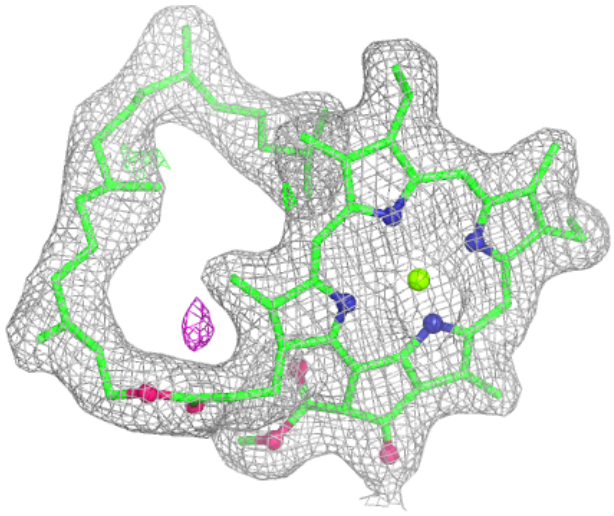
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

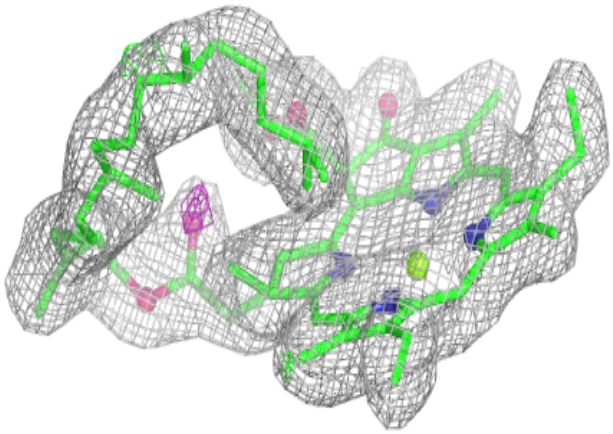


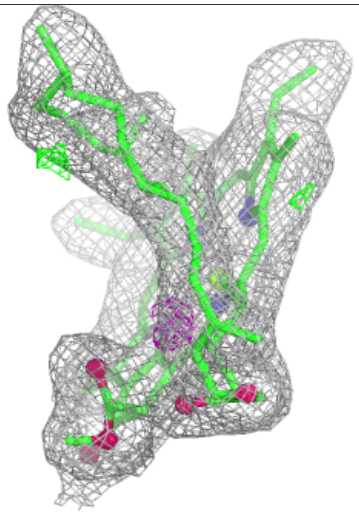


Electron density around CLA B 616:

