Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:46 AM UTC

PDB ID	:	4IXQ / pdb_00004ixq
Title	:	RT fs X-ray diffraction of Photosystem II, dark state
Authors	:	Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.
Deposited on	:	2013-01-27
Resolution	:	5.70 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:

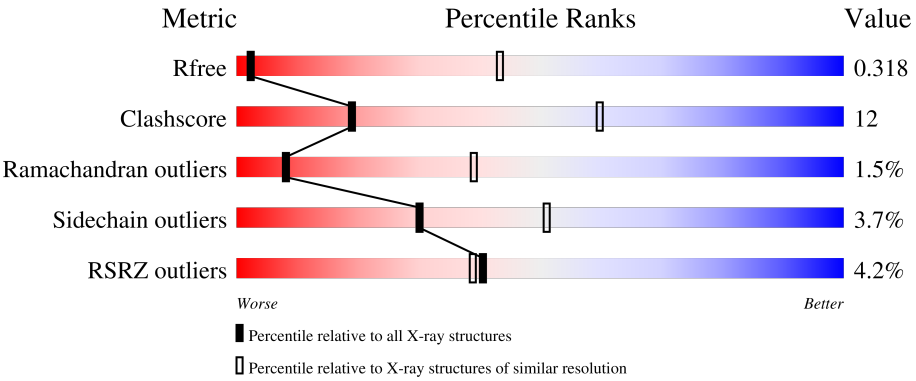
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)

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 5.70 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	1109 (7.40-4.00)
Clashscore	190562	1170 (7.40-4.00)
Ramachandran outliers	187476	1005 (7.40-4.00)
Sidechain outliers	187428	1035 (7.40-3.96)
RSRZ outliers	180081	1102 (7.40-4.00)

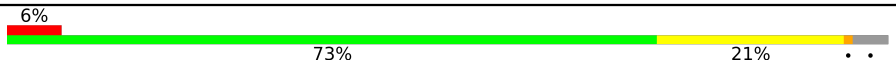
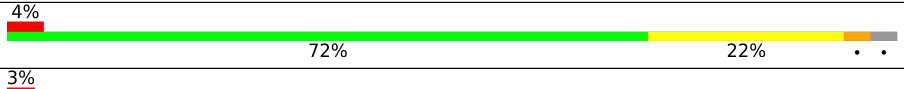
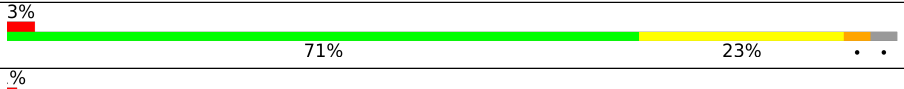
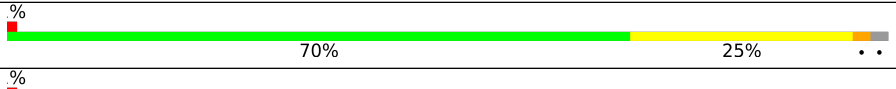
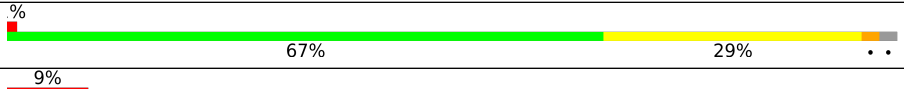
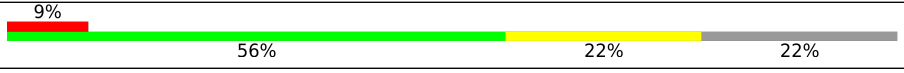
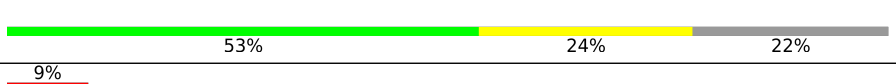
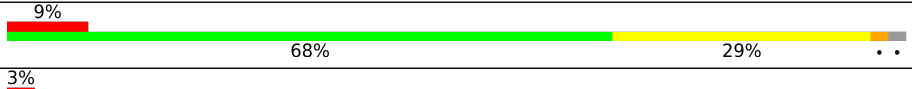
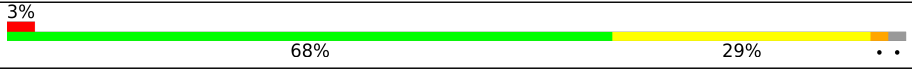
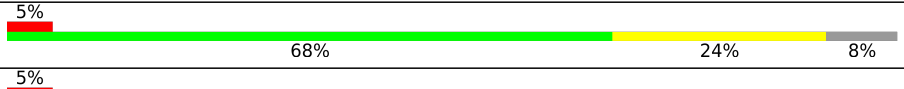
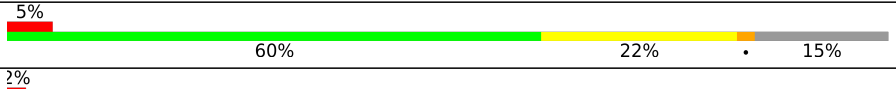
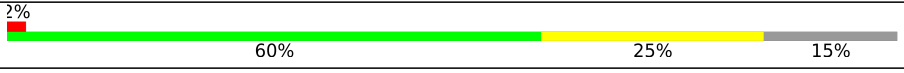
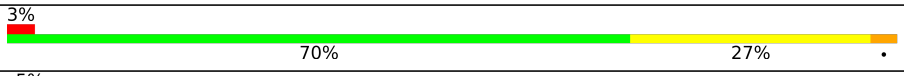
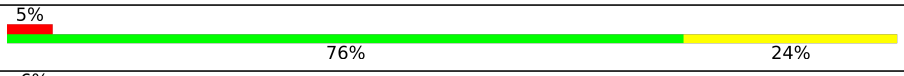
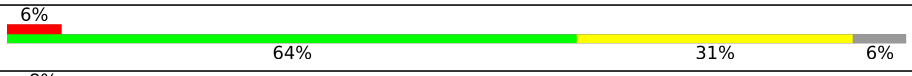
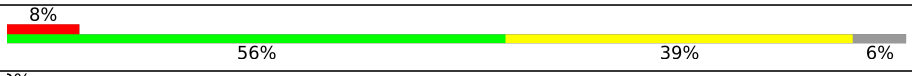
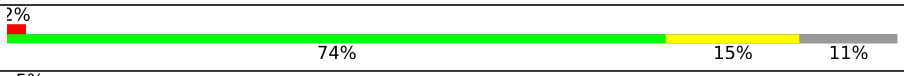
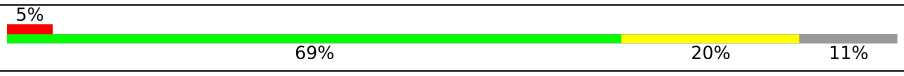
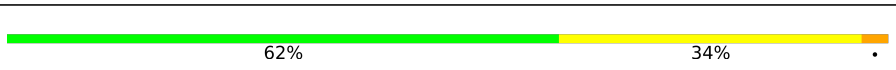
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	4% 65% 27% · 7%
1	a	360	3% 66% 26% · 7%

Continued on next page...

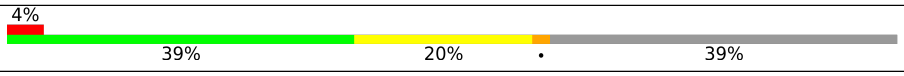
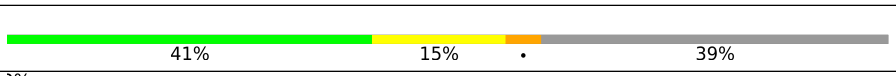
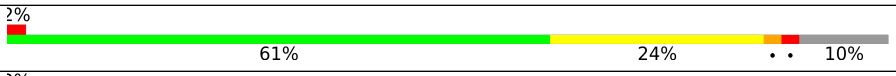
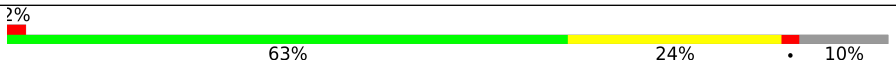
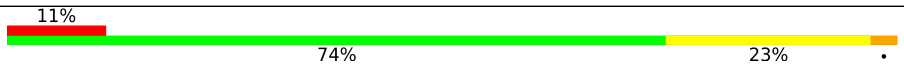
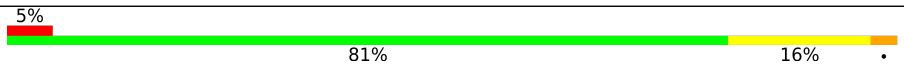
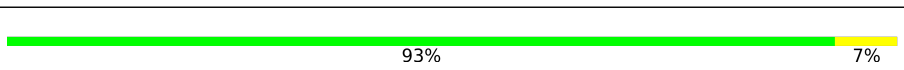
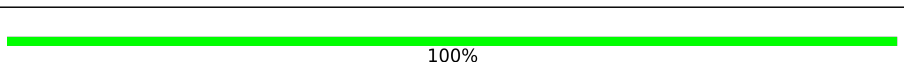
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	G	28	
20	Y	28	

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
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	PL9	J	101	-	-	-	X

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 50232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	15			
1	a	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total 666	C 434	N 108	O 124	0	0	0
5	e	82	Total 666	C 434	N 108	O 124	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total 282	C 192	N 46	O 43	S 1	0	0	0
6	f	35	Total 282	C 192	N 46	O 43	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total 507	C 338	N 81	O 86	S 2	0	0	0
7	h	65	Total 507	C 338	N 81	O 86	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total 286	C 195	N 45	O 45	S 1	0	0	0
8	i	35	Total 286	C 195	N 45	O 45	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	34	Total 249	C 170	N 38	O 40	S 1	0	0	0
9	j	34	Total 249	C 170	N 38	O 40	S 1	0	0	0

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total 304	C 202	N 48	O 53	S 1	0	0	0
11	l	37	Total 304	C 202	N 48	O 53	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total 267	C 178	N 40	O 48	S 1	0	0	0
12	m	34	Total 267	C 178	N 40	O 48	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total 1845	C 1154	N 308	O 379	S 4	0	0	0
13	o	243	Total 1845	C 1154	N 308	O 379	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total 275	C 192	N 40	O 41	S 2	0	0	0
14	t	32	Total 275	C 192	N 40	O 41	S 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	0	0	0
			270	182	41	47			
18	x	37	Total	C	N	O	0	0	0
			270	182	41	47			

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

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

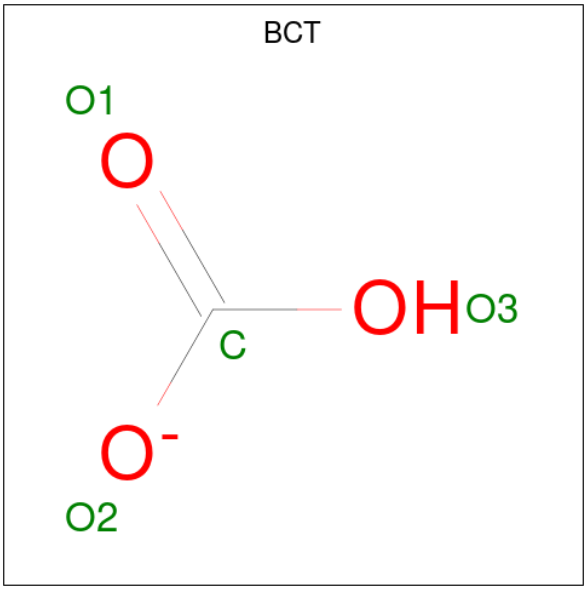
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Y	28	Total	C	N	O	0	0	0
			140	84	28	28			
20	G	28	Total	C	N	O	0	0	0
			140	84	28	28			

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

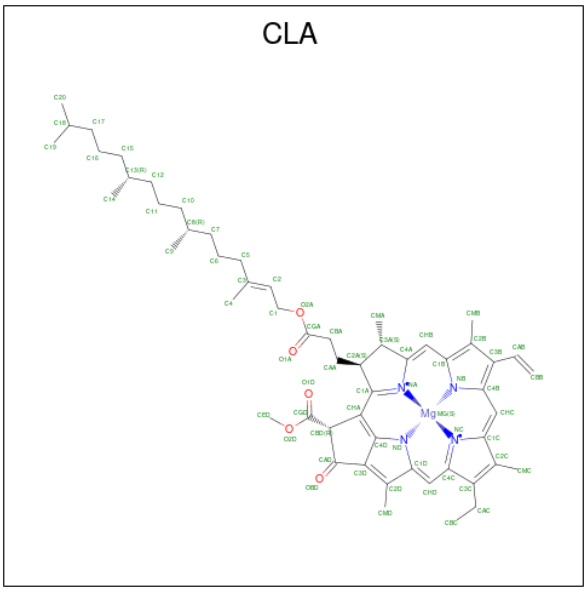
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total Fe 1 1	0	0
21	a	1	Total Fe 1 1	0	0

- Molecule 22 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	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
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

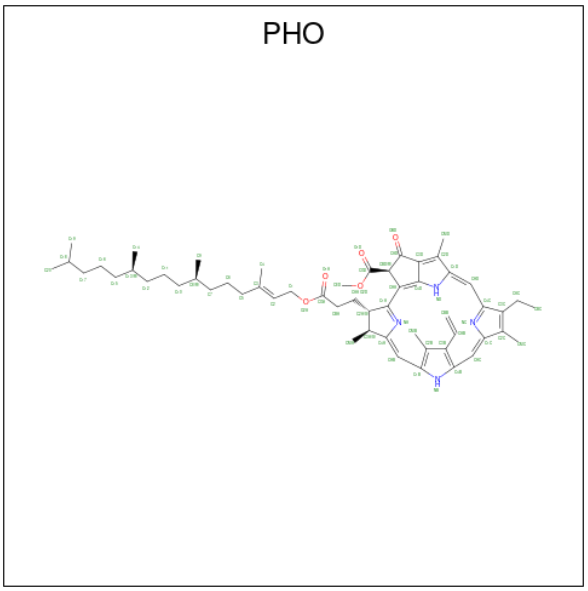
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

Continued on next page...

Continued from previous page...

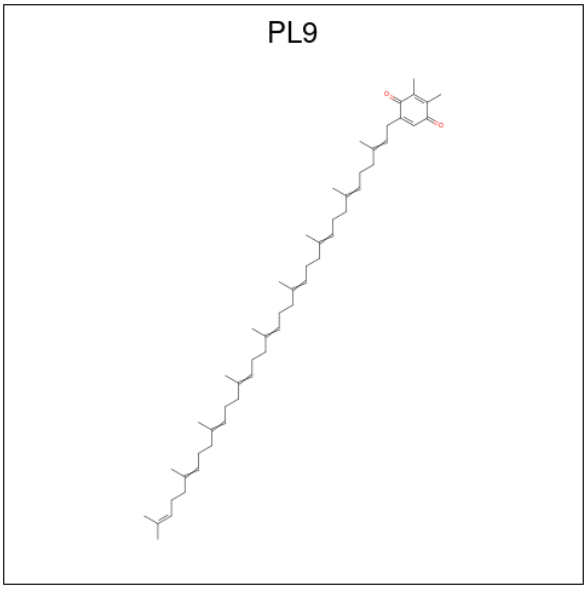
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



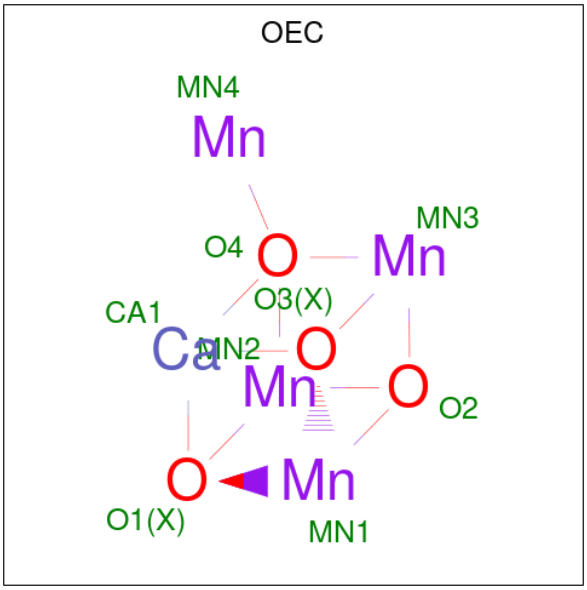
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



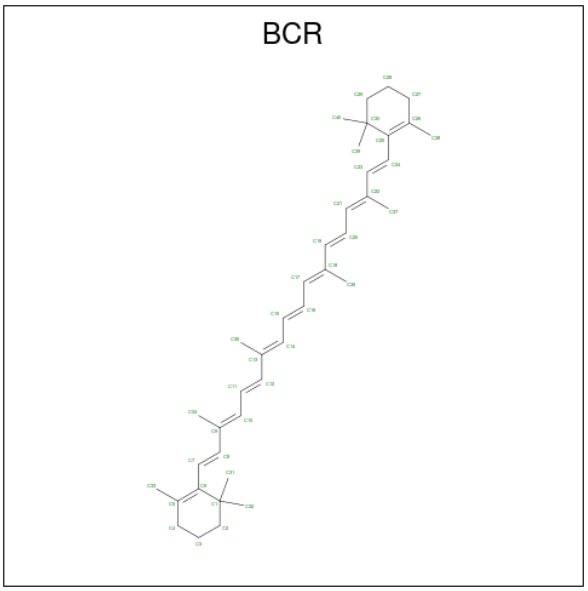
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 45 43 2	0	0
25	D	1	Total C O 55 53 2	0	0
25	J	1	Total C O 35 33 2	0	0
25	a	1	Total C O 45 43 2	0	0
25	d	1	Total C O 55 53 2	0	0
25	j	1	Total C O 35 33 2	0	0

- Molecule 26 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: $CaMn_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total Ca Mn 5 1 4	0	0
26	a	1	Total Ca Mn 5 1 4	0	0

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



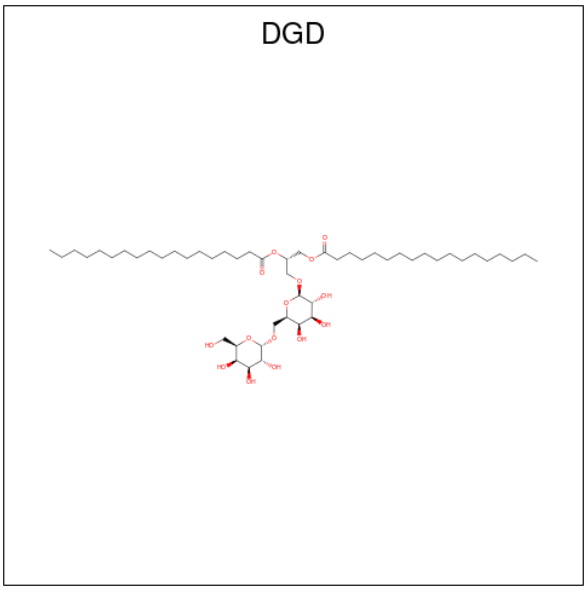
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	K	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	f	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	x	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



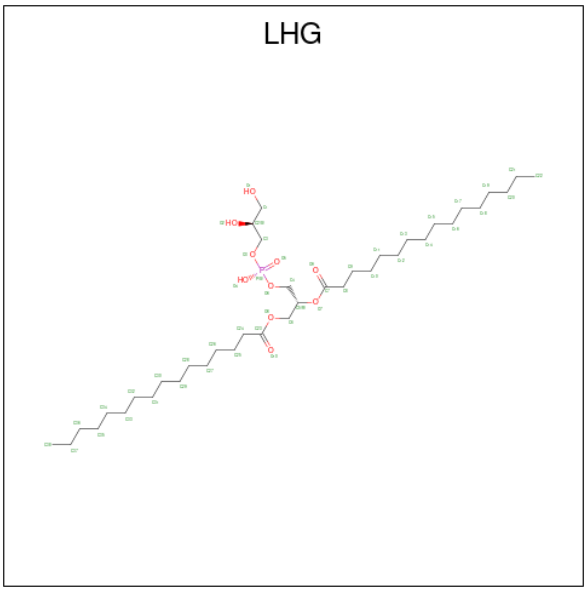
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 56 41 15	0	0

Continued on next page...

