Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:30 PM UTC

PDB ID	:	7YQ2 / pdb_00007yq2
Title	:	Crystal structure of photosystem II expressing psbA2 gene only
Authors	:	Nakajima, Y.; Suga, M.; Shen, J.R.
Deposited on	:	2022-08-05
Resolution	:	1.90 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:

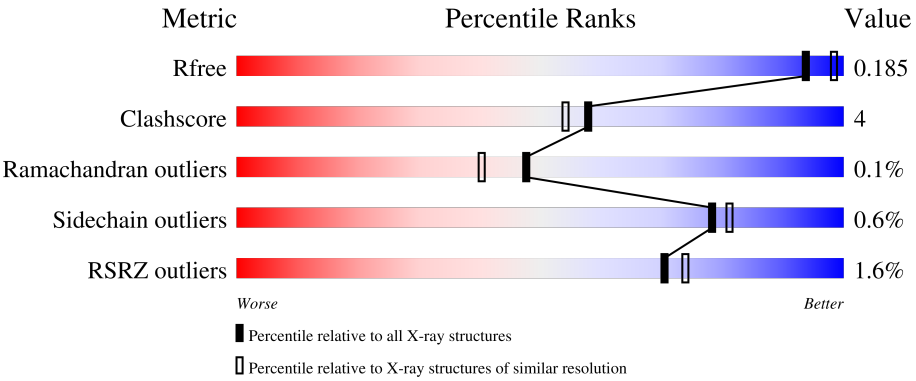
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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.



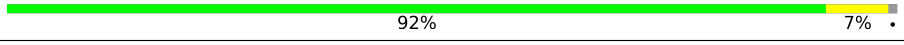
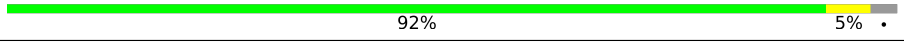
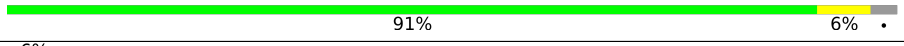
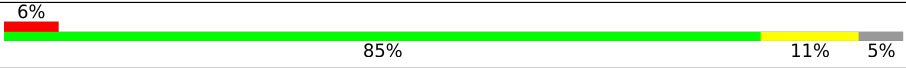
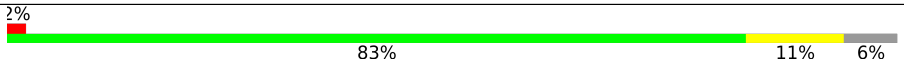
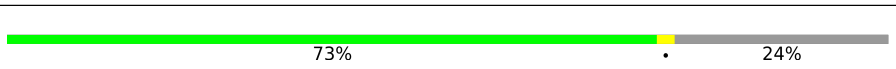
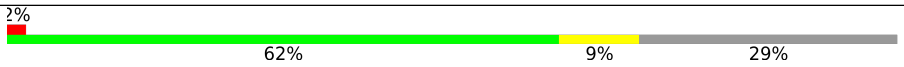
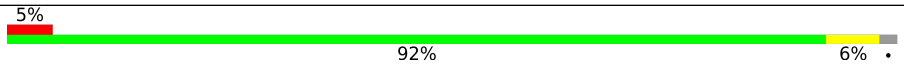
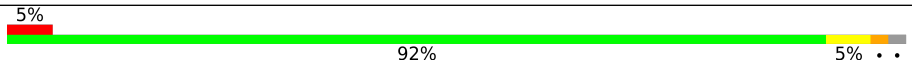
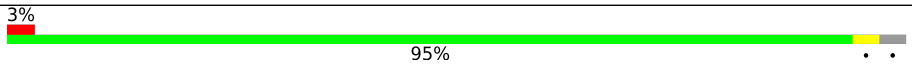
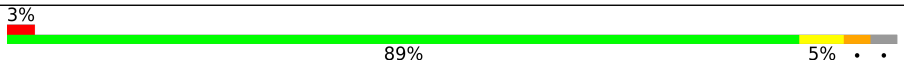
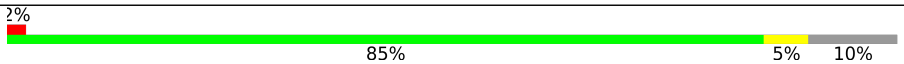
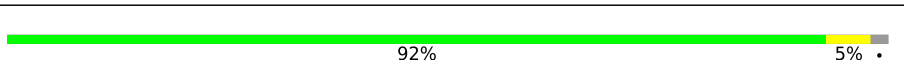
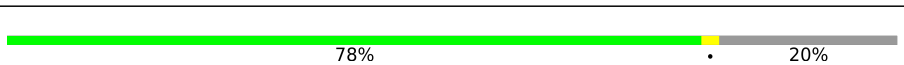
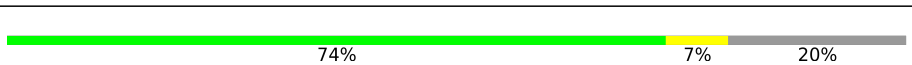
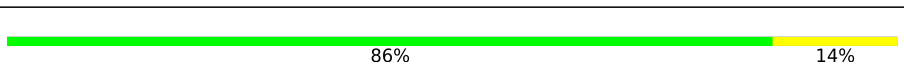
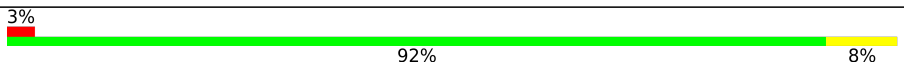
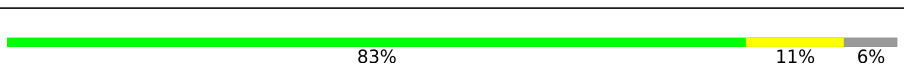
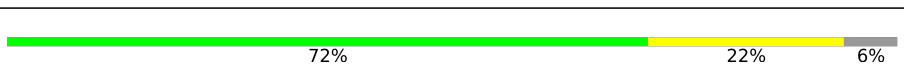
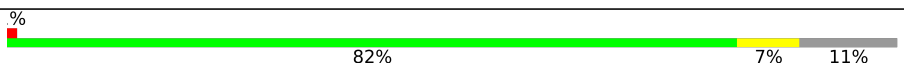
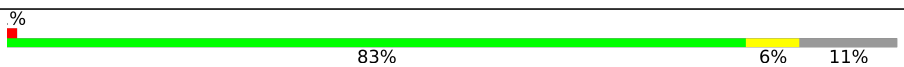
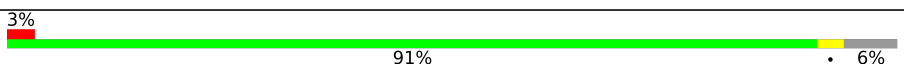
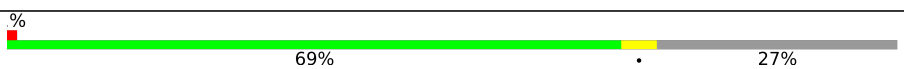
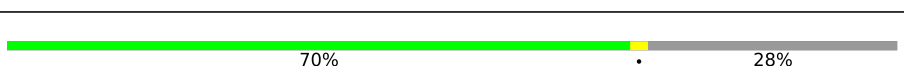
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	360	% 87% 6% 7%
1	a	360	% 85% 9% 7%
2	B	510	93% 6% •
2	b	510	3% 93% 6% •
3	C	461	92% 6% •

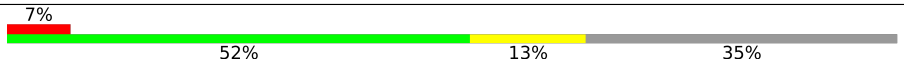
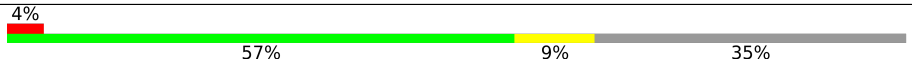
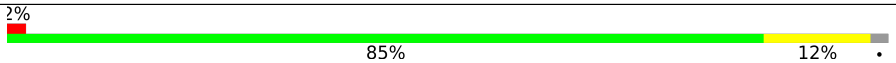
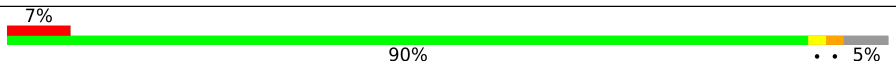
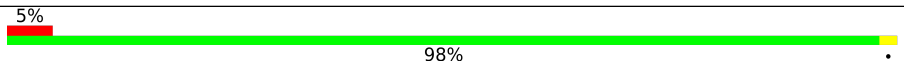
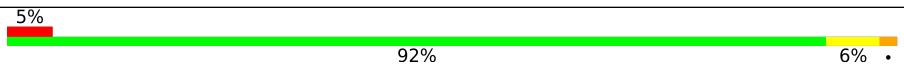
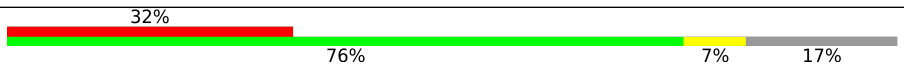
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	413	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	903	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	c	914	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 55630 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	2	0
			2607	1712	427	455	13			
1	a	336	Total	C	N	O	S	0	3	0
			2632	1727	431	461	13			

- 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	8	0
			3995	2623	665	694	13			
2	b	504	Total	C	N	O	S	0	9	0
			3961	2600	656	692	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	6	0
			3507	2295	586	613	13			
3	c	456	Total	C	N	O	S	0	3	0
			3532	2314	589	616	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2713	1799	439	463	12			
4	d	342	Total	C	N	O	S	0	2	0
			2724	1806	442	463	13			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total 629	C 413	N 102	O 114	0	1	0
5	e	79	Total 644	C 423	N 102	O 119	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total 275	C 187	N 45	O 42	S 1	0	0	0
6	f	32	Total 263	C 179	N 44	O 39	S 1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total 505	C 336	N 81	O 86	S 2	0	0	0
7	h	65	Total 516	C 343	N 85	O 86	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	37	Total 301	C 205	N 47	O 48	S 1	0	0	0
8	i	37	Total 297	C 203	N 47	O 46	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	39	Total 270	C 182	N 40	O 46	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 289	C 201	N 42	O 46	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total 289	C 201	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	37	Total 311	C 209	N 49	O 52	S 1	0	2	0
11	l	37	Total 305	C 205	N 48	O 51	S 1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total 270	C 182	N 39	O 48	S 1	0	1	0
12	m	34	Total 274	C 184	N 40	O 49	S 1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total 1895	C 1190	N 313	O 388	S 4	0	10	0
13	o	243	Total 1879	C 1177	N 311	O 387	S 4	0	5	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total 767	C 487	N 129	O 151	0	0	0
15	u	97	Total 774	C 491	N 129	O 154	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	4	0
			1089	691	181	213	4			
16	v	137	Total	C	N	O	S	0	2	0
			1070	678	178	210	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			218	144	35	36	3			
17	y	30	Total	C	N	O	S	0	1	0
			229	152	38	36	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	0	0	0
			286	191	46	49			
18	x	39	Total	C	N	O	0	0	0
			286	191	46	49			

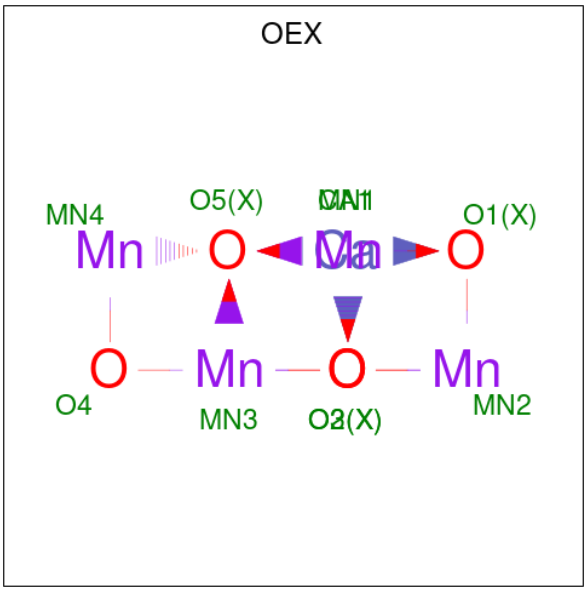
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			458	317	67	72	2			
19	z	62	Total	C	N	O	S	0	0	0
			455	312	67	74	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			228	150	41	37			

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

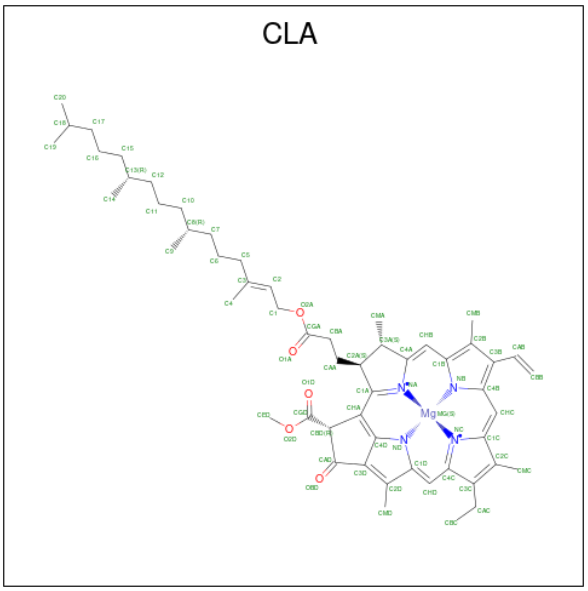
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

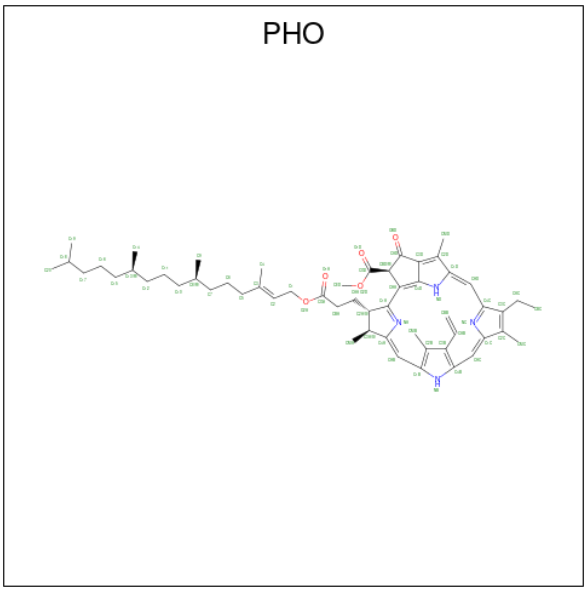
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

Continued on next page...

Continued from previous page...

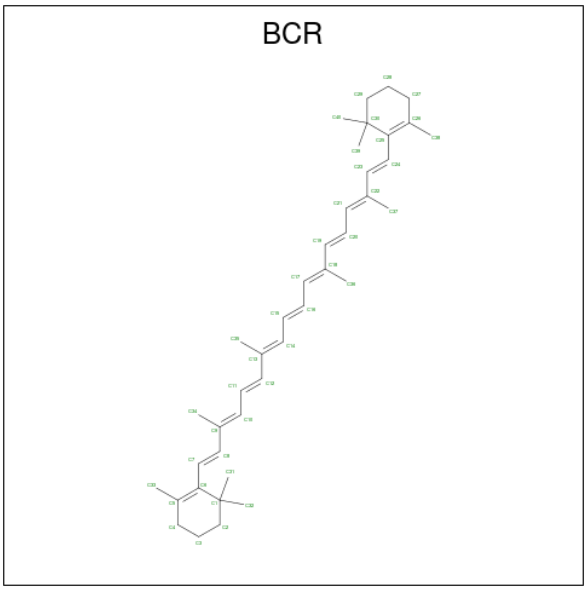
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



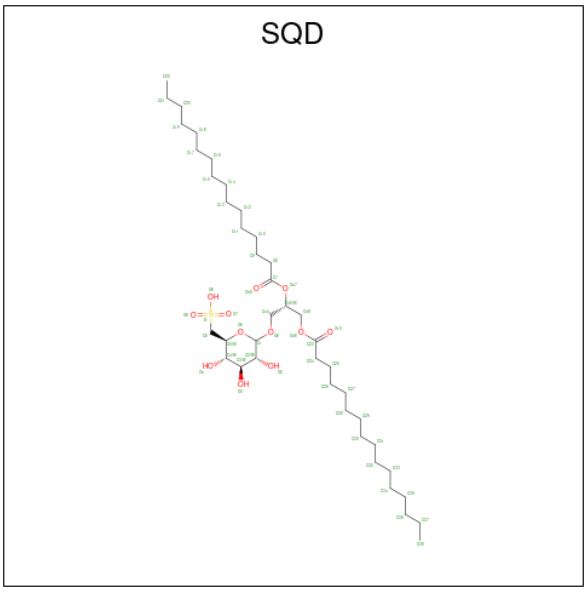
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



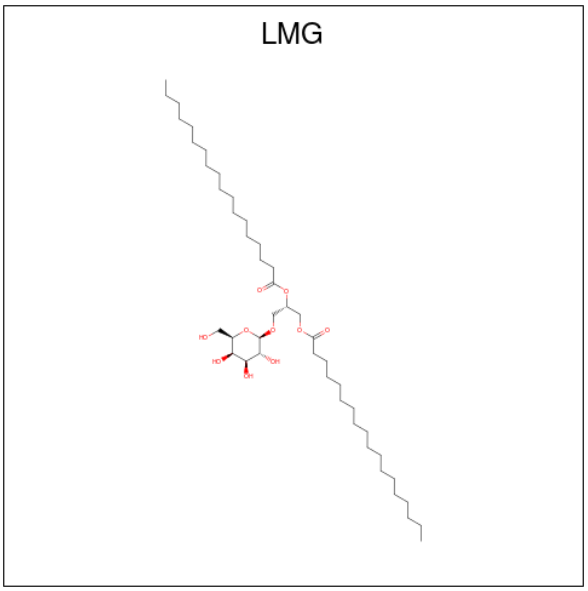
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

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



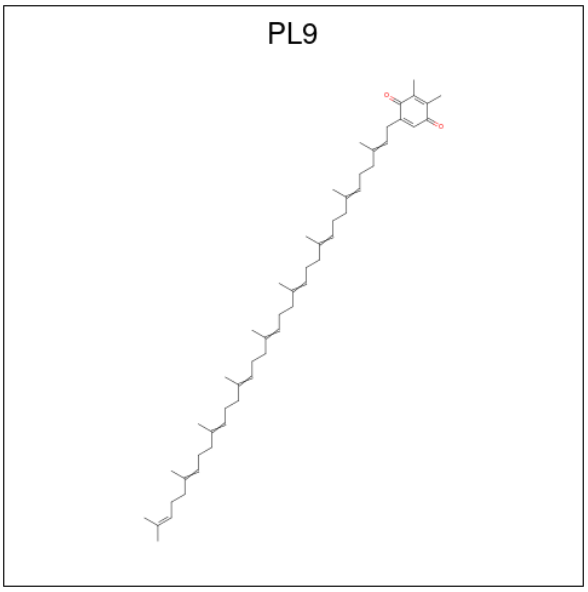
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			37	25	11	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		
27	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 51 41 10	0	0
28	B	1	Total C O 51 41 10	0	0
28	C	1	Total C O 51 41 10	0	0
28	C	1	Total C O 51 41 10	0	0
28	D	1	Total C O 51 41 10	0	0
28	a	1	Total C O 51 41 10	0	0
28	b	1	Total C O 51 41 10	0	0
28	c	1	Total C O 51 41 10	0	0
28	c	1	Total C O 51 41 10	0	0
28	d	1	Total C O 51 41 10	0	0

- Molecule 29 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



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

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

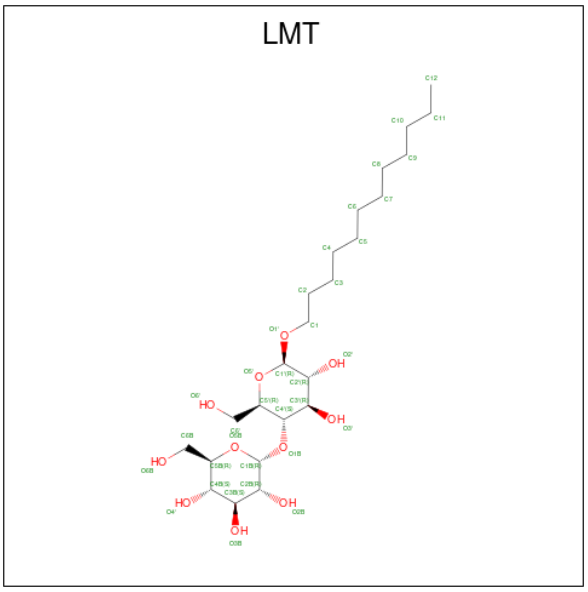
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	4	Total C O 57 52 5	0	0
30	B	4	Total C 24 24	0	0
30	C	3	Total C O 54 49 5	0	0
30	D	3	Total C O 60 55 5	0	0
30	E	4	Total C 22 22	0	0
30	H	2	Total C O 24 22 2	0	0
30	I	7	Total C 79 79	0	0
30	J	3	Total C 36 36	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	T	1	Total C 15 15	0	0
30	X	1	Total C 16 16	0	0
30	Z	3	Total C 20 20	0	0
30	a	2	Total C O 45 40 5	0	0
30	b	8	Total C O 87 85 2	0	0
30	c	6	Total C O 47 45 2	0	0
30	d	3	Total C O 65 58 7	0	0
30	e	2	Total C 15 15	0	0
30	h	3	Total C 29 29	0	0
30	i	5	Total C O 66 64 2	0	0
30	j	3	Total C 15 15	0	0
30	k	2	Total C O 39 34 5	0	0
30	l	1	Total C 13 13	0	0
30	m	1	Total C 11 11	0	0
30	t	1	Total C 12 12	0	0
30	y	1	Total C 4 4	0	0
30	x	4	Total C O 39 37 2	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



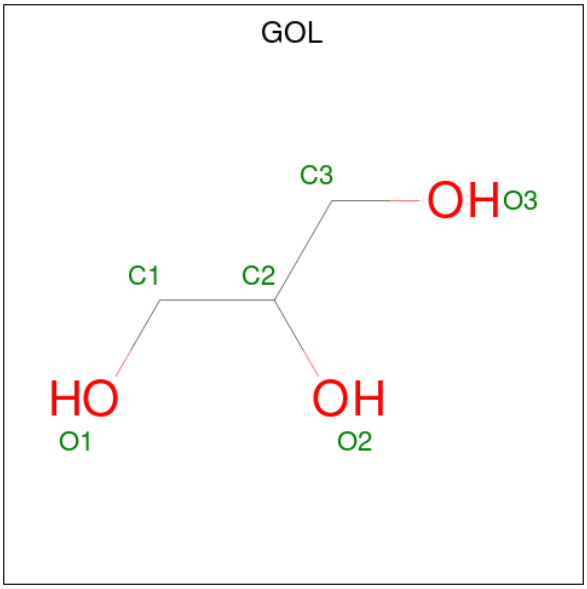
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total 35	C 24	O 11	0	0
31	A	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 24	C 18	O 6	0	0
31	F	1	Total 24	C 18	O 6	0	0
31	J	1	Total 24	C 18	O 6	0	0
31	M	1	Total 35	C 24	O 11	0	0
31	M	1	Total 25	C 19	O 6	0	0
31	Z	1	Total 35	C 24	O 11	0	0
31	a	1	Total 35	C 24	O 11	0	0
31	b	1	Total 35	C 24	O 11	0	0
31	c	1	Total 35	C 24	O 11	0	0
31	c	1	Total 35	C 24	O 11	0	0
31	e	1	Total 24	C 18	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	j	1	Total C O 24 18 6	0	0
31	m	1	Total C O 35 24 11	0	0
31	m	1	Total C O 35 24 11	0	0
31	t	1	Total C O 23 18 5	0	0
31	t	1	Total C O 35 24 11	0	0

- Molecule 32 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



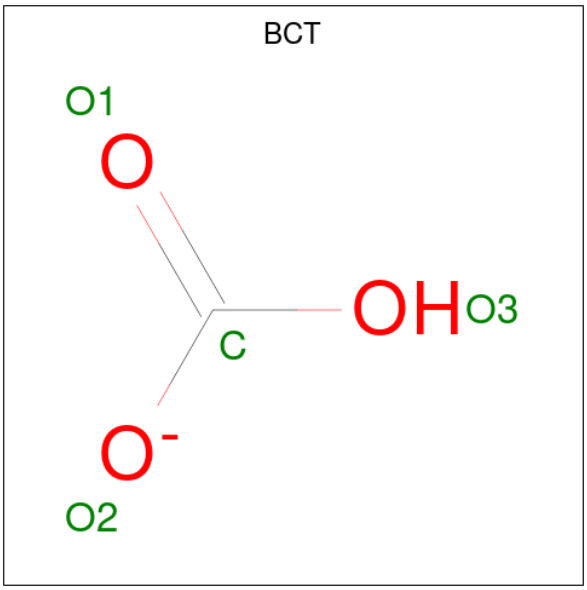
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 6 3 3	0	0
32	B	1	Total C O 6 3 3	0	0
32	B	1	Total C O 6 3 3	0	0
32	C	1	Total C O 6 3 3	0	0
32	O	1	Total C O 6 3 3	0	0
32	V	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

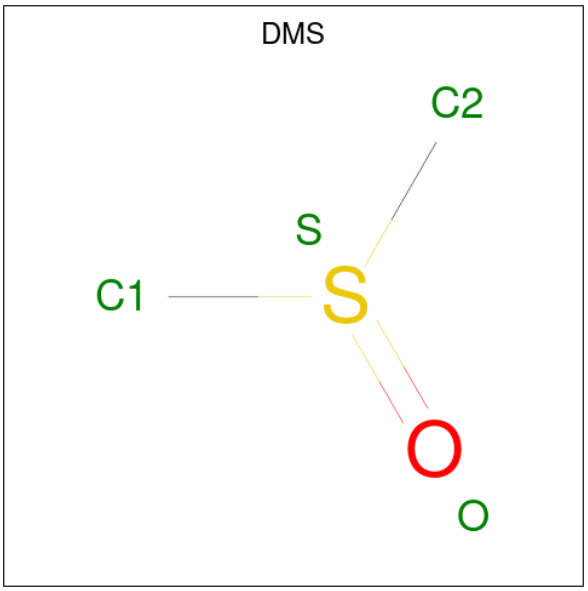
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	V	1	Total C O 6 3 3	0	0
32	a	1	Total C O 6 3 3	0	0
32	b	1	Total C O 6 3 3	0	0
32	c	1	Total C O 6 3 3	0	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 34 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	B	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	C	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	D	1	Total	C	O	S	0	0
			4	2	1	1		
34	H	1	Total	C	O	S	0	0
			4	2	1	1		
34	K	1	Total	C	O	S	0	0
			4	2	1	1		
34	L	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	O	1	Total	C	O	S	0	0
			4	2	1	1		
34	T	1	Total	C	O	S	0	0
			4	2	1	1		
34	U	1	Total	C	O	S	0	0
			4	2	1	1		
34	U	1	Total	C	O	S	0	0
			4	2	1	1		
34	U	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		
34	V	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

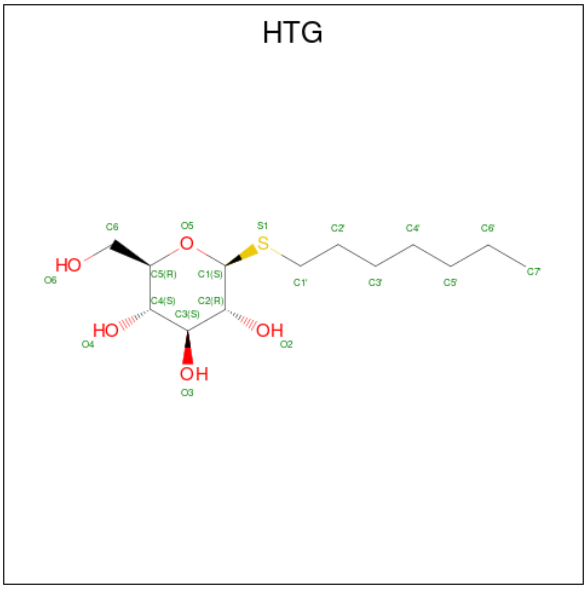
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0

Continued on next page...

Continued from previous page...

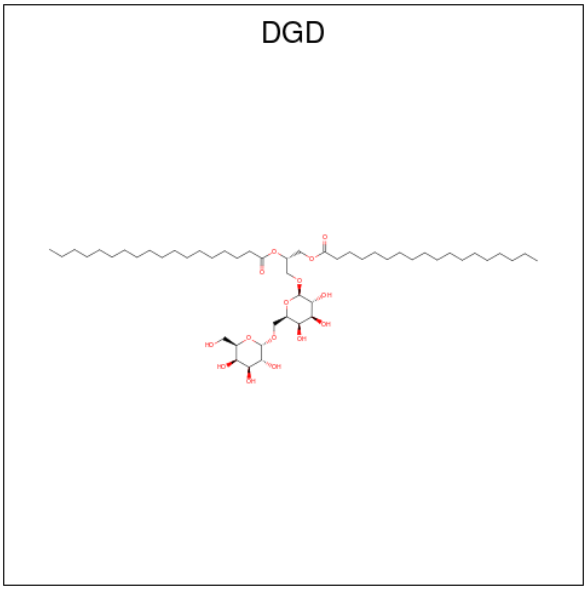
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	D	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	O	1	Total	C	O	S	0	0
			19	13	5	1		
36	U	1	Total	C			0	0
			4	4				
36	V	1	Total	C	O	S	0	0
			13	7	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			17	11	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	d	1	Total C O S 19 13 5 1	0	0
36	d	1	Total C O S 19 13 5 1	0	0
36	d	1	Total C O S 19 13 5 1	0	0
36	v	1	Total C O S 19 13 5 1	0	0
36	y	1	Total C O S 19 13 5 1	0	0

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



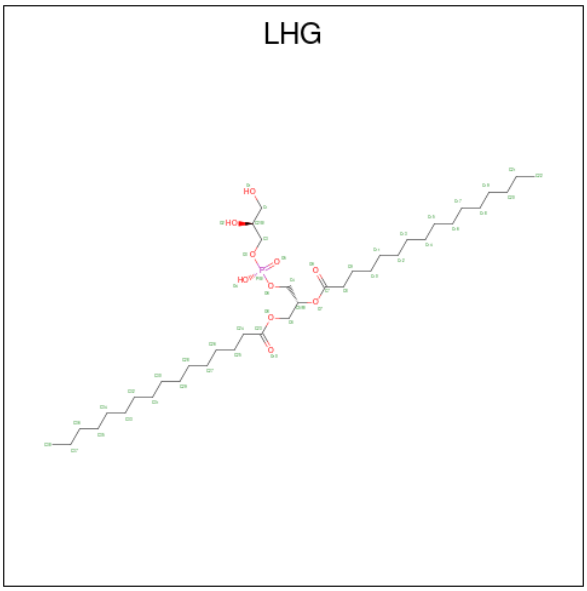
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	C	1	Total C O 62 47 15	0	0
37	C	1	Total C O 62 47 15	0	0
37	C	1	Total C O 62 47 15	0	0
37	D	1	Total C O 52 42 10	0	0
37	H	1	Total C O 62 47 15	0	0
37	c	1	Total C O 62 47 15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	c	1	Total C O 62 47 15	0	0
37	c	1	Total C O 62 47 15	0	0
37	d	1	Total C O 50 41 9	0	0
37	h	1	Total C O 62 47 15	0	0

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



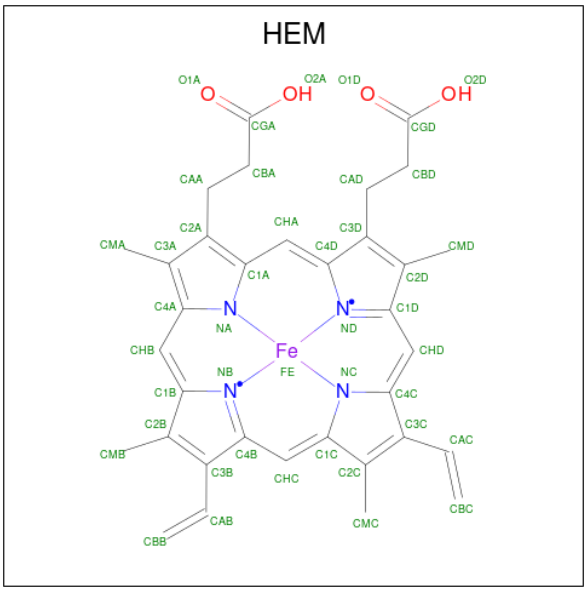
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 46 35 10 1	0	0
38	E	1	Total C O P 42 31 10 1	0	0
38	L	1	Total C O P 49 38 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0

Continued on next page...

Continued from previous page...

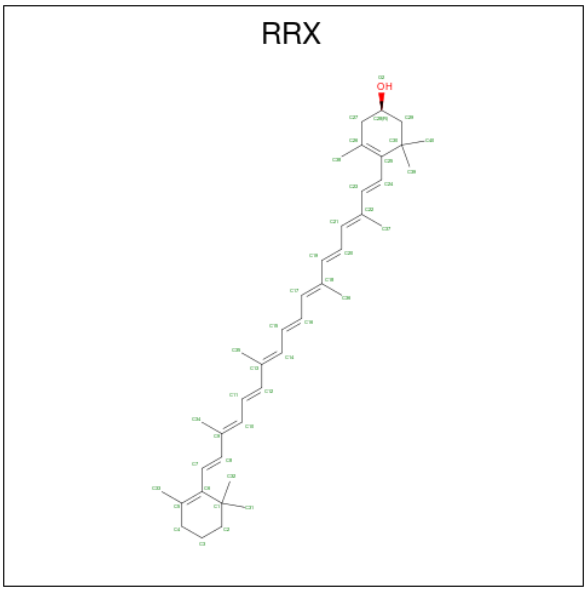
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	d	1	Total	C	O	P	0	0
			47	36	10	1		
38	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

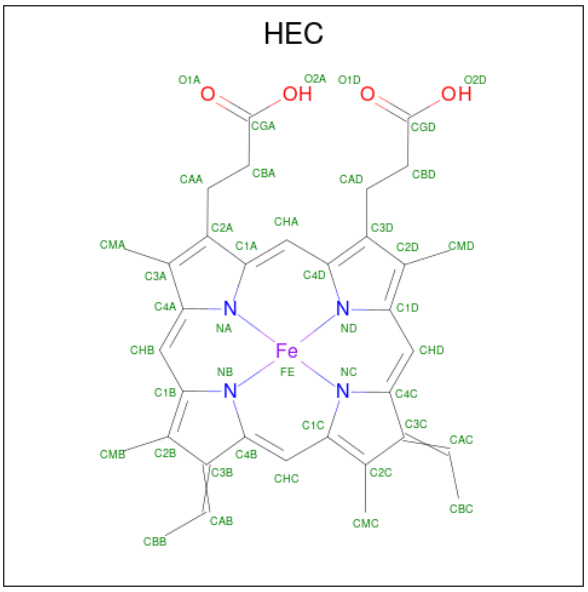


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	H	1	Total C O 41 40 1	0	0
40	h	1	Total C O 41 40 1	0	0

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 42 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
43	A	158	Total	O	0	1
			159	159		
43	B	406	Total	O	0	6
			411	411		
43	C	293	Total	O	0	2
			295	295		
43	D	173	Total	O	0	4
			177	177		
43	E	35	Total	O	0	0
			35	35		
43	F	15	Total	O	0	0
			15	15		
43	H	51	Total	O	0	0
			51	51		
43	I	11	Total	O	0	0
			11	11		
43	J	15	Total	O	0	0
			15	15		
43	K	9	Total	O	0	0
			9	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	L	16	Total O 16 16	0	0
43	M	20	Total O 20 20	0	0
43	O	217	Total O 224 224	0	7
43	T	14	Total O 14 14	0	0
43	U	116	Total O 117 117	0	1
43	V	153	Total O 157 157	0	4
43	Y	6	Total O 6 6	0	0
43	X	22	Total O 22 22	0	0
43	Z	4	Total O 4 4	0	0
43	a	157	Total O 159 159	0	2
43	b	394	Total O 399 399	0	5
43	c	316	Total O 320 320	0	5
43	d	170	Total O 172 172	0	2
43	e	38	Total O 39 39	0	1
43	f	12	Total O 12 12	0	0
43	h	51	Total O 52 52	0	1
43	i	12	Total O 12 12	0	0
43	j	12	Total O 12 12	0	0
43	k	6	Total O 6 6	0	0
43	l	20	Total O 20 20	0	0
43	m	20	Total O 20 20	0	0

Continued on next page...

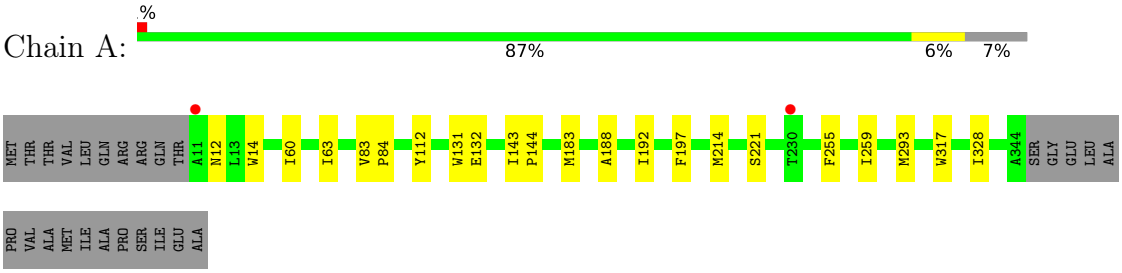
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	o	194	Total O 198 198	0	4
43	t	23	Total O 24 24	0	1
43	u	117	Total O 119 119	0	2
43	v	116	Total O 118 118	0	2
43	y	8	Total O 8 8	0	0
43	x	14	Total O 14 14	0	0
43	z	6	Total O 6 6	0	0

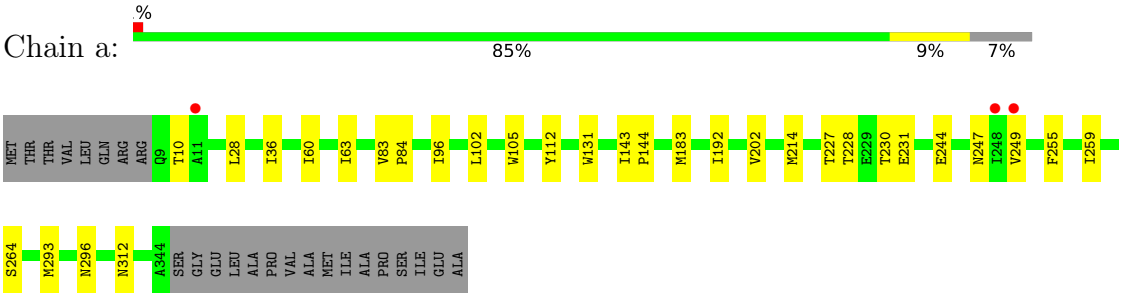
3 Residue-property plots (i)

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.

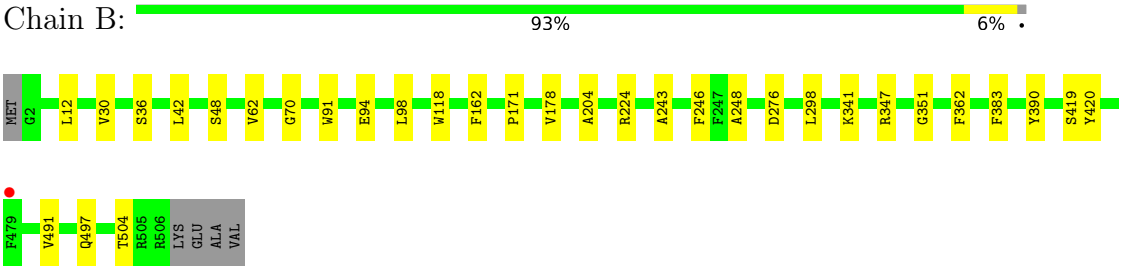
• Molecule 1: Photosystem II protein D1 2



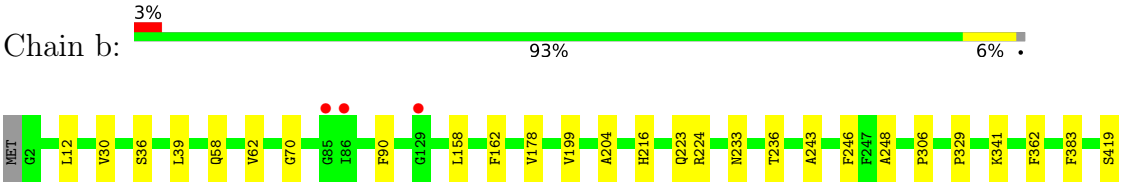
• Molecule 1: Photosystem II protein D1 2

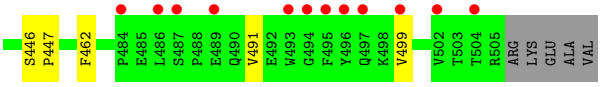


• Molecule 2: Photosystem II CP47 reaction center protein



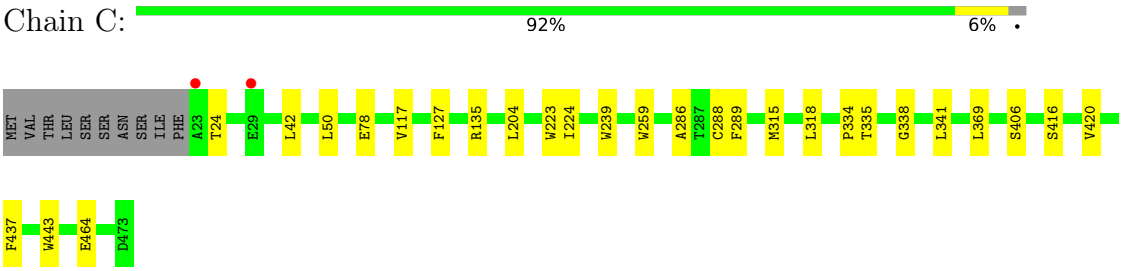
• Molecule 2: Photosystem II CP47 reaction center protein





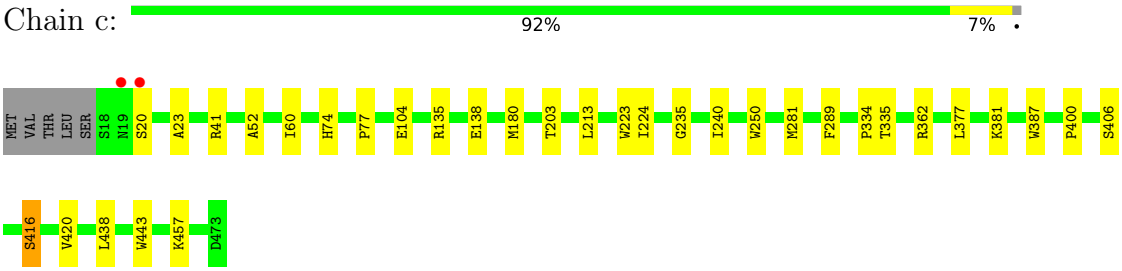
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



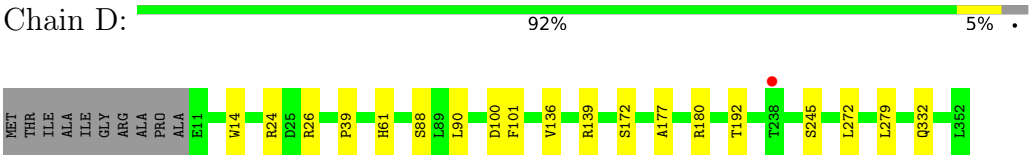
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



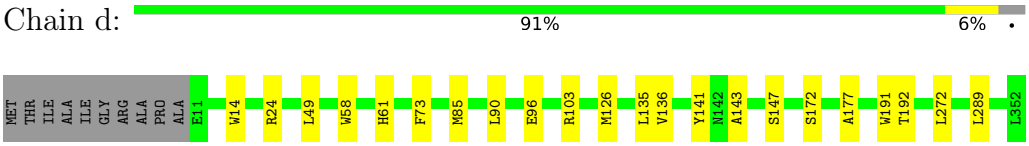
• Molecule 4: Photosystem II D2 protein

Chain D:



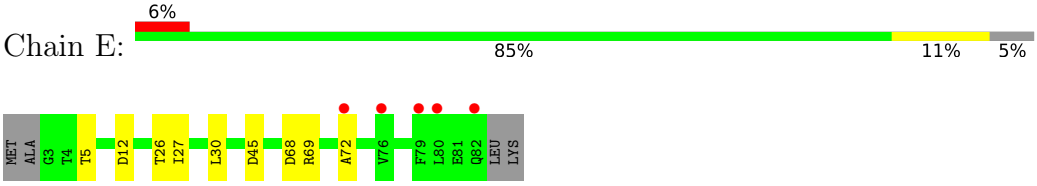
• Molecule 4: Photosystem II D2 protein

Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

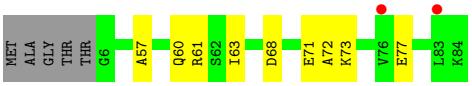
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

Chain e:





• Molecule 6: Cytochrome b559 subunit beta

Chain F:

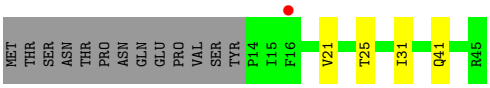




• Molecule 6: Cytochrome b559 subunit beta

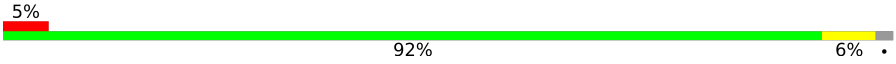
Chain f:





• Molecule 7: Photosystem II reaction center protein H

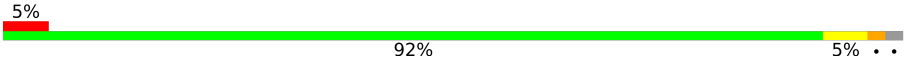
Chain H:

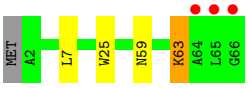




• Molecule 7: Photosystem II reaction center protein H

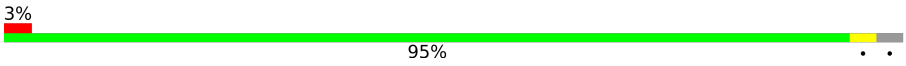
Chain h:





• Molecule 8: Photosystem II reaction center protein I

Chain I:

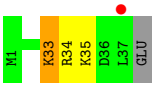




• Molecule 8: Photosystem II reaction center protein I

Chain i:

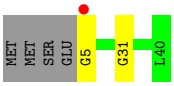




• Molecule 9: Photosystem II reaction center protein J

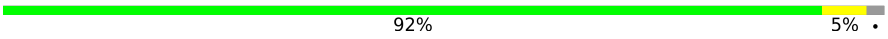
Chain J:

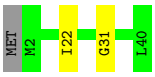




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

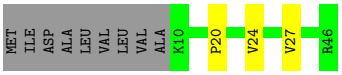




• Molecule 10: Photosystem II reaction center protein K

Chain k:

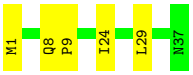




• Molecule 11: Photosystem II reaction center protein L

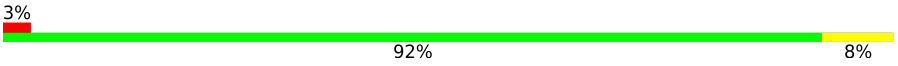
Chain L:

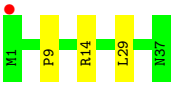




• Molecule 11: Photosystem II reaction center protein L

Chain l:

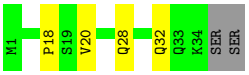




• Molecule 12: Photosystem II reaction center protein M

Chain M:

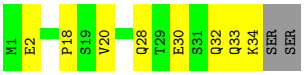




• Molecule 12: Photosystem II reaction center protein M

Chain m:

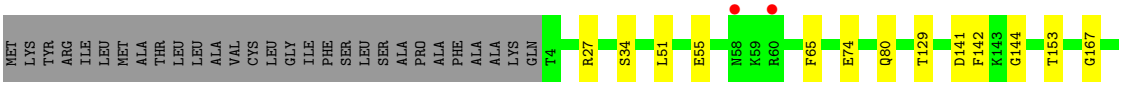




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



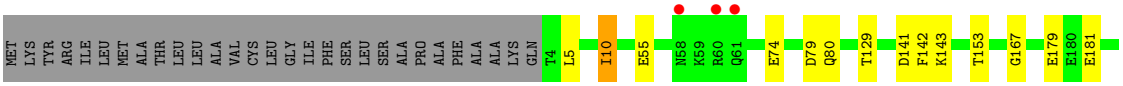


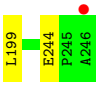


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

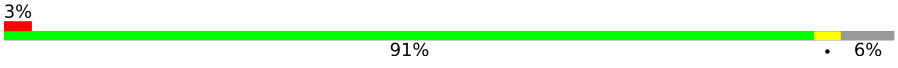


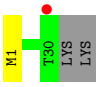




• Molecule 14: Photosystem II reaction center protein T

Chain T:

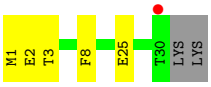




• Molecule 14: Photosystem II reaction center protein T

Chain t:

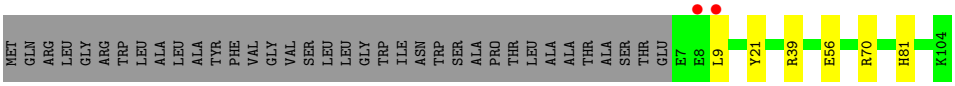




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

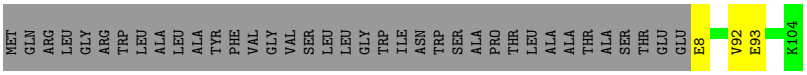




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:

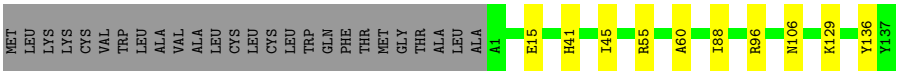




• Molecule 16: Cytochrome c-550

Chain V:

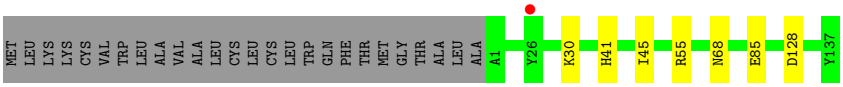




• Molecule 16: Cytochrome c-550

Chain v:

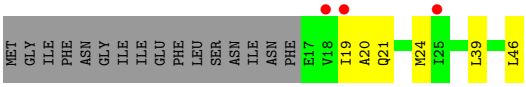




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:

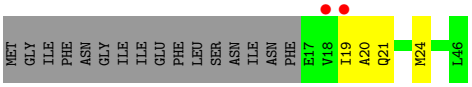




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:

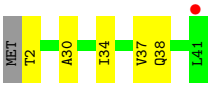




• Molecule 18: Photosystem II reaction center X protein

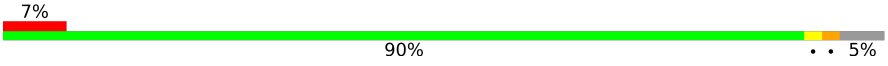
Chain X:





• Molecule 18: Photosystem II reaction center X protein

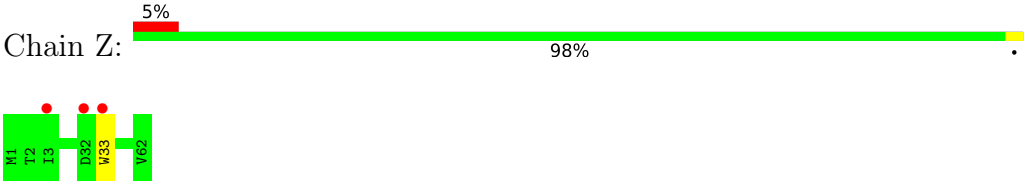
Chain x:





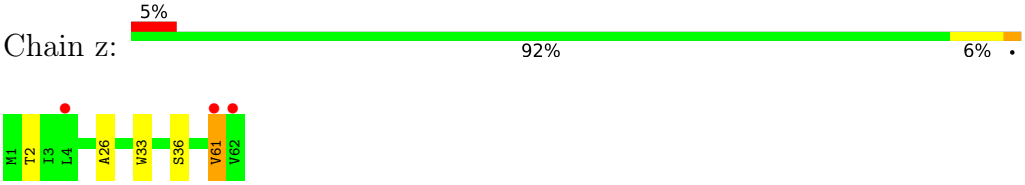
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



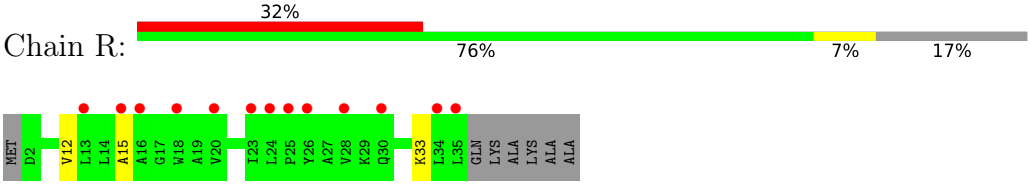
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.14Å 228.17Å 286.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.90) 99.6 (20.00-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, REFMAC 5.8.0103	Depositor
R, R_{free}	0.151 , 0.184 0.151 , 0.185	Depositor DCC
R_{free} test set	31121 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 76.4	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	0.98	EDS
Total number of atoms	55630	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.38	0/2693	0.53	0/3680
1	a	0.37	0/2723	0.52	0/3719
2	B	0.34	0/4156	0.51	2/5665 (0.0%)
2	b	0.32	0/4122	0.48	0/5623
3	C	0.30	0/3638	0.46	0/4954
3	c	0.29	0/3655	0.46	0/4976
4	D	0.38	0/2811	0.51	0/3833
4	d	0.36	0/2825	0.49	0/3850
5	E	0.26	0/651	0.43	0/892
5	e	0.22	0/669	0.41	0/913
6	F	0.25	0/284	0.43	0/387
6	f	0.27	0/274	0.47	0/372
7	H	0.26	0/518	0.44	0/706
7	h	0.24	0/532	0.42	0/723
8	I	0.21	0/298	0.39	0/403
8	i	0.24	0/294	0.41	0/398
9	J	0.24	0/257	0.43	0/349
9	j	0.24	0/276	0.42	0/374
10	K	0.24	0/299	0.42	0/412
10	k	0.23	0/299	0.39	0/412
11	L	0.40	0/324	0.48	0/441
11	l	0.37	0/315	0.47	0/428
12	M	0.34	0/266	0.49	0/363
12	m	0.31	0/270	0.47	0/368
13	O	0.30	0/1956	0.50	0/2653
13	o	0.29	0/1925	0.50	0/2611
14	T	0.37	0/266	0.42	0/362
14	t	0.35	0/266	0.43	0/362
15	U	0.31	0/778	0.49	0/1057
15	u	0.32	0/785	0.47	0/1064
16	V	0.32	0/1122	0.46	0/1522

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.24	0/1097	0.42	0/1491
17	Y	0.20	0/219	0.34	0/294
17	y	0.19	0/233	0.36	0/312
18	X	0.19	0/289	0.31	0/391
18	x	0.18	0/289	0.33	0/391
19	Z	0.19	0/459	0.33	0/630
19	z	0.16	0/456	0.28	0/626
20	R	0.18	0/232	0.37	0/321
All	All	0.32	0/42821	0.48	2/58328 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	48	SER	CA-C-N	-7.62	115.57	122.28
2	B	48	SER	C-N-CA	-7.62	115.57	122.28

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	2607	0	2508	15	0
1	a	2632	0	2551	21	0
2	B	3995	0	3853	28	0
2	b	3961	0	3794	25	0
3	C	3507	0	3436	23	0
3	c	3532	0	3456	30	0
4	D	2713	0	2606	16	0
4	d	2724	0	2626	19	0
5	E	629	0	601	8	0
5	e	644	0	619	8	0
6	F	275	0	282	1	0
6	f	263	0	277	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	505	0	514	6	0
7	h	516	0	536	4	0
8	I	301	0	320	0	0
8	i	297	0	316	2	0
9	J	251	0	257	2	0
9	j	270	0	273	2	0
10	K	289	0	294	1	0
10	k	289	0	294	2	0
11	L	311	0	331	5	0
11	l	305	0	323	4	0
12	M	270	0	293	5	0
12	m	274	0	299	7	0
13	O	1895	0	1877	16	0
13	o	1879	0	1848	11	0
14	T	264	0	267	0	0
14	t	264	0	267	4	0
15	U	767	0	756	6	0
15	u	774	0	773	2	0
16	V	1089	0	1104	9	0
16	v	1070	0	1070	5	0
17	Y	218	0	241	4	0
17	y	229	0	263	2	0
18	X	286	0	309	4	0
18	x	286	0	314	2	0
19	Z	458	0	479	1	0
19	z	455	0	463	3	0
20	R	228	0	201	3	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	260	0	288	11	0
24	B	1040	0	1152	35	0
24	C	845	0	936	36	0
24	D	130	0	144	1	0
24	a	195	0	216	10	0
24	b	1040	0	1152	33	0
24	c	845	0	936	22	0
24	d	195	0	216	4	0
25	A	128	0	148	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	a	128	0	148	2	0
26	A	40	0	56	0	0
26	B	160	0	224	10	0
26	C	80	0	112	4	0
26	D	40	0	56	0	0
26	K	40	0	56	1	0
26	T	40	0	56	4	0
26	Y	40	0	56	2	0
26	a	40	0	56	2	0
26	b	120	0	168	7	0
26	c	80	0	112	4	0
26	d	40	0	56	2	0
26	k	80	0	112	2	0
27	A	108	0	156	2	0
27	F	37	0	46	2	0
27	a	108	0	156	9	0
27	b	54	0	78	1	0
27	f	43	0	53	0	0
27	l	54	0	78	1	0
28	A	51	0	72	3	0
28	B	51	0	72	1	0
28	C	102	0	144	6	0
28	D	51	0	72	1	0
28	a	51	0	72	1	0
28	b	51	0	72	1	0
28	c	102	0	144	3	0
28	d	51	0	72	3	0
29	A	55	0	80	4	0
29	D	55	0	80	1	0
29	a	55	0	80	3	0
29	d	55	0	80	3	0
30	A	57	0	0	0	0
30	B	24	0	0	0	0
30	C	54	0	0	0	0
30	D	60	0	0	0	0
30	E	22	0	0	0	0
30	H	24	0	0	0	0
30	I	79	0	0	0	0
30	J	36	0	0	0	0
30	T	15	0	0	0	0
30	X	16	0	0	0	0
30	Z	20	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	45	0	0	0	0
30	b	87	0	0	0	0
30	c	47	0	0	0	0
30	d	65	0	0	1	0
30	e	15	0	0	0	0
30	h	29	0	0	0	0
30	i	66	0	0	0	0
30	j	15	0	0	0	0
30	k	39	0	0	0	0
30	l	13	0	0	0	0
30	m	11	0	0	0	0
30	t	12	0	0	0	0
30	x	39	0	0	0	0
30	y	4	0	0	0	0
31	A	70	0	92	7	0
31	B	59	0	81	2	0
31	F	24	0	35	0	0
31	J	24	0	35	0	0
31	M	60	0	81	3	0
31	Z	35	0	46	1	0
31	a	35	0	46	2	0
31	b	35	0	46	2	0
31	c	70	0	92	1	0
31	e	24	0	35	0	0
31	j	24	0	35	2	0
31	m	70	0	92	2	0
31	t	58	0	80	0	0
32	A	6	0	8	0	0
32	B	12	0	16	4	0
32	C	6	0	8	0	0
32	O	6	0	8	0	0
32	V	12	0	16	2	0
32	a	6	0	8	0	0
32	b	6	0	8	0	0
32	c	6	0	8	2	0
33	A	4	0	0	0	0
33	a	4	0	0	0	0
33	d	4	0	0	0	0
34	A	20	0	30	1	0
34	B	48	0	72	4	0
34	C	44	0	66	1	0
34	D	16	0	24	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	H	4	0	6	0	0
34	K	4	0	6	0	0
34	L	4	0	6	1	0
34	O	48	0	72	5	0
34	T	4	0	6	0	0
34	U	12	0	18	3	0
34	V	36	0	54	1	0
34	a	24	0	36	1	0
34	b	48	0	72	2	0
34	c	48	0	72	8	0
34	d	16	0	24	1	0
34	e	12	0	18	0	0
34	h	4	0	6	2	0
34	i	4	0	6	0	0
34	o	24	0	36	2	0
34	u	8	0	12	0	0
34	v	32	0	48	0	0
34	y	4	0	6	2	0
35	B	1	0	0	0	0
35	O	1	0	0	0	0
35	V	1	0	0	0	0
35	b	1	0	0	0	0
35	c	1	0	0	0	0
35	o	1	0	0	0	0
35	v	1	0	0	0	0
36	B	114	0	156	7	0
36	C	76	0	104	4	0
36	D	19	0	26	2	0
36	O	38	0	52	1	0
36	U	4	0	4	1	0
36	V	32	0	37	1	0
36	b	76	0	104	4	0
36	c	112	0	149	4	0
36	d	57	0	78	5	0
36	v	19	0	26	2	0
36	y	19	0	26	0	0
37	C	186	0	246	4	0
37	D	52	0	71	7	0
37	H	62	0	82	1	0
37	c	186	0	246	3	0
37	d	50	0	69	4	0
37	h	62	0	82	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	D	144	0	213	9	0
38	E	42	0	57	1	0
38	L	49	0	74	3	0
38	d	145	0	215	10	0
38	l	49	0	74	2	0
39	F	43	0	30	2	0
39	f	43	0	30	3	0
40	H	41	0	56	3	0
40	h	41	0	56	2	0
41	J	1	0	0	0	0
41	j	1	0	0	0	0
42	V	43	0	30	0	0
42	v	43	0	30	0	0
43	A	159	0	0	1	0
43	B	411	0	0	1	0
43	C	295	0	0	0	0
43	D	177	0	0	1	0
43	E	35	0	0	0	0
43	F	15	0	0	0	0
43	H	51	0	0	1	0
43	I	11	0	0	0	0
43	J	15	0	0	0	0
43	K	9	0	0	0	0
43	L	16	0	0	0	0
43	M	20	0	0	0	0
43	O	224	0	0	3	0
43	T	14	0	0	0	0
43	U	117	0	0	2	0
43	V	157	0	0	4	0
43	X	22	0	0	0	0
43	Y	6	0	0	0	0
43	Z	4	0	0	0	0
43	a	159	0	0	1	0
43	b	399	0	0	0	0
43	c	320	0	0	2	0
43	d	172	0	0	1	0
43	e	39	0	0	0	0
43	f	12	0	0	0	0
43	h	52	0	0	2	0
43	i	12	0	0	0	0
43	j	12	0	0	0	0
43	k	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	l	20	0	0	0	0
43	m	20	0	0	0	0
43	o	198	0	0	3	0
43	t	24	0	0	0	0
43	u	119	0	0	0	0
43	v	118	0	0	3	0
43	x	14	0	0	0	0
43	y	8	0	0	1	0
43	z	6	0	0	0	0
All	All	55630	0	52949	469	0

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

All (469) 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)
24:a:413:CLA:H152	24:c:907:CLA:H142	1.62	0.80
4:D:101:PHE:H	37:D:405:DGD:HB31	1.48	0.78
2:B:347[B]:ARG:NH1	32:B:637:GOL:O2	2.19	0.76
37:D:405:DGD:HD5	5:E:45:ASP:HB3	1.70	0.72
38:D:408:LHG:H141	38:D:408:LHG:H342	1.72	0.72
13:O:194:LYS:NZ	43:O:403:HOH:O	2.22	0.72
34:C:534:DMS:H22	36:C:537:HTG:H5	1.72	0.71
3:c:438:LEU:HD11	24:c:906:CLA:HBB1	1.73	0.70
34:A:426:DMS:H23	4:D:332:GLN:HG2	1.72	0.70
34:V:210:DMS:H13	34:V:211:DMS:H12	1.74	0.69
28:c:920:LMG:H241	31:j:102:LMT:H112	1.73	0.69
16:v:85:GLU:OE2	43:v:301:HOH:O	2.10	0.69
3:c:457:LYS:HZ3	32:c:929:GOL:H11	1.57	0.69
13:o:55:GLU:H	34:o:307:DMS:H23	1.56	0.69
2:b:224:ARG:NH1	31:b:625:LMT:O2'	2.23	0.69
24:C:512:CLA:H143	24:C:513:CLA:H142	1.75	0.68
27:a:415:SQD:H381	9:j:22:ILE:HD11	1.76	0.68
13:O:55:GLU:H	34:O:315:DMS:H12	1.60	0.67
36:v:211:HTG:S1	43:v:302:HOH:O	2.54	0.66
1:a:244:GLU:OE2	43:a:501:HOH:O	2.14	0.66
27:a:415:SQD:H182	38:d:411:LHG:H201	1.78	0.65
24:C:501:CLA:H202	24:C:507:CLA:HBB1	1.78	0.64
16:V:55[B]:ARG:NH1	43:V:303:HOH:O	2.31	0.64
37:D:405:DGD:HA42	37:D:405:DGD:HBT2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:74[B]:GLU:OE1	43:o:401:HOH:O	2.14	0.64
29:d:407:PL9:H401	38:d:410:LHG:H202	1.80	0.63
24:C:511:CLA:H41	17:Y:39:LEU:HD13	1.81	0.62
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.82	0.62
5:E:27:ILE:HG12	39:F:102:HEM:HMC3	1.81	0.62
24:B:615:CLA:H42	31:m:102:LMT:H61	1.80	0.61
3:C:78:GLU:OE2	16:V:106[B]:ASN:ND2	2.33	0.61
31:M:101:LMT:H6'2	11:l:9:PRO:HB3	1.81	0.61
13:O:80[B]:GLN:OE1	43:O:401:HOH:O	2.16	0.61
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.35	0.61
26:B:636:BCR:H321	26:B:636:BCR:HC8	1.80	0.61
15:U:56:GLU:HG2	34:U:204:DMS:H11	1.83	0.61
24:A:407:CLA:H122	29:A:414:PL9:H252	1.82	0.61
1:A:12:ASN:HD21	1:A:14:TRP:HB3	1.66	0.60
1:a:228:THR:HG23	1:a:230:THR:H	1.66	0.60
39:f:101:HEM:HBC2	39:f:101:HEM:HMC2	1.81	0.60
16:V:136:TYR:OH	43:V:301:HOH:O	2.11	0.60
2:B:347[B]:ARG:NH2	2:B:351:GLY:O	2.35	0.60
36:d:419:HTG:H1	7:h:25:TRP:CD1	2.37	0.59
24:b:619:CLA:H2	24:b:620:CLA:HBB2	1.84	0.59
2:B:171:PRO:HB3	7:H:63:LYS:HA	1.82	0.59
2:B:497:GLN:NE2	18:X:38:GLN:O	2.35	0.59
26:B:619:BCR:H363	26:B:636:BCR:H19C	1.83	0.59
2:b:36[A]:SER:OG	26:b:622:BCR:H362	2.03	0.59
24:b:610:CLA:HBB1	24:b:610:CLA:HMB1	1.84	0.59
37:D:405:DGD:HBF1	37:D:405:DGD:HB92	1.84	0.58
1:a:84:PRO:HA	1:a:112:TYR:CG	2.38	0.58
24:B:604:CLA:HAB	24:B:606:CLA:H171	1.85	0.58
24:b:615:CLA:H142	38:l:103:LHG:H362	1.84	0.58
16:V:88:ILE:HA	32:V:206:GOL:H12	1.85	0.58
4:d:192:THR:HG23	24:d:404:CLA:HBC2	1.84	0.58
28:D:409:LMG:H292	28:D:409:LMG:H141	1.86	0.58
15:U:39:ARG:NH1	16:V:60:ALA:O	2.37	0.58
29:d:407:PL9:H412	11:l:29:LEU:HD23	1.86	0.58
39:F:102:HEM:HBB2	39:F:102:HEM:HMB2	1.86	0.57
2:b:341:LYS:NZ	36:b:626:HTG:S1	2.77	0.57
24:C:504:CLA:H152	24:C:508:CLA:H143	1.86	0.57
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.39	0.57
38:d:411:LHG:H341	38:d:411:LHG:H132	1.86	0.57
3:C:464:GLU:OE2	4:D:245:SER:OG	2.22	0.57
43:c:1194[B]:HOH:O	13:o:79:ASP:OD2	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.86	0.56
26:B:618:BCR:H383	27:l:101:SQD:H101	1.87	0.56
37:d:408:DGD:HAF1	37:d:408:DGD:HBH1	1.87	0.56
26:k:102:BCR:H321	26:k:102:BCR:HC8	1.87	0.56
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.56
24:c:909:CLA:H201	28:c:920:LMG:H242	1.88	0.56
37:c:918:DGD:HA21	31:j:102:LMT:H61	1.86	0.56
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.41	0.56
24:B:614:CLA:H51	38:D:406:LHG:H351	1.87	0.56
26:Y:101:BCR:H321	26:Y:101:BCR:HC8	1.87	0.56
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.06	0.56
27:a:401:SQD:H372	27:a:401:SQD:H132	1.88	0.55
37:c:918:DGD:HA82	37:c:918:DGD:HAF1	1.88	0.55
1:a:183:MET:HA	24:a:409:CLA:HMD1	1.87	0.55
24:c:906:CLA:H93	24:c:906:CLA:HAB	1.88	0.55
24:c:902:CLA:H202	24:c:908:CLA:HBB1	1.89	0.55
24:A:410:CLA:H61	24:C:505:CLA:H201	1.88	0.55
2:B:118:TRP:NE1	32:B:638:GOL:H2	2.22	0.55
24:C:506:CLA:HMC2	24:C:507:CLA:H102	1.88	0.55
31:M:101:LMT:H6D	11:l:9:PRO:HA	1.88	0.54
13:O:144:GLY:HA2	34:O:314:DMS:H12	1.90	0.54
1:a:228:THR:HG22	1:a:231:GLU:HG2	1.90	0.54
24:A:410:CLA:H151	24:C:506:CLA:H13	1.89	0.54
24:C:508:CLA:HBC3	24:C:510:CLA:H71	1.90	0.54
26:T:101:BCR:H19C	26:b:622:BCR:H363	1.89	0.54
28:A:413:LMG:H392	37:C:516:DGD:HB51	1.88	0.54
24:a:413:CLA:H62	24:c:906:CLA:H191	1.90	0.54
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.43	0.54
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.37	0.54
3:c:60:ILE:HG22	24:c:904:CLA:HHD	1.90	0.54
31:A:421:LMT:H102	24:C:506:CLA:H71	1.89	0.54
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.88	0.54
27:b:601:SQD:H1	27:b:601:SQD:H462	1.90	0.54
24:b:615:CLA:H141	38:l:103:LHG:H383	1.90	0.54
24:b:617:CLA:H18	38:d:409:LHG:H202	1.89	0.54
2:B:341:LYS:NZ	36:B:624:HTG:S1	2.81	0.53
5:E:12[B]:ASP:OD1	9:J:5:GLY:N	2.42	0.53
26:T:101:BCR:H321	26:T:101:BCR:HC8	1.89	0.53
1:a:247:ASN:HA	34:a:424:DMS:H12	1.90	0.53
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.90	0.53
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:24:ARG:HD3	18:x:37:VAL:HG12	1.90	0.53
4:d:58:TRP:CH2	5:e:63:ILE:HD12	2.43	0.53
24:A:410:CLA:H41	24:A:410:CLA:H71	1.91	0.52
2:B:248:ALA:HA	24:B:604:CLA:H42	1.92	0.52
24:C:513:CLA:HAB	26:C:514:BCR:H24C	1.90	0.52
37:d:408:DGD:HA42	37:d:408:DGD:HB21	1.91	0.52
36:B:623:HTG:H3	31:a:402:LMT:H12	1.90	0.52
36:D:412:HTG:H1	7:H:25:TRP:CD1	2.44	0.52
3:c:250:TRP:CZ3	36:c:941:HTG:H3'1	2.45	0.52
4:d:141:TYR:CE1	34:d:415:DMS:H23	2.44	0.52
31:A:421:LMT:H11	3:C:259:TRP:HB2	1.92	0.52
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.92	0.52
5:E:68:ASP:O	5:E:72:ALA:HB2	2.10	0.52
28:A:413:LMG:H111	24:C:505:CLA:H193	1.92	0.52
28:c:920:LMG:H172	28:c:920:LMG:H301	1.92	0.52
24:C:503:CLA:C3B	28:C:523:LMG:H221	2.40	0.51
27:a:401:SQD:H301	27:a:401:SQD:H362	1.92	0.51
24:C:511:CLA:H42	17:Y:46:LEU:HA	1.92	0.51
3:c:138:GLU:HB2	34:c:934:DMS:H22	1.91	0.51
24:A:406:CLA:HBB1	24:A:406:CLA:HMB1	1.93	0.51
29:A:414:PL9:H512	27:F:101:SQD:H152	1.91	0.51
13:O:27:ARG:NH1	13:O:202:ALA:O	2.44	0.51
16:v:30:LYS:NZ	43:v:303:HOH:O	2.36	0.51
36:B:623:HTG:H1	31:a:402:LMT:H22	1.92	0.51
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.46	0.51
27:A:416:SQD:H292	26:b:623:BCR:H363	1.93	0.51
31:A:417:LMT:H62	2:b:39:LEU:HD22	1.91	0.51
24:B:608:CLA:HMB1	24:B:608:CLA:HBB1	1.93	0.51
3:c:406:SER:HA	3:c:420:VAL:HG23	1.92	0.51
2:B:91:TRP:HE1	31:B:626:LMT:H2'	1.76	0.50
3:c:457:LYS:NZ	32:c:929:GOL:H11	2.25	0.50
2:B:62:VAL:HB	24:B:606:CLA:HED3	1.93	0.50
4:D:192:THR:HG23	24:D:401:CLA:HBC2	1.93	0.50
13:o:80[B]:GLN:OE1	43:o:402:HOH:O	2.19	0.50
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.94	0.50
5:e:57:ALA:H	5:e:60:GLN:NE2	2.10	0.50
24:B:605:CLA:H43	24:B:606:CLA:H2	1.93	0.50
36:U:201:HTG:H3'2	34:U:204:DMS:H23	1.93	0.50
27:a:401:SQD:H162	38:d:410:LHG:H382	1.94	0.50
16:V:96:ARG:NH2	36:V:215:HTG:S1	2.84	0.50
24:B:615:CLA:H151	14:t:8:PHE:HE1	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.47	0.50
5:e:73:LYS:NZ	5:e:77[B]:GLU:OE2	2.42	0.50
24:a:409:CLA:HBB1	24:a:409:CLA:HMB3	1.93	0.50
37:d:408:DGD:HB51	36:d:414:HTG:H3'1	1.93	0.50
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.94	0.50
3:C:286:ALA:HB2	24:C:502:CLA:HMD2	1.94	0.50
2:b:248:ALA:HA	24:b:607:CLA:H42	1.93	0.50
31:A:417:LMT:H111	36:O:303:HTG:H6'2	1.94	0.49
2:b:90:PHE:CE2	24:b:610:CLA:H151	2.47	0.49
32:B:638:GOL:H32	11:L:1:MET:HB3	1.94	0.49
26:c:915:BCR:H382	36:c:928:HTG:H7'3	1.95	0.49
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.92	0.49
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.94	0.49
2:b:12:LEU:HB2	24:b:616:CLA:HMC2	1.95	0.49
3:c:213[A]:LEU:HD21	26:c:916:BCR:C20	2.42	0.49
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.94	0.49
3:C:239:TRP:CE2	36:C:536:HTG:H7'2	2.46	0.49
10:k:20:PRO:HB3	17:y:21:GLN:HG3	1.94	0.49
18:X:30:ALA:O	18:X:34:ILE:HG12	2.13	0.49
25:A:409:PHO:HBC3	4:D:279:LEU:HD22	1.95	0.49
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.95	0.49
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.43	0.49
24:C:501:CLA:C3D	24:C:503:CLA:H2	2.43	0.49
24:b:619:CLA:H2	24:b:620:CLA:CBB	2.42	0.49
38:d:411:LHG:H152	38:d:411:LHG:H332	1.95	0.48
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.95	0.48
24:C:504:CLA:H151	24:C:504:CLA:H111	1.51	0.48
5:E:26:THR:HA	20:R:15:ALA:HB1	1.95	0.48
15:U:70:ARG:HG3	34:U:202:DMS:H12	1.94	0.48
10:k:24:VAL:O	10:k:27:VAL:HG22	2.13	0.48
24:b:609:CLA:HHC	24:b:609:CLA:HBB1	1.95	0.48
3:c:443:TRP:CZ2	24:c:909:CLA:HMD1	2.48	0.48
4:d:61:HIS:HD2	43:d:512[B]:HOH:O	1.96	0.48
27:a:415:SQD:H271	38:d:411:LHG:H142	1.94	0.48
29:A:414:PL9:H502	4:D:39:PRO:HG3	1.96	0.48
38:E:101:LHG:H171	38:E:101:LHG:H142	1.71	0.48
31:c:927:LMT:O2B	43:c:1001:HOH:O	2.20	0.48
39:f:101:HEM:HBB2	39:f:101:HEM:HMB2	1.94	0.48
1:A:221:SER:HB2	4:D:139:ARG:O	2.14	0.48
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.49	0.48
24:B:602:CLA:H152	24:B:602:CLA:H52	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:625:LMT:H1B	31:b:625:LMT:H3'	1.41	0.47
1:A:188:ALA:HB2	1:A:328:ILE:HB	1.96	0.47
38:D:408:LHG:H331	38:D:408:LHG:H172	1.96	0.47
15:U:81:HIS:HE1	43:U:394:HOH:O	1.95	0.47
1:a:312:ASN:OD1	5:e:61:ARG:NH1	2.44	0.47
3:c:41:ARG:NH1	24:c:912:CLA:HMD1	2.29	0.47
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.13	0.47
26:b:621:BCR:H12C	28:b:624:LMG:C43	2.45	0.47
24:c:907:CLA:H71	26:c:916:BCR:H10C	1.96	0.47
24:B:611:CLA:H122	24:B:616:CLA:HAA1	1.96	0.47
4:D:61:HIS:HD2	43:D:533[B]:HOH:O	1.97	0.47
16:v:68:ASN:ND2	36:v:211:HTG:O3	2.44	0.47
2:B:98:LEU:HB2	36:B:623:HTG:H7'3	1.96	0.47
3:C:135[A]:ARG:HH21	19:Z:33:TRP:NE1	2.12	0.47
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.97	0.47
34:h:105:DMS:O	43:h:201:HOH:O	2.21	0.47
24:C:501:CLA:H42	24:C:502:CLA:HMD3	1.97	0.47
4:d:14:TRP:CD1	36:d:419:HTG:H61	2.49	0.47
13:O:34:SER:HB2	34:O:311:DMS:H11	1.97	0.47
36:d:419:HTG:H1	7:h:25:TRP:CG	2.50	0.47
24:C:505:CLA:HBB1	24:C:505:CLA:HHC	1.97	0.47
24:C:508:CLA:H172	28:C:519:LMG:H201	1.96	0.47
11:L:9:PRO:HA	31:m:102:LMT:H6D	1.96	0.47
13:O:231:HIS:HE1	34:O:315:DMS:H22	1.79	0.47
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.95	0.46
24:b:609:CLA:H8	24:b:616:CLA:H191	1.97	0.46
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.15	0.46
12:m:30:GLU:O	12:m:34:LYS:NZ	2.48	0.46
17:y:20:ALA:O	17:y:24:MET:HG2	2.16	0.46
1:A:63:ILE:HB	3:C:335:THR:HG21	1.97	0.46
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.50	0.46
24:c:910:CLA:H142	24:c:910:CLA:H112	1.81	0.46
2:B:162:PHE:O	24:B:607:CLA:HHD	2.16	0.46
13:O:129:THR:HA	13:O:141:ASP:O	2.15	0.46
24:c:910:CLA:HMB1	24:c:910:CLA:HBB1	1.97	0.46
8:i:33:LYS:O	8:i:35:LYS:HG3	2.15	0.46
13:O:74[B]:GLU:OE1	43:O:402:HOH:O	2.21	0.46
17:Y:20:ALA:O	17:Y:24:MET:HG2	2.16	0.46
19:z:2:THR:HG23	19:z:61:VAL:HG11	1.98	0.46
3:C:443:TRP:CE2	24:C:508:CLA:HMD2	2.51	0.46
12:M:28:GLN:O	12:M:32:GLN:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:413:CLA:H102	24:a:413:CLA:H61	1.67	0.46
24:d:401:CLA:H91	29:d:407:PL9:H402	1.96	0.46
2:b:204:ALA:HA	36:b:627:HTG:H6'2	1.98	0.46
24:b:610:CLA:H102	24:b:610:CLA:H61	1.72	0.46
24:A:410:CLA:H172	24:C:506:CLA:H142	1.96	0.46
24:B:606:CLA:H143	24:B:611:CLA:HED2	1.97	0.46
24:B:616:CLA:H121	24:B:617:CLA:H112	1.98	0.46
3:C:406:SER:HA	3:C:420:VAL:HG23	1.97	0.46
36:c:942:HTG:H2'2	15:u:92:VAL:HG23	1.98	0.46
26:B:619:BCR:H331	26:B:619:BCR:C8	2.44	0.46
2:b:499:VAL:HG12	4:d:135:LEU:HB3	1.97	0.46
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.51	0.46
3:c:334:PRO:HA	13:o:153:THR:OG1	2.16	0.46
34:h:105:DMS:O	43:h:202:HOH:O	2.21	0.46
31:A:421:LMT:H81	24:C:506:CLA:H52	1.98	0.45
3:C:288:CYS:SG	37:C:516:DGD:HB32	2.56	0.45
24:a:409:CLA:CBD	24:d:401:CLA:HAC2	2.45	0.45
2:b:30:VAL:HG12	24:b:609:CLA:HHD	1.98	0.45
6:f:21:VAL:O	6:f:25:THR:HG23	2.16	0.45
24:C:504:CLA:H192	28:C:519:LMG:H241	1.99	0.45
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.98	0.45
26:B:620:BCR:H331	26:B:620:BCR:C8	2.47	0.45
24:b:613:CLA:NC	40:h:101:RRX:H56	2.31	0.45
7:h:59:ASN:ND2	7:h:63:LYS:O	2.49	0.45
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.98	0.45
1:a:28:LEU:HB2	27:a:401:SQD:H102	1.99	0.45
34:B:634:DMS:H23	43:B:928:HOH:O	2.16	0.45
16:V:129:LYS:HD3	43:V:386:HOH:O	2.16	0.45
2:b:216:HIS:HE1	24:b:613:CLA:C1A	2.30	0.45
26:k:103:BCR:H24C	26:k:103:BCR:H371	1.76	0.45
3:C:338:GLY:HA3	3:C:341:LEU:O	2.16	0.45
24:B:603:CLA:H171	37:H:102:DGD:HA91	1.98	0.45
24:B:615:CLA:H151	14:t:8:PHE:CE1	2.52	0.45
24:b:608:CLA:H43	24:b:609:CLA:H2	1.99	0.45
3:c:281:MET:HE1	37:c:917:DGD:HAN1	1.97	0.45
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.52	0.45
25:a:412:PHO:ND	25:a:412:PHO:NC	2.65	0.44
3:C:117:VAL:HG12	28:C:523:LMG:H211	1.98	0.44
15:U:9:LEU:HA	43:U:352[B]:HOH:O	2.17	0.44
5:e:68:ASP:O	5:e:72:ALA:HB2	2.16	0.44
7:H:20:LYS:NZ	43:H:201:HOH:O	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:K:101:BCR:H24C	26:K:101:BCR:H371	1.79	0.44
2:b:233:ASN:O	2:b:236:THR:HG22	2.17	0.44
13:o:74[A]:GLU:OE1	43:o:403:HOH:O	2.20	0.44
29:A:414:PL9:H471	27:F:101:SQD:H141	2.00	0.44
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.53	0.44
3:c:223:TRP:CG	3:c:224:ILE:H	2.36	0.44
38:d:409:LHG:H212	12:m:18:PRO:HG3	1.98	0.44
5:e:68:ASP:OD2	5:e:71:GLU:HB2	2.17	0.44
25:A:409:PHO:NC	25:A:409:PHO:ND	2.63	0.44
1:a:296:ASN:HB2	3:c:400:PRO:O	2.18	0.44
3:c:362:ARG:HD3	34:c:940:DMS:O	2.18	0.44
4:d:49:LEU:HD13	26:d:406:BCR:C15	2.48	0.44
4:d:141:TYR:OH	38:d:409:LHG:O4	2.26	0.44
1:A:12:ASN:ND2	1:A:14:TRP:HB3	2.32	0.44
31:A:417:LMT:H71	31:M:102:LMT:H62	1.99	0.44
1:a:131:TRP:CH2	24:c:906:CLA:HAA2	2.51	0.44
3:c:387:TRP:CE2	34:c:932:DMS:H12	2.53	0.44
29:D:404:PL9:H411	11:L:29:LEU:HD23	1.99	0.44
40:H:101:RRX:H32	40:H:101:RRX:H28	1.89	0.44
20:R:33:LYS:HE2	20:R:33:LYS:HB3	1.77	0.44
24:A:406:CLA:H203	24:A:406:CLA:H162	1.79	0.44
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	1.98	0.44
24:a:410:CLA:H141	28:d:412:LMG:H362	2.00	0.44
26:Y:101:BCR:H15C	26:Y:101:BCR:H351	1.91	0.44
1:a:227:THR:HB	1:a:231:GLU:HG3	2.00	0.44
24:b:613:CLA:HMA3	24:b:614:CLA:C1C	2.48	0.44
3:c:52:ALA:HB2	24:c:912:CLA:HMA2	1.99	0.44
11:L:8[B]:GLN:NE2	34:L:102:DMS:O	2.51	0.43
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.00	0.43
27:a:401:SQD:H192	27:a:401:SQD:H161	1.92	0.43
34:b:647:DMS:H21	12:m:2:GLU:HB3	2.00	0.43
24:B:607:CLA:H141	36:B:630:HTG:H7'2	2.00	0.43
13:O:216:GLU:CD	13:O:234:LYS:HD2	2.44	0.43
24:c:909:CLA:HBC3	24:c:911:CLA:H71	2.00	0.43
26:b:621:BCR:H24C	26:b:621:BCR:H371	1.81	0.43
24:c:906:CLA:HAA1	24:c:906:CLA:HBD	2.01	0.43
26:B:636:BCR:H20C	26:B:636:BCR:H361	1.91	0.43
24:c:909:CLA:C9	38:d:411:LHG:H151	2.49	0.43
24:A:406:CLA:C4A	24:A:406:CLA:HBA1	2.49	0.43
28:A:413:LMG:H211	28:A:413:LMG:H242	1.67	0.43
24:C:505:CLA:HBC2	26:C:515:BCR:H341	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100:ASP:HA	37:D:405:DGD:HB22	2.00	0.43
28:a:416:LMG:HC8	28:a:416:LMG:H111	1.56	0.43
36:c:942:HTG:H2'1	15:u:93:GLU:OE1	2.18	0.43
2:B:298:LEU:HD21	32:B:637:GOL:H12	2.00	0.43
24:B:617:CLA:H61	24:B:617:CLA:H92	1.64	0.43
3:C:42:LEU:HD21	24:C:511:CLA:H2A	2.01	0.43
3:C:223:TRP:CG	3:C:224:ILE:H	2.37	0.43
2:b:62:VAL:HB	24:b:609:CLA:HED3	1.99	0.43
2:b:162:PHE:O	24:b:610:CLA:HHD	2.18	0.43
13:o:129:THR:HA	13:o:141:ASP:O	2.19	0.43
13:o:244:GLU:HA	34:o:303:DMS:H21	2.01	0.43
38:D:408:LHG:H162	38:D:408:LHG:H191	1.90	0.43
24:a:410:CLA:HBB1	24:a:410:CLA:HMB1	2.01	0.43
24:b:619:CLA:H161	7:h:7:LEU:HD21	1.99	0.43
3:c:20:SER:HB3	3:c:23:ALA:HB2	2.01	0.43
13:o:142:PHE:HB2	13:o:199:LEU:HB2	2.01	0.43
1:A:197:PHE:CZ	37:C:517:DGD:HBN2	2.53	0.43
24:B:607:CLA:H201	31:B:626:LMT:O2'	2.19	0.43
24:b:620:CLA:H152	24:b:620:CLA:H18	1.85	0.43
3:C:204:LEU:HB3	36:C:536:HTG:H4'2	1.99	0.43
3:C:318:LEU:C	3:C:318:LEU:HD23	2.44	0.43
25:a:411:PHO:NC	25:a:411:PHO:ND	2.66	0.43
24:B:615:CLA:H93	24:B:615:CLA:H111	1.87	0.43
24:C:508:CLA:HBC2	38:D:408:LHG:H171	2.01	0.43
16:V:41:HIS:HA	16:V:45:ILE:O	2.19	0.43
24:b:616:CLA:H122	24:b:616:CLA:H162	1.85	0.43
26:b:621:BCR:H15C	26:b:621:BCR:H351	1.81	0.43
2:B:204:ALA:CB	24:B:603:CLA:HAB	2.49	0.42
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.49	0.42
26:T:101:BCR:H11C	26:T:101:BCR:H341	1.92	0.42
2:b:306:PRO:HG3	34:b:639:DMS:H12	2.01	0.42
6:f:31:ILE:HG13	39:f:101:HEM:HMC2	2.01	0.42
13:o:5:LEU:HD13	13:o:10:ILE:HD11	2.01	0.42
4:D:26:ARG:HA	5:E:5:THR:HB	2.01	0.42
40:H:101:RRX:H43	40:H:101:RRX:H47	1.82	0.42
24:c:902:CLA:H42	24:c:903:CLA:HMD3	2.01	0.42
2:B:419[A]:SER:OG	36:B:624:HTG:H2'1	2.19	0.42
24:B:603:CLA:H111	24:B:603:CLA:H91	1.83	0.42
1:a:264:SER:OG	29:a:417:PL9:O2	2.34	0.42
24:b:605:CLA:HBD	24:b:605:CLA:H42	2.01	0.42
24:B:615:CLA:H101	26:B:618:BCR:H362	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.42
26:c:915:BCR:H15C	26:c:915:BCR:H351	1.84	0.42
8:i:33:LYS:HB3	8:i:34:ARG:H	1.62	0.42
3:C:50:LEU:HD11	24:C:513:CLA:HBB1	2.02	0.42
34:y:101:DMS:H23	43:y:202:HOH:O	2.19	0.42
3:C:334:PRO:HA	13:O:153:THR:OG1	2.20	0.42
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.49	0.42
1:a:63:ILE:HB	3:c:335:THR:HG21	2.00	0.42
12:m:28:GLN:O	12:m:32:GLN:HG3	2.20	0.42
2:B:390:TYR:OH	34:B:639:DMS:O	2.20	0.42
18:x:15:LEU:HD12	18:x:15:LEU:HA	1.86	0.42
24:B:616:CLA:H2	24:B:617:CLA:HBB2	2.02	0.42
3:C:315:MET:HE1	3:C:369:LEU:HD11	2.01	0.42
38:D:406:LHG:O9	38:L:101:LHG:HC81	2.20	0.42
24:B:603:CLA:H41	7:H:46:LEU:HA	2.02	0.42
3:C:443:TRP:CD2	24:C:508:CLA:HMD2	2.55	0.42
40:H:101:RRX:H3	18:X:2:THR:N	2.18	0.42
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	2.01	0.42
1:a:36:ILE:HG21	24:c:906:CLA:H143	2.02	0.42
24:a:409:CLA:CAD	24:d:401:CLA:HAC2	2.50	0.42
26:b:623:BCR:H15C	26:b:623:BCR:H351	1.90	0.42
3:c:104:GLU:HB2	34:c:933:DMS:H21	2.01	0.42
1:A:143:ILE:N	1:A:144:PRO:HD2	2.35	0.42
24:C:513:CLA:HBA1	24:C:513:CLA:H3A	1.65	0.42
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.01	0.42
2:b:419[A]:SER:OG	36:b:626:HTG:H2'1	2.20	0.42
24:b:614:CLA:H192	24:b:614:CLA:H161	1.64	0.42
3:c:74:HIS:CE1	34:y:101:DMS:H11	2.55	0.42
19:z:26:ALA:HB1	19:z:36:SER:HB3	2.02	0.42
2:B:42:LEU:HD13	2:B:94:GLU:HG3	2.02	0.41
24:C:510:CLA:H41	38:D:408:LHG:H151	2.02	0.41
4:D:14:TRP:CD1	36:D:412:HTG:H61	2.55	0.41
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.01	0.41
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.75	0.41
3:C:127:PHE:CZ	31:Z:101:LMT:H42	2.55	0.41
24:b:610:CLA:H111	24:b:610:CLA:H142	1.81	0.41
36:b:626:HTG:H2'1	36:b:626:HTG:H5'2	1.88	0.41
3:c:135[A]:ARG:HH21	19:z:33:TRP:NE1	2.18	0.41
2:B:276:ASP:O	34:B:632:DMS:H22	2.20	0.41
2:B:420:TYR:CE1	36:B:624:HTG:H3'2	2.56	0.41
24:B:607:CLA:H102	24:B:607:CLA:H61	1.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:515:BCR:H351	26:C:515:BCR:H15C	1.82	0.41
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.03	0.41
13:O:180:GLU:CD	13:O:180:GLU:H	2.26	0.41
26:a:414:BCR:H15C	26:a:414:BCR:H351	1.91	0.41
24:b:615:CLA:H72	24:b:615:CLA:H112	1.92	0.41
4:d:103:ARG:HE	5:e:77[B]:GLU:HG3	1.85	0.41
1:a:102:LEU:HD23	1:a:102:LEU:HA	1.92	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.86	0.41
3:c:362:ARG:NH1	34:c:940:DMS:O	2.47	0.41
4:d:85:MET:HE1	4:d:96:GLU:HG2	2.01	0.41
40:h:101:RRX:H26	40:h:101:RRX:H22	1.89	0.41
26:B:636:BCR:HC7	26:B:636:BCR:H331	1.61	0.41
38:D:406:LHG:HC12	38:L:101:LHG:O5	2.20	0.41
32:V:207:GOL:H32	43:V:343:HOH:O	2.19	0.41
1:a:143:ILE:N	1:a:144:PRO:HD2	2.35	0.41
1:A:60:ILE:HB	1:A:83:VAL:CG1	2.50	0.41
24:B:603:CLA:H203	24:B:603:CLA:H162	1.91	0.41
37:D:405:DGD:HD2	37:D:405:DGD:HG32	1.69	0.41
24:b:614:CLA:HHC	24:b:614:CLA:HBB1	2.01	0.41
4:d:73:PHE:CZ	28:d:412:LMG:H181	2.55	0.41
24:A:405:CLA:H192	24:A:405:CLA:H161	1.82	0.41
37:D:405:DGD:HB82	37:D:405:DGD:HB51	1.84	0.41
2:b:58:GLN:C	2:b:329:PRO:HB3	2.45	0.41
24:b:606:CLA:H111	24:b:606:CLA:H91	1.90	0.41
24:b:620:CLA:HBB1	24:b:620:CLA:HMB3	2.02	0.41
3:c:180:MET:HE2	3:c:180:MET:HB3	1.88	0.41
3:c:387:TRP:CZ3	34:c:932:DMS:H23	2.55	0.41
4:d:73:PHE:CE2	28:d:412:LMG:H181	2.56	0.41
24:B:611:CLA:HHC	24:B:611:CLA:CBB	2.50	0.41
34:D:416:DMS:H21	16:V:129:LYS:HE3	2.02	0.41
29:a:417:PL9:H28	30:d:421:UNL:C37	2.50	0.41
1:A:131:TRP:CD2	1:A:131:TRP:C	2.98	0.41
27:A:416:SQD:H361	24:b:610:CLA:H93	2.03	0.41
2:B:497:GLN:HB2	2:B:504:THR:HB	2.03	0.41
24:B:604:CLA:HBB1	24:B:604:CLA:HMB3	2.03	0.41
24:C:508:CLA:CBC	38:D:408:LHG:H171	2.51	0.41
28:C:523:LMG:H292	28:C:523:LMG:H321	1.82	0.41
11:L:24[B]:ILE:CD1	12:M:18:PRO:HB2	2.51	0.41
1:a:202:VAL:HG11	24:a:410:CLA:C3D	2.50	0.41
27:a:401:SQD:H301	27:a:401:SQD:H272	1.85	0.41
24:c:903:CLA:H102	24:c:904:CLA:CHB	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:905:CLA:H143	24:c:905:CLA:H111	1.81	0.41
4:d:126[A]:MET:HE3	4:d:143:ALA:O	2.21	0.41
16:v:55[B]:ARG:NH2	16:v:128:ASP:OD1	2.54	0.41
3:C:437:PHE:CE2	24:C:510:CLA:HMB2	2.56	0.41
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	2.03	0.41
26:C:514:BCR:H382	36:C:537:HTG:H6'1	2.03	0.41
2:b:462:PHE:CE2	24:b:617:CLA:HMB2	2.56	0.41
3:c:362:ARG:NH2	34:c:930:DMS:H13	2.36	0.41
4:d:126[B]:MET:HE1	4:d:147:SER:HA	2.03	0.41
14:t:2:GLU:HG2	14:t:3:THR:N	2.35	0.41
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.57	0.40
24:A:405:CLA:CBD	24:A:406:CLA:HAC2	2.51	0.40
34:B:633:DMS:H13	15:U:21:TYR:CZ	2.56	0.40
29:a:417:PL9:H13	29:a:417:PL9:H172	1.88	0.40
2:b:446:SER:HB2	2:b:447:PRO:HD2	2.02	0.40
24:b:607:CLA:H3A	24:b:607:CLA:CGA	2.51	0.40
3:c:77:PRO:HG2	34:c:937:DMS:H12	2.03	0.40
24:c:905:CLA:HBD	24:c:905:CLA:HAA1	2.04	0.40
16:v:41:HIS:HA	16:v:45:ILE:O	2.21	0.40
24:B:610:CLA:HBA1	24:B:610:CLA:H3A	1.90	0.40
24:B:612:CLA:H142	38:L:101:LHG:H362	2.04	0.40
24:B:614:CLA:H122	28:B:621:LMG:H232	2.02	0.40
1:a:60:ILE:HB	1:a:83:VAL:CG1	2.51	0.40
26:a:414:BCR:H24C	26:a:414:BCR:H371	1.88	0.40
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.57	0.40
37:C:518:DGD:HB92	37:C:518:DGD:HBW1	1.87	0.40
13:O:194:LYS:HE3	34:O:306:DMS:H21	2.03	0.40
37:d:408:DGD:O1B	36:d:414:HTG:O6	2.24	0.40
24:b:619:CLA:H61	24:b:619:CLA:H92	1.76	0.40
11:l:14:ARG:HB3	14:t:25[A]:GLU:CG	2.51	0.40
31:A:421:LMT:O4'	43:A:501:HOH:O	2.21	0.40
3:C:437:PHE:CZ	24:C:510:CLA:HMB2	2.57	0.40
28:C:519:LMG:H212	28:C:519:LMG:H242	1.91	0.40
26:T:101:BCR:H331	26:T:101:BCR:HC7	1.59	0.40
26:d:406:BCR:H15C	26:d:406:BCR:H351	1.91	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	334/360 (93%)	329 (98%)	4 (1%)	1 (0%)	36	29
1	a	337/360 (94%)	332 (98%)	4 (1%)	1 (0%)	36	29
2	B	511/510 (100%)	503 (98%)	8 (2%)	0	100	100
2	b	511/510 (100%)	503 (98%)	8 (2%)	0	100	100
3	C	455/461 (99%)	445 (98%)	8 (2%)	2 (0%)	30	22
3	c	457/461 (99%)	446 (98%)	10 (2%)	1 (0%)	43	36
4	D	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
4	d	342/352 (97%)	335 (98%)	7 (2%)	0	100	100
5	E	79/84 (94%)	79 (100%)	0	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	31/45 (69%)	31 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
8	I	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
8	i	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	37/37 (100%)	37 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	251/272 (92%)	246 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	246/272 (90%)	241 (98%)	5 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	96/134 (72%)	93 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	139/163 (85%)	136 (98%)	3 (2%)	0	100	100
16	v	137/163 (84%)	134 (98%)	3 (2%)	0	100	100
17	Y	28/46 (61%)	28 (100%)	0	0	100	100
17	y	29/46 (63%)	29 (100%)	0	0	100	100
18	X	38/41 (93%)	37 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5292/5691 (93%)	5194 (98%)	93 (2%)	5 (0%)	48	40

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/290 (92%)	266 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	271/290 (93%)	269 (99%)	2 (1%)	76 78
2	B	405/407 (100%)	404 (100%)	1 (0%)	87 90
2	b	397/407 (98%)	395 (100%)	2 (0%)	81 84
3	C	357/362 (99%)	355 (99%)	2 (1%)	78 81
3	c	358/362 (99%)	356 (99%)	2 (1%)	78 81
4	D	275/283 (97%)	273 (99%)	2 (1%)	76 78
4	d	277/283 (98%)	275 (99%)	2 (1%)	76 78
5	E	65/73 (89%)	65 (100%)	0	100 100
5	e	68/73 (93%)	68 (100%)	0	100 100
6	F	28/39 (72%)	28 (100%)	0	100 100
6	f	27/39 (69%)	27 (100%)	0	100 100
7	H	52/55 (94%)	52 (100%)	0	100 100
7	h	54/55 (98%)	53 (98%)	1 (2%)	50 47
8	I	32/34 (94%)	31 (97%)	1 (3%)	35 29
8	i	31/34 (91%)	30 (97%)	1 (3%)	34 27
9	J	23/28 (82%)	23 (100%)	0	100 100
9	j	25/28 (89%)	25 (100%)	0	100 100
10	K	29/37 (78%)	29 (100%)	0	100 100
10	k	29/37 (78%)	29 (100%)	0	100 100
11	L	36/35 (103%)	36 (100%)	0	100 100
11	l	35/35 (100%)	35 (100%)	0	100 100
12	M	30/32 (94%)	30 (100%)	0	100 100
12	m	31/32 (97%)	30 (97%)	1 (3%)	34 27
13	O	211/228 (92%)	211 (100%)	0	100 100
13	o	208/228 (91%)	203 (98%)	5 (2%)	43 38
14	T	27/28 (96%)	27 (100%)	0	100 100
14	t	27/28 (96%)	27 (100%)	0	100 100
15	U	81/112 (72%)	81 (100%)	0	100 100
15	u	84/112 (75%)	83 (99%)	1 (1%)	63 63
16	V	121/138 (88%)	119 (98%)	2 (2%)	53 52
16	v	117/138 (85%)	117 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	Y	22/37 (60%)	21 (96%)	1 (4%)	24 17
17	y	24/37 (65%)	23 (96%)	1 (4%)	26 19
18	X	30/34 (88%)	30 (100%)	0	100 100
18	x	31/34 (91%)	30 (97%)	1 (3%)	34 27
19	Z	45/51 (88%)	45 (100%)	0	100 100
19	z	44/51 (86%)	43 (98%)	1 (2%)	44 40
20	R	16/33 (48%)	16 (100%)	0	100 100
All	All	4289/4639 (92%)	4260 (99%)	29 (1%)	78 78

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	PHE
3	C	24	THR
3	C	289	PHE
4	D	90	LEU
4	D	272	LEU
8	I	2	GLU
16	V	15[A]	GLU
16	V	15[B]	GLU
17	Y	19	ILE
1	a	10	THR
1	a	249	VAL
2	b	223	GLN
2	b	362	PHE
3	c	289	PHE
3	c	416	SER
4	d	90	LEU
4	d	272	LEU
7	h	63	LYS
8	i	33	LYS
12	m	33	GLN
13	o	10	ILE
13	o	143	LYS
13	o	179[A]	GLU
13	o	179[B]	GLU
13	o	181	GLU
15	u	8	GLU
17	y	19	ILE
18	x	37	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	z	61	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	75	ASN
1	A	165	GLN
2	B	374	ASN
3	C	44	ASN
3	C	415	ASN
4	D	61	HIS
4	D	186	GLN
4	D	332	GLN
13	O	147	ASN
15	U	37	GLN
15	U	78	ASN
1	a	165	GLN
3	c	44	ASN
3	c	415	ASN
4	d	186	GLN
4	d	301	GLN
13	o	155	ASN
15	u	78	ASN
15	u	81	HIS
16	v	86	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	0.95	0	8,9,11	0.86	0
19	FME	z	1	19	8,9,10	0.93	0	8,9,11	1.04	0
8	FME	I	1	8	8,9,10	0.95	0	8,9,11	0.90	0
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	0.78	0
14	FME	t	1	14	8,9,10	1.01	0	8,9,11	1.36	1 (12%)
19	FME	Z	1	19	8,9,10	0.95	0	8,9,11	1.02	0
12	FME	M	1	12	8,9,10	1.01	0	8,9,11	0.52	0
14	FME	T	1	14	8,9,10	1.02	0	8,9,11	1.28	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
19	FME	z	1	19	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-
19	FME	Z	1	19	-	2/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	C-CA-N	2.54	114.41	109.50
14	t	1	FME	C-CA-N	2.10	113.55	109.50

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	t	1	FME	O-C-CA-CB
19	Z	1	FME	CA-CB-CG-SD
19	z	1	FME	CA-CB-CG-SD
19	Z	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	C-CA-CB-CG
14	t	1	FME	CB-CG-SD-CE
19	z	1	FME	C-CA-CB-CG

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 414 ligands modelled in this entry, 15 are monoatomic and 77 are unknown - leaving 322 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	$\#\|Z\| > 2$
27	SQD	a	401	-	52,54,54	0.98	2 (3%)	62,65,65	1.08	3 (4%)
34	DMS	T	103	-	3,3,3	2.71	1 (33%)	3,3,3	0.53	0
32	GOL	V	207	-	5,5,5	1.05	0	5,5,5	0.93	0
28	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.13	4 (6%)
36	HTG	O	316	-	19,19,19	0.82	1 (5%)	23,24,24	1.21	2 (8%)
24	CLA	C	504	43	69,73,73	2.29	22 (31%)	82,113,113	2.44	29 (35%)
34	DMS	u	201	-	3,3,3	2.73	1 (33%)	3,3,3	0.84	0
26	BCR	K	101	-	41,41,41	0.76	0	56,56,56	1.35	7 (12%)
26	BCR	b	623	-	41,41,41	0.78	1 (2%)	56,56,56	1.48	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.08	3 (6%)
31	LMT	c	927	-	36,36,36	0.43	0	47,47,47	0.91	3 (6%)
25	PHO	A	408	-	58,69,69	2.57	12 (20%)	55,99,99	3.00	16 (29%)
34	DMS	c	940	-	3,3,3	2.70	1 (33%)	3,3,3	0.48	0
34	DMS	C	527	-	3,3,3	2.70	1 (33%)	3,3,3	0.51	0
24	CLA	c	914	-	69,73,73	2.48	23 (33%)	82,113,113	2.29	26 (31%)
34	DMS	o	305	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
24	CLA	D	402	-	69,73,73	2.31	22 (31%)	82,113,113	2.41	28 (34%)
34	DMS	C	530	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
24	CLA	B	602	43	69,73,73	2.34	26 (37%)	82,113,113	2.36	29 (35%)
24	CLA	c	910	-	69,73,73	2.40	23 (33%)	82,113,113	2.41	32 (39%)
36	HTG	V	204	-	12,13,19	0.60	0	17,18,24	2.08	5 (29%)
34	DMS	V	212	-	3,3,3	2.74	1 (33%)	3,3,3	0.66	0
34	DMS	a	423	-	3,3,3	2.75	1 (33%)	3,3,3	0.68	0
34	DMS	c	932	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
24	CLA	C	509	-	69,73,73	2.43	24 (34%)	82,113,113	2.43	29 (35%)
34	DMS	c	938	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
34	DMS	B	633	-	3,3,3	2.66	1 (33%)	3,3,3	0.38	0
37	DGD	c	917	-	63,63,67	0.85	2 (3%)	77,77,81	1.13	6 (7%)
36	HTG	C	536	-	19,19,19	0.99	2 (10%)	23,24,24	1.14	1 (4%)
32	GOL	A	419	-	5,5,5	1.01	0	5,5,5	1.08	1 (20%)
24	CLA	d	401	43	69,73,73	2.34	21 (30%)	82,113,113	2.56	33 (40%)
34	DMS	c	936	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
24	CLA	B	608	43	69,73,73	2.24	22 (31%)	82,113,113	2.40	28 (34%)
37	DGD	d	408	-	50,50,67	0.96	2 (4%)	58,58,81	1.39	8 (13%)
24	CLA	A	405	-	69,73,73	2.50	22 (31%)	82,113,113	2.38	29 (35%)
24	CLA	b	618	-	69,73,73	2.36	23 (33%)	82,113,113	2.55	29 (35%)
28	LMG	D	409	41	51,51,55	0.83	2 (3%)	59,59,63	0.90	3 (5%)
31	LMT	M	102	-	25,25,36	0.48	0	30,30,47	0.93	1 (3%)
34	DMS	b	632	-	3,3,3	2.69	1 (33%)	3,3,3	0.47	0
34	DMS	V	201	-	3,3,3	2.70	1 (33%)	3,3,3	0.47	0
36	HTG	b	626	-	19,19,19	0.79	1 (5%)	23,24,24	1.22	3 (13%)
24	CLA	a	410	43	69,73,73	2.28	24 (34%)	82,113,113	2.56	29 (35%)
31	LMT	t	102	-	36,36,36	0.43	0	47,47,47	0.87	1 (2%)
34	DMS	B	641	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	C	515	-	41,41,41	0.73	0	56,56,56	1.47	7 (12%)
34	DMS	a	425	-	3,3,3	2.75	1 (33%)	3,3,3	0.54	0
36	HTG	c	928	-	19,19,19	0.98	2 (10%)	23,24,24	1.38	3 (13%)
34	DMS	O	307	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
34	DMS	e	102	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
36	HTG	v	211	-	19,19,19	0.96	2 (10%)	23,24,24	1.55	4 (17%)
29	PL9	d	407	-	55,55,55	0.77	1 (1%)	68,69,69	1.49	12 (17%)
24	CLA	B	617	-	69,73,73	2.34	22 (31%)	82,113,113	2.51	32 (39%)
34	DMS	o	307	-	3,3,3	2.74	1 (33%)	3,3,3	0.66	0
36	HTG	U	201	-	3,3,19	0.32	0	2,2,24	0.73	0
34	DMS	c	939	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
24	CLA	C	508	-	69,73,73	2.56	23 (33%)	82,113,113	2.37	27 (32%)
36	HTG	b	603	-	19,19,19	0.94	2 (10%)	23,24,24	1.27	3 (13%)
26	BCR	d	406	-	41,41,41	0.85	0	56,56,56	1.73	11 (19%)
32	GOL	V	206	-	5,5,5	0.88	0	5,5,5	1.04	0
24	CLA	C	513	-	69,73,73	2.37	25 (36%)	82,113,113	2.37	28 (34%)
34	DMS	D	414	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
34	DMS	v	210	-	3,3,3	2.76	1 (33%)	3,3,3	0.55	0
34	DMS	U	204	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
27	SQD	A	412	-	52,54,54	0.89	2 (3%)	62,65,65	1.68	12 (19%)
36	HTG	C	537	-	19,19,19	0.91	1 (5%)	23,24,24	1.38	3 (13%)
34	DMS	C	529	-	3,3,3	2.72	1 (33%)	3,3,3	0.46	0
34	DMS	O	313	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	0
29	PL9	D	404	-	55,55,55	0.74	2 (3%)	68,69,69	1.53	13 (19%)
38	LHG	l	103	-	48,48,48	0.89	2 (4%)	51,54,54	1.05	4 (7%)
34	DMS	a	421	-	3,3,3	2.71	1 (33%)	3,3,3	0.48	0
36	HTG	O	303	-	19,19,19	1.01	1 (5%)	23,24,24	1.08	2 (8%)
26	BCR	B	619	-	41,41,41	0.90	0	56,56,56	1.16	6 (10%)
38	LHG	d	409	-	48,48,48	0.89	3 (6%)	51,54,54	1.17	5 (9%)
32	GOL	a	419	-	5,5,5	1.15	0	5,5,5	0.71	0
34	DMS	L	102	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
36	HTG	c	943	-	17,17,19	0.96	1 (5%)	21,22,24	1.27	1 (4%)
34	DMS	B	632	-	3,3,3	2.51	1 (33%)	3,3,3	0.39	0
31	LMT	m	102	-	36,36,36	0.44	0	47,47,47	0.89	0
34	DMS	c	934	-	3,3,3	2.76	1 (33%)	3,3,3	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	a	422	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
24	CLA	C	511	3	69,73,73	2.52	23 (33%)	82,113,113	2.31	28 (34%)
26	BCR	c	915	-	41,41,41	0.76	0	56,56,56	1.38	7 (12%)
24	CLA	C	506	-	69,73,73	2.51	24 (34%)	82,113,113	2.38	29 (35%)
34	DMS	c	933	-	3,3,3	2.73	1 (33%)	3,3,3	0.50	0
34	DMS	O	315	-	3,3,3	2.77	1 (33%)	3,3,3	0.62	0
24	CLA	C	502	-	69,73,73	2.50	24 (34%)	82,113,113	2.44	28 (34%)
34	DMS	A	423	-	3,3,3	2.47	1 (33%)	3,3,3	0.75	0
32	GOL	c	929	-	5,5,5	1.03	0	5,5,5	1.00	0
26	BCR	b	622	-	41,41,41	0.87	0	56,56,56	1.09	3 (5%)
34	DMS	i	106	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
29	PL9	a	417	-	55,55,55	0.64	2 (3%)	68,69,69	1.82	18 (26%)
37	DGD	C	518	-	63,63,67	0.83	3 (4%)	77,77,81	0.99	4 (5%)
34	DMS	V	205	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
36	HTG	B	629	-	19,19,19	0.92	2 (10%)	23,24,24	1.33	3 (13%)
26	BCR	A	411	-	41,41,41	0.79	0	56,56,56	1.35	5 (8%)
34	DMS	v	203	-	3,3,3	2.69	1 (33%)	3,3,3	0.42	0
28	LMG	C	523	-	51,51,55	0.95	2 (3%)	59,59,63	1.28	8 (13%)
24	CLA	b	607	-	69,73,73	2.37	24 (34%)	82,113,113	2.42	28 (34%)
24	CLA	B	605	-	69,73,73	2.28	20 (28%)	82,113,113	2.49	28 (34%)
34	DMS	B	646	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
24	CLA	b	616	-	69,73,73	2.23	21 (30%)	82,113,113	2.55	29 (35%)
24	CLA	C	501	-	69,73,73	2.28	22 (31%)	82,113,113	2.42	27 (32%)
34	DMS	u	202	-	3,3,3	2.67	1 (33%)	3,3,3	0.74	0
36	HTG	C	520	-	19,19,19	0.92	2 (10%)	23,24,24	1.15	1 (4%)
36	HTG	d	419	-	19,19,19	0.96	2 (10%)	23,24,24	1.12	1 (4%)
24	CLA	b	613	-	69,73,73	2.54	23 (33%)	82,113,113	2.28	27 (32%)
25	PHO	a	411	-	58,69,69	2.54	12 (20%)	55,99,99	2.89	17 (30%)
24	CLA	C	503	-	69,73,73	2.63	20 (28%)	82,113,113	2.33	24 (29%)
34	DMS	e	104	-	3,3,3	2.76	1 (33%)	3,3,3	0.58	0
32	GOL	b	637	-	5,5,5	0.94	0	5,5,5	1.04	0
21	OEX	A	401	3,1,43	0,15,15	-	-	-		
32	GOL	B	637	-	5,5,5	0.99	0	5,5,5	0.97	0
36	HTG	B	623	-	19,19,19	1.01	1 (5%)	23,24,24	1.15	1 (4%)
34	DMS	v	209	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	609	-	69,73,73	2.27	24 (34%)	82,113,113	2.52	30 (36%)
36	HTG	C	521	-	19,19,19	0.96	2 (10%)	23,24,24	1.36	2 (8%)
34	DMS	b	647	-	3,3,3	2.73	1 (33%)	3,3,3	0.62	0
24	CLA	B	613	-	69,73,73	2.29	21 (30%)	82,113,113	2.32	24 (29%)
36	HTG	c	924	-	19,19,19	0.95	2 (10%)	23,24,24	1.17	2 (8%)
34	DMS	B	647	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
31	LMT	F	103	-	24,24,36	0.46	0	29,29,47	0.58	0
38	LHG	D	407	-	48,48,48	0.88	3 (6%)	51,54,54	0.92	3 (5%)
34	DMS	b	640	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0
34	DMS	V	210	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
26	BCR	c	916	-	41,41,41	0.79	0	56,56,56	1.38	7 (12%)
28	LMG	C	519	-	51,51,55	0.91	3 (5%)	59,59,63	1.20	6 (10%)
34	DMS	y	101	-	3,3,3	2.72	1 (33%)	3,3,3	0.56	0
24	CLA	b	611	43	69,73,73	2.30	21 (30%)	82,113,113	2.33	29 (35%)
24	CLA	B	612	-	69,73,73	2.41	20 (28%)	82,113,113	2.54	32 (39%)
34	DMS	v	207	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
24	CLA	B	611	43	69,73,73	2.49	24 (34%)	82,113,113	2.43	31 (37%)
25	PHO	a	412	-	58,69,69	2.72	12 (20%)	55,99,99	3.00	15 (27%)
24	CLA	b	610	-	69,73,73	2.42	21 (30%)	82,113,113	2.39	29 (35%)
33	BCT	A	422	22	3,3,3	0.52	0	2,3,3	0.61	0
36	HTG	c	941	-	19,19,19	0.92	1 (5%)	23,24,24	1.76	5 (21%)
31	LMT	j	102	-	24,24,36	0.55	1 (4%)	29,29,47	0.89	0
34	DMS	O	309	-	3,3,3	2.70	1 (33%)	3,3,3	0.48	0
34	DMS	b	641	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
24	CLA	B	615	-	69,73,73	2.19	20 (28%)	82,113,113	2.56	30 (36%)
27	SQD	f	102	-	41,43,54	1.12	2 (4%)	51,54,65	1.47	6 (11%)
27	SQD	A	416	-	52,54,54	0.98	2 (3%)	62,65,65	1.09	4 (6%)
28	LMG	c	921	-	51,51,55	0.97	2 (3%)	59,59,63	1.20	6 (10%)
36	HTG	y	102	-	19,19,19	0.98	2 (10%)	23,24,24	1.08	1 (4%)
34	DMS	C	532	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
34	DMS	C	534	-	3,3,3	2.71	1 (33%)	3,3,3	0.44	0
26	BCR	D	403	-	41,41,41	0.86	0	56,56,56	1.71	9 (16%)
36	HTG	B	625	-	19,19,19	0.93	1 (5%)	23,24,24	1.74	3 (13%)
24	CLA	B	607	-	69,73,73	2.46	22 (31%)	82,113,113	2.42	30 (36%)
29	PL9	A	414	-	55,55,55	0.62	1 (1%)	68,69,69	1.92	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	616	-	69,73,73	2.42	23 (33%)	82,113,113	2.43	29 (35%)
24	CLA	b	620	-	69,73,73	2.43	22 (31%)	82,113,113	2.48	27 (32%)
34	DMS	c	935	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
34	DMS	O	314	-	3,3,3	2.73	1 (33%)	3,3,3	0.66	0
34	DMS	V	211	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
34	DMS	o	306	-	3,3,3	2.76	1 (33%)	3,3,3	0.68	0
34	DMS	d	416	-	3,3,3	2.72	1 (33%)	3,3,3	0.44	0
34	DMS	C	524	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
24	CLA	c	909	-	69,73,73	2.36	24 (34%)	82,113,113	2.58	30 (36%)
26	BCR	B	618	-	41,41,41	0.78	0	56,56,56	1.34	6 (10%)
34	DMS	O	305	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
37	DGD	c	918	-	63,63,67	0.83	2 (3%)	77,77,81	1.00	4 (5%)
34	DMS	b	642	-	3,3,3	2.74	1 (33%)	3,3,3	0.55	0
38	LHG	d	410	-	48,48,48	0.86	2 (4%)	51,54,54	0.93	3 (5%)
34	DMS	D	415	-	3,3,3	2.77	1 (33%)	3,3,3	0.56	0
38	LHG	d	411	-	46,46,48	0.88	2 (4%)	49,52,54	1.03	4 (8%)
36	HTG	b	627	-	19,19,19	1.02	2 (10%)	23,24,24	1.56	4 (17%)
26	BCR	T	101	-	41,41,41	0.73	0	56,56,56	1.71	12 (21%)
34	DMS	V	209	-	3,3,3	2.66	1 (33%)	3,3,3	0.60	0
34	DMS	b	645	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
34	DMS	v	208	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
33	BCT	a	408[A]	22	3,3,3	0.52	0	2,3,3	0.72	0
27	SQD	b	601	-	52,54,54	1.00	3 (5%)	62,65,65	1.58	12 (19%)
24	CLA	c	906	-	69,73,73	2.36	22 (31%)	82,113,113	2.31	30 (36%)
37	DGD	C	516	-	63,63,67	0.83	3 (4%)	77,77,81	1.11	5 (6%)
31	LMT	A	417	-	36,36,36	0.47	0	47,47,47	1.21	3 (6%)
26	BCR	Y	101	-	41,41,41	0.81	0	56,56,56	1.55	10 (17%)
42	HEC	v	202	16	46,50,50	2.03	8 (17%)	58,82,82	1.31	6 (10%)
26	BCR	k	103	-	41,41,41	0.74	0	56,56,56	1.30	6 (10%)
34	DMS	B	634	-	3,3,3	2.76	1 (33%)	3,3,3	0.75	0
36	HTG	d	414	-	19,19,19	0.95	1 (5%)	23,24,24	1.52	3 (13%)
31	LMT	e	101	-	24,24,36	0.47	0	29,29,47	0.64	0
34	DMS	A	425	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
24	CLA	c	908	43	69,73,73	2.41	21 (30%)	82,113,113	2.53	31 (37%)
34	DMS	D	416	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	RRX	H	101	-	42,42,42	0.72	0	56,58,58	1.33	6 (10%)
34	DMS	b	646	-	3,3,3	2.79	1 (33%)	3,3,3	0.62	0
36	HTG	V	215	-	19,19,19	0.95	1 (5%)	23,24,24	1.92	3 (13%)
26	BCR	B	636	-	41,41,41	0.74	0	56,56,56	1.61	12 (21%)
34	DMS	b	639	-	3,3,3	2.73	1 (33%)	3,3,3	0.61	0
39	HEM	F	102	5,6	50,50,50	1.88	9 (18%)	67,82,82	1.31	5 (7%)
24	CLA	c	903	-	69,73,73	2.40	22 (31%)	82,113,113	2.35	26 (31%)
34	DMS	b	631	-	3,3,3	2.43	1 (33%)	3,3,3	0.43	0
24	CLA	b	619	-	69,73,73	2.37	23 (33%)	82,113,113	2.33	29 (35%)
34	DMS	C	528	-	3,3,3	2.75	1 (33%)	3,3,3	0.59	0
31	LMT	Z	101	-	36,36,36	0.42	0	47,47,47	0.92	1 (2%)
36	HTG	B	631	-	19,19,19	0.90	1 (5%)	23,24,24	1.57	2 (8%)
36	HTG	d	420	-	19,19,19	0.92	1 (5%)	23,24,24	1.29	2 (8%)
24	CLA	C	510	-	69,73,73	2.48	25 (36%)	82,113,113	2.46	34 (41%)
34	DMS	V	213	-	3,3,3	2.73	1 (33%)	3,3,3	0.64	0
24	CLA	B	610	-	69,73,73	2.50	21 (30%)	82,113,113	2.31	29 (35%)
24	CLA	C	512	-	69,73,73	2.56	24 (34%)	82,113,113	2.35	30 (36%)
34	DMS	e	103	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
39	HEM	f	101	5,6	50,50,50	1.89	8 (16%)	67,82,82	1.34	7 (10%)
31	LMT	c	922	-	36,36,36	0.50	1 (2%)	47,47,47	1.26	4 (8%)
34	DMS	v	205	-	3,3,3	2.73	1 (33%)	3,3,3	0.58	0
24	CLA	b	605	43	69,73,73	2.46	23 (33%)	82,113,113	2.33	27 (32%)
24	CLA	c	911	-	69,73,73	2.43	24 (34%)	82,113,113	2.38	26 (31%)
42	HEC	V	203	16	46,50,50	1.96	7 (15%)	58,82,82	1.45	5 (8%)
34	DMS	A	427	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0
34	DMS	O	310	-	3,3,3	2.73	1 (33%)	3,3,3	0.50	0
34	DMS	C	526	-	3,3,3	2.69	1 (33%)	3,3,3	0.41	0
31	LMT	t	101	-	23,23,36	0.47	0	26,27,47	0.97	1 (3%)
34	DMS	U	203	-	3,3,3	2.75	1 (33%)	3,3,3	0.88	0
34	DMS	O	302	-	3,3,3	2.74	1 (33%)	3,3,3	0.64	0
28	LMG	A	413	-	51,51,55	0.95	2 (3%)	59,59,63	1.17	6 (10%)
24	CLA	c	902	-	69,73,73	2.40	22 (31%)	82,113,113	2.57	30 (36%)
34	DMS	B	643	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
34	DMS	K	102	-	3,3,3	2.71	1 (33%)	3,3,3	0.47	0
32	GOL	O	304	-	5,5,5	0.85	0	5,5,5	1.14	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	HTG	b	602	-	19,19,19	0.93	2 (10%)	23,24,24	1.29	3 (13%)
24	CLA	b	617	-	69,73,73	2.44	22 (31%)	82,113,113	2.45	30 (36%)
36	HTG	D	412	-	19,19,19	0.96	1 (5%)	23,24,24	1.33	3 (13%)
24	CLA	b	612	-	69,73,73	2.71	23 (33%)	82,113,113	2.33	26 (31%)
38	LHG	D	408	-	45,45,48	0.91	2 (4%)	48,51,54	0.97	4 (8%)
34	DMS	V	208	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
34	DMS	a	424	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
34	DMS	o	304	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
25	PHO	A	409	-	58,69,69	2.81	13 (22%)	55,99,99	3.10	15 (27%)
24	CLA	b	608	-	69,73,73	2.66	22 (31%)	82,113,113	2.47	28 (34%)
34	DMS	A	424	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
31	LMT	B	626	-	24,24,36	0.47	0	29,29,47	1.13	2 (6%)
34	DMS	C	535	-	3,3,3	2.77	1 (33%)	3,3,3	0.58	0
31	LMT	a	402	-	36,36,36	0.43	0	47,47,47	1.14	4 (8%)
24	CLA	b	615	-	69,73,73	2.40	22 (31%)	82,113,113	2.37	32 (39%)
28	LMG	B	621	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	4 (6%)
21	OEX	a	404	3,1,43	0,15,15	-	-	-		
37	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.90	3 (3%)
34	DMS	C	531	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
32	GOL	B	638	-	5,5,5	1.09	0	5,5,5	1.29	1 (20%)
36	HTG	B	624	-	19,19,19	0.73	1 (5%)	23,24,24	1.34	2 (8%)
24	CLA	A	410	-	69,73,73	2.18	22 (31%)	82,113,113	2.52	31 (37%)
34	DMS	h	105	-	3,3,3	2.71	1 (33%)	3,3,3	0.38	0
31	LMT	m	103	-	36,36,36	0.41	0	47,47,47	0.81	1 (2%)
34	DMS	O	308	-	3,3,3	2.71	1 (33%)	3,3,3	0.48	0
26	BCR	b	621	-	41,41,41	0.76	0	56,56,56	1.49	9 (16%)
24	CLA	d	404	-	69,73,73	2.48	23 (33%)	82,113,113	2.47	31 (37%)
28	LMG	a	416	-	51,51,55	0.96	3 (5%)	59,59,63	1.29	9 (15%)
34	DMS	c	926	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
34	DMS	H	104	-	3,3,3	2.71	1 (33%)	3,3,3	0.58	0
26	BCR	B	620	-	41,41,41	0.69	0	56,56,56	1.27	8 (14%)
24	CLA	B	603	-	69,73,73	2.34	24 (34%)	82,113,113	2.55	31 (37%)
24	CLA	c	904	-	69,73,73	2.65	24 (34%)	82,113,113	2.21	29 (35%)
26	BCR	C	514	-	41,41,41	0.77	0	56,56,56	1.36	7 (12%)
24	CLA	C	507	43	69,73,73	2.55	22 (31%)	82,113,113	2.47	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	614	-	69,73,73	2.25	21 (30%)	82,113,113	2.47	31 (37%)
38	LHG	D	406	-	48,48,48	0.83	2 (4%)	51,54,54	1.21	7 (13%)
24	CLA	d	405	-	69,73,73	2.27	22 (31%)	82,113,113	2.53	32 (39%)
34	DMS	B	640	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
26	BCR	a	414	-	41,41,41	0.80	0	56,56,56	1.28	5 (8%)
32	GOL	C	525	-	5,5,5	0.95	0	5,5,5	1.04	0
34	DMS	o	302	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
34	DMS	d	417	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
24	CLA	B	609	-	69,73,73	2.37	23 (33%)	82,113,113	2.28	27 (32%)
24	CLA	C	505	-	69,73,73	2.66	22 (31%)	82,113,113	2.22	25 (30%)
24	CLA	b	614	43	69,73,73	2.26	22 (31%)	82,113,113	2.38	29 (35%)
24	CLA	c	907	-	69,73,73	2.43	24 (34%)	82,113,113	2.39	27 (32%)
34	DMS	A	426	-	3,3,3	2.73	1 (33%)	3,3,3	0.62	0
24	CLA	c	905	43	69,73,73	2.19	24 (34%)	82,113,113	2.56	32 (39%)
34	DMS	a	420	-	3,3,3	2.57	1 (33%)	3,3,3	0.43	0
27	SQD	a	415	-	52,54,54	0.89	2 (3%)	62,65,65	1.66	11 (17%)
24	CLA	c	912	3	69,73,73	2.36	22 (31%)	82,113,113	2.37	30 (36%)
33	BCT	d	402[B]	22	3,3,3	0.55	0	2,3,3	0.43	0
34	DMS	d	415	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
28	LMG	d	412	41	51,51,55	0.90	2 (3%)	59,59,63	0.89	3 (5%)
34	DMS	O	311	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0
36	HTG	c	923	-	19,19,19	0.94	2 (10%)	23,24,24	1.39	3 (13%)
34	DMS	U	202	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
28	LMG	b	624	-	51,51,55	0.95	2 (3%)	59,59,63	1.08	4 (6%)
34	DMS	v	206	-	3,3,3	2.78	1 (33%)	3,3,3	0.57	0
24	CLA	D	401	-	69,73,73	2.16	24 (34%)	82,113,113	2.61	29 (35%)
27	SQD	l	101	-	52,54,54	0.97	3 (5%)	62,65,65	1.32	5 (8%)
24	CLA	a	413	-	69,73,73	2.15	23 (33%)	82,113,113	2.47	32 (39%)
34	DMS	B	645	-	3,3,3	2.74	1 (33%)	3,3,3	0.64	0
34	DMS	b	643	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
34	DMS	D	413	-	3,3,3	2.65	1 (33%)	3,3,3	0.49	0
31	LMT	b	625	-	36,36,36	0.39	0	47,47,47	1.28	7 (14%)
38	LHG	L	101	-	48,48,48	0.96	2 (4%)	51,54,54	1.13	4 (7%)
34	DMS	d	418	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0
26	BCR	k	102	-	41,41,41	0.78	0	56,56,56	1.55	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	DMS	c	931	-	3,3,3	2.69	1 (33%)	3,3,3	0.50	0
34	DMS	C	533	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
31	LMT	J	102	-	24,24,36	0.51	0	29,29,47	0.76	0
24	CLA	c	913	-	69,73,73	2.57	23 (33%)	82,113,113	2.46	29 (35%)
37	DGD	D	405	-	52,52,67	0.93	2 (3%)	60,60,81	1.18	6 (10%)
36	HTG	B	630	-	19,19,19	0.92	2 (10%)	23,24,24	1.25	2 (8%)
31	LMT	M	101	-	36,36,36	0.39	0	47,47,47	0.83	1 (2%)
34	DMS	O	312	-	3,3,3	2.74	1 (33%)	3,3,3	0.50	0
24	CLA	A	406	43	69,73,73	2.29	24 (34%)	82,113,113	2.60	27 (32%)
37	DGD	c	919	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	4 (5%)
24	CLA	A	407	43	69,73,73	2.15	20 (28%)	82,113,113	2.60	32 (39%)
40	RRX	h	101	-	42,42,42	0.74	0	56,58,58	1.32	7 (12%)
27	SQD	F	101	-	35,37,54	0.90	1 (2%)	44,47,65	1.89	9 (20%)
34	DMS	b	638	-	3,3,3	2.80	1 (33%)	3,3,3	0.69	0
34	DMS	V	214	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
31	LMT	A	421	-	36,36,36	0.43	0	47,47,47	1.01	1 (2%)
24	CLA	a	409	-	69,73,73	2.39	23 (33%)	82,113,113	2.45	28 (34%)
34	DMS	B	639	-	3,3,3	2.70	1 (33%)	3,3,3	0.49	0
24	CLA	b	606	-	69,73,73	2.43	24 (34%)	82,113,113	2.44	30 (36%)
34	DMS	c	930	-	3,3,3	2.59	1 (33%)	3,3,3	0.37	0
24	CLA	B	606	-	69,73,73	2.28	23 (33%)	82,113,113	2.43	30 (36%)
34	DMS	o	303	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0
34	DMS	v	204	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
34	DMS	B	642	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
31	LMT	B	622	-	36,36,36	0.43	0	47,47,47	1.60	12 (25%)
37	DGD	H	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.99	7 (9%)
34	DMS	b	644	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
34	DMS	O	306	-	3,3,3	2.73	1 (33%)	3,3,3	0.48	0
37	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.06	6 (7%)
34	DMS	B	644	-	3,3,3	2.65	1 (33%)	3,3,3	0.33	0
24	CLA	B	604	-	69,73,73	2.26	24 (34%)	82,113,113	2.55	28 (34%)
36	HTG	c	942	-	19,19,19	0.93	2 (10%)	23,24,24	1.21	3 (13%)
34	DMS	c	937	-	3,3,3	2.70	1 (33%)	3,3,3	0.58	0

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
29	PL9	a	417	-	-	11/53/73/73	0/1/1/1
37	DGD	C	518	-	-	10/51/91/95	0/2/2/2
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
24	CLA	C	507	43	1/1/15/20	8/39/115/115	-
27	SQD	a	401	-	-	20/49/69/69	0/1/1/1
36	HTG	B	629	-	-	2/10/30/30	0/1/1/1
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
32	GOL	V	207	-	-	1/4/4/4	-
28	LMG	c	920	-	-	8/46/66/70	0/1/1/1
36	HTG	O	316	-	-	1/10/30/30	0/1/1/1
24	CLA	B	614	-	1/1/15/20	5/39/115/115	-
24	CLA	C	504	43	1/1/15/20	4/39/115/115	-
38	LHG	D	406	-	-	8/53/53/53	-
24	CLA	d	405	-	1/1/15/20	4/39/115/115	-
40	RRX	H	101	-	-	2/29/65/65	0/2/2/2
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
28	LMG	C	523	-	-	9/46/66/70	0/1/1/1
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
24	CLA	b	607	-	1/1/15/20	1/39/115/115	-
24	CLA	B	605	-	1/1/15/20	0/39/115/115	-
26	BCR	B	636	-	-	1/29/63/63	0/2/2/2
26	BCR	a	414	-	-	0/29/63/63	0/2/2/2
36	HTG	V	215	-	-	1/10/30/30	0/1/1/1
38	LHG	E	101	-	-	10/46/46/53	-
24	CLA	b	616	-	1/1/15/20	3/39/115/115	-
32	GOL	C	525	-	-	0/4/4/4	-
39	HEM	F	102	5,6	-	2/14/54/54	-
31	LMT	c	927	-	-	11/21/61/61	0/2/2/2
24	CLA	c	903	-	1/1/15/20	5/39/115/115	-
25	PHO	A	408	-	-	0/37/103/103	0/5/6/6
24	CLA	C	501	-	1/1/15/20	3/39/115/115	-
24	CLA	b	619	-	1/1/15/20	7/39/115/115	-
31	LMT	Z	101	-	-	7/21/61/61	0/2/2/2
36	HTG	C	520	-	-	3/10/30/30	0/1/1/1
36	HTG	d	419	-	-	1/10/30/30	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	B	631	-	-	1/10/30/30	0/1/1/1
24	CLA	b	613	-	1/1/15/20	2/39/115/115	-
24	CLA	B	609	-	-	2/39/115/115	-
24	CLA	C	505	-	1/1/15/20	1/39/115/115	-
36	HTG	d	420	-	-	3/10/30/30	0/1/1/1
25	PHO	a	411	-	-	2/37/103/103	0/5/6/6
24	CLA	C	510	-	1/1/15/20	3/39/115/115	-
24	CLA	b	614	43	1/1/15/20	2/39/115/115	-
24	CLA	c	914	-	1/1/15/20	2/39/115/115	-
24	CLA	C	503	-	1/1/15/20	4/39/115/115	-
24	CLA	D	402	-	1/1/15/20	5/39/115/115	-
32	GOL	b	637	-	-	0/4/4/4	-
24	CLA	B	602	43	1/1/15/20	12/39/115/115	-
24	CLA	c	907	-	1/1/15/20	8/39/115/115	-
32	GOL	B	637	-	-	4/4/4/4	-
36	HTG	B	623	-	-	2/10/30/30	0/1/1/1
24	CLA	c	910	-	1/1/15/20	6/39/115/115	-
24	CLA	b	609	-	1/1/15/20	3/39/115/115	-
36	HTG	C	521	-	-	1/10/30/30	0/1/1/1
36	HTG	V	204	-	-	3/4/24/30	0/1/1/1
24	CLA	c	905	43	1/1/15/20	4/39/115/115	-
24	CLA	B	610	-	1/1/15/20	5/39/115/115	-
24	CLA	C	512	-	1/1/15/20	3/39/115/115	-
27	SQD	a	415	-	-	6/49/69/69	0/1/1/1
24	CLA	B	613	-	1/1/15/20	1/39/115/115	-
36	HTG	c	924	-	-	0/10/30/30	0/1/1/1
31	LMT	F	103	-	-	4/15/35/61	0/1/1/2
24	CLA	c	912	3	-	0/39/115/115	-
39	HEM	f	101	5,6	-	0/14/54/54	-
38	LHG	D	407	-	-	4/53/53/53	-
31	LMT	c	922	-	-	5/21/61/61	0/2/2/2
24	CLA	C	509	-	1/1/15/20	8/39/115/115	-
26	BCR	c	916	-	-	3/29/63/63	0/2/2/2
28	LMG	C	519	-	-	14/46/66/70	0/1/1/1
24	CLA	b	611	43	1/1/15/20	1/39/115/115	-
24	CLA	B	612	-	1/1/15/20	1/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	605	43	1/1/15/20	3/39/115/115	-
24	CLA	B	611	43	1/1/15/20	2/39/115/115	-
25	PHO	a	412	-	-	1/37/103/103	0/5/6/6
28	LMG	d	412	41	-	8/46/66/70	0/1/1/1
24	CLA	c	911	-	1/1/15/20	2/39/115/115	-
36	HTG	c	923	-	-	0/10/30/30	0/1/1/1
24	CLA	b	610	-	1/1/15/20	2/39/115/115	-
42	HEC	V	203	16	-	6/14/54/54	-
37	DGD	c	917	-	-	13/51/91/95	0/2/2/2
36	HTG	C	536	-	-	1/10/30/30	0/1/1/1
28	LMG	b	624	-	-	11/46/66/70	0/1/1/1
24	CLA	D	401	-	1/1/15/20	4/39/115/115	-
27	SQD	l	101	-	-	21/49/69/69	0/1/1/1
32	GOL	A	419	-	-	2/4/4/4	-
36	HTG	c	941	-	-	1/10/30/30	0/1/1/1
31	LMT	t	101	-	-	3/15/31/61	0/1/1/2
24	CLA	a	413	-	1/1/15/20	6/39/115/115	-
24	CLA	d	401	43	1/1/15/20	3/39/115/115	-
24	CLA	B	608	43	1/1/15/20	1/39/115/115	-
37	DGD	d	408	-	-	20/44/64/95	0/1/1/2
24	CLA	A	405	-	1/1/15/20	2/39/115/115	-
24	CLA	b	618	-	1/1/15/20	11/39/115/115	-
28	LMG	D	409	41	-	3/46/66/70	0/1/1/1
28	LMG	A	413	-	-	16/46/66/70	0/1/1/1
31	LMT	j	102	-	-	3/15/35/61	0/1/1/2
24	CLA	c	902	-	1/1/15/20	3/39/115/115	-
31	LMT	b	625	-	-	8/21/61/61	0/2/2/2
31	LMT	M	102	-	-	7/17/37/61	0/1/1/2
32	GOL	O	304	-	-	2/4/4/4	-
38	LHG	L	101	-	-	13/53/53/53	-
24	CLA	B	615	-	1/1/15/20	2/39/115/115	-
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
36	HTG	b	602	-	-	2/10/30/30	0/1/1/1
24	CLA	a	410	43	-	2/39/115/115	-
31	LMT	t	102	-	-	9/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	617	-	1/1/15/20	2/39/115/115	-
27	SQD	A	416	-	-	11/49/69/69	0/1/1/1
28	LMG	c	921	-	-	1/46/66/70	0/1/1/1
36	HTG	b	626	-	-	2/10/30/30	0/1/1/1
36	HTG	y	102	-	-	3/10/30/30	0/1/1/1
26	BCR	C	515	-	-	1/29/63/63	0/2/2/2
36	HTG	D	412	-	-	3/10/30/30	0/1/1/1
36	HTG	c	928	-	-	0/10/30/30	0/1/1/1
24	CLA	b	612	-	-	2/39/115/115	-
26	BCR	k	102	-	-	4/29/63/63	0/2/2/2
38	LHG	D	408	-	-	8/50/50/53	-
26	BCR	D	403	-	-	6/29/63/63	0/2/2/2
36	HTG	v	211	-	-	1/10/30/30	0/1/1/1
31	LMT	J	102	-	-	3/15/35/61	0/1/1/2
36	HTG	B	625	-	-	3/10/30/30	0/1/1/1
24	CLA	B	607	-	1/1/15/20	5/39/115/115	-
24	CLA	c	913	-	1/1/15/20	4/39/115/115	-
37	DGD	D	405	-	-	20/47/67/95	0/1/1/2
29	PL9	A	414	-	-	11/53/73/73	0/1/1/1
24	CLA	B	616	-	1/1/15/20	10/39/115/115	-
24	CLA	b	620	-	1/1/15/20	9/39/115/115	-
29	PL9	d	407	-	-	6/53/73/73	0/1/1/1
24	CLA	B	617	-	1/1/15/20	10/39/115/115	-
25	PHO	A	409	-	-	0/37/103/103	0/5/6/6
24	CLA	b	608	-	1/1/15/20	4/39/115/115	-
36	HTG	U	201	-	-	0/1/1/30	-
24	CLA	C	508	-	1/1/15/20	4/39/115/115	-
36	HTG	b	603	-	-	0/10/30/30	0/1/1/1
26	BCR	d	406	-	-	4/29/63/63	0/2/2/2
32	GOL	V	206	-	-	4/4/4/4	-
36	HTG	B	630	-	-	1/10/30/30	0/1/1/1
31	LMT	B	626	-	-	9/15/35/61	0/1/1/2
31	LMT	M	101	-	-	3/21/61/61	0/2/2/2
24	CLA	C	513	-	-	9/39/115/115	-
24	CLA	c	909	-	1/1/15/20	7/39/115/115	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	a	402	-	-	7/21/61/61	0/2/2/2
24	CLA	A	406	43	-	3/39/115/115	-
37	DGD	c	919	-	-	9/51/91/95	0/2/2/2
37	DGD	c	918	-	-	15/51/91/95	0/2/2/2
24	CLA	b	615	-	1/1/15/20	2/39/115/115	-
28	LMG	B	621	-	-	13/46/66/70	0/1/1/1
27	SQD	A	412	-	-	9/49/69/69	0/1/1/1
36	HTG	C	537	-	-	2/10/30/30	0/1/1/1
37	DGD	h	102	-	-	10/51/91/95	0/2/2/2
24	CLA	A	407	43	-	2/39/115/115	-
38	LHG	d	410	-	-	9/53/53/53	-
38	LHG	d	411	-	-	9/51/51/53	-
36	HTG	b	627	-	-	3/10/30/30	0/1/1/1
40	RRX	h	101	-	-	1/29/65/65	0/2/2/2
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
32	GOL	B	638	-	-	4/4/4/4	-
27	SQD	F	101	-	-	8/31/51/69	0/1/1/1
36	HTG	B	624	-	-	2/10/30/30	0/1/1/1
29	PL9	D	404	-	-	1/53/73/73	0/1/1/1
38	LHG	l	103	-	-	13/53/53/53	-
27	SQD	b	601	-	-	17/49/69/69	0/1/1/1
24	CLA	A	410	-	-	8/39/115/115	-
36	HTG	O	303	-	-	2/10/30/30	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	c	906	-	1/1/15/20	6/39/115/115	-
37	DGD	C	516	-	-	14/51/91/95	0/2/2/2
38	LHG	d	409	-	-	6/53/53/53	-
31	LMT	m	103	-	-	2/21/61/61	0/2/2/2
31	LMT	A	417	-	-	6/21/61/61	0/2/2/2
32	GOL	a	419	-	-	2/4/4/4	-
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
31	LMT	A	421	-	-	8/21/61/61	0/2/2/2
36	HTG	c	943	-	-	2/8/28/30	0/1/1/1
42	HEC	v	202	16	-	6/14/54/54	-
24	CLA	a	409	-	1/1/15/20	3/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2
24	CLA	b	606	-	1/1/15/20	5/39/115/115	-
31	LMT	m	102	-	-	3/21/61/61	0/2/2/2
24	CLA	B	606	-	1/1/15/20	4/39/115/115	-
24	CLA	C	511	3	1/1/15/20	3/39/115/115	-
26	BCR	c	915	-	-	0/29/63/63	0/2/2/2
26	BCR	k	103	-	-	0/29/63/63	0/2/2/2
24	CLA	C	506	-	1/1/15/20	5/39/115/115	-
24	CLA	d	404	-	1/1/15/20	5/39/115/115	-
28	LMG	a	416	-	-	18/46/66/70	0/1/1/1
31	LMT	B	622	-	-	6/21/61/61	0/2/2/2
24	CLA	C	502	-	-	4/39/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
36	HTG	d	414	-	-	4/10/30/30	0/1/1/1
24	CLA	B	603	-	1/1/15/20	4/39/115/115	-
37	DGD	H	102	-	-	10/51/91/95	0/2/2/2
32	GOL	c	929	-	-	2/4/4/4	-
31	LMT	e	101	-	-	3/15/35/61	0/1/1/2
37	DGD	C	517	-	-	14/51/91/95	0/2/2/2
24	CLA	B	604	-	1/1/15/20	3/39/115/115	-
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
36	HTG	c	942	-	-	2/10/30/30	0/1/1/1
24	CLA	c	908	43	1/1/15/20	5/39/115/115	-
24	CLA	c	904	-	1/1/15/20	3/39/115/115	-