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

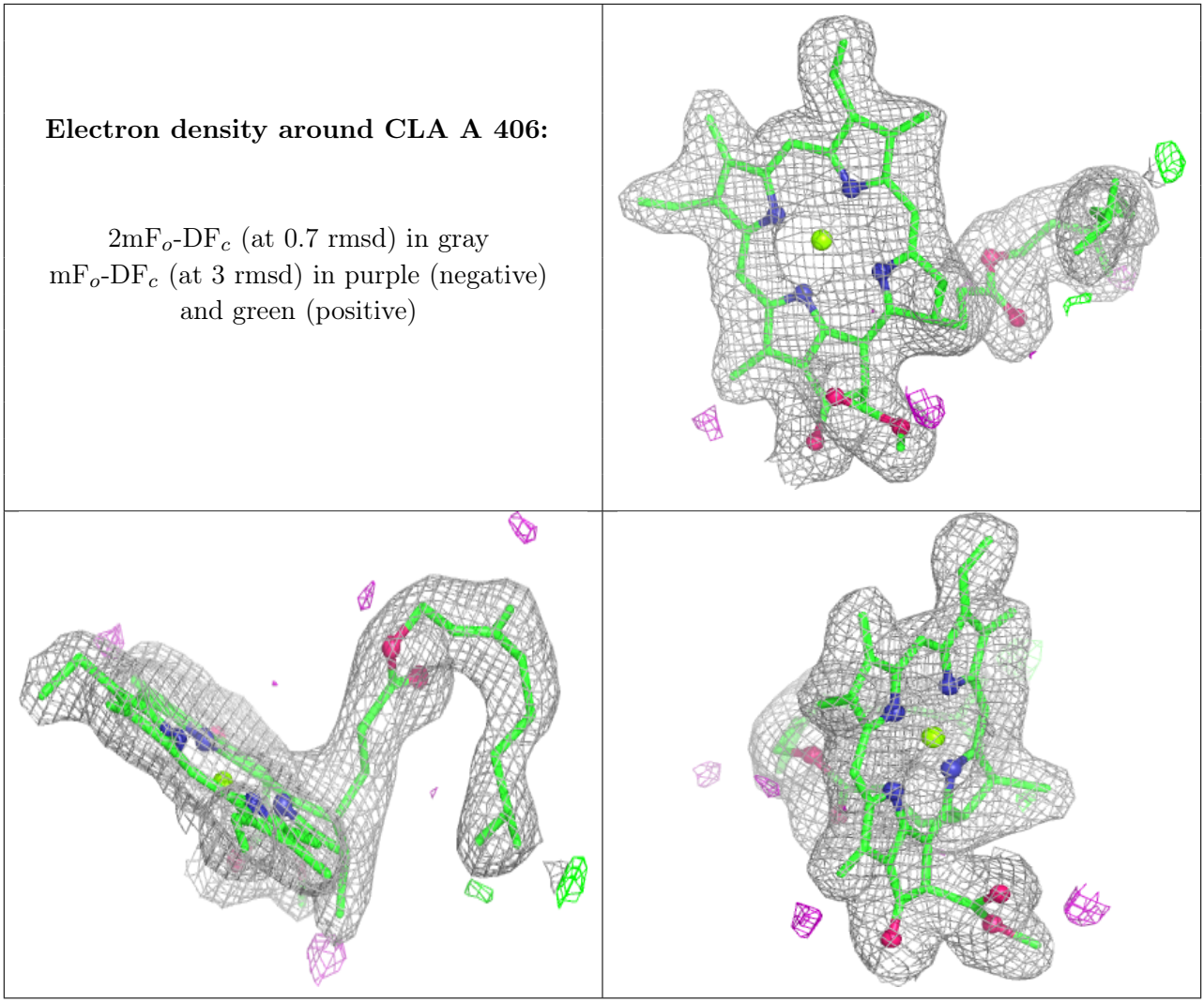






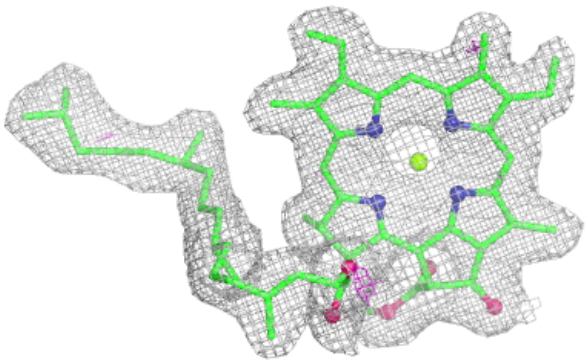
Electron density around CLA A 406:

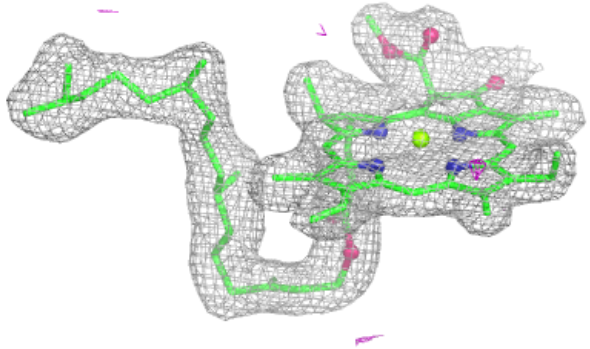
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

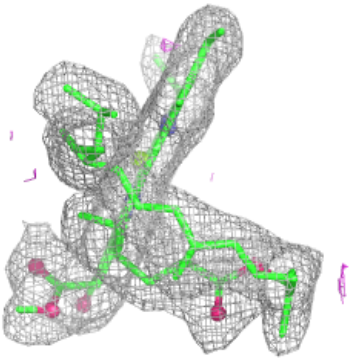


Electron density around CLA a 408:

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

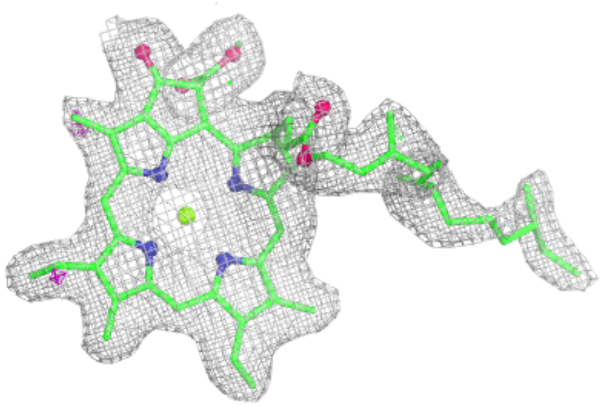


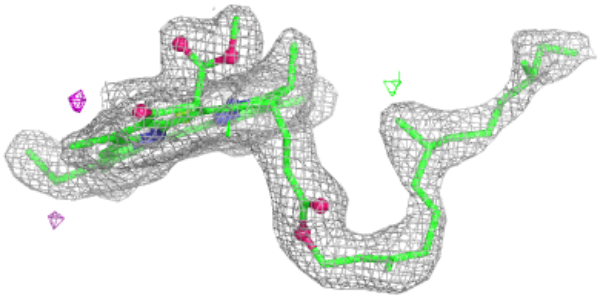


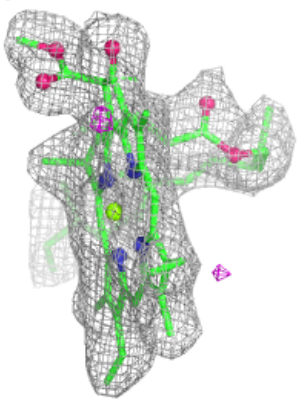


Electron density around CLA a 409:

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

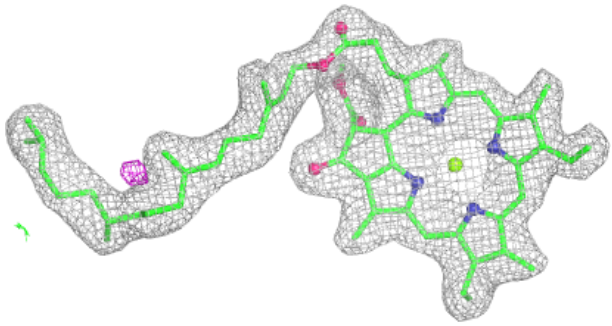


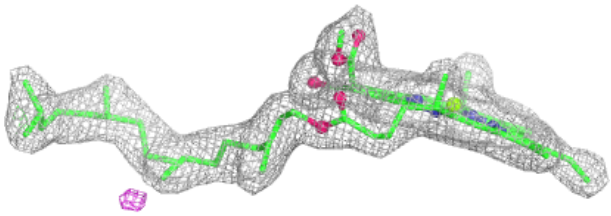




Electron density around CLA B 603:

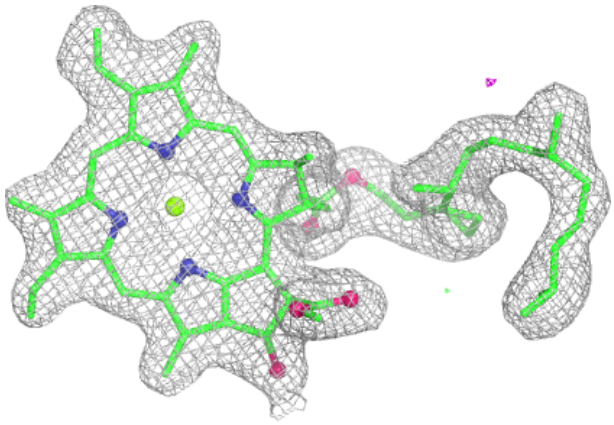
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

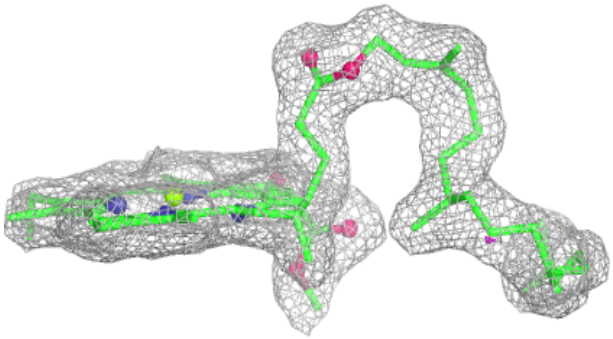


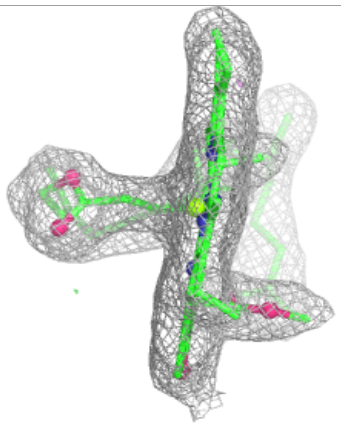


Electron density around CLA b 613:

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

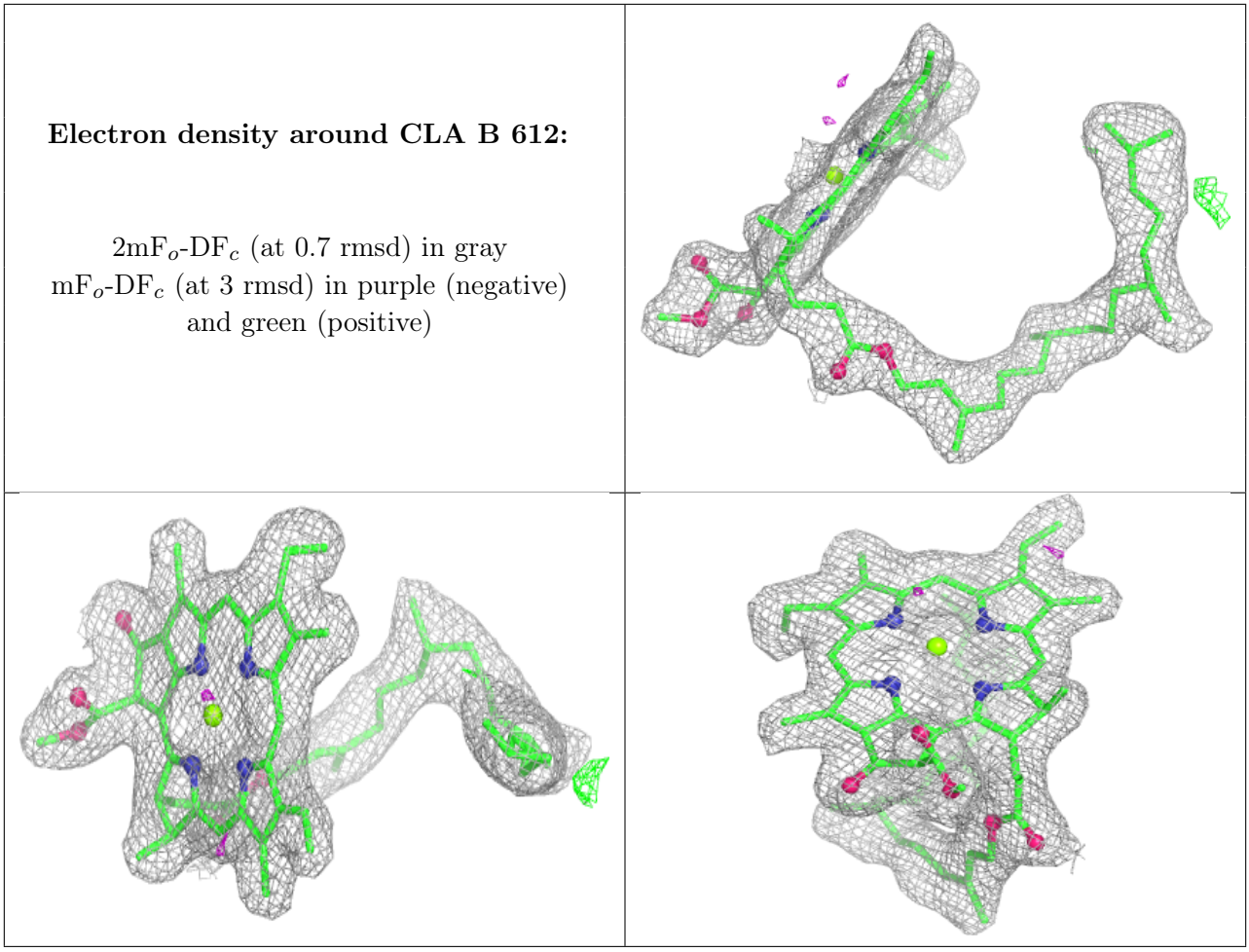






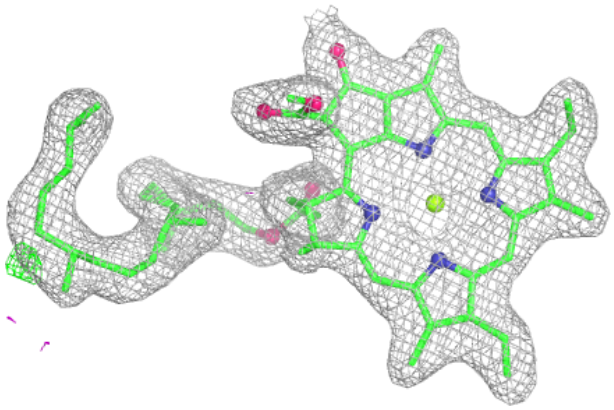
Electron density around CLA B 612:

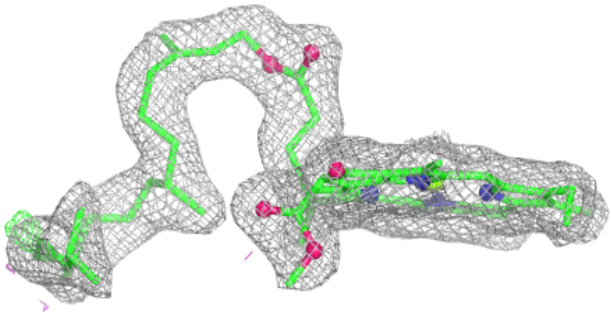
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

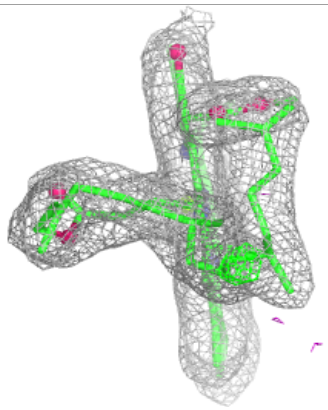


Electron density around CLA B 613:

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

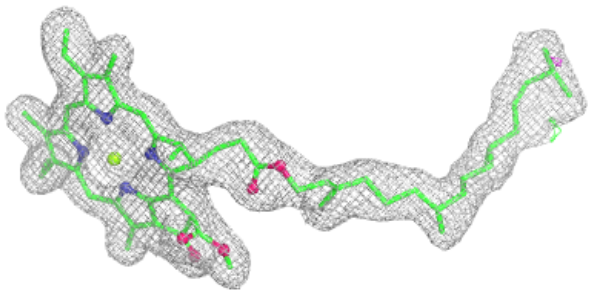


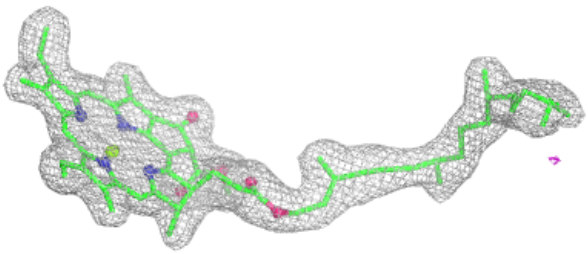


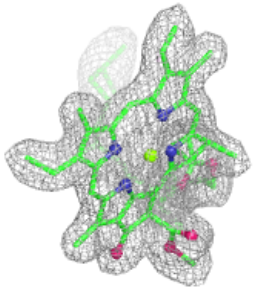


Electron density around CLA A 405:

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

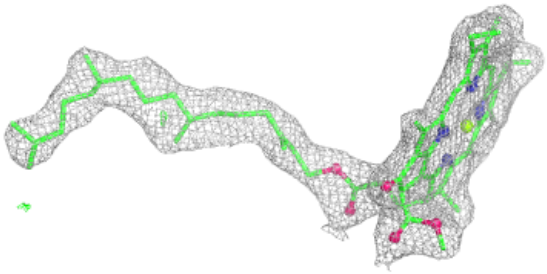


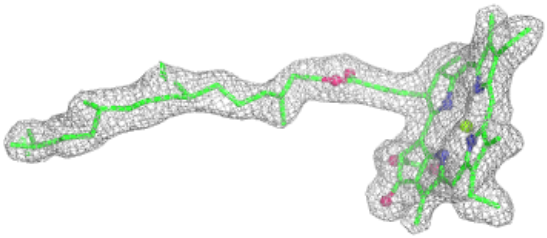


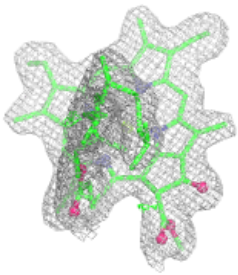


Electron density around CLA b 605:

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

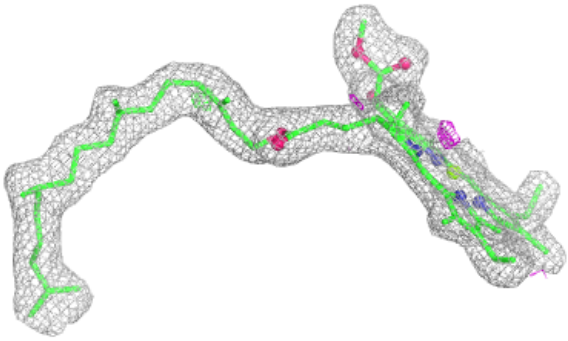


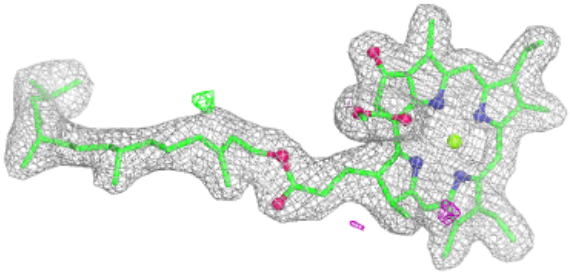


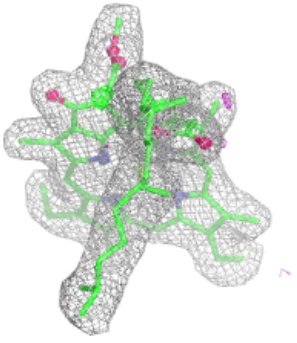


Electron density around CLA d 402:

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

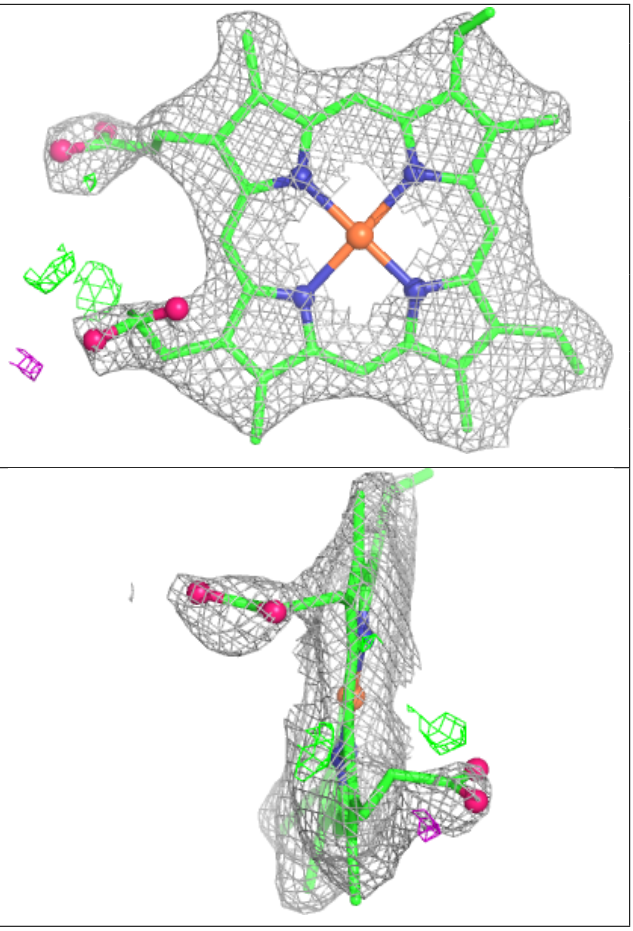






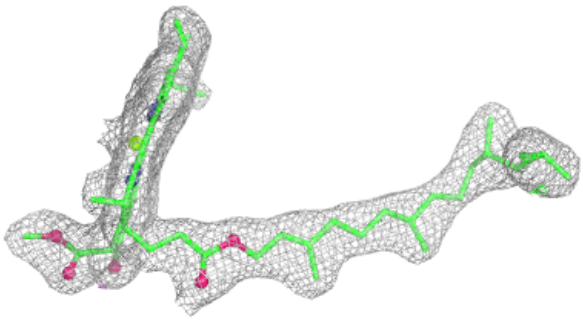
Electron density around HEM e 101:

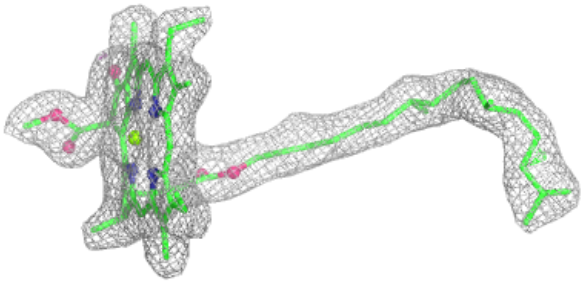
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

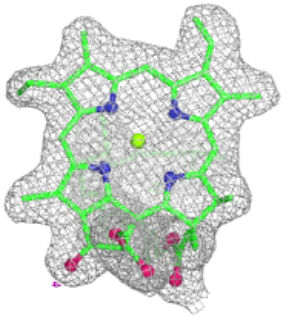


Electron density around CLA b 606:

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

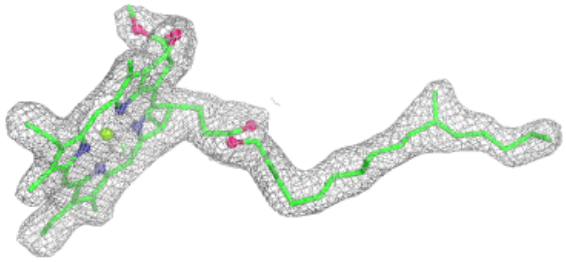


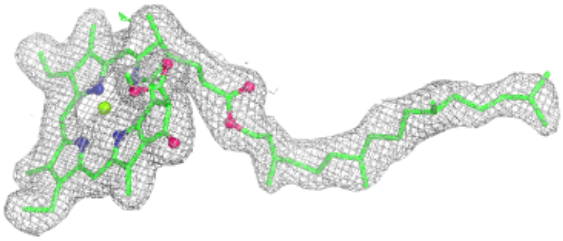


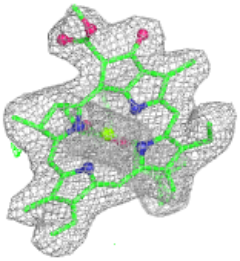


Electron density around CLA c 903:

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

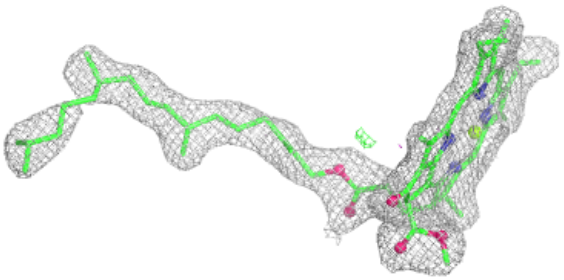


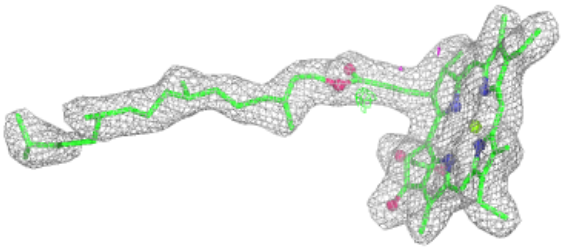


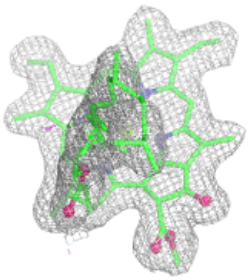


Electron density around CLA B 605:

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

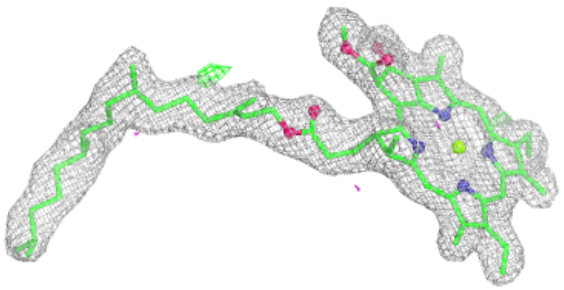


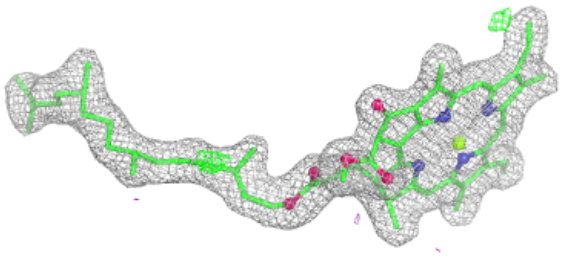


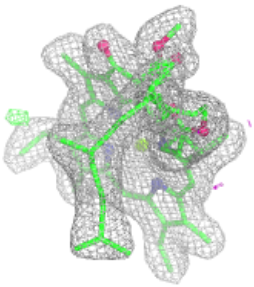


Electron density around CLA a 407:

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

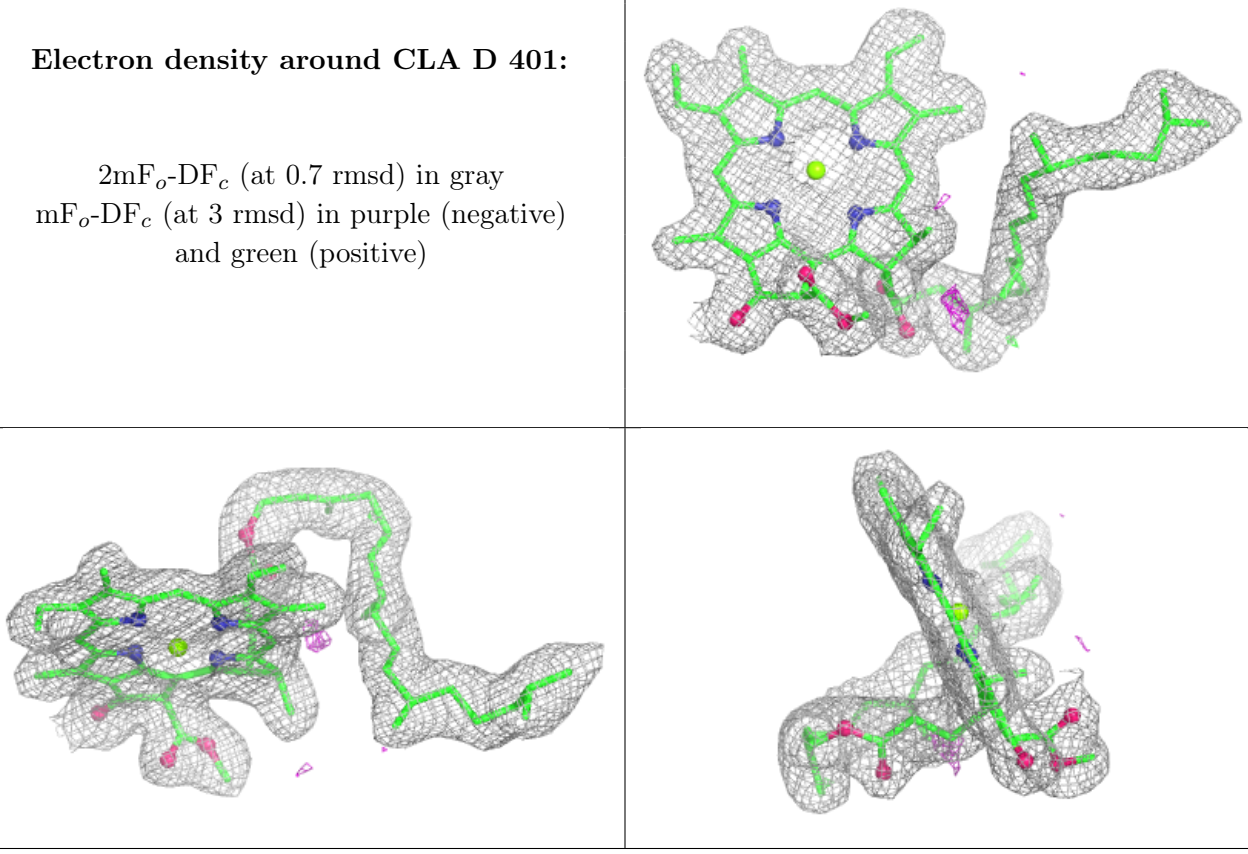






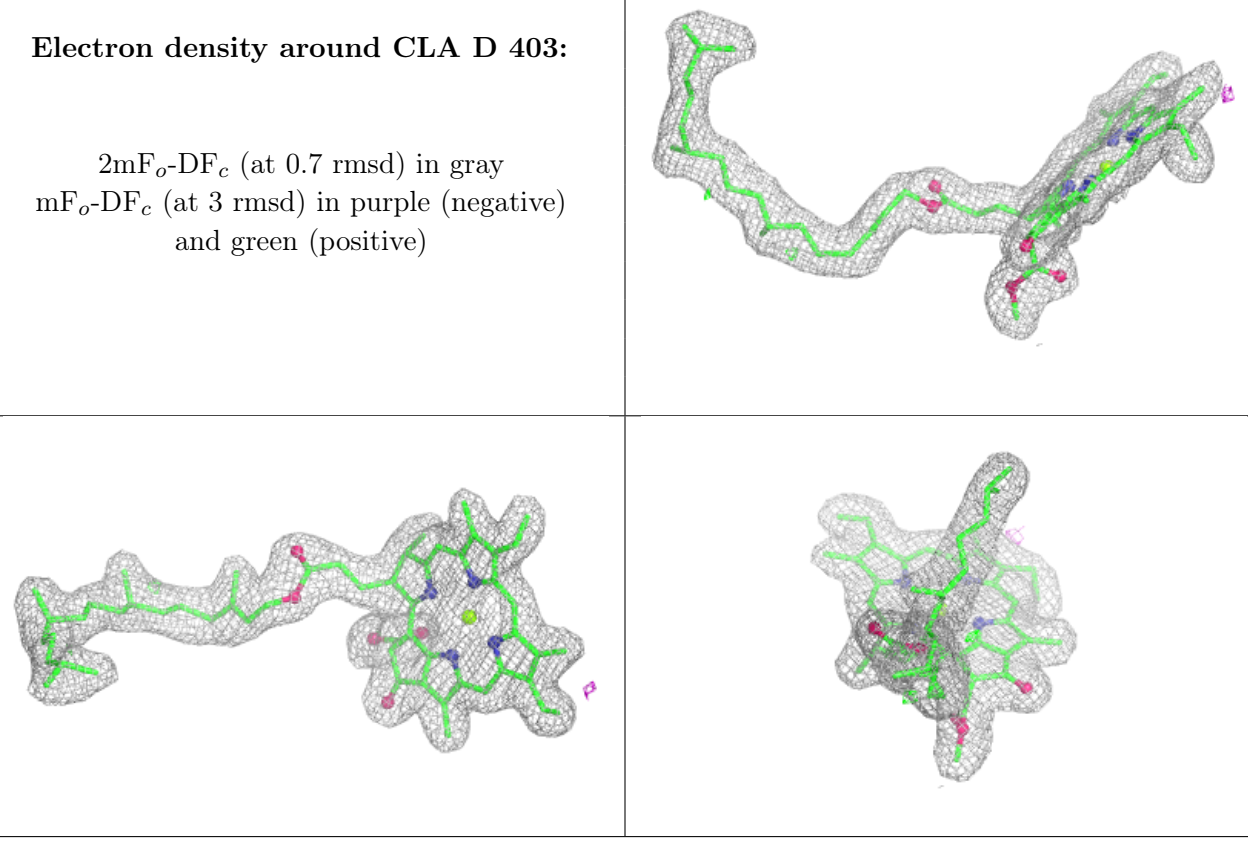
Electron density around CLA D 401:

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



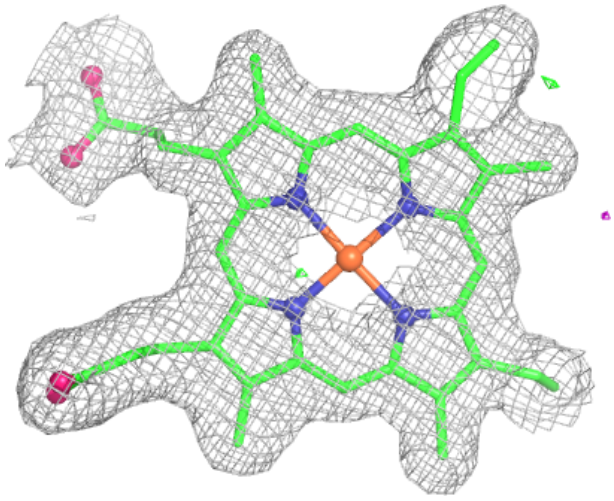
Electron density around CLA D 403:

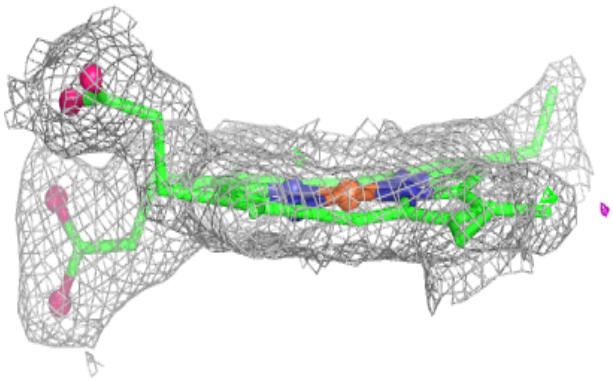
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

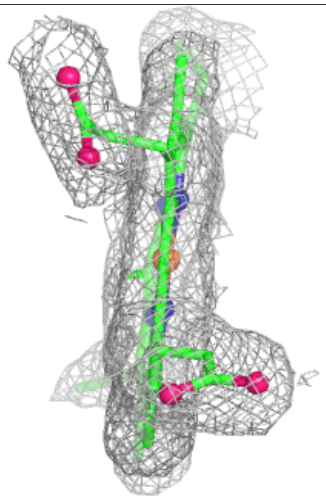


Electron density around HEC V 202:

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

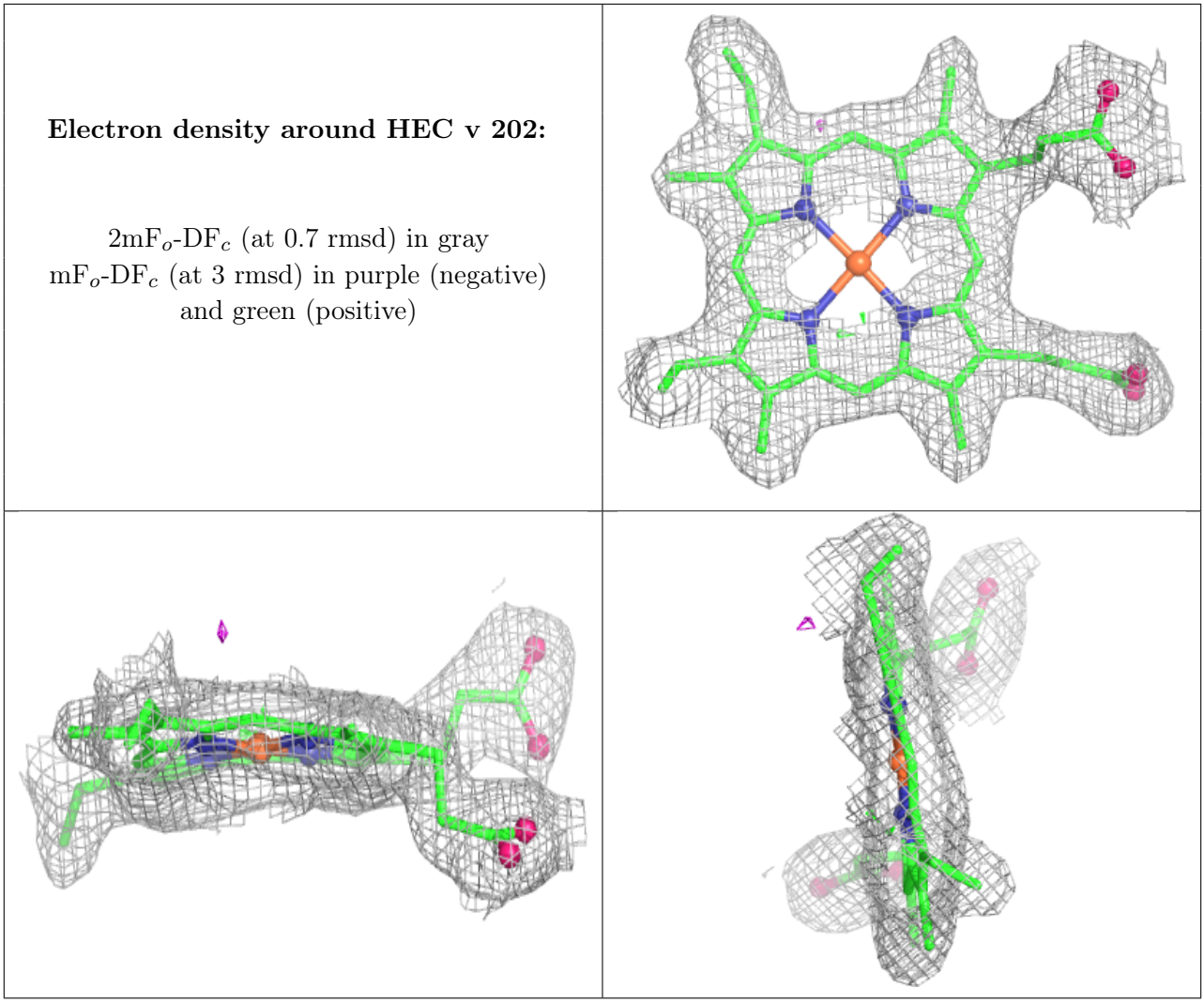






Electron density around HEC v 202:

$2mF_o$-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.