Continued from previous page...

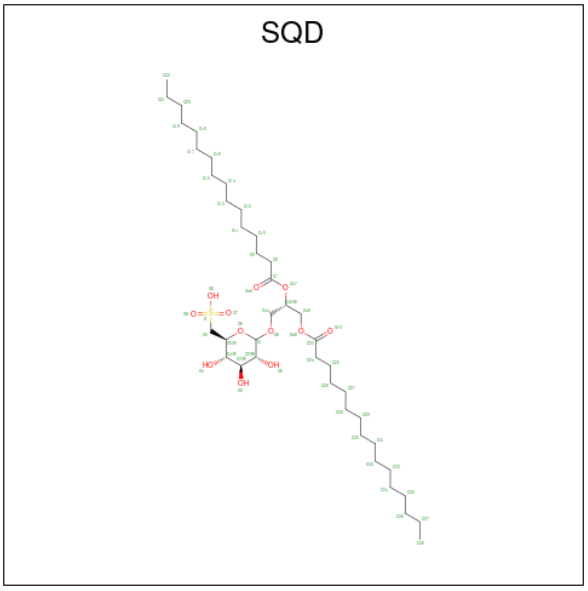
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	B	1	Total C O 58 43 15	0	0
28	B	1	Total C O 52 37 15	0	0
28	C	1	Total C O 53 38 15	0	0
28	C	1	Total C O 62 47 15	0	0
28	C	1	Total C O 66 51 15	0	0
28	D	1	Total C O 63 48 15	0	0
28	a	1	Total C O 56 41 15	0	0
28	b	1	Total C O 52 37 15	0	0
28	b	1	Total C O 58 43 15	0	0
28	c	1	Total C O 53 38 15	0	0
28	c	1	Total C O 62 47 15	0	0
28	c	1	Total C O 66 51 15	0	0
28	d	1	Total C O 63 48 15	0	0

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



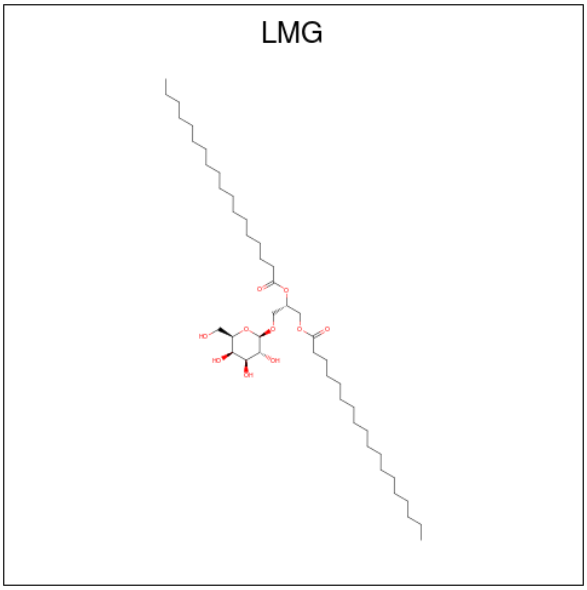
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			39	28	10	1		
29	A	1	Total	C	O	P	0	0
			37	26	10	1		
29	a	1	Total	C	O	P	0	0
			39	28	10	1		
29	a	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 30 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
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			51	41	10		

Continued on next page...

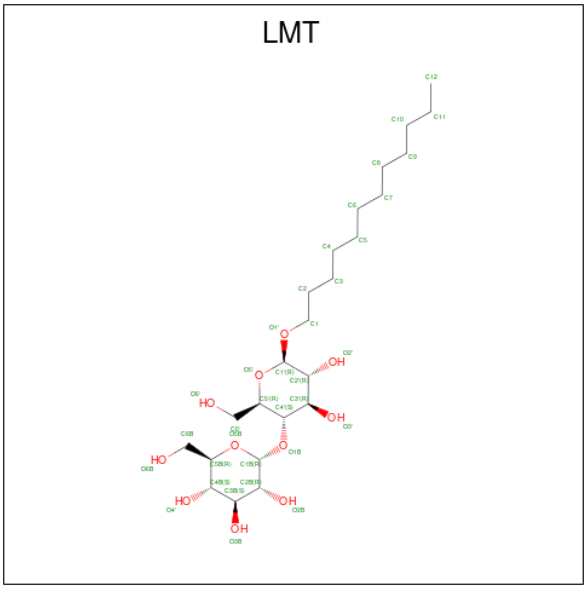
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 42 32 10	0	0
31	B	1	Total C O 49 39 10	0	0
31	C	1	Total C O 48 38 10	0	0
31	C	1	Total C O 45 35 10	0	0
31	D	1	Total C O 46 36 10	0	0
31	D	1	Total C O 49 39 10	0	0
31	D	1	Total C O 48 38 10	0	0
31	E	1	Total C O 44 34 10	0	0
31	I	1	Total C O 43 33 10	0	0
31	M	1	Total C O 42 32 10	0	0
31	M	1	Total C O 42 32 10	0	0
31	a	1	Total C O 42 32 10	0	0
31	a	1	Total C O 51 41 10	0	0
31	b	1	Total C O 49 39 10	0	0
31	b	1	Total C O 49 39 10	0	0
31	c	1	Total C O 45 35 10	0	0
31	d	1	Total C O 46 36 10	0	0
31	d	1	Total C O 48 38 10	0	0
31	e	1	Total C O 44 34 10	0	0
31	i	1	Total C O 43 33 10	0	0
31	k	1	Total C O 48 38 10	0	0

- Molecule 32 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total Cl 1 1	0	0
32	d	1	Total Cl 1 1	0	0

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



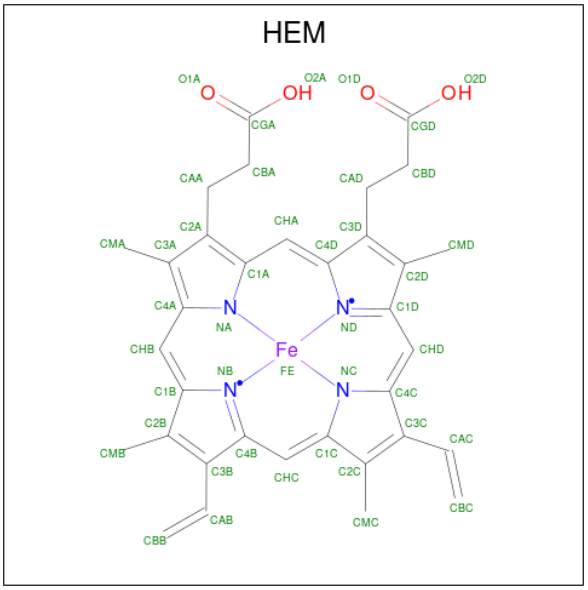
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	D	1	Total C O 31 20 11	0	0
33	I	1	Total C O 35 24 11	0	0
33	M	1	Total C O 35 24 11	0	0
33	T	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	b	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0
33	i	1	Total C O 35 24 11	0	0
33	m	1	Total C O 35 24 11	0	0
33	x	1	Total C O 31 20 11	0	0

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



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

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

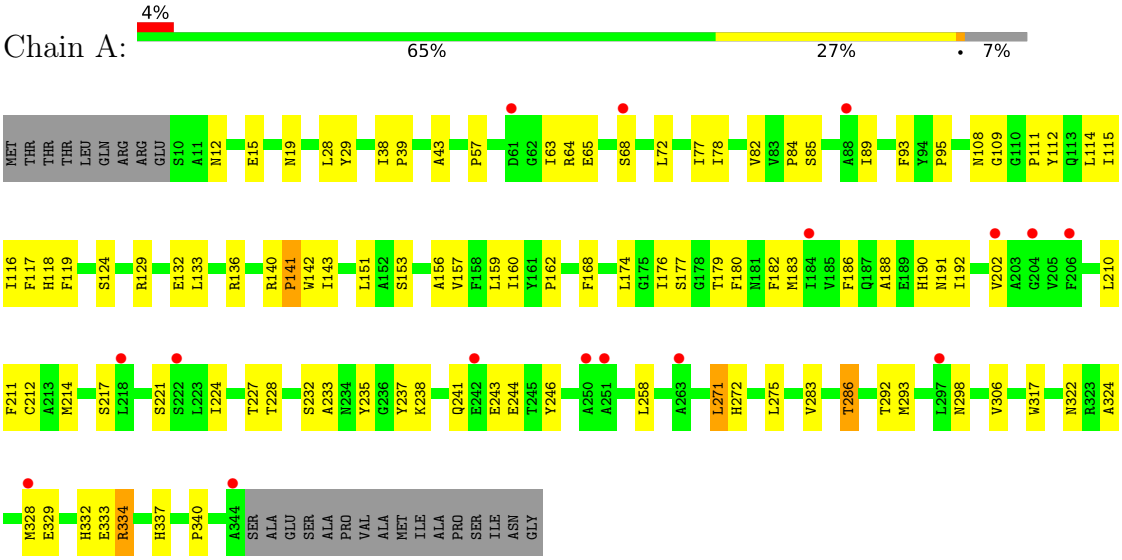
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	K	1	Total Ca 1 1	0	0
35	O	1	Total Ca 1 1	0	0
35	k	1	Total Ca 1 1	0	0
35	o	1	Total Ca 1 1	0	0

3 Residue-property plots (i)

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

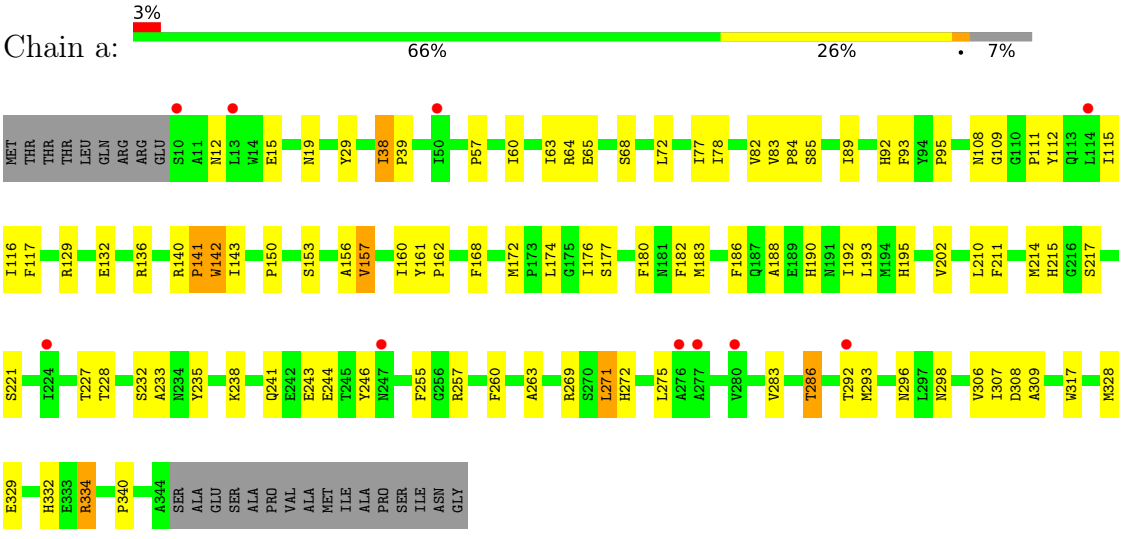
• Molecule 1: Photosystem Q(B) protein 1

Chain A:



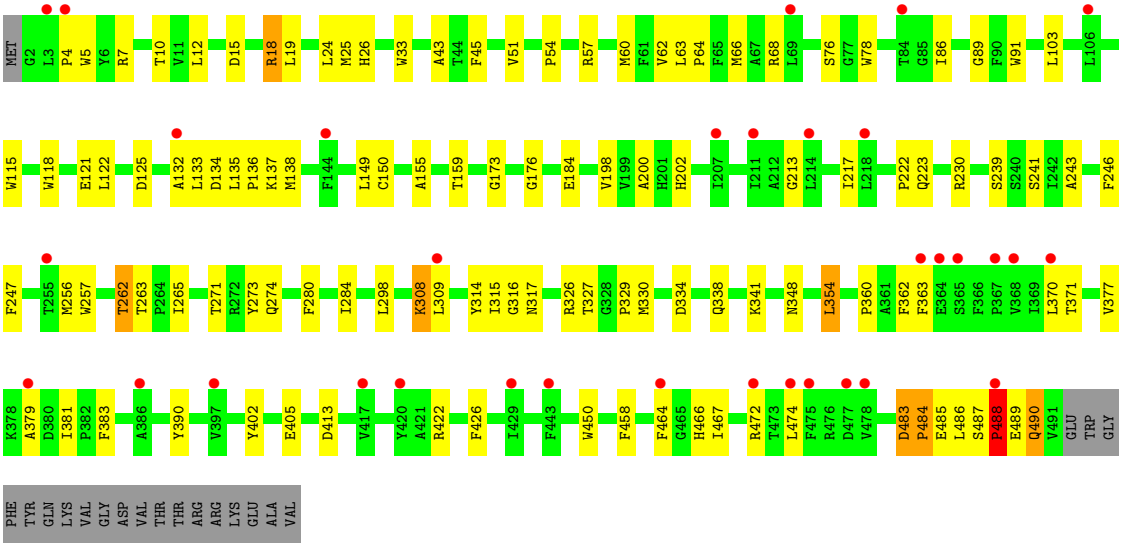
• Molecule 1: Photosystem Q(B) protein 1

Chain a:



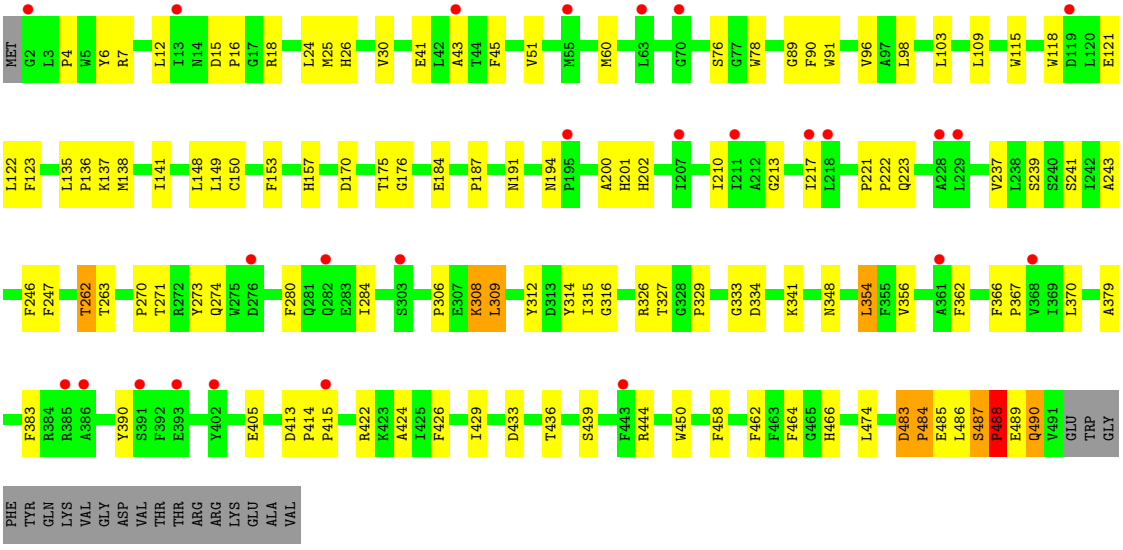
• Molecule 2: Photosystem II core light harvesting protein

Chain B:



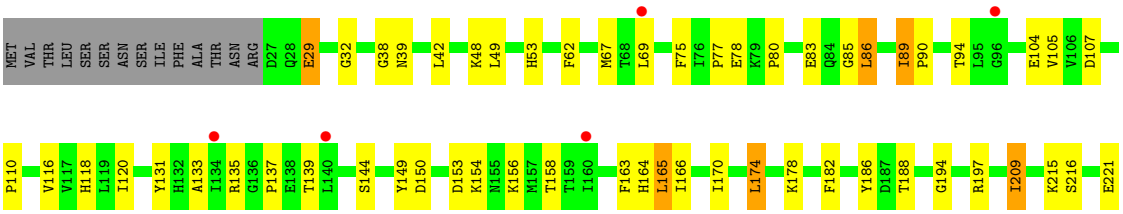
• Molecule 2: Photosystem II core light harvesting protein

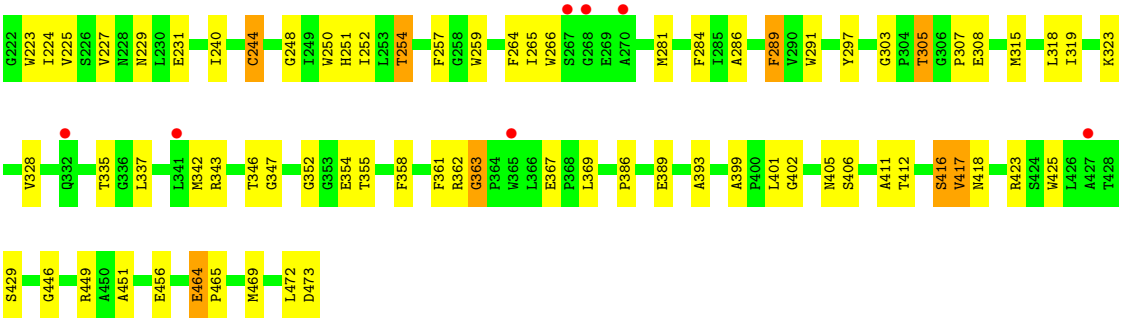
Chain b:



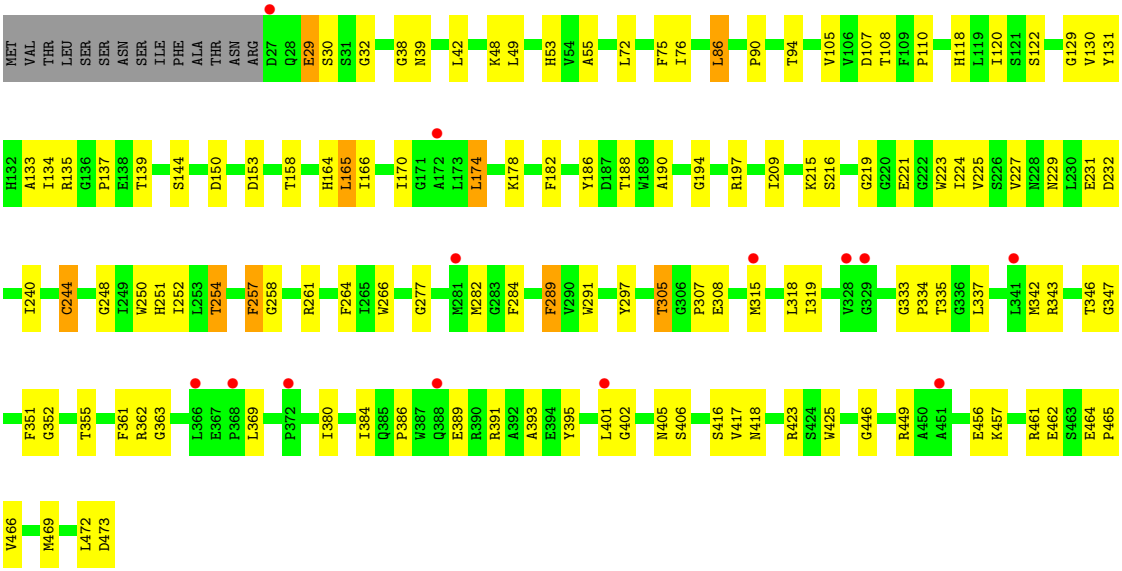
• Molecule 3: Photosystem II CP43 protein

Chain C:

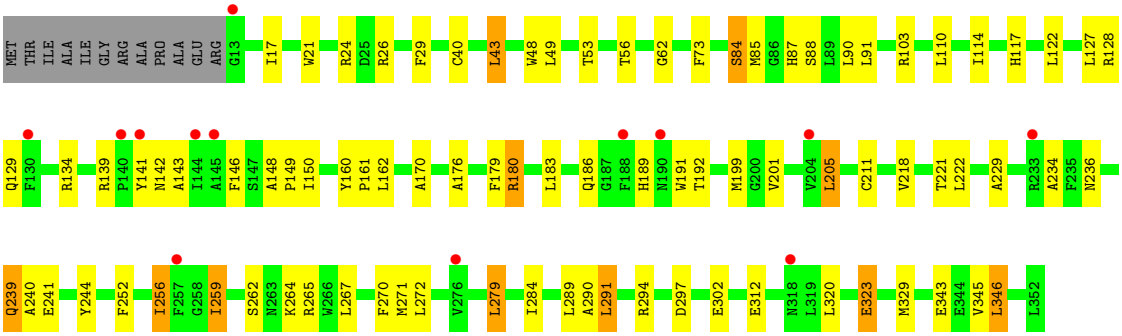




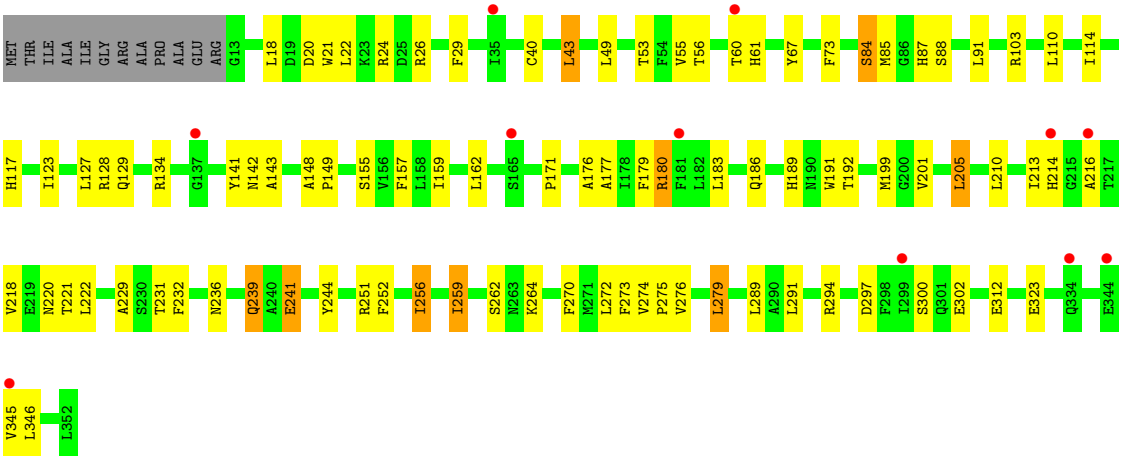
• Molecule 3: Photosystem II CP43 protein



• Molecule 4: Photosystem II D2 protein

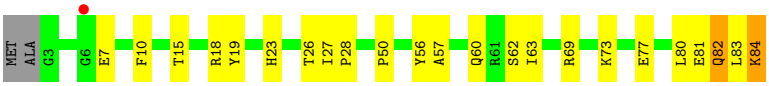


• Molecule 4: Photosystem II D2 protein



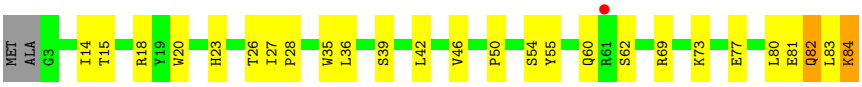
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



• Molecule 6: Cytochrome b559 subunit beta

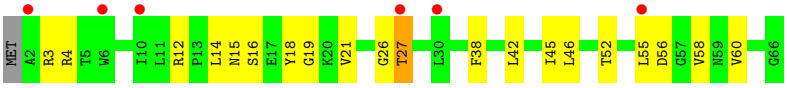
Chain F:

• Molecule 6: Cytochrome b559 subunit beta

Chain f:

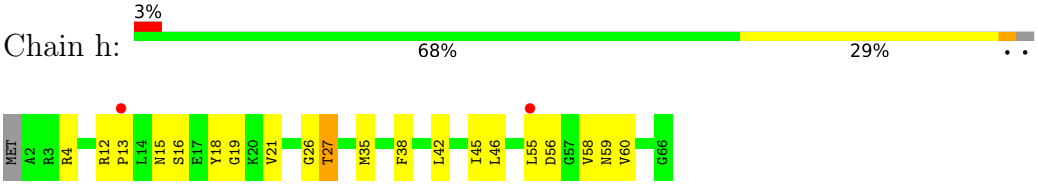
• Molecule 7: Photosystem II reaction center protein H

Chain H:



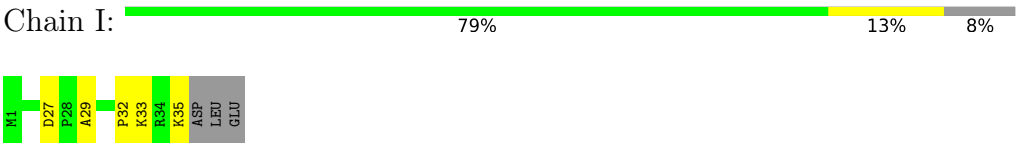
• Molecule 7: Photosystem II reaction center protein H

Chain h:



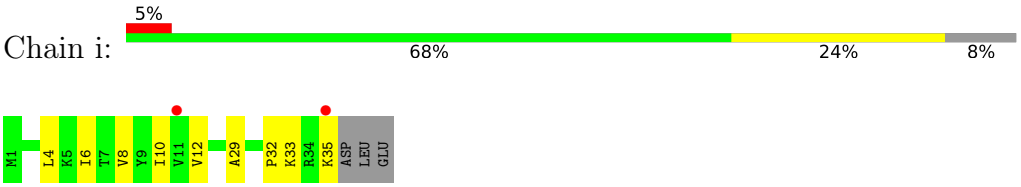
• Molecule 8: Photosystem II reaction center protein I

Chain I:



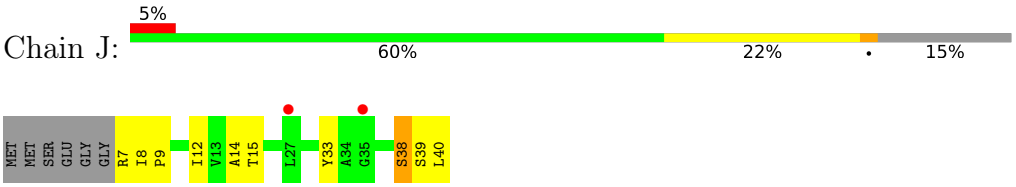
• Molecule 8: Photosystem II reaction center protein I

Chain i:



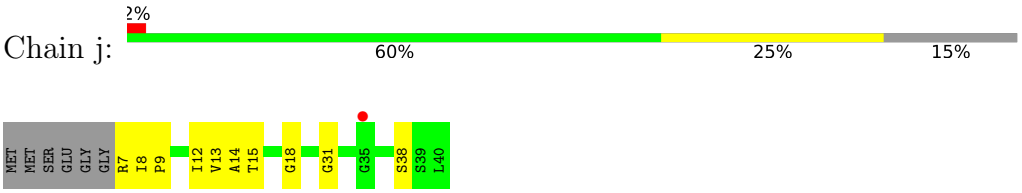
• Molecule 9: Photosystem II reaction center protein J

Chain J:



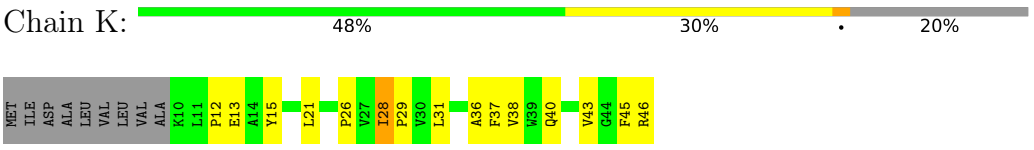
• Molecule 9: Photosystem II reaction center protein J

Chain j:



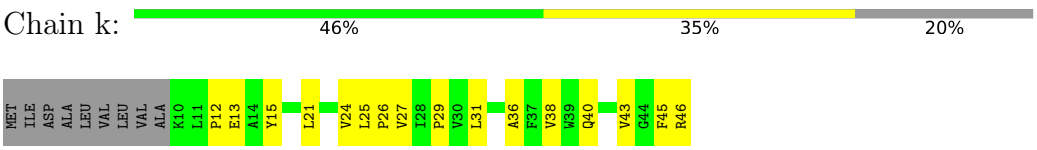
• Molecule 10: Photosystem II reaction center protein K

Chain K:



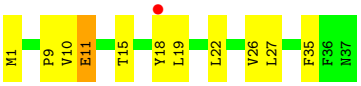
• Molecule 10: Photosystem II reaction center protein K

Chain k:



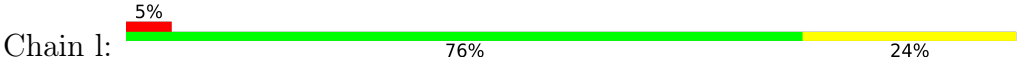
• Molecule 11: Photosystem II reaction center protein L

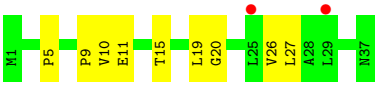
Chain L:



• Molecule 11: Photosystem II reaction center protein L

Chain l:



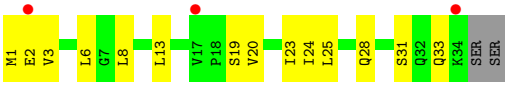


• Molecule 12: Photosystem II reaction center protein M

Chain M:

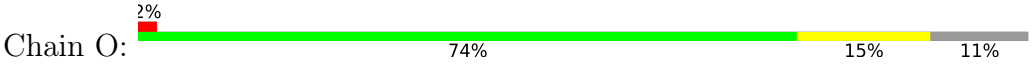
• Molecule 12: Photosystem II reaction center protein M

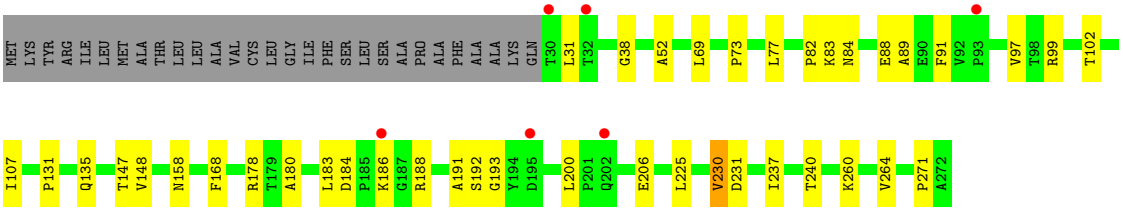
Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

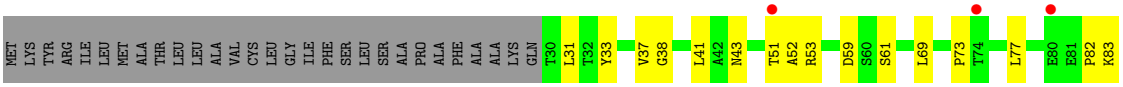
Chain O:

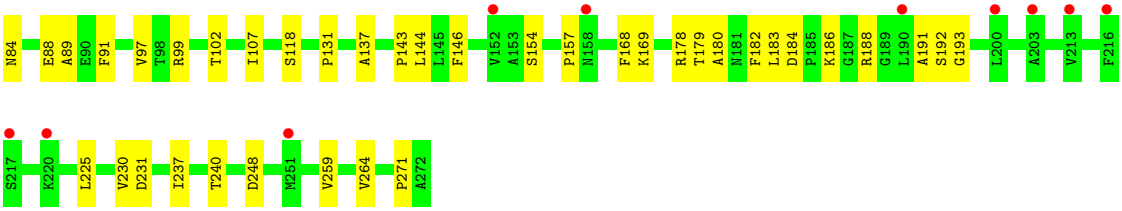




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

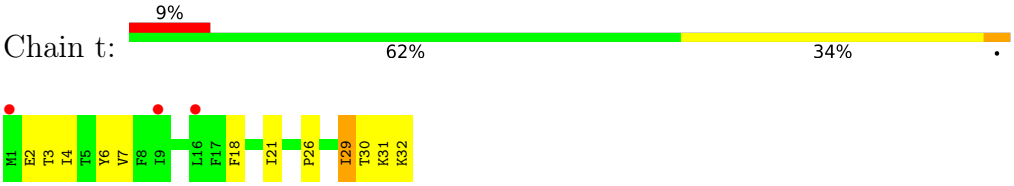
Chain o:



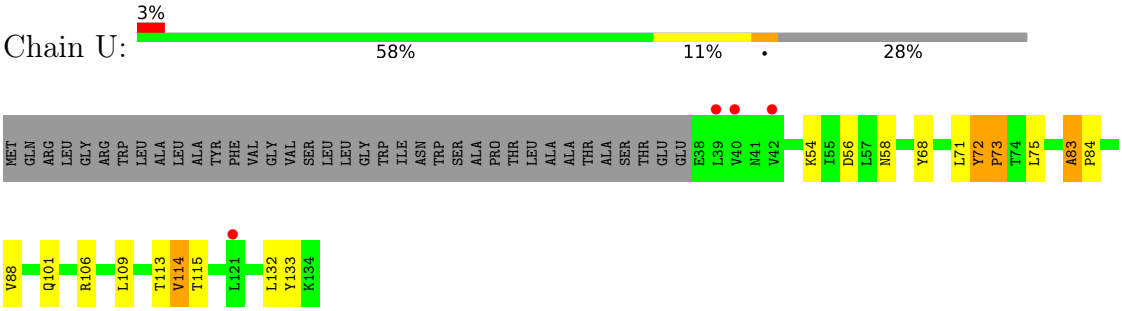


• Molecule 14: Photosystem II reaction center protein T

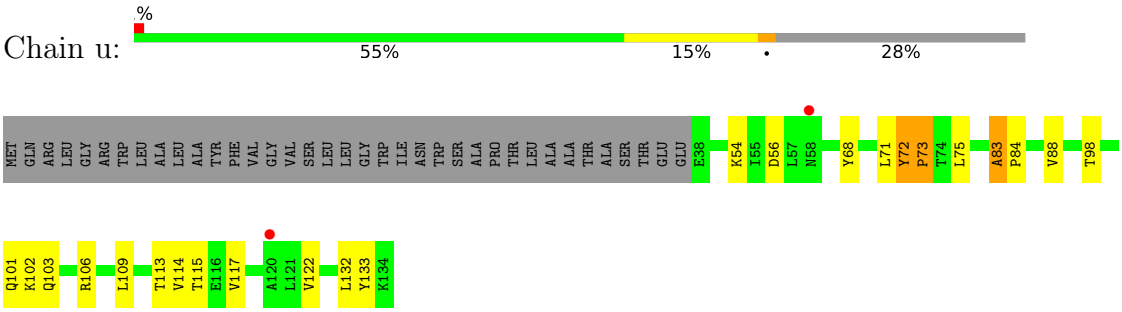
• Molecule 14: Photosystem II reaction center protein T



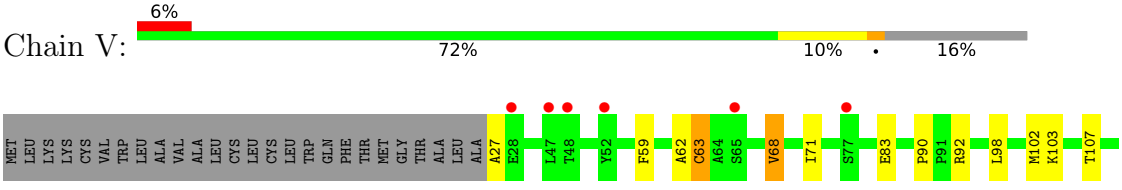
• Molecule 15: Photosystem II 12 kDa extrinsic protein

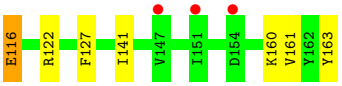


• Molecule 15: Photosystem II 12 kDa extrinsic protein



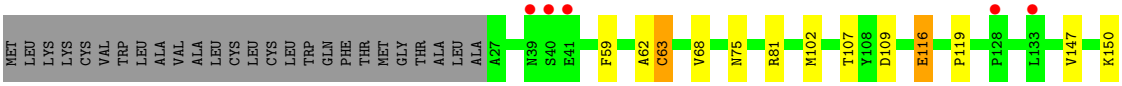
• Molecule 16: Cytochrome c-550





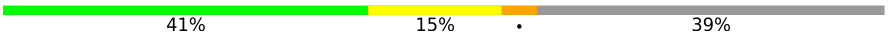
• Molecule 16: Cytochrome c-550

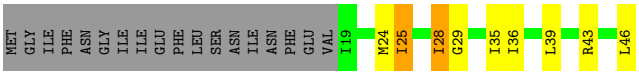
Chain v:



• Molecule 17: Photosystem II reaction center protein ycf12

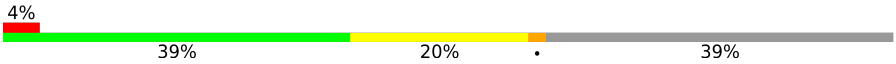
Chain y:

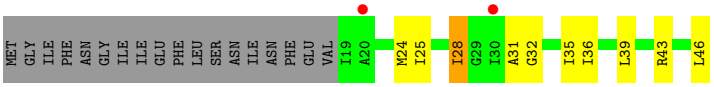




• Molecule 17: Photosystem II reaction center protein ycf12

Chain g:





• Molecule 18: Photosystem II reaction center X protein

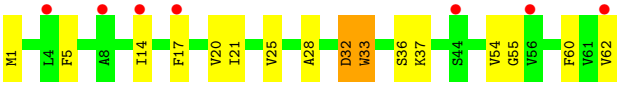
Chain X:

• Molecule 18: Photosystem II reaction center X protein

Chain x:

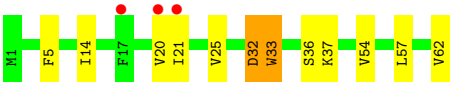
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



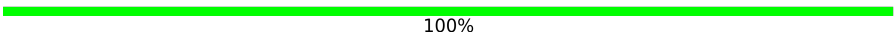
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II reaction center protein Y

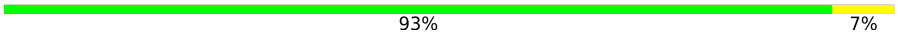
Chain Y:

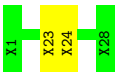


There are no outlier residues recorded for this chain.