All (1918) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	904	CLA	MG-NA	10.97	2.32	2.06
24	C	507	CLA	MG-NA	10.43	2.31	2.06
24	C	511	CLA	MG-NA	10.27	2.30	2.06
24	C	503	CLA	MG-NA	10.00	2.30	2.06
24	b	612	CLA	MG-ND	-9.99	1.86	2.05
24	b	608	CLA	MG-ND	-9.58	1.86	2.05
24	B	607	CLA	MG-NA	9.53	2.28	2.06
24	b	615	CLA	MG-NA	9.28	2.28	2.06
24	b	608	CLA	MG-NA	9.03	2.27	2.06
25	a	412	PHO	C3B-C4B	8.96	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C1D-C2D	8.95	1.49	1.39
24	c	908	CLA	MG-NA	8.91	2.27	2.06
24	c	913	CLA	MG-ND	-8.91	1.88	2.05
24	B	616	CLA	MG-NA	8.89	2.27	2.06
24	b	613	CLA	MG-NA	8.85	2.27	2.06
24	A	405	CLA	MG-ND	-8.82	1.88	2.05
25	a	411	PHO	C1D-C2D	8.74	1.49	1.39
25	A	409	PHO	C1D-C2D	8.73	1.49	1.39
25	a	412	PHO	C1D-C2D	8.67	1.49	1.39
24	C	506	CLA	MG-NA	8.63	2.26	2.06
25	A	409	PHO	C1B-C2B	8.57	1.48	1.39
24	b	619	CLA	MG-NA	8.52	2.26	2.06
24	B	612	CLA	MG-NA	8.50	2.26	2.06
25	A	409	PHO	C3B-C4B	8.48	1.50	1.41
24	C	510	CLA	MG-ND	-8.46	1.89	2.05
24	C	505	CLA	MG-ND	-8.42	1.89	2.05
24	C	508	CLA	MG-ND	-8.30	1.89	2.05
24	d	404	CLA	MG-ND	-8.30	1.89	2.05
24	c	910	CLA	MG-NA	8.30	2.26	2.06
24	b	610	CLA	MG-NA	8.21	2.25	2.06
25	a	412	PHO	C1B-C2B	8.02	1.48	1.39
24	C	512	CLA	MG-NA	7.96	2.25	2.06
24	d	401	CLA	MG-ND	-7.92	1.90	2.05
24	B	611	CLA	MG-ND	-7.76	1.90	2.05
24	C	505	CLA	MG-NA	7.74	2.24	2.06
24	c	914	CLA	MG-NC	7.72	2.24	2.06
39	f	101	HEM	C3D-C2D	7.65	1.53	1.36
24	c	913	CLA	MG-NA	7.65	2.24	2.06
24	b	620	CLA	MG-NA	7.65	2.24	2.06
24	C	502	CLA	MG-ND	-7.61	1.90	2.05
25	a	411	PHO	C1B-C2B	7.59	1.47	1.39
24	c	902	CLA	MG-ND	-7.57	1.90	2.05
24	b	620	CLA	MG-ND	-7.52	1.90	2.05
24	c	909	CLA	MG-ND	-7.45	1.91	2.05
39	F	102	HEM	C3D-C2D	7.43	1.52	1.36
25	A	408	PHO	C1B-C2B	7.41	1.47	1.39
24	B	617	CLA	MG-NA	7.40	2.23	2.06
24	c	912	CLA	MG-NA	7.29	2.23	2.06
24	B	610	CLA	MG-NC	7.28	2.23	2.06
24	b	617	CLA	MG-ND	-7.24	1.91	2.05
24	B	609	CLA	MG-NA	7.22	2.23	2.06
24	c	911	CLA	MG-ND	-7.16	1.91	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	911	CLA	MG-NC	7.15	2.23	2.06
24	B	610	CLA	MG-NA	7.14	2.23	2.06
24	c	907	CLA	MG-ND	-7.12	1.91	2.05
24	b	612	CLA	MG-NA	7.12	2.23	2.06
24	b	617	CLA	MG-NA	7.09	2.23	2.06
25	A	409	PHO	C4D-CHA	7.04	1.50	1.39
24	b	612	CLA	MG-NC	7.01	2.22	2.06
24	C	512	CLA	MG-ND	-6.99	1.91	2.05
25	A	408	PHO	C3B-C4B	6.98	1.48	1.41
24	B	612	CLA	MG-ND	-6.96	1.92	2.05
24	b	618	CLA	MG-ND	-6.88	1.92	2.05
24	C	501	CLA	MG-NA	6.86	2.22	2.06
25	a	411	PHO	C4D-CHA	6.86	1.49	1.39
24	A	406	CLA	MG-ND	-6.77	1.92	2.05
24	B	610	CLA	MG-ND	-6.76	1.92	2.05
24	C	509	CLA	MG-NC	6.72	2.22	2.06
24	b	609	CLA	MG-NA	6.65	2.22	2.06
25	A	409	PHO	C3B-C2B	6.64	1.49	1.40
24	c	906	CLA	MG-NA	6.64	2.22	2.06
24	d	404	CLA	MG-NA	6.62	2.22	2.06
25	a	411	PHO	C3B-C4B	6.62	1.48	1.41
24	b	605	CLA	MG-NC	6.62	2.22	2.06
24	B	602	CLA	MG-NA	6.62	2.22	2.06
24	c	904	CLA	MG-NC	6.61	2.22	2.06
24	C	503	CLA	MG-NC	6.59	2.21	2.06
24	c	903	CLA	MG-NA	6.56	2.21	2.06
24	b	613	CLA	MG-NC	6.54	2.21	2.06
25	A	408	PHO	C4D-CHA	6.52	1.49	1.39
24	b	606	CLA	MG-ND	-6.51	1.92	2.05
24	C	502	CLA	MG-NA	6.50	2.21	2.06
42	v	202	HEC	CAC-C3C	6.45	1.55	1.35
24	c	902	CLA	MG-NA	6.43	2.21	2.06
24	b	616	CLA	MG-ND	-6.43	1.93	2.05
24	C	513	CLA	MG-ND	-6.40	1.93	2.05
42	V	203	HEC	CAB-C3B	6.37	1.55	1.35
24	B	614	CLA	MG-NA	6.36	2.21	2.06
24	b	607	CLA	MG-NC	6.35	2.21	2.06
24	d	404	CLA	MG-NC	6.34	2.21	2.06
42	V	203	HEC	CAC-C3C	6.34	1.55	1.35
42	v	202	HEC	CAB-C3B	6.33	1.55	1.35
24	C	510	CLA	MG-NA	6.31	2.21	2.06
24	D	401	CLA	MG-NA	6.29	2.21	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	412	PHO	C4D-CHA	6.26	1.48	1.39
24	a	409	CLA	MG-ND	-6.17	1.93	2.05
24	B	613	CLA	MG-NA	6.16	2.20	2.06
24	B	603	CLA	MG-NA	6.13	2.20	2.06
24	B	616	CLA	MG-ND	-6.12	1.93	2.05
24	C	503	CLA	MG-ND	-6.12	1.93	2.05
24	b	605	CLA	MG-NA	6.11	2.20	2.06
25	A	408	PHO	C3B-C2B	6.08	1.48	1.40
24	C	504	CLA	MG-NA	6.08	2.20	2.06
25	a	411	PHO	C3B-C2B	6.05	1.48	1.40
24	a	410	CLA	MG-NA	6.04	2.20	2.06
24	B	615	CLA	MG-NA	6.01	2.20	2.06
24	C	511	CLA	MG-ND	-6.00	1.93	2.05
24	a	410	CLA	MG-ND	-5.99	1.93	2.05
24	C	506	CLA	MG-ND	-5.99	1.93	2.05
24	c	914	CLA	MG-ND	-5.96	1.94	2.05
24	b	607	CLA	MG-NA	5.96	2.20	2.06
24	c	903	CLA	MG-ND	-5.94	1.94	2.05
24	B	605	CLA	MG-NC	5.92	2.20	2.06
24	B	605	CLA	MG-ND	-5.90	1.94	2.05
39	F	102	HEM	FE-ND	5.89	2.13	1.94
24	C	502	CLA	C1D-ND	5.88	1.45	1.37
24	B	606	CLA	MG-NA	5.87	2.20	2.06
24	b	606	CLA	MG-NC	5.86	2.20	2.06
24	C	505	CLA	MG-NC	5.83	2.20	2.06
24	C	503	CLA	C1D-ND	5.83	1.45	1.37
24	B	607	CLA	C3C-C2C	5.82	1.49	1.36
24	c	913	CLA	C3C-C2C	5.80	1.49	1.36
24	b	612	CLA	C3C-C2C	5.79	1.49	1.36
24	b	606	CLA	MG-NA	5.76	2.20	2.06
24	a	409	CLA	MG-NA	5.76	2.20	2.06
24	b	605	CLA	C3C-C2C	5.75	1.49	1.36
24	A	406	CLA	MG-NA	5.74	2.19	2.06
24	B	611	CLA	C3C-C2C	5.73	1.49	1.36
24	c	909	CLA	MG-NC	5.72	2.19	2.06
24	C	512	CLA	C3C-C2C	5.71	1.49	1.36
24	C	504	CLA	MG-ND	-5.69	1.94	2.05
24	C	508	CLA	C3C-C2C	5.68	1.49	1.36
24	a	413	CLA	C3C-C2C	5.68	1.49	1.36
24	b	608	CLA	MG-NC	5.67	2.19	2.06
24	C	509	CLA	C3C-C2C	5.67	1.49	1.36
24	b	614	CLA	MG-NA	5.66	2.19	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	MG-NA	5.65	2.19	2.06
24	c	909	CLA	C3C-C2C	5.65	1.49	1.36
24	b	608	CLA	C3C-C2C	5.64	1.48	1.36
24	C	509	CLA	C1D-ND	5.64	1.45	1.37
24	d	401	CLA	MG-NA	5.64	2.19	2.06
24	c	914	CLA	C3C-C2C	5.63	1.48	1.36
24	c	907	CLA	MG-NA	5.63	2.19	2.06
24	c	911	CLA	C3C-C2C	5.62	1.48	1.36
24	D	402	CLA	C3C-C2C	5.62	1.48	1.36
24	c	907	CLA	C3C-C2C	5.61	1.48	1.36
39	f	101	HEM	FE-ND	5.61	2.12	1.94
24	A	405	CLA	MG-NC	5.60	2.19	2.06
24	b	610	CLA	MG-NC	5.60	2.19	2.06
24	b	605	CLA	C1D-ND	5.59	1.45	1.37
24	B	610	CLA	C1D-ND	5.59	1.45	1.37
24	A	405	CLA	MG-NA	5.59	2.19	2.06
24	b	606	CLA	C3C-C2C	5.58	1.48	1.36
24	C	508	CLA	MG-NC	5.57	2.19	2.06
24	b	614	CLA	C3C-C2C	5.57	1.48	1.36
24	b	606	CLA	C1D-ND	5.56	1.45	1.37
24	B	602	CLA	C3C-C2C	5.56	1.48	1.36
24	C	508	CLA	MG-NB	5.56	2.16	2.05
24	B	608	CLA	MG-NA	5.56	2.19	2.06
24	B	605	CLA	C1D-ND	5.55	1.45	1.37
24	C	503	CLA	C3C-C2C	5.55	1.48	1.36
24	B	608	CLA	C3C-C2C	5.54	1.48	1.36
24	d	405	CLA	MG-ND	-5.53	1.94	2.05
42	v	202	HEC	C3D-C2D	5.53	1.53	1.38
24	B	603	CLA	MG-ND	-5.52	1.94	2.05
24	c	914	CLA	C1D-ND	5.52	1.45	1.37
24	B	603	CLA	C3C-C2C	5.52	1.48	1.36
24	C	509	CLA	MG-NA	5.52	2.19	2.06
24	b	610	CLA	C3C-C2C	5.50	1.48	1.36
25	a	412	PHO	C3D-C2D	5.48	1.49	1.39
24	c	907	CLA	C1D-ND	5.48	1.45	1.37
24	b	613	CLA	C3C-C2C	5.48	1.48	1.36
24	b	607	CLA	C3C-C2C	5.46	1.48	1.36
24	C	506	CLA	C3C-C2C	5.46	1.48	1.36
24	C	506	CLA	C1D-ND	5.45	1.45	1.37
24	b	608	CLA	C1D-ND	5.44	1.45	1.37
24	B	606	CLA	C3C-C2C	5.44	1.48	1.36
24	B	604	CLA	C3C-C2C	5.44	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C1D-ND	5.43	1.45	1.37
24	B	617	CLA	MG-ND	-5.43	1.95	2.05
24	B	607	CLA	MG-NC	5.42	2.19	2.06
24	B	611	CLA	MG-NC	5.42	2.19	2.06
24	b	611	CLA	C3C-C2C	5.42	1.48	1.36
24	c	912	CLA	C3C-C2C	5.41	1.48	1.36
24	C	505	CLA	C1D-ND	5.40	1.45	1.37
24	A	405	CLA	C3C-C2C	5.40	1.48	1.36
24	b	612	CLA	C1D-ND	5.40	1.45	1.37
24	C	513	CLA	C3C-C2C	5.39	1.48	1.36
24	B	612	CLA	C1D-ND	5.39	1.44	1.37
24	B	613	CLA	C3C-C2C	5.38	1.48	1.36
24	b	618	CLA	C3C-C2C	5.38	1.48	1.36
24	C	507	CLA	C3C-C2C	5.38	1.48	1.36
24	c	903	CLA	C3C-C2C	5.38	1.48	1.36
24	C	505	CLA	C3C-C2C	5.38	1.48	1.36
24	B	605	CLA	MG-NA	5.37	2.19	2.06
24	C	502	CLA	C3C-C2C	5.37	1.48	1.36
24	a	409	CLA	C3C-C2C	5.36	1.48	1.36
24	c	910	CLA	C3C-C2C	5.35	1.48	1.36
24	d	401	CLA	C3C-C2C	5.35	1.48	1.36
24	c	909	CLA	C1D-ND	5.35	1.44	1.37
24	b	605	CLA	CHC-C1C	5.34	1.49	1.38
24	B	604	CLA	MG-ND	-5.34	1.95	2.05
24	a	409	CLA	C1D-ND	5.33	1.44	1.37
24	A	410	CLA	C3C-C2C	5.33	1.48	1.36
24	b	613	CLA	C1D-ND	5.31	1.44	1.37
24	B	604	CLA	MG-NC	5.31	2.18	2.06
24	b	619	CLA	C3C-C2C	5.31	1.48	1.36
24	c	904	CLA	C1D-ND	5.31	1.44	1.37
24	c	908	CLA	C3C-C2C	5.30	1.48	1.36
25	a	412	PHO	C3B-C2B	5.30	1.47	1.40
24	B	617	CLA	C3C-C2C	5.29	1.48	1.36
24	b	617	CLA	C3C-C2C	5.28	1.48	1.36
24	c	904	CLA	C3C-C2C	5.26	1.48	1.36
24	d	404	CLA	C3C-C2C	5.26	1.48	1.36
24	B	609	CLA	C1D-ND	5.25	1.44	1.37
24	B	611	CLA	C1D-ND	5.25	1.44	1.37
24	b	611	CLA	MG-NA	5.25	2.18	2.06
24	A	410	CLA	MG-NA	5.25	2.18	2.06
24	D	402	CLA	MG-ND	-5.25	1.95	2.05
42	V	203	HEC	C3D-C2D	5.25	1.52	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	CLA	C3C-C2C	5.25	1.48	1.36
24	d	404	CLA	C1D-ND	5.23	1.44	1.37
24	c	904	CLA	CHC-C1C	5.23	1.49	1.38
24	C	507	CLA	MG-NB	-5.23	1.95	2.05
24	d	405	CLA	C3C-C2C	5.23	1.48	1.36
24	D	402	CLA	MG-NC	5.22	2.18	2.06
24	C	512	CLA	MG-NC	5.22	2.18	2.06
24	B	609	CLA	C3C-C2C	5.21	1.48	1.36
24	C	501	CLA	C1D-ND	5.20	1.44	1.37
25	A	409	PHO	C3D-C2D	5.20	1.48	1.39
24	B	611	CLA	CHC-C1C	5.19	1.48	1.38
24	c	906	CLA	MG-ND	-5.19	1.95	2.05
24	C	506	CLA	O2D-CGD	5.17	1.45	1.33
24	B	617	CLA	CHC-C1C	5.17	1.48	1.38
24	a	410	CLA	C3C-C2C	5.17	1.47	1.36
24	D	402	CLA	CHC-C1C	5.16	1.48	1.38
24	c	902	CLA	C1D-ND	5.16	1.44	1.37
24	b	617	CLA	C1D-ND	5.16	1.44	1.37
24	b	613	CLA	O2D-CGD	5.16	1.45	1.33
24	B	602	CLA	CHC-C1C	5.16	1.48	1.38
24	a	413	CLA	CHC-C1C	5.15	1.48	1.38
24	b	609	CLA	CHC-C1C	5.15	1.48	1.38
24	b	609	CLA	C3C-C2C	5.15	1.47	1.36
24	b	616	CLA	C3C-C2C	5.15	1.47	1.36
25	A	408	PHO	C3D-C2D	5.15	1.48	1.39
24	c	905	CLA	C3C-C2C	5.15	1.47	1.36
24	b	614	CLA	CHC-C1C	5.15	1.48	1.38
24	A	405	CLA	C1D-ND	5.14	1.44	1.37
24	b	620	CLA	C3C-C2C	5.13	1.47	1.36
24	c	905	CLA	MG-NA	5.13	2.18	2.06
24	B	615	CLA	C3C-C2C	5.12	1.47	1.36
24	c	906	CLA	C1D-ND	5.12	1.44	1.37
24	a	413	CLA	O2D-CGD	5.12	1.45	1.33
24	C	512	CLA	CHC-C1C	5.11	1.48	1.38
24	c	906	CLA	C3C-C2C	5.11	1.47	1.36
24	C	502	CLA	MG-NC	5.11	2.18	2.06
24	B	606	CLA	C1D-ND	5.11	1.44	1.37
24	B	605	CLA	C3C-C2C	5.11	1.47	1.36
24	C	510	CLA	C3C-C2C	5.10	1.47	1.36
24	c	903	CLA	O2D-CGD	5.10	1.45	1.33
24	B	603	CLA	CHC-C1C	5.09	1.48	1.38
24	c	912	CLA	C1D-ND	5.09	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C3C-C2C	5.09	1.47	1.36
24	c	911	CLA	C1D-ND	5.09	1.44	1.37
24	c	913	CLA	C1D-ND	5.08	1.44	1.37
24	b	619	CLA	C1D-ND	5.08	1.44	1.37
24	C	503	CLA	CHC-C1C	5.08	1.48	1.38
24	c	902	CLA	C3C-C2C	5.07	1.47	1.36
24	c	905	CLA	O2D-CGD	5.07	1.45	1.33
24	B	613	CLA	CHC-C1C	5.07	1.48	1.38
24	C	502	CLA	O2D-CGD	5.07	1.45	1.33
24	C	512	CLA	C1D-ND	5.06	1.44	1.37
24	C	513	CLA	C1D-ND	5.04	1.44	1.37
24	B	607	CLA	CHC-C1C	5.04	1.48	1.38
24	B	616	CLA	C1D-ND	5.04	1.44	1.37
24	A	406	CLA	C3C-C2C	5.04	1.47	1.36
24	A	407	CLA	C3C-C2C	5.04	1.47	1.36
24	B	615	CLA	C1D-ND	5.04	1.44	1.37
24	C	505	CLA	CHD-C1D	5.03	1.48	1.38
24	b	605	CLA	O2D-CGD	5.03	1.45	1.33
24	c	904	CLA	CHD-C1D	5.02	1.48	1.38
24	B	607	CLA	C1D-ND	5.02	1.44	1.37
24	C	510	CLA	C1D-ND	5.02	1.44	1.37
24	c	914	CLA	CHC-C1C	5.02	1.48	1.38
24	B	609	CLA	MG-NC	5.02	2.18	2.06
24	B	606	CLA	O2D-CGD	5.01	1.45	1.33
24	C	511	CLA	C3C-C2C	5.01	1.47	1.36
24	B	602	CLA	C1D-ND	5.01	1.44	1.37
24	B	604	CLA	C1D-ND	5.01	1.44	1.37
25	A	409	PHO	OBD-CAD	5.01	1.28	1.22
24	B	610	CLA	C3C-C2C	5.01	1.47	1.36
24	C	501	CLA	C3C-C2C	5.01	1.47	1.36
25	a	412	PHO	O2D-CGD	5.01	1.45	1.33
25	a	411	PHO	C3D-C2D	5.00	1.48	1.39
24	b	618	CLA	CHC-C1C	5.00	1.48	1.38
24	c	907	CLA	MG-NC	5.00	2.18	2.06
24	a	409	CLA	MG-NC	5.00	2.18	2.06
24	C	505	CLA	CHC-C1C	5.00	1.48	1.38
24	B	612	CLA	C3C-C2C	4.98	1.47	1.36
24	b	618	CLA	MG-NA	4.98	2.18	2.06
24	B	616	CLA	CHC-C1C	4.97	1.48	1.38
24	D	402	CLA	O2D-CGD	4.97	1.45	1.33
24	d	405	CLA	MG-NA	4.96	2.18	2.06
24	C	506	CLA	MG-NC	4.96	2.18	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	MG-NC	4.96	2.18	2.06
24	c	914	CLA	MG-NA	4.95	2.18	2.06
25	A	409	PHO	O2D-CGD	4.95	1.45	1.33
24	B	614	CLA	C3C-C2C	4.94	1.47	1.36
24	d	404	CLA	CHC-C1C	4.94	1.48	1.38
24	b	612	CLA	O2D-CGD	4.93	1.45	1.33
24	b	611	CLA	CHD-C1D	4.93	1.48	1.38
24	B	606	CLA	CHC-C1C	4.93	1.48	1.38
24	C	509	CLA	O2D-CGD	4.93	1.45	1.33
24	B	614	CLA	MG-ND	-4.92	1.96	2.05
24	b	615	CLA	C3C-C2C	4.92	1.47	1.36
24	b	610	CLA	CHC-C1C	4.92	1.48	1.38
24	b	617	CLA	MG-NC	4.92	2.18	2.06
24	c	906	CLA	MG-NC	4.92	2.18	2.06
24	b	614	CLA	C1D-ND	4.92	1.44	1.37
24	B	610	CLA	O2D-CGD	4.91	1.45	1.33
24	B	606	CLA	MG-NC	4.91	2.17	2.06
24	b	620	CLA	O2D-CGD	4.91	1.45	1.33
24	C	508	CLA	C1D-ND	4.91	1.44	1.37
24	a	410	CLA	CHC-C1C	4.91	1.48	1.38
24	c	910	CLA	C1D-ND	4.91	1.44	1.37
24	B	609	CLA	MG-ND	-4.90	1.96	2.05
24	C	504	CLA	MG-NC	4.90	2.17	2.06
24	b	607	CLA	CHD-C1D	4.90	1.48	1.38
24	b	612	CLA	CHC-C1C	4.89	1.48	1.38
24	C	508	CLA	CHC-C1C	4.89	1.48	1.38
24	C	506	CLA	CHC-C1C	4.88	1.48	1.38
24	C	502	CLA	CHC-C1C	4.87	1.48	1.38
24	B	602	CLA	O2D-CGD	4.87	1.45	1.33
24	c	907	CLA	O2D-CGD	4.87	1.45	1.33
24	B	613	CLA	MG-ND	-4.87	1.96	2.05
24	A	410	CLA	CHC-C1C	4.86	1.48	1.38
24	C	511	CLA	O2D-CGD	4.86	1.45	1.33
24	B	612	CLA	CHC-C1C	4.85	1.48	1.38
24	B	616	CLA	C3C-C2C	4.85	1.47	1.36
24	B	603	CLA	C1D-ND	4.84	1.44	1.37
24	c	912	CLA	CHC-C1C	4.84	1.48	1.38
24	C	501	CLA	CHC-C1C	4.83	1.48	1.38
24	c	903	CLA	CHC-C1C	4.83	1.48	1.38
24	c	913	CLA	CHC-C1C	4.83	1.48	1.38
24	C	513	CLA	O2D-CGD	4.83	1.45	1.33
24	b	616	CLA	O2D-CGD	4.83	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	906	CLA	CHD-C1D	4.83	1.47	1.38
24	b	611	CLA	MG-NC	4.83	2.17	2.06
24	b	614	CLA	MG-ND	-4.83	1.96	2.05
24	C	508	CLA	MG-NA	4.82	2.17	2.06
24	B	614	CLA	CHC-C1C	4.82	1.48	1.38
24	B	607	CLA	O2D-CGD	4.81	1.45	1.33
24	B	609	CLA	CHD-C1D	4.81	1.47	1.38
24	c	910	CLA	CHC-C1C	4.81	1.48	1.38
24	C	509	CLA	CHD-C1D	4.81	1.47	1.38
24	c	907	CLA	CHC-C1C	4.80	1.48	1.38
24	a	413	CLA	MG-NA	4.80	2.17	2.06
24	b	620	CLA	C1D-ND	4.80	1.44	1.37
24	b	607	CLA	O2D-CGD	4.80	1.45	1.33
24	c	914	CLA	CHD-C1D	4.80	1.47	1.38
24	B	609	CLA	CHC-C1C	4.80	1.48	1.38
24	C	511	CLA	CHC-C1C	4.80	1.48	1.38
24	c	904	CLA	O2D-CGD	4.80	1.45	1.33
24	b	613	CLA	CHD-C1D	4.79	1.47	1.38
24	b	609	CLA	C1D-ND	4.79	1.44	1.37
24	A	407	CLA	O2D-CGD	4.78	1.45	1.33
24	b	617	CLA	O2D-CGD	4.78	1.45	1.33
24	B	617	CLA	O2D-CGD	4.78	1.45	1.33
24	b	615	CLA	O2D-CGD	4.78	1.45	1.33
24	d	405	CLA	C1D-ND	4.77	1.44	1.37
24	b	606	CLA	O2D-CGD	4.77	1.45	1.33
24	c	912	CLA	CHD-C1D	4.77	1.47	1.38
24	b	619	CLA	CHC-C1C	4.76	1.48	1.38
24	b	608	CLA	CHC-C1C	4.76	1.48	1.38
24	B	608	CLA	MG-NC	4.75	2.17	2.06
24	b	616	CLA	CHC-C1C	4.75	1.48	1.38
24	b	611	CLA	MG-ND	-4.75	1.96	2.05
24	c	905	CLA	C1D-ND	4.75	1.44	1.37
24	C	504	CLA	CHC-C1C	4.75	1.48	1.38
24	C	513	CLA	CHC-C1C	4.74	1.48	1.38
24	c	909	CLA	CHC-C1C	4.74	1.48	1.38
24	c	911	CLA	O2D-CGD	4.74	1.44	1.33
24	b	610	CLA	MG-ND	-4.73	1.96	2.05
24	c	903	CLA	C1D-ND	4.73	1.44	1.37
24	b	612	CLA	CHD-C1D	4.73	1.47	1.38
24	B	617	CLA	C1D-ND	4.72	1.44	1.37
25	A	408	PHO	O2D-CGD	4.72	1.44	1.33
24	b	607	CLA	MG-ND	-4.72	1.96	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	908	CLA	C1D-ND	4.72	1.44	1.37
24	B	614	CLA	C1D-ND	4.72	1.44	1.37
24	b	608	CLA	O2D-CGD	4.72	1.44	1.33
24	c	902	CLA	O2D-CGD	4.72	1.44	1.33
24	b	617	CLA	CHC-C1C	4.72	1.47	1.38
24	d	405	CLA	O2D-CGD	4.71	1.44	1.33
24	B	604	CLA	O2D-CGD	4.71	1.44	1.33
24	c	906	CLA	CHC-C1C	4.70	1.47	1.38
24	B	614	CLA	O2D-CGD	4.70	1.44	1.33
24	C	505	CLA	CHB-C1B	4.69	1.49	1.39
24	b	605	CLA	CHD-C1D	4.69	1.47	1.38
24	C	509	CLA	CHC-C1C	4.68	1.47	1.38
24	b	613	CLA	CHC-C1C	4.68	1.47	1.38
34	b	638	DMS	O-S	4.68	1.81	1.50
24	B	611	CLA	MG-NB	4.68	2.15	2.05
24	c	910	CLA	CHB-C1B	4.68	1.49	1.39
24	b	609	CLA	O2D-CGD	4.67	1.44	1.33
24	b	615	CLA	CHD-C1D	4.67	1.47	1.38
24	c	906	CLA	O2D-CGD	4.67	1.44	1.33
34	b	646	DMS	O-S	4.67	1.81	1.50
24	d	401	CLA	CHC-C1C	4.67	1.47	1.38
24	B	608	CLA	CHC-C1C	4.67	1.47	1.38
24	b	615	CLA	CHB-C1B	4.67	1.49	1.39
34	D	415	DMS	O-S	4.66	1.81	1.50
24	c	903	CLA	CHB-C1B	4.66	1.49	1.39
24	B	603	CLA	O2D-CGD	4.66	1.44	1.33
24	B	604	CLA	CHC-C1C	4.65	1.47	1.38
24	C	507	CLA	O2D-CGD	4.65	1.44	1.33
24	B	613	CLA	O2D-CGD	4.65	1.44	1.33
24	c	911	CLA	CHC-C1C	4.65	1.47	1.38
34	v	206	DMS	O-S	4.65	1.80	1.50
34	O	315	DMS	O-S	4.65	1.80	1.50
34	o	306	DMS	O-S	4.64	1.80	1.50
34	C	535	DMS	O-S	4.64	1.80	1.50
34	e	104	DMS	O-S	4.64	1.80	1.50
24	b	611	CLA	CHC-C1C	4.64	1.47	1.38
24	B	611	CLA	MG-NA	4.64	2.17	2.06
24	C	510	CLA	O2D-CGD	4.63	1.44	1.33
24	B	613	CLA	CHB-C1B	4.63	1.49	1.39
24	A	410	CLA	C1D-ND	4.63	1.43	1.37
34	v	210	DMS	O-S	4.63	1.80	1.50
24	b	610	CLA	C1D-ND	4.63	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	416	DMS	O-S	4.63	1.80	1.50
24	c	914	CLA	O2D-CGD	4.63	1.44	1.33
34	c	934	DMS	O-S	4.62	1.80	1.50
24	c	908	CLA	MG-ND	-4.62	1.96	2.05
24	B	610	CLA	CHC-C1C	4.62	1.47	1.38
34	c	939	DMS	O-S	4.62	1.80	1.50
24	b	610	CLA	O2D-CGD	4.62	1.44	1.33
34	C	528	DMS	O-S	4.62	1.80	1.50
24	b	611	CLA	O2D-CGD	4.62	1.44	1.33
24	C	508	CLA	O2D-CGD	4.62	1.44	1.33
34	a	425	DMS	O-S	4.62	1.80	1.50
34	V	211	DMS	O-S	4.62	1.80	1.50
34	B	634	DMS	O-S	4.61	1.80	1.50
24	b	609	CLA	MG-ND	-4.61	1.96	2.05
34	a	423	DMS	O-S	4.61	1.80	1.50
24	A	410	CLA	O2D-CGD	4.61	1.44	1.33
34	A	425	DMS	O-S	4.61	1.80	1.50
24	c	908	CLA	O2D-CGD	4.61	1.44	1.33
34	b	641	DMS	O-S	4.61	1.80	1.50
34	d	417	DMS	O-S	4.61	1.80	1.50
34	A	427	DMS	O-S	4.60	1.80	1.50
34	b	642	DMS	O-S	4.60	1.80	1.50
34	o	307	DMS	O-S	4.60	1.80	1.50
24	c	907	CLA	CHD-C1D	4.60	1.47	1.38
34	C	532	DMS	O-S	4.60	1.80	1.50
24	B	602	CLA	CHD-C1D	4.60	1.47	1.38
24	b	615	CLA	CHC-C1C	4.60	1.47	1.38
34	A	426	DMS	O-S	4.60	1.80	1.50
25	a	412	PHO	OBD-CAD	4.60	1.28	1.22
24	b	606	CLA	CHC-C1C	4.60	1.47	1.38
34	V	212	DMS	O-S	4.60	1.80	1.50
34	c	933	DMS	O-S	4.60	1.80	1.50
34	O	307	DMS	O-S	4.60	1.80	1.50
24	D	402	CLA	C1D-ND	4.60	1.43	1.37
34	b	643	DMS	O-S	4.60	1.80	1.50
24	b	606	CLA	CHD-C1D	4.60	1.47	1.38
34	O	313	DMS	O-S	4.59	1.80	1.50
34	O	302	DMS	O-S	4.59	1.80	1.50
34	O	312	DMS	O-S	4.59	1.80	1.50
34	C	530	DMS	O-S	4.59	1.80	1.50
24	b	615	CLA	C1D-ND	4.59	1.43	1.37
34	B	645	DMS	O-S	4.59	1.80	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	529	DMS	O-S	4.59	1.80	1.50
24	C	504	CLA	O2D-CGD	4.59	1.44	1.33
24	C	505	CLA	O2D-CGD	4.59	1.44	1.33
34	e	103	DMS	O-S	4.59	1.80	1.50
24	c	905	CLA	CHC-C1C	4.59	1.47	1.38
34	C	531	DMS	O-S	4.59	1.80	1.50
34	U	204	DMS	O-S	4.59	1.80	1.50
34	A	424	DMS	O-S	4.59	1.80	1.50
34	O	310	DMS	O-S	4.59	1.80	1.50
34	v	207	DMS	O-S	4.58	1.80	1.50
34	V	210	DMS	O-S	4.58	1.80	1.50
34	c	938	DMS	O-S	4.58	1.80	1.50
34	i	106	DMS	O-S	4.58	1.80	1.50
24	b	616	CLA	C1D-ND	4.58	1.43	1.37
34	e	102	DMS	O-S	4.58	1.80	1.50
34	d	416	DMS	O-S	4.58	1.80	1.50
34	c	926	DMS	O-S	4.58	1.80	1.50
34	V	213	DMS	O-S	4.58	1.80	1.50
34	a	422	DMS	O-S	4.58	1.80	1.50
34	B	646	DMS	O-S	4.58	1.80	1.50
24	b	608	CLA	CHD-C1D	4.58	1.47	1.38
24	c	902	CLA	CHC-C1C	4.58	1.47	1.38
24	b	618	CLA	C1D-ND	4.58	1.43	1.37
34	c	936	DMS	O-S	4.58	1.80	1.50
34	b	639	DMS	O-S	4.58	1.80	1.50
24	A	407	CLA	OBD-CAD	4.58	1.30	1.22
34	B	640	DMS	O-S	4.58	1.80	1.50
34	U	202	DMS	O-S	4.58	1.80	1.50
34	c	935	DMS	O-S	4.58	1.80	1.50
34	O	305	DMS	O-S	4.58	1.80	1.50
34	C	534	DMS	O-S	4.58	1.80	1.50
34	B	643	DMS	O-S	4.58	1.80	1.50
34	y	101	DMS	O-S	4.58	1.80	1.50
34	O	306	DMS	O-S	4.57	1.80	1.50
34	b	647	DMS	O-S	4.57	1.80	1.50
34	C	524	DMS	O-S	4.57	1.80	1.50
34	B	647	DMS	O-S	4.57	1.80	1.50
34	C	533	DMS	O-S	4.57	1.80	1.50
24	c	904	CLA	CHB-C1B	4.57	1.49	1.39
24	B	608	CLA	O2D-CGD	4.57	1.44	1.33
34	D	414	DMS	O-S	4.57	1.80	1.50
34	c	932	DMS	O-S	4.57	1.80	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	205	DMS	O-S	4.57	1.80	1.50
34	V	208	DMS	O-S	4.57	1.80	1.50
34	V	214	DMS	O-S	4.57	1.80	1.50
24	C	512	CLA	O2D-CGD	4.57	1.44	1.33
34	d	418	DMS	O-S	4.57	1.80	1.50
34	U	203	DMS	O-S	4.57	1.80	1.50
34	B	642	DMS	O-S	4.57	1.80	1.50
24	b	611	CLA	C1D-ND	4.57	1.43	1.37
34	v	205	DMS	O-S	4.57	1.80	1.50
24	B	610	CLA	CHB-C1B	4.57	1.49	1.39
34	O	314	DMS	O-S	4.57	1.80	1.50
34	H	104	DMS	O-S	4.57	1.80	1.50
34	a	424	DMS	O-S	4.56	1.80	1.50
34	o	303	DMS	O-S	4.56	1.80	1.50
34	v	204	DMS	O-S	4.56	1.80	1.50
34	b	640	DMS	O-S	4.56	1.80	1.50
34	o	304	DMS	O-S	4.56	1.80	1.50
34	L	102	DMS	O-S	4.56	1.80	1.50
34	O	311	DMS	O-S	4.56	1.80	1.50
34	B	641	DMS	O-S	4.56	1.80	1.50
24	B	603	CLA	CHD-C1D	4.56	1.47	1.38
34	v	209	DMS	O-S	4.56	1.80	1.50
34	v	208	DMS	O-S	4.56	1.80	1.50
34	O	308	DMS	O-S	4.56	1.80	1.50
24	d	405	CLA	CHC-C1C	4.56	1.47	1.38
34	a	421	DMS	O-S	4.56	1.80	1.50
24	A	407	CLA	CHC-C1C	4.55	1.47	1.38
34	o	302	DMS	O-S	4.55	1.80	1.50
24	B	617	CLA	CHB-C1B	4.55	1.49	1.39
34	o	305	DMS	O-S	4.55	1.80	1.50
24	c	912	CLA	O2D-CGD	4.55	1.44	1.33
34	K	102	DMS	O-S	4.55	1.80	1.50
34	T	103	DMS	O-S	4.55	1.80	1.50
24	C	512	CLA	CHD-C1D	4.55	1.47	1.38
24	B	610	CLA	CHD-C1D	4.54	1.47	1.38
34	C	527	DMS	O-S	4.54	1.80	1.50
34	B	639	DMS	O-S	4.54	1.80	1.50
24	c	908	CLA	CHC-C1C	4.54	1.47	1.38
24	b	616	CLA	MG-NA	4.54	2.17	2.06
34	b	632	DMS	O-S	4.54	1.80	1.50
34	h	105	DMS	O-S	4.54	1.80	1.50
34	u	201	DMS	O-S	4.54	1.80	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	CHB-C1B	4.53	1.49	1.39
24	d	401	CLA	O2D-CGD	4.53	1.44	1.33
24	A	405	CLA	CHC-C1C	4.53	1.47	1.38
34	c	937	DMS	O-S	4.53	1.80	1.50
24	C	501	CLA	O2D-CGD	4.53	1.44	1.33
24	C	506	CLA	CHD-C1D	4.53	1.47	1.38
24	B	616	CLA	O2D-CGD	4.53	1.44	1.33
27	A	416	SQD	O48-C23	4.53	1.46	1.33
34	c	931	DMS	O-S	4.53	1.80	1.50
24	a	410	CLA	C1D-ND	4.53	1.43	1.37
34	b	645	DMS	O-S	4.53	1.80	1.50
34	V	201	DMS	O-S	4.52	1.80	1.50
34	v	203	DMS	O-S	4.52	1.80	1.50
34	O	309	DMS	O-S	4.52	1.80	1.50
34	d	415	DMS	O-S	4.52	1.80	1.50
34	c	940	DMS	O-S	4.52	1.80	1.50
24	a	409	CLA	CHD-C1D	4.52	1.47	1.38
25	a	411	PHO	O2D-CGD	4.52	1.44	1.33
34	C	526	DMS	O-S	4.51	1.80	1.50
34	b	644	DMS	O-S	4.51	1.80	1.50
24	c	909	CLA	CHD-C1D	4.51	1.47	1.38
24	b	620	CLA	CHD-C1D	4.50	1.47	1.38
24	C	513	CLA	MG-NC	4.50	2.17	2.06
24	b	607	CLA	C1D-ND	4.50	1.43	1.37
24	a	409	CLA	OBD-CAD	4.50	1.30	1.22
34	B	633	DMS	O-S	4.49	1.79	1.50
24	C	509	CLA	CHB-C1B	4.49	1.49	1.39
28	b	624	LMG	O8-C28	4.49	1.46	1.33
24	b	614	CLA	O2D-CGD	4.49	1.44	1.33
34	D	413	DMS	O-S	4.49	1.79	1.50
24	C	503	CLA	CHC-C4B	4.48	1.49	1.39
24	b	607	CLA	CHC-C1C	4.48	1.47	1.38
24	c	910	CLA	O2D-CGD	4.48	1.44	1.33
24	B	612	CLA	O2D-CGD	4.48	1.44	1.33
28	B	621	LMG	O8-C28	4.48	1.46	1.33
24	b	618	CLA	O2D-CGD	4.47	1.44	1.33
24	b	608	CLA	CHB-C1B	4.47	1.49	1.39
24	b	620	CLA	CHB-C1B	4.47	1.49	1.39
24	d	404	CLA	O2A-CGA	4.47	1.46	1.33
24	B	607	CLA	CHD-C1D	4.47	1.47	1.38
24	B	606	CLA	CHD-C1D	4.47	1.47	1.38
34	u	202	DMS	O-S	4.47	1.79	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	209	DMS	O-S	4.46	1.79	1.50
24	C	507	CLA	CHD-C1D	4.46	1.47	1.38
24	A	406	CLA	C1D-ND	4.46	1.43	1.37
24	c	912	CLA	CHB-C1B	4.46	1.49	1.39
24	A	410	CLA	CHB-C1B	4.46	1.49	1.39
24	b	605	CLA	O2A-CGA	4.45	1.46	1.33
24	B	608	CLA	C1D-ND	4.45	1.43	1.37
27	f	102	SQD	O47-C7	4.45	1.46	1.34
24	C	506	CLA	O2A-CGA	4.45	1.46	1.33
24	b	616	CLA	CHB-C1B	4.45	1.49	1.39
38	E	101	LHG	O8-C23	4.45	1.46	1.33
24	C	513	CLA	CHD-C1D	4.44	1.47	1.38
24	B	612	CLA	CHD-C1D	4.44	1.47	1.38
24	b	618	CLA	CHD-C1D	4.44	1.47	1.38
24	C	504	CLA	C1D-ND	4.44	1.43	1.37
24	B	607	CLA	CHC-C4B	4.44	1.49	1.39
24	C	503	CLA	CHB-C1B	4.44	1.49	1.39
24	D	401	CLA	O2D-CGD	4.44	1.44	1.33
24	c	903	CLA	CHD-C1D	4.43	1.47	1.38
34	B	644	DMS	O-S	4.43	1.79	1.50
24	b	605	CLA	CHC-C4B	4.43	1.49	1.39
24	a	409	CLA	O2D-CGD	4.43	1.44	1.33
24	A	405	CLA	O2D-CGD	4.42	1.44	1.33
24	A	406	CLA	O2D-CGD	4.42	1.44	1.33
24	B	605	CLA	CHC-C1C	4.42	1.47	1.38
24	C	503	CLA	O2D-CGD	4.42	1.44	1.33
24	c	910	CLA	CHD-C1D	4.42	1.47	1.38
24	c	908	CLA	CHD-C1D	4.42	1.47	1.38
27	b	601	SQD	O47-C7	4.42	1.46	1.34
24	C	504	CLA	CHD-C1D	4.41	1.47	1.38
24	b	617	CLA	CHB-C1B	4.41	1.49	1.39
24	C	510	CLA	CHC-C1C	4.40	1.47	1.38
27	a	401	SQD	O48-C23	4.40	1.46	1.33
24	b	613	CLA	MG-ND	-4.40	1.97	2.05
24	C	502	CLA	CHB-C1B	4.40	1.49	1.39
24	b	614	CLA	CHD-C1D	4.40	1.47	1.38
24	B	615	CLA	CHC-C1C	4.39	1.47	1.38
24	B	615	CLA	CHB-C1B	4.38	1.49	1.39
24	c	908	CLA	O2A-CGA	4.38	1.46	1.33
24	c	913	CLA	CHD-C1D	4.38	1.47	1.38
24	C	512	CLA	O2A-CGA	4.37	1.46	1.33
24	c	913	CLA	O2D-CGD	4.37	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	CLA	CHD-C1D	4.36	1.46	1.38
34	c	930	DMS	O-S	4.35	1.78	1.50
24	B	611	CLA	CHB-C1B	4.35	1.49	1.39
24	b	620	CLA	CHC-C1C	4.35	1.47	1.38
24	a	409	CLA	CHC-C1C	4.35	1.47	1.38
24	C	510	CLA	CHD-C1D	4.34	1.46	1.38
24	b	620	CLA	O2A-CGA	4.34	1.46	1.33
24	B	602	CLA	O2A-CGA	4.34	1.46	1.33
24	C	509	CLA	O2A-CGA	4.33	1.46	1.33
28	c	921	LMG	O8-C28	4.33	1.46	1.33
24	C	503	CLA	CHD-C1D	4.32	1.46	1.38
24	B	614	CLA	CHC-C4B	4.32	1.49	1.39
24	c	911	CLA	CHD-C1D	4.31	1.46	1.38
24	b	619	CLA	MG-NC	4.31	2.16	2.06
24	B	615	CLA	O2D-CGD	4.31	1.43	1.33
27	l	101	SQD	O47-C7	4.31	1.46	1.34
24	b	619	CLA	O2D-CGD	4.30	1.43	1.33
27	a	401	SQD	O47-C7	4.30	1.46	1.34
24	a	409	CLA	CHB-C1B	4.30	1.49	1.39
24	B	604	CLA	O2A-CGA	4.30	1.45	1.33
24	C	505	CLA	CHC-C4B	4.30	1.49	1.39
24	b	610	CLA	CHB-C1B	4.30	1.49	1.39
34	a	420	DMS	O-S	4.30	1.78	1.50
24	B	609	CLA	O2D-CGD	4.29	1.43	1.33
24	C	511	CLA	CHB-C1B	4.29	1.49	1.39
27	f	102	SQD	O48-C23	4.29	1.45	1.33
28	A	413	LMG	O7-C10	4.28	1.46	1.34
27	A	416	SQD	O47-C7	4.28	1.46	1.34
24	b	617	CLA	CHD-C1D	4.28	1.46	1.38
24	c	909	CLA	O2D-CGD	4.28	1.43	1.33
24	C	512	CLA	CHB-C1B	4.28	1.49	1.39
24	b	607	CLA	O2A-CGA	4.27	1.45	1.33
24	d	401	CLA	CHD-C1D	4.27	1.46	1.38
24	C	507	CLA	O2A-CGA	4.27	1.45	1.33
24	C	508	CLA	CHB-C1B	4.27	1.49	1.39
24	b	619	CLA	CHD-C1D	4.27	1.46	1.38
24	d	401	CLA	C1D-ND	4.27	1.43	1.37
24	A	406	CLA	CHD-C1D	4.27	1.46	1.38
28	C	523	LMG	O8-C28	4.26	1.45	1.33
24	c	903	CLA	MG-NC	4.26	2.16	2.06
24	D	402	CLA	CHB-C1B	4.26	1.49	1.39
24	c	910	CLA	MG-ND	-4.26	1.97	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	413	LMG	O8-C28	4.26	1.45	1.33
24	B	614	CLA	MG-NC	4.25	2.16	2.06
24	a	413	CLA	C1D-ND	4.25	1.43	1.37
28	c	921	LMG	O7-C10	4.25	1.46	1.34
24	c	912	CLA	MG-NC	4.25	2.16	2.06
24	C	511	CLA	C1D-ND	4.25	1.43	1.37
24	C	502	CLA	CHD-C1D	4.25	1.46	1.38
24	c	907	CLA	O2A-CGA	4.25	1.45	1.33
24	c	912	CLA	O2A-CGA	4.25	1.45	1.33
24	C	508	CLA	O2A-CGA	4.24	1.45	1.33
24	B	608	CLA	MG-ND	-4.24	1.97	2.05
24	B	606	CLA	CHB-C1B	4.24	1.48	1.39
24	C	501	CLA	CHB-C1B	4.23	1.48	1.39
24	c	908	CLA	CHB-C1B	4.23	1.48	1.39
24	B	611	CLA	CHD-C1D	4.23	1.46	1.38
24	c	905	CLA	MG-NC	4.22	2.16	2.06
24	C	507	CLA	OBD-CAD	4.22	1.29	1.22
24	C	501	CLA	CHD-C1D	4.22	1.46	1.38
24	B	604	CLA	CHD-C1D	4.22	1.46	1.38
24	b	611	CLA	CHB-C1B	4.22	1.48	1.39
34	B	632	DMS	O-S	4.21	1.78	1.50
24	a	410	CLA	CHB-C1B	4.21	1.48	1.39
24	B	613	CLA	CHD-C1D	4.21	1.46	1.38
24	c	906	CLA	CHB-C1B	4.21	1.48	1.39
24	C	502	CLA	O2A-CGA	4.21	1.45	1.33
24	B	613	CLA	OBD-CAD	4.21	1.29	1.22
24	c	909	CLA	O2A-CGA	4.21	1.45	1.33
24	C	510	CLA	CHB-C1B	4.21	1.48	1.39
28	a	416	LMG	O7-C10	4.20	1.46	1.34
24	c	902	CLA	CHB-C1B	4.20	1.48	1.39
24	c	904	CLA	CHC-C4B	4.20	1.48	1.39
24	B	605	CLA	O2D-CGD	4.20	1.43	1.33
37	D	405	DGD	O1G-C1A	4.20	1.45	1.33
24	b	619	CLA	CHB-C1B	4.20	1.48	1.39
24	c	913	CLA	MG-NC	4.20	2.16	2.06
24	C	511	CLA	O2A-CGA	4.20	1.45	1.33
28	c	920	LMG	O8-C28	4.19	1.45	1.33
24	c	902	CLA	CHD-C1D	4.19	1.46	1.38
28	C	523	LMG	O7-C10	4.19	1.46	1.34
24	B	602	CLA	CHD-C4C	4.19	1.48	1.39
24	b	605	CLA	CHB-C1B	4.19	1.48	1.39
24	c	911	CLA	CHB-C1B	4.19	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	CHC-C4B	4.19	1.48	1.39
27	b	601	SQD	O48-C23	4.19	1.45	1.33
24	C	507	CLA	CHC-C1C	4.18	1.46	1.38
27	F	101	SQD	O47-C7	4.18	1.46	1.34
24	c	914	CLA	O2A-CGA	4.18	1.45	1.33
24	B	613	CLA	MG-NC	4.18	2.16	2.06
24	d	404	CLA	O2D-CGD	4.18	1.43	1.33
24	B	604	CLA	MG-NA	4.18	2.16	2.06
24	B	603	CLA	CHB-C1B	4.17	1.48	1.39
24	b	609	CLA	CHD-C1D	4.17	1.46	1.38
24	B	611	CLA	O2D-CGD	4.17	1.43	1.33
24	c	902	CLA	MG-NC	4.17	2.16	2.06
24	D	401	CLA	O2A-CGA	4.17	1.45	1.33
24	A	407	CLA	MG-ND	-4.17	1.97	2.05
24	D	401	CLA	MG-ND	-4.16	1.97	2.05
28	a	416	LMG	O8-C28	4.16	1.45	1.33
24	c	905	CLA	CHD-C1D	4.16	1.46	1.38
37	d	408	DGD	O1G-C1A	4.16	1.45	1.33
38	L	101	LHG	O7-C7	4.16	1.46	1.34
24	B	609	CLA	O2A-CGA	4.16	1.45	1.33
24	b	613	CLA	CHB-C1B	4.16	1.48	1.39
24	b	615	CLA	MG-ND	-4.16	1.97	2.05
24	b	610	CLA	O2A-CGA	4.16	1.45	1.33
24	B	602	CLA	CHB-C1B	4.15	1.48	1.39
28	c	920	LMG	O7-C10	4.15	1.46	1.34
24	b	613	CLA	CHC-C4B	4.15	1.48	1.39
24	D	401	CLA	CHD-C1D	4.15	1.46	1.38
24	C	513	CLA	CHB-C1B	4.15	1.48	1.39
24	C	505	CLA	MG-NB	4.15	2.14	2.05
24	B	608	CLA	CHD-C1D	4.14	1.46	1.38
24	D	401	CLA	CHB-C1B	4.14	1.48	1.39
24	d	405	CLA	O2A-CGA	4.14	1.45	1.33
24	B	603	CLA	CHC-C4B	4.14	1.48	1.39
34	A	423	DMS	O-S	4.14	1.77	1.50
42	v	202	HEC	CBC-CAC	-4.13	1.34	1.49
37	d	408	DGD	O2G-C1B	4.13	1.46	1.34
24	d	401	CLA	O2A-CGA	4.13	1.45	1.33
28	b	624	LMG	O7-C10	4.13	1.45	1.34
24	D	402	CLA	CHD-C1D	4.13	1.46	1.38
24	b	606	CLA	CHB-C1B	4.13	1.48	1.39
24	B	608	CLA	CHD-C4C	4.12	1.48	1.39
24	d	401	CLA	OBD-CAD	4.12	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	905	CLA	MG-ND	-4.11	1.97	2.05
24	c	906	CLA	CHC-C4B	4.11	1.48	1.39
24	a	413	CLA	O2A-CGA	4.11	1.45	1.33
24	c	902	CLA	O2A-CGA	4.11	1.45	1.33
24	C	506	CLA	CHB-C1B	4.11	1.48	1.39
24	d	404	CLA	CHB-C1B	4.11	1.48	1.39
24	a	410	CLA	O2D-CGD	4.11	1.43	1.33
24	a	413	CLA	CHB-C1B	4.11	1.48	1.39
37	D	405	DGD	O2G-C1B	4.11	1.45	1.34
24	C	508	CLA	CHD-C1D	4.10	1.46	1.38
24	B	602	CLA	CHC-C4B	4.10	1.48	1.39
24	C	509	CLA	MG-ND	-4.10	1.97	2.05
24	c	910	CLA	O2A-CGA	4.10	1.45	1.33
24	B	617	CLA	O2A-CGA	4.10	1.45	1.33
38	d	409	LHG	O8-C23	4.09	1.45	1.33
24	C	501	CLA	MG-NC	4.09	2.16	2.06
28	C	519	LMG	O8-C28	4.08	1.45	1.33
24	C	510	CLA	MG-NB	4.08	2.13	2.05
24	C	504	CLA	C3D-C2D	4.08	1.50	1.39
24	B	613	CLA	O2A-CGA	4.08	1.45	1.33
24	A	410	CLA	CHD-C1D	4.08	1.46	1.38
38	L	101	LHG	O8-C23	4.07	1.45	1.33
24	c	914	CLA	CHC-C4B	4.07	1.48	1.39
24	d	405	CLA	CHD-C1D	4.07	1.46	1.38
38	E	101	LHG	O7-C7	4.07	1.45	1.34
37	C	516	DGD	O2G-C1B	4.07	1.45	1.34
24	b	610	CLA	CHC-C4B	4.07	1.48	1.39
24	C	501	CLA	OBD-CAD	4.06	1.29	1.22
34	b	631	DMS	O-S	4.06	1.77	1.50
24	B	616	CLA	CHD-C1D	4.06	1.46	1.38
24	B	611	CLA	CHC-C4B	4.06	1.48	1.39
27	l	101	SQD	O48-C23	4.06	1.45	1.33
24	c	907	CLA	CHD-C4C	4.06	1.48	1.39
24	A	406	CLA	O2A-CGA	4.06	1.45	1.33
24	B	612	CLA	CHB-C1B	4.05	1.48	1.39
24	b	617	CLA	O2A-CGA	4.05	1.45	1.33
24	C	507	CLA	CHB-C1B	4.04	1.48	1.39
24	D	402	CLA	CHC-C4B	4.04	1.48	1.39
24	c	906	CLA	OBD-CAD	4.04	1.29	1.22
24	C	509	CLA	CHC-C4B	4.04	1.48	1.39
24	c	908	CLA	CHC-C4B	4.04	1.48	1.39
24	B	614	CLA	CHD-C1D	4.04	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	903	CLA	C3D-C2D	4.04	1.50	1.39
24	B	617	CLA	CHD-C1D	4.04	1.46	1.38
24	c	902	CLA	CHC-C4B	4.03	1.48	1.39
24	c	913	CLA	O2A-CGA	4.03	1.45	1.33
24	b	618	CLA	CHB-C1B	4.03	1.48	1.39
24	b	613	CLA	OBD-CAD	4.03	1.29	1.22
37	H	102	DGD	O1G-C1A	4.03	1.45	1.33
24	D	402	CLA	MG-NB	4.03	2.13	2.05
24	C	513	CLA	O2A-CGA	4.03	1.45	1.33
24	B	616	CLA	CHB-C1B	4.02	1.48	1.39
24	b	605	CLA	MG-ND	-4.02	1.97	2.05
24	b	605	CLA	CHD-C4C	4.02	1.48	1.39
24	b	613	CLA	O2A-CGA	4.02	1.45	1.33
24	A	405	CLA	CHB-C1B	4.02	1.48	1.39
24	B	616	CLA	CHC-C4B	4.02	1.48	1.39
24	c	911	CLA	CHC-C4B	4.01	1.48	1.39
28	B	621	LMG	O7-C10	4.01	1.45	1.34
24	c	912	CLA	CHD-C4C	4.01	1.48	1.39
24	C	508	CLA	OBD-CAD	4.01	1.29	1.22
24	B	610	CLA	CHC-C4B	4.01	1.48	1.39
24	B	602	CLA	MG-NC	4.01	2.15	2.06
24	B	617	CLA	C3D-C2D	4.01	1.49	1.39
24	a	410	CLA	CHD-C1D	4.00	1.46	1.38
24	B	611	CLA	O2A-CGA	4.00	1.45	1.33
24	b	607	CLA	CHB-C1B	4.00	1.48	1.39
24	A	406	CLA	CHB-C1B	4.00	1.48	1.39
24	d	404	CLA	CHD-C1D	4.00	1.46	1.38
24	b	614	CLA	CHC-C4B	4.00	1.48	1.39
24	C	510	CLA	CHC-C4B	4.00	1.48	1.39
38	l	103	LHG	O7-C7	4.00	1.45	1.34
24	C	501	CLA	CHD-C4C	4.00	1.48	1.39
24	A	407	CLA	MG-NC	3.99	2.15	2.06
24	d	405	CLA	MG-NC	3.99	2.15	2.06
24	D	401	CLA	CHC-C1C	3.99	1.46	1.38
24	c	914	CLA	C3D-C2D	3.99	1.49	1.39
24	C	506	CLA	CHC-C4B	3.99	1.48	1.39
24	b	619	CLA	OBD-CAD	3.99	1.29	1.22
24	b	605	CLA	C3D-C2D	3.99	1.49	1.39
27	a	415	SQD	O48-C23	3.98	1.45	1.33
24	B	605	CLA	CHD-C1D	3.98	1.46	1.38
24	B	607	CLA	CHB-C1B	3.98	1.48	1.39
24	C	511	CLA	CHD-C1D	3.98	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	O2A-CGA	3.98	1.44	1.33
24	b	616	CLA	O2A-CGA	3.98	1.44	1.33
24	c	908	CLA	CHD-C4C	3.98	1.48	1.39
24	b	618	CLA	C3D-C2D	3.97	1.49	1.39
24	C	502	CLA	CHC-C4B	3.97	1.48	1.39
24	a	410	CLA	OBD-CAD	3.97	1.29	1.22
24	c	912	CLA	C3D-C2D	3.97	1.49	1.39
24	C	511	CLA	C3D-C2D	3.97	1.49	1.39
24	b	607	CLA	CHD-C4C	3.97	1.48	1.39
37	h	102	DGD	O2G-C1B	3.97	1.45	1.34
24	A	405	CLA	O2A-CGA	3.97	1.44	1.33
24	A	410	CLA	O2A-CGA	3.97	1.44	1.33
24	C	507	CLA	MG-ND	-3.97	1.97	2.05
24	b	612	CLA	O2A-CGA	3.97	1.44	1.33
24	B	603	CLA	OBD-CAD	3.96	1.29	1.22
24	B	616	CLA	O2A-CGA	3.96	1.44	1.33
24	B	604	CLA	CHC-C4B	3.96	1.48	1.39
24	b	618	CLA	CHC-C4B	3.96	1.48	1.39
24	B	608	CLA	O2A-CGA	3.96	1.44	1.33
24	b	606	CLA	O2A-CGA	3.96	1.44	1.33
37	c	917	DGD	O2G-C1B	3.96	1.45	1.34
24	C	504	CLA	CHD-C4C	3.96	1.48	1.39
24	c	904	CLA	MG-ND	-3.95	1.98	2.05
24	d	405	CLA	CHB-C1B	3.95	1.48	1.39
24	C	513	CLA	CHC-C4B	3.95	1.48	1.39
39	f	101	HEM	FE-NB	3.95	2.07	1.94
24	c	903	CLA	CHC-C4B	3.94	1.48	1.39
24	B	615	CLA	C3D-C2D	3.94	1.49	1.39
24	c	904	CLA	O2A-CGA	3.94	1.44	1.33
24	A	406	CLA	OBD-CAD	3.94	1.29	1.22
24	b	609	CLA	CHC-C4B	3.94	1.48	1.39
24	C	508	CLA	C3D-C2D	3.94	1.49	1.39
24	b	606	CLA	C3D-C2D	3.93	1.49	1.39
24	b	619	CLA	C3D-C2D	3.93	1.49	1.39
24	a	409	CLA	CHD-C4C	3.93	1.48	1.39
24	B	610	CLA	OBD-CAD	3.93	1.29	1.22
24	b	613	CLA	CHD-C4C	3.93	1.48	1.39
24	b	615	CLA	CHC-C4B	3.93	1.48	1.39
24	c	912	CLA	OBD-CAD	3.93	1.29	1.22
24	c	914	CLA	CHD-C4C	3.93	1.48	1.39
24	A	406	CLA	CHC-C4B	3.92	1.48	1.39
24	d	401	CLA	CHB-C1B	3.92	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C3D-C2D	3.92	1.49	1.39
24	A	407	CLA	MG-NA	3.92	2.15	2.06
24	b	610	CLA	CHD-C1D	3.92	1.46	1.38
24	c	914	CLA	CHB-C1B	3.92	1.48	1.39
24	a	410	CLA	O2A-CGA	3.91	1.44	1.33
37	c	919	DGD	O1G-C1A	3.91	1.44	1.33
24	C	505	CLA	OBD-CAD	3.91	1.29	1.22
24	b	611	CLA	C3D-C2D	3.91	1.49	1.39
28	d	412	LMG	O7-C10	3.91	1.45	1.34
24	B	605	CLA	CHC-C4B	3.91	1.48	1.39
24	c	910	CLA	C3D-C2D	3.91	1.49	1.39
24	B	616	CLA	OBD-CAD	3.91	1.29	1.22
24	C	501	CLA	O2A-CGA	3.91	1.44	1.33
24	C	504	CLA	CHB-C1B	3.90	1.48	1.39
24	B	614	CLA	CHB-C1B	3.90	1.48	1.39
24	B	615	CLA	CHD-C1D	3.90	1.46	1.38
24	C	510	CLA	CHD-C4C	3.90	1.48	1.39
24	A	405	CLA	CHD-C1D	3.90	1.46	1.38
24	c	906	CLA	O2A-CGA	3.90	1.44	1.33
24	c	905	CLA	O2A-CGA	3.89	1.44	1.33
24	d	405	CLA	CHC-C4B	3.89	1.48	1.39
24	A	407	CLA	C1D-ND	3.89	1.43	1.37
24	B	605	CLA	CHB-C1B	3.89	1.48	1.39
24	b	609	CLA	O2A-CGA	3.89	1.44	1.33
24	C	506	CLA	CHD-C4C	3.89	1.48	1.39
24	c	911	CLA	MG-NA	3.89	2.15	2.06
24	b	612	CLA	CHC-C4B	3.89	1.48	1.39
24	c	913	CLA	MG-NB	3.88	2.13	2.05
24	b	619	CLA	O2A-CGA	3.88	1.44	1.33
24	b	616	CLA	OBD-CAD	3.88	1.29	1.22
24	c	904	CLA	C3D-C2D	3.88	1.49	1.39
24	b	608	CLA	CHC-C4B	3.88	1.48	1.39
24	a	413	CLA	CHD-C1D	3.88	1.46	1.38
24	c	913	CLA	C3D-C2D	3.88	1.49	1.39
38	d	411	LHG	O7-C7	3.87	1.45	1.34
24	C	509	CLA	C3D-C2D	3.87	1.49	1.39
24	b	606	CLA	CHD-C4C	3.87	1.48	1.39
24	B	606	CLA	O2A-CGA	3.87	1.44	1.33
24	C	508	CLA	CHC-C4B	3.87	1.48	1.39
24	C	511	CLA	CHC-C4B	3.87	1.48	1.39
24	C	502	CLA	C3D-C2D	3.87	1.49	1.39
24	b	619	CLA	MG-ND	-3.87	1.98	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	OBD-CAD	3.87	1.29	1.22
37	H	102	DGD	O2G-C1B	3.86	1.45	1.34
24	c	910	CLA	CHD-C4C	3.86	1.48	1.39
24	B	609	CLA	CHB-C1B	3.86	1.48	1.39
25	a	411	PHO	O2A-CGA	3.86	1.44	1.33
24	c	910	CLA	OBD-CAD	3.86	1.29	1.22
24	c	913	CLA	CHB-C1B	3.86	1.48	1.39
37	c	919	DGD	O2G-C1B	3.86	1.45	1.34
27	A	412	SQD	O48-C23	3.85	1.44	1.33
24	C	509	CLA	CHD-C4C	3.85	1.48	1.39
24	b	609	CLA	CHB-C1B	3.85	1.48	1.39
28	d	412	LMG	O8-C28	3.85	1.44	1.33
27	a	415	SQD	O47-C7	3.85	1.45	1.34
24	B	609	CLA	CHC-C4B	3.85	1.48	1.39
24	C	503	CLA	O2A-CGA	3.84	1.44	1.33
24	A	406	CLA	CHC-C1C	3.84	1.46	1.38
24	A	410	CLA	CHC-C4B	3.84	1.48	1.39
24	C	512	CLA	MG-NB	3.84	2.13	2.05
27	A	412	SQD	O47-C7	3.84	1.45	1.34
24	b	618	CLA	O2A-CGA	3.84	1.44	1.33
24	b	611	CLA	O2A-CGA	3.84	1.44	1.33
24	C	512	CLA	C3D-C2D	3.84	1.49	1.39
24	a	413	CLA	C3D-C2D	3.83	1.49	1.39
37	h	102	DGD	O1G-C1A	3.83	1.44	1.33
24	B	606	CLA	C3D-C2D	3.83	1.49	1.39
25	a	412	PHO	O2A-CGA	3.83	1.44	1.33
24	C	507	CLA	CHC-C4B	3.83	1.48	1.39
24	C	506	CLA	C3D-C2D	3.83	1.49	1.39
24	C	508	CLA	CHD-C4C	3.83	1.47	1.39
24	c	905	CLA	CHB-C1B	3.83	1.48	1.39
24	D	402	CLA	O2A-CGA	3.83	1.44	1.33
25	A	409	PHO	O2A-CGA	3.83	1.44	1.33
24	B	607	CLA	CHD-C4C	3.83	1.47	1.39
24	b	612	CLA	OBD-CAD	3.82	1.29	1.22
24	B	611	CLA	C3D-C2D	3.82	1.49	1.39
24	C	503	CLA	C3D-C2D	3.82	1.49	1.39
24	B	603	CLA	MG-NC	3.82	2.15	2.06
24	c	907	CLA	CHB-C1B	3.82	1.48	1.39
24	A	407	CLA	CHB-C1B	3.82	1.48	1.39
24	c	912	CLA	CHC-C4B	3.82	1.48	1.39
24	c	909	CLA	CHB-C1B	3.82	1.48	1.39
24	C	510	CLA	MG-NC	3.81	2.15	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	O	303	HTG	C1'-S1	-3.81	1.76	1.81
24	c	905	CLA	C3D-C2D	3.81	1.49	1.39
24	c	909	CLA	OBD-CAD	3.81	1.29	1.22
24	a	410	CLA	C3D-C2D	3.81	1.49	1.39
24	B	602	CLA	C3D-C2D	3.81	1.49	1.39
24	A	405	CLA	CHC-C4B	3.81	1.48	1.39
24	B	608	CLA	CHC-C4B	3.80	1.47	1.39
24	b	615	CLA	O2A-CGA	3.80	1.44	1.33
28	C	519	LMG	O7-C10	3.79	1.45	1.34
24	c	903	CLA	CHD-C4C	3.79	1.47	1.39
24	C	513	CLA	CHD-C4C	3.79	1.47	1.39
24	c	909	CLA	C3D-C2D	3.79	1.49	1.39
24	A	405	CLA	C3D-C2D	3.79	1.49	1.39
24	b	605	CLA	OBD-CAD	3.79	1.29	1.22
24	b	611	CLA	C1B-NB	-3.79	1.32	1.37
24	C	512	CLA	CHD-C4C	3.79	1.47	1.39
24	C	502	CLA	OBD-CAD	3.79	1.29	1.22
24	C	501	CLA	CHC-C4B	3.78	1.47	1.39
24	b	607	CLA	CHC-C4B	3.78	1.47	1.39
24	b	619	CLA	CHC-C4B	3.78	1.47	1.39
24	c	907	CLA	C3D-C2D	3.78	1.49	1.39
42	V	203	HEC	CBC-CAC	-3.77	1.35	1.49
24	C	511	CLA	OBD-CAD	3.77	1.29	1.22
24	C	504	CLA	CHC-C4B	3.77	1.47	1.39
24	c	908	CLA	C3D-C2D	3.77	1.49	1.39
24	B	608	CLA	CHB-C1B	3.77	1.47	1.39
24	b	614	CLA	CHB-C1B	3.77	1.47	1.39
24	D	401	CLA	C1D-ND	3.77	1.42	1.37
24	b	608	CLA	O2A-CGA	3.76	1.44	1.33
24	D	401	CLA	CHC-C4B	3.76	1.47	1.39
24	C	510	CLA	C3D-C2D	3.76	1.49	1.39
42	v	202	HEC	CBB-CAB	-3.76	1.35	1.49
24	d	405	CLA	C3D-C2D	3.76	1.49	1.39
24	B	607	CLA	OBD-CAD	3.76	1.29	1.22
37	c	917	DGD	O1G-C1A	3.75	1.44	1.33
24	B	612	CLA	CHC-C4B	3.75	1.47	1.39
37	C	518	DGD	O2G-C1B	3.75	1.44	1.34
24	B	613	CLA	C1D-ND	3.75	1.42	1.37
24	b	616	CLA	CHC-C4B	3.75	1.47	1.39
38	D	406	LHG	O8-C23	3.75	1.44	1.33
24	b	618	CLA	CHD-C4C	3.75	1.47	1.39
38	D	407	LHG	O8-C23	3.74	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	CLA	O2A-CGA	3.73	1.44	1.33
24	B	614	CLA	C3D-C2D	3.73	1.49	1.39
24	C	511	CLA	CHD-C4C	3.73	1.47	1.39
24	C	510	CLA	OBD-CAD	3.73	1.28	1.22
24	B	615	CLA	OBD-CAD	3.73	1.28	1.22
24	B	610	CLA	C3D-C2D	3.73	1.49	1.39
24	C	507	CLA	MG-NC	3.72	2.15	2.06
24	b	617	CLA	CHC-C4B	3.72	1.47	1.39
24	b	615	CLA	CHD-C4C	3.72	1.47	1.39
24	A	410	CLA	OBD-CAD	3.72	1.28	1.22
24	b	619	CLA	CHD-C4C	3.72	1.47	1.39
38	D	408	LHG	O8-C23	3.72	1.44	1.33
24	b	616	CLA	CHD-C1D	3.72	1.45	1.38
24	c	914	CLA	OBD-CAD	3.72	1.28	1.22
24	D	402	CLA	C3D-C2D	3.71	1.49	1.39
24	b	610	CLA	C3D-C2D	3.71	1.49	1.39
24	c	913	CLA	CHD-C4C	3.71	1.47	1.39
39	F	102	HEM	FE-NA	3.71	2.07	1.95
24	c	908	CLA	MG-NC	3.71	2.15	2.06
24	B	613	CLA	C3D-C2D	3.71	1.49	1.39
24	B	615	CLA	CHC-C4B	3.71	1.47	1.39
24	c	913	CLA	CHC-C4B	3.71	1.47	1.39
24	c	903	CLA	O2A-CGA	3.71	1.44	1.33
24	B	603	CLA	C3D-C2D	3.71	1.49	1.39
24	B	606	CLA	CHC-C4B	3.71	1.47	1.39
24	c	908	CLA	OBD-CAD	3.71	1.28	1.22
24	b	606	CLA	CHC-C4B	3.70	1.47	1.39
24	C	513	CLA	OBD-CAD	3.70	1.28	1.22
24	a	410	CLA	CHD-C4C	3.70	1.47	1.39
24	A	410	CLA	CHD-C4C	3.70	1.47	1.39
24	C	505	CLA	CHD-C4C	3.70	1.47	1.39
24	b	607	CLA	C3D-C2D	3.70	1.49	1.39
24	a	409	CLA	O2A-CGA	3.70	1.44	1.33
24	C	505	CLA	O2A-CGA	3.69	1.44	1.33
24	B	604	CLA	CHB-C1B	3.69	1.47	1.39
24	b	611	CLA	CHC-C4B	3.69	1.47	1.39
24	D	402	CLA	OBD-CAD	3.69	1.28	1.22
24	B	609	CLA	CHD-C4C	3.69	1.47	1.39
24	B	614	CLA	O2A-CGA	3.69	1.44	1.33
28	D	409	LMG	O8-C28	3.69	1.44	1.33
24	C	501	CLA	C3D-C2D	3.69	1.49	1.39
37	c	918	DGD	O2G-C1B	3.69	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	CHD-C4C	3.68	1.47	1.39
36	B	623	HTG	C1'-S1	-3.68	1.76	1.81
24	b	615	CLA	C3D-C2D	3.68	1.49	1.39
24	c	911	CLA	C3D-C2D	3.68	1.49	1.39
24	C	513	CLA	C3D-C2D	3.68	1.49	1.39
24	A	407	CLA	C3D-C2D	3.68	1.49	1.39
37	c	918	DGD	O1G-C1A	3.68	1.44	1.33
24	B	603	CLA	CHD-C4C	3.67	1.47	1.39
24	d	405	CLA	CHD-C4C	3.67	1.47	1.39
24	B	612	CLA	CHD-C4C	3.67	1.47	1.39
24	b	610	CLA	CHD-C4C	3.67	1.47	1.39
24	c	906	CLA	CHD-C4C	3.66	1.47	1.39
24	B	609	CLA	C3D-C2D	3.66	1.49	1.39
24	b	609	CLA	C3D-C2D	3.66	1.49	1.39
37	C	517	DGD	O2G-C1B	3.66	1.44	1.34
24	c	904	CLA	CHD-C4C	3.66	1.47	1.39
24	c	911	CLA	O2A-CGA	3.66	1.44	1.33
24	b	611	CLA	CHD-C4C	3.66	1.47	1.39
25	A	408	PHO	OBD-CAD	3.65	1.27	1.22
24	c	911	CLA	CHD-C4C	3.65	1.47	1.39
24	B	605	CLA	OBD-CAD	3.65	1.28	1.22
24	b	620	CLA	OBD-CAD	3.65	1.28	1.22
38	l	103	LHG	O8-C23	3.65	1.44	1.33
38	d	410	LHG	O8-C23	3.64	1.44	1.33
24	c	907	CLA	CHC-C4B	3.64	1.47	1.39
24	B	612	CLA	O2A-CGA	3.64	1.44	1.33
24	A	410	CLA	C3D-C2D	3.64	1.48	1.39
24	c	902	CLA	CHD-C4C	3.64	1.47	1.39
24	D	402	CLA	CHD-C4C	3.63	1.47	1.39
24	B	606	CLA	MG-ND	-3.63	1.98	2.05
24	C	507	CLA	CHD-C4C	3.63	1.47	1.39
24	c	905	CLA	CHD-C4C	3.63	1.47	1.39
24	c	902	CLA	C3D-C2D	3.63	1.48	1.39
24	B	617	CLA	CHC-C4B	3.62	1.47	1.39
24	C	502	CLA	CHD-C4C	3.62	1.47	1.39
24	c	903	CLA	OBD-CAD	3.62	1.28	1.22
38	D	408	LHG	O7-C7	3.62	1.44	1.34
24	C	507	CLA	C3D-C2D	3.61	1.48	1.39
24	d	401	CLA	CHC-C4B	3.61	1.47	1.39
24	b	609	CLA	CHD-C4C	3.61	1.47	1.39
24	B	605	CLA	CHD-C4C	3.61	1.47	1.39
24	B	603	CLA	O2A-CGA	3.60	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C3D-C2D	3.60	1.48	1.39
24	b	614	CLA	CHD-C4C	3.60	1.47	1.39
24	b	620	CLA	CHC-C4B	3.60	1.47	1.39
24	d	401	CLA	C3D-C2D	3.60	1.48	1.39
24	c	910	CLA	CHC-C4B	3.60	1.47	1.39
24	b	614	CLA	C3D-C2D	3.60	1.48	1.39
24	b	617	CLA	OBD-CAD	3.59	1.28	1.22
24	D	401	CLA	CHD-C4C	3.59	1.47	1.39
24	B	617	CLA	MG-NC	3.59	2.14	2.06
38	d	410	LHG	O7-C7	3.59	1.44	1.34
24	a	413	CLA	CHC-C4B	3.58	1.47	1.39
36	b	627	HTG	C1'-S1	-3.58	1.76	1.81
24	B	612	CLA	OBD-CAD	3.58	1.28	1.22
24	b	620	CLA	C3D-C2D	3.58	1.48	1.39
38	D	407	LHG	O7-C7	3.58	1.44	1.34
24	C	505	CLA	C3D-C2D	3.58	1.48	1.39
24	b	609	CLA	MG-NC	3.58	2.14	2.06
24	B	610	CLA	O2A-CGA	3.57	1.43	1.33
24	A	405	CLA	OBD-CAD	3.57	1.28	1.22
24	a	409	CLA	CHC-C4B	3.57	1.47	1.39
24	C	503	CLA	CHD-C4C	3.56	1.47	1.39
24	b	608	CLA	C3D-C2D	3.56	1.48	1.39
25	a	411	PHO	OBD-CAD	3.56	1.27	1.22
24	d	404	CLA	CHD-C4C	3.56	1.47	1.39
24	b	617	CLA	C3D-C2D	3.55	1.48	1.39
25	A	408	PHO	O2A-CGA	3.55	1.43	1.33
24	B	615	CLA	MG-ND	-3.55	1.98	2.05
24	C	512	CLA	OBD-CAD	3.54	1.28	1.22
24	c	905	CLA	CHC-C4B	3.54	1.47	1.39
24	d	401	CLA	MG-NB	3.54	2.12	2.05
24	d	401	CLA	CHD-C4C	3.54	1.47	1.39
24	A	407	CLA	CHD-C4C	3.53	1.47	1.39
24	b	612	CLA	C3D-C2D	3.53	1.48	1.39
24	d	405	CLA	OBD-CAD	3.53	1.28	1.22
24	b	616	CLA	C3D-C2D	3.53	1.48	1.39
24	c	909	CLA	CHD-C4C	3.53	1.47	1.39
24	B	607	CLA	C3D-C2D	3.52	1.48	1.39
24	B	604	CLA	C3D-C2D	3.52	1.48	1.39
24	b	614	CLA	O2A-CGA	3.52	1.43	1.33
24	B	602	CLA	OBD-CAD	3.52	1.28	1.22
24	C	505	CLA	C1B-NB	-3.52	1.33	1.37
24	B	613	CLA	CHD-C4C	3.52	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	CHD-C4C	3.52	1.47	1.39
24	c	906	CLA	C3D-C2D	3.52	1.48	1.39
37	C	517	DGD	O1G-C1A	3.52	1.43	1.33
24	C	510	CLA	O2A-CGA	3.51	1.43	1.33
24	C	509	CLA	OBD-CAD	3.51	1.28	1.22
24	B	609	CLA	OBD-CAD	3.51	1.28	1.22
24	c	902	CLA	OBD-CAD	3.51	1.28	1.22
24	b	617	CLA	CHD-C4C	3.51	1.47	1.39
24	A	407	CLA	CHC-C4B	3.50	1.47	1.39
24	B	607	CLA	O2A-CGA	3.50	1.43	1.33
24	c	909	CLA	CHC-C4B	3.50	1.47	1.39
24	b	612	CLA	CHD-C4C	3.50	1.47	1.39
24	B	608	CLA	C3D-C2D	3.50	1.48	1.39
24	A	405	CLA	CHD-C4C	3.50	1.47	1.39
24	B	613	CLA	CHC-C4B	3.49	1.47	1.39
24	c	913	CLA	OBD-CAD	3.49	1.28	1.22
24	b	618	CLA	MG-NB	3.48	2.12	2.05
24	C	501	CLA	MG-ND	-3.48	1.98	2.05
24	a	413	CLA	CHD-C4C	3.48	1.47	1.39
24	a	409	CLA	C1B-NB	-3.47	1.33	1.37
24	B	606	CLA	OBD-CAD	3.47	1.28	1.22
24	B	614	CLA	CHD-C4C	3.46	1.47	1.39
36	D	412	HTG	C1'-S1	-3.46	1.76	1.81
24	b	606	CLA	OBD-CAD	3.46	1.28	1.22
24	C	506	CLA	OBD-CAD	3.46	1.28	1.22
36	y	102	HTG	C1'-S1	-3.45	1.76	1.81
38	d	411	LHG	O8-C23	3.45	1.43	1.33
24	B	612	CLA	C3D-C2D	3.44	1.48	1.39
24	c	904	CLA	OBD-CAD	3.44	1.28	1.22
24	d	404	CLA	CHC-C4B	3.44	1.47	1.39
24	B	613	CLA	C1B-NB	-3.44	1.33	1.37
24	b	616	CLA	MG-NC	3.44	2.14	2.06
36	d	419	HTG	C1'-S1	-3.43	1.76	1.81
24	b	614	CLA	MG-NC	3.43	2.14	2.06
24	B	604	CLA	CHD-C4C	3.43	1.47	1.39
24	C	510	CLA	C1B-NB	-3.43	1.33	1.37
24	b	615	CLA	MG-NC	3.43	2.14	2.06
24	A	407	CLA	C1B-NB	-3.43	1.33	1.37
36	C	521	HTG	C1'-S1	-3.42	1.76	1.81
37	C	518	DGD	O1G-C1A	3.42	1.43	1.33
24	B	617	CLA	CHD-C4C	3.42	1.47	1.39
24	b	607	CLA	OBD-CAD	3.42	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	908	CLA	C4D-CHA	3.42	1.50	1.38
24	C	504	CLA	O2A-CGA	3.42	1.43	1.33
24	c	907	CLA	OBD-CAD	3.41	1.28	1.22
24	B	605	CLA	C3D-C2D	3.41	1.48	1.39
24	B	614	CLA	OBD-CAD	3.41	1.28	1.22
37	C	516	DGD	O1G-C1A	3.40	1.43	1.33
24	c	911	CLA	OBD-CAD	3.40	1.28	1.22
36	c	924	HTG	C1'-S1	-3.40	1.76	1.81
24	A	406	CLA	CHD-C4C	3.39	1.46	1.39
36	C	536	HTG	C1'-S1	-3.38	1.76	1.81
24	b	620	CLA	CHD-C4C	3.38	1.46	1.39
24	b	608	CLA	C4D-CHA	3.38	1.50	1.38
24	A	410	CLA	MG-NC	3.38	2.14	2.06
24	b	614	CLA	C1B-NB	-3.38	1.33	1.37
24	C	504	CLA	OBD-CAD	3.37	1.28	1.22
24	c	904	CLA	C4D-CHA	3.37	1.49	1.38
24	B	611	CLA	OBD-CAD	3.36	1.28	1.22
24	a	413	CLA	MG-NC	3.36	2.14	2.06
25	A	409	PHO	CHA-CBD	-3.36	1.47	1.51
24	A	406	CLA	C3D-C2D	3.36	1.48	1.39
24	b	615	CLA	OBD-CAD	3.35	1.28	1.22
28	D	409	LMG	O7-C10	3.35	1.43	1.34
24	d	404	CLA	C3D-C2D	3.34	1.48	1.39
36	c	928	HTG	C1'-S1	-3.34	1.76	1.81
36	d	414	HTG	C1'-S1	-3.34	1.76	1.81
24	D	401	CLA	OBD-CAD	3.34	1.28	1.22
24	C	507	CLA	C4D-CHA	3.33	1.49	1.38
24	c	905	CLA	OBD-CAD	3.32	1.28	1.22
36	d	420	HTG	C1'-S1	-3.32	1.76	1.81
36	v	211	HTG	C1'-S1	-3.32	1.76	1.81
24	a	410	CLA	CHC-C4B	3.32	1.46	1.39
24	d	404	CLA	OBD-CAD	3.31	1.28	1.22
24	B	611	CLA	CHD-C4C	3.31	1.46	1.39
24	c	907	CLA	C1B-NB	-3.30	1.33	1.37
36	V	215	HTG	C1'-S1	-3.30	1.76	1.81
24	B	615	CLA	CHD-C4C	3.29	1.46	1.39
24	C	508	CLA	C1B-NB	-3.28	1.33	1.37
24	b	616	CLA	C1B-NB	-3.28	1.33	1.37
39	f	101	HEM	CAB-C3B	3.28	1.56	1.47
24	d	405	CLA	C4B-NB	-3.27	1.33	1.37
38	d	409	LHG	O7-C7	3.27	1.43	1.34
24	b	618	CLA	OBD-CAD	3.26	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	943	HTG	C1'-S1	-3.26	1.76	1.81
24	C	503	CLA	C4D-CHA	3.26	1.49	1.38
24	a	410	CLA	C4B-NB	-3.25	1.33	1.37
42	V	203	HEC	CBB-CAB	-3.25	1.37	1.49
24	D	401	CLA	C3D-C2D	3.25	1.47	1.39
24	B	605	CLA	O2A-CGA	3.25	1.42	1.33
24	B	608	CLA	OBD-CAD	3.24	1.28	1.22
24	b	612	CLA	C1B-NB	-3.23	1.33	1.37
24	B	615	CLA	MG-NC	3.22	2.13	2.06
24	b	608	CLA	OBD-CAD	3.22	1.28	1.22
24	B	616	CLA	C1B-NB	-3.22	1.33	1.37
24	b	611	CLA	C1B-C2B	3.22	1.50	1.43
24	B	610	CLA	CHD-C4C	3.21	1.46	1.39
36	c	923	HTG	C1'-S1	-3.20	1.76	1.81
24	B	604	CLA	OBD-CAD	3.20	1.28	1.22
36	b	603	HTG	C1'-S1	-3.20	1.76	1.81
24	d	405	CLA	C1B-NB	-3.19	1.33	1.37
24	b	608	CLA	CHD-C4C	3.19	1.46	1.39
24	c	910	CLA	C1B-C2B	3.19	1.50	1.43
24	A	405	CLA	C4B-NB	-3.19	1.33	1.37
24	B	605	CLA	C4D-CHA	3.19	1.49	1.38
24	B	616	CLA	C1B-C2B	3.18	1.50	1.43
36	B	630	HTG	C1'-S1	-3.18	1.76	1.81
24	c	910	CLA	C1B-NB	-3.18	1.33	1.37
24	c	910	CLA	C4D-CHA	3.18	1.49	1.38
24	b	619	CLA	C4D-CHA	3.18	1.49	1.38
24	A	406	CLA	MG-NC	3.18	2.13	2.06
24	B	606	CLA	C1B-C2B	3.16	1.50	1.43
24	B	617	CLA	OBD-CAD	3.16	1.27	1.22
24	D	402	CLA	MG-NA	3.16	2.13	2.06
24	c	912	CLA	C1B-C2B	3.16	1.50	1.43
24	C	511	CLA	C4D-CHA	3.16	1.49	1.38
24	b	614	CLA	OBD-CAD	3.15	1.27	1.22
36	b	602	HTG	C1'-S1	-3.15	1.77	1.81
36	C	537	HTG	C1'-S1	-3.15	1.77	1.81
25	A	408	PHO	CHA-CBD	-3.15	1.48	1.51
24	A	405	CLA	C1B-NB	-3.15	1.33	1.37
36	B	625	HTG	C1'-S1	-3.14	1.77	1.81
36	B	631	HTG	C1'-S1	-3.14	1.77	1.81
24	a	410	CLA	C1B-C2B	3.14	1.50	1.43
36	c	942	HTG	C1'-S1	-3.13	1.77	1.81
36	c	941	HTG	C1'-S1	-3.13	1.77	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	f	101	HEM	FE-NA	3.13	2.05	1.95
24	B	612	CLA	C4D-CHA	3.13	1.49	1.38
24	C	509	CLA	C4B-NB	-3.13	1.33	1.37
24	c	911	CLA	C1B-NB	-3.13	1.33	1.37
24	a	409	CLA	C3D-C2D	3.12	1.47	1.39
24	b	610	CLA	C4D-CHA	3.12	1.49	1.38
24	c	913	CLA	C1B-C2B	3.11	1.50	1.43
36	C	520	HTG	C1'-S1	-3.11	1.77	1.81
36	B	629	HTG	C1'-S1	-3.10	1.77	1.81
24	B	616	CLA	C4D-CHA	3.10	1.49	1.38
24	a	409	CLA	C4B-NB	-3.10	1.33	1.37
24	b	612	CLA	C4D-CHA	3.10	1.49	1.38
24	b	620	CLA	C1B-C2B	3.10	1.50	1.43
24	c	908	CLA	C4B-NB	-3.10	1.33	1.37
24	B	617	CLA	C4B-NB	-3.10	1.33	1.37
24	a	413	CLA	MG-ND	-3.09	1.99	2.05
24	c	903	CLA	MG-NB	3.09	2.11	2.05
24	b	615	CLA	C1B-NB	-3.09	1.33	1.37
24	d	405	CLA	C1B-C2B	3.09	1.50	1.43
24	c	910	CLA	MG-NC	3.09	2.13	2.06
24	C	503	CLA	OBD-CAD	3.08	1.27	1.22
38	D	406	LHG	O7-C7	3.08	1.43	1.34
24	C	512	CLA	C4D-CHA	3.08	1.48	1.38
24	b	606	CLA	C4D-CHA	3.08	1.48	1.38
24	c	906	CLA	C1B-C2B	3.07	1.50	1.43
24	a	413	CLA	OBD-CAD	3.07	1.27	1.22
24	C	511	CLA	C1B-C2B	3.07	1.50	1.43
24	B	608	CLA	C1B-C2B	3.07	1.50	1.43
24	B	615	CLA	C4B-NB	-3.06	1.33	1.37
39	F	102	HEM	CAB-C3B	3.06	1.55	1.47
24	c	908	CLA	C1B-C2B	3.05	1.50	1.43
24	B	607	CLA	C4D-CHA	3.05	1.48	1.38
24	B	616	CLA	C4B-NB	-3.05	1.33	1.37
24	c	913	CLA	C4D-CHA	3.05	1.48	1.38
24	b	609	CLA	OBD-CAD	3.04	1.27	1.22
24	C	512	CLA	C1B-C2B	3.04	1.50	1.43
24	c	912	CLA	C4D-CHA	3.03	1.48	1.38
24	C	505	CLA	C4D-CHA	3.03	1.48	1.38
24	b	611	CLA	MG-NB	3.02	2.11	2.05
24	b	620	CLA	MG-NC	3.01	2.13	2.06
25	a	412	PHO	C3A-C2A	-3.01	1.52	1.54
24	b	610	CLA	C1B-C2B	3.01	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	C4B-NB	-3.01	1.33	1.37
24	b	605	CLA	C4D-CHA	3.01	1.48	1.38
24	c	903	CLA	C1B-C2B	3.00	1.50	1.43
24	C	506	CLA	C4D-CHA	3.00	1.48	1.38
24	b	616	CLA	C4B-NB	-3.00	1.33	1.37
24	B	608	CLA	C1B-NB	-3.00	1.33	1.37
24	A	405	CLA	C4D-CHA	3.00	1.48	1.38
24	B	611	CLA	C1B-C2B	2.99	1.50	1.43
24	B	602	CLA	C4D-CHA	2.99	1.48	1.38
24	C	502	CLA	C4D-CHA	2.99	1.48	1.38
24	B	609	CLA	C4C-C3C	2.99	1.50	1.45
24	D	401	CLA	MG-NC	2.99	2.13	2.06
24	b	615	CLA	C4D-CHA	2.98	1.48	1.38
24	B	609	CLA	C4D-CHA	2.98	1.48	1.38
24	b	611	CLA	OBD-CAD	2.98	1.27	1.22
24	B	614	CLA	C4D-CHA	2.98	1.48	1.38
24	b	611	CLA	C4D-CHA	2.97	1.48	1.38
24	c	909	CLA	C1B-NB	-2.97	1.34	1.37
24	B	603	CLA	C1B-C2B	2.97	1.50	1.43
24	B	611	CLA	C1B-NB	-2.96	1.34	1.37
39	F	102	HEM	FE-NC	2.96	2.04	1.95
24	c	903	CLA	C1B-NB	-2.96	1.34	1.37
24	C	509	CLA	C4D-CHA	2.96	1.48	1.38
24	b	620	CLA	C4B-NB	-2.95	1.34	1.37
24	c	905	CLA	C1B-NB	-2.95	1.34	1.37
24	b	614	CLA	C4D-CHA	2.95	1.48	1.38
24	C	502	CLA	C1B-C2B	2.94	1.50	1.43
24	c	905	CLA	C4D-CHA	2.94	1.48	1.38
24	c	904	CLA	C1B-C2B	2.94	1.50	1.43
39	f	101	HEM	CAC-C3C	2.94	1.55	1.47
24	B	609	CLA	C1B-NB	-2.94	1.34	1.37
24	a	413	CLA	C1B-C2B	2.94	1.50	1.43
24	b	618	CLA	C1B-NB	-2.93	1.34	1.37
24	A	406	CLA	C4B-NB	-2.93	1.34	1.37
24	A	410	CLA	C4D-CHA	2.93	1.48	1.38
24	B	610	CLA	C4D-CHA	2.93	1.48	1.38
24	B	615	CLA	C1B-C2B	2.92	1.50	1.43
24	C	505	CLA	C1B-C2B	2.92	1.50	1.43
24	B	604	CLA	C1B-C2B	2.92	1.50	1.43
24	b	616	CLA	C1B-C2B	2.92	1.50	1.43
24	A	410	CLA	C1B-C2B	2.92	1.50	1.43
24	B	612	CLA	C4B-NB	-2.92	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C4D-CHA	2.92	1.48	1.38
24	B	613	CLA	C1B-C2B	2.91	1.50	1.43
24	c	902	CLA	C4D-CHA	2.90	1.48	1.38
24	C	501	CLA	C4D-CHA	2.90	1.48	1.38
24	b	613	CLA	C4D-CHA	2.90	1.48	1.38
24	C	501	CLA	C1B-C2B	2.89	1.49	1.43
24	a	409	CLA	MG-NB	2.89	2.11	2.05
24	A	410	CLA	C4B-NB	-2.89	1.34	1.37
24	B	617	CLA	C1B-C2B	2.89	1.49	1.43
24	d	401	CLA	C1B-NB	-2.88	1.34	1.37
24	C	509	CLA	C1B-C2B	2.88	1.49	1.43
24	D	402	CLA	C1B-NB	-2.88	1.34	1.37
39	F	102	HEM	CAC-C3C	2.88	1.55	1.47
24	B	615	CLA	C1B-NB	-2.88	1.34	1.37
24	b	619	CLA	C1B-C2B	2.87	1.49	1.43
24	D	402	CLA	C4D-CHA	2.87	1.48	1.38
24	d	405	CLA	C4D-CHA	2.87	1.48	1.38
24	B	609	CLA	C4B-NB	-2.87	1.34	1.37
24	D	402	CLA	C1B-C2B	2.87	1.49	1.43
24	b	609	CLA	C1B-NB	-2.87	1.34	1.37
24	c	914	CLA	C1B-C2B	2.87	1.49	1.43
24	b	606	CLA	C4B-NB	-2.87	1.34	1.37
24	c	911	CLA	C4D-CHA	2.86	1.48	1.38
24	B	605	CLA	C1B-NB	-2.86	1.34	1.37
24	c	911	CLA	C1B-C2B	2.86	1.49	1.43
24	d	404	CLA	C4D-CHA	2.86	1.48	1.38
24	C	507	CLA	C1B-C2B	2.86	1.49	1.43
24	c	906	CLA	C4D-CHA	2.86	1.48	1.38
24	B	617	CLA	C4D-CHA	2.85	1.48	1.38
24	b	614	CLA	C1B-C2B	2.85	1.49	1.43
24	b	613	CLA	MG-NB	-2.85	2.00	2.05
24	C	511	CLA	C1B-NB	-2.84	1.34	1.37
24	c	914	CLA	C4D-CHA	2.84	1.48	1.38
24	c	903	CLA	C4B-NB	-2.83	1.34	1.37
24	A	410	CLA	MG-ND	-2.83	2.00	2.05
24	b	616	CLA	CHD-C4C	2.83	1.45	1.39
24	C	513	CLA	C1B-C2B	2.83	1.49	1.43
24	B	607	CLA	C1B-C2B	2.83	1.49	1.43
24	C	510	CLA	C4D-CHA	2.83	1.48	1.38
24	A	406	CLA	C1B-C2B	2.83	1.49	1.43
24	A	406	CLA	C4D-CHA	2.82	1.48	1.38
24	B	608	CLA	C4D-CHA	2.82	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C1C-C2C	2.82	1.50	1.44
24	c	909	CLA	MG-NA	2.81	2.13	2.06
24	C	504	CLA	C1B-NB	-2.81	1.34	1.37
24	B	613	CLA	C4D-CHA	2.81	1.48	1.38
24	b	620	CLA	C4D-CHA	2.81	1.48	1.38
25	a	412	PHO	C4B-NB	-2.80	1.33	1.38
24	C	504	CLA	C4D-CHA	2.80	1.48	1.38
24	B	610	CLA	C1B-C2B	2.80	1.49	1.43
24	b	609	CLA	C1B-C2B	2.80	1.49	1.43
24	b	617	CLA	C1C-NC	-2.80	1.33	1.37
24	b	617	CLA	C4D-CHA	2.80	1.48	1.38
24	A	407	CLA	C1B-C2B	2.79	1.49	1.43
24	B	611	CLA	C4D-CHA	2.79	1.48	1.38
24	A	406	CLA	C1B-NB	-2.79	1.34	1.37
24	C	510	CLA	C1B-C2B	2.79	1.49	1.43
24	c	903	CLA	C4D-CHA	2.78	1.47	1.38
24	b	609	CLA	C4D-CHA	2.78	1.47	1.38
24	B	602	CLA	C1B-C2B	2.78	1.49	1.43
24	a	410	CLA	C4D-CHA	2.77	1.47	1.38
24	C	513	CLA	C4D-CHA	2.77	1.47	1.38
24	c	902	CLA	C1B-C2B	2.77	1.49	1.43
24	b	607	CLA	C4D-CHA	2.77	1.47	1.38
24	b	617	CLA	C1B-C2B	2.77	1.49	1.43
24	B	604	CLA	C1B-NB	-2.77	1.34	1.37
24	c	905	CLA	C1B-C2B	2.76	1.49	1.43
24	B	603	CLA	C4D-CHA	2.76	1.47	1.38
24	c	909	CLA	C4B-NB	-2.76	1.34	1.37
24	c	912	CLA	MG-ND	-2.76	2.00	2.05
24	c	904	CLA	C1C-C2C	2.76	1.50	1.44
24	c	907	CLA	C4D-CHA	2.76	1.47	1.38
29	a	417	PL9	C6-C5	2.75	1.48	1.35
24	a	409	CLA	C4D-CHA	2.74	1.47	1.38
24	C	510	CLA	C4B-NB	-2.74	1.34	1.37
36	b	626	HTG	C1'-S1	-2.74	1.77	1.81
24	a	413	CLA	C4D-CHA	2.73	1.47	1.38
24	d	401	CLA	C1B-C2B	2.73	1.49	1.43
24	b	618	CLA	C1B-C2B	2.73	1.49	1.43
24	B	602	CLA	C4B-NB	-2.72	1.34	1.37
24	B	613	CLA	C4B-NB	-2.72	1.34	1.37
24	B	607	CLA	C1B-NB	-2.72	1.34	1.37
24	b	606	CLA	C1B-C2B	2.72	1.49	1.43
37	h	102	DGD	O5D-C1E	2.71	1.44	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	912	CLA	C1B-NB	-2.71	1.34	1.37
24	B	610	CLA	C1C-NC	-2.71	1.33	1.37
24	B	612	CLA	MG-NC	2.71	2.12	2.06
24	b	615	CLA	C1B-C2B	2.71	1.49	1.43
24	a	410	CLA	C1B-NB	-2.70	1.34	1.37
24	C	512	CLA	C1B-NB	-2.70	1.34	1.37
42	V	203	HEC	CMC-C2C	2.70	1.56	1.50
24	A	405	CLA	C1C-C2C	2.70	1.50	1.44
24	B	605	CLA	C1B-C2B	2.70	1.49	1.43
24	C	511	CLA	MG-NB	2.69	2.11	2.05
24	b	615	CLA	MG-NB	2.69	2.11	2.05
24	c	906	CLA	C4C-C3C	2.69	1.49	1.45
24	B	614	CLA	C4B-NB	-2.68	1.34	1.37
24	C	508	CLA	C1B-C2B	2.67	1.49	1.43
24	b	608	CLA	C4B-NB	-2.67	1.34	1.37
24	A	407	CLA	C4D-CHA	2.67	1.47	1.38
24	b	606	CLA	C1B-NB	-2.67	1.34	1.37
24	c	904	CLA	C4C-C3C	2.66	1.49	1.45
24	b	620	CLA	C1B-NB	-2.66	1.34	1.37
24	A	407	CLA	C4B-NB	-2.66	1.34	1.37
24	b	616	CLA	C4D-CHA	2.66	1.47	1.38
24	C	503	CLA	C1B-C2B	2.66	1.49	1.43
24	B	602	CLA	MG-ND	-2.66	2.00	2.05
24	d	404	CLA	C1C-NC	-2.65	1.33	1.37
24	a	410	CLA	MG-NC	2.65	2.12	2.06
36	B	624	HTG	C1'-S1	-2.65	1.77	1.81
24	c	909	CLA	C1B-C2B	2.65	1.49	1.43
24	b	618	CLA	C4D-CHA	2.65	1.47	1.38
24	b	607	CLA	C1B-C2B	2.65	1.49	1.43
24	C	512	CLA	C4B-NB	-2.64	1.34	1.37
24	C	513	CLA	MG-NB	2.64	2.11	2.05
24	c	910	CLA	MG-NB	2.64	2.11	2.05
24	b	610	CLA	C1B-NB	-2.64	1.34	1.37
24	c	914	CLA	C1C-C2C	2.64	1.49	1.44
24	D	401	CLA	MG-NB	-2.64	2.00	2.05
29	d	407	PL9	C6-C5	2.64	1.48	1.35
24	C	502	CLA	C1B-NB	-2.64	1.34	1.37
24	C	505	CLA	C4C-C3C	2.64	1.49	1.45
24	c	906	CLA	C1B-NB	-2.64	1.34	1.37
24	B	611	CLA	C4B-NB	-2.63	1.34	1.37
24	c	913	CLA	C1B-NB	-2.63	1.34	1.37
24	D	401	CLA	C1B-C2B	2.63	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	411	PHO	C4B-NB	-2.63	1.33	1.38
24	A	410	CLA	C1B-NB	-2.62	1.34	1.37
24	c	910	CLA	C4B-NB	-2.62	1.34	1.37
24	C	502	CLA	C1C-C2C	2.62	1.49	1.44
24	b	605	CLA	C3B-C4B	2.62	1.50	1.42
24	C	507	CLA	C4B-NB	-2.62	1.34	1.37
24	b	605	CLA	C1B-NB	-2.61	1.34	1.37
36	O	316	HTG	C1'-S1	-2.61	1.77	1.81
24	C	506	CLA	C1B-NB	-2.61	1.34	1.37
29	A	414	PL9	C6-C5	2.61	1.48	1.35
24	C	501	CLA	C4B-NB	-2.61	1.34	1.37
24	b	615	CLA	C4B-NB	-2.60	1.34	1.37
29	D	404	PL9	C6-C5	2.60	1.48	1.35
24	B	603	CLA	C4B-NB	-2.60	1.34	1.37
24	b	619	CLA	C1B-NB	-2.60	1.34	1.37
24	c	902	CLA	C1C-C2C	2.60	1.49	1.44
24	B	609	CLA	C1B-C2B	2.60	1.49	1.43
24	b	613	CLA	C1C-NC	-2.60	1.33	1.37
24	b	614	CLA	C4C-C3C	2.60	1.49	1.45
24	B	612	CLA	C1B-NB	-2.59	1.34	1.37
24	b	610	CLA	C1C-C2C	2.59	1.49	1.44
24	C	508	CLA	C4B-NB	-2.59	1.34	1.37
24	D	402	CLA	C3B-C4B	2.58	1.50	1.42
24	B	603	CLA	C1B-NB	-2.58	1.34	1.37
37	H	102	DGD	O5D-C1E	2.58	1.44	1.40
24	c	902	CLA	C4B-NB	-2.57	1.34	1.37
24	a	413	CLA	C1B-NB	-2.57	1.34	1.37
24	b	620	CLA	C1C-NC	-2.56	1.33	1.37
24	b	615	CLA	C3B-C2B	2.56	1.49	1.41
24	b	612	CLA	C1C-NC	-2.56	1.33	1.37
24	a	409	CLA	C1B-C2B	2.56	1.49	1.43
24	b	619	CLA	C4B-NB	-2.56	1.34	1.37
24	c	908	CLA	C1C-C2C	2.56	1.49	1.44
24	B	611	CLA	C4C-C3C	2.56	1.49	1.45
24	B	608	CLA	C3D-C4D	-2.55	1.38	1.44
24	d	404	CLA	C4B-NB	-2.54	1.34	1.37
24	C	508	CLA	C4C-C3C	2.54	1.49	1.45
24	b	605	CLA	C1C-C2C	2.54	1.49	1.44
24	C	513	CLA	C1C-C2C	2.54	1.49	1.44
24	d	401	CLA	C4D-CHA	2.54	1.47	1.38
24	B	606	CLA	C4D-CHA	2.54	1.47	1.38
24	B	607	CLA	MG-ND	-2.53	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	C1B-C2B	2.53	1.49	1.43
24	C	510	CLA	C3D-C4D	-2.52	1.38	1.44
24	C	501	CLA	C1B-NB	-2.52	1.34	1.37
24	b	614	CLA	C4B-NB	-2.52	1.34	1.37
24	b	618	CLA	C4B-NB	-2.52	1.34	1.37
24	D	401	CLA	C4B-NB	-2.51	1.34	1.37
24	a	413	CLA	C4B-NB	-2.51	1.34	1.37
24	B	611	CLA	C3B-C4B	2.51	1.50	1.42
25	a	411	PHO	CHA-CBD	-2.51	1.48	1.51
24	b	620	CLA	C3B-C2B	2.51	1.49	1.41
24	d	405	CLA	C1C-C2C	2.51	1.49	1.44
24	C	508	CLA	C4D-CHA	2.51	1.47	1.38
24	c	912	CLA	C4B-NB	-2.51	1.34	1.37
25	A	408	PHO	C4B-NB	-2.51	1.34	1.38
24	B	614	CLA	C1C-C2C	2.51	1.49	1.44
24	b	612	CLA	C1B-C2B	2.51	1.49	1.43
24	b	617	CLA	C1B-NB	-2.50	1.34	1.37
24	C	509	CLA	C1B-NB	-2.50	1.34	1.37
24	b	608	CLA	C1C-C2C	2.49	1.49	1.44
24	d	404	CLA	C1B-C2B	2.49	1.49	1.43
24	A	405	CLA	MG-NB	2.48	2.10	2.05
24	b	608	CLA	C1C-NC	-2.48	1.34	1.37
24	b	607	CLA	C4B-NB	-2.48	1.34	1.37
24	c	914	CLA	C1B-NB	-2.47	1.34	1.37
24	c	911	CLA	C4B-NB	-2.47	1.34	1.37
24	c	909	CLA	C4D-CHA	2.47	1.46	1.38
24	C	505	CLA	C3B-C4B	2.47	1.49	1.42
24	b	612	CLA	C1C-C2C	2.47	1.49	1.44
24	b	617	CLA	C4C-C3C	2.46	1.49	1.45
24	c	907	CLA	C1C-NC	-2.46	1.34	1.37
24	C	503	CLA	C1C-NC	-2.46	1.34	1.37
24	C	513	CLA	C1B-NB	-2.46	1.34	1.37
24	B	614	CLA	C1B-NB	-2.46	1.34	1.37
24	D	401	CLA	C4D-CHA	2.45	1.46	1.38
24	C	506	CLA	C1B-C2B	2.45	1.48	1.43
24	C	505	CLA	C1C-C2C	2.45	1.49	1.44
24	C	512	CLA	C1C-C2C	2.45	1.49	1.44
24	c	906	CLA	C4B-NB	-2.45	1.34	1.37
24	B	607	CLA	C1C-C2C	2.45	1.49	1.44
24	B	602	CLA	C1C-C2C	2.44	1.49	1.44
24	d	404	CLA	C1B-NB	-2.44	1.34	1.37
24	b	614	CLA	C3B-C4B	2.44	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C3B-C2B	2.44	1.49	1.41
24	c	910	CLA	C3B-C2B	2.44	1.49	1.41
24	C	513	CLA	C3B-C2B	2.44	1.49	1.41
24	A	405	CLA	C1B-C2B	2.44	1.48	1.43
24	B	606	CLA	C3B-C2B	2.44	1.49	1.41
24	c	908	CLA	C3B-C2B	2.44	1.49	1.41
24	B	602	CLA	C3B-C4B	2.44	1.49	1.42
24	B	606	CLA	C4B-NB	-2.43	1.34	1.37
24	c	912	CLA	C4C-C3C	2.43	1.49	1.45
24	c	913	CLA	C4B-NB	-2.43	1.34	1.37
24	b	607	CLA	C1C-NC	-2.43	1.34	1.37
24	B	617	CLA	C3B-C2B	2.43	1.49	1.41
24	B	602	CLA	C1B-NB	-2.43	1.34	1.37
24	B	614	CLA	C1B-C2B	2.43	1.48	1.43
24	C	504	CLA	C1B-C2B	2.43	1.48	1.43
24	b	609	CLA	C3B-C4B	2.43	1.49	1.42
24	C	509	CLA	C1C-NC	-2.43	1.34	1.37
24	d	405	CLA	C4C-C3C	2.42	1.49	1.45
24	b	607	CLA	C4C-C3C	2.42	1.49	1.45
24	C	509	CLA	C4C-C3C	2.42	1.49	1.45
36	C	536	HTG	C1-S1	-2.42	1.76	1.80
24	c	914	CLA	C4C-C3C	2.42	1.49	1.45
24	A	405	CLA	C3B-C2B	2.41	1.49	1.41
24	D	402	CLA	C3D-C4D	-2.40	1.38	1.44
24	B	604	CLA	C4D-CHA	2.40	1.46	1.38
24	C	511	CLA	C1C-C2C	2.39	1.49	1.44
25	A	408	PHO	C1D-ND	-2.39	1.34	1.38
24	B	612	CLA	C1B-C2B	2.39	1.48	1.43
24	C	508	CLA	C3B-C4B	2.39	1.49	1.42
24	A	406	CLA	C3B-C2B	2.39	1.49	1.41
24	B	617	CLA	C1C-NC	-2.39	1.34	1.37
24	b	618	CLA	C4C-C3C	2.38	1.49	1.45
24	b	608	CLA	C1B-C2B	2.38	1.48	1.43
24	b	612	CLA	C3D-C4D	-2.38	1.38	1.44
24	B	602	CLA	C3B-C2B	2.38	1.49	1.41
24	A	406	CLA	MG-NB	2.38	2.10	2.05
24	B	606	CLA	C1B-NB	-2.38	1.34	1.37
24	b	610	CLA	C4B-NB	-2.37	1.34	1.37
24	c	907	CLA	C3D-C4D	-2.37	1.38	1.44
24	B	606	CLA	C1C-C2C	2.37	1.49	1.44
24	C	511	CLA	C3B-C2B	2.37	1.49	1.41
24	c	911	CLA	C3D-C4D	-2.37	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	C4B-NB	-2.37	1.34	1.37
24	C	509	CLA	C1C-C2C	2.37	1.49	1.44
24	C	504	CLA	C4B-NB	-2.37	1.34	1.37
24	B	606	CLA	C1C-NC	-2.37	1.34	1.37
24	b	606	CLA	C1C-NC	-2.37	1.34	1.37
24	C	507	CLA	C1C-NC	-2.36	1.34	1.37
24	c	906	CLA	C1C-C2C	2.36	1.49	1.44
24	c	914	CLA	C4B-NB	-2.36	1.34	1.37
24	b	607	CLA	C1C-C2C	2.36	1.49	1.44
24	A	406	CLA	C4C-C3C	2.36	1.49	1.45
24	b	617	CLA	C1C-C2C	2.35	1.49	1.44
24	c	909	CLA	C1C-NC	-2.35	1.34	1.37
24	b	614	CLA	C3D-C4D	-2.35	1.38	1.44
24	D	401	CLA	C4C-C3C	2.35	1.49	1.45
24	B	603	CLA	MG-NB	2.35	2.10	2.05
24	D	402	CLA	C4B-NB	-2.35	1.34	1.37
24	D	401	CLA	C1C-NC	-2.34	1.34	1.37
24	B	615	CLA	C4C-C3C	2.34	1.49	1.45
24	B	603	CLA	C1C-C2C	2.34	1.49	1.44
24	c	902	CLA	C3B-C2B	2.34	1.49	1.41
24	C	509	CLA	C3B-C2B	2.34	1.49	1.41
24	c	905	CLA	C1C-NC	-2.34	1.34	1.37
25	A	409	PHO	C4B-NB	-2.34	1.34	1.38
24	C	510	CLA	C4C-C3C	2.34	1.49	1.45
24	B	602	CLA	MG-NB	2.33	2.10	2.05
24	c	908	CLA	C1C-NC	-2.33	1.34	1.37
24	C	501	CLA	C1C-C2C	2.33	1.49	1.44
24	A	406	CLA	C1C-NC	-2.33	1.34	1.37
24	B	611	CLA	C1C-C2C	2.33	1.49	1.44
24	C	502	CLA	C4C-C3C	2.33	1.49	1.45
24	A	410	CLA	C1C-C2C	2.33	1.49	1.44
24	c	913	CLA	C1C-C2C	2.33	1.49	1.44
24	B	608	CLA	C4B-NB	-2.32	1.34	1.37
25	a	412	PHO	CHA-CBD	-2.32	1.48	1.51
24	c	907	CLA	C1B-C2B	2.32	1.48	1.43
24	b	607	CLA	C1B-NB	-2.32	1.34	1.37
24	a	410	CLA	C4C-C3C	2.32	1.49	1.45
24	B	609	CLA	C3B-C2B	2.32	1.49	1.41
24	c	903	CLA	C3D-C4D	-2.32	1.39	1.44
24	a	410	CLA	MG-NB	2.32	2.10	2.05
24	c	909	CLA	C3B-C4B	2.32	1.49	1.42
24	B	604	CLA	C3B-C2B	2.32	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	902	CLA	C1B-NB	-2.32	1.34	1.37
24	A	406	CLA	C1C-C2C	2.31	1.49	1.44
24	A	410	CLA	C3B-C2B	2.31	1.49	1.41
24	C	504	CLA	C3D-C4D	-2.31	1.39	1.44
24	b	610	CLA	C3B-C2B	2.31	1.48	1.41
24	a	409	CLA	C4C-C3C	2.30	1.48	1.45
24	C	508	CLA	C3B-C2B	2.30	1.48	1.41
24	b	611	CLA	C4C-C3C	2.30	1.48	1.45
24	B	611	CLA	C1C-NC	-2.30	1.34	1.37
24	b	620	CLA	C3D-C4D	-2.30	1.39	1.44
24	b	606	CLA	C3B-C2B	2.30	1.48	1.41
24	c	913	CLA	C3B-C2B	2.30	1.48	1.41
24	C	501	CLA	C1C-NC	-2.30	1.34	1.37
24	B	610	CLA	C1B-NB	-2.30	1.34	1.37
24	B	613	CLA	C1C-NC	-2.30	1.34	1.37
24	C	510	CLA	C1C-C2C	2.30	1.49	1.44
24	c	905	CLA	C3D-C4D	-2.29	1.39	1.44
24	b	619	CLA	C3B-C2B	2.29	1.48	1.41
24	b	616	CLA	C1C-C2C	2.29	1.49	1.44
24	C	507	CLA	C3B-C2B	2.29	1.48	1.41
36	v	211	HTG	C1-S1	-2.29	1.76	1.80
24	C	507	CLA	C4C-C3C	2.29	1.48	1.45
24	a	413	CLA	C3B-C2B	2.29	1.48	1.41
24	C	505	CLA	C3B-C2B	2.29	1.48	1.41
24	c	914	CLA	C3B-C2B	2.29	1.48	1.41
24	c	905	CLA	C1C-C2C	2.29	1.49	1.44
24	c	913	CLA	C4C-C3C	2.28	1.48	1.45
24	B	614	CLA	C3B-C2B	2.28	1.48	1.41
36	b	602	HTG	C1-S1	-2.28	1.76	1.80
24	A	407	CLA	C3D-C4D	-2.28	1.39	1.44
24	b	616	CLA	C1C-NC	-2.28	1.34	1.37
24	d	401	CLA	C4B-NB	-2.28	1.34	1.37
24	C	513	CLA	C4B-NB	-2.27	1.34	1.37
24	B	604	CLA	C3D-C4D	-2.27	1.39	1.44
24	C	506	CLA	C1C-NC	-2.27	1.34	1.37
24	c	904	CLA	C4B-NB	-2.27	1.34	1.37
24	c	911	CLA	C4C-C3C	2.27	1.48	1.45
24	c	905	CLA	C4C-C3C	2.26	1.48	1.45
24	B	602	CLA	C4C-C3C	2.26	1.48	1.45
24	d	404	CLA	C1C-C2C	2.26	1.49	1.44
24	c	909	CLA	MG-NB	2.26	2.10	2.05
42	v	202	HEC	CMC-C2C	2.26	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	906	CLA	C3B-C4B	2.26	1.49	1.42
24	b	612	CLA	C4B-NB	-2.25	1.34	1.37
24	C	506	CLA	C4C-C3C	2.25	1.48	1.45
24	b	606	CLA	C4C-C3C	2.25	1.48	1.45
24	a	410	CLA	C3B-C4B	2.25	1.49	1.42
24	b	608	CLA	C4C-C3C	2.25	1.48	1.45
24	C	506	CLA	C4B-NB	-2.25	1.34	1.37
24	B	605	CLA	C1C-C2C	2.25	1.49	1.44
24	D	402	CLA	C1C-C2C	2.25	1.49	1.44
24	C	511	CLA	C4C-C3C	2.24	1.48	1.45
24	B	606	CLA	C3D-C4D	-2.24	1.39	1.44
24	d	404	CLA	C3B-C2B	2.24	1.48	1.41
24	b	613	CLA	C1C-C2C	2.24	1.49	1.44
24	b	614	CLA	C3B-C2B	2.24	1.48	1.41
24	b	609	CLA	C1C-NC	-2.24	1.34	1.37
24	B	610	CLA	C1C-C2C	2.24	1.49	1.44
36	c	942	HTG	C1-S1	-2.23	1.77	1.80
24	d	404	CLA	C4C-C3C	2.23	1.48	1.45
24	C	512	CLA	C3B-C4B	2.23	1.49	1.42
24	C	504	CLA	C3B-C2B	2.23	1.48	1.41
24	D	401	CLA	C3D-C4D	-2.23	1.39	1.44
24	c	904	CLA	C3B-C2B	2.23	1.48	1.41
24	B	604	CLA	C1C-NC	-2.22	1.34	1.37
24	C	512	CLA	C3B-C2B	2.22	1.48	1.41
24	b	607	CLA	C3D-C4D	-2.22	1.39	1.44
24	c	912	CLA	C3B-C2B	2.22	1.48	1.41
36	C	520	HTG	C1-S1	-2.22	1.77	1.80
24	C	502	CLA	C3D-C4D	-2.22	1.39	1.44
24	b	605	CLA	C3B-C2B	2.22	1.48	1.41
24	c	911	CLA	C1C-NC	-2.22	1.34	1.37
24	B	607	CLA	MG-NB	-2.21	2.01	2.05
36	B	629	HTG	C1-S1	-2.21	1.77	1.80
26	b	623	BCR	C30-C25	-2.21	1.50	1.53
24	B	607	CLA	C3B-C2B	2.21	1.48	1.41
24	b	609	CLA	C1C-C2C	2.21	1.49	1.44
24	b	618	CLA	C3B-C2B	2.21	1.48	1.41
39	f	101	HEM	CMB-C2B	2.21	1.55	1.50
24	b	617	CLA	C4B-NB	-2.21	1.35	1.37
42	v	202	HEC	CMD-C2D	2.21	1.55	1.50
24	c	903	CLA	C3B-C2B	2.21	1.48	1.41
24	d	401	CLA	C3B-C4B	2.21	1.49	1.42
25	A	409	PHO	C1D-ND	-2.21	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C3D-C4D	-2.20	1.39	1.44
24	C	510	CLA	C3B-C2B	2.20	1.48	1.41
24	b	613	CLA	C1D-C2D	2.20	1.49	1.45
36	c	928	HTG	C1-S1	-2.20	1.77	1.80
24	B	617	CLA	C3D-C4D	-2.20	1.39	1.44
24	C	513	CLA	C3B-C4B	2.19	1.49	1.42
24	B	603	CLA	C4C-C3C	2.19	1.48	1.45
28	a	416	LMG	O1-C1	2.19	1.43	1.40
24	c	904	CLA	C1C-NC	-2.19	1.34	1.37
24	A	407	CLA	C1C-NC	-2.19	1.34	1.37
24	B	615	CLA	C3D-C4D	-2.19	1.39	1.44
24	B	608	CLA	C4C-C3C	2.19	1.48	1.45
24	b	612	CLA	C4C-C3C	2.19	1.48	1.45
24	b	606	CLA	C1C-C2C	2.19	1.49	1.44
24	B	617	CLA	C4C-C3C	2.19	1.48	1.45
24	B	613	CLA	C1C-C2C	2.19	1.49	1.44
24	C	501	CLA	C4C-C3C	2.19	1.48	1.45
24	b	605	CLA	C1C-NC	-2.19	1.34	1.37
24	C	503	CLA	C3B-C2B	2.19	1.48	1.41
24	b	613	CLA	C1B-C2B	2.19	1.48	1.43
24	a	413	CLA	C1C-C2C	2.19	1.49	1.44
24	c	907	CLA	C3B-C2B	2.19	1.48	1.41
24	C	506	CLA	C1C-C2C	2.19	1.49	1.44
24	B	603	CLA	C3B-C2B	2.18	1.48	1.41
39	f	101	HEM	FE-NC	2.18	2.02	1.95
24	c	913	CLA	C3D-C4D	-2.18	1.39	1.44
24	a	410	CLA	C3D-C4D	-2.18	1.39	1.44
24	C	511	CLA	C3D-C4D	-2.18	1.39	1.44
31	j	102	LMT	O1'-C1'	2.18	1.43	1.40
36	d	419	HTG	C1-S1	-2.18	1.77	1.80
24	C	508	CLA	C1C-C2C	2.17	1.48	1.44
24	c	912	CLA	C3B-C4B	2.17	1.49	1.42
24	B	616	CLA	C4C-C3C	2.17	1.48	1.45
24	B	604	CLA	C1C-C2C	2.17	1.48	1.44
36	c	923	HTG	C1-S1	-2.17	1.77	1.80
24	c	910	CLA	C4C-C3C	2.17	1.48	1.45
24	c	903	CLA	C1C-C2C	2.17	1.48	1.44
24	c	911	CLA	C3B-C4B	2.17	1.49	1.42
24	B	602	CLA	C3D-C4D	-2.17	1.39	1.44
24	b	619	CLA	C3B-C4B	2.17	1.49	1.42
24	D	401	CLA	C1B-NB	-2.17	1.35	1.37
24	a	413	CLA	C1C-NC	-2.17	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C3D-C4D	-2.16	1.39	1.44
24	D	401	CLA	C1C-C2C	2.16	1.48	1.44
24	A	410	CLA	C3B-C4B	2.16	1.49	1.42
24	c	909	CLA	C3B-C2B	2.16	1.48	1.41
24	c	912	CLA	C1C-C2C	2.16	1.48	1.44
24	c	911	CLA	C3B-C2B	2.16	1.48	1.41
36	b	603	HTG	C1-S1	-2.16	1.77	1.80
24	B	605	CLA	C3D-C4D	-2.16	1.39	1.44
24	B	608	CLA	C3B-C2B	2.16	1.48	1.41
24	C	506	CLA	C3D-C4D	-2.16	1.39	1.44
24	b	607	CLA	C3B-C4B	2.16	1.49	1.42
24	B	612	CLA	C3B-C2B	2.16	1.48	1.41
24	b	619	CLA	C3D-C4D	-2.16	1.39	1.44
24	C	502	CLA	C4B-NB	-2.16	1.35	1.37
24	A	406	CLA	C3D-C4D	-2.15	1.39	1.44
24	D	401	CLA	C3B-C2B	2.15	1.48	1.41
24	B	604	CLA	C4B-NB	-2.15	1.35	1.37
24	b	613	CLA	C3D-C4D	-2.15	1.39	1.44
24	b	609	CLA	MG-NB	2.15	2.10	2.05
24	A	405	CLA	C1C-NC	-2.15	1.34	1.37
24	b	606	CLA	C3D-C4D	-2.15	1.39	1.44
24	B	606	CLA	C4C-C3C	2.15	1.48	1.45
24	B	602	CLA	C1D-C2D	2.15	1.49	1.45
24	B	603	CLA	C3D-C4D	-2.15	1.39	1.44
24	c	907	CLA	C4B-NB	-2.15	1.35	1.37
27	b	601	SQD	O6-C1	2.14	1.43	1.40
24	B	608	CLA	C3B-C4B	2.14	1.49	1.42
31	c	922	LMT	O1'-C1'	2.14	1.43	1.40
24	b	606	CLA	C3B-C4B	2.14	1.49	1.42
24	C	509	CLA	C3D-C4D	-2.14	1.39	1.44
24	b	607	CLA	C3B-C2B	2.14	1.48	1.41
24	B	607	CLA	C3D-C4D	-2.13	1.39	1.44
24	b	619	CLA	C4C-C3C	2.13	1.48	1.45
24	a	410	CLA	C1C-NC	-2.13	1.34	1.37
25	A	409	PHO	C1B-NB	-2.13	1.34	1.38
24	c	907	CLA	C3B-C4B	2.13	1.48	1.42
24	c	907	CLA	C1C-C2C	2.13	1.48	1.44
24	c	904	CLA	C1B-NB	-2.13	1.35	1.37
24	B	611	CLA	C3B-C2B	2.12	1.48	1.41
24	b	615	CLA	C3D-C4D	-2.12	1.39	1.44
24	B	603	CLA	C3B-C4B	2.12	1.48	1.42
24	B	613	CLA	C3B-C2B	2.12	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	C4C-C3C	2.12	1.48	1.45
24	b	608	CLA	C3D-C4D	-2.12	1.39	1.44
38	d	409	LHG	O7-C5	-2.12	1.41	1.46
24	c	910	CLA	C1C-C2C	2.12	1.48	1.44
37	C	516	DGD	O5D-C1E	2.12	1.43	1.40
24	B	609	CLA	C3D-C4D	-2.11	1.39	1.44
24	b	613	CLA	C4C-C3C	2.11	1.48	1.45
24	B	602	CLA	C1C-NC	-2.11	1.34	1.37
24	B	616	CLA	C3B-C2B	2.11	1.48	1.41
24	c	910	CLA	C1C-NC	-2.11	1.34	1.37
24	a	409	CLA	C1C-C2C	2.11	1.48	1.44
24	B	607	CLA	C4C-C3C	2.10	1.48	1.45
24	B	612	CLA	C3B-C4B	2.10	1.48	1.42
36	b	627	HTG	C1-S1	-2.10	1.77	1.80
24	C	513	CLA	C1C-NC	-2.10	1.34	1.37
24	B	610	CLA	C3B-C2B	2.10	1.48	1.41
24	C	509	CLA	C3B-C4B	2.10	1.48	1.42
24	c	914	CLA	C1C-NC	-2.10	1.34	1.37
24	d	401	CLA	C3D-C4D	-2.10	1.39	1.44
24	b	611	CLA	C3D-C4D	-2.10	1.39	1.44
24	c	907	CLA	C4C-C3C	2.10	1.48	1.45
24	B	614	CLA	C4C-C3C	2.09	1.48	1.45
24	B	605	CLA	C4C-C3C	2.09	1.48	1.45
24	b	611	CLA	C3B-C2B	2.09	1.48	1.41
24	b	605	CLA	C3D-C4D	-2.09	1.39	1.44
24	c	905	CLA	C3B-C4B	2.09	1.48	1.42
37	C	518	DGD	O2G-C2G	-2.09	1.41	1.46
24	b	617	CLA	C3B-C2B	2.09	1.48	1.41
24	B	610	CLA	C4B-NB	-2.09	1.35	1.37
24	a	409	CLA	C3B-C2B	2.08	1.48	1.41
24	B	616	CLA	C3B-C4B	2.08	1.48	1.42
24	C	512	CLA	C3D-C4D	-2.08	1.39	1.44
24	C	506	CLA	C3B-C4B	2.08	1.48	1.42
24	c	905	CLA	C4B-NB	-2.07	1.35	1.37
24	b	618	CLA	C1C-C2C	2.07	1.48	1.44
24	C	511	CLA	C3B-C4B	2.07	1.48	1.42
27	l	101	SQD	O6-C1	2.07	1.43	1.40
42	V	203	HEC	CMB-C2B	2.07	1.55	1.50
29	D	404	PL9	C2-C3	2.07	1.39	1.34
24	C	501	CLA	C3B-C2B	2.07	1.48	1.41
24	B	604	CLA	C3B-C4B	2.07	1.48	1.42
36	C	521	HTG	C1-S1	-2.07	1.77	1.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	904	CLA	C3B-C4B	2.07	1.48	1.42
24	c	908	CLA	C1A-CHA	2.07	1.51	1.43
36	y	102	HTG	C1-S1	-2.07	1.77	1.80
24	C	504	CLA	C1C-C2C	2.07	1.48	1.44
24	a	409	CLA	C1C-NC	-2.07	1.34	1.37
24	b	609	CLA	C3B-C2B	2.06	1.48	1.41
39	F	102	HEM	CMA-C3A	2.06	1.55	1.50
24	C	513	CLA	C3D-C4D	-2.06	1.39	1.44
24	d	405	CLA	C3D-C4D	-2.06	1.39	1.44
24	b	613	CLA	C3B-C4B	2.06	1.48	1.42
39	F	102	HEM	CMC-C2C	2.06	1.55	1.50
24	a	413	CLA	C4C-C3C	2.05	1.48	1.45
24	A	410	CLA	C1C-NC	-2.05	1.34	1.37
24	a	410	CLA	C3B-C2B	2.05	1.48	1.41
24	b	612	CLA	C3B-C4B	2.05	1.48	1.42
36	c	924	HTG	C1-S1	-2.05	1.77	1.80
24	c	905	CLA	C3B-C2B	2.05	1.48	1.41
24	d	404	CLA	C3D-C4D	-2.05	1.39	1.44
37	c	919	DGD	O2G-C2G	-2.05	1.41	1.46
24	C	507	CLA	C1C-C2C	2.05	1.48	1.44
25	a	411	PHO	CBD-CGD	-2.05	1.49	1.52
24	C	504	CLA	C3B-C4B	2.05	1.48	1.42
38	D	407	LHG	O7-C5	-2.05	1.41	1.46
24	b	610	CLA	C3B-C4B	2.05	1.48	1.42
24	B	604	CLA	C4C-C3C	2.04	1.48	1.45
24	b	605	CLA	C4B-NB	-2.04	1.35	1.37
24	B	616	CLA	MG-NC	2.04	2.11	2.06
24	C	502	CLA	C1C-NC	-2.04	1.34	1.37
29	a	417	PL9	C2-C3	2.04	1.39	1.34
24	C	510	CLA	C3B-C4B	2.04	1.48	1.42
36	B	630	HTG	C1-S1	-2.04	1.77	1.80
24	B	616	CLA	MG-NB	2.03	2.09	2.05
24	C	506	CLA	C3B-C2B	2.03	1.48	1.41
24	C	502	CLA	MG-NB	2.03	2.09	2.05
42	v	202	HEC	C3B-C2B	-2.03	1.34	1.41
24	c	902	CLA	MG-NB	2.03	2.09	2.05
24	c	911	CLA	C1C-C2C	2.03	1.48	1.44
28	C	519	LMG	O1-C1	2.03	1.43	1.40
24	B	609	CLA	C1C-C2C	2.02	1.48	1.44
24	B	617	CLA	C1B-NB	-2.02	1.35	1.37
24	b	619	CLA	C1C-C2C	2.02	1.48	1.44
24	c	914	CLA	C3B-C4B	2.02	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	904	CLA	C1A-CHA	2.02	1.51	1.43
24	b	608	CLA	C3B-C4B	2.02	1.48	1.42
24	B	609	CLA	C3B-C4B	2.02	1.48	1.42
24	c	909	CLA	C1C-C2C	2.02	1.48	1.44
24	d	401	CLA	C3B-C2B	2.02	1.48	1.41
24	a	413	CLA	C3B-C4B	2.01	1.48	1.42
24	C	510	CLA	C1C-NC	-2.01	1.34	1.37
24	d	405	CLA	C3B-C2B	2.01	1.47	1.41
24	b	616	CLA	C3D-C4D	-2.01	1.39	1.44
24	b	609	CLA	C3D-C4D	-2.01	1.39	1.44
24	C	512	CLA	C1C-NC	-2.01	1.34	1.37
24	c	902	CLA	C4C-C3C	2.00	1.48	1.45
24	C	513	CLA	C4C-C3C	2.00	1.48	1.45
24	c	909	CLA	C3D-C4D	-2.00	1.39	1.44
24	C	503	CLA	C4B-NB	-2.00	1.35	1.37
39	F	102	HEM	CMB-C2B	2.00	1.54	1.50
24	b	620	CLA	MG-NB	2.00	2.09	2.05
24	c	906	CLA	C3B-C2B	2.00	1.47	1.41