• Molecule 20: Photosystem II reaction center protein Y

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	131.86Å 227.51Å 307.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.94 – 5.70 82.94 – 5.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (82.94-5.70) 98.3 (82.94-5.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.277 , 0.314 0.281 , 0.318	Depositor DCC
R_{free} test set	1325 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	3.698	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 64.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OEC, CL, PL9, CLA, BCT, FE2, LMT, DGD, HEM, BCR, CA, LMG, LHG, PHO, SQD

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	0.39	0/2712	0.85	0/3700
1	a	0.38	0/2712	0.86	5/3700 (0.1%)
2	B	0.39	0/3986	0.86	8/5433 (0.1%)
2	b	0.38	0/3986	0.87	10/5433 (0.2%)
3	C	0.38	0/3556	0.84	5/4842 (0.1%)
3	c	0.39	0/3556	0.85	8/4842 (0.2%)
4	D	0.36	0/2801	0.82	0/3818
4	d	0.37	0/2801	0.83	1/3818 (0.0%)
5	E	0.36	0/685	0.88	0/933
5	e	0.36	0/685	0.87	0/933
6	F	0.39	0/291	0.83	0/397
6	f	0.41	0/291	0.82	0/397
7	H	0.37	0/520	0.77	1/709 (0.1%)
7	h	0.37	0/520	0.78	0/709
8	I	0.36	0/293	0.82	0/395
8	i	0.37	0/293	0.87	0/395
9	J	0.35	0/255	0.89	0/346
9	j	0.42	0/255	0.94	0/346
10	K	0.43	0/303	0.92	1/416 (0.2%)
10	k	0.46	0/303	0.93	0/416
11	L	0.38	0/311	0.75	0/422
11	l	0.33	0/311	0.78	0/422
12	M	0.53	0/270	1.07	0/367
12	m	0.53	0/270	1.08	0/367
13	O	0.33	0/1876	0.74	2/2548 (0.1%)
13	o	0.36	0/1876	0.77	0/2548
14	T	0.38	0/284	0.84	0/381
14	t	0.40	0/284	0.81	0/381
15	U	0.37	0/785	0.84	0/1064
15	u	0.43	0/785	0.91	0/1064
16	V	0.39	0/1081	0.86	2/1468 (0.1%)
16	v	0.38	0/1081	0.82	2/1468 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	g	0.39	0/202	0.88	0/272
17	y	0.40	0/202	0.82	0/272
18	X	0.47	0/273	0.85	0/370
18	x	0.47	0/273	0.89	0/370
19	Z	0.36	0/490	0.86	0/669
19	z	0.35	0/490	0.86	0/669
All	All	0.38	0/41948	0.84	45/57100 (0.1%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	483	ASP	CA-C-N	10.80	133.34	119.84
2	b	483	ASP	C-N-CA	10.80	133.34	119.84
2	B	483	ASP	CA-C-N	10.41	132.85	119.84
2	B	483	ASP	C-N-CA	10.41	132.85	119.84
2	b	194	ASN	CA-C-N	6.55	126.32	119.05
2	b	194	ASN	C-N-CA	6.55	126.32	119.05
3	C	363	GLY	CA-C-N	6.26	125.76	119.24
3	C	363	GLY	C-N-CA	6.26	125.76	119.24
2	B	413	ASP	CA-C-N	6.10	126.66	120.38
2	B	413	ASP	C-N-CA	6.10	126.66	120.38
3	c	363	GLY	CA-C-N	6.03	125.51	119.24
3	c	363	GLY	C-N-CA	6.03	125.51	119.24
2	B	381	ILE	CA-C-N	6.01	125.92	119.85
2	B	381	ILE	C-N-CA	6.01	125.92	119.85
2	b	413	ASP	CA-C-N	5.84	126.40	120.38
2	b	413	ASP	C-N-CA	5.84	126.40	120.38
16	V	127	PHE	CA-C-N	5.65	126.03	119.47
16	V	127	PHE	C-N-CA	5.65	126.03	119.47
10	K	28	ILE	CB-CA-C	-5.61	108.37	113.70
2	b	15	ASP	CA-C-N	5.59	125.69	119.32
2	b	15	ASP	C-N-CA	5.59	125.69	119.32
3	C	464	GLU	CA-C-N	5.43	126.62	119.84
3	C	464	GLU	C-N-CA	5.43	126.62	119.84
3	c	333	GLY	CA-C-N	5.43	126.62	119.84
3	c	333	GLY	C-N-CA	5.43	126.62	119.84
3	c	190	ALA	CA-C-N	5.39	124.85	119.24
3	c	190	ALA	C-N-CA	5.39	124.85	119.24
16	v	75	ASN	CA-C-N	5.30	125.02	119.82
16	v	75	ASN	C-N-CA	5.30	125.02	119.82
2	B	15	ASP	CA-C-N	5.30	125.36	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	15	ASP	C-N-CA	5.30	125.36	119.32
1	a	195	HIS	CA-C-N	5.17	124.62	119.24
1	a	195	HIS	C-N-CA	5.17	124.62	119.24
13	O	200	LEU	CA-C-N	5.15	125.45	119.47
13	O	200	LEU	C-N-CA	5.15	125.45	119.47
3	c	76	ILE	CA-C-N	5.14	124.59	119.24
3	c	76	ILE	C-N-CA	5.14	124.59	119.24
2	b	487	SER	CA-C-N	5.12	126.24	119.84
2	b	487	SER	C-N-CA	5.12	126.24	119.84
1	a	38	ILE	CB-CA-C	-5.07	108.88	113.70
1	a	60	ILE	N-CA-C	5.06	115.28	110.42
7	H	52	THR	N-CA-C	-5.04	106.99	113.23
3	C	89	ILE	CB-CA-C	-5.01	109.04	114.35
4	d	273	PHE	N-CA-C	5.01	116.43	110.97
1	a	83	VAL	N-CA-C	5.01	112.94	108.63

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	2627	0	2524	87	0
1	a	2627	0	2524	84	0
2	B	3850	0	3718	82	0
2	b	3850	0	3718	89	0
3	C	3444	0	3365	95	0
3	c	3444	0	3365	90	0
4	D	2706	0	2608	71	0
4	d	2706	0	2608	78	0
5	E	666	0	651	15	0
5	e	666	0	651	19	0
6	F	282	0	291	8	0
6	f	282	0	291	10	0
7	H	507	0	521	16	0
7	h	507	0	521	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	286	0	308	3	0
8	i	286	0	308	4	0
9	J	249	0	262	7	0
9	j	249	0	262	7	0
10	K	293	0	305	11	0
10	k	293	0	305	14	0
11	L	304	0	316	11	0
11	l	304	0	316	8	0
12	M	267	0	289	13	0
12	m	267	0	289	16	0
13	O	1845	0	1801	24	0
13	o	1845	0	1801	35	0
14	T	275	0	288	10	0
14	t	275	0	288	10	0
15	U	774	0	773	11	0
15	u	774	0	773	10	0
16	V	1060	0	1068	13	0
16	v	1060	0	1068	10	0
17	g	201	0	226	8	0
17	y	201	0	226	5	0
18	X	270	0	299	10	0
18	x	270	0	299	9	0
19	Z	479	0	516	15	0
19	z	479	0	516	9	0
20	G	140	0	32	1	0
20	Y	140	0	32	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	4	0	1	0	0
22	d	4	0	1	0	0
23	A	260	0	288	29	0
23	B	1040	0	1152	73	0
23	C	845	0	936	36	0
23	D	130	0	144	11	0
23	a	260	0	288	32	0
23	b	1040	0	1152	73	0
23	c	845	0	936	38	0
23	d	130	0	144	12	0
24	A	64	0	74	5	0
24	D	64	0	74	7	0
24	a	128	0	148	14	0
25	A	45	0	61	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	D	55	0	80	5	0
25	J	35	0	45	2	0
25	a	45	0	61	5	0
25	d	55	0	80	7	0
25	j	35	0	45	0	0
26	A	5	0	0	0	0
26	a	5	0	0	0	0
27	A	40	0	56	5	0
27	B	160	0	224	24	0
27	C	80	0	112	16	0
27	D	40	0	56	3	0
27	H	40	0	56	2	0
27	J	40	0	56	5	0
27	K	40	0	56	9	0
27	T	80	0	112	14	0
27	Z	40	0	56	4	0
27	a	40	0	56	2	0
27	b	80	0	112	12	0
27	c	120	0	168	14	0
27	f	40	0	56	3	0
27	j	40	0	56	4	0
27	k	40	0	56	7	0
27	x	40	0	56	4	0
28	A	56	0	70	1	0
28	B	110	0	136	5	0
28	C	181	0	245	14	0
28	D	63	0	87	3	0
28	a	56	0	70	0	0
28	b	110	0	136	8	0
28	c	181	0	245	11	0
28	d	63	0	87	0	0
29	A	76	0	95	6	0
29	a	76	0	95	7	0
30	A	105	0	147	12	0
30	B	47	0	61	1	0
30	D	43	0	50	3	0
30	F	45	0	54	2	0
30	a	105	0	147	6	0
30	b	47	0	61	2	0
30	d	43	0	50	4	0
30	f	45	0	54	2	0
31	A	93	0	124	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	B	49	0	67	4	0
31	C	93	0	124	4	0
31	D	143	0	194	10	0
31	E	44	0	57	1	0
31	I	43	0	55	3	0
31	M	84	0	107	6	0
31	a	93	0	124	7	0
31	b	98	0	134	7	0
31	c	45	0	59	2	0
31	d	94	0	126	9	0
31	e	44	0	58	0	0
31	i	43	0	55	2	0
31	k	48	0	66	2	0
32	A	1	0	0	0	0
32	d	1	0	0	0	0
33	B	140	0	184	4	0
33	D	31	0	35	1	0
33	I	35	0	46	2	0
33	M	35	0	46	0	0
33	T	35	0	46	2	0
33	b	105	0	138	6	0
33	i	35	0	46	1	0
33	m	35	0	46	0	0
33	x	31	0	35	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	4	0
34	v	43	0	30	5	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50232	0	51358	1198	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 12.

All (1198) 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)
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.50	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ASN:HB2	23:C:508:CLA:HBA1	1.51	0.89
4:d:26:ARG:HD3	6:f:18:VAL:HG11	1.54	0.89
3:C:362:ARG:H	28:C:516:DGD:HE4	1.40	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.57	0.85
13:o:82:PRO:HG3	13:o:89:ALA:HB2	1.59	0.84
3:c:39:ASN:HB2	23:c:508:CLA:HBA1	1.61	0.82
3:c:362:ARG:H	28:c:517:DGD:HE4	1.43	0.82
34:V:201:HEM:HBC2	34:V:201:HEM:HHD	1.62	0.82
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.62	0.80
4:d:199:MET:HG2	25:d:404:PL9:H322	1.65	0.79
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.65	0.78
24:a:408:PHO:HBC3	4:d:279:LEU:HG	1.65	0.78
27:T:102:BCR:H383	30:b:601:SQD:H92	1.65	0.77
23:B:606:CLA:H72	27:B:620:BCR:H311	1.68	0.75
12:M:28:GLN:HA	12:m:28:GLN:HA	1.66	0.75
1:A:63:ILE:HB	3:C:335:THR:HG21	1.67	0.75
14:T:18:PHE:HB2	27:T:103:BCR:H10C	1.67	0.75
1:a:192:ILE:HA	1:a:293:MET:HE1	1.67	0.74
1:a:190:HIS:HB3	1:a:293:MET:HE2	1.68	0.74
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.68	0.74
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.69	0.74
3:c:297:TYR:O	3:c:423:ARG:NH2	2.21	0.73
1:a:214:MET:HE2	1:a:214:MET:HA	1.70	0.73
3:C:449:ARG:HE	23:C:505:CLA:HED1	1.54	0.73
4:d:29:PHE:O	4:d:128:ARG:NH2	2.21	0.73
23:b:609:CLA:H72	27:b:621:BCR:H311	1.71	0.72
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.71	0.72
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.71	0.72
30:d:407:SQD:H171	30:d:407:SQD:H301	1.70	0.72
3:c:216:SER:HB3	3:c:221:GLU:HB2	1.71	0.72
5:e:60:GLN:OE1	5:e:84:LYS:NZ	2.23	0.71
13:o:69:LEU:HB3	13:o:107:ILE:HB	1.71	0.71
1:A:192:ILE:HA	1:A:293:MET:HE1	1.71	0.71
23:c:508:CLA:HBC3	23:c:510:CLA:H92	1.72	0.71
4:d:236:ASN:ND2	4:d:239:GLN:O	2.23	0.71
12:m:25:LEU:O	12:m:28:GLN:HG3	1.91	0.71
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.72	0.71
23:b:611:CLA:H42	4:d:127:LEU:HD11	1.72	0.70
1:a:174:LEU:HD22	24:a:407:PHO:H151	1.74	0.70
3:c:405:ASN:HB2	28:c:519:DGD:HG31	1.73	0.70
3:C:250:TRP:O	3:C:254:THR:OG1	2.08	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:602:DGD:HB22	33:b:603:LMT:H72	1.74	0.70
24:A:406:PHO:HBC3	4:D:279:LEU:HG	1.73	0.70
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.57	0.69
4:D:236:ASN:ND2	4:D:239:GLN:O	2.24	0.69
23:B:602:CLA:H42	7:H:45:ILE:HD11	1.73	0.69
2:b:262:THR:HG22	2:b:263:THR:HG23	1.72	0.69
2:B:271:THR:HG22	2:B:273:TYR:H	1.56	0.69
23:a:405:CLA:HED1	25:d:404:PL9:H372	1.73	0.69
23:C:507:CLA:H112	27:C:515:BCR:H362	1.74	0.69
10:K:21:LEU:HD13	17:y:24:MET:HE2	1.74	0.69
1:A:64:ARG:O	13:O:178:ARG:NH2	2.26	0.68
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.26	0.68
10:k:21:LEU:HD13	17:g:24:MET:HE2	1.75	0.68
34:v:201:HEM:HBC2	34:v:201:HEM:HHD	1.75	0.68
23:C:503:CLA:H172	23:C:510:CLA:HBB2	1.74	0.68
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.68
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.74	0.68
1:a:63:ILE:HB	3:c:335:THR:HG21	1.76	0.68
1:a:129:ARG:HH21	4:d:256:ILE:HD12	1.58	0.68
17:y:35:ILE:HG22	19:Z:21:ILE:HG23	1.75	0.68
1:A:15:GLU:O	1:A:19:ASN:ND2	2.26	0.68
4:D:29:PHE:O	4:D:128:ARG:NH2	2.26	0.68
27:T:103:BCR:H19C	27:b:620:BCR:H363	1.76	0.68
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.75	0.68
27:T:102:BCR:H23C	2:b:25:MET:HE3	1.75	0.68
24:a:408:PHO:H151	23:d:402:CLA:H172	1.76	0.68
27:B:618:BCR:H10C	14:t:18:PHE:HB2	1.76	0.67
17:g:35:ILE:HG22	19:z:21:ILE:HG23	1.76	0.67
2:b:24:LEU:HD21	23:b:619:CLA:HAB	1.75	0.67
1:a:29:TYR:O	1:a:129:ARG:NH1	2.26	0.67
23:D:403:CLA:H43	18:X:23:LEU:HA	1.77	0.67
23:A:403:CLA:H71	23:A:404:CLA:HAB	1.76	0.67
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.59	0.67
3:C:291:TRP:O	3:C:305:THR:OG1	2.13	0.67
3:C:303:GLY:O	3:C:423:ARG:NE	2.23	0.66
1:A:183:MET:HB3	23:A:403:CLA:HBC2	1.77	0.66
23:B:608:CLA:H42	4:D:127:LEU:HD11	1.76	0.66
2:B:25:MET:HE3	27:B:617:BCR:H23C	1.77	0.66
27:B:617:BCR:H383	30:B:625:SQD:H92	1.77	0.65
6:F:17:THR:HG23	6:F:20:TRP:H	1.61	0.65
23:B:608:CLA:HBA2	30:D:409:SQD:H101	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:259:ILE:HG12	31:d:406:LMG:H292	1.78	0.65
23:A:404:CLA:HED1	25:D:404:PL9:H372	1.78	0.65
2:B:262:THR:HG22	2:B:263:THR:HG23	1.79	0.65
3:C:49:LEU:O	3:C:53:HIS:ND1	2.29	0.65
23:B:603:CLA:H193	7:H:42:LEU:HD12	1.78	0.65
1:a:329:GLU:O	1:a:332:HIS:ND1	2.30	0.65
23:b:607:CLA:HBD	23:b:608:CLA:H43	1.77	0.64
27:c:514:BCR:H391	10:k:36:ALA:HB2	1.79	0.64
12:M:25:LEU:O	12:M:28:GLN:HG3	1.97	0.64
29:A:415:LHG:H271	29:A:415:LHG:H101	1.78	0.64
11:L:9:PRO:HB3	31:M:102:LMG:HC61	1.80	0.64
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.79	0.64
23:b:608:CLA:HBB1	23:b:609:CLA:H51	1.79	0.64
14:T:21:ILE:HD12	27:T:103:BCR:H332	1.80	0.64
23:c:513:CLA:HAB	27:c:515:BCR:H24C	1.79	0.64
1:a:64:ARG:O	13:o:178:ARG:NH2	2.30	0.64
3:C:118:HIS:CE1	31:C:520:LMG:H192	2.33	0.63
3:C:48:LYS:NZ	3:C:133:ALA:O	2.31	0.63
4:D:186:GLN:HB2	23:D:401:CLA:HBC1	1.79	0.63
4:D:199:MET:HG2	25:D:404:PL9:H322	1.79	0.63
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.80	0.63
4:D:259:ILE:HG12	31:D:408:LMG:H292	1.79	0.63
2:B:149:LEU:HG	23:B:603:CLA:HBC1	1.79	0.63
23:C:511:CLA:HMB1	27:C:514:BCR:H382	1.79	0.63
1:a:214:MET:HE1	4:d:142:ASN:HD21	1.63	0.63
4:d:186:GLN:HB2	23:d:402:CLA:HBC1	1.79	0.63
2:B:24:LEU:HD21	23:B:616:CLA:HAB	1.79	0.63
23:C:508:CLA:HBC3	23:C:510:CLA:H92	1.80	0.63
23:b:606:CLA:H193	7:h:42:LEU:HD12	1.80	0.63
30:D:409:SQD:H301	30:D:409:SQD:H171	1.81	0.63
12:M:20:VAL:O	12:M:24:ILE:HG13	1.98	0.63
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.81	0.62
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.62
3:c:49:LEU:O	3:c:53:HIS:ND1	2.33	0.62
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.80	0.62
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.24	0.62
23:A:404:CLA:H203	24:D:402:PHO:H71	1.81	0.62
31:A:418:LMG:H112	2:b:43:ALA:HA	1.80	0.62
30:a:415:SQD:H311	23:c:508:CLA:H71	1.82	0.62
23:d:403:CLA:H43	18:x:23:LEU:HA	1.82	0.62
3:c:165:LEU:HD21	23:c:506:CLA:HAB	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:20:VAL:O	12:m:24:ILE:HG13	2.00	0.61
23:B:608:CLA:H151	23:B:609:CLA:H203	1.82	0.61
27:B:618:BCR:H19C	27:B:619:BCR:H363	1.81	0.61
31:a:416:LMG:H231	25:d:404:PL9:H352	1.81	0.61
4:d:21:TRP:O	4:d:26:ARG:NH2	2.32	0.61
1:A:329:GLU:O	1:A:332:HIS:ND1	2.32	0.61
3:c:250:TRP:O	3:c:254:THR:OG1	2.16	0.61
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.83	0.61
23:A:403:CLA:H122	24:D:402:PHO:H3A	1.83	0.61
23:A:405:CLA:H142	23:D:401:CLA:H151	1.82	0.61
1:a:217:SER:HA	4:d:272:LEU:HD12	1.83	0.61
23:a:405:CLA:H42	25:d:404:PL9:H162	1.83	0.61
3:c:118:HIS:CE1	31:c:520:LMG:H192	2.36	0.61
23:d:403:CLA:H42	18:x:26:GLY:HA3	1.83	0.61
3:c:215:LYS:HB3	3:c:223:TRP:HA	1.83	0.61
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.35	0.60
3:c:449:ARG:HE	23:c:505:CLA:HED1	1.66	0.60
23:D:403:CLA:H42	18:X:26:GLY:HA3	1.82	0.60
2:b:271:THR:HG22	2:b:273:TYR:H	1.65	0.60
1:A:140:ARG:HH22	29:A:412:LHG:P	2.23	0.60
7:H:38:PHE:HB2	27:H:101:BCR:H10C	1.82	0.60
34:F:101:HEM:HBC2	34:F:101:HEM:HMC2	1.84	0.60
11:L:10:VAL:O	12:M:28:GLN:NE2	2.29	0.60
31:A:414:LMG:H231	25:D:404:PL9:H352	1.82	0.60
23:b:606:CLA:C2D	23:b:608:CLA:H2	2.32	0.60
10:k:26:PRO:O	10:k:29:PRO:HD2	2.02	0.60
2:B:43:ALA:HA	31:a:402:LMG:H112	1.84	0.60
1:a:84:PRO:HA	1:a:112:TYR:CG	2.37	0.60
23:b:605:CLA:H42	7:h:45:ILE:HD11	1.84	0.60
1:A:29:TYR:O	1:A:129:ARG:NH1	2.34	0.59
4:D:24:ARG:NH2	18:X:44:ASP:O	2.35	0.59
1:a:183:MET:HB3	23:a:404:CLA:HBC2	1.83	0.59
3:c:48:LYS:NZ	3:c:133:ALA:O	2.35	0.59
1:A:132:GLU:O	1:A:136:ARG:HG2	2.02	0.59
3:c:284:PHE:HB3	28:c:517:DGD:HA51	1.84	0.59
30:A:413:SQD:H311	23:C:508:CLA:H71	1.84	0.59
2:B:222:PRO:HG3	7:H:27:THR:H	1.67	0.59
23:B:602:CLA:HBD	23:B:602:CLA:H2	1.82	0.59
23:A:403:CLA:H202	23:A:404:CLA:H93	1.83	0.59
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.85	0.59
23:C:513:CLA:HAB	27:Z:101:BCR:H24C	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:610:CLA:HBB1	31:b:624:LMG:H341	1.84	0.59
1:a:153:SER:HB3	23:a:404:CLA:HED1	1.83	0.59
9:j:15:THR:HG21	10:k:38:VAL:HG13	1.84	0.59
23:C:509:CLA:H121	23:C:509:CLA:HBD	1.84	0.59
6:f:17:THR:HG23	6:f:20:TRP:H	1.68	0.59
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.84	0.59
23:c:501:CLA:H193	23:c:507:CLA:H111	1.85	0.59
13:o:178:ARG:HG3	13:o:178:ARG:HH11	1.67	0.59
23:b:606:CLA:C3D	23:b:608:CLA:H2	2.32	0.59
13:o:77:LEU:HB3	13:o:91:PHE:HB3	1.84	0.58
2:B:458:PHE:HB3	23:B:604:CLA:HBC2	1.85	0.58
7:h:55:LEU:HB2	7:h:58:VAL:HG12	1.85	0.58
2:b:271:THR:HB	2:b:274:GLN:HG3	1.85	0.58
16:v:62:ALA:O	34:v:201:HEM:HAB	2.03	0.58
23:b:611:CLA:HBA2	30:d:407:SQD:H101	1.85	0.58
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.37	0.58
3:C:361:PHE:HD1	28:C:516:DGD:HE61	1.68	0.58
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.85	0.58
12:M:31:SER:HA	31:M:101:LMG:HC1	1.86	0.58
23:b:608:CLA:H202	23:b:612:CLA:HBB2	1.85	0.58
30:A:413:SQD:H223	28:C:518:DGD:HAE1	1.85	0.58
3:c:305:THR:HG22	3:c:308:GLU:HB2	1.85	0.58
1:A:227:THR:HG21	1:A:233:ALA:HA	1.85	0.57
3:C:405:ASN:HB2	28:C:518:DGD:HG31	1.86	0.57
16:V:62:ALA:O	34:V:201:HEM:HAB	2.03	0.57
23:b:605:CLA:H2	23:b:605:CLA:HBD	1.85	0.57
1:A:214:MET:HA	1:A:214:MET:HE2	1.85	0.57
31:M:102:LMG:HC1	12:m:31:SER:HA	1.86	0.57
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.86	0.57
2:b:383:PHE:CZ	13:o:193:GLY:HA2	2.39	0.57
1:A:174:LEU:HD22	24:D:402:PHO:H151	1.85	0.57
3:C:165:LEU:HD21	23:C:506:CLA:HAB	1.86	0.57
13:O:73:PRO:HG2	13:O:102:THR:HB	1.85	0.57
23:B:615:CLA:H172	23:B:615:CLA:H111	1.85	0.57
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.85	0.57
15:u:54:LYS:HD2	15:u:113:THR:HG23	1.87	0.57
28:D:410:DGD:HO4E	28:D:410:DGD:HO5E	1.52	0.57
2:b:149:LEU:HG	23:b:606:CLA:HBC1	1.85	0.57
1:A:72:LEU:HD13	31:A:418:LMG:H111	1.87	0.57
23:C:501:CLA:C2D	23:C:503:CLA:H2	2.34	0.57
1:a:78:ILE:O	1:a:176:ILE:HB	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:HD12	23:A:404:CLA:HED3	1.86	0.57
23:A:404:CLA:HAA1	25:D:404:PL9:H362	1.86	0.56
2:B:271:THR:HB	2:B:274:GLN:HG3	1.87	0.56
3:C:342:MET:HE3	3:C:352:GLY:HA2	1.86	0.56
2:b:270:PRO:HG3	2:b:312:TYR:HD2	1.70	0.56
3:c:229:ASN:HD22	3:c:231:GLU:HB2	1.70	0.56
18:x:12:ILE:HA	18:x:16:LEU:HD12	1.86	0.56
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.69	0.56
4:d:221:THR:HG23	4:d:244:TYR:HB2	1.86	0.56
23:C:511:CLA:H171	19:Z:20:VAL:HA	1.88	0.56
23:a:404:CLA:HHC	23:a:404:CLA:HBB1	1.86	0.56
23:a:406:CLA:H142	23:d:402:CLA:H151	1.86	0.56
3:C:361:PHE:HA	28:C:516:DGD:HE62	1.86	0.56
19:Z:33:TRP:O	19:Z:37:LYS:HB2	2.04	0.56
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.87	0.56
1:A:244:GLU:HG3	1:A:246:TYR:H	1.69	0.56
23:A:405:CLA:H93	23:D:401:CLA:H152	1.88	0.56
3:c:158:THR:O	3:c:251:HIS:HB3	2.06	0.56
2:b:458:PHE:HB3	23:b:607:CLA:HBC2	1.86	0.56
1:a:132:GLU:O	1:a:136:ARG:HG2	2.06	0.56
2:b:433:ASP:OD2	2:b:436:THR:OG1	2.22	0.56
15:u:56:ASP:OD2	15:u:115:THR:OG1	2.15	0.56
1:a:215:HIS:ND1	25:a:410:PL9:O1	2.39	0.56
2:b:327:THR:HG21	31:b:624:LMG:H111	1.87	0.56
34:f:101:HEM:HBC2	34:f:101:HEM:HMC2	1.88	0.56
15:u:72:TYR:HB3	15:u:73:PRO:HD3	1.88	0.56
16:v:160:LYS:HA	16:v:163:TYR:CD2	2.41	0.56
1:A:78:ILE:O	1:A:176:ILE:HB	2.05	0.55
31:D:408:LMG:H111	11:L:19:LEU:HD21	1.88	0.55
31:I:101:LMG:H181	33:I:102:LMT:H42	1.88	0.55
2:b:329:PRO:HB3	23:b:610:CLA:HED1	1.87	0.55
13:o:73:PRO:HG2	13:o:102:THR:HB	1.88	0.55
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.88	0.55
3:c:405:ASN:CB	28:c:519:DGD:HG31	2.35	0.55
23:c:505:CLA:H11	27:c:516:BCR:H312	1.89	0.55
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.71	0.55
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.89	0.55
23:c:503:CLA:H172	23:c:510:CLA:HBB2	1.88	0.55
13:o:118:SER:HB3	13:o:157:PRO:HA	1.87	0.55
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.89	0.55
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:THR:HG21	31:B:622:LMG:H111	1.88	0.55
1:a:15:GLU:O	1:a:19:ASN:ND2	2.37	0.55
2:b:122:LEU:O	7:h:15:ASN:ND2	2.39	0.55
3:c:406:SER:O	3:c:418:ASN:ND2	2.39	0.55
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.87	0.54
1:a:244:GLU:HG3	1:a:246:TYR:H	1.72	0.54
1:a:328:MET:HE1	4:d:183:LEU:HD22	1.89	0.54
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.23	0.54
2:B:329:PRO:HB3	23:B:607:CLA:HED1	1.89	0.54
28:C:517:DGD:HA41	31:C:519:LMG:H391	1.89	0.54
29:a:417:LHG:H271	29:a:417:LHG:H101	1.90	0.54
4:d:84:SER:HB2	4:d:85:MET:HE2	1.89	0.54
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.89	0.54
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.89	0.54