All (2680) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	409	PHO	C2D-C1D-ND	12.48	118.45	109.43
25	A	408	PHO	C2D-C1D-ND	12.25	118.28	109.43
24	c	909	CLA	C1D-ND-C4D	-11.41	98.31	106.31
24	D	401	CLA	C1D-ND-C4D	-11.32	98.37	106.31
25	a	411	PHO	C2D-C1D-ND	11.18	117.51	109.43
24	b	616	CLA	C1D-ND-C4D	-10.96	98.62	106.31
25	a	412	PHO	C2D-C1D-ND	10.96	117.35	109.43
24	A	406	CLA	C1D-ND-C4D	-10.84	98.71	106.31
24	c	902	CLA	C1D-ND-C4D	-10.77	98.75	106.31
24	d	401	CLA	C1D-ND-C4D	-10.59	98.88	106.31
24	a	409	CLA	C1D-ND-C4D	-10.42	99.00	106.31
24	B	605	CLA	C1D-ND-C4D	-10.38	99.03	106.31
24	a	410	CLA	C1D-ND-C4D	-10.35	99.05	106.31
24	d	404	CLA	C1D-ND-C4D	-10.34	99.06	106.31
24	B	604	CLA	C1D-ND-C4D	-10.27	99.11	106.31
24	b	617	CLA	C1D-ND-C4D	-10.25	99.12	106.31
24	A	407	CLA	C1D-ND-C4D	-10.24	99.13	106.31
24	B	612	CLA	C1D-ND-C4D	-10.10	99.23	106.31
24	B	614	CLA	C1D-ND-C4D	-10.08	99.24	106.31
24	B	615	CLA	C1D-ND-C4D	-9.97	99.32	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	502	CLA	C1D-ND-C4D	-9.96	99.32	106.31
24	b	609	CLA	C1D-ND-C4D	-9.96	99.33	106.31
24	B	613	CLA	C1D-ND-C4D	-9.93	99.34	106.31
24	A	410	CLA	C1D-ND-C4D	-9.91	99.36	106.31
24	c	905	CLA	C1D-ND-C4D	-9.87	99.39	106.31
24	b	612	CLA	C1D-ND-C4D	-9.77	99.46	106.31
24	A	405	CLA	C1D-ND-C4D	-9.74	99.48	106.31
24	d	405	CLA	C1D-ND-C4D	-9.72	99.49	106.31
24	B	606	CLA	C1D-ND-C4D	-9.71	99.50	106.31
24	C	508	CLA	C1D-ND-C4D	-9.69	99.51	106.31
24	b	608	CLA	C1D-ND-C4D	-9.69	99.52	106.31
24	B	610	CLA	C1D-ND-C4D	-9.68	99.52	106.31
24	B	608	CLA	C1D-ND-C4D	-9.64	99.55	106.31
24	C	513	CLA	C1D-ND-C4D	-9.64	99.55	106.31
24	B	616	CLA	C1D-ND-C4D	-9.62	99.56	106.31
24	B	617	CLA	C1D-ND-C4D	-9.62	99.56	106.31
24	b	618	CLA	C1D-ND-C4D	-9.53	99.62	106.31
24	b	620	CLA	C1D-ND-C4D	-9.51	99.64	106.31
24	C	504	CLA	C1D-ND-C4D	-9.50	99.65	106.31
24	B	603	CLA	C1D-ND-C4D	-9.45	99.68	106.31
24	D	402	CLA	C1D-ND-C4D	-9.43	99.69	106.31
24	C	501	CLA	C1D-ND-C4D	-9.36	99.74	106.31
24	c	911	CLA	C1D-ND-C4D	-9.34	99.76	106.31
24	c	913	CLA	C1D-ND-C4D	-9.30	99.78	106.31
24	c	903	CLA	C1D-ND-C4D	-9.30	99.79	106.31
24	c	907	CLA	C1D-ND-C4D	-9.30	99.79	106.31
24	B	611	CLA	C1D-ND-C4D	-9.14	99.90	106.31
24	C	510	CLA	C1D-ND-C4D	-9.13	99.91	106.31
24	b	613	CLA	C1D-ND-C4D	-8.97	100.02	106.31
24	C	512	CLA	C1D-ND-C4D	-8.95	100.03	106.31
24	b	614	CLA	C1D-ND-C4D	-8.92	100.06	106.31
24	c	910	CLA	C1D-ND-C4D	-8.90	100.07	106.31
24	a	413	CLA	C1D-ND-C4D	-8.88	100.08	106.31
24	c	908	CLA	C1D-ND-C4D	-8.86	100.09	106.31
24	b	606	CLA	C1D-ND-C4D	-8.83	100.11	106.31
24	c	914	CLA	C1D-ND-C4D	-8.82	100.12	106.31
24	C	506	CLA	C1D-ND-C4D	-8.81	100.13	106.31
24	c	912	CLA	C1D-ND-C4D	-8.80	100.14	106.31
24	b	610	CLA	C1D-ND-C4D	-8.76	100.17	106.31
24	B	607	CLA	C1D-ND-C4D	-8.75	100.17	106.31
24	b	607	CLA	C1D-ND-C4D	-8.73	100.19	106.31
24	B	609	CLA	C1D-ND-C4D	-8.73	100.19	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	503	CLA	C1D-ND-C4D	-8.73	100.19	106.31
24	C	509	CLA	C1D-ND-C4D	-8.72	100.19	106.31
24	C	507	CLA	C1D-ND-C4D	-8.58	100.29	106.31
24	b	615	CLA	C1D-ND-C4D	-8.56	100.31	106.31
24	c	906	CLA	C1D-ND-C4D	-8.54	100.32	106.31
24	b	605	CLA	C1D-ND-C4D	-8.49	100.35	106.31
24	C	511	CLA	C1D-ND-C4D	-8.47	100.37	106.31
24	b	619	CLA	C1D-ND-C4D	-8.47	100.37	106.31
24	C	505	CLA	C1D-ND-C4D	-8.47	100.37	106.31
24	b	611	CLA	C1D-ND-C4D	-8.41	100.41	106.31
24	B	602	CLA	C1D-ND-C4D	-8.32	100.47	106.31
25	a	411	PHO	O2D-CGD-CBD	8.29	120.05	110.95
25	a	411	PHO	C3B-C4B-NB	8.20	112.81	107.46
25	a	412	PHO	O2D-CGD-CBD	7.91	119.64	110.95
25	a	412	PHO	C2B-C1B-NB	7.87	115.12	109.43
25	A	408	PHO	O2D-CGD-CBD	7.80	119.52	110.95
24	b	618	CLA	C1-C2-C3	-7.71	113.56	126.20
25	A	408	PHO	C3B-C4B-NB	7.68	112.47	107.46
25	a	412	PHO	C3B-C4B-NB	7.58	112.41	107.46
25	A	409	PHO	C2B-C1B-NB	7.54	114.88	109.43
24	c	904	CLA	C1D-ND-C4D	-7.51	101.04	106.31
25	A	409	PHO	O2D-CGD-CBD	7.51	119.19	110.95
24	D	401	CLA	C2D-C1D-ND	7.38	117.43	110.13
36	V	215	HTG	C1'-S1-C1	7.34	116.31	100.45
24	B	614	CLA	C2D-C1D-ND	7.25	117.30	110.13
24	c	908	CLA	O2D-CGD-CBD	7.20	123.82	111.23
25	A	409	PHO	C3B-C4B-NB	7.20	112.16	107.46
24	c	909	CLA	C2D-C1D-ND	7.18	117.23	110.13
24	b	616	CLA	C2D-C1D-ND	7.17	117.22	110.13
24	A	406	CLA	C2D-C1D-ND	7.11	117.17	110.13
25	A	408	PHO	C2B-C1B-NB	6.88	114.40	109.43
24	B	602	CLA	CMD-C2D-C1D	6.88	136.84	124.73
24	c	902	CLA	C2D-C1D-ND	6.83	116.88	110.13
25	a	411	PHO	C2B-C1B-NB	6.82	114.36	109.43
24	b	609	CLA	C2D-C1D-ND	6.79	116.85	110.13
24	A	410	CLA	C2D-C1D-ND	6.78	116.84	110.13
24	B	615	CLA	C2D-C1D-ND	6.75	116.81	110.13
24	b	617	CLA	C2D-C1D-ND	6.75	116.81	110.13
24	B	607	CLA	CMD-C2D-C1D	6.73	136.59	124.73
24	B	617	CLA	C2D-C1D-ND	6.73	116.78	110.13
27	F	101	SQD	O6-C1-C2	6.70	118.45	108.27
24	b	608	CLA	C2D-C1D-ND	6.69	116.75	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	C2D-C1D-ND	6.67	116.72	110.13
24	B	612	CLA	C2D-C1D-ND	6.62	116.68	110.13
24	d	405	CLA	C2D-C1D-ND	6.61	116.67	110.13
24	C	506	CLA	CMD-C2D-C1D	6.59	136.33	124.73
24	B	611	CLA	C2D-C1D-ND	6.56	116.62	110.13
24	d	401	CLA	C2D-C1D-ND	6.54	116.60	110.13
24	a	410	CLA	C2D-C1D-ND	6.53	116.59	110.13
24	B	605	CLA	C2D-C1D-ND	6.51	116.56	110.13
24	b	608	CLA	O2D-CGD-CBD	6.44	122.49	111.23
24	B	605	CLA	CMD-C2D-C1D	6.43	136.06	124.73
24	B	612	CLA	CMD-C2D-C1D	6.43	136.05	124.73
24	d	404	CLA	CMD-C2D-C1D	6.41	136.02	124.73
25	A	409	PHO	C4D-ND-C1D	-6.41	101.19	108.87
24	B	613	CLA	C2D-C1D-ND	6.41	116.47	110.13
24	C	507	CLA	CMD-C2D-C1D	6.40	135.99	124.73
24	c	907	CLA	CMD-C2D-C1D	6.39	135.99	124.73
24	D	401	CLA	CMD-C2D-C1D	6.39	135.99	124.73
24	C	509	CLA	CMD-C2D-C1D	6.37	135.94	124.73
24	d	404	CLA	C2D-C1D-ND	6.35	116.41	110.13
24	C	503	CLA	CMD-C2D-C1D	6.33	135.87	124.73
25	A	408	PHO	C4D-ND-C1D	-6.32	101.30	108.87
24	A	407	CLA	C2D-C1D-ND	6.31	116.37	110.13
24	c	905	CLA	CMD-C2D-C1D	6.30	135.83	124.73
24	c	910	CLA	C2D-C1D-ND	6.30	116.36	110.13
25	a	412	PHO	C4D-ND-C1D	-6.26	101.37	108.87
24	C	508	CLA	C2D-C1D-ND	6.26	116.32	110.13
24	C	511	CLA	C2D-C1D-ND	6.24	116.30	110.13
24	b	620	CLA	C2D-C1D-ND	6.24	116.30	110.13
24	c	905	CLA	C2D-C1D-ND	6.23	116.29	110.13
24	b	606	CLA	CMD-C2D-C1D	6.23	135.69	124.73
24	C	504	CLA	C2D-C1D-ND	6.22	116.28	110.13
24	B	603	CLA	CMD-C2D-C1D	6.22	135.68	124.73
24	c	906	CLA	CMD-C2D-C1D	6.22	135.67	124.73
24	a	413	CLA	C2D-C1D-ND	6.21	116.27	110.13
24	a	409	CLA	C2D-C1D-ND	6.20	116.26	110.13
24	B	606	CLA	C2D-C1D-ND	6.20	116.26	110.13
24	c	913	CLA	C2D-C1D-ND	6.19	116.26	110.13
24	D	402	CLA	CMD-C2D-C1D	6.17	135.60	124.73
24	b	618	CLA	C2D-C1D-ND	6.16	116.22	110.13
36	B	631	HTG	C1'-S1-C1	6.16	113.75	100.45
24	C	502	CLA	C2D-C1D-ND	6.15	116.22	110.13
24	A	405	CLA	C2D-C1D-ND	6.15	116.21	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	503	CLA	C2D-C1D-ND	6.15	116.21	110.13
24	C	510	CLA	CMD-C2D-C1D	6.12	135.51	124.73
24	B	604	CLA	C2D-C1D-ND	6.09	116.16	110.13
24	c	908	CLA	C2D-C1D-ND	6.07	116.13	110.13
24	b	605	CLA	O2D-CGD-CBD	6.06	121.82	111.23
24	B	610	CLA	C2D-C1D-ND	6.06	116.12	110.13
24	b	613	CLA	CMD-C2D-C1D	6.05	135.39	124.73
24	c	902	CLA	CMD-C2D-C1D	6.05	135.39	124.73
24	b	614	CLA	C2D-C1D-ND	6.05	116.12	110.13
24	C	501	CLA	C2D-C1D-ND	6.05	116.12	110.13
24	b	610	CLA	C2D-C1D-ND	6.05	116.12	110.13
24	B	604	CLA	O2D-CGD-CBD	6.04	121.79	111.23
27	a	415	SQD	O6-C1-C2	6.04	117.45	108.27
24	C	507	CLA	C2D-C1D-ND	6.04	116.11	110.13
24	b	611	CLA	C2D-C1D-ND	6.02	116.09	110.13
24	C	501	CLA	O2D-CGD-CBD	6.02	121.75	111.23
24	C	510	CLA	O2D-CGD-CBD	6.01	121.73	111.23
24	C	501	CLA	CMD-C2D-C1D	6.00	135.29	124.73
24	b	617	CLA	CMD-C2D-C1D	5.99	135.27	124.73
24	b	620	CLA	O2D-CGD-CBD	5.97	121.67	111.23
24	C	507	CLA	O2D-CGD-CBD	5.97	121.66	111.23
24	b	609	CLA	CMD-C2D-C1D	5.96	135.23	124.73
24	b	608	CLA	CMD-C2D-C1D	5.96	135.22	124.73
24	b	614	CLA	CMD-C2D-C1D	5.93	135.18	124.73
24	c	903	CLA	C2D-C1D-ND	5.93	115.99	110.13
24	b	619	CLA	CMD-C2D-C1D	5.91	135.13	124.73
24	b	615	CLA	C2D-C1D-ND	5.90	115.96	110.13
24	B	608	CLA	C2D-C1D-ND	5.89	115.96	110.13
24	b	605	CLA	CMD-C2D-C1D	5.89	135.10	124.73
24	C	513	CLA	C2D-C1D-ND	5.88	115.94	110.13
24	C	512	CLA	C2D-C1D-ND	5.86	115.93	110.13
36	B	625	HTG	C1'-S1-C1	5.85	113.09	100.45
24	B	608	CLA	CMD-C2D-C1D	5.84	135.01	124.73
25	a	412	PHO	C3D-C4D-ND	5.83	115.18	107.71
24	B	602	CLA	O2D-CGD-CBD	5.81	121.39	111.23
24	B	609	CLA	C2D-C1D-ND	5.81	115.87	110.13
24	b	611	CLA	CMD-C2D-C1D	5.80	134.95	124.73
24	C	504	CLA	CMD-C2D-C1D	5.80	134.94	124.73
24	B	607	CLA	C2D-C1D-ND	5.80	115.86	110.13
27	b	601	SQD	O6-C1-C2	5.80	117.08	108.27
24	c	904	CLA	C2D-C1D-ND	5.78	115.85	110.13
24	D	402	CLA	C2D-C1D-ND	5.77	115.84	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	513	CLA	CMD-C2D-C1D	5.77	134.90	124.73
24	b	619	CLA	C2D-C1D-ND	5.77	115.83	110.13
24	c	911	CLA	CMD-C2D-C1D	5.76	134.88	124.73
24	B	604	CLA	CMD-C2D-C1D	5.75	134.86	124.73
25	a	411	PHO	C4D-ND-C1D	-5.74	102.00	108.87
24	B	603	CLA	C2D-C1D-ND	5.73	115.80	110.13
24	C	505	CLA	CMD-C2D-C1D	5.72	134.81	124.73
24	b	607	CLA	O2D-CGD-CBD	5.72	121.23	111.23
25	A	409	PHO	C1-C2-C3	-5.71	116.84	126.20
24	B	617	CLA	O2D-CGD-CBD	5.70	121.20	111.23
24	A	407	CLA	CMD-C2D-C1D	5.70	134.76	124.73
24	c	912	CLA	CMD-C2D-C1D	5.69	134.75	124.73
24	A	406	CLA	CMD-C2D-C1D	5.68	134.74	124.73
24	a	409	CLA	CMD-C2D-C1D	5.67	134.71	124.73
24	C	506	CLA	C2D-C1D-ND	5.65	115.72	110.13
24	c	905	CLA	O2D-CGD-CBD	5.65	121.10	111.23
25	A	408	PHO	C3D-C4D-ND	5.63	114.93	107.71
24	b	606	CLA	C2D-C1D-ND	5.61	115.68	110.13
24	B	615	CLA	CMD-C2D-C1D	5.61	134.60	124.73
24	d	401	CLA	CMD-C2D-C1D	5.60	134.59	124.73
24	b	612	CLA	C2D-C1D-ND	5.60	115.67	110.13
24	A	410	CLA	CMD-C2D-C1D	5.60	134.58	124.73
24	c	904	CLA	CMD-C2D-C1D	5.59	134.57	124.73
24	c	907	CLA	C2D-C1D-ND	5.55	115.62	110.13
42	V	203	HEC	CBB-CAB-C3B	-5.54	116.36	127.43
24	b	610	CLA	CMD-C2D-C1D	5.53	134.47	124.73
24	c	903	CLA	O2D-CGD-CBD	5.53	120.89	111.23
27	A	412	SQD	O6-C1-C2	5.52	116.66	108.27
24	B	603	CLA	O2D-CGD-CBD	5.52	120.87	111.23
24	B	616	CLA	CMD-C2D-C1D	5.50	134.41	124.73
24	c	910	CLA	CMD-C2D-C1D	5.49	134.40	124.73
24	C	502	CLA	CMD-C2D-C1D	5.49	134.39	124.73
24	B	614	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	C	509	CLA	O2D-CGD-CBD	5.47	120.78	111.23
24	c	912	CLA	C2D-C1D-ND	5.46	115.53	110.13
24	A	405	CLA	CMD-C2D-C1D	5.46	134.35	124.73
24	b	607	CLA	CMD-C2D-C1D	5.44	134.31	124.73
24	a	413	CLA	C1-C2-C3	-5.44	117.28	126.20
24	C	510	CLA	C2D-C1D-ND	5.44	115.51	110.13
24	C	511	CLA	CMD-C2D-C1D	5.44	134.30	124.73
24	B	610	CLA	CMD-C2D-C1D	5.43	134.28	124.73
24	d	405	CLA	CMD-C2D-C1D	5.43	134.28	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	502	CLA	O2D-CGD-CBD	5.43	120.71	111.23
24	b	612	CLA	CMD-C2D-C1D	5.40	134.24	124.73
24	c	913	CLA	O2D-CGD-CBD	5.40	120.67	111.23
25	A	409	PHO	C3D-C4D-ND	5.38	114.61	107.71
24	c	908	CLA	CMD-C2D-C1D	5.36	134.16	124.73
24	b	610	CLA	O2D-CGD-CBD	5.35	120.59	111.23
27	f	102	SQD	O47-C7-C8	5.35	123.05	111.48
24	b	605	CLA	C2D-C1D-ND	5.34	115.42	110.13
24	c	914	CLA	C2D-C1D-ND	5.34	115.41	110.13
24	B	611	CLA	O2D-CGD-CBD	5.34	120.56	111.23
24	c	911	CLA	C2D-C1D-ND	5.31	115.38	110.13
24	c	906	CLA	O2D-CGD-CBD	5.31	120.51	111.23
24	c	913	CLA	CMD-C2D-C1D	5.30	134.06	124.73
24	B	614	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
24	b	606	CLA	O2D-CGD-CBD	5.27	120.44	111.23
24	C	509	CLA	C2D-C1D-ND	5.26	115.33	110.13
24	d	405	CLA	C1-C2-C3	-5.25	117.59	126.20
24	b	616	CLA	CHD-C4C-C3C	-5.24	117.13	124.77
36	V	204	HTG	C1-O5-C5	5.21	121.91	112.56
24	b	618	CLA	CMD-C2D-C1D	5.20	133.88	124.73
26	d	406	BCR	C38-C26-C25	-5.18	118.83	124.48
24	B	611	CLA	CMD-C2D-C1D	5.17	133.84	124.73
24	C	512	CLA	CMD-C2D-C1D	5.17	133.84	124.73
24	a	410	CLA	CMD-C2D-C1D	5.17	133.83	124.73
24	b	615	CLA	CMD-C2D-C1D	5.17	133.83	124.73
24	b	613	CLA	C2D-C1D-ND	5.16	115.23	110.13
24	B	617	CLA	CMD-C2D-C1D	5.14	133.79	124.73
24	b	620	CLA	CMD-C2D-C1D	5.13	133.77	124.73
36	d	414	HTG	C1'-S1-C1	5.13	111.53	100.45
24	b	609	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
24	B	605	CLA	O2D-CGD-CBD	5.07	120.09	111.23
24	C	505	CLA	C2D-C1D-ND	5.05	115.13	110.13
24	c	902	CLA	O2D-CGD-CBD	5.05	120.06	111.23
24	B	602	CLA	C2D-C1D-ND	5.05	115.12	110.13
24	c	906	CLA	C2D-C1D-ND	5.04	115.12	110.13
24	c	914	CLA	CMD-C2D-C1D	5.03	133.59	124.73
24	A	410	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
24	B	611	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	A	406	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	B	616	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
24	A	407	CLA	C3D-C4D-ND	4.99	118.10	109.99
24	B	606	CLA	CHD-C4C-C3C	-4.99	117.50	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	908	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
24	a	410	CLA	O2D-CGD-CBD	4.98	119.93	111.23
24	b	611	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
24	C	508	CLA	CMD-C2D-C1D	4.97	133.48	124.73
24	C	507	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
24	b	614	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
37	d	408	DGD	C3D-C4D-C5D	4.95	117.34	109.81
24	B	617	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
24	C	509	CLA	C1-C2-C3	-4.93	118.12	126.20
27	A	412	SQD	O47-C7-C8	4.91	122.10	111.48
24	c	914	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
24	a	410	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
24	B	615	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
24	D	401	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
24	c	913	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
24	C	503	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	b	608	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	d	405	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
24	D	402	CLA	O2D-CGD-CBD	4.87	119.74	111.23
24	d	405	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
24	b	607	CLA	C2D-C1D-ND	4.85	114.93	110.13
24	c	909	CLA	C3D-C4D-ND	4.85	117.87	109.99
24	C	503	CLA	C1-C2-C3	-4.85	118.25	126.20
24	B	615	CLA	CHD-C4C-C3C	-4.85	117.71	124.77
36	d	420	HTG	C1'-S1-C1	4.84	110.91	100.45
36	c	941	HTG	C1-O5-C5	4.84	121.25	112.56
24	B	612	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	b	615	CLA	O2D-CGD-CBD	4.83	119.68	111.23
24	B	609	CLA	CMD-C2D-C1D	4.83	133.23	124.73
24	C	511	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
24	b	617	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
24	a	413	CLA	CMD-C2D-C1D	4.81	133.20	124.73
24	b	616	CLA	CMD-C2D-C1D	4.81	133.19	124.73
25	a	411	PHO	C3D-C4D-ND	4.80	113.86	107.71
24	B	615	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
24	a	410	CLA	C3D-C4D-ND	4.80	117.78	109.99
24	C	509	CLA	C3B-C2B-C1B	-4.80	101.52	107.17
24	c	902	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
24	a	413	CLA	O2D-CGD-CBD	4.76	119.54	111.23
39	f	101	HEM	C4D-ND-C1D	4.75	110.84	105.21
24	c	904	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
24	C	507	CLA	C3D-C2D-C1D	-4.75	99.35	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	401	CLA	C3D-C4D-ND	4.73	117.68	109.99
24	d	405	CLA	O2D-CGD-CBD	4.73	119.50	111.23
26	d	406	BCR	C24-C23-C22	-4.73	119.24	126.23
24	C	502	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
29	a	417	PL9	C7-C8-C9	-4.73	118.69	126.83
26	k	102	BCR	C33-C5-C6	-4.73	119.33	124.48
24	C	512	CLA	O2D-CGD-CBD	4.72	119.49	111.23
24	D	401	CLA	C3D-C4D-ND	4.71	117.65	109.99
24	b	619	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
27	b	601	SQD	O47-C7-C8	4.71	121.67	111.48
26	T	101	BCR	C33-C5-C6	-4.71	119.35	124.48
24	C	512	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
24	c	909	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
24	A	406	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
24	c	909	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
24	B	606	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	B	605	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	b	606	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	B	608	CLA	C3B-C2B-C1B	-4.67	101.67	107.17
24	c	905	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	606	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
24	B	609	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
36	c	923	HTG	C1'-S1-C1	4.64	110.47	100.45
24	c	910	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	B	614	CLA	CHD-C4C-C3C	-4.63	118.02	124.77
29	A	414	PL9	C7-C8-C9	-4.63	118.85	126.83
24	c	909	CLA	C2B-C1B-NB	4.62	115.12	110.33
24	a	413	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
24	A	407	CLA	O2D-CGD-CBD	4.60	119.28	111.23
24	B	612	CLA	CHD-C4C-C3C	-4.60	118.06	124.77
24	b	618	CLA	C3B-C2B-C1B	-4.60	101.74	107.17
24	B	616	CLA	CHD-C4C-C3C	-4.60	118.06	124.77
24	B	607	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	c	909	CLA	O2D-CGD-CBD	4.60	119.27	111.23
28	C	519	LMG	O7-C10-C11	4.60	121.43	111.48
36	C	521	HTG	C1'-S1-C1	4.60	110.38	100.45
24	b	616	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
37	c	917	DGD	O2G-C1B-C2B	4.59	121.41	111.48
24	c	907	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
24	C	508	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
28	C	523	LMG	O7-C10-C11	4.58	121.40	111.48
24	C	506	CLA	C3D-C2D-C1D	-4.58	99.58	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	403	BCR	C38-C26-C25	-4.57	119.49	124.48
24	A	405	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
24	b	620	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
24	B	604	CLA	C3D-C4D-ND	4.57	117.41	109.99
24	B	606	CLA	CMD-C2D-C1D	4.57	132.77	124.73
24	A	406	CLA	C2C-C1C-NC	4.56	114.78	109.98
24	b	610	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
24	A	406	CLA	C1C-C2C-C3C	-4.55	102.19	106.98
24	D	402	CLA	C3D-C4D-ND	4.55	117.38	109.99
27	a	415	SQD	O47-C7-C8	4.55	121.32	111.48
24	b	616	CLA	C3D-C4D-ND	4.55	117.38	109.99
24	c	902	CLA	C3B-C2B-C1B	-4.54	101.81	107.17
24	C	508	CLA	O2D-CGD-CBD	4.54	119.17	111.23
24	C	502	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
24	d	404	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	B	614	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	b	610	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	B	616	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	c	902	CLA	C3D-C4D-ND	4.52	117.34	109.99
24	c	903	CLA	CHD-C4C-C3C	-4.52	118.18	124.77
24	b	615	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
24	A	410	CLA	CHD-C4C-C3C	-4.51	118.19	124.77
24	D	402	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
24	C	503	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
24	C	508	CLA	C3D-C4D-ND	4.50	117.31	109.99
24	B	608	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
24	c	908	CLA	C4A-NA-C1A	4.50	108.73	106.68
24	b	606	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
24	B	606	CLA	C3D-C4D-ND	4.50	117.30	109.99
24	B	608	CLA	C1C-C2C-C3C	-4.50	102.25	106.98
24	B	607	CLA	CHD-C4C-C3C	-4.49	118.22	124.77
26	C	515	BCR	C7-C8-C9	-4.49	119.59	126.23
24	C	501	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	B	617	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
24	B	603	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
24	B	607	CLA	O2D-CGD-CBD	4.49	119.08	111.23
24	C	504	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
26	b	623	BCR	C24-C23-C22	-4.49	119.60	126.23
24	c	905	CLA	C3D-C4D-ND	4.49	117.28	109.99
24	A	410	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
24	B	608	CLA	C3D-C4D-ND	4.48	117.27	109.99
26	D	403	BCR	C24-C23-C22	-4.47	119.62	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	513	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
24	a	410	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	B	613	CLA	C3D-C4D-ND	4.47	117.25	109.99
31	c	922	LMT	O5'-C5'-C4'	4.47	118.95	109.72
24	A	407	CLA	C3B-C2B-C1B	-4.46	101.91	107.17
24	C	503	CLA	CHD-C4C-C3C	-4.46	118.27	124.77
37	D	405	DGD	O2G-C1B-C2B	4.46	121.13	111.48
24	A	406	CLA	C3D-C4D-ND	4.46	117.23	109.99
27	l	101	SQD	O47-C7-C8	4.45	121.11	111.48
24	a	409	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
24	d	401	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	B	602	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
24	B	609	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
29	D	404	PL9	C40-C39-C41	4.45	122.95	115.23
24	b	607	CLA	C3D-C4D-ND	4.44	117.21	109.99
24	c	911	CLA	C3D-C4D-ND	4.44	117.21	109.99
31	A	417	LMT	C1'-O5'-C5'	4.44	122.39	113.72
28	a	416	LMG	O7-C10-C11	4.44	121.08	111.48
24	B	604	CLA	C3B-C2B-C1B	-4.43	101.94	107.17
24	A	405	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
24	b	615	CLA	C1-C2-C3	-4.43	118.94	126.20
24	b	619	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
36	c	943	HTG	C1'-S1-C1	4.43	110.01	100.45
24	b	618	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
24	a	413	CLA	CHD-C4C-C3C	-4.42	118.33	124.77
24	c	912	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
24	C	513	CLA	C3D-C4D-ND	4.42	117.17	109.99
28	c	921	LMG	O7-C10-C11	4.42	121.03	111.48
24	B	615	CLA	C2C-C1C-NC	4.41	114.62	109.98
24	b	618	CLA	C3D-C4D-ND	4.41	117.16	109.99
24	c	913	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
24	B	603	CLA	C3D-C4D-ND	4.40	117.14	109.99
26	B	636	BCR	C33-C5-C6	-4.39	119.69	124.48
24	B	610	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	c	903	CLA	CMD-C2D-C1D	4.39	132.46	124.73
24	B	612	CLA	C3B-C2B-C1B	-4.38	102.00	107.17
36	D	412	HTG	C1'-S1-C1	4.38	109.92	100.45
24	B	613	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
24	b	609	CLA	CHD-C4C-C3C	-4.37	118.40	124.77
24	b	614	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
24	d	405	CLA	CHD-C4C-C3C	-4.36	118.42	124.77
29	a	417	PL9	C22-C23-C24	-4.36	117.65	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	613	CLA	C3D-C4D-ND	4.35	117.06	109.99
24	c	908	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
24	B	602	CLA	CHD-C4C-C3C	-4.35	118.42	124.77
24	b	607	CLA	C1C-C2C-C3C	-4.35	102.40	106.98
27	l	101	SQD	O6-C1-C2	4.35	114.88	108.27
27	A	412	SQD	C1-O5-C5	-4.35	105.23	113.72
24	A	405	CLA	C3D-C4D-ND	4.35	117.06	109.99
26	B	636	BCR	C15-C16-C17	-4.35	114.62	123.52
39	F	102	HEM	C4D-ND-C1D	4.34	110.35	105.21
24	C	507	CLA	CHD-C4C-C3C	-4.34	118.44	124.77
24	c	903	CLA	C3D-C4D-ND	4.34	117.04	109.99
24	C	505	CLA	O2D-CGD-CBD	4.34	118.82	111.23
24	C	504	CLA	C3D-C4D-ND	4.33	117.03	109.99
24	B	613	CLA	O2D-CGD-CBD	4.33	118.80	111.23
24	C	504	CLA	O2D-CGD-CBD	4.32	118.79	111.23
24	c	902	CLA	CHD-C4C-C3C	-4.32	118.47	124.77
24	C	513	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
27	a	401	SQD	O47-C7-C8	4.32	120.82	111.48
24	C	512	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
24	b	605	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
24	a	409	CLA	C3D-C4D-ND	4.31	117.00	109.99
24	C	510	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
24	D	401	CLA	C2C-C1C-NC	4.31	114.51	109.98
24	b	609	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
24	B	609	CLA	O2D-CGD-CBD	4.31	118.76	111.23
24	B	605	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
36	B	629	HTG	C1'-S1-C1	4.31	109.75	100.45
24	B	615	CLA	C3D-C4D-ND	4.31	116.98	109.99
24	C	502	CLA	C3D-C4D-ND	4.30	116.98	109.99
24	a	413	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
24	A	407	CLA	CHD-C4C-C3C	-4.30	118.51	124.77
24	c	903	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
36	b	627	HTG	C1'-S1-C1	4.29	109.72	100.45
28	A	413	LMG	O7-C10-C11	4.29	120.75	111.48
37	C	516	DGD	O2G-C1B-C2B	4.29	120.75	111.48
24	b	615	CLA	CHD-C4C-C3C	-4.28	118.53	124.77
24	b	607	CLA	CAA-C2A-C3A	-4.27	101.45	113.00
24	c	904	CLA	C3B-C2B-C1B	-4.27	102.13	107.17
24	B	604	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
37	d	408	DGD	O2G-C1B-C2B	4.27	120.72	111.48
24	C	511	CLA	C3B-C2B-C1B	-4.27	102.14	107.17
24	B	603	CLA	C3D-C2D-C1D	-4.27	100.01	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	907	CLA	C3D-C4D-ND	4.27	116.92	109.99
36	d	419	HTG	C1'-S1-C1	4.27	109.66	100.45
24	C	504	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
24	b	620	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
24	a	409	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
24	c	906	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
24	A	407	CLA	C2B-C1B-NB	4.26	114.74	110.33
24	B	607	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
24	A	407	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
24	C	509	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
24	b	605	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
24	B	602	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
24	d	404	CLA	C3D-C4D-ND	4.25	116.89	109.99
24	b	618	CLA	O2D-CGD-CBD	4.25	118.65	111.23
24	b	612	CLA	C3D-C4D-ND	4.24	116.88	109.99
24	B	611	CLA	CAC-C3C-C4C	4.23	130.29	124.79
24	C	501	CLA	C3B-C2B-C1B	-4.23	102.18	107.17
24	d	401	CLA	C3B-C2B-C1B	-4.23	102.18	107.17
24	c	910	CLA	CHD-C4C-C3C	-4.23	118.61	124.77
24	A	406	CLA	CHD-C4C-C3C	-4.22	118.61	124.77
24	b	607	CLA	O2D-CGD-O1D	-4.22	115.63	123.85
24	c	908	CLA	CHD-C4C-C3C	-4.22	118.62	124.77
24	B	608	CLA	C2C-C1C-NC	4.22	114.42	109.98
24	b	616	CLA	C3C-C4C-NC	4.21	115.83	110.43
26	D	403	BCR	C7-C8-C9	-4.21	120.00	126.23
24	C	502	CLA	C1-C2-C3	-4.21	119.30	126.20
24	b	616	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
24	a	410	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	c	914	CLA	C3D-C4D-ND	4.20	116.82	109.99
24	A	407	CLA	C3B-C4B-NB	4.20	114.28	110.53
25	a	412	PHO	C1-C2-C3	-4.19	119.33	126.20
24	d	405	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
24	B	612	CLA	O2D-CGD-CBD	4.19	118.56	111.23
36	b	603	HTG	C1'-S1-C1	4.19	109.50	100.45
24	c	912	CLA	CHD-C4C-C3C	-4.19	118.67	124.77
24	c	902	CLA	O2D-CGD-O1D	-4.19	115.69	123.85
24	C	507	CLA	C2C-C1C-NC	4.18	114.37	109.98
24	c	912	CLA	O2D-CGD-CBD	4.18	118.54	111.23
28	c	920	LMG	O7-C10-C11	4.18	120.53	111.48
24	d	401	CLA	CHD-C4C-C3C	-4.18	118.68	124.77
24	b	620	CLA	CHD-C4C-C3C	-4.18	118.68	124.77
24	C	506	CLA	O2D-CGD-CBD	4.18	118.54	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	621	BCR	C15-C14-C13	-4.18	121.42	127.28
24	c	909	CLA	CHD-C4C-C3C	-4.18	118.69	124.77
24	c	911	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
24	b	620	CLA	C3B-C4B-NB	4.17	114.25	110.53
24	b	617	CLA	C3D-C4D-ND	4.17	116.76	109.99
24	c	911	CLA	O2D-CGD-CBD	4.17	118.51	111.23
24	b	609	CLA	C3D-C4D-ND	4.16	116.75	109.99
24	C	504	CLA	C3B-C2B-C1B	-4.16	102.26	107.17
24	B	615	CLA	C1C-C2C-C3C	-4.16	102.60	106.98
24	c	902	CLA	C1C-C2C-C3C	-4.16	102.61	106.98
24	c	912	CLA	C3D-C4D-ND	4.15	116.74	109.99
24	b	607	CLA	C3B-C2B-C1B	-4.15	102.28	107.17
29	A	414	PL9	C22-C23-C24	-4.15	118.12	127.62
24	B	609	CLA	CMA-C3A-C4A	-4.15	100.62	111.77
24	C	510	CLA	C3D-C4D-ND	4.15	116.73	109.99
24	C	512	CLA	CHD-C4C-C3C	-4.15	118.73	124.77
24	D	402	CLA	CHD-C4C-C3C	-4.15	118.73	124.77
24	B	604	CLA	CHD-C4C-C3C	-4.14	118.73	124.77
26	Y	101	BCR	C33-C5-C6	-4.14	119.96	124.48
24	c	914	CLA	O2D-CGD-CBD	4.14	118.47	111.23
24	B	611	CLA	C4C-C3C-C2C	-4.14	100.86	106.89
24	b	613	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
24	b	614	CLA	O2D-CGD-CBD	4.14	118.46	111.23
24	A	407	CLA	C1C-C2C-C3C	-4.14	102.63	106.98
24	A	410	CLA	C3D-C4D-ND	4.14	116.71	109.99
24	b	612	CLA	CMA-C3A-C4A	-4.14	100.66	111.77
24	C	511	CLA	CHD-C4C-C3C	-4.13	118.75	124.77
24	D	402	CLA	C3B-C2B-C1B	-4.13	102.30	107.17
27	a	415	SQD	C1-O5-C5	-4.13	105.65	113.72
36	C	520	HTG	C1'-S1-C1	4.13	109.36	100.45
24	C	509	CLA	C1C-C2C-C3C	-4.13	102.64	106.98
24	c	908	CLA	C1C-C2C-C3C	-4.13	102.64	106.98
31	B	622	LMT	C1-O1'-C1'	-4.12	106.64	113.68
24	d	404	CLA	O2D-CGD-CBD	4.12	118.44	111.23
39	F	102	HEM	CBD-CAD-C3D	-4.12	101.13	112.53
24	C	508	CLA	C3B-C2B-C1B	-4.11	102.32	107.17
36	C	536	HTG	C1'-S1-C1	4.11	109.33	100.45
24	b	609	CLA	O2D-CGD-CBD	4.11	118.42	111.23
24	C	510	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
24	c	905	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
24	A	407	CLA	CBC-CAC-C3C	-4.11	101.28	112.42
24	d	401	CLA	C1C-C2C-C3C	-4.11	102.66	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	903	CLA	C3B-C2B-C1B	-4.10	102.33	107.17
24	c	914	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
24	C	505	CLA	CAC-C3C-C4C	4.10	130.13	124.79
27	F	101	SQD	C1-C2-C3	-4.10	101.39	110.01
24	c	903	CLA	C1C-C2C-C3C	-4.10	102.67	106.98
24	d	401	CLA	C2C-C1C-NC	4.09	114.28	109.98
24	B	617	CLA	C3D-C4D-ND	4.09	116.64	109.99
24	C	501	CLA	O2D-CGD-O1D	-4.09	115.88	123.85
24	b	605	CLA	CHD-C4C-C3C	-4.09	118.81	124.77
24	c	909	CLA	CMD-C2D-C1D	4.09	131.93	124.73
24	B	613	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
24	C	507	CLA	C1C-C2C-C3C	-4.09	102.68	106.98
24	b	607	CLA	C2C-C1C-NC	4.09	114.27	109.98
24	B	603	CLA	CAA-C2A-C3A	-4.07	101.99	113.00
37	c	918	DGD	O2G-C1B-C2B	4.07	120.29	111.48
24	c	905	CLA	CHD-C4C-C3C	-4.07	118.83	124.77
24	c	910	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
24	C	501	CLA	C3D-C4D-ND	4.07	116.60	109.99
24	c	911	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
24	b	608	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
24	B	603	CLA	O2D-CGD-O1D	-4.06	115.94	123.85
24	B	608	CLA	C2B-C1B-NB	4.06	114.54	110.33
24	b	619	CLA	CHD-C4C-C3C	-4.06	118.86	124.77
24	B	610	CLA	C3D-C4D-ND	4.06	116.58	109.99
24	b	615	CLA	C3B-C2B-C1B	-4.06	102.39	107.17
24	c	913	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
24	C	513	CLA	CHD-C4C-C3C	-4.05	118.86	124.77
24	A	407	CLA	C2C-C1C-NC	4.05	114.24	109.98
24	B	613	CLA	CHD-C4C-C3C	-4.05	118.87	124.77
24	B	607	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
24	C	506	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
24	a	413	CLA	C3D-C4D-ND	4.04	116.55	109.99
24	B	603	CLA	CHD-C4C-C3C	-4.03	118.89	124.77
24	C	508	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
24	B	614	CLA	C3D-C4D-ND	4.03	116.54	109.99
24	d	405	CLA	C3D-C4D-ND	4.03	116.54	109.99
24	b	611	CLA	CHD-C4C-C3C	-4.03	118.90	124.77
24	b	612	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
36	c	924	HTG	C1'-S1-C1	4.03	109.15	100.45
42	v	202	HEC	CBB-CAB-C3B	-4.02	119.41	127.43
24	A	410	CLA	C1C-C2C-C3C	-4.02	102.76	106.98
26	T	101	BCR	C15-C16-C17	-4.01	115.31	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	C2C-C1C-NC	4.01	114.20	109.98
24	C	509	CLA	C3D-C4D-ND	4.01	116.50	109.99
24	b	616	CLA	O2D-CGD-CBD	4.01	118.24	111.23
24	c	912	CLA	C3D-C2D-C1D	-4.01	100.36	105.83
36	c	941	HTG	C1'-S1-C1	4.01	109.11	100.45
31	t	101	LMT	C1-O1'-C1'	-4.01	106.84	113.68
24	B	607	CLA	C4-C3-C5	4.01	122.18	115.23
24	c	903	CLA	O2D-CGD-O1D	-4.00	116.06	123.85
24	B	612	CLA	C3D-C4D-ND	4.00	116.49	109.99
24	B	602	CLA	C3D-C4D-ND	3.99	116.48	109.99
24	B	616	CLA	C1D-CHD-C4C	-3.99	117.54	126.02
24	a	409	CLA	C2C-C1C-NC	3.99	114.17	109.98
24	a	409	CLA	CAC-C3C-C4C	3.99	129.98	124.79
24	D	401	CLA	C3B-C2B-C1B	-3.98	102.47	107.17
27	A	412	SQD	C45-O47-C7	-3.98	108.26	117.80
24	b	613	CLA	C3B-C2B-C1B	-3.98	102.48	107.17
24	b	620	CLA	C1D-CHD-C4C	-3.98	117.57	126.02
24	C	509	CLA	O2D-CGD-O1D	-3.98	116.11	123.85
24	c	914	CLA	C1-C2-C3	-3.97	119.69	126.20
24	c	902	CLA	CMC-C2C-C1C	3.97	131.24	125.03
24	C	503	CLA	C1C-C2C-C3C	-3.97	102.81	106.98
24	A	407	CLA	C1-C2-C3	-3.96	119.70	126.20
24	B	606	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
24	c	914	CLA	C2B-C1B-NB	3.96	114.43	110.33
24	b	606	CLA	C3D-C4D-ND	3.96	116.42	109.99
36	b	627	HTG	O5-C1-C2	3.96	115.77	110.32
36	V	204	HTG	C1-C2-C3	-3.96	102.81	110.55
24	b	614	CLA	CHD-C4C-C3C	-3.96	119.01	124.77
24	B	609	CLA	C2C-C1C-NC	3.95	114.14	109.98
24	c	906	CLA	C3D-C4D-ND	3.95	116.42	109.99
29	A	414	PL9	C32-C33-C34	-3.95	118.58	127.62
24	B	605	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
24	a	413	CLA	C2C-C1C-NC	3.95	114.13	109.98
24	d	405	CLA	C2C-C1C-NC	3.94	114.12	109.98
24	b	620	CLA	C3D-C4D-ND	3.94	116.40	109.99
26	Y	101	BCR	C38-C26-C25	-3.94	120.18	124.48
24	B	613	CLA	CMD-C2D-C1D	3.94	131.67	124.73
24	B	605	CLA	C3D-C4D-ND	3.94	116.39	109.99
24	A	410	CLA	CBC-CAC-C3C	-3.94	101.75	112.42
36	C	537	HTG	C1'-S1-C1	3.93	108.94	100.45
24	a	410	CLA	CHD-C4C-C3C	-3.93	119.04	124.77
26	K	101	BCR	C33-C5-C6	-3.93	120.20	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	401	CLA	C2B-C1B-NB	3.93	114.40	110.33
36	v	211	HTG	C1-C2-C3	-3.93	102.87	110.55
24	d	404	CLA	C3B-C2B-C1B	-3.92	102.54	107.17
24	B	606	CLA	O2D-CGD-CBD	3.92	118.09	111.23
24	A	406	CLA	C2B-C1B-NB	3.92	114.39	110.33
24	c	912	CLA	C4-C3-C5	3.92	122.03	115.23
24	b	610	CLA	C4-C3-C5	3.92	122.03	115.23
24	B	614	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
24	A	410	CLA	C4-C3-C5	3.92	122.03	115.23
24	C	513	CLA	O2D-CGD-CBD	3.91	118.07	111.23
24	c	913	CLA	CHD-C4C-C3C	-3.91	119.07	124.77
24	b	610	CLA	CHD-C4C-C3C	-3.91	119.08	124.77
24	D	401	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
24	B	610	CLA	C3B-C2B-C1B	-3.90	102.58	107.17
24	b	614	CLA	C2B-C1B-NB	3.90	114.37	110.33
24	c	911	CLA	C3D-C2D-C1D	-3.89	100.52	105.83
24	B	615	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
26	c	915	BCR	C33-C5-C6	-3.89	120.24	124.48
24	B	611	CLA	CHD-C4C-C3C	-3.89	119.10	124.77
24	c	906	CLA	C3D-C2D-C1D	-3.89	100.53	105.83
24	B	612	CLA	C2B-C1B-NB	3.89	114.36	110.33
24	a	409	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
24	c	909	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
27	f	102	SQD	C1-O5-C5	3.88	121.29	113.72
24	b	606	CLA	O2D-CGD-O1D	-3.88	116.30	123.85
24	b	605	CLA	C3D-C4D-ND	3.88	116.29	109.99
24	c	913	CLA	C3D-C4D-ND	3.87	116.28	109.99
24	c	911	CLA	C2C-C1C-NC	3.87	114.05	109.98
24	B	615	CLA	C2B-C1B-NB	3.87	114.34	110.33
24	b	614	CLA	C3D-C4D-ND	3.87	116.28	109.99
24	B	617	CLA	CHD-C4C-C3C	-3.86	119.14	124.77
24	B	617	CLA	O2A-CGA-CBA	3.86	123.59	111.83
24	B	603	CLA	C1-C2-C3	-3.85	119.88	126.20
26	A	411	BCR	C33-C5-C6	-3.85	120.28	124.48
24	b	611	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
24	D	401	CLA	CHD-C4C-C3C	-3.84	119.17	124.77
27	F	101	SQD	C44-O6-C1	-3.84	105.57	113.80
24	C	512	CLA	C3D-C4D-ND	3.83	116.22	109.99
26	b	621	BCR	C7-C8-C9	-3.83	120.56	126.23
24	b	611	CLA	C3D-C4D-ND	3.83	116.22	109.99
24	b	609	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
24	b	617	CLA	C2C-C1C-NC	3.83	114.01	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	C2C-C1C-NC	3.83	114.00	109.98
36	c	941	HTG	O5-C5-C4	3.83	116.59	109.70
24	b	606	CLA	C2B-C1B-NB	3.82	114.29	110.33
24	b	605	CLA	C2B-C1B-NB	3.82	114.29	110.33
24	B	609	CLA	C3D-C4D-ND	3.82	116.20	109.99
24	C	506	CLA	C3D-C4D-ND	3.82	116.19	109.99
24	B	612	CLA	CMC-C2C-C1C	3.81	131.00	125.03
24	c	909	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
24	B	611	CLA	C3C-C4C-NC	3.81	115.31	110.43
24	C	506	CLA	C3B-C2B-C1B	-3.81	102.68	107.17
24	B	605	CLA	C2B-C1B-NB	3.81	114.27	110.33
24	c	913	CLA	CBA-CAA-C2A	-3.81	102.47	113.79
24	c	913	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
24	a	413	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
24	c	911	CLA	C1-C2-C3	-3.80	119.98	126.20
36	B	625	HTG	O5-C1-C2	3.80	115.55	110.32
29	D	404	PL9	C42-C43-C44	-3.80	118.94	127.62
24	B	604	CLA	C1C-C2C-C3C	-3.79	102.99	106.98
24	C	501	CLA	C1C-C2C-C3C	-3.79	102.99	106.98
24	c	910	CLA	C1C-C2C-C3C	-3.79	102.99	106.98
31	a	402	LMT	C1B-O5B-C5B	3.79	121.13	113.72
24	B	610	CLA	CHD-C4C-C3C	-3.79	119.24	124.77
29	a	417	PL9	C32-C33-C34	-3.79	118.94	127.62
24	b	618	CLA	CAC-C3C-C4C	3.79	129.72	124.79
24	b	610	CLA	C1C-C2C-C3C	-3.79	103.00	106.98
24	B	605	CLA	CHD-C4C-C3C	-3.79	119.25	124.77
24	c	910	CLA	O2D-CGD-CBD	3.79	117.85	111.23
24	a	409	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
24	c	903	CLA	C2C-C1C-NC	3.78	113.95	109.98
24	A	406	CLA	CBC-CAC-C3C	-3.78	102.18	112.42
24	b	618	CLA	CHD-C4C-C3C	-3.78	119.27	124.77
24	c	906	CLA	CHD-C4C-C3C	-3.78	119.27	124.77
24	b	608	CLA	C3B-C2B-C1B	-3.78	102.72	107.17
24	b	609	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
36	B	624	HTG	C1'-S1-C1	3.78	108.60	100.45
24	B	611	CLA	C3B-C2B-C1B	-3.77	102.72	107.17
26	T	101	BCR	C7-C8-C9	-3.77	120.66	126.23
24	C	506	CLA	C2C-C1C-NC	3.76	113.94	109.98
29	A	414	PL9	C37-C38-C39	-3.76	119.01	127.62
26	k	102	BCR	C15-C14-C13	-3.76	122.00	127.28
24	c	906	CLA	C2C-C1C-NC	3.76	113.93	109.98
24	c	913	CLA	C2B-C1B-NB	3.76	114.22	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	609	CLA	CHD-C1D-ND	-3.76	119.51	124.80
24	b	619	CLA	C2B-C1B-NB	3.76	114.22	110.33
38	E	101	LHG	O7-C7-C8	3.76	119.61	111.48
24	B	612	CLA	C1D-CHD-C4C	-3.76	118.04	126.02
27	F	101	SQD	O47-C7-C8	3.75	119.59	111.48
24	B	617	CLA	C1D-CHD-C4C	-3.75	118.06	126.02
26	B	618	BCR	C33-C5-C6	-3.74	120.40	124.48
24	C	509	CLA	C2C-C1C-NC	3.74	113.92	109.98
24	b	613	CLA	O2D-CGD-CBD	3.74	117.78	111.23
24	A	405	CLA	CAA-C2A-C3A	-3.74	102.88	113.00
24	c	905	CLA	C3B-C2B-C1B	-3.74	102.76	107.17
24	c	910	CLA	C2C-C1C-NC	3.74	113.91	109.98
37	C	517	DGD	O2G-C1B-C2B	3.74	119.57	111.48
24	C	510	CLA	C2B-C1B-NB	3.73	114.20	110.33
24	B	616	CLA	C3D-C4D-ND	3.73	116.05	109.99
26	d	406	BCR	C33-C5-C6	-3.73	120.41	124.48
24	b	619	CLA	C3D-C4D-ND	3.73	116.05	109.99
24	b	619	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
24	c	907	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
24	b	610	CLA	C3D-C4D-ND	3.73	116.04	109.99
28	C	519	LMG	C8-O7-C10	-3.72	108.88	117.80
24	C	502	CLA	O2D-CGD-O1D	-3.72	116.60	123.85
24	c	907	CLA	CHD-C4C-C3C	-3.72	119.35	124.77
24	B	604	CLA	C2B-C1B-NB	3.72	114.18	110.33
24	c	905	CLA	CBC-CAC-C3C	-3.72	102.35	112.42
24	C	509	CLA	C2B-C1B-NB	3.71	114.18	110.33
24	b	617	CLA	C3B-C2B-C1B	-3.71	102.80	107.17
24	B	611	CLA	C3D-C4D-ND	3.71	116.01	109.99
26	C	514	BCR	C33-C5-C6	-3.71	120.44	124.48
24	b	609	CLA	C2B-C1B-NB	3.70	114.17	110.33
24	c	914	CLA	C1D-CHD-C4C	-3.70	118.15	126.02
24	b	606	CLA	C2C-C1C-NC	3.70	113.87	109.98
24	B	614	CLA	C2B-C1B-NB	3.70	114.16	110.33
24	c	908	CLA	C3D-C4D-ND	3.70	115.99	109.99
24	c	903	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
24	b	619	CLA	C2C-C1C-NC	3.69	113.86	109.98
24	A	406	CLA	C3B-C4B-NB	3.69	113.83	110.53
24	c	910	CLA	C3D-C4D-ND	3.69	115.99	109.99
40	H	101	RRX	C24-C23-C22	-3.69	120.78	126.23
24	c	905	CLA	C2C-C1C-NC	3.69	113.86	109.98
24	C	505	CLA	C3D-C4D-ND	3.69	115.98	109.99
24	C	511	CLA	C2C-C1C-NC	3.68	113.85	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	401	CLA	C1D-CHD-C4C	-3.68	118.19	126.02
24	c	911	CLA	C1-O2A-CGA	3.68	125.56	116.65
31	c	922	LMT	C1'-O5'-C5'	3.68	120.91	113.72
38	L	101	LHG	O7-C7-C8	3.68	119.44	111.48
24	C	508	CLA	C2C-C1C-NC	3.68	113.85	109.98
24	A	410	CLA	C2C-C1C-NC	3.68	113.84	109.98
24	c	912	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
24	d	404	CLA	C2C-C1C-NC	3.67	113.84	109.98
24	b	617	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	a	410	CLA	C2C-C1C-NC	3.67	113.84	109.98
24	C	510	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	c	913	CLA	CBC-CAC-C3C	-3.67	102.47	112.42
24	b	612	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	C	506	CLA	CHD-C4C-C3C	-3.67	119.43	124.77
24	C	501	CLA	CHD-C4C-C3C	-3.66	119.44	124.77
24	c	905	CLA	C3B-C4B-NB	3.66	113.80	110.53
24	c	907	CLA	CAA-C2A-C3A	-3.65	103.12	113.00
24	C	507	CLA	C4A-NA-C1A	3.65	108.35	106.68
24	B	603	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
24	b	611	CLA	C2C-C1C-NC	3.65	113.81	109.98
24	B	604	CLA	O2D-CGD-O1D	-3.65	116.75	123.85
31	B	622	LMT	O1B-C4'-C3'	3.64	116.49	107.23
36	c	928	HTG	O5-C1-C2	3.64	115.34	110.32
24	b	615	CLA	C3D-C4D-ND	3.64	115.91	109.99
24	c	907	CLA	C2C-C1C-NC	3.64	113.81	109.98
24	C	502	CLA	CHD-C4C-C3C	-3.64	119.47	124.77
24	C	505	CLA	C3D-C2D-C1D	-3.64	100.87	105.83
24	D	401	CLA	O2D-CGD-CBD	3.64	117.59	111.23
24	b	618	CLA	C2C-C1C-NC	3.64	113.80	109.98
24	C	501	CLA	CBC-CAC-C3C	-3.64	102.56	112.42
24	B	609	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	d	404	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	B	612	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	C	502	CLA	C1C-C2C-C3C	-3.63	103.17	106.98
24	c	907	CLA	C1D-CHD-C4C	-3.62	118.31	126.02
37	c	919	DGD	O2G-C1B-C2B	3.62	119.32	111.48
24	A	406	CLA	CMA-C3A-C4A	-3.62	102.04	111.77
24	C	510	CLA	C2C-C1C-NC	3.62	113.78	109.98
24	b	608	CLA	C2C-C1C-NC	3.62	113.78	109.98
24	B	614	CLA	C1-C2-C3	-3.62	120.27	126.20
24	C	510	CLA	CHD-C4C-C3C	-3.62	119.50	124.77
24	D	401	CLA	CHD-C1D-ND	-3.62	119.71	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	912	CLA	C1-O2A-CGA	3.62	125.40	116.65
24	b	615	CLA	C4A-NA-C1A	3.61	108.33	106.68
24	b	605	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
24	b	619	CLA	C4-C3-C5	3.61	121.50	115.23
24	C	512	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
24	c	911	CLA	CMA-C3A-C4A	-3.61	102.07	111.77
24	C	511	CLA	C3D-C4D-ND	3.61	115.86	109.99
24	A	405	CLA	C2B-C1B-NB	3.61	114.07	110.33
29	A	414	PL9	C27-C28-C29	-3.61	119.37	127.62
24	c	911	CLA	C2B-C1B-NB	3.60	114.06	110.33
36	B	630	HTG	C1'-S1-C1	3.60	108.22	100.45
26	D	403	BCR	C28-C27-C26	-3.60	107.64	114.06
24	C	501	CLA	C2C-C1C-NC	3.60	113.76	109.98
24	D	401	CLA	C1-C2-C3	-3.59	120.31	126.20
24	B	616	CLA	O2D-CGD-CBD	3.59	117.51	111.23
24	A	410	CLA	O2D-CGD-CBD	3.59	117.50	111.23
24	B	616	CLA	C2C-C1C-NC	3.59	113.75	109.98
36	b	602	HTG	C1'-S1-C1	3.59	108.20	100.45
24	C	513	CLA	C1D-CHD-C4C	-3.59	118.39	126.02
31	A	417	LMT	O5'-C5'-C4'	3.58	117.13	109.72
24	c	905	CLA	C2B-C1B-NB	3.58	114.04	110.33
24	B	615	CLA	O2D-CGD-CBD	3.58	117.49	111.23
37	C	518	DGD	O2G-C1B-C2B	3.58	119.23	111.48
24	d	405	CLA	C2B-C1B-NB	3.58	114.04	110.33
24	B	606	CLA	C3C-C4C-NC	3.58	115.01	110.43
31	B	626	LMT	C1'-O5'-C5'	3.58	120.71	113.72
24	A	405	CLA	C1D-CHD-C4C	-3.58	118.42	126.02
24	b	607	CLA	C3D-C2D-C1D	-3.58	100.95	105.83
24	C	504	CLA	C2B-C1B-NB	3.58	114.03	110.33
24	C	507	CLA	C2B-C1B-NB	3.58	114.03	110.33
24	c	913	CLA	C2C-C1C-NC	3.57	113.73	109.98
24	b	609	CLA	CMB-C2B-C1B	3.57	130.86	125.42
38	d	409	LHG	O8-C23-C24	3.57	122.72	111.83
24	C	513	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
24	B	608	CLA	CBC-CAC-C3C	-3.57	102.75	112.42
24	B	612	CLA	CBC-CAC-C3C	-3.57	102.75	112.42
24	b	609	CLA	C1-C2-C3	-3.57	120.35	126.20
24	C	511	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
26	B	618	BCR	C7-C8-C9	-3.56	120.96	126.23
24	A	410	CLA	C2B-C1B-NB	3.56	114.02	110.33
24	b	619	CLA	C1D-CHD-C4C	-3.56	118.44	126.02
24	d	401	CLA	CBC-CAC-C3C	-3.56	102.76	112.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	616	CLA	C2B-C1B-NB	3.56	114.02	110.33
24	c	912	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
24	b	616	CLA	C2C-C1C-NC	3.56	113.72	109.98
24	d	404	CLA	C1-C2-C3	-3.56	120.36	126.20
24	A	405	CLA	CHD-C4C-C3C	-3.56	119.58	124.77
39	f	101	HEM	CBD-CAD-C3D	-3.56	102.69	112.53
42	V	203	HEC	CBC-CAC-C3C	-3.56	120.32	127.43
24	C	507	CLA	C1D-CHD-C4C	-3.56	118.46	126.02
24	C	512	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
24	c	904	CLA	CHD-C4C-C3C	-3.55	119.59	124.77
24	c	907	CLA	C4B-C3B-C2B	-3.55	102.89	107.30
24	B	602	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
24	A	407	CLA	C4-C3-C5	3.55	121.39	115.23
24	B	616	CLA	CMB-C2B-C1B	3.55	130.82	125.42
24	a	410	CLA	C3B-C4B-NB	3.55	113.70	110.53
27	a	415	SQD	C1-C2-C3	-3.55	102.55	110.01
24	b	620	CLA	C3C-C4C-NC	3.55	114.97	110.43
24	c	904	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
27	A	416	SQD	O47-C7-C8	3.54	119.15	111.48
29	d	407	PL9	C37-C38-C39	-3.54	119.52	127.62
24	b	620	CLA	C4C-C3C-C2C	-3.54	101.74	106.89
24	B	610	CLA	C1D-CHD-C4C	-3.54	118.50	126.02
24	B	611	CLA	CAA-C2A-C3A	-3.54	103.44	113.00
24	b	616	CLA	C3B-C4B-NB	3.54	113.69	110.53
24	B	607	CLA	C1D-CHD-C4C	-3.53	118.51	126.02
24	B	604	CLA	CAA-C2A-C3A	-3.53	103.46	113.00
24	C	513	CLA	C2B-C1B-NB	3.53	113.99	110.33
24	b	616	CLA	C1D-CHD-C4C	-3.53	118.52	126.02
24	C	505	CLA	C3B-C2B-C1B	-3.53	103.01	107.17
24	c	908	CLA	C2C-C1C-NC	3.53	113.69	109.98
24	C	504	CLA	C2C-C1C-NC	3.53	113.69	109.98
27	b	601	SQD	C3-C4-C5	3.53	116.63	110.23
36	c	942	HTG	C1'-S1-C1	3.53	108.07	100.45
24	b	606	CLA	C1C-C2C-C3C	-3.53	103.27	106.98
24	c	907	CLA	O2D-CGD-CBD	3.53	117.39	111.23
24	C	508	CLA	CHD-C4C-C3C	-3.52	119.64	124.77
24	C	504	CLA	CMC-C2C-C1C	3.52	130.54	125.03
24	b	618	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
24	C	511	CLA	CAC-C3C-C4C	3.52	129.37	124.79
24	c	910	CLA	C4A-NA-C1A	3.52	108.28	106.68
24	c	910	CLA	C1D-CHD-C4C	-3.52	118.55	126.02
24	b	617	CLA	C3B-C4B-NB	3.51	113.67	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	C2B-C1B-NB	3.51	113.97	110.33
24	a	410	CLA	CBC-CAC-C3C	-3.51	102.90	112.42
24	b	614	CLA	C1D-CHD-C4C	-3.51	118.56	126.02
24	c	912	CLA	C2C-C1C-NC	3.51	113.67	109.98
24	A	410	CLA	CMA-C3A-C4A	-3.51	102.34	111.77
27	A	416	SQD	O48-C23-C24	3.51	122.53	111.83
24	B	617	CLA	C1-C2-C3	-3.51	120.45	126.20
24	b	613	CLA	C1C-C2C-C3C	-3.50	103.29	106.98
24	c	912	CLA	C4A-NA-C1A	3.50	108.28	106.68
24	C	511	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
28	b	624	LMG	O7-C10-C11	3.50	119.06	111.48
26	B	618	BCR	C24-C23-C22	-3.50	121.06	126.23
24	D	402	CLA	C2B-C1B-NB	3.50	113.95	110.33
37	d	408	DGD	O6D-C5D-C4D	3.50	115.85	109.55
24	B	613	CLA	C2B-C1B-NB	3.50	113.95	110.33
26	C	515	BCR	C15-C14-C13	-3.49	122.38	127.28
24	C	507	CLA	C1-C2-C3	-3.49	120.47	126.20
27	F	101	SQD	O7-S-C6	3.49	111.97	106.76
24	B	606	CLA	C2C-C1C-NC	3.49	113.65	109.98
24	b	618	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
24	B	608	CLA	O2D-CGD-CBD	3.49	117.33	111.23
24	b	615	CLA	CAC-C3C-C4C	3.49	129.33	124.79
24	b	617	CLA	CHD-C4C-C3C	-3.49	119.69	124.77
24	A	405	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
24	B	602	CLA	C1D-CHD-C4C	-3.48	118.61	126.02
24	c	908	CLA	CMB-C2B-C1B	3.48	130.72	125.42
24	b	614	CLA	C2C-C1C-NC	3.48	113.64	109.98
24	B	608	CLA	CAC-C3C-C4C	3.48	129.32	124.79
24	c	906	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
24	a	410	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
24	a	409	CLA	C2B-C1B-NB	3.48	113.93	110.33
24	C	504	CLA	CHD-C4C-C3C	-3.48	119.71	124.77
24	B	607	CLA	C3D-C4D-ND	3.47	115.64	109.99
24	A	405	CLA	C3C-C4C-NC	3.47	114.88	110.43
24	B	603	CLA	C2B-C1B-NB	3.47	113.93	110.33
24	a	413	CLA	CBC-CAC-C3C	-3.47	103.01	112.42
24	c	910	CLA	C3B-C4B-NB	3.47	113.63	110.53
24	B	603	CLA	C2C-C1C-NC	3.47	113.63	109.98
24	c	904	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
24	c	914	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
24	c	913	CLA	C1-O2A-CGA	3.47	125.05	116.65
24	B	602	CLA	C2B-C1B-NB	3.47	113.92	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	909	CLA	C2C-C1C-NC	3.47	113.62	109.98
24	b	620	CLA	CBC-CAC-C3C	-3.47	103.02	112.42
24	c	902	CLA	C2C-C1C-NC	3.47	113.62	109.98
24	b	611	CLA	C3B-C2B-C1B	-3.47	103.08	107.17
24	B	616	CLA	C2B-C1B-NB	3.47	113.92	110.33
24	B	604	CLA	C1D-CHD-C4C	-3.46	118.66	126.02
27	f	102	SQD	O5-C5-C4	3.46	115.93	109.70
24	b	616	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
24	B	606	CLA	C4C-C3C-C2C	-3.45	101.87	106.89
29	A	414	PL9	C53-C6-C1	3.45	122.34	115.28
24	A	410	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
24	B	610	CLA	C2C-C1C-NC	3.45	113.61	109.98
24	b	617	CLA	C4-C3-C5	3.45	121.21	115.23
24	c	909	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
24	B	609	CLA	C2B-C1B-NB	3.45	113.90	110.33
24	c	907	CLA	C3B-C2B-C1B	-3.45	103.11	107.17
24	b	611	CLA	O2D-CGD-CBD	3.44	117.25	111.23
24	C	512	CLA	C2B-C1B-NB	3.44	113.89	110.33
24	C	508	CLA	C2B-C1B-NB	3.44	113.89	110.33
24	b	611	CLA	C1D-CHD-C4C	-3.43	118.72	126.02
24	C	503	CLA	C1D-CHD-C4C	-3.43	118.73	126.02
24	A	405	CLA	C2C-C1C-NC	3.43	113.58	109.98
24	C	502	CLA	C2B-C1B-NB	3.43	113.88	110.33
25	A	408	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
24	C	503	CLA	O2D-CGD-CBD	3.42	117.22	111.23
29	d	407	PL9	C7-C8-C9	-3.42	120.93	126.83
24	b	616	CLA	C4C-C3C-C2C	-3.42	101.91	106.89
38	d	409	LHG	O8-C23-O10	-3.42	115.07	123.63
24	a	409	CLA	CAA-C2A-C1A	-3.42	100.76	111.97
25	A	409	PHO	C4-C3-C5	3.42	121.17	115.23
27	a	415	SQD	C45-O47-C7	-3.42	109.61	117.80
24	b	608	CLA	C3D-C4D-ND	3.42	115.55	109.99
24	b	615	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
28	B	621	LMG	O7-C10-C11	3.42	118.88	111.48
24	c	907	CLA	C2B-C1B-NB	3.42	113.87	110.33
24	d	405	CLA	C1D-CHD-C4C	-3.42	118.76	126.02
24	B	602	CLA	CHD-C1D-ND	-3.41	120.00	124.80
36	c	928	HTG	C1-O5-C5	3.41	118.68	112.56
24	B	611	CLA	CMA-C3A-C4A	-3.41	102.61	111.77
24	B	616	CLA	C1C-C2C-C3C	-3.41	103.40	106.98
24	B	614	CLA	C2C-C1C-NC	3.41	113.56	109.98
24	b	611	CLA	O2A-CGA-O1A	-3.40	115.11	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	416	LMG	C7-O1-C1	-3.40	106.50	113.80
24	c	903	CLA	O2A-CGA-O1A	-3.40	115.12	123.63
24	b	613	CLA	C2B-C1B-NB	3.40	113.85	110.33
24	B	606	CLA	C4-C3-C5	3.40	121.13	115.23
24	b	612	CLA	C3B-C2B-C1B	-3.40	103.16	107.17
24	a	410	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
24	c	905	CLA	C4-C3-C5	3.40	121.12	115.23
24	a	413	CLA	CAA-C2A-C3A	-3.40	103.82	113.00
24	b	615	CLA	C1D-CHD-C4C	-3.39	118.81	126.02
24	B	615	CLA	O2A-CGA-O1A	-3.39	115.14	123.63
24	b	608	CLA	C1D-CHD-C4C	-3.39	118.81	126.02
24	C	505	CLA	CHD-C4C-C3C	-3.39	119.83	124.77
24	b	611	CLA	C4B-C3B-C2B	-3.39	103.09	107.30
24	b	605	CLA	C1C-C2C-C3C	-3.39	103.42	106.98
26	c	915	BCR	C38-C26-C25	-3.39	120.79	124.48
24	b	607	CLA	O2A-CGA-CBA	3.38	122.15	111.83
24	B	617	CLA	C4C-C3C-C2C	-3.38	101.97	106.89
24	C	509	CLA	CHD-C4C-C3C	-3.38	119.85	124.77
24	c	906	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
24	b	607	CLA	CBC-CAC-C3C	-3.38	103.26	112.42
24	B	607	CLA	C2C-C1C-NC	3.38	113.53	109.98
42	v	202	HEC	CBC-CAC-C3C	-3.38	120.68	127.43
26	a	414	BCR	C33-C5-C6	-3.38	120.80	124.48
24	b	620	CLA	C2C-C1C-NC	3.38	113.53	109.98
24	b	607	CLA	C2B-C1B-NB	3.38	113.83	110.33
24	b	610	CLA	C2C-C1C-NC	3.37	113.53	109.98
36	C	537	HTG	C1-O5-C5	3.37	118.61	112.56
24	D	402	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
24	b	610	CLA	C3C-C4C-NC	3.37	114.75	110.43
24	b	606	CLA	CAA-C2A-C3A	-3.37	103.89	113.00
24	A	406	CLA	O2D-CGD-CBD	3.37	117.12	111.23
36	y	102	HTG	C1'-S1-C1	3.37	107.72	100.45
24	C	506	CLA	CBC-CAC-C3C	-3.37	103.30	112.42
24	d	404	CLA	C2B-C1B-NB	3.37	113.82	110.33
26	K	101	BCR	C24-C23-C22	-3.36	121.26	126.23
24	B	615	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
24	c	905	CLA	C1D-CHD-C4C	-3.36	118.88	126.02
24	D	401	CLA	C3C-C4C-NC	3.36	114.73	110.43
42	V	203	HEC	C4D-ND-C1D	3.36	111.30	105.82
24	C	504	CLA	O2A-CGA-O1A	-3.36	115.23	123.63
24	b	607	CLA	C4-C3-C5	3.36	121.05	115.23
24	A	406	CLA	C1D-CHD-C4C	-3.35	118.89	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	C3B-C4B-NB	3.35	113.52	110.53
24	c	904	CLA	C2C-C1C-NC	3.35	113.50	109.98
24	b	610	CLA	C1D-CHD-C4C	-3.35	118.89	126.02
24	C	504	CLA	C4-C3-C5	3.35	121.04	115.23
24	B	613	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
24	b	615	CLA	C2C-C1C-NC	3.35	113.50	109.98
24	C	501	CLA	C1D-CHD-C4C	-3.35	118.90	126.02
24	b	606	CLA	C1D-CHD-C4C	-3.35	118.90	126.02
24	b	615	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
24	b	608	CLA	CMB-C2B-C1B	3.35	130.52	125.42
24	B	603	CLA	CMA-C3A-C4A	-3.35	102.78	111.77
24	B	610	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
24	c	908	CLA	C1D-CHD-C4C	-3.34	118.92	126.02
24	c	912	CLA	C2B-C1B-NB	3.34	113.79	110.33
24	B	603	CLA	C1D-CHD-C4C	-3.34	118.92	126.02
24	c	904	CLA	C4A-NA-C1A	3.34	108.20	106.68
26	T	101	BCR	C12-C13-C14	-3.34	113.76	119.01
24	C	505	CLA	C1D-CHD-C4C	-3.33	118.94	126.02
26	C	514	BCR	C7-C8-C9	-3.33	121.31	126.23
24	b	620	CLA	CAC-C3C-C4C	3.33	129.12	124.79
24	B	609	CLA	C1D-CHD-C4C	-3.33	118.95	126.02
38	l	103	LHG	O7-C7-C8	3.32	118.67	111.48
24	c	909	CLA	C3B-C4B-NB	3.32	113.49	110.53
29	a	417	PL9	C17-C18-C19	-3.32	120.03	127.62
25	a	412	PHO	C4-C3-C5	3.32	120.98	115.23
24	B	606	CLA	C2B-C1B-NB	3.32	113.77	110.33
24	C	505	CLA	C4C-C3C-C2C	-3.31	102.07	106.89
24	b	616	CLA	C4-C3-C5	3.31	120.98	115.23
24	b	606	CLA	CHD-C4C-C3C	-3.31	119.94	124.77
24	c	904	CLA	O2D-CGD-CBD	3.31	117.02	111.23
24	B	608	CLA	CAA-C2A-C3A	-3.31	104.06	113.00
24	c	911	CLA	CHD-C4C-C3C	-3.31	119.95	124.77
24	c	905	CLA	C4B-C3B-C2B	-3.31	103.19	107.30
25	A	408	PHO	CBC-CAC-C3C	-3.30	108.15	112.87
31	B	622	LMT	C6'-C5'-C4'	-3.30	104.09	113.38
24	a	409	CLA	C3B-C4B-NB	3.30	113.47	110.53
24	b	611	CLA	C3B-C4B-NB	3.30	113.47	110.53
40	h	101	RRX	C38-C26-C25	-3.30	120.89	124.48
24	A	407	CLA	CHD-C1D-ND	-3.29	120.17	124.80
24	b	609	CLA	C2C-C1C-NC	3.29	113.44	109.98
24	C	511	CLA	CBC-CAC-C3C	-3.29	103.49	112.42
24	a	413	CLA	C2B-C1B-NB	3.29	113.74	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	C3C-C4C-NC	3.29	114.64	110.43
24	c	906	CLA	C2B-C1B-NB	3.29	113.74	110.33
24	d	405	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
29	a	417	PL9	C37-C38-C39	-3.29	120.10	127.62
26	C	515	BCR	C38-C26-C25	-3.28	120.90	124.48
24	b	610	CLA	C2B-C1B-NB	3.28	113.73	110.33
24	C	506	CLA	C1D-CHD-C4C	-3.28	119.04	126.02
24	D	402	CLA	C4-C3-C5	3.28	120.92	115.23
24	b	620	CLA	O2A-CGA-CBA	3.28	121.84	111.83
24	B	617	CLA	C3B-C4B-NB	3.27	113.45	110.53
24	c	914	CLA	CHD-C4C-C3C	-3.27	120.01	124.77
24	b	613	CLA	CHD-C4C-C3C	-3.27	120.01	124.77
24	C	510	CLA	C3B-C4B-NB	3.27	113.44	110.53
24	D	401	CLA	CAA-C2A-C3A	-3.26	104.18	113.00
24	C	504	CLA	CHD-C1D-ND	-3.26	120.21	124.80
42	v	202	HEC	C4D-ND-C1D	3.26	111.14	105.82
26	B	636	BCR	C21-C20-C19	-3.26	113.75	123.20
24	b	612	CLA	C2C-C1C-NC	3.26	113.40	109.98
38	d	411	LHG	O7-C7-C8	3.26	118.53	111.48
24	D	401	CLA	C2B-C1B-NB	3.26	113.70	110.33
24	B	615	CLA	C3B-C4B-NB	3.26	113.44	110.53
24	b	612	CLA	C4B-C3B-C2B	-3.25	103.25	107.30
24	B	613	CLA	C3C-C4C-NC	3.25	114.60	110.43
24	b	612	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
24	c	902	CLA	CHD-C1D-ND	-3.25	120.22	124.80
24	c	911	CLA	C1D-CHD-C4C	-3.25	119.11	126.02
24	C	512	CLA	CMB-C2B-C1B	3.25	130.37	125.42
24	C	510	CLA	C4-C3-C5	3.25	120.87	115.23
38	L	101	LHG	O8-C23-C24	3.25	121.74	111.83
24	D	401	CLA	C3B-C4B-NB	3.25	113.43	110.53
24	C	506	CLA	C2B-C1B-NB	3.25	113.69	110.33
24	c	910	CLA	C4B-C3B-C2B	-3.24	103.27	107.30
24	C	510	CLA	C1D-CHD-C4C	-3.24	119.12	126.02
24	c	902	CLA	C2B-C1B-NB	3.24	113.69	110.33
37	d	408	DGD	C2G-O2G-C1B	-3.24	110.04	117.80
24	c	908	CLA	CMC-C2C-C1C	3.24	130.10	125.03
24	b	612	CLA	C3C-C4C-NC	3.24	114.58	110.43
24	B	613	CLA	C3B-C4B-NB	3.24	113.42	110.53
26	k	103	BCR	C33-C5-C6	-3.24	120.95	124.48
24	b	609	CLA	C4-C3-C5	3.24	120.84	115.23
24	b	620	CLA	C4B-C3B-C2B	-3.24	103.28	107.30
24	C	502	CLA	C1D-CHD-C4C	-3.23	119.14	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	BCR	C2-C1-C6	3.23	115.14	110.44
24	C	503	CLA	C2B-C1B-NB	3.23	113.68	110.33
24	b	608	CLA	CHD-C4C-C3C	-3.22	120.07	124.77
42	V	203	HEC	CBD-CAD-C3D	-3.22	103.62	112.53
24	b	613	CLA	CMB-C2B-C1B	3.22	130.33	125.42
24	A	410	CLA	CHD-C1D-ND	-3.22	120.27	124.80
24	C	502	CLA	C2C-C1C-NC	3.22	113.37	109.98
24	c	910	CLA	C16-C15-C13	-3.22	105.26	115.97
24	C	511	CLA	C3C-C4C-NC	3.22	114.55	110.43
27	A	412	SQD	C1-C2-C3	-3.22	103.24	110.01
37	C	516	DGD	O3G-C3G-C2G	-3.22	102.99	110.82
24	b	613	CLA	C2C-C1C-NC	3.22	113.36	109.98
24	D	402	CLA	C1C-C2C-C3C	-3.21	103.60	106.98
24	b	617	CLA	C2B-C1B-NB	3.21	113.66	110.33
24	c	910	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
24	C	504	CLA	C1D-CHD-C4C	-3.21	119.19	126.02
24	d	404	CLA	C3B-C4B-NB	3.21	113.40	110.53
24	b	607	CLA	C1D-CHD-C4C	-3.21	119.20	126.02
24	b	614	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
24	C	503	CLA	C3D-C4D-ND	3.21	115.20	109.99
24	B	608	CLA	C3B-C4B-NB	3.21	113.39	110.53
24	B	607	CLA	C2B-C1B-NB	3.21	113.65	110.33
24	B	612	CLA	C1-C2-C3	-3.21	120.94	126.20
29	a	417	PL9	C42-C43-C44	-3.21	120.28	127.62
27	l	101	SQD	O7-S-C6	3.21	111.54	106.76
24	c	906	CLA	C3C-C4C-NC	3.20	114.53	110.43
36	v	211	HTG	O5-C1-C2	-3.20	105.90	110.32
24	c	907	CLA	CBC-CAC-C3C	-3.20	103.75	112.42
24	C	503	CLA	CMB-C2B-C1B	3.20	130.29	125.42
24	c	908	CLA	C2B-C1B-NB	3.20	113.64	110.33
25	a	412	PHO	C1A-C2A-C3A	-3.20	99.80	102.84
24	b	608	CLA	C3C-C4C-NC	3.20	114.53	110.43
24	b	617	CLA	C4C-C3C-C2C	-3.19	102.24	106.89
24	d	404	CLA	C3C-C4C-NC	3.19	114.52	110.43
27	b	601	SQD	O48-C23-C24	3.19	121.57	111.83
24	a	410	CLA	CAC-C3C-C4C	3.19	128.94	124.79
24	B	607	CLA	O2A-CGA-O1A	-3.19	115.65	123.63
28	c	921	LMG	C3-C4-C5	3.19	116.01	110.23
24	C	505	CLA	C3C-C4C-NC	3.19	114.51	110.43
24	a	410	CLA	C3C-C4C-NC	3.18	114.51	110.43
24	B	610	CLA	CAC-C3C-C4C	3.18	128.93	124.79
24	C	510	CLA	C1-C2-C3	-3.18	120.98	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
24	d	405	CLA	CMB-C2B-C1B	3.18	130.26	125.42
26	b	621	BCR	C33-C5-C6	-3.18	121.02	124.48
25	a	412	PHO	CMB-C2B-C3B	3.18	131.03	124.68
24	c	913	CLA	CMB-C2B-C1B	3.18	130.26	125.42
24	C	504	CLA	CBC-CAC-C3C	-3.17	103.82	112.42
24	B	617	CLA	CMB-C2B-C1B	3.17	130.25	125.42
24	b	608	CLA	C2B-C1B-NB	3.17	113.62	110.33
24	c	912	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
24	B	616	CLA	C3B-C4B-NB	3.17	113.36	110.53
29	a	417	PL9	C27-C28-C29	-3.17	120.37	127.62
40	H	101	RRX	C38-C26-C25	-3.17	121.03	124.48
29	A	414	PL9	C10-C9-C11	3.17	120.73	115.23
24	b	612	CLA	C1D-CHD-C4C	-3.17	119.29	126.02
26	c	916	BCR	C38-C26-C25	-3.16	121.03	124.48
26	k	103	BCR	C24-C23-C22	-3.16	121.55	126.23
24	C	505	CLA	C2C-C1C-NC	3.16	113.31	109.98
26	d	406	BCR	C7-C8-C9	-3.16	121.56	126.23
24	A	406	CLA	C3C-C4C-NC	3.16	114.48	110.43
36	V	204	HTG	C4-C3-C2	-3.16	105.28	110.83
24	c	903	CLA	O2A-CGA-CBA	3.16	121.47	111.83
40	H	101	RRX	C7-C8-C9	-3.16	121.56	126.23
24	A	407	CLA	CMC-C2C-C1C	3.16	129.97	125.03
24	B	617	CLA	CAC-C3C-C4C	3.16	128.90	124.79
29	d	407	PL9	C10-C9-C11	3.16	120.71	115.23
24	B	617	CLA	C2B-C1B-NB	3.16	113.60	110.33
36	V	204	HTG	O5-C5-C4	3.15	115.38	109.70
24	c	909	CLA	C1-C2-C3	-3.15	121.03	126.20
26	C	515	BCR	C33-C5-C6	-3.15	121.05	124.48
24	c	914	CLA	C2C-C1C-NC	3.15	113.29	109.98
24	d	401	CLA	C3C-C4C-NC	3.15	114.47	110.43
29	D	404	PL9	C7-C8-C9	-3.15	121.41	126.83
26	T	101	BCR	C35-C13-C12	3.15	122.90	118.09
25	A	409	PHO	C1A-C2A-C3A	-3.15	99.84	102.84
24	C	501	CLA	CAC-C3C-C4C	3.15	128.89	124.79
24	B	604	CLA	C3C-C4C-NC	3.15	114.46	110.43
24	c	910	CLA	C1-C2-C3	-3.15	121.04	126.20
26	D	403	BCR	C33-C5-C6	-3.15	121.05	124.48
24	c	908	CLA	O1D-CGD-CBD	-3.15	118.31	124.52
24	b	617	CLA	C3C-C4C-NC	3.15	114.46	110.43
24	c	908	CLA	CBC-CAC-C3C	-3.15	103.89	112.42
24	B	612	CLA	C2C-C1C-NC	3.15	113.29	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	620	CLA	C2B-C1B-NB	3.14	113.59	110.33
25	A	409	PHO	CMB-C2B-C3B	3.14	130.96	124.68
24	c	907	CLA	C3B-C4B-NB	3.14	113.33	110.53
24	c	908	CLA	C4-C3-C5	3.14	120.68	115.23
24	d	404	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
26	c	915	BCR	C7-C8-C9	-3.14	121.59	126.23
24	C	505	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
24	b	607	CLA	O2A-CGA-O1A	-3.14	115.78	123.63
24	b	612	CLA	O2A-CGA-CBA	3.14	121.40	111.83
28	B	621	LMG	O8-C28-C29	3.14	121.40	111.83
24	A	407	CLA	C1D-CHD-C4C	-3.14	119.35	126.02
24	B	613	CLA	C4C-C3C-C2C	-3.14	102.33	106.89
24	C	503	CLA	CMC-C2C-C1C	3.13	129.93	125.03
26	D	403	BCR	C29-C30-C25	3.13	114.99	110.44
24	B	611	CLA	CMB-C2B-C1B	3.13	130.19	125.42
24	C	513	CLA	C2C-C1C-NC	3.13	113.27	109.98
24	A	406	CLA	CHD-C1D-ND	-3.13	120.40	124.80
24	b	617	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
24	B	614	CLA	C3C-C4C-NC	3.13	114.44	110.43
24	B	612	CLA	CAC-C3C-C4C	3.13	128.86	124.79
36	B	623	HTG	C1'-S1-C1	3.13	107.20	100.45
24	b	609	CLA	C1D-CHD-C4C	-3.12	119.38	126.02
24	b	619	CLA	C3B-C4B-NB	3.12	113.32	110.53
24	B	613	CLA	C2C-C1C-NC	3.12	113.26	109.98
24	C	509	CLA	C1D-CHD-C4C	-3.12	119.39	126.02
24	B	616	CLA	CHA-C1A-NA	-3.12	119.33	126.39
24	c	902	CLA	CBC-CAC-C3C	-3.12	103.96	112.42
24	B	612	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
31	B	622	LMT	O5'-C1'-O1'	-3.12	102.68	110.04
24	b	614	CLA	CAC-C3C-C4C	3.12	128.85	124.79
28	B	621	LMG	C9-C8-C7	-3.11	104.52	111.78
24	c	902	CLA	C1D-CHD-C4C	-3.11	119.40	126.02
26	c	915	BCR	C15-C14-C13	-3.11	122.91	127.28
24	A	406	CLA	CAA-C2A-C3A	-3.11	104.59	113.00
24	B	611	CLA	C1D-CHD-C4C	-3.11	119.41	126.02
27	F	101	SQD	C1-O5-C5	-3.11	107.65	113.72
24	C	507	CLA	C3D-C4D-ND	3.11	115.04	109.99
24	c	904	CLA	C3C-C4C-NC	3.11	114.41	110.43
36	c	928	HTG	C1'-S1-C1	3.10	107.15	100.45
24	d	405	CLA	CMC-C2C-C1C	3.10	129.88	125.03
26	c	916	BCR	C33-C5-C6	-3.10	121.10	124.48
24	A	407	CLA	O2A-CGA-O1A	-3.10	115.87	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	H	101	RRX	C10-C11-C12	-3.10	114.22	123.20
24	d	404	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
24	a	413	CLA	C3C-C4C-NC	3.10	114.40	110.43
24	D	402	CLA	CHD-C1D-ND	-3.09	120.45	124.80
36	V	215	HTG	O5-C1-C2	3.09	114.58	110.32
24	B	615	CLA	C4-C3-C5	3.09	120.59	115.23
24	B	606	CLA	C1C-C2C-C3C	-3.09	103.73	106.98
24	c	906	CLA	CAC-C3C-C4C	3.09	128.81	124.79
24	a	410	CLA	C4C-C3C-C2C	-3.09	102.40	106.89
24	B	602	CLA	C2C-C1C-NC	3.09	113.22	109.98
24	b	606	CLA	C3B-C4B-NB	3.09	113.29	110.53
27	b	601	SQD	C1-C2-C3	-3.09	103.52	110.01
24	C	502	CLA	C3C-C4C-NC	3.08	114.38	110.43
24	C	506	CLA	C1-C2-C3	-3.08	121.14	126.20
36	d	414	HTG	O5-C1-C2	3.08	114.56	110.32
24	C	509	CLA	O2A-CGA-CBA	3.08	121.23	111.83
24	A	410	CLA	CMA-C3A-C2A	-3.08	102.08	113.98
24	d	401	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
24	C	504	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
24	c	908	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
24	A	405	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
27	f	102	SQD	O7-S-C6	3.07	111.34	106.76
24	C	501	CLA	CHD-C1D-ND	-3.07	120.49	124.80
24	b	606	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
28	c	921	LMG	O6-C5-C4	3.06	115.22	109.70
24	b	610	CLA	O2A-CGA-O1A	-3.06	115.97	123.63
37	C	517	DGD	O1G-C1A-C2A	3.06	121.17	111.83
24	B	604	CLA	C3B-C4B-NB	3.06	113.26	110.53
24	B	603	CLA	C3C-C4C-NC	3.06	114.35	110.43
24	c	909	CLA	C3C-C4C-NC	3.06	114.35	110.43
24	B	606	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
24	B	614	CLA	CHD-C1D-ND	-3.06	120.50	124.80
24	D	401	CLA	C4C-C3C-C2C	-3.05	102.44	106.89
26	C	514	BCR	C38-C26-C25	-3.05	121.15	124.48
24	c	911	CLA	C3B-C4B-NB	3.05	113.25	110.53
26	T	101	BCR	C15-C14-C13	3.05	131.56	127.28
24	b	614	CLA	C1C-C2C-C3C	-3.05	103.77	106.98
24	d	401	CLA	C3B-C4B-NB	3.05	113.25	110.53
24	C	511	CLA	C1-O2A-CGA	3.05	124.03	116.65
24	B	605	CLA	O2A-CGA-O1A	-3.05	116.00	123.63
24	C	501	CLA	C2B-C1B-NB	3.05	113.49	110.33
24	C	510	CLA	C4B-C3B-C2B	-3.05	103.51	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
26	c	916	BCR	C7-C8-C9	-3.05	121.73	126.23
24	b	618	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
31	B	626	LMT	O5'-C5'-C4'	3.04	115.19	109.70
24	d	401	CLA	CHD-C1D-ND	-3.04	120.52	124.80
24	D	401	CLA	O2A-CGA-CBA	3.04	121.12	111.83
24	B	616	CLA	CBC-CAC-C3C	-3.04	104.17	112.42
24	b	612	CLA	CHD-C4C-C3C	-3.04	120.34	124.77
24	B	605	CLA	C1D-CHD-C4C	-3.04	119.56	126.02
24	d	401	CLA	O2D-CGD-CBD	3.04	116.55	111.23
24	B	617	CLA	O2A-CGA-O1A	-3.04	116.02	123.63
24	a	410	CLA	C4-C3-C5	3.04	120.50	115.23
24	C	508	CLA	C1D-CHD-C4C	-3.04	119.56	126.02
24	c	904	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
24	C	511	CLA	CMC-C2C-C1C	3.03	129.78	125.03
24	b	607	CLA	CHD-C4C-C3C	-3.03	120.35	124.77
24	a	410	CLA	C1-C2-C3	-3.03	121.23	126.20
28	A	413	LMG	C1-O6-C5	3.03	119.64	113.72
24	C	507	CLA	CBC-CAC-C3C	-3.03	104.20	112.42
29	a	417	PL9	C20-C19-C21	3.03	120.49	115.23
24	C	507	CLA	C3C-C4C-NC	3.03	114.31	110.43
24	d	401	CLA	CMB-C2B-C1B	3.03	130.03	125.42
24	A	407	CLA	CAA-C2A-C3A	-3.03	104.82	113.00
24	C	510	CLA	C1-O2A-CGA	3.03	123.97	116.65
24	c	903	CLA	C3C-C4C-NC	3.03	114.31	110.43
24	C	505	CLA	C1C-C2C-C3C	-3.02	103.80	106.98
24	b	617	CLA	C4A-NA-C1A	3.02	108.06	106.68
24	d	405	CLA	CHD-C1D-ND	-3.02	120.55	124.80
24	b	613	CLA	CBC-CAC-C3C	-3.02	104.23	112.42
24	b	608	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
28	c	920	LMG	C8-O7-C10	-3.02	110.58	117.80
24	d	404	CLA	C4B-C3B-C2B	-3.01	103.55	107.30
24	a	409	CLA	CAA-C2A-C3A	-3.01	104.85	113.00
24	D	402	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
29	A	414	PL9	C20-C19-C21	3.01	120.45	115.23
24	c	911	CLA	CBC-CAC-C3C	-3.01	104.26	112.42
24	A	410	CLA	C3B-C4B-NB	3.01	113.22	110.53
26	Y	101	BCR	C15-C14-C13	-3.01	123.06	127.28
24	c	907	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
24	b	610	CLA	CMC-C2C-C1C	3.00	129.73	125.03
24	B	602	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
24	b	613	CLA	C4C-C3C-C2C	-3.00	102.52	106.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	608	CLA	C3B-C4B-NB	3.00	113.21	110.53
24	c	904	CLA	CMB-C2B-C1B	3.00	129.99	125.42
24	C	508	CLA	O2A-CGA-O1A	-3.00	116.12	123.63
31	A	421	LMT	C1B-O5B-C5B	3.00	119.58	113.72
29	a	417	PL9	C30-C29-C31	3.00	120.44	115.23
40	H	101	RRX	C16-C17-C18	-3.00	123.07	127.28
36	C	521	HTG	C1-O5-C5	3.00	117.94	112.56
24	b	616	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
24	c	910	CLA	C2B-C1B-NB	3.00	113.43	110.33
24	c	906	CLA	C4C-C3C-C2C	-2.99	102.53	106.89
24	D	402	CLA	C3C-C4C-NC	2.99	114.27	110.43
29	d	407	PL9	C42-C43-C44	-2.99	120.78	127.62
26	a	414	BCR	C7-C8-C9	-2.99	121.81	126.23
24	C	505	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
24	b	606	CLA	C4-C3-C5	2.99	120.42	115.23
24	b	619	CLA	CHA-C1A-NA	-2.99	119.62	126.39
24	C	512	CLA	C3C-C4C-NC	2.99	114.26	110.43
24	C	507	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
24	c	909	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
24	c	914	CLA	C4C-C3C-C2C	-2.99	102.55	106.89
24	C	510	CLA	O1D-CGD-CBD	-2.99	118.63	124.52
24	C	511	CLA	O2D-CGD-CBD	2.98	116.45	111.23
24	B	605	CLA	C3C-C4C-NC	2.98	114.25	110.43
24	b	609	CLA	C3C-C4C-NC	2.98	114.25	110.43
26	B	636	BCR	C11-C10-C9	-2.98	123.09	127.28
24	B	617	CLA	C3C-C4C-NC	2.98	114.25	110.43
24	B	603	CLA	O2A-CGA-O1A	-2.98	116.17	123.63
24	B	617	CLA	C2C-C1C-NC	2.98	113.11	109.98
24	B	609	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
24	C	503	CLA	C2C-C1C-NC	2.98	113.11	109.98
28	C	523	LMG	C8-O7-C10	-2.98	110.67	117.80
24	b	606	CLA	C3C-C4C-NC	2.98	114.24	110.43
24	d	404	CLA	O2A-CGA-CBA	2.98	120.91	111.83
24	C	511	CLA	C4-C3-C5	2.97	120.39	115.23
24	a	409	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
24	b	612	CLA	C2B-C1B-NB	2.97	113.41	110.33
24	B	615	CLA	C1-O2A-CGA	2.97	123.84	116.65
24	C	508	CLA	C3C-C4C-NC	2.97	114.23	110.43
24	c	912	CLA	CBC-CAC-C3C	-2.97	104.37	112.42
24	C	508	CLA	O2A-CGA-CBA	2.97	120.88	111.83
37	h	102	DGD	O2G-C1B-C2B	2.97	117.90	111.48
24	B	613	CLA	C1D-CHD-C4C	-2.97	119.72	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	405	DGD	O1G-C1A-C2A	2.96	120.86	111.83
24	D	402	CLA	CMB-C2B-C1B	2.96	129.93	125.42
24	C	511	CLA	C2B-C1B-NB	2.96	113.39	110.33
28	C	523	LMG	C1-O6-C5	2.96	119.50	113.72
24	C	506	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
24	c	911	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
38	D	406	LHG	C5-O7-C7	-2.96	110.72	117.80
36	v	211	HTG	C1'-S1-C1	2.96	106.83	100.45
24	C	503	CLA	C3C-C4C-NC	2.96	114.22	110.43
24	B	610	CLA	CBC-CAC-C3C	-2.95	104.41	112.42
24	C	511	CLA	C3B-C4B-NB	2.95	113.17	110.53
24	b	614	CLA	C3C-C4C-NC	2.95	114.21	110.43
24	a	409	CLA	CHD-C4C-C3C	-2.95	120.47	124.77
24	b	612	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
24	c	904	CLA	CHA-C1A-NA	-2.95	119.71	126.39
24	c	906	CLA	CMB-C2B-C1B	2.95	129.91	125.42
24	C	512	CLA	C1-O2A-CGA	2.95	123.79	116.65
24	B	615	CLA	CBC-CAC-C3C	-2.95	104.42	112.42
24	C	511	CLA	CHA-C1A-NA	-2.95	119.72	126.39
24	B	608	CLA	C1-O2A-CGA	2.95	123.78	116.65
24	a	413	CLA	C3B-C4B-NB	2.95	113.16	110.53
24	C	508	CLA	CAA-C2A-C3A	-2.94	105.05	113.00
24	B	609	CLA	CHD-C4C-C3C	-2.94	120.48	124.77
26	b	623	BCR	C3-C4-C5	-2.94	108.81	114.06
24	c	907	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
36	b	626	HTG	C1'-S1-C1	2.94	106.80	100.45
24	c	914	CLA	C3C-C4C-NC	2.94	114.19	110.43
24	C	508	CLA	C4B-C3B-C2B	-2.94	103.65	107.30
24	B	616	CLA	CAC-C3C-C4C	2.93	128.61	124.79
24	d	405	CLA	C3C-C4C-NC	2.93	114.19	110.43
36	b	602	HTG	C1-O5-C5	2.93	117.82	112.56
24	b	619	CLA	C7-C6-C5	-2.93	105.45	113.26
24	c	908	CLA	C3B-C4B-NB	2.93	113.15	110.53
24	b	605	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
24	B	611	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
24	D	401	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	B	613	CLA	CAC-C3C-C4C	2.93	128.60	124.79
24	b	614	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
24	A	405	CLA	CMA-C3A-C2A	-2.93	102.67	113.98
24	c	909	CLA	CAA-C2A-C3A	-2.92	105.10	113.00
24	B	604	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
24	a	413	CLA	C1D-CHD-C4C	-2.92	119.81	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	910	CLA	CBC-CAC-C3C	-2.92	104.50	112.42
27	a	401	SQD	O8-S-C6	2.92	111.61	105.97
24	b	605	CLA	C4-C3-C5	2.92	120.30	115.23
27	f	102	SQD	O48-C23-C24	2.92	120.74	111.83
24	C	513	CLA	C3C-C4C-NC	2.92	114.17	110.43
24	B	606	CLA	O2A-CGA-O1A	-2.92	116.32	123.63
28	c	920	LMG	O8-C28-C29	2.92	120.74	111.83
24	C	502	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
24	B	609	CLA	O2A-CGA-CBA	2.92	120.74	111.83
24	B	603	CLA	CHD-C1D-ND	-2.92	120.69	124.80
26	K	101	BCR	C7-C8-C9	-2.92	121.92	126.23
24	C	501	CLA	CMC-C2C-C1C	2.92	129.59	125.03
26	B	636	BCR	C35-C13-C12	2.91	122.54	118.09
24	a	413	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
27	A	412	SQD	O9-S-C6	2.91	111.11	106.76
38	d	411	LHG	O8-C23-O10	-2.91	116.34	123.63
24	C	503	CLA	CBC-CAC-C3C	-2.91	104.53	112.42
24	b	618	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
24	C	512	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
24	B	614	CLA	C1D-CHD-C4C	-2.91	119.84	126.02
24	b	610	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
24	b	615	CLA	C4B-C3B-C2B	-2.91	103.69	107.30
24	c	904	CLA	C3D-C4D-ND	2.91	114.71	109.99
24	B	605	CLA	C1-C2-C3	-2.90	121.44	126.20
24	B	602	CLA	C1-C2-C3	-2.90	121.44	126.20
28	C	519	LMG	O8-C28-C29	2.90	120.68	111.83
24	B	609	CLA	CAC-C3C-C4C	2.90	128.56	124.79
24	c	911	CLA	C4-C3-C5	2.90	120.26	115.23
24	C	513	CLA	O2A-CGA-CBA	2.90	120.67	111.83
24	b	606	CLA	CBC-CAC-C3C	-2.90	104.57	112.42
24	B	607	CLA	CHD-C1D-ND	-2.90	120.73	124.80
24	B	610	CLA	CMB-C2B-C1B	2.89	129.83	125.42
24	c	904	CLA	C2B-C1B-NB	2.89	113.33	110.33
24	a	409	CLA	O2A-CGA-CBA	2.89	120.66	111.83
24	C	505	CLA	CHA-C1A-NA	-2.89	119.84	126.39
24	C	510	CLA	CBC-CAC-C3C	-2.89	104.58	112.42
24	a	413	CLA	CMA-C3A-C2A	-2.89	102.81	113.98
24	b	619	CLA	C1-O2A-CGA	2.89	123.64	116.65
24	b	613	CLA	C1D-CHD-C4C	-2.88	119.89	126.02
24	C	509	CLA	C3B-C4B-NB	2.88	113.11	110.53
24	c	907	CLA	O2A-CGA-O1A	-2.88	116.42	123.63
24	d	404	CLA	CAA-C2A-C3A	-2.88	105.22	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	405	CLA	CMC-C2C-C1C	2.88	129.53	125.03
24	A	407	CLA	CMB-C2B-C1B	2.88	129.80	125.42
24	B	612	CLA	C3B-C4B-NB	2.88	113.10	110.53
24	d	401	CLA	CMA-C3A-C2A	-2.87	102.87	113.98
24	A	405	CLA	CAA-C2A-C1A	-2.87	102.56	111.97
24	c	909	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
24	C	510	CLA	C3C-C4C-NC	2.87	114.11	110.43
24	B	613	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
24	C	502	CLA	CBC-CAC-C3C	-2.87	104.64	112.42
24	B	605	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
24	b	606	CLA	CMA-C3A-C2A	-2.87	102.89	113.98
24	b	618	CLA	CBC-CAC-C3C	-2.87	104.64	112.42
38	d	409	LHG	O7-C7-C8	2.87	117.69	111.48
24	c	904	CLA	C1-C2-C3	-2.87	121.50	126.20
24	C	507	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
24	C	512	CLA	C2C-C1C-NC	2.87	112.99	109.98
24	c	905	CLA	CHD-C1D-ND	-2.87	120.77	124.80
24	b	614	CLA	C1-C2-C3	-2.86	121.50	126.20
24	A	406	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
24	A	405	CLA	CMA-C3A-C4A	-2.86	104.08	111.77
24	b	612	CLA	C3B-C4B-NB	2.86	113.09	110.53
38	d	411	LHG	O8-C23-C24	2.86	120.56	111.83
24	C	511	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
24	D	402	CLA	C1D-CHD-C4C	-2.86	119.94	126.02
24	C	505	CLA	C4A-NA-C1A	2.86	107.98	106.68
24	B	611	CLA	C2C-C1C-NC	2.86	112.99	109.98
24	c	911	CLA	C3C-C4C-NC	2.86	114.09	110.43
24	c	907	CLA	C3C-C4C-NC	2.86	114.09	110.43
24	B	611	CLA	O2A-CGA-CBA	2.86	120.54	111.83
40	h	101	RRX	C10-C11-C12	-2.85	114.93	123.20
24	b	617	CLA	CAC-C3C-C4C	2.85	128.50	124.79
24	B	612	CLA	C4A-NA-C1A	2.85	107.98	106.68
26	c	915	BCR	C16-C17-C18	-2.85	123.28	127.28
24	c	913	CLA	C3C-C4C-NC	2.85	114.08	110.43
24	c	908	CLA	CHD-C1D-ND	-2.85	120.79	124.80
26	k	102	BCR	C10-C11-C12	-2.85	114.95	123.20
24	C	502	CLA	CAC-C3C-C4C	2.85	128.49	124.79
24	A	407	CLA	C3C-C4C-NC	2.85	114.08	110.43
24	a	410	CLA	CHD-C1D-ND	-2.84	120.80	124.80
24	B	609	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
36	b	626	HTG	C1-C2-C3	2.84	116.10	110.55
24	A	410	CLA	CAA-C2A-C3A	-2.84	105.33	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	913	CLA	C4-C3-C5	2.84	120.15	115.23
24	B	611	CLA	C1-C2-C3	-2.84	121.55	126.20
27	a	415	SQD	O8-S-C6	2.84	111.45	105.97
36	B	630	HTG	C1-O5-C5	2.84	117.65	112.56
24	c	906	CLA	CBC-CAC-C3C	-2.84	104.73	112.42
24	B	615	CLA	CAC-C3C-C4C	2.84	128.48	124.79
24	B	613	CLA	CMC-C2C-C1C	2.83	129.46	125.03
24	C	512	CLA	C1-C2-C3	-2.83	121.56	126.20
24	B	604	CLA	CMA-C3A-C2A	-2.83	103.03	113.98
24	c	905	CLA	O2A-CGA-O1A	-2.83	116.54	123.63
31	A	417	LMT	C1B-O1B-C4'	-2.83	111.27	117.98
24	b	611	CLA	CBC-CAC-C3C	-2.83	104.74	112.42
24	A	406	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
24	D	401	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
24	B	602	CLA	O2A-CGA-CBA	2.83	120.47	111.83
24	C	511	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
29	A	414	PL9	C45-C44-C46	2.83	120.14	115.23
24	c	904	CLA	CMC-C2C-C1C	2.83	129.45	125.03
24	c	911	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
24	b	608	CLA	O1D-CGD-CBD	-2.83	118.94	124.52
24	d	401	CLA	C4B-C3B-C2B	-2.83	103.79	107.30
24	C	512	CLA	CBC-CAC-C3C	-2.82	104.76	112.42
24	C	510	CLA	CAC-C3C-C4C	2.82	128.46	124.79
37	C	517	DGD	O1G-C1A-O1A	-2.82	116.56	123.63
24	C	502	CLA	CED-O2D-CGD	2.82	122.32	115.92
36	B	624	HTG	C1-C2-C3	2.82	116.07	110.55
29	A	414	PL9	C37-C36-C34	-2.82	103.84	113.19
24	B	608	CLA	C1D-CHD-C4C	-2.82	120.03	126.02
24	b	605	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
24	b	618	CLA	C3C-C4C-NC	2.82	114.04	110.43
24	b	613	CLA	C4-C3-C5	2.82	120.12	115.23
24	b	609	CLA	O2A-CGA-O1A	-2.82	116.58	123.63
24	b	616	CLA	CMB-C2B-C1B	2.82	129.71	125.42
24	C	513	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
24	B	610	CLA	C3B-C4B-NB	2.82	113.04	110.53
26	C	515	BCR	C23-C24-C25	-2.81	119.48	127.00
24	C	505	CLA	C2B-C1B-NB	2.81	113.24	110.33
29	a	417	PL9	C53-C6-C1	2.81	121.03	115.28
31	a	402	LMT	O5B-C5B-C4B	2.81	114.76	109.70
24	d	405	CLA	C3B-C4B-NB	2.81	113.04	110.53
26	b	621	BCR	C3-C4-C5	-2.80	109.06	114.06
24	c	910	CLA	C3C-C4C-NC	2.80	114.02	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	603	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
24	b	620	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
24	D	402	CLA	C2C-C1C-NC	2.80	112.92	109.98
40	h	101	RRX	C7-C8-C9	-2.80	122.09	126.23
24	b	620	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
24	a	409	CLA	O2A-CGA-O1A	-2.80	116.63	123.63
25	a	411	PHO	O2D-CGD-O1D	-2.80	118.40	123.85
24	c	912	CLA	C1-C2-C3	-2.80	121.61	126.20
24	B	615	CLA	C3C-C4C-NC	2.80	114.01	110.43
24	b	613	CLA	C3C-C4C-NC	2.80	114.01	110.43
24	c	912	CLA	CMB-C2B-C1B	2.80	129.68	125.42
24	A	406	CLA	CMA-C3A-C2A	-2.79	103.18	113.98
24	a	410	CLA	CMB-C2B-C1B	2.79	129.67	125.42
24	d	401	CLA	CAA-C2A-C3A	-2.79	105.45	113.00
24	B	605	CLA	CMB-C2B-C1B	2.79	129.67	125.42
24	d	404	CLA	C4-C3-C5	2.79	120.08	115.23
24	b	620	CLA	C1-C2-C3	-2.79	121.62	126.20
26	B	619	BCR	C11-C10-C9	-2.79	123.36	127.28
24	b	619	CLA	CBC-CAC-C3C	-2.79	104.85	112.42
26	B	636	BCR	C12-C13-C14	-2.79	114.62	119.01
24	C	502	CLA	CMB-C2B-C1B	2.79	129.67	125.42
27	a	415	SQD	O47-C7-O49	-2.79	117.19	123.70
24	b	605	CLA	C1-O2A-CGA	2.79	123.39	116.65
24	C	503	CLA	C4C-C3C-C2C	-2.79	102.84	106.89
24	C	507	CLA	C3B-C4B-NB	2.79	113.02	110.53
24	c	902	CLA	C3B-C4B-NB	2.79	113.02	110.53
29	A	414	PL9	C17-C18-C19	-2.79	121.25	127.62
28	b	624	LMG	C9-C8-C7	-2.79	105.29	111.78
24	C	504	CLA	CAC-C3C-C4C	2.78	128.41	124.79
24	b	612	CLA	CHA-C1A-NA	-2.78	120.09	126.39
24	b	606	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
37	C	518	DGD	O3G-C3G-C2G	-2.78	104.06	110.82
24	B	615	CLA	O2A-CGA-CBA	2.78	120.31	111.83
24	C	506	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
24	a	413	CLA	C4-C3-C5	2.78	120.05	115.23
24	c	902	CLA	C3C-C4C-NC	2.78	113.99	110.43
24	B	614	CLA	C1-O2A-CGA	2.78	123.37	116.65
24	b	619	CLA	C4B-C3B-C2B	-2.78	103.85	107.30
24	B	603	CLA	O2A-CGA-CBA	2.77	120.29	111.83
27	A	412	SQD	O47-C7-O49	-2.77	117.22	123.70
26	T	101	BCR	C21-C20-C19	-2.77	115.17	123.20
24	B	606	CLA	C3B-C4B-NB	2.77	113.00	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	508	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
24	B	616	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
24	b	609	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
26	k	103	BCR	C8-C7-C6	-2.77	119.60	127.00
24	A	405	CLA	C3B-C4B-NB	2.77	113.00	110.53
24	C	510	CLA	CMA-C3A-C4A	-2.77	104.33	111.77
24	B	611	CLA	C2B-C1B-NB	2.77	113.20	110.33
24	C	513	CLA	CBC-CAC-C3C	-2.77	104.92	112.42
37	H	102	DGD	O1G-C1A-C2A	2.76	120.27	111.83
24	B	616	CLA	C4B-C3B-C2B	-2.76	103.86	107.30
24	c	904	CLA	C1-O2A-CGA	2.76	123.34	116.65
24	B	611	CLA	CAA-CBA-CGA	-2.76	105.36	113.21
24	A	405	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
24	B	604	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
24	a	410	CLA	O2A-CGA-O1A	-2.76	116.72	123.63
37	c	917	DGD	C2G-O2G-C1B	-2.76	111.19	117.80
27	a	415	SQD	C44-O6-C1	-2.75	107.89	113.80
24	B	616	CLA	C3C-C4C-NC	2.75	113.96	110.43
24	B	605	CLA	O2A-CGA-CBA	2.75	120.23	111.83
25	a	412	PHO	C4D-CHA-CBD	2.75	109.78	108.45
24	a	410	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
24	C	506	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
37	C	516	DGD	C3G-C2G-C1G	-2.75	105.37	111.78
24	a	410	CLA	CAA-C2A-C3A	-2.75	105.57	113.00
29	a	417	PL9	C15-C14-C16	2.75	120.00	115.23
24	b	609	CLA	CBC-CAC-C3C	-2.75	104.97	112.42
27	a	401	SQD	O48-C23-C24	2.75	120.21	111.83
24	C	513	CLA	C4-C3-C5	2.75	120.00	115.23
24	c	912	CLA	C3B-C4B-NB	2.75	112.98	110.53
24	d	401	CLA	C4-C3-C5	2.75	119.99	115.23
24	B	605	CLA	CHD-C1D-ND	-2.74	120.94	124.80
24	C	506	CLA	CHD-C1D-ND	-2.74	120.94	124.80
26	C	515	BCR	C21-C20-C19	-2.74	115.25	123.20
24	B	616	CLA	C11-C10-C8	-2.74	106.85	115.97
24	B	614	CLA	CBC-CAC-C3C	-2.74	104.99	112.42
24	c	913	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
24	c	902	CLA	CMB-C2B-C1B	2.74	129.59	125.42
36	O	316	HTG	C1'-S1-C1	2.74	106.37	100.45
24	C	504	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
24	B	612	CLA	CHD-C1D-ND	-2.74	120.95	124.80
26	b	623	BCR	C32-C1-C6	-2.74	105.95	110.24
29	D	404	PL9	C12-C13-C14	-2.74	121.36	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	f	101	HEM	CHC-C1C-NC	2.74	127.43	124.45
40	h	101	RRX	C20-C21-C22	-2.74	123.44	127.28
24	c	914	CLA	C4-C3-C5	2.73	119.97	115.23
24	B	612	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
24	a	413	CLA	CHD-C1D-ND	-2.73	120.96	124.80
24	b	608	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
27	F	101	SQD	C3-C4-C5	2.73	115.18	110.23
29	d	407	PL9	C12-C13-C14	-2.73	121.38	127.62
24	A	410	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
24	A	410	CLA	C3C-C4C-NC	2.73	113.92	110.43
24	B	617	CLA	C6-C5-C3	-2.73	106.82	113.47
24	B	617	CLA	CBC-CAC-C3C	-2.73	105.03	112.42
24	c	905	CLA	CAC-C3C-C4C	2.73	128.34	124.79
24	b	619	CLA	CHD-C1D-ND	-2.73	120.97	124.80
24	B	617	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
29	A	414	PL9	C15-C14-C16	2.72	119.96	115.23
24	C	510	CLA	C4C-C3C-C2C	-2.72	102.93	106.89
24	C	504	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
38	D	408	LHG	O7-C7-C8	2.72	117.37	111.48
29	A	414	PL9	C42-C43-C44	-2.72	121.39	127.62
24	B	613	CLA	C4-C3-C5	2.72	119.95	115.23
24	c	910	CLA	C4C-C3C-C2C	-2.72	102.93	106.89
24	D	401	CLA	C1D-CHD-C4C	-2.72	120.24	126.02
24	B	614	CLA	CED-O2D-CGD	2.72	122.08	115.92
24	b	608	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
38	D	406	LHG	O8-C23-O10	-2.72	116.83	123.63
24	a	409	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
24	B	610	CLA	CMC-C2C-C1C	2.72	129.28	125.03
37	c	919	DGD	O1G-C1A-C2A	2.72	120.12	111.83
24	B	607	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
24	C	502	CLA	CMC-C2C-C1C	2.71	129.28	125.03
24	B	602	CLA	CAA-C2A-C3A	-2.71	105.67	113.00
24	c	903	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
40	h	101	RRX	C24-C23-C22	-2.71	122.22	126.23
26	A	411	BCR	C38-C26-C25	-2.71	121.53	124.48
24	b	611	CLA	C3C-C4C-NC	2.71	113.90	110.43
25	a	411	PHO	C4A-C3A-C2A	-2.71	100.26	102.84
24	b	608	CLA	O2A-CGA-CBA	2.71	120.09	111.83
24	C	513	CLA	CMB-C2B-C1B	2.71	129.54	125.42
24	b	606	CLA	CHD-C1D-ND	-2.71	120.99	124.80
28	c	921	LMG	O8-C28-C29	2.71	120.09	111.83
24	d	404	CLA	CAC-C3C-C4C	2.71	128.31	124.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	415	SQD	O9-S-C6	2.71	110.80	106.76
24	b	611	CLA	CMC-C2C-C1C	2.71	129.26	125.03
24	c	913	CLA	C3B-C4B-NB	2.70	112.94	110.53
24	a	410	CLA	O2A-CGA-CBA	2.70	120.08	111.83
24	B	614	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
24	C	506	CLA	C3C-C4C-NC	2.70	113.89	110.43
24	D	402	CLA	CAC-C3C-C4C	2.70	128.31	124.79
24	A	410	CLA	CMC-C2C-C1C	2.70	129.26	125.03
24	B	610	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	B	617	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
24	C	505	CLA	CMB-C2B-C1B	2.70	129.53	125.42
24	b	605	CLA	CBC-CAC-C3C	-2.70	105.11	112.42
29	d	407	PL9	C15-C14-C16	2.70	119.91	115.23
24	B	611	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
24	B	610	CLA	C2B-C1B-NB	2.70	113.12	110.33
24	c	903	CLA	C2B-C1B-NB	2.70	113.12	110.33
24	b	615	CLA	C4C-C3C-C2C	-2.69	102.97	106.89
24	C	505	CLA	CMC-C2C-C1C	2.69	129.24	125.03
31	c	927	LMT	C1B-O1B-C4'	-2.69	111.60	117.98
24	B	602	CLA	C4C-C3C-C2C	-2.69	102.97	106.89
24	b	608	CLA	CHA-C1A-NA	-2.69	120.30	126.39
26	B	636	BCR	C16-C15-C14	2.69	129.01	123.52
24	B	615	CLA	CMC-C2C-C1C	2.69	129.23	125.03
24	c	905	CLA	CMC-C2C-C1C	2.68	129.23	125.03
24	B	616	CLA	C4C-C3C-C2C	-2.68	102.98	106.89
24	A	410	CLA	O2A-CGA-CBA	2.68	120.02	111.83
24	A	410	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
25	A	408	PHO	CMA-C3A-C4A	-2.68	108.83	114.61
24	b	618	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
27	b	601	SQD	O7-S-C6	2.68	110.76	106.76
24	D	402	CLA	CMC-C2C-C1C	2.68	129.22	125.03
24	B	608	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
24	b	617	CLA	CMB-C2B-C1B	2.68	129.50	125.42
36	O	303	HTG	C1'-S1-C1	2.68	106.24	100.45
24	d	404	CLA	C1D-CHD-C4C	-2.68	120.33	126.02
24	a	413	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
24	C	506	CLA	C4C-C3C-C2C	-2.68	103.00	106.89
24	C	512	CLA	CMA-C3A-C4A	-2.67	104.59	111.77
38	E	101	LHG	O8-C23-C24	2.67	119.98	111.83
24	b	617	CLA	O2A-CGA-CBA	2.67	119.98	111.83
24	B	614	CLA	CMC-C2C-C1C	2.67	129.21	125.03
38	D	406	LHG	O8-C23-C24	2.67	119.98	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	609	CLA	CMC-C2C-C1C	2.67	129.21	125.03
24	b	605	CLA	C2C-C1C-NC	2.67	112.79	109.98
24	B	604	CLA	O2A-CGA-CBA	2.67	119.98	111.83
25	a	412	PHO	C4A-C3A-C2A	-2.67	100.30	102.84
24	B	602	CLA	CBC-CAC-C3C	-2.67	105.18	112.42
24	B	607	CLA	C3C-C4C-NC	2.67	113.85	110.43
24	C	504	CLA	OBD-CAD-C3D	-2.67	122.18	128.42
24	b	611	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
24	B	614	CLA	CMA-C3A-C4A	-2.67	104.61	111.77
24	c	914	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
25	A	409	PHO	C4A-C3A-C2A	-2.67	100.30	102.84
24	b	612	CLA	CMA-C3A-C2A	-2.67	103.67	113.98
26	C	514	BCR	C11-C10-C9	-2.67	123.54	127.28
24	b	615	CLA	C2B-C1B-NB	2.67	113.09	110.33
24	C	503	CLA	CHA-C1A-NA	-2.67	120.36	126.39
24	C	513	CLA	CAC-C3C-C4C	2.66	128.26	124.79
26	K	101	BCR	C38-C26-C25	-2.66	121.58	124.48
24	b	607	CLA	CMA-C3A-C2A	-2.66	103.69	113.98
27	F	101	SQD	C45-O47-C7	-2.66	111.43	117.80
24	B	609	CLA	C3C-C4C-NC	2.66	113.84	110.43
24	b	611	CLA	C2B-C1B-NB	2.66	113.08	110.33
24	B	603	CLA	C3B-C4B-NB	2.66	112.91	110.53
26	b	623	BCR	C38-C26-C25	-2.66	121.58	124.48
24	c	910	CLA	CMC-C2C-C1C	2.66	129.19	125.03
25	A	408	PHO	CBA-CAA-C2A	-2.66	105.95	113.78
24	b	618	CLA	O2A-CGA-CBA	2.65	119.93	111.83
24	A	407	CLA	CAC-C3C-C4C	2.65	128.24	124.79
24	b	614	CLA	CMA-C3A-C4A	-2.65	104.65	111.77
24	D	401	CLA	CMB-C2B-C1B	2.65	129.45	125.42
24	b	614	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
24	B	616	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
24	a	410	CLA	CMA-C3A-C2A	-2.65	103.74	113.98
24	b	610	CLA	CAC-C3C-C4C	2.65	128.24	124.79
24	B	604	CLA	CBC-CAC-C3C	-2.65	105.24	112.42
28	c	921	LMG	C8-O7-C10	-2.65	111.46	117.80
24	B	606	CLA	C1-C2-C3	-2.65	121.86	126.20
24	b	617	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
25	a	411	PHO	C1A-C2A-C3A	-2.64	100.32	102.84
24	C	509	CLA	C4C-C3C-C2C	-2.64	103.04	106.89
24	c	908	CLA	C3C-C4C-NC	2.64	113.82	110.43
24	b	611	CLA	CAA-C2A-C1A	-2.64	103.32	111.97
24	A	406	CLA	O2D-CGD-O1D	-2.64	118.71	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	912	CLA	CHD-C1D-ND	-2.64	121.09	124.80
24	c	913	CLA	CHA-C1A-NA	-2.64	120.42	126.39
26	b	622	BCR	C8-C7-C6	-2.64	119.95	127.00
24	b	619	CLA	C3C-C4C-NC	2.64	113.81	110.43
36	B	631	HTG	C1-O5-C5	2.64	117.29	112.56
24	B	616	CLA	CMC-C2C-C1C	2.64	129.15	125.03
24	C	501	CLA	C3B-C4B-NB	2.63	112.88	110.53
24	C	504	CLA	C3C-C4C-NC	2.63	113.80	110.43
26	k	102	BCR	C16-C17-C18	-2.63	123.59	127.28
38	D	406	LHG	O7-C7-C8	2.63	117.17	111.48
24	b	610	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
24	C	512	CLA	CHA-C1A-NA	-2.63	120.44	126.39
24	d	404	CLA	CHD-C4C-C3C	-2.63	120.94	124.77
36	C	537	HTG	O5-C5-C4	2.63	114.43	109.70
24	c	910	CLA	CHD-C1D-ND	-2.63	121.11	124.80
24	B	604	CLA	CAC-C3C-C4C	2.63	128.21	124.79
27	a	415	SQD	O48-C23-C24	2.63	119.84	111.83
24	b	616	CLA	O2A-CGA-CBA	2.63	119.84	111.83
28	a	416	LMG	O6-C5-C4	2.62	114.43	109.70
36	O	316	HTG	C6-C5-C4	-2.62	106.58	113.02
40	H	101	RRX	C20-C21-C22	-2.62	123.60	127.28
26	b	622	BCR	C38-C26-C25	-2.62	121.62	124.48
26	k	102	BCR	C38-C26-C25	-2.62	121.63	124.48
24	b	619	CLA	C4C-C3C-C2C	-2.62	103.08	106.89
24	d	401	CLA	C6-C5-C3	-2.62	107.09	113.47
27	A	412	SQD	O48-C23-C24	2.62	119.81	111.83
24	b	616	CLA	CMC-C2C-C1C	2.62	129.12	125.03
24	b	606	CLA	C1-C2-C3	-2.61	121.91	126.20
24	B	617	CLA	C4B-C3B-C2B	-2.61	104.05	107.30
24	B	607	CLA	O2A-CGA-CBA	2.61	119.80	111.83
24	c	910	CLA	CAC-C3C-C4C	2.61	128.19	124.79
24	c	907	CLA	CHD-C1D-ND	-2.61	121.13	124.80
26	B	636	BCR	C1-C6-C7	2.61	122.73	115.65
26	B	636	BCR	C23-C24-C25	-2.61	120.03	127.00
24	C	512	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
24	a	410	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
24	c	906	CLA	C1-O2A-CGA	2.61	122.96	116.65
26	K	101	BCR	C10-C11-C12	-2.61	115.65	123.20
24	b	615	CLA	CBC-CAC-C3C	-2.61	105.35	112.42
29	A	414	PL9	C25-C24-C26	2.61	119.75	115.23
24	b	617	CLA	CMA-C3A-C4A	-2.61	104.77	111.77
24	B	612	CLA	C3C-C4C-NC	2.60	113.77	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	CHA-C1A-NA	-2.60	120.49	126.39
26	b	623	BCR	C15-C14-C13	-2.60	123.63	127.28
24	B	609	CLA	C4B-C3B-C2B	-2.60	104.06	107.30
24	B	614	CLA	C4C-C3C-C2C	-2.60	103.10	106.89
31	b	625	LMT	O5'-C1'-C2'	-2.60	105.02	110.37
24	A	406	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
24	b	605	CLA	C3C-C4C-NC	2.60	113.76	110.43
24	a	413	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
24	d	404	CLA	CHA-C1A-NA	-2.60	120.51	126.39
24	d	405	CLA	CAA-C2A-C3A	-2.60	105.98	113.00
26	A	411	BCR	C20-C21-C22	-2.60	123.64	127.28
24	B	612	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
24	c	912	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
24	C	513	CLA	C1-C2-C3	-2.60	121.94	126.20
24	B	603	CLA	C4-C3-C5	2.59	119.73	115.23
42	v	202	HEC	CBD-CAD-C3D	-2.59	105.36	112.53
24	a	413	CLA	CMA-C3A-C4A	-2.59	104.80	111.77
24	b	607	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
24	a	413	CLA	O2A-CGA-CBA	2.59	119.74	111.83
24	b	618	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
24	C	506	CLA	C4-C3-C5	2.59	119.73	115.23
29	a	417	PL9	C10-C9-C11	2.59	119.72	115.23
26	B	636	BCR	C15-C14-C13	2.59	130.91	127.28
24	C	508	CLA	CMC-C2C-C1C	2.59	129.08	125.03
24	b	613	CLA	C1-C2-C3	-2.59	121.95	126.20
26	k	103	BCR	C20-C21-C22	-2.59	123.65	127.28
24	B	603	CLA	CBC-CAC-C3C	-2.59	105.40	112.42
24	b	608	CLA	C4A-NA-C1A	2.59	107.86	106.68
24	B	604	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
24	b	617	CLA	CHD-C1D-ND	-2.59	121.16	124.80
24	B	614	CLA	C3B-C4B-NB	2.59	112.84	110.53
24	c	903	CLA	C3B-C4B-NB	2.59	112.84	110.53
26	c	916	BCR	C21-C20-C19	-2.59	115.71	123.20
24	b	614	CLA	C3B-C4B-NB	2.58	112.84	110.53
24	B	615	CLA	C7-C6-C5	-2.58	106.38	113.26
24	c	912	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
26	k	103	BCR	C11-C10-C9	-2.58	123.66	127.28
26	b	623	BCR	C2-C1-C6	2.58	114.19	110.44
37	C	518	DGD	O6E-C1E-O5D	-2.58	103.94	110.04
25	a	411	PHO	CMB-C2B-C3B	2.58	129.84	124.68
37	C	516	DGD	O1G-C1A-O1A	-2.58	117.17	123.63
26	b	621	BCR	C24-C23-C22	-2.58	122.42	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	611	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
24	b	607	CLA	C3B-C4B-NB	2.58	112.83	110.53
24	D	401	CLA	CBC-CAC-C3C	-2.58	105.44	112.42
24	B	614	CLA	O2A-CGA-CBA	2.58	119.69	111.83
24	D	402	CLA	C1-C2-C3	-2.57	121.98	126.20
24	d	404	CLA	CMA-C3A-C2A	-2.57	104.03	113.98
24	d	405	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
24	c	908	CLA	O2A-CGA-CBA	2.57	119.68	111.83
24	D	402	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
24	b	607	CLA	C3C-C4C-NC	2.57	113.72	110.43
24	c	905	CLA	C3C-C4C-NC	2.57	113.72	110.43
24	c	914	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
24	c	907	CLA	O2A-CGA-CBA	2.57	119.67	111.83
38	d	410	LHG	O8-C23-C24	2.57	119.66	111.83
26	a	414	BCR	C15-C14-C13	-2.57	123.68	127.28
24	b	614	CLA	CHC-C1C-C2C	-2.56	119.66	126.95
38	D	408	LHG	O8-C23-O10	-2.56	117.21	123.63
27	l	101	SQD	O48-C23-C24	2.56	119.65	111.83
24	c	903	CLA	C4C-C3C-C2C	-2.56	103.16	106.89
38	d	410	LHG	O8-C23-O10	-2.56	117.22	123.63
24	B	602	CLA	CMB-C2B-C1B	2.56	129.32	125.42
25	A	408	PHO	CMC-C2C-C1C	2.56	129.34	124.73
24	b	615	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
24	A	405	CLA	CAC-C3C-C4C	2.56	128.12	124.79
24	b	611	CLA	CAA-C2A-C3A	-2.56	106.08	113.00
24	B	615	CLA	CHD-C4C-NC	2.56	128.20	124.23
38	d	410	LHG	O7-C7-C8	2.56	117.01	111.48
38	E	101	LHG	C5-O7-C7	-2.56	111.68	117.80
24	d	401	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
37	h	102	DGD	C6D-C5D-C4D	2.56	117.43	112.07
37	H	102	DGD	O2G-C1B-C2B	2.55	117.01	111.48
24	C	501	CLA	CMB-C2B-C1B	2.55	129.31	125.42
37	c	917	DGD	O2G-C1B-O1B	-2.55	117.74	123.70
24	c	905	CLA	C4C-C3C-C2C	-2.55	103.18	106.89
29	d	407	PL9	C25-C24-C26	2.55	119.65	115.23
24	b	610	CLA	CHA-C1A-NA	-2.55	120.62	126.39
29	A	414	PL9	C30-C29-C31	2.55	119.65	115.23
24	d	401	CLA	CAC-C3C-C4C	2.55	128.10	124.79
24	c	906	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
24	c	909	CLA	CBC-CAC-C3C	-2.55	105.52	112.42
24	b	615	CLA	C3C-C4C-NC	2.55	113.69	110.43
24	c	912	CLA	CMC-C2C-C1C	2.55	129.01	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	606	CLA	CMA-C3A-C4A	-2.55	104.93	111.77
26	d	406	BCR	C3-C4-C5	-2.55	109.52	114.06
27	A	416	SQD	O9-S-C6	2.55	110.56	106.76
26	T	101	BCR	C7-C6-C5	-2.55	115.69	121.56
24	b	606	CLA	CHA-C1A-NA	-2.54	120.63	126.39
28	a	416	LMG	O1-C1-C2	2.54	112.14	108.27
24	c	902	CLA	C1-C2-C3	-2.54	122.03	126.20
24	d	401	CLA	CMA-C3A-C4A	-2.54	104.94	111.77
26	A	411	BCR	C15-C14-C13	-2.54	123.72	127.28
24	c	906	CLA	CHA-C1A-NA	-2.54	120.64	126.39
24	C	510	CLA	CMC-C2C-C1C	2.54	129.00	125.03
24	d	401	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
24	c	905	CLA	O1D-CGD-CBD	-2.54	119.52	124.52
24	b	611	CLA	CHD-C1D-ND	-2.53	121.23	124.80
24	B	603	CLA	CMA-C3A-C2A	-2.53	104.18	113.98
24	C	509	CLA	C16-C15-C13	-2.53	107.54	115.97
24	C	504	CLA	C3B-C4B-NB	2.53	112.79	110.53
24	a	409	CLA	C4C-C3C-C2C	-2.53	103.21	106.89
24	B	612	CLA	CHA-C1A-NA	-2.53	120.66	126.39
24	d	405	CLA	CAC-C3C-C4C	2.53	128.08	124.79
24	C	513	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
24	a	409	CLA	C3C-C4C-NC	2.53	113.67	110.43
24	d	405	CLA	C4-C3-C5	2.53	119.61	115.23
24	C	510	CLA	CHC-C1C-C2C	-2.53	119.77	126.95
24	C	507	CLA	CMB-C2B-C1B	2.53	129.26	125.42
24	c	909	CLA	C4-C3-C5	2.53	119.61	115.23
24	C	511	CLA	CHD-C1D-ND	-2.53	121.25	124.80
25	a	412	PHO	O2D-CGD-O1D	-2.52	118.93	123.85
24	b	609	CLA	C4B-C3B-C2B	-2.52	104.16	107.30
28	d	412	LMG	O8-C28-O10	-2.52	117.31	123.63
24	C	509	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
24	B	615	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
24	b	613	CLA	CHD-C1D-ND	-2.52	121.25	124.80
24	B	607	CLA	CMC-C2C-C1C	2.52	128.97	125.03
24	b	618	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
24	b	611	CLA	O2A-CGA-CBA	2.52	119.52	111.83
24	B	606	CLA	CMC-C2C-C1C	2.52	128.97	125.03
24	C	510	CLA	C11-C10-C8	-2.52	107.60	115.97
24	b	607	CLA	C4C-C3C-C2C	-2.52	103.23	106.89
24	d	405	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
27	f	102	SQD	O47-C7-O49	-2.52	117.82	123.70
24	c	904	CLA	CAC-C3C-C4C	2.51	128.06	124.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	101	BCR	C16-C17-C18	-2.51	123.75	127.28
24	A	410	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
24	b	613	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
38	D	407	LHG	O7-C7-C8	2.51	116.92	111.48
24	B	610	CLA	C4B-C3B-C2B	-2.51	104.18	107.30
24	d	404	CLA	CMB-C2B-C1B	2.51	129.24	125.42
24	C	513	CLA	CMC-C2C-C1C	2.51	128.95	125.03
24	b	613	CLA	CHA-C1A-NA	-2.50	120.72	126.39
24	b	616	CLA	C16-C15-C13	-2.50	107.64	115.97
24	b	610	CLA	CBC-CAC-C3C	-2.50	105.63	112.42
26	B	619	BCR	C29-C28-C27	-2.50	105.77	111.28
31	Z	101	LMT	C1B-O1B-C4'	-2.50	112.04	117.98
24	c	914	CLA	C3B-C4B-NB	2.50	112.77	110.53
24	B	607	CLA	C4C-C3C-C2C	-2.50	103.25	106.89
24	C	506	CLA	C3B-C4B-NB	2.50	112.76	110.53
24	B	609	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
24	c	913	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
24	C	509	CLA	C3C-C4C-NC	2.50	113.63	110.43
26	T	101	BCR	C1-C6-C7	2.50	122.43	115.65
24	b	617	CLA	C1D-CHD-C4C	-2.50	120.71	126.02
24	a	409	CLA	CMA-C3A-C2A	-2.50	104.32	113.98
24	B	614	CLA	CMB-C2B-C1B	2.50	129.22	125.42
24	B	616	CLA	C6-C7-C8	-2.50	107.66	115.97
24	B	602	CLA	C3C-C4C-NC	2.50	113.63	110.43
24	c	902	CLA	CAC-C3C-C4C	2.49	128.03	124.79
24	C	509	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
24	C	513	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
29	D	404	PL9	C30-C29-C31	2.49	119.55	115.23
25	a	411	PHO	C1-C2-C3	-2.49	122.12	126.20
24	c	906	CLA	C3B-C4B-NB	2.49	112.75	110.53
25	a	411	PHO	CBA-CAA-C2A	-2.49	106.46	113.78
24	c	914	CLA	CED-O2D-CGD	2.49	121.55	115.92
24	C	502	CLA	C1-O2A-CGA	2.48	122.67	116.65
24	D	402	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
26	Y	101	BCR	C10-C11-C12	-2.48	116.01	123.20
24	C	503	CLA	C4A-NA-C1A	2.48	107.81	106.68
24	B	602	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
24	b	619	CLA	CAC-C3C-C4C	2.48	128.02	124.79
24	D	401	CLA	CAC-C3C-C4C	2.48	128.01	124.79
26	B	620	BCR	C15-C14-C13	-2.48	123.80	127.28
24	B	612	CLA	CHD-C4C-NC	2.48	128.07	124.23
24	b	611	CLA	CMB-C2B-C1B	2.48	129.19	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	619	CLA	O2D-CGD-CBD	2.48	115.56	111.23
26	c	916	BCR	C3-C4-C5	-2.47	109.64	114.06
24	B	614	CLA	C4-C3-C5	2.47	119.52	115.23
26	B	636	BCR	C7-C6-C5	-2.47	115.86	121.56
24	b	617	CLA	O2D-CGD-CBD	2.47	115.55	111.23
36	c	924	HTG	C1-O5-C5	2.47	117.00	112.56
24	d	405	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
24	B	605	CLA	C4C-C3C-C2C	-2.47	103.30	106.89
24	c	913	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
24	c	908	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
24	c	906	CLA	CMC-C2C-C1C	2.47	128.89	125.03
24	A	405	CLA	CMB-C2B-C3B	2.47	132.35	126.55
37	D	405	DGD	O2G-C1B-O1B	-2.47	117.94	123.70
24	c	910	CLA	C11-C12-C13	-2.47	107.77	115.97
24	C	507	CLA	O2A-CGA-CBA	2.46	119.35	111.83
24	c	912	CLA	C3C-C4C-NC	2.46	113.59	110.43
24	A	407	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
24	C	509	CLA	CBC-CAC-C3C	-2.46	105.75	112.42
31	c	922	LMT	C1B-O5B-C5B	2.46	118.53	113.72
24	b	615	CLA	C3B-C4B-NB	2.46	112.73	110.53
24	C	501	CLA	C3C-C4C-NC	2.46	113.58	110.43
36	b	602	HTG	O5-C5-C4	2.46	114.13	109.70
36	B	629	HTG	O5-C5-C4	2.46	114.13	109.70
25	A	409	PHO	O2D-CGD-O1D	-2.46	119.06	123.85
26	c	916	BCR	C15-C14-C13	-2.46	123.83	127.28
31	b	625	LMT	C3'-C4'-C5'	2.45	116.37	110.93
24	a	410	CLA	CHC-C1C-C2C	-2.45	119.98	126.95
24	b	610	CLA	O2A-CGA-CBA	2.45	119.31	111.83
24	b	605	CLA	C1-C2-C3	-2.45	122.18	126.20
24	A	410	CLA	C4C-C3C-C2C	-2.45	103.33	106.89
28	C	523	LMG	O8-C28-C29	2.45	119.30	111.83
24	d	401	CLA	CAA-CBA-CGA	2.45	120.16	113.21
24	C	501	CLA	C4C-C3C-C2C	-2.45	103.33	106.89
24	B	609	CLA	C3B-C4B-NB	2.45	112.72	110.53
24	B	603	CLA	C4B-C3B-C2B	-2.45	104.26	107.30
24	a	409	CLA	O2D-CGD-CBD	2.44	115.50	111.23
24	c	906	CLA	C4B-C3B-C2B	-2.44	104.26	107.30
24	b	612	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
24	C	508	CLA	C4-C3-C5	2.44	119.47	115.23
37	D	405	DGD	O6D-C5D-C4D	2.44	114.10	109.70
24	A	407	CLA	O2A-CGA-CBA	2.44	119.28	111.83
24	C	506	CLA	CHA-C1A-NA	-2.44	120.86	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	D	408	LHG	O8-C23-C24	2.44	119.28	111.83
38	D	407	LHG	O8-C23-C24	2.44	119.28	111.83
24	b	612	CLA	CBC-CAC-C3C	-2.44	105.80	112.42
24	b	619	CLA	CED-O2D-CGD	2.44	121.45	115.92
24	B	614	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
24	C	503	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
27	b	601	SQD	O8-S-C6	2.44	110.68	105.97
24	b	605	CLA	CAA-C2A-C3A	-2.44	106.41	113.00
24	c	907	CLA	CGD-CBD-CAD	-2.44	102.95	110.85
24	b	605	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
24	b	608	CLA	CHD-C1D-C2D	-2.44	120.42	125.49
27	b	601	SQD	O5-C5-C4	2.43	114.09	109.70
24	c	908	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
24	b	613	CLA	CED-O2D-CGD	2.43	121.44	115.92
24	c	910	CLA	O2A-CGA-CBA	2.43	119.25	111.83
24	C	501	CLA	C4B-C3B-C2B	-2.43	104.28	107.30
38	L	101	LHG	O8-C23-O10	-2.43	117.55	123.63
24	c	912	CLA	O2A-CGA-CBA	2.43	119.24	111.83
24	B	608	CLA	CHC-C1C-C2C	-2.43	120.06	126.95
24	C	508	CLA	CHC-C1C-C2C	-2.43	120.06	126.95
24	b	619	CLA	CMC-C2C-C1C	2.43	128.82	125.03
24	B	608	CLA	CHD-C1D-ND	-2.42	121.39	124.80
36	c	923	HTG	C1-O5-C5	2.42	116.91	112.56
24	B	605	CLA	C6-C5-C3	-2.42	107.56	113.47
24	c	914	CLA	O2A-CGA-CBA	2.42	119.22	111.83
26	d	406	BCR	C15-C14-C13	-2.42	123.88	127.28
24	B	611	CLA	CHA-C1A-NA	-2.42	120.91	126.39
27	b	601	SQD	O47-C7-O49	-2.42	118.05	123.70
29	D	404	PL9	C20-C19-C21	2.42	119.43	115.23
38	D	407	LHG	O8-C23-O10	-2.42	117.58	123.63
28	C	523	LMG	O6-C5-C4	2.42	114.06	109.70
25	A	409	PHO	CMC-C2C-C1C	2.42	129.09	124.73
24	D	402	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
24	C	513	CLA	CHD-C1D-ND	-2.42	121.40	124.80
39	F	102	HEM	CBA-CAA-C2A	-2.42	105.85	112.53
24	c	910	CLA	C16-C17-C18	-2.42	105.16	115.94
24	B	616	CLA	CHD-C1D-ND	-2.41	121.41	124.80
24	C	506	CLA	CHB-C1B-C2B	-2.41	120.42	127.43
24	C	508	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
24	b	615	CLA	CMC-C2C-C1C	2.41	128.80	125.03
24	a	409	CLA	C4-C3-C5	2.41	119.41	115.23
24	D	401	CLA	CHC-C1C-C2C	-2.41	120.09	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	101	BCR	C24-C23-C22	-2.41	122.67	126.23
24	c	907	CLA	C4-C3-C5	2.41	119.41	115.23
26	B	618	BCR	C21-C20-C19	-2.41	116.22	123.20
24	B	610	CLA	CED-O2D-CGD	2.41	121.38	115.92
24	b	619	CLA	C1-C2-C3	-2.41	122.25	126.20
36	D	412	HTG	O5-C5-C4	2.41	114.04	109.70
31	b	625	LMT	O1'-C1'-C2'	-2.41	104.62	108.27
31	B	622	LMT	O2'-C2'-C1'	-2.40	104.34	110.08
24	B	615	CLA	C4B-C3B-C2B	-2.40	104.31	107.30
24	b	607	CLA	CHD-C1D-ND	-2.40	121.42	124.80
24	C	501	CLA	C1-O2A-CGA	2.40	122.47	116.65
24	a	409	CLA	CHD-C1D-ND	-2.40	121.42	124.80
24	c	909	CLA	CHD-C1D-C2D	-2.40	120.49	125.49
24	b	608	CLA	C6-C7-C8	-2.40	107.98	115.97
31	t	102	LMT	O1B-C1B-C2B	2.40	114.00	108.09
26	C	514	BCR	C23-C24-C25	-2.40	120.58	127.00
24	c	907	CLA	CHC-C1C-C2C	-2.40	120.12	126.95
24	B	615	CLA	C4C-C3C-C2C	-2.40	103.40	106.89
24	B	613	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
24	C	513	CLA	C11-C10-C8	-2.40	107.99	115.97
24	c	903	CLA	CMB-C2B-C1B	2.40	129.07	125.42
24	c	904	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
24	B	616	CLA	C4-C3-C5	2.40	119.39	115.23
24	b	618	CLA	CMB-C2B-C1B	2.40	129.07	125.42
24	c	902	CLA	C4-C3-C5	2.39	119.38	115.23
24	B	602	CLA	C4-C3-C5	2.39	119.38	115.23
40	h	101	RRX	C16-C15-C14	-2.39	118.62	123.52
24	B	602	CLA	CHD-C4C-NC	2.39	127.94	124.23
24	b	620	CLA	CHC-C1C-C2C	-2.39	120.15	126.95
25	A	408	PHO	CMB-C2B-C3B	2.39	129.46	124.68
28	a	416	LMG	C1-O6-C5	2.39	118.39	113.72
38	D	406	LHG	O7-C7-O9	-2.39	118.11	123.70
24	C	507	CLA	CHB-C1B-C2B	-2.39	120.49	127.43
28	d	412	LMG	O7-C10-C11	2.39	116.65	111.48
37	C	518	DGD	C2G-O2G-C1B	-2.39	112.08	117.80
24	b	613	CLA	CHB-C1B-C2B	-2.39	120.49	127.43
31	b	625	LMT	O2'-C2'-C1'	2.39	115.77	110.08
24	b	612	CLA	OBD-CAD-C3D	-2.39	122.83	128.42
37	C	516	DGD	O6D-C5D-C6D	2.39	111.43	106.69
37	D	405	DGD	C2G-O2G-C1B	-2.39	112.08	117.80
24	B	612	CLA	C4C-C3C-C2C	-2.39	103.42	106.89
24	B	608	CLA	CHD-C4C-C3C	-2.39	121.29	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	909	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
24	B	606	CLA	C4B-C3B-C2B	-2.38	104.34	107.30
24	c	903	CLA	CMC-C2C-C1C	2.38	128.76	125.03
24	b	611	CLA	CAA-CBA-CGA	2.38	119.97	113.21
24	b	612	CLA	C11-C10-C8	-2.38	108.05	115.97
24	C	512	CLA	C4-C3-C5	2.38	119.36	115.23
24	b	614	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
24	c	912	CLA	CHC-C1C-C2C	-2.38	120.18	126.95
24	C	512	CLA	O2A-CGA-CBA	2.38	119.10	111.83
24	B	610	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
36	b	603	HTG	C1-O5-C5	2.38	116.83	112.56
24	B	607	CLA	CBC-CAC-C3C	-2.38	105.97	112.42
26	T	101	BCR	C23-C24-C25	-2.38	120.64	127.00
24	C	512	CLA	CBA-CAA-C2A	-2.38	106.71	113.79
37	c	918	DGD	O1G-C1A-C2A	2.38	119.09	111.83
24	C	506	CLA	CMC-C2C-C1C	2.38	128.75	125.03
26	k	102	BCR	C23-C24-C25	-2.38	120.65	127.00
24	b	605	CLA	CHA-C1A-NA	-2.37	121.02	126.39
28	D	409	LMG	C9-C8-C7	-2.37	106.25	111.78
24	c	910	CLA	CMB-C2B-C1B	2.37	129.03	125.42
24	C	510	CLA	CHD-C1D-ND	-2.37	121.47	124.80
24	c	912	CLA	CAC-C3C-C4C	2.37	127.87	124.79
24	B	603	CLA	CAA-CBA-CGA	-2.37	106.49	113.21
24	B	603	CLA	C11-C10-C8	-2.37	108.10	115.97
24	B	607	CLA	CHA-C1A-NA	-2.37	121.03	126.39
24	b	611	CLA	CAC-C3C-C4C	2.36	127.87	124.79
24	C	501	CLA	C1-C2-C3	-2.36	122.32	126.20
42	v	202	HEC	C2A-C1A-NA	-2.36	108.04	110.32
28	C	523	LMG	C3-C4-C5	2.36	114.51	110.23
24	A	405	CLA	O2A-CGA-CBA	2.36	119.03	111.83
24	c	902	CLA	C4C-C3C-C2C	-2.36	103.45	106.89
24	c	908	CLA	CHA-C1A-NA	-2.36	121.05	126.39
24	c	904	CLA	C4-C3-C5	2.36	119.33	115.23
24	C	513	CLA	C3B-C4B-NB	2.36	112.64	110.53
29	D	404	PL9	C27-C28-C29	-2.36	122.22	127.62
37	c	918	DGD	O1G-C1A-O1A	-2.36	117.72	123.63
36	c	941	HTG	C3-C4-C5	2.36	114.51	110.23
31	B	622	LMT	O2B-C2B-C1B	-2.36	104.45	110.08
24	b	616	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
24	C	508	CLA	C1-C2-C3	-2.36	122.33	126.20
24	b	620	CLA	CHA-C1A-NA	-2.36	121.05	126.39
37	H	102	DGD	C3G-C2G-C1G	-2.36	106.29	111.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	909	CLA	CHB-C4A-NA	2.36	127.80	124.40
29	A	414	PL9	C12-C13-C14	-2.35	122.23	127.62
24	B	607	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
24	B	607	CLA	CHD-C4C-NC	2.35	127.88	124.23
24	b	609	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
24	b	615	CLA	CHD-C1D-ND	-2.35	121.49	124.80
24	b	620	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
25	A	408	PHO	O1D-CGD-CBD	-2.35	121.16	124.72
24	B	612	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
26	B	619	BCR	C15-C16-C17	-2.35	118.71	123.52
31	a	402	LMT	C3B-C4B-C5B	2.35	114.49	110.23
24	A	410	CLA	CHD-C4C-NC	2.35	127.87	124.23
24	B	605	CLA	CHA-C1A-NA	-2.35	121.08	126.39
29	D	404	PL9	C36-C37-C38	-2.35	100.41	112.02
24	b	616	CLA	CED-O2D-CGD	2.34	121.23	115.92
28	D	409	LMG	O7-C10-C11	2.34	116.55	111.48
26	T	101	BCR	C3-C4-C5	-2.34	109.88	114.06
26	k	103	BCR	C3-C4-C5	-2.34	109.88	114.06
24	C	505	CLA	C1-O2A-CGA	2.34	122.32	116.65
26	Y	101	BCR	C21-C20-C19	-2.34	116.41	123.20
37	d	408	DGD	O1G-C1A-C2A	2.34	118.98	111.83
24	A	406	CLA	CMB-C2B-C1B	2.34	128.99	125.42
24	b	611	CLA	C1-C2-C3	-2.34	122.36	126.20
24	b	606	CLA	CAC-C3C-C4C	2.34	127.84	124.79
24	c	909	CLA	CMB-C2B-C1B	2.34	128.99	125.42
38	D	406	LHG	O8-C6-C5	-2.34	101.65	108.40
36	O	303	HTG	O2-C2-C3	-2.34	104.86	110.38
24	B	611	CLA	C4-C3-C5	2.34	119.29	115.23
24	c	911	CLA	CHC-C1C-C2C	-2.34	120.30	126.95
24	b	618	CLA	CMA-C3A-C4A	-2.34	105.48	111.77
37	C	517	DGD	O2G-C1B-O1B	-2.34	118.24	123.70
24	b	618	CLA	C3B-C4B-NB	2.34	112.62	110.53
24	b	605	CLA	CMB-C2B-C1B	2.34	128.98	125.42
36	d	414	HTG	C1-C2-C3	2.34	115.12	110.55
24	b	618	CLA	CED-O2D-CGD	2.34	121.21	115.92
37	H	102	DGD	O1G-C1A-O1A	-2.34	117.79	123.63
26	T	101	BCR	C11-C10-C9	-2.33	124.00	127.28
25	A	409	PHO	CAC-C3C-C4C	2.33	130.03	124.03
24	c	908	CLA	C1-C2-C3	-2.33	122.37	126.20
24	b	610	CLA	C6-C5-C3	-2.33	107.79	113.47
29	d	407	PL9	O1-C4-C3	-2.33	118.27	120.73
24	d	401	CLA	O2D-CGD-O1D	-2.33	119.31	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	609	CLA	CHA-C1A-NA	-2.33	121.11	126.39
24	C	509	CLA	CHD-C1D-ND	-2.33	121.52	124.80
24	c	902	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
24	B	606	CLA	CMA-C3A-C2A	-2.33	104.98	113.98
24	b	618	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
24	B	603	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
26	k	102	BCR	C34-C9-C8	2.33	121.64	118.09
24	b	610	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
26	B	619	BCR	C2-C1-C6	2.33	113.82	110.44
24	c	902	CLA	C1-O2A-CGA	2.33	122.28	116.65
24	b	620	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
25	A	408	PHO	O2D-CGD-O1D	-2.32	119.32	123.85
26	B	620	BCR	C23-C24-C25	-2.32	120.79	127.00
24	c	906	CLA	CHD-C1D-ND	-2.32	121.53	124.80
27	A	412	SQD	O48-C23-O10	-2.32	117.82	123.63
24	B	606	CLA	CMB-C2B-C1B	2.32	128.96	125.42
24	c	905	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
24	C	507	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	b	610	CLA	C3B-C4B-NB	2.32	112.60	110.53
31	b	625	LMT	O5B-C5B-C4B	2.32	113.88	109.70
24	B	609	CLA	CMA-C3A-C2A	-2.32	105.01	113.98
29	a	417	PL9	C40-C39-C41	2.32	119.25	115.23
26	B	620	BCR	C24-C23-C22	-2.32	122.80	126.23
24	b	606	CLA	C7-C6-C5	-2.32	107.08	113.26
24	B	610	CLA	CHA-C1A-NA	-2.32	121.14	126.39
24	B	604	CLA	CHD-C1D-ND	-2.31	121.55	124.80
24	a	409	CLA	CMA-C3A-C4A	-2.31	105.55	111.77
24	B	614	CLA	CMA-C3A-C2A	-2.31	105.04	113.98
24	C	503	CLA	O2A-CGA-CBA	2.31	118.89	111.83
24	C	511	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
24	c	905	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
24	c	914	CLA	CMC-C2C-C1C	2.31	128.65	125.03
26	b	621	BCR	C11-C10-C9	-2.31	124.04	127.28
24	c	903	CLA	CHD-C1D-ND	-2.31	121.55	124.80
24	C	506	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
24	c	904	CLA	O2A-CGA-CBA	2.31	118.87	111.83
24	d	405	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
24	C	501	CLA	C4-C3-C5	2.30	119.23	115.23
24	c	902	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
39	F	102	HEM	C3B-C2B-C1B	2.30	108.14	106.41
24	c	910	CLA	CHC-C1C-C2C	-2.30	120.40	126.95
24	B	617	CLA	CMA-C3A-C4A	-2.30	105.59	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
24	B	602	CLA	CMC-C2C-C1C	2.30	128.63	125.03
26	D	403	BCR	C38-C26-C27	2.30	118.50	113.60
24	d	401	CLA	O2A-CGA-CBA	2.30	118.85	111.83
24	D	401	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
38	d	409	LHG	C5-O7-C7	-2.30	112.29	117.80
24	D	402	CLA	O2A-CGA-CBA	2.30	118.84	111.83
24	B	607	CLA	C4B-C3B-C2B	-2.30	104.44	107.30
24	B	610	CLA	CMA-C3A-C4A	-2.30	105.60	111.77
26	D	403	BCR	C30-C25-C24	2.30	121.88	115.65
29	a	417	PL9	C45-C44-C46	2.30	119.21	115.23
28	A	413	LMG	O8-C28-C29	2.29	118.83	111.83
24	C	504	CLA	C4C-C3C-C2C	-2.29	103.55	106.89
26	d	406	BCR	C38-C26-C27	2.29	118.48	113.60
28	A	413	LMG	O6-C5-C4	2.29	113.83	109.70
24	c	903	CLA	CHA-C1A-NA	-2.29	121.20	126.39
24	C	507	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
29	D	404	PL9	C25-C24-C26	2.29	119.20	115.23
24	b	615	CLA	OBD-CAD-C3D	-2.29	123.06	128.42
24	B	617	CLA	CAA-CBA-CGA	-2.29	106.71	113.21
26	K	101	BCR	C11-C10-C9	-2.29	124.07	127.28
24	d	404	CLA	CMA-C3A-C4A	-2.29	105.62	111.77
24	B	608	CLA	C4C-C3C-C2C	-2.29	103.56	106.89
29	A	414	PL9	C51-C49-C50	2.29	119.85	114.59
38	l	103	LHG	O8-C23-C24	2.28	118.80	111.83
24	B	608	CLA	CMC-C2C-C1C	2.28	128.60	125.03
24	b	612	CLA	O2D-CGD-CBD	2.28	115.22	111.23
29	a	417	PL9	C35-C34-C36	2.28	119.19	115.23
24	B	613	CLA	CHD-C1D-ND	-2.28	121.59	124.80
28	C	519	LMG	O8-C28-O10	-2.28	117.92	123.63
24	a	409	CLA	CBC-CAC-C3C	-2.28	106.24	112.42
26	B	618	BCR	C15-C14-C13	-2.28	124.08	127.28
24	b	607	CLA	CMB-C2B-C1B	2.28	128.89	125.42
36	b	603	HTG	O5-C1-C2	2.28	113.46	110.32
24	b	615	CLA	CMA-C3A-C4A	-2.28	105.65	111.77
37	c	919	DGD	O3G-C3G-C2G	-2.28	105.28	110.82
24	c	910	CLA	CHA-C1A-NA	-2.28	121.24	126.39
38	l	103	LHG	O4-P-O5	2.28	123.03	112.44
24	b	605	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
24	c	906	CLA	O2A-CGA-CBA	2.27	118.77	111.83
24	b	619	CLA	C11-C10-C8	-2.27	108.41	115.97
24	B	613	CLA	O2A-CGA-CBA	2.27	118.76	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	608	CLA	C4-C3-C5	2.27	119.17	115.23
24	b	616	CLA	CAC-C3C-C4C	2.27	127.75	124.79
24	B	608	CLA	CMB-C2B-C1B	2.27	128.88	125.42
24	a	413	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
32	B	638	GOL	C3-C2-C1	-2.26	103.49	111.80
24	B	614	CLA	C7-C6-C5	-2.26	107.23	113.26
24	D	402	CLA	CMA-C3A-C2A	-2.26	105.23	113.98
24	c	914	CLA	CAC-C3C-C4C	2.26	127.73	124.79
24	b	605	CLA	CHD-C1D-ND	-2.26	121.62	124.80
24	A	405	CLA	O2D-CGD-CBD	2.26	115.19	111.23
25	A	408	PHO	C4-C3-C5	2.26	119.16	115.23
28	C	523	LMG	O6-C1-C2	2.26	115.02	110.37
24	C	510	CLA	CHA-C1A-NA	-2.26	121.27	126.39
24	B	605	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
24	B	607	CLA	C3B-C4B-NB	2.26	112.55	110.53
26	Y	101	BCR	C1-C6-C7	2.26	121.78	115.65
24	C	506	CLA	O2A-CGA-CBA	2.26	118.73	111.83
24	C	508	CLA	CAC-C3C-C4C	2.26	127.73	124.79
26	C	515	BCR	C37-C22-C23	2.26	121.54	118.09
24	B	608	CLA	C3C-C4C-NC	2.26	113.32	110.43
24	B	607	CLA	CHB-C1B-C2B	-2.26	120.87	127.43
24	b	615	CLA	O2A-CGA-CBA	2.26	118.71	111.83
36	V	215	HTG	C1-C2-C3	2.26	114.96	110.55
28	B	621	LMG	O7-C10-O9	-2.26	118.43	123.70
24	b	614	CLA	O2A-CGA-CBA	2.26	118.71	111.83
31	c	922	LMT	C1'-C2'-C3'	-2.26	105.27	110.01
24	B	605	CLA	CHC-C1C-C2C	-2.25	120.55	126.95
24	b	617	CLA	CMC-C2C-C1C	2.25	128.55	125.03
24	D	401	CLA	CMA-C3A-C2A	-2.25	105.28	113.98
24	B	615	CLA	CMA-C3A-C2A	-2.25	105.28	113.98
24	A	407	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
24	A	406	CLA	O2A-CGA-CBA	2.25	118.69	111.83
29	a	417	PL9	C51-C49-C50	2.25	119.77	114.59
24	c	907	CLA	CHA-C1A-NA	-2.25	121.30	126.39
26	B	619	BCR	C3-C4-C5	-2.25	110.05	114.06
24	b	616	CLA	C5-C3-C2	-2.25	116.12	121.17
26	b	623	BCR	C8-C7-C6	-2.25	121.00	127.00
38	d	409	LHG	O7-C7-O9	-2.24	118.46	123.70
24	B	610	CLA	C4-C3-C5	2.24	119.12	115.23
24	b	609	CLA	CHA-C1A-NA	-2.24	121.31	126.39
24	a	413	CLA	CED-O2D-CGD	2.24	121.00	115.92
24	b	620	CLA	C4-C3-C5	2.24	119.12	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	617	CLA	CBC-CAC-C3C	-2.24	106.34	112.42
24	b	614	CLA	CHD-C1D-ND	-2.24	121.65	124.80
37	H	102	DGD	C6D-C5D-C4D	2.24	116.77	112.07
37	c	917	DGD	O6D-C1D-O3G	-2.24	104.75	110.04
24	b	620	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
24	d	404	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
24	c	903	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
24	B	604	CLA	C1-O2A-CGA	2.24	122.07	116.65
24	b	614	CLA	C11-C12-C13	-2.24	108.53	115.97
24	B	609	CLA	OBD-CAD-C3D	-2.24	123.19	128.42
27	b	601	SQD	C44-O6-C1	-2.24	109.00	113.80
24	d	404	CLA	CHD-C1D-ND	-2.23	121.66	124.80
29	A	414	PL9	C2-C1-C6	2.23	121.65	119.00
24	c	905	CLA	C11-C10-C8	-2.23	108.54	115.97
28	C	523	LMG	O7-C10-O9	-2.23	118.48	123.70
24	B	608	CLA	CAA-CBA-CGA	2.23	119.55	113.21
27	a	415	SQD	O48-C23-O10	-2.23	118.04	123.63
24	C	511	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
26	b	623	BCR	C21-C20-C19	-2.23	116.73	123.20
26	c	915	BCR	C21-C20-C19	-2.23	116.73	123.20
24	C	508	CLA	C3B-C4B-NB	2.23	112.52	110.53
24	b	616	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
24	C	513	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
26	B	620	BCR	C28-C27-C26	-2.23	110.08	114.06
24	B	617	CLA	C4-C3-C5	2.23	119.09	115.23
26	d	406	BCR	C16-C15-C14	-2.23	118.97	123.52
24	b	618	CLA	CMC-C2C-C1C	2.23	128.51	125.03
28	b	624	LMG	C30-C29-C28	-2.22	105.54	113.69
29	D	404	PL9	C51-C49-C50	2.22	119.71	114.59
24	b	617	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
24	d	401	CLA	CHB-C4A-NA	2.22	127.61	124.40
24	c	908	CLA	C7-C6-C5	-2.22	107.34	113.26
24	C	504	CLA	O2A-CGA-CBA	2.22	118.61	111.83
24	B	617	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
31	B	622	LMT	O1B-C4'-C5'	-2.22	103.65	109.48
31	B	622	LMT	C3B-C4B-C5B	2.22	114.25	110.23
24	B	604	CLA	CMC-C2C-C1C	2.22	128.50	125.03
24	d	401	CLA	CHA-C1A-NA	-2.22	121.37	126.39
28	b	624	LMG	O8-C28-C29	2.22	118.59	111.83
24	B	604	CLA	C4-C3-C5	2.22	119.08	115.23
24	b	613	CLA	CMA-C3A-C4A	-2.22	105.81	111.77
28	a	416	LMG	C3-C4-C5	2.22	114.25	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	910	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
24	c	913	CLA	C4B-C3B-C2B	-2.21	104.55	107.30
25	A	408	PHO	C4A-C3A-C2A	-2.21	100.73	102.84
28	c	920	LMG	O7-C10-O9	-2.21	118.53	123.70
24	c	912	CLA	CHD-C4C-NC	2.21	127.66	124.23
24	b	619	CLA	C5-C3-C2	-2.21	116.20	121.17
31	c	927	LMT	O1B-C1B-C2B	2.21	113.53	108.09
24	b	613	CLA	CAC-C3C-C4C	2.21	127.67	124.79
24	b	608	CLA	C1-C2-C3	-2.21	122.58	126.20
24	b	615	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
36	v	211	HTG	C1-O5-C5	-2.21	108.60	112.56
24	A	410	CLA	CMB-C2B-C1B	2.21	128.78	125.42
39	f	101	HEM	CHD-C4C-NC	2.21	126.86	124.45
24	C	502	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
38	D	406	LHG	C25-C24-C23	-2.21	105.61	113.69
37	H	102	DGD	C3B-C2B-C1B	-2.20	105.62	113.69
24	d	405	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
27	A	416	SQD	O48-C23-O10	-2.20	118.12	123.63
24	B	606	CLA	CAC-C3C-C4C	2.20	127.66	124.79
24	B	616	CLA	CHD-C4C-NC	2.20	127.65	124.23
24	a	413	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
27	b	601	SQD	O48-C23-O10	-2.20	118.12	123.63
29	d	407	PL9	C53-C6-C1	2.20	119.79	115.28
24	b	619	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
24	A	405	CLA	CHA-C1A-NA	-2.20	121.41	126.39
26	b	621	BCR	C10-C11-C12	-2.20	116.83	123.20
24	A	405	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
24	b	615	CLA	C7-C6-C5	-2.20	107.40	113.26
24	A	407	CLA	CHC-C1C-C2C	-2.20	120.70	126.95
36	D	412	HTG	C1-O5-C5	2.20	116.50	112.56
24	b	609	CLA	C3B-C4B-NB	2.20	112.49	110.53
29	A	414	PL9	C25-C24-C23	-2.20	117.98	123.63
24	C	510	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
24	B	604	CLA	CHC-C1C-C2C	-2.19	120.71	126.95
24	C	513	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
36	B	629	HTG	C3-C4-C5	2.19	114.21	110.23
24	B	611	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
28	C	519	LMG	O7-C10-O9	-2.19	118.58	123.70
24	D	402	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	b	610	CLA	C1-C2-C3	-2.19	122.61	126.20
24	c	904	CLA	CBC-CAC-C3C	-2.19	106.48	112.42
24	b	615	CLA	CHA-C1A-NA	-2.19	121.44	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	CHC-C4B-NB	2.19	127.33	124.05
24	c	904	CLA	CHD-C1D-ND	-2.19	121.72	124.80
26	d	406	BCR	C10-C11-C12	-2.19	116.86	123.20
29	d	407	PL9	C35-C34-C36	2.19	119.02	115.23
25	a	411	PHO	CMA-C3A-C4A	-2.19	109.90	114.61
24	b	607	CLA	CHB-C1B-C2B	-2.19	121.08	127.43
24	B	609	CLA	CHC-C1C-C2C	-2.19	120.74	126.95
26	k	102	BCR	C1-C6-C7	2.19	121.58	115.65
24	C	512	CLA	C4A-NA-C1A	2.19	107.68	106.68
24	b	607	CLA	C1-O2A-CGA	2.19	121.94	116.65
24	b	606	CLA	CHC-C1C-C2C	-2.18	120.74	126.95
37	h	102	DGD	O1G-C1A-O1A	-2.18	118.16	123.63
24	c	902	CLA	O2A-CGA-CBA	2.18	118.48	111.83
24	B	617	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
24	b	608	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
24	c	904	CLA	C7-C6-C5	-2.18	107.45	113.26
31	B	622	LMT	C1B-O5B-C5B	2.18	117.98	113.72
24	C	511	CLA	O2A-CGA-CBA	2.18	118.48	111.83
25	a	412	PHO	O1D-CGD-CBD	-2.18	121.42	124.72
24	B	617	CLA	CHD-C1D-ND	-2.18	121.74	124.80
24	d	405	CLA	O2A-CGA-CBA	2.18	118.47	111.83
24	B	602	CLA	CHA-C1A-NA	-2.18	121.47	126.39
42	v	202	HEC	CMD-C2D-C1D	2.18	128.73	125.42
24	b	613	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
39	f	101	HEM	CBA-CAA-C2A	-2.17	106.52	112.53
24	b	616	CLA	CHD-C1D-C2D	-2.17	120.97	125.49
24	C	509	CLA	CMB-C2B-C1B	2.17	128.73	125.42
24	c	909	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
24	B	611	CLA	C3B-C4B-NB	2.17	112.47	110.53
24	C	502	CLA	CHA-C1A-NA	-2.17	121.48	126.39
24	B	607	CLA	C6-C7-C8	-2.17	108.75	115.97
24	d	405	CLA	C6-C7-C8	-2.17	108.76	115.97
29	D	404	PL9	O2-C1-C6	-2.17	117.03	120.48
26	c	916	BCR	C23-C24-C25	-2.17	121.21	127.00
24	C	506	CLA	CAC-C3C-C4C	2.17	127.61	124.79
24	b	614	CLA	CHA-C1A-NA	-2.17	121.48	126.39
24	c	911	CLA	CMB-C2B-C1B	2.17	128.72	125.42
24	B	608	CLA	C2A-C1A-CHA	-2.17	120.11	123.87
24	b	606	CLA	O2A-CGA-CBA	2.17	118.44	111.83
38	l	103	LHG	O8-C23-O10	-2.17	118.21	123.63
39	f	101	HEM	C3B-C2B-C1B	2.17	108.04	106.41
26	D	403	BCR	C29-C28-C27	-2.16	106.52	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	506	CLA	CHC-C1C-C2C	-2.16	120.80	126.95
24	A	410	CLA	C4-C3-C2	-2.16	118.07	123.63
24	c	904	CLA	C4B-C3B-C2B	-2.16	104.61	107.30
24	a	413	CLA	OBD-CAD-C3D	-2.16	123.36	128.42
36	B	625	HTG	C1-C2-C3	2.16	114.78	110.55
24	B	602	CLA	CHC-C1C-C2C	-2.16	120.81	126.95
24	A	407	CLA	CHC-C4B-NB	2.16	127.29	124.05
26	b	623	BCR	C16-C15-C14	-2.16	119.10	123.52
24	c	905	CLA	CMB-C2B-C1B	2.16	128.71	125.42
24	b	616	CLA	CHC-C1C-C2C	-2.16	120.81	126.95
24	A	407	CLA	CMA-C3A-C2A	-2.16	105.64	113.98
24	C	501	CLA	CHC-C1C-C2C	-2.16	120.81	126.95
24	c	907	CLA	CHB-C1B-C2B	-2.16	121.16	127.43
29	A	414	PL9	O1-C4-C3	-2.16	118.46	120.73
31	M	102	LMT	C1-O1'-C1'	-2.16	110.00	113.68
24	C	512	CLA	C4B-C3B-C2B	-2.16	104.62	107.30
24	b	617	CLA	CHA-C1A-NA	-2.16	121.51	126.39
26	B	620	BCR	C7-C8-C9	-2.16	123.05	126.23
24	b	610	CLA	CHD-C1D-ND	-2.16	121.77	124.80
24	c	906	CLA	CHC-C1C-C2C	-2.16	120.82	126.95
28	d	412	LMG	O8-C28-C29	2.16	118.41	111.83
24	C	507	CLA	C1-O2A-CGA	2.16	121.87	116.65
28	a	416	LMG	C8-O7-C10	-2.15	112.64	117.80
24	B	603	CLA	CHA-C1A-NA	-2.15	121.52	126.39
26	b	623	BCR	C28-C27-C26	-2.15	110.22	114.06
24	B	610	CLA	O2D-CGD-CBD	2.15	114.99	111.23
24	C	508	CLA	CHD-C1D-ND	-2.15	121.78	124.80
39	F	102	HEM	C1B-NB-C4B	2.15	107.75	105.21
24	B	606	CLA	OBD-CAD-C3D	-2.15	123.40	128.42
24	a	413	CLA	CMB-C2B-C1B	2.15	128.69	125.42
37	c	918	DGD	O2G-C1B-O1B	-2.15	118.69	123.70
24	c	906	CLA	CMA-C3A-C4A	-2.15	106.00	111.77
24	b	605	CLA	CMC-C2C-C1C	2.14	128.38	125.03
24	b	617	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
38	D	408	LHG	O4-P-O5	2.14	122.42	112.44
24	c	905	CLA	OBD-CAD-C3D	-2.14	123.41	128.42
24	b	606	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
36	b	626	HTG	C1-O5-C5	2.14	116.40	112.56
24	C	510	CLA	OBD-CAD-C3D	-2.14	123.41	128.42
24	B	610	CLA	CHD-C1D-C2D	-2.14	121.04	125.49
27	l	101	SQD	O47-C7-O49	-2.14	118.70	123.70
24	C	512	CLA	CHC-C1C-C2C	-2.14	120.87	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	905	CLA	C1-O2A-CGA	2.14	121.83	116.65
24	B	614	CLA	CHA-C1A-NA	-2.14	121.55	126.39
26	B	636	BCR	C3-C4-C5	-2.14	110.25	114.06
24	C	502	CLA	C4B-C3B-C2B	-2.14	104.64	107.30
24	b	616	CLA	CHD-C1D-ND	-2.14	121.80	124.80
27	b	601	SQD	O6-C44-C45	2.14	116.01	110.82
24	B	611	CLA	C1C-C2C-C3C	-2.14	104.73	106.98
24	B	606	CLA	CMA-C3A-C4A	-2.14	106.03	111.77
24	B	603	CLA	CMB-C2B-C1B	2.13	128.67	125.42
24	A	406	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
24	C	505	CLA	CHC-C1C-C2C	-2.13	120.89	126.95
24	B	605	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
24	C	512	CLA	CMC-C2C-C1C	2.13	128.36	125.03
37	d	408	DGD	O2G-C1B-O1B	-2.13	118.72	123.70
36	d	420	HTG	C1-O5-C5	2.13	116.38	112.56
36	V	204	HTG	O2-C2-C1	2.13	114.08	110.30
24	b	609	CLA	C7-C6-C5	-2.13	107.59	113.26
24	c	909	CLA	CMC-C2C-C1C	2.13	128.36	125.03
24	C	505	CLA	C1-C2-C3	-2.13	122.71	126.20
37	H	102	DGD	O4D-C4D-C3D	-2.13	105.36	110.38
24	B	610	CLA	C1-O2A-CGA	2.13	121.80	116.65
24	B	615	CLA	CHD-C1D-ND	-2.13	121.81	124.80
24	b	615	CLA	CHD-C4C-NC	2.13	127.53	124.23
24	c	909	CLA	C6-C7-C8	-2.13	108.90	115.97
28	a	416	LMG	O8-C28-C29	2.12	118.31	111.83
26	B	619	BCR	C38-C26-C25	-2.12	122.17	124.48
24	B	612	CLA	C1-O2A-CGA	2.12	121.79	116.65
28	a	416	LMG	O7-C10-O9	-2.12	118.75	123.70
24	c	914	CLA	C4B-C3B-C2B	-2.12	104.66	107.30
27	A	412	SQD	C44-O6-C1	-2.12	109.25	113.80
24	a	410	CLA	CHA-C1A-NA	-2.12	121.59	126.39
36	c	941	HTG	C1-C2-C3	-2.12	106.41	110.55
24	C	504	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
24	b	614	CLA	CAA-CBA-CGA	-2.12	107.20	113.21
26	a	414	BCR	C24-C23-C22	-2.12	123.10	126.23
24	b	609	CLA	O2A-CGA-CBA	2.12	118.29	111.83
29	a	417	PL9	C25-C24-C26	2.12	118.90	115.23
31	c	927	LMT	O5B-C1B-C2B	-2.12	106.02	110.37
24	C	511	CLA	CMB-C2B-C1B	2.12	128.64	125.42
37	d	408	DGD	C4D-C3D-C2D	2.12	114.54	110.83
24	c	902	CLA	CHC-C1C-C2C	-2.11	120.94	126.95
31	m	103	LMT	C1B-O1B-C4'	-2.11	112.97	117.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	409	CLA	CMC-C2C-C1C	2.11	128.34	125.03
24	C	501	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
38	d	411	LHG	O7-C7-O9	-2.11	118.76	123.70
24	c	913	CLA	O2D-CGD-O1D	-2.11	119.73	123.85
24	c	905	CLA	O2A-CGA-CBA	2.11	118.27	111.83
24	B	611	CLA	CHD-C1D-C2D	-2.11	121.10	125.49
26	b	622	BCR	C29-C28-C27	-2.11	106.64	111.28
26	C	514	BCR	C20-C21-C22	-2.11	124.32	127.28
26	b	623	BCR	C11-C10-C9	-2.11	124.32	127.28
24	B	615	CLA	CMB-C2B-C1B	2.11	128.63	125.42
24	B	612	CLA	C4-C3-C5	2.11	118.89	115.23
24	b	607	CLA	CHC-C1C-C2C	-2.11	120.96	126.95
24	B	614	CLA	CHD-C4C-NC	2.10	127.50	124.23
24	c	911	CLA	CHA-C1A-NA	-2.10	121.62	126.39
24	B	612	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
24	D	401	CLA	C2A-C1A-CHA	-2.10	120.22	123.87
26	b	621	BCR	C28-C27-C26	-2.10	110.30	114.06
24	C	509	CLA	CHC-C1C-C2C	-2.10	120.97	126.95
26	B	620	BCR	C10-C11-C12	-2.10	117.11	123.20
37	C	517	DGD	O6E-C5E-C6E	2.10	111.65	106.44
24	b	610	CLA	C5-C3-C2	-2.10	116.45	121.17
24	B	611	CLA	CHB-C4A-NA	2.10	127.43	124.40
24	d	401	CLA	CHC-C1C-NC	2.10	127.48	124.31
28	A	413	LMG	C8-O7-C10	-2.10	112.77	117.80
24	B	613	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
24	B	605	CLA	CMC-C2C-C1C	2.10	128.32	125.03
24	c	912	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
24	B	617	CLA	CHA-C1A-NA	-2.10	121.64	126.39
24	c	908	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
24	b	608	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
25	a	411	PHO	O1D-CGD-CBD	-2.10	121.54	124.72
24	B	606	CLA	CHD-C4C-NC	2.10	127.48	124.23
28	C	519	LMG	C12-C11-C10	-2.10	106.01	113.69
24	B	612	CLA	C7-C6-C5	-2.10	107.68	113.26
37	d	408	DGD	C3G-C2G-C1G	-2.10	106.90	111.78
36	c	942	HTG	O5-C5-C4	2.10	113.47	109.70
28	c	921	LMG	O7-C10-O9	-2.09	118.81	123.70
25	a	411	PHO	OBD-CAD-C3D	-2.09	124.63	127.89
27	A	412	SQD	O9-S-O7	-2.09	107.02	113.82
24	c	906	CLA	C6-C7-C8	-2.09	109.01	115.97
28	D	409	LMG	O8-C28-O10	-2.09	118.40	123.63
27	F	101	SQD	O9-S-C6	2.09	109.87	106.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	615	CLA	C11-C12-C13	-2.09	109.03	115.97
24	C	507	CLA	CHC-C4B-NB	2.09	127.18	124.05
26	d	406	BCR	C21-C20-C19	-2.09	117.16	123.20
24	C	502	CLA	C3B-C4B-NB	2.08	112.39	110.53
31	b	625	LMT	C1'-C2'-C3'	2.08	114.39	110.01
24	A	406	CLA	CAA-C2A-C1A	-2.08	105.15	111.97
31	B	622	LMT	C3'-C4'-C5'	2.08	115.54	110.93
24	b	609	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
24	A	405	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
24	C	512	CLA	OBD-CAD-C3D	-2.08	123.56	128.42
24	C	510	CLA	C6-C7-C8	-2.08	109.06	115.97
32	O	304	GOL	C3-C2-C1	-2.08	104.18	111.80
24	D	402	CLA	CHC-C1C-C2C	-2.08	121.05	126.95
24	A	405	CLA	CHB-C1B-C2B	-2.08	121.40	127.43
26	B	618	BCR	C10-C11-C12	-2.08	117.19	123.20
24	b	613	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
24	b	609	CLA	CAA-C2A-C3A	-2.07	107.39	113.00
24	C	503	CLA	CHB-C1B-C2B	-2.07	121.40	127.43
31	a	402	LMT	O5'-C5'-C4'	2.07	114.01	109.72
28	A	413	LMG	O7-C10-O9	-2.07	118.86	123.70
24	c	913	CLA	CAC-C3C-C2C	2.07	131.36	127.56
24	B	613	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
26	Y	101	BCR	C37-C22-C23	2.07	121.25	118.09
24	c	914	CLA	CHA-C1A-NA	-2.07	121.70	126.39
24	b	617	CLA	C1-C2-C3	-2.07	122.81	126.20
24	c	903	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
31	B	622	LMT	O1B-C1B-O5B	-2.07	105.26	110.69
24	c	909	CLA	O2A-CGA-CBA	2.07	118.14	111.83
24	C	510	CLA	CMB-C2B-C1B	2.07	128.56	125.42
24	C	505	CLA	O2A-CGA-CBA	2.07	118.13	111.83
24	C	509	CLA	CMC-C2C-C1C	2.07	128.26	125.03
24	B	602	CLA	C3B-C4B-NB	2.07	112.37	110.53
24	C	509	CLA	CAC-C3C-C4C	2.07	127.48	124.79
24	b	605	CLA	CHD-C4C-NC	2.06	127.43	124.23
24	A	407	CLA	CHC-C4B-C3B	-2.06	118.43	127.37
24	B	605	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
24	b	614	CLA	CMB-C2B-C1B	2.06	128.55	125.42
24	c	906	CLA	C1-C2-C3	-2.06	122.83	126.20
25	A	409	PHO	C4-C3-C2	-2.06	118.34	123.63
26	B	620	BCR	C3-C4-C5	-2.06	110.39	114.06
26	A	411	BCR	C10-C11-C12	-2.06	117.24	123.20
29	d	407	PL9	C51-C49-C50	2.06	119.32	114.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	404	CLA	CMC-C2C-C1C	2.06	128.25	125.03
24	C	502	CLA	OBD-CAD-C3D	-2.06	123.61	128.42
24	c	911	CLA	C6-C7-C8	-2.06	109.13	115.97
24	C	504	CLA	CAA-CBA-CGA	2.06	119.04	113.21
24	c	914	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
24	b	610	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
27	A	412	SQD	O8-S-C6	2.05	109.93	105.97
37	c	919	DGD	O1G-C1A-O1A	-2.05	118.50	123.63
26	C	514	BCR	C8-C7-C6	-2.05	121.52	127.00
24	A	407	CLA	CHD-C4C-NC	2.05	127.41	124.23
24	B	614	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
24	c	913	CLA	CHB-C4A-NA	2.05	127.36	124.40
37	D	405	DGD	C3G-C2G-C1G	-2.05	107.01	111.78
24	B	606	CLA	O2A-CGA-CBA	2.05	118.08	111.83
24	B	607	CLA	CMB-C2B-C1B	2.05	128.54	125.42
24	b	611	CLA	O2D-CGD-O1D	-2.05	119.87	123.85
24	B	609	CLA	CHB-C1B-C2B	-2.05	121.49	127.43
26	d	406	BCR	C40-C30-C25	-2.05	107.03	110.24
24	a	413	CLA	CAC-C3C-C4C	2.05	127.45	124.79
24	c	905	CLA	C11-C12-C13	-2.05	109.17	115.97
24	C	511	CLA	C4A-NA-C1A	2.05	107.61	106.68
24	c	902	CLA	CHD-C4C-NC	2.04	127.40	124.23
24	d	405	CLA	CMA-C3A-C2A	-2.04	106.08	113.98
25	a	412	PHO	CAC-C3C-C4C	2.04	129.28	124.03
24	c	909	CLA	CAC-C3C-C2C	2.04	131.31	127.56
24	C	507	CLA	CMC-C2C-C1C	2.04	128.22	125.03
32	A	419	GOL	C3-C2-C1	-2.04	104.31	111.80
31	M	101	LMT	C1'-O5'-C5'	-2.04	109.73	113.72
24	c	913	CLA	C1-C2-C3	-2.04	122.85	126.20
24	C	510	CLA	CAA-CBA-CGA	-2.04	107.41	113.21
24	C	510	CLA	C4-C3-C2	-2.04	118.39	123.63
26	b	623	BCR	C33-C5-C6	-2.04	122.26	124.48
31	B	622	LMT	O1'-C1'-C2'	2.04	111.37	108.27
37	C	517	DGD	C9B-C8B-C7B	-2.04	104.06	114.37
24	B	606	CLA	C7-C6-C5	-2.04	107.83	113.26
24	d	404	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
24	c	906	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
24	B	608	CLA	C1-C2-C3	-2.04	122.86	126.20
38	L	101	LHG	O4-P-O5	2.04	121.92	112.44
40	h	101	RRX	C33-C5-C6	-2.04	122.26	124.48
24	C	503	CLA	C4-C3-C5	2.03	118.76	115.23
26	b	621	BCR	C16-C17-C18	-2.03	124.43	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	CHA-C1A-NA	-2.03	121.79	126.39
24	B	608	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
24	B	617	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
24	B	602	CLA	CAC-C3C-C4C	2.03	127.43	124.79
24	c	908	CLA	CAC-C3C-C4C	2.03	127.43	124.79
24	C	502	CLA	CBB-CAB-C3B	-2.03	117.40	127.53
24	c	905	CLA	C2A-C1A-CHA	-2.03	120.35	123.87
26	Y	101	BCR	C16-C15-C14	-2.03	119.38	123.52
24	c	902	CLA	CHA-C1A-NA	-2.03	121.81	126.39
24	C	509	CLA	C4-C3-C5	2.03	118.74	115.23
29	d	407	PL9	C50-C49-C48	-2.02	116.58	122.66
24	C	507	CLA	CHC-C1C-C2C	-2.02	121.20	126.95
29	a	417	PL9	C2-C1-C6	2.02	121.40	119.00
24	c	908	CLA	CHD-C4C-NC	2.02	127.37	124.23
24	B	606	CLA	CHD-C1D-ND	-2.02	121.96	124.80
24	A	405	CLA	CHC-C1C-C2C	-2.02	121.20	126.95
24	C	508	CLA	CHA-C1A-NA	-2.02	121.81	126.39
24	c	904	CLA	C3B-C4B-NB	2.02	112.33	110.53
24	c	903	CLA	CHD-C4C-NC	2.02	127.37	124.23
42	V	203	HEC	CHA-C1A-NA	2.02	126.65	124.45
24	C	512	CLA	C3B-C4B-NB	2.02	112.33	110.53
24	d	405	CLA	CMA-C3A-C4A	-2.02	106.34	111.77
24	b	612	CLA	CHD-C1D-C2D	-2.02	121.29	125.49
24	d	404	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
24	D	401	CLA	OBD-CAD-C3D	-2.02	123.70	128.42
24	A	410	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
26	a	414	BCR	C8-C7-C6	-2.02	121.61	127.00
24	C	504	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
39	f	101	HEM	C1B-NB-C4B	2.01	107.59	105.21
24	B	609	CLA	CBC-CAC-C3C	-2.01	106.96	112.42
29	D	404	PL9	C10-C9-C11	2.01	118.72	115.23
24	b	614	CLA	CMA-C3A-C2A	-2.01	106.20	113.98
25	a	411	PHO	C7-C6-C5	-2.01	107.90	113.26
36	c	942	HTG	C3-C4-C5	2.01	113.88	110.23
24	B	616	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
26	K	101	BCR	C20-C21-C22	-2.01	124.46	127.28
37	c	917	DGD	O6D-C5D-C6D	2.01	110.68	106.69
24	c	913	CLA	CMA-C3A-C4A	-2.01	106.37	111.77
24	c	910	CLA	CHD-C4C-NC	2.01	127.34	124.23
24	B	611	CLA	CHC-C1C-C2C	-2.01	121.25	126.95
24	a	413	CLA	CHB-C4A-NA	2.01	127.30	124.40
36	c	923	HTG	O5-C5-C4	2.01	113.31	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	405	CLA	CHD-C4C-NC	2.01	127.34	124.23
36	b	627	HTG	C1-C2-C3	2.01	114.47	110.55
24	B	607	CLA	C10-C8-C7	-2.00	101.92	112.07
24	b	618	CLA	OBD-CAD-C3D	-2.00	123.73	128.42
31	b	625	LMT	O5'-C5'-C4'	2.00	113.87	109.72
24	B	611	CLA	CMC-C2C-C1C	2.00	128.16	125.03
24	B	612	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
24	c	911	CLA	O2A-CGA-CBA	2.00	117.94	111.83
25	a	411	PHO	O2A-CGA-CBA	2.00	117.94	111.83
37	c	917	DGD	O1G-C1A-O1A	-2.00	118.62	123.63
26	c	915	BCR	C37-C22-C23	2.00	121.15	118.09
29	D	404	PL9	C15-C14-C16	2.00	118.70	115.23
24	A	410	CLA	C2A-C1A-CHA	-2.00	120.39	123.87
36	b	627	HTG	C3-C4-C5	-2.00	106.60	110.23

All (61) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	608	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	B	617	CLA	ND
24	C	501	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	D	401	CLA	ND
24	D	402	CLA	ND
24	a	409	CLA	ND
24	a	413	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	609	CLA	ND
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	b	618	CLA	ND
24	b	619	CLA	ND
24	b	620	CLA	ND
24	c	902	CLA	ND
24	c	903	CLA	ND
24	c	904	CLA	ND
24	c	905	CLA	ND
24	c	906	CLA	ND
24	c	907	CLA	ND
24	c	908	CLA	ND
24	c	909	CLA	ND
24	c	910	CLA	ND
24	c	911	CLA	ND
24	c	913	CLA	ND
24	c	914	CLA	ND
24	d	401	CLA	ND
24	d	404	CLA	ND
24	d	405	CLA	ND

All (967) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	513	CLA	C1A-C2A-CAA-CBA
24	C	513	CLA	C3A-C2A-CAA-CBA
24	b	618	CLA	CAD-CBD-CGD-O1D
24	b	618	CLA	CAD-CBD-CGD-O2D
24	c	908	CLA	CHA-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O2D
24	d	405	CLA	C2-C3-C5-C6
24	d	405	CLA	C4-C3-C5-C6
26	D	403	BCR	C21-C22-C23-C24
26	D	403	BCR	C37-C22-C23-C24
26	Y	101	BCR	C21-C22-C23-C24
26	d	406	BCR	C37-C22-C23-C24
27	A	416	SQD	O6-C44-C45-O47
27	A	416	SQD	C5-C6-S-O8
27	a	401	SQD	O6-C44-C45-O47
27	a	401	SQD	O5-C5-C6-S
27	b	601	SQD	O5-C1-O6-C44
27	b	601	SQD	O49-C7-O47-C45
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O9
27	l	101	SQD	O5-C1-O6-C44
27	l	101	SQD	O49-C7-O47-C45
28	a	416	LMG	O9-C10-O7-C8
28	a	416	LMG	C11-C10-O7-C8
29	A	414	PL9	C14-C16-C17-C18
31	B	626	LMT	C2'-C1'-O1'-C1
31	B	626	LMT	O5'-C1'-O1'-C1
31	a	402	LMT	O5'-C1'-O1'-C1
31	b	625	LMT	C3'-C4'-O1B-C1B
31	b	625	LMT	C2'-C1'-O1'-C1
31	b	625	LMT	O5'-C1'-O1'-C1
31	j	102	LMT	C2'-C1'-O1'-C1
31	t	102	LMT	C2'-C1'-O1'-C1
32	A	419	GOL	O1-C1-C2-C3
32	B	637	GOL	C1-C2-C3-O3
32	V	206	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	419	GOL	O1-C1-C2-C3
32	c	929	GOL	O1-C1-C2-C3
36	B	625	HTG	O5-C1-S1-C1'
36	V	204	HTG	O5-C1-S1-C1'
36	V	215	HTG	O5-C1-S1-C1'
36	b	627	HTG	O5-C1-S1-C1'
36	c	942	HTG	O5-C1-S1-C1'
37	D	405	DGD	C2B-C1B-O2G-C2G
37	D	405	DGD	O1B-C1B-O2G-C2G
37	d	408	DGD	C2B-C1B-O2G-C2G
38	E	101	LHG	C4-O6-P-O3
38	E	101	LHG	O7-C5-C6-O8
38	L	101	LHG	C4-O6-P-O3
38	L	101	LHG	C4-O6-P-O4
38	L	101	LHG	C4-O6-P-O5
38	d	409	LHG	O1-C1-C2-C3
38	l	103	LHG	C4-O6-P-O3
38	l	103	LHG	C4-O6-P-O4
38	l	103	LHG	C4-O6-P-O5
42	V	203	HEC	C2B-C3B-CAB-CBB
42	V	203	HEC	C4B-C3B-CAB-CBB
42	V	203	HEC	C2C-C3C-CAC-CBC
42	V	203	HEC	C4C-C3C-CAC-CBC
42	v	202	HEC	C2B-C3B-CAB-CBB
42	v	202	HEC	C4B-C3B-CAB-CBB
42	v	202	HEC	C2C-C3C-CAC-CBC
42	v	202	HEC	C4C-C3C-CAC-CBC
31	t	102	LMT	O5B-C1B-O1B-C4'
31	B	622	LMT	C3'-C4'-O1B-C1B
31	t	102	LMT	C2B-C1B-O1B-C4'
37	d	408	DGD	O1A-C1A-O1G-C1G
37	d	408	DGD	O1B-C1B-O2G-C2G
27	b	601	SQD	C8-C7-O47-C45
27	l	101	SQD	C8-C7-O47-C45
24	B	606	CLA	C4-C3-C5-C6
29	A	414	PL9	C25-C24-C26-C27
29	a	417	PL9	C30-C29-C31-C32
24	B	606	CLA	C2-C3-C5-C6
29	a	417	PL9	C28-C29-C31-C32
37	d	408	DGD	C2A-C1A-O1G-C1G
26	B	636	BCR	C13-C14-C15-C16
26	T	101	BCR	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	927	LMT	O5B-C5B-C6B-O6B
24	D	402	CLA	C3-C5-C6-C7
31	m	103	LMT	C1-C2-C3-C4
37	D	405	DGD	O6D-C5D-C6D-O5D
31	t	102	LMT	O5'-C5'-C6'-O6'
37	D	405	DGD	C4D-C5D-C6D-O5D
29	a	417	PL9	C20-C19-C21-C22
29	a	417	PL9	C18-C19-C21-C22
29	D	404	PL9	C39-C41-C42-C43
36	d	420	HTG	O5-C5-C6-O6
28	A	413	LMG	O6-C1-O1-C7
31	A	417	LMT	O5'-C1'-O1'-C1
31	A	421	LMT	O5'-C1'-O1'-C1
31	F	103	LMT	O5'-C1'-O1'-C1
31	J	102	LMT	O5'-C1'-O1'-C1
31	M	102	LMT	O5'-C1'-O1'-C1
31	c	922	LMT	O5'-C1'-O1'-C1
31	c	927	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
31	j	102	LMT	O5'-C1'-O1'-C1
31	t	102	LMT	O5'-C1'-O1'-C1
37	d	408	DGD	O6D-C1D-O3G-C3G
31	M	101	LMT	O5B-C5B-C6B-O6B
36	B	625	HTG	O5-C5-C6-O6
36	V	204	HTG	O5-C5-C6-O6
36	b	627	HTG	O5-C5-C6-O6
24	B	604	CLA	C5-C6-C7-C8
31	c	927	LMT	C4B-C5B-C6B-O6B
24	c	904	CLA	C10-C11-C12-C13
24	b	618	CLA	C4-C3-C5-C6
24	b	618	CLA	C2-C3-C5-C6
29	A	414	PL9	C23-C24-C26-C27
24	A	410	CLA	C11-C12-C13-C14
24	B	617	CLA	C14-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C9
24	c	910	CLA	C6-C7-C8-C9
36	B	625	HTG	C4-C5-C6-O6
36	b	627	HTG	C4-C5-C6-O6
28	A	413	LMG	C2-C1-O1-C7
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	421	LMT	C2'-C1'-O1'-C1
31	F	103	LMT	C2'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	J	102	LMT	C2'-C1'-O1'-C1
31	M	102	LMT	C2'-C1'-O1'-C1
31	c	922	LMT	C2'-C1'-O1'-C1
31	c	927	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
37	d	408	DGD	C2D-C1D-O3G-C3G
26	D	403	BCR	C7-C8-C9-C34
26	Y	101	BCR	C37-C22-C23-C24
26	d	406	BCR	C21-C22-C23-C24
27	F	101	SQD	C7-C8-C9-C10
27	l	101	SQD	C23-C24-C25-C26
37	c	918	DGD	C1A-C2A-C3A-C4A
24	A	410	CLA	C13-C15-C16-C17
32	O	304	GOL	O2-C2-C3-O3
38	d	409	LHG	O1-C1-C2-O2
27	l	101	SQD	C7-C8-C9-C10
37	C	518	DGD	C1A-C2A-C3A-C4A
24	c	907	CLA	C13-C15-C16-C17
36	d	414	HTG	O5-C5-C6-O6
24	C	504	CLA	C10-C11-C12-C13
27	f	102	SQD	C23-C24-C25-C26
37	d	408	DGD	C1B-C2B-C3B-C4B
24	B	617	CLA	C5-C6-C7-C8
24	C	507	CLA	C15-C16-C17-C18
24	b	618	CLA	C5-C6-C7-C8
24	b	619	CLA	C5-C6-C7-C8
24	c	907	CLA	C15-C16-C17-C18
31	t	102	LMT	C4'-C5'-C6'-O6'
24	B	607	CLA	C2A-CAA-CBA-CGA
28	a	416	LMG	C10-C11-C12-C13
37	d	408	DGD	C1A-C2A-C3A-C4A
31	Z	101	LMT	O5'-C1'-O1'-C1
24	B	616	CLA	C5-C6-C7-C8
24	C	508	CLA	C5-C6-C7-C8
24	c	908	CLA	C5-C6-C7-C8
36	V	204	HTG	C4-C5-C6-O6
24	D	402	CLA	C8-C10-C11-C12
31	c	927	LMT	O5B-C1B-O1B-C4'
24	c	910	CLA	C8-C10-C11-C12
24	B	617	CLA	C10-C11-C12-C13
24	c	904	CLA	C5-C6-C7-C8
29	A	414	PL9	C20-C19-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	C2C-C3C-CAC-CBC
31	Z	101	LMT	C2'-C1'-O1'-C1
24	B	602	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C2A-CAA-CBA-CGA
32	B	637	GOL	O1-C1-C2-C3
32	B	638	GOL	O1-C1-C2-C3
32	B	638	GOL	C1-C2-C3-O3
32	O	304	GOL	C1-C2-C3-O3
32	V	206	GOL	O1-C1-C2-C3
38	D	406	LHG	O1-C1-C2-C3
38	d	411	LHG	O1-C1-C2-C3
31	B	626	LMT	O1'-C1-C2-C3
31	j	102	LMT	O1'-C1-C2-C3
24	C	510	CLA	C8-C10-C11-C12
24	C	508	CLA	C13-C15-C16-C17
27	f	102	SQD	C7-C8-C9-C10
24	D	402	CLA	C16-C17-C18-C19
31	M	102	LMT	O1'-C1-C2-C3
28	C	519	LMG	C30-C31-C32-C33
31	Z	101	LMT	C4-C5-C6-C7
38	l	103	LHG	C14-C15-C16-C17
28	C	519	LMG	C37-C38-C39-C40
31	Z	101	LMT	C3-C4-C5-C6
37	c	918	DGD	CAA-CBA-CCA-CDA
37	c	919	DGD	CBA-CCA-CDA-CEA
38	L	101	LHG	C14-C15-C16-C17
28	B	621	LMG	C33-C34-C35-C36
28	D	409	LMG	C20-C21-C22-C23
37	c	917	DGD	C9A-CAA-CBA-CCA
38	D	406	LHG	C29-C30-C31-C32
38	L	101	LHG	C27-C28-C29-C30
31	c	927	LMT	C2-C1-O1'-C1'
31	m	102	LMT	C2-C1-O1'-C1'
31	t	101	LMT	C2-C1-O1'-C1'
32	A	419	GOL	O1-C1-C2-O2
32	B	637	GOL	O1-C1-C2-O2
32	B	638	GOL	O1-C1-C2-O2
32	a	419	GOL	O1-C1-C2-O2
32	c	929	GOL	O1-C1-C2-O2
28	B	621	LMG	C17-C18-C19-C20
28	b	624	LMG	C17-C18-C19-C20
37	D	405	DGD	C8B-C9B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	H	102	DGD	C9A-CAA-CBA-CCA
37	h	102	DGD	C6A-C7A-C8A-C9A
24	C	513	CLA	C4B-C3B-CAB-CBB
24	c	913	CLA	C4B-C3B-CAB-CBB
36	c	941	HTG	C1'-C2'-C3'-C4'
37	C	517	DGD	C9A-CAA-CBA-CCA
37	H	102	DGD	C6A-C7A-C8A-C9A
28	b	624	LMG	C33-C34-C35-C36
24	C	504	CLA	C11-C12-C13-C15
24	C	506	CLA	C6-C7-C8-C10
37	H	102	DGD	CCA-CDA-CEA-CFA
24	B	602	CLA	CBA-CGA-O2A-C1
24	B	607	CLA	C13-C15-C16-C17
24	b	620	CLA	C10-C11-C12-C13
31	A	421	LMT	O5B-C5B-C6B-O6B
28	d	412	LMG	C15-C16-C17-C18
38	l	103	LHG	C27-C28-C29-C30
24	a	413	CLA	C3-C5-C6-C7
24	B	610	CLA	C3A-C2A-CAA-CBA
29	a	417	PL9	C25-C24-C26-C27
28	C	519	LMG	C17-C18-C19-C20
28	d	412	LMG	C20-C21-C22-C23
36	b	626	HTG	C3'-C4'-C5'-C6'
38	d	411	LHG	C29-C30-C31-C32
31	c	927	LMT	C1-C2-C3-C4
27	A	412	SQD	C9-C10-C11-C12
31	c	927	LMT	O1'-C1-C2-C3
31	c	927	LMT	C2B-C1B-O1B-C4'
28	A	413	LMG	C13-C14-C15-C16
29	a	417	PL9	C9-C11-C12-C13
38	d	409	LHG	C29-C30-C31-C32
27	a	401	SQD	C33-C34-C35-C36
28	A	413	LMG	C37-C38-C39-C40
28	B	621	LMG	C15-C16-C17-C18
36	B	624	HTG	C3'-C4'-C5'-C6'
37	D	405	DGD	C6B-C7B-C8B-C9B
37	c	918	DGD	CCB-CDB-CEB-CFB
28	A	413	LMG	C38-C39-C40-C41
31	t	102	LMT	C5-C6-C7-C8
37	C	516	DGD	C3B-C4B-C5B-C6B
38	d	411	LHG	C30-C31-C32-C33
31	B	622	LMT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	625	LMT	C1-C2-C3-C4
37	D	405	DGD	C7B-C8B-C9B-CAB
38	d	410	LHG	C30-C31-C32-C33
24	b	613	CLA	C2B-C3B-CAB-CBB
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C26
26	d	406	BCR	C23-C24-C25-C30
26	k	102	BCR	C1-C6-C7-C8
26	k	102	BCR	C5-C6-C7-C8
27	a	415	SQD	C34-C35-C36-C37
38	E	101	LHG	C8-C7-O7-C5
27	A	416	SQD	C16-C17-C18-C19
28	b	624	LMG	C15-C16-C17-C18
37	D	405	DGD	C3B-C4B-C5B-C6B
27	A	416	SQD	C14-C15-C16-C17
27	f	102	SQD	C28-C29-C30-C31
38	d	409	LHG	C30-C31-C32-C33
29	A	414	PL9	C18-C19-C21-C22
28	c	920	LMG	C36-C37-C38-C39
37	h	102	DGD	C7A-C8A-C9A-CAA
36	D	412	HTG	C1'-C2'-C3'-C4'
24	C	504	CLA	C11-C10-C8-C9
27	l	101	SQD	C28-C29-C30-C31
37	C	517	DGD	CAB-CBB-CCB-CDB
38	L	101	LHG	C13-C14-C15-C16
24	c	909	CLA	C13-C15-C16-C17
38	D	406	LHG	C28-C29-C30-C31
28	B	621	LMG	C29-C30-C31-C32
37	c	918	DGD	C3A-C4A-C5A-C6A
38	l	103	LHG	C13-C14-C15-C16
38	d	409	LHG	C27-C28-C29-C30
27	F	101	SQD	C9-C10-C11-C12
37	C	518	DGD	C3A-C4A-C5A-C6A
38	D	406	LHG	C25-C26-C27-C28
28	A	413	LMG	C11-C10-O7-C8
28	C	519	LMG	C11-C10-O7-C8
24	B	616	CLA	C10-C11-C12-C13
27	b	601	SQD	C13-C14-C15-C16
27	a	401	SQD	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	c	919	DGD	C2A-C3A-C4A-C5A
38	L	101	LHG	C31-C32-C33-C34
31	J	102	LMT	O1'-C1-C2-C3
28	b	624	LMG	C39-C40-C41-C42
37	C	518	DGD	CBA-CCA-CDA-CEA
37	c	917	DGD	C6A-C7A-C8A-C9A
28	A	413	LMG	C11-C12-C13-C14
31	A	417	LMT	C2-C3-C4-C5
27	b	601	SQD	C15-C16-C17-C18
24	B	602	CLA	O1A-CGA-O2A-C1
36	B	629	HTG	O5-C5-C6-O6
24	b	607	CLA	C5-C6-C7-C8
31	B	626	LMT	C1-C2-C3-C4
37	C	517	DGD	C6A-C7A-C8A-C9A
37	c	918	DGD	CBA-CCA-CDA-CEA
31	c	922	LMT	O5'-C5'-C6'-O6'
28	B	621	LMG	C35-C36-C37-C38
24	b	618	CLA	C10-C11-C12-C13
24	D	402	CLA	C16-C17-C18-C20
28	B	621	LMG	C39-C40-C41-C42
27	a	401	SQD	C30-C31-C32-C33
28	b	624	LMG	C35-C36-C37-C38
38	l	103	LHG	C31-C32-C33-C34
37	D	405	DGD	CAB-CBB-CCB-CDB
36	B	630	HTG	O5-C5-C6-O6
28	B	621	LMG	C14-C15-C16-C17
31	A	417	LMT	C3-C4-C5-C6
37	C	516	DGD	O6E-C5E-C6E-O5E
27	a	415	SQD	C12-C13-C14-C15
28	C	519	LMG	O9-C10-O7-C8
38	D	407	LHG	C1-C2-C3-O3
37	c	917	DGD	O6E-C5E-C6E-O5E
27	F	101	SQD	C11-C10-C9-C8
31	c	927	LMT	C4-C5-C6-C7
37	d	408	DGD	CBB-CCB-CDB-CEB
32	B	638	GOL	O2-C2-C3-O3
27	f	102	SQD	C33-C34-C35-C36
24	B	602	CLA	C1A-C2A-CAA-CBA
24	B	610	CLA	C1A-C2A-CAA-CBA
24	B	612	CLA	C1A-C2A-CAA-CBA
24	C	511	CLA	C1A-C2A-CAA-CBA
24	c	907	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	a	416	LMG	O6-C1-O1-C7
27	a	401	SQD	C34-C35-C36-C37
28	b	624	LMG	C14-C15-C16-C17
31	m	103	LMT	C11-C10-C9-C8
38	L	101	LHG	O6-C4-C5-C6
38	E	101	LHG	O9-C7-O7-C5
27	b	601	SQD	C31-C32-C33-C34
31	F	103	LMT	C4-C5-C6-C7
24	C	508	CLA	C11-C10-C8-C7
24	C	509	CLA	C12-C13-C15-C16
24	b	620	CLA	C11-C12-C13-C15
24	c	909	CLA	C12-C13-C15-C16
28	a	416	LMG	C13-C14-C15-C16
37	C	516	DGD	C1B-C2B-C3B-C4B
24	B	602	CLA	C4-C3-C5-C6
29	a	417	PL9	C15-C14-C16-C17
29	a	417	PL9	C13-C14-C16-C17
29	a	417	PL9	C23-C24-C26-C27
31	M	101	LMT	C4B-C5B-C6B-O6B
24	B	602	CLA	C6-C7-C8-C9
24	B	604	CLA	C6-C7-C8-C9
24	B	617	CLA	C11-C10-C8-C9
24	C	507	CLA	C14-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C9
24	c	907	CLA	C14-C13-C15-C16
24	c	908	CLA	C11-C10-C8-C9
28	C	519	LMG	C35-C36-C37-C38
28	a	416	LMG	O6-C5-C6-O5
38	D	406	LHG	C7-C8-C9-C10
37	D	405	DGD	CDA-CEA-CFA-CGA
24	B	603	CLA	C15-C16-C17-C18
37	D	405	DGD	C2D-C1D-O3G-C3G
36	C	537	HTG	C3'-C4'-C5'-C6'
37	c	918	DGD	C9A-CAA-CBA-CCA
36	b	602	HTG	O5-C5-C6-O6
27	A	416	SQD	O6-C44-C45-C46
27	a	401	SQD	O6-C44-C45-C46
28	C	523	LMG	C4-C5-C6-O5
31	M	102	LMT	C4-C5-C6-C7
37	C	516	DGD	O6D-C5D-C6D-O5D
37	h	102	DGD	C5B-C6B-C7B-C8B
24	c	911	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	415	SQD	C11-C12-C13-C14
28	a	416	LMG	C36-C37-C38-C39
28	d	412	LMG	O6-C5-C6-O5
27	a	415	SQD	C15-C16-C17-C18
37	D	405	DGD	C2B-C3B-C4B-C5B
24	C	503	CLA	C15-C16-C17-C18
37	c	919	DGD	C6B-C7B-C8B-C9B
24	B	602	CLA	C2-C3-C5-C6
36	b	626	HTG	C2'-C3'-C4'-C5'
26	k	102	BCR	C37-C22-C23-C24
28	a	416	LMG	C15-C16-C17-C18
28	D	409	LMG	O6-C5-C6-O5
31	B	626	LMT	O5'-C5'-C6'-O6'
36	D	412	HTG	O5-C5-C6-O6
26	D	403	BCR	C7-C8-C9-C10
26	k	102	BCR	C21-C22-C23-C24
36	C	536	HTG	C1'-C2'-C3'-C4'
28	c	920	LMG	C28-C29-C30-C31
37	H	102	DGD	C7A-C8A-C9A-CAA
27	A	416	SQD	C13-C14-C15-C16
31	c	927	LMT	C5-C6-C7-C8
37	C	518	DGD	C9A-CAA-CBA-CCA
37	C	518	DGD	CAA-CBA-CCA-CDA
28	D	409	LMG	C11-C12-C13-C14
36	C	520	HTG	C2'-C3'-C4'-C5'
31	B	626	LMT	C6-C7-C8-C9
31	M	102	LMT	C1-C2-C3-C4
28	C	519	LMG	O1-C7-C8-O7
28	a	416	LMG	O7-C8-C9-O8
38	D	407	LHG	O2-C2-C3-O3
36	v	211	HTG	C4'-C5'-C6'-C7'
37	C	516	DGD	C4B-C5B-C6B-C7B
36	d	414	HTG	C4-C5-C6-O6
36	d	420	HTG	C4-C5-C6-O6
37	C	517	DGD	C1B-C2B-C3B-C4B
24	b	620	CLA	C4-C3-C5-C6
29	A	414	PL9	C30-C29-C31-C32
29	d	407	PL9	C40-C39-C41-C42
28	a	416	LMG	C40-C41-C42-C43
28	C	523	LMG	C17-C18-C19-C20
28	A	413	LMG	O9-C10-O7-C8
31	a	402	LMT	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	625	LMT	C2-C1-O1'-C1'
32	V	206	GOL	O2-C2-C3-O3
24	C	509	CLA	C14-C13-C15-C16
24	b	619	CLA	C11-C10-C8-C9
24	b	620	CLA	C11-C12-C13-C14
24	c	909	CLA	C14-C13-C15-C16
24	B	606	CLA	C4B-C3B-CAB-CBB
24	C	503	CLA	C4B-C3B-CAB-CBB
24	b	613	CLA	C4B-C3B-CAB-CBB
24	d	404	CLA	C4B-C3B-CAB-CBB
37	D	405	DGD	CBB-CCB-CDB-CEB
37	c	918	DGD	C7A-C8A-C9A-CAA
31	a	402	LMT	C3-C4-C5-C6
27	l	101	SQD	C9-C10-C11-C12
38	l	103	LHG	O6-C4-C5-C6
37	c	919	DGD	CBB-CCB-CDB-CEB
38	l	103	LHG	C28-C29-C30-C31
36	D	412	HTG	C4'-C5'-C6'-C7'
37	c	918	DGD	CDB-CEB-CFB-CGB
37	h	102	DGD	CDA-CEA-CFA-CGA
24	B	602	CLA	C6-C7-C8-C10
24	B	604	CLA	C6-C7-C8-C10
24	B	616	CLA	C12-C13-C15-C16
24	B	617	CLA	C11-C10-C8-C7
24	C	507	CLA	C12-C13-C15-C16
24	C	513	CLA	C12-C13-C15-C16
24	b	618	CLA	C6-C7-C8-C10
24	b	619	CLA	C11-C10-C8-C7
24	c	907	CLA	C12-C13-C15-C16
24	c	908	CLA	C11-C10-C8-C7
24	c	913	CLA	C12-C13-C15-C16
38	d	410	LHG	C35-C36-C37-C38
37	d	408	DGD	CDB-CEB-CFB-CGB
29	A	414	PL9	C15-C14-C16-C17
37	C	516	DGD	C2A-C3A-C4A-C5A
38	d	410	LHG	C11-C10-C9-C8
29	A	414	PL9	C13-C14-C16-C17
29	d	407	PL9	C43-C44-C46-C47
38	L	101	LHG	C28-C29-C30-C31
28	B	621	LMG	C40-C41-C42-C43
37	C	516	DGD	CDA-CEA-CFA-CGA
28	c	920	LMG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	D	408	LHG	C30-C31-C32-C33
37	C	518	DGD	C7A-C8A-C9A-CAA
27	b	601	SQD	C44-C45-C46-O48
27	f	102	SQD	C44-C45-C46-O48
27	l	101	SQD	C44-C45-C46-O48
28	a	416	LMG	C7-C8-C9-O8
27	a	401	SQD	C11-C10-C9-C8
24	c	914	CLA	C10-C11-C12-C13
24	d	401	CLA	C2C-C3C-CAC-CBC
37	c	917	DGD	CBA-CCA-CDA-CEA
28	C	523	LMG	C29-C30-C31-C32
29	d	407	PL9	C45-C44-C46-C47
28	d	412	LMG	C14-C15-C16-C17
37	H	102	DGD	C5B-C6B-C7B-C8B
29	A	414	PL9	C28-C29-C31-C32
26	D	403	BCR	C23-C24-C25-C30
38	d	411	LHG	C28-C29-C30-C31
27	b	601	SQD	C26-C27-C28-C29
24	b	612	CLA	C13-C15-C16-C17
27	A	412	SQD	O6-C44-C45-O47
27	f	102	SQD	O47-C45-C46-O48
36	y	102	HTG	O5-C1-S1-C1'
31	a	402	LMT	C9-C10-C11-C12
37	c	919	DGD	C5B-C6B-C7B-C8B
24	b	620	CLA	C2-C3-C5-C6
31	M	102	LMT	C11-C10-C9-C8
37	C	518	DGD	CDB-CEB-CFB-CGB
28	C	519	LMG	C36-C37-C38-C39
24	b	618	CLA	C14-C13-C15-C16
24	c	913	CLA	C14-C13-C15-C16
37	C	516	DGD	C4A-C5A-C6A-C7A
37	H	102	DGD	CDA-CEA-CFA-CGA
37	c	919	DGD	C9B-CAB-CBB-CCB
27	F	101	SQD	O47-C45-C46-O48
38	D	406	LHG	O1-C1-C2-O2
38	d	410	LHG	C28-C29-C30-C31
28	B	621	LMG	C18-C19-C20-C21
36	O	316	HTG	C2'-C3'-C4'-C5'
24	B	617	CLA	C8-C10-C11-C12
24	a	413	CLA	C5-C6-C7-C8
27	F	101	SQD	C12-C13-C14-C15
37	d	408	DGD	CCB-CDB-CEB-CFB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	607	CLA	C8-C10-C11-C12
24	B	616	CLA	C6-C7-C8-C10
24	C	506	CLA	C12-C13-C15-C16
24	a	413	CLA	C11-C10-C8-C7
24	b	618	CLA	C12-C13-C15-C16
31	b	625	LMT	C11-C10-C9-C8
28	c	920	LMG	C20-C21-C22-C23
27	f	102	SQD	C5-C6-S-O8
37	C	517	DGD	C2G-C3G-O3G-C1D
37	C	517	DGD	C5D-C6D-O5D-C1E
37	c	918	DGD	C5D-C6D-O5D-C1E
24	a	413	CLA	C8-C10-C11-C12
24	b	614	CLA	C2A-CAA-CBA-CGA
36	B	623	HTG	C4-C5-C6-O6
38	d	409	LHG	C23-C24-C25-C26
27	A	416	SQD	C24-C23-O48-C46
27	F	101	SQD	C11-C12-C13-C14
27	b	601	SQD	C46-C45-O47-C7
28	b	624	LMG	C18-C19-C20-C21
24	c	909	CLA	C16-C17-C18-C20
37	C	517	DGD	C7A-C8A-C9A-CAA
38	D	407	LHG	C32-C33-C34-C35
37	h	102	DGD	O2G-C1B-C2B-C3B
28	c	920	LMG	C14-C15-C16-C17
37	H	102	DGD	CAA-CBA-CCA-CDA
37	c	917	DGD	O6D-C5D-C6D-O5D
28	C	519	LMG	C7-C8-C9-O8
38	E	101	LHG	C4-C5-C6-O8
28	B	621	LMG	C36-C37-C38-C39
36	C	521	HTG	S1-C1'-C2'-C3'
37	C	516	DGD	C4D-C5D-C6D-O5D
29	d	407	PL9	C38-C39-C41-C42
36	c	942	HTG	C2-C1-S1-C1'
36	y	102	HTG	C2-C1-S1-C1'
31	B	622	LMT	C11-C10-C9-C8
27	b	601	SQD	O47-C45-C46-O48
27	l	101	SQD	O47-C45-C46-O48
24	A	410	CLA	C6-C7-C8-C9
24	C	513	CLA	C14-C13-C15-C16
24	c	903	CLA	C16-C17-C18-C20
37	C	516	DGD	C7B-C8B-C9B-CAB
28	A	413	LMG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	523	LMG	C16-C17-C18-C19
27	b	601	SQD	C11-C10-C9-C8
28	b	624	LMG	C28-C29-C30-C31
37	H	102	DGD	O2G-C1B-C2B-C3B
27	F	101	SQD	C13-C14-C15-C16
24	C	509	CLA	C2-C1-O2A-CGA
28	d	412	LMG	C36-C37-C38-C39
31	a	402	LMT	C6-C7-C8-C9
24	B	602	CLA	C5-C6-C7-C8
36	C	520	HTG	S1-C1'-C2'-C3'
24	C	511	CLA	O1A-CGA-O2A-C1
27	A	416	SQD	O10-C23-O48-C46
36	C	537	HTG	C2'-C3'-C4'-C5'
38	D	408	LHG	C28-C29-C30-C31
37	C	517	DGD	C8A-C9A-CAA-CBA
27	l	101	SQD	C24-C25-C26-C27
31	a	402	LMT	C4-C5-C6-C7
32	B	637	GOL	O2-C2-C3-O3
24	c	906	CLA	C4B-C3B-CAB-CBB
24	c	909	CLA	C1A-C2A-CAA-CBA
37	H	102	DGD	C6B-C7B-C8B-C9B
31	m	102	LMT	O1'-C1-C2-C3
37	C	517	DGD	C6B-C7B-C8B-C9B
31	b	625	LMT	C6-C7-C8-C9
31	Z	101	LMT	O1'-C1-C2-C3
24	b	619	CLA	C8-C10-C11-C12
31	B	626	LMT	C7-C8-C9-C10
27	A	416	SQD	C5-C6-S-O7
24	A	410	CLA	C6-C7-C8-C10
24	C	507	CLA	C11-C10-C8-C7
24	b	617	CLA	C12-C13-C15-C16
24	c	906	CLA	C12-C13-C15-C16
24	c	907	CLA	C11-C10-C8-C7
27	a	401	SQD	C25-C26-C27-C28
36	b	602	HTG	C2'-C3'-C4'-C5'
31	M	101	LMT	C1-C2-C3-C4
27	A	412	SQD	C7-C8-C9-C10
38	L	101	LHG	O6-C4-C5-O7
38	l	103	LHG	O6-C4-C5-O7
37	C	518	DGD	CAB-CBB-CCB-CDB
36	B	629	HTG	C4'-C5'-C6'-C7'
31	F	103	LMT	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C2C-C3C-CAC-CBC
24	B	616	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C10-C8-C9
24	a	413	CLA	C11-C10-C8-C9
24	b	618	CLA	C6-C7-C8-C9
24	b	608	CLA	C13-C15-C16-C17
37	d	408	DGD	CAA-CBA-CCA-CDA
24	B	617	CLA	C16-C17-C18-C19
37	h	102	DGD	CDB-CEB-CFB-CGB
24	B	614	CLA	C15-C16-C17-C18
28	a	416	LMG	C17-C18-C19-C20
36	B	624	HTG	C2'-C3'-C4'-C5'
27	a	415	SQD	O6-C44-C45-O47
27	b	601	SQD	O6-C44-C45-O47
28	A	413	LMG	O1-C7-C8-O7
28	C	519	LMG	O7-C8-C9-O8
31	B	622	LMT	C5'-C4'-O1B-C1B
27	a	401	SQD	C28-C29-C30-C31
36	d	419	HTG	C2'-C3'-C4'-C5'
28	d	412	LMG	C35-C36-C37-C38
28	A	413	LMG	O1-C7-C8-C9
38	D	406	LHG	C11-C10-C9-C8
36	c	943	HTG	C1'-C2'-C3'-C4'
24	C	502	CLA	CAD-CBD-CGD-O2D
24	b	605	CLA	CAD-CBD-CGD-O2D
24	c	903	CLA	CAD-CBD-CGD-O2D
24	b	610	CLA	C10-C11-C12-C13
37	C	518	DGD	CBB-CCB-CDB-CEB
28	c	920	LMG	C39-C40-C41-C42
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	605	CLA	CAD-CBD-CGD-O1D
24	b	609	CLA	CAD-CBD-CGD-O1D
24	b	620	CLA	CHA-CBD-CGD-O1D
24	b	620	CLA	CHA-CBD-CGD-O2D
24	c	903	CLA	CAD-CBD-CGD-O1D
24	c	907	CLA	CHA-CBD-CGD-O1D
38	D	407	LHG	C3-O3-P-O5
38	E	101	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	b	619	CLA	C16-C17-C18-C19
37	c	917	DGD	C8A-C9A-CAA-CBA
24	C	503	CLA	C2B-C3B-CAB-CBB
24	C	513	CLA	C2B-C3B-CAB-CBB
24	c	913	CLA	C2B-C3B-CAB-CBB
27	a	401	SQD	C15-C16-C17-C18
38	D	408	LHG	C2-C3-O3-P
38	d	411	LHG	C2-C3-O3-P
37	c	918	DGD	CBB-CCB-CDB-CEB
38	D	408	LHG	C14-C15-C16-C17
24	A	406	CLA	C4C-C3C-CAC-CBC
32	V	206	GOL	O1-C1-C2-O2
38	d	411	LHG	O1-C1-C2-O2
24	a	409	CLA	C2C-C3C-CAC-CBC
29	A	414	PL9	C4-C3-C7-C8
29	a	417	PL9	C4-C3-C7-C8
32	V	207	GOL	O1-C1-C2-C3
27	l	101	SQD	C11-C10-C9-C8
27	l	101	SQD	C46-C45-O47-C7
36	d	420	HTG	C2'-C3'-C4'-C5'
37	c	917	DGD	C4D-C5D-C6D-O5D
24	b	615	CLA	C16-C17-C18-C19
24	c	909	CLA	C16-C17-C18-C19
37	c	918	DGD	C5A-C6A-C7A-C8A
24	C	512	CLA	C11-C12-C13-C14
24	c	904	CLA	C11-C10-C8-C9
28	A	413	LMG	C35-C36-C37-C38
28	C	523	LMG	O6-C1-O1-C7
27	l	101	SQD	C16-C17-C18-C19
24	A	410	CLA	C4-C3-C5-C6
37	C	517	DGD	C2A-C3A-C4A-C5A
37	D	405	DGD	CAA-CBA-CCA-CDA
27	a	401	SQD	C19-C20-C21-C22
28	a	416	LMG	C16-C17-C18-C19
37	d	408	DGD	CCA-CDA-CEA-CFA
31	t	101	LMT	O1'-C1-C2-C3
37	d	408	DGD	C3A-C4A-C5A-C6A
28	C	523	LMG	O1-C7-C8-O7
27	A	412	SQD	C11-C12-C13-C14
27	A	412	SQD	C8-C7-O47-C45
28	B	621	LMG	C11-C10-O7-C8
27	l	101	SQD	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	523	LMG	C35-C36-C37-C38
24	b	606	CLA	C8-C10-C11-C12
36	d	414	HTG	C4'-C5'-C6'-C7'
27	A	412	SQD	O49-C7-O47-C45
28	C	519	LMG	O1-C7-C8-C9
27	l	101	SQD	C12-C13-C14-C15
37	c	917	DGD	C2A-C3A-C4A-C5A
37	C	517	DGD	C3A-C4A-C5A-C6A
24	b	615	CLA	C16-C17-C18-C20
28	B	621	LMG	O9-C10-O7-C8
37	C	516	DGD	C5D-C6D-O5D-C1E
37	c	917	DGD	C5D-C6D-O5D-C1E
38	E	101	LHG	C14-C15-C16-C17
24	B	613	CLA	C13-C15-C16-C17
37	c	918	DGD	CAB-CBB-CCB-CDB
28	a	416	LMG	O8-C28-C29-C30
27	a	401	SQD	C9-C10-C11-C12
28	c	921	LMG	O6-C5-C6-O5
31	a	402	LMT	C11-C10-C9-C8
27	b	601	SQD	C9-C10-C11-C12
31	Z	101	LMT	C2-C1-O1'-C1'
24	c	907	CLA	C11-C10-C8-C9
24	C	502	CLA	C4B-C3B-CAB-CBB
24	B	616	CLA	C16-C17-C18-C19
28	A	413	LMG	C21-C22-C23-C24
24	B	616	CLA	C8-C10-C11-C12
27	a	401	SQD	C2-C1-O6-C44
24	b	619	CLA	C16-C17-C18-C20
37	D	405	DGD	CCA-CDA-CEA-CFA
37	d	408	DGD	C2A-C3A-C4A-C5A
24	B	617	CLA	C12-C13-C15-C16
24	D	401	CLA	C12-C13-C15-C16
27	b	601	SQD	C16-C17-C18-C19
27	b	601	SQD	C35-C36-C37-C38
27	A	412	SQD	C30-C31-C32-C33
24	B	617	CLA	C16-C17-C18-C20
37	D	405	DGD	O1G-C1G-C2G-O2G
37	h	102	DGD	CBB-CCB-CDB-CEB
24	b	611	CLA	C3A-C2A-CAA-CBA
24	b	612	CLA	C3A-C2A-CAA-CBA
24	C	505	CLA	C2-C3-C5-C6
24	C	509	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	a	412	PHO	C2C-C3C-CAC-CBC
27	b	601	SQD	C10-C11-C12-C13
31	A	417	LMT	C4-C5-C6-C7
36	O	303	HTG	C2'-C3'-C4'-C5'
40	H	101	RRX	C9-C10-C11-C12
40	h	101	RRX	C9-C10-C11-C12
38	l	103	LHG	C17-C18-C19-C20
31	t	102	LMT	O5B-C5B-C6B-O6B
31	A	417	LMT	C4'-C5'-C6'-O6'
38	d	410	LHG	C1-C2-C3-O3
27	a	415	SQD	O6-C44-C45-C46
24	A	410	CLA	C3-C5-C6-C7
24	B	617	CLA	C6-C7-C8-C9
24	C	506	CLA	C14-C13-C15-C16
24	b	617	CLA	C14-C13-C15-C16
24	b	620	CLA	C11-C10-C8-C9
31	A	421	LMT	C7-C8-C9-C10
24	b	616	CLA	C8-C10-C11-C12
37	C	516	DGD	C8A-C9A-CAA-CBA
38	L	101	LHG	C17-C18-C19-C20
27	F	101	SQD	C44-C45-C46-O48
36	d	414	HTG	C2'-C3'-C4'-C5'
27	a	401	SQD	C23-C24-C25-C26
27	a	401	SQD	C18-C19-C20-C21
31	M	102	LMT	C7-C8-C9-C10
37	c	917	DGD	CAB-CBB-CCB-CDB
38	l	103	LHG	C12-C13-C14-C15
24	b	606	CLA	C3-C5-C6-C7
28	A	413	LMG	O6-C5-C6-O5
28	c	920	LMG	C37-C38-C39-C40
38	l	103	LHG	C10-C11-C12-C13
31	c	922	LMT	O1'-C1-C2-C3
24	B	603	CLA	C2B-C3B-CAB-CBB
24	C	502	CLA	C2B-C3B-CAB-CBB
24	b	608	CLA	C2B-C3B-CAB-CBB
24	c	906	CLA	C2B-C3B-CAB-CBB
26	D	403	BCR	C23-C24-C25-C26
26	b	621	BCR	C1-C6-C7-C8
26	c	916	BCR	C1-C6-C7-C8
40	H	101	RRX	C23-C24-C25-C30
38	d	410	LHG	O2-C2-C3-O3
24	B	616	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	417	PL9	C45-C44-C46-C47
37	c	917	DGD	C6B-C7B-C8B-C9B
24	A	407	CLA	C12-C13-C15-C16
24	B	611	CLA	C11-C10-C8-C7
24	a	410	CLA	C11-C10-C8-C7
24	b	606	CLA	C6-C7-C8-C10
24	c	910	CLA	C12-C13-C15-C16
36	O	303	HTG	C3'-C4'-C5'-C6'
28	C	523	LMG	C14-C15-C16-C17
28	B	621	LMG	C31-C32-C33-C34
37	h	102	DGD	C9B-CAB-CBB-CCB
38	L	101	LHG	C10-C11-C12-C13
42	v	202	HEC	CAD-CBD-CGD-O2D
24	C	506	CLA	C4-C3-C5-C6
24	c	914	CLA	C4-C3-C5-C6
31	e	101	LMT	C1-C2-C3-C4
28	A	413	LMG	C31-C32-C33-C34
31	B	626	LMT	C5-C6-C7-C8
24	B	609	CLA	C13-C15-C16-C17
38	L	101	LHG	C12-C13-C14-C15
42	V	203	HEC	CAD-CBD-CGD-O2D
38	d	411	LHG	C11-C10-C9-C8
31	t	102	LMT	C6-C7-C8-C9
24	A	405	CLA	C4C-C3C-CAC-CBC
24	B	616	CLA	C4-C3-C5-C6
24	C	513	CLA	C4-C3-C5-C6
24	B	603	CLA	C8-C10-C11-C12
36	B	623	HTG	O5-C5-C6-O6
27	A	412	SQD	O6-C44-C45-C46
37	D	405	DGD	O1G-C1G-C2G-C3G
28	b	624	LMG	C40-C41-C42-C43
42	v	202	HEC	CAD-CBD-CGD-O1D
24	d	401	CLA	C4C-C3C-CAC-CBC
24	b	609	CLA	C8-C10-C11-C12
24	b	606	CLA	C13-C15-C16-C17
31	B	622	LMT	C2-C1-O1'-C1'
38	d	410	LHG	O1-C1-C2-O2
24	D	402	CLA	C4-C3-C5-C6
24	c	905	CLA	C4-C3-C5-C6
24	B	603	CLA	C4B-C3B-CAB-CBB
24	D	401	CLA	C4B-C3B-CAB-CBB
24	c	902	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	b	606	CLA	C15-C16-C17-C18
38	E	101	LHG	O10-C23-O8-C6
28	C	519	LMG	C34-C35-C36-C37
38	D	408	LHG	O10-C23-O8-C6
42	V	203	HEC	CAD-CBD-CGD-O1D
31	A	421	LMT	C3-C4-C5-C6
24	c	903	CLA	C16-C17-C18-C19
24	B	614	CLA	C10-C11-C12-C13
28	A	413	LMG	C18-C19-C20-C21
38	d	411	LHG	C33-C34-C35-C36
24	A	410	CLA	C11-C12-C13-C15
28	b	624	LMG	C31-C32-C33-C34
27	l	101	SQD	C27-C28-C29-C30
24	B	607	CLA	C11-C12-C13-C14
24	C	507	CLA	C11-C10-C8-C9
24	a	410	CLA	C6-C7-C8-C9
24	c	905	CLA	C14-C13-C15-C16
37	c	918	DGD	C2G-C3G-O3G-C1D
24	B	614	CLA	C2-C1-O2A-CGA
24	d	404	CLA	C2-C1-O2A-CGA
37	d	408	DGD	C4A-C5A-C6A-C7A
24	C	511	CLA	CBA-CGA-O2A-C1
28	b	624	LMG	O9-C10-O7-C8
24	B	609	CLA	C3A-C2A-CAA-CBA
27	f	102	SQD	C25-C26-C27-C28
37	d	408	DGD	CDA-CEA-CFA-CGA
37	C	517	DGD	C2E-C1E-O5D-C6D
27	l	101	SQD	C24-C23-O48-C46
28	a	416	LMG	C32-C33-C34-C35
27	a	401	SQD	O5-C1-O6-C44
37	C	516	DGD	C9A-CAA-CBA-CCA
28	C	523	LMG	O1-C7-C8-C9
37	h	102	DGD	C9A-CAA-CBA-CCA
27	l	101	SQD	O10-C23-O48-C46
37	c	917	DGD	C1B-C2B-C3B-C4B
24	c	910	CLA	C16-C17-C18-C20
31	B	626	LMT	C3-C4-C5-C6
37	C	516	DGD	C7A-C8A-C9A-CAA
27	l	101	SQD	O48-C23-C24-C25
37	D	405	DGD	O2G-C1B-C2B-C3B
24	c	906	CLA	C14-C13-C15-C16
24	c	910	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	h	102	DGD	C6B-C7B-C8B-C9B
38	d	410	LHG	C33-C34-C35-C36
28	C	519	LMG	C38-C39-C40-C41
31	A	421	LMT	C11-C10-C9-C8
38	E	101	LHG	C26-C27-C28-C29
24	c	905	CLA	C12-C13-C15-C16
24	B	606	CLA	C2B-C3B-CAB-CBB
24	C	501	CLA	C2B-C3B-CAB-CBB
24	D	401	CLA	C2B-C3B-CAB-CBB
24	b	620	CLA	C2B-C3B-CAB-CBB
24	c	902	CLA	C2B-C3B-CAB-CBB
24	d	404	CLA	C2B-C3B-CAB-CBB
26	C	515	BCR	C23-C24-C25-C30
26	b	621	BCR	C5-C6-C7-C8
26	c	916	BCR	C5-C6-C7-C8
37	d	408	DGD	O1G-C1A-C2A-C3A
29	d	407	PL9	C39-C41-C42-C43
37	c	918	DGD	O6E-C1E-O5D-C6D
25	a	411	PHO	C2-C3-C5-C6
24	B	607	CLA	C10-C11-C12-C13
24	C	513	CLA	O1A-CGA-O2A-C1
36	C	520	HTG	C2'-C1'-S1-C1
36	y	102	HTG	C2'-C1'-S1-C1
24	a	409	CLA	C4C-C3C-CAC-CBC
28	a	416	LMG	C21-C22-C23-C24
24	C	504	CLA	C15-C16-C17-C18
36	B	631	HTG	C3'-C4'-C5'-C6'
38	D	408	LHG	C19-C20-C21-C22
37	c	919	DGD	O1G-C1A-C2A-C3A
28	C	519	LMG	C19-C20-C21-C22
27	a	401	SQD	C4-C5-C6-S
24	A	406	CLA	C15-C16-C17-C18
24	A	410	CLA	C2-C3-C5-C6
24	B	610	CLA	C2-C3-C5-C6
24	B	611	CLA	C2A-CAA-CBA-CGA
24	a	413	CLA	C10-C11-C12-C13
24	b	614	CLA	C11-C12-C13-C14
24	c	903	CLA	C14-C13-C15-C16
38	D	406	LHG	O8-C23-C24-C25
28	d	412	LMG	C13-C14-C15-C16
27	b	601	SQD	O6-C44-C45-C46
24	B	602	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	C	501	CLA	C4B-C3B-CAB-CBB
24	b	605	CLA	C1A-C2A-CAA-CBA
24	b	608	CLA	C4B-C3B-CAB-CBB
31	Z	101	LMT	C5-C6-C7-C8
25	a	411	PHO	C4-C3-C5-C6
37	C	517	DGD	O6E-C1E-O5D-C6D
31	B	622	LMT	C6-C7-C8-C9
27	f	102	SQD	O6-C44-C45-O47
29	d	407	PL9	C11-C12-C13-C14
28	d	412	LMG	C16-C17-C18-C19
26	c	916	BCR	C7-C8-C9-C10
38	D	408	LHG	C24-C23-O8-C6
28	a	416	LMG	O7-C10-C11-C12
37	c	917	DGD	O2G-C1B-C2B-C3B
27	A	416	SQD	C28-C29-C30-C31
24	C	512	CLA	CAA-CBA-CGA-O2A
27	A	416	SQD	C5-C6-S-O9
27	l	101	SQD	C5-C6-S-O9
24	B	610	CLA	C4-C3-C5-C6
24	a	409	CLA	C2-C1-O2A-CGA
38	D	408	LHG	C17-C18-C19-C20
24	C	509	CLA	C11-C10-C8-C7
24	c	909	CLA	C11-C10-C8-C7
24	c	910	CLA	C6-C7-C8-C10
24	d	404	CLA	C11-C12-C13-C15
24	d	405	CLA	C12-C13-C15-C16
31	m	102	LMT	O5'-C5'-C6'-O6'
24	B	614	CLA	CAA-CBA-CGA-O2A
37	d	408	DGD	CBA-CCA-CDA-CEA
38	E	101	LHG	C24-C23-O8-C6
31	t	101	LMT	C2-C3-C4-C5
24	C	501	CLA	C2A-CAA-CBA-CGA
37	D	405	DGD	C1B-C2B-C3B-C4B
39	F	102	HEM	CAD-CBD-CGD-O1D
31	b	625	LMT	C5'-C4'-O1B-C1B
29	A	414	PL9	C45-C44-C46-C47
31	A	421	LMT	C4-C5-C6-C7
24	d	404	CLA	C16-C17-C18-C20
37	H	102	DGD	C9B-CAB-CBB-CCB
24	C	510	CLA	CAA-CBA-CGA-O2A
37	C	517	DGD	O2G-C1B-C2B-C3B
37	c	919	DGD	O1A-C1A-C2A-C3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	C	507	CLA	C2A-CAA-CBA-CGA
24	b	618	CLA	C2A-CAA-CBA-CGA
24	c	902	CLA	C2A-CAA-CBA-CGA
24	A	407	CLA	C14-C13-C15-C16
24	B	616	CLA	C6-C7-C8-C9
27	a	401	SQD	O48-C23-C24-C25
24	C	503	CLA	C10-C11-C12-C13
24	b	619	CLA	C10-C11-C12-C13
27	f	102	SQD	O5-C5-C6-S
36	c	943	HTG	C2'-C3'-C4'-C5'
37	c	919	DGD	CDB-CEB-CFB-CGB
28	a	416	LMG	O9-C10-C11-C12
24	C	512	CLA	CAA-CBA-CGA-O1A
24	d	401	CLA	C15-C16-C17-C18
27	a	401	SQD	C45-C44-O6-C1
27	l	101	SQD	O10-C23-C24-C25
37	d	408	DGD	O1A-C1A-C2A-C3A
38	d	410	LHG	C26-C27-C28-C29
24	b	616	CLA	CAA-CBA-CGA-O2A
24	c	906	CLA	CAA-CBA-CGA-O2A
37	C	518	DGD	CDA-CEA-CFA-CGA
24	B	608	CLA	CAD-CBD-CGD-O2D
24	c	905	CLA	CAD-CBD-CGD-O2D
24	d	405	CLA	CAD-CBD-CGD-O2D
31	A	421	LMT	C5-C6-C7-C8
37	c	918	DGD	CDA-CEA-CFA-CGA
27	A	412	SQD	C13-C14-C15-C16
37	D	405	DGD	C2A-C3A-C4A-C5A
24	b	609	CLA	C10-C11-C12-C13
39	F	102	HEM	CAA-CBA-CGA-O1A
31	c	922	LMT	C2-C3-C4-C5
24	b	608	CLA	C10-C11-C12-C13
24	C	513	CLA	C11-C10-C8-C7
24	c	911	CLA	CAA-CBA-CGA-O2A
27	f	102	SQD	O47-C7-C8-C9
38	d	411	LHG	O8-C23-C24-C25
24	D	401	CLA	C2C-C3C-CAC-CBC
24	C	510	CLA	CAA-CBA-CGA-O1A
24	b	616	CLA	CAA-CBA-CGA-O1A
24	c	906	CLA	CAA-CBA-CGA-O1A
28	c	920	LMG	O7-C10-C11-C12
24	B	614	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