30:A:413:SQD:H241	29:A:415:LHG:HC81	1.89	0.54
1:a:221:SER:HB3	4:d:141:TYR:HB2	1.90	0.54
23:b:610:CLA:HBC3	27:b:620:BCR:HC8	1.89	0.54
1:a:255:PHE:CE2	25:a:410:PL9:H111	2.43	0.54
30:a:401:SQD:H311	27:a:412:BCR:H342	1.89	0.54
3:c:346:THR:HG21	13:o:38:GLY:HA2	1.90	0.54
19:z:33:TRP:O	19:z:37:LYS:HB2	2.06	0.54
23:B:608:CLA:H18	23:B:609:CLA:H192	1.89	0.54
1:A:141:PRO:O	1:A:143:ILE:N	2.40	0.54
23:B:607:CLA:H192	31:D:407:LMG:H342	1.89	0.54
23:b:614:CLA:H41	23:b:617:CLA:HBC3	1.89	0.54
4:d:274:VAL:HA	25:d:404:PL9:H253	1.89	0.54
23:B:605:CLA:HBB1	23:B:606:CLA:H51	1.89	0.54
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.43	0.54
14:T:7:VAL:HG12	33:T:101:LMT:H122	1.90	0.54
1:a:183:MET:HE1	23:a:405:CLA:HMD2	1.88	0.54
2:b:241:SER:HB3	23:b:615:CLA:HED3	1.88	0.54
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.88	0.54
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.90	0.54
23:B:603:CLA:C2D	23:B:605:CLA:H2	2.38	0.53
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.08	0.53
31:M:101:LMG:HC61	11:l:9:PRO:HB3	1.90	0.53
2:b:121:GLU:O	7:h:12:ARG:NH2	2.41	0.53
23:C:504:CLA:H121	28:C:517:DGD:HBE2	1.89	0.53
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.08	0.53
12:M:31:SER:OG	12:m:28:GLN:O	2.22	0.53
23:a:404:CLA:H122	24:a:407:PHO:H3A	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:GLU:H	2:B:200:ALA:HB2	1.73	0.53
13:o:180:ALA:HB1	13:o:191:ALA:HB2	1.91	0.53
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.91	0.53
23:B:604:CLA:HBB1	23:B:607:CLA:CBB	2.39	0.53
31:D:408:LMG:O6	11:L:15:THR:HG21	2.09	0.53
13:O:83:LYS:HG2	13:O:84:ASN:H	1.73	0.53
23:a:405:CLA:CHA	23:a:405:CLA:HBA1	2.38	0.53
2:b:150:CYS:HA	23:b:606:CLA:HBC2	1.91	0.53
23:b:618:CLA:H111	23:b:618:CLA:H172	1.90	0.53
3:c:361:PHE:HD1	28:c:517:DGD:HE61	1.74	0.53
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.43	0.53
2:b:96:VAL:HG22	23:b:609:CLA:HBA1	1.90	0.53
4:d:56:THR:HG21	5:e:50:PRO:HD3	1.91	0.53
23:B:608:CLA:H51	23:B:609:CLA:H101	1.91	0.53
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.90	0.53
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.91	0.53
2:b:474:LEU:O	4:d:134:ARG:NH1	2.41	0.53
31:d:406:LMG:H111	11:l:19:LEU:HD21	1.91	0.53
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.74	0.53
16:v:59:PHE:HA	16:v:63:CYS:SG	2.49	0.53
24:a:408:PHO:HMC3	4:d:279:LEU:HD21	1.91	0.53
4:d:49:LEU:HD13	27:f:102:BCR:C15	2.39	0.53
23:A:403:CLA:HHC	23:A:403:CLA:HBB1	1.90	0.53
9:J:9:PRO:HB2	9:J:12:ILE:HG13	1.91	0.53
31:d:406:LMG:O6	11:l:15:THR:HG21	2.08	0.53
13:o:83:LYS:HG2	13:o:84:ASN:H	1.74	0.53
1:A:298:ASN:ND2	3:C:402:GLY:O	2.42	0.52
2:B:122:LEU:O	7:H:15:ASN:ND2	2.41	0.52
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.74	0.52
4:d:24:ARG:NH2	18:x:44:ASP:O	2.42	0.52
9:j:14:ALA:O	9:j:18:GLY:N	2.41	0.52
3:C:158:THR:O	3:C:251:HIS:HB3	2.10	0.52
1:a:190:HIS:O	1:a:298:ASN:HB3	2.09	0.52
13:o:230:VAL:HG12	13:o:231:ASP:H	1.74	0.52
1:A:232:SER:OG	31:A:414:LMG:O3	2.25	0.52
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.45	0.52
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.91	0.52
23:b:611:CLA:HAB	4:d:123:ILE:HG23	1.92	0.52
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.92	0.52
4:d:189:HIS:HA	4:d:294:ARG:HD2	1.92	0.52
3:c:337:LEU:HA	13:o:131:PRO:HG3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:230:VAL:HG12	13:O:231:ASP:H	1.75	0.52
2:b:103:LEU:HD21	23:b:608:CLA:HMC2	1.92	0.52
1:A:140:ARG:NH2	29:A:412:LHG:O5	2.40	0.52
2:B:239:SER:O	2:B:466:HIS:ND1	2.43	0.52
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.90	0.52
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.92	0.52
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.44	0.52
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.90	0.52
23:c:504:CLA:H202	28:c:519:DGD:HAF2	1.92	0.52
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.52
27:A:410:BCR:H311	30:A:417:SQD:H351	1.91	0.52
23:C:504:CLA:H202	28:C:518:DGD:HAF2	1.92	0.52
4:D:192:THR:HG23	23:D:401:CLA:HBC2	1.92	0.52
16:V:59:PHE:HA	16:V:63:CYS:SG	2.49	0.52
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.91	0.52
3:c:229:ASN:ND2	3:c:232:ASP:OD1	2.38	0.52
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.92	0.52
3:C:284:PHE:HB3	28:C:516:DGD:HA51	1.91	0.51
1:a:334:ARG:NH1	13:o:183:LEU:O	2.43	0.51
23:c:511:CLA:H171	19:z:20:VAL:HA	1.91	0.51
4:d:222:LEU:HD23	4:d:244:TYR:HB3	1.92	0.51
1:A:177:SER:HA	1:A:180:PHE:CD2	2.45	0.51
30:A:417:SQD:H332	23:b:609:CLA:H203	1.91	0.51
3:C:164:HIS:ND1	23:C:507:CLA:OBD	2.37	0.51
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.92	0.51
15:u:98:THR:O	15:u:102:LYS:HG3	2.11	0.51
23:B:607:CLA:H193	11:L:27:LEU:HD11	1.92	0.51
2:b:201:HIS:HD2	2:b:202:HIS:CE1	2.28	0.51
3:c:393:ALA:HB1	34:v:201:HEM:HBC1	1.93	0.51
15:u:117:VAL:HG13	15:u:122:VAL:HG21	1.93	0.51
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.91	0.51
16:V:98:LEU:O	16:V:102:MET:HG3	2.11	0.51
1:a:317:TRP:CZ3	4:d:180:ARG:HD3	2.46	0.51
23:a:405:CLA:H203	24:a:407:PHO:H71	1.92	0.51
23:b:611:CLA:H151	23:b:612:CLA:H203	1.92	0.51
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.44	0.51
16:v:119:PRO:HG2	34:v:201:HEM:HMC2	1.91	0.51
1:A:217:SER:HA	4:D:272:LEU:HD12	1.91	0.51
28:A:411:DGD:HAT2	3:C:281:MET:HG3	1.93	0.51
30:A:413:SQD:H171	25:J:101:PL9:H522	1.93	0.51
1:a:65:GLU:OE2	1:a:334:ARG:NH2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:404:CLA:H151	24:a:407:PHO:H72	1.92	0.51
1:a:85:SER:HA	1:a:109:GLY:HA3	1.93	0.51
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.46	0.51
2:b:464:PHE:HD2	23:b:614:CLA:HAC2	1.75	0.51
3:c:342:MET:HE3	3:c:352:GLY:HA2	1.92	0.51
23:c:507:CLA:H112	27:c:516:BCR:H362	1.92	0.51
23:B:603:CLA:C3D	23:B:605:CLA:H2	2.41	0.51
17:y:39:LEU:HD21	19:Z:25:VAL:HA	1.93	0.51
1:a:271:LEU:HD11	25:a:410:PL9:C4	2.41	0.51
2:b:26:HIS:CE1	23:b:615:CLA:HMA2	2.45	0.51
2:B:68:ARG:HH22	23:B:604:CLA:HED1	1.75	0.51
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.93	0.51
3:c:282:MET:HG2	23:c:501:CLA:H61	1.93	0.51
3:C:451:ALA:HA	3:C:456:GLU:CD	2.36	0.51
4:D:84:SER:HB2	4:D:85:MET:HE2	1.93	0.51
2:b:341:LYS:HA	2:b:405:GLU:HB2	1.92	0.51
1:A:211:PHE:HA	1:A:214:MET:HB2	1.93	0.50
27:B:618:BCR:H352	27:B:619:BCR:H382	1.92	0.50
2:b:18:ARG:NH1	2:b:115:TRP:O	2.37	0.50
17:g:39:LEU:HD21	19:z:25:VAL:HA	1.92	0.50
19:z:32:ASP:CG	19:z:33:TRP:H	2.19	0.50
3:c:380:ILE:HA	3:c:384:ILE:HD11	1.94	0.50
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.93	0.50
27:B:618:BCR:H381	14:t:4:ILE:HD13	1.92	0.50
30:F:102:SQD:H162	18:X:33:THR:HA	1.94	0.50
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.94	0.50
2:b:184:GLU:H	2:b:200:ALA:HB2	1.75	0.50
3:c:224:ILE:O	3:c:227:VAL:HG23	2.10	0.50
2:B:213:GLY:O	2:B:217:ILE:HG13	2.12	0.50
2:B:371:THR:HG22	2:B:377:VAL:HA	1.93	0.50
23:a:404:CLA:H51	24:a:407:PHO:C3B	2.41	0.50
23:b:611:CLA:CHA	23:b:611:CLA:HBA1	2.41	0.50
13:o:240:THR:HG22	13:o:264:VAL:HG12	1.93	0.50
24:A:406:PHO:H151	23:D:401:CLA:H172	1.93	0.50
27:B:618:BCR:H332	14:t:21:ILE:HD12	1.94	0.50
10:K:21:LEU:HD21	27:K:102:BCR:HC31	1.92	0.50
1:A:153:SER:HB3	23:A:403:CLA:HED1	1.93	0.50
23:A:404:CLA:H42	25:D:404:PL9:H162	1.93	0.50
4:D:49:LEU:HD13	27:D:405:BCR:C15	2.41	0.50
27:T:102:BCR:H333	12:m:13:LEU:HD12	1.93	0.50
1:a:176:ILE:HD12	23:a:405:CLA:HED3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:361:PHE:HA	28:c:517:DGD:HE62	1.93	0.50
4:d:244:TYR:OH	4:d:264:LYS:HE3	2.12	0.50
28:B:626:DGD:HB22	33:B:628:LMT:H72	1.93	0.50
27:T:103:BCR:H352	27:b:620:BCR:H382	1.93	0.50
3:c:130:VAL:O	3:c:134:ILE:HG12	2.12	0.50
3:c:223:TRP:CG	3:c:224:ILE:H	2.30	0.50
4:d:129:GLN:OE1	4:d:143:ALA:HA	2.11	0.50
10:k:27:VAL:HG23	31:k:103:LMG:H322	1.94	0.50
23:b:610:CLA:H193	11:l:27:LEU:HD11	1.94	0.50
2:B:121:GLU:O	7:H:12:ARG:NH2	2.45	0.50
23:C:505:CLA:H11	27:C:515:BCR:H312	1.94	0.50
31:D:408:LMG:H392	27:T:103:BCR:HC32	1.94	0.50
1:a:140:ARG:HH22	29:a:414:LHG:P	2.34	0.50
23:B:616:CLA:H12	23:B:616:CLA:H72	1.92	0.49
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.77	0.49
28:D:410:DGD:O5E	28:D:410:DGD:O4E	2.29	0.49
1:a:141:PRO:O	1:a:143:ILE:N	2.43	0.49
3:c:131:TYR:HE1	3:c:135:ARG:HD2	1.77	0.49
16:v:102:MET:HE3	34:v:201:HEM:HBB2	1.94	0.49
17:g:31:ALA:O	17:g:35:ILE:HG23	2.12	0.49
2:B:137:LYS:HD2	7:H:14:LEU:O	2.12	0.49
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.47	0.49
23:B:611:CLA:H41	23:B:614:CLA:HBC3	1.92	0.49
30:F:102:SQD:H131	18:X:36:VAL:HG11	1.95	0.49
19:Z:33:TRP:HA	19:Z:36:SER:HB3	1.94	0.49
3:c:164:HIS:ND1	23:c:507:CLA:OBD	2.37	0.49
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.94	0.49
13:o:230:VAL:HG13	13:o:237:ILE:HG22	1.94	0.49
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.94	0.49
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.93	0.49
3:c:461:ARG:NH1	4:d:241:GLU:OE1	2.45	0.49
30:f:103:SQD:H162	18:x:33:THR:HA	1.95	0.49
23:C:505:CLA:HBA1	23:C:505:CLA:HBD	1.94	0.49
6:F:21:VAL:O	6:F:25:THR:HG23	2.12	0.49
30:a:415:SQD:H241	29:a:417:LHG:HC81	1.93	0.49
23:c:505:CLA:HBD	23:c:505:CLA:HBA1	1.95	0.49
27:K:102:BCR:H332	19:Z:17:PHE:CD1	2.48	0.49
16:V:90:PRO:O	16:V:92:ARG:HD3	2.13	0.49
29:a:414:LHG:HC41	4:d:232:PHE:CE2	2.47	0.49
3:c:305:THR:HG23	3:c:307:PRO:HD2	1.95	0.49
2:B:78:TRP:HB3	13:o:137:ALA:HB1	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.95	0.49
1:a:161:TYR:HB3	1:a:162:PRO:HD3	1.94	0.49
2:B:5:TRP:HZ3	23:B:611:CLA:H51	1.77	0.49
4:D:49:LEU:O	4:D:53:THR:HG23	2.12	0.49
10:K:31:LEU:HB3	27:K:102:BCR:C15	2.43	0.49
33:B:627:LMT:H122	14:t:7:VAL:HG12	1.94	0.49
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.46	0.49
27:T:102:BCR:C23	2:b:25:MET:HG2	2.43	0.49
23:b:606:CLA:C1D	23:b:608:CLA:H52	2.43	0.49
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.94	0.49
6:f:27:ALA:HB1	34:f:101:HEM:CAC	2.43	0.49
15:u:75:LEU:HD21	15:u:101:GLN:HB3	1.94	0.49
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.95	0.49
3:C:223:TRP:CG	3:C:224:ILE:H	2.30	0.49
3:C:406:SER:O	3:C:418:ASN:ND2	2.43	0.49
4:D:146:PHE:C	4:D:149:PRO:HD2	2.38	0.49
6:F:27:ALA:HB1	34:F:101:HEM:CAC	2.42	0.49
23:b:605:CLA:H152	28:b:622:DGD:HAW2	1.94	0.49
23:c:512:CLA:H143	23:c:513:CLA:H162	1.94	0.49
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.47	0.49
2:B:25:MET:HG2	27:B:617:BCR:C23	2.43	0.49
2:B:326:ARG:NH2	4:D:297:ASP:OD2	2.45	0.49
2:B:474:LEU:O	4:D:134:ARG:NH1	2.46	0.49
3:C:363:GLY:O	3:C:367:GLU:HG2	2.13	0.49
15:U:54:LYS:HD2	15:U:113:THR:HG23	1.94	0.49
13:o:184:ASP:OD2	13:o:188:ARG:HB2	2.13	0.49
1:A:283:VAL:O	1:A:286:THR:HG22	2.13	0.48
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.93	0.48
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.48	0.48
5:e:15:THR:HG23	9:j:8:ILE:O	2.13	0.48
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.95	0.48
2:B:241:SER:HB3	23:B:612:CLA:HED3	1.95	0.48
23:B:606:CLA:H203	30:a:401:SQD:H332	1.95	0.48
13:O:77:LEU:HB2	13:O:260:LYS:HB3	1.95	0.48
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.23	0.48
3:c:197:ARG:NH2	3:c:231:GLU:OE2	2.45	0.48
3:C:425:TRP:CE2	23:C:504:CLA:HBA1	2.49	0.48
12:M:9:ILE:HD12	12:m:8:LEU:HG	1.95	0.48
23:a:404:CLA:H71	23:a:405:CLA:HAB	1.94	0.48
23:a:405:CLA:H51	23:a:405:CLA:H11	1.62	0.48
2:b:341:LYS:HD2	2:b:429:ILE:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:514:BCR:H311	27:c:514:BCR:H343	1.94	0.48
1:A:114:LEU:O	1:A:118:HIS:ND1	2.47	0.48
23:A:404:CLA:HBA1	23:A:404:CLA:CHA	2.42	0.48
2:B:280:PHE:O	2:B:284:ILE:HG13	2.14	0.48
5:E:15:THR:HG23	9:J:8:ILE:O	2.13	0.48
16:V:83:GLU:H	16:V:83:GLU:CD	2.21	0.48
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.95	0.48
23:B:603:CLA:CBB	23:B:605:CLA:H152	2.42	0.48
23:a:406:CLA:H93	23:d:402:CLA:H152	1.94	0.48
2:b:222:PRO:HG3	7:h:27:THR:H	1.79	0.48
23:A:405:CLA:HAB	23:D:401:CLA:H72	1.95	0.48
1:a:57:PRO:HG3	1:a:68:SER:HB3	1.95	0.48
2:b:91:TRP:HE1	33:b:625:LMT:H12	1.78	0.48
3:c:75:PHE:HD1	3:c:86:LEU:HD21	1.77	0.48
3:c:291:TRP:O	3:c:305:THR:OG1	2.32	0.48
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.94	0.48
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.95	0.48
23:b:605:CLA:H162	23:b:605:CLA:H122	1.50	0.48
2:B:25:MET:HG2	27:B:617:BCR:H23C	1.95	0.48
2:B:26:HIS:CE1	23:B:612:CLA:HMA2	2.49	0.48
23:b:604:CLA:HMB2	27:x:101:BCR:H281	1.96	0.48
23:b:606:CLA:H61	23:b:606:CLA:H41	1.66	0.48
23:b:611:CLA:H51	23:b:612:CLA:H101	1.95	0.48
3:c:166:ILE:O	3:c:170:ILE:HG13	2.13	0.48
3:c:391:ARG:HD2	3:c:395:TYR:CZ	2.48	0.48
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.95	0.48
33:D:411:LMT:H72	18:X:26:GLY:HA2	1.96	0.48
5:E:7:GLU:H	5:E:7:GLU:CD	2.22	0.48
1:a:72:LEU:HD13	31:a:402:LMG:H111	1.96	0.48
3:c:29:GLU:HB3	10:k:46:ARG:HH11	1.79	0.48
7:h:19:GLY:O	7:h:21:VAL:HG13	2.14	0.48
23:A:404:CLA:H101	31:D:408:LMG:H221	1.96	0.48
2:B:317:ASN:HA	2:B:330:MET:HE1	1.96	0.48
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.96	0.48
1:A:337:HIS:NE2	3:C:354:GLU:OE1	2.47	0.47
23:C:504:CLA:H151	28:C:517:DGD:HBW1	1.96	0.47
4:D:320:LEU:HD23	4:D:323:GLU:OE1	2.14	0.47
19:Z:32:ASP:CG	19:Z:33:TRP:H	2.22	0.47
30:f:103:SQD:H131	18:x:36:VAL:HG11	1.96	0.47
16:v:81:ARG:CZ	16:v:157:GLY:HA3	2.43	0.47
2:B:89:GLY:HA2	28:B:626:DGD:HE1	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:464:PHE:HD2	23:B:611:CLA:HAC2	1.79	0.47
4:D:267:LEU:O	4:D:271:MET:HG3	2.14	0.47
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.48	0.47
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.79	0.47
3:C:315:MET:HE1	3:C:369:LEU:HD12	1.96	0.47
1:a:317:TRP:HZ3	4:d:180:ARG:HD3	1.79	0.47
23:a:409:CLA:HBC1	31:i:101:LMG:H341	1.96	0.47
2:b:18:ARG:HD3	2:b:118:TRP:HB3	1.96	0.47
2:b:315:ILE:HG22	2:b:426:PHE:HB3	1.96	0.47
3:c:223:TRP:CD2	3:c:224:ILE:HG13	2.50	0.47
7:h:38:PHE:HB2	27:x:101:BCR:H10C	1.95	0.47
2:B:91:TRP:CH2	23:B:606:CLA:H12	2.49	0.47
33:T:101:LMT:H3'	33:T:101:LMT:H1B	1.56	0.47
27:T:102:BCR:H23C	2:b:25:MET:HG2	1.96	0.47
3:c:315:MET:HE1	3:c:369:LEU:HD12	1.96	0.47
17:g:24:MET:O	17:g:28:ILE:HG23	2.14	0.47
30:A:417:SQD:H152	27:T:103:BCR:HC22	1.97	0.47
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.49	0.47
28:b:602:DGD:O1B	28:b:602:DGD:O2D	2.32	0.47
2:B:348:ASN:HB3	2:B:354:LEU:HD21	1.97	0.47
23:B:604:CLA:HBB1	23:B:607:CLA:HBB2	1.95	0.47
27:B:620:BCR:H15C	27:B:620:BCR:H351	1.80	0.47
23:a:405:CLA:HAA1	25:d:404:PL9:H362	1.97	0.47
2:B:257:TRP:CD2	4:D:291:LEU:HD12	2.50	0.47
23:B:606:CLA:H18	23:B:616:CLA:H121	1.96	0.47
23:B:611:CLA:HBC2	31:D:407:LMG:H222	1.96	0.47
3:C:297:TYR:O	3:C:423:ARG:NH2	2.48	0.47
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.95	0.47
2:b:213:GLY:O	2:b:217:ILE:HG13	2.15	0.47
2:b:326:ARG:HB3	2:b:444:ARG:HG2	1.96	0.47
3:c:425:TRP:CE2	23:c:504:CLA:HBA1	2.50	0.47
13:o:154:SER:N	13:o:169:LYS:O	2.46	0.47
1:A:116:ILE:HG13	1:A:117:PHE:N	2.29	0.47
27:B:617:BCR:H341	27:B:618:BCR:H24C	1.96	0.47
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.79	0.47
3:C:240:ILE:HD11	27:C:515:BCR:H372	1.97	0.47
30:D:409:SQD:H241	30:D:409:SQD:H111	1.97	0.47
1:a:156:ALA:HA	1:a:160:ILE:HB	1.97	0.47
1:A:156:ALA:HA	1:A:160:ILE:HB	1.97	0.47
30:A:413:SQD:H112	29:A:415:LHG:H111	1.97	0.47
12:M:19:SER:O	12:M:23:ILE:HG13	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:407:SQD:H241	30:d:407:SQD:H111	1.96	0.47
24:A:406:PHO:H161	4:D:48:TRP:CE2	2.50	0.47
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.97	0.47
2:B:450:TRP:NE1	23:B:607:CLA:HBA1	2.30	0.47
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.97	0.47
27:J:102:BCR:H341	27:J:102:BCR:H11C	1.71	0.47
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.14	0.47
5:e:60:GLN:HG2	5:e:62:SER:H	1.80	0.47
23:B:603:CLA:H92	23:B:603:CLA:HBB2	1.97	0.46
3:C:209:ILE:HG23	27:C:515:BCR:H382	1.97	0.46
14:T:4:ILE:HD13	27:T:103:BCR:H381	1.96	0.46
1:a:260:PHE:CZ	1:a:263:ALA:HB2	2.50	0.46
31:i:101:LMG:H181	33:i:102:LMT:H42	1.97	0.46
10:k:12:PRO:HB2	10:k:15:TYR:HD2	1.80	0.46
24:D:402:PHO:H92	24:D:402:PHO:H61	1.75	0.46
6:F:45:ARG:NH2	9:J:40:LEU:O	2.48	0.46
10:K:26:PRO:O	10:K:29:PRO:HD2	2.15	0.46
3:c:229:ASN:ND2	3:c:231:GLU:HB2	2.30	0.46
4:d:252:PHE:O	4:d:256:ILE:HG22	2.15	0.46
16:v:147:VAL:O	16:v:150:LYS:HB2	2.16	0.46
17:g:32:GLY:O	17:g:35:ILE:HG12	2.15	0.46
1:A:111:PRO:O	1:A:115:ILE:HG13	2.15	0.46
23:B:614:CLA:H112	23:B:614:CLA:H91	1.73	0.46
17:y:25:ILE:O	17:y:29:GLY:N	2.49	0.46
1:a:214:MET:HE1	4:d:142:ASN:ND2	2.28	0.46
2:b:348:ASN:HB3	2:b:354:LEU:HD21	1.97	0.46
4:d:214:HIS:ND1	25:d:404:PL9:O2	2.33	0.46
10:k:40:GLN:HA	10:k:43:VAL:HG12	1.97	0.46
23:B:603:CLA:H41	23:B:603:CLA:H61	1.67	0.46
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.97	0.46
14:T:1:MET:HE2	12:m:6:LEU:HD21	1.97	0.46
1:a:157:VAL:HG13	1:a:172:MET:HB3	1.97	0.46
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.51	0.46
1:a:317:TRP:CD1	4:d:177:ALA:HB2	2.50	0.46
24:a:408:PHO:CHB	23:d:402:CLA:H101	2.46	0.46
3:c:150:ASP:HB3	3:c:153:ASP:HB2	1.98	0.46
3:c:277:GLY:C	23:c:505:CLA:HBC2	2.41	0.46
3:c:466:VAL:HG13	4:d:251:ARG:HD2	1.97	0.46
23:C:510:CLA:H2	23:C:510:CLA:H61	1.67	0.46
27:C:514:BCR:H343	27:C:514:BCR:H311	1.98	0.46
27:C:515:BCR:H11C	27:C:515:BCR:H341	1.82	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:333:GLY:O	2:b:439:SER:HB3	2.16	0.46
23:b:609:CLA:H71	27:b:621:BCR:H342	1.98	0.46
23:c:509:CLA:H121	23:c:509:CLA:HBD	1.97	0.46
5:e:81:GLU:C	5:e:83:LEU:H	2.24	0.46
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.48	0.46
23:C:511:CLA:H141	19:Z:20:VAL:HG13	1.98	0.46
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.98	0.46
9:J:33:TYR:HB3	27:J:102:BCR:H383	1.97	0.46
27:J:102:BCR:H15C	27:J:102:BCR:H351	1.63	0.46
13:O:192:SER:OG	13:O:193:GLY:N	2.49	0.46
2:b:12:LEU:HB2	23:b:615:CLA:HMC2	1.97	0.46
2:b:450:TRP:NE1	23:b:610:CLA:HBA1	2.31	0.46
28:c:518:DGD:HAW2	28:c:518:DGD:HA91	1.76	0.46
4:d:216:ALA:O	4:d:220:ASN:ND2	2.45	0.46
7:H:19:GLY:O	7:H:21:VAL:HG13	2.15	0.46
1:a:334:ARG:NH2	4:d:312:GLU:OE2	2.48	0.46
4:D:146:PHE:O	4:D:149:PRO:HD2	2.16	0.46
1:a:153:SER:HB2	23:a:404:CLA:H43	1.97	0.46
30:a:415:SQD:H172	29:a:417:LHG:H172	1.97	0.46
13:o:51:THR:O	13:o:53:ARG:N	2.49	0.46
3:C:429:SER:HB3	28:C:517:DGD:HA81	1.97	0.46
31:C:520:LMG:H292	31:C:520:LMG:H111	1.98	0.46
1:a:129:ARG:NH2	4:d:256:ILE:HD12	2.29	0.46
2:b:135:LEU:HA	2:b:138:MET:HE3	1.97	0.46
23:b:606:CLA:HBB2	23:b:606:CLA:H92	1.98	0.46
23:b:615:CLA:H122	23:b:615:CLA:H162	1.75	0.46
3:c:38:GLY:HA3	23:c:511:CLA:HMD2	1.98	0.46
27:c:514:BCR:H353	27:k:102:BCR:H321	1.97	0.46
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.44	0.46
23:B:608:CLA:CHA	23:B:608:CLA:HBA1	2.46	0.46
27:B:617:BCR:H24C	27:B:617:BCR:H371	1.74	0.46
33:B:628:LMT:H62	8:i:4:LEU:HD22	1.97	0.46
23:C:501:CLA:C1D	23:C:503:CLA:H2	2.46	0.46
4:D:221:THR:HG23	4:D:244:TYR:HB2	1.98	0.46
3:c:174:LEU:HD13	23:c:502:CLA:H111	1.98	0.46
3:c:257:PHE:HB3	3:c:258:GLY:H	1.62	0.46
1:A:183:MET:HE1	23:A:404:CLA:HMD2	1.97	0.45
1:A:214:MET:HE1	4:D:142:ASN:HD21	1.81	0.45
1:A:244:GLU:CD	4:D:264:LYS:HZ3	2.23	0.45
27:A:410:BCR:H342	30:A:417:SQD:H311	1.98	0.45
11:L:18:TYR:CE2	14:T:20:ALA:HA	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:302:GLU:OE1	13:o:186:LYS:NZ	2.44	0.45
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.97	0.45
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.98	0.45
1:A:235:TYR:C	1:A:237:TYR:H	2.25	0.45
23:A:403:CLA:H62	23:A:403:CLA:H102	1.79	0.45
23:B:614:CLA:H72	31:M:102:LMG:H352	1.98	0.45
3:C:163:PHE:CG	23:C:512:CLA:HAB	2.52	0.45
9:J:38:SER:OG	9:J:39:SER:N	2.49	0.45
2:b:326:ARG:NH2	4:d:297:ASP:OD2	2.50	0.45
27:c:515:BCR:H15C	27:c:515:BCR:H351	1.70	0.45
23:d:403:CLA:H41	23:d:403:CLA:H61	1.78	0.45
27:k:102:BCR:H333	17:g:28:ILE:HG22	1.98	0.45
2:B:198:VAL:O	2:B:202:HIS:ND1	2.42	0.45
19:Z:1:MET:HE3	19:Z:60:PHE:CG	2.51	0.45
1:a:180:PHE:HA	1:a:183:MET:HE3	1.98	0.45
2:b:7:ARG:HH21	31:b:623:LMG:HC3	1.82	0.45
4:d:87:HIS:CD2	4:d:162:LEU:HD23	2.51	0.45
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.81	0.45
3:C:337:LEU:HA	13:O:131:PRO:HG3	1.97	0.45
4:D:252:PHE:O	4:D:256:ILE:HG22	2.15	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.45
19:z:33:TRP:HA	19:z:36:SER:HB3	1.98	0.45
23:A:403:CLA:H191	31:D:408:LMG:H352	1.98	0.45
2:B:103:LEU:HD21	23:B:605:CLA:HMC2	1.99	0.45
2:B:487:SER:N	2:B:488:PRO:HD2	2.32	0.45
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.78	0.45
14:T:1:MET:HB3	14:T:2:GLU:OE2	2.17	0.45
1:a:140:ARG:NH2	29:a:414:LHG:O5	2.46	0.45
24:a:407:PHO:H92	24:a:407:PHO:H61	1.76	0.45
2:b:137:LYS:O	2:b:141:ILE:HG13	2.17	0.45
2:b:247:PHE:HE1	23:b:605:CLA:H101	1.82	0.45
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.51	0.45
4:D:148:ALA:HB1	4:D:279:LEU:HB2	1.99	0.45
1:a:150:PRO:HB2	23:a:404:CLA:H61	1.99	0.45
27:c:514:BCR:H331	27:c:514:BCR:HC7	1.53	0.45
8:i:8:VAL:O	8:i:12:VAL:HG23	2.17	0.45
13:o:168:PHE:HB2	13:o:225:LEU:HB2	1.97	0.45
23:A:404:CLA:H71	31:D:408:LMG:H202	1.98	0.45
29:A:412:LHG:HC32	4:D:229:ALA:O	2.16	0.45
31:B:622:LMG:H421	4:D:284:ILE:HD13	1.99	0.45
5:E:81:GLU:C	5:E:83:LEU:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:106:ARG:HA	15:U:109:LEU:HG	1.99	0.45
30:a:415:SQD:H223	28:c:519:DGD:HAE1	1.98	0.45
2:b:243:ALA:HB2	2:b:466:HIS:CE1	2.51	0.45
3:c:120:ILE:HD11	27:c:514:BCR:HC8	1.98	0.45
23:A:403:CLA:H3A	23:A:403:CLA:HBA1	1.57	0.45
23:A:403:CLA:H51	24:D:402:PHO:C3B	2.47	0.45
2:B:135:LEU:HA	2:B:138:MET:HE3	1.97	0.45
3:C:319:ILE:HG21	3:C:389:GLU:HG3	1.99	0.45
27:D:405:BCR:H11C	27:D:405:BCR:H341	1.75	0.45
5:E:19:TYR:O	5:E:23:HIS:ND1	2.41	0.45
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.99	0.45
27:J:102:BCR:H361	27:J:102:BCR:H20C	1.85	0.45
27:T:102:BCR:H371	27:T:102:BCR:H24C	1.73	0.45
2:b:239:SER:O	2:b:466:HIS:ND1	2.49	0.45
2:b:487:SER:N	2:b:488:PRO:HD2	2.31	0.45
23:b:614:CLA:H52	23:b:617:CLA:HBC3	1.99	0.45
3:c:318:LEU:HD13	3:c:351:PHE:HE1	1.82	0.45
2:B:125:ASP:HB2	2:B:132:ALA:HB3	1.99	0.45
2:B:135:LEU:HD23	2:B:138:MET:HE3	1.99	0.45
2:B:256:MET:HA	2:B:263:THR:HG21	1.99	0.45
23:B:605:CLA:H202	23:B:609:CLA:HBB2	1.99	0.45
27:B:618:BCR:H11C	27:B:618:BCR:H341	1.70	0.45
3:C:405:ASN:CB	28:C:518:DGD:HG31	2.46	0.45
23:C:512:CLA:H143	23:C:513:CLA:H162	1.99	0.45
3:c:137:PRO:HB2	3:c:139:THR:O	2.17	0.45
3:c:240:ILE:O	3:c:244:CYS:HB2	2.17	0.45
5:e:55:TYR:O	5:e:84:LYS:HE3	2.17	0.45
27:B:618:BCR:HC32	31:d:406:LMG:H392	1.99	0.45
3:C:154:LYS:HE3	3:C:266:TRP:CE2	2.51	0.45
3:C:248:GLY:O	3:C:252:ILE:HG12	2.16	0.45
31:a:416:LMG:H172	4:d:270:PHE:HE1	1.82	0.45
2:b:16:PRO:HG2	2:b:123:PHE:HB3	1.98	0.45
5:e:42:LEU:O	5:e:46:VAL:HG23	2.17	0.45
1:A:124:SER:HA	1:A:151:LEU:HD21	1.99	0.44
2:B:155:ALA:O	2:B:159:THR:OG1	2.22	0.44
2:B:354:LEU:HB3	2:B:370:LEU:HB3	1.98	0.44
1:a:238:LYS:HD2	14:t:32:LYS:HB3	1.98	0.44
2:b:247:PHE:HB2	23:b:611:CLA:HBC1	1.97	0.44
3:c:343:ARG:NH1	3:c:347:GLY:O	2.50	0.44
10:k:21:LEU:HD21	27:k:102:BCR:HC31	1.99	0.44
2:B:150:CYS:HA	23:B:603:CLA:HBC2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	1.99	0.44
1:a:271:LEU:HD21	25:a:410:PL9:HC71	1.98	0.44
3:c:86:LEU:HB3	3:c:90:PRO:HD3	1.98	0.44
3:c:248:GLY:O	3:c:252:ILE:HG12	2.17	0.44
23:d:402:CLA:H41	23:d:402:CLA:H61	1.71	0.44
1:A:190:HIS:O	1:A:298:ASN:HB3	2.18	0.44
1:A:210:LEU:HG	24:A:406:PHO:NC	2.32	0.44
1:A:224:ILE:O	4:D:265:ARG:NH2	2.50	0.44
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.83	0.44
4:D:40:CYS:HB3	4:D:117:HIS:O	2.18	0.44
1:a:89:ILE:HG12	13:o:99:ARG:NH2	2.32	0.44
1:a:232:SER:OG	31:a:416:LMG:O3	2.20	0.44
2:b:89:GLY:HA2	28:b:602:DGD:HD61	1.98	0.44
2:b:201:HIS:HD2	2:b:202:HIS:ND1	2.15	0.44
23:b:605:CLA:H41	23:b:605:CLA:H62	1.53	0.44
23:b:605:CLA:H193	28:b:622:DGD:HA71	1.98	0.44
23:c:509:CLA:H11	23:c:509:CLA:H51	1.68	0.44
2:B:89:GLY:HA2	28:B:626:DGD:HD61	1.98	0.44
23:B:607:CLA:HBB1	31:B:622:LMG:H341	2.00	0.44
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.81	0.44
6:F:17:THR:OG1	6:F:18:VAL:N	2.50	0.44
23:b:605:CLA:H72	7:h:46:LEU:HD13	2.00	0.44
3:c:319:ILE:HG21	3:c:389:GLU:HG3	1.99	0.44
13:o:240:THR:HA	13:o:264:VAL:HA	1.99	0.44
15:u:68:TYR:HB2	15:u:71:LEU:HD12	1.99	0.44
30:A:413:SQD:H162	25:J:101:PL9:H533	1.99	0.44
23:B:602:CLA:H93	23:B:602:CLA:H62	1.90	0.44
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.00	0.44
19:Z:33:TRP:O	19:Z:33:TRP:CD1	2.71	0.44
23:b:606:CLA:H2	23:b:608:CLA:H93	2.00	0.44
23:b:607:CLA:HBB1	23:b:610:CLA:CBB	2.47	0.44
23:b:615:CLA:H171	23:b:616:CLA:HBB2	1.99	0.44
2:b:488:PRO:O	2:b:490:GLN:N	2.44	0.44
23:b:616:CLA:H191	27:b:620:BCR:H333	2.00	0.44
3:c:456:GLU:HG2	3:c:457:LYS:HG3	2.00	0.44
4:d:275:PRO:O	4:d:279:LEU:HD23	2.17	0.44
27:j:102:BCR:H271	31:k:103:LMG:HC62	2.00	0.44
10:k:12:PRO:HB2	10:k:15:TYR:CD2	2.53	0.44
1:A:28:LEU:HB2	30:A:417:SQD:H91	1.99	0.44
1:A:43:ALA:HB1	27:A:410:BCR:H362	2.00	0.44
2:B:338:GLN:HB3	13:o:84:ASN:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:76:SER:HG	2:b:78:TRP:CD1	2.36	0.44
27:b:621:BCR:H331	33:b:625:LMT:H122	1.99	0.44
7:h:12:ARG:O	7:h:12:ARG:HD3	2.17	0.44
1:A:238:LYS:O	1:A:241:GLN:HG3	2.18	0.44
2:B:360:PRO:HB2	2:B:363:PHE:HD2	1.83	0.44
3:C:343:ARG:NH1	3:C:347:GLY:O	2.51	0.44
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.98	0.44
23:a:404:CLA:H172	24:a:407:PHO:H43	1.99	0.44
29:a:414:LHG:HC32	4:d:229:ALA:O	2.18	0.44
2:b:4:PRO:HD2	2:b:7:ARG:HD2	2.00	0.44
2:b:191:ASN:HD21	7:h:59:ASN:C	2.26	0.44
2:b:414:PRO:HB2	2:b:415:PRO:HD3	2.00	0.44
23:b:619:CLA:H143	23:b:619:CLA:H111	1.78	0.44
16:v:107:THR:OG1	16:v:109:ASP:OD1	2.35	0.44
23:B:607:CLA:C4A	23:B:607:CLA:HBA2	2.44	0.44
3:C:240:ILE:O	3:C:244:CYS:HB2	2.18	0.44
27:C:514:BCR:H11C	27:K:102:BCR:H322	2.00	0.44
4:D:110:LEU:O	4:D:114:ILE:HG13	2.18	0.44
24:D:402:PHO:H13	24:D:402:PHO:H102	1.77	0.44
9:J:14:ALA:HB3	27:K:102:BCR:H393	2.00	0.44
3:c:464:GLU:HA	3:c:465:PRO:HD2	1.84	0.44
5:e:23:HIS:HA	5:e:26:THR:OG1	2.17	0.44
12:m:1:MET:HG2	12:m:2:GLU:H	1.83	0.44
24:A:406:PHO:HMC3	4:D:279:LEU:HD21	2.00	0.43
23:B:602:CLA:H162	23:B:602:CLA:H122	1.57	0.43
3:C:38:GLY:HA3	23:C:511:CLA:HMD2	2.00	0.43
3:C:85:GLY:N	28:C:517:DGD:HE4	2.33	0.43
27:C:514:BCR:H353	27:K:102:BCR:H321	2.00	0.43
16:V:103:LYS:O	16:V:122:ARG:HG2	2.19	0.43
2:b:109:LEU:O	27:b:621:BCR:H21C	2.18	0.43
23:b:609:CLA:HMD3	33:b:625:LMT:H1'	2.00	0.43
3:c:347:GLY:HA3	13:o:43:ASN:HB2	1.99	0.43
2:B:488:PRO:O	2:B:490:GLN:N	2.43	0.43
23:B:604:CLA:HBD	23:B:605:CLA:H43	2.00	0.43
23:B:610:CLA:H12	23:B:610:CLA:H51	1.82	0.43
23:B:613:CLA:H191	27:B:619:BCR:H333	1.99	0.43
27:B:619:BCR:H15C	27:B:619:BCR:H351	1.78	0.43
3:C:86:LEU:HB3	3:C:90:PRO:HD3	2.00	0.43
1:a:141:PRO:HB2	1:a:142:TRP:H	1.64	0.43
24:a:407:PHO:H41	24:a:407:PHO:H62	1.37	0.43
2:b:280:PHE:O	2:b:284:ILE:HG13	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:619:CLA:H72	23:b:619:CLA:H12	1.98	0.43
3:c:72:LEU:HD11	3:c:108:THR:HB	1.99	0.43
12:m:19:SER:O	12:m:23:ILE:HG13	2.18	0.43
1:A:191:ASN:HB2	3:C:411:ALA:HB1	1.99	0.43
1:A:340:PRO:HD3	15:U:133:TYR:CZ	2.54	0.43
27:A:410:BCR:H24C	27:A:410:BCR:H371	1.84	0.43
31:A:414:LMG:H172	4:D:270:PHE:HE1	1.83	0.43
23:B:603:CLA:H2	23:B:605:CLA:H93	2.01	0.43
27:B:617:BCR:H15C	27:B:617:BCR:H351	1.76	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.18	0.43
27:C:514:BCR:H24C	27:C:514:BCR:H371	1.84	0.43
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.89	0.43
27:D:405:BCR:H15C	27:D:405:BCR:H351	1.82	0.43
27:K:102:BCR:H15C	27:K:102:BCR:H351	1.84	0.43
2:b:366:PHE:CG	2:b:367:PRO:HD2	2.53	0.43
13:o:143:PRO:HG2	13:o:248:ASP:HB3	2.01	0.43
13:o:192:SER:OG	13:o:193:GLY:N	2.50	0.43
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.52	0.43
1:A:159:LEU:C	1:A:162:PRO:HD2	2.43	0.43
1:A:271:LEU:HD11	25:A:408:PL9:C4	2.48	0.43
23:A:404:CLA:H202	23:A:404:CLA:H162	1.72	0.43
23:C:501:CLA:H193	23:C:507:CLA:H111	2.00	0.43
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.48	0.43
5:E:60:GLN:HG2	5:E:62:SER:H	1.83	0.43
19:Z:1:MET:HE3	19:Z:60:PHE:CD2	2.53	0.43
1:a:257:ARG:HH22	2:b:488:PRO:C	2.27	0.43
23:b:613:CLA:HBB1	27:x:101:BCR:HC32	1.98	0.43
3:c:473:ASP:HB2	14:t:26:PRO:HB3	2.00	0.43
4:d:67:TYR:CD1	31:d:405:LMG:HC72	2.53	0.43
4:d:157:PHE:CE1	4:d:171:PRO:HG2	2.53	0.43
4:d:176:ALA:HA	4:d:179:PHE:CD2	2.54	0.43
1:A:179:THR:HG22	1:A:183:MET:HE2	2.01	0.43
1:A:232:SER:HB3	1:A:235:TYR:HD1	1.83	0.43
3:C:80:PRO:HB2	3:C:83:GLU:HG3	1.99	0.43
3:C:166:ILE:O	3:C:170:ILE:HG13	2.17	0.43
27:C:514:BCR:H331	27:C:514:BCR:HC7	1.60	0.43
31:a:416:LMG:H211	11:l:26:VAL:HG21	2.00	0.43
2:b:30:VAL:HG12	23:b:608:CLA:HHD	2.00	0.43
2:b:462:PHE:HA	23:b:614:CLA:HMC2	2.01	0.43
31:A:414:LMG:H211	11:L:26:VAL:HG21	2.01	0.43
23:B:603:CLA:HBB2	23:B:605:CLA:H152	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:PHE:CD2	23:C:512:CLA:HAB	2.53	0.43
13:O:240:THR:HA	13:O:264:VAL:HA	1.99	0.43
1:a:227:THR:HG21	1:a:233:ALA:HA	2.00	0.43
3:c:90:PRO:O	3:c:94:THR:HG23	2.18	0.43
23:c:504:CLA:H151	28:c:518:DGD:HBW1	1.99	0.43
23:c:507:CLA:H92	23:c:507:CLA:H62	1.70	0.43
27:c:514:BCR:H353	27:k:102:BCR:C32	2.49	0.43
1:A:182:PHE:O	1:A:186:PHE:HB2	2.18	0.43
1:A:221:SER:HB2	4:D:139:ARG:O	2.18	0.43
23:B:606:CLA:H71	27:B:620:BCR:H342	2.00	0.43
1:a:141:PRO:HG3	3:c:446:GLY:C	2.43	0.43
2:b:354:LEU:HB3	2:b:370:LEU:HB3	2.01	0.43
3:c:186:TYR:HE2	3:c:188:THR:HG22	1.82	0.43
10:k:31:LEU:HB3	27:k:102:BCR:C15	2.49	0.43
1:A:334:ARG:NH1	13:O:183:LEU:O	2.52	0.43
4:D:239:GLN:HB3	4:D:240:ALA:H	1.55	0.43
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.43
27:K:102:BCR:H11C	27:K:102:BCR:H341	1.90	0.43
4:d:40:CYS:HB3	4:d:117:HIS:O	2.19	0.43
4:d:73:PHE:CZ	31:d:405:LMG:H172	2.54	0.43
4:d:110:LEU:O	4:d:114:ILE:HG13	2.19	0.43
2:B:76:SER:HG	2:B:78:TRP:CD1	2.36	0.43
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.53	0.43
2:B:247:PHE:HB2	23:B:608:CLA:HBC1	2.00	0.43
23:D:401:CLA:H41	23:D:401:CLA:H61	1.66	0.43
31:I:101:LMG:H221	33:I:102:LMT:H81	2.00	0.43
10:K:37:PHE:HB3	27:K:102:BCR:C40	2.48	0.43
15:U:58:ASN:ND2	15:U:114:VAL:HG13	2.34	0.43
18:X:34:PHE:O	18:X:38:ILE:HG12	2.18	0.43
1:a:116:ILE:HG13	1:a:117:PHE:N	2.34	0.43
2:b:366:PHE:CD1	2:b:367:PRO:HD2	2.54	0.43
23:b:607:CLA:H202	23:b:607:CLA:H161	1.83	0.43
27:f:102:BCR:H351	27:f:102:BCR:H15C	1.74	0.43
8:i:6:ILE:O	8:i:10:ILE:HG12	2.19	0.43
27:x:101:BCR:H371	27:x:101:BCR:H24C	1.77	0.43
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.54	0.43
23:B:611:CLA:H52	23:B:614:CLA:HBC3	2.01	0.43
3:C:89:ILE:N	3:C:90:PRO:HD2	2.34	0.43
23:C:513:CLA:H3A	23:C:513:CLA:HBA2	1.76	0.43
11:L:22:LEU:O	11:L:26:VAL:HG22	2.19	0.43
1:a:193:LEU:HD11	23:a:404:CLA:HMC2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:269:ARG:NH1	4:d:231:THR:HB	2.33	0.43
23:a:404:CLA:H191	31:d:406:LMG:H352	2.00	0.43
2:b:483:ASP:CB	2:b:484:PRO:HD2	2.49	0.43
33:b:626:LMT:H102	7:h:35:MET:SD	2.59	0.43
4:d:88:SER:HB2	5:e:69:ARG:NH2	2.34	0.43
19:z:33:TRP:O	19:z:33:TRP:CD1	2.72	0.43
2:B:18:ARG:HD3	2:B:118:TRP:HB3	2.01	0.42
3:C:62:PHE:HZ	10:K:28:ILE:HD12	1.83	0.42
3:C:137:PRO:HB2	3:C:139:THR:O	2.19	0.42
27:Z:101:BCR:H24C	27:Z:101:BCR:H371	1.77	0.42
27:a:412:BCR:H11C	27:a:412:BCR:H341	1.82	0.42
4:d:85:MET:HA	5:e:69:ARG:HB3	2.01	0.42
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.49	0.42
27:k:102:BCR:H351	27:k:102:BCR:H15C	1.74	0.42
13:o:41:LEU:HD12	13:o:41:LEU:HA	1.89	0.42
1:A:258:LEU:O	4:D:128:ARG:NH1	2.52	0.42
2:B:472:ARG:NE	23:B:611:CLA:HED3	2.34	0.42
3:C:265:ILE:HG12	23:C:505:CLA:HED1	2.00	0.42
3:C:416:SER:OG	3:C:417:VAL:N	2.52	0.42
1:a:82:VAL:HB	1:a:174:LEU:HB2	2.00	0.42
23:c:501:CLA:C2D	23:c:503:CLA:H2	2.49	0.42
27:c:515:BCR:H24C	27:c:515:BCR:H371	1.87	0.42
9:j:9:PRO:HB2	9:j:12:ILE:HG13	2.01	0.42
23:B:602:CLA:H72	7:H:46:LEU:HD13	2.01	0.42
23:B:608:CLA:H143	23:B:608:CLA:H161	1.86	0.42
23:C:511:CLA:H151	19:Z:20:VAL:O	2.20	0.42
5:E:10:PHE:N	31:E:101:LMG:O3	2.51	0.42
11:L:11:GLU:HA	12:M:29:THR:OG1	2.18	0.42
1:a:309:ALA:HA	6:f:45:ARG:HB2	2.00	0.42
2:b:148:LEU:HA	2:b:210:ILE:HD11	2.00	0.42
27:b:620:BCR:H20C	27:b:620:BCR:H361	1.88	0.42
5:e:50:PRO:HB3	5:e:54:SER:O	2.19	0.42
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.54	0.42
23:B:602:CLA:H61	7:H:46:LEU:HB2	2.01	0.42
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.00	0.42
6:F:22:ALA:O	6:F:25:THR:OG1	2.37	0.42
7:H:12:ARG:O	7:H:12:ARG:HD3	2.19	0.42
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.54	0.42
2:b:334:ASP:OD1	2:b:334:ASP:N	2.51	0.42
23:c:506:CLA:H161	23:c:506:CLA:H202	1.80	0.42
27:j:102:BCR:H15C	27:j:102:BCR:H351	1.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:106:ARG:HA	15:u:109:LEU:HG	2.02	0.42
1:A:119:PHE:HZ	23:A:403:CLA:H8	1.84	0.42
1:A:322:ASN:OD1	3:C:412:THR:HA	2.20	0.42
2:B:7:ARG:O	2:B:10:THR:OG1	2.31	0.42
27:B:620:BCR:H331	33:B:623:LMT:H122	2.01	0.42
3:C:120:ILE:HD11	27:C:514:BCR:HC8	2.01	0.42
27:C:514:BCR:H15C	27:C:514:BCR:H351	1.69	0.42
1:a:92:HIS:CD2	3:c:219:GLY:HA3	2.55	0.42
8:i:29:ALA:HA	8:i:35:LYS:HB2	2.00	0.42
23:A:405:CLA:H143	23:A:405:CLA:H161	1.89	0.42
23:B:614:CLA:H43	31:M:102:LMG:H332	2.00	0.42
1:a:129:ARG:NH2	4:d:256:ILE:HA	2.34	0.42
1:a:238:LYS:O	1:a:241:GLN:HG3	2.20	0.42
2:b:135:LEU:HD22	2:b:237:VAL:HG21	2.02	0.42
2:b:170:ASP:OD1	2:b:175:THR:N	2.48	0.42
3:c:29:GLU:HB2	3:c:30:SER:H	1.63	0.42
23:c:509:CLA:H92	23:c:509:CLA:H62	1.67	0.42
27:c:514:BCR:H351	27:c:514:BCR:H15C	1.63	0.42
4:d:60:THR:HG23	4:d:61:HIS:CD2	2.55	0.42
5:e:14:ILE:HG22	9:j:13:VAL:HG11	2.01	0.42
19:z:5:PHE:CE1	19:z:54:VAL:HG13	2.55	0.42
23:A:404:CLA:H92	23:A:404:CLA:H61	1.77	0.42
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.42
31:B:622:LMG:H142	11:L:35:PHE:CE1	2.54	0.42
1:a:296:ASN:HB3	3:c:401:LEU:HD13	2.02	0.42
23:b:614:CLA:H141	23:b:614:CLA:H162	1.77	0.42
5:e:26:THR:HB	34:f:101:HEM:CAB	2.49	0.42
27:j:102:BCR:H20C	27:j:102:BCR:H361	1.79	0.42
13:o:33:TYR:O	13:o:37:VAL:HG23	2.20	0.42
1:A:324:ALA:HB2	4:D:329:MET:SD	2.60	0.42
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.55	0.42
27:B:619:BCR:H11C	27:B:619:BCR:H341	1.85	0.42
28:B:626:DGD:O1B	28:B:626:DGD:O2D	2.37	0.42
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.01	0.42
3:C:174:LEU:HD13	23:C:502:CLA:H111	2.01	0.42
27:C:514:BCR:H11C	27:C:514:BCR:H341	1.79	0.42
16:V:102:MET:HE1	16:V:141:ILE:HD12	2.02	0.42
23:b:610:CLA:H122	31:b:624:LMG:H412	2.02	0.42
3:c:261:ARG:HA	3:c:266:TRP:CZ2	2.55	0.42
3:c:334:PRO:HA	13:o:179:THR:OG1	2.20	0.42
3:c:425:TRP:CZ2	23:c:504:CLA:HBA1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:300:SER:O	12:m:1:MET:HE3	2.20	0.42
27:k:102:BCR:H14C	17:g:28:ILE:O	2.20	0.42
1:A:141:PRO:C	1:A:143:ILE:H	2.27	0.42
2:B:133:LEU:HB3	2:B:138:MET:CE	2.50	0.42
8:I:29:ALA:HA	8:I:35:LYS:HB2	2.01	0.42
13:O:147:THR:OG1	13:O:148:VAL:N	2.53	0.42
15:U:83:ALA:HB1	15:U:84:PRO:HD2	2.00	0.42
19:Z:55:GLY:HA2	27:Z:101:BCR:H312	2.01	0.42
2:b:41:GLU:HB3	2:b:60:MET:SD	2.60	0.42
3:c:318:LEU:HD21	3:c:380:ILE:HG23	2.00	0.42
3:c:386:PRO:HB3	16:v:116:GLU:HG2	2.01	0.42
23:c:509:CLA:H141	23:c:512:CLA:HMD3	2.02	0.42
31:c:520:LMG:H292	31:c:520:LMG:H111	2.01	0.42
27:j:102:BCR:H341	27:j:102:BCR:H11C	1.74	0.42
14:t:3:THR:O	14:t:7:VAL:HG23	2.20	0.42
1:A:183:MET:HA	23:A:403:CLA:HMD2	2.02	0.42
23:B:615:CLA:H72	23:B:616:CLA:HBB1	2.02	0.42
27:C:514:BCR:H391	10:K:36:ALA:HB2	2.02	0.42
27:Z:101:BCR:H351	27:Z:101:BCR:H15C	1.75	0.42
1:a:232:SER:HB3	1:a:235:TYR:HD1	1.85	0.42
1:a:340:PRO:HG3	15:u:133:TYR:CG	2.55	0.42
3:c:261:ARG:HA	3:c:266:TRP:HZ2	1.85	0.42
23:c:502:CLA:CGA	23:c:503:CLA:H42	2.50	0.42
27:c:514:BCR:H24C	27:c:514:BCR:H371	1.88	0.42
4:d:148:ALA:HB1	4:d:279:LEU:HB2	2.02	0.42
10:k:25:LEU:HB2	10:k:26:PRO:HD3	2.01	0.42
11:l:10:VAL:O	12:m:28:GLN:NE2	2.38	0.42
13:o:144:LEU:HD13	13:o:259:VAL:HG11	2.02	0.42
1:A:85:SER:HA	1:A:109:GLY:HA3	2.02	0.41
1:A:271:LEU:HD21	25:A:408:PL9:HC71	2.00	0.41
2:B:45:PHE:HB2	2:B:60:MET:SD	2.59	0.41
3:C:69:LEU:HD21	3:C:116:VAL:HG13	2.02	0.41
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.02	0.41
5:E:26:THR:HB	34:F:101:HEM:CAB	2.50	0.41
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.85	0.41
15:U:73:PRO:HG2	16:V:107:THR:HB	2.01	0.41
23:b:606:CLA:H192	23:b:606:CLA:H162	1.76	0.41
23:c:511:CLA:H93	23:c:511:CLA:H61	1.82	0.41
5:e:35:TRP:CD2	6:f:39:ALA:HB2	2.55	0.41
23:B:612:CLA:H162	23:B:612:CLA:H122	1.82	0.41
27:B:620:BCR:H11C	27:B:620:BCR:H341	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:TRP:CD1	3:C:259:TRP:H	2.37	0.41
27:T:102:BCR:H351	27:T:102:BCR:H15C	1.75	0.41
1:a:211:PHE:HA	1:a:214:MET:HB2	2.01	0.41
23:a:404:CLA:HBD	23:a:405:CLA:HAC2	2.02	0.41
2:b:98:LEU:HD11	28:b:602:DGD:HB92	2.02	0.41
2:b:306:PRO:HG2	2:b:309:LEU:HB2	2.02	0.41
31:d:405:LMG:H171	27:f:102:BCR:H383	2.01	0.41
13:o:73:PRO:HG3	13:o:146:PHE:CE2	2.55	0.41
2:b:118:TRP:CH2	11:l:5:PRO:HD2	2.55	0.41
23:b:610:CLA:C4A	23:b:610:CLA:HBA2	2.49	0.41
23:b:618:CLA:H52	23:b:618:CLA:H12	1.79	0.41
3:c:457:LYS:HG2	4:d:229:ALA:HA	2.02	0.41
10:k:43:VAL:HG22	10:k:46:ARG:HE	1.86	0.41
16:v:160:LYS:HA	16:v:163:TYR:CG	2.56	0.41
1:A:77:ILE:HD11	14:T:6:TYR:HB3	2.03	0.41
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.29	0.41
27:A:410:BCR:H15C	27:A:410:BCR:H351	1.78	0.41
23:B:609:CLA:HMD1	7:H:27:THR:HB	2.03	0.41
23:B:615:CLA:H52	23:B:615:CLA:H12	1.74	0.41
3:C:107:ASP:O	3:C:110:PRO:HD2	2.20	0.41
3:C:386:PRO:HB3	16:V:116:GLU:HG2	2.01	0.41
4:D:73:PHE:CZ	31:D:406:LMG:H172	2.56	0.41
23:D:403:CLA:H41	23:D:403:CLA:H61	1.88	0.41
12:M:28:GLN:O	12:m:31:SER:OG	2.33	0.41
1:a:172:MET:HE1	23:a:405:CLA:CHC	2.49	0.41
1:a:210:LEU:HG	24:a:408:PHO:NC	2.36	0.41
23:a:405:CLA:H202	23:a:405:CLA:H162	1.75	0.41
23:a:406:CLA:HAB	23:d:402:CLA:H72	2.02	0.41
24:a:407:PHO:H13	24:a:407:PHO:H102	1.82	0.41
2:b:18:ARG:NH2	30:b:601:SQD:O9	2.53	0.41
2:b:135:LEU:HB2	2:b:136:PRO:HD3	2.01	0.41
23:b:605:CLA:H61	7:h:46:LEU:HB2	2.03	0.41
1:A:141:PRO:HG3	3:C:446:GLY:C	2.45	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
2:B:247:PHE:HE1	23:B:602:CLA:H101	1.86	0.41
31:C:519:LMG:H112	27:J:102:BCR:H373	2.02	0.41
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.36	0.41
7:H:3:ARG:NH2	11:L:1:MET:HE1	2.36	0.41
7:H:55:LEU:O	7:H:58:