185 monomers are involved in 327 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	401	SQD	6	0
32	V	207	GOL	1	0
28	c	920	LMG	3	0
24	C	504	CLA	3	0
26	K	101	BCR	1	0
26	b	623	BCR	2	0
38	E	101	LHG	1	0
31	c	927	LMT	1	0
34	c	940	DMS	2	0
24	B	602	CLA	1	0
24	c	910	CLA	2	0
34	c	932	DMS	2	0
24	C	509	CLA	1	0
34	B	633	DMS	1	0
37	c	917	DGD	1	0
36	C	536	HTG	2	0
24	d	401	CLA	3	0
24	B	608	CLA	1	0
37	d	408	DGD	4	0
24	A	405	CLA	3	0
28	D	409	LMG	1	0
31	M	102	LMT	1	0
36	b	626	HTG	3	0
24	a	410	CLA	3	0
26	C	515	BCR	2	0
36	c	928	HTG	1	0
36	v	211	HTG	2	0
29	d	407	PL9	3	0
24	B	617	CLA	3	0
34	o	307	DMS	1	0
36	U	201	HTG	1	0
24	C	508	CLA	7	0
26	d	406	BCR	2	0
32	V	206	GOL	1	0
24	C	513	CLA	4	0
34	U	204	DMS	2	0
36	C	537	HTG	2	0
29	D	404	PL9	1	0
38	l	103	LHG	2	0
36	O	303	HTG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	619	BCR	3	0
38	d	409	LHG	3	0
34	L	102	DMS	1	0
34	B	632	DMS	1	0
31	m	102	LMT	2	0
34	c	934	DMS	1	0
24	C	511	CLA	3	0
26	c	915	BCR	2	0
24	C	506	CLA	5	0
34	c	933	DMS	1	0
34	O	315	DMS	2	0
24	C	502	CLA	2	0
32	c	929	GOL	2	0
26	b	622	BCR	2	0
29	a	417	PL9	3	0
37	C	518	DGD	1	0
28	C	523	LMG	3	0
24	b	607	CLA	2	0
24	B	605	CLA	1	0
24	b	616	CLA	3	0
24	C	501	CLA	4	0
36	d	419	HTG	3	0
24	b	613	CLA	3	0
25	a	411	PHO	1	0
24	C	503	CLA	3	0
32	B	637	GOL	2	0
36	B	623	HTG	3	0
24	b	609	CLA	5	0
34	b	647	DMS	1	0
24	B	613	CLA	1	0
34	V	210	DMS	1	0
26	c	916	BCR	2	0
28	C	519	LMG	3	0
34	y	101	DMS	2	0
24	B	612	CLA	1	0
24	B	611	CLA	5	0
25	a	412	PHO	1	0
24	b	610	CLA	6	0
36	c	941	HTG	1	0
31	j	102	LMT	2	0
24	B	615	CLA	5	0
27	A	416	SQD	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	534	DMS	1	0
24	B	607	CLA	4	0
29	A	414	PL9	4	0
24	B	616	CLA	3	0
24	b	620	CLA	4	0
34	O	314	DMS	1	0
34	V	211	DMS	1	0
24	c	909	CLA	4	0
26	B	618	BCR	3	0
37	c	918	DGD	2	0
38	d	410	LHG	2	0
38	d	411	LHG	5	0
36	b	627	HTG	1	0
26	T	101	BCR	4	0
27	b	601	SQD	1	0
24	c	906	CLA	6	0
37	C	516	DGD	2	0
31	A	417	LMT	3	0
26	Y	101	BCR	2	0
26	k	103	BCR	1	0
34	B	634	DMS	1	0
36	d	414	HTG	2	0
24	c	908	CLA	1	0
34	D	416	DMS	1	0
40	H	101	RRX	3	0
36	V	215	HTG	1	0
26	B	636	BCR	4	0
34	b	639	DMS	1	0
39	F	102	HEM	2	0
24	c	903	CLA	2	0
24	b	619	CLA	4	0
31	Z	101	LMT	1	0
24	C	510	CLA	4	0
24	B	610	CLA	1	0
24	C	512	CLA	1	0
39	f	101	HEM	3	0
24	b	605	CLA	1	0
24	c	911	CLA	1	0
28	A	413	LMG	3	0
24	c	902	CLA	2	0
24	b	617	CLA	2	0
36	D	412	HTG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	D	408	LHG	6	0
34	a	424	DMS	1	0
25	A	409	PHO	2	0
24	b	608	CLA	1	0
31	B	626	LMT	2	0
31	a	402	LMT	2	0
24	b	615	CLA	3	0
28	B	621	LMG	1	0
32	B	638	GOL	2	0
36	B	624	HTG	3	0
24	A	410	CLA	4	0
34	h	105	DMS	2	0
26	b	621	BCR	3	0
24	d	404	CLA	1	0
28	a	416	LMG	1	0
26	B	620	BCR	1	0
24	B	603	CLA	5	0
24	c	904	CLA	2	0
26	C	514	BCR	2	0
24	C	507	CLA	2	0
24	B	614	CLA	2	0
38	D	406	LHG	3	0
26	a	414	BCR	2	0
24	C	505	CLA	5	0
24	b	614	CLA	3	0
24	c	907	CLA	2	0
34	A	426	DMS	1	0
24	c	905	CLA	2	0
27	a	415	SQD	3	0
24	c	912	CLA	2	0
34	d	415	DMS	1	0
28	d	412	LMG	3	0
34	O	311	DMS	1	0
34	U	202	DMS	1	0
28	b	624	LMG	1	0
24	D	401	CLA	1	0
27	l	101	SQD	1	0
24	a	413	CLA	3	0
31	b	625	LMT	2	0
38	L	101	LHG	3	0
26	k	102	BCR	1	0
37	D	405	DGD	7	0

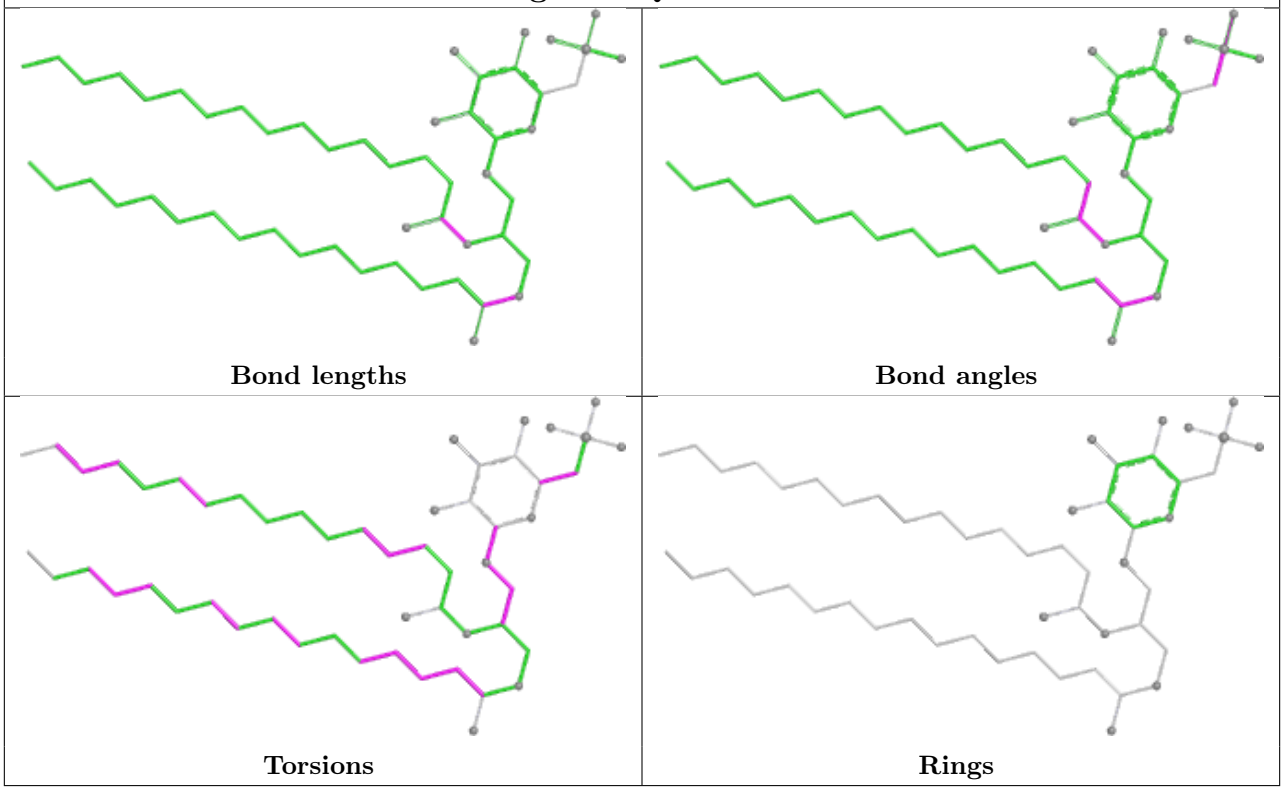
Continued on next page...

Continued from previous page...

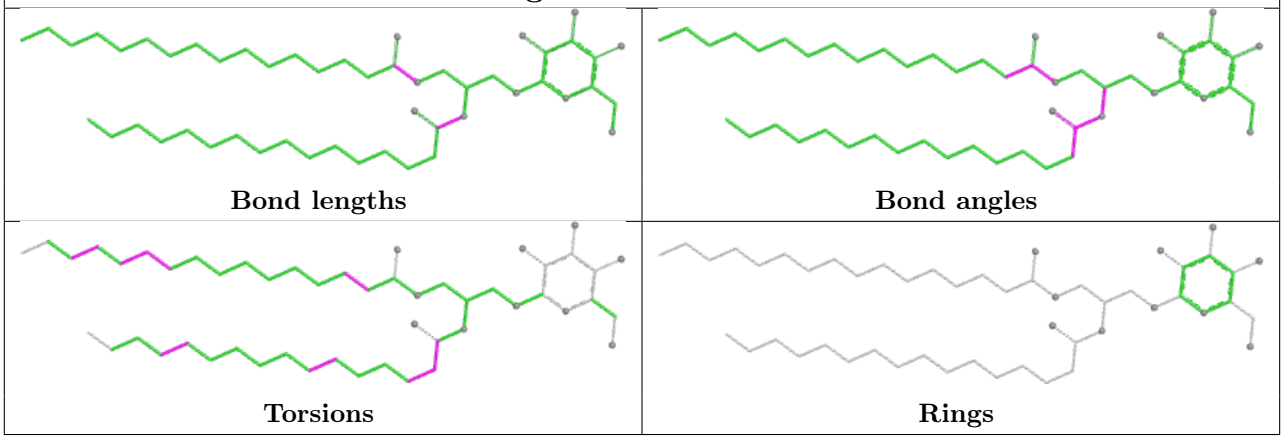
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	B	630	HTG	1	0
31	M	101	LMT	2	0
24	A	406	CLA	4	0
24	A	407	CLA	1	0
40	h	101	RRX	2	0
27	F	101	SQD	2	0
31	A	421	LMT	4	0
24	a	409	CLA	4	0
34	B	639	DMS	1	0
24	b	606	CLA	1	0
34	c	930	DMS	1	0
24	B	606	CLA	6	0
34	o	303	DMS	1	0
37	H	102	DGD	1	0
34	O	306	DMS	1	0
37	C	517	DGD	1	0
24	B	604	CLA	3	0
36	c	942	HTG	2	0
34	c	937	DMS	1	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.

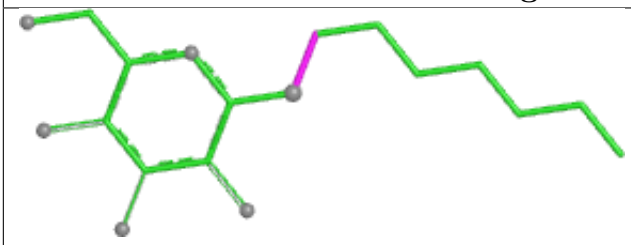
Ligand SQD a 401



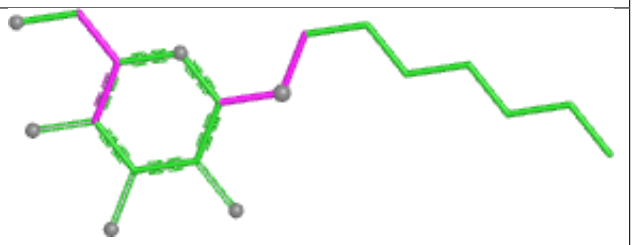
Ligand LMG c 920



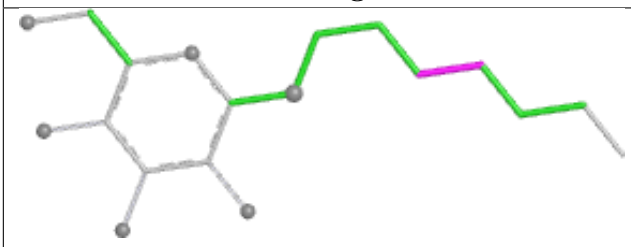
Ligand HTG O 316



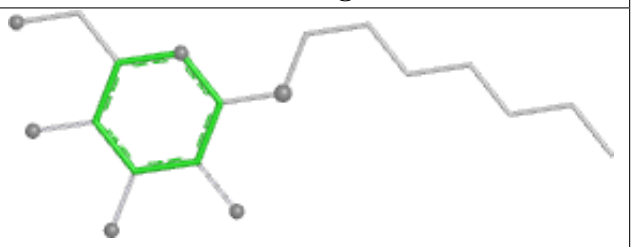
Bond lengths



Bond angles

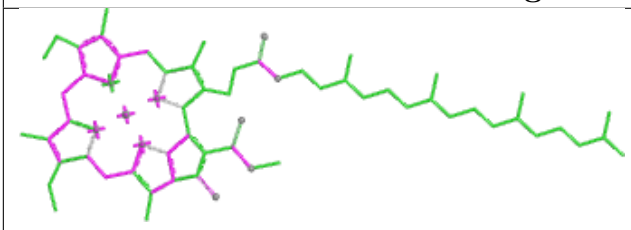


Torsions

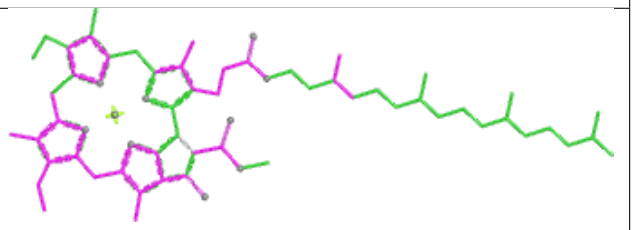


Rings

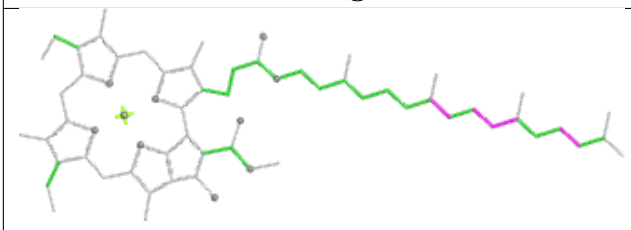
Ligand CLA C 504



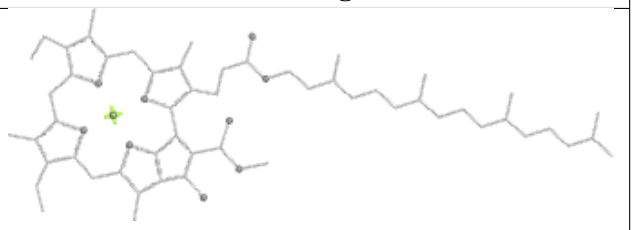
Bond lengths



Bond angles



Torsions

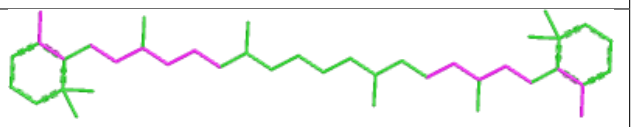


Rings

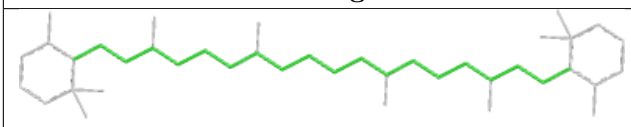
Ligand BCR K 101



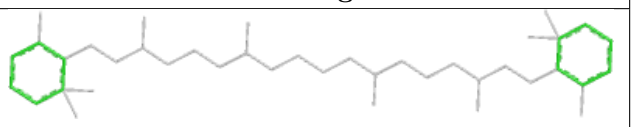
Bond lengths



Bond angles

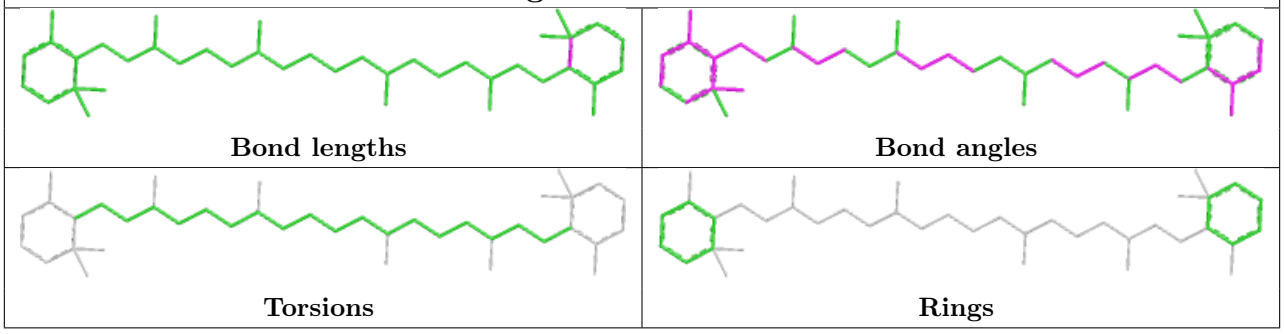


Torsions

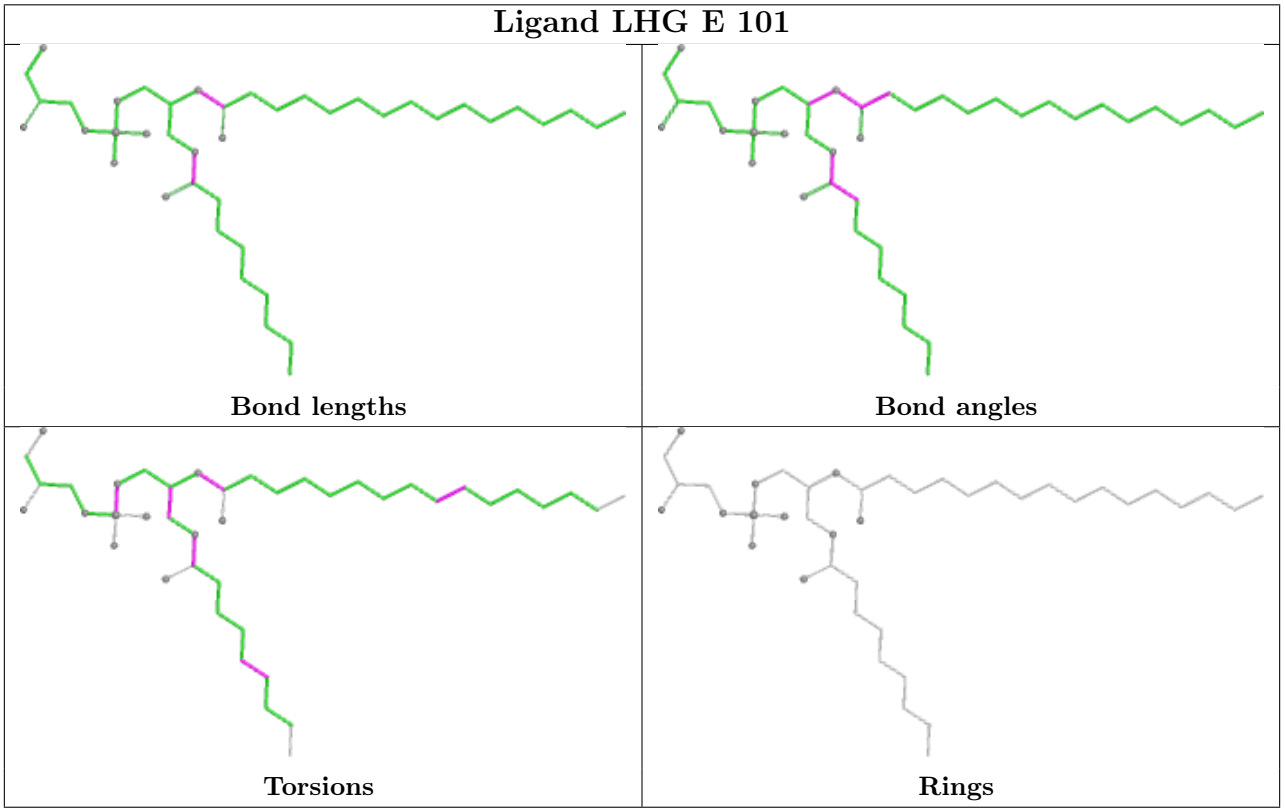


Rings

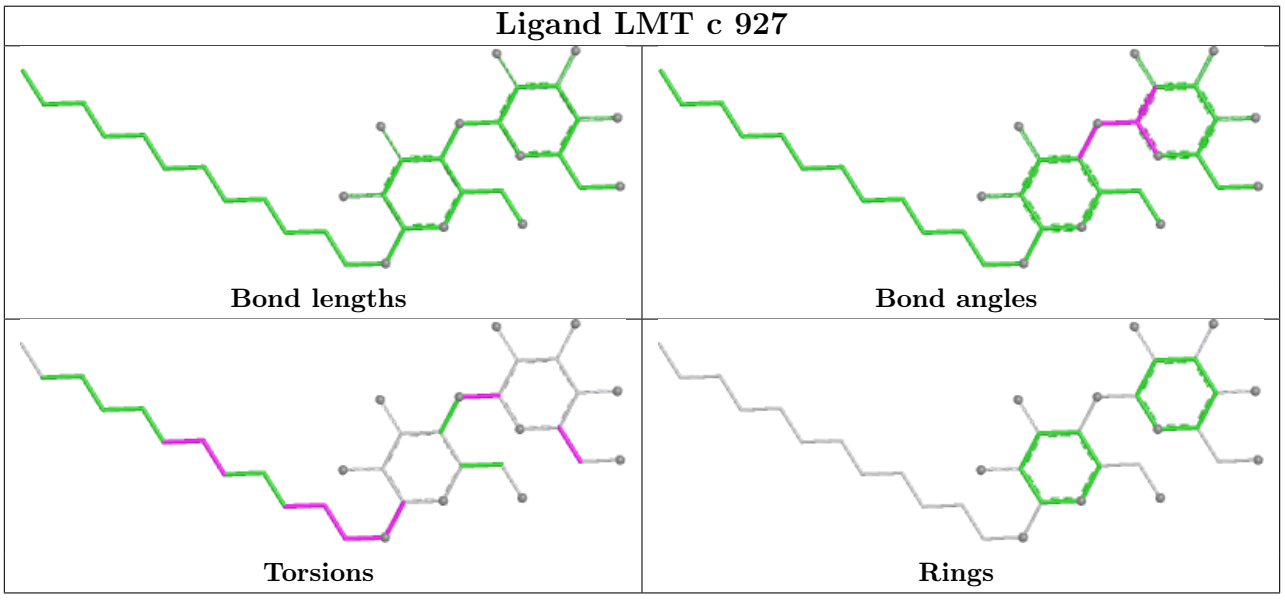
Ligand BCR b 623



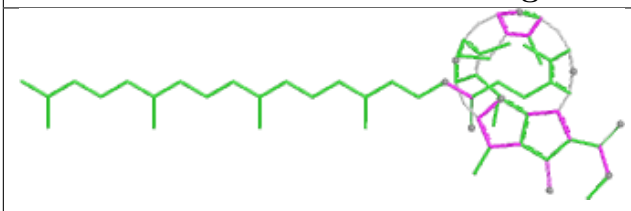
Ligand LHG E 101



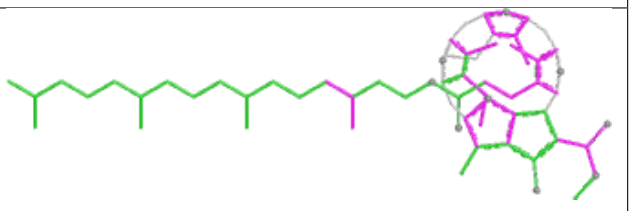
Ligand LMT c 927



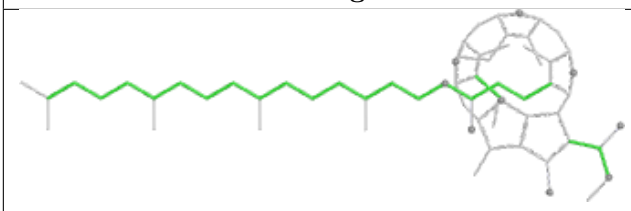
Ligand PHO A 408



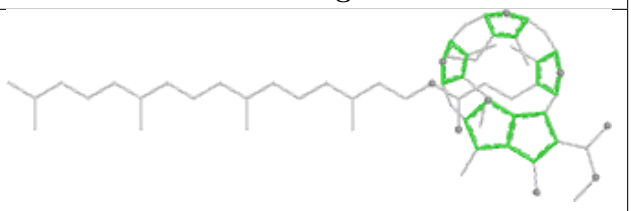
Bond lengths



Bond angles

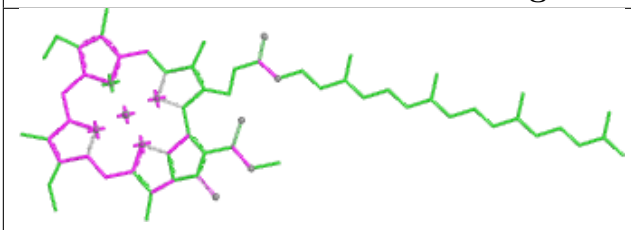


Torsions

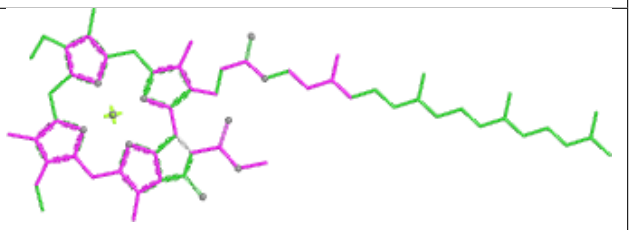


Rings

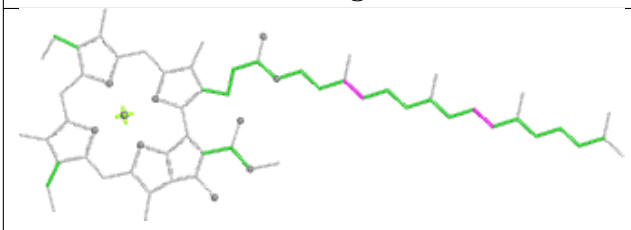
Ligand CLA c 914



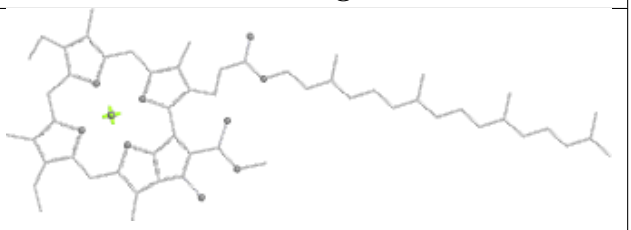
Bond lengths



Bond angles

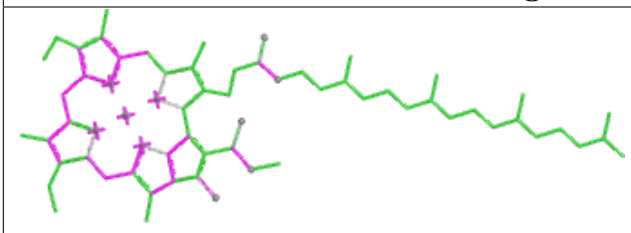


Torsions

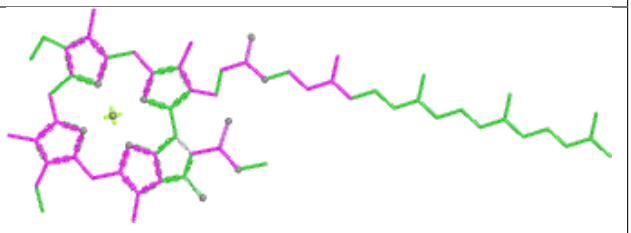


Rings

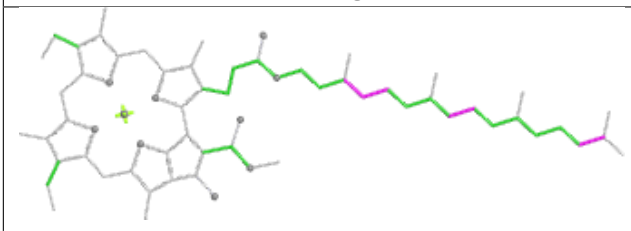
Ligand CLA D 402



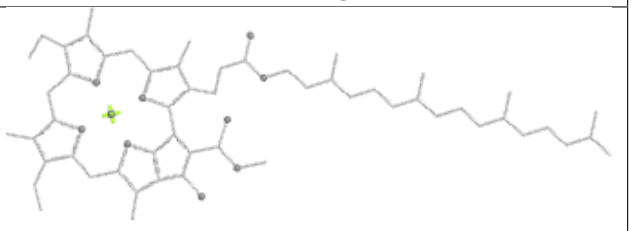
Bond lengths



Bond angles

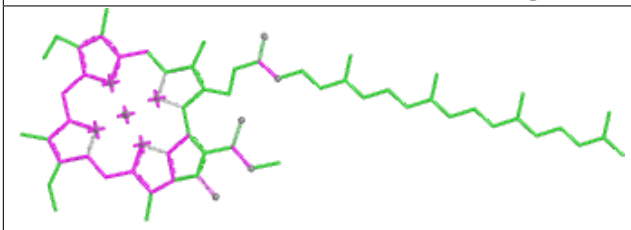


Torsions

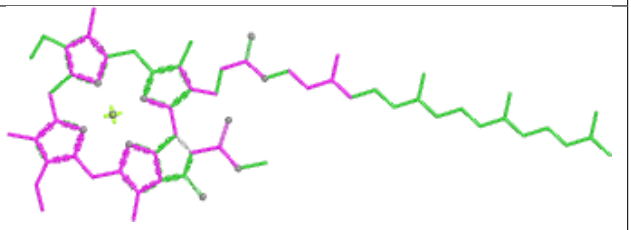


Rings

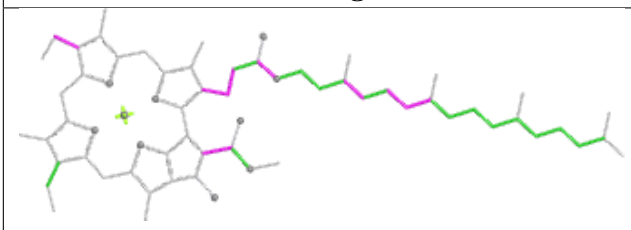
Ligand CLA B 602



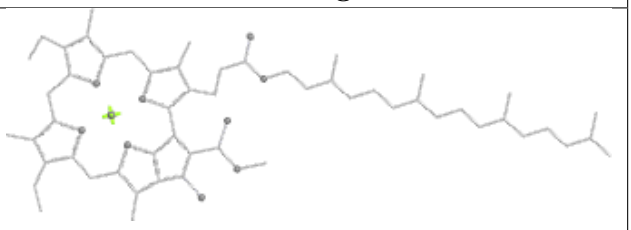
Bond lengths



Bond angles

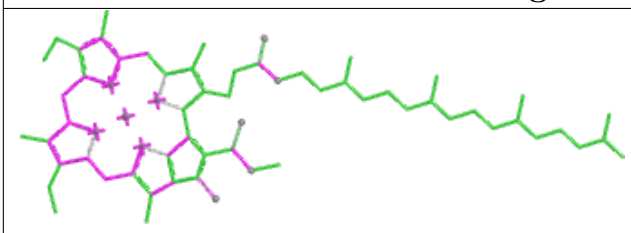


Torsions

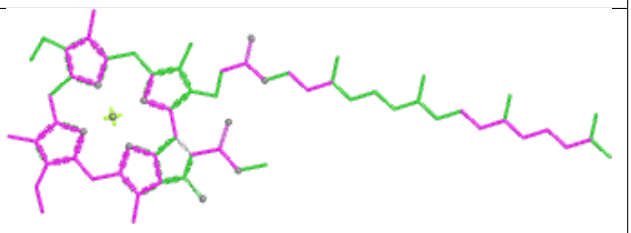


Rings

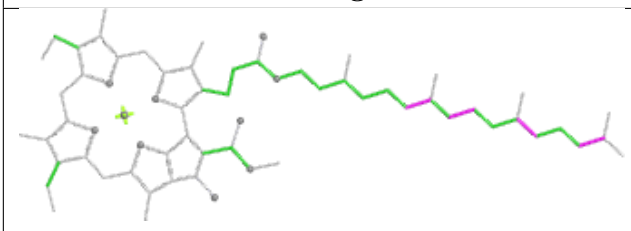
Ligand CLA c 910



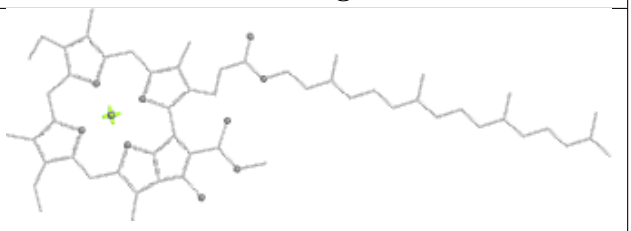
Bond lengths



Bond angles

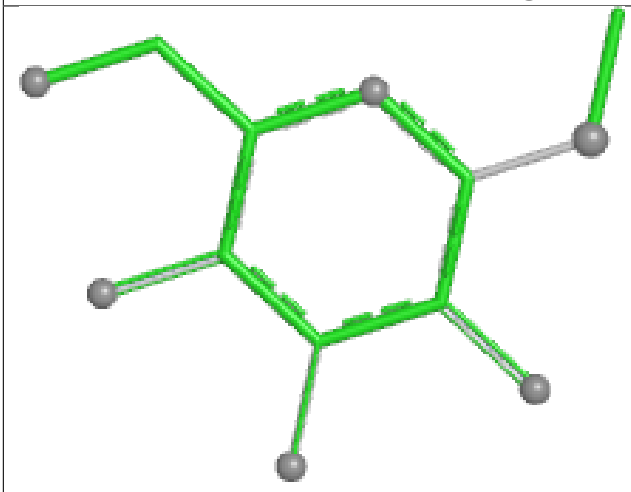


Torsions

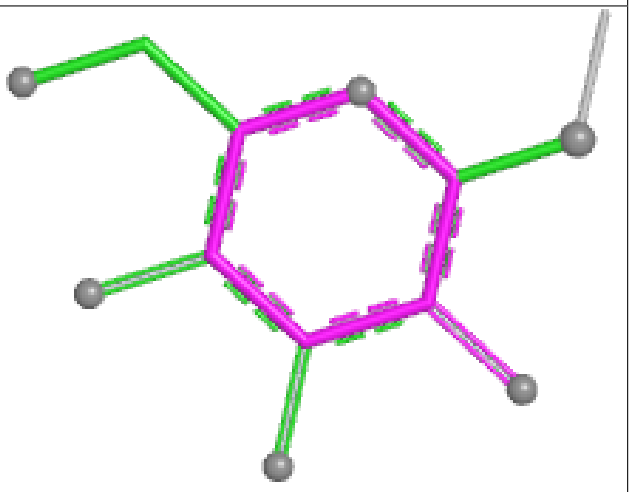


Rings

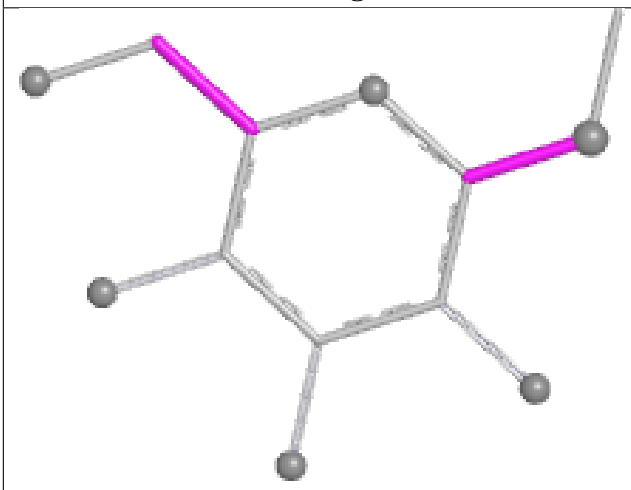
Ligand HTG V 204



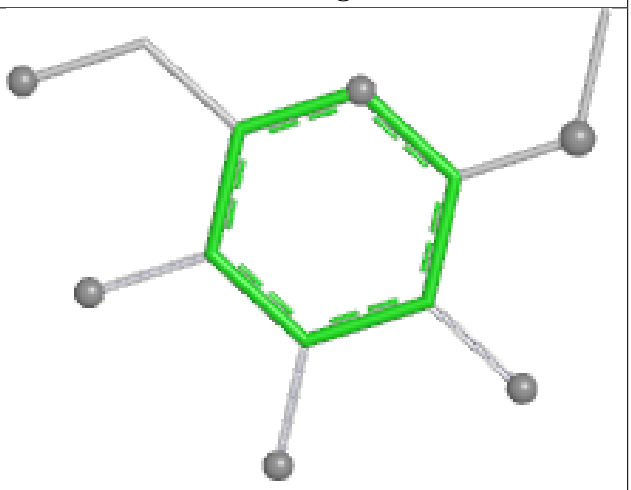
Bond lengths



Bond angles

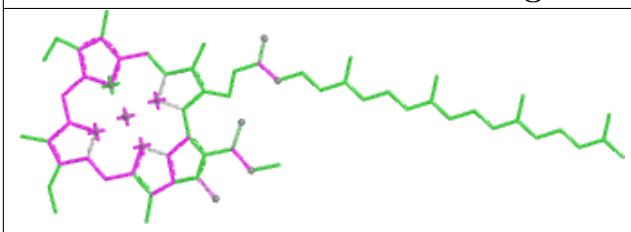


Torsions

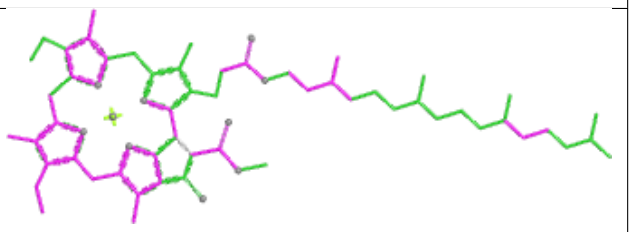


Rings

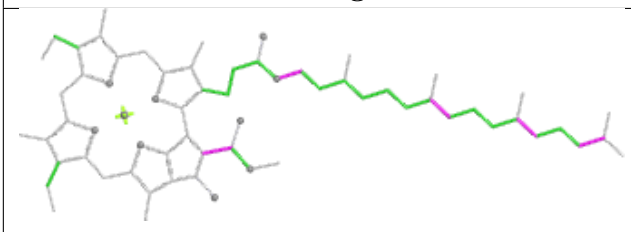
Ligand CLA C 509



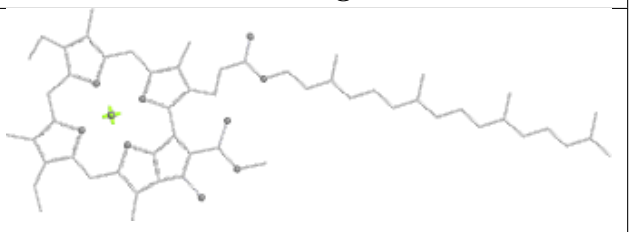
Bond lengths



Bond angles

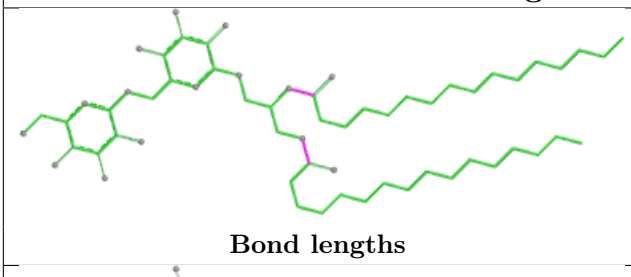


Torsions

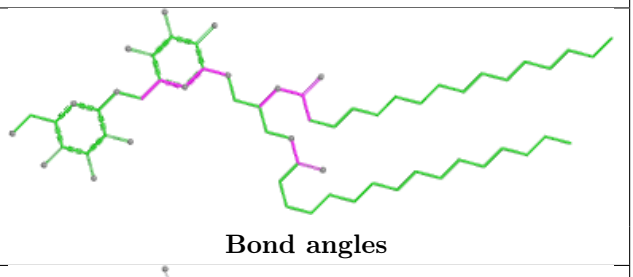


Rings

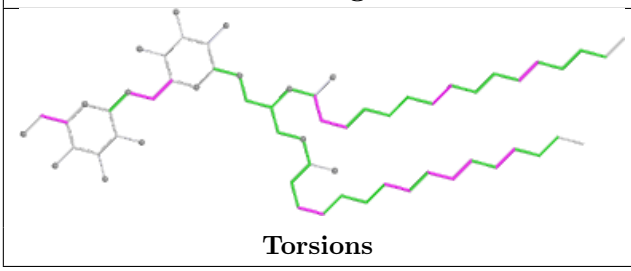
Ligand DGD c 917



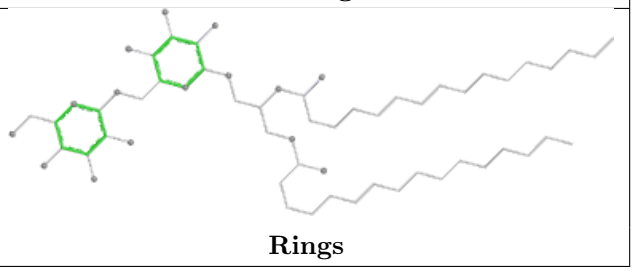
Bond lengths



Bond angles

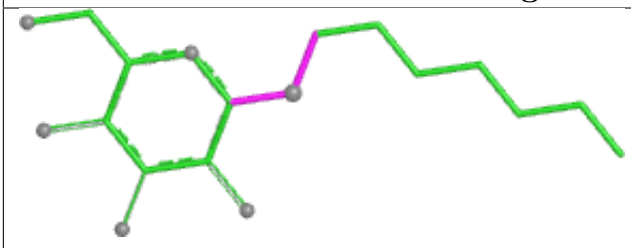


Torsions

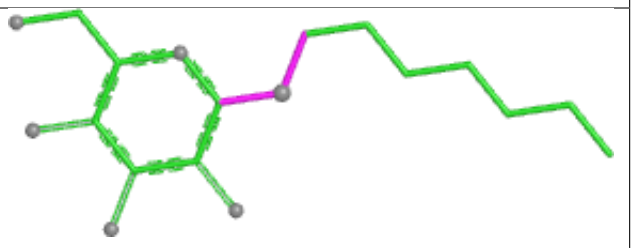


Rings

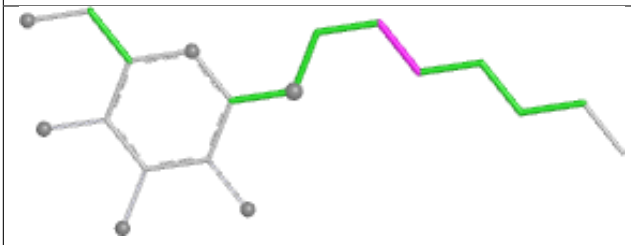
Ligand HTG C 536



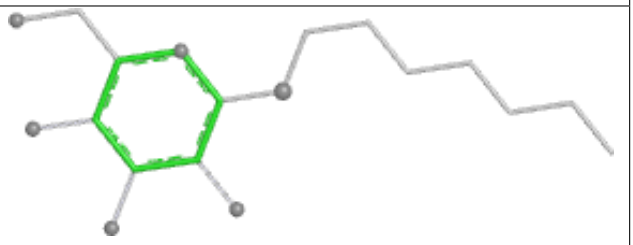
Bond lengths



Bond angles

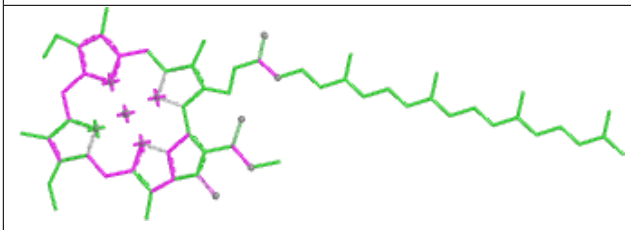


Torsions

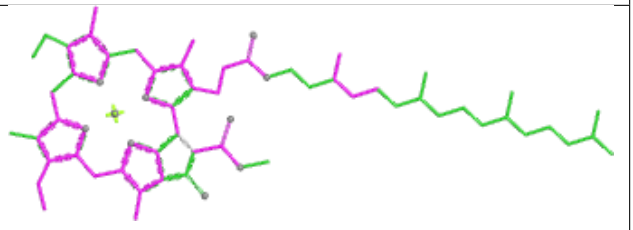


Rings

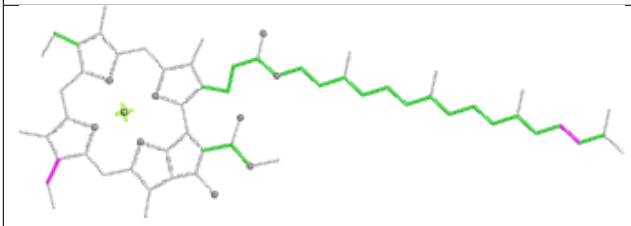
Ligand CLA d 401



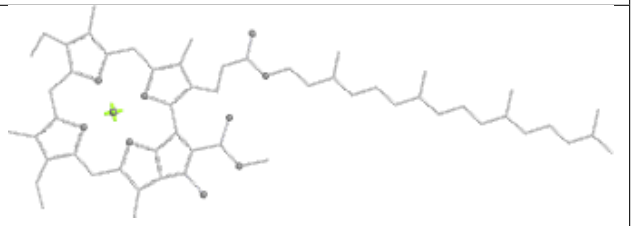
Bond lengths



Bond angles

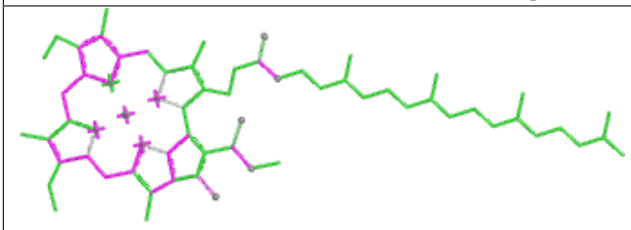


Torsions

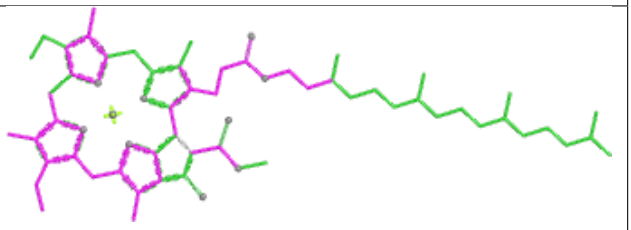


Rings

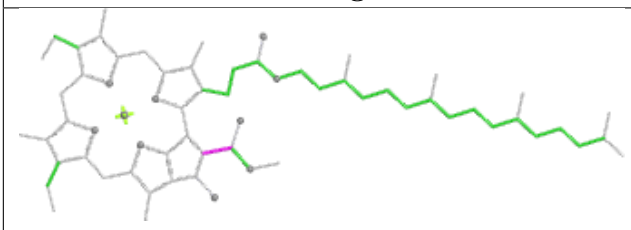
Ligand CLA B 608



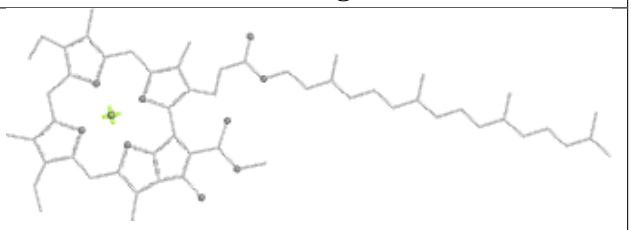
Bond lengths



Bond angles

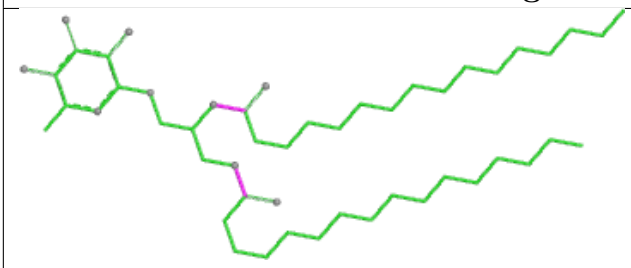


Torsions

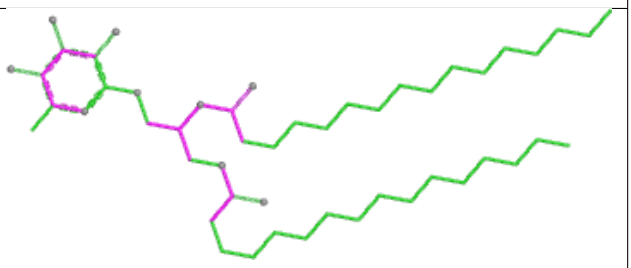


Rings

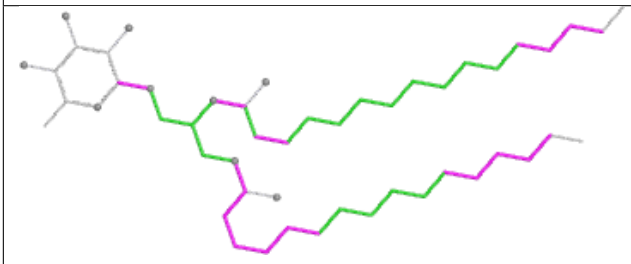
Ligand DGD d 408



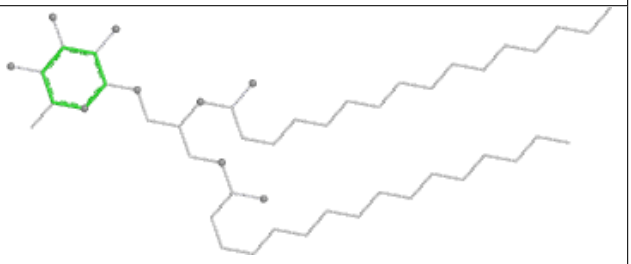
Bond lengths



Bond angles

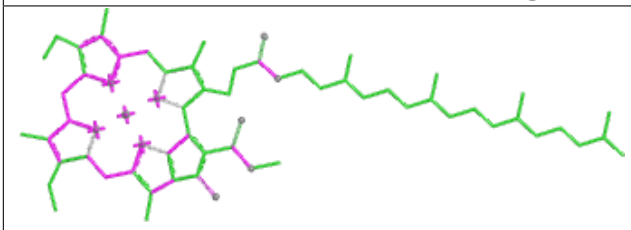


Torsions

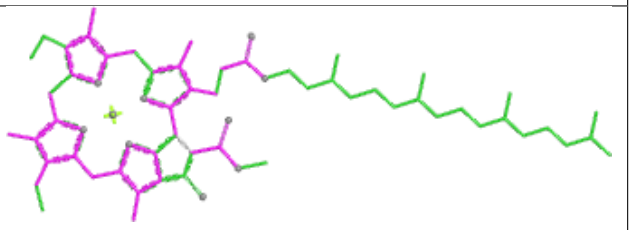


Rings

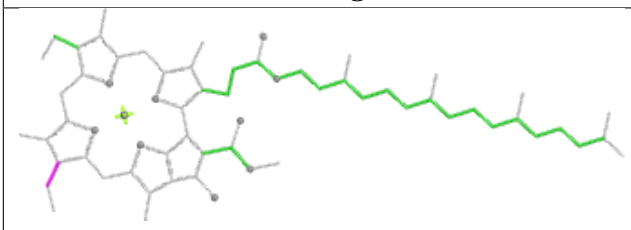
Ligand CLA A 405



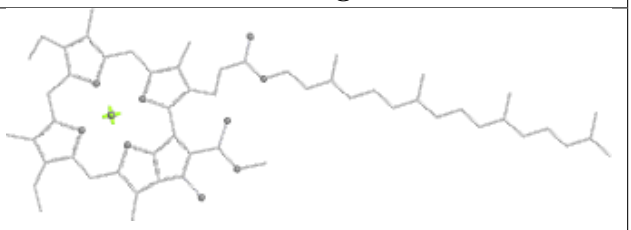
Bond lengths



Bond angles

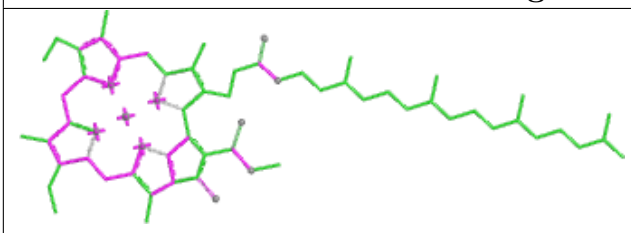


Torsions

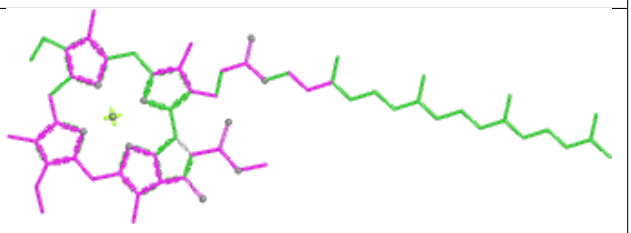


Rings

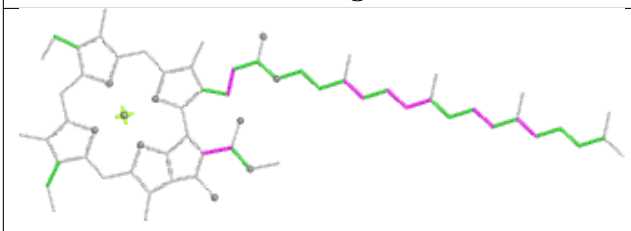
Ligand CLA b 618



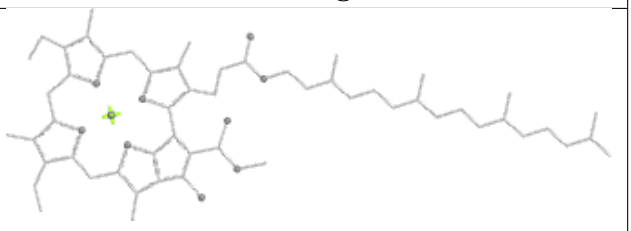
Bond lengths



Bond angles

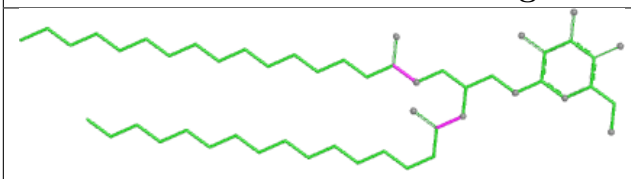


Torsions

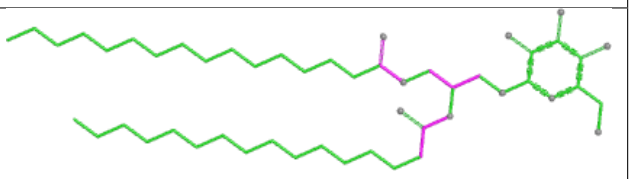


Rings

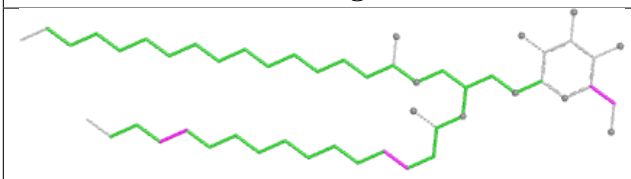
Ligand LMG D 409



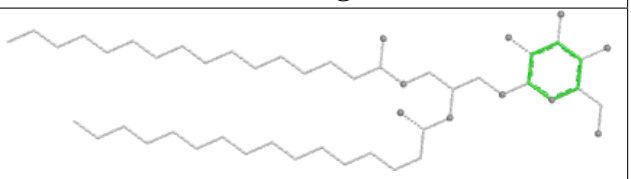
Bond lengths



Bond angles

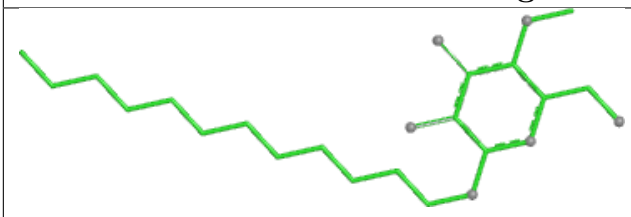


Torsions

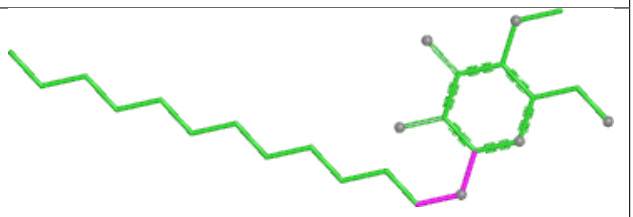


Rings

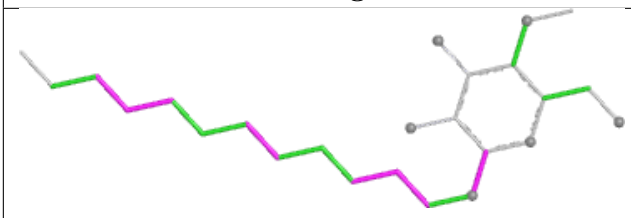
Ligand LMT M 102



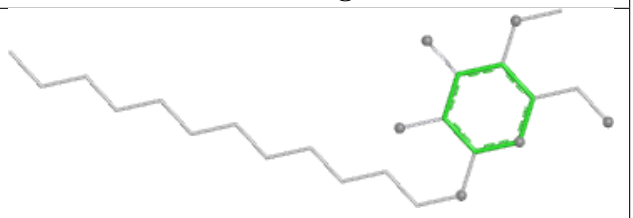
Bond lengths



Bond angles

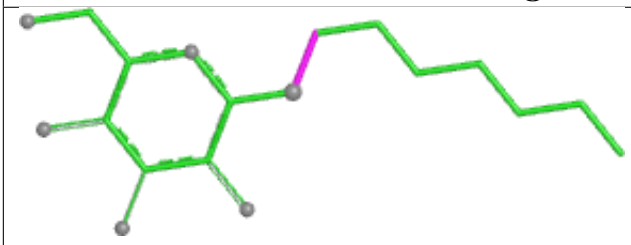


Torsions

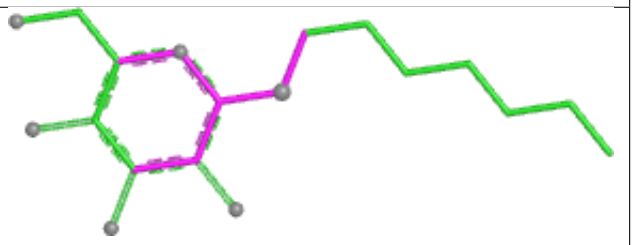


Rings

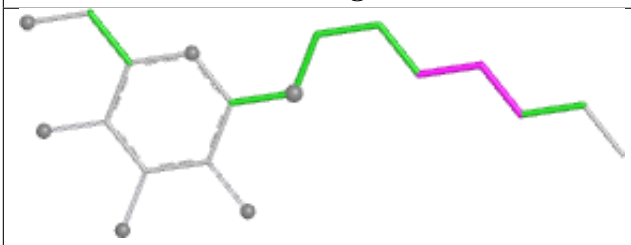
Ligand HTG b 626



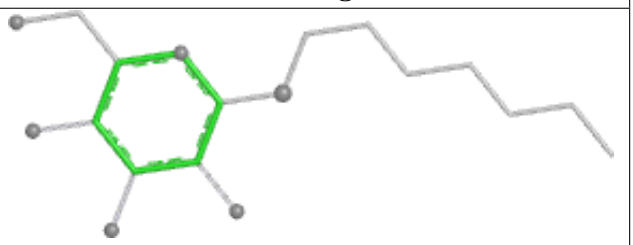
Bond lengths



Bond angles

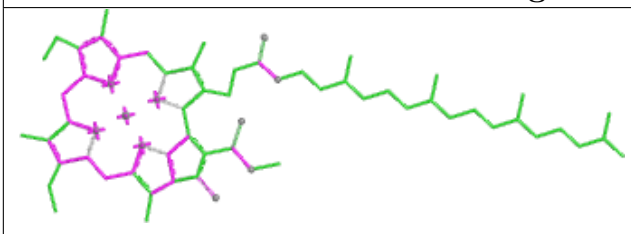


Torsions

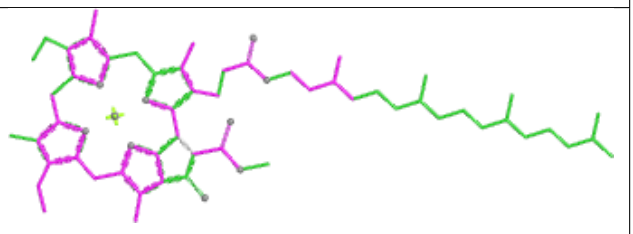


Rings

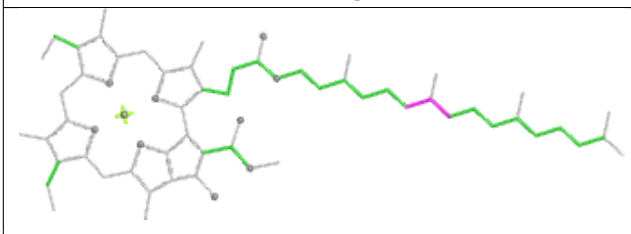
Ligand CLA a 410



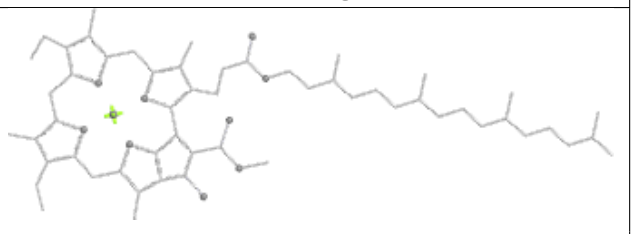
Bond lengths



Bond angles

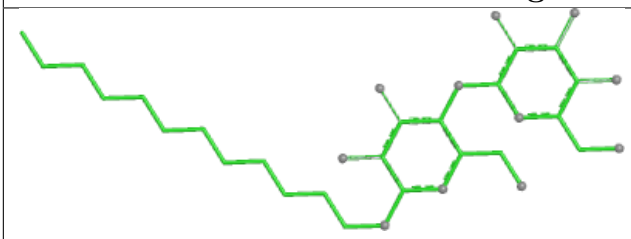


Torsions

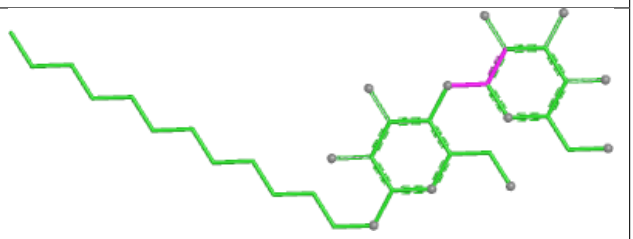


Rings

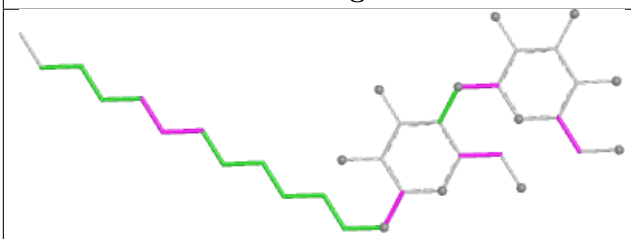
Ligand LMT t 102



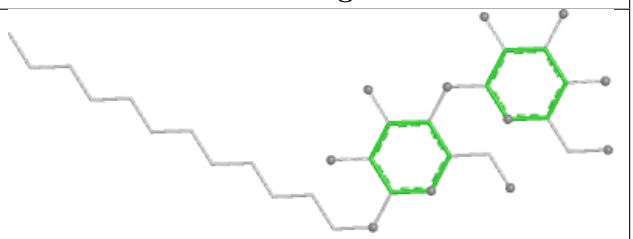
Bond lengths



Bond angles

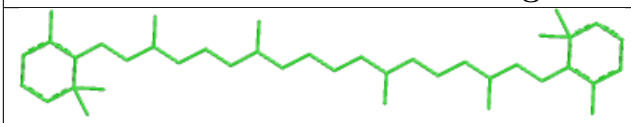


Torsions

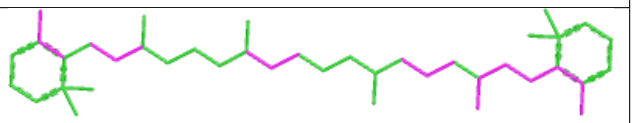


Rings

Ligand BCR C 515



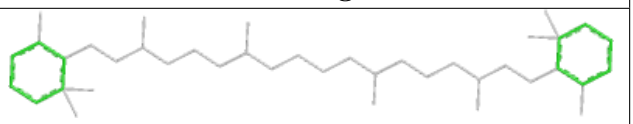
Bond lengths



Bond angles

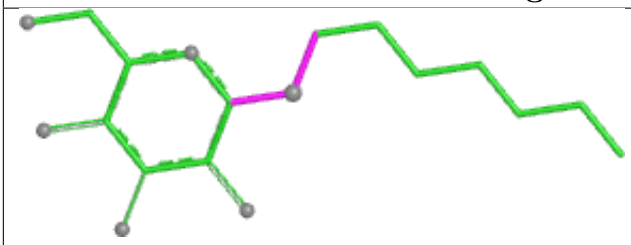


Torsions

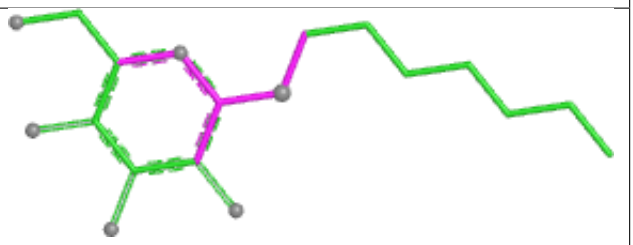


Rings

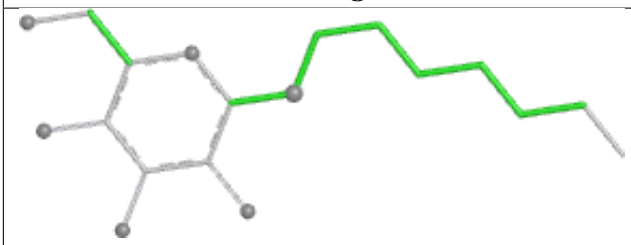
Ligand HTG c 928



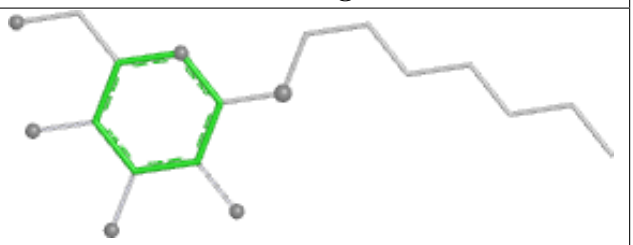
Bond lengths



Bond angles

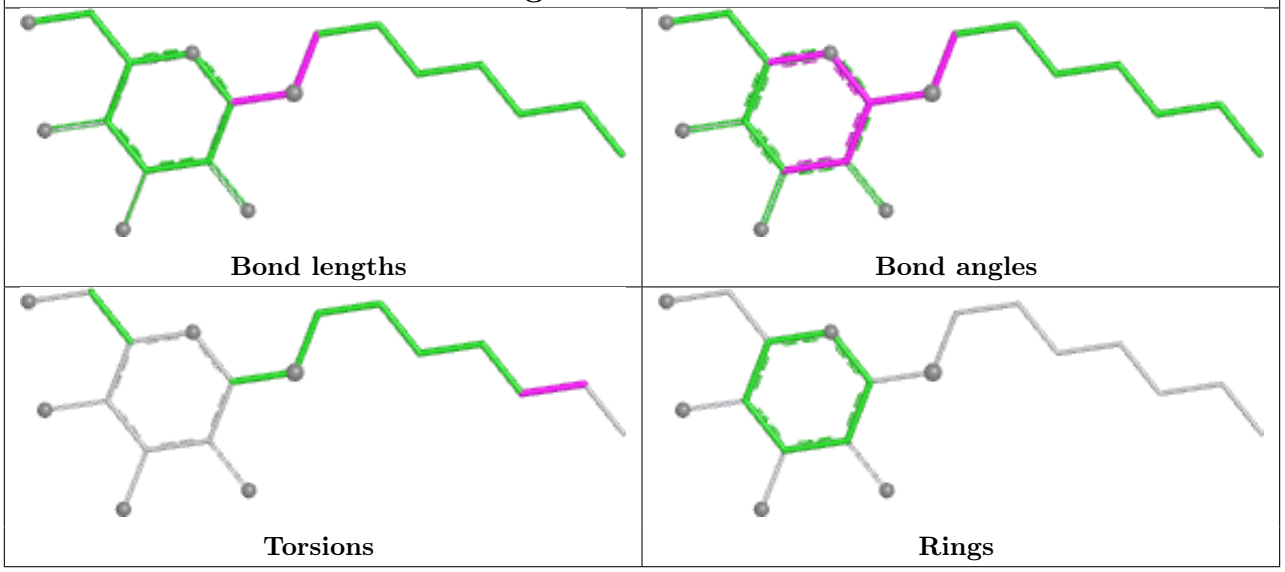


Torsions



Rings

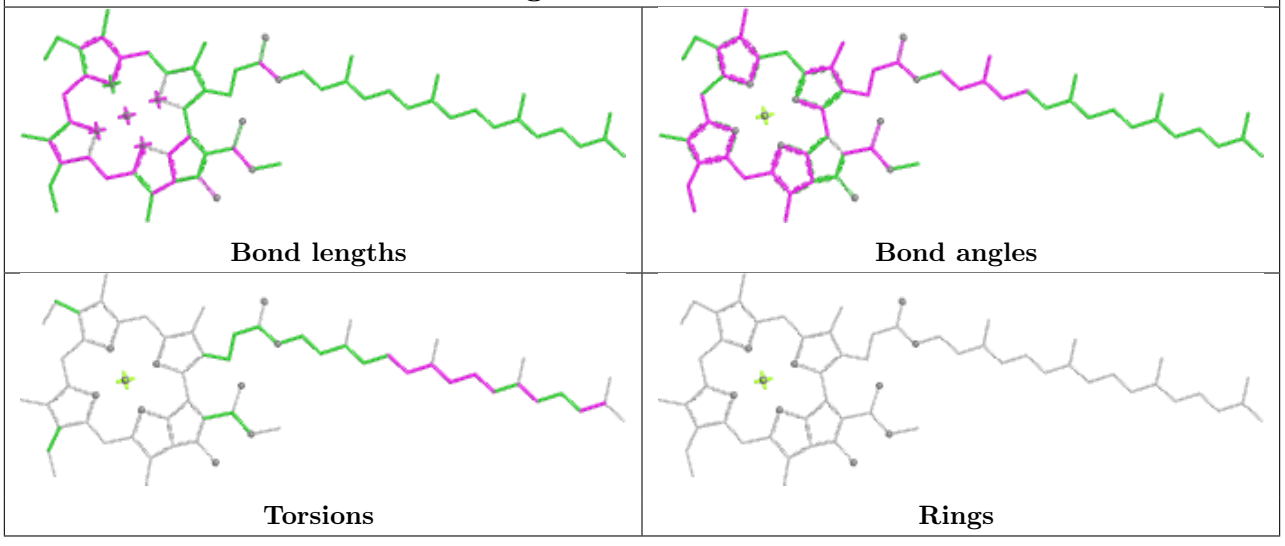
Ligand HTG v 211



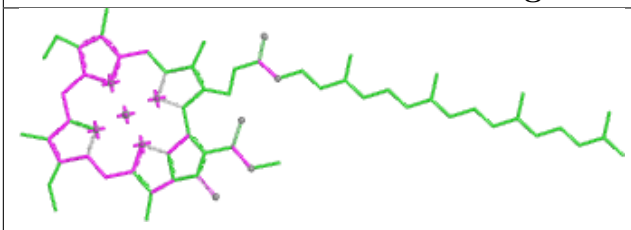
Ligand PL9 d 407



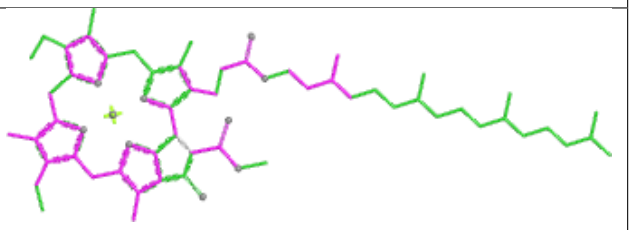
Ligand CLA B 617



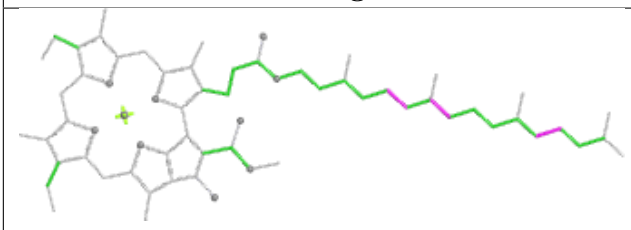
Ligand CLA C 508



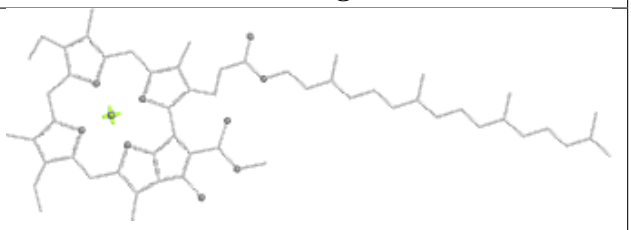
Bond lengths



Bond angles

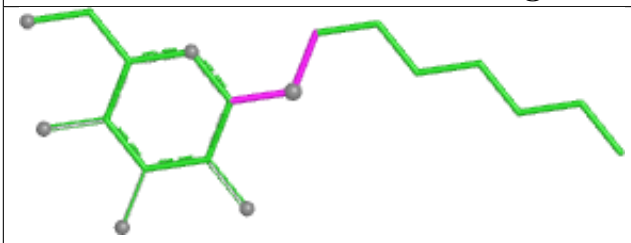


Torsions

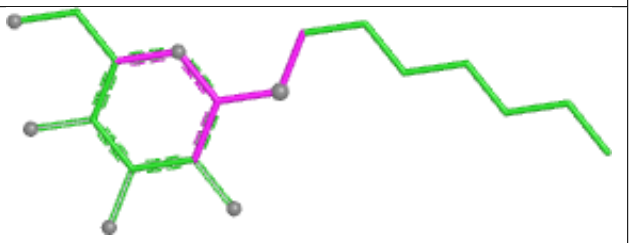


Rings

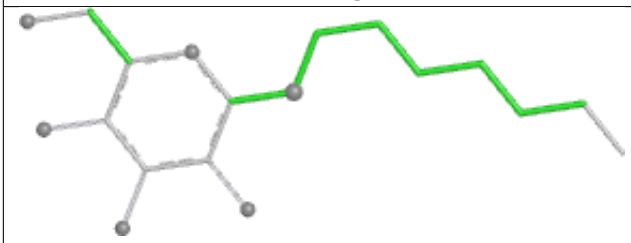
Ligand HTG b 603



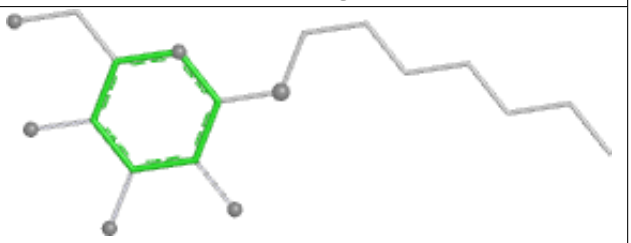
Bond lengths



Bond angles

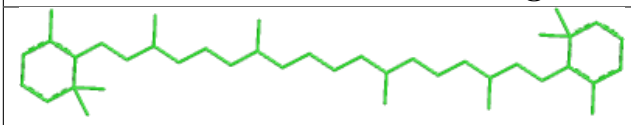


Torsions

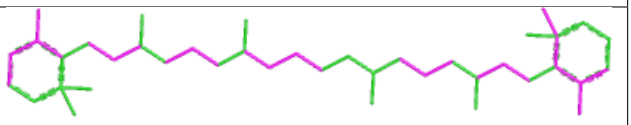


Rings

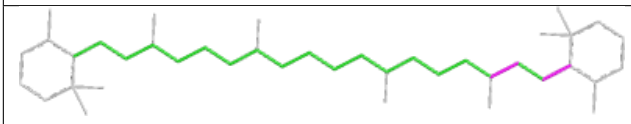
Ligand BCR d 406



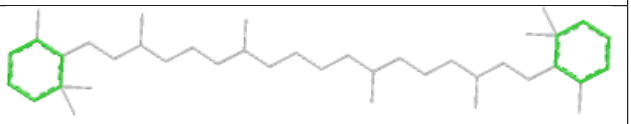
Bond lengths



Bond angles

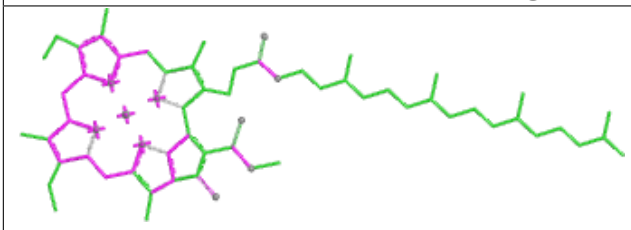


Torsions

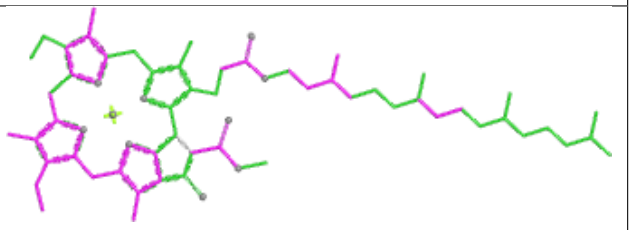


Rings

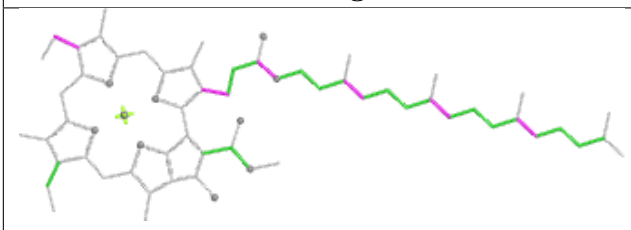
Ligand CLA C 513



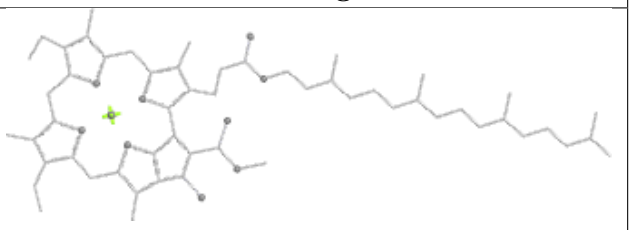
Bond lengths



Bond angles

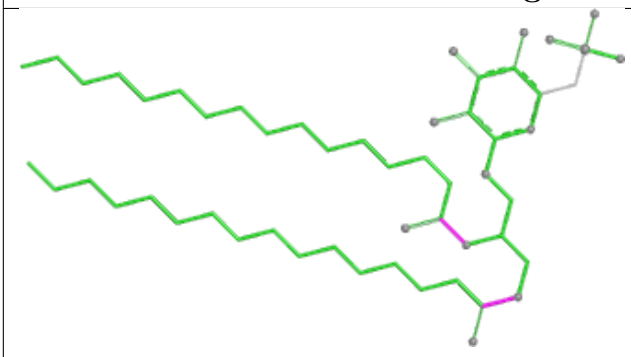


Torsions

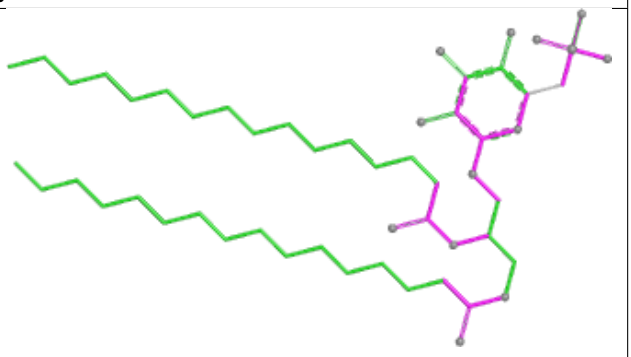


Rings

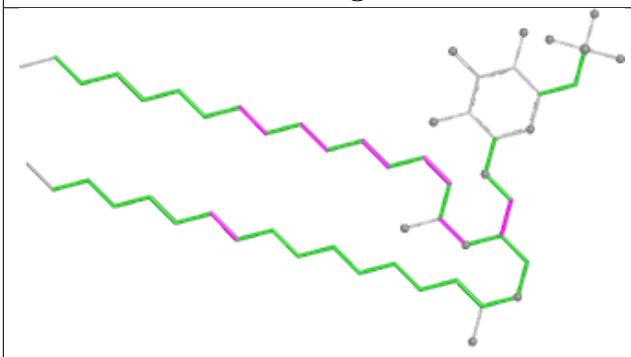
Ligand SQD A 412



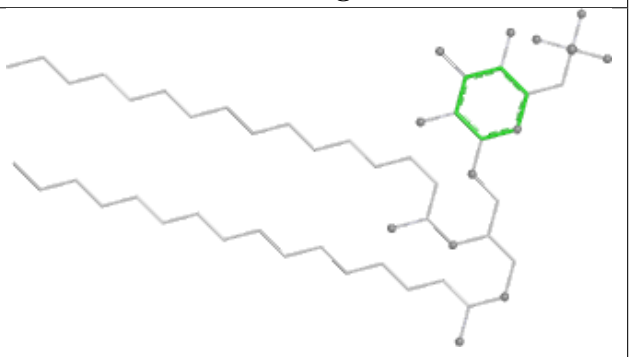
Bond lengths



Bond angles

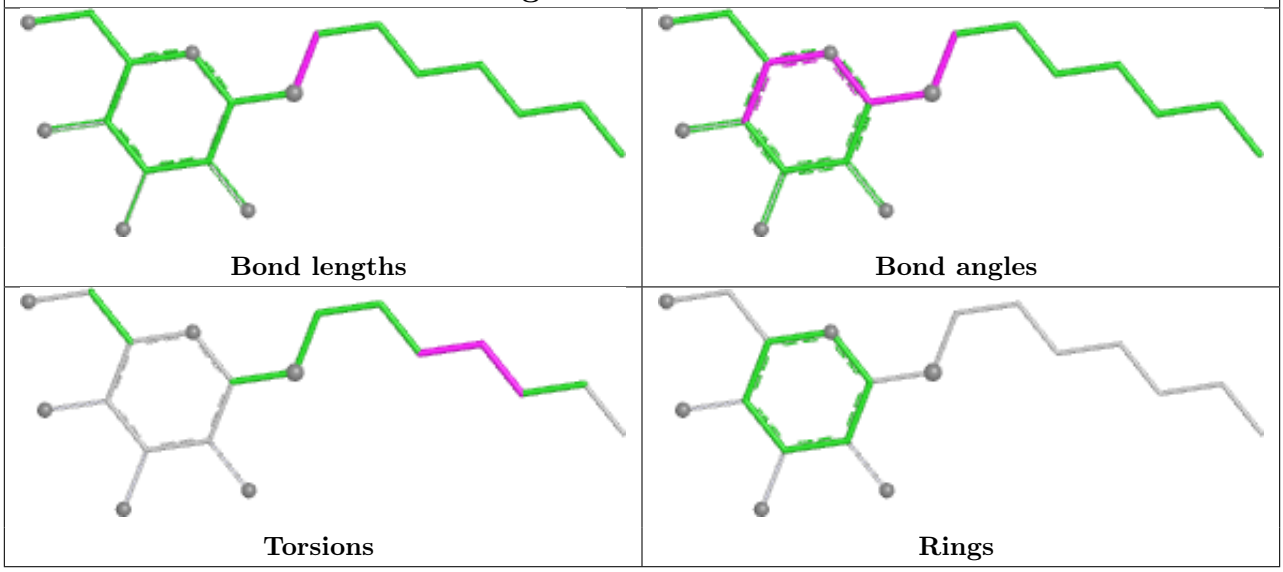


Torsions

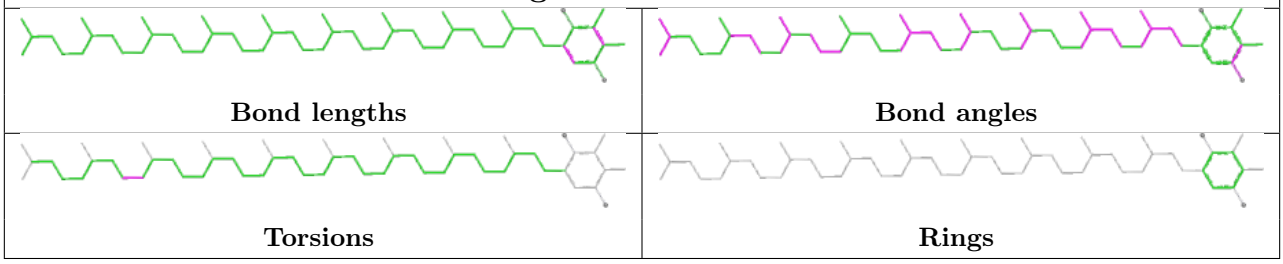


Rings

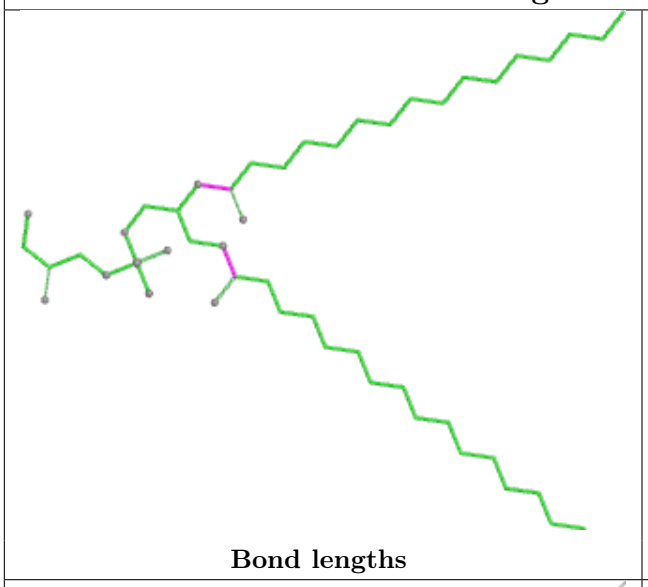
Ligand HTG C 537



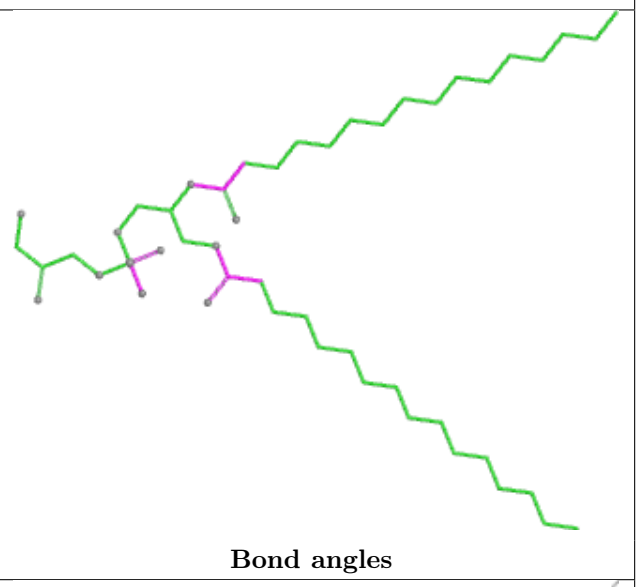
Ligand PL9 D 404



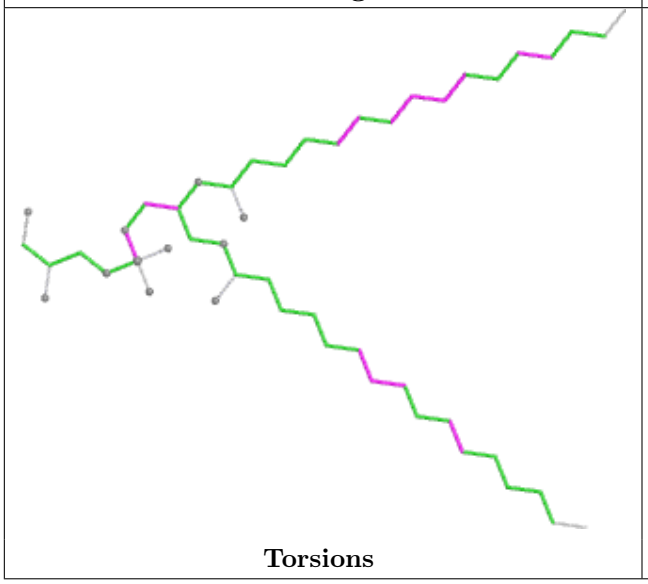
Ligand LHG l 103



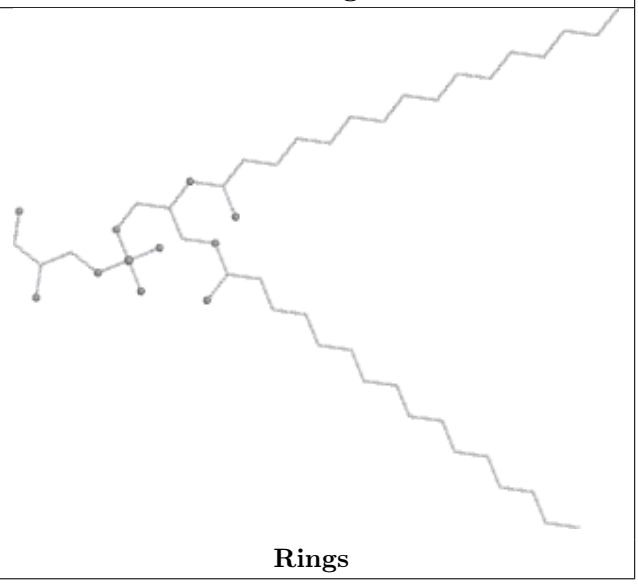
Bond lengths



Bond angles

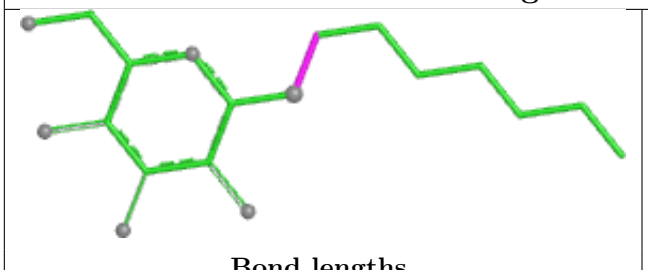


Torsions

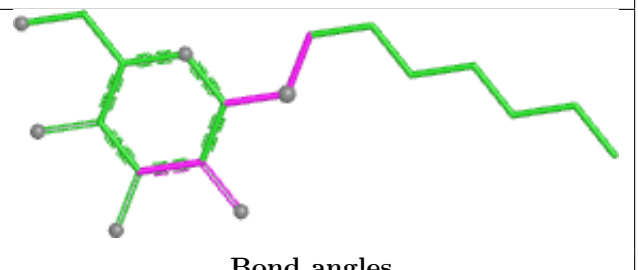


Rings

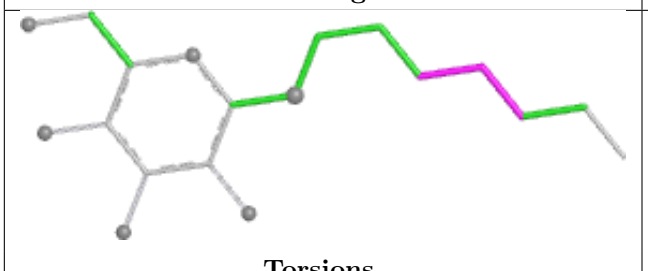
Ligand HTG O 303



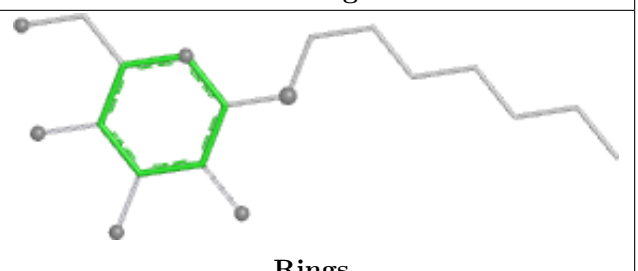
Bond lengths



Bond angles

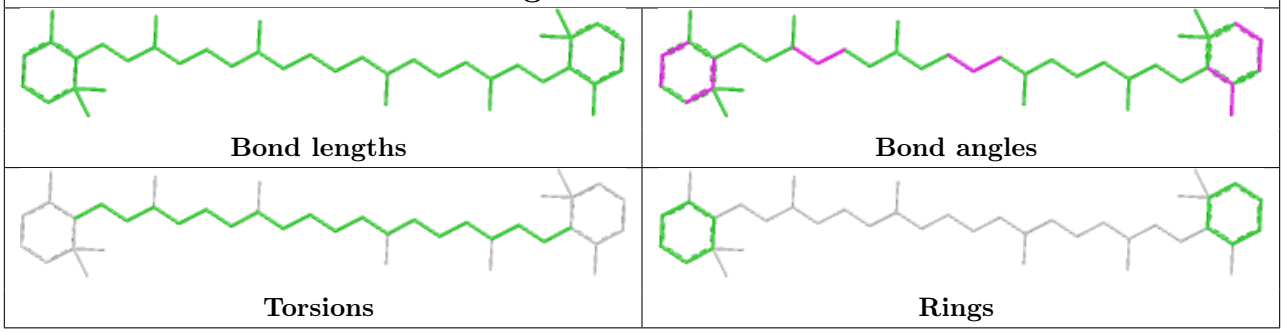


Torsions

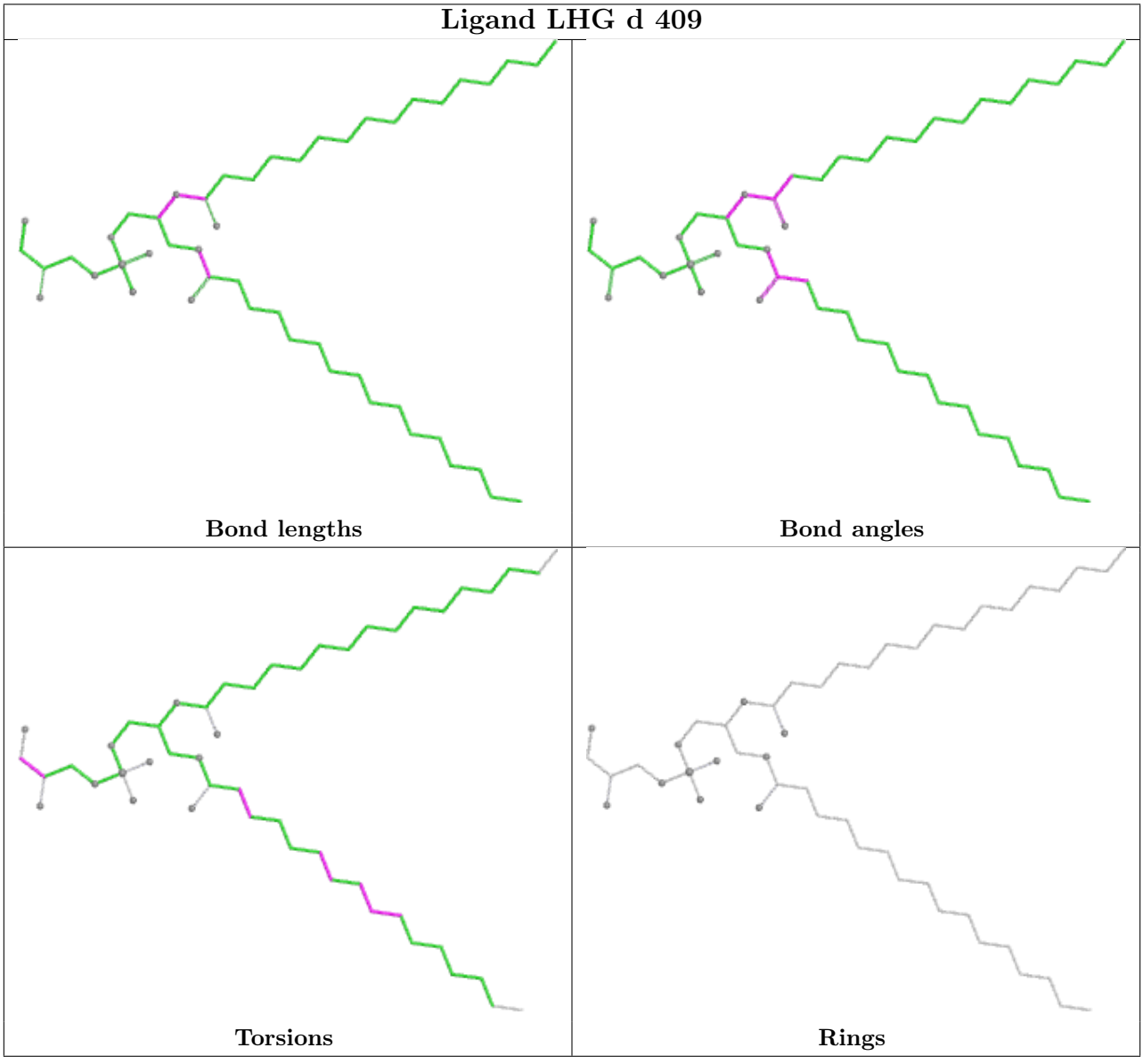


Rings

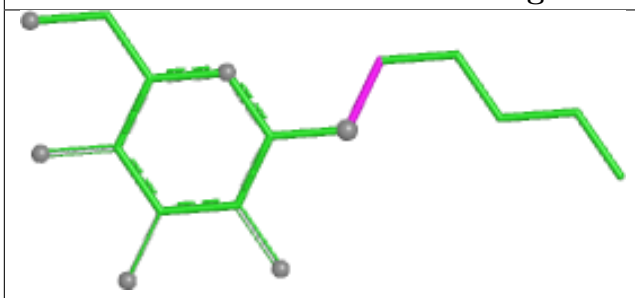
Ligand BCR B 619



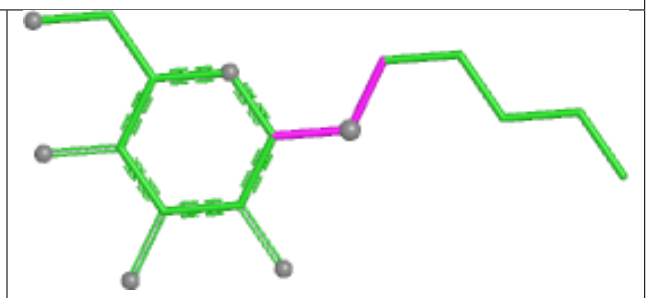
Ligand LHG d 409



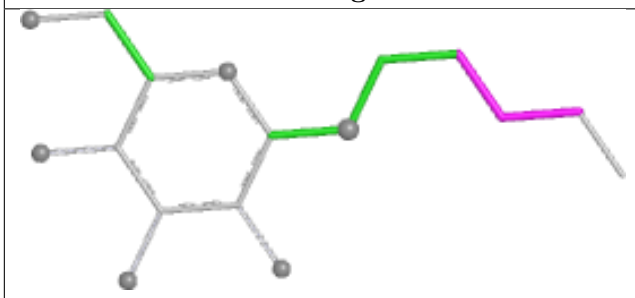
Ligand HTG c 943



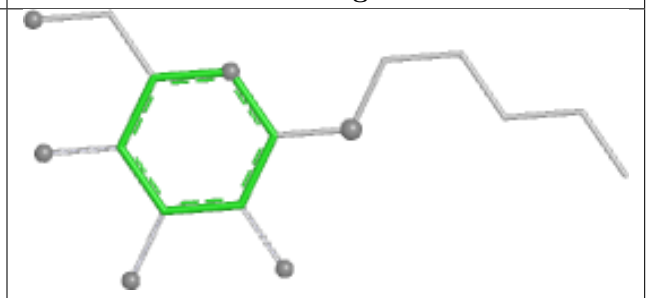
Bond lengths



Bond angles

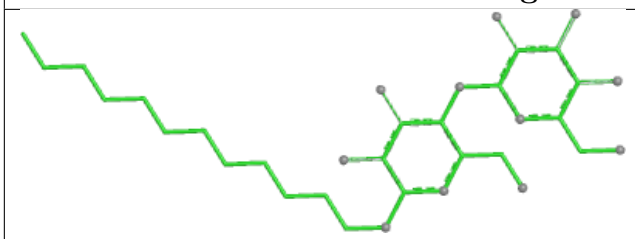


Torsions

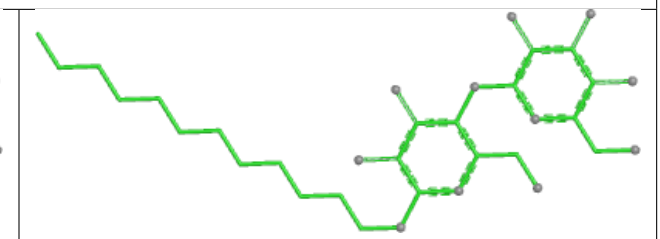


Rings

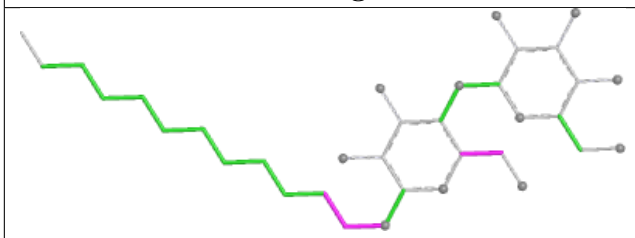
Ligand LMT m 102



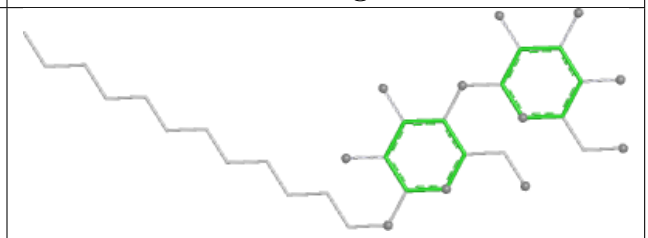
Bond lengths



Bond angles

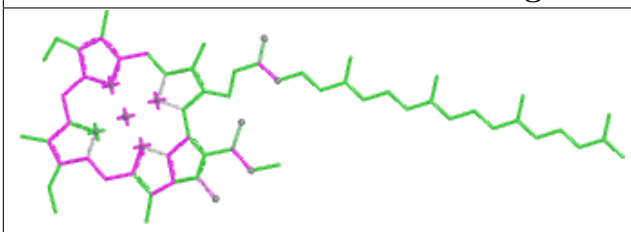


Torsions

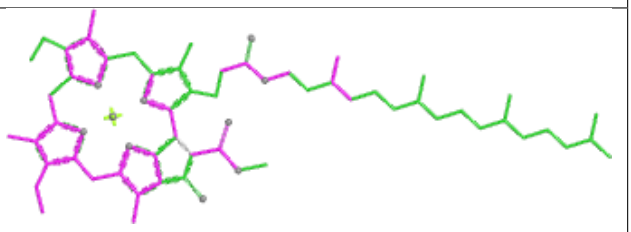


Rings

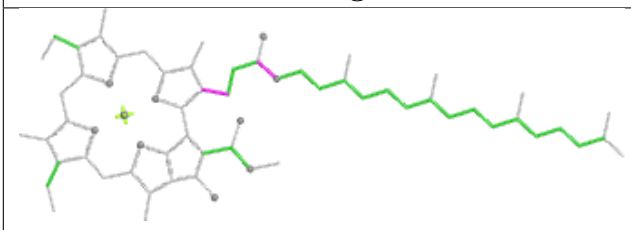
Ligand CLA C 511



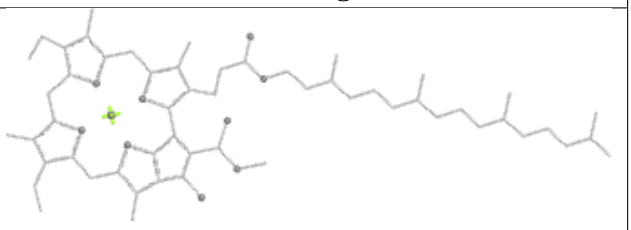
Bond lengths



Bond angles



Torsions

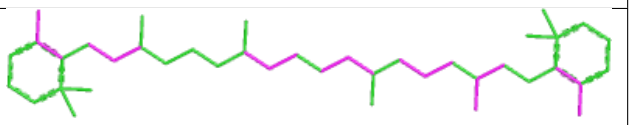


Rings

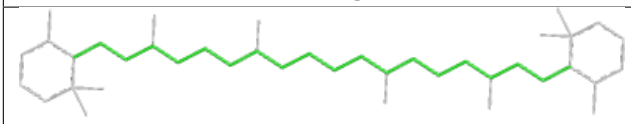
Ligand BCR c 915



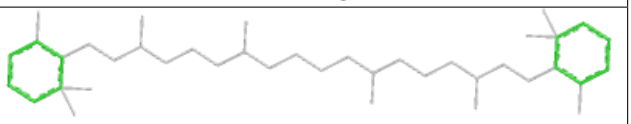
Bond lengths



Bond angles

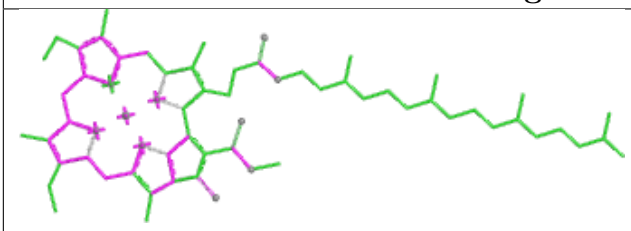


Torsions

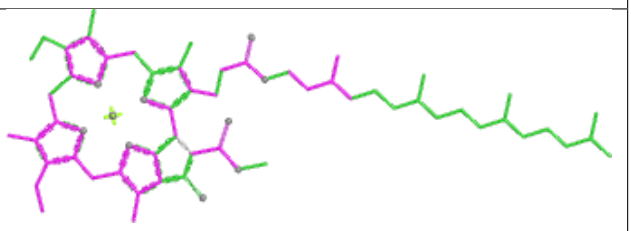


Rings

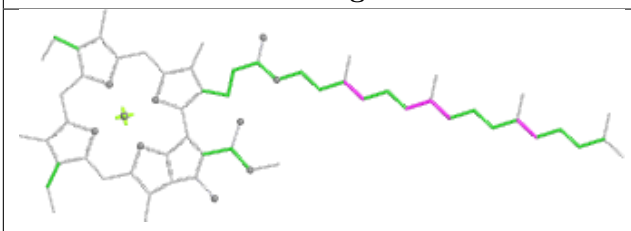
Ligand CLA C 506



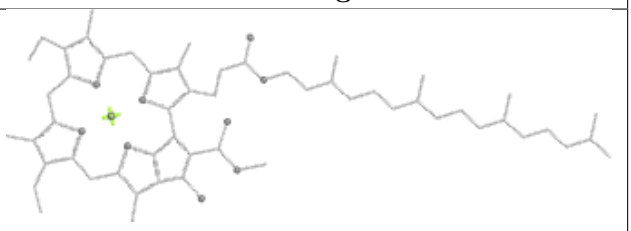
Bond lengths



Bond angles

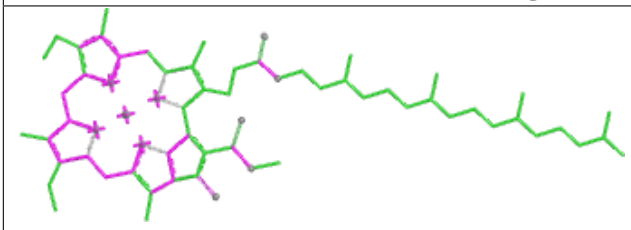


Torsions

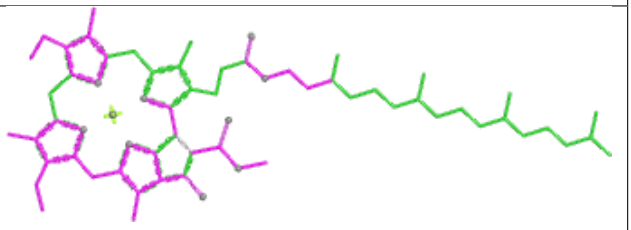


Rings

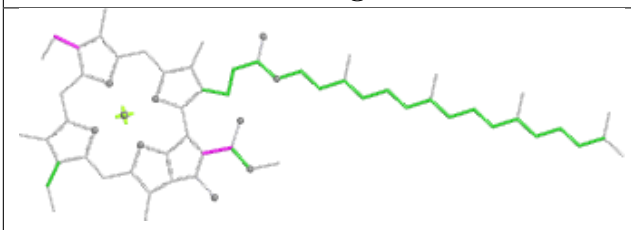
Ligand CLA C 502



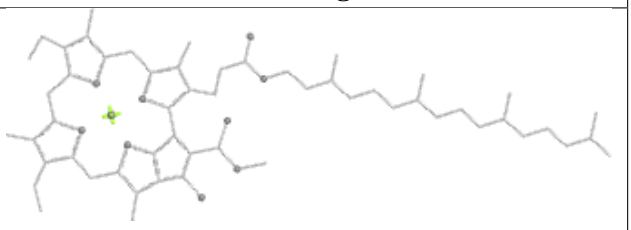
Bond lengths



Bond angles



Torsions

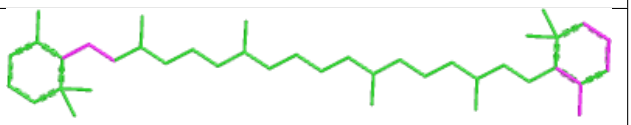


Rings

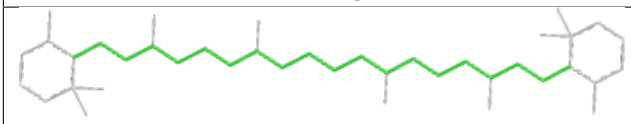
Ligand BCR b 622



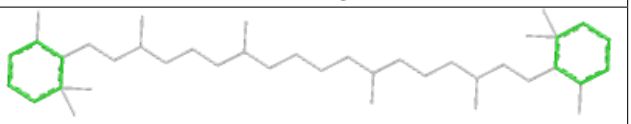
Bond lengths



Bond angles

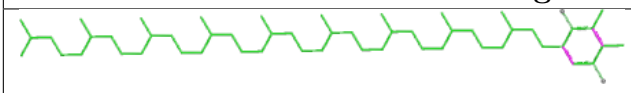


Torsions

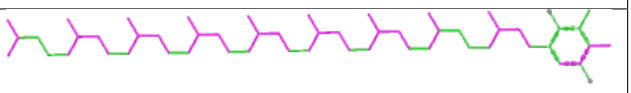


Rings

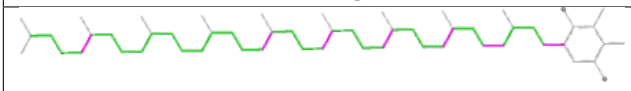
Ligand PL9 a 417



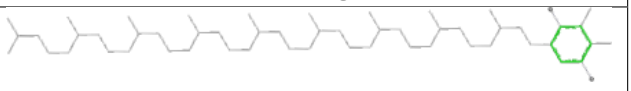
Bond lengths



Bond angles

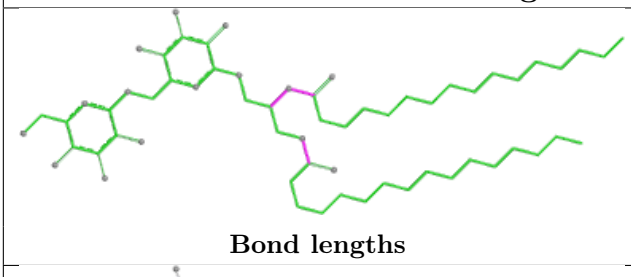


Torsions

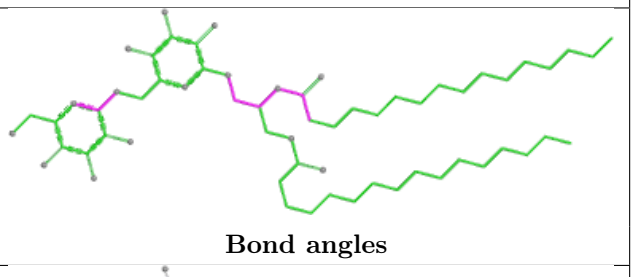


Rings

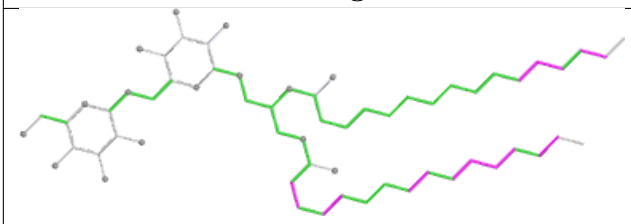
Ligand DGD C 518



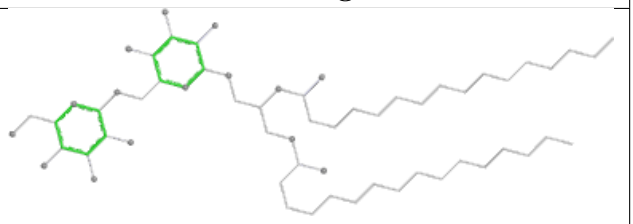
Bond lengths



Bond angles

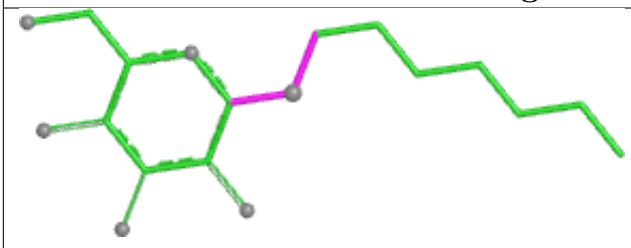


Torsions

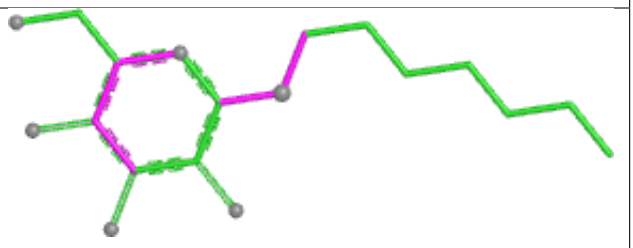


Rings

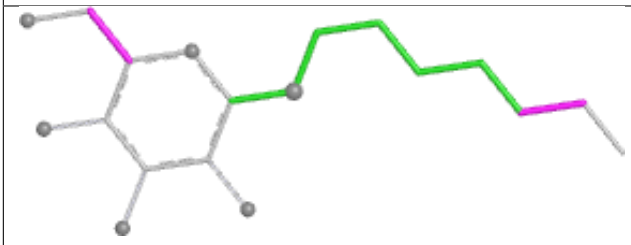
Ligand HTG B 629



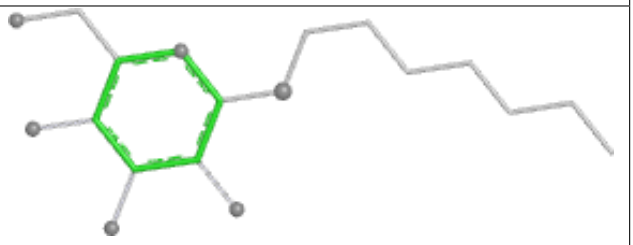
Bond lengths



Bond angles



Torsions

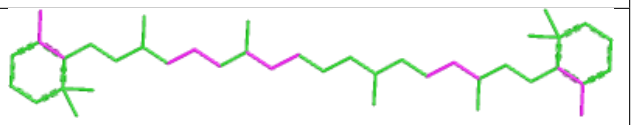


Rings

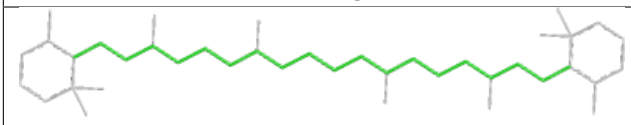
Ligand BCR A 411



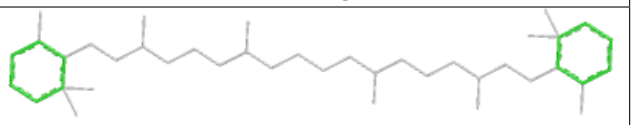
Bond lengths



Bond angles

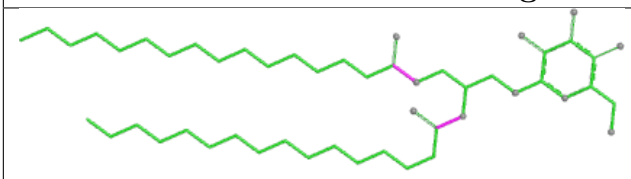


Torsions

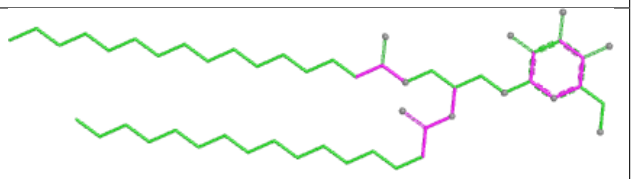


Rings

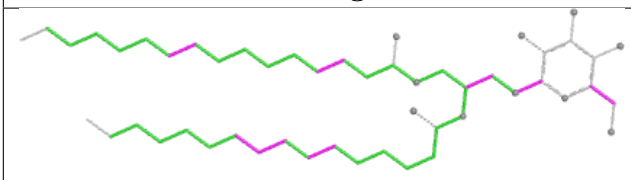
Ligand LMG C 523



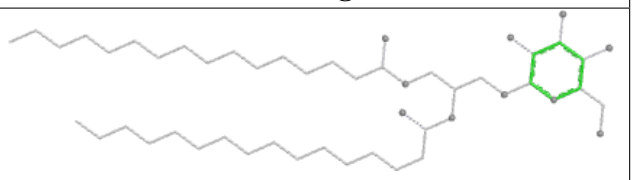
Bond lengths



Bond angles

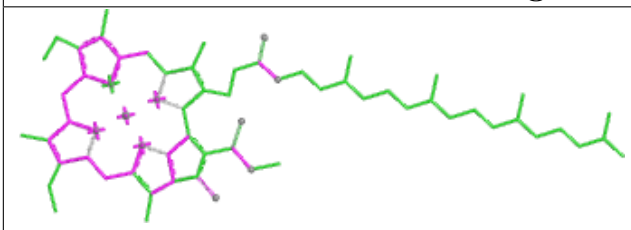


Torsions

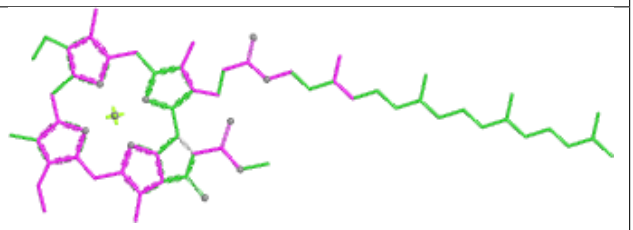


Rings

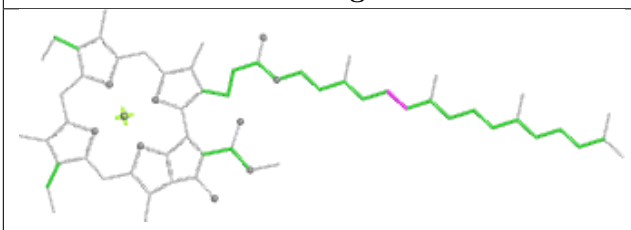
Ligand CLA b 607



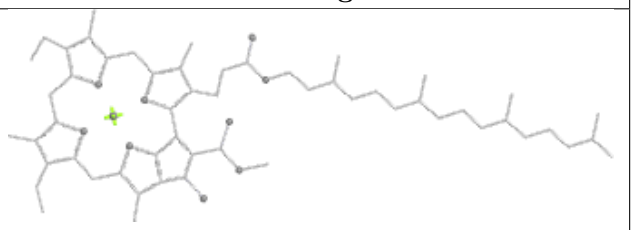
Bond lengths



Bond angles

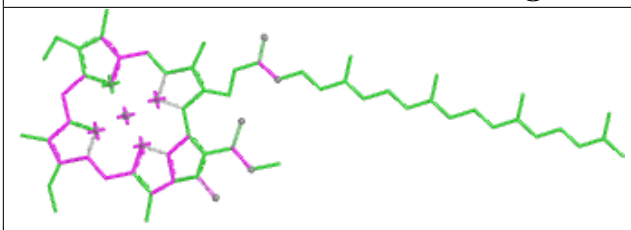


Torsions

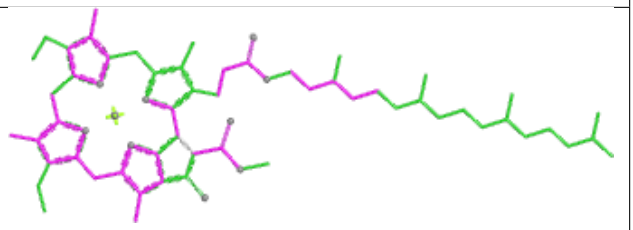


Rings

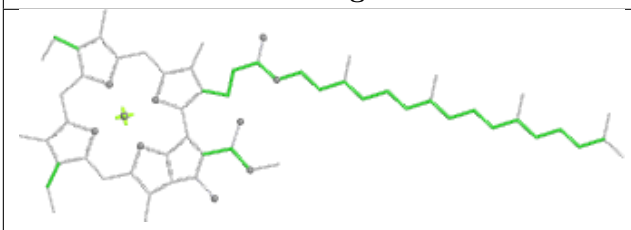
Ligand CLA B 605



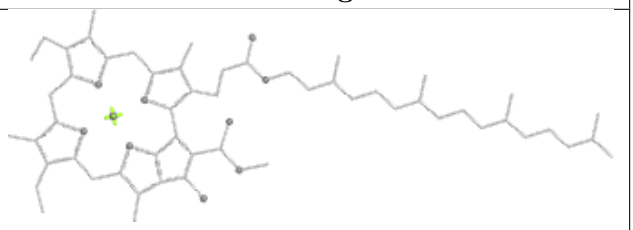
Bond lengths



Bond angles

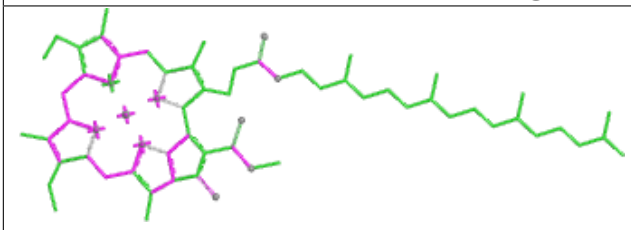


Torsions

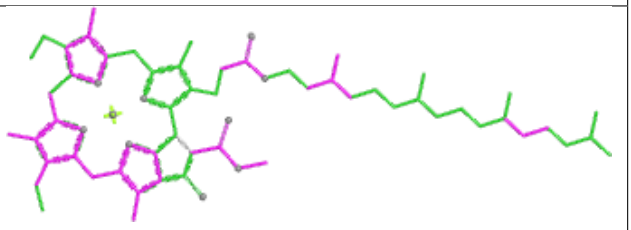


Rings

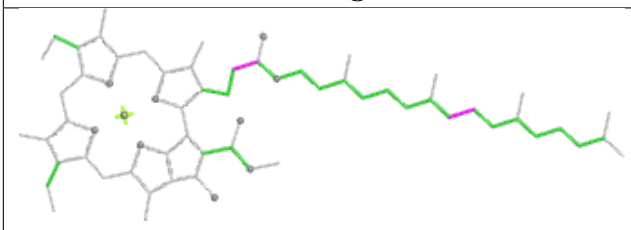
Ligand CLA b 616



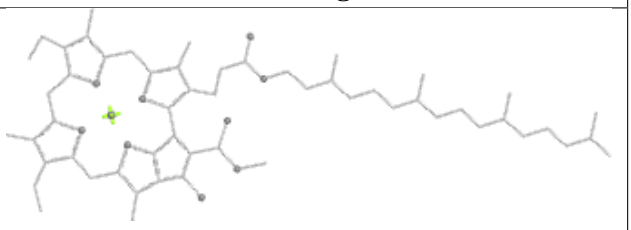
Bond lengths



Bond angles

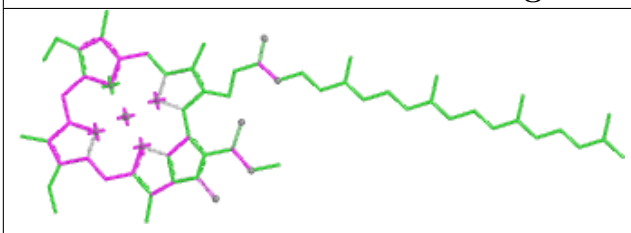


Torsions

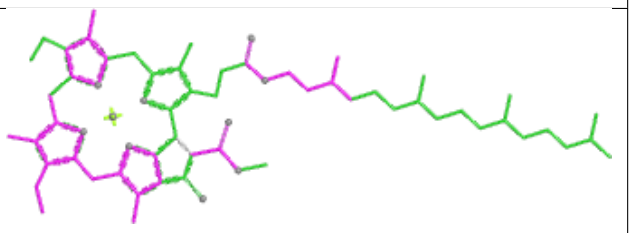


Rings

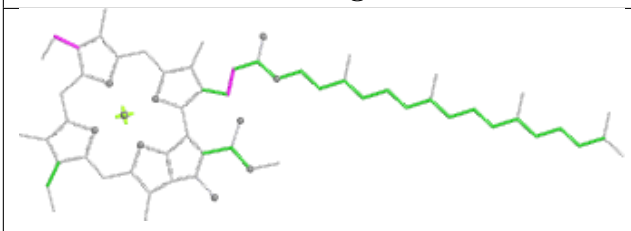
Ligand CLA C 501



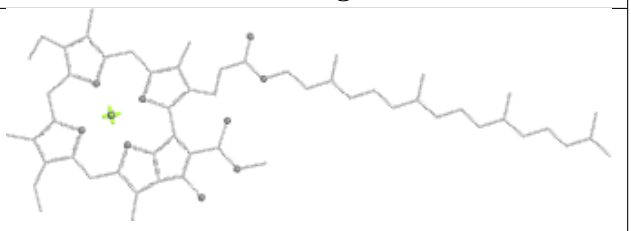
Bond lengths



Bond angles

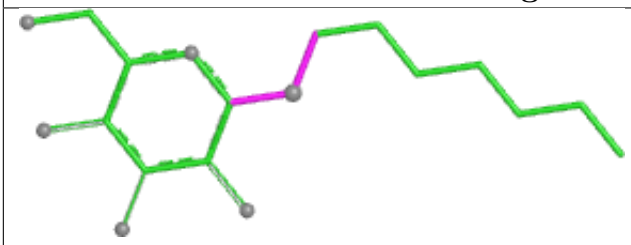


Torsions

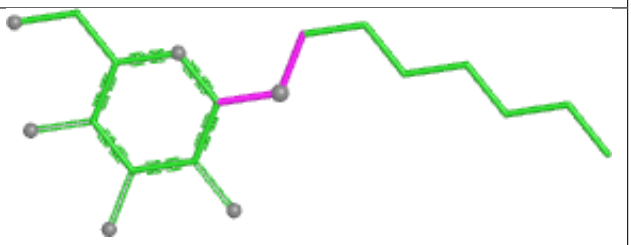


Rings

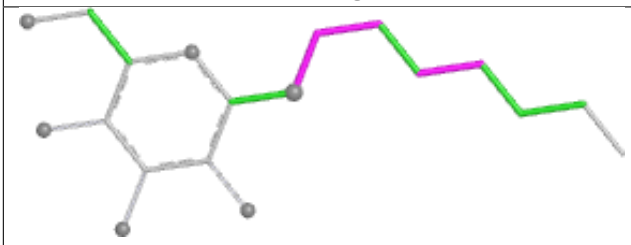
Ligand HTG C 520



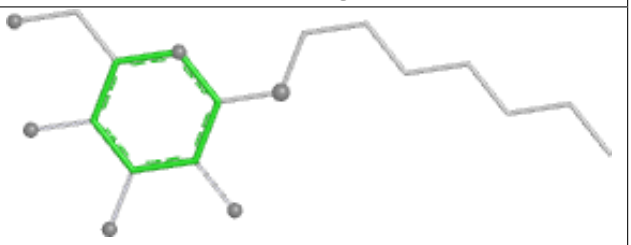
Bond lengths



Bond angles

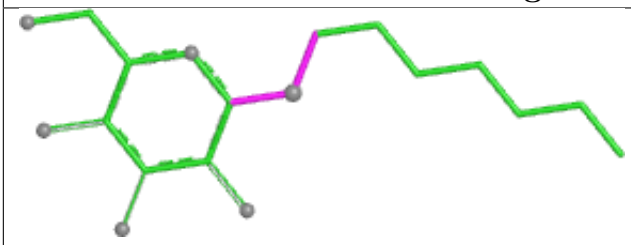


Torsions

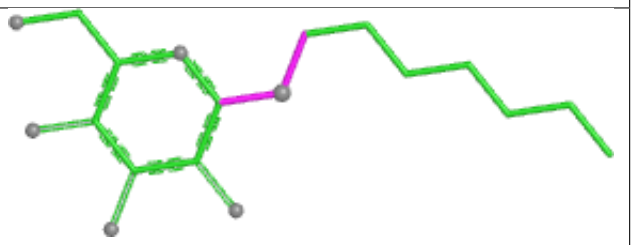


Rings

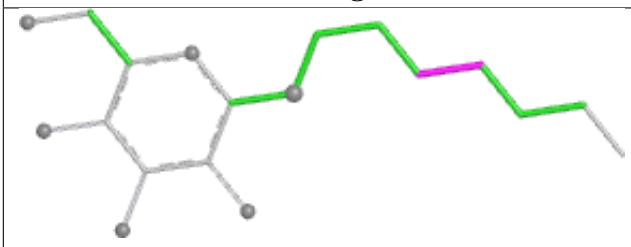
Ligand HTG d 419



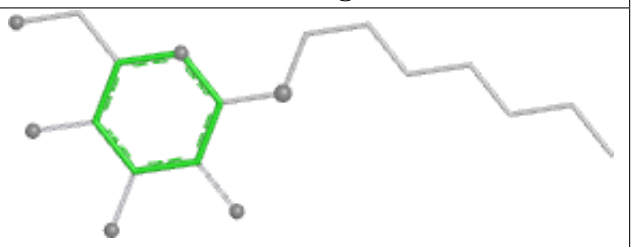
Bond lengths



Bond angles

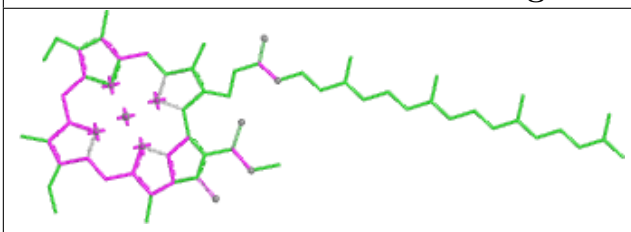


Torsions

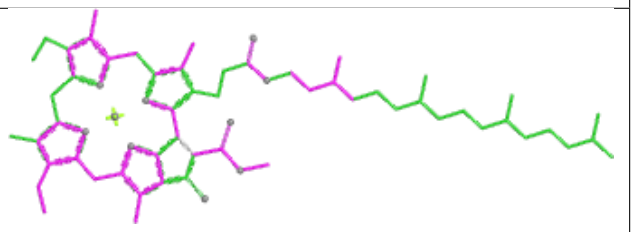


Rings

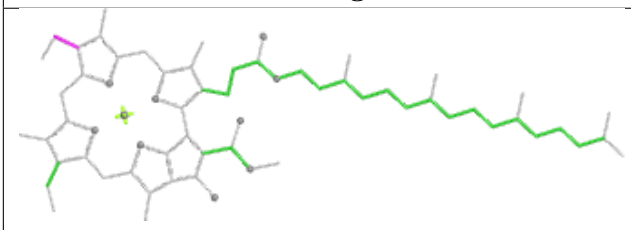
Ligand CLA b 613



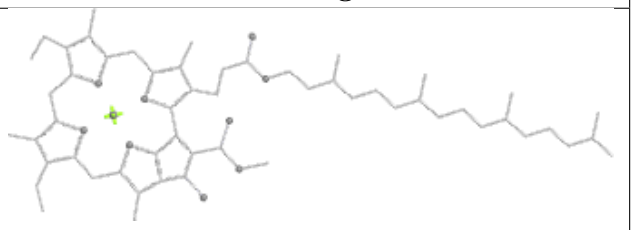
Bond lengths



Bond angles

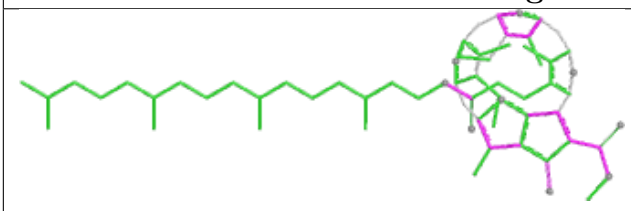


Torsions

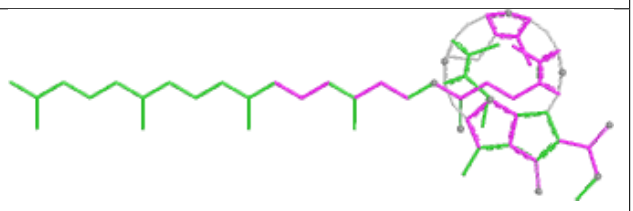


Rings

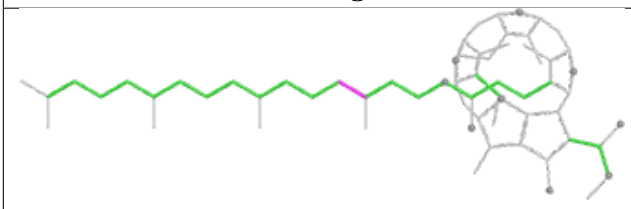
Ligand PHO a 411



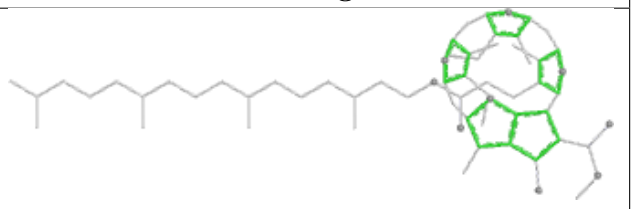
Bond lengths



Bond angles

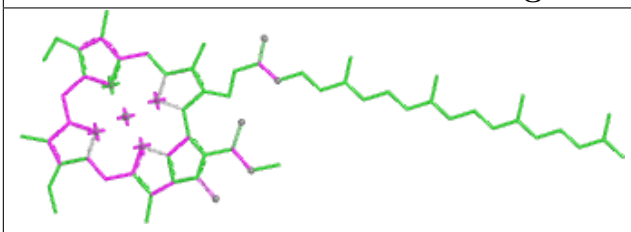


Torsions

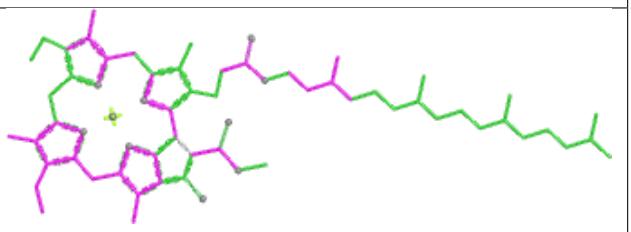


Rings

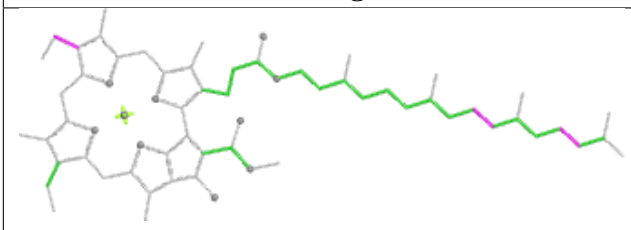
Ligand CLA C 503



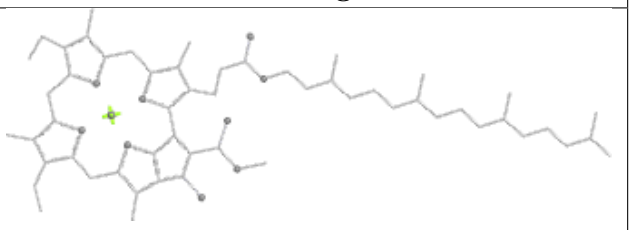
Bond lengths



Bond angles

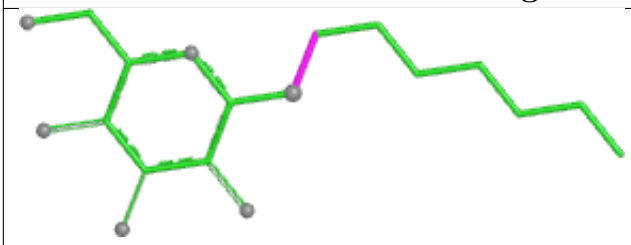


Torsions

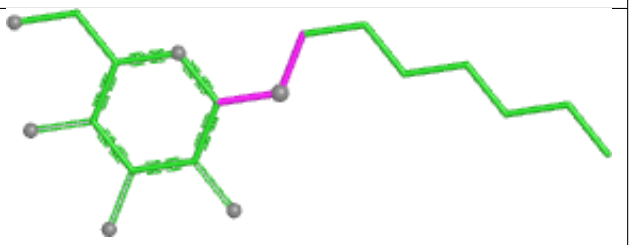


Rings

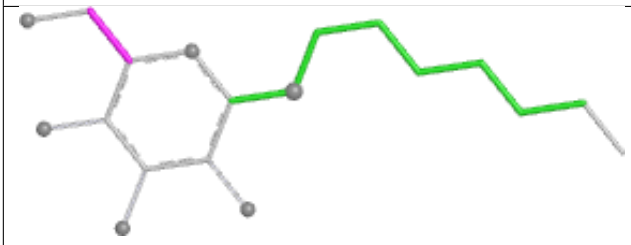
Ligand HTG B 623



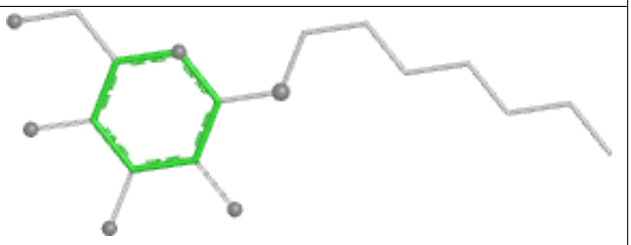
Bond lengths



Bond angles

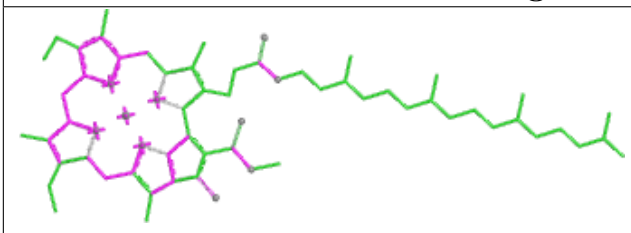


Torsions

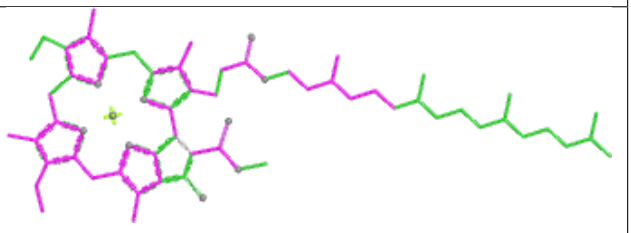


Rings

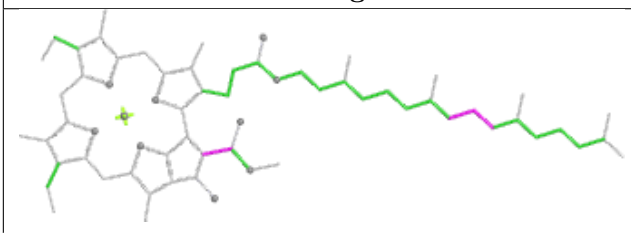
Ligand CLA b 609



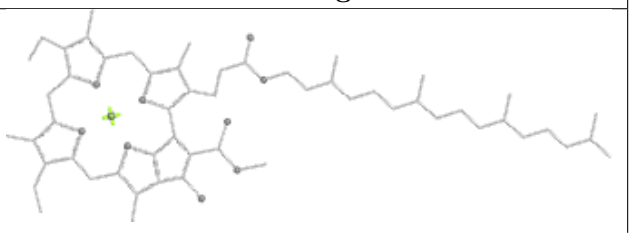
Bond lengths



Bond angles

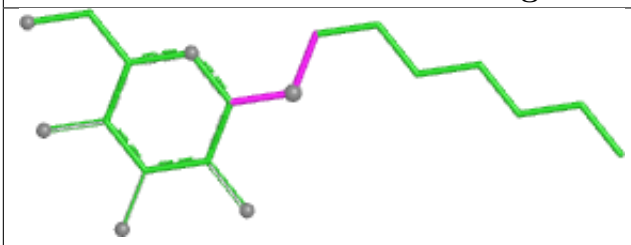


Torsions

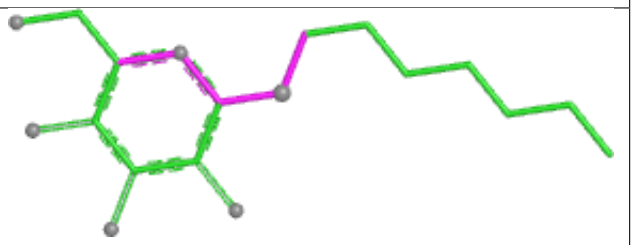


Rings

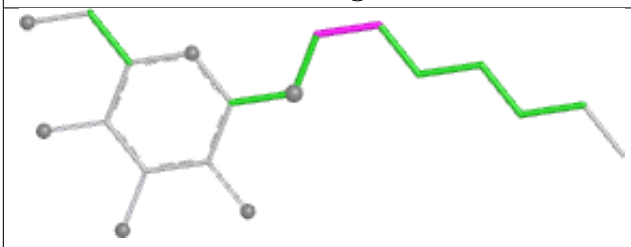
Ligand HTG C 521



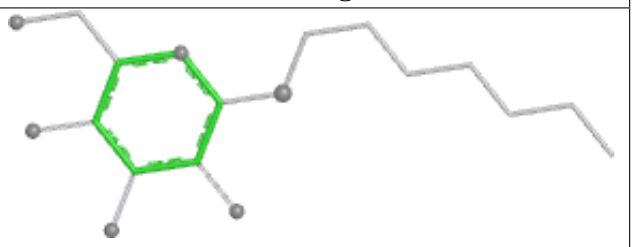
Bond lengths



Bond angles

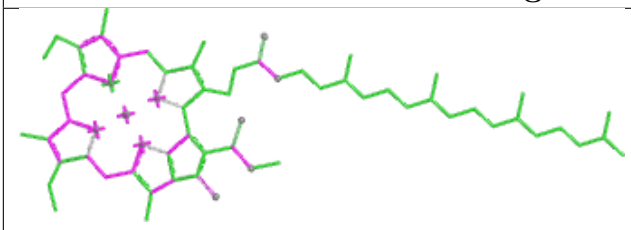


Torsions

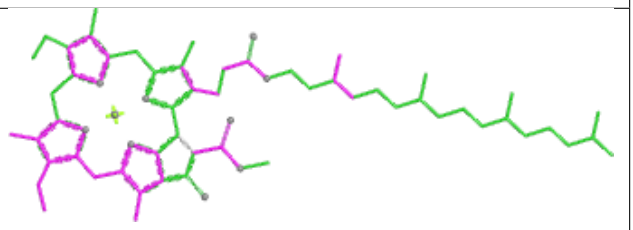


Rings

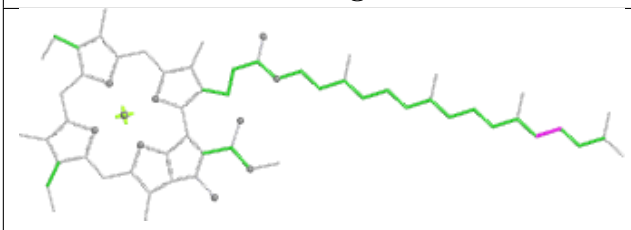
Ligand CLA B 613



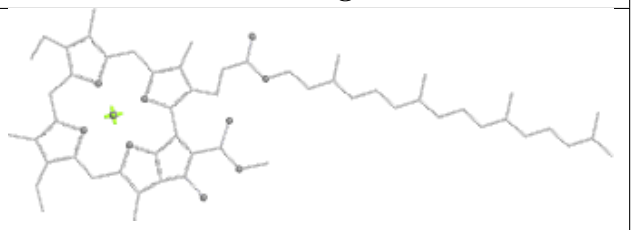
Bond lengths



Bond angles

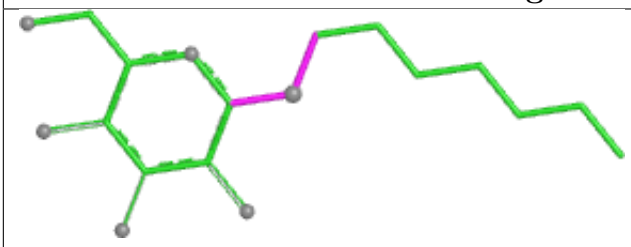


Torsions

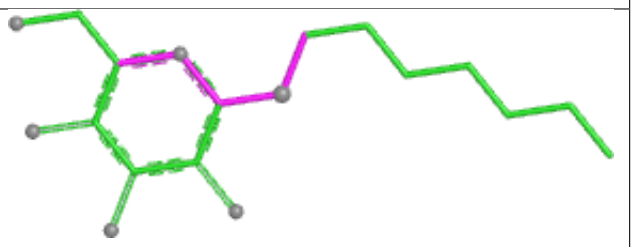


Rings

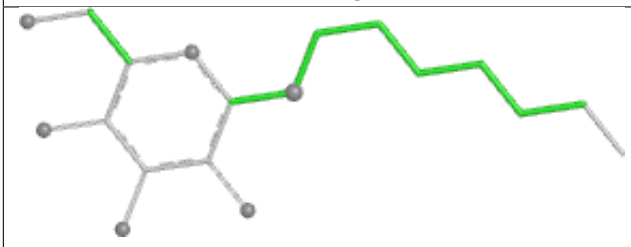
Ligand HTG c 924



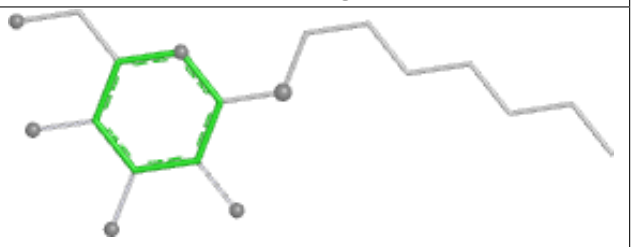
Bond lengths



Bond angles

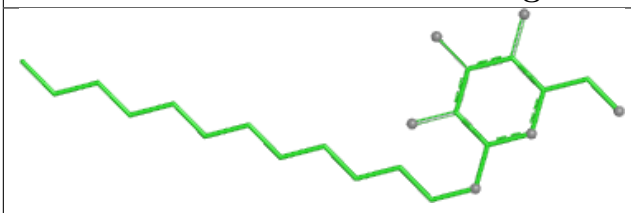


Torsions

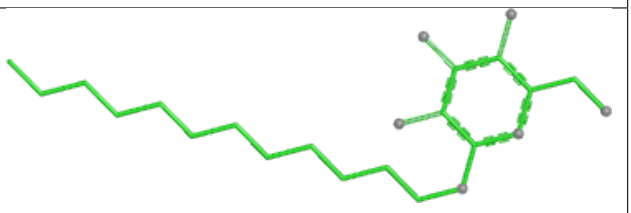


Rings

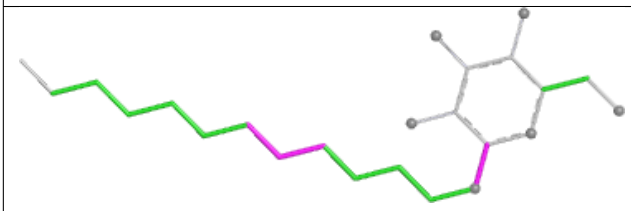
Ligand LMT F 103



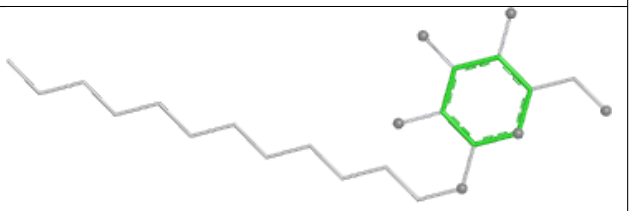
Bond lengths



Bond angles

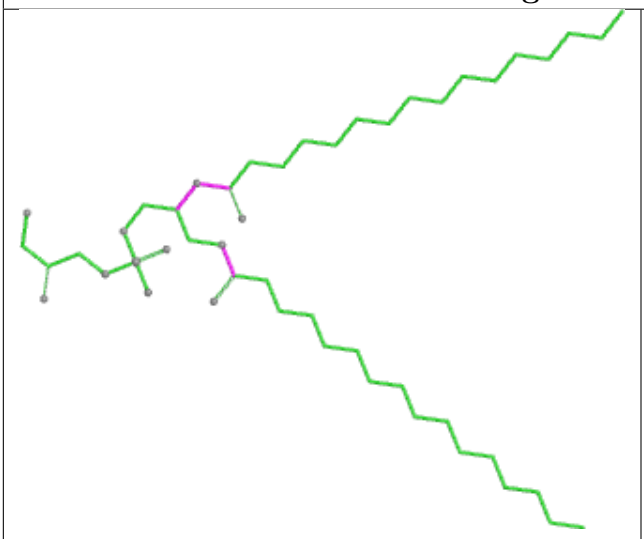


Torsions

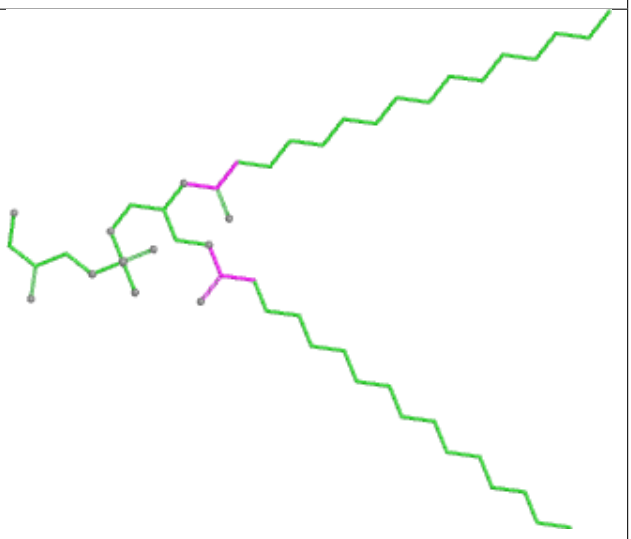


Rings

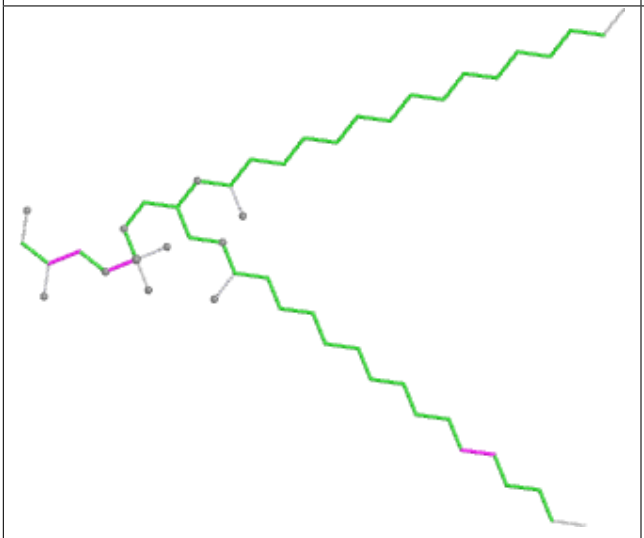
Ligand LHG D 407



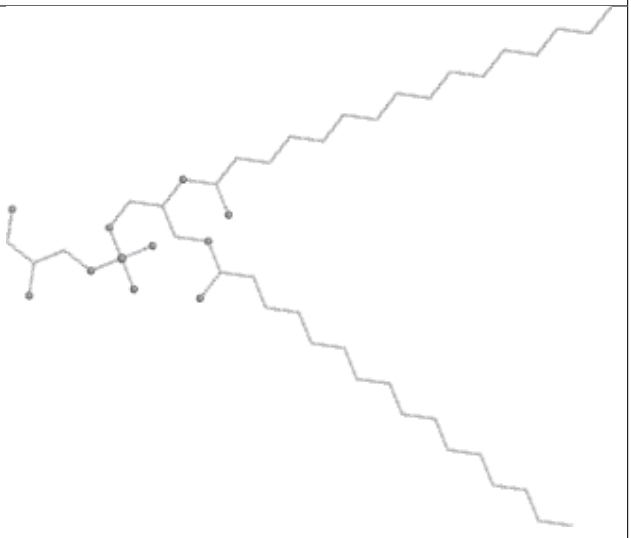
Bond lengths



Bond angles

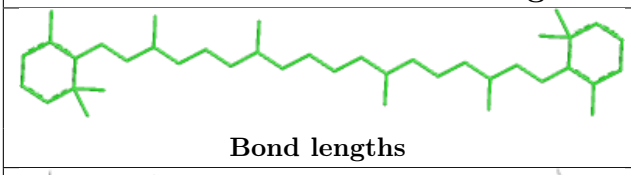


Torsions

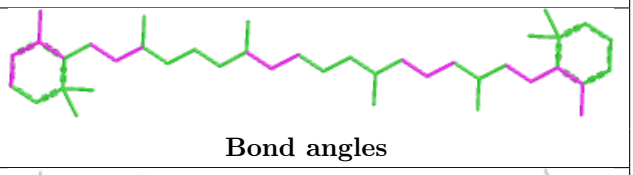


Rings

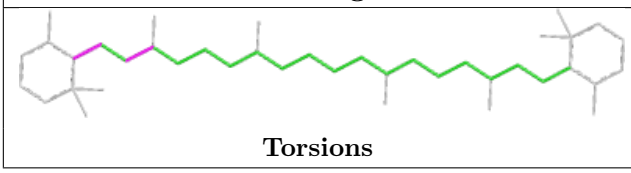
Ligand BCR c 916



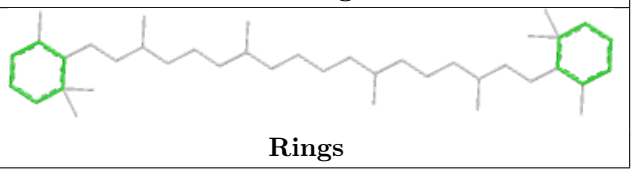
Bond lengths



Bond angles

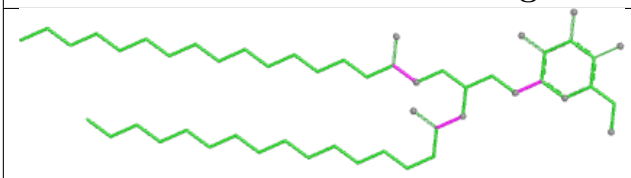


Torsions

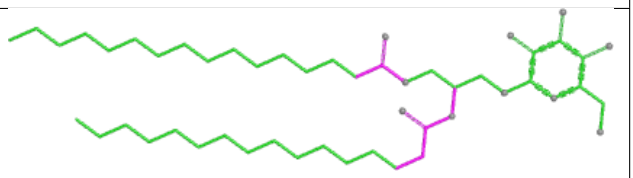


Rings

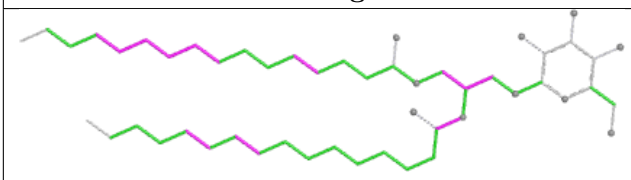
Ligand LMG C 519



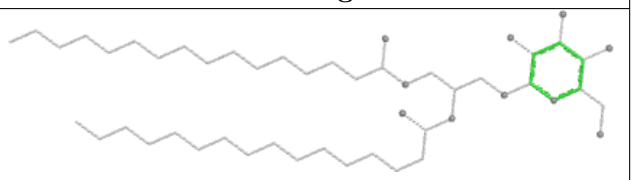
Bond lengths



Bond angles

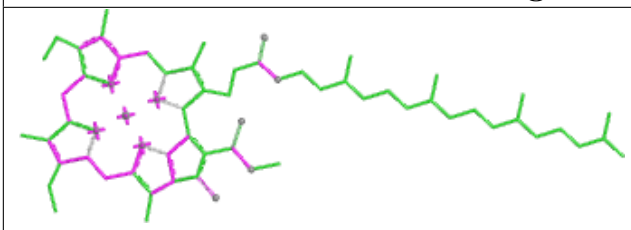


Torsions

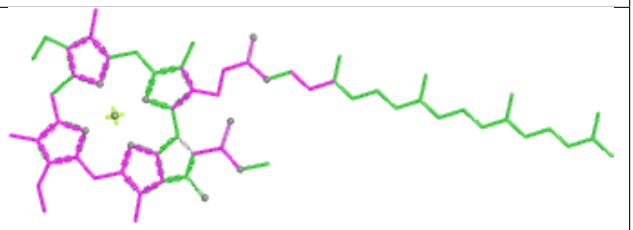


Rings

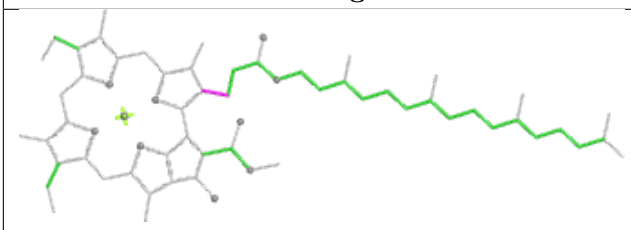
Ligand CLA b 611



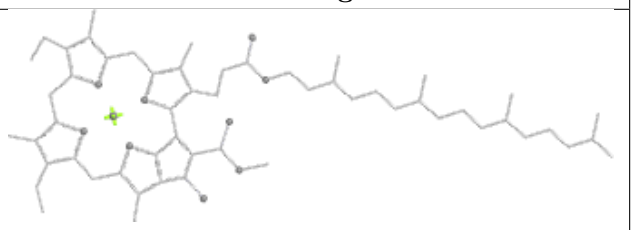
Bond lengths



Bond angles

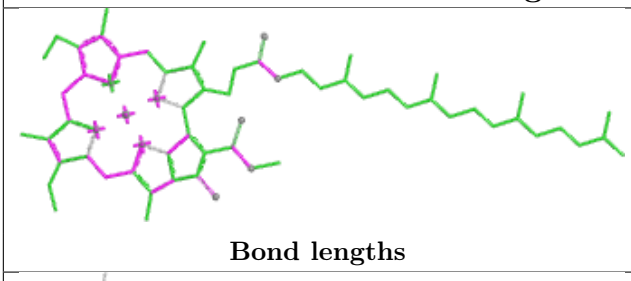


Torsions

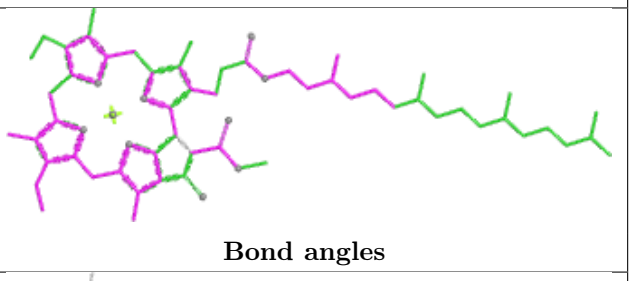


Rings

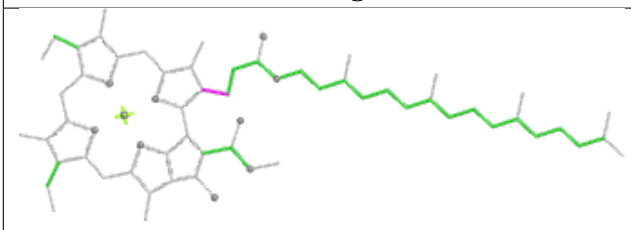
Ligand CLA B 612



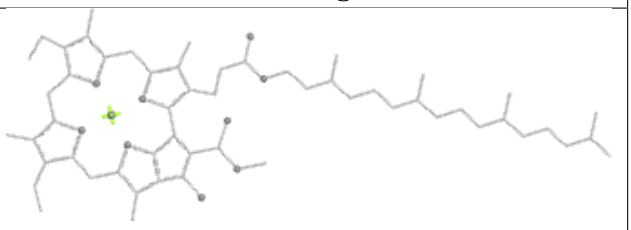
Bond lengths



Bond angles

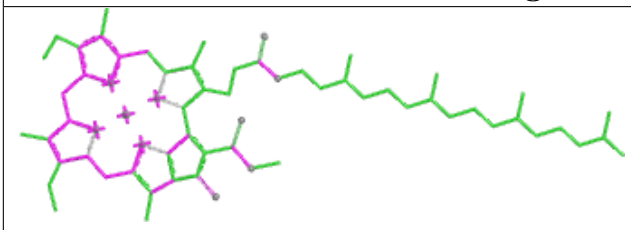


Torsions

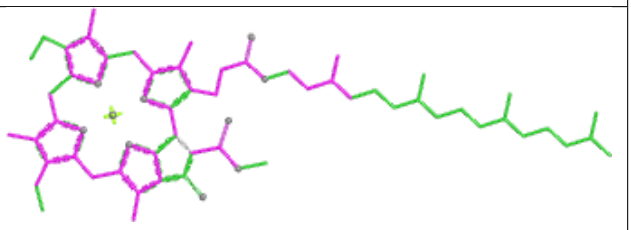


Rings

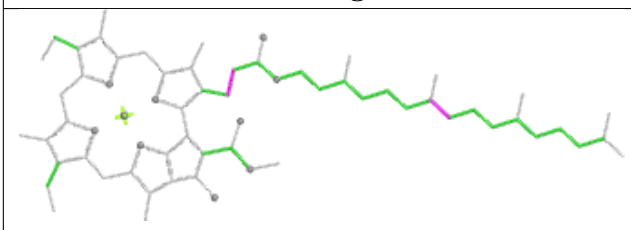
Ligand CLA B 611



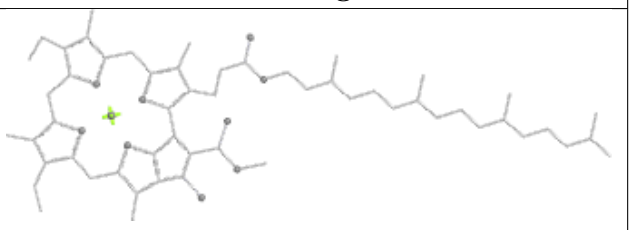
Bond lengths



Bond angles

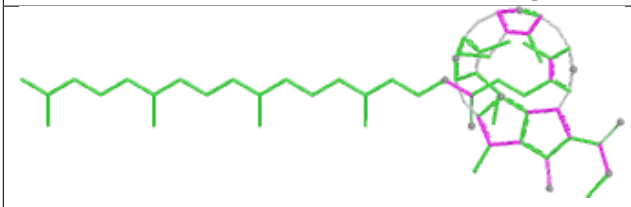


Torsions

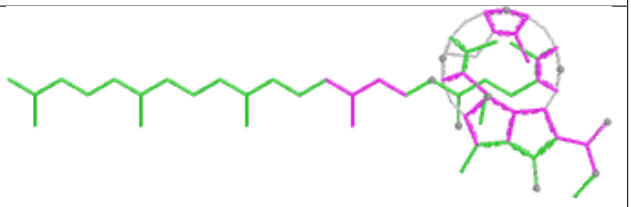


Rings

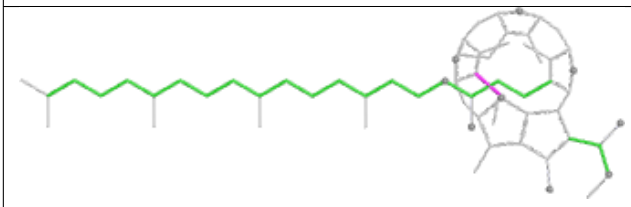
Ligand PHO a 412



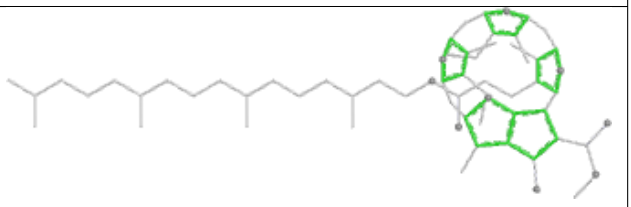
Bond lengths



Bond angles

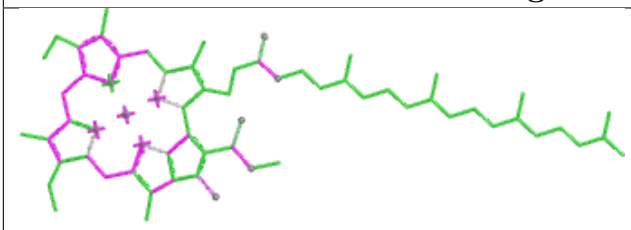


Torsions

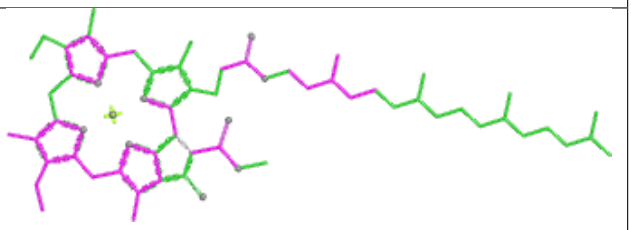


Rings

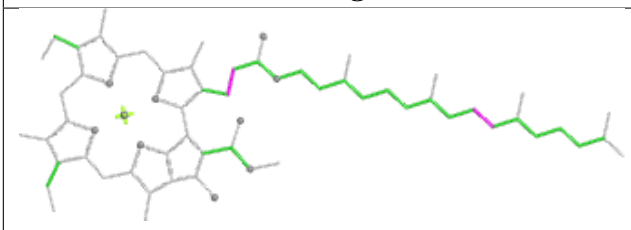
Ligand CLA b 610



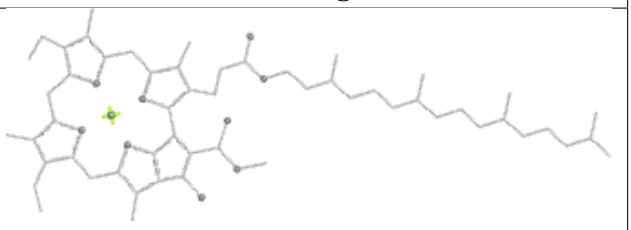
Bond lengths



Bond angles

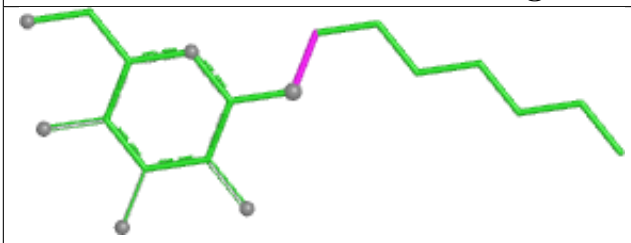


Torsions

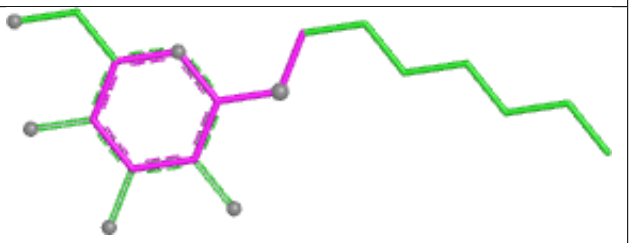


Rings

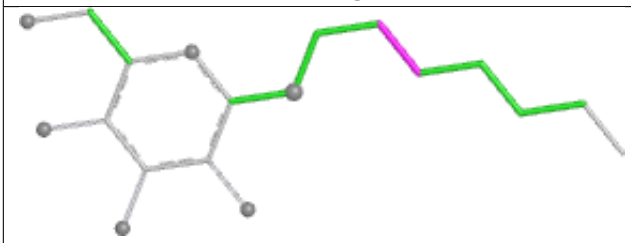
Ligand HTG c 941



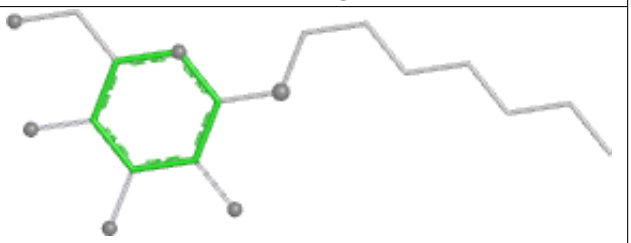
Bond lengths



Bond angles

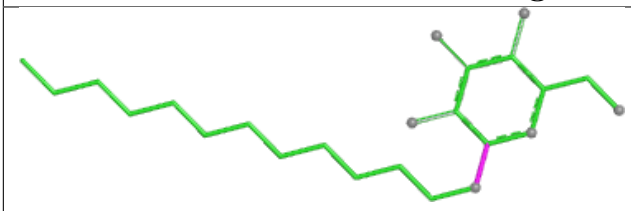


Torsions

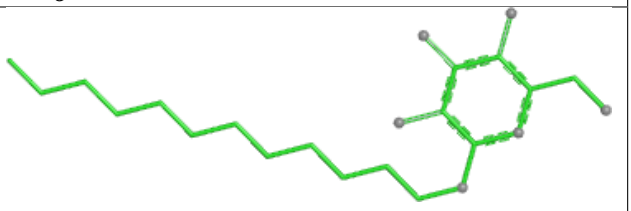


Rings

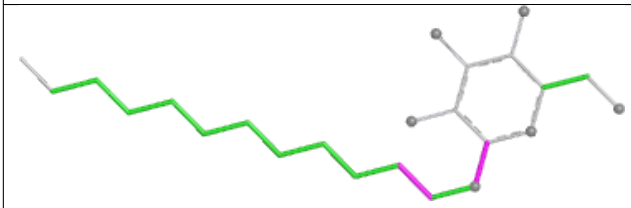
Ligand LMT j 102



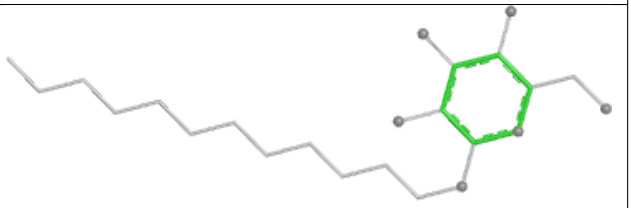
Bond lengths



Bond angles

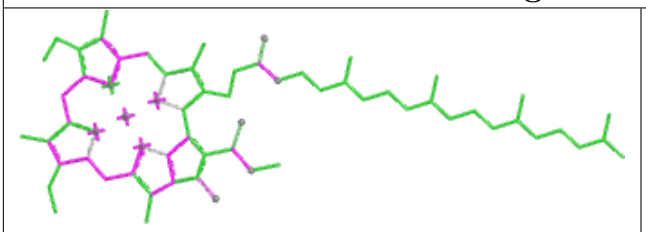


Torsions

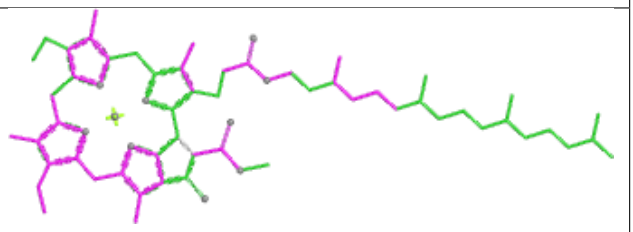


Rings

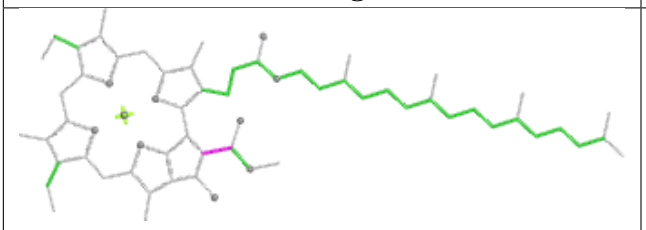
Ligand CLA B 615



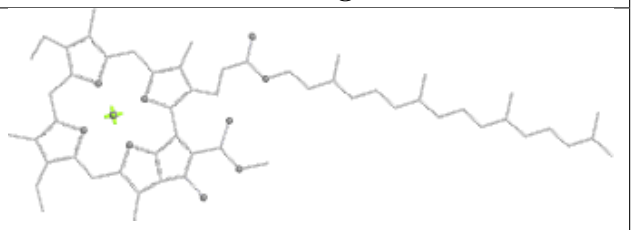
Bond lengths



Bond angles

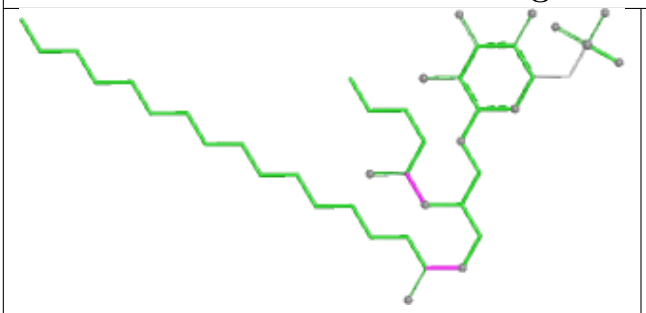


Torsions

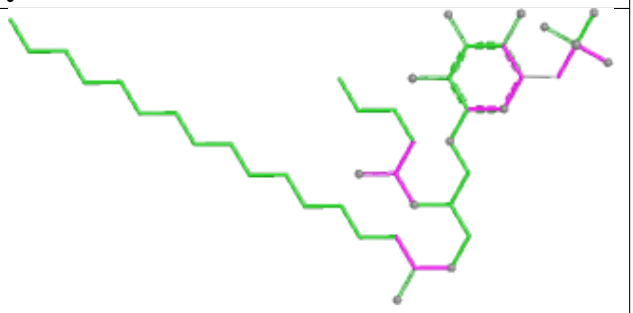


Rings

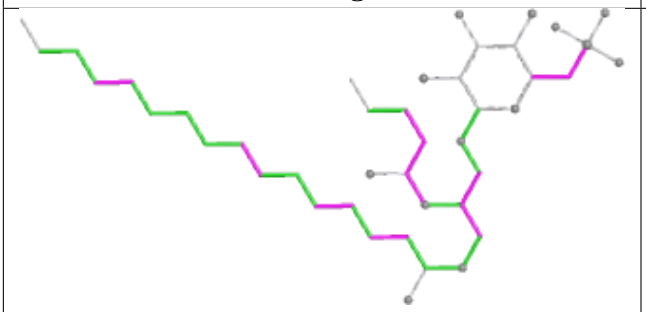
Ligand SQD f 102



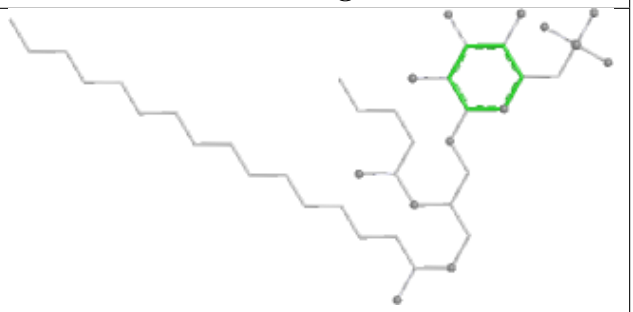
Bond lengths



Bond angles

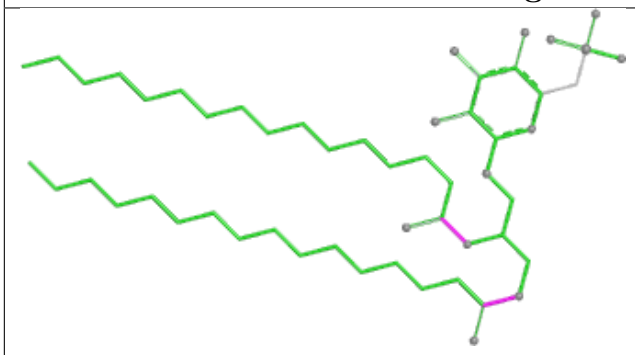


Torsions

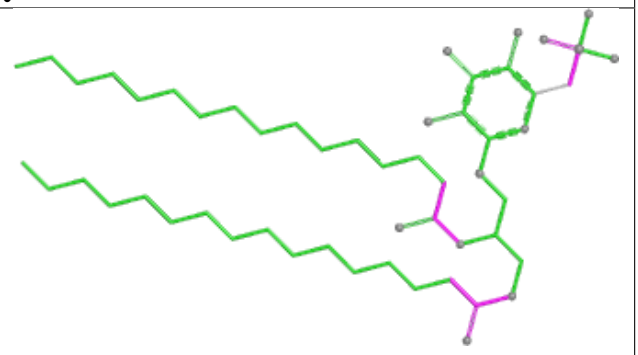


Rings

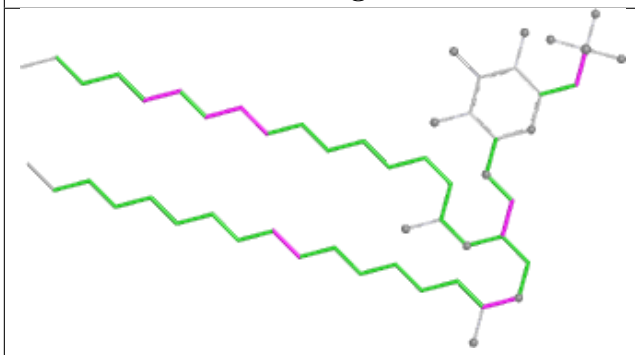
Ligand SQD A 416



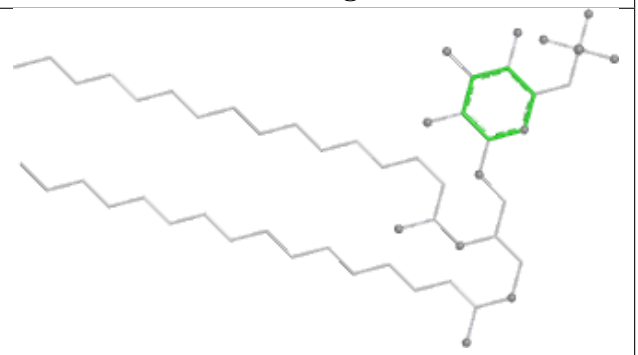
Bond lengths



Bond angles

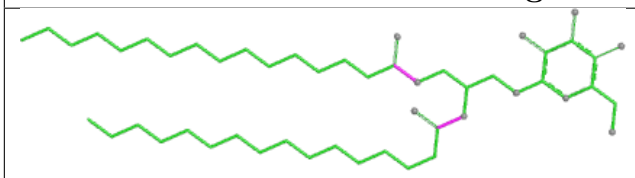


Torsions

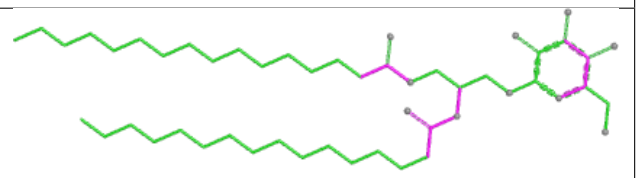


Rings

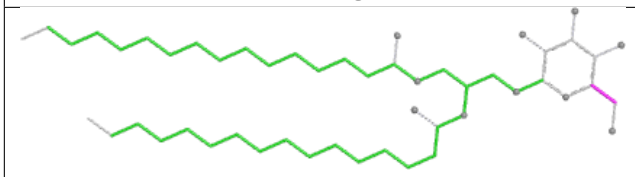
Ligand LMG c 921



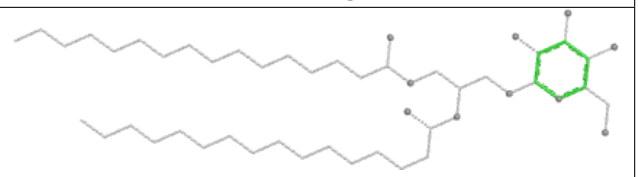
Bond lengths



Bond angles

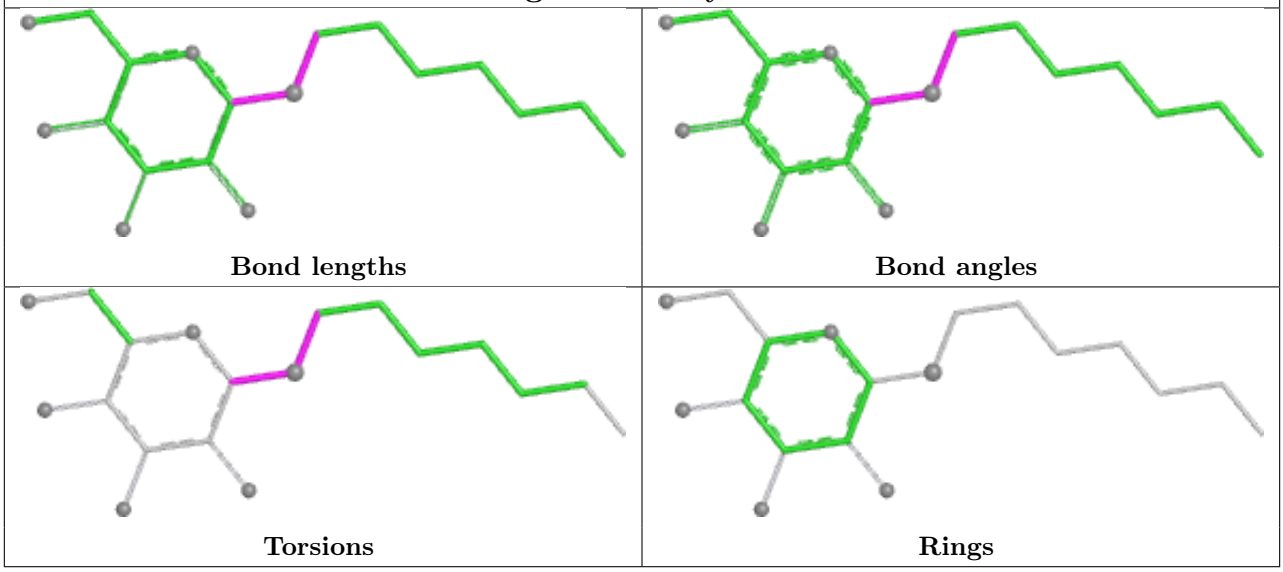


Torsions

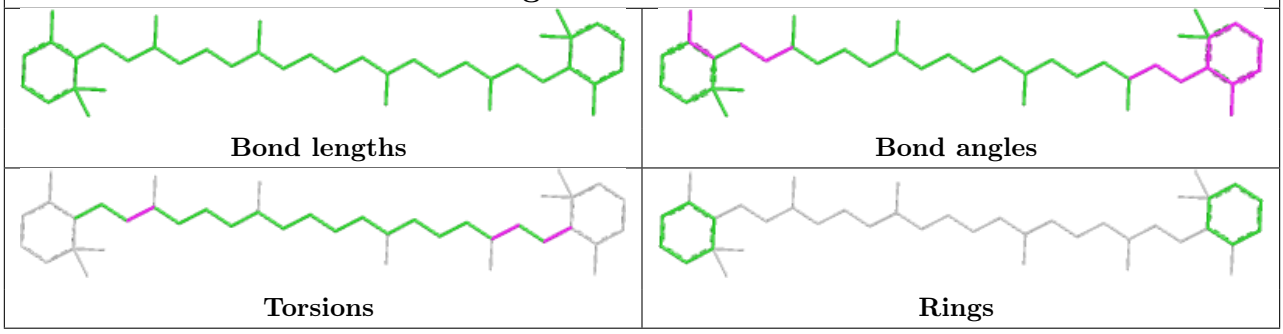


Rings

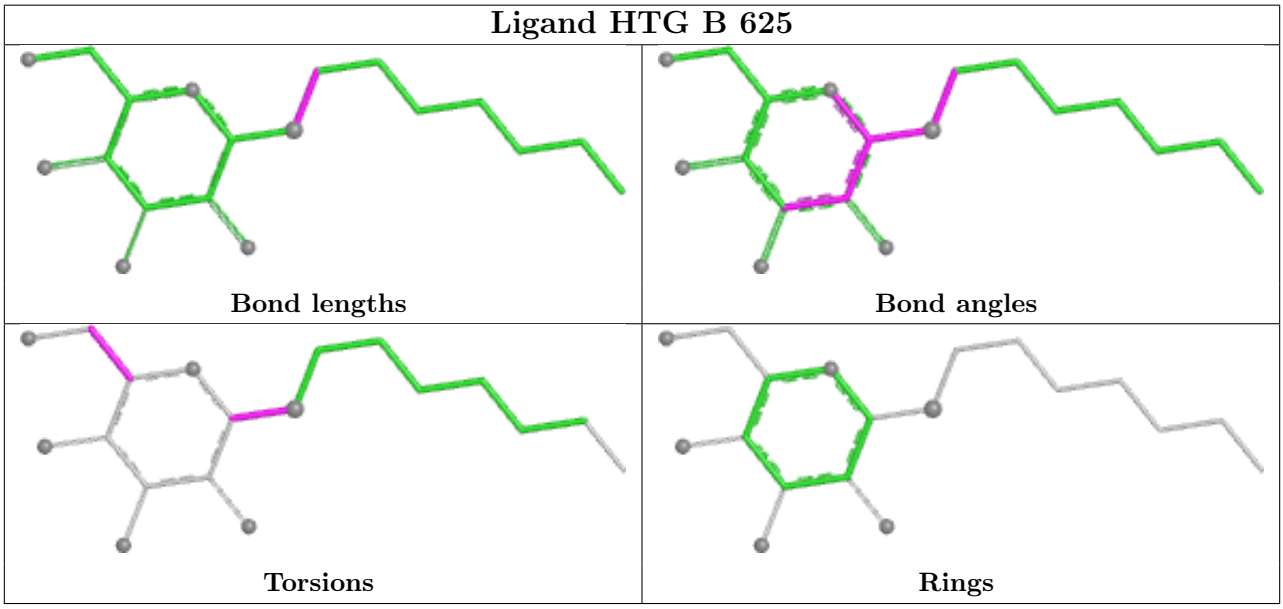
Ligand HTG y 102



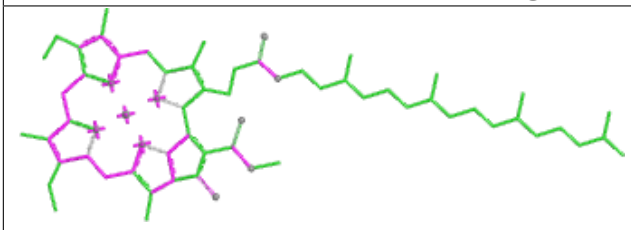
Ligand BCR D 403



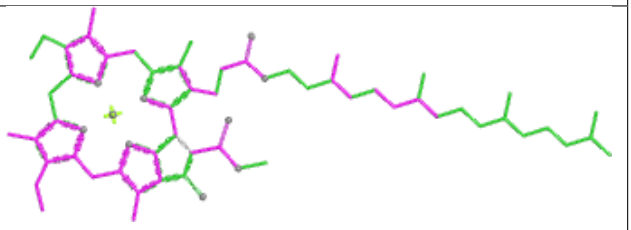
Ligand HTG B 625



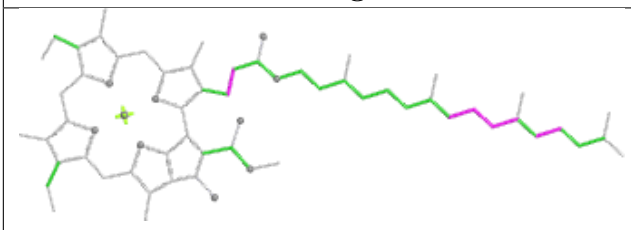
Ligand CLA B 607



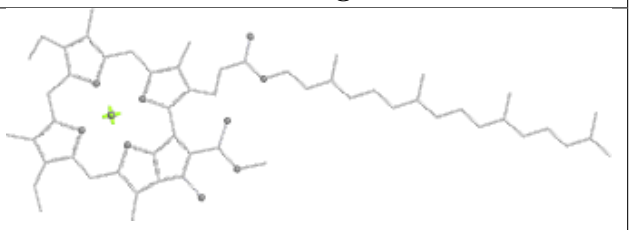
Bond lengths



Bond angles



Torsions

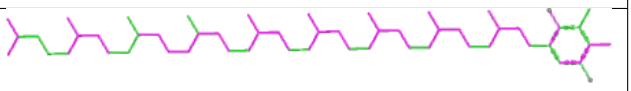


Rings

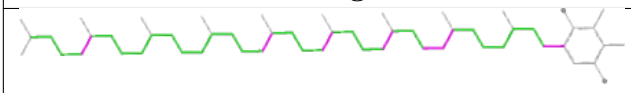
Ligand PL9 A 414



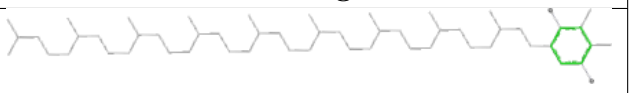
Bond lengths



Bond angles

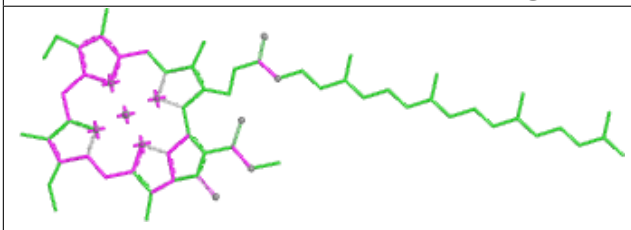


Torsions

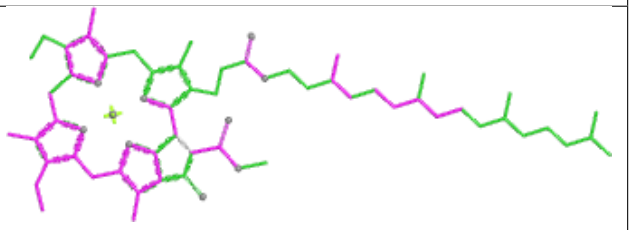


Rings

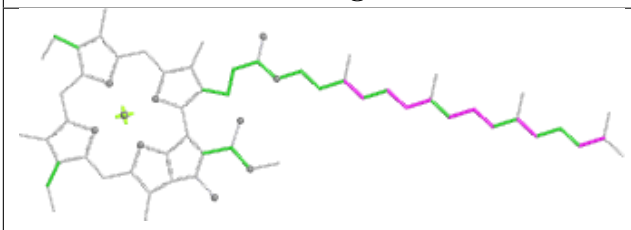
Ligand CLA B 616



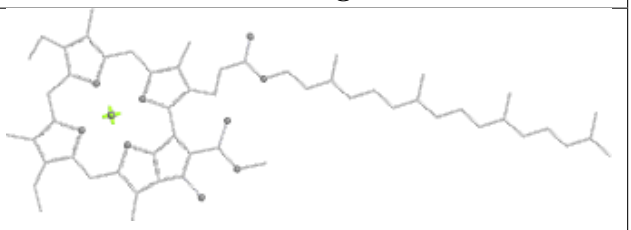
Bond lengths



Bond angles

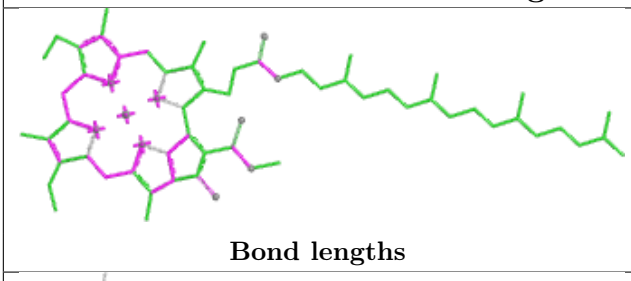


Torsions

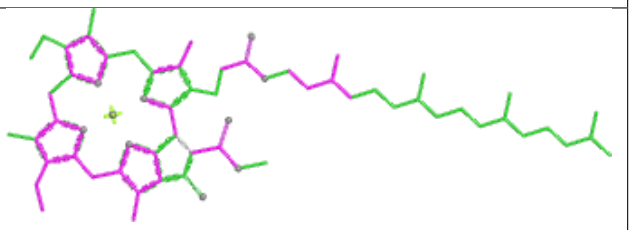


Rings

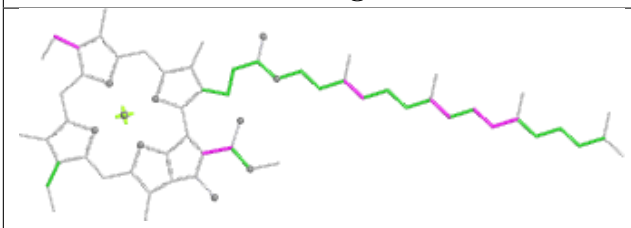
Ligand CLA b 620



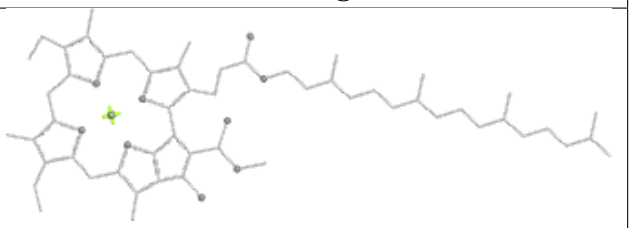
Bond lengths



Bond angles

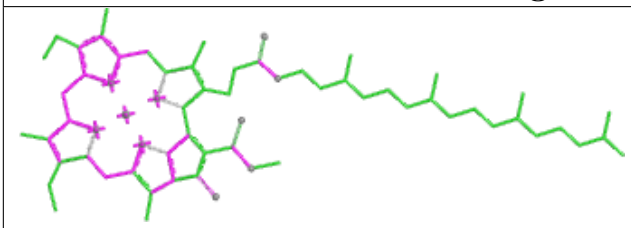


Torsions

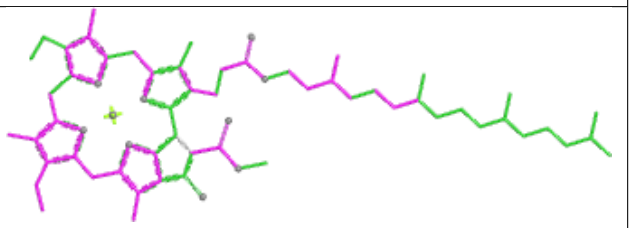


Rings

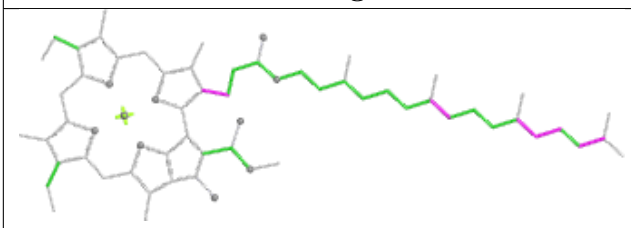
Ligand CLA c 909



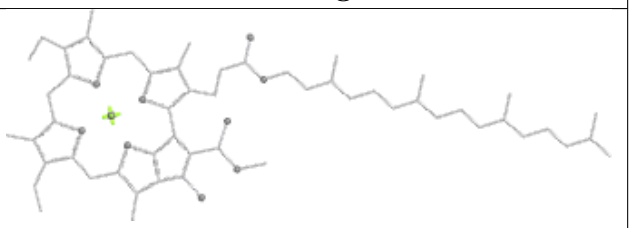
Bond lengths



Bond angles

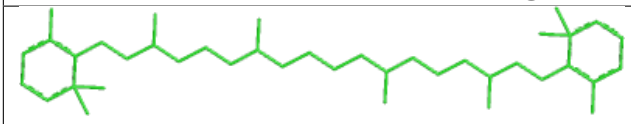


Torsions

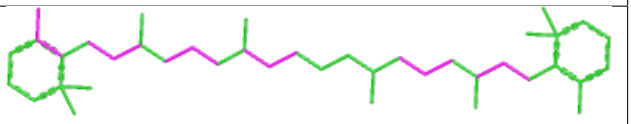


Rings

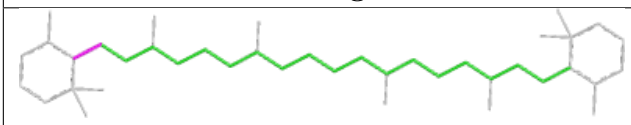
Ligand BCR B 618



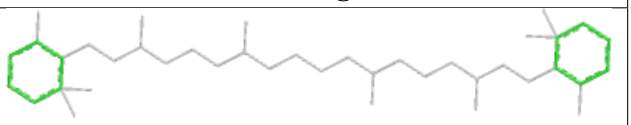
Bond lengths



Bond angles

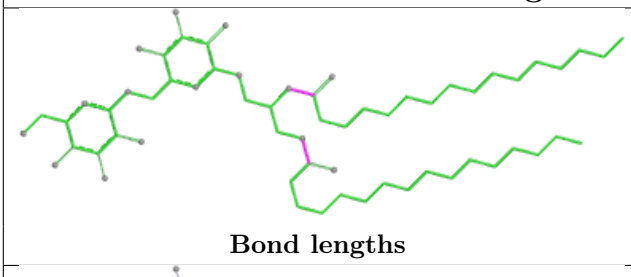


Torsions

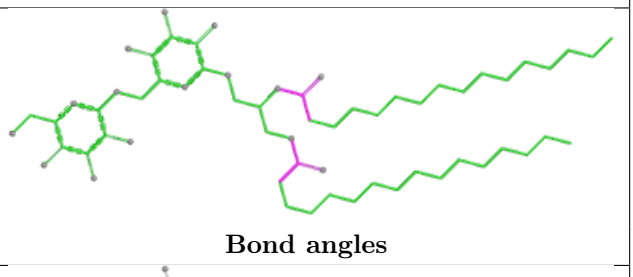


Rings

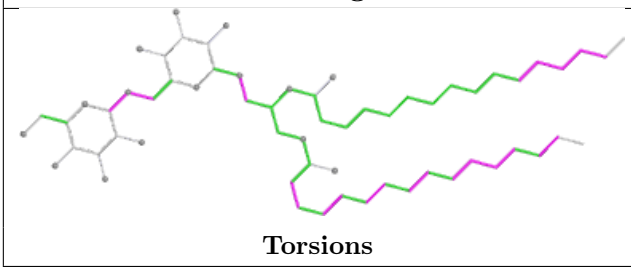
Ligand DGD c 918



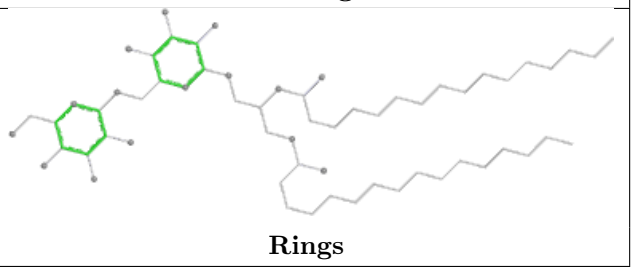
Bond lengths



Bond angles

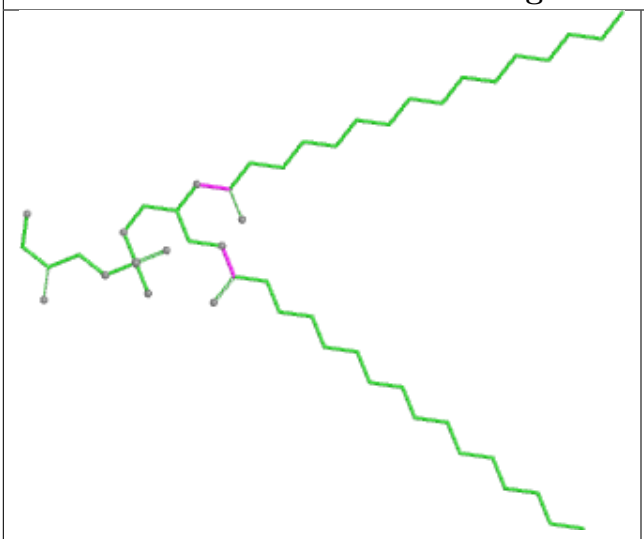


Torsions

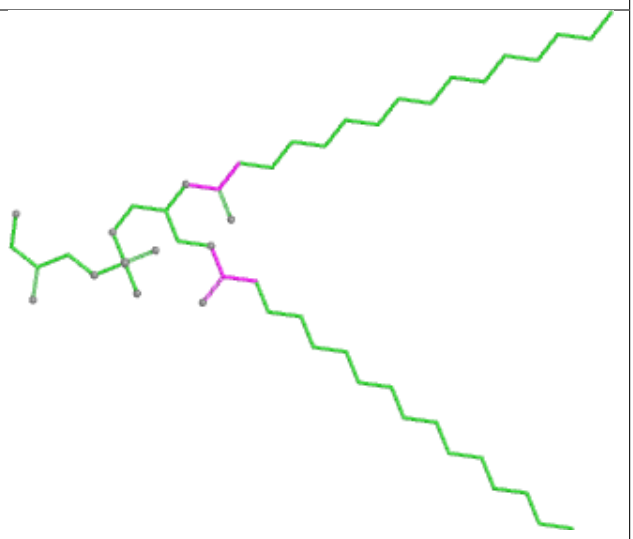


Rings

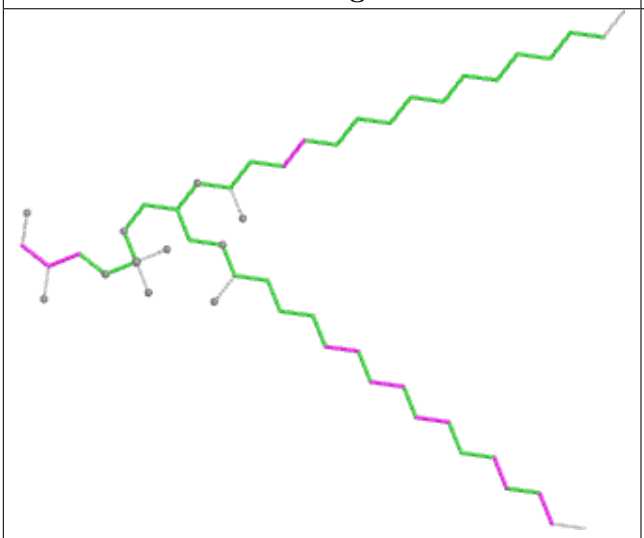
Ligand LHG d 410



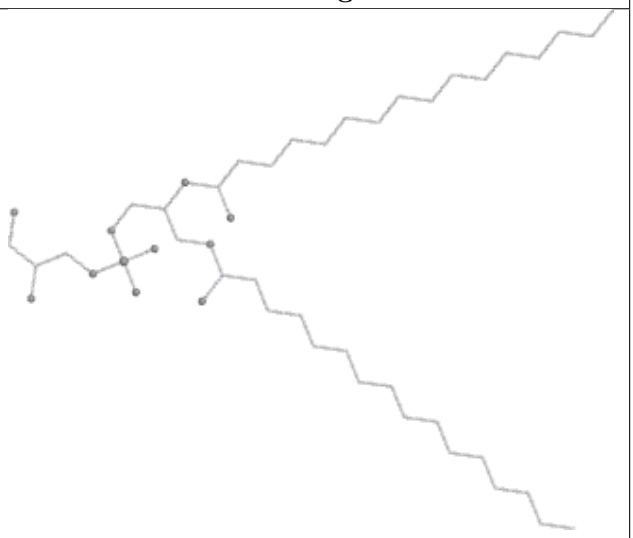
Bond lengths



Bond angles

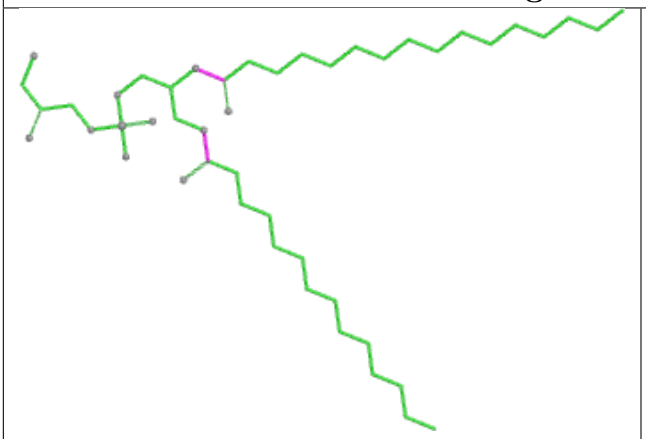


Torsions

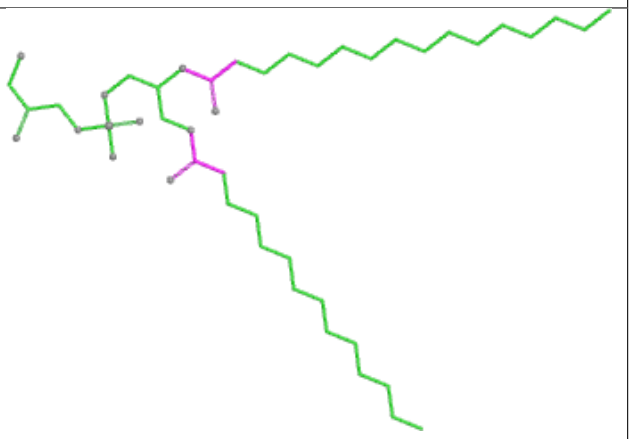


Rings

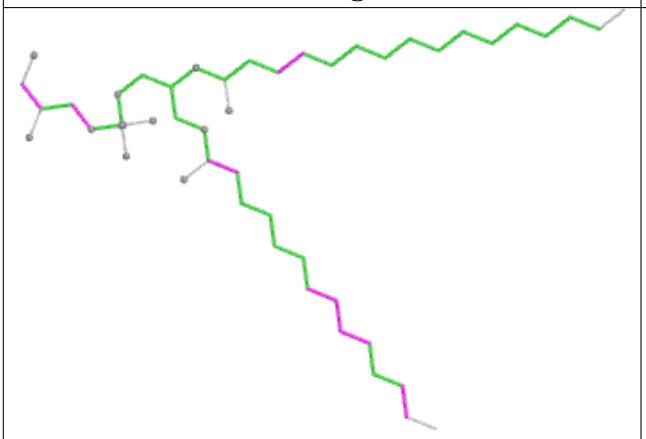
Ligand LHG d 411



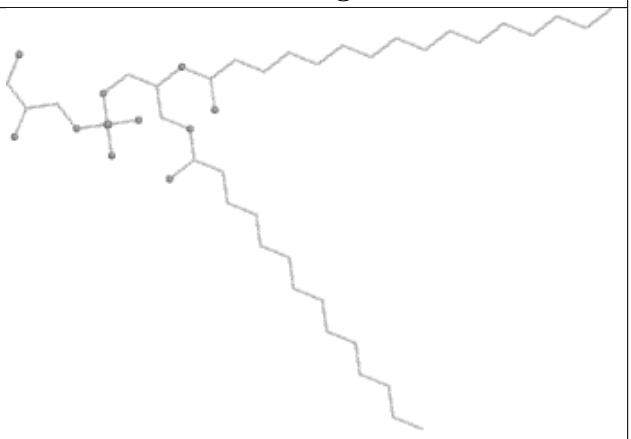
Bond lengths



Bond angles

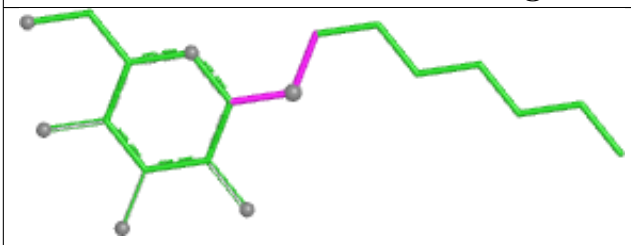


Torsions

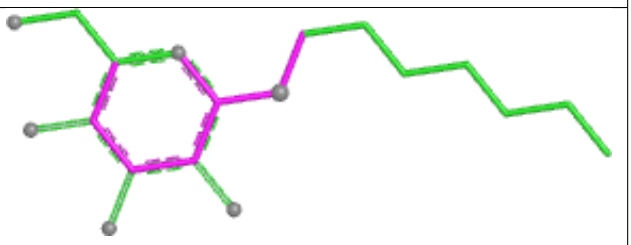


Rings

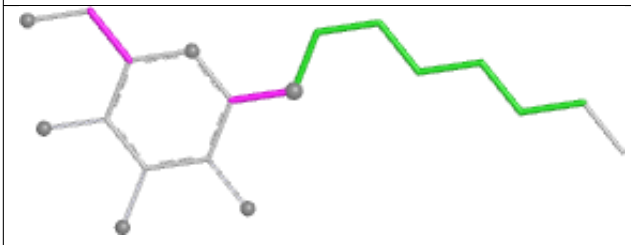
Ligand HTG b 627



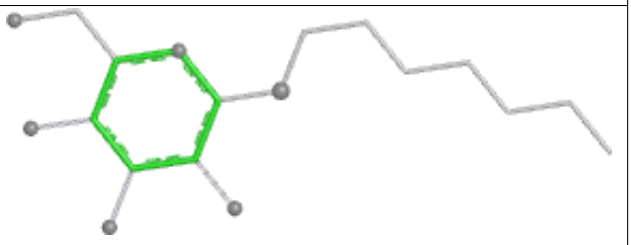
Bond lengths



Bond angles

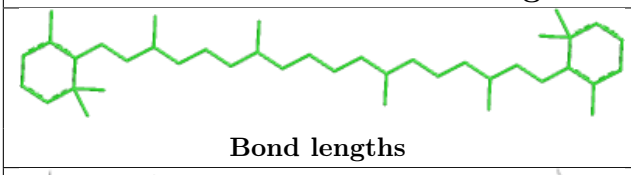


Torsions

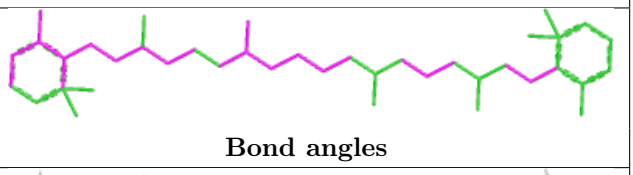


Rings

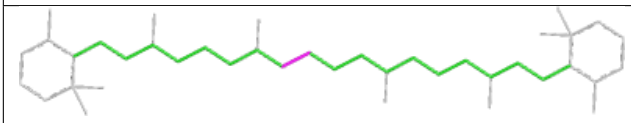
Ligand BCR T 101



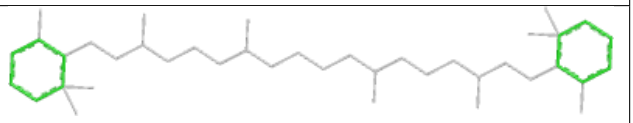
Bond lengths



Bond angles

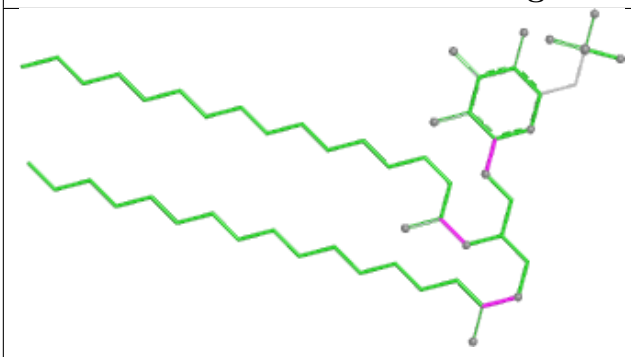


Torsions

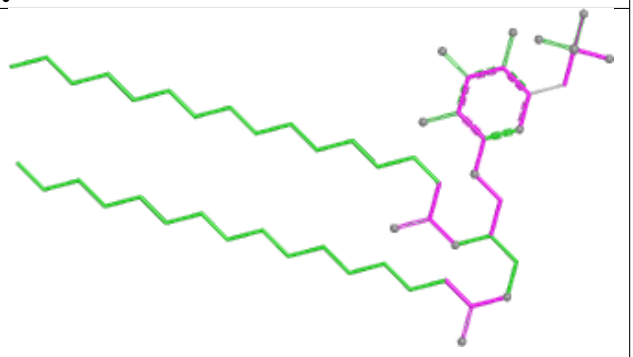


Rings

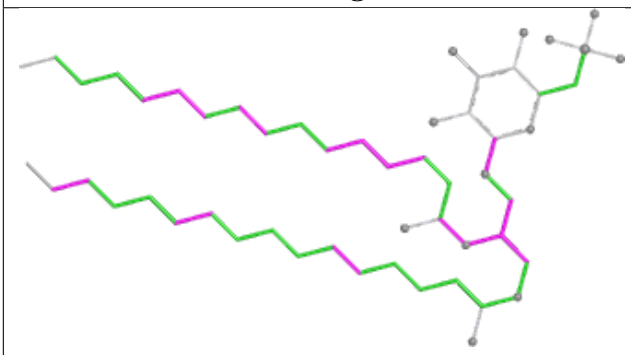
Ligand SQD b 601



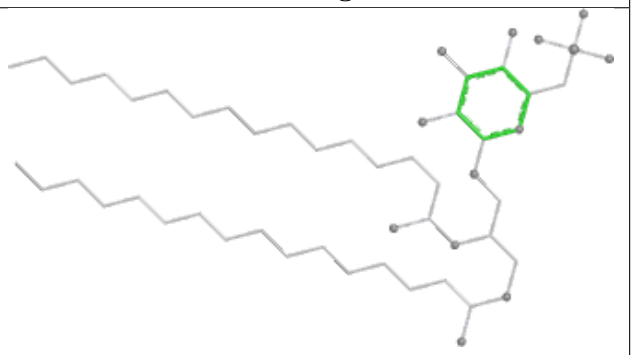
Bond lengths



Bond angles

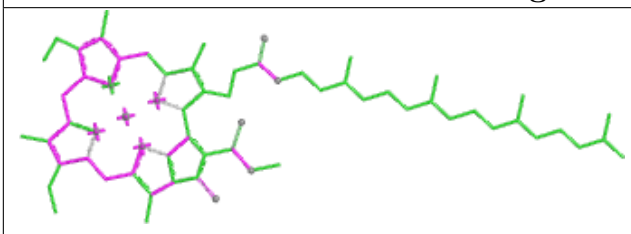


Torsions

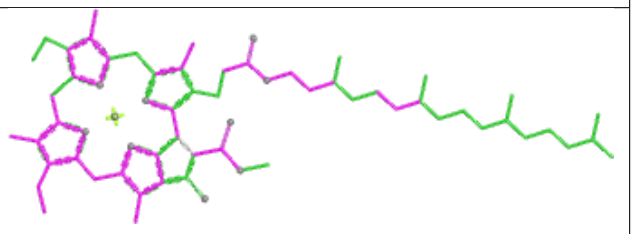


Rings

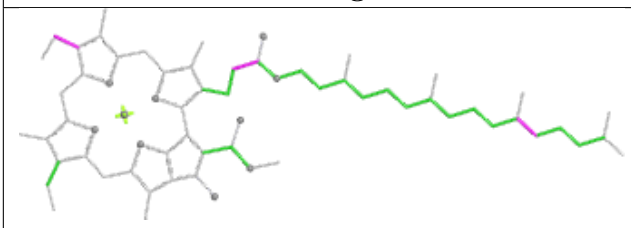
Ligand CLA c 906



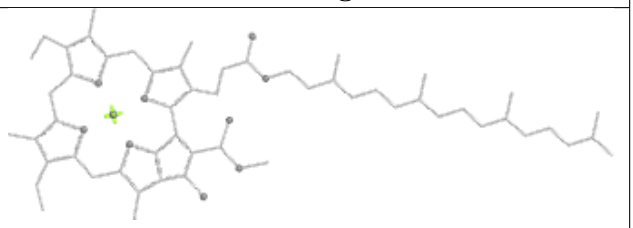
Bond lengths



Bond angles

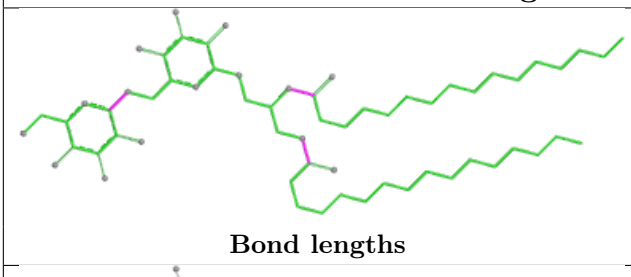


Torsions

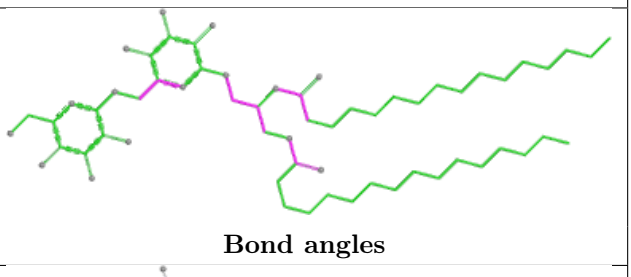


Rings

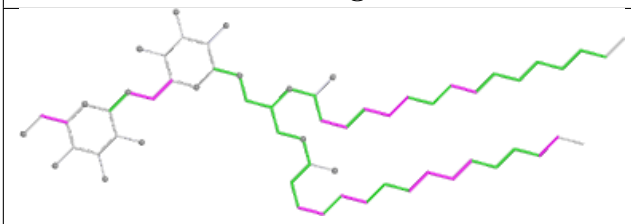
Ligand DGD C 516



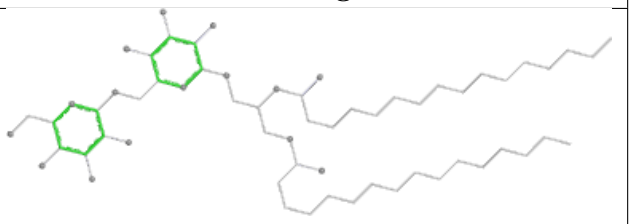
Bond lengths



Bond angles

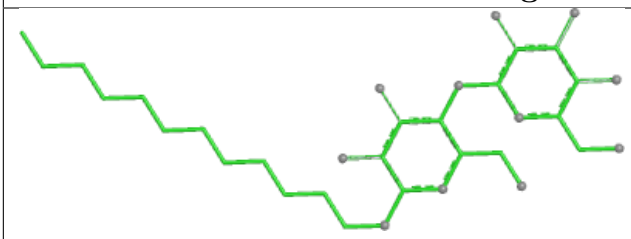


Torsions

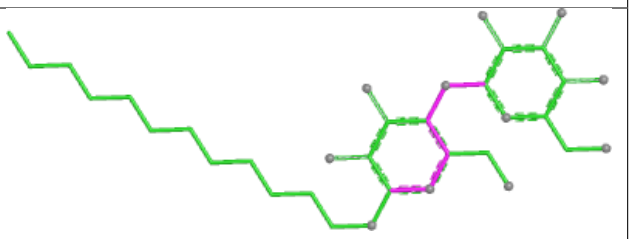


Rings

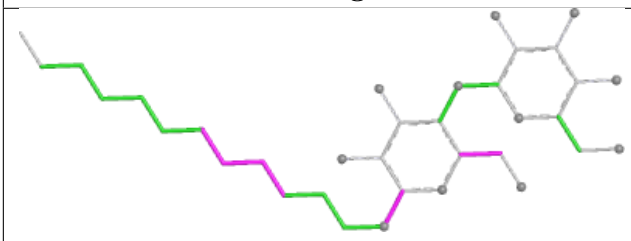
Ligand LMT A 417



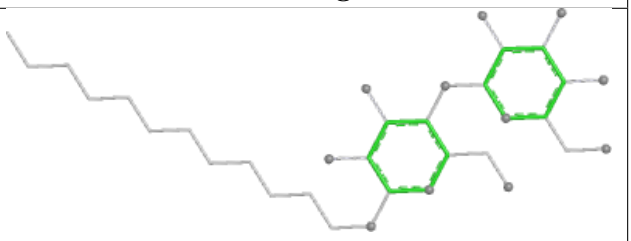
Bond lengths



Bond angles

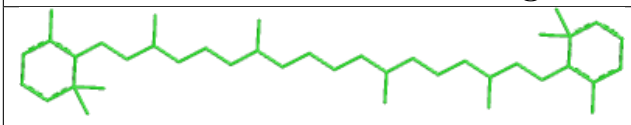


Torsions

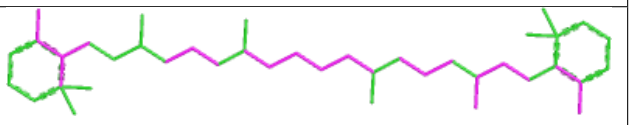


Rings

Ligand BCR Y 101



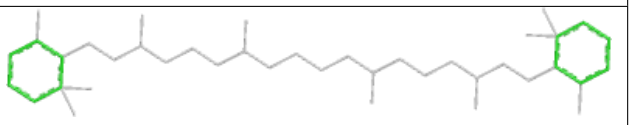
Bond lengths



Bond angles

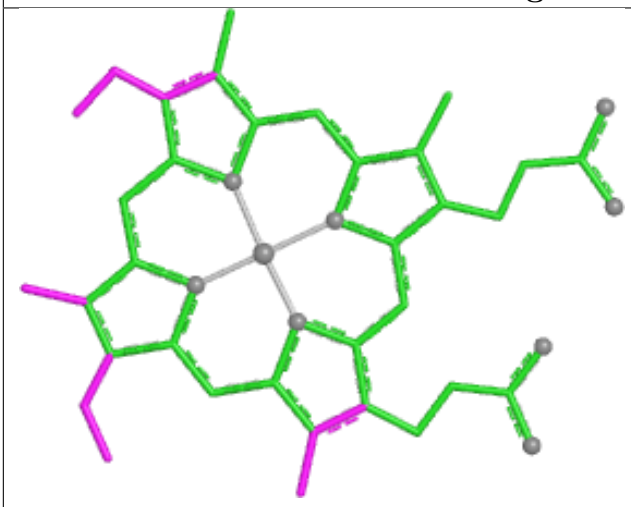


Torsions

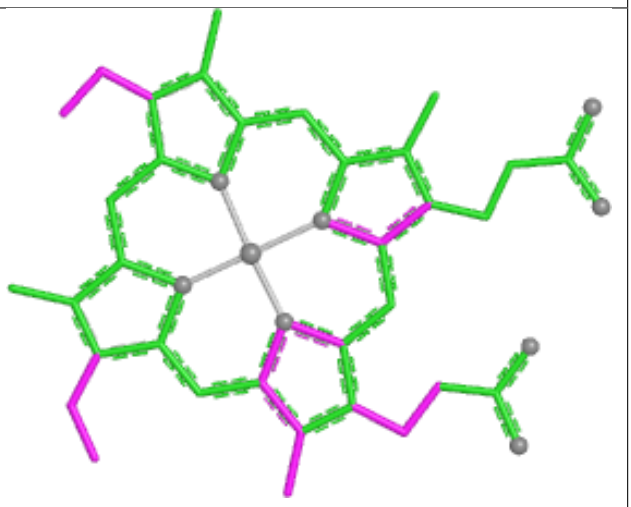


Rings

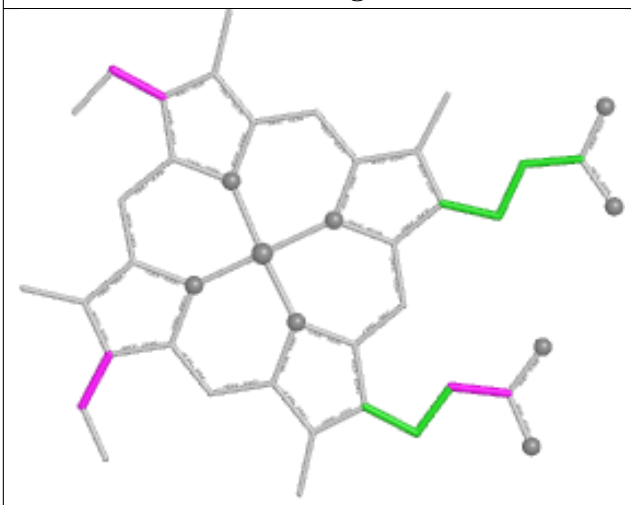
Ligand HEC v 202



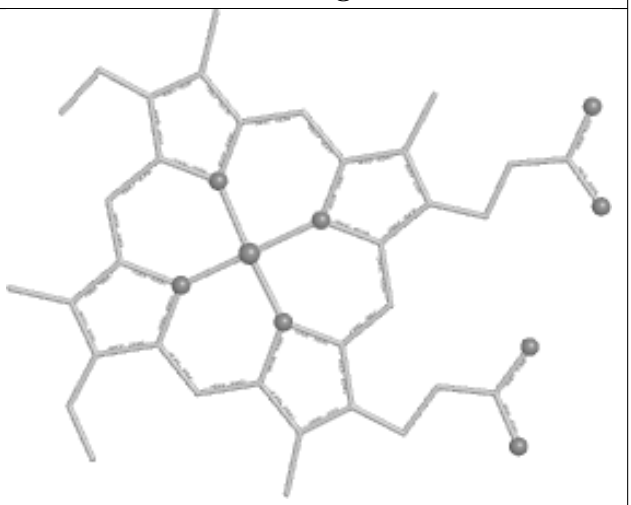
Bond lengths



Bond angles



Torsions

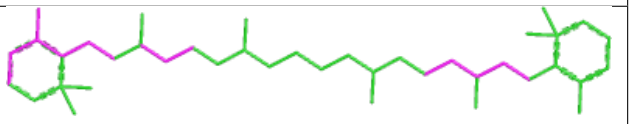


Rings

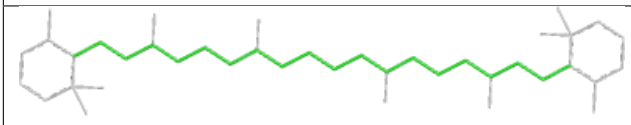
Ligand BCR k 103



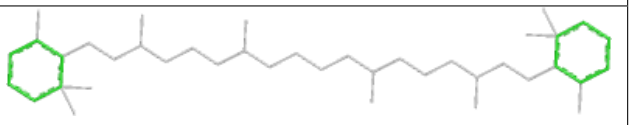
Bond lengths



Bond angles

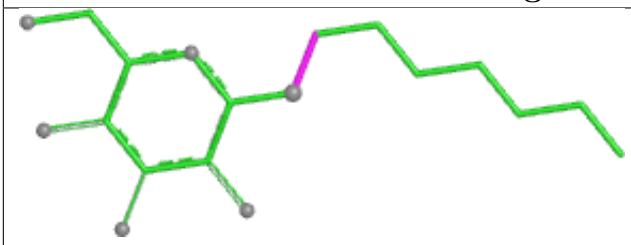


Torsions

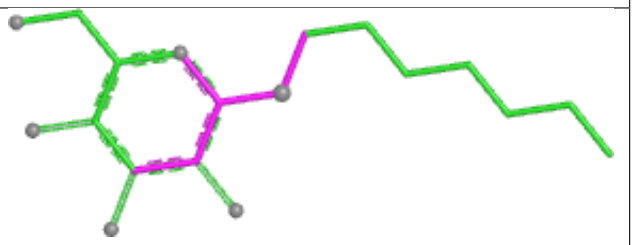


Rings

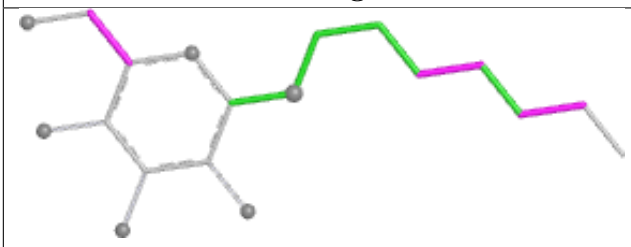
Ligand HTG d 414



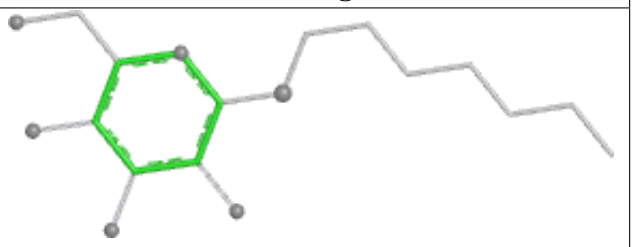
Bond lengths



Bond angles

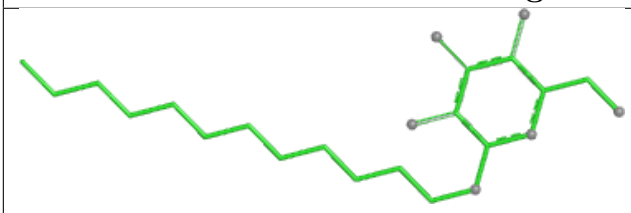


Torsions

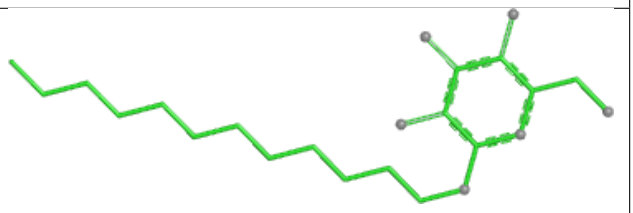


Rings

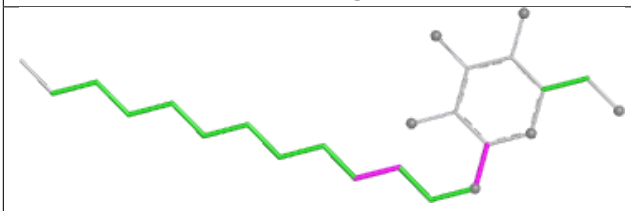
Ligand LMT e 101



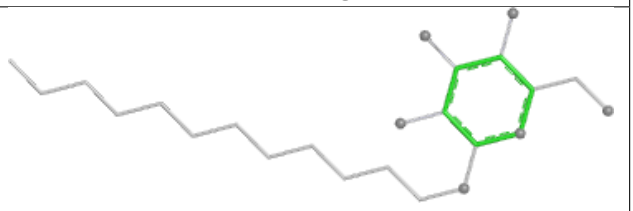
Bond lengths



Bond angles

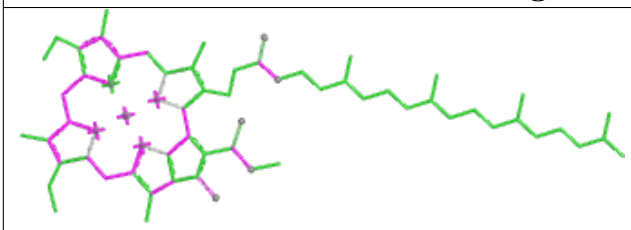


Torsions

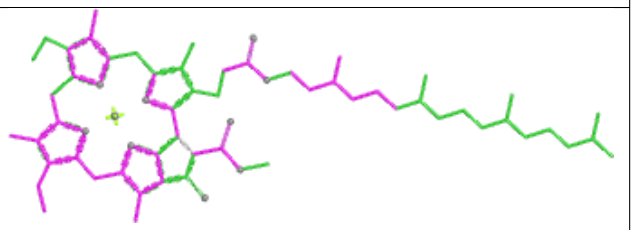


Rings

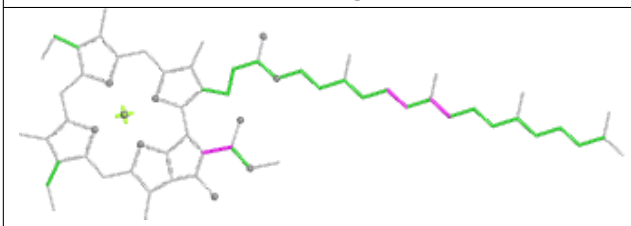
Ligand CLA c 908



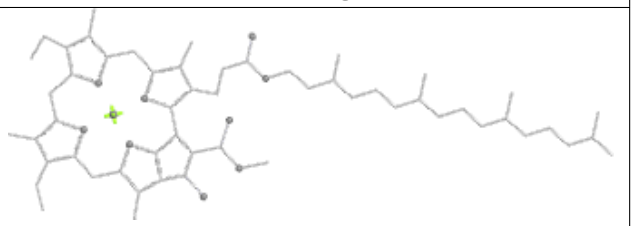
Bond lengths



Bond angles

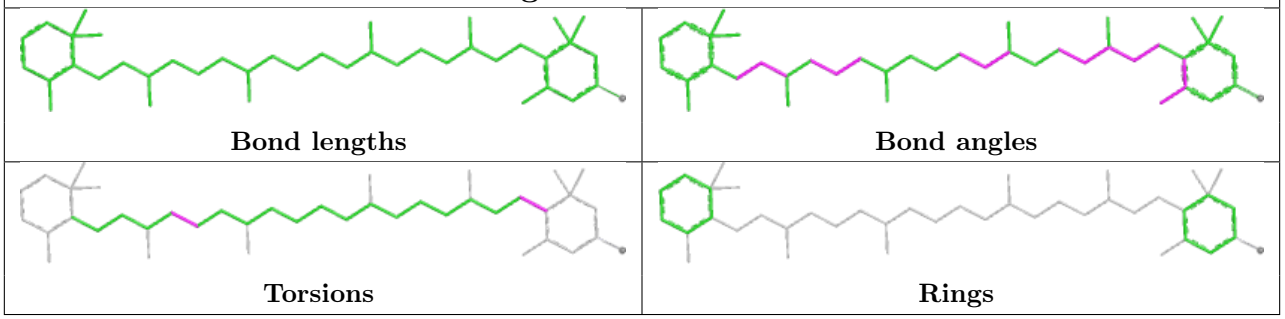


Torsions

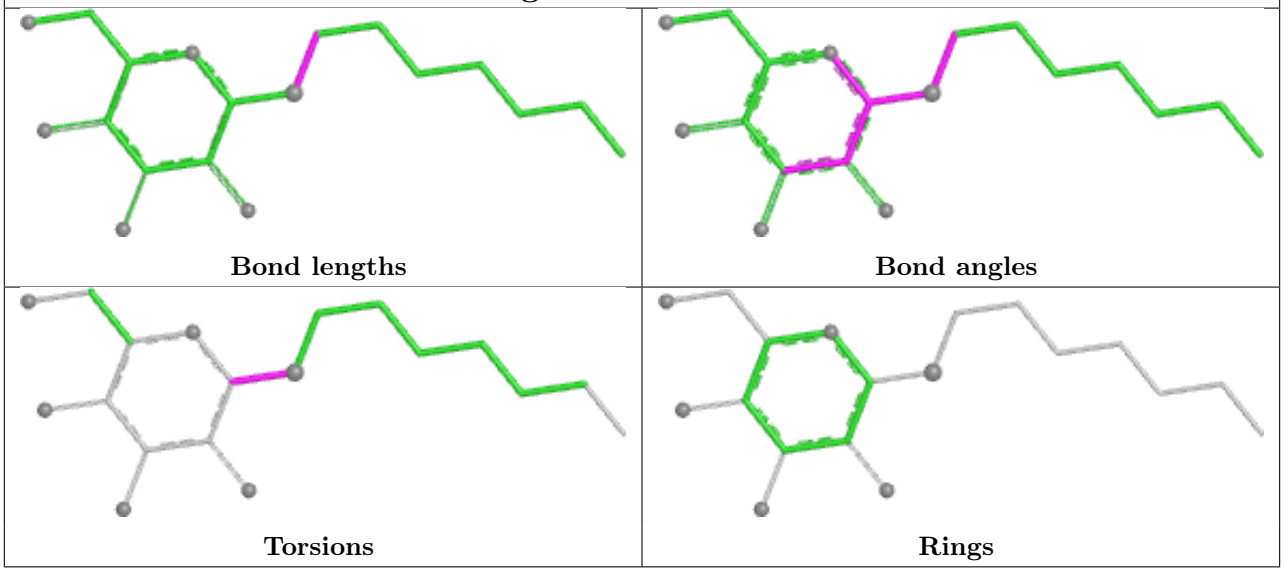


Rings

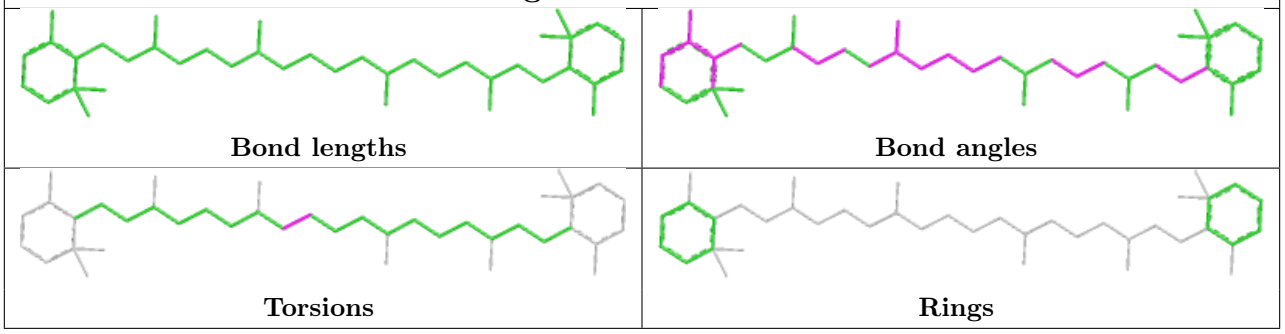
Ligand RRX H 101



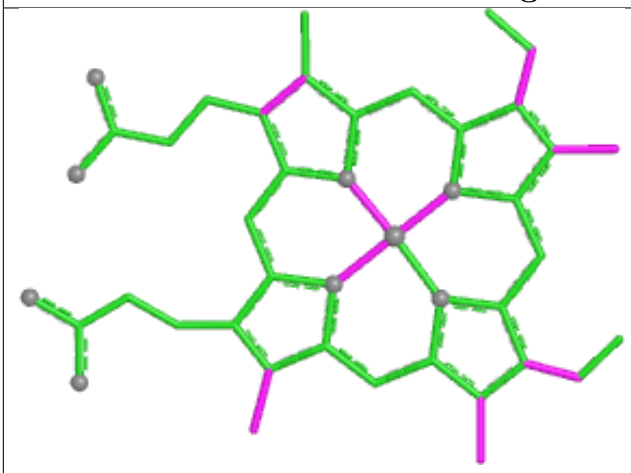
Ligand HTG V 215



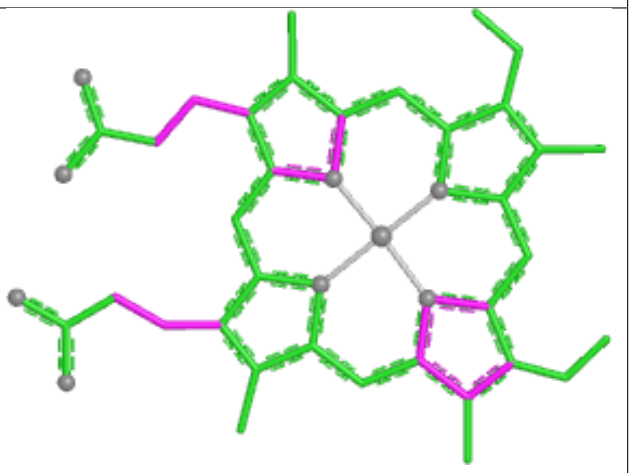
Ligand BCR B 636



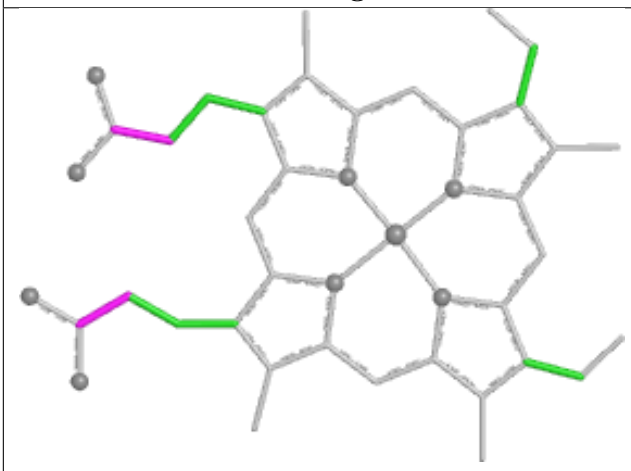
Ligand HEM F 102



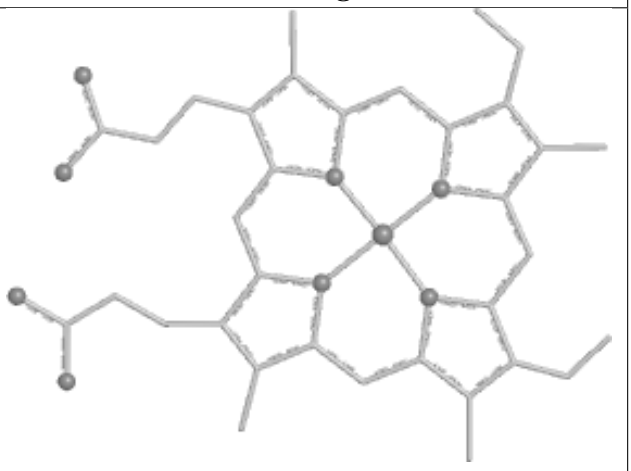
Bond lengths



Bond angles

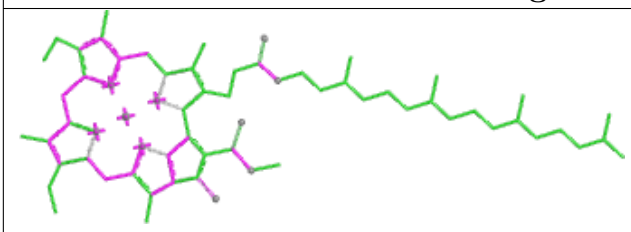


Torsions

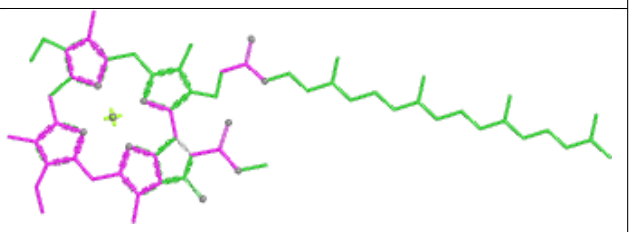


Rings

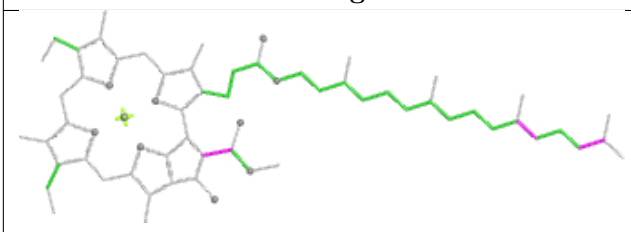
Ligand CLA c 903



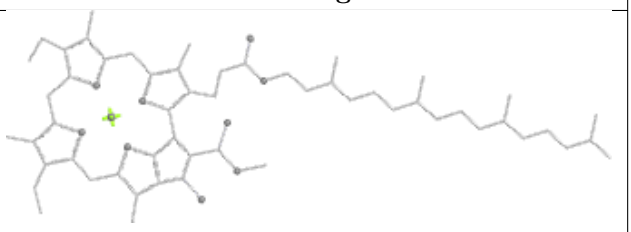
Bond lengths



Bond angles

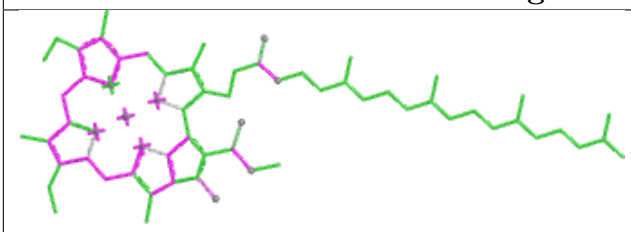


Torsions

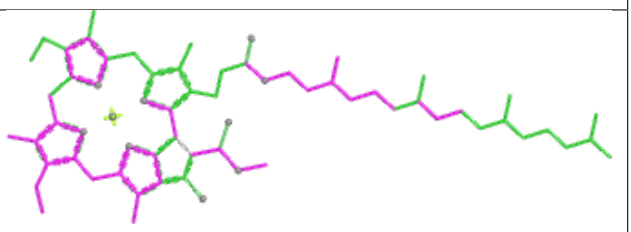


Rings

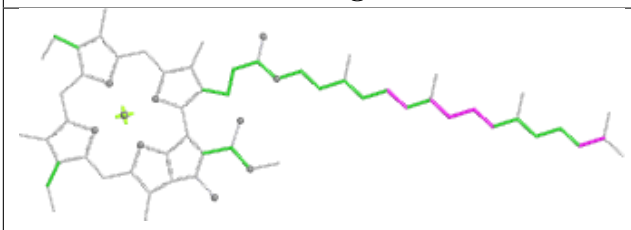
Ligand CLA b 619



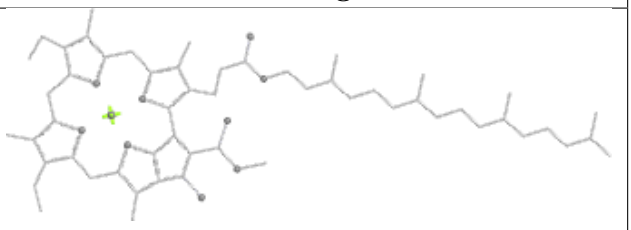
Bond lengths



Bond angles

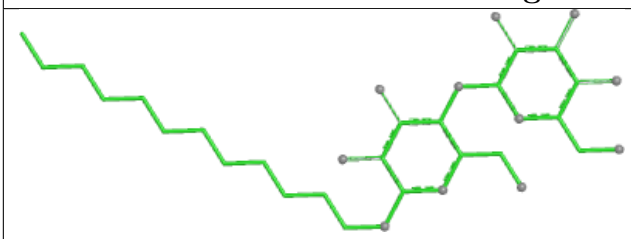


Torsions

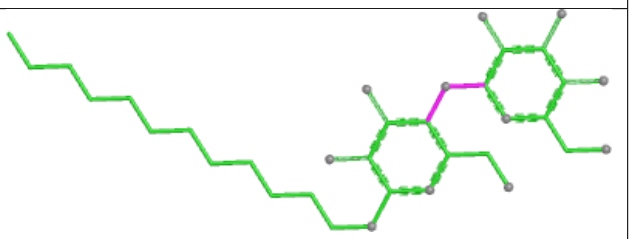


Rings

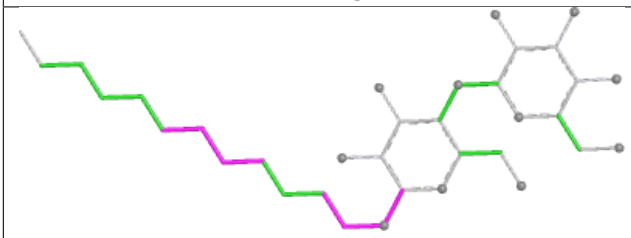
Ligand LMT Z 101



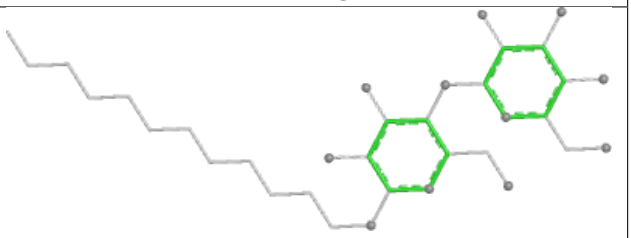
Bond lengths



Bond angles

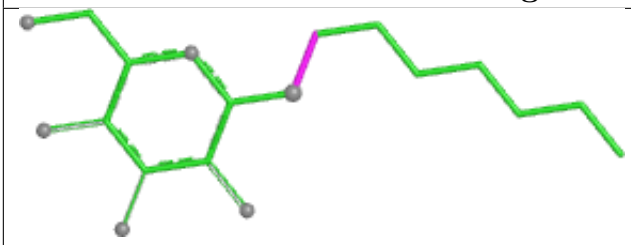


Torsions

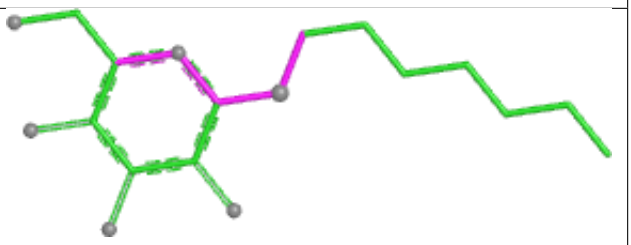


Rings

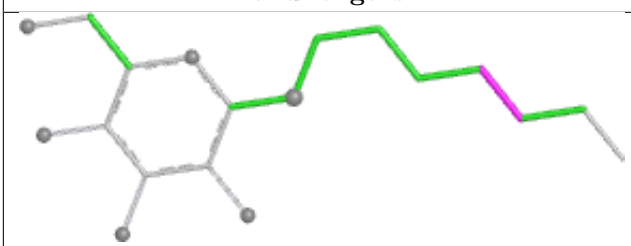
Ligand HTG B 631



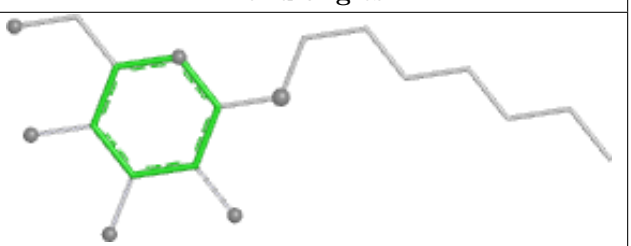
Bond lengths



Bond angles

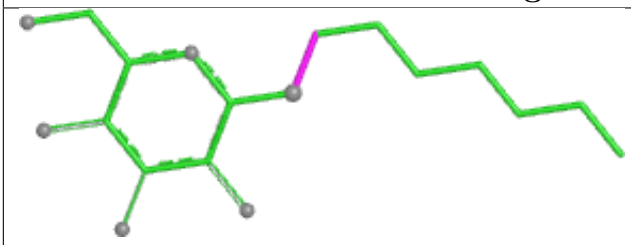


Torsions

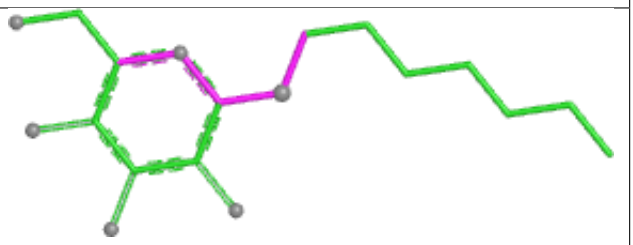


Rings

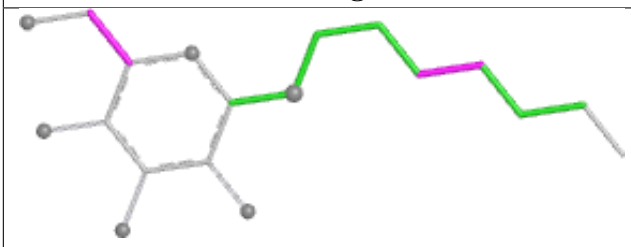
Ligand HTG d 420



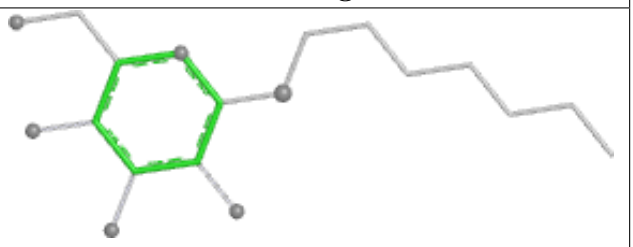
Bond lengths



Bond angles

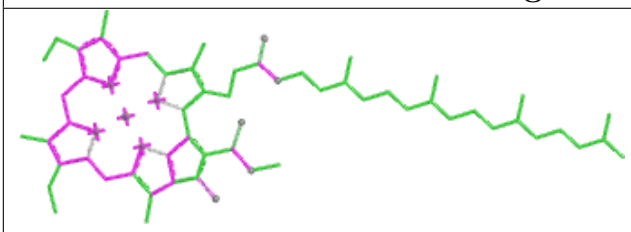


Torsions

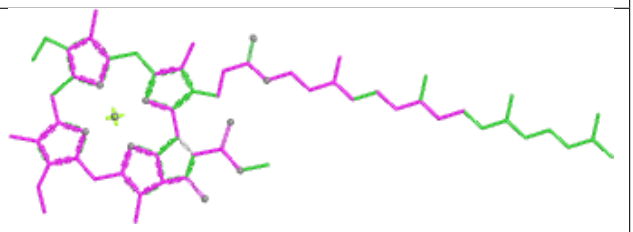


Rings

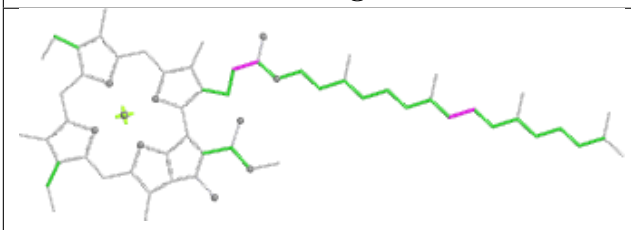
Ligand CLA C 510



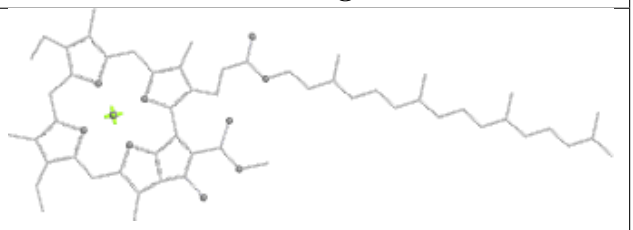
Bond lengths



Bond angles

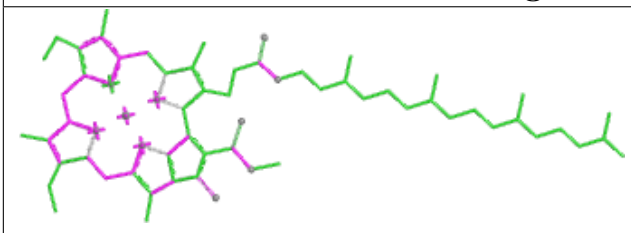


Torsions

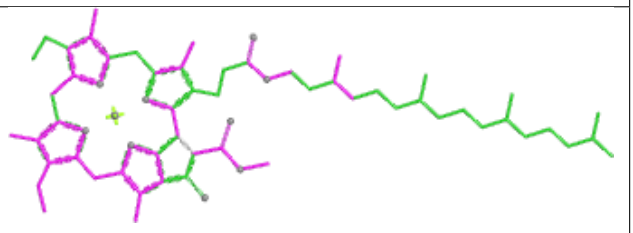


Rings

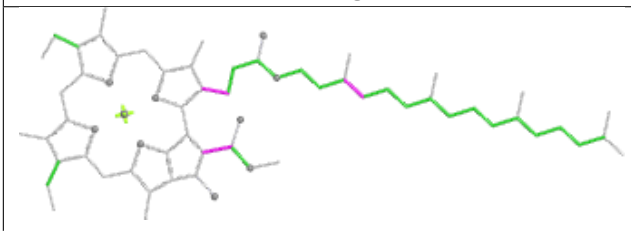
Ligand CLA B 610



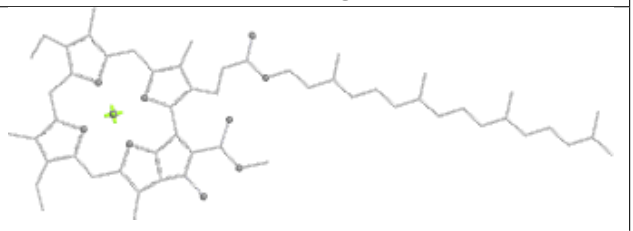
Bond lengths



Bond angles

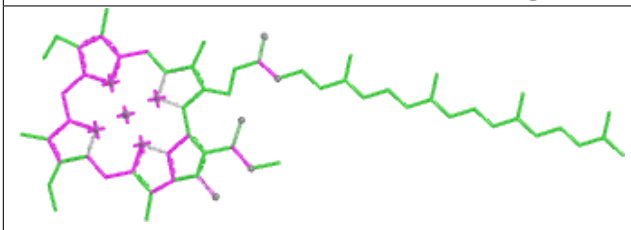


Torsions

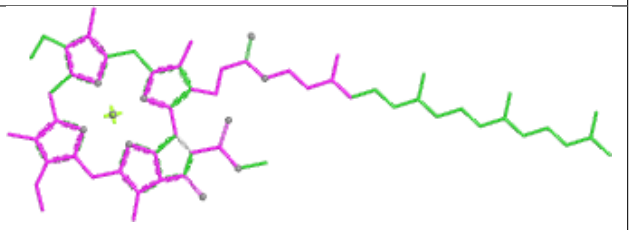


Rings

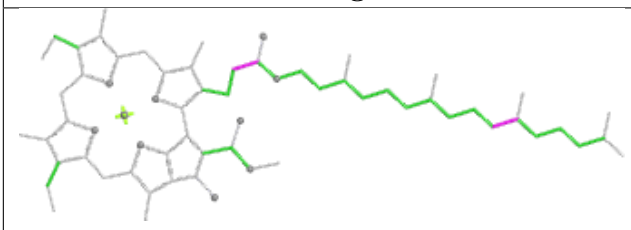
Ligand CLA C 512



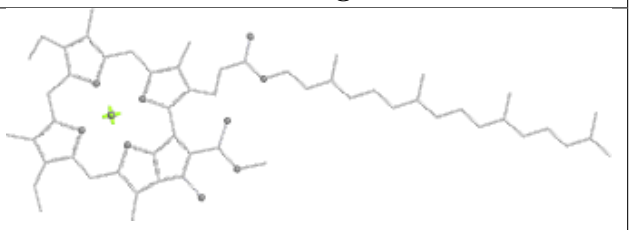
Bond lengths



Bond angles

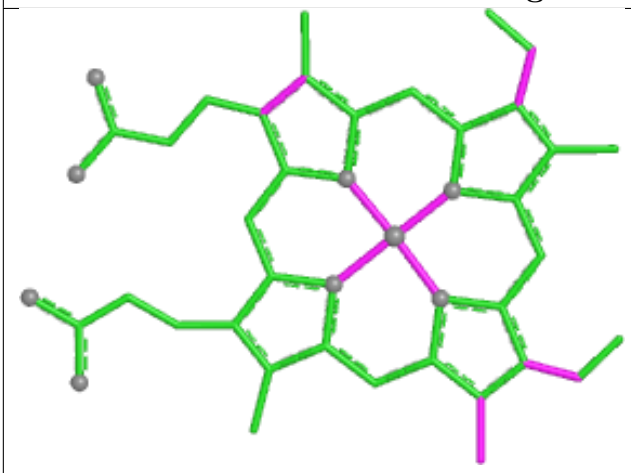


Torsions

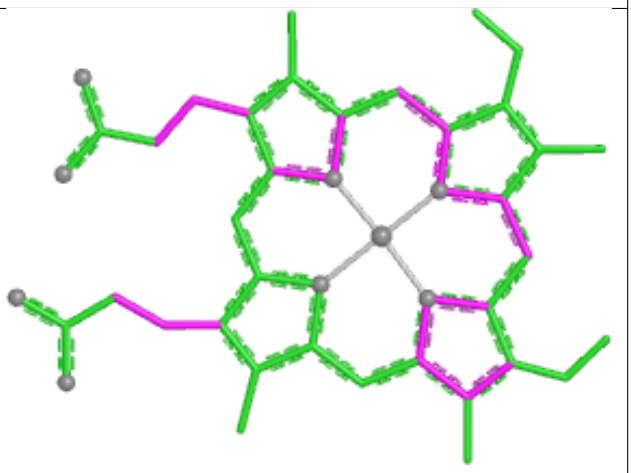


Rings

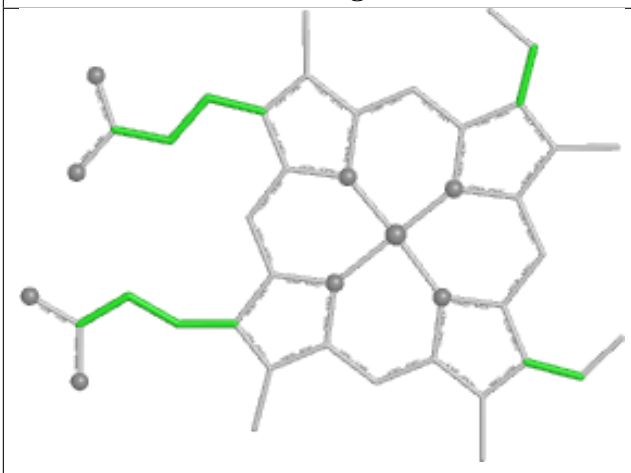
Ligand HEM f 101



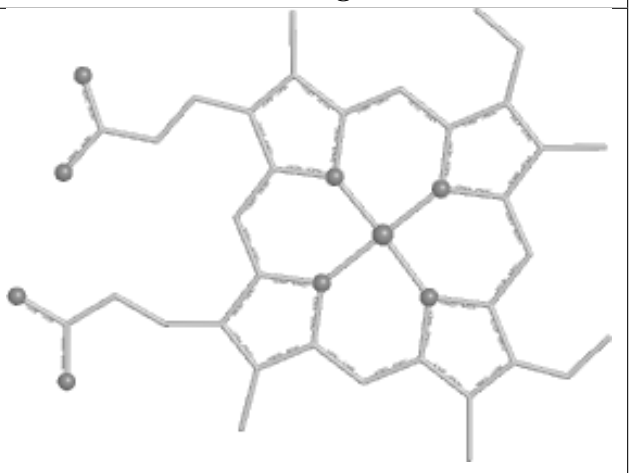
Bond lengths



Bond angles

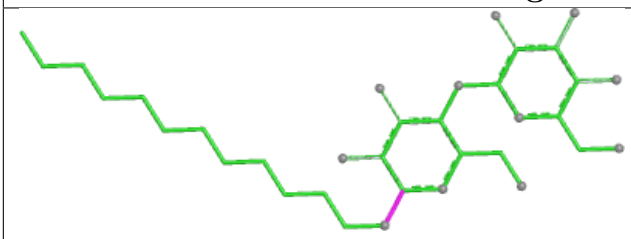


Torsions

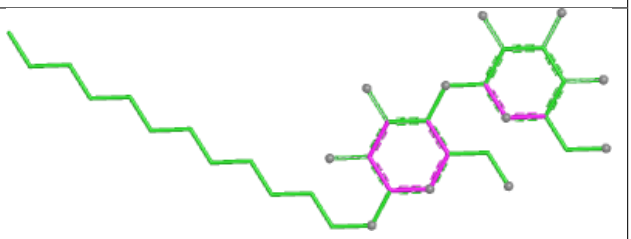


Rings

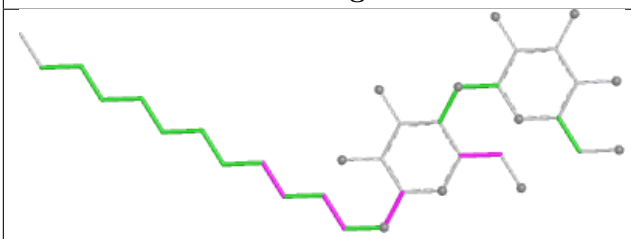
Ligand LMT c 922



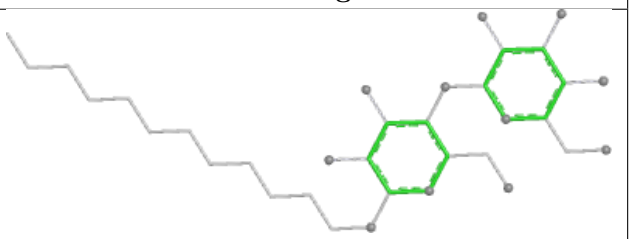
Bond lengths



Bond angles

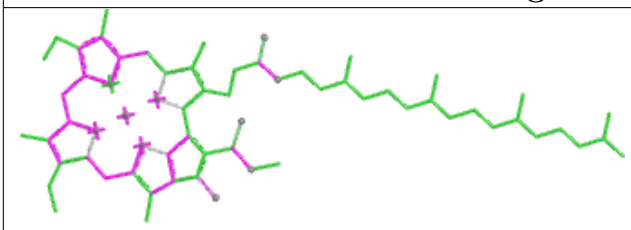


Torsions

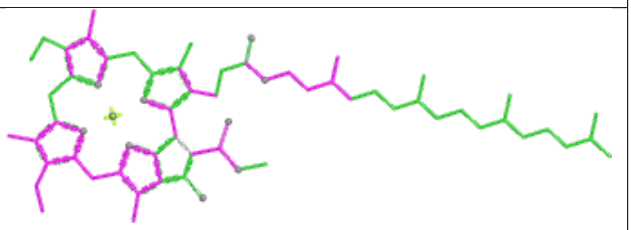


Rings

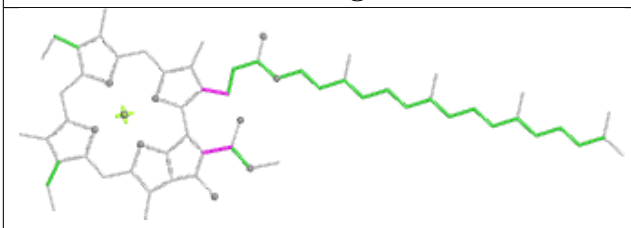
Ligand CLA b 605



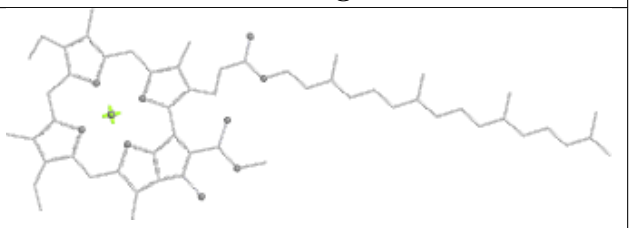
Bond lengths



Bond angles

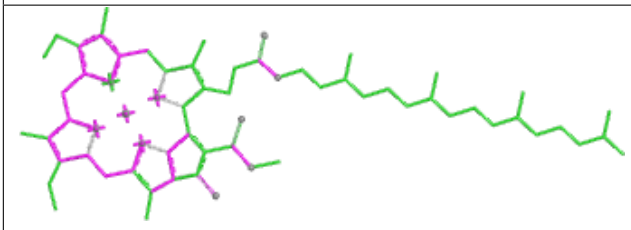


Torsions

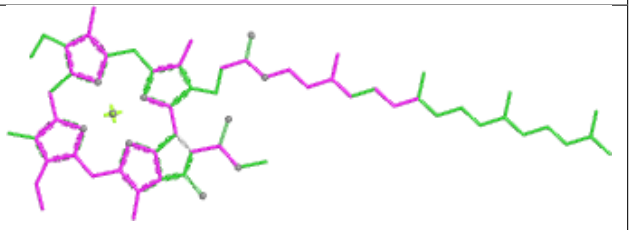


Rings

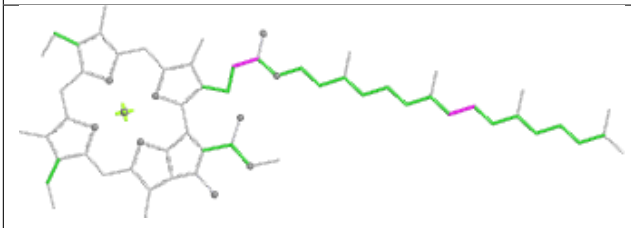
Ligand CLA c 911



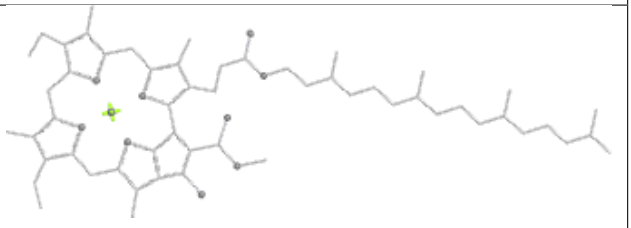
Bond lengths



Bond angles

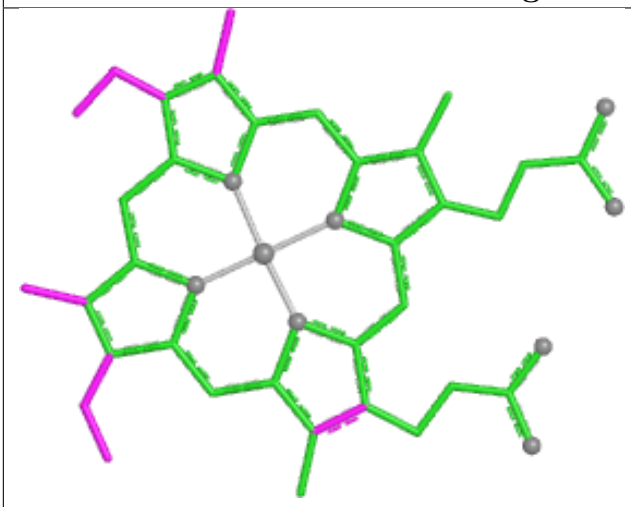


Torsions

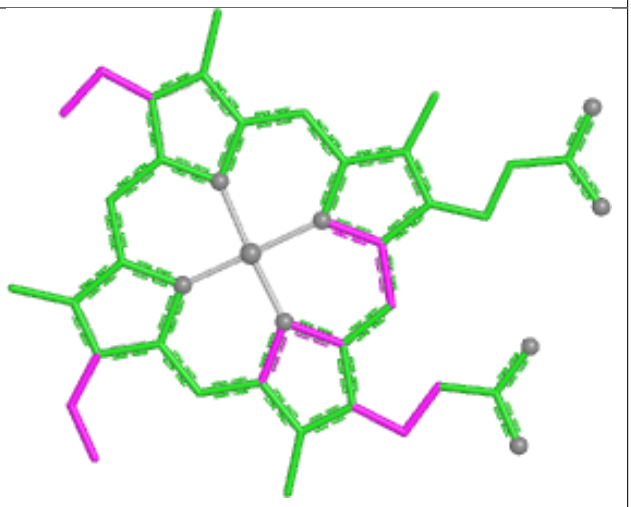


Rings

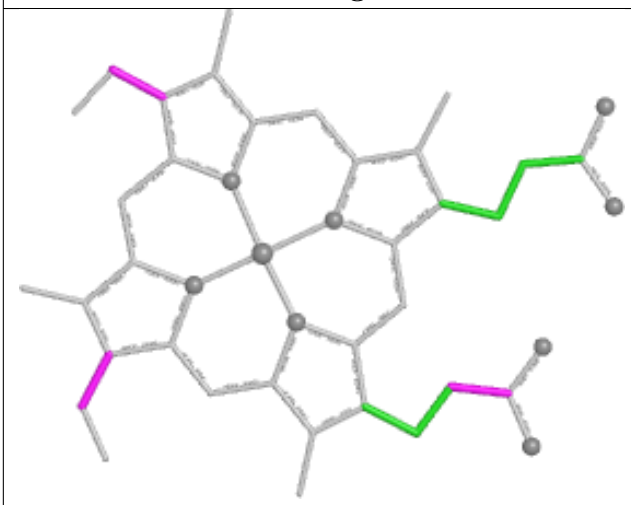
Ligand HEC V 203



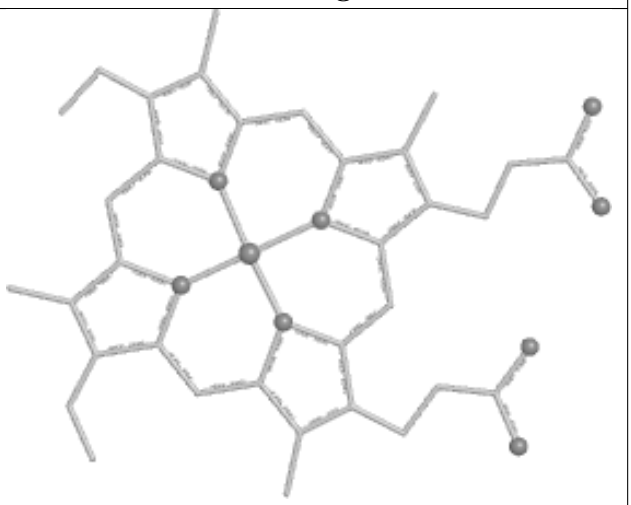
Bond lengths



Bond angles



Torsions

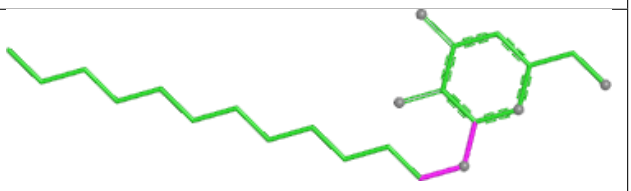


Rings

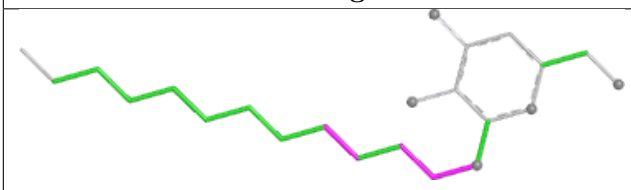
Ligand LMT t 101



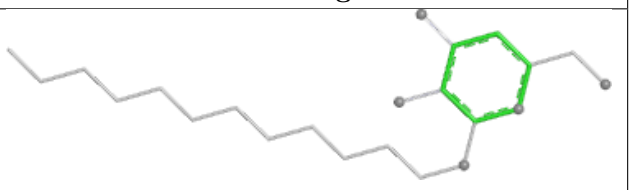
Bond lengths



Bond angles

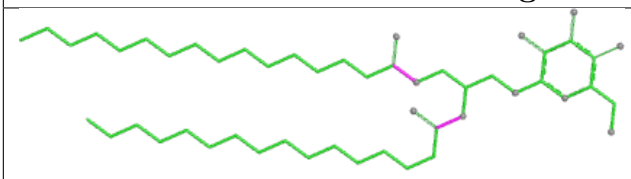


Torsions

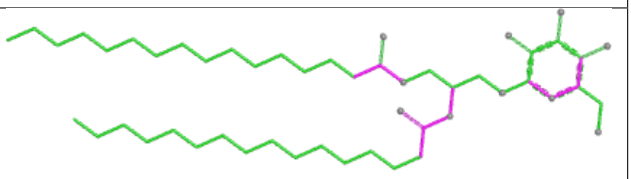


Rings

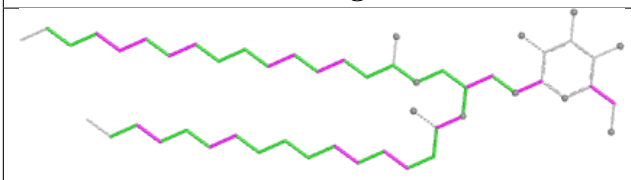
Ligand LMG A 413



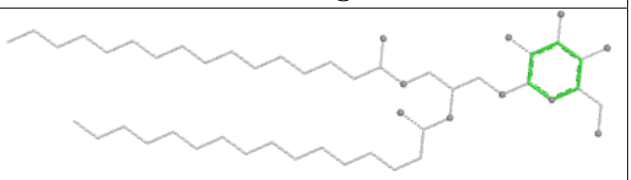
Bond lengths



Bond angles

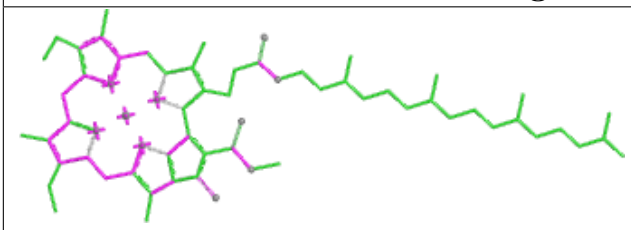


Torsions

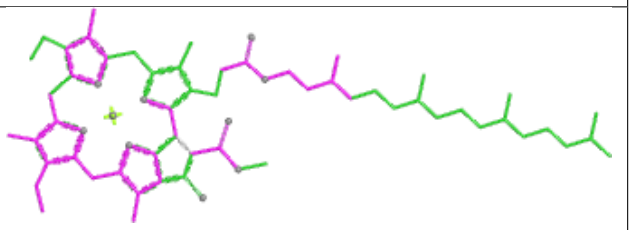


Rings

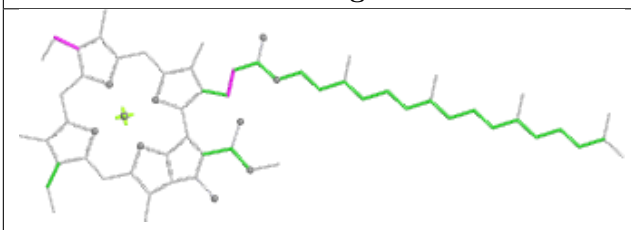
Ligand CLA c 902



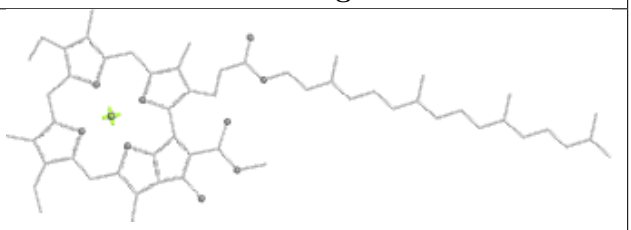
Bond lengths



Bond angles

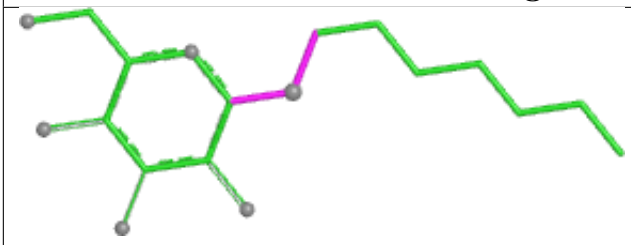


Torsions

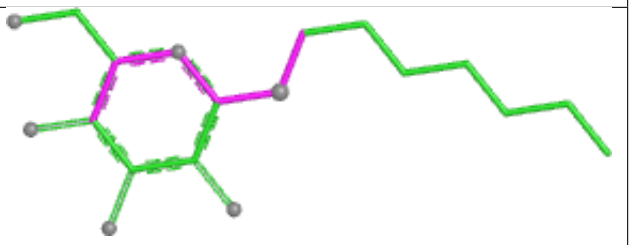


Rings

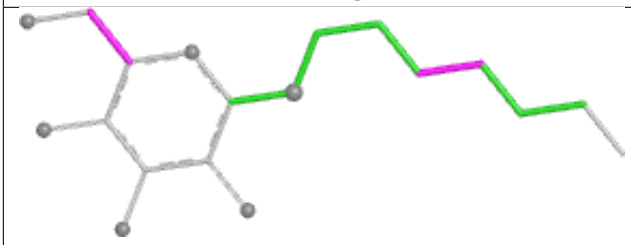
Ligand HTG b 602



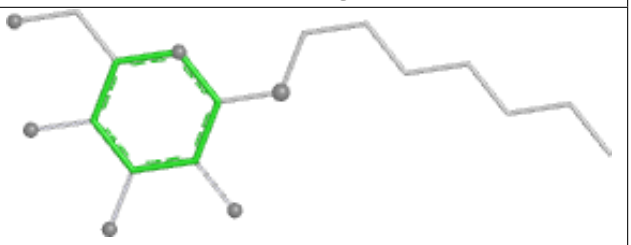
Bond lengths



Bond angles

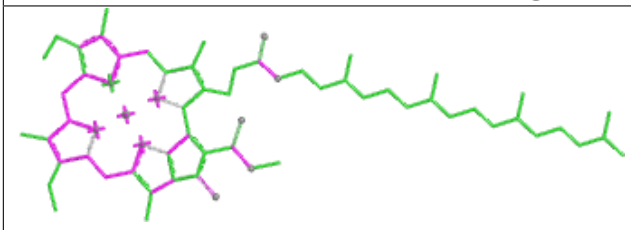


Torsions

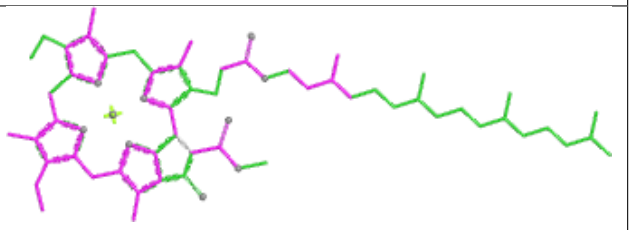


Rings

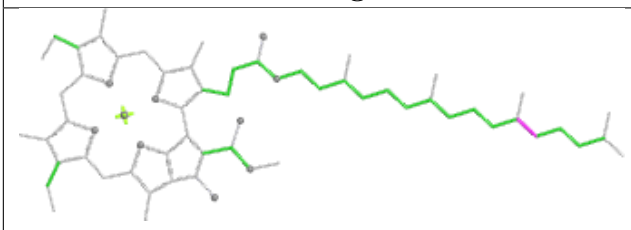
Ligand CLA b 617



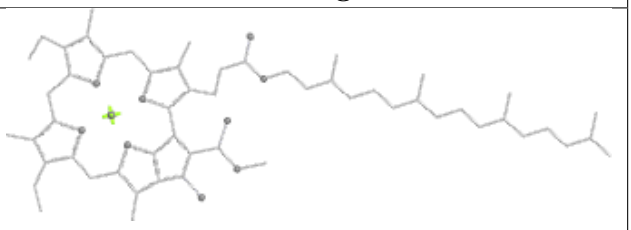
Bond lengths



Bond angles

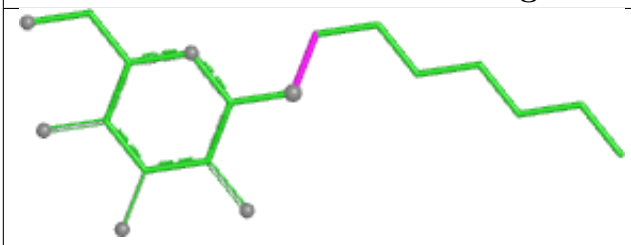


Torsions

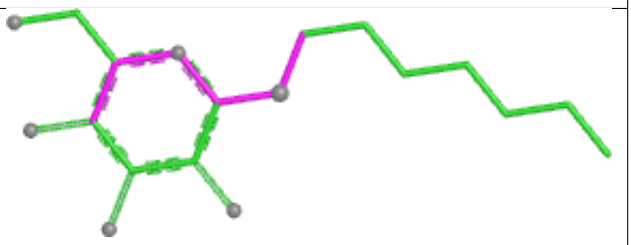


Rings

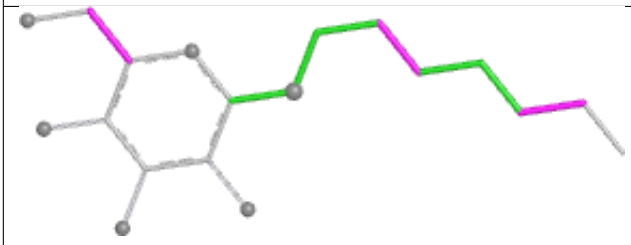
Ligand HTG D 412



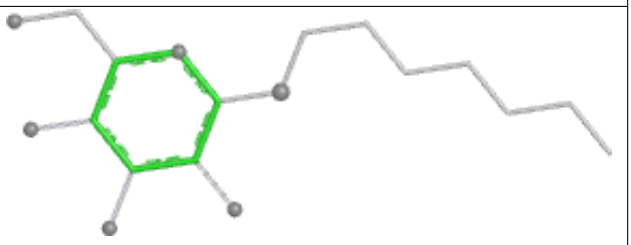
Bond lengths



Bond angles

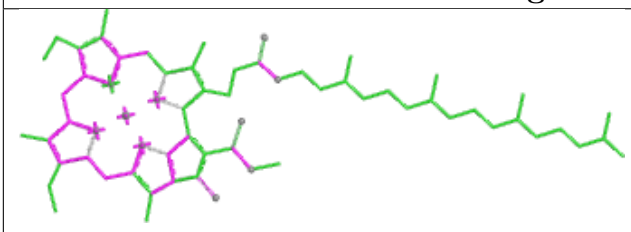


Torsions

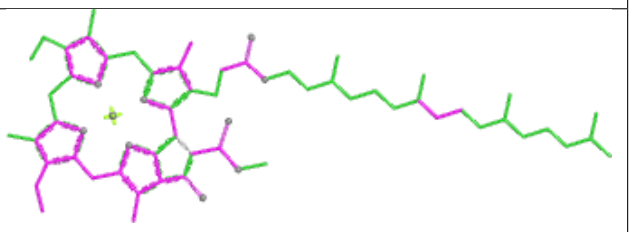


Rings

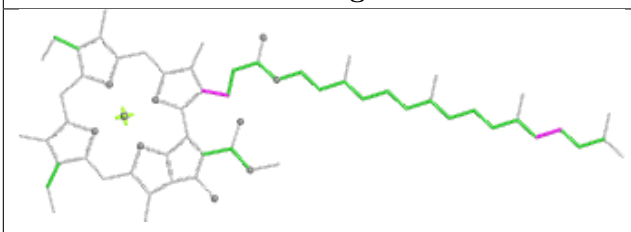
Ligand CLA b 612



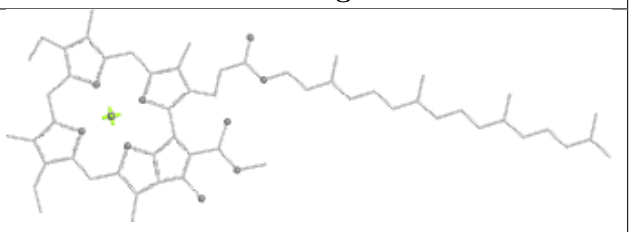
Bond lengths



Bond angles

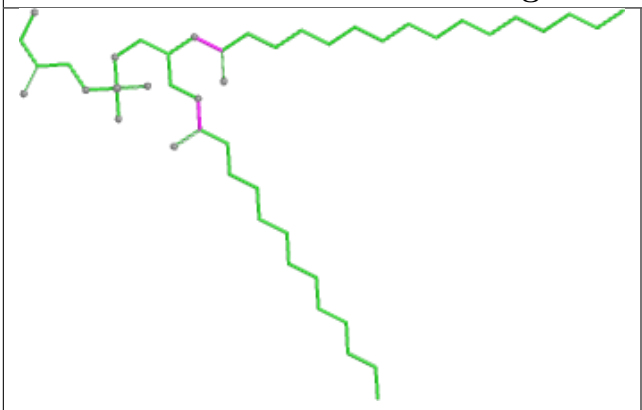


Torsions

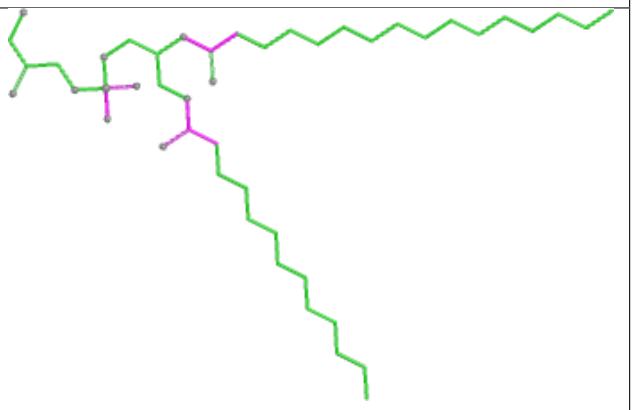


Rings

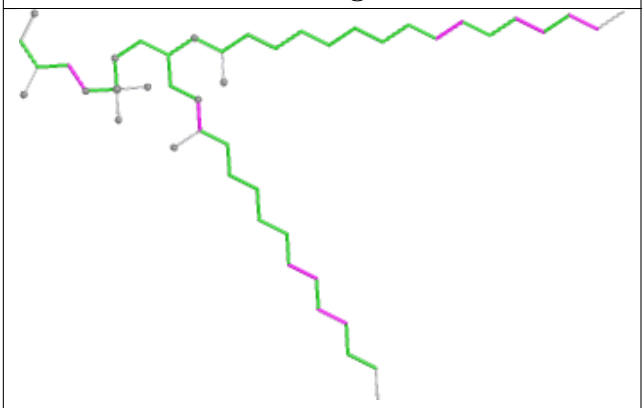
Ligand LHG D 408



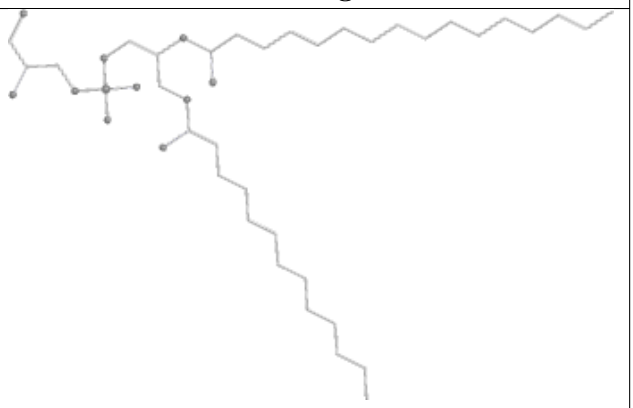
Bond lengths



Bond angles

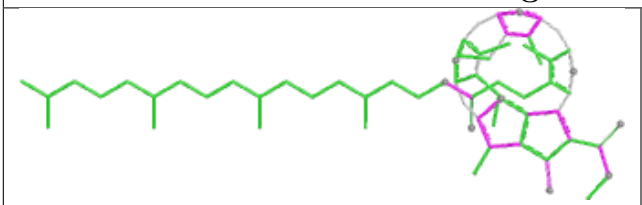


Torsions

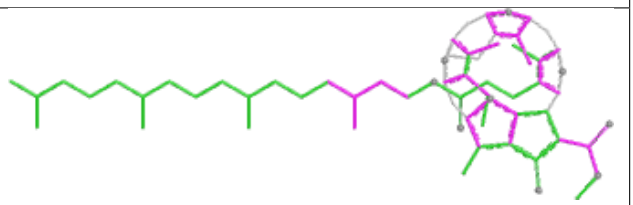


Rings

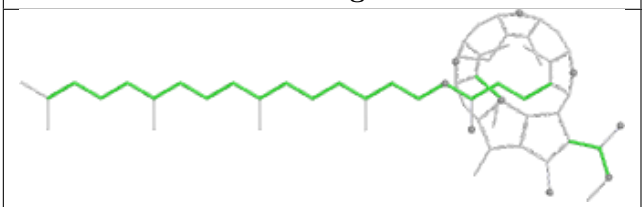
Ligand PHO A 409



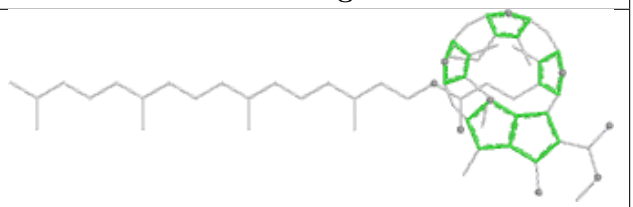
Bond lengths



Bond angles

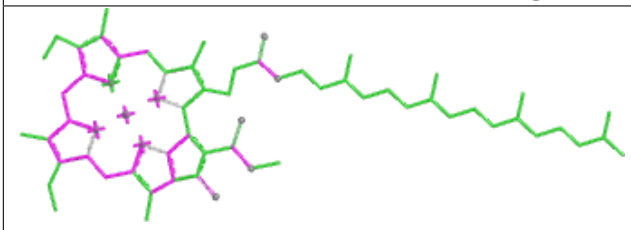


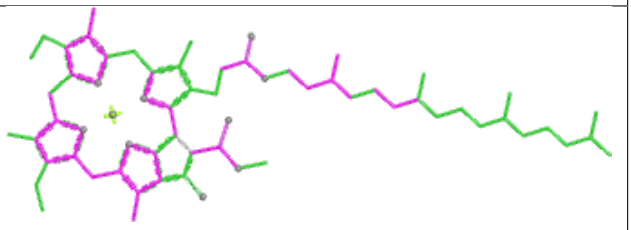
Torsions

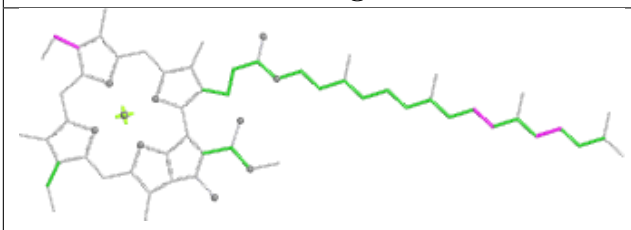


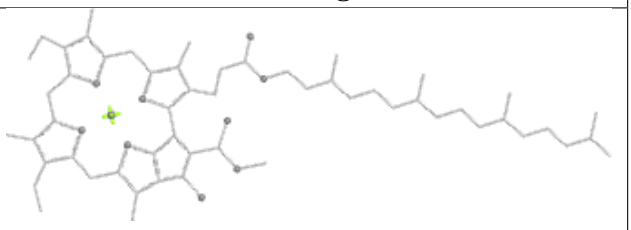
Rings

Ligand CLA b 608


Bond lengths


Bond angles

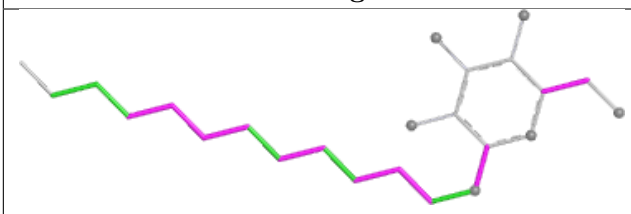

Torsions

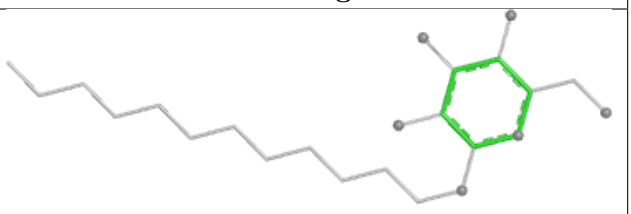

Rings

Ligand LMT B 626

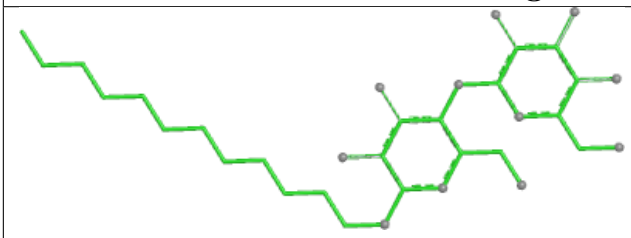

Bond lengths

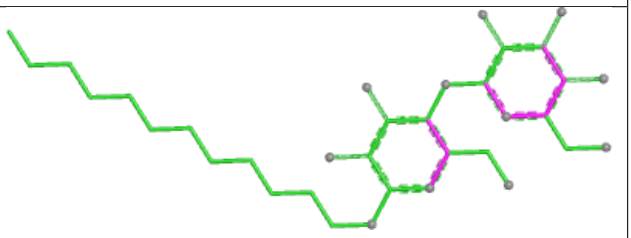

Bond angles

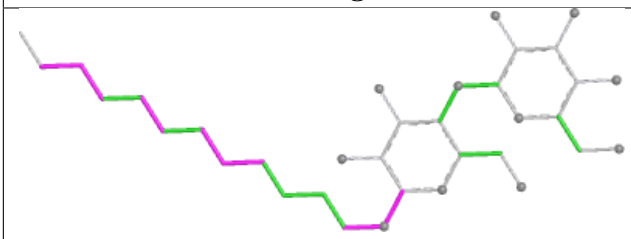

Torsions

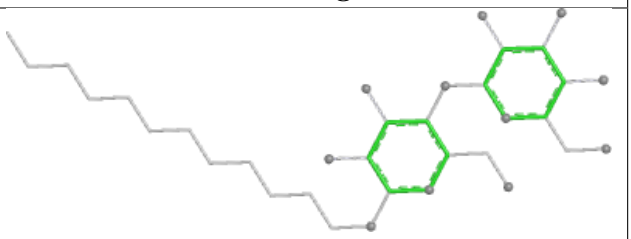

Rings

Ligand LMT a 402

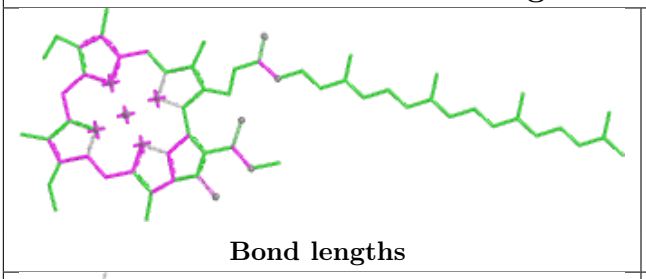

Bond lengths


Bond angles

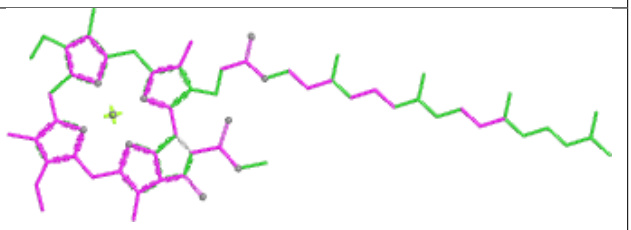

Torsions


Rings

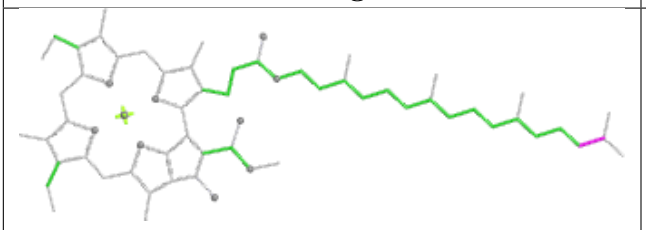
Ligand CLA b 615



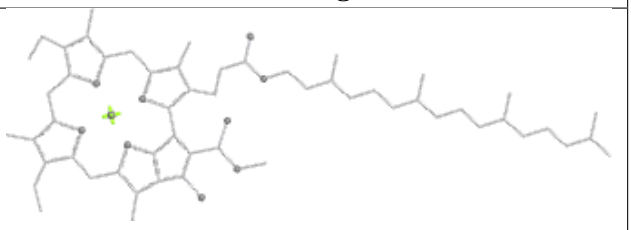
Bond lengths



Bond angles

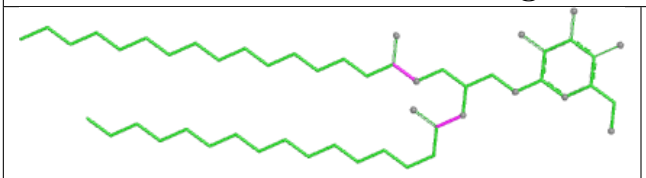


Torsions

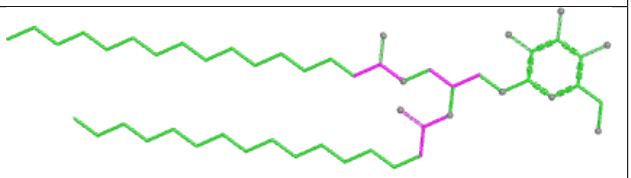


Rings

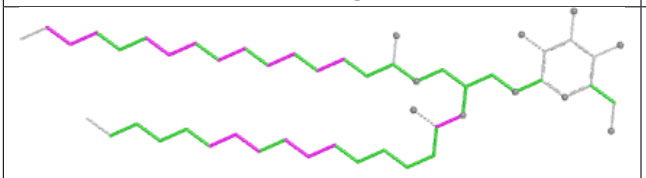
Ligand LMG B 621



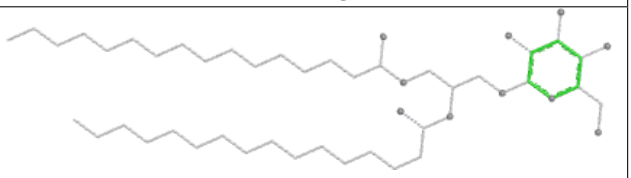
Bond lengths



Bond angles

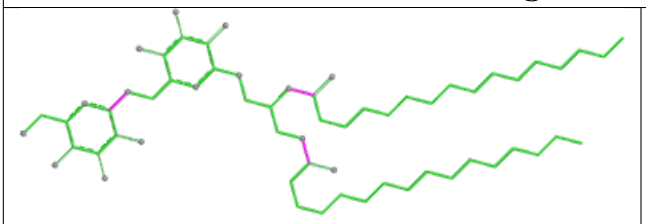


Torsions

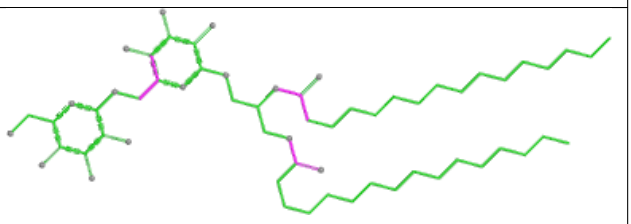


Rings

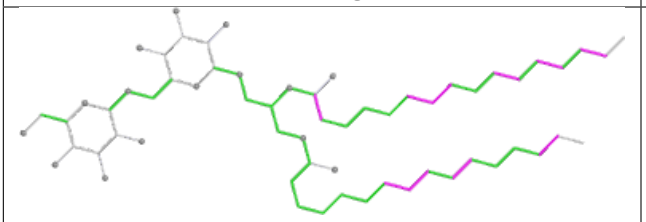
Ligand DGD h 102



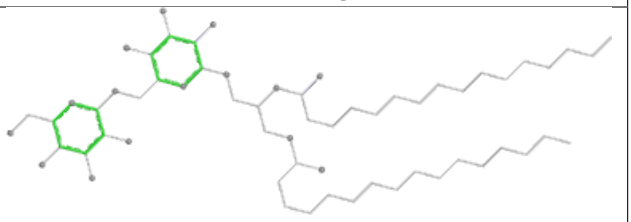
Bond lengths



Bond angles

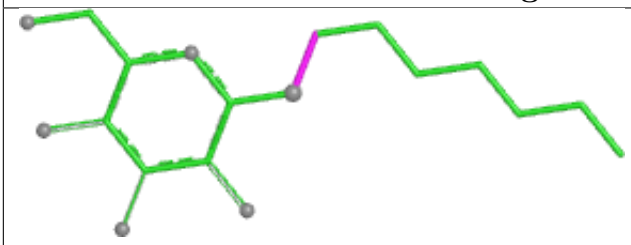


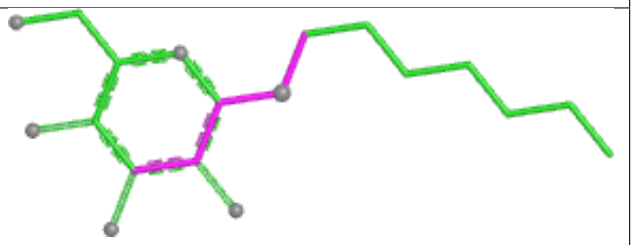
Torsions

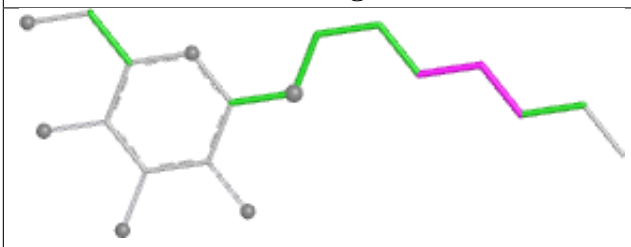


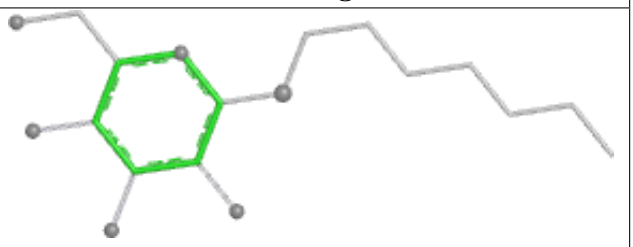
Rings

Ligand HTG B 624

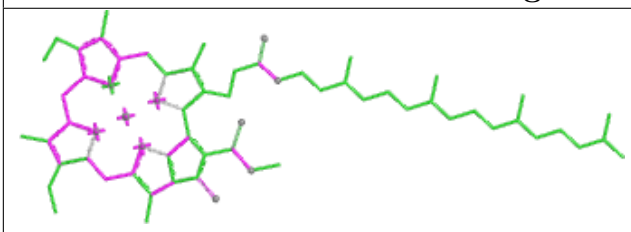

Bond lengths

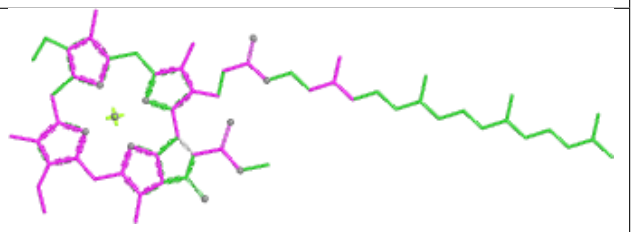

Bond angles

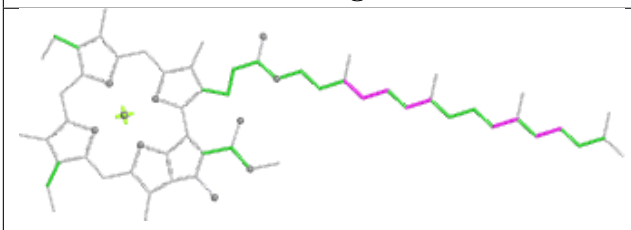

Torsions

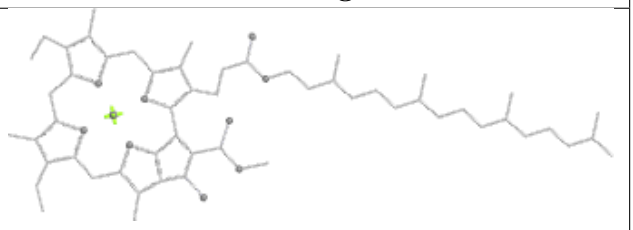

Rings

Ligand CLA A 410

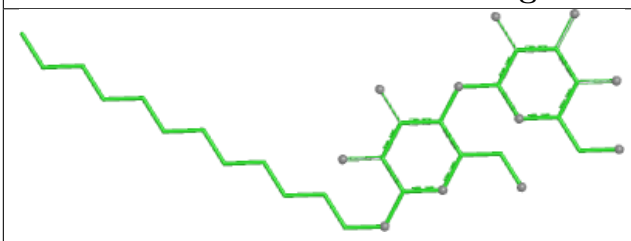

Bond lengths

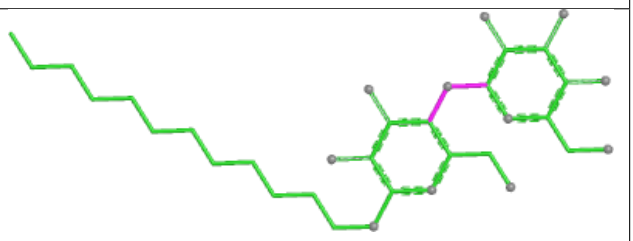

Bond angles

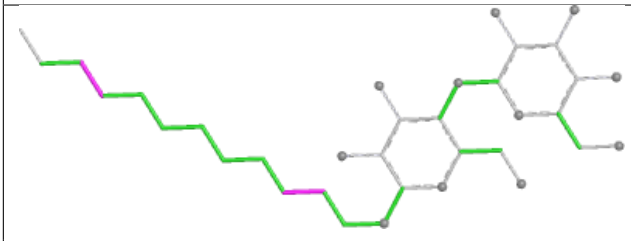

Torsions

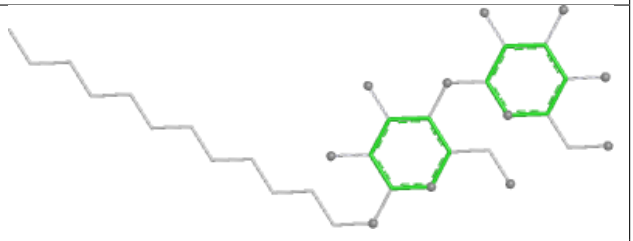

Rings

Ligand LMT m 103

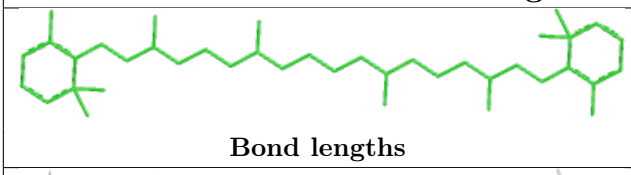

Bond lengths


Bond angles

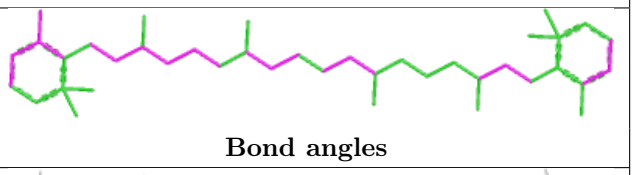

Torsions


Rings

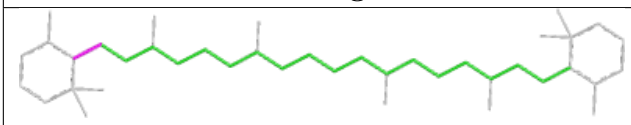
Ligand BCR b 621



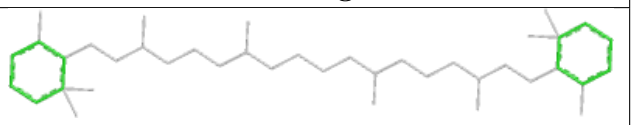
Bond lengths



Bond angles

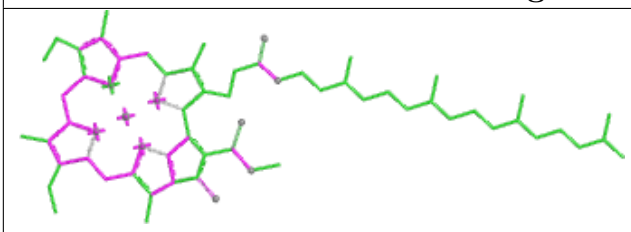


Torsions

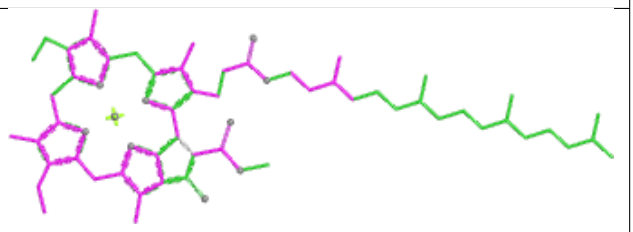


Rings

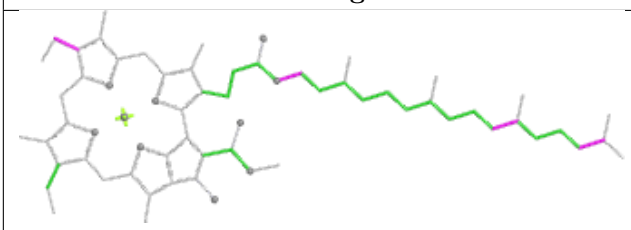
Ligand CLA d 404



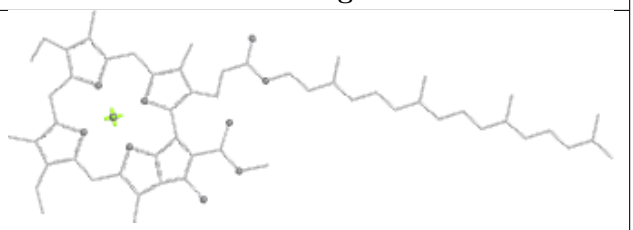
Bond lengths



Bond angles

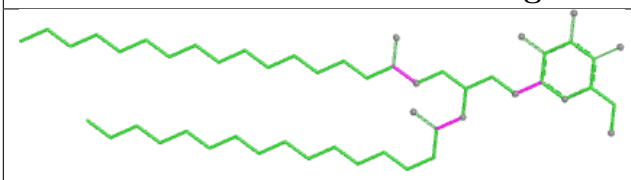


Torsions

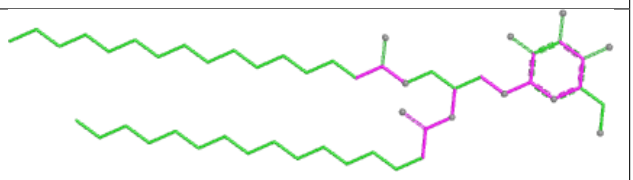


Rings

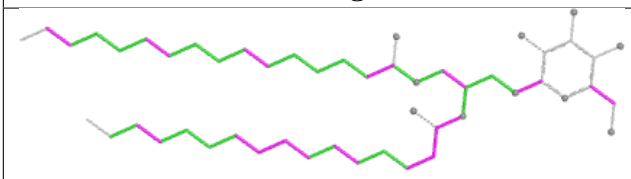
Ligand LMG a 416



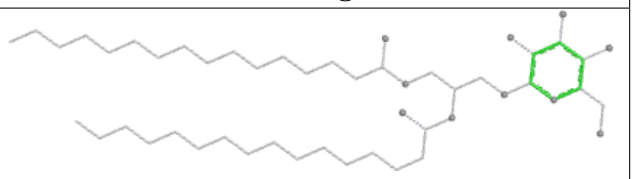
Bond lengths



Bond angles

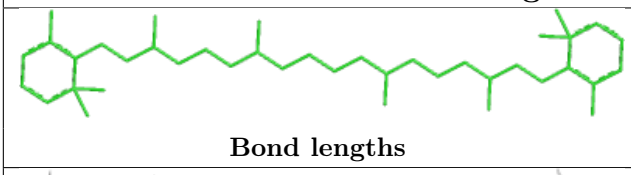


Torsions

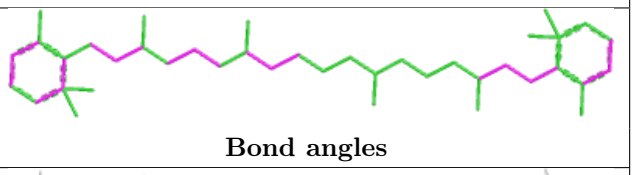


Rings

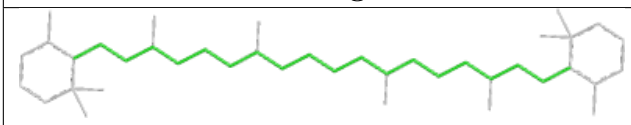
Ligand BCR B 620



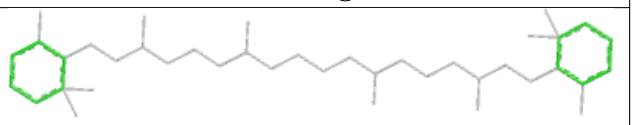
Bond lengths



Bond angles

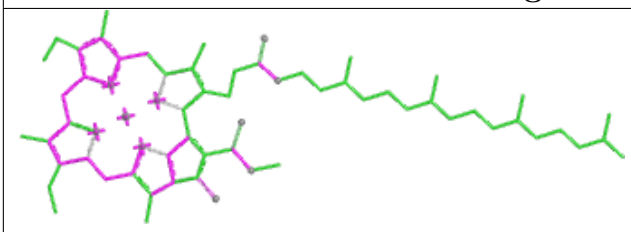


Torsions

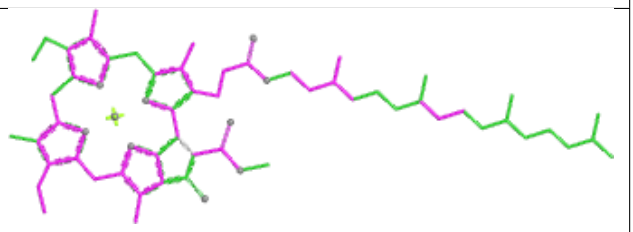


Rings

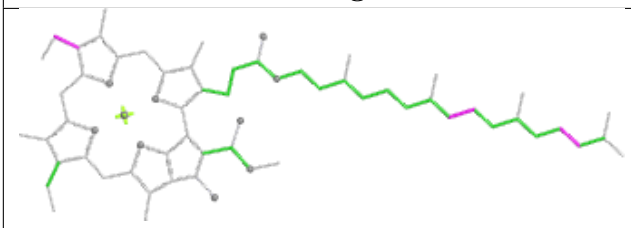
Ligand CLA B 603



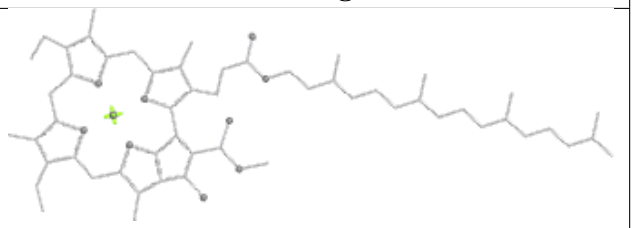
Bond lengths



Bond angles

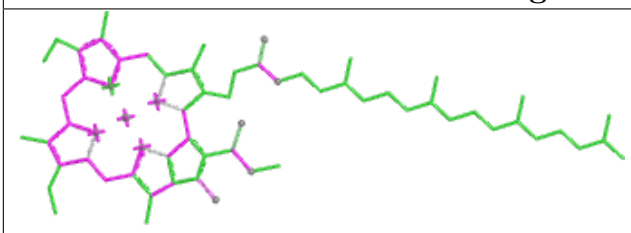


Torsions

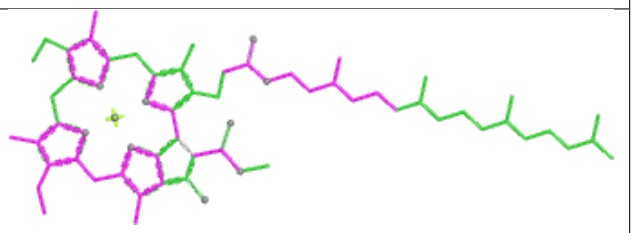


Rings

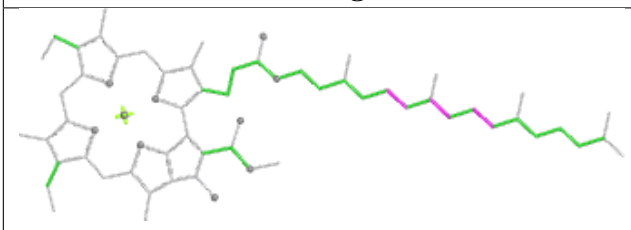
Ligand CLA c 904



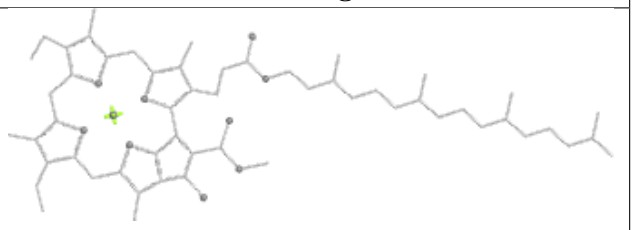
Bond lengths



Bond angles

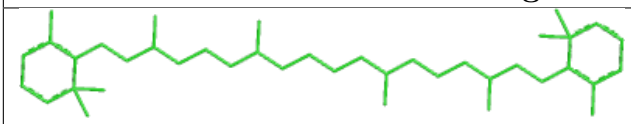


Torsions

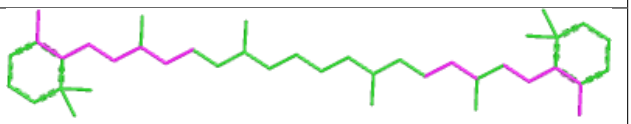


Rings

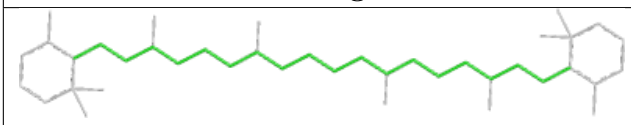
Ligand BCR C 514



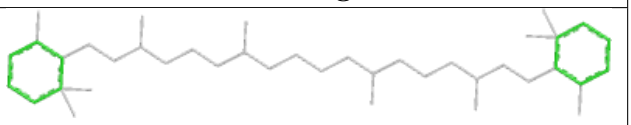
Bond lengths



Bond angles

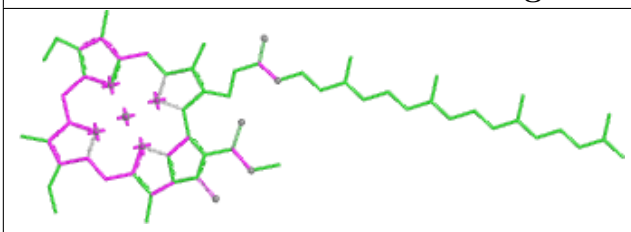


Torsions

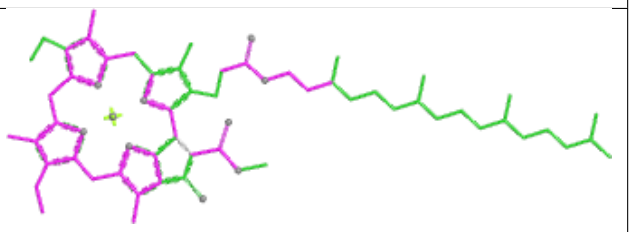


Rings

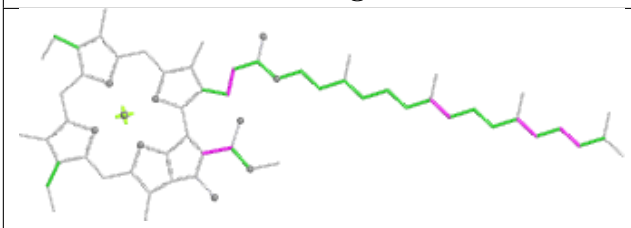
Ligand CLA C 507



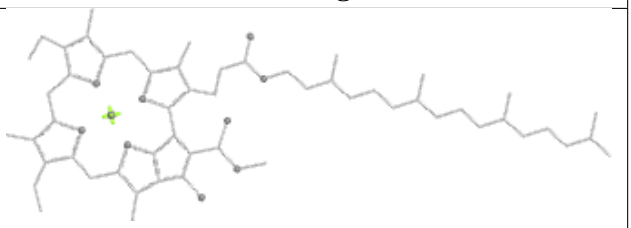
Bond lengths



Bond angles

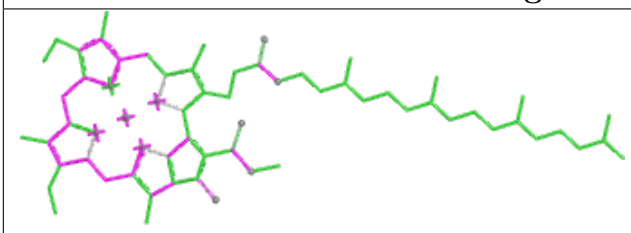


Torsions

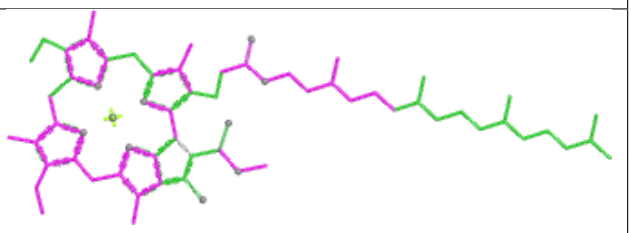


Rings

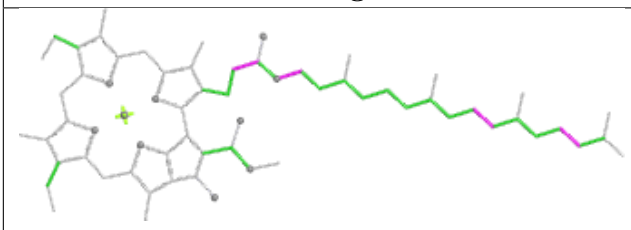
Ligand CLA B 614



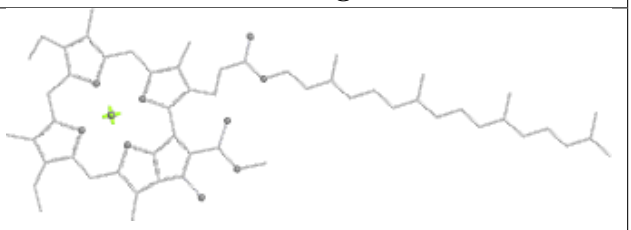
Bond lengths



Bond angles

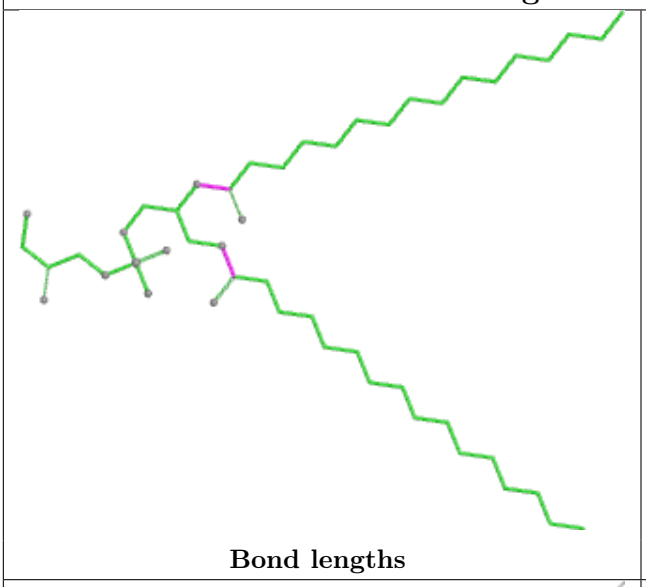


Torsions

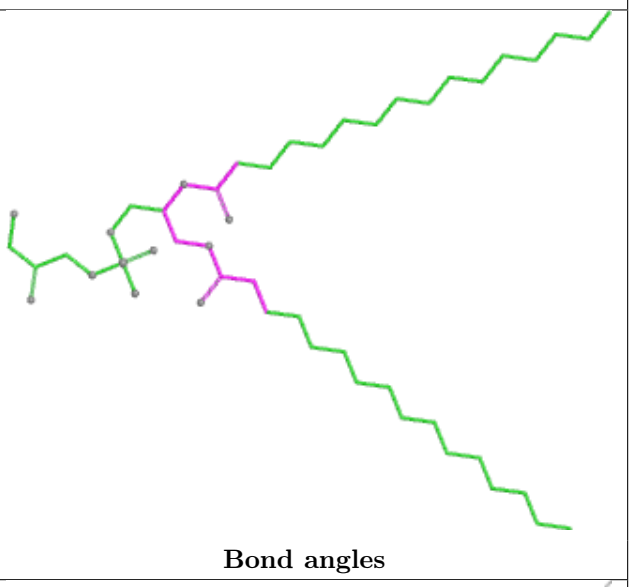


Rings

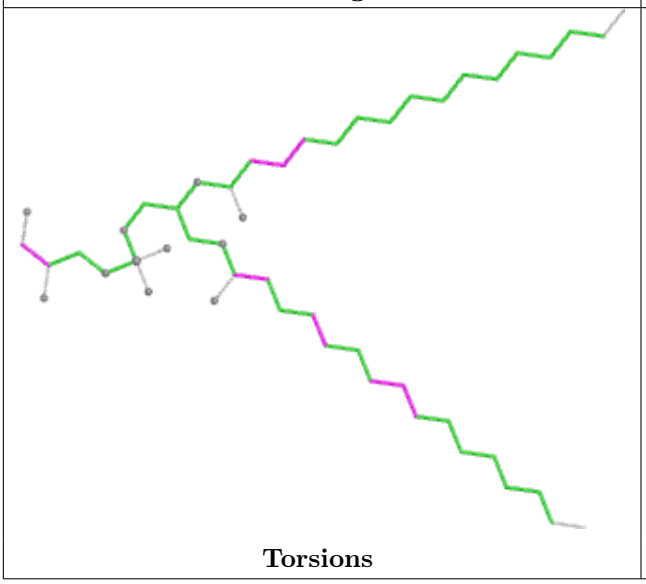
Ligand LHG D 406



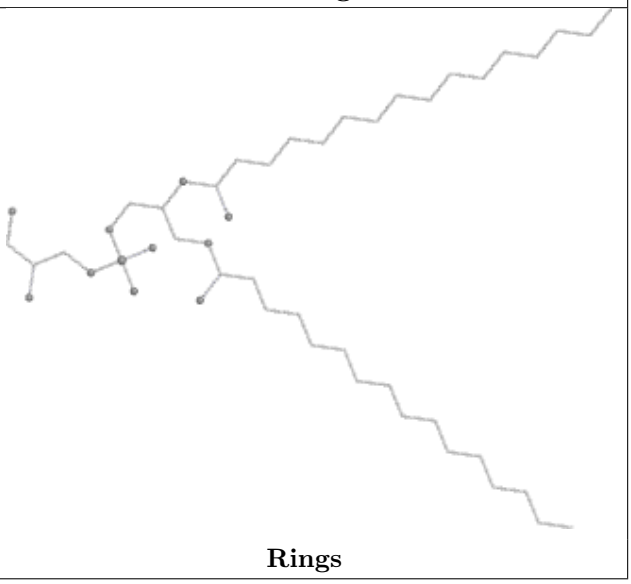
Bond lengths



Bond angles

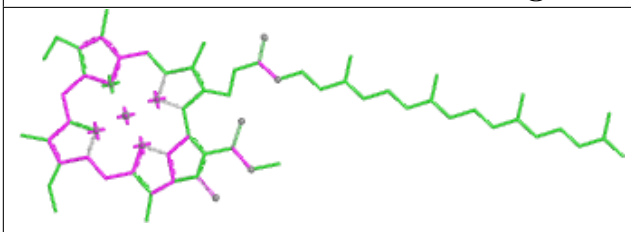


Torsions

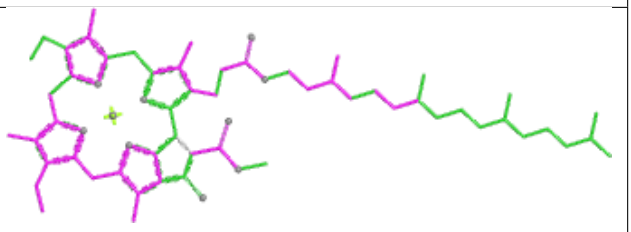


Rings

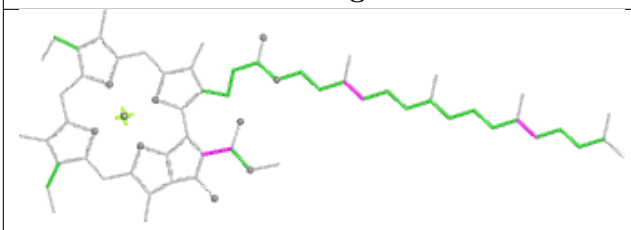
Ligand CLA d 405



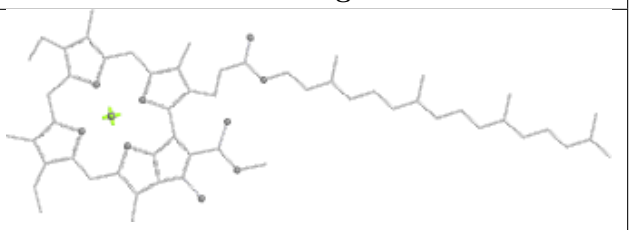
Bond lengths



Bond angles

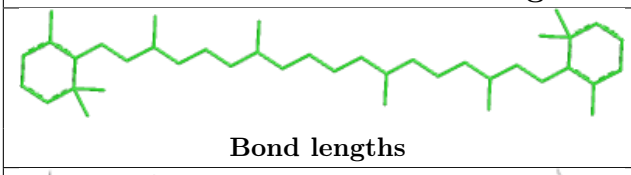


Torsions

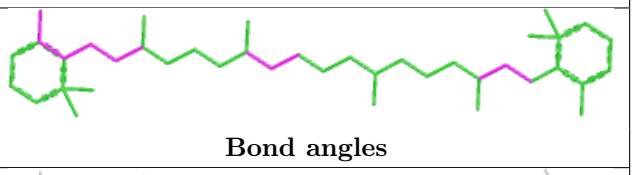


Rings

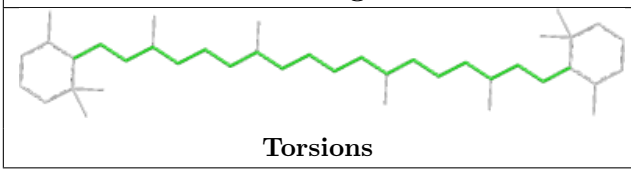
Ligand BCR a 414



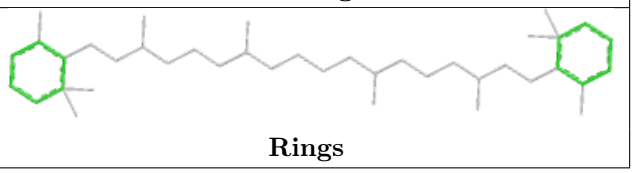
Bond lengths



Bond angles

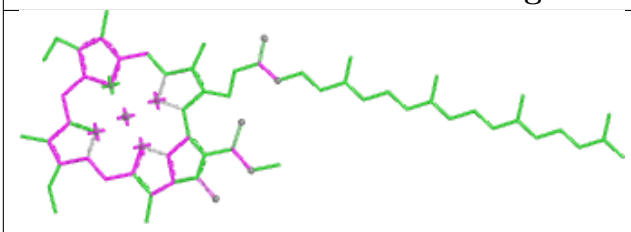


Torsions

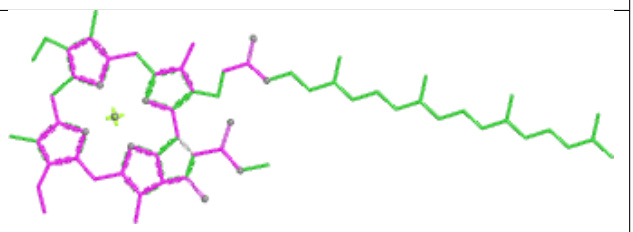


Rings

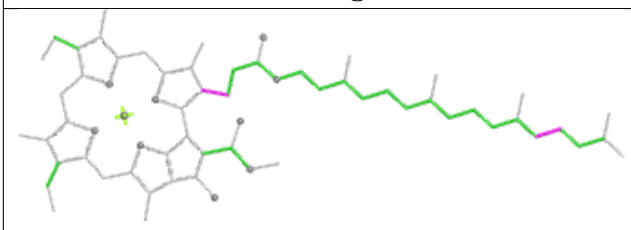
Ligand CLA B 609



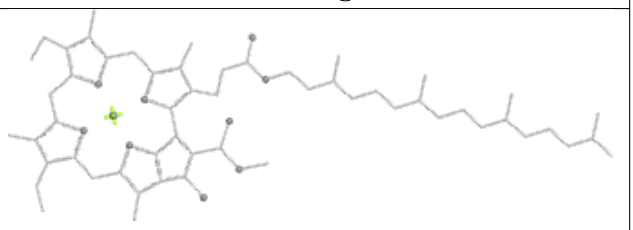
Bond lengths



Bond angles

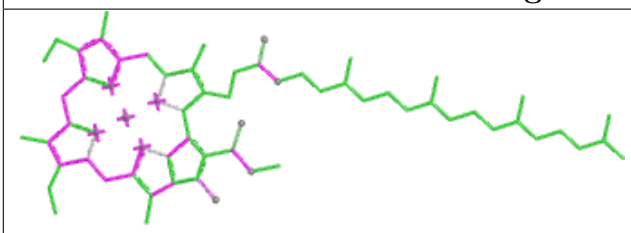


Torsions

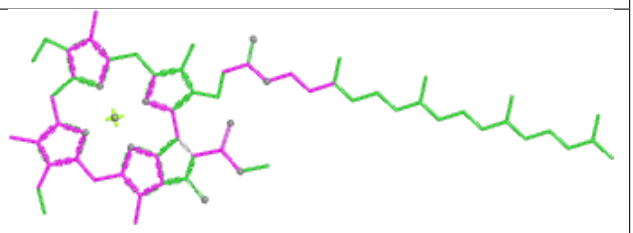


Rings

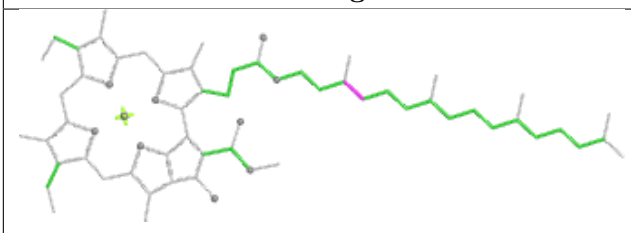
Ligand CLA C 505



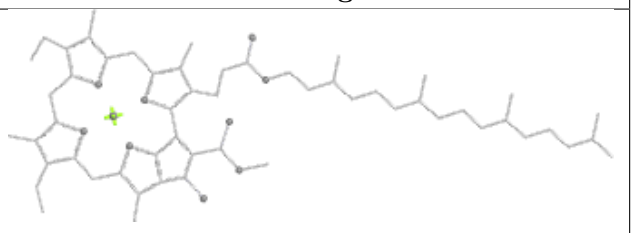
Bond lengths



Bond angles

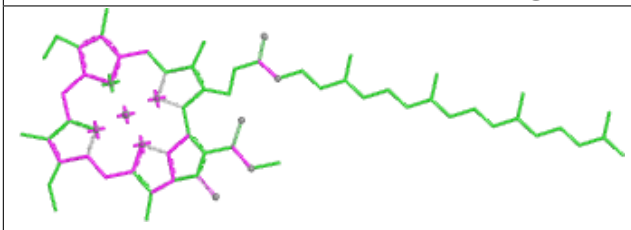


Torsions

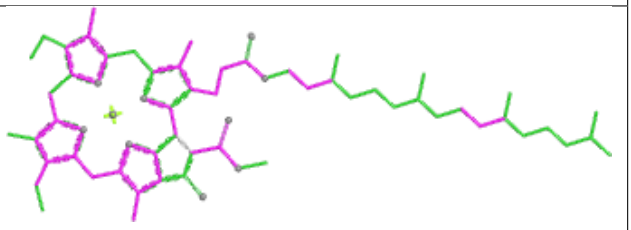


Rings

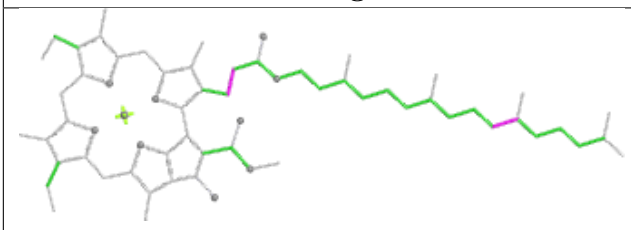
Ligand CLA b 614



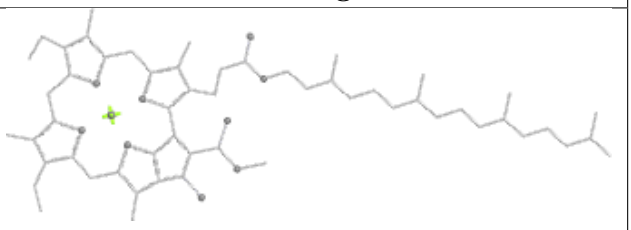
Bond lengths



Bond angles

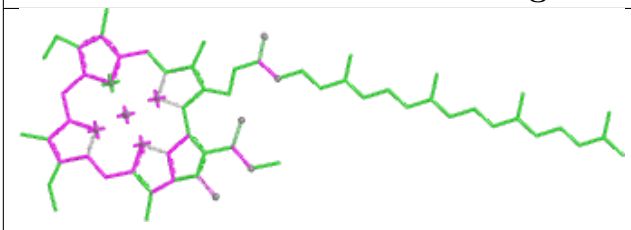


Torsions

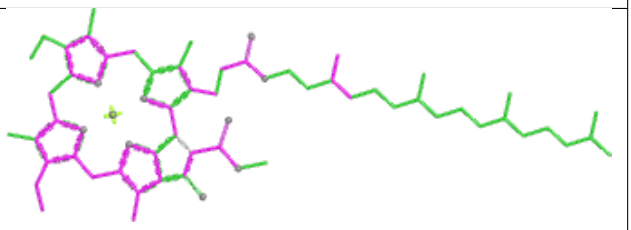


Rings

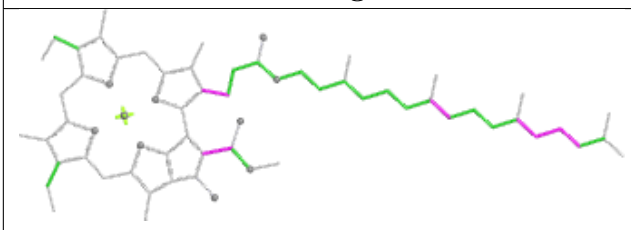
Ligand CLA c 907



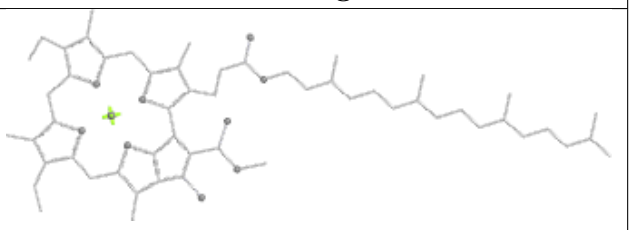
Bond lengths



Bond angles

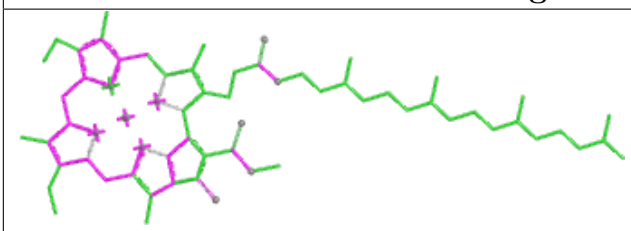


Torsions

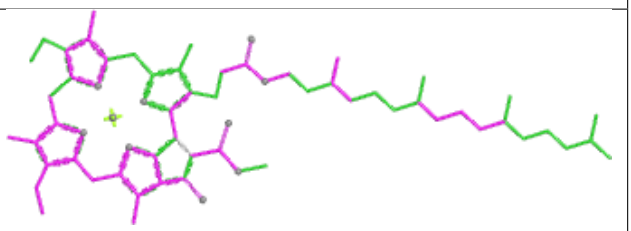


Rings

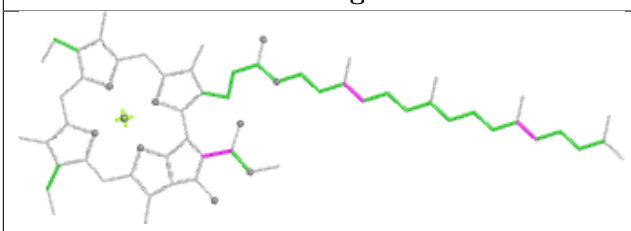
Ligand CLA c 905



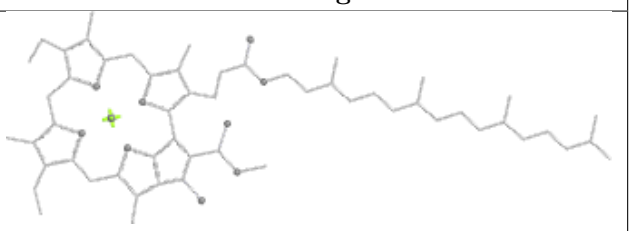
Bond lengths



Bond angles

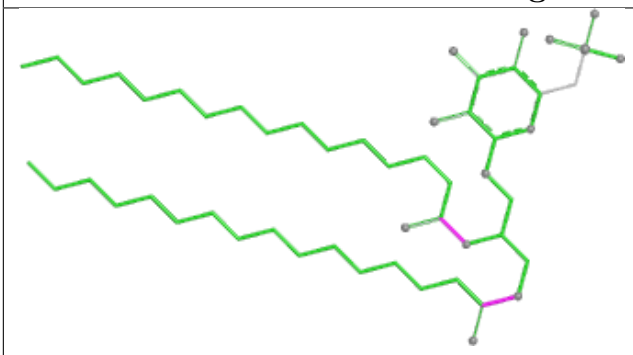


Torsions

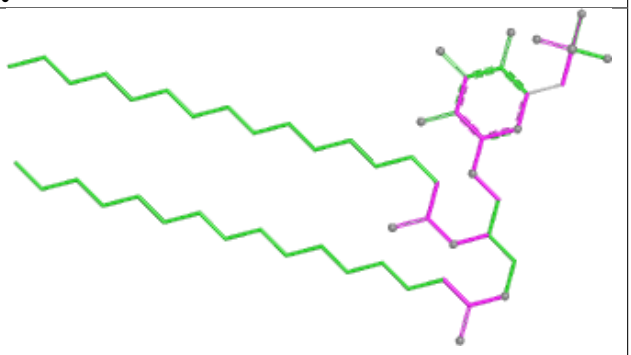


Rings

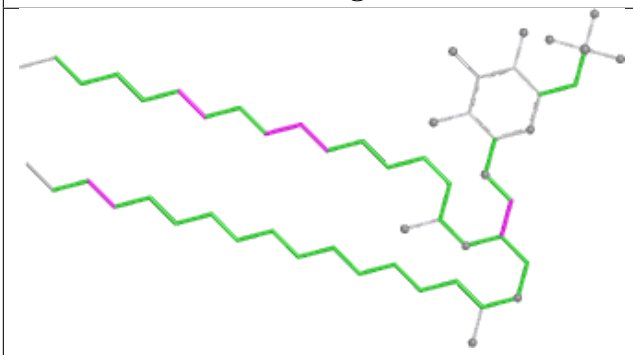
Ligand SQD a 415



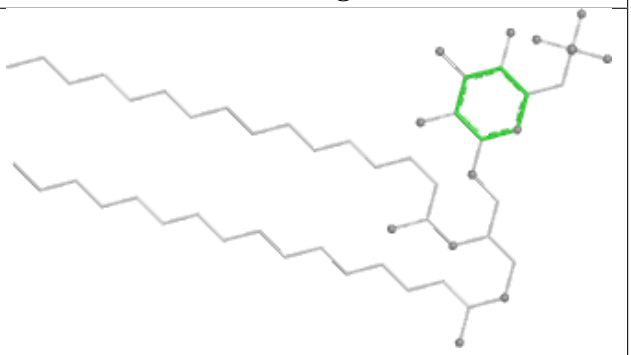
Bond lengths



Bond angles

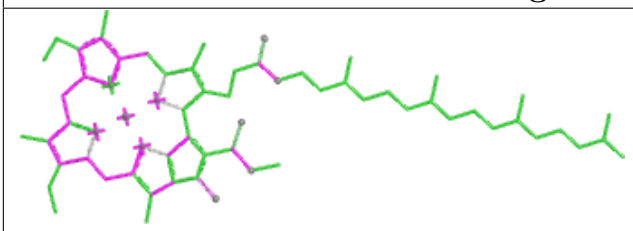


Torsions

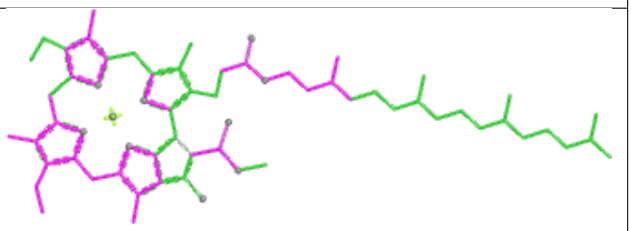


Rings

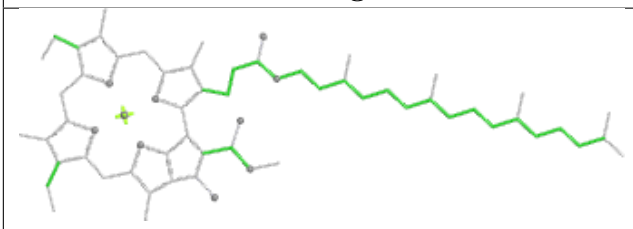
Ligand CLA c 912



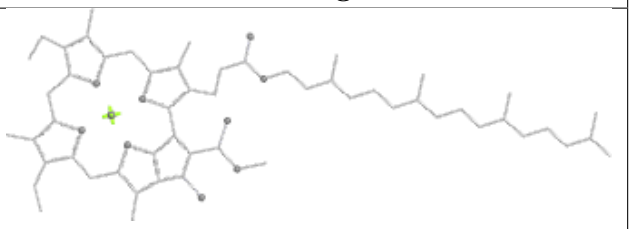
Bond lengths



Bond angles

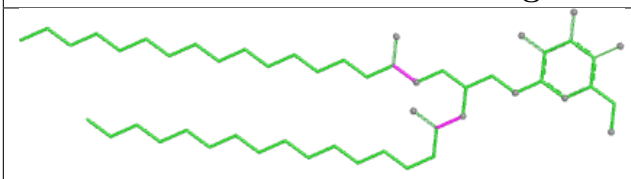


Torsions

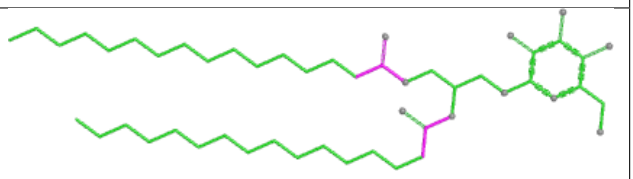


Rings

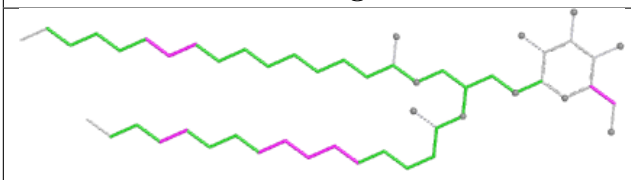
Ligand LMG d 412



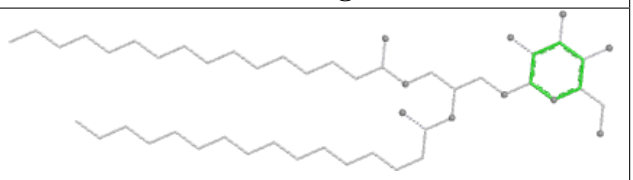
Bond lengths



Bond angles

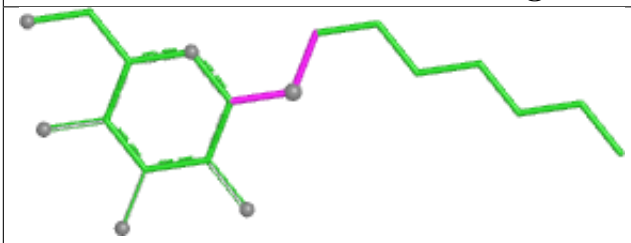


Torsions

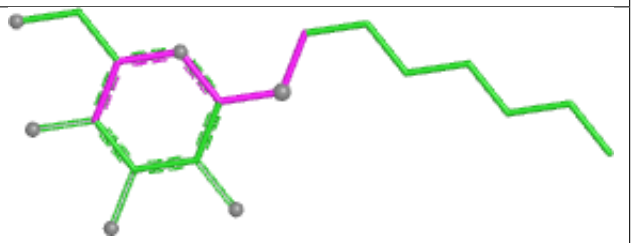


Rings

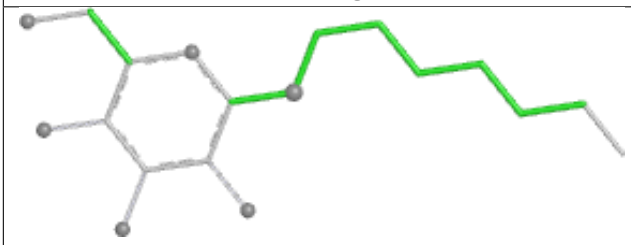
Ligand HTG c 923



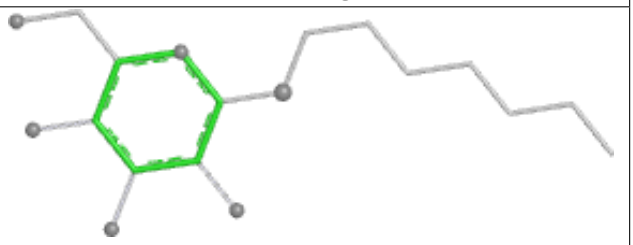
Bond lengths



Bond angles

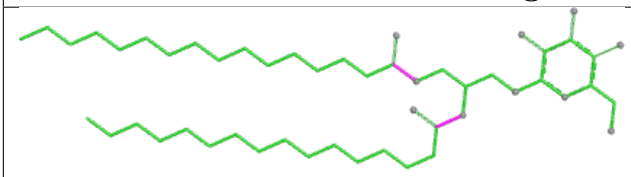


Torsions

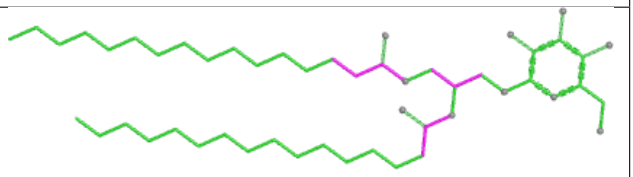


Rings

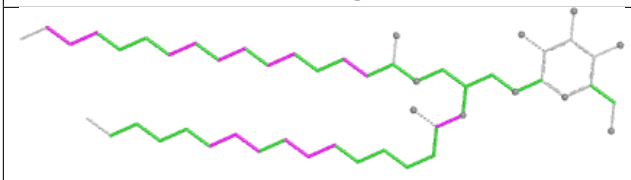
Ligand LMG b 624



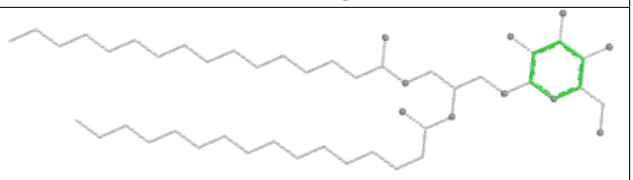
Bond lengths



Bond angles

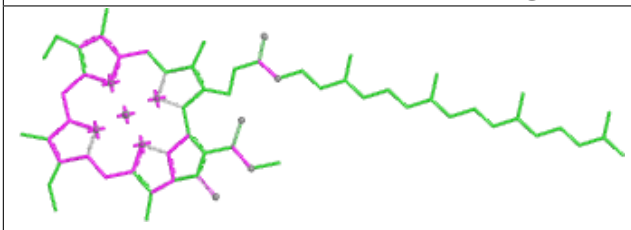


Torsions

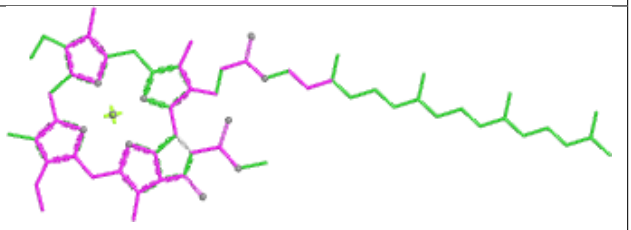


Rings

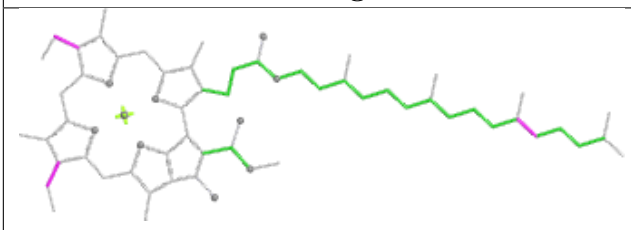
Ligand CLA D 401



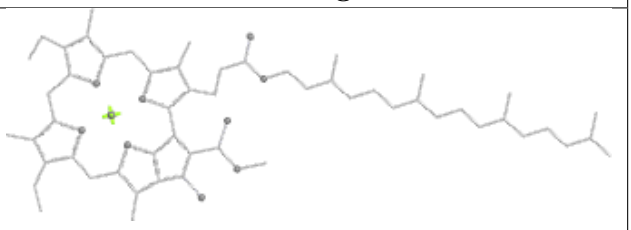
Bond lengths



Bond angles

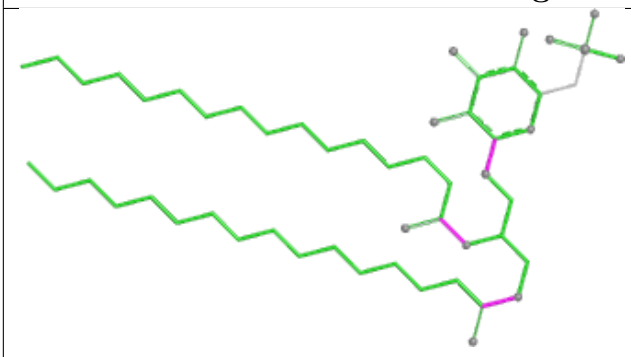


Torsions

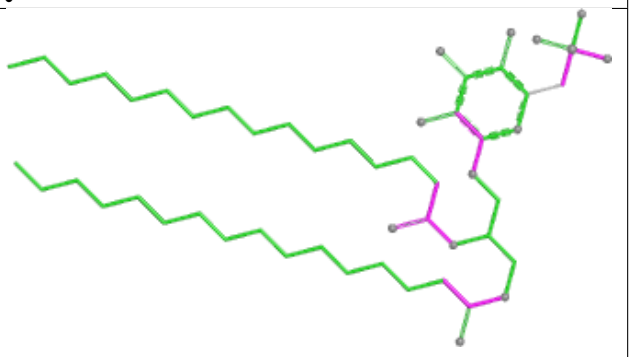


Rings

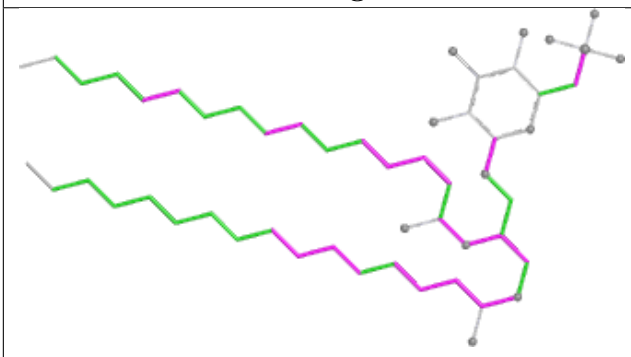
Ligand SQD l 101



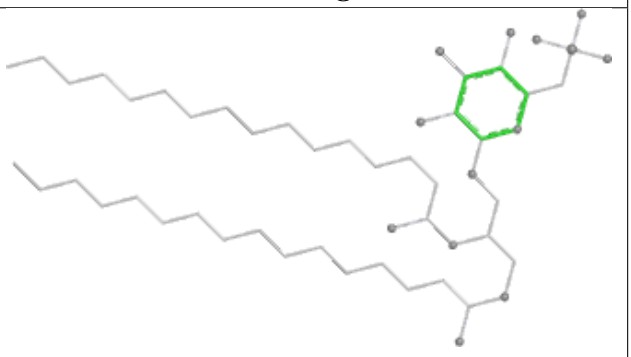
Bond lengths



Bond angles

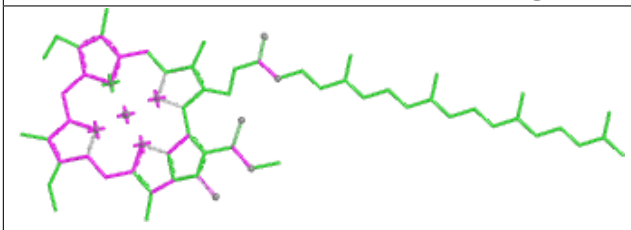


Torsions

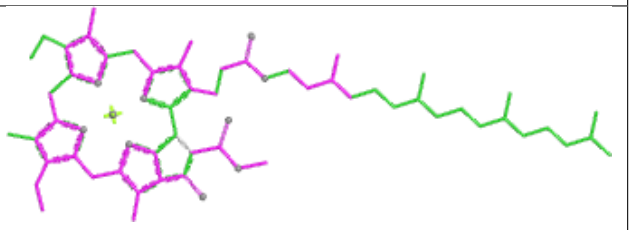


Rings

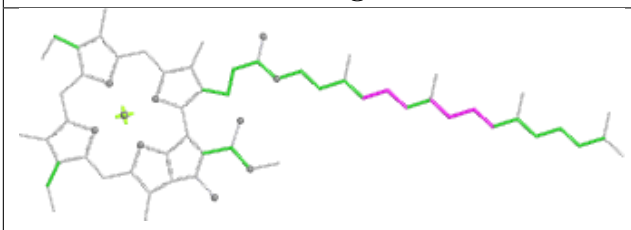
Ligand CLA a 413



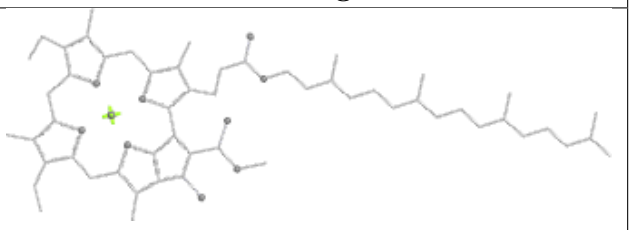
Bond lengths



Bond angles

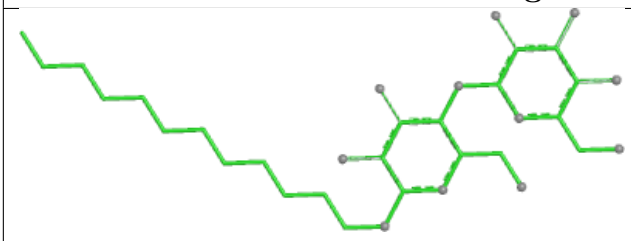


Torsions

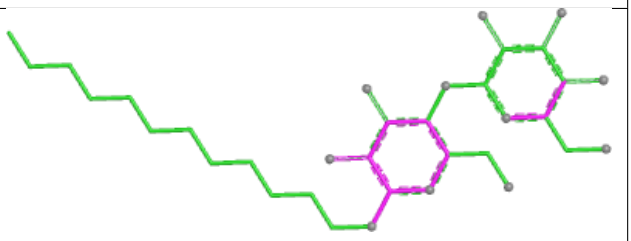


Rings

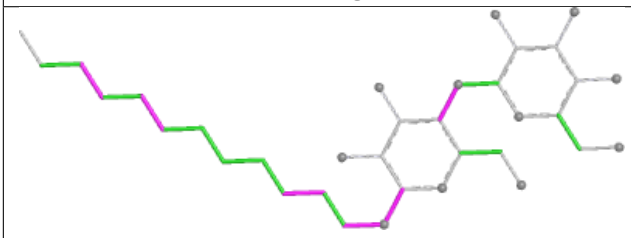
Ligand LMT b 625



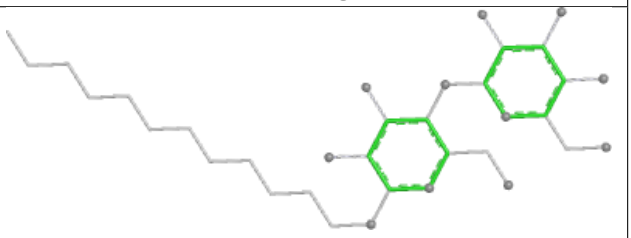
Bond lengths



Bond angles

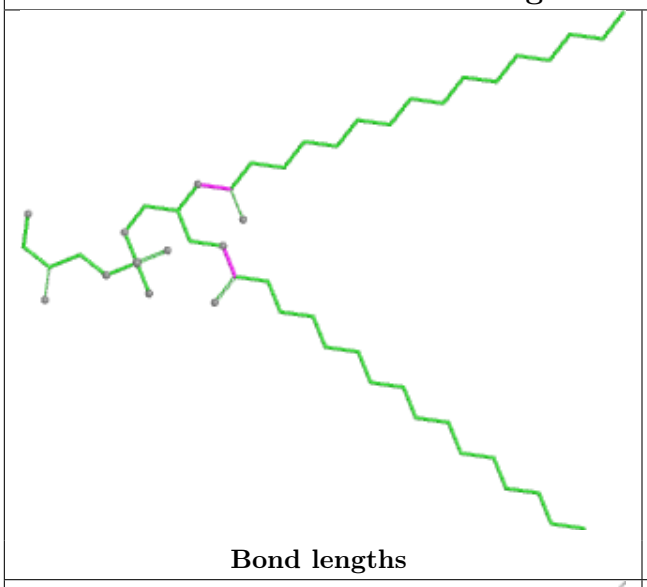


Torsions

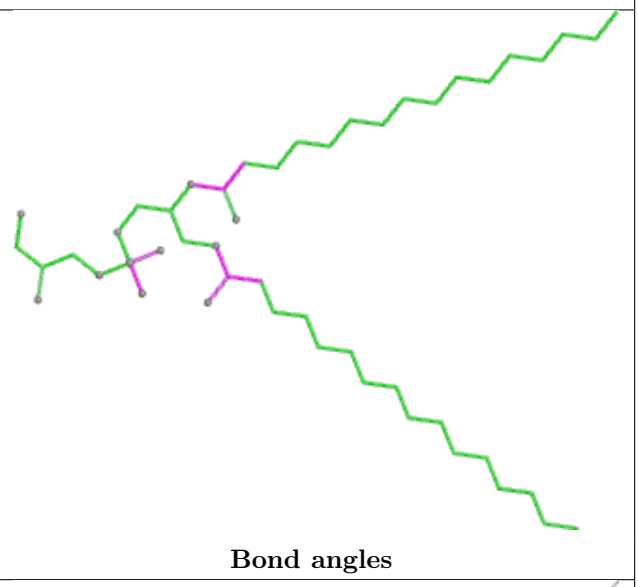


Rings

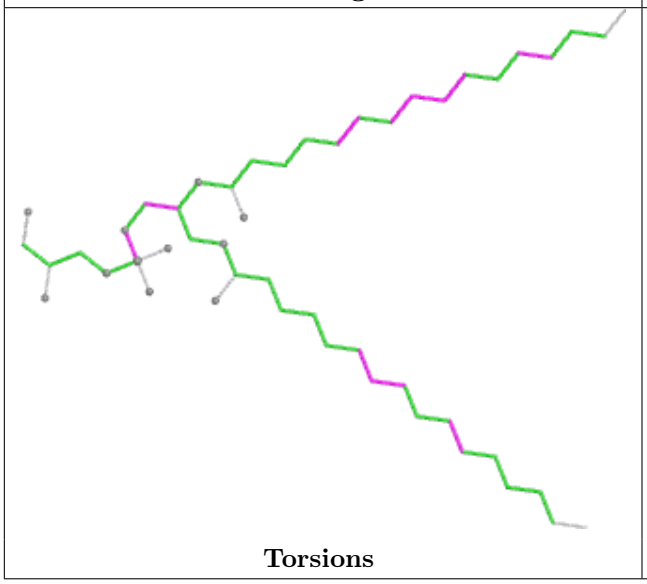
Ligand LHG L 101



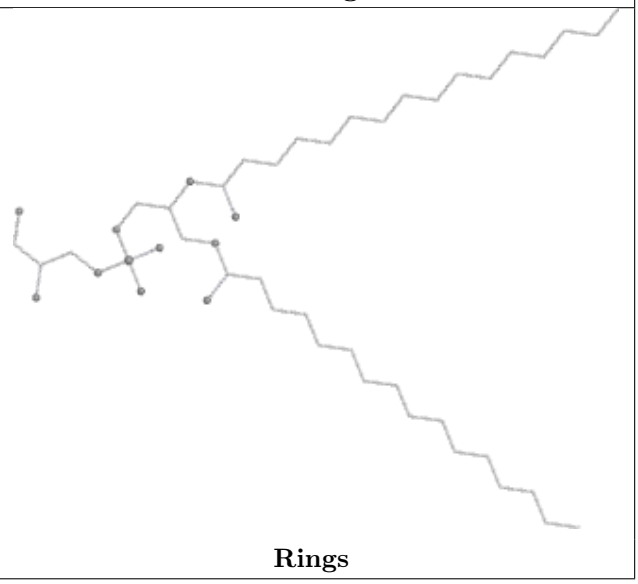
Bond lengths



Bond angles



Torsions

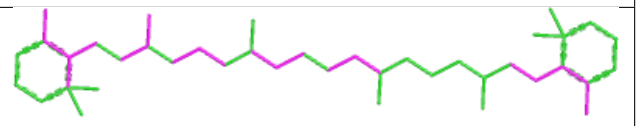


Rings

Ligand BCR k 102



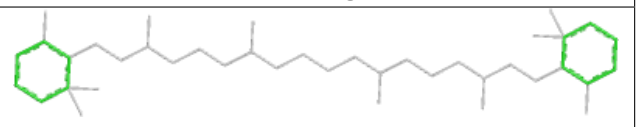
Bond lengths



Bond angles

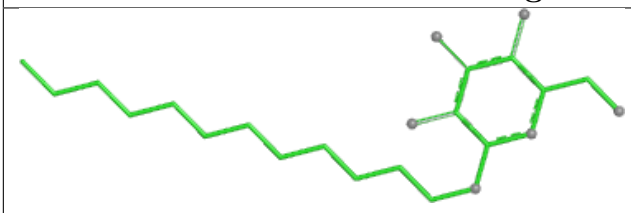


Torsions

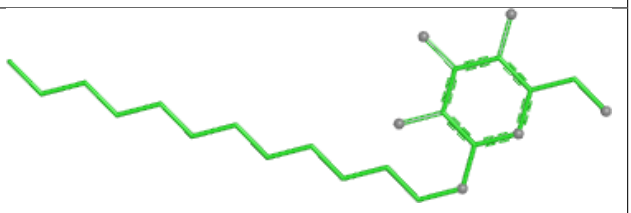


Rings

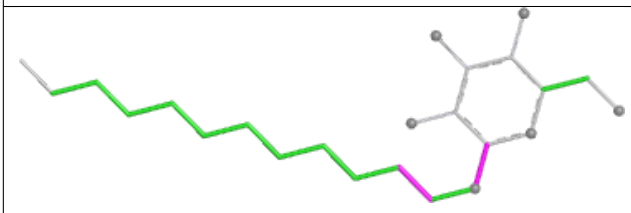
Ligand LMT J 102



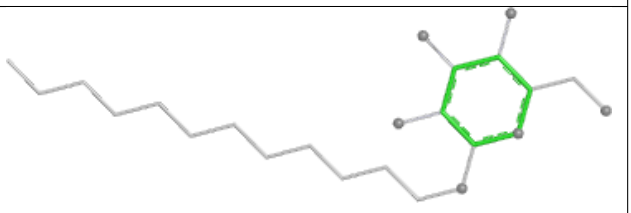
Bond lengths



Bond angles

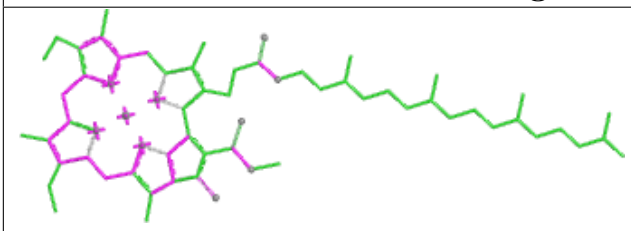


Torsions

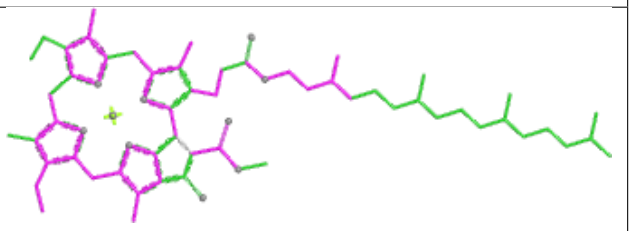


Rings

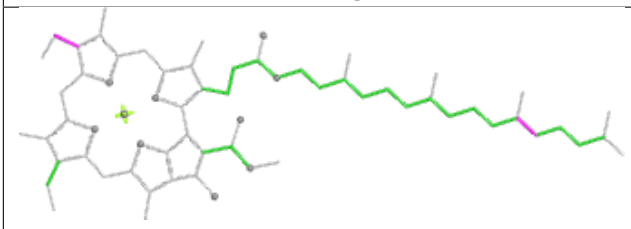
Ligand CLA c 913



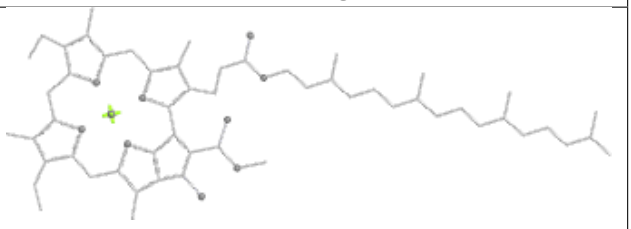
Bond lengths



Bond angles

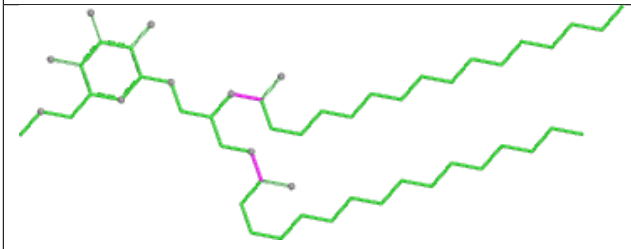


Torsions

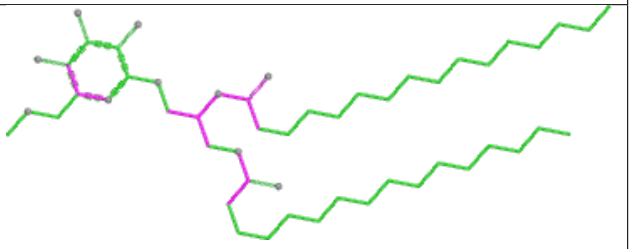


Rings

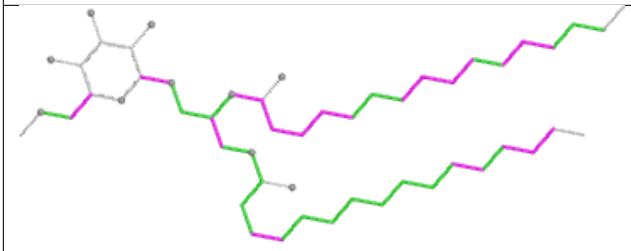
Ligand DGD D 405



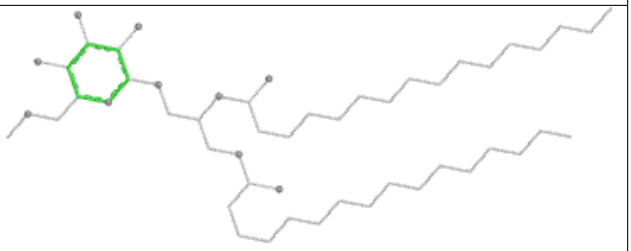
Bond lengths



Bond angles

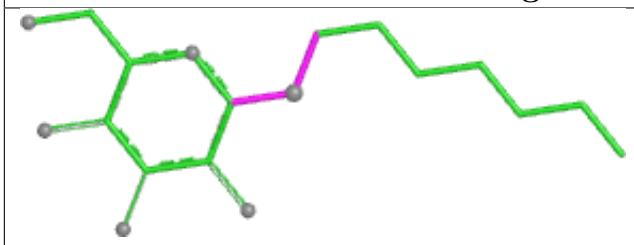


Torsions

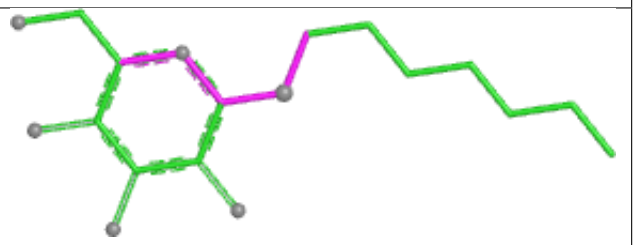


Rings

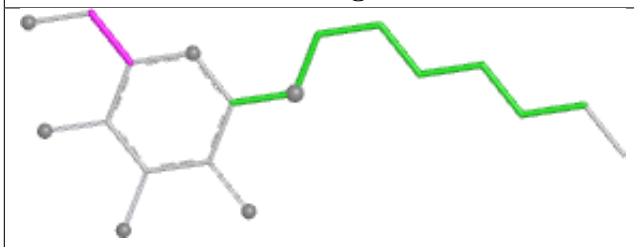
Ligand HTG B 630



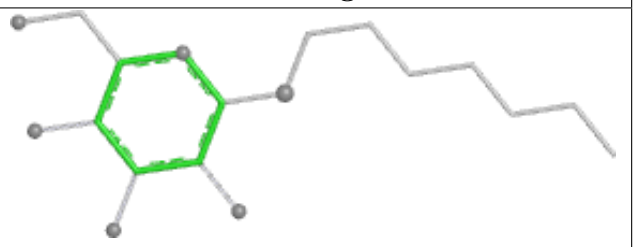
Bond lengths



Bond angles

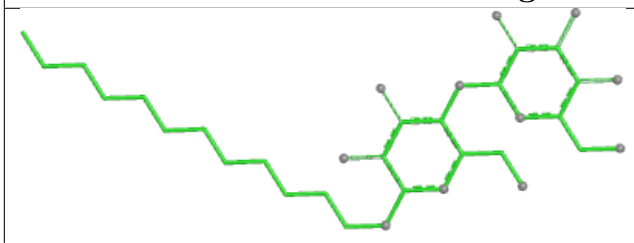


Torsions

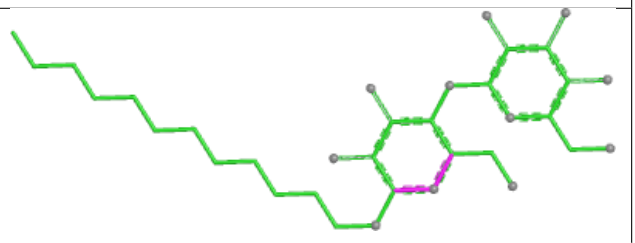


Rings

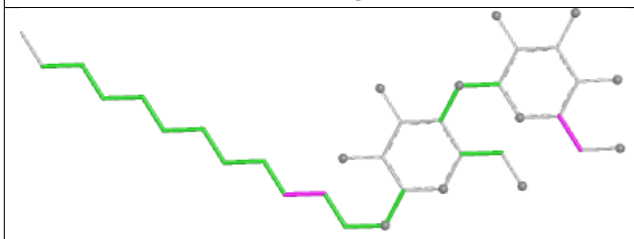
Ligand LMT M 101



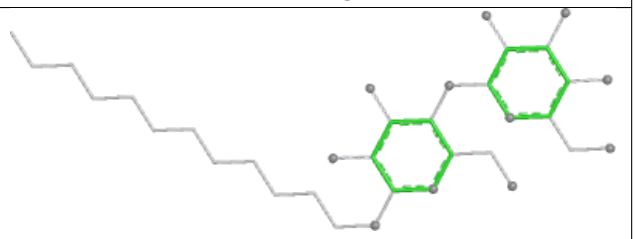
Bond lengths



Bond angles

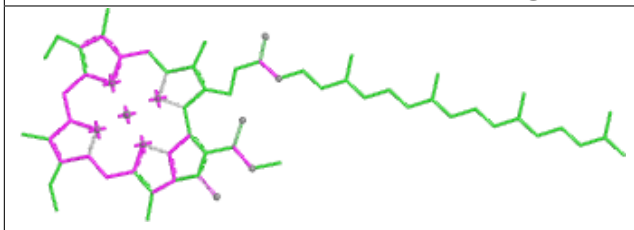


Torsions

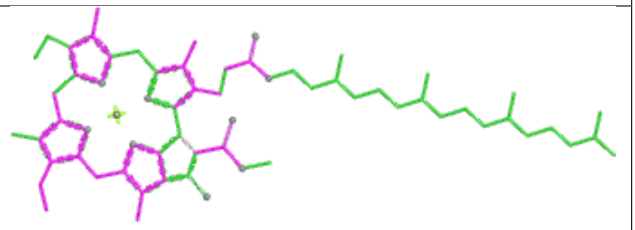


Rings

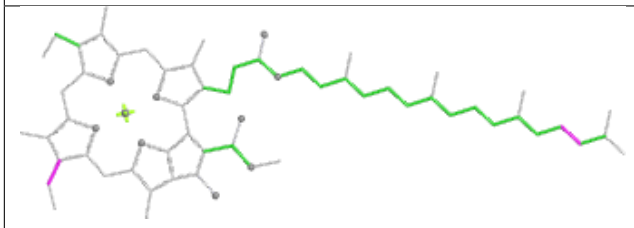
Ligand CLA A 406



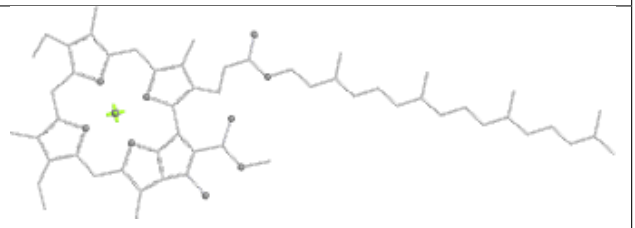
Bond lengths



Bond angles

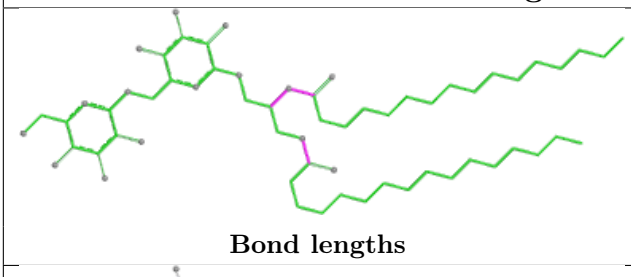


Torsions

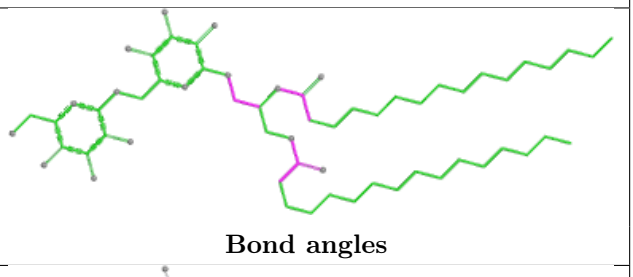


Rings

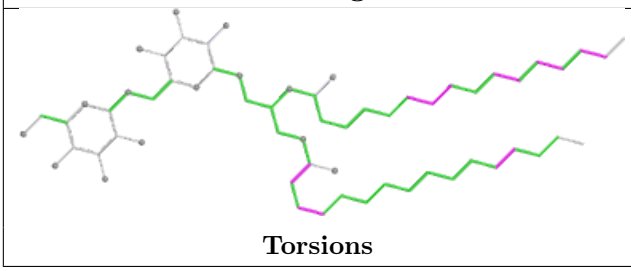
Ligand DGD c 919



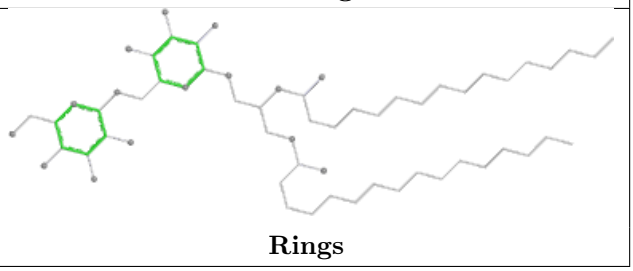
Bond lengths



Bond angles

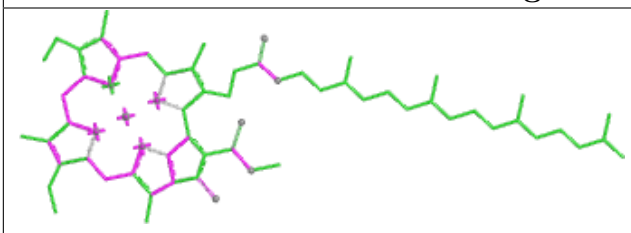


Torsions

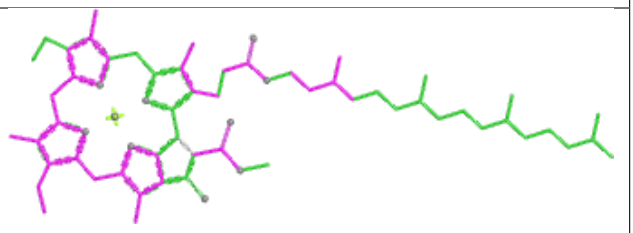


Rings

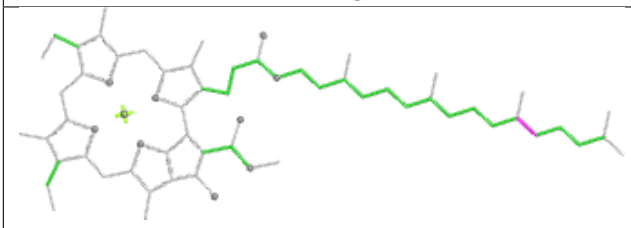
Ligand CLA A 407



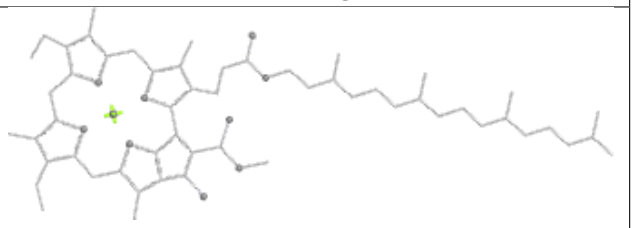
Bond lengths



Bond angles

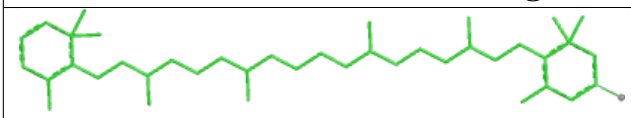


Torsions

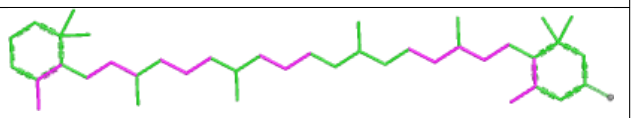


Rings

Ligand RRX h 101



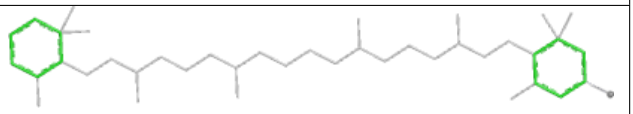
Bond lengths



Bond angles

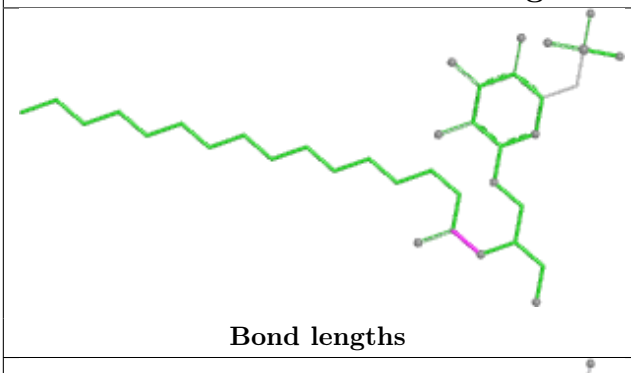


Torsions

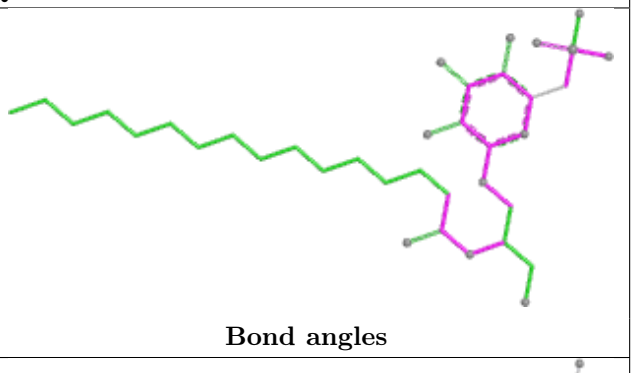


Rings

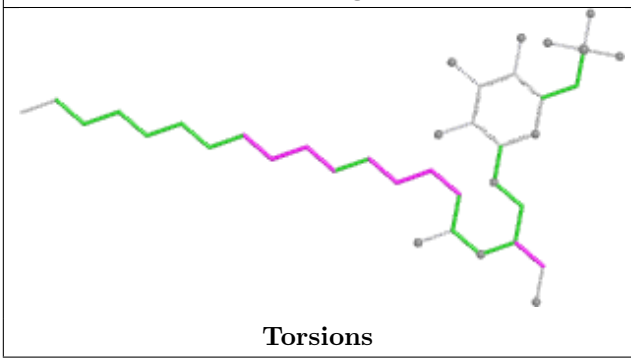
Ligand SQD F 101



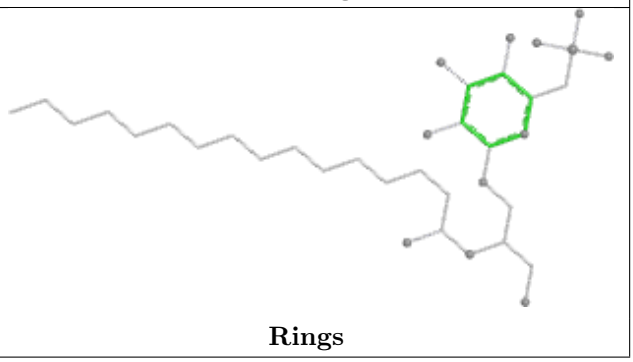
Bond lengths



Bond angles

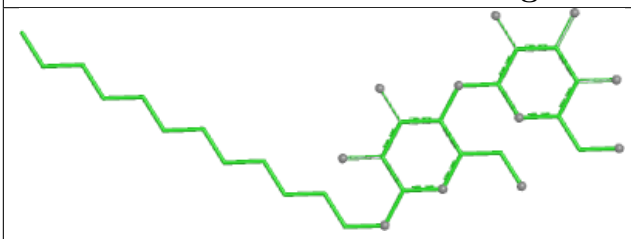


Torsions

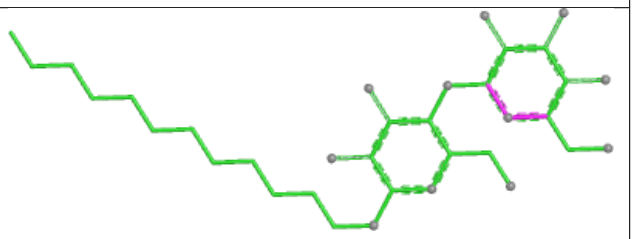


Rings

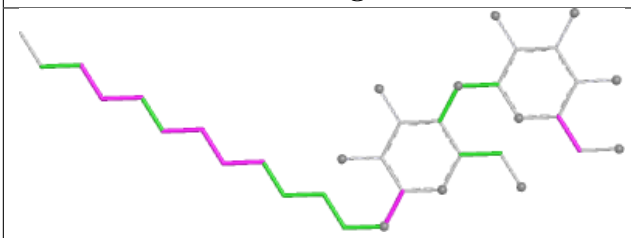
Ligand LMT A 421



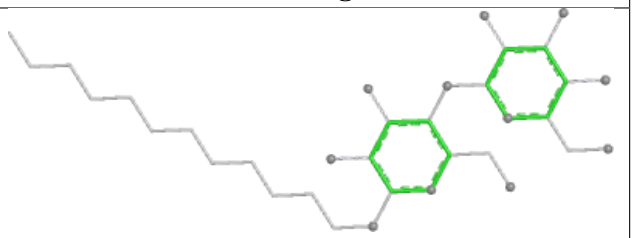
Bond lengths



Bond angles

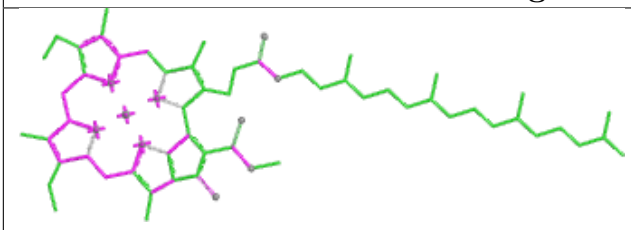


Torsions

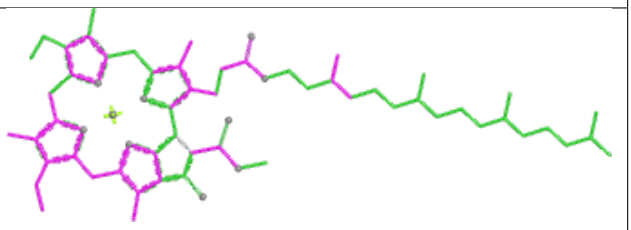


Rings

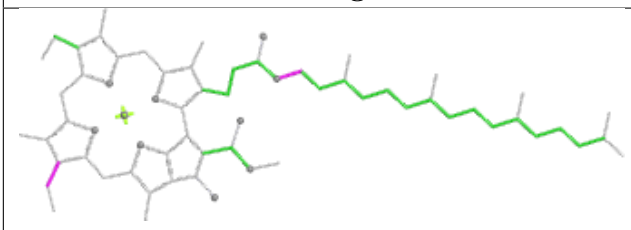
Ligand CLA a 409



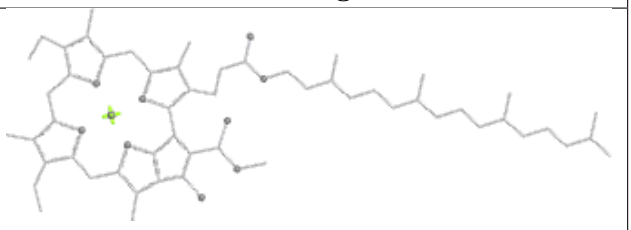
Bond lengths



Bond angles

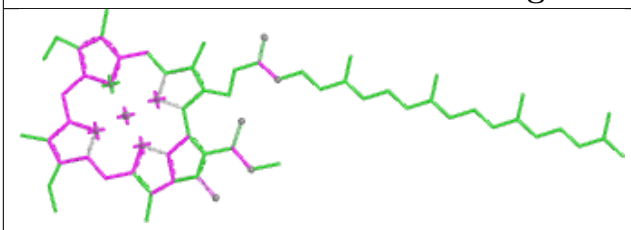


Torsions

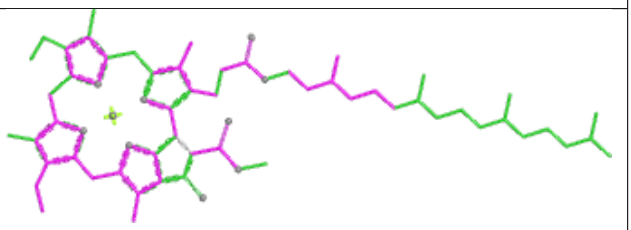


Rings

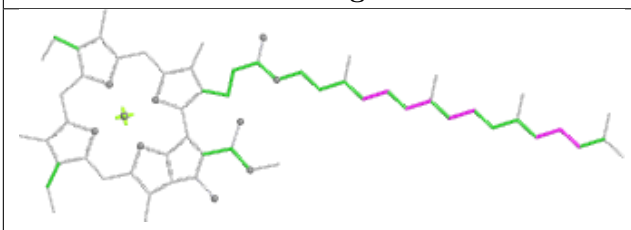
Ligand CLA b 606



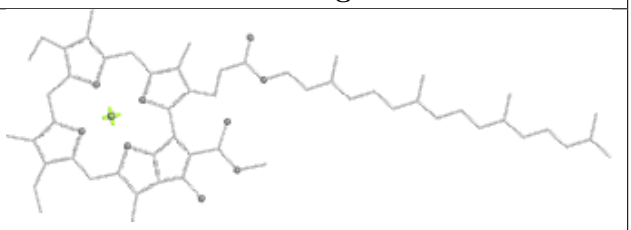
Bond lengths



Bond angles

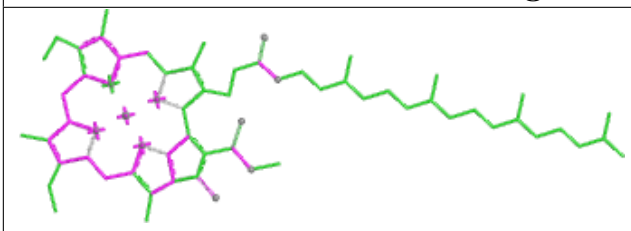


Torsions

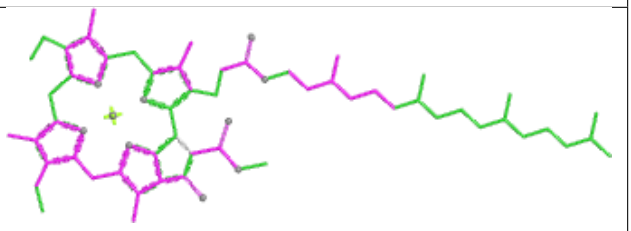


Rings

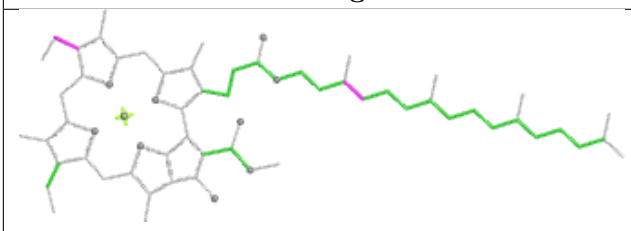
Ligand CLA B 606



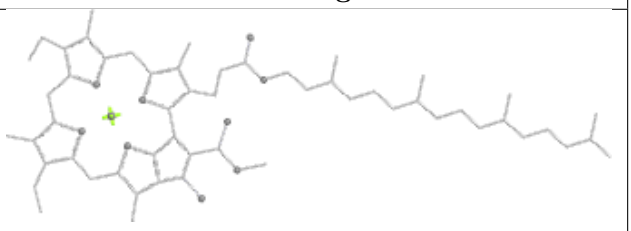
Bond lengths



Bond angles

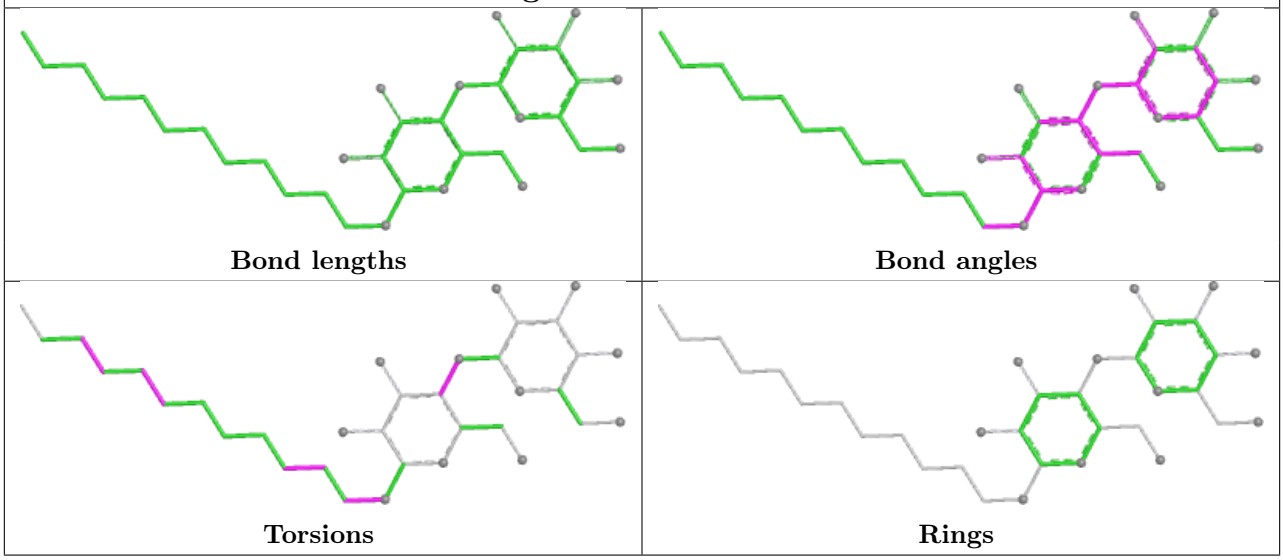


Torsions

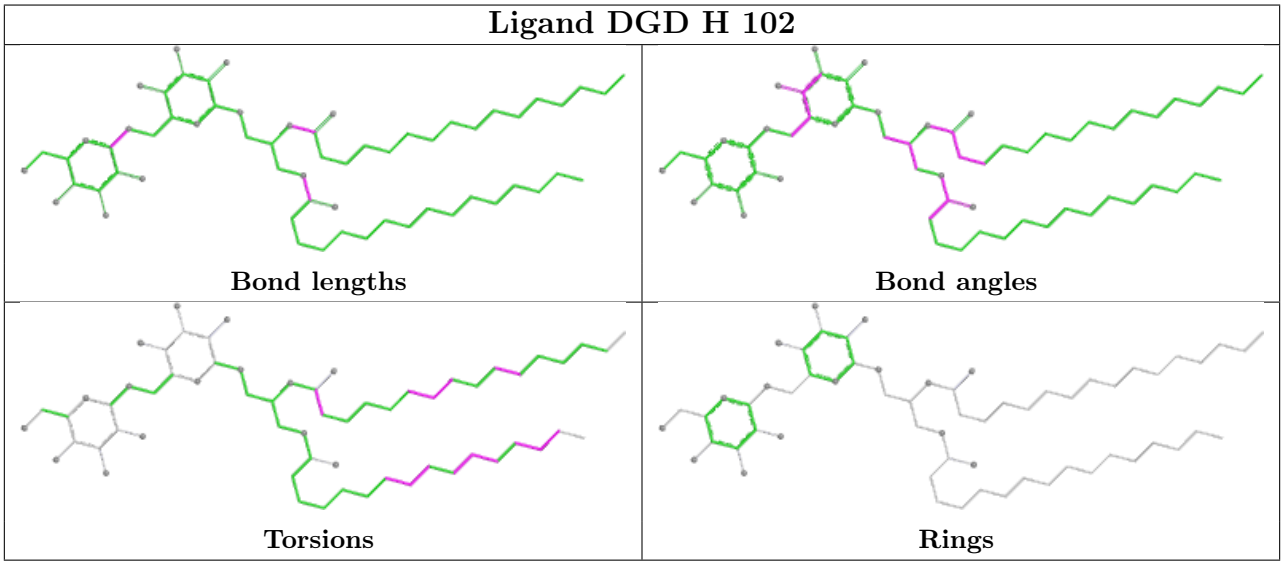


Rings

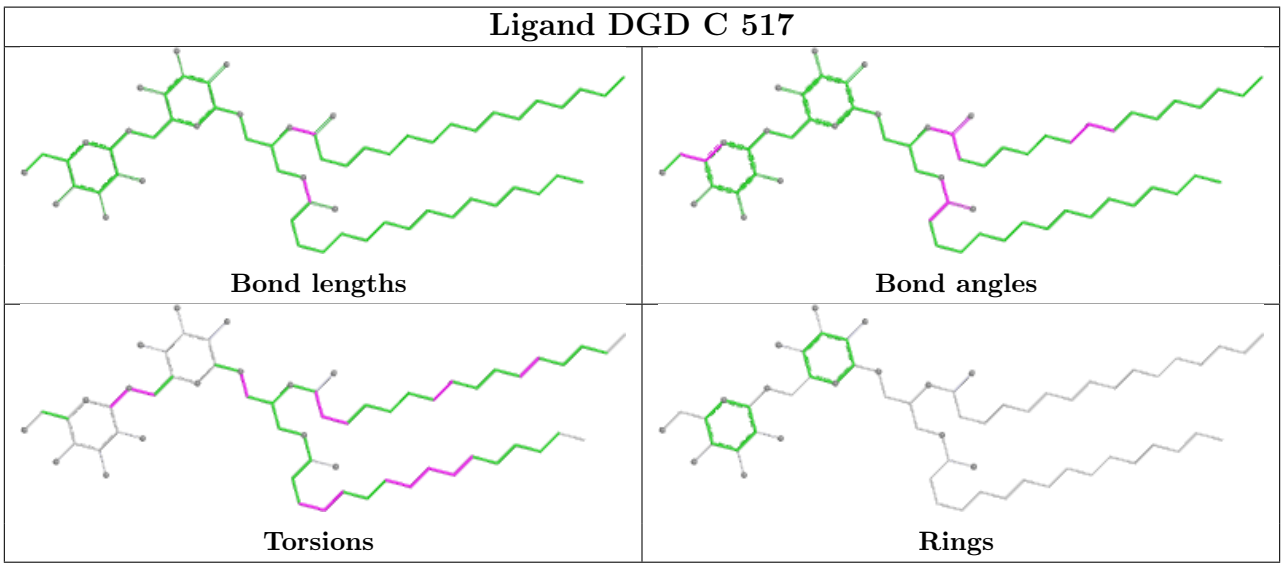
Ligand LMT B 622



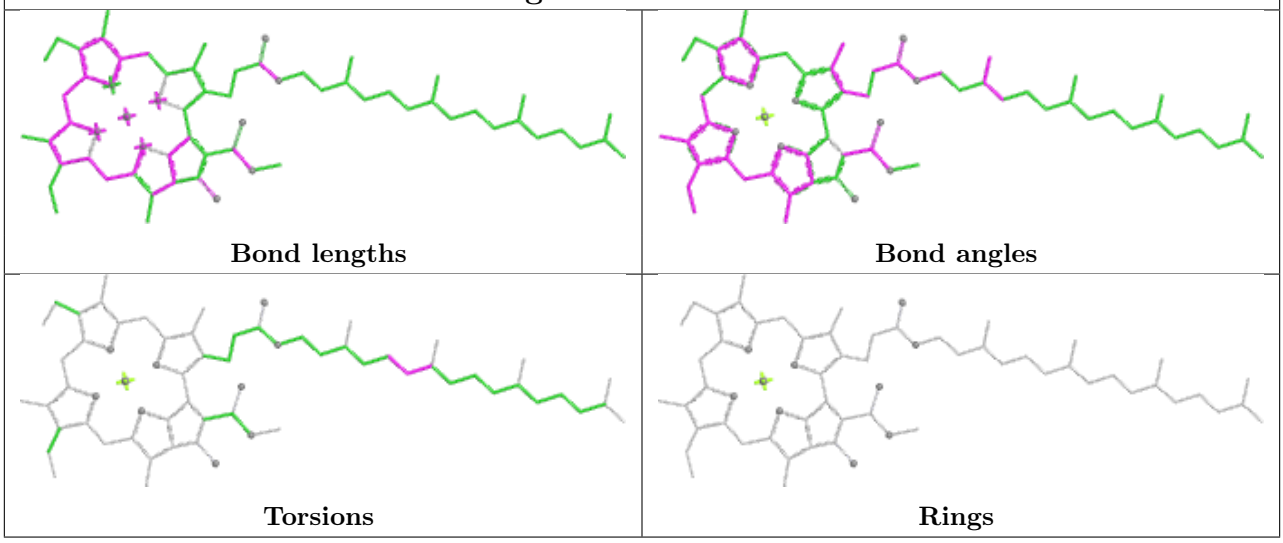
Ligand DGD H 102



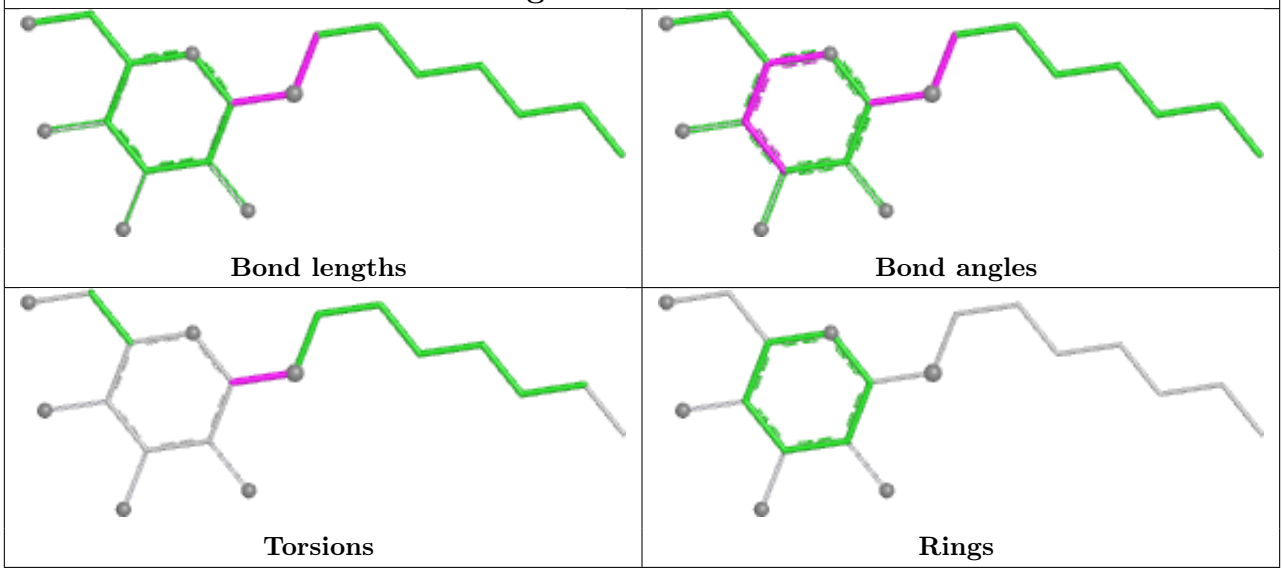
Ligand DGD C 517



Ligand CLA B 604



Ligand HTG c 942



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	334/360 (92%)	-0.64	2 (0%) 85 87	19, 30, 52, 108	2 (0%)
1	a	336/360 (93%)	-0.52	3 (0%) 81 83	24, 32, 66, 131	3 (0%)
2	B	505/510 (99%)	-0.52	1 (0%) 91 92	18, 35, 61, 93	8 (1%)
2	b	504/510 (98%)	-0.39	15 (2%) 52 56	19, 37, 70, 153	9 (1%)
3	C	451/461 (97%)	-0.49	2 (0%) 88 90	25, 40, 56, 104	6 (1%)
3	c	456/461 (98%)	-0.42	2 (0%) 88 90	25, 43, 59, 112	3 (0%)
4	D	342/352 (97%)	-0.70	1 (0%) 90 91	18, 31, 48, 116	1 (0%)
4	d	342/352 (97%)	-0.62	0 100 100	19, 34, 52, 104	2 (0%)
5	E	80/84 (95%)	0.33	5 (6%) 26 27	33, 53, 100, 124	1 (1%)
5	e	79/84 (94%)	0.12	2 (2%) 58 62	31, 52, 98, 121	2 (2%)
6	F	34/45 (75%)	-0.31	0 100 100	35, 42, 64, 94	0
6	f	32/45 (71%)	-0.23	1 (3%) 51 55	33, 43, 82, 101	1 (3%)
7	H	65/66 (98%)	-0.16	3 (4%) 37 40	32, 43, 64, 121	0
7	h	65/66 (98%)	-0.15	3 (4%) 37 40	34, 47, 62, 133	1 (1%)
8	I	36/38 (94%)	0.14	1 (2%) 55 59	39, 46, 115, 133	0
8	i	36/38 (94%)	-0.18	1 (2%) 55 59	37, 45, 86, 108	0
9	J	36/40 (90%)	-0.19	1 (2%) 55 59	33, 46, 85, 103	0
9	j	39/40 (97%)	-0.15	0 100 100	38, 49, 64, 71	0
10	K	37/46 (80%)	-0.39	0 100 100	40, 46, 61, 68	0
10	k	37/46 (80%)	0.02	0 100 100	40, 50, 69, 82	0
11	L	37/37 (100%)	-0.58	0 100 100	15, 29, 75, 116	2 (5%)
11	l	37/37 (100%)	-0.49	1 (2%) 56 60	17, 30, 83, 121	1 (2%)
12	M	33/36 (91%)	-0.51	0 100 100	19, 32, 75, 105	1 (3%)
12	m	33/36 (91%)	-0.51	0 100 100	18, 33, 73, 86	1 (3%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	-0.32	2 (0%) 82 85	22, 41, 69, 115	10 (4%)
13	o	243/272 (89%)	-0.25	4 (1%) 70 74	24, 44, 80, 109	5 (2%)
14	T	29/32 (90%)	-0.55	1 (3%) 48 51	25, 30, 51, 120	1 (3%)
14	t	29/32 (90%)	-0.46	1 (3%) 48 51	25, 31, 59, 101	1 (3%)
15	U	98/134 (73%)	-0.41	2 (2%) 65 69	30, 38, 61, 115	0
15	u	97/134 (72%)	-0.38	0 100 100	34, 44, 61, 123	0
16	V	137/163 (84%)	-0.52	0 100 100	20, 37, 55, 70	4 (2%)
16	v	137/163 (84%)	-0.31	1 (0%) 84 86	25, 50, 70, 87	2 (1%)
17	Y	30/46 (65%)	0.40	3 (10%) 12 13	47, 60, 102, 111	0
17	y	30/46 (65%)	0.55	2 (6%) 24 25	35, 64, 96, 105	1 (3%)
18	X	40/41 (97%)	0.04	1 (2%) 58 62	41, 50, 92, 125	0
18	x	39/41 (95%)	0.27	3 (7%) 19 21	44, 52, 113, 137	0
19	Z	61/62 (98%)	0.35	3 (4%) 35 37	45, 55, 85, 112	0
19	z	61/62 (98%)	0.52	3 (4%) 35 37	51, 64, 105, 121	0
20	R	34/41 (82%)	1.84	13 (38%) 1 0	60, 94, 119, 124	0
All	All	5294/5691 (93%)	-0.38	83 (1%) 70 74	15, 39, 72, 153	68 (1%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	I	37	LEU	6.8
7	H	65	LEU	5.1
13	o	58	ASN	4.6
18	x	37	VAL	4.6
7	h	65	LEU	4.5
20	R	26	TYR	4.4
2	b	495	PHE	4.1
2	b	499	VAL	4.1
2	B	479	PHE	4.0
2	b	486	LEU	3.7
20	R	35	LEU	3.7
20	R	24	LEU	3.6
5	E	72	ALA	3.4
2	b	484	PRO	3.4
7	H	64	ALA	3.3
2	b	504	THR	3.2
20	R	34	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	T	30	THR	3.2
9	J	5	GLY	3.2
5	E	79	PHE	3.2
2	b	493	TRP	3.1
13	o	246	ALA	3.1
5	E	80	LEU	3.0
5	E	76	VAL	3.0
19	z	62	VAL	3.0
20	R	16	ALA	3.0
1	A	11	ALA	3.0
20	R	23	ILE	2.9
13	O	58	ASN	2.8
17	y	18	VAL	2.8
19	Z	33	TRP	2.8
20	R	28	VAL	2.8
2	b	496	TYR	2.7
3	c	20	SER	2.7
5	e	76	VAL	2.7
17	Y	18	VAL	2.7
20	R	13	LEU	2.6
3	c	19	ASN	2.6
2	b	497	GLN	2.6
2	b	487	SER	2.5
4	D	238	THR	2.5
20	R	30	GLN	2.5
19	Z	32	ASP	2.4
2	b	489	GLU	2.4
17	Y	25	ILE	2.4
18	x	2	THR	2.4
6	f	16	PHE	2.4
7	h	64	ALA	2.4
20	R	15	ALA	2.4
15	U	8	GLU	2.4
18	X	41	LEU	2.3
20	R	25	PRO	2.3
11	l	1	MET	2.3
7	h	66	GLY	2.3
20	R	18	TRP	2.3
3	C	29	GLU	2.3
5	E	82	GLN	2.3
2	b	502	VAL	2.3
5	e	83	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	129	GLY	2.2
7	H	66	GLY	2.2
3	C	23	ALA	2.2
17	Y	19	ILE	2.2
19	z	61	VAL	2.2
8	i	37	LEU	2.2
13	o	61	GLN	2.2
17	y	19	ILE	2.2
13	O	60	ARG	2.2
2	b	85	GLY	2.2
2	b	494	GLY	2.2
15	U	9	LEU	2.2
19	z	4	LEU	2.2
1	A	230	THR	2.1
1	a	249	VAL	2.1
1	a	248	ILE	2.1
19	Z	3	ILE	2.1
20	R	20	VAL	2.1
1	a	11	ALA	2.1
13	o	60	ARG	2.1
18	x	40	SER	2.0
16	v	26	TYR	2.0
14	t	30	THR	2.0
2	b	86	ILE	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
19	FME	z	1	10/11	0.84	0.10	98,112,120,122	0
19	FME	Z	1	10/11	0.88	0.12	68,82,98,101	0
14	FME	T	1	10/11	0.95	0.08	30,39,62,64	0
14	FME	t	1	10/11	0.96	0.07	30,34,59,63	0
12	FME	M	1	10/11	0.97	0.07	31,40,71,76	0
12	FME	m	1	10/11	0.97	0.07	33,42,69,78	0
8	FME	i	1	10/11	0.98	0.07	31,40,44,47	0
8	FME	I	1	10/11	0.98	0.06	34,43,49,50	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
36	HTG	V	215	19/19	0.54	0.19	100,116,127,128	0
30	UNL	h	103	9/-	0.59	0.20	81,86,109,110	0
30	UNL	b	634	9/-	0.60	0.15	99,103,113,114	0
30	UNL	h	106	11/-	0.63	0.18	72,75,78,79	0
30	UNL	C	538	4/-	0.65	0.15	74,76,77,82	0
36	HTG	c	941	19/19	0.65	0.15	67,133,141,142	0
34	DMS	B	646	4/4	0.66	0.20	109,114,115,116	0
34	DMS	c	939	4/4	0.66	0.19	112,114,119,120	0
30	UNL	A	420	9/-	0.66	0.14	85,95,111,112	0
30	UNL	i	105	12/-	0.66	0.15	77,86,88,89	0
34	DMS	i	106	4/4	0.67	0.22	125,125,125,127	0
30	UNL	h	104	9/-	0.67	0.18	68,74,84,85	0
34	DMS	e	103	4/4	0.67	0.22	106,108,108,111	0
30	UNL	I	105	9/-	0.68	0.14	70,73,81,83	0
31	LMT	A	417	35/35	0.68	0.18	55,92,108,115	0
30	UNL	c	947	6/-	0.69	0.19	71,80,83,85	0
30	UNL	J	105	8/-	0.69	0.16	80,94,98,99	0
30	UNL	a	418	40/-	0.69	0.17	79,99,122,125	0
30	UNL	A	415	36/-	0.69	0.17	75,99,113,114	0
37	DGD	d	408	50/66	0.69	0.15	81,99,121,130	0
36	HTG	B	631	19/19	0.70	0.14	71,107,118,120	0
31	LMT	m	103	35/35	0.71	0.16	53,125,136,137	0
34	DMS	v	210	4/4	0.71	0.20	119,119,120,120	0
37	DGD	D	405	52/66	0.71	0.18	74,102,120,124	0
31	LMT	c	922	35/35	0.71	0.15	85,117,122,126	0
34	DMS	A	425	4/4	0.72	0.19	94,101,101,104	0
30	UNL	y	103	4/-	0.72	0.14	81,82,84,85	0
34	DMS	O	307	4/4	0.72	0.20	113,113,115,121	0
30	UNL	c	944	4/-	0.72	0.16	76,77,78,81	0
30	UNL	b	633	9/-	0.72	0.18	76,81,87,88	0
30	UNL	A	428	4/-	0.72	0.15	64,66,70,71	0
31	LMT	e	101	24/35	0.73	0.15	94,101,125,127	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	U	202	4/4	0.73	0.18	105,108,108,110	0
34	DMS	V	214	4/4	0.73	0.20	102,102,104,106	0
31	LMT	a	402	35/35	0.73	0.16	49,96,119,123	0
31	LMT	b	625	35/35	0.73	0.16	59,119,133,139	0
30	UNL	Z	104	8/-	0.73	0.20	69,83,102,103	0
34	DMS	d	417	4/4	0.74	0.20	106,109,109,110	0
34	DMS	b	646	4/4	0.74	0.22	74,83,84,85	0
31	LMT	A	421	35/35	0.74	0.14	84,100,131,132	0
30	UNL	C	522	34/-	0.75	0.15	68,94,102,106	0
32	GOL	O	304	6/6	0.75	0.12	89,90,92,96	0
32	GOL	V	207	6/6	0.75	0.13	78,85,88,96	0
30	UNL	l	102	13/-	0.75	0.16	55,61,77,83	0
34	DMS	B	645	4/4	0.75	0.21	103,104,107,107	0
36	HTG	c	943	17/19	0.75	0.13	76,122,129,130	0
30	UNL	J	104	16/-	0.75	0.21	75,83,91,91	0
34	DMS	C	532	4/4	0.75	0.19	96,99,100,102	0
30	UNL	b	635	9/-	0.76	0.16	59,82,90,90	0
34	DMS	c	936	4/4	0.76	0.18	119,124,124,124	0
34	DMS	B	642	4/4	0.76	0.21	104,106,109,111	0
34	DMS	O	315	4/4	0.76	0.24	96,96,98,99	0
36	HTG	c	942	19/19	0.76	0.17	52,78,94,100	0
30	UNL	j	105	5/-	0.76	0.14	66,67,73,74	0
31	LMT	j	102	24/35	0.76	0.14	66,84,120,122	0
34	DMS	o	307	4/4	0.76	0.21	89,91,91,93	0
30	UNL	b	636	11/-	0.77	0.18	70,77,83,83	0
36	HTG	B	625	19/19	0.77	0.12	64,112,121,124	0
31	LMT	t	101	23/35	0.77	0.16	60,95,135,138	0
36	HTG	C	520	19/19	0.77	0.13	81,93,101,105	0
34	DMS	B	647	4/4	0.77	0.22	107,108,110,113	0
36	HTG	c	924	19/19	0.77	0.13	69,99,118,118	0
30	UNL	I	106	9/-	0.77	0.17	76,80,87,87	0
34	DMS	D	415	4/4	0.77	0.22	83,93,97,99	0
30	UNL	I	107	11/-	0.77	0.17	65,78,88,88	0
36	HTG	y	102	19/19	0.77	0.14	84,115,122,124	0
30	UNL	B	627	8/-	0.77	0.14	63,68,78,83	0
31	LMT	F	103	24/35	0.77	0.13	85,90,119,121	0
34	DMS	T	103	4/4	0.78	0.26	112,112,112,112	0
34	DMS	c	926	4/4	0.78	0.20	107,110,110,111	0
30	UNL	c	946	4/-	0.78	0.14	83,83,83,84	0
30	UNL	e	106	11/-	0.78	0.13	83,87,92,94	0
34	DMS	b	639	4/4	0.78	0.19	90,100,102,102	0
30	UNL	c	945	4/-	0.79	0.14	77,77,77,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	HTG	C	521	19/19	0.79	0.12	58,93,110,117	0
30	UNL	A	418	8/-	0.79	0.12	70,75,82,82	0
36	HTG	b	603	19/19	0.79	0.12	64,103,118,120	0
34	DMS	U	204	4/4	0.79	0.15	134,135,136,136	0
34	DMS	C	533	4/4	0.79	0.14	121,122,123,125	0
34	DMS	C	534	4/4	0.79	0.18	112,116,117,120	0
27	SQD	b	601	54/54	0.79	0.13	46,73,108,111	0
34	DMS	y	101	4/4	0.79	0.20	116,122,123,124	0
30	UNL	x	104	9/-	0.79	0.17	93,95,99,102	0
30	UNL	I	103	12/-	0.79	0.14	60,63,84,84	0
38	LHG	E	101	42/49	0.79	0.14	53,100,110,112	0
30	UNL	c	948	18/-	0.80	0.16	79,89,113,114	0
30	UNL	b	628	18/-	0.80	0.14	51,61,81,95	0
34	DMS	A	424	4/4	0.80	0.20	95,98,100,101	0
30	UNL	J	103	12/-	0.80	0.16	69,79,83,84	0
31	LMT	J	102	24/35	0.80	0.14	64,86,118,120	0
30	UNL	I	104	12/-	0.80	0.14	70,80,92,93	0
27	SQD	a	401	54/54	0.80	0.12	55,80,106,110	0
30	UNL	T	102	15/-	0.80	0.16	78,86,92,93	0
36	HTG	c	923	19/19	0.80	0.11	84,98,100,102	0
34	DMS	c	935	4/4	0.80	0.13	101,101,101,102	0
34	DMS	C	530	4/4	0.80	0.14	89,96,97,99	0
30	UNL	Z	103	6/-	0.80	0.14	73,84,87,88	0
30	UNL	H	103	6/-	0.80	0.14	65,66,79,81	0
36	HTG	d	419	19/19	0.80	0.12	75,100,110,113	0
36	HTG	v	211	19/19	0.80	0.14	63,84,98,102	0
30	UNL	a	403	5/-	0.80	0.13	73,73,74,75	0
27	SQD	l	101	54/54	0.80	0.14	48,77,116,117	0
32	GOL	B	637	6/6	0.80	0.13	61,67,75,80	0
34	DMS	v	207	4/4	0.80	0.15	111,114,114,114	0
28	LMG	C	523	51/55	0.81	0.13	47,94,109,114	0
34	DMS	o	306	4/4	0.81	0.19	84,85,89,90	0
34	DMS	C	535	4/4	0.81	0.19	66,79,83,89	0
34	DMS	v	205	4/4	0.81	0.16	90,95,98,106	0
30	UNL	i	104	16/-	0.81	0.13	65,72,83,83	0
34	DMS	O	302	4/4	0.81	0.22	101,104,107,108	0
30	UNL	d	403	36/-	0.81	0.14	47,67,99,107	0
36	HTG	d	414	19/19	0.81	0.11	67,100,117,120	0
34	DMS	C	524	4/4	0.81	0.15	105,107,108,108	0
36	HTG	B	630	19/19	0.81	0.11	56,109,116,118	0
30	UNL	I	102	12/-	0.81	0.17	70,82,95,98	0
30	UNL	D	417	4/-	0.81	0.21	57,66,66,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	E	104	5/-	0.81	0.16	59,64,67,69	0
36	HTG	D	412	19/19	0.81	0.13	68,112,130,130	0
34	DMS	c	938	4/4	0.82	0.14	97,97,100,104	0
30	UNL	t	103	12/-	0.82	0.12	64,74,83,86	0
34	DMS	A	427	4/4	0.82	0.16	82,88,89,89	0
31	LMT	B	622	35/35	0.82	0.12	48,85,97,99	0
30	UNL	b	648	5/-	0.82	0.16	73,74,76,77	0
29	PL9	a	417	55/55	0.82	0.15	50,78,101,105	0
32	GOL	b	637	6/6	0.82	0.12	92,92,94,96	0
36	HTG	O	316	19/19	0.82	0.15	47,71,81,84	0
32	GOL	c	929	6/6	0.82	0.16	77,89,93,94	0
34	DMS	O	312	4/4	0.82	0.14	101,103,104,106	0
30	UNL	b	629	16/-	0.82	0.17	59,83,97,99	0
36	HTG	C	537	19/19	0.83	0.11	84,109,123,126	0
30	UNL	i	102	18/-	0.83	0.13	44,68,93,96	0
34	DMS	O	314	4/4	0.83	0.16	81,87,87,88	0
30	UNL	x	102	8/-	0.83	0.13	77,80,86,88	0
34	DMS	C	531	4/4	0.83	0.16	109,111,113,116	0
36	HTG	b	627	19/19	0.83	0.13	69,113,125,128	0
30	UNL	b	630	10/-	0.83	0.16	71,82,85,85	0
30	UNL	D	410	40/-	0.83	0.13	46,67,103,106	0
36	HTG	c	928	19/19	0.83	0.12	74,98,122,126	0
34	DMS	V	212	4/4	0.83	0.15	86,96,99,99	0
30	UNL	C	539	16/-	0.83	0.15	76,79,102,107	0
34	DMS	a	425	4/4	0.83	0.15	116,120,120,121	0
30	UNL	k	101	30/-	0.83	0.13	62,90,106,111	0
36	HTG	B	624	19/19	0.83	0.15	34,53,75,76	0
36	HTG	d	420	19/19	0.83	0.11	85,115,118,118	0
30	UNL	k	104	9/-	0.83	0.15	69,82,89,90	0
30	UNL	E	102	5/-	0.83	0.14	76,76,76,77	0
30	UNL	i	101	8/-	0.83	0.13	63,67,75,81	0
34	DMS	O	309	4/4	0.83	0.18	98,101,102,105	0
34	DMS	O	311	4/4	0.83	0.16	93,96,97,98	0
29	PL9	A	414	55/55	0.84	0.14	53,68,102,104	0
34	DMS	V	211	4/4	0.84	0.16	94,94,96,99	0
34	DMS	B	643	4/4	0.84	0.12	100,104,106,106	0
34	DMS	H	104	4/4	0.84	0.23	109,109,112,116	0
34	DMS	a	424	4/4	0.84	0.17	102,104,105,105	0
34	DMS	v	209	4/4	0.84	0.20	110,110,110,111	0
34	DMS	L	102	4/4	0.84	0.16	106,110,111,112	0
30	UNL	c	925	11/-	0.84	0.12	74,77,85,85	0
34	DMS	b	640	4/4	0.84	0.14	69,91,92,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	i	103	12/-	0.84	0.14	67,75,83,87	0
30	UNL	e	105	4/-	0.84	0.18	74,77,79,82	0
32	GOL	a	419	6/6	0.84	0.12	55,59,59,60	0
27	SQD	A	416	54/54	0.84	0.11	50,70,89,95	0
31	LMT	c	927	35/35	0.84	0.13	49,97,104,111	0
30	UNL	E	105	4/-	0.84	0.13	60,62,69,72	0
28	LMG	a	416	51/55	0.84	0.12	54,73,92,98	0
28	LMG	c	921	51/55	0.84	0.12	47,94,101,104	0
30	UNL	m	101	11/-	0.85	0.13	56,67,78,84	0
34	DMS	D	416	4/4	0.85	0.18	93,94,97,98	0
30	UNL	B	628	6/-	0.85	0.14	68,69,79,82	0
30	UNL	H	105	18/-	0.85	0.12	51,67,98,103	0
34	DMS	o	305	4/4	0.85	0.18	94,102,106,107	0
31	LMT	m	102	35/35	0.85	0.11	34,64,85,88	0
34	DMS	b	645	4/4	0.85	0.17	103,110,111,111	0
34	DMS	U	203	4/4	0.85	0.19	40,60,64,66	0
30	UNL	Z	102	6/-	0.85	0.14	61,72,75,77	0
34	DMS	v	208	4/4	0.85	0.13	86,89,94,98	0
31	LMT	B	626	24/35	0.85	0.12	47,73,114,118	0
31	LMT	t	102	35/35	0.85	0.11	43,91,116,118	0
34	DMS	V	213	4/4	0.85	0.14	76,84,85,86	0
36	HTG	b	626	19/19	0.86	0.15	41,52,95,99	0
30	UNL	B	648	4/-	0.86	0.13	66,70,70,71	0
34	DMS	a	422	4/4	0.86	0.15	91,94,96,98	0
36	HTG	B	623	19/19	0.86	0.13	46,59,69,72	0
30	UNL	E	103	8/-	0.86	0.15	65,78,79,79	0
34	DMS	K	102	4/4	0.86	0.16	95,106,107,109	0
34	DMS	e	104	4/4	0.86	0.15	88,94,96,98	0
34	DMS	B	641	4/4	0.86	0.18	107,108,110,110	0
30	UNL	j	103	6/-	0.86	0.12	72,80,86,88	0
30	UNL	j	104	4/-	0.86	0.12	74,75,76,78	0
36	HTG	C	536	19/19	0.86	0.10	66,106,124,126	0
34	DMS	V	205	4/4	0.86	0.19	94,98,98,100	0
28	LMG	A	413	51/55	0.86	0.12	49,74,97,102	0
34	DMS	c	934	4/4	0.86	0.13	73,80,82,84	0
33	BCT	a	408[A]	4/4	0.86	0.11	31,38,39,41	4
30	UNL	B	635	6/-	0.86	0.14	70,73,75,79	0
34	DMS	b	638	4/4	0.87	0.14	58,80,83,83	0
31	LMT	Z	101	35/35	0.87	0.13	52,104,121,123	0
34	DMS	O	313	4/4	0.87	0.12	101,106,108,111	0
34	DMS	b	641	4/4	0.87	0.18	89,91,92,95	0
34	DMS	b	643	4/4	0.87	0.20	113,118,118,120	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	B	639	4/4	0.87	0.15	87,90,93,95	0
27	SQD	f	102	43/54	0.87	0.13	50,91,111,117	0
31	LMT	M	101	35/35	0.87	0.11	42,70,85,89	0
34	DMS	D	414	4/4	0.87	0.16	102,104,106,107	0
31	LMT	M	102	25/35	0.87	0.12	40,67,106,110	0
34	DMS	B	644	4/4	0.87	0.16	56,75,78,78	0
30	UNL	d	421	11/-	0.88	0.13	77,88,95,95	0
34	DMS	d	418	4/4	0.88	0.15	74,75,76,78	0
34	DMS	c	933	4/4	0.88	0.15	108,111,113,114	0
34	DMS	C	529	4/4	0.88	0.20	100,103,104,105	0
30	UNL	x	103	4/-	0.88	0.13	74,75,83,84	0
34	DMS	o	304	4/4	0.88	0.12	83,88,90,94	0
35	CA	v	201	1/1	0.88	0.09	104,104,104,104	0
34	DMS	O	306	4/4	0.88	0.14	78,82,86,86	0
32	GOL	A	419	6/6	0.88	0.14	59,61,62,66	0
34	DMS	b	647	4/4	0.88	0.16	72,73,79,79	0
34	DMS	u	202	4/4	0.88	0.16	68,80,81,86	0
34	DMS	v	203	4/4	0.88	0.17	87,94,95,96	0
32	GOL	C	525	6/6	0.89	0.12	89,91,92,93	0
36	HTG	V	204	13/19	0.89	0.09	49,59,79,86	0
30	UNL	I	101	14/-	0.89	0.10	46,53,70,73	0
36	HTG	O	303	19/19	0.89	0.12	46,56,64,64	0
36	HTG	B	629	19/19	0.90	0.10	46,70,92,97	0
28	LMG	B	621	51/55	0.90	0.10	39,54,71,82	0
32	GOL	V	206	6/6	0.90	0.09	58,69,71,83	0
34	DMS	a	423	4/4	0.90	0.13	63,76,79,85	0
26	BCR	B	636	40/40	0.90	0.08	29,41,59,59	0
34	DMS	e	102	4/4	0.90	0.12	95,95,96,99	0
34	DMS	V	201	4/4	0.90	0.13	75,76,79,88	0
30	UNL	d	413	18/-	0.90	0.11	42,57,77,85	0
26	BCR	T	101	40/40	0.90	0.07	29,42,60,63	0
34	DMS	o	302	4/4	0.90	0.14	71,74,78,80	0
36	HTG	U	201	4/19	0.90	0.19	49,51,51,56	0
34	DMS	o	303	4/4	0.90	0.11	92,94,95,101	0
30	UNL	D	411	16/-	0.90	0.10	44,51,73,74	0
28	LMG	b	624	51/55	0.90	0.10	44,56,78,89	0
38	LHG	D	406	49/49	0.90	0.11	36,50,67,81	0
34	DMS	c	937	4/4	0.90	0.11	99,101,103,103	0
38	LHG	d	409	49/49	0.90	0.10	38,50,61,67	0
28	LMG	C	519	51/55	0.91	0.11	36,80,92,97	0
36	HTG	b	602	19/19	0.91	0.09	51,67,78,83	0
34	DMS	h	105	4/4	0.91	0.13	52,53,61,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	v	206	4/4	0.91	0.12	55,68,74,84	0
34	DMS	A	426	4/4	0.91	0.15	81,86,86,88	0
34	DMS	O	305	4/4	0.91	0.13	81,82,85,88	0
34	DMS	a	421	4/4	0.91	0.13	78,84,85,89	0
34	DMS	u	201	4/4	0.92	0.16	52,64,66,70	0
27	SQD	a	415	54/54	0.92	0.10	35,65,85,87	0
34	DMS	B	640	4/4	0.92	0.10	77,78,82,86	0
27	SQD	A	412	54/54	0.92	0.10	35,64,79,85	0
24	CLA	C	506	65/65	0.92	0.09	37,52,90,94	0
34	DMS	O	308	4/4	0.92	0.12	80,83,84,90	0
27	SQD	F	101	37/54	0.92	0.10	45,71,88,92	0
34	DMS	O	310	4/4	0.92	0.12	88,89,90,94	0
30	UNL	x	101	18/-	0.92	0.13	51,65,90,92	0
33	BCT	d	402[B]	4/4	0.92	0.09	34,37,37,40	4
35	CA	V	202	1/1	0.92	0.06	89,89,89,89	0
32	GOL	B	638	6/6	0.92	0.10	39,58,69,73	0
30	UNL	X	101	16/-	0.92	0.11	48,57,70,73	0
26	BCR	c	915	40/40	0.92	0.08	47,58,64,66	0
34	DMS	C	528	4/4	0.92	0.12	81,81,83,83	0
28	LMG	c	920	51/55	0.92	0.09	41,72,98,99	0
26	BCR	Y	101	40/40	0.93	0.07	40,44,48,54	0
34	DMS	V	210	4/4	0.93	0.09	69,71,76,76	0
26	BCR	b	622	40/40	0.93	0.07	31,39,57,64	0
26	BCR	B	619	40/40	0.93	0.07	28,37,54,62	0
26	BCR	d	406	40/40	0.93	0.08	34,41,69,72	0
24	CLA	c	907	65/65	0.93	0.08	39,48,81,85	0
26	BCR	K	101	40/40	0.93	0.08	34,43,48,49	0
24	CLA	c	914	65/65	0.93	0.09	41,53,89,96	0
34	DMS	b	644	4/4	0.93	0.15	63,65,67,78	0
34	DMS	c	940	4/4	0.94	0.20	58,63,64,66	0
34	DMS	d	415	4/4	0.94	0.14	63,66,70,74	0
24	CLA	b	618	65/65	0.94	0.08	24,33,88,91	0
26	BCR	a	414	40/40	0.94	0.06	27,33,39,41	0
24	CLA	B	617	65/65	0.94	0.09	30,36,105,109	0
24	CLA	c	913	65/65	0.94	0.08	40,49,84,89	0
34	DMS	b	642	4/4	0.94	0.09	57,63,69,73	0
24	CLA	B	602	65/65	0.94	0.08	35,52,105,110	0
28	LMG	D	409	51/55	0.94	0.09	32,43,99,106	0
24	CLA	C	512	65/65	0.94	0.08	43,50,90,92	0
33	BCT	A	422	4/4	0.94	0.09	37,37,48,55	0
24	CLA	C	513	65/65	0.94	0.08	43,54,86,88	0
26	BCR	C	514	40/40	0.94	0.07	41,49,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	DMS	c	931	4/4	0.94	0.16	88,88,89,92	0
26	BCR	C	515	40/40	0.94	0.06	33,42,50,54	0
28	LMG	d	412	51/55	0.94	0.09	35,45,89,94	0
37	DGD	C	517	62/66	0.94	0.08	31,43,92,101	0
26	BCR	D	403	40/40	0.94	0.07	33,41,69,73	0
37	DGD	H	102	62/66	0.94	0.07	27,40,51,53	0
24	CLA	b	605	65/65	0.94	0.08	40,54,102,107	0
37	DGD	h	102	62/66	0.94	0.08	34,42,51,63	0
34	DMS	B	633	4/4	0.94	0.13	48,49,56,58	0
34	DMS	B	634	4/4	0.94	0.11	63,64,64,65	0
24	CLA	b	610	65/65	0.94	0.08	29,37,71,80	0
40	RRX	h	101	41/41	0.94	0.07	31,44,61,71	0
24	CLA	c	902	65/65	0.95	0.07	33,42,54,60	0
24	CLA	c	905	65/65	0.95	0.07	32,40,72,81	0
24	CLA	B	607	65/65	0.95	0.07	28,34,65,71	0
34	DMS	V	209	4/4	0.95	0.13	50,59,66,67	0
24	CLA	c	908	65/65	0.95	0.07	32,42,59,61	0
24	CLA	C	503	65/65	0.95	0.06	32,39,46,56	0
24	CLA	B	615	65/65	0.95	0.08	24,32,86,95	0
34	DMS	c	932	4/4	0.95	0.11	80,88,88,89	0
34	DMS	C	527	4/4	0.95	0.11	72,74,75,77	0
24	CLA	d	405	65/65	0.95	0.08	33,39,102,107	0
26	BCR	c	916	40/40	0.95	0.06	38,43,54,57	0
26	BCR	A	411	40/40	0.95	0.06	27,33,41,45	0
37	DGD	C	516	62/66	0.95	0.07	27,38,90,95	0
26	BCR	k	102	40/40	0.95	0.06	40,45,54,55	0
34	DMS	v	204	4/4	0.95	0.10	55,57,58,64	0
26	BCR	B	618	40/40	0.95	0.06	27,35,41,41	0
37	DGD	c	917	62/66	0.95	0.07	28,39,84,88	0
37	DGD	c	918	62/66	0.95	0.08	36,44,99,109	0
24	CLA	C	507	65/65	0.95	0.07	36,42,57,66	0
24	CLA	b	614	65/65	0.95	0.06	30,36,42,61	0
24	CLA	C	508	65/65	0.95	0.07	28,37,95,108	0
29	PL9	D	404	55/55	0.95	0.06	23,29,38,51	0
38	LHG	L	101	49/49	0.95	0.07	30,41,64,71	0
24	CLA	b	620	65/65	0.95	0.08	30,41,98,102	0
38	LHG	l	103	49/49	0.95	0.07	32,42,66,69	0
29	PL9	d	407	55/55	0.95	0.06	22,29,43,56	0
24	CLA	C	505	65/65	0.96	0.06	32,39,57,63	0
26	BCR	b	623	40/40	0.96	0.06	32,41,55,58	0
24	CLA	B	610	65/65	0.96	0.06	30,36,43,46	0
24	CLA	c	904	65/65	0.96	0.06	35,44,50,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	611	65/65	0.96	0.06	26,35,43,50	0
24	CLA	B	604	65/65	0.96	0.06	28,33,40,42	0
26	BCR	k	103	40/40	0.96	0.06	37,46,54,59	0
24	CLA	C	510	65/65	0.96	0.06	31,39,51,58	0
24	CLA	c	909	65/65	0.96	0.06	31,37,91,96	0
24	CLA	c	910	65/65	0.96	0.07	34,40,58,64	0
24	CLA	c	912	65/65	0.96	0.07	34,43,52,58	0
24	CLA	C	511	65/65	0.96	0.07	33,44,51,54	0
24	CLA	B	616	65/65	0.96	0.06	26,35,53,65	0
24	CLA	A	410	65/65	0.96	0.08	26,35,99,104	0
34	DMS	C	526	4/4	0.96	0.09	44,46,46,50	0
25	PHO	A	409	64/64	0.96	0.05	24,30,37,42	0
24	CLA	D	402	65/65	0.96	0.07	29,37,102,104	0
24	CLA	a	413	65/65	0.96	0.08	26,34,107,111	0
24	CLA	C	501	65/65	0.96	0.06	30,39,53,61	0
37	DGD	C	518	62/66	0.96	0.07	28,37,80,85	0
26	BCR	B	620	40/40	0.96	0.06	30,37,52,55	0
24	CLA	b	606	65/65	0.96	0.06	31,36,46,56	0
24	CLA	C	502	65/65	0.96	0.06	29,36,48,63	0
24	CLA	b	611	65/65	0.96	0.05	23,31,44,50	0
37	DGD	c	919	62/66	0.96	0.07	32,40,76,82	0
24	CLA	b	613	65/65	0.96	0.06	32,38,44,57	0
34	DMS	D	413	4/4	0.96	0.13	62,65,67,73	0
24	CLA	B	608	65/65	0.96	0.06	23,29,44,50	0
38	LHG	D	408	46/49	0.96	0.07	32,39,72,77	0
24	CLA	b	616	65/65	0.96	0.06	25,33,41,42	0
24	CLA	b	617	65/65	0.96	0.06	25,31,71,77	0
24	CLA	C	504	65/65	0.96	0.07	27,35,80,83	0
38	LHG	d	410	49/49	0.96	0.07	27,33,53,64	0
38	LHG	d	411	47/49	0.96	0.08	32,39,87,92	0
26	BCR	b	621	40/40	0.96	0.05	31,37,48,53	0
40	RRX	H	101	41/41	0.96	0.06	30,41,56,63	0
34	DMS	b	632	4/4	0.96	0.12	61,63,64,65	0
24	CLA	a	409	65/65	0.97	0.05	23,28,37,50	0
24	CLA	a	410	65/65	0.97	0.06	26,32,89,95	0
24	CLA	c	903	65/65	0.97	0.06	29,38,50,61	0
24	CLA	B	613	65/65	0.97	0.05	24,31,37,41	0
35	CA	b	604	1/1	0.97	0.06	52,52,52,52	0
35	CA	c	901	1/1	0.97	0.05	52,52,52,52	0
24	CLA	B	614	65/65	0.97	0.06	21,30,67,76	0
34	DMS	d	416	4/4	0.97	0.09	62,64,65,72	0
24	CLA	c	906	65/65	0.97	0.06	30,37,66,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	606	65/65	0.97	0.06	25,30,43,46	0
24	CLA	b	607	65/65	0.97	0.05	28,35,41,44	0
24	CLA	b	608	65/65	0.97	0.06	25,31,69,74	0
24	CLA	b	609	65/65	0.97	0.06	25,33,44,49	0
24	CLA	c	911	65/65	0.97	0.06	30,39,51,61	0
24	CLA	A	407	65/65	0.97	0.06	21,29,89,95	0
24	CLA	C	509	65/65	0.97	0.07	34,41,63,67	0
24	CLA	b	612	65/65	0.97	0.05	28,35,42,45	0
24	CLA	d	401	65/65	0.97	0.05	21,27,41,51	0
24	CLA	d	404	65/65	0.97	0.05	23,28,50,57	0
24	CLA	B	603	65/65	0.97	0.05	27,34,44,49	0
38	LHG	D	407	49/49	0.97	0.06	25,34,48,65	0
24	CLA	B	609	65/65	0.97	0.05	27,33,40,44	0
25	PHO	a	411	64/64	0.97	0.05	24,28,33,38	0
25	PHO	a	412	64/64	0.97	0.05	26,33,41,43	0
24	CLA	b	615	65/65	0.97	0.05	25,31,51,55	0
24	CLA	A	406	65/65	0.97	0.04	20,26,38,53	0
34	DMS	V	208	4/4	0.97	0.08	50,53,56,57	0
24	CLA	B	605	65/65	0.97	0.06	23,29,61,62	0
39	HEM	f	101	43/43	0.97	0.08	42,50,65,84	0
24	CLA	B	612	65/65	0.97	0.05	25,30,46,54	0
24	CLA	b	619	65/65	0.97	0.06	29,37,58,65	0
25	PHO	A	408	64/64	0.98	0.04	21,28,33,36	0
24	CLA	A	405	65/65	0.98	0.04	22,26,33,54	0
34	DMS	a	420	4/4	0.98	0.07	34,35,35,42	0
34	DMS	b	631	4/4	0.98	0.07	34,34,37,43	0
34	DMS	c	930	4/4	0.98	0.07	46,49,49,50	0
39	HEM	F	102	43/43	0.98	0.06	38,48,56,60	0
24	CLA	D	401	65/65	0.98	0.05	20,26,41,46	0
35	CA	B	601	1/1	0.98	0.09	51,51,51,51	0
34	DMS	B	632	4/4	0.98	0.07	28,31,33,34	0
41	MG	j	101	1/1	0.98	0.12	44,44,44,44	0
42	HEC	v	202	43/43	0.98	0.06	35,41,47,48	0
23	CL	A	403	1/1	0.99	0.03	26,26,26,26	0
21	OEX	a	404	10/10	0.99	0.03	29,32,33,34	0
35	CA	o	301	1/1	0.99	0.03	55,55,55,55	0
41	MG	J	101	1/1	0.99	0.09	36,36,36,36	0
35	CA	O	301	1/1	0.99	0.06	56,56,56,56	0
42	HEC	V	203	43/43	0.99	0.05	27,31,37,40	0
34	DMS	A	423	4/4	0.99	0.06	31,34,37,48	0
23	CL	a	406	1/1	1.00	0.02	29,29,29,29	0
23	CL	a	407	1/1	1.00	0.03	34,34,34,34	0

Continued on next page...

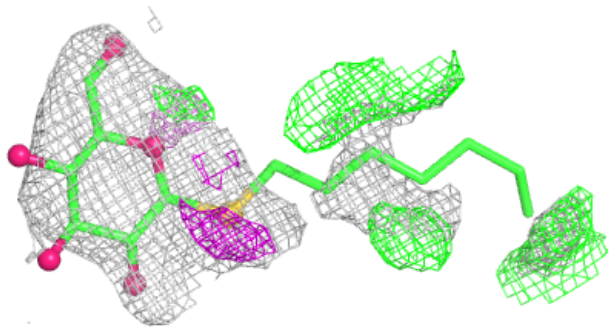
Continued from previous page...

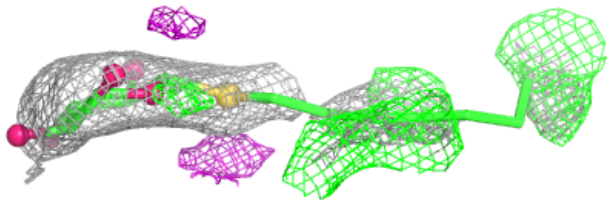
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	FE2	A	402	1/1	1.00	0.01	33,33,33,33	0
22	FE2	a	405	1/1	1.00	0.02	33,33,33,33	0
21	OEX	A	401	10/10	1.00	0.03	25,28,31,31	0
23	CL	A	404	1/1	1.00	0.02	29,29,29,29	0

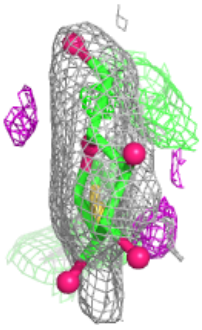
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG V 215:

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

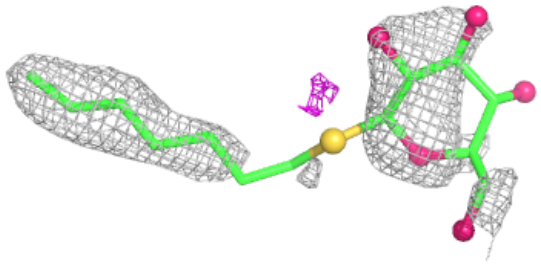


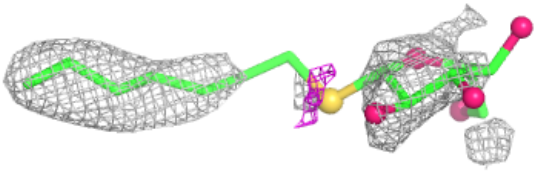


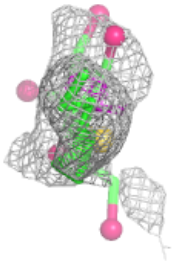


Electron density around HTG c 941:

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

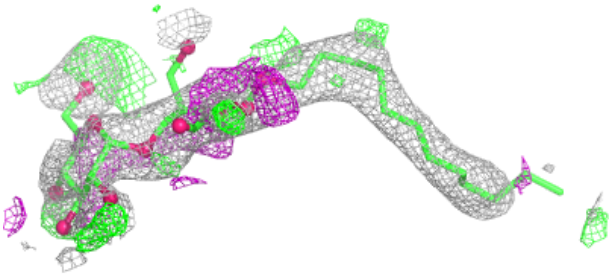


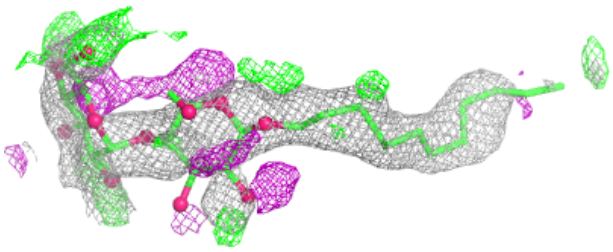


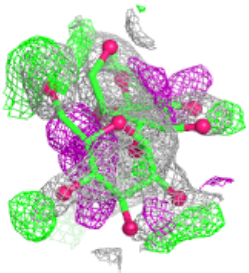


Electron density around LMT A 417:

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

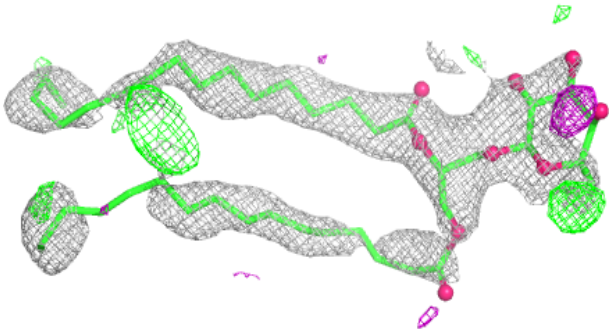


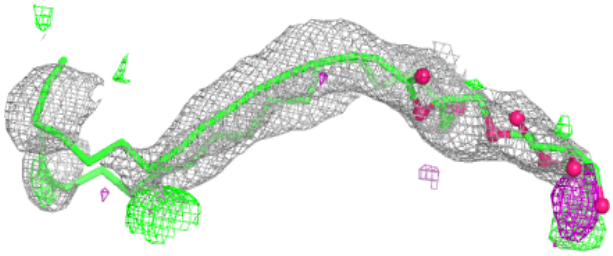


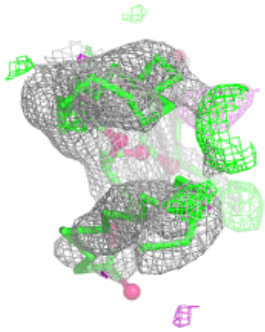


Electron density around DGD d 408:

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

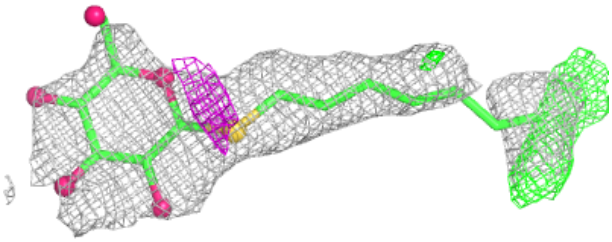


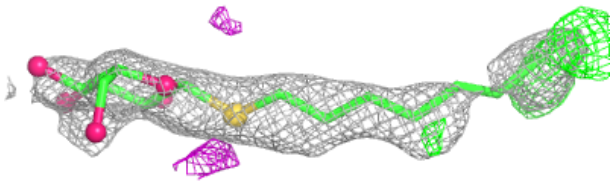


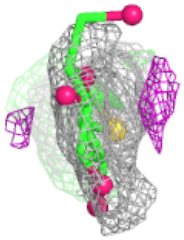


Electron density around HTG B 631:

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

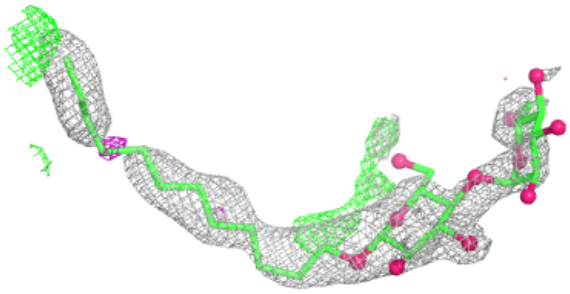


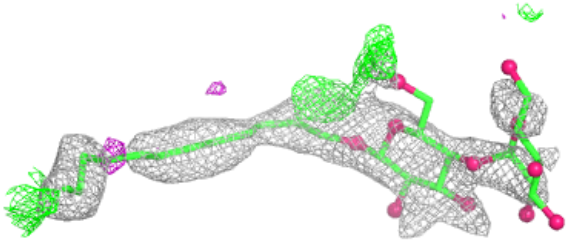


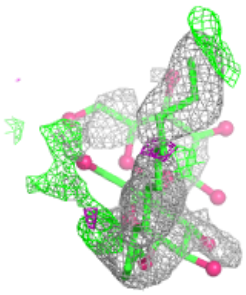


Electron density around LMT m 103:

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

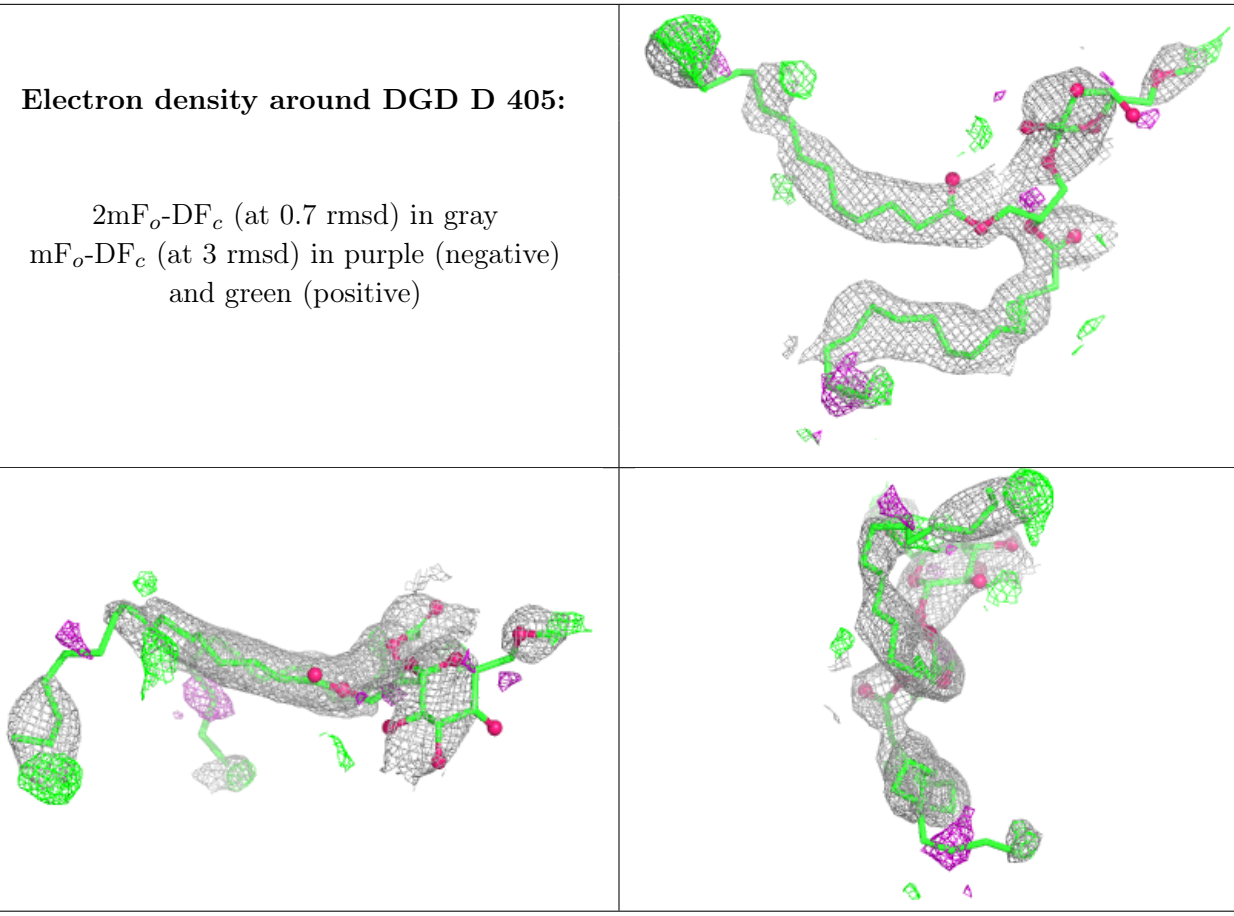






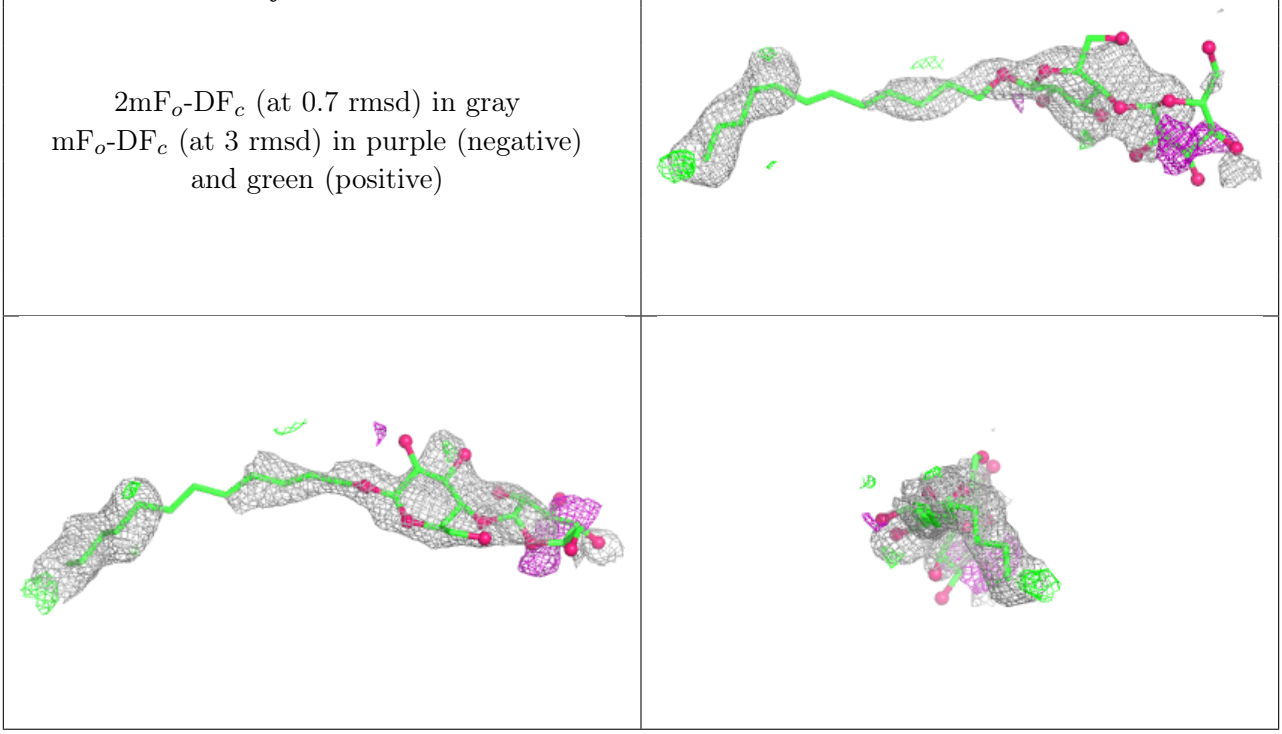
Electron density around DGD D 405:

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



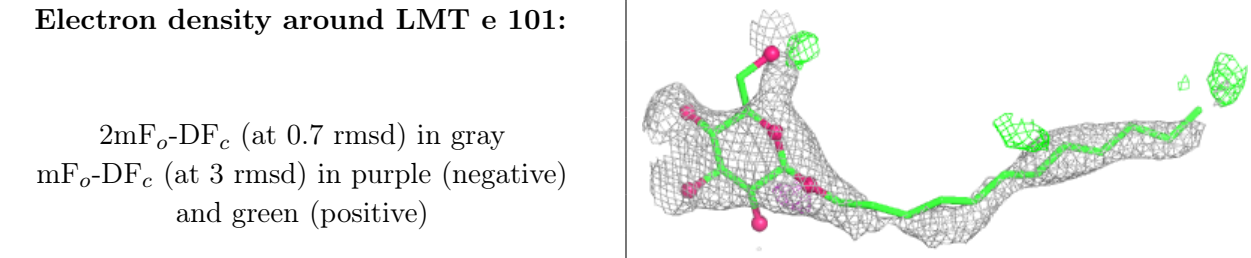
Electron density around LMT c 922:

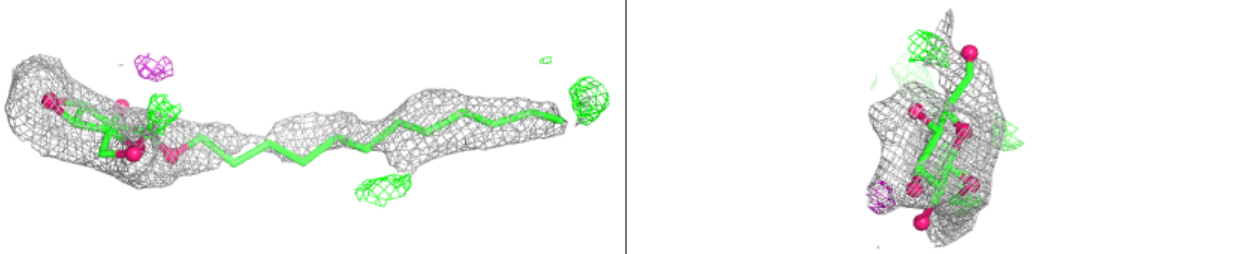
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT e 101:

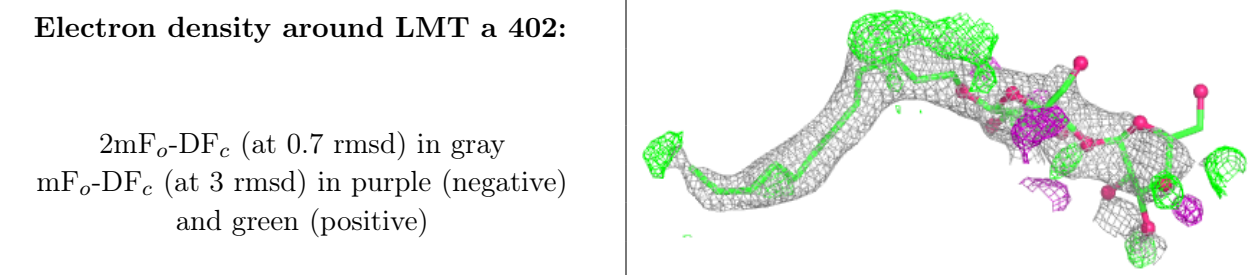
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

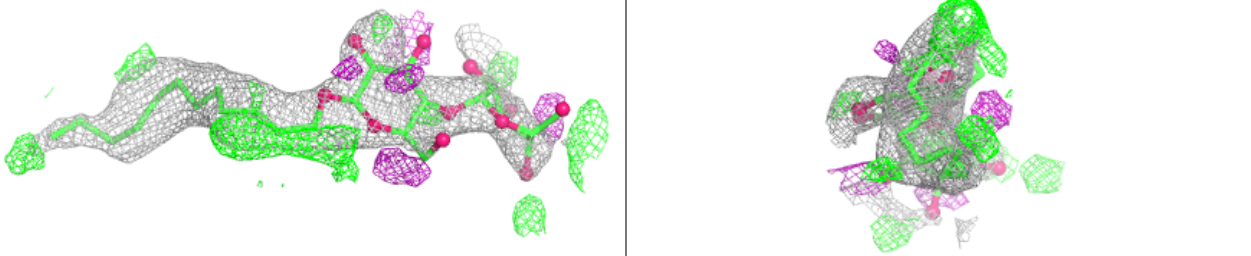




Electron density around LMT a 402:

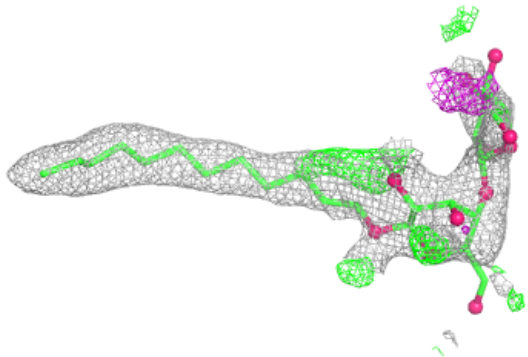
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

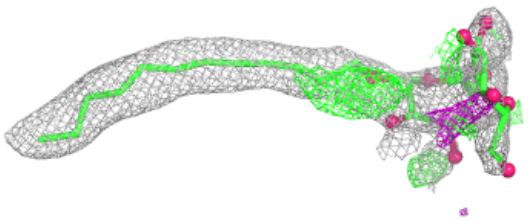


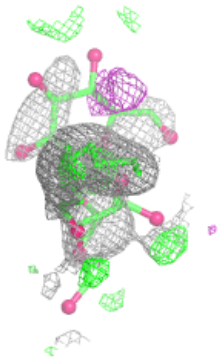


Electron density around LMT b 625:

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

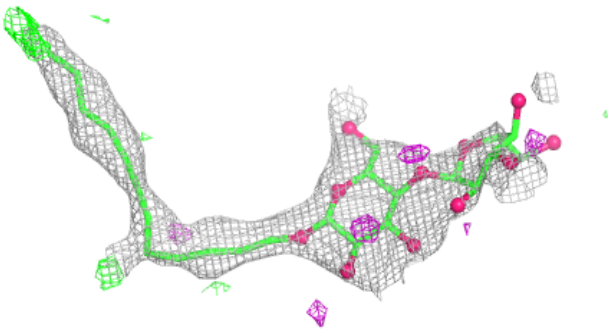


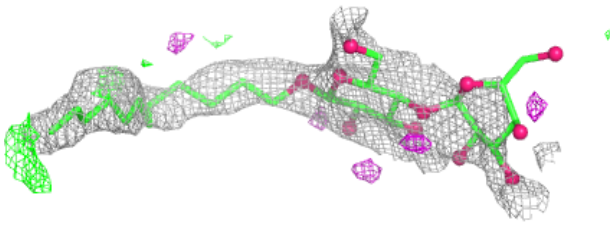


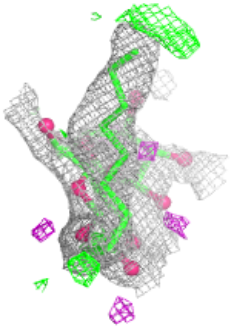


Electron density around LMT A 421:

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

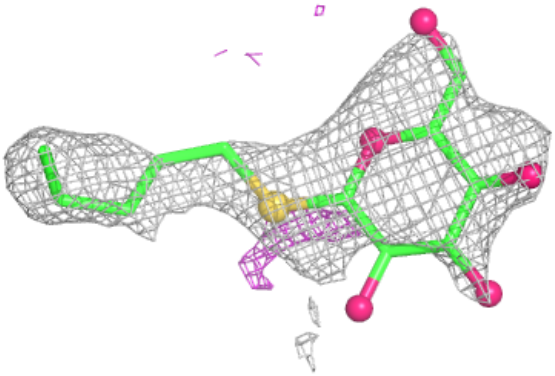


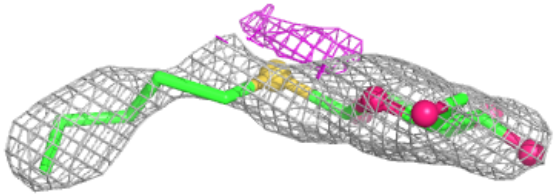


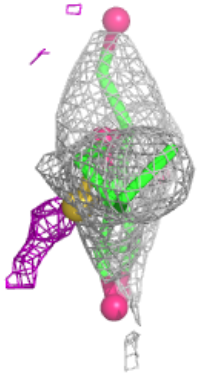


Electron density around HTG c 943:

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

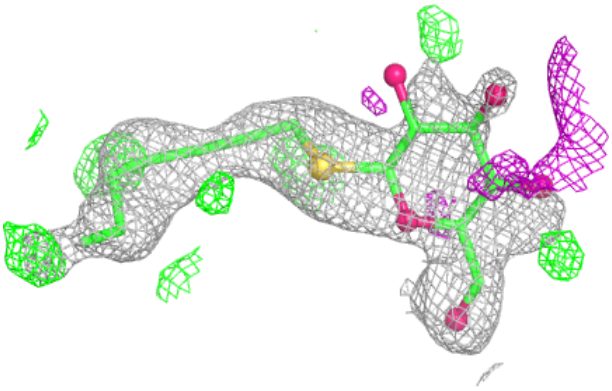


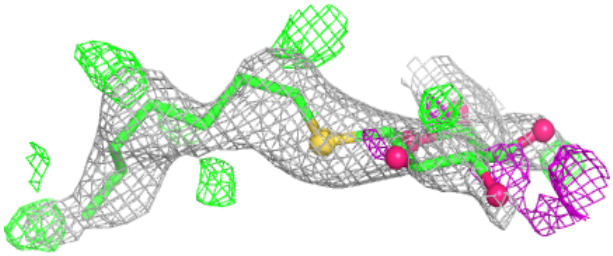


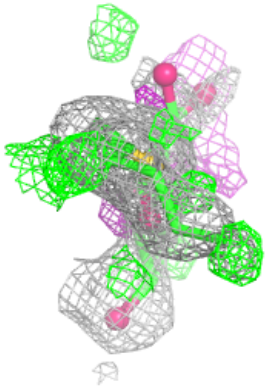


Electron density around HTG c 942:

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

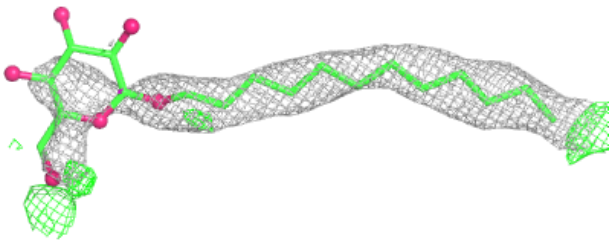


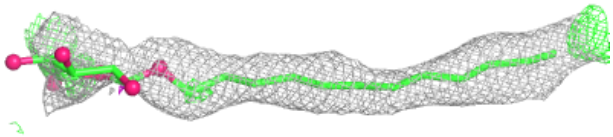


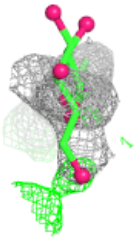


Electron density around LMT j 102:

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

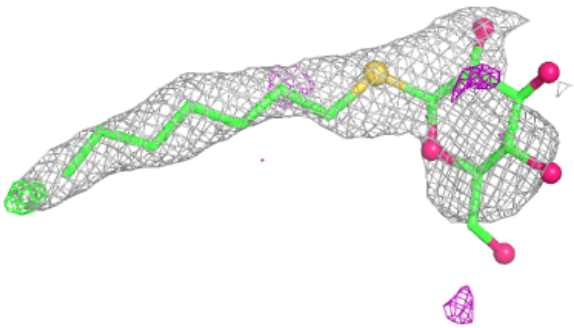


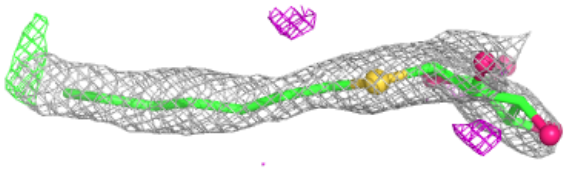


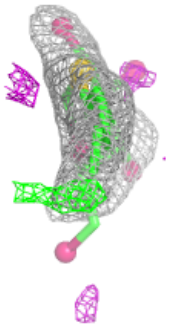


Electron density around HTG B 625:

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

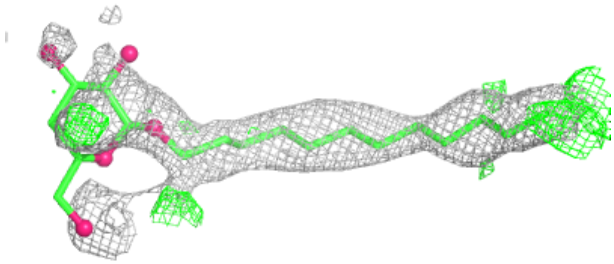


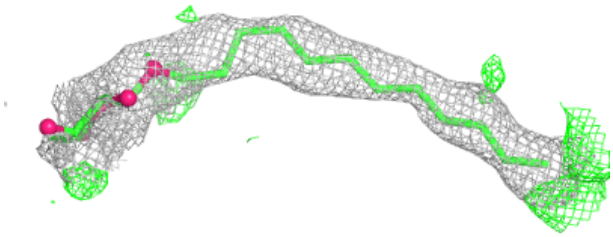


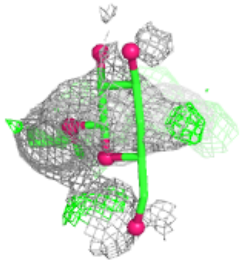


Electron density around LMT t 101:

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

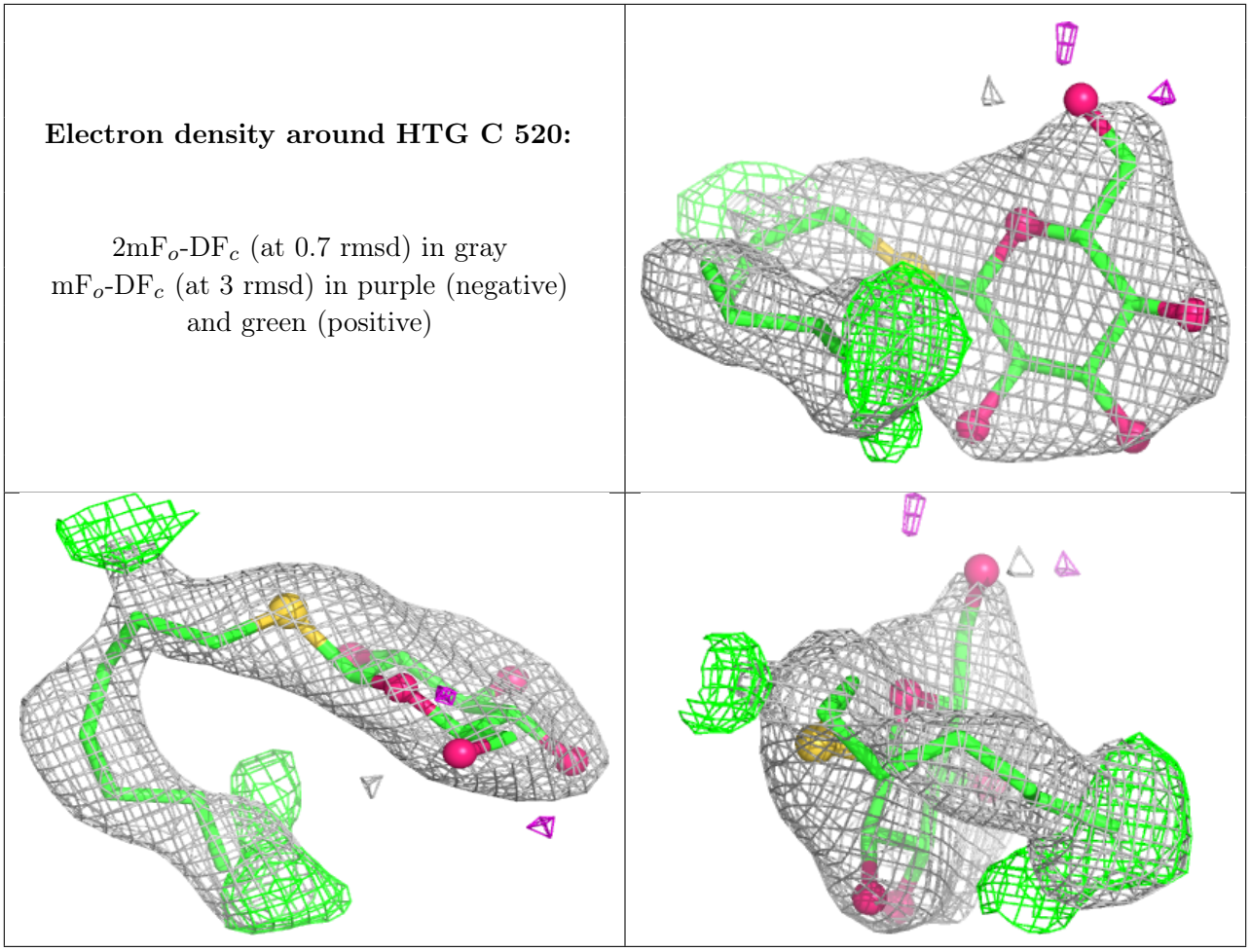






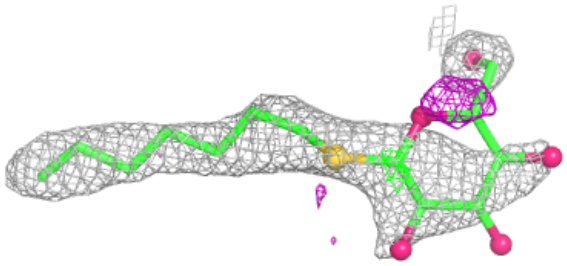
Electron density around HTG C 520:

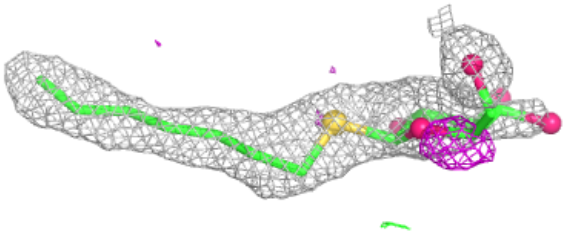
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

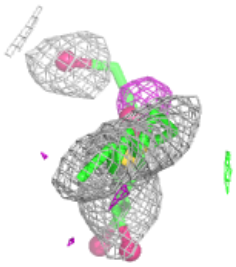


Electron density around HTG c 924:

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

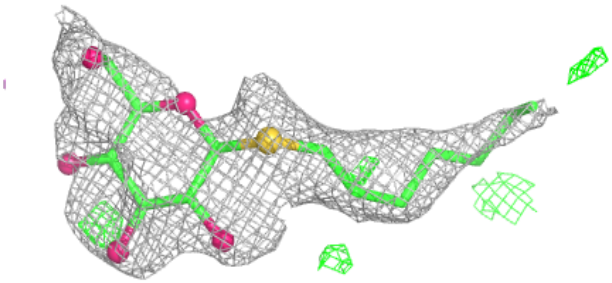


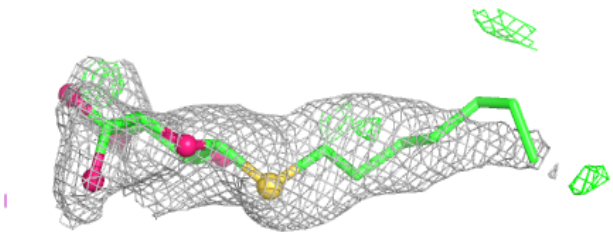


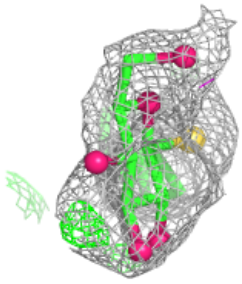


Electron density around HTG y 102:

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

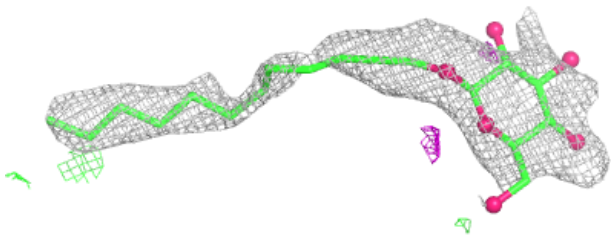


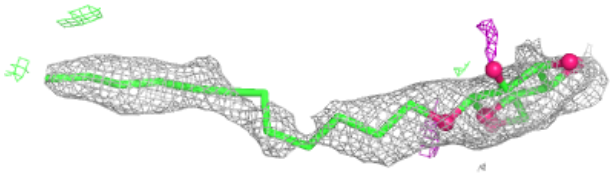


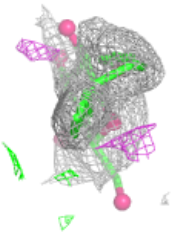


Electron density around LMT F 103:

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

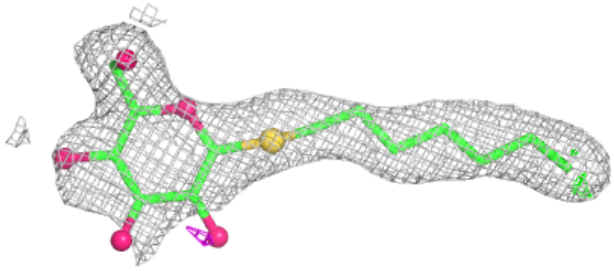


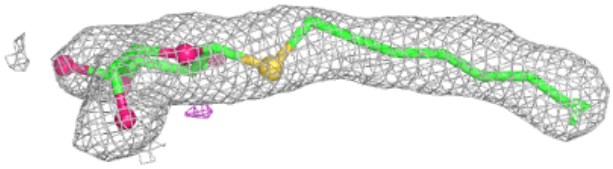


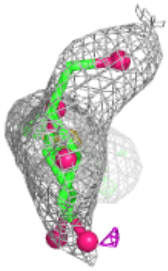


Electron density around HTG C 521:

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

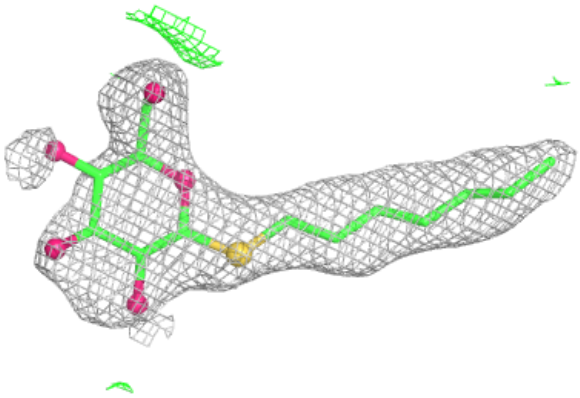


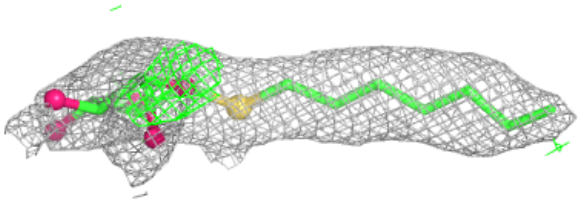


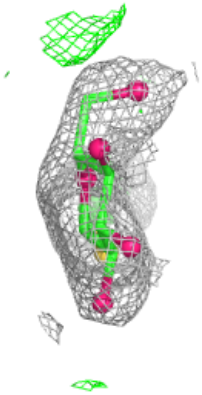


Electron density around HTG b 603:

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

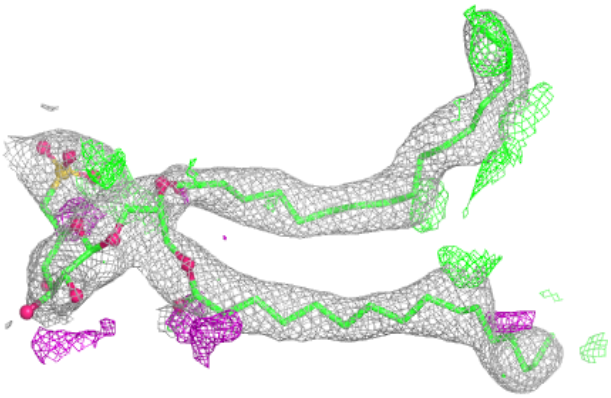


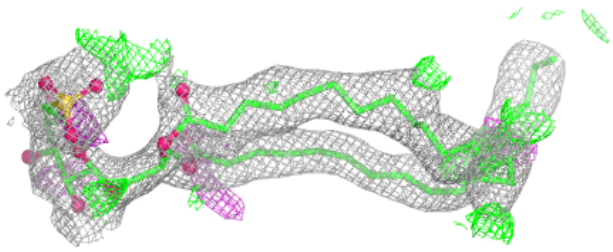


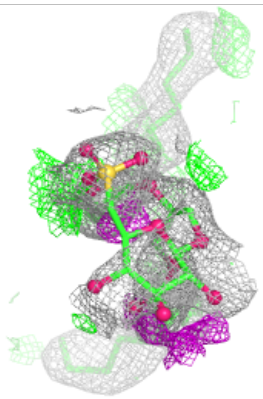


Electron density around SQD b 601:

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

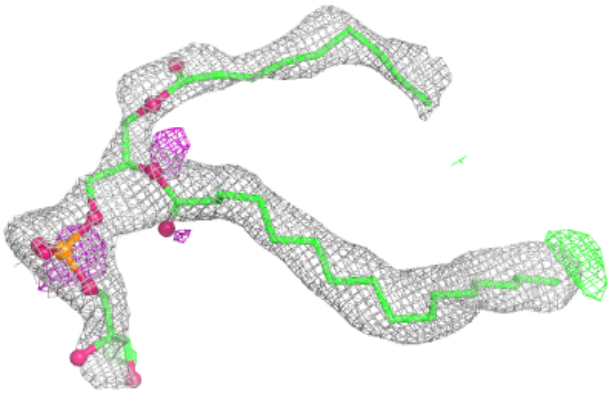


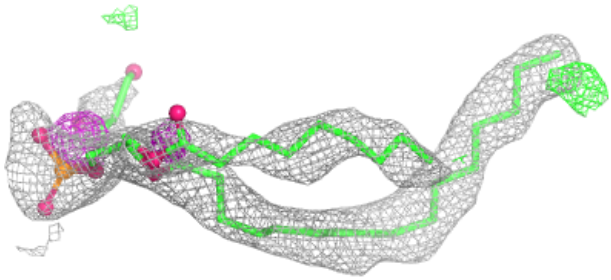


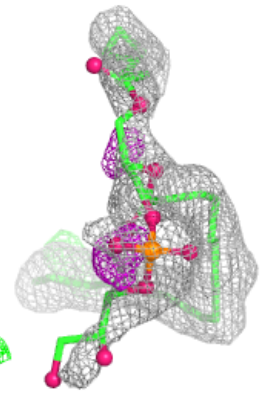


Electron density around LHG E 101:

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

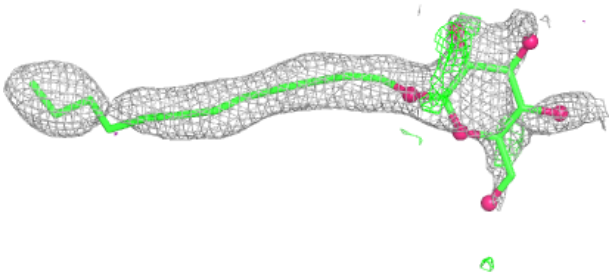


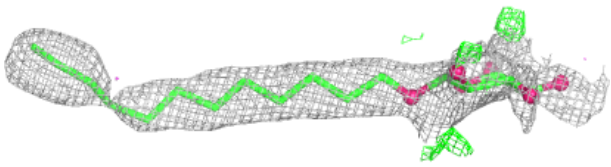


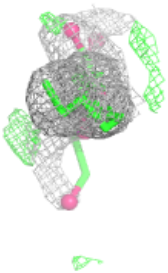


Electron density around LMT J 102:

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

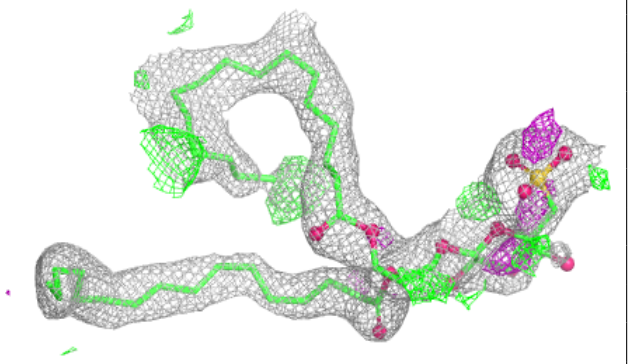


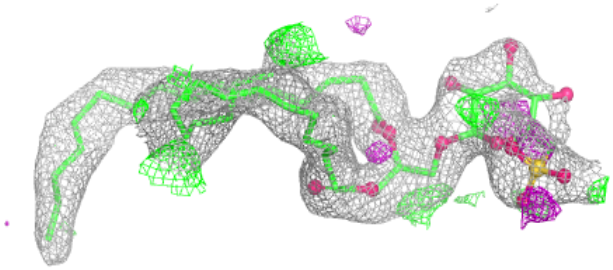


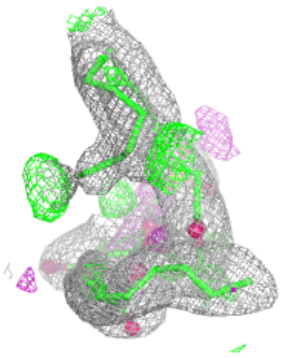


Electron density around SQD a 401:

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

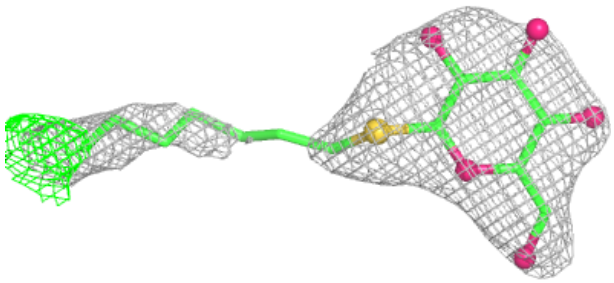


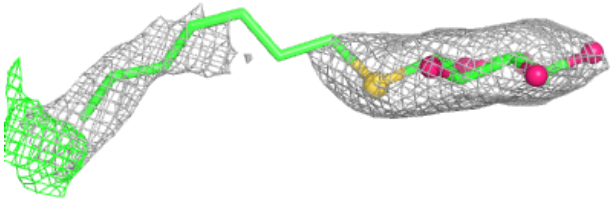


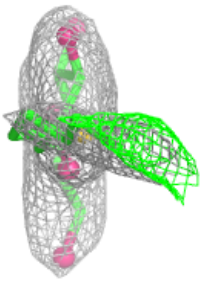


Electron density around HTG c 923:

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

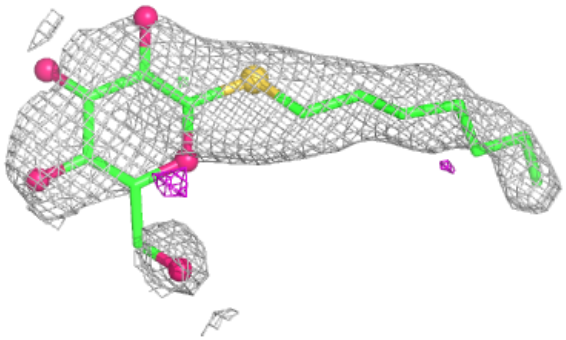


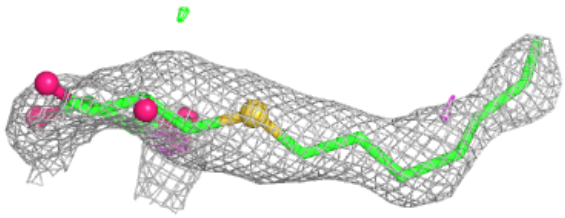


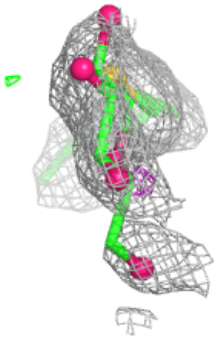


Electron density around HTG d 419:

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

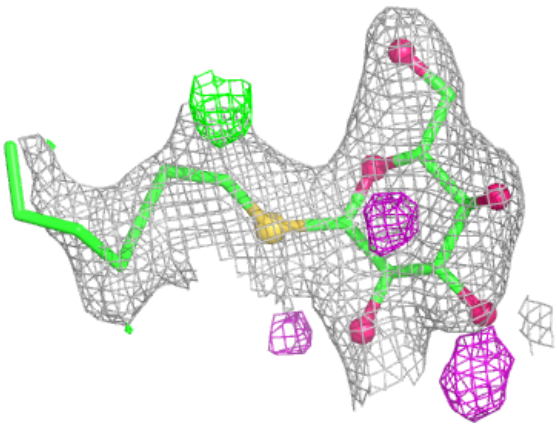


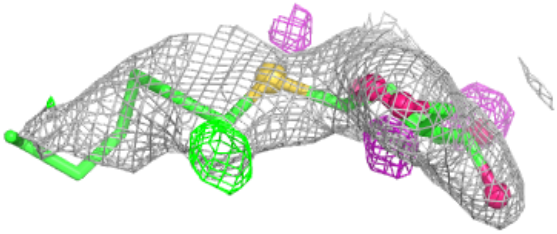


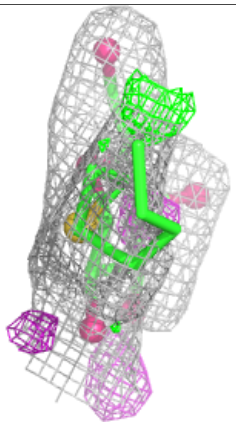


Electron density around HTG v 211:

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

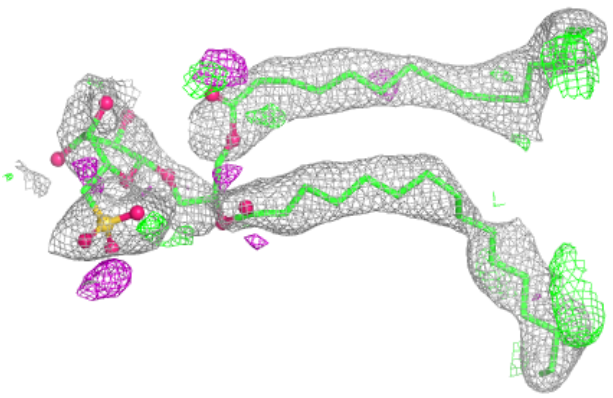


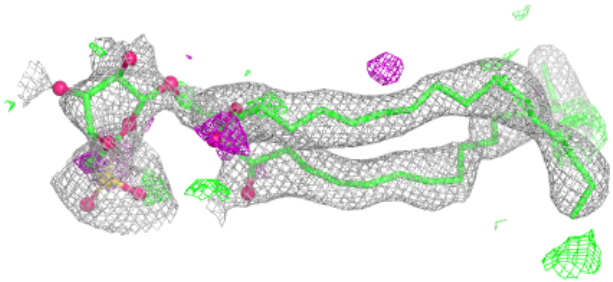


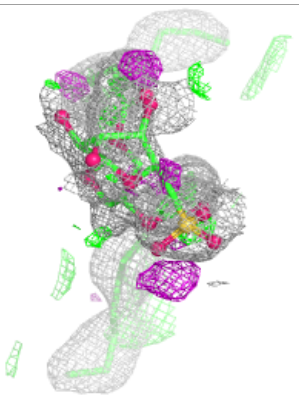


Electron density around SQD l 101:

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

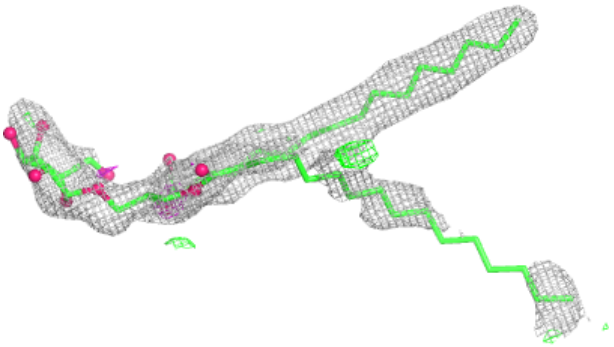


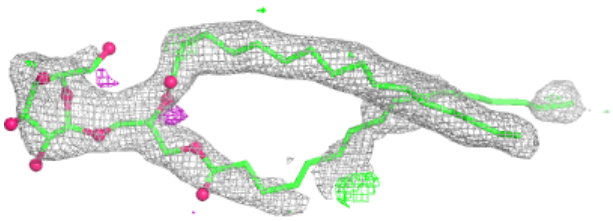


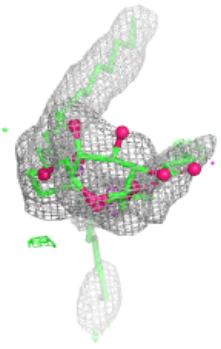


Electron density around LMG C 523:

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

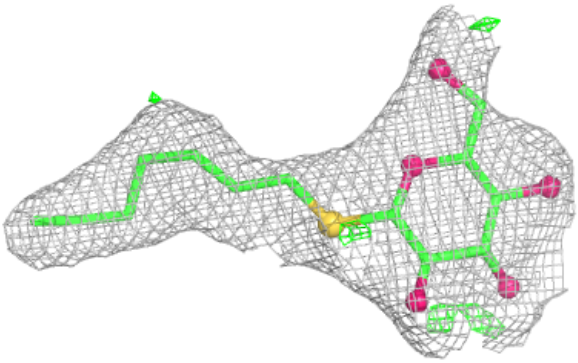


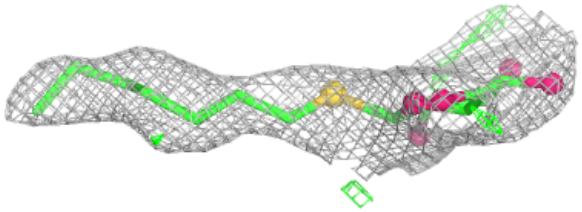


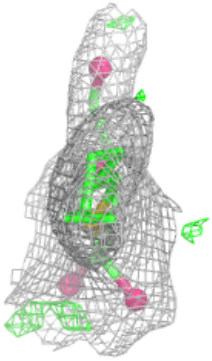


Electron density around HTG d 414:

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

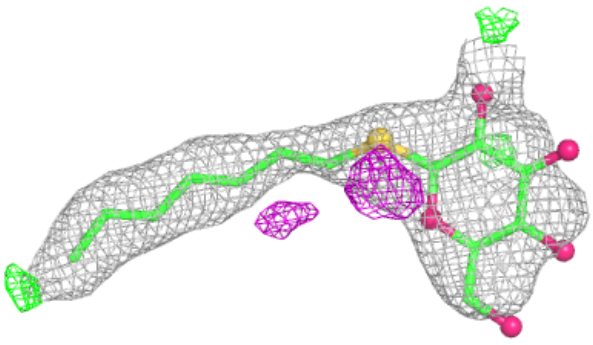


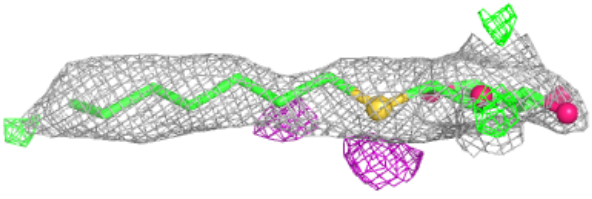


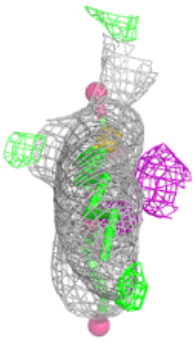


Electron density around HTG B 630:

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

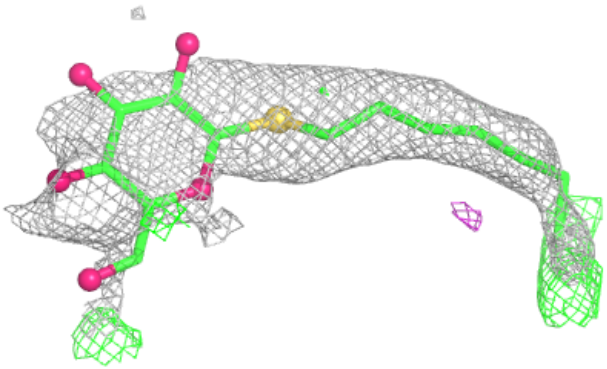


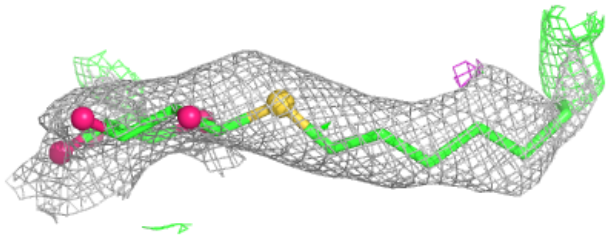


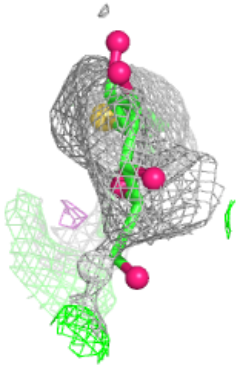


Electron density around HTG D 412:

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

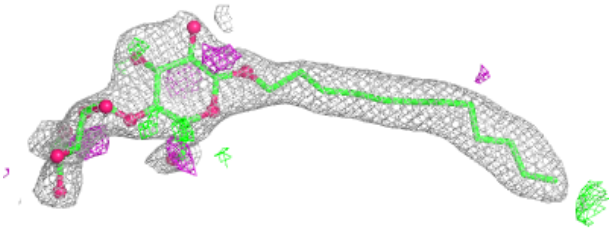


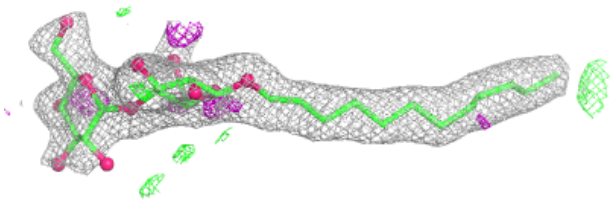


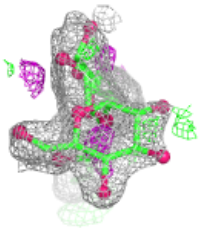


Electron density around LMT B 622:

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

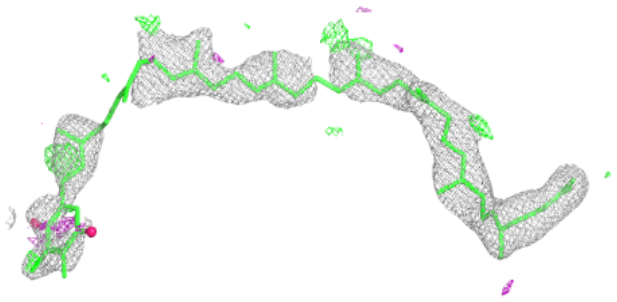


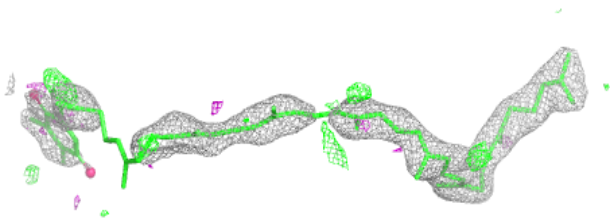


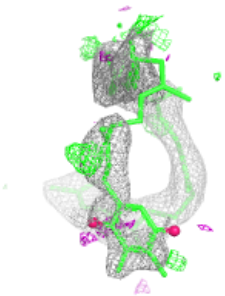


Electron density around PL9 a 417:

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

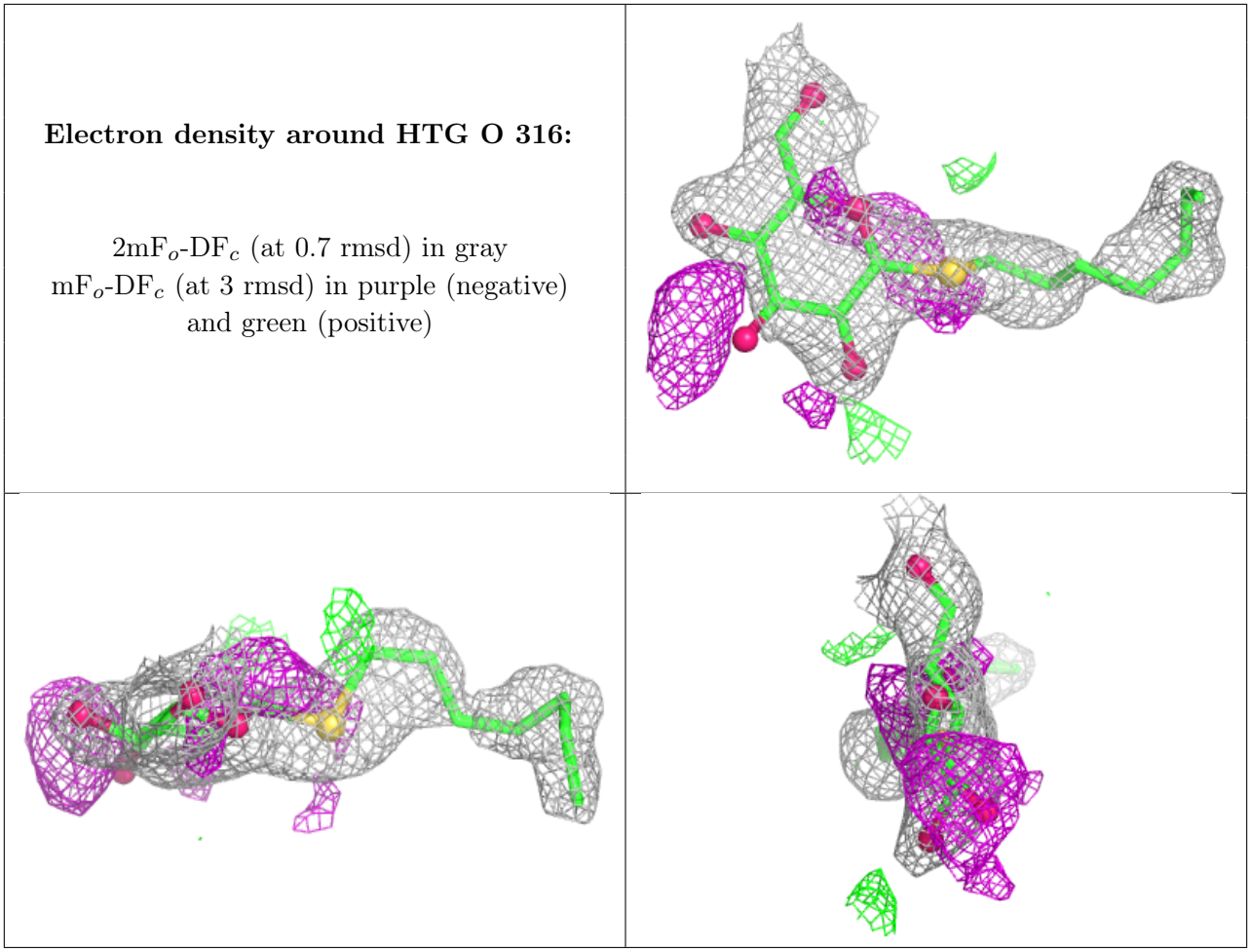






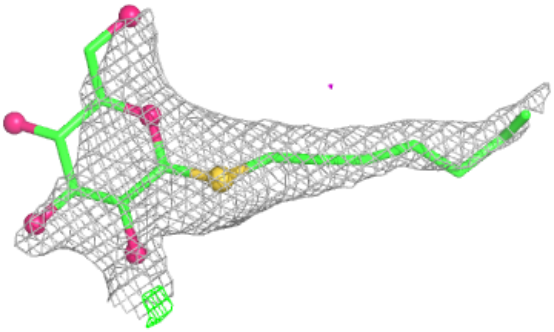
Electron density around HTG O 316:

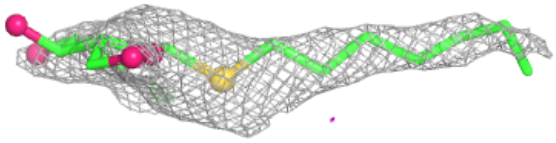
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HTG C 537:

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

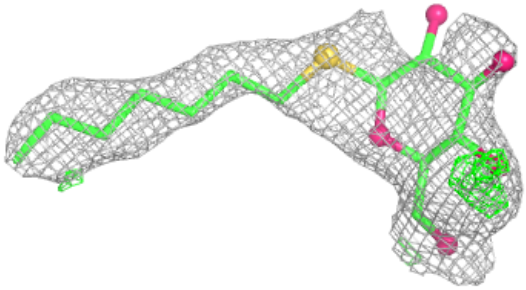


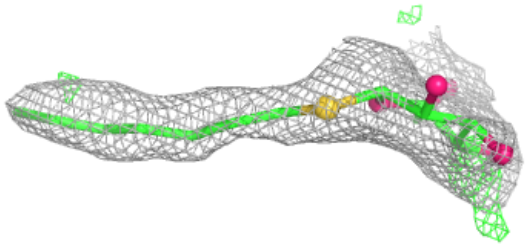


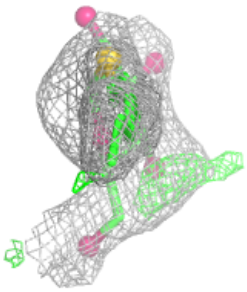


Electron density around HTG b 627:

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

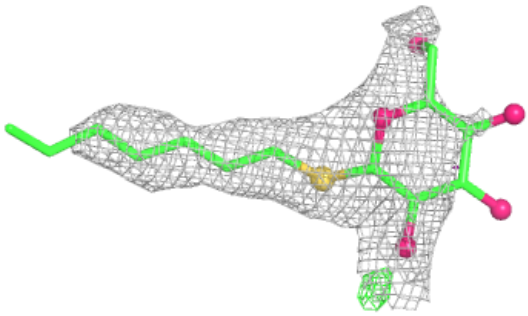


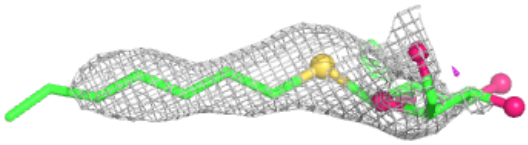


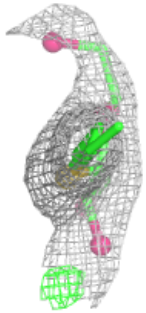


Electron density around HTG c 928:

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

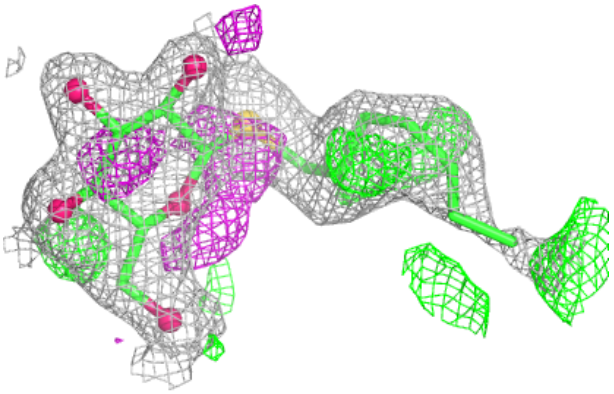


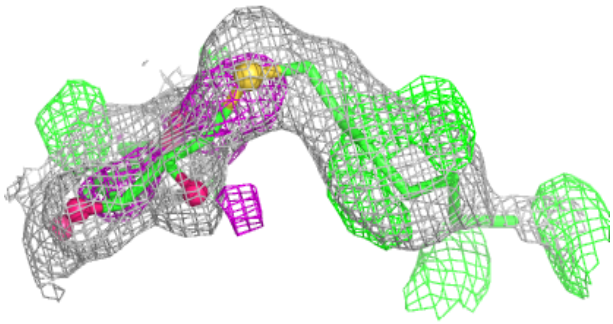


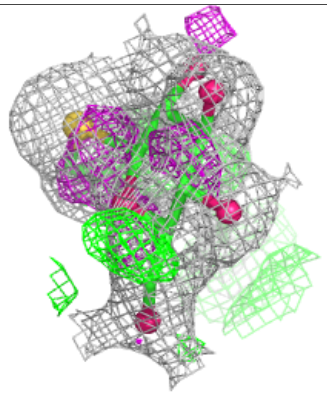


Electron density around HTG B 624:

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

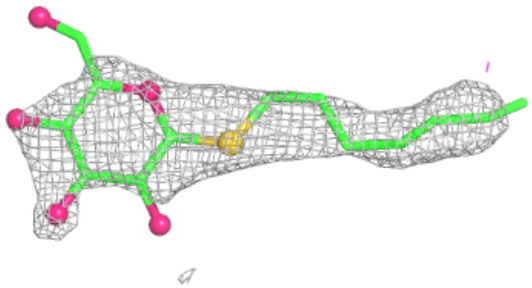


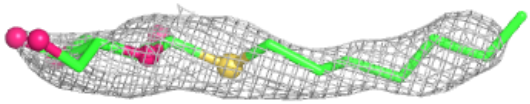


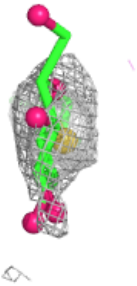


Electron density around HTG d 420:

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

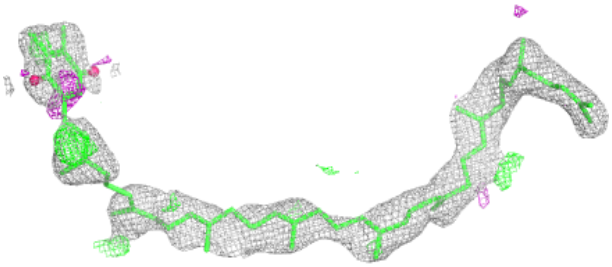


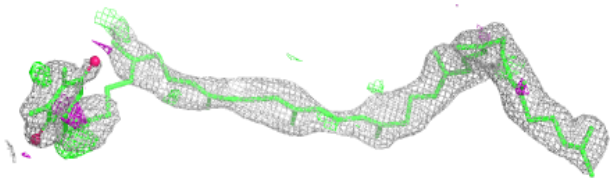


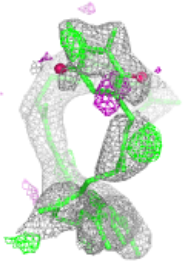


Electron density around PL9 A 414:

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



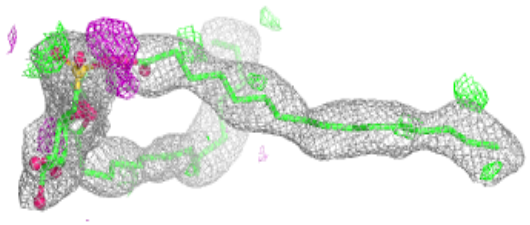


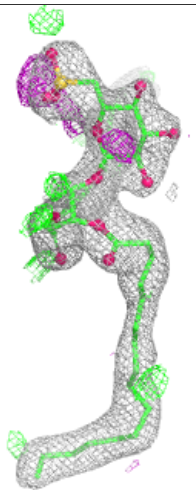


Electron density around SQD A 416:

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

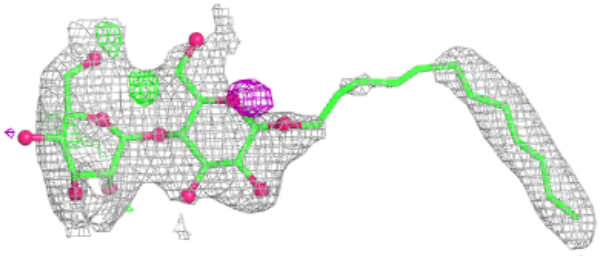


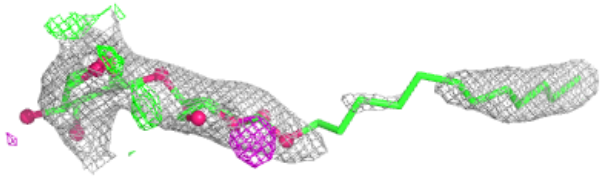


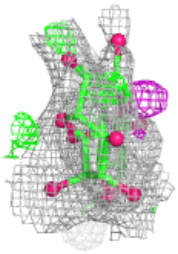


Electron density around LMT c 927:

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

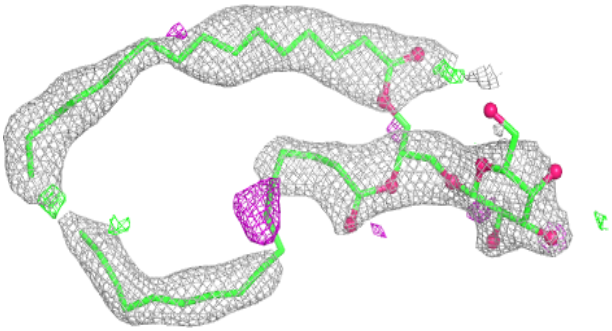


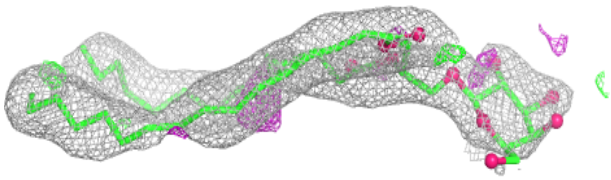


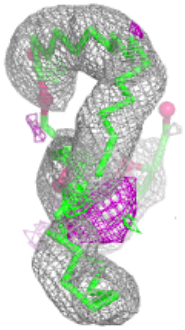


Electron density around LMG a 416:

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

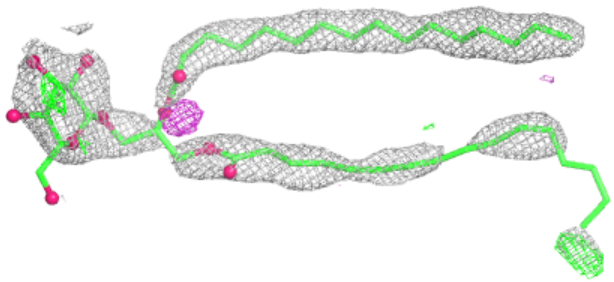


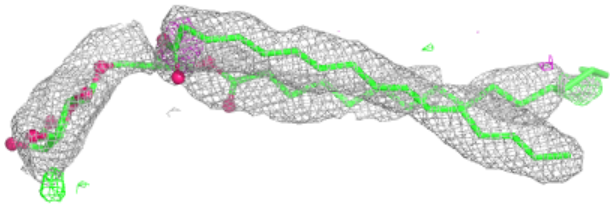


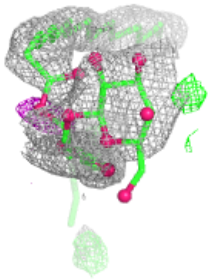


Electron density around LMG c 921:

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

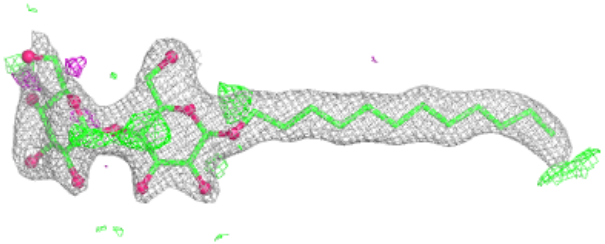


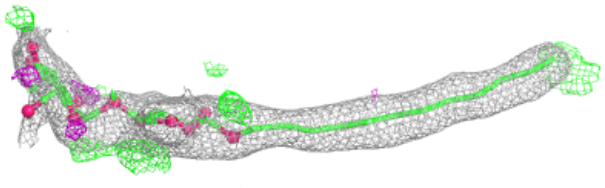


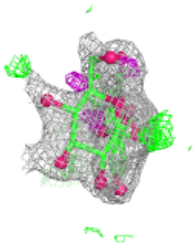


Electron density around LMT m 102:

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

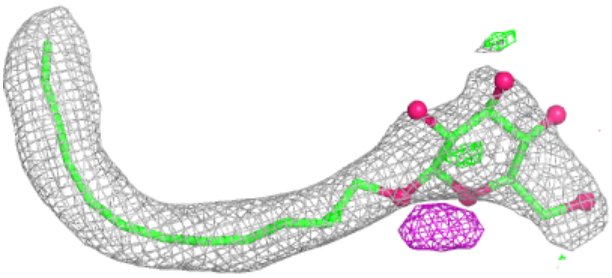


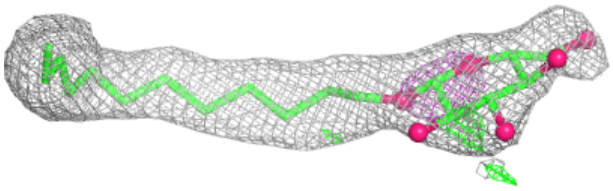


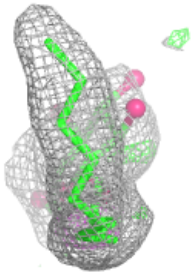


Electron density around LMT B 626:

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

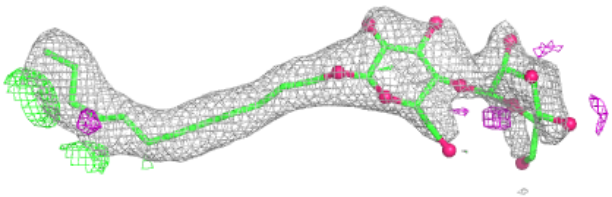


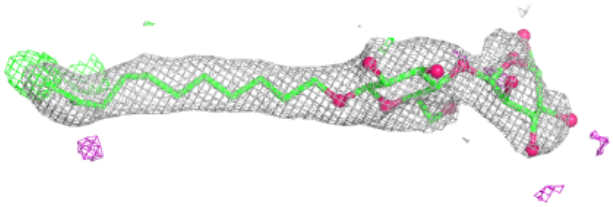


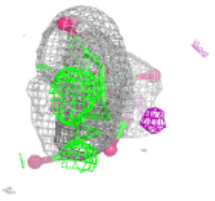


Electron density around LMT t 102:

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

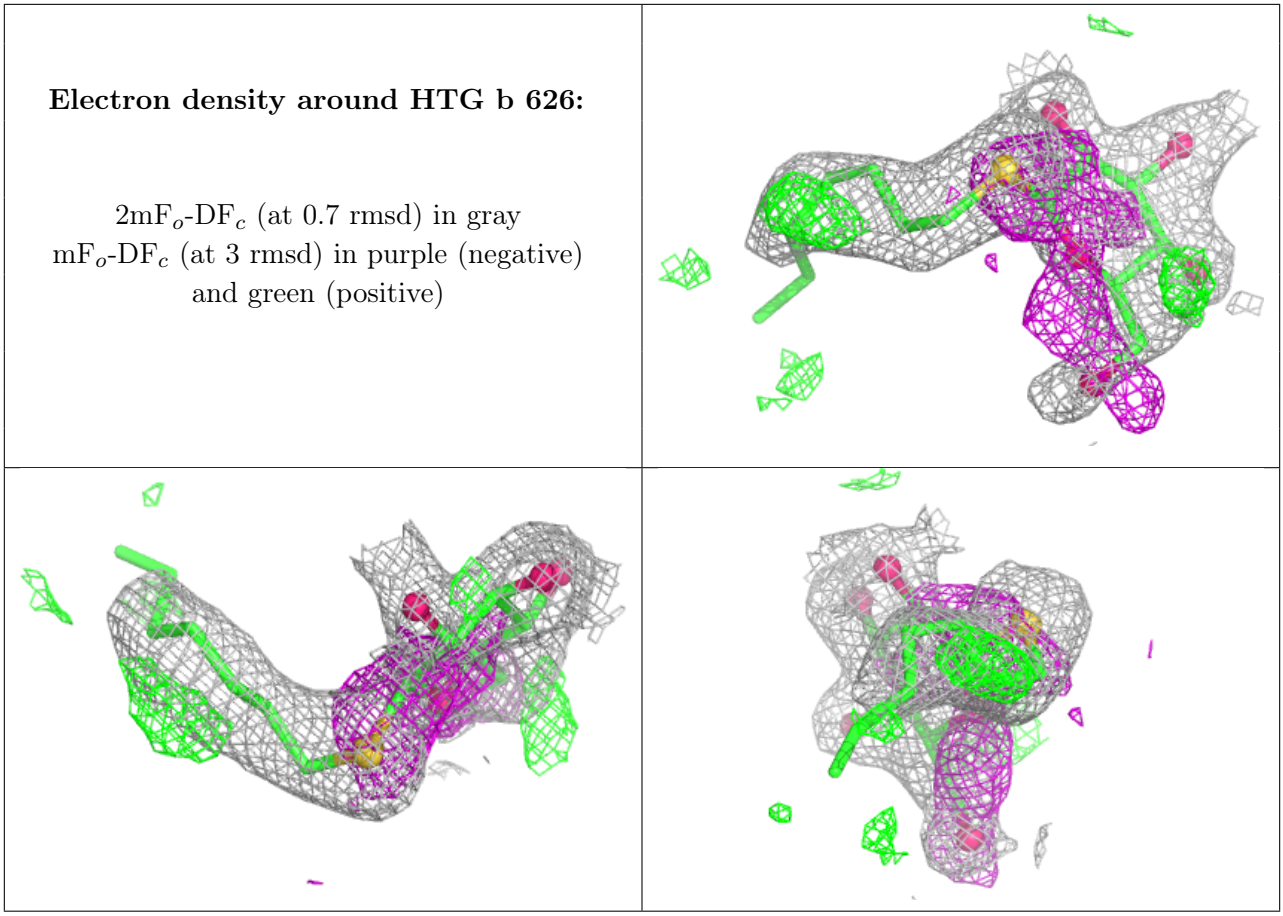






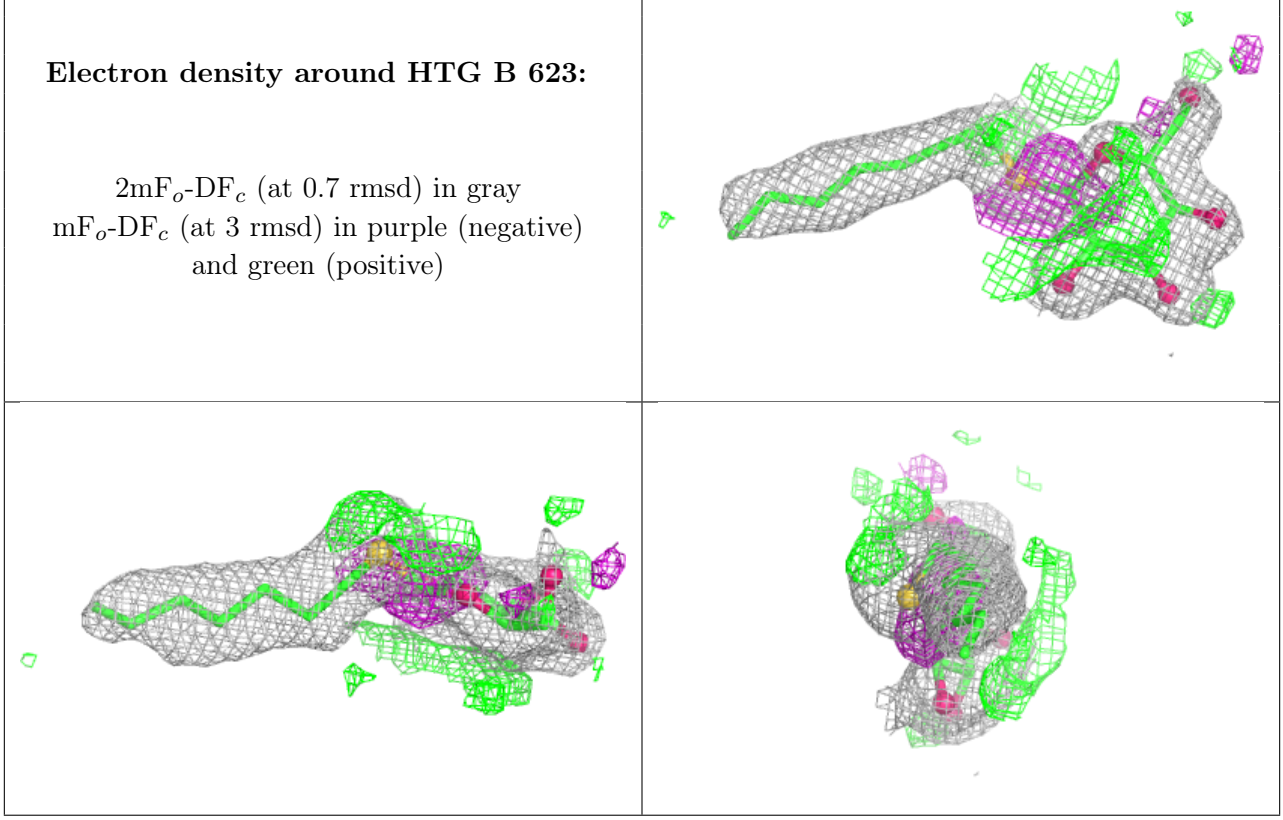
Electron density around HTG b 626:

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



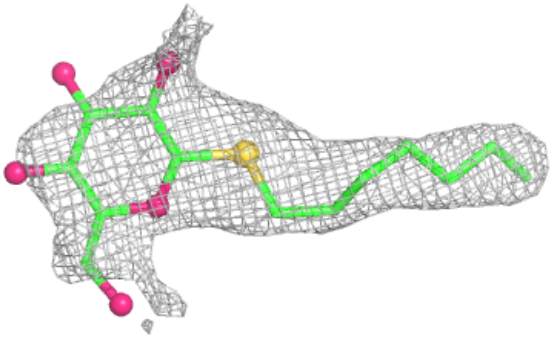
Electron density around HTG B 623:

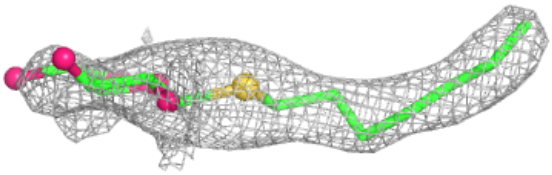
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

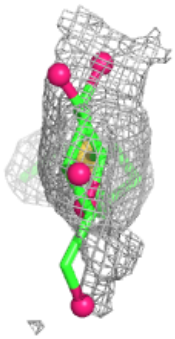


Electron density around HTG C 536:

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

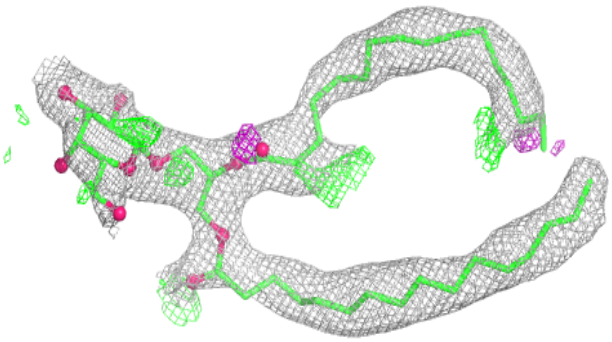


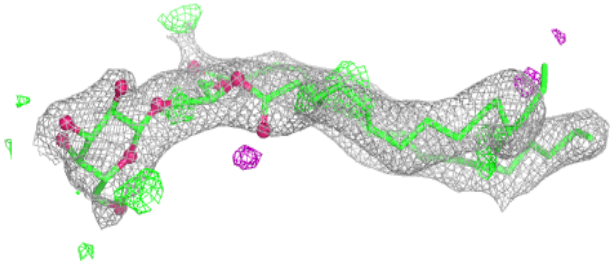


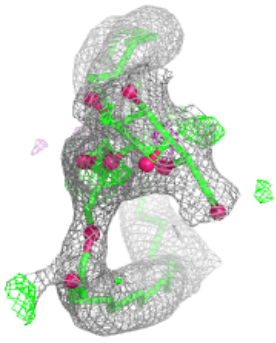


Electron density around LMG A 413:

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

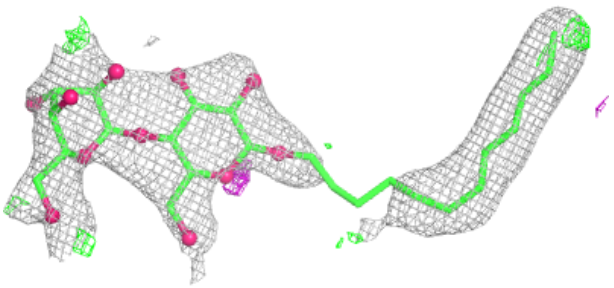


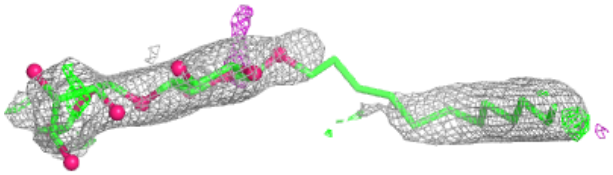


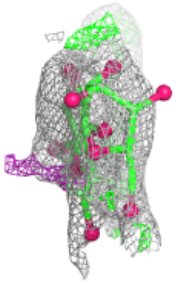


Electron density around LMT Z 101:

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

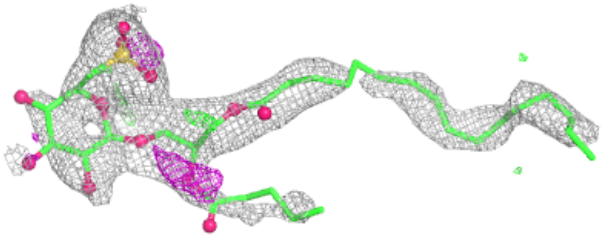


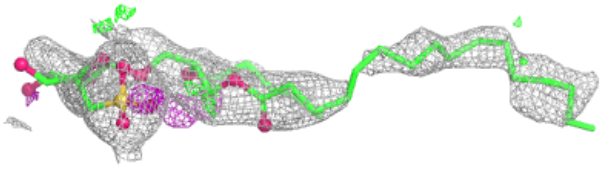


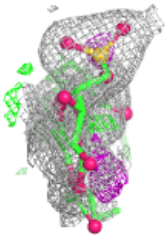


Electron density around SQD f 102:

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

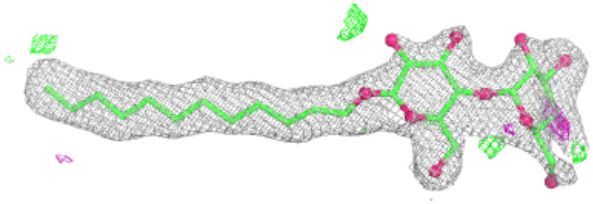


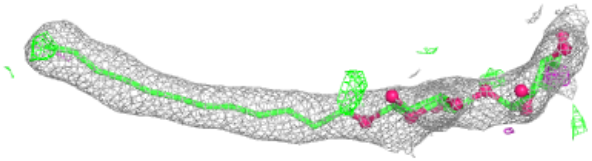


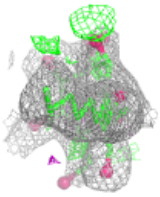


Electron density around LMT M 101:

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

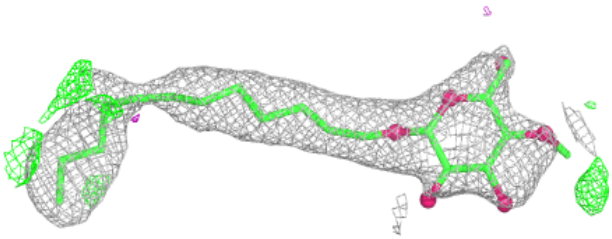


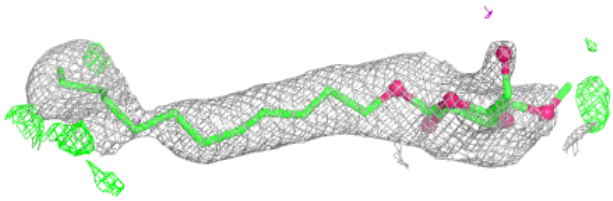


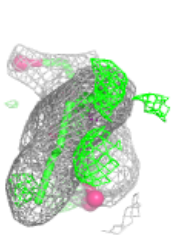


Electron density around LMT M 102:

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

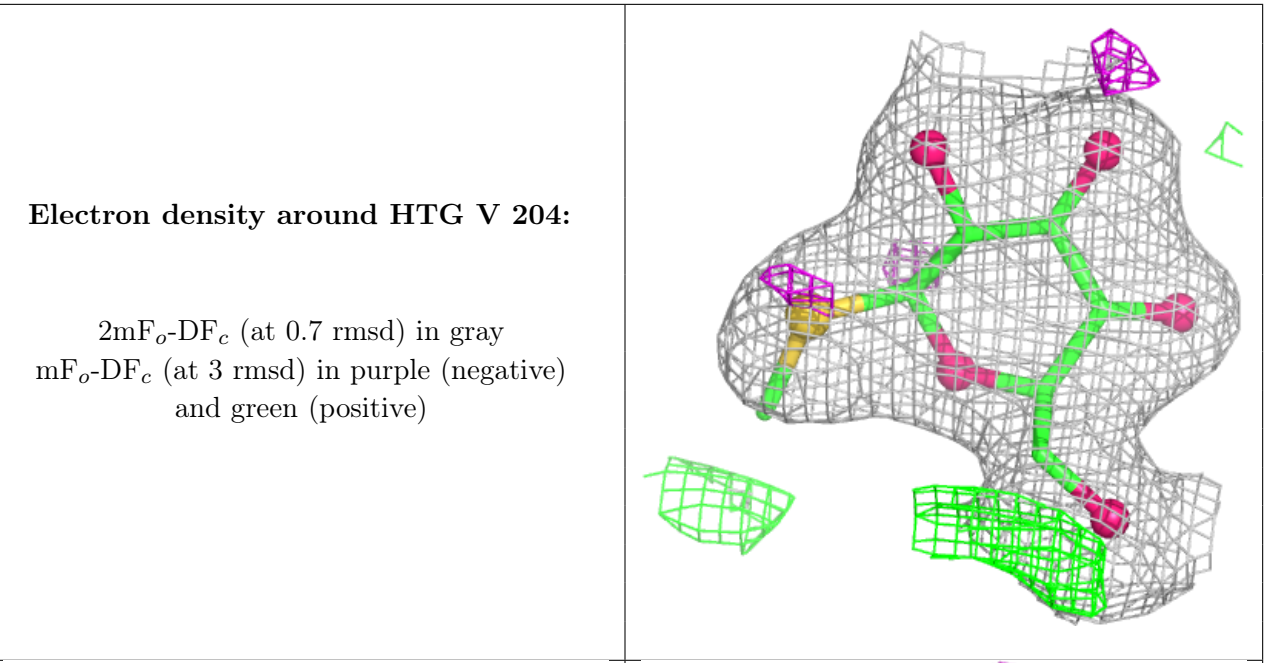


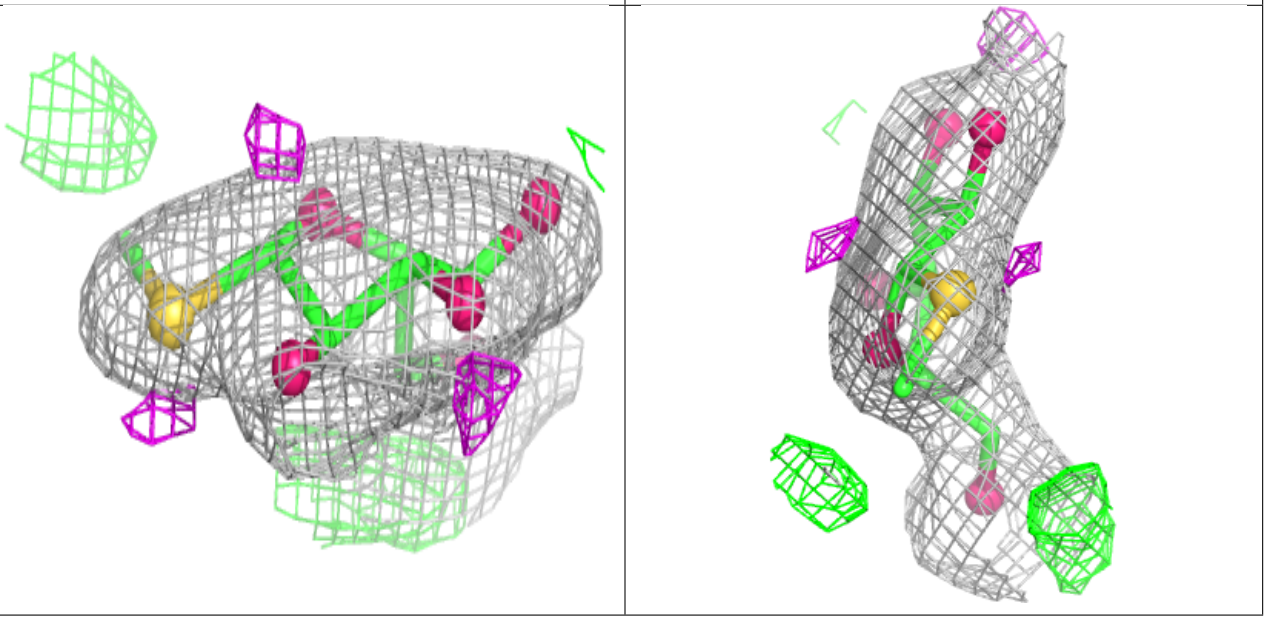




Electron density around HTG V 204:

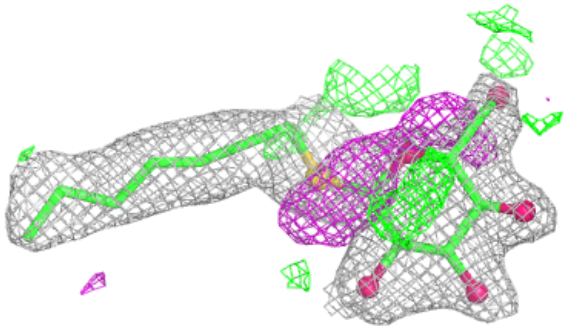
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

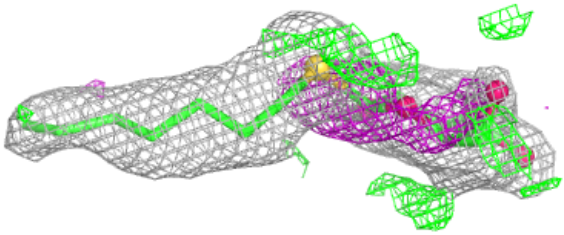


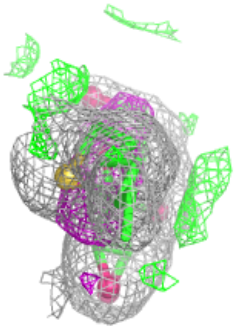


Electron density around HTG O 303:

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

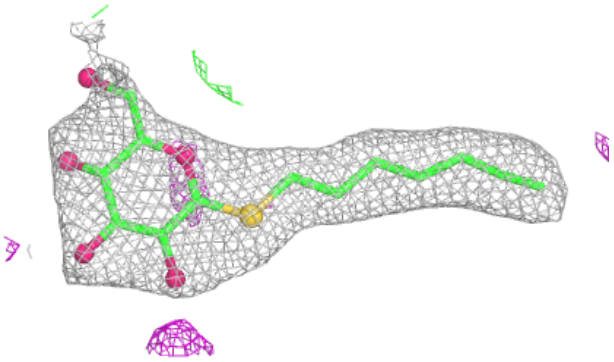


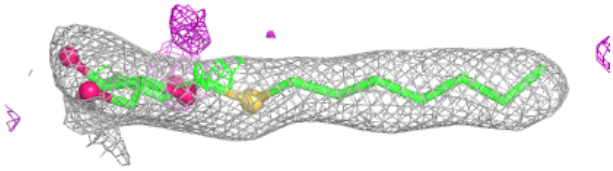


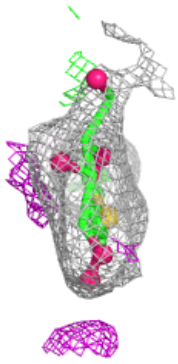


Electron density around HTG B 629:

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

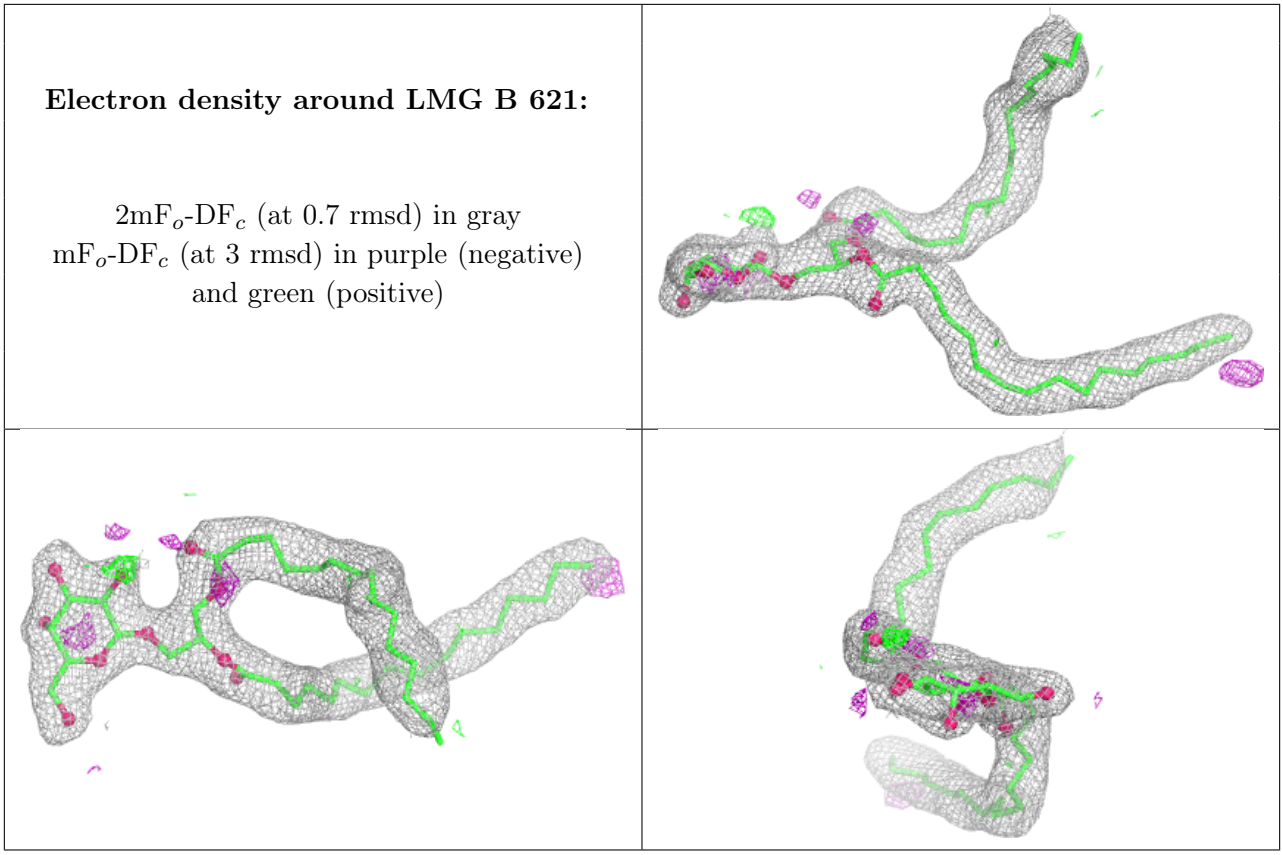






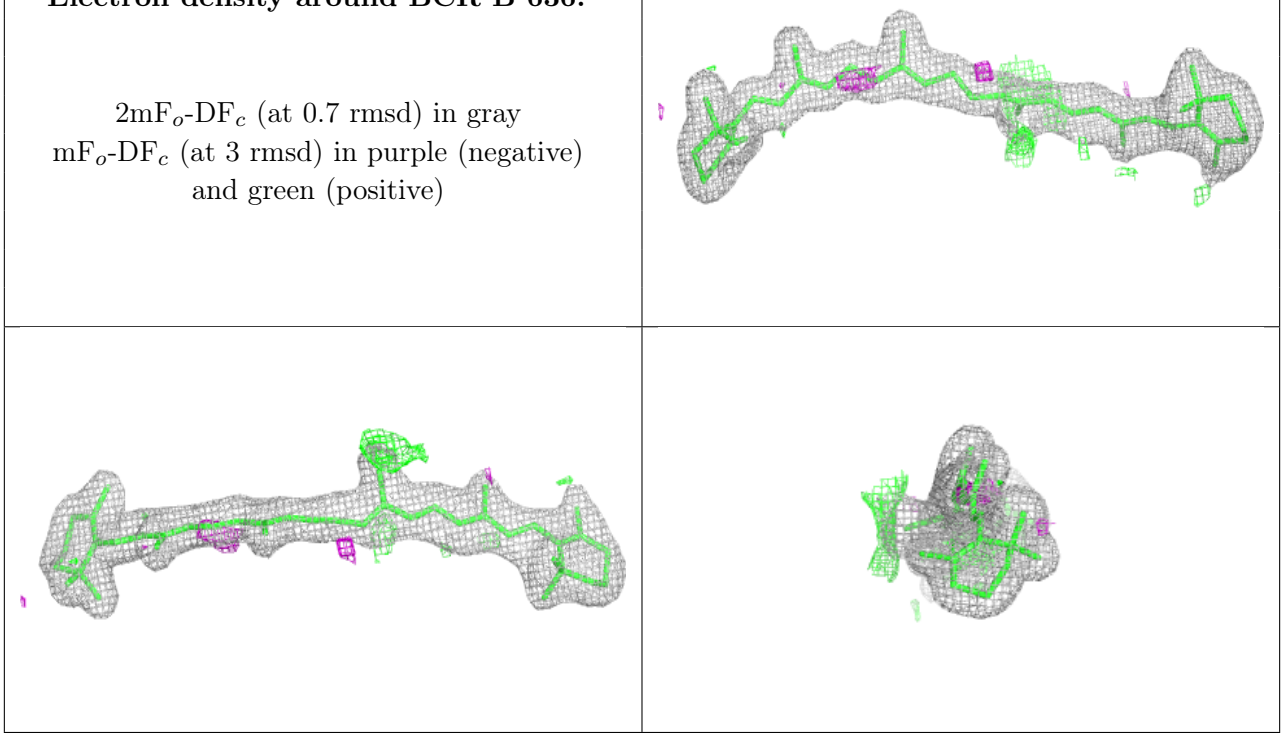
Electron density around LMG B 621:

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



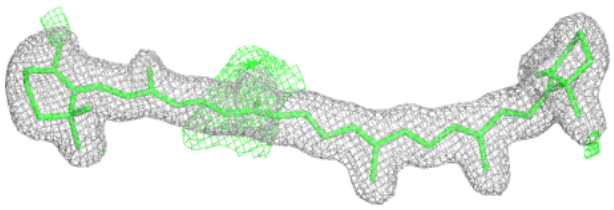
Electron density around BCR B 636:

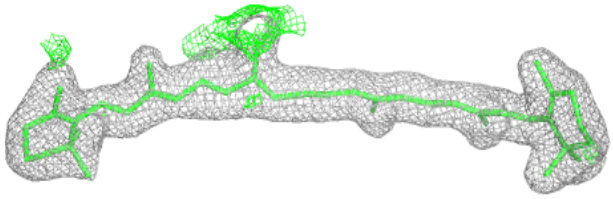
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

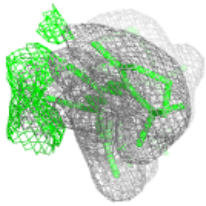


Electron density around BCR T 101:

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

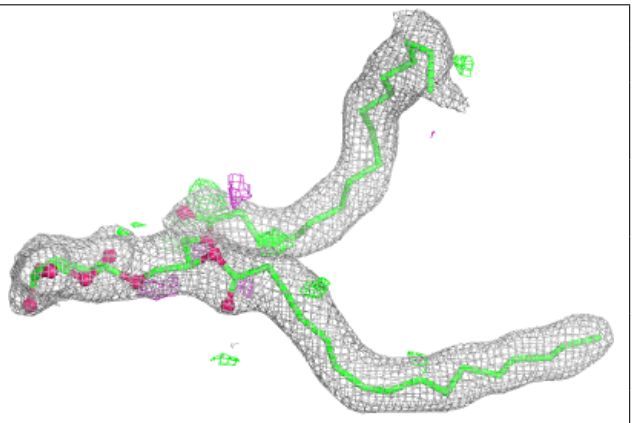


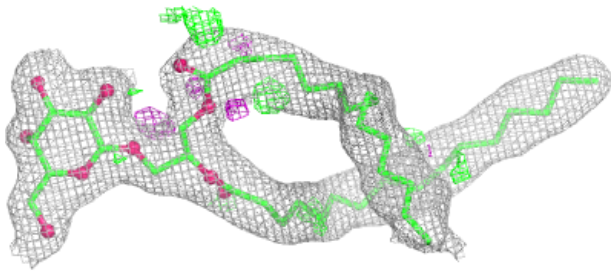


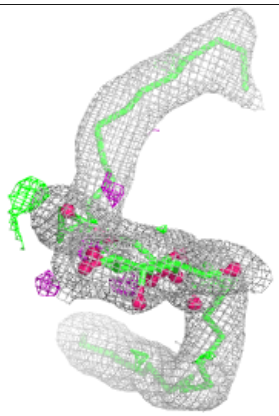


Electron density around LMG b 624:

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

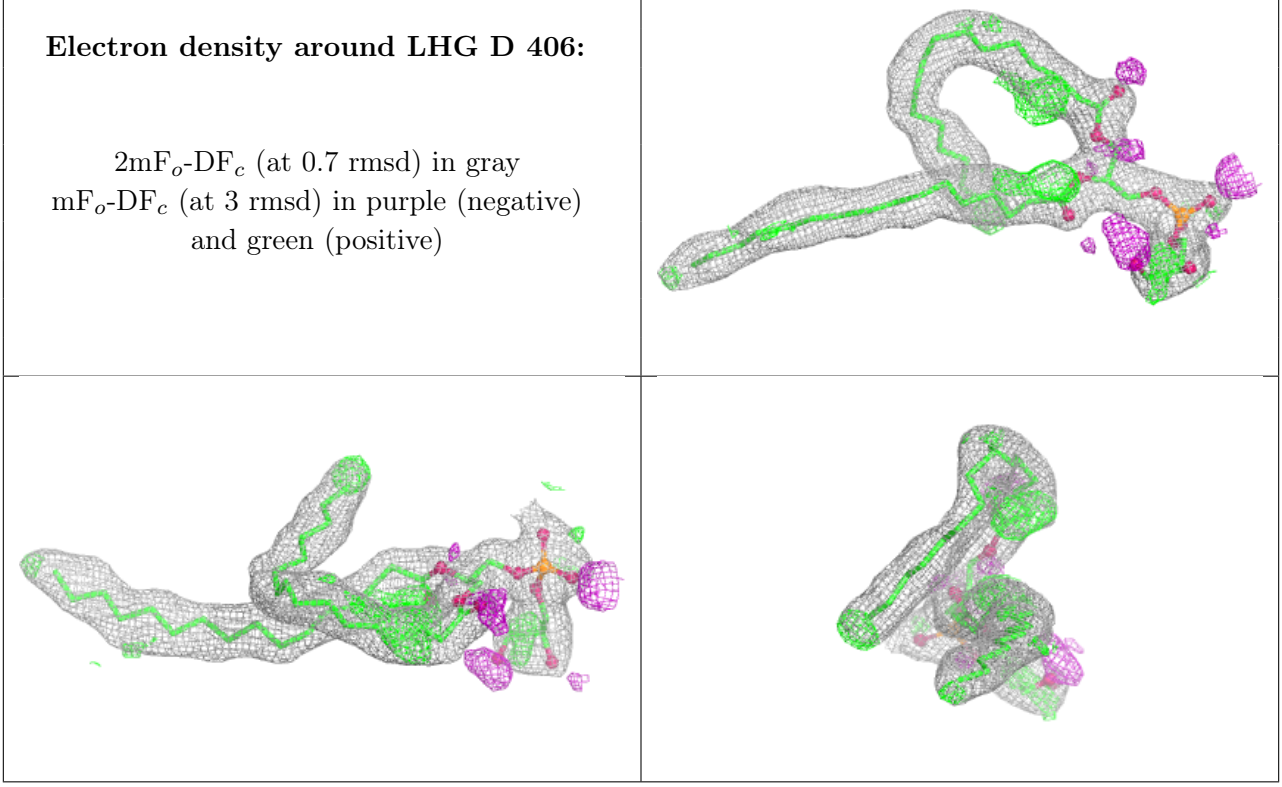






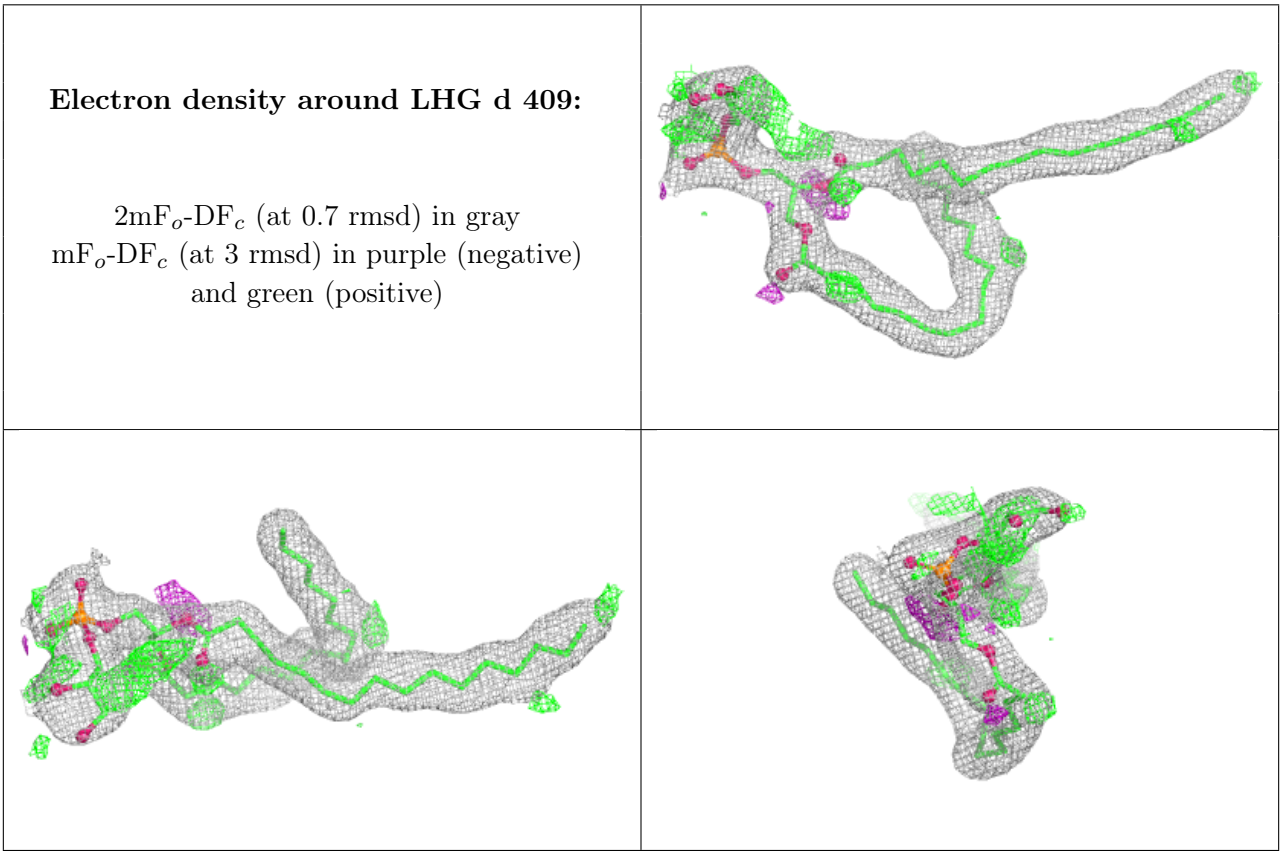
Electron density around LHG D 406:

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



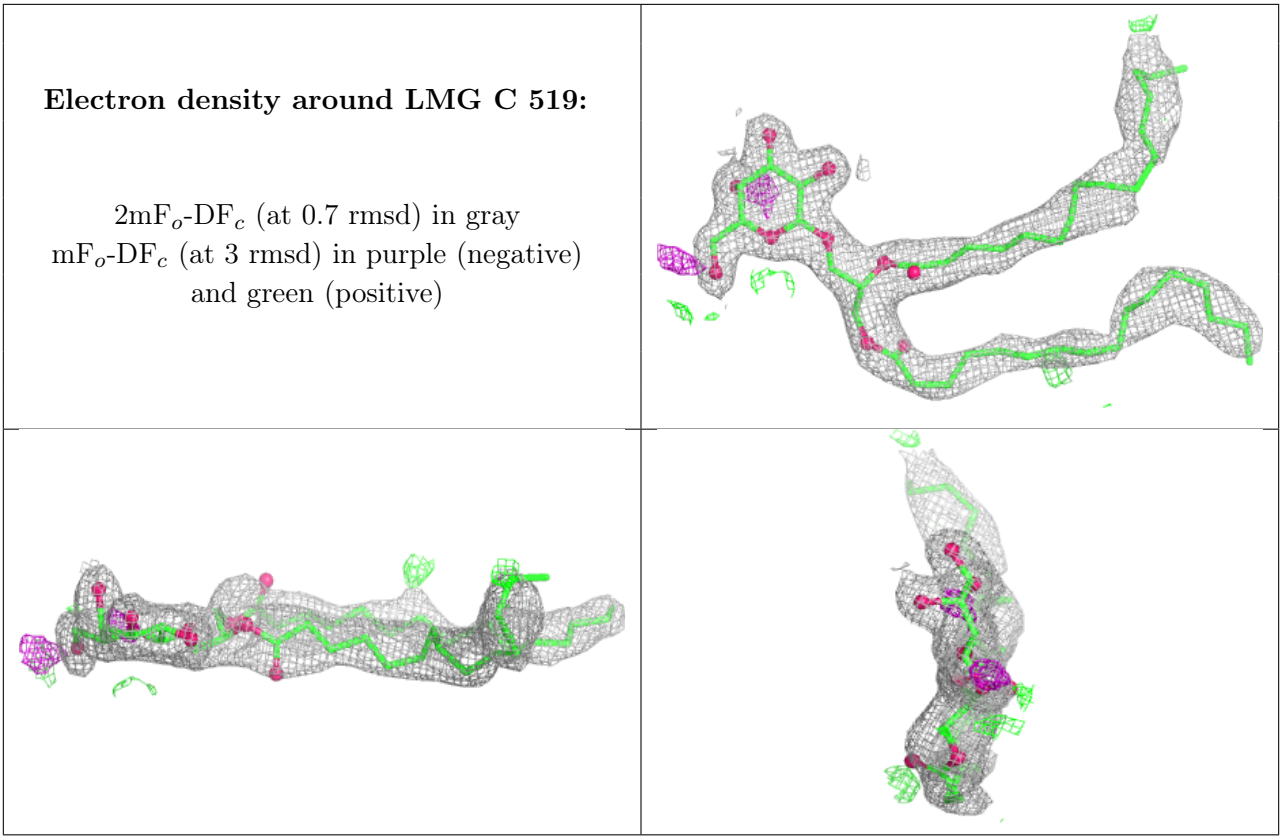
Electron density around LHG d 409:

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



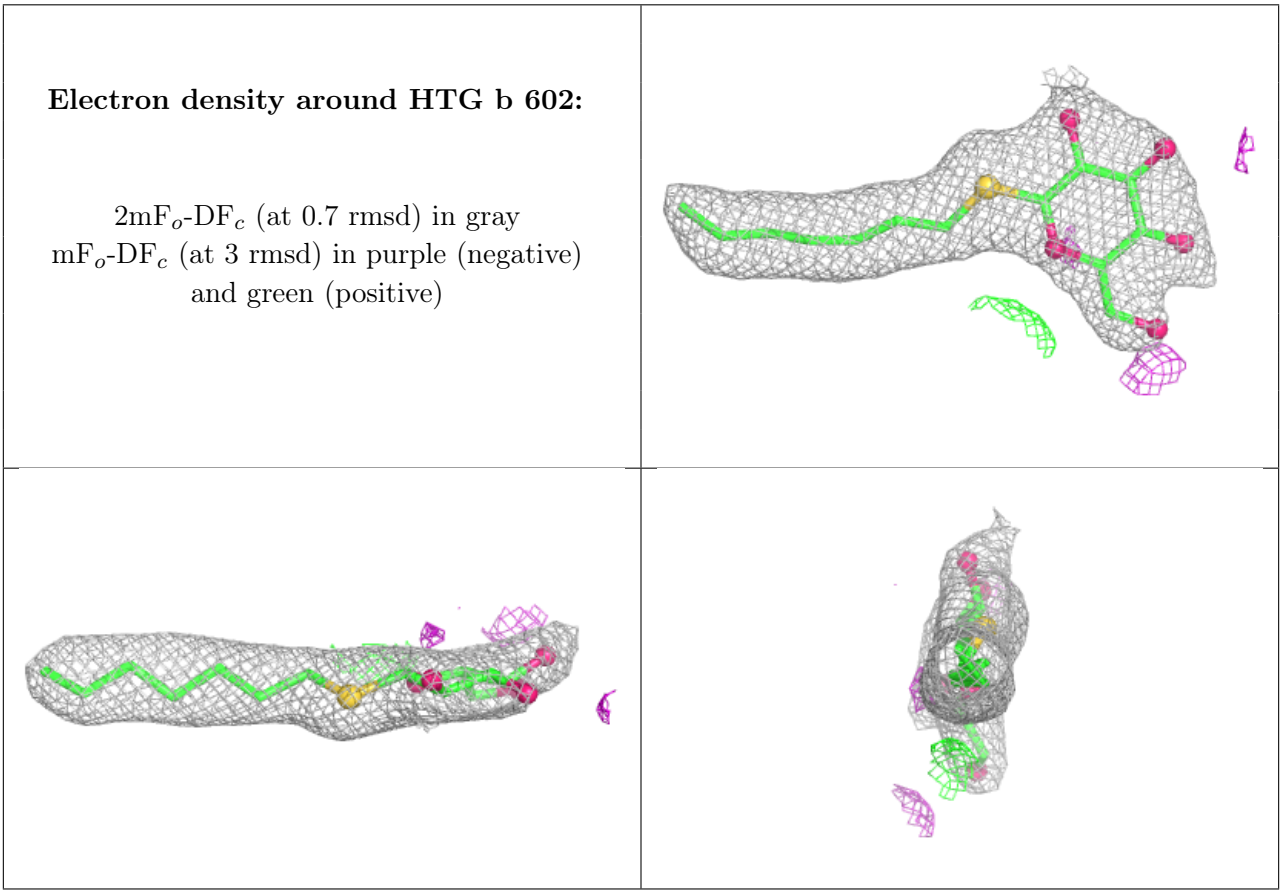
Electron density around LMG C 519:

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



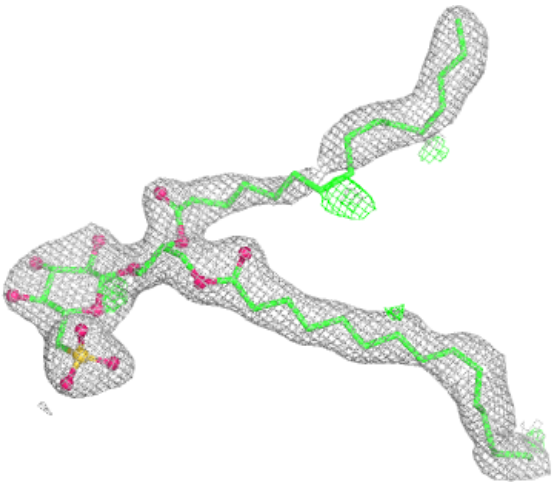
Electron density around HTG b 602:

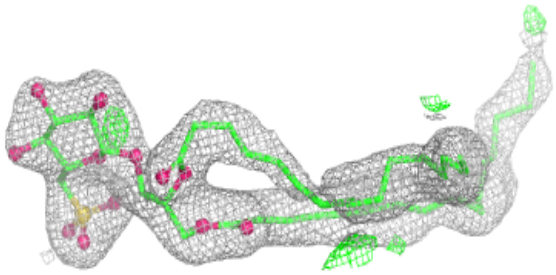
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

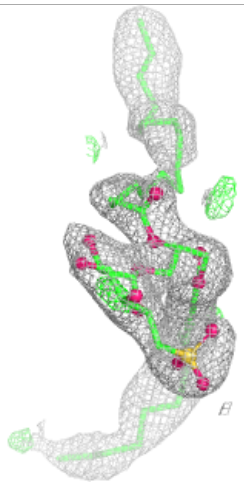


Electron density around SQD a 415:

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

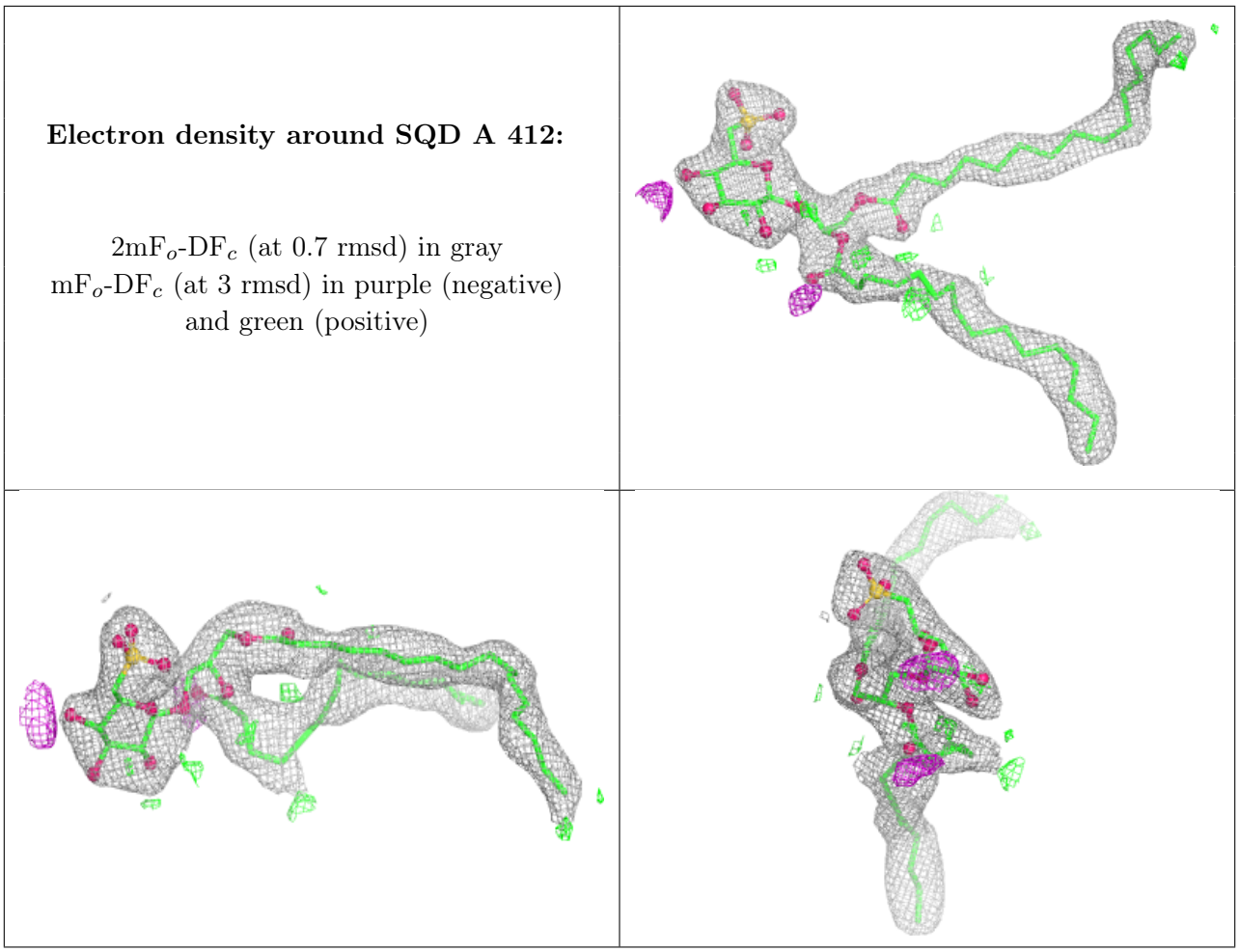






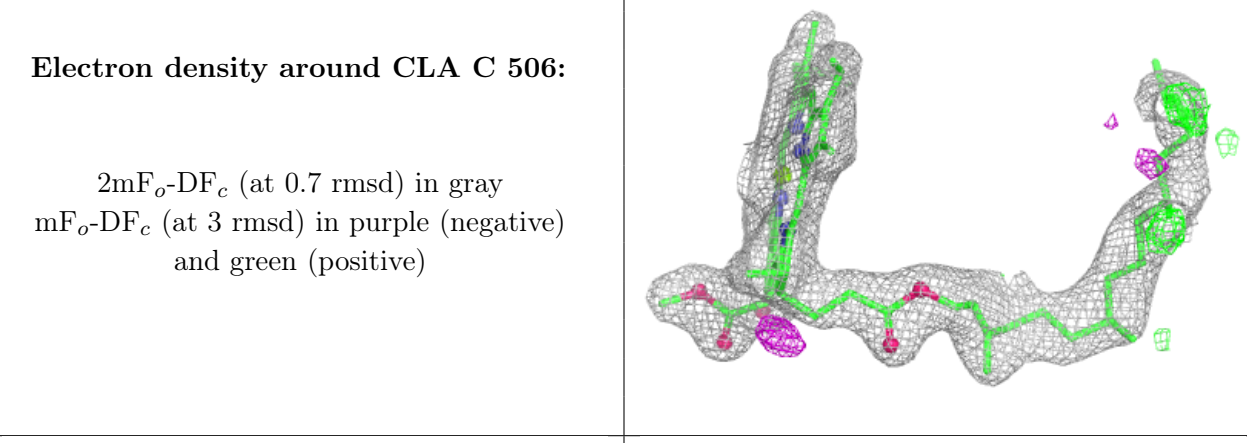
Electron density around SQD A 412:

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



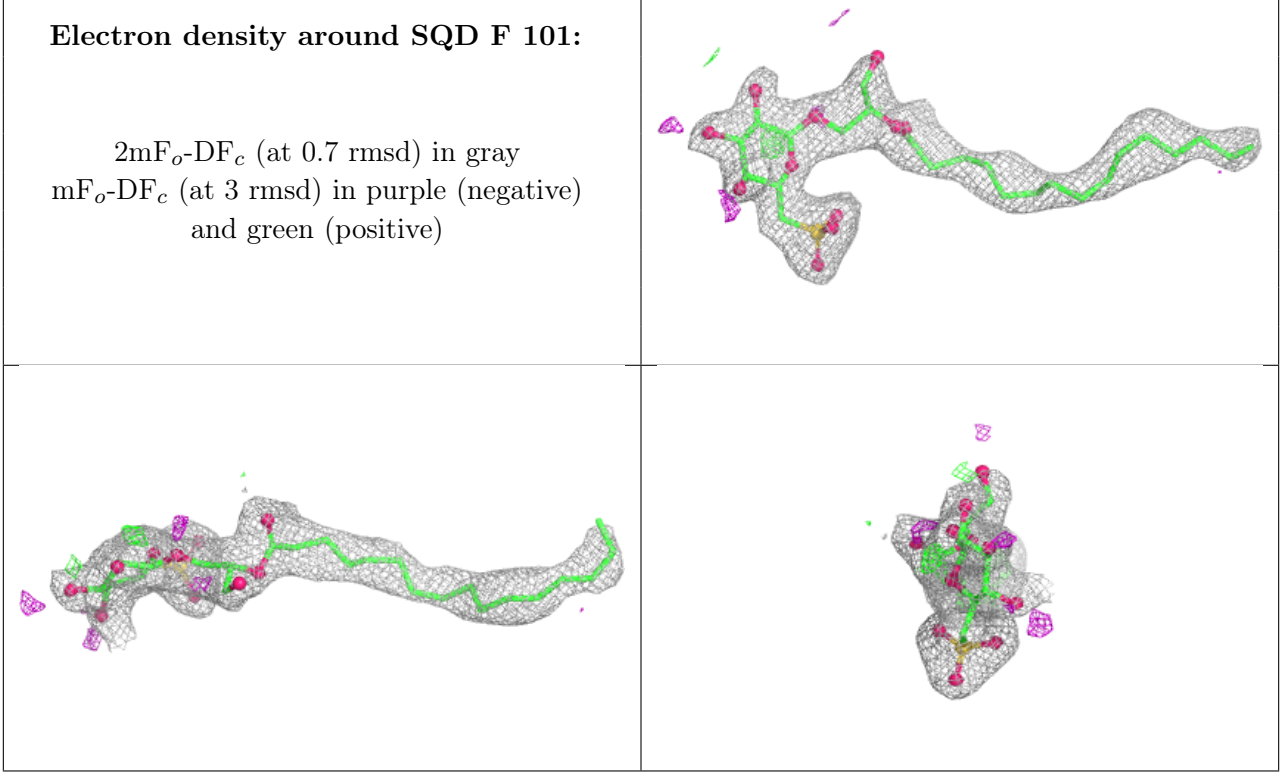
Electron density around CLA C 506:

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



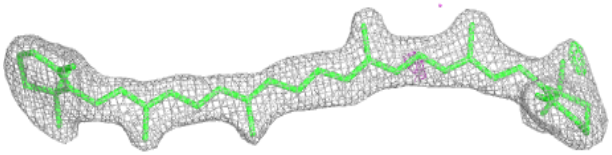
Electron density around SQD F 101:

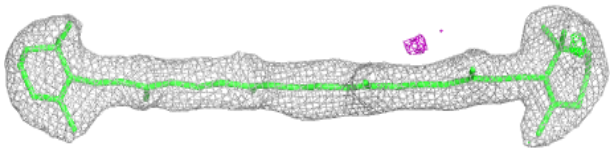
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

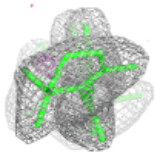


Electron density around BCR c 915:

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

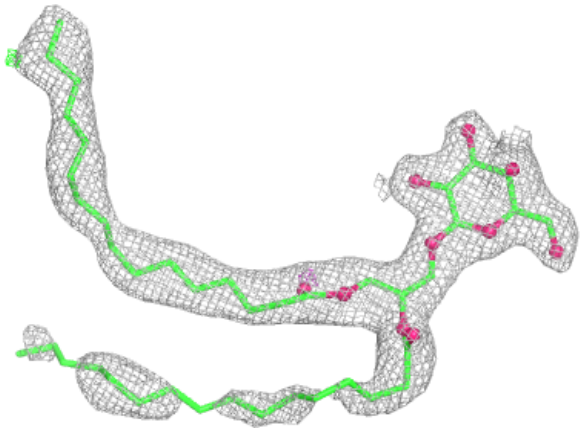


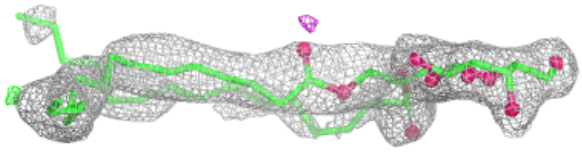


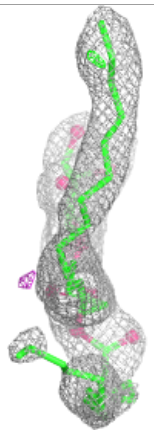


Electron density around LMG c 920:

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

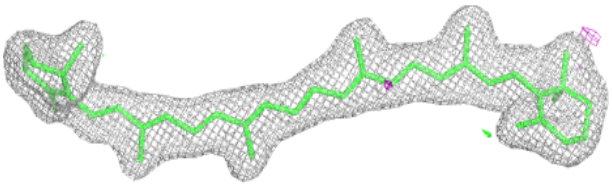


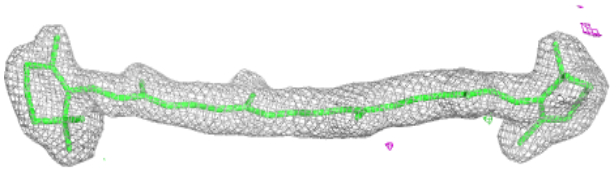


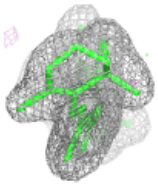


Electron density around BCR Y 101:

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

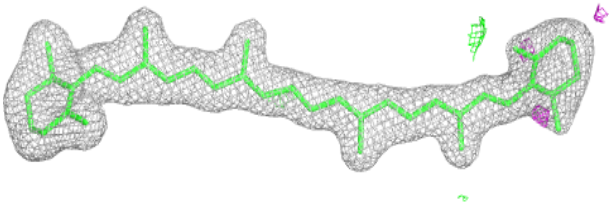


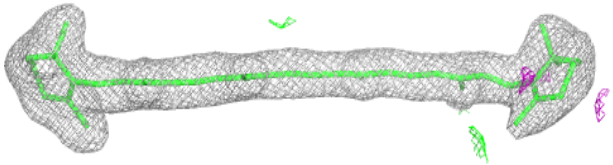


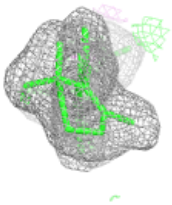


Electron density around BCR b 622:

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

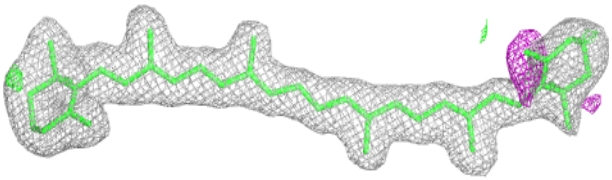


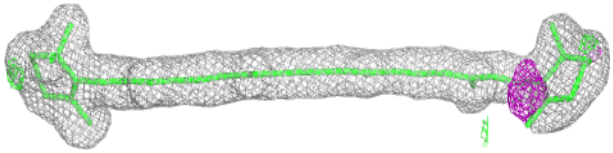


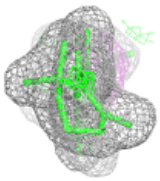


Electron density around BCR B 619:

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

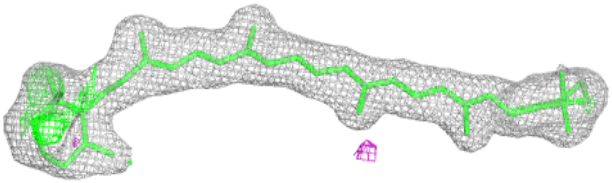


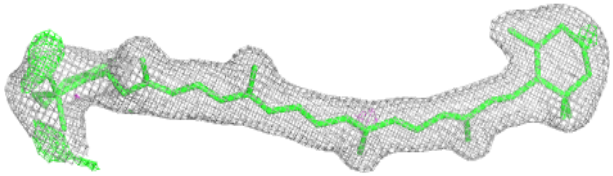


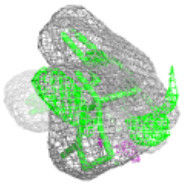


Electron density around BCR d 406:

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

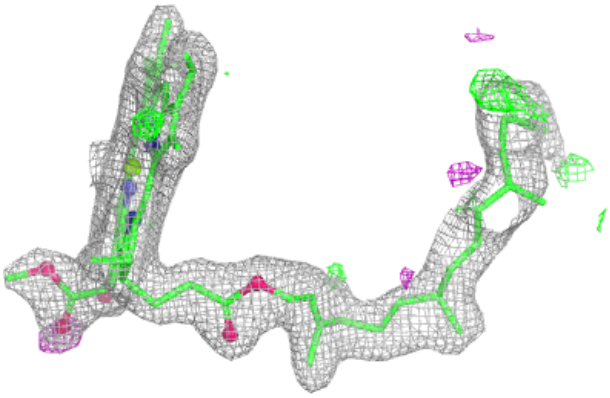


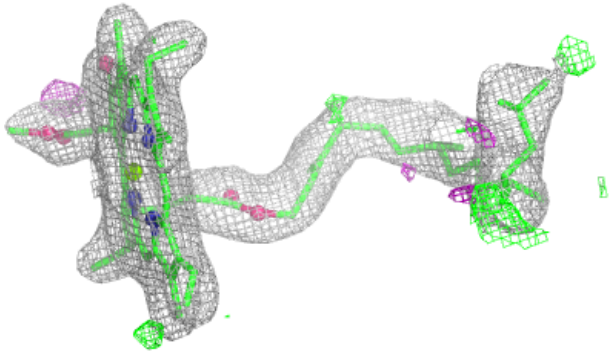


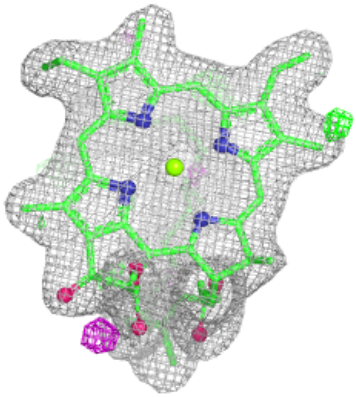


Electron density around CLA c 907:

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

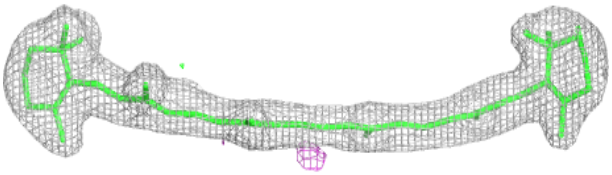


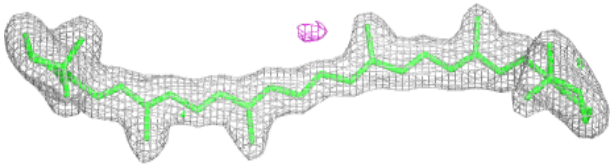


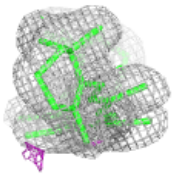


Electron density around BCR K 101:

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

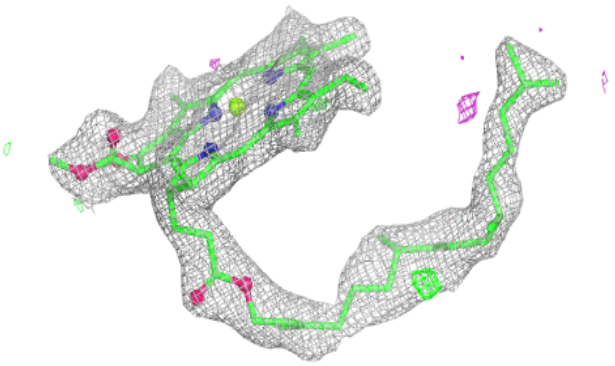


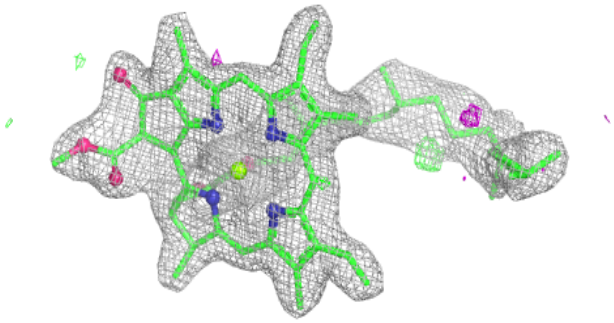


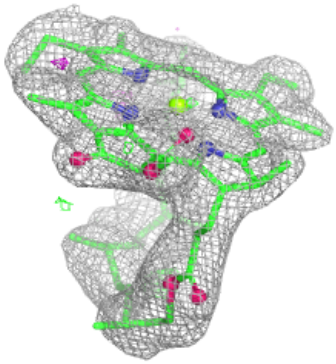


Electron density around CLA c 914:

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

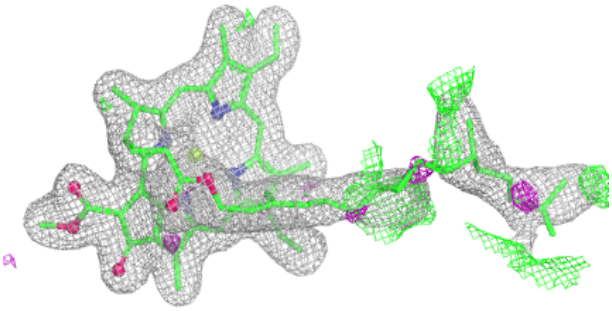


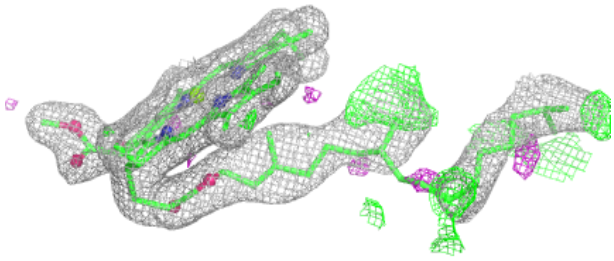


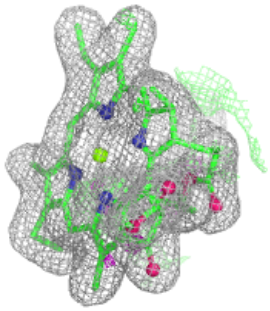


Electron density around CLA b 618:

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

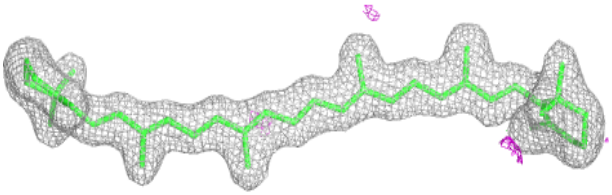


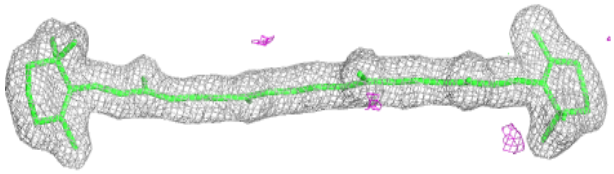


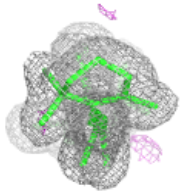


Electron density around BCR a 414:

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

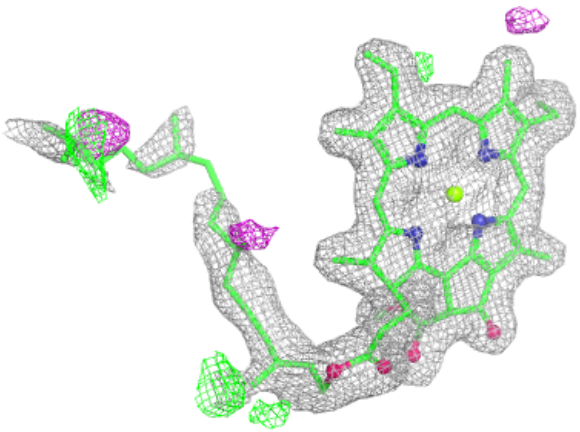


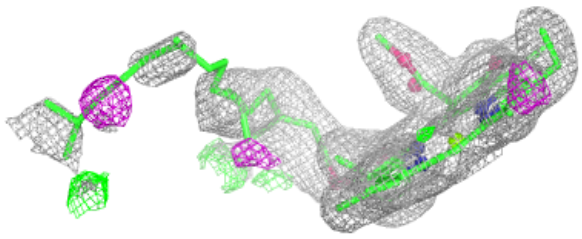


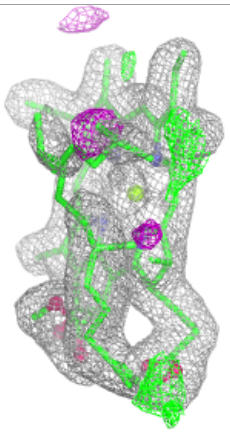


Electron density around CLA B 617:

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

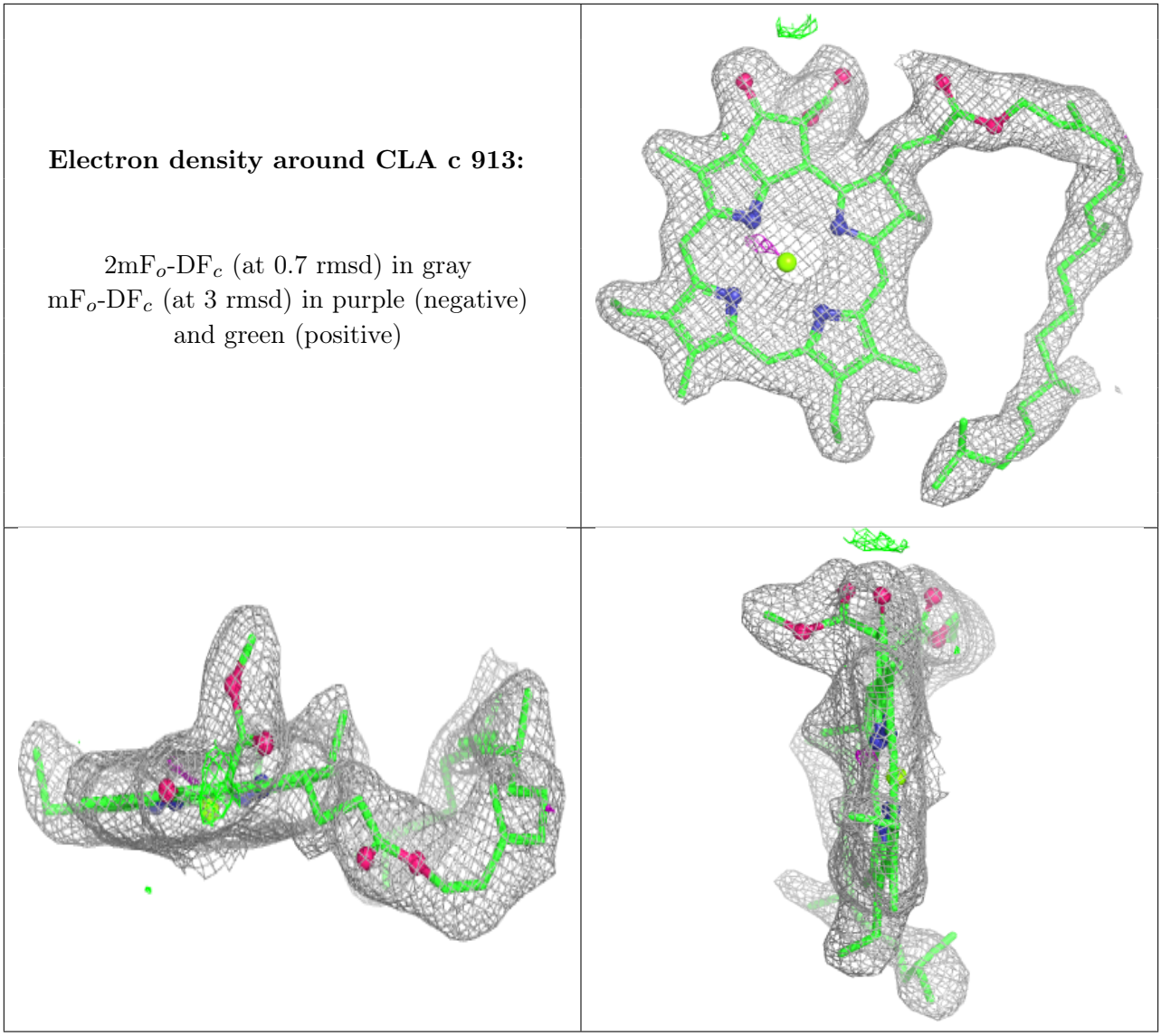






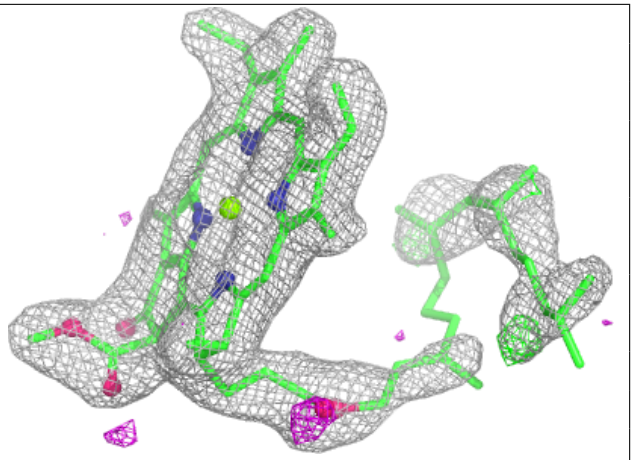
Electron density around CLA c 913:

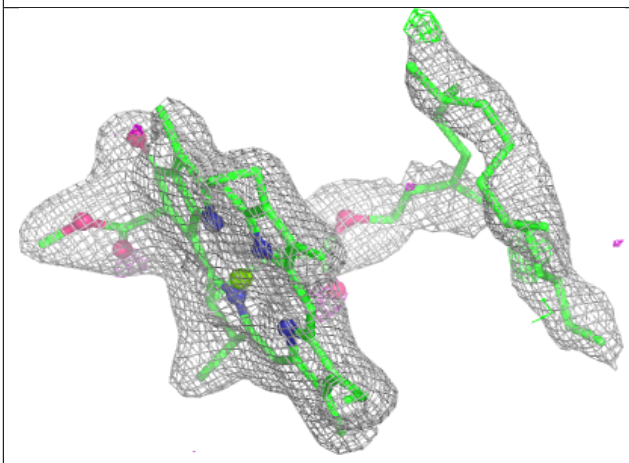
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

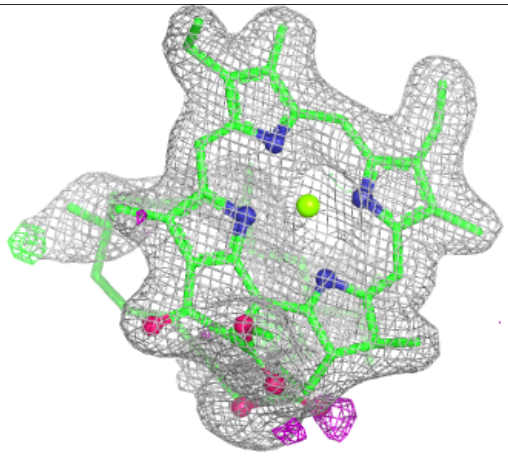


Electron density around CLA B 602:

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

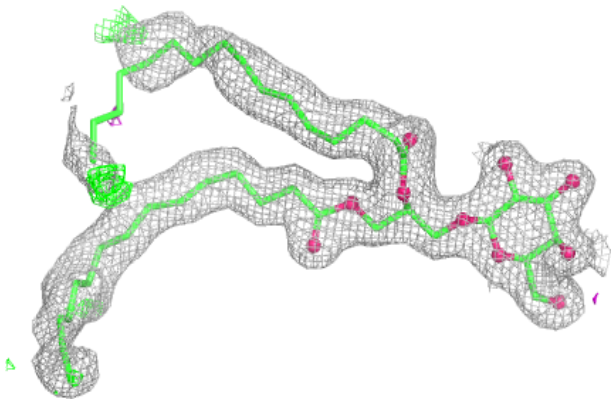


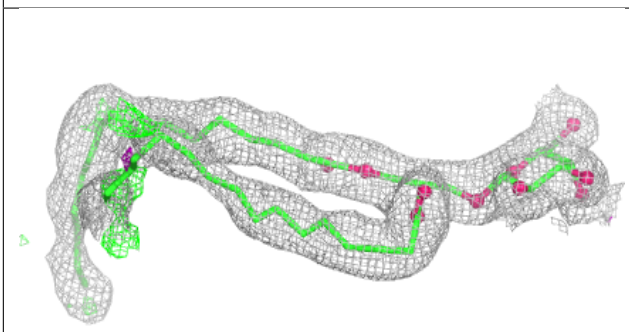


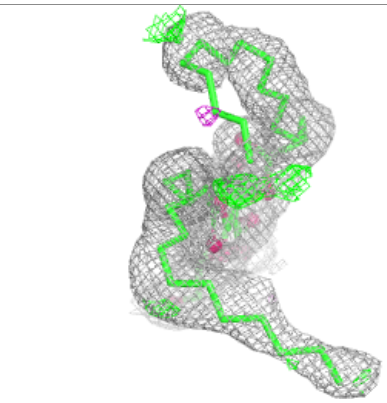


Electron density around LMG D 409:

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

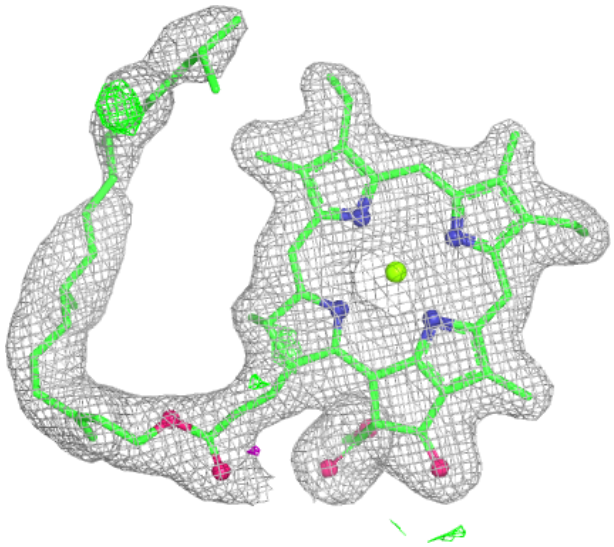


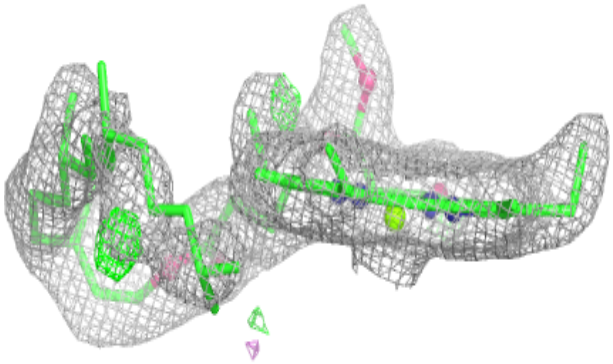


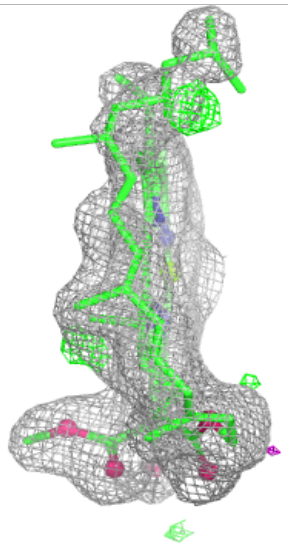


Electron density around CLA C 512:

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

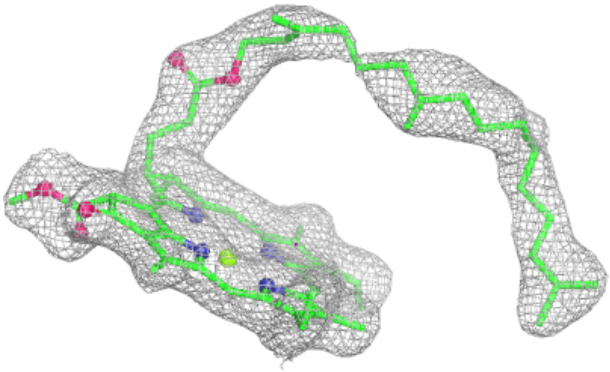


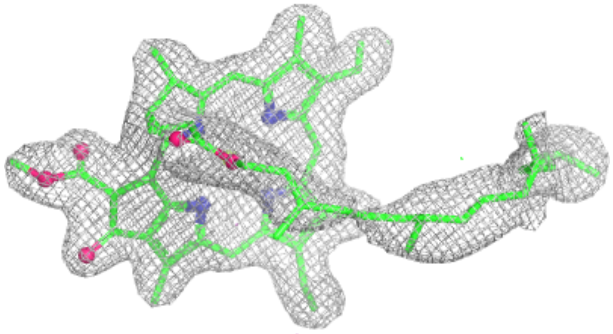


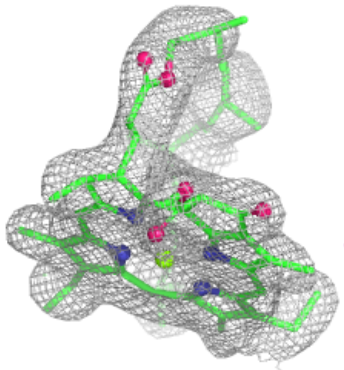


Electron density around CLA C 513:

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

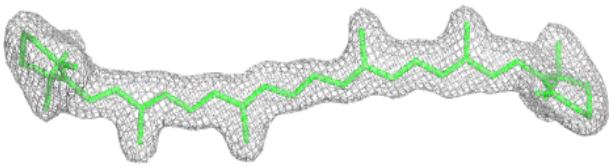


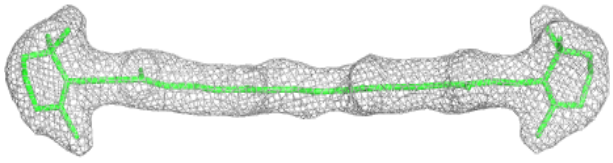


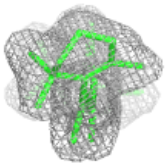


Electron density around BCR C 514:

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

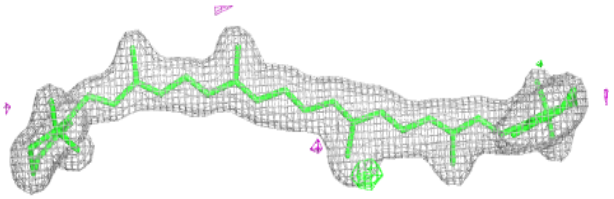


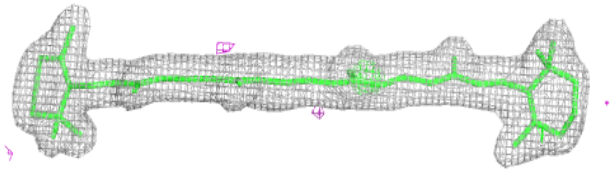


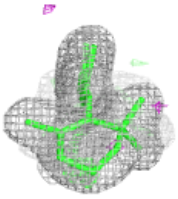


Electron density around BCR C 515:

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

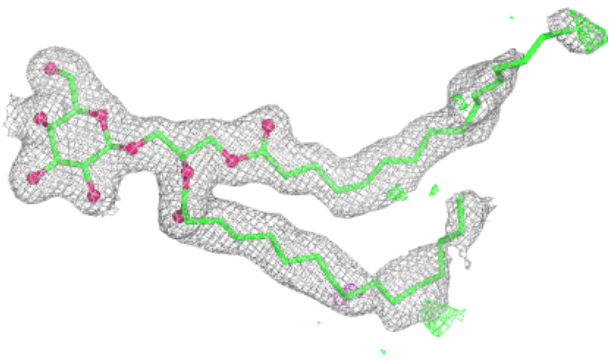


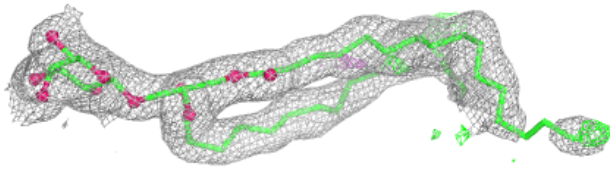


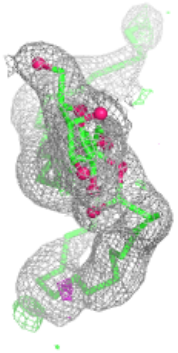


Electron density around LMG d 412:

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

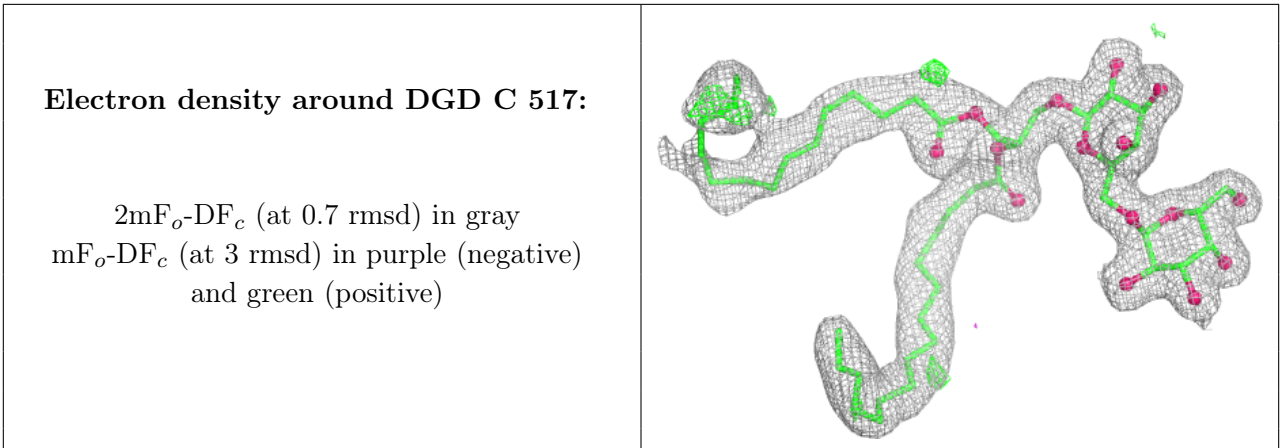






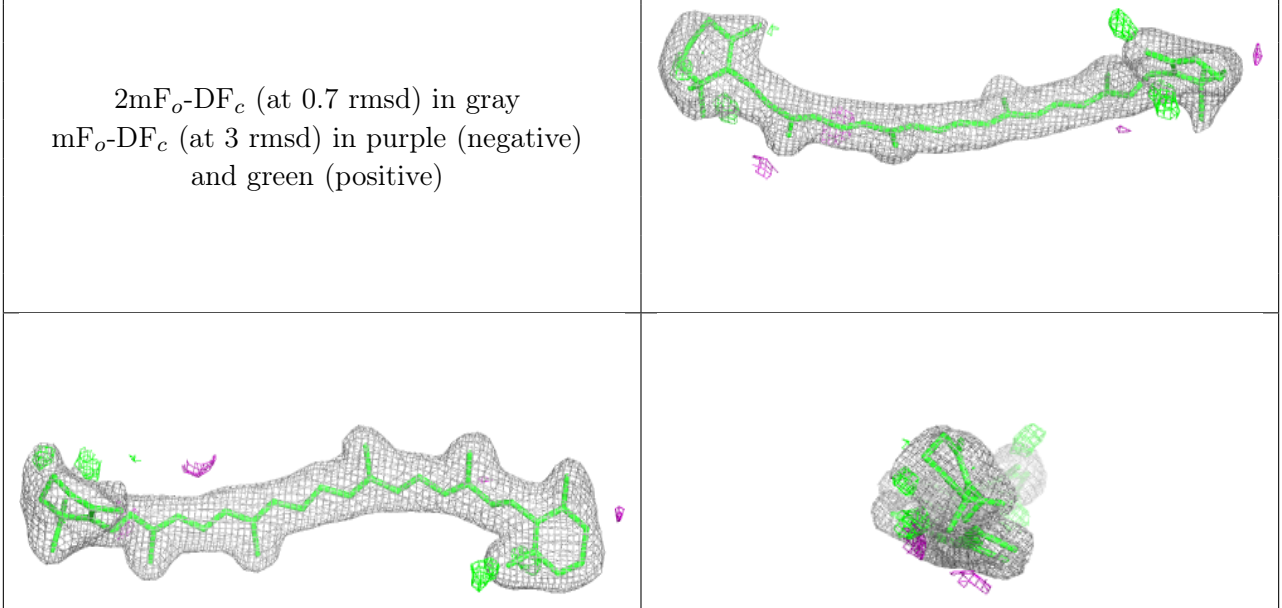
Electron density around DGD C 517:

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



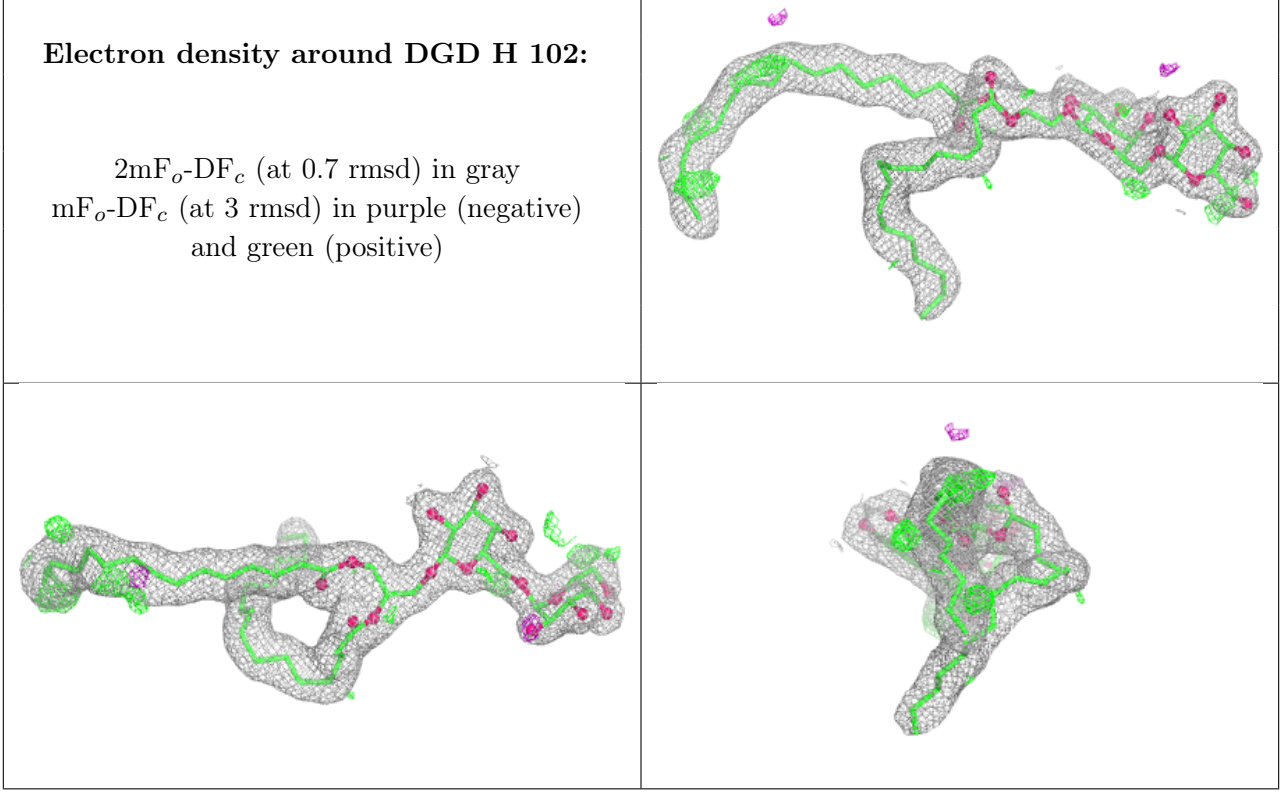
Electron density around BCR D 403:

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



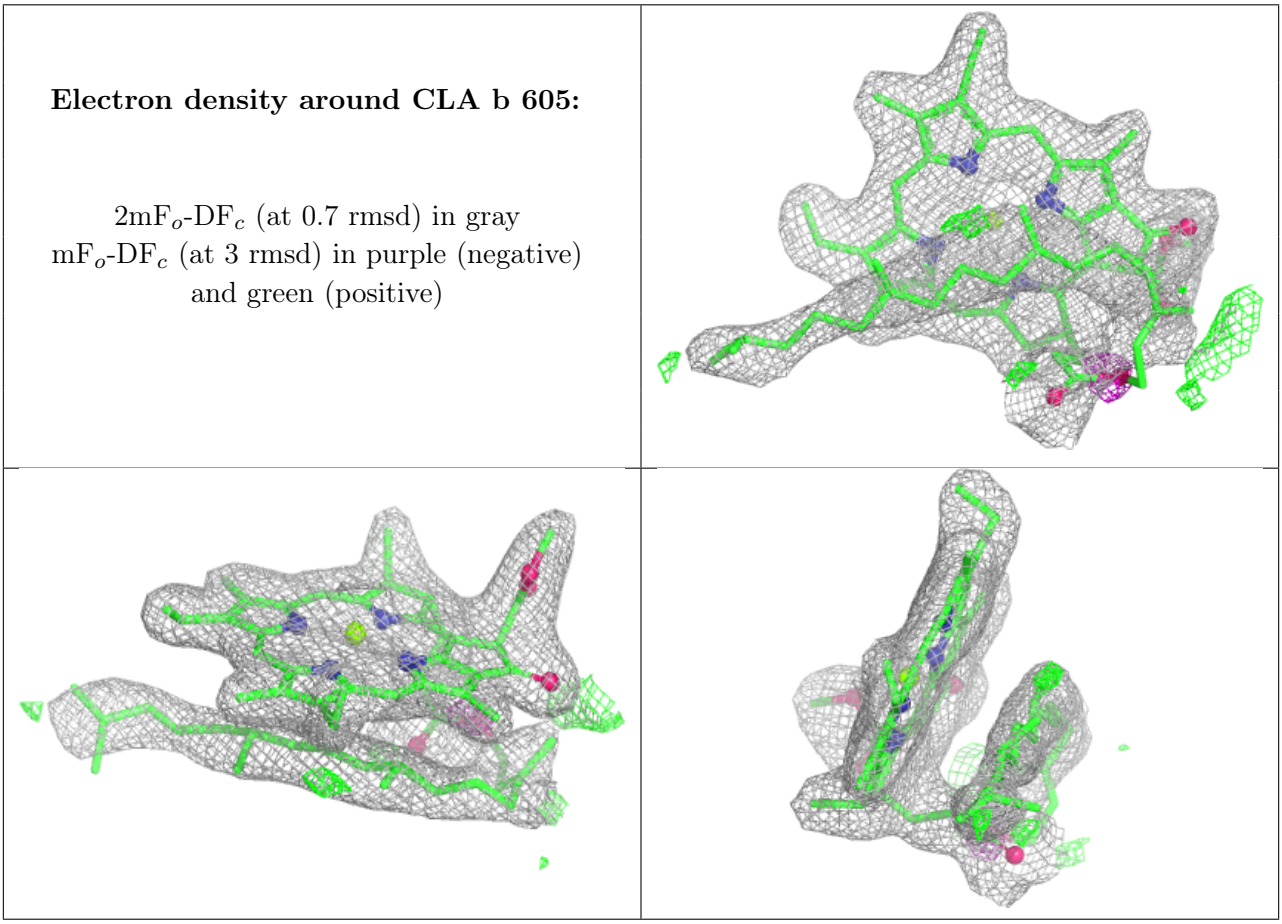
Electron density around DGD H 102:

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



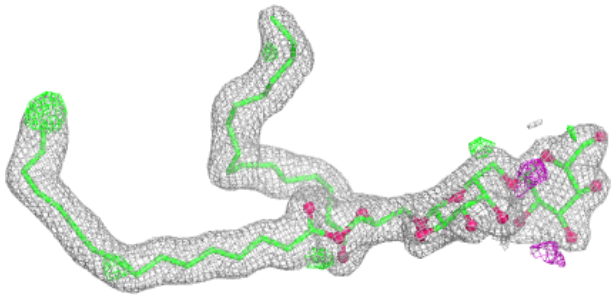
Electron density around CLA b 605:

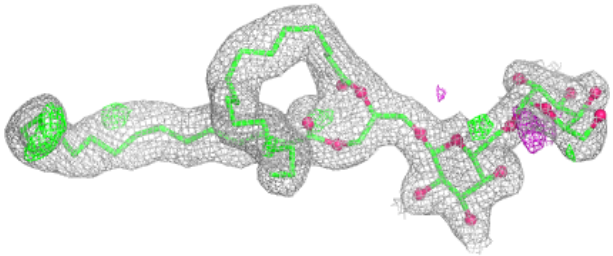
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD 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)

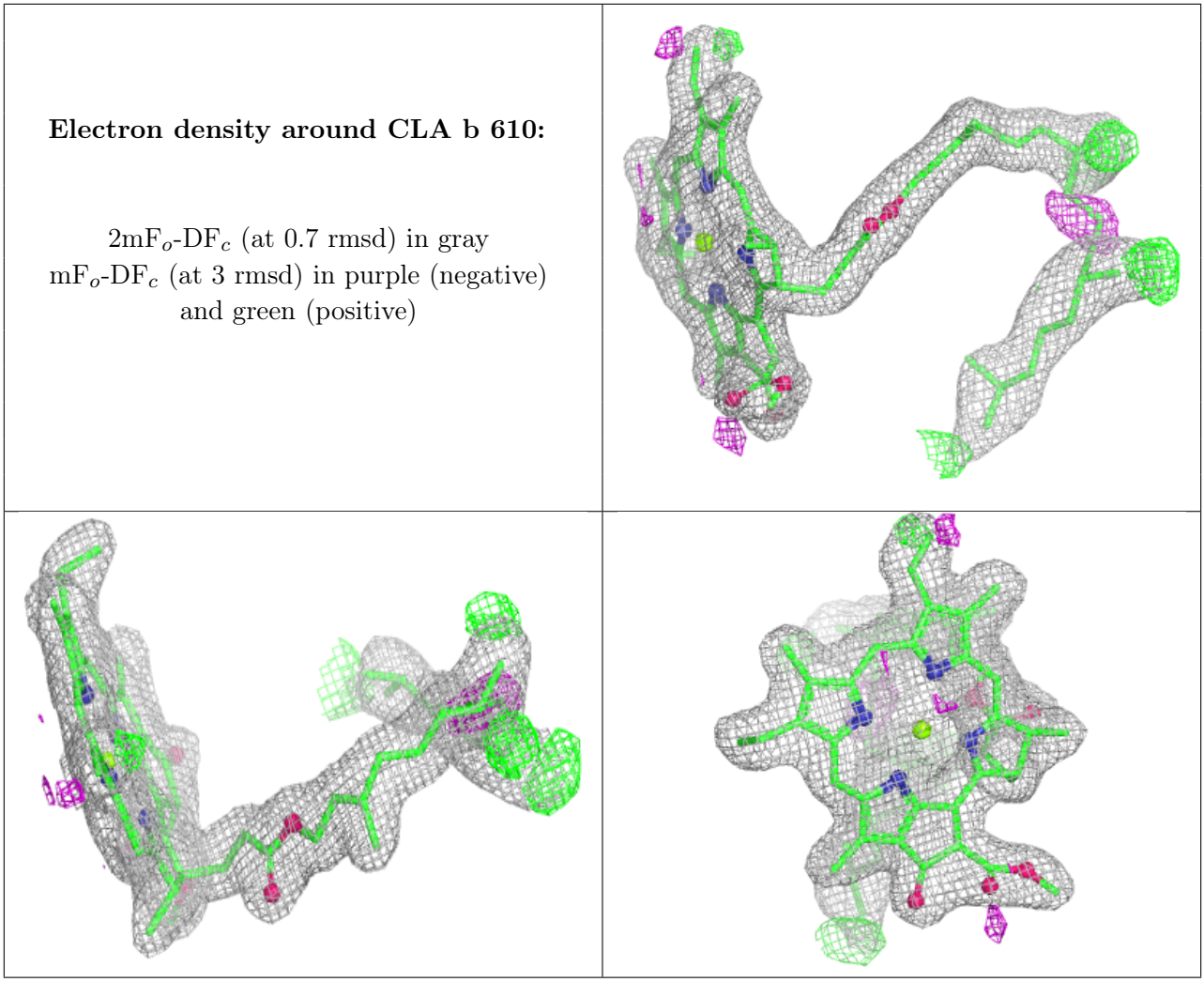






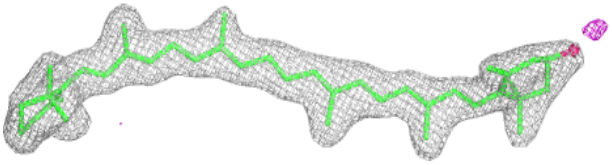
Electron density around CLA b 610:

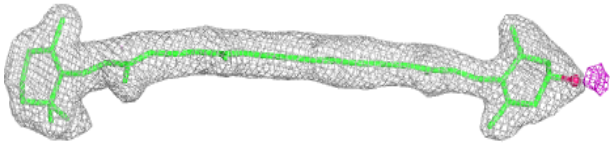
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

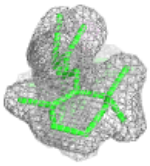


Electron density around RRX h 101:

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

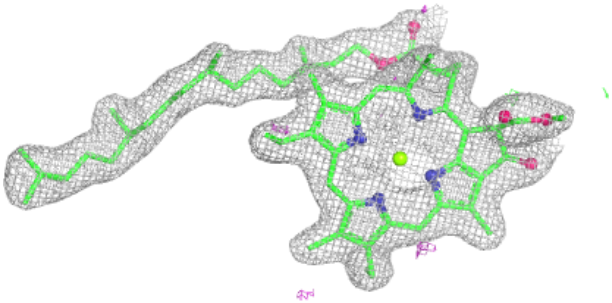


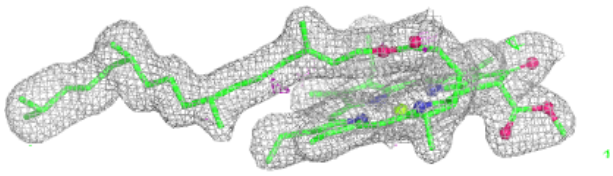


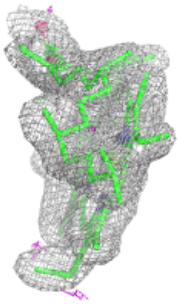


Electron density around CLA c 902:

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

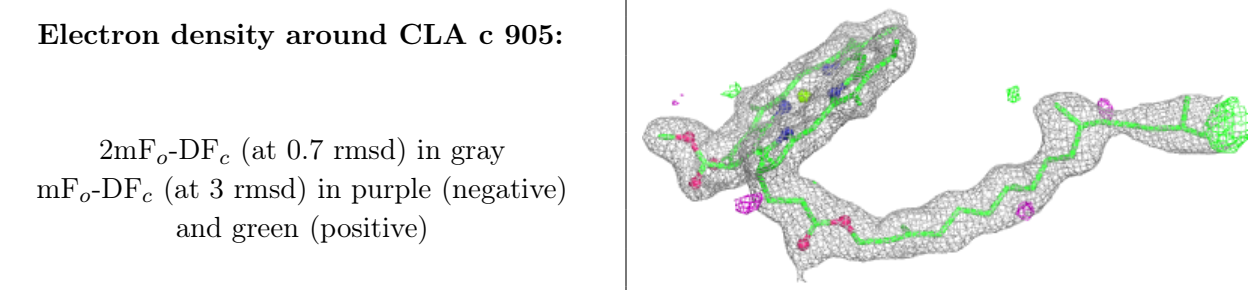


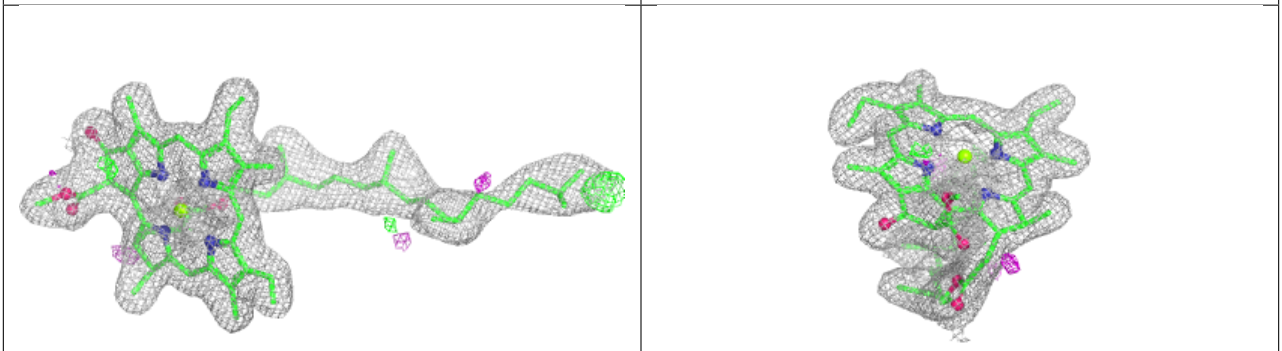




Electron density around CLA c 905:

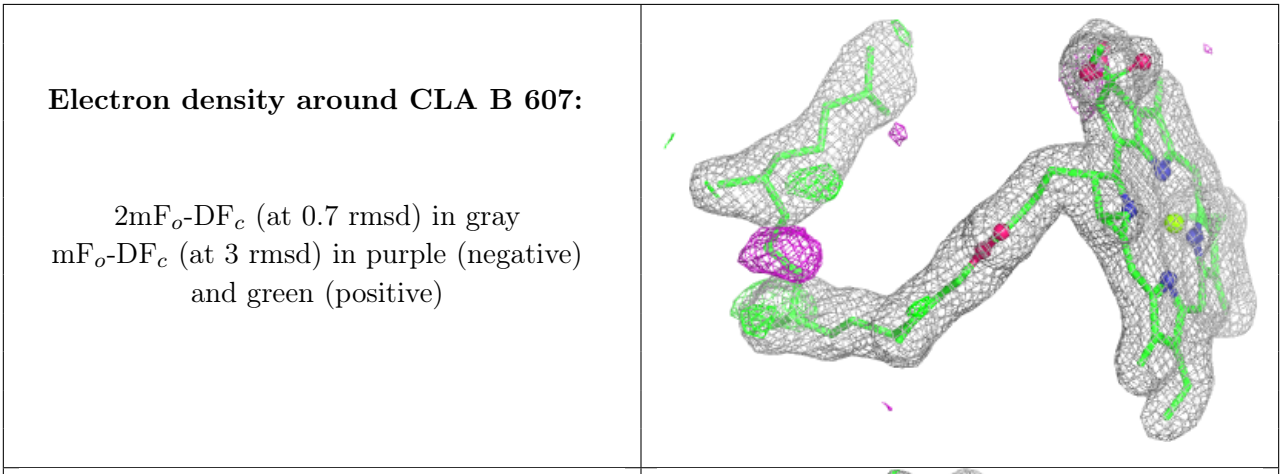
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

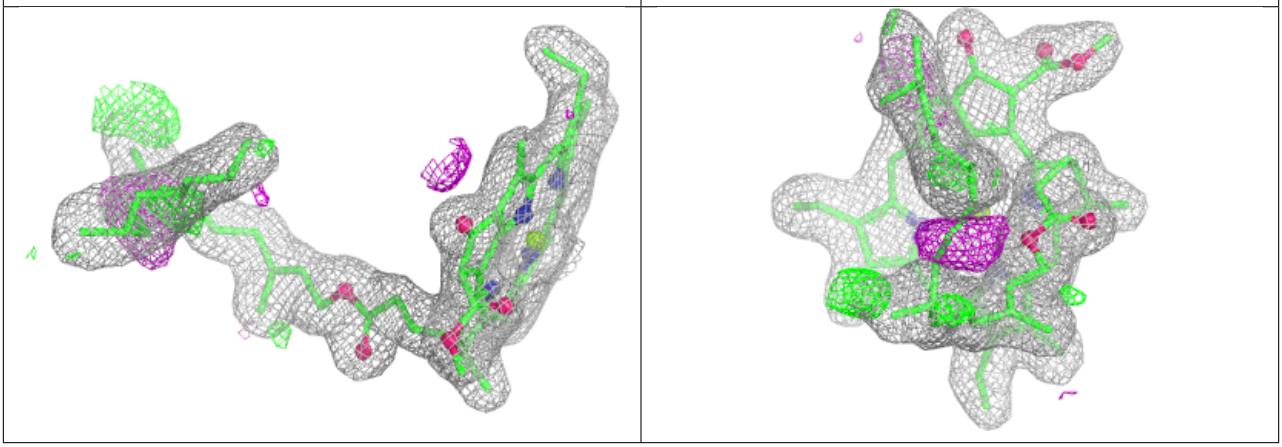




Electron density around CLA B 607:

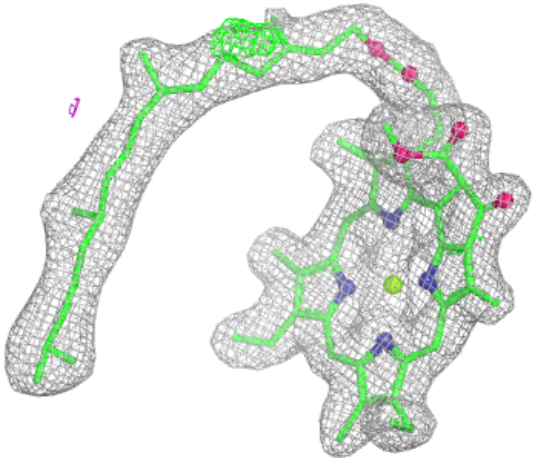
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

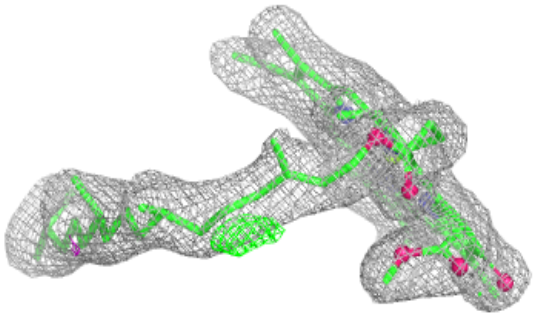


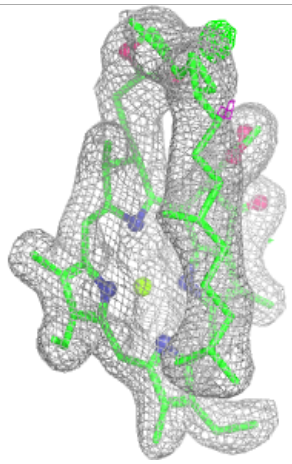


Electron density around CLA c 908:

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

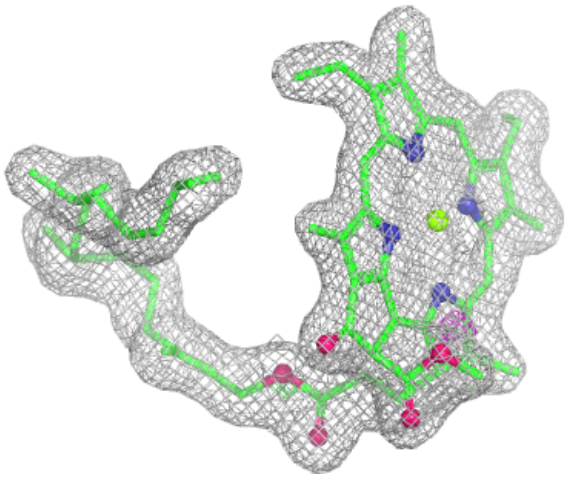


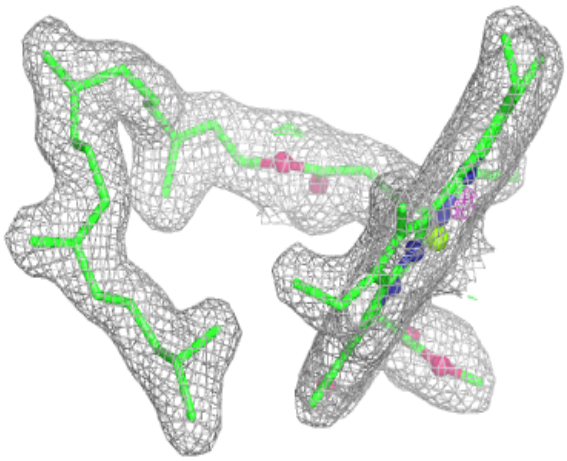


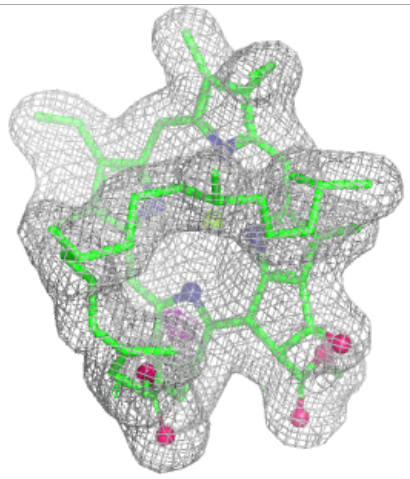


Electron density around CLA C 503:

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

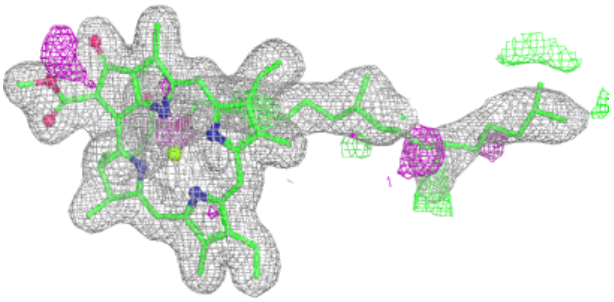


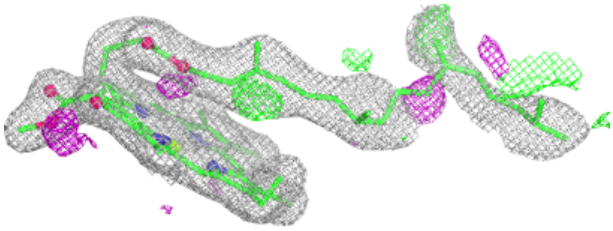


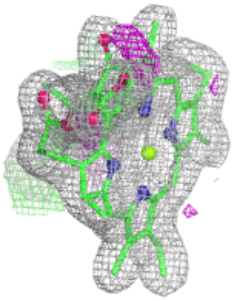


Electron density around CLA B 615:

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

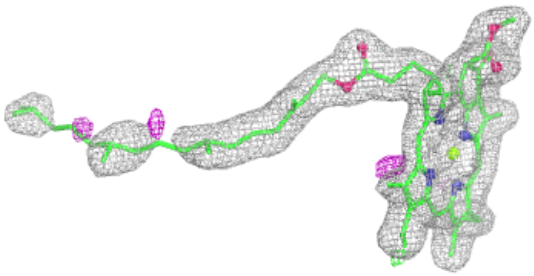


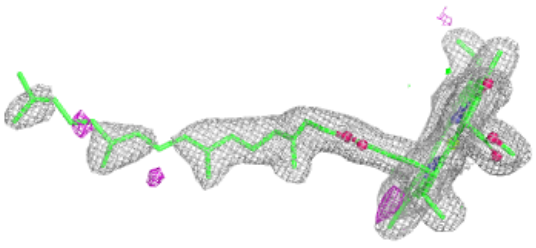


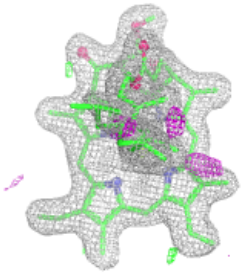


Electron density around CLA d 405:

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

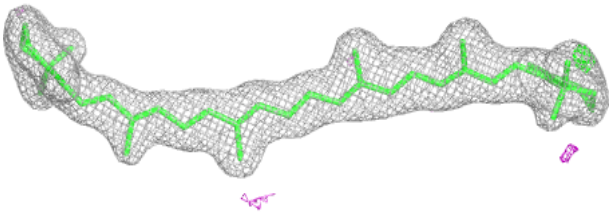


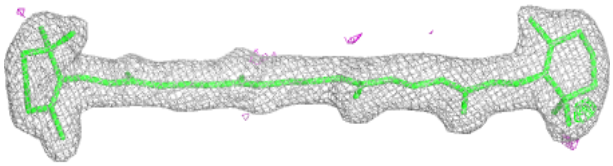




Electron density around BCR c 916:

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

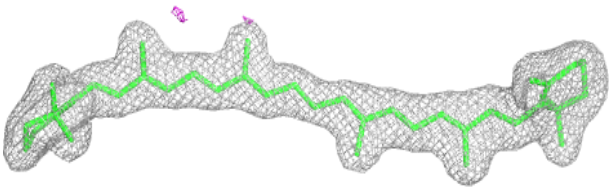


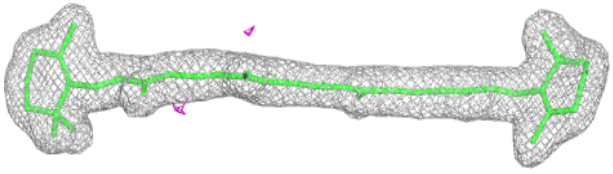


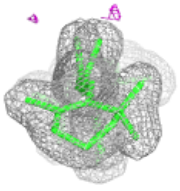


Electron density around BCR A 411:

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

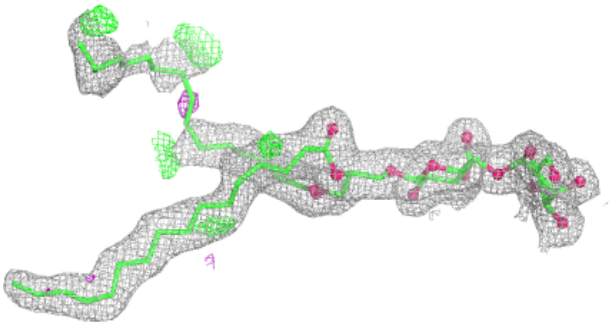


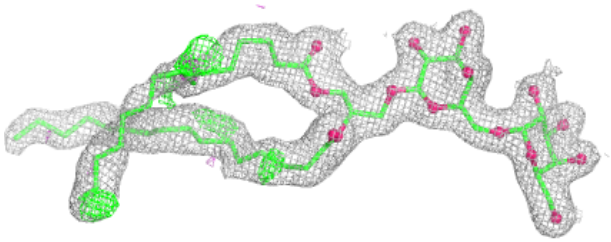


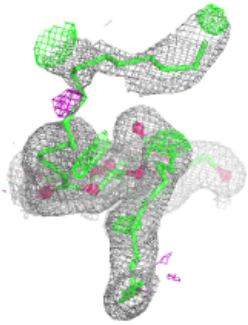


Electron density around DGD C 516:

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

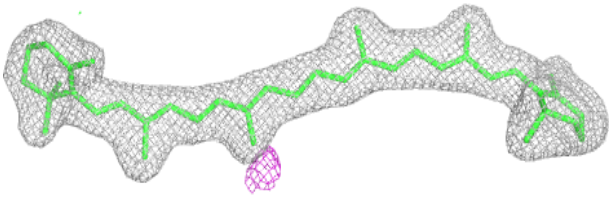


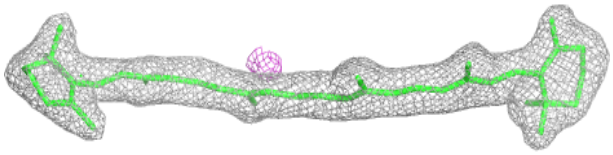


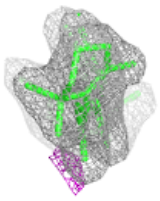


Electron density around BCR k 102:

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

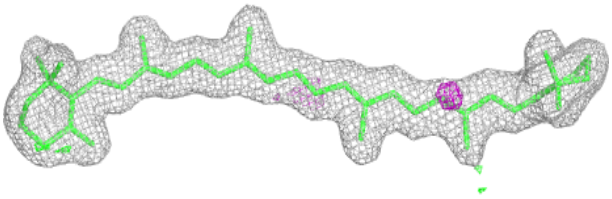


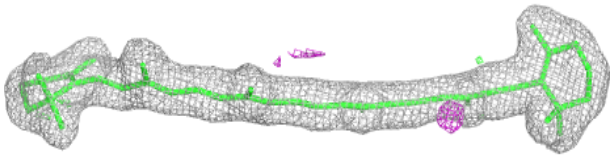


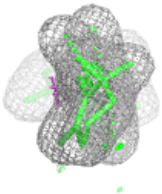


Electron density around BCR B 618:

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

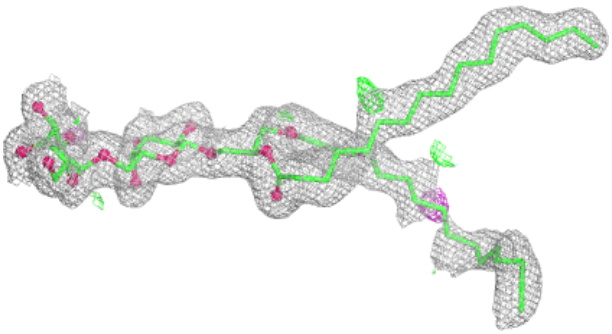


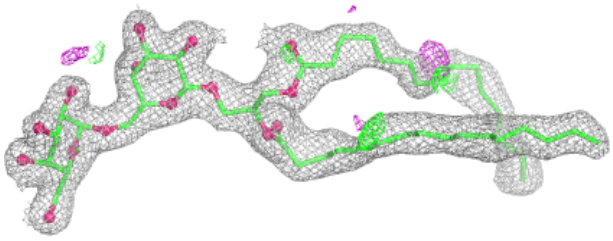


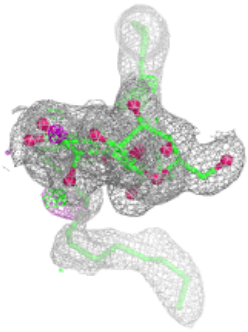


Electron density around DGD c 917:

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

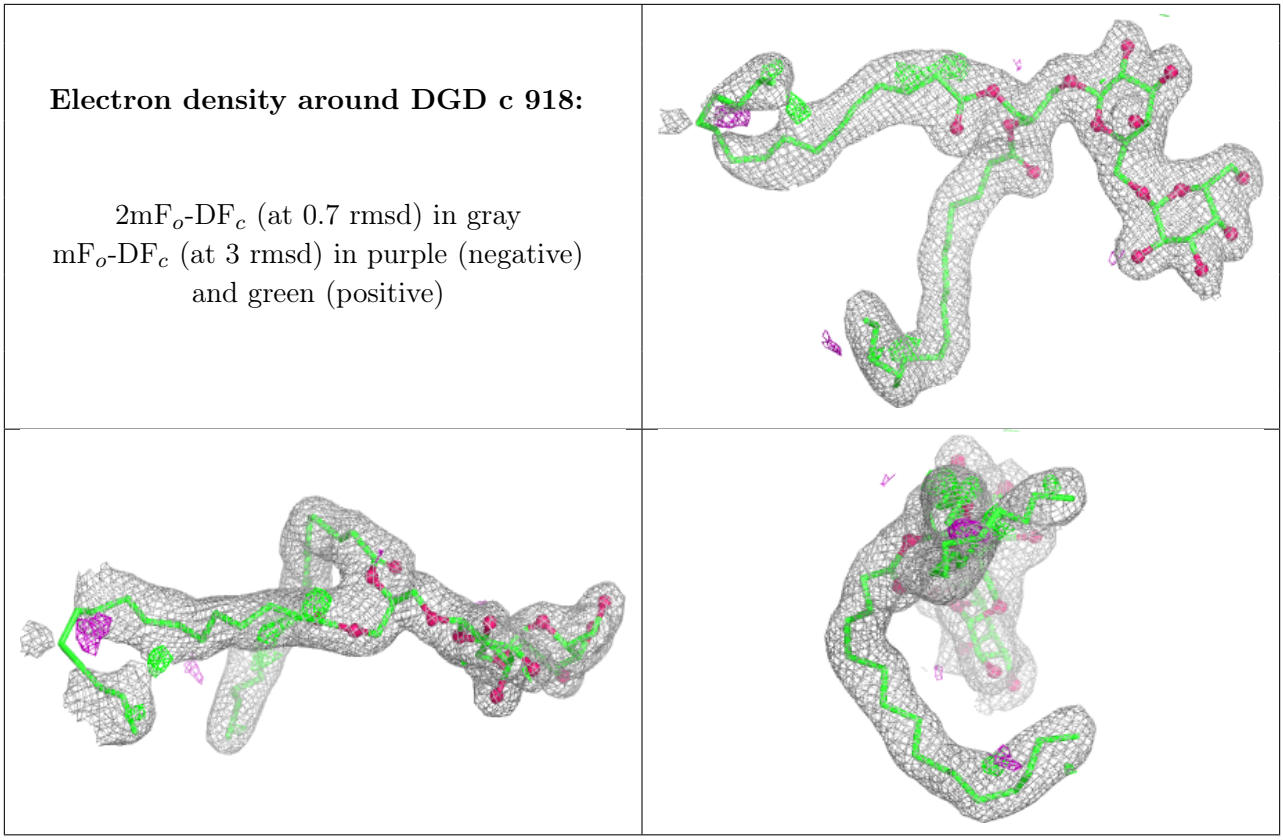






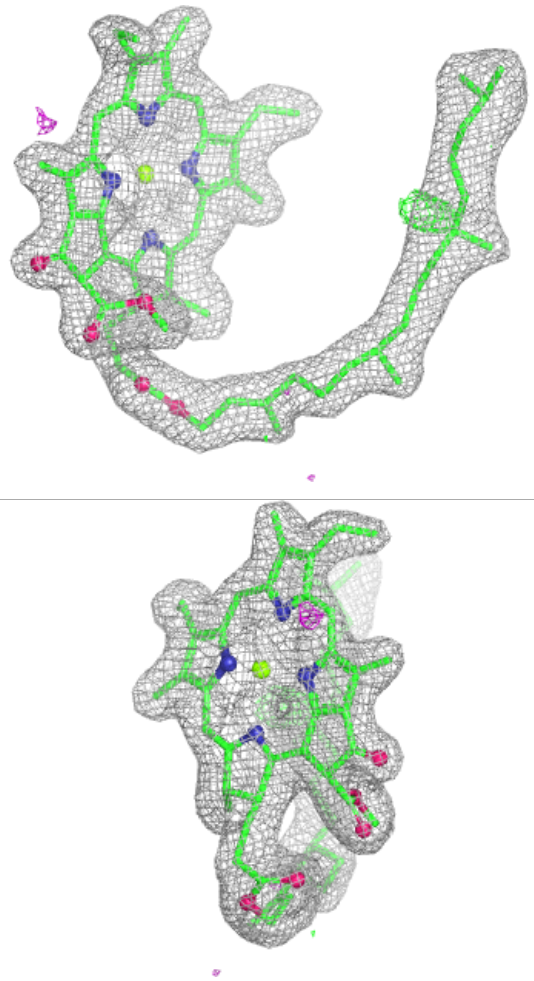
Electron density around DGD c 918:

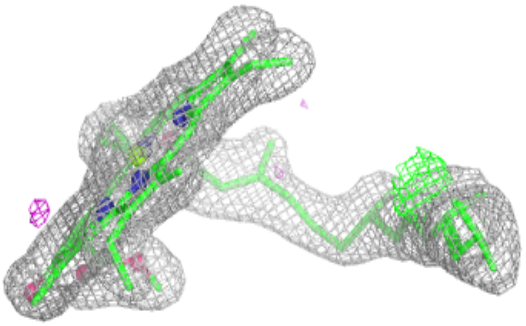
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA C 507:

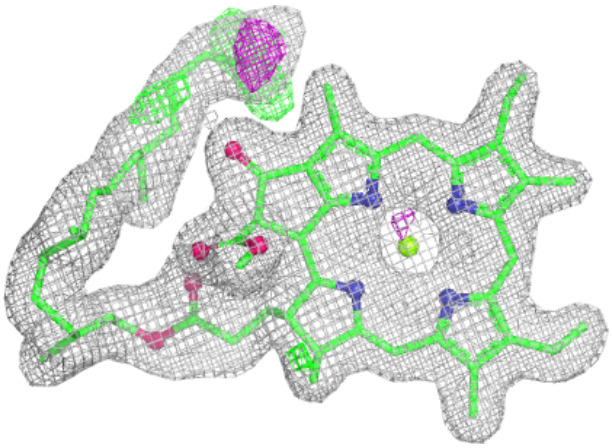
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

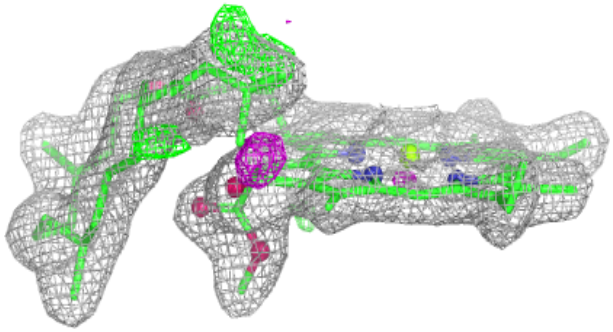


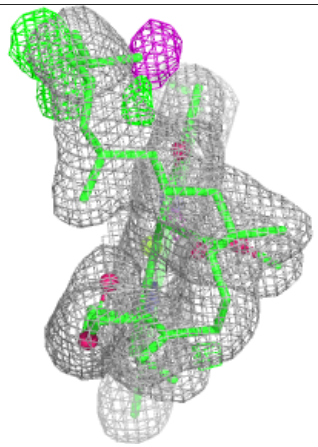


Electron density around CLA b 614:

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

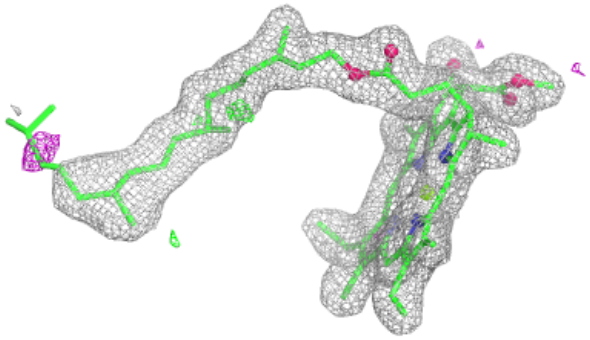


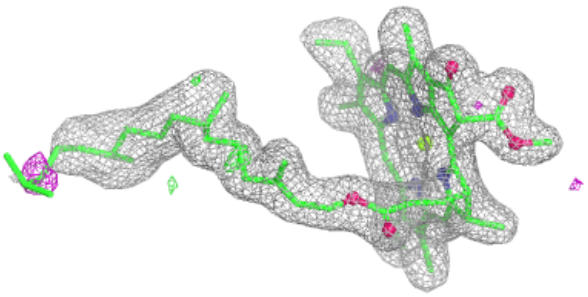


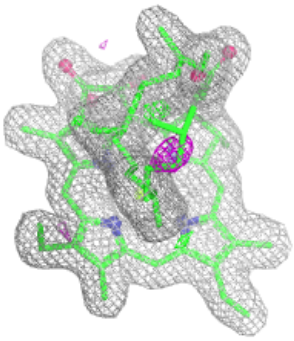


Electron density around CLA C 508:

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

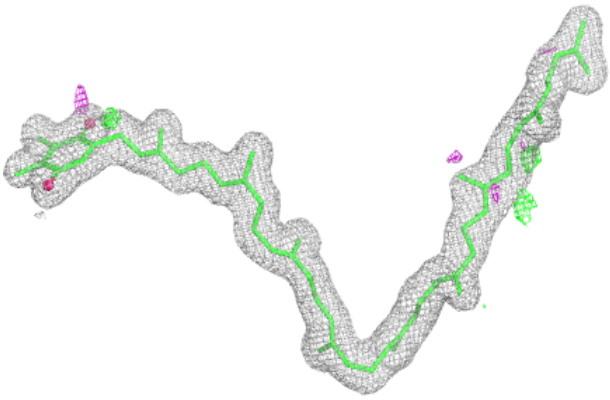


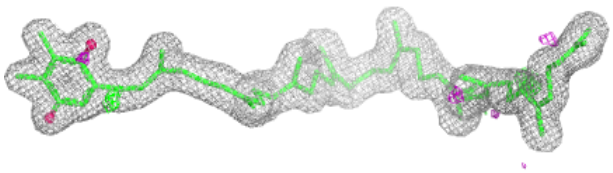


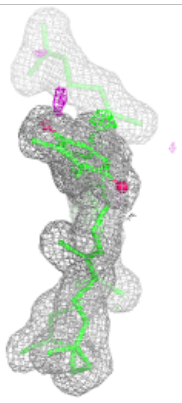


Electron density around PL9 D 404:

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

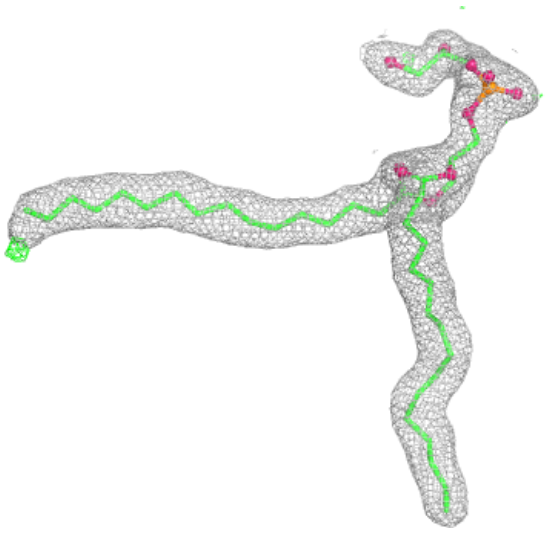


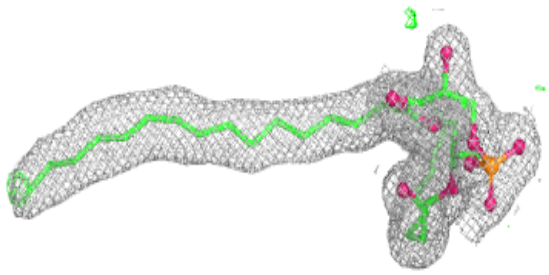


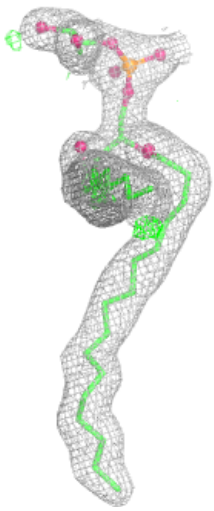


Electron density around LHG L 101:

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

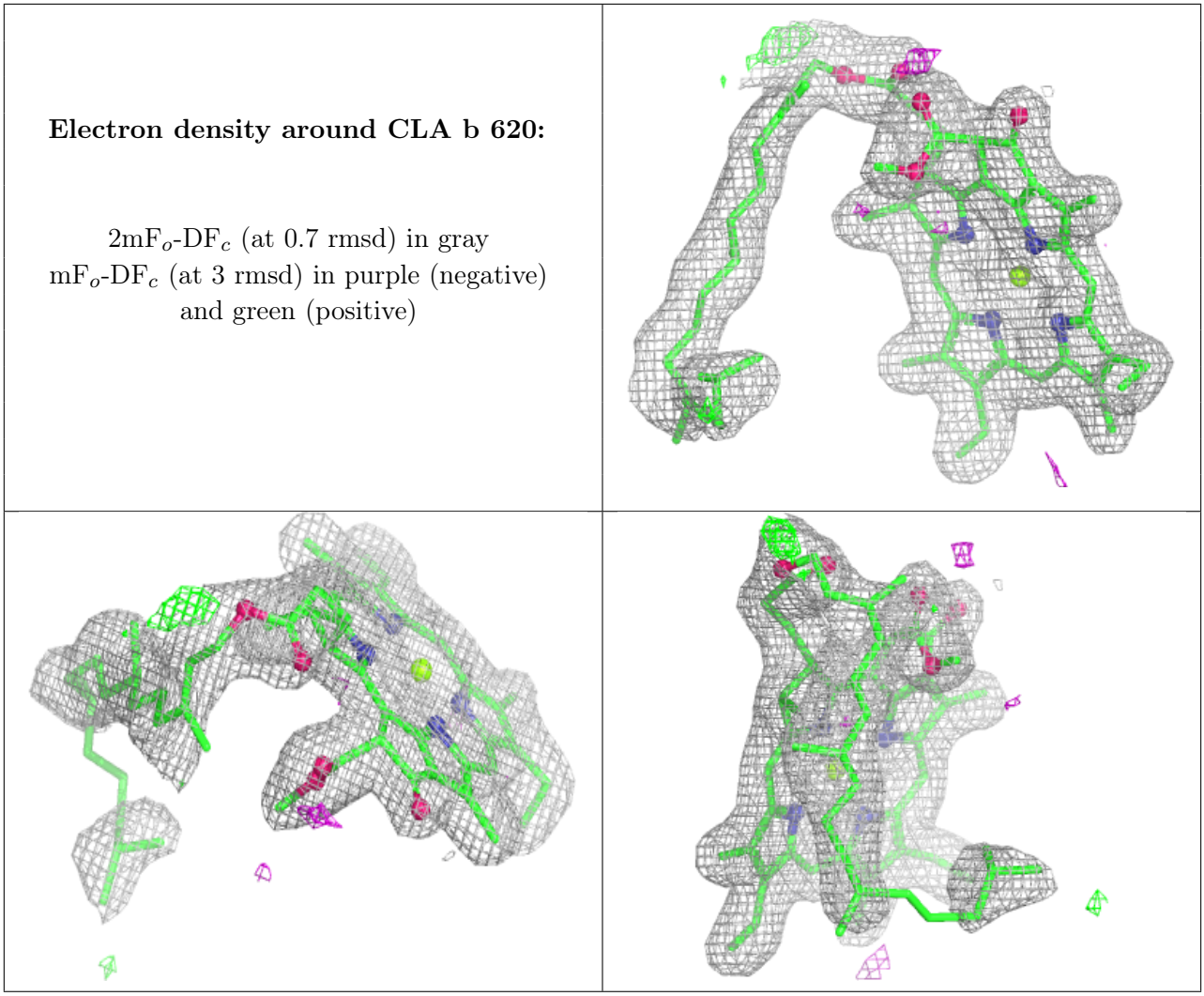






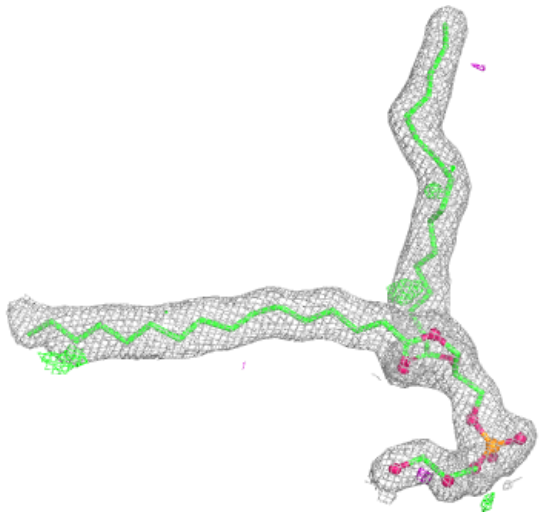
Electron density around CLA b 620:

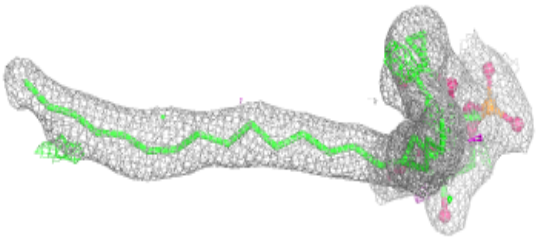
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

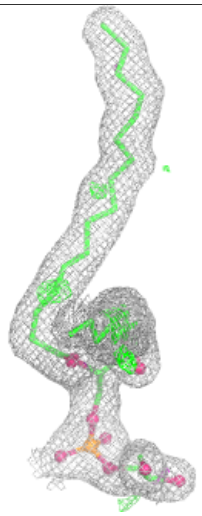


Electron density around LHG l 103:

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

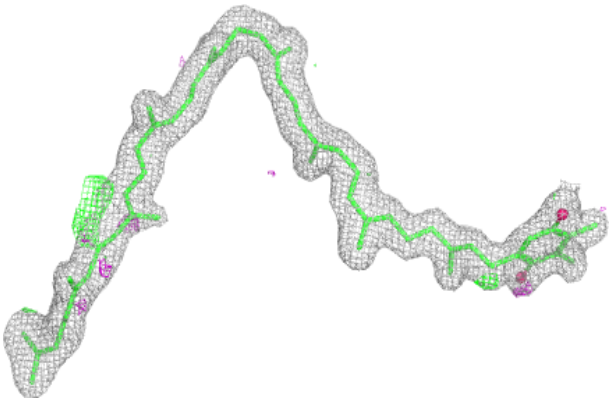


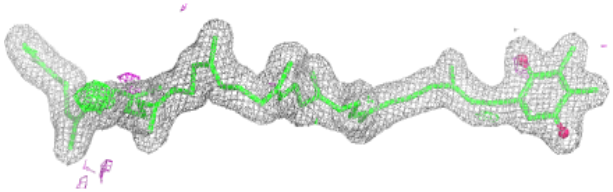


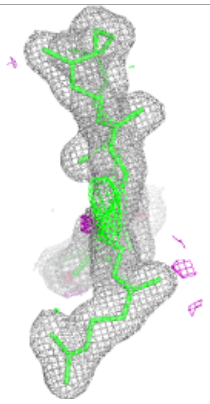


Electron density around PL9 d 407:

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

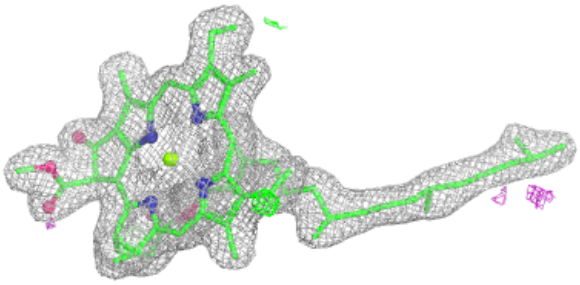


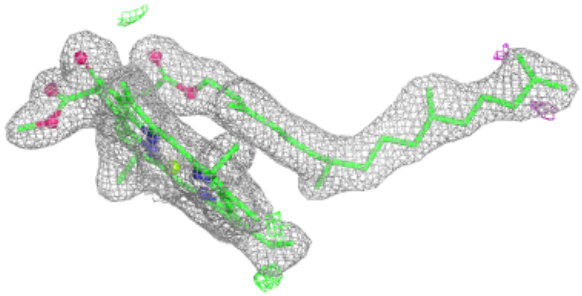


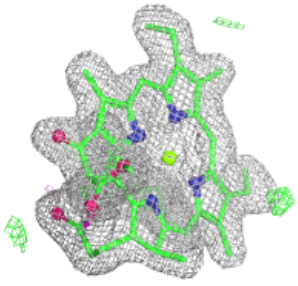


Electron density around CLA C 505:

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

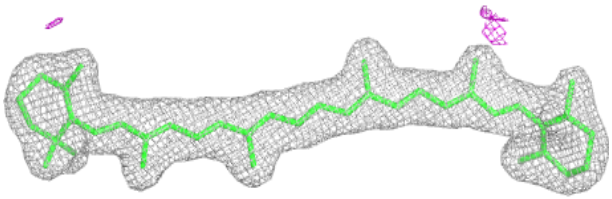


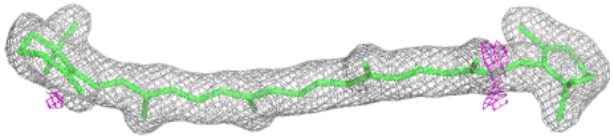


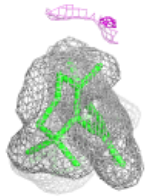


Electron density around BCR b 623:

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

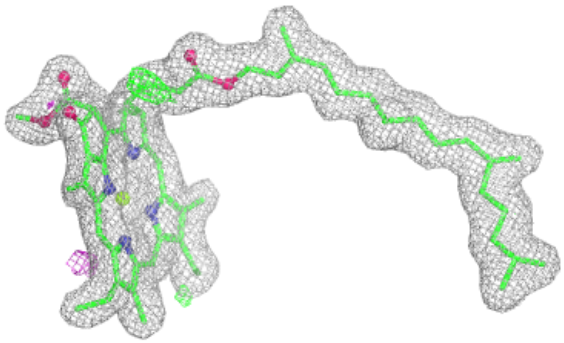


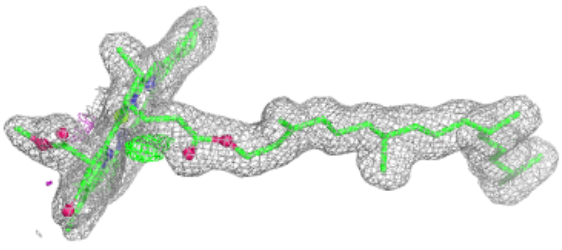


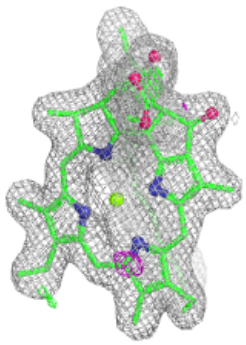


Electron density around CLA B 610:

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

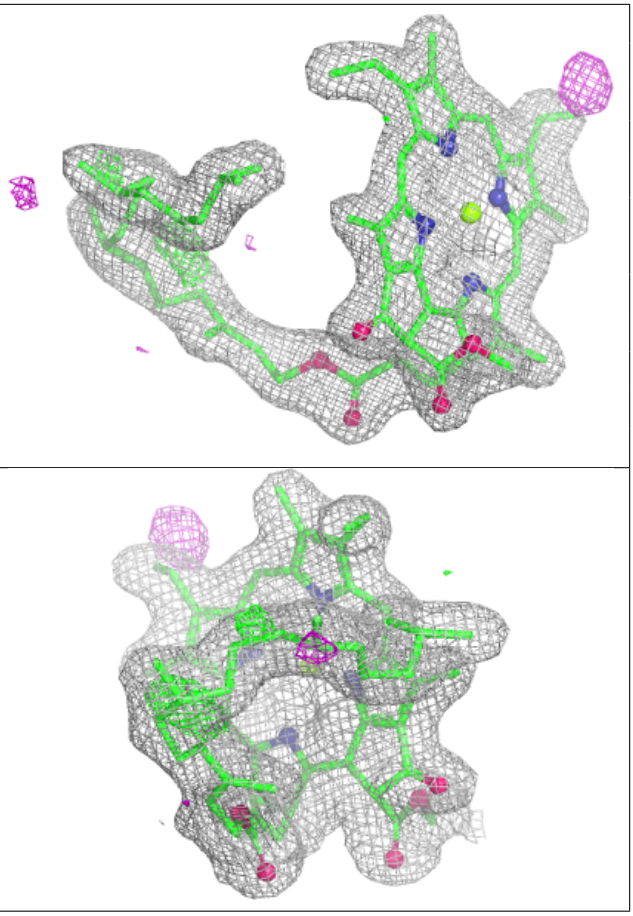






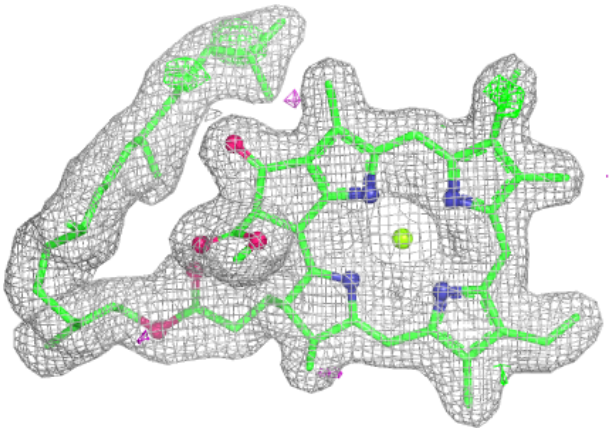
Electron density around CLA c 904:

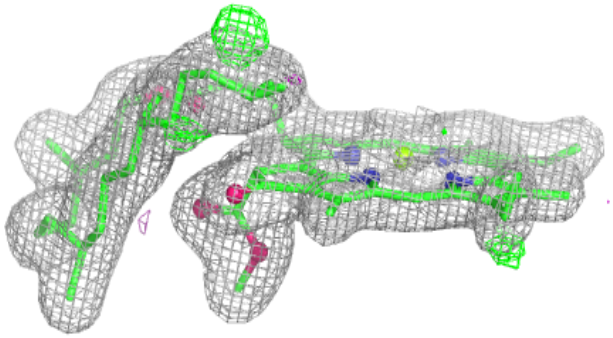
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

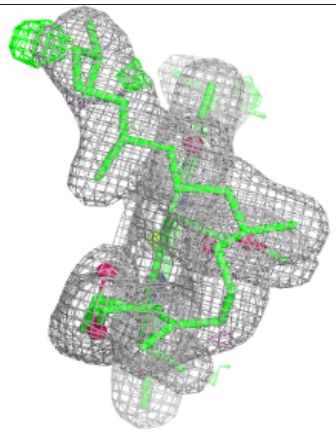


Electron density around CLA B 611:

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

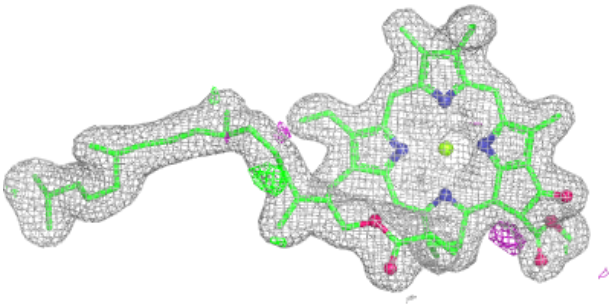


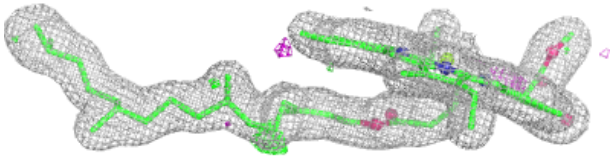


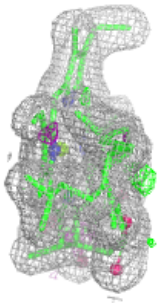


Electron density around CLA B 604:

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

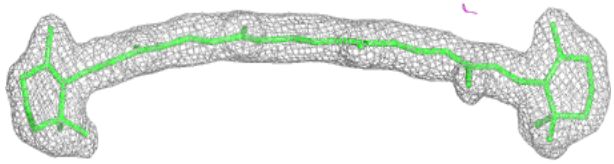


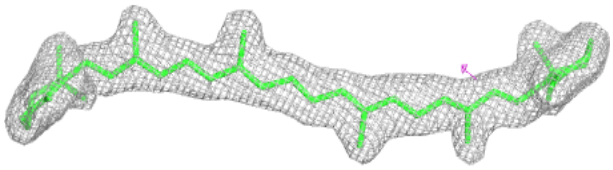


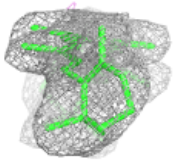


Electron density around BCR k 103:

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

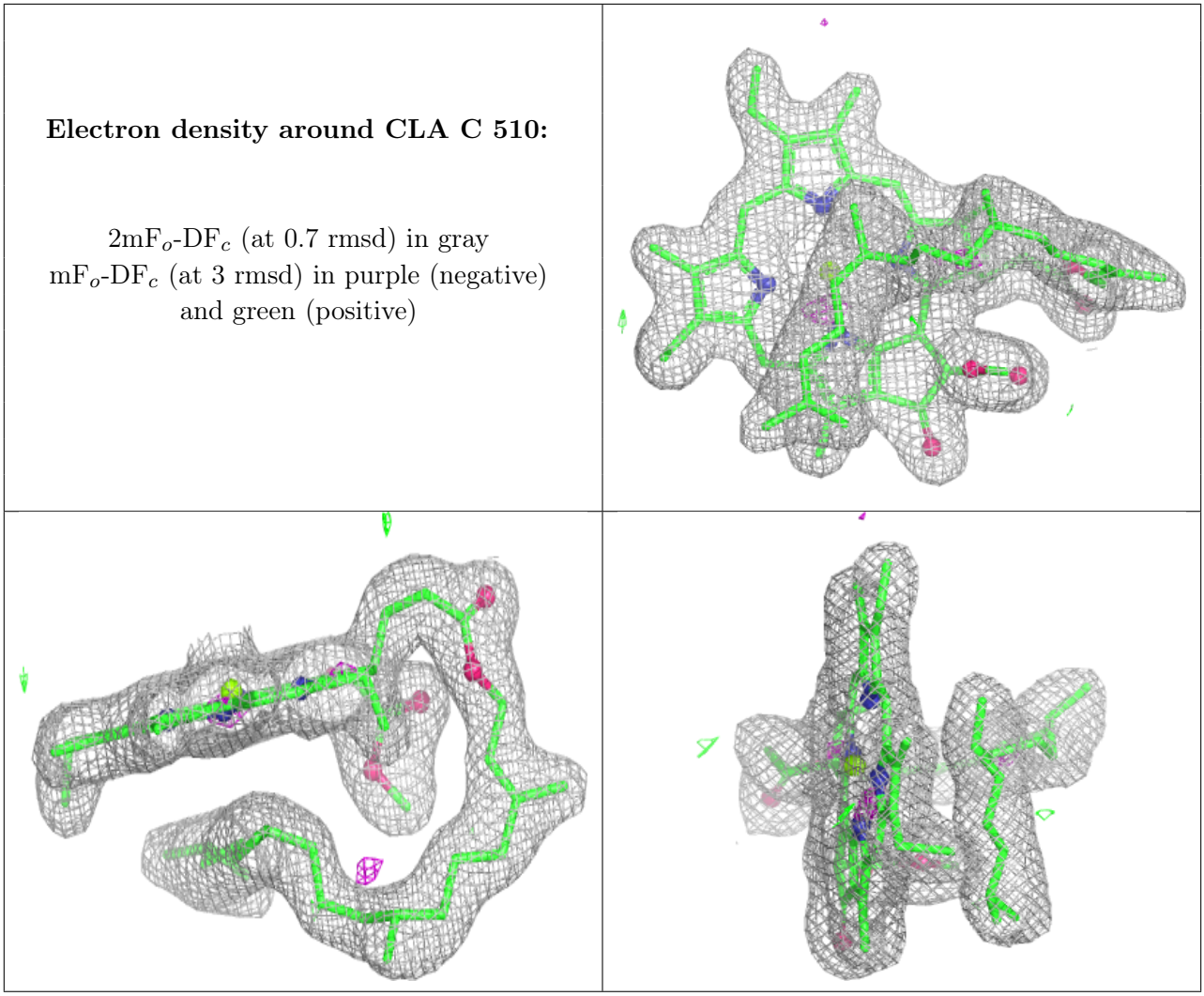






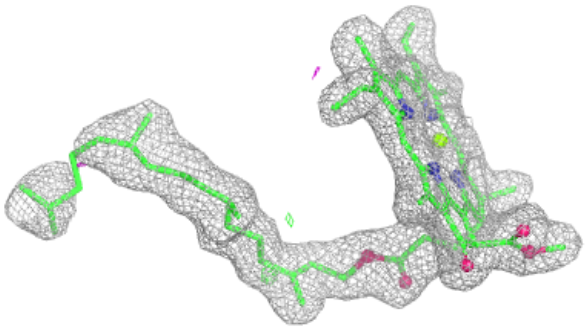
Electron density around CLA C 510:

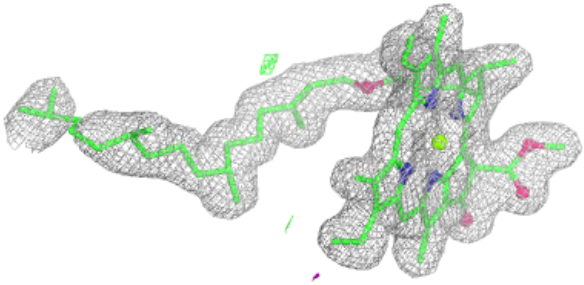
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

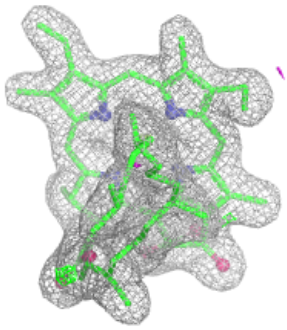


Electron density around CLA c 909:

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

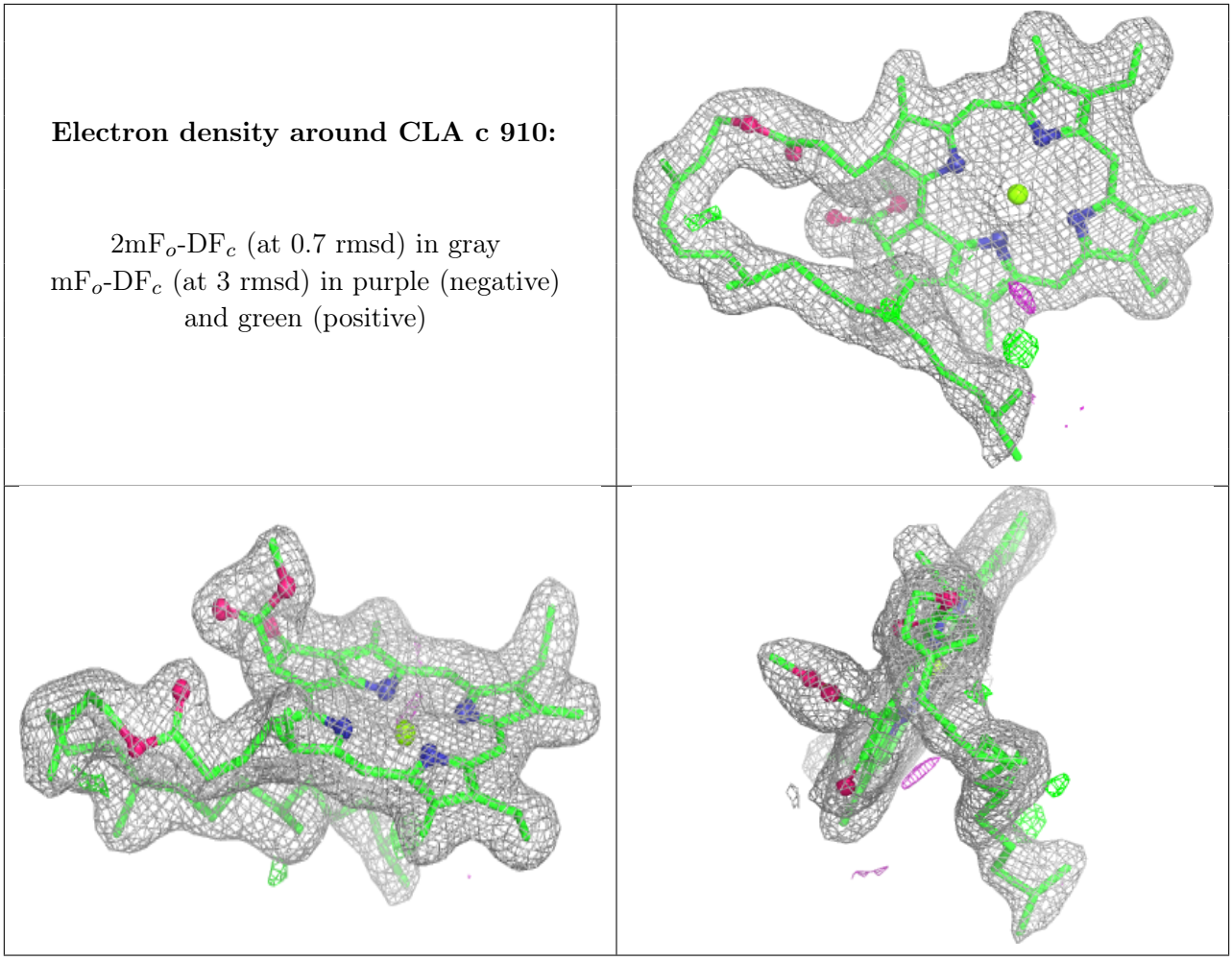






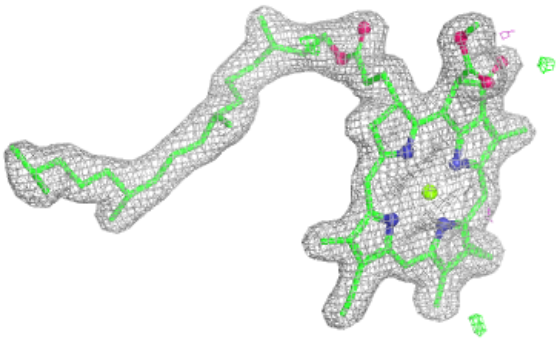
Electron density around CLA c 910:

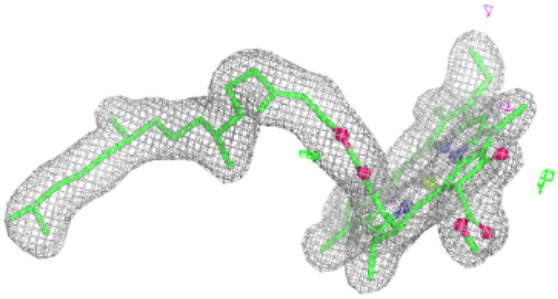
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

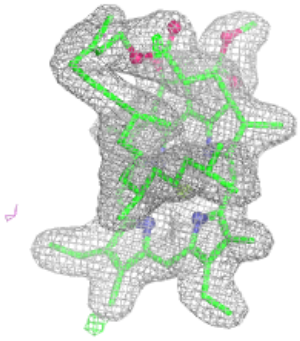


Electron density around CLA c 912:

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

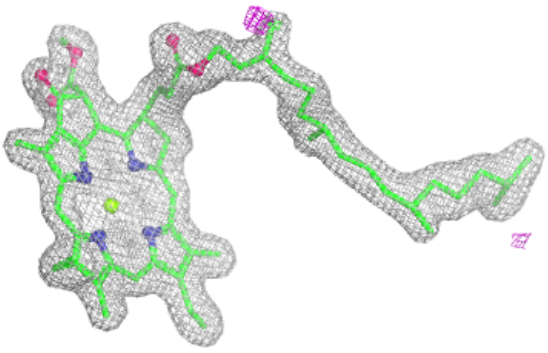


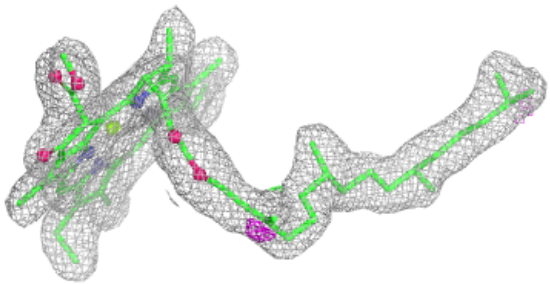


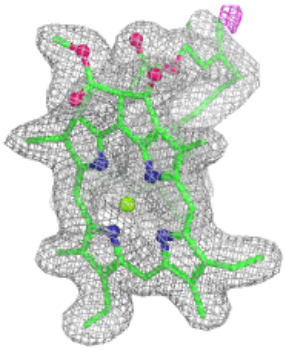


Electron density around CLA C 511:

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

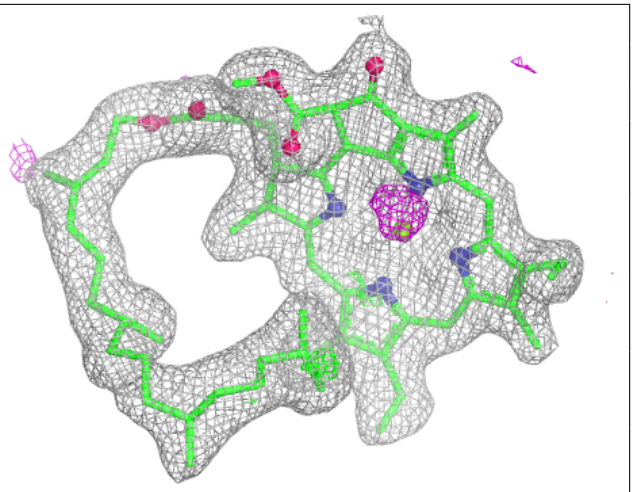


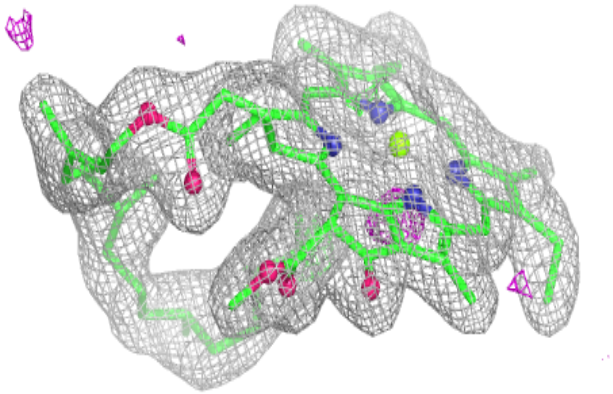


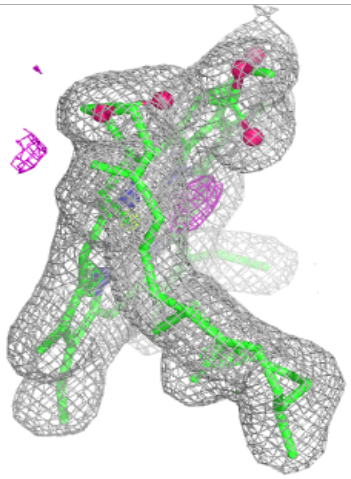


Electron density around CLA B 616:

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

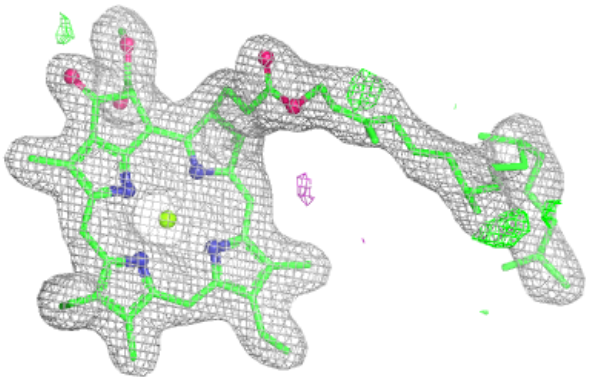


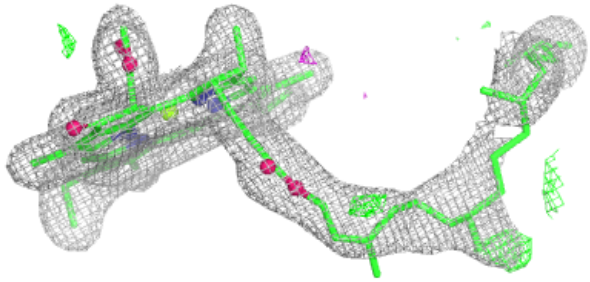


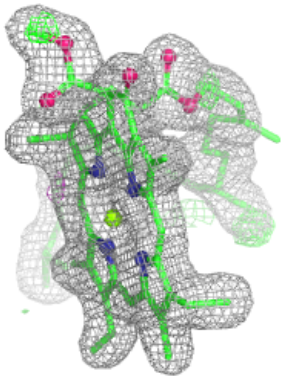


Electron density around CLA A 410:

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

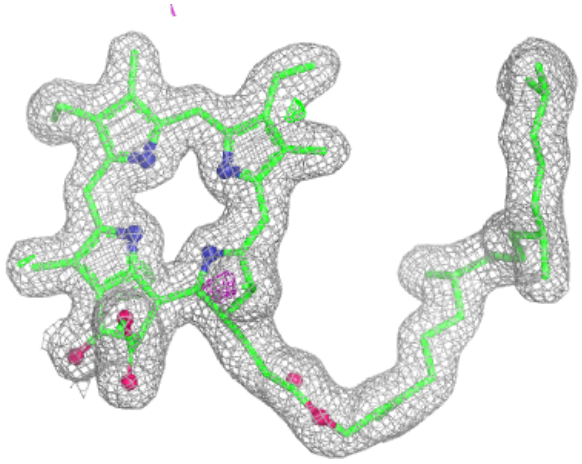


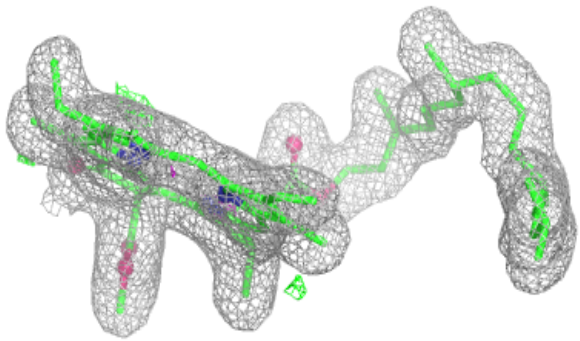


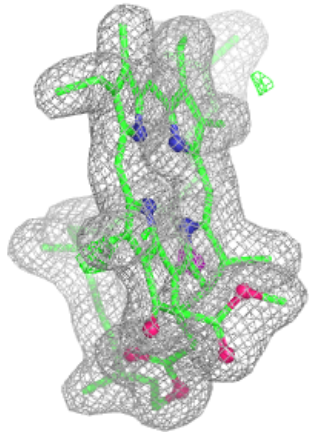


Electron density around PHO A 409:

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

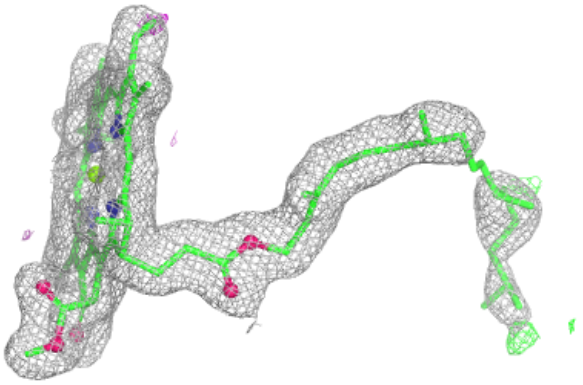


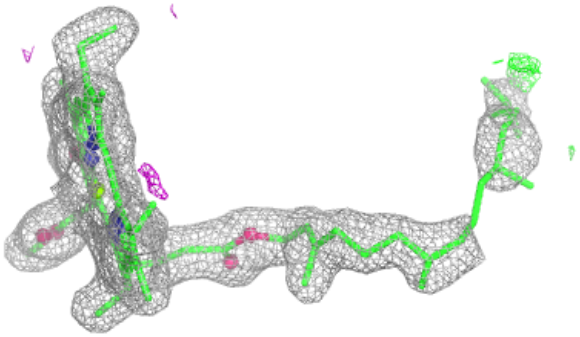


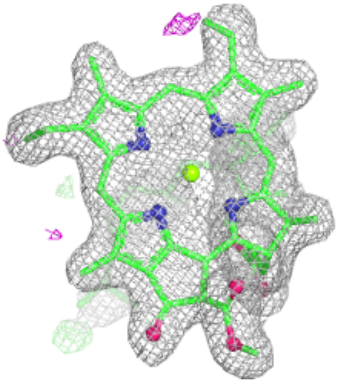


Electron density around CLA D 402:

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

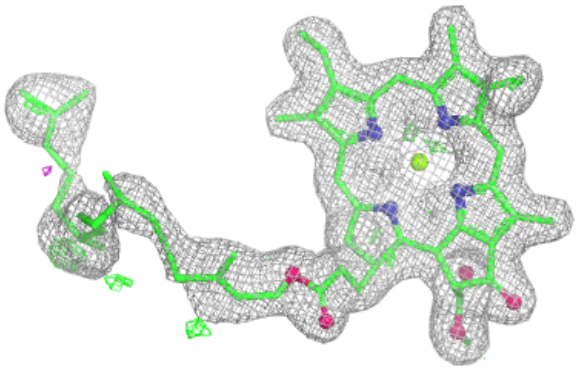


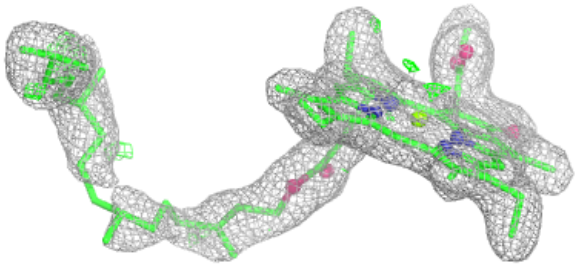


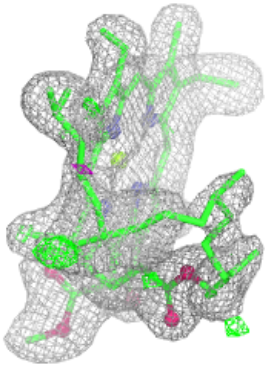


Electron density around CLA a 413:

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

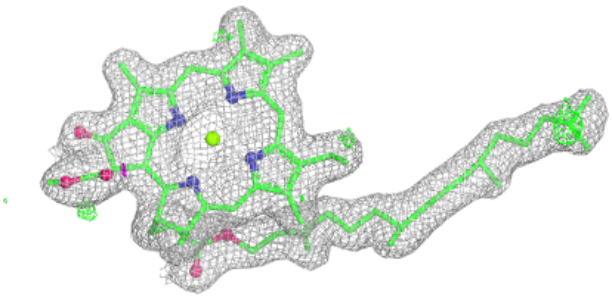


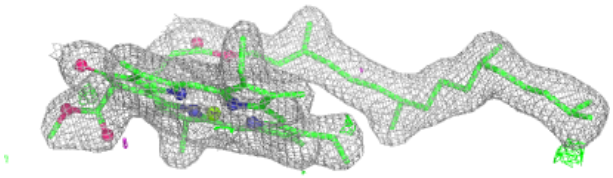


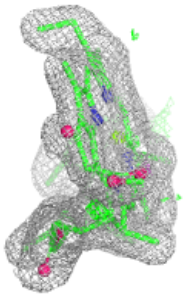


Electron density around CLA C 501:

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

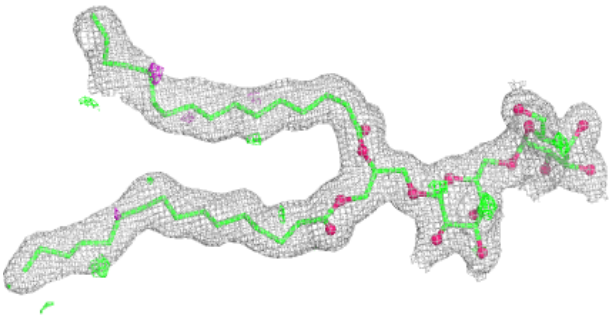


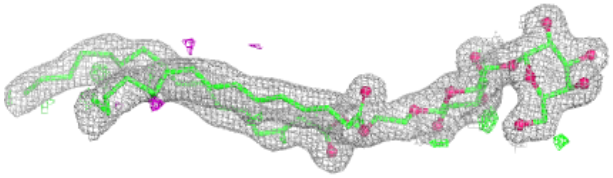


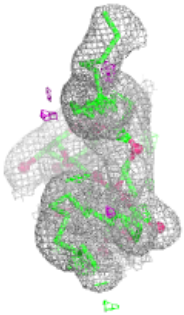


Electron density around DGD C 518:

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

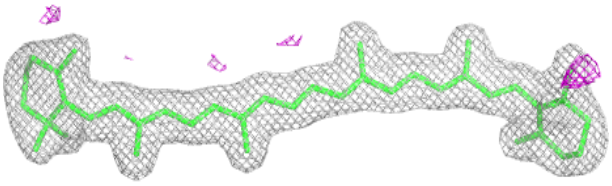


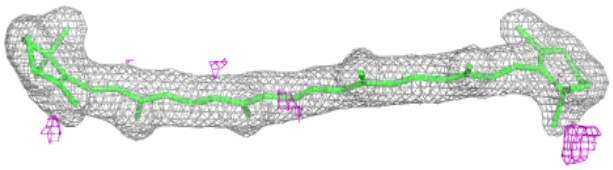


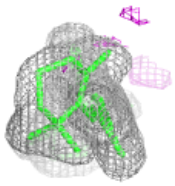


Electron density around BCR B 620:

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

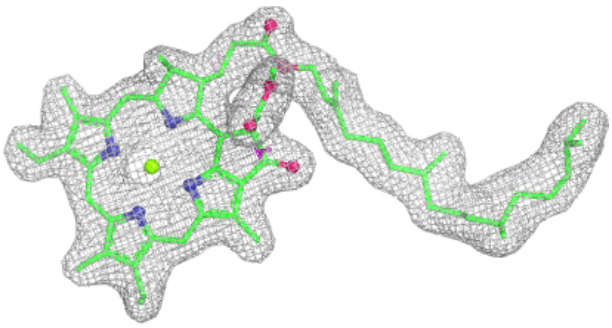


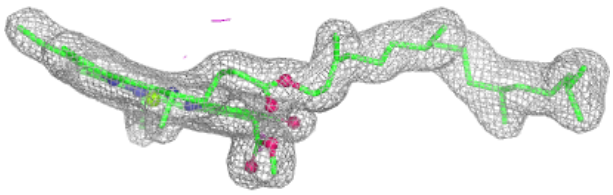


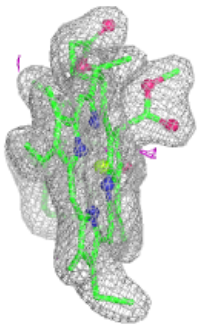


Electron density around CLA b 606:

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

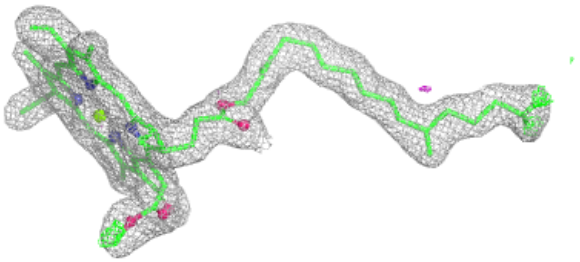


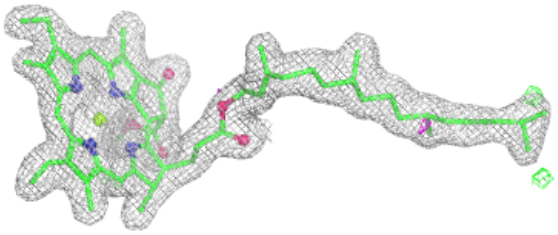


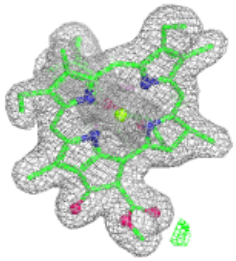


Electron density around CLA C 502:

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

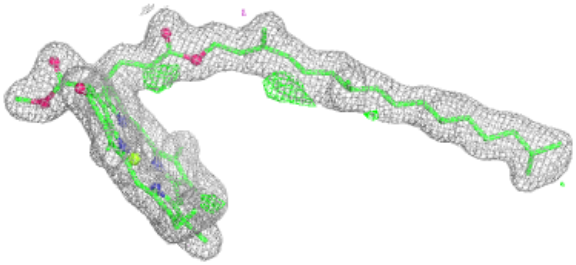


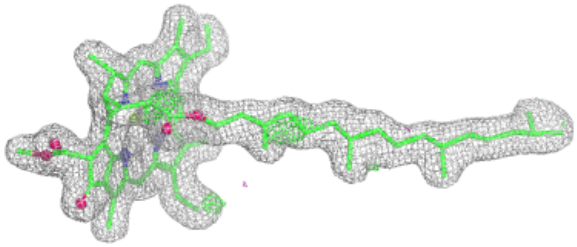


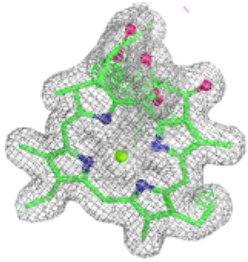


Electron density around CLA b 611:

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

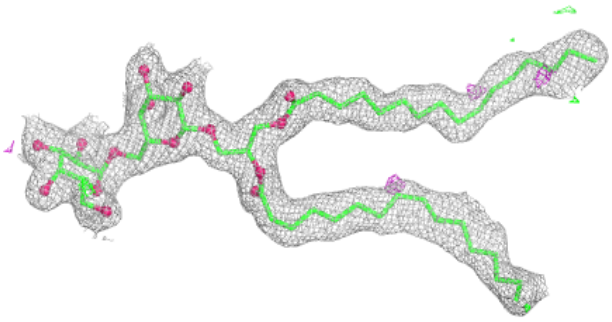


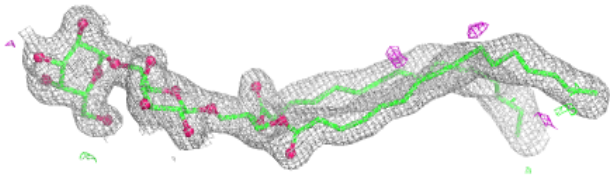


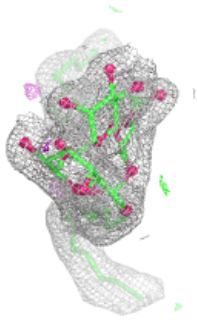


Electron density around DGD c 919:

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

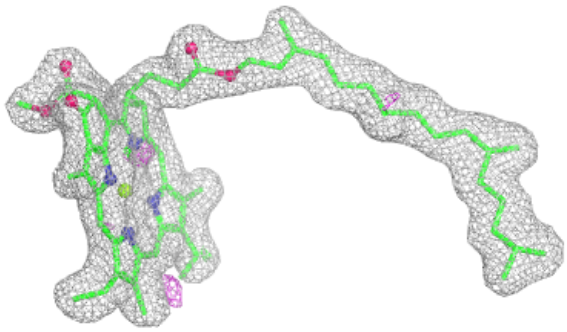


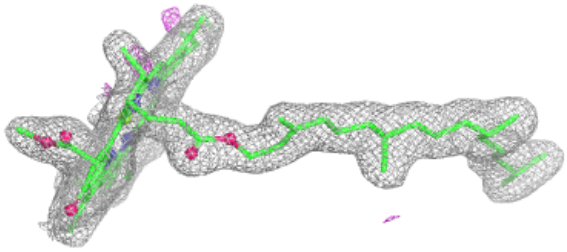


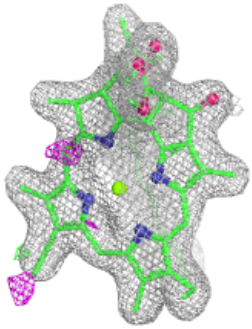


Electron density around CLA b 613:

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

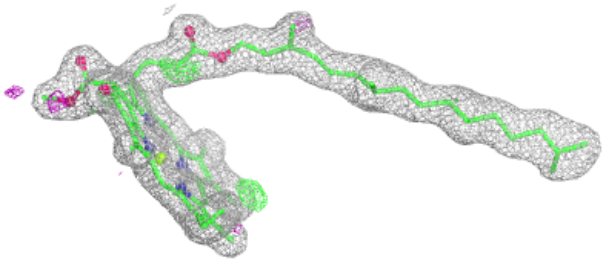


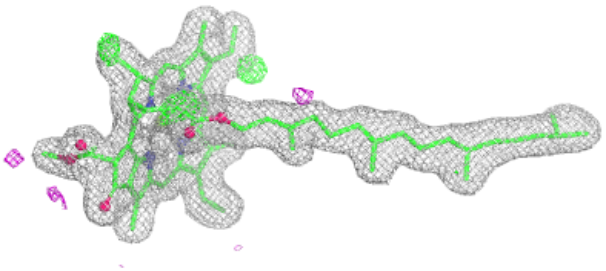


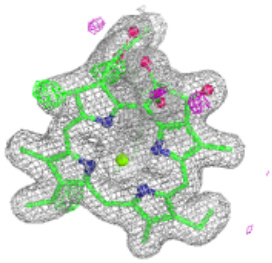


Electron density around CLA B 608:

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

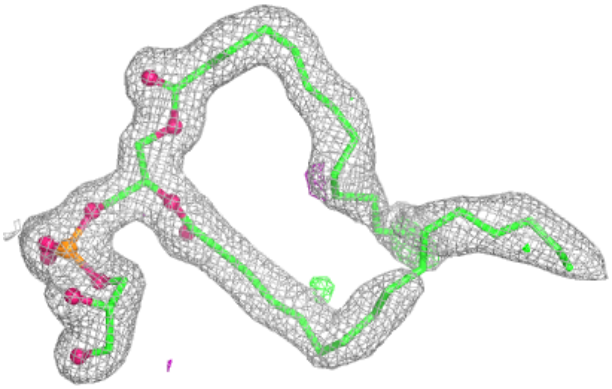


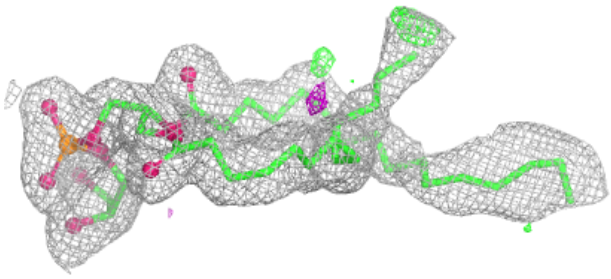


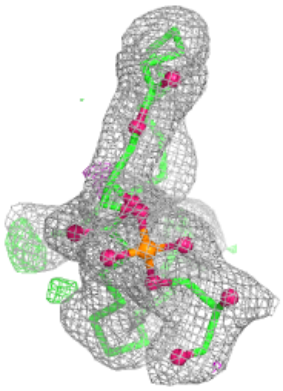


Electron density around LHG D 408:

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

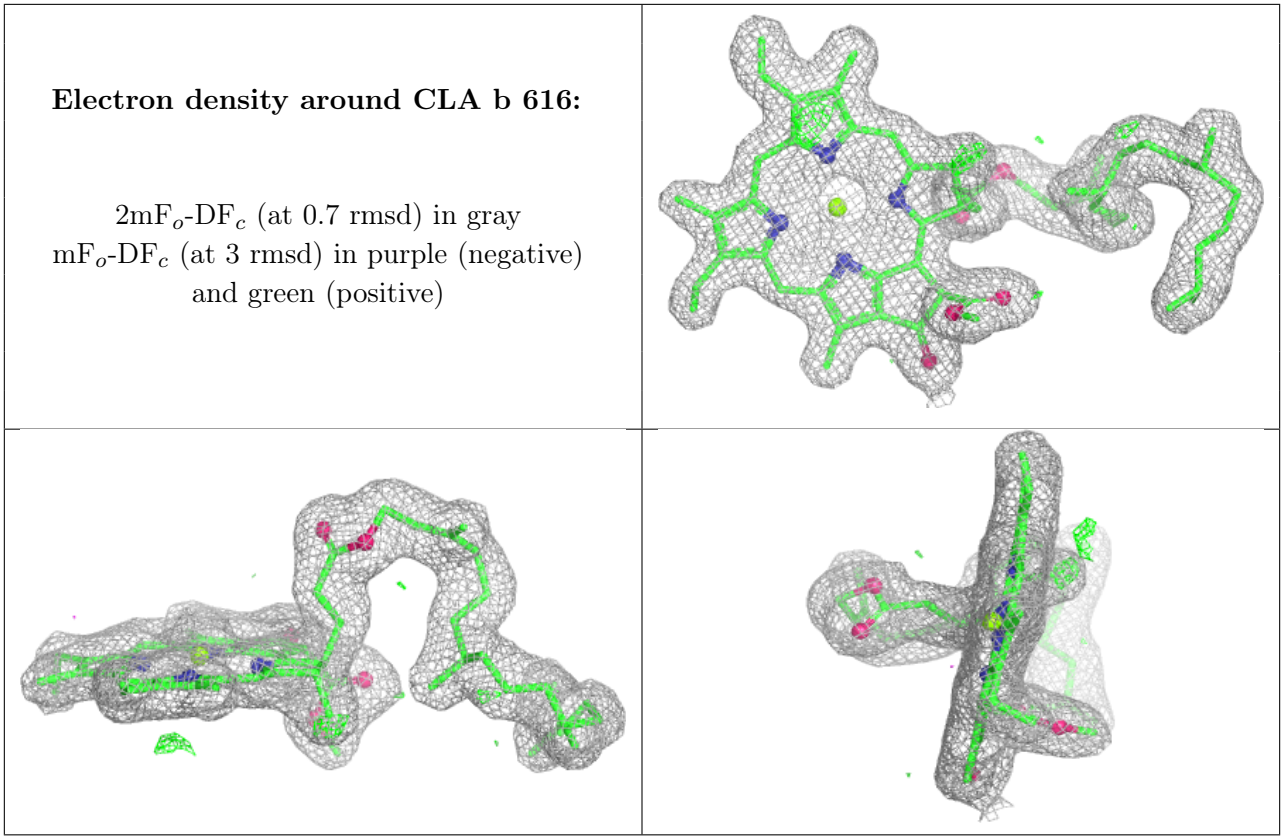






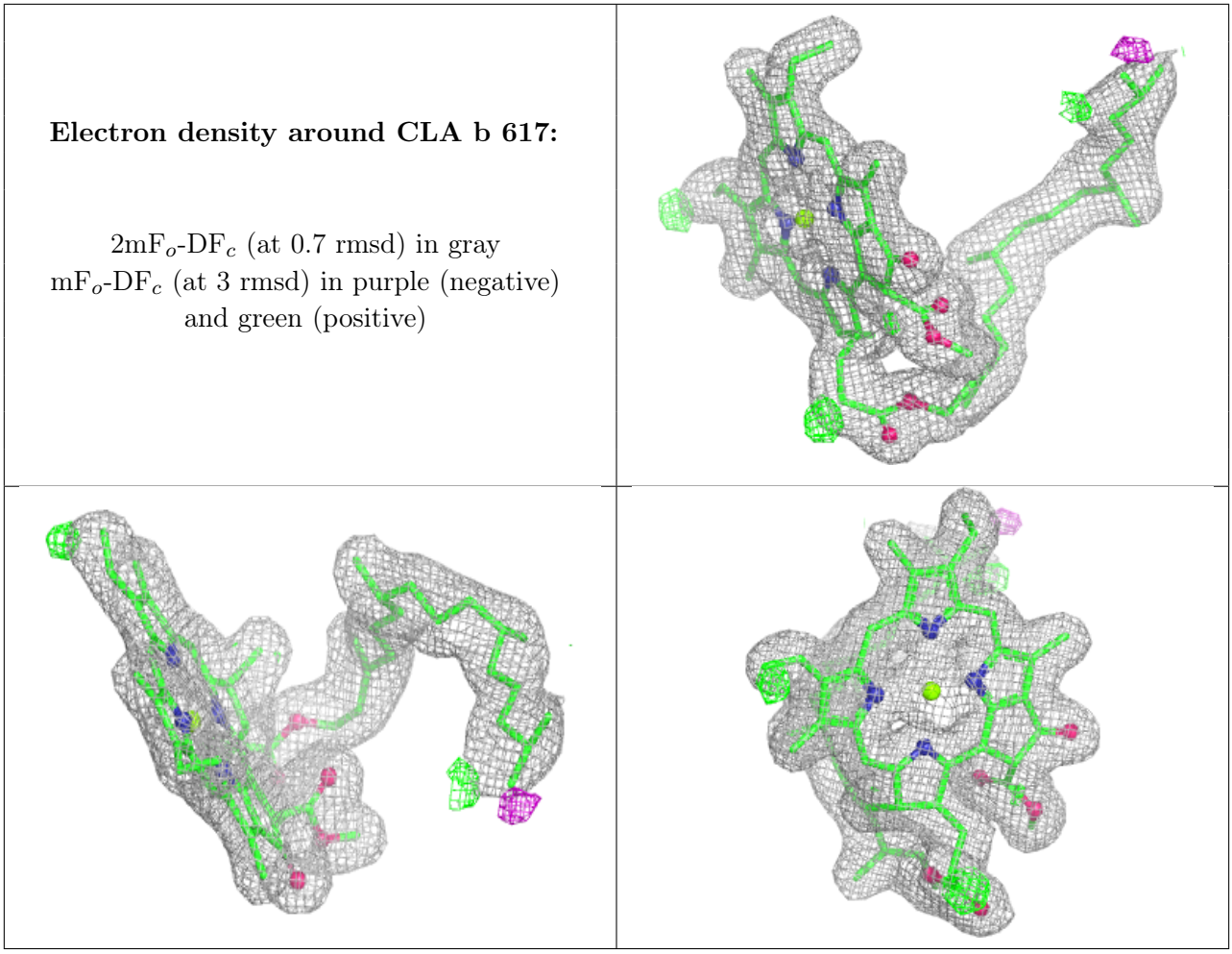
Electron density around CLA b 616:

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



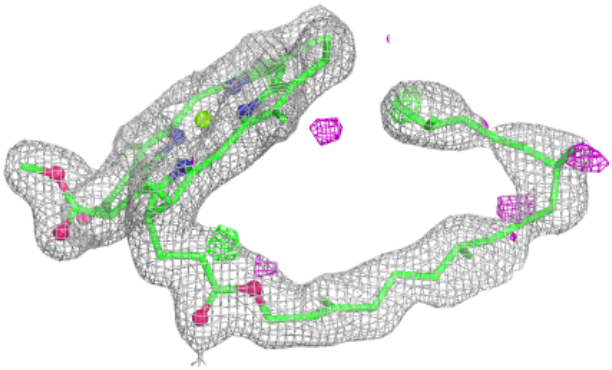
Electron density around CLA b 617:

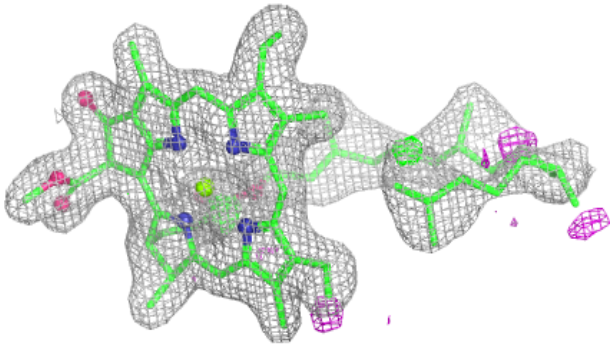
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

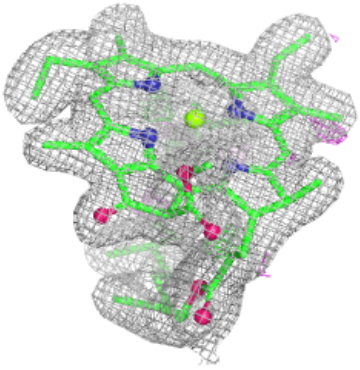


Electron density around CLA C 504:

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

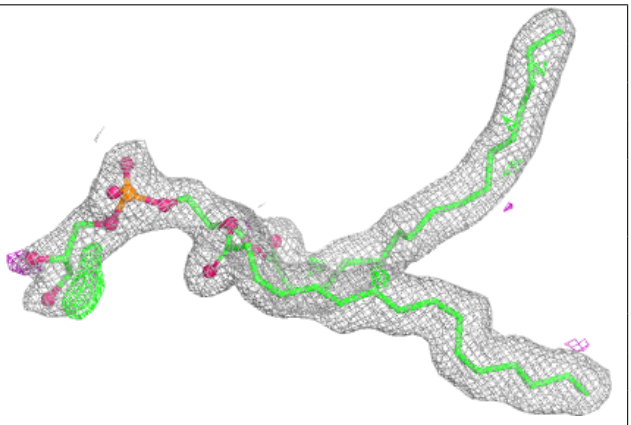


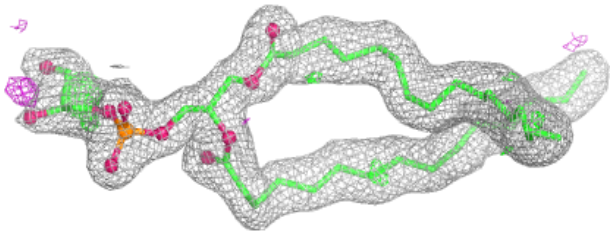


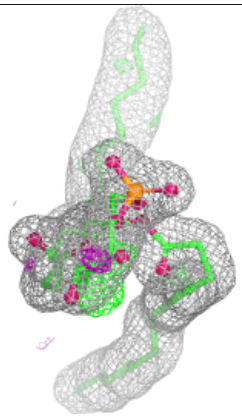


Electron density around LHG d 410:

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

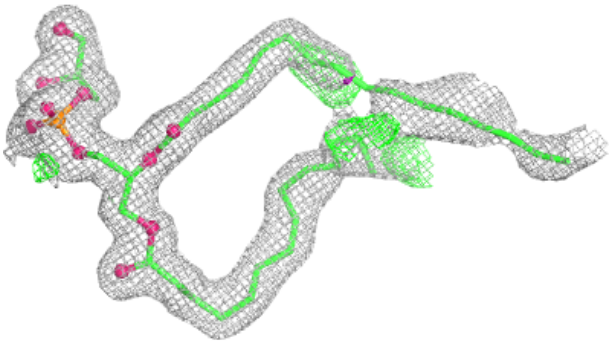


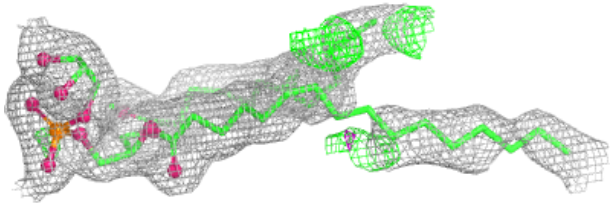


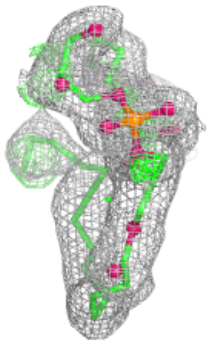


Electron density around LHG d 411:

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

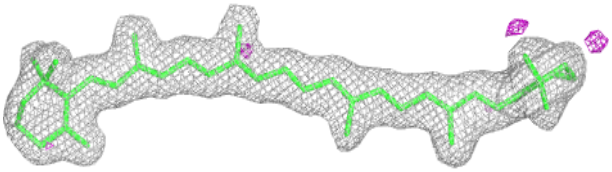


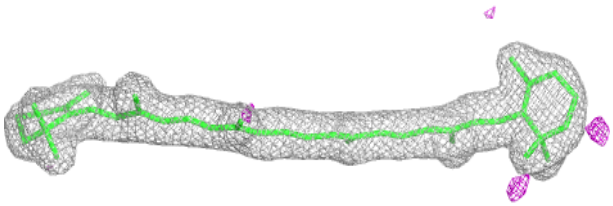


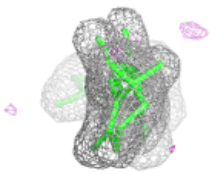


Electron density around BCR b 621:

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

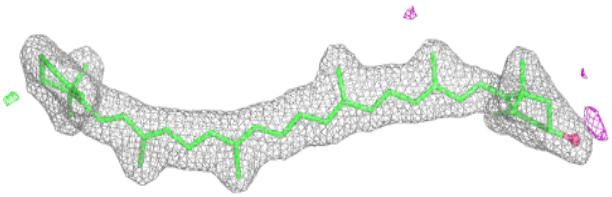


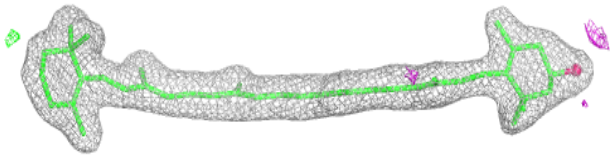


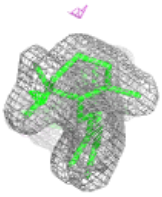


Electron density around RRX H 101:

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

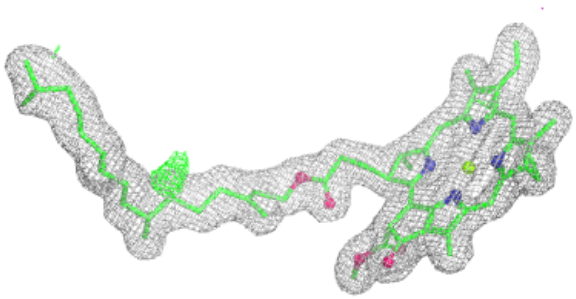


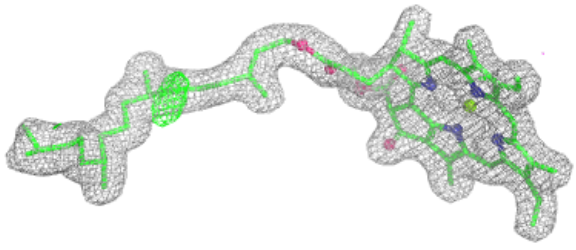


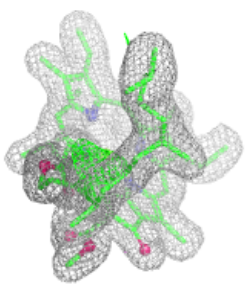


Electron density around CLA a 409:

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

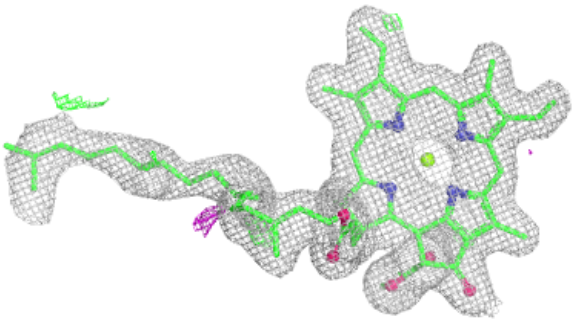


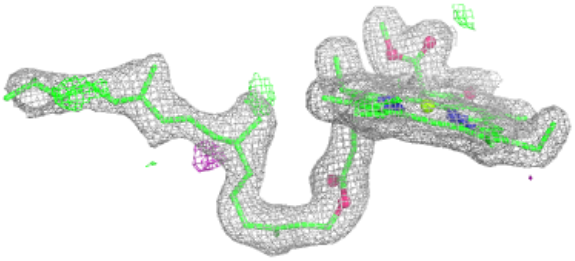


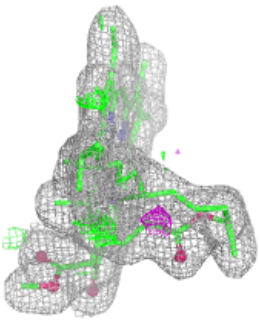


Electron density around CLA a 410:

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

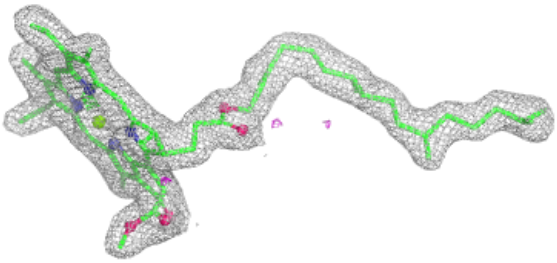


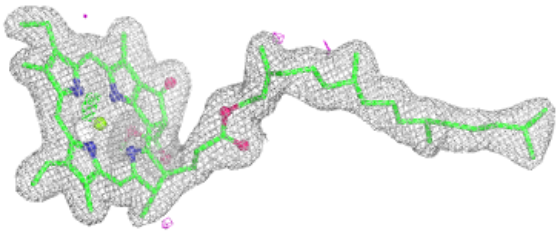


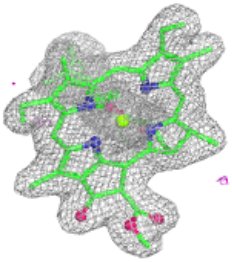


Electron density around CLA c 903:

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

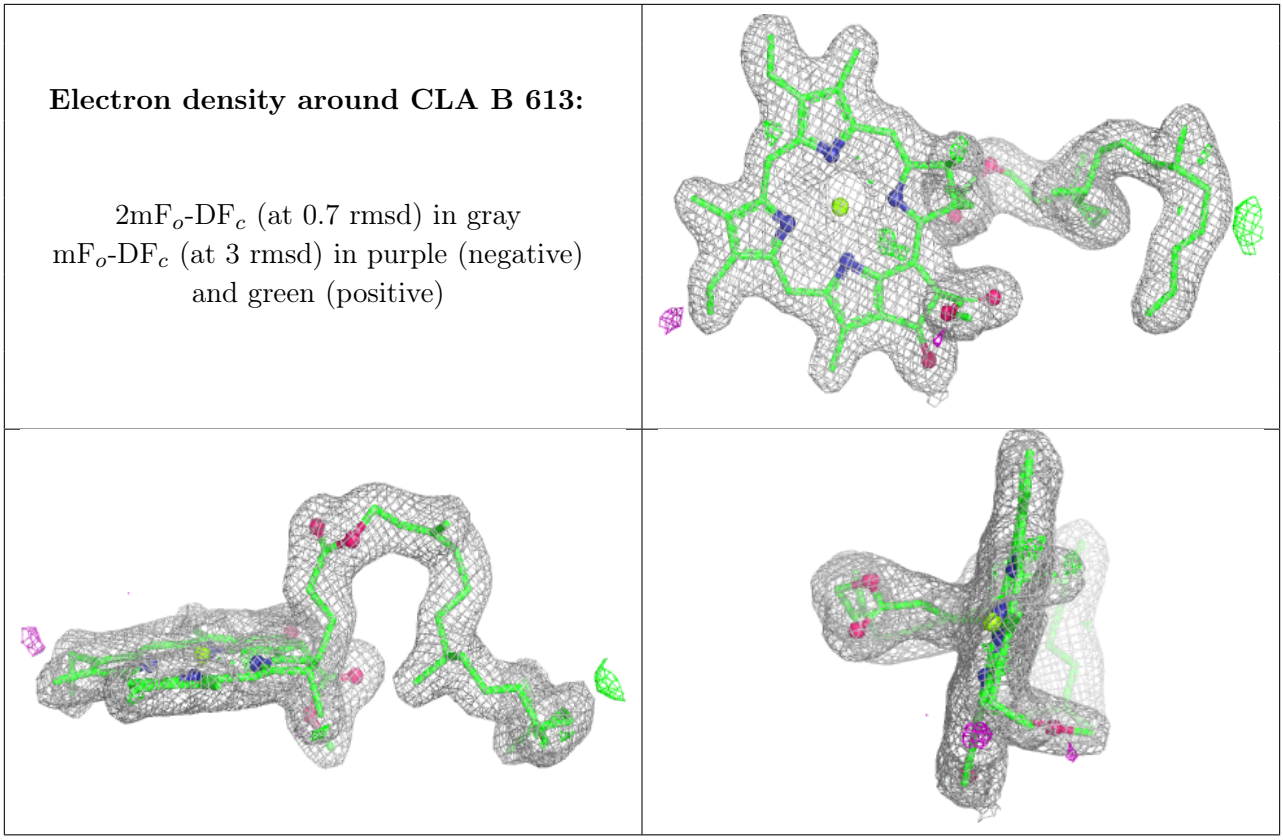






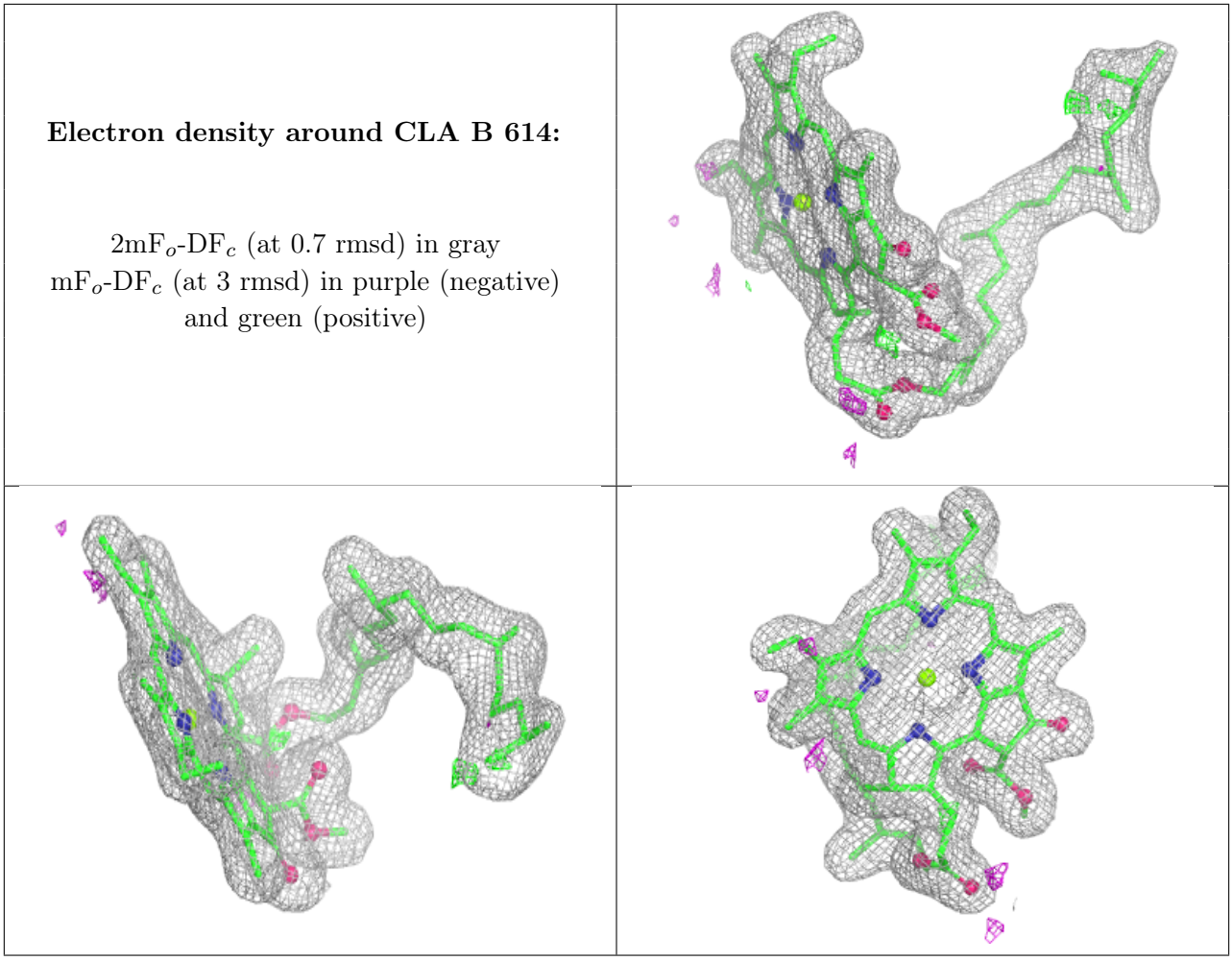
Electron density around CLA B 613:

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



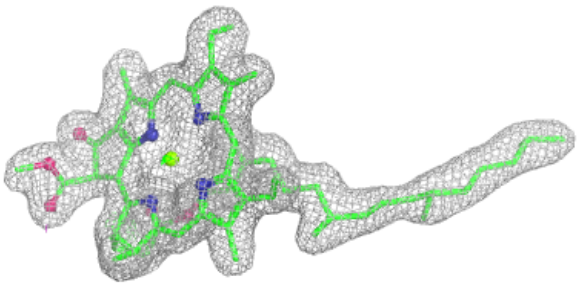
Electron density around CLA B 614:

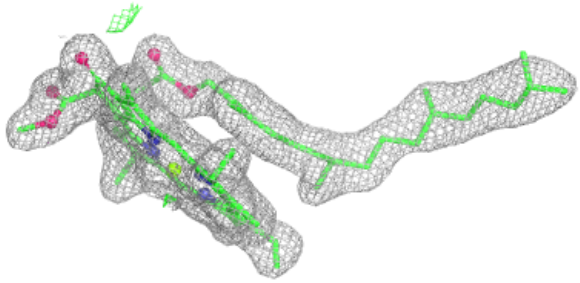
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

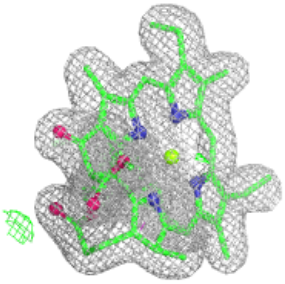


Electron density around CLA c 906:

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

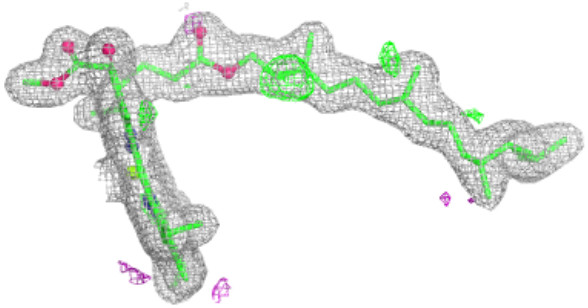


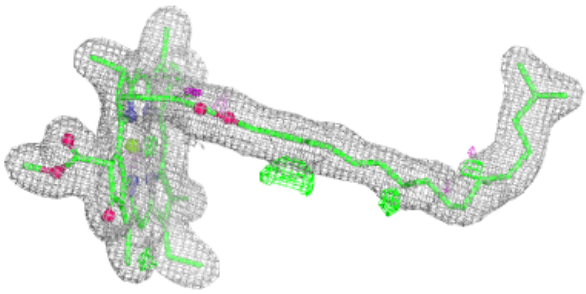


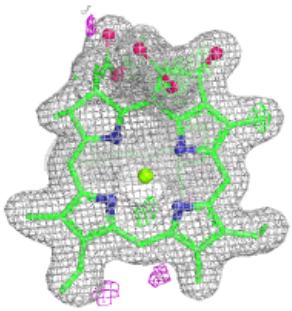


Electron density around CLA B 606:

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

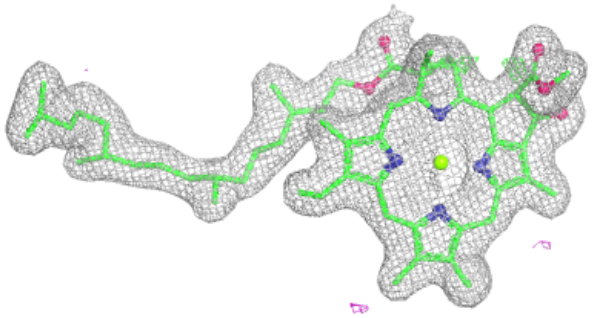


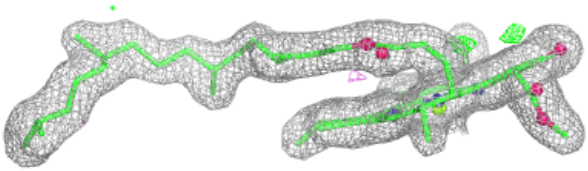


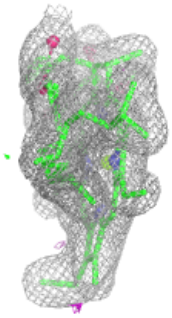


Electron density around CLA b 607:

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

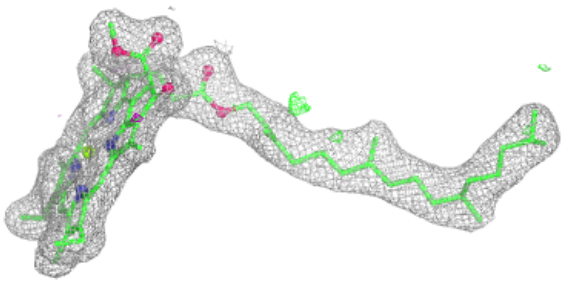


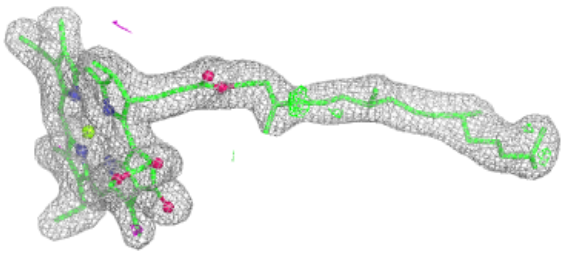


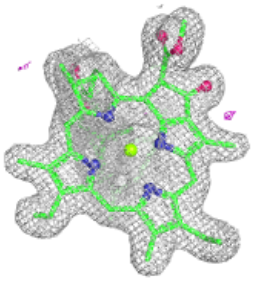


Electron density around CLA b 608:

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

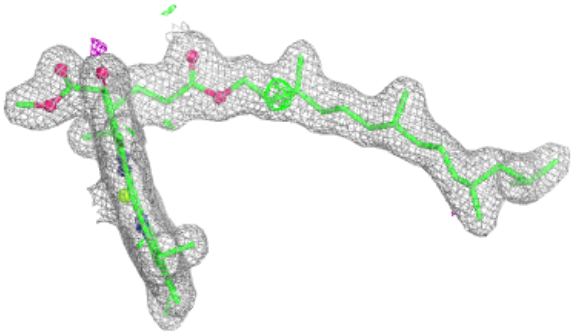


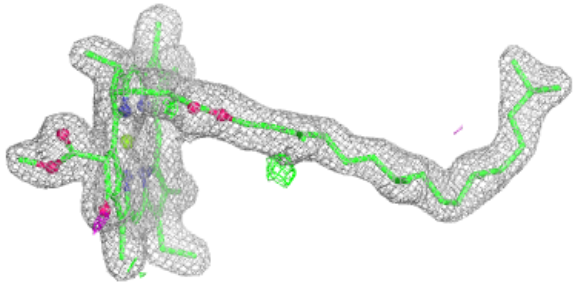


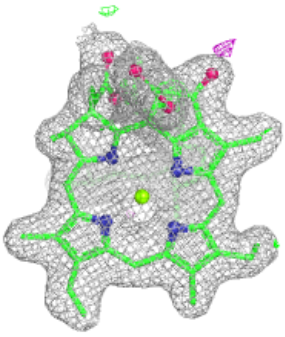


Electron density around CLA b 609:

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

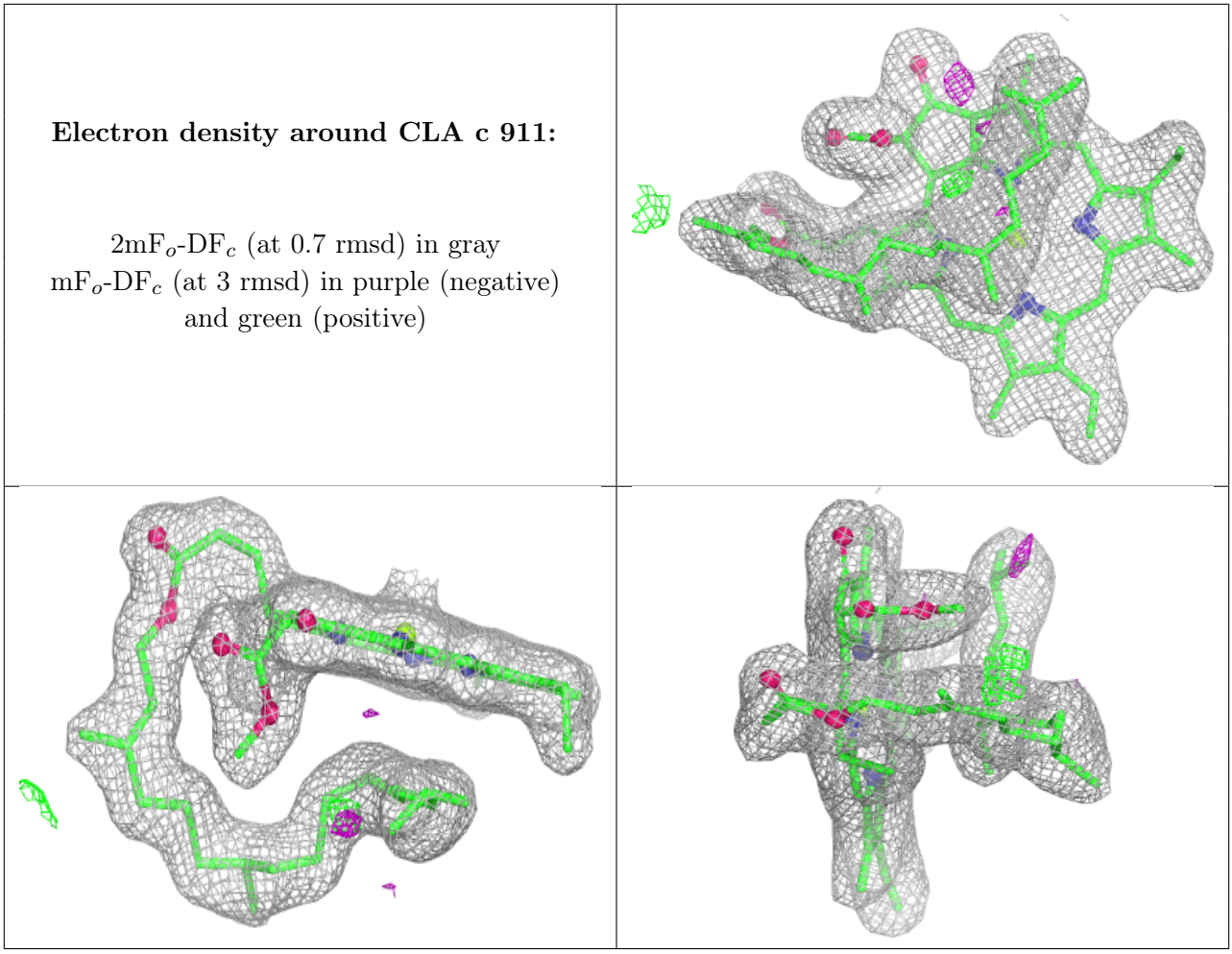






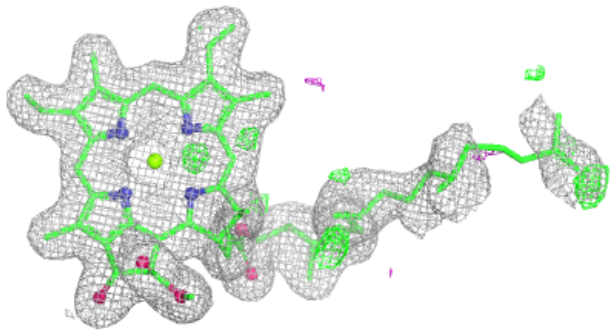
Electron density around CLA c 911:

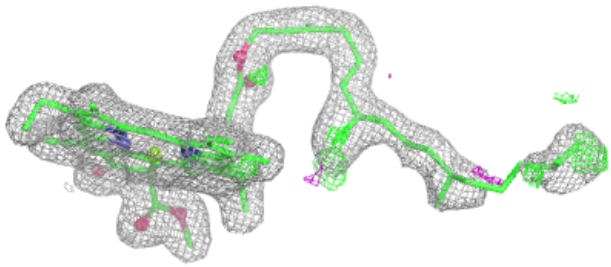
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

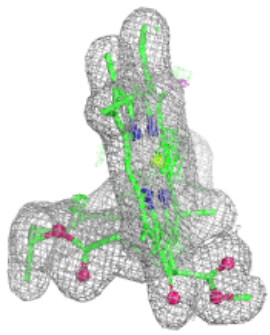


Electron density around CLA A 407:

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

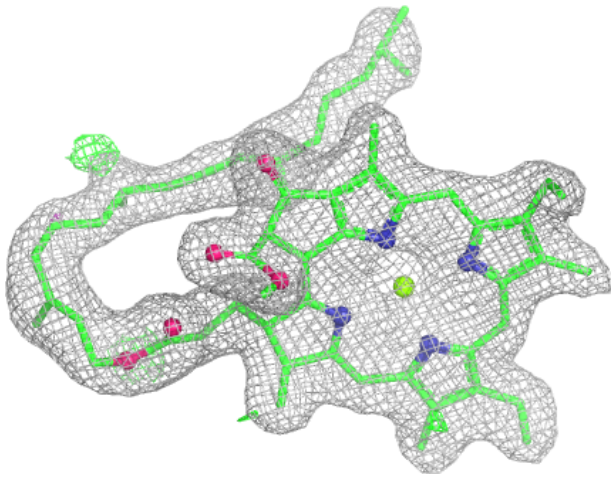


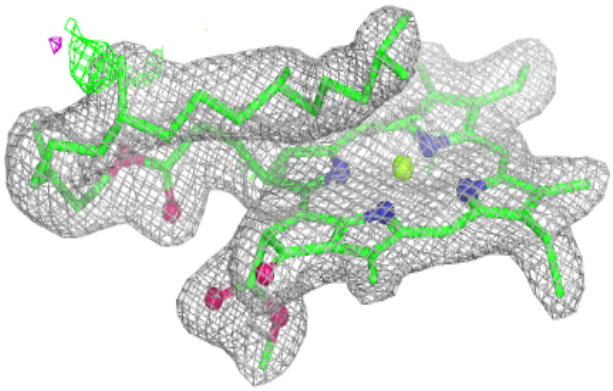


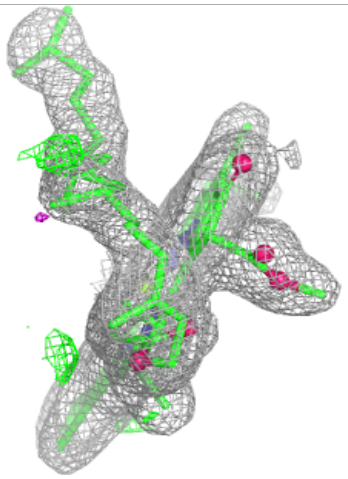


Electron density around CLA C 509:

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

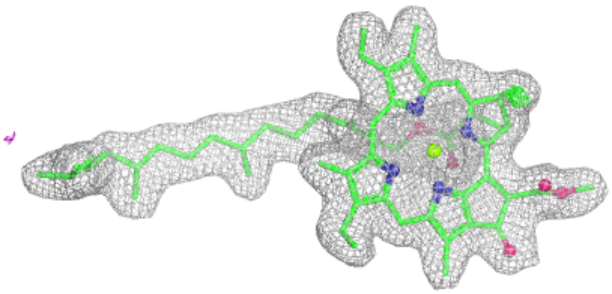


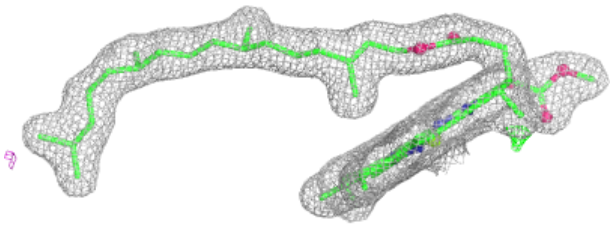


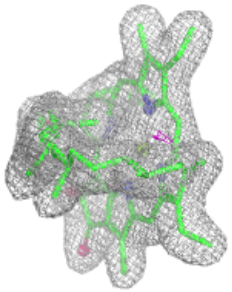


Electron density around CLA b 612:

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

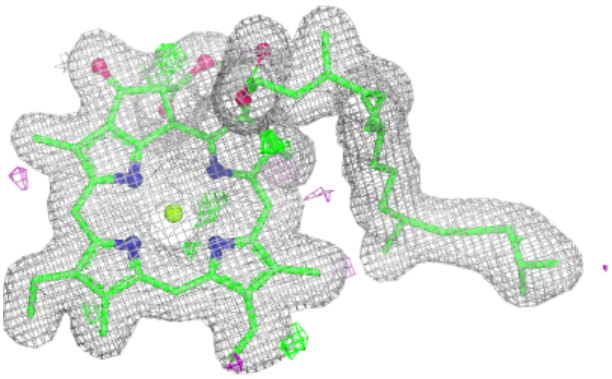


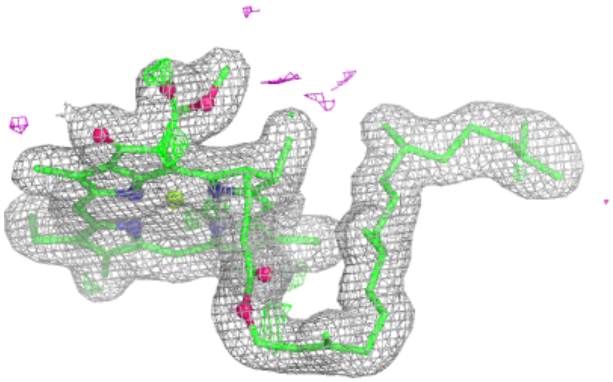


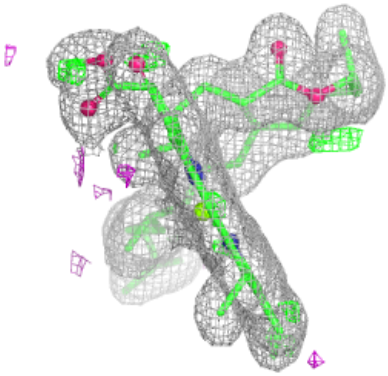


Electron density around CLA d 401:

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

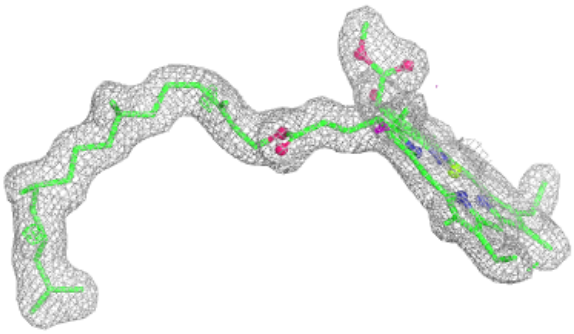


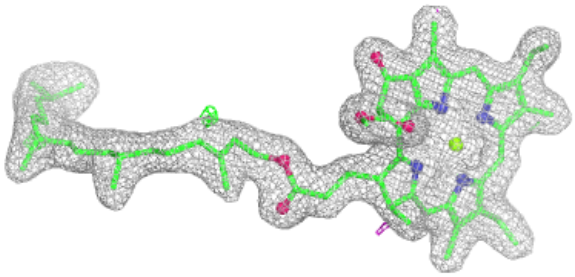


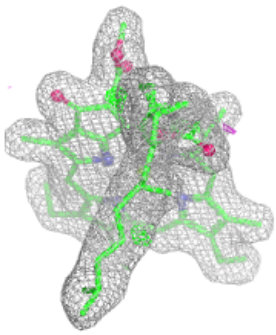


Electron density around CLA d 404:

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

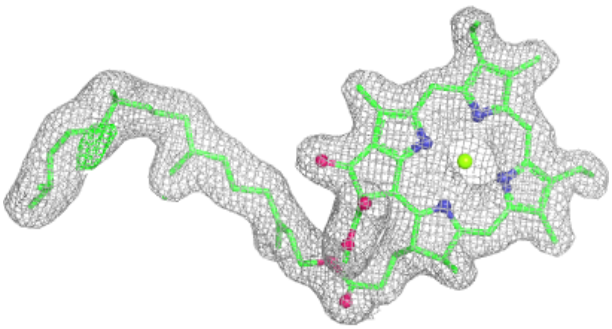


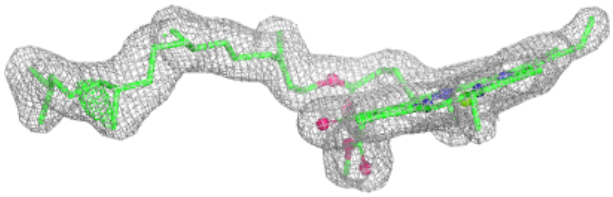


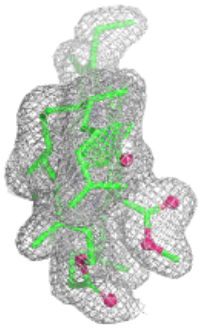


Electron density around CLA B 603:

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

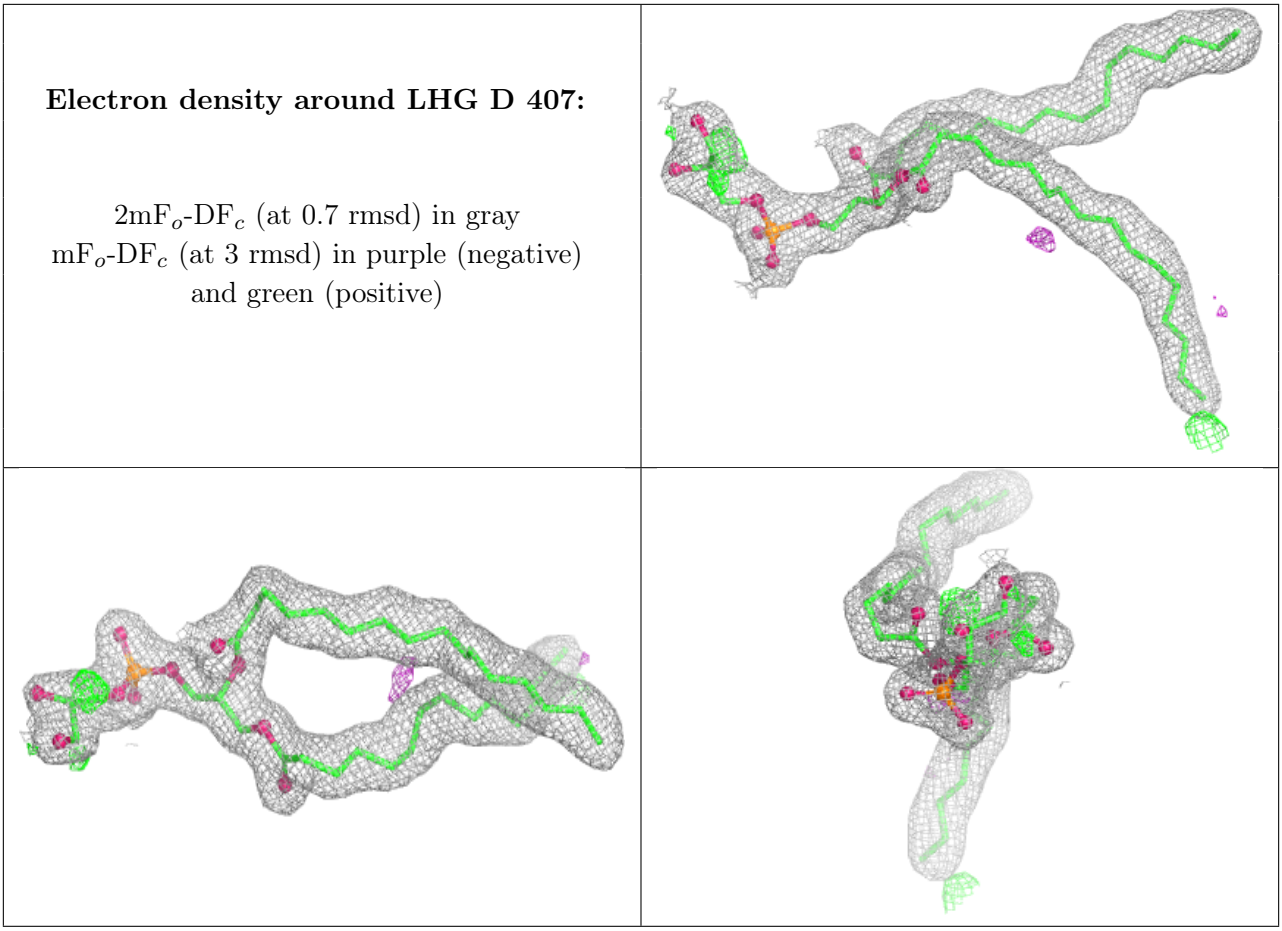






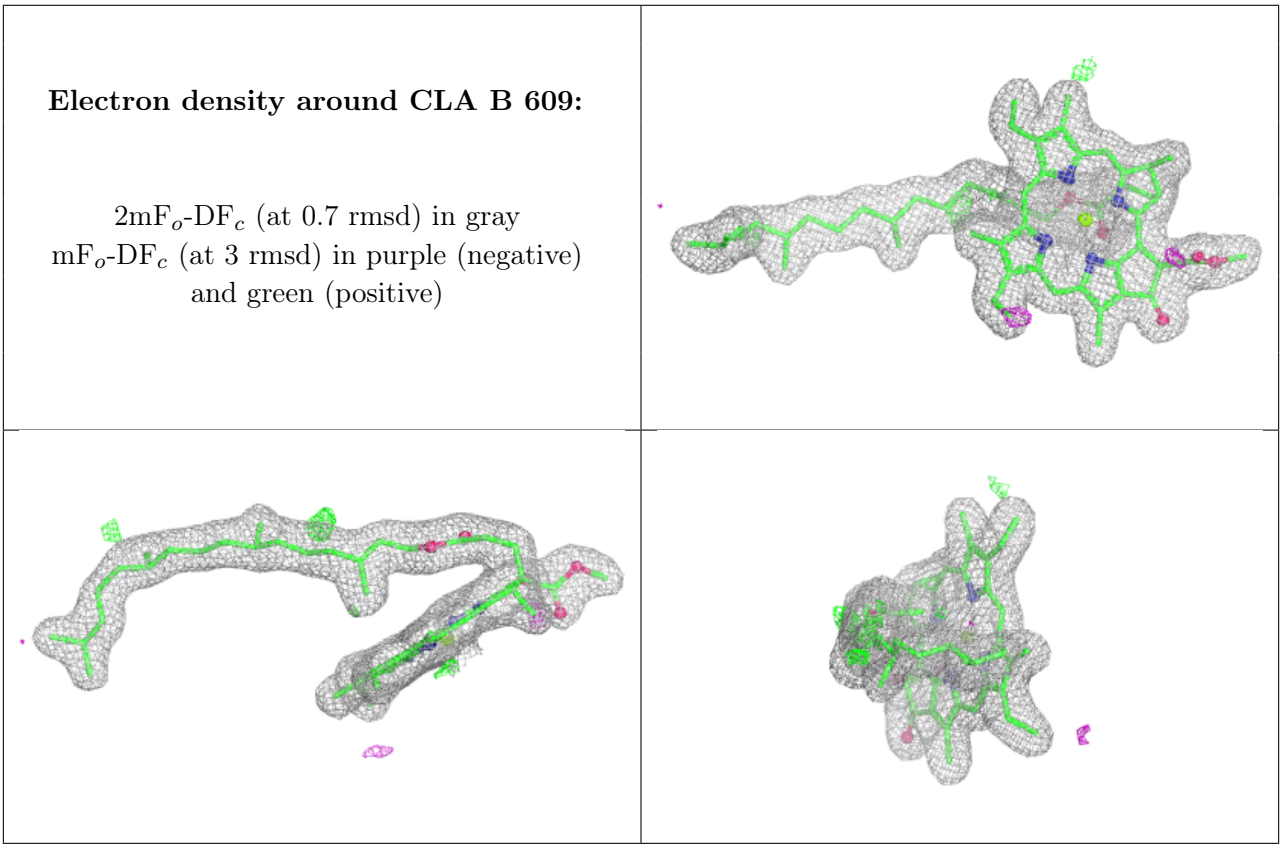
Electron density around LHG D 407:

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



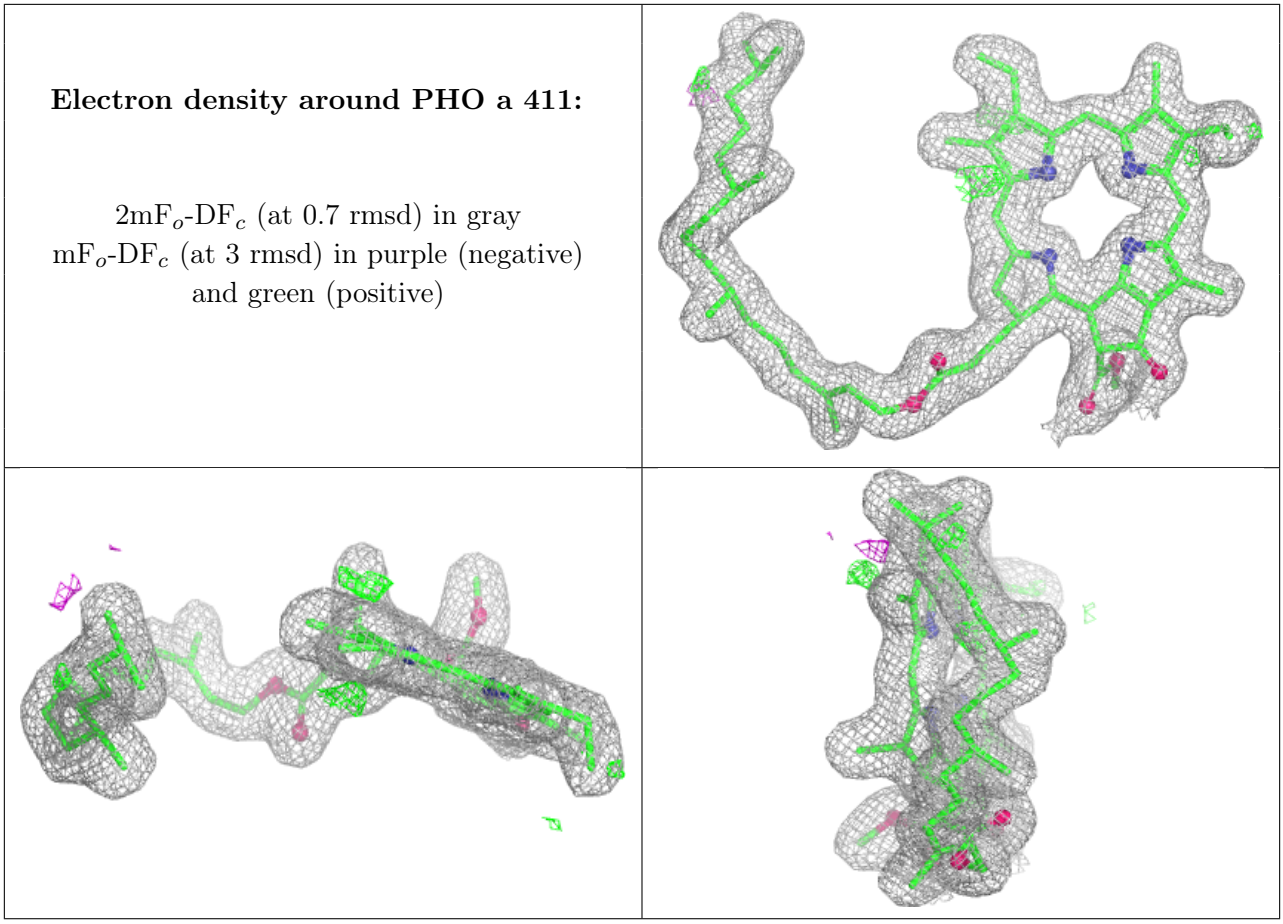
Electron density around CLA B 609:

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



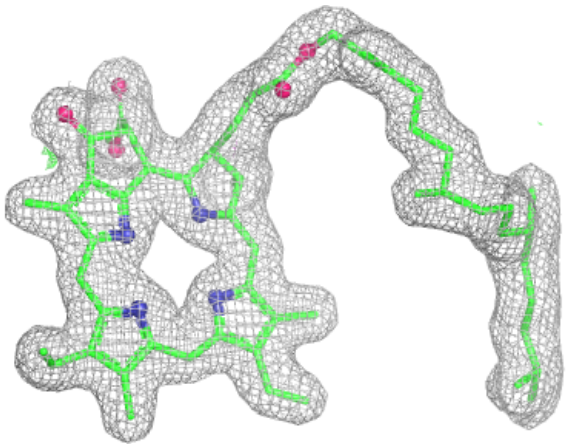
Electron density around PHO a 411:

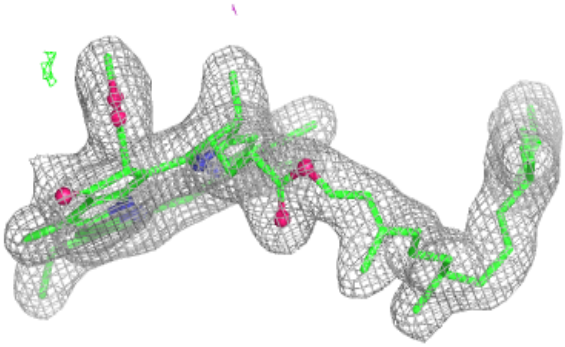
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

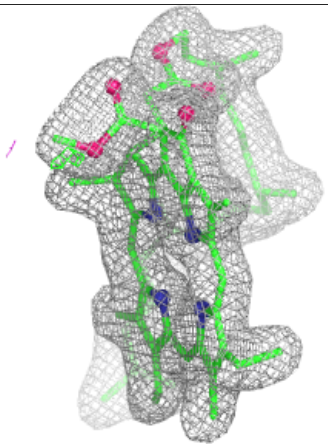


Electron density around PHO a 412:

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

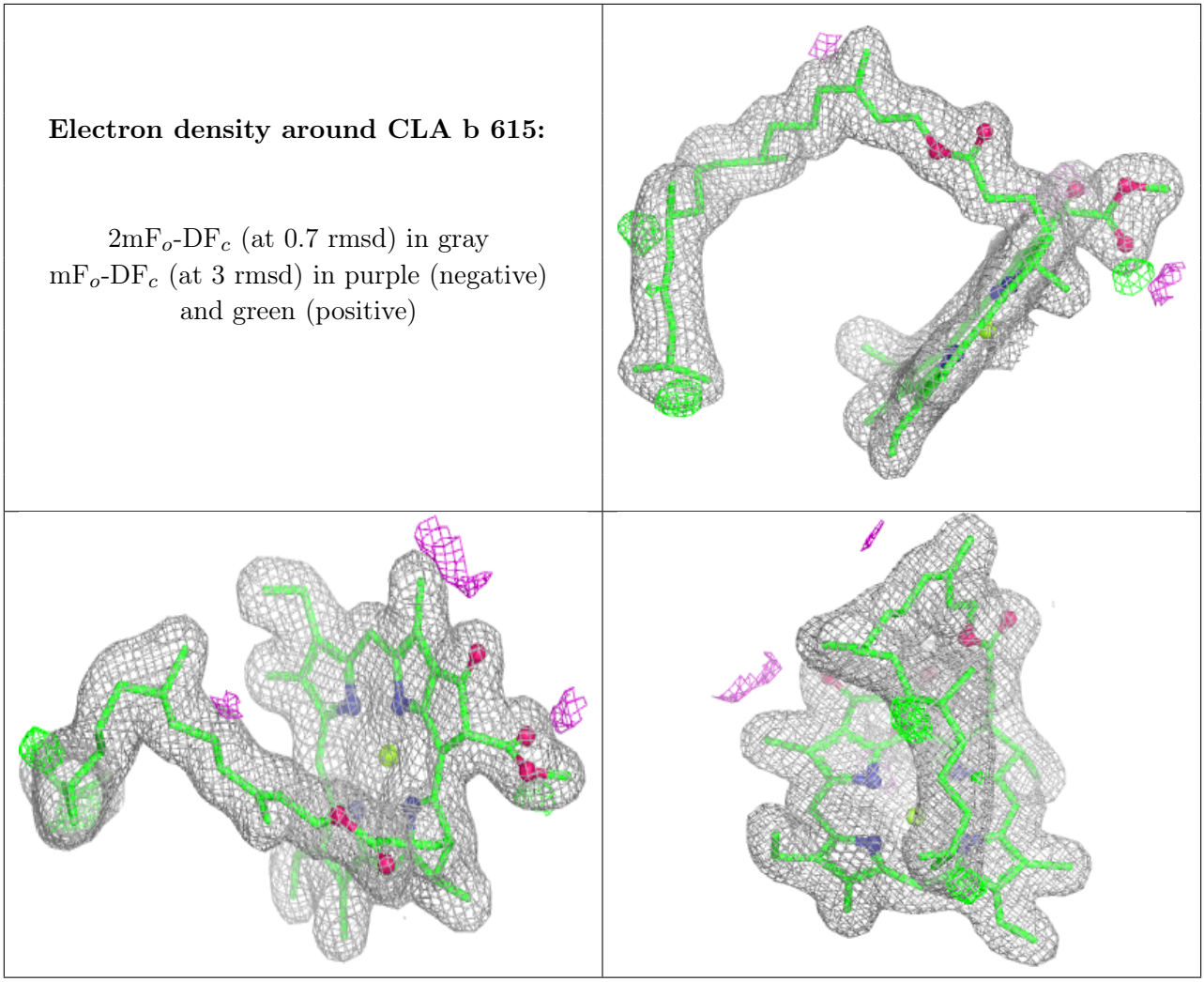






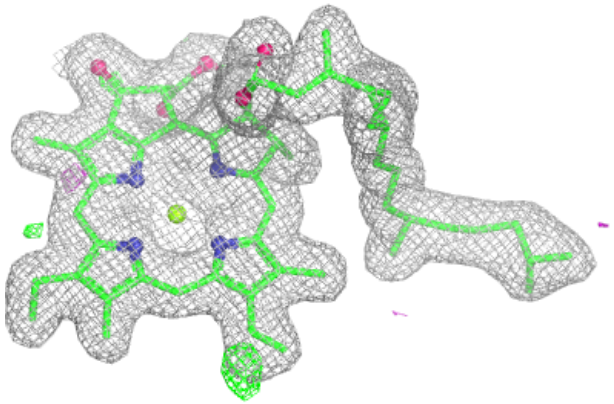
Electron density around CLA b 615:

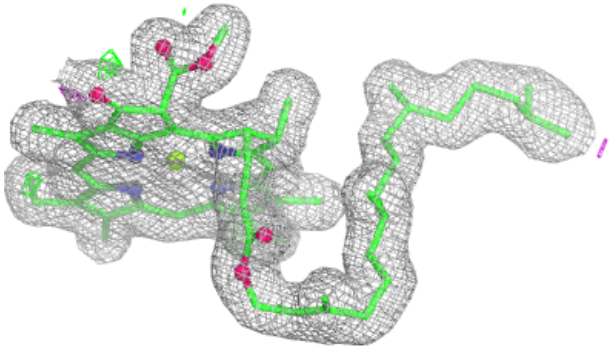
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

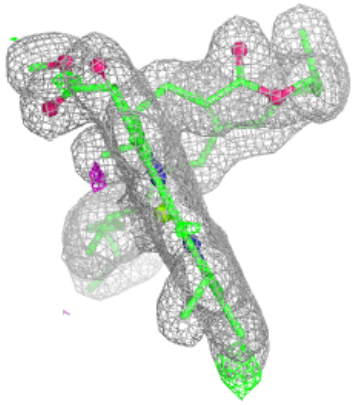


Electron density around CLA A 406:

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

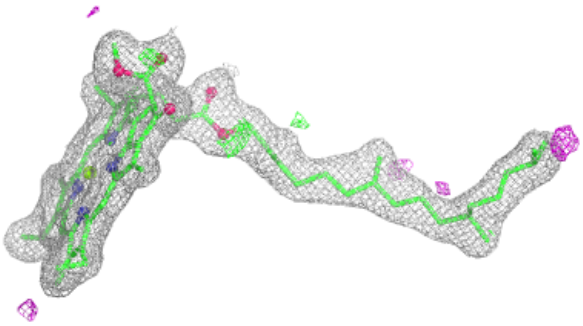


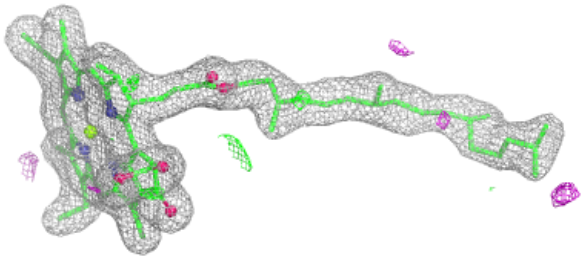


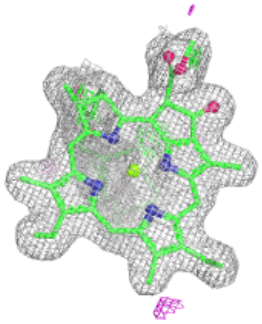


Electron density around CLA B 605:

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

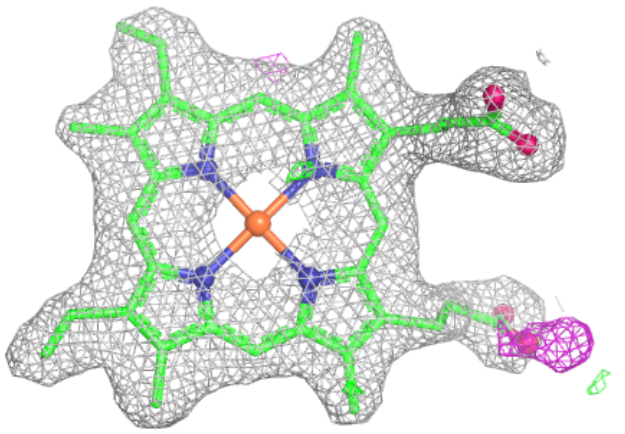


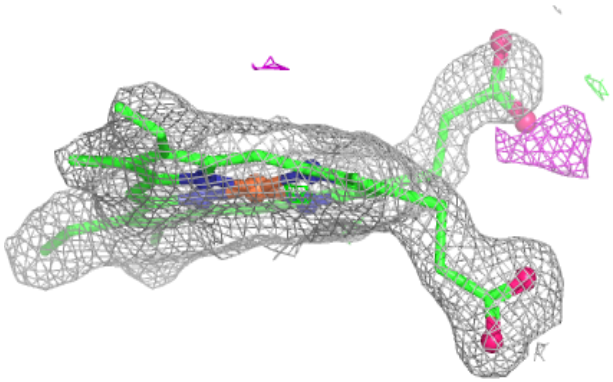


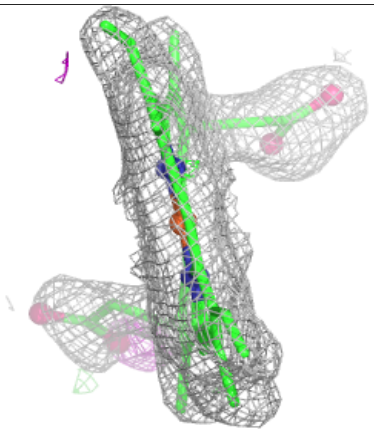


Electron density around HEM f 101:

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

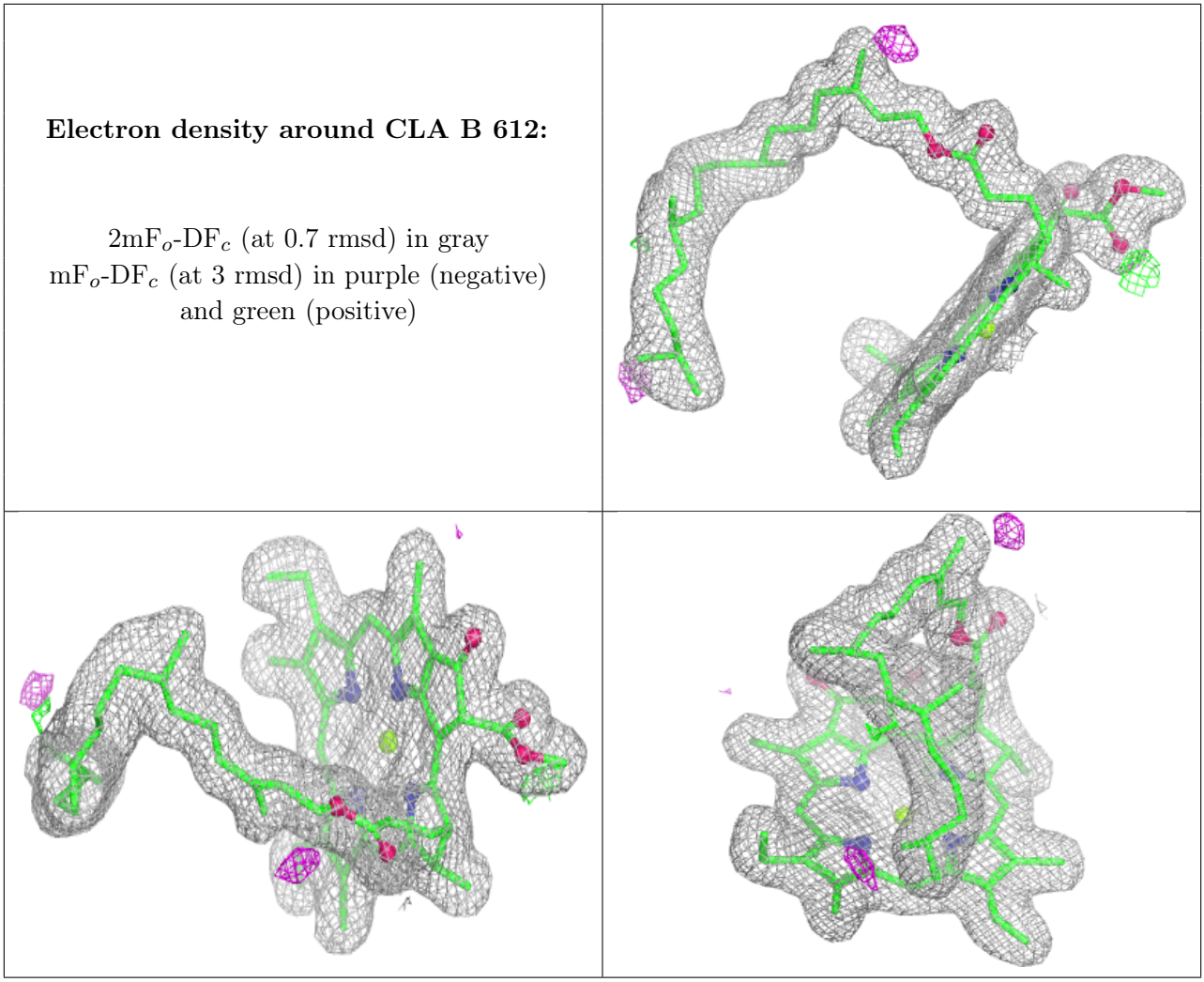






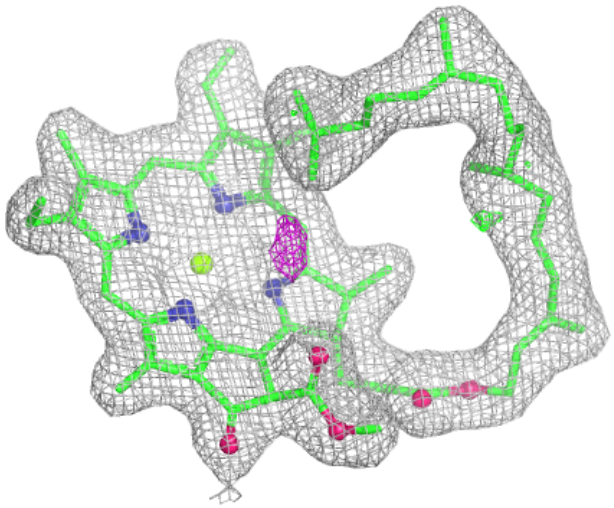
Electron density around CLA B 612:

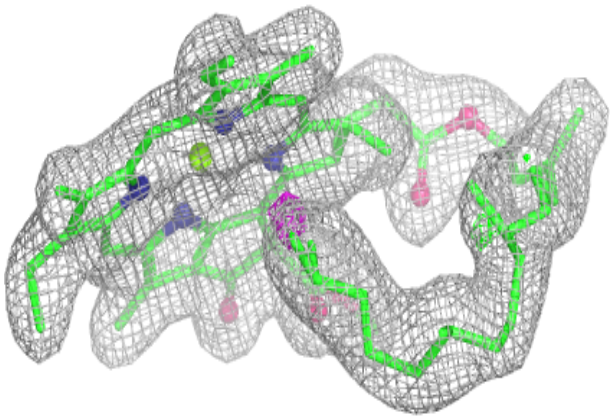
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

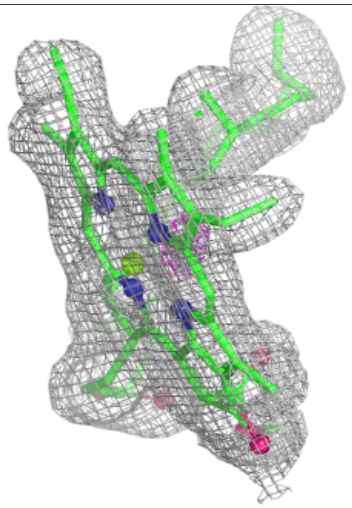


Electron density around CLA b 619:

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

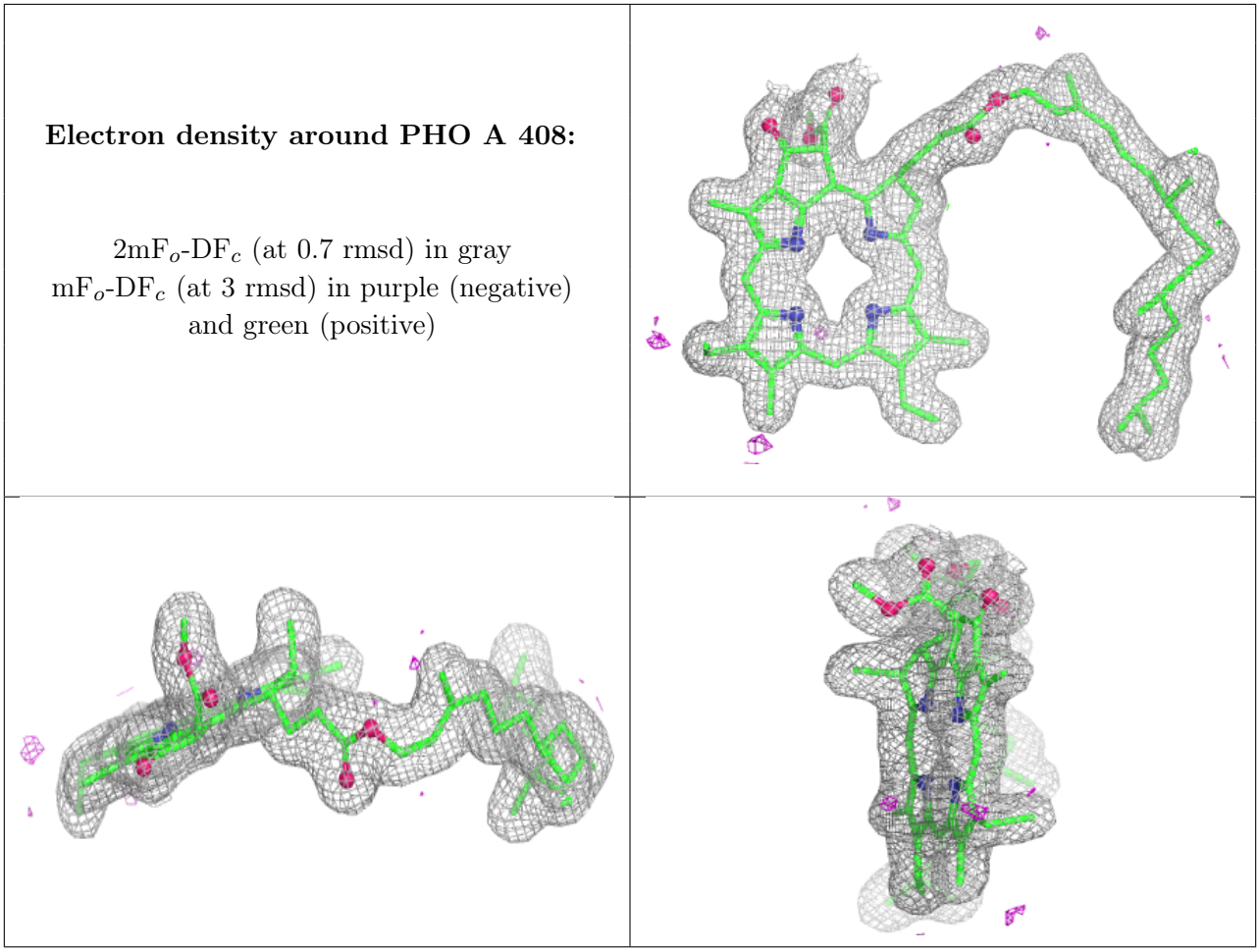






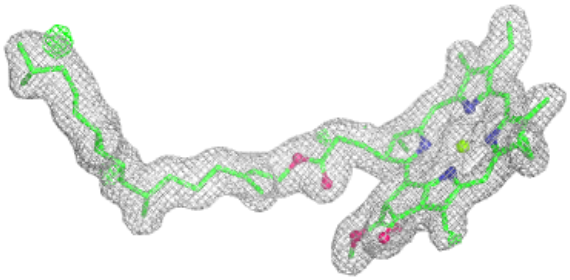
Electron density around PHO A 408:

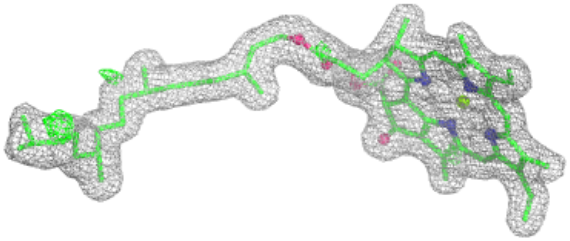
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

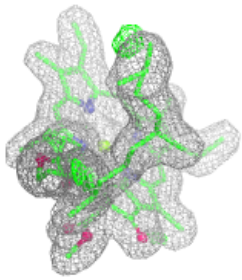


Electron density around CLA A 405:

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

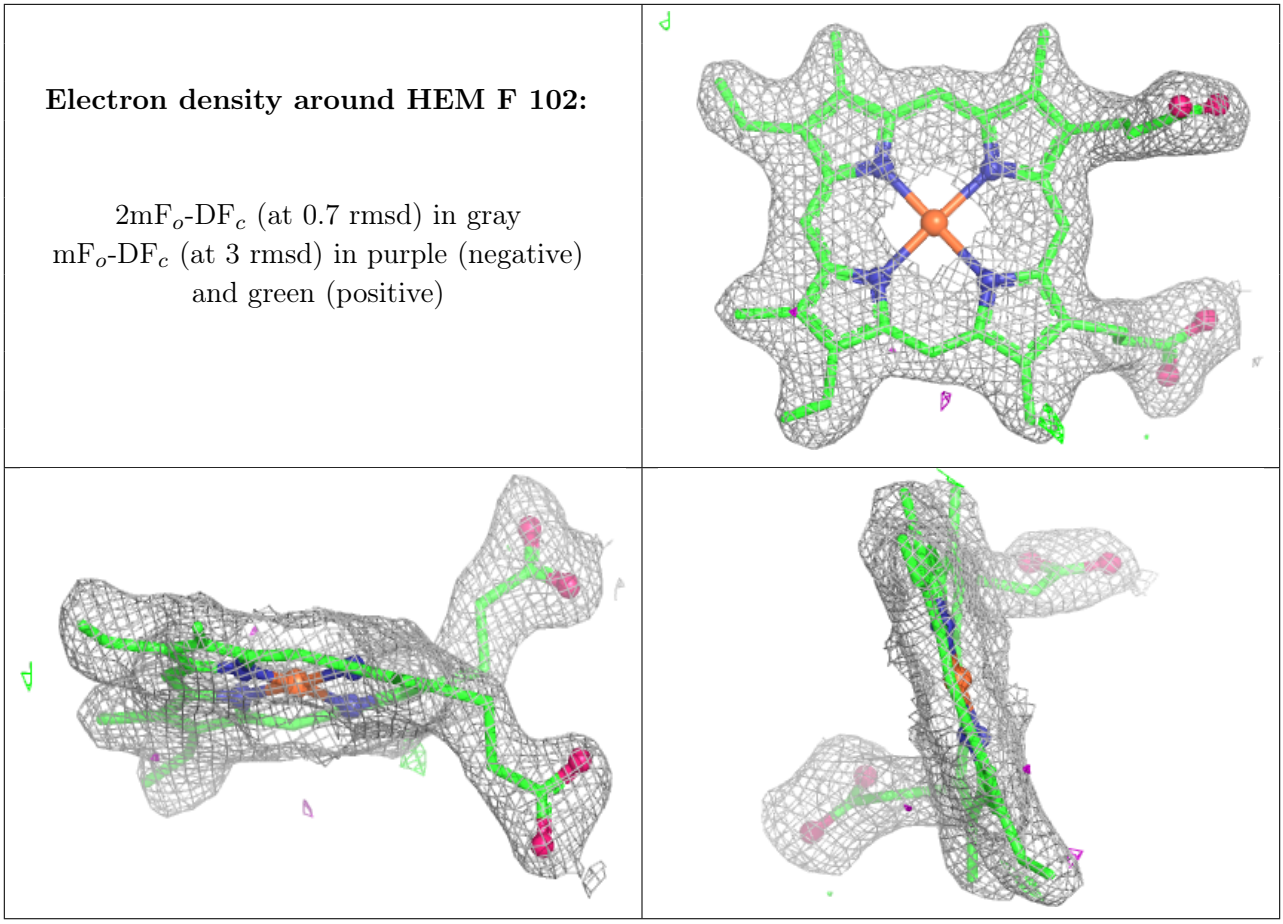






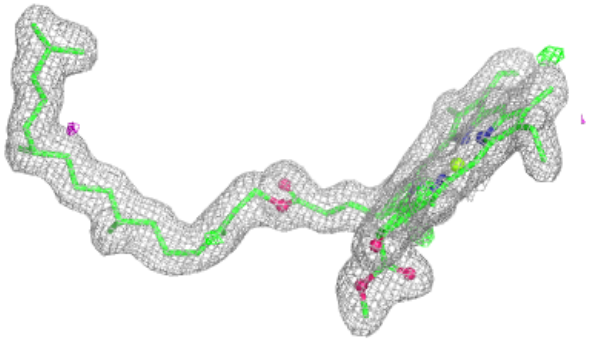
Electron density around HEM F 102:

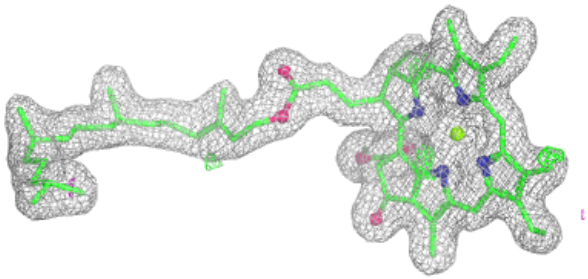
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

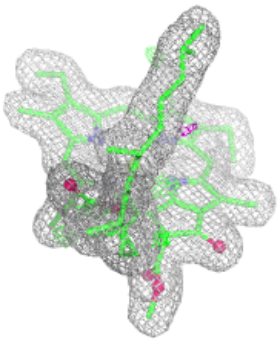


Electron density around CLA D 401:

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

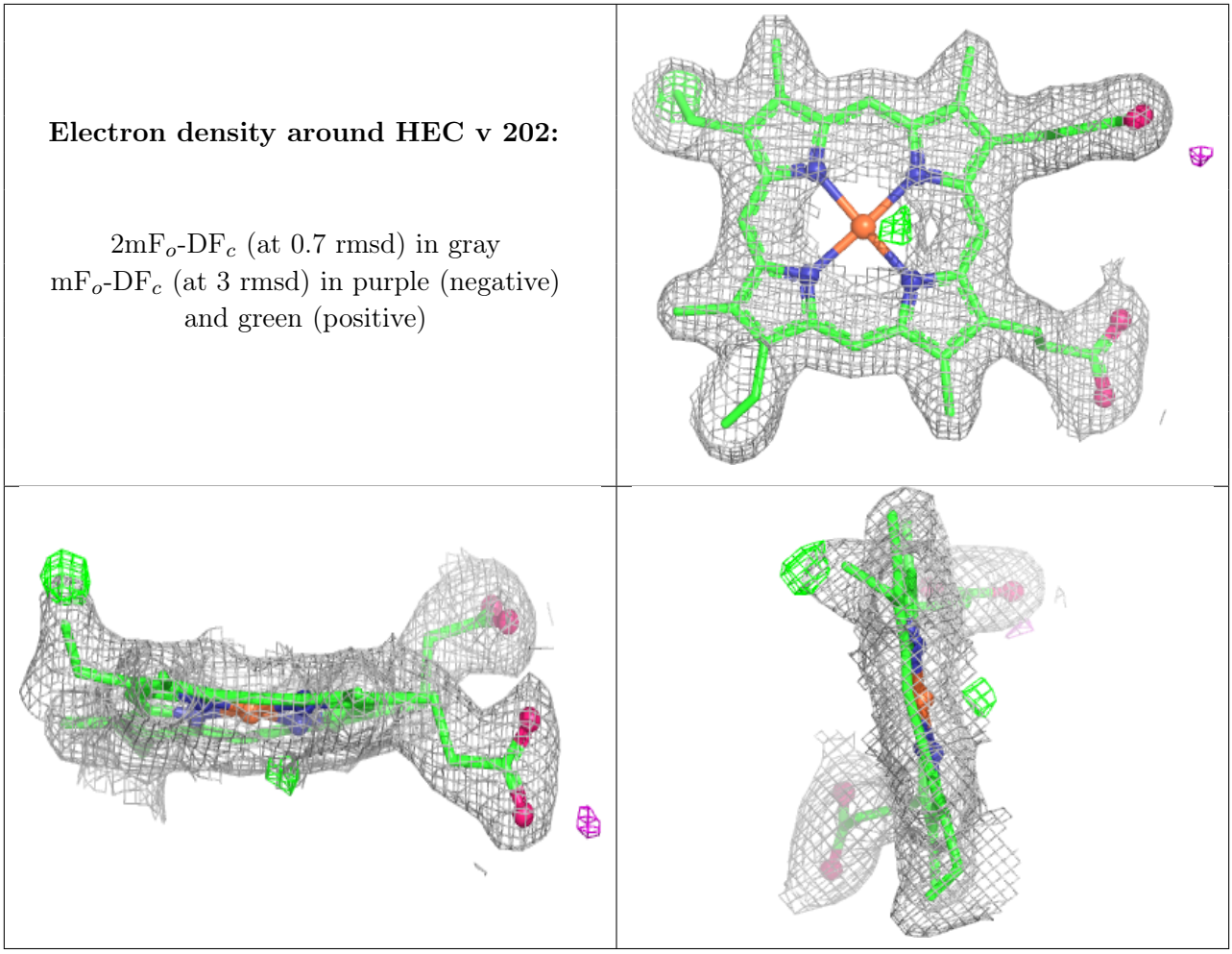






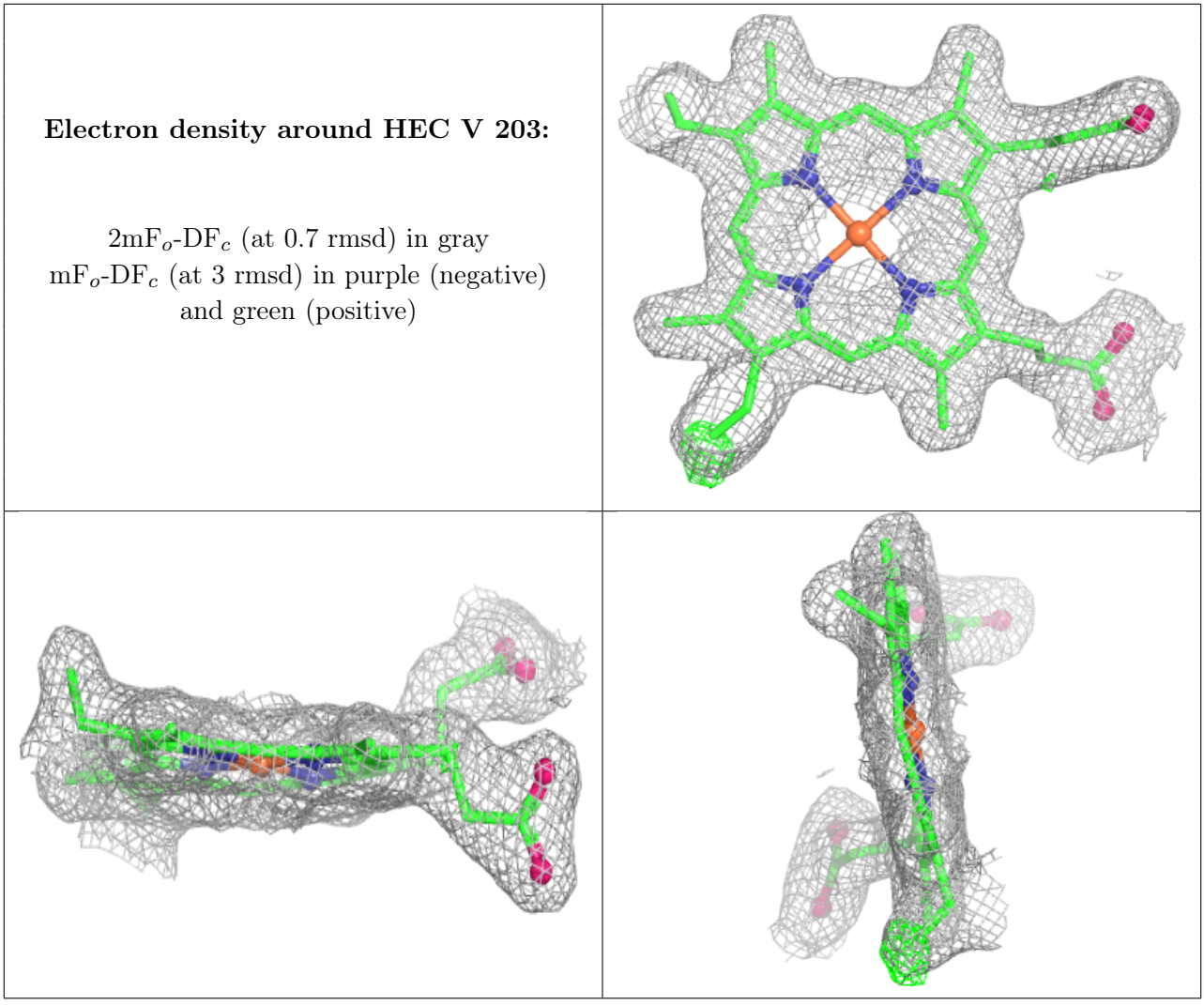
Electron density around HEC v 202:

$2mF_o$-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 203:

$2mF_o$-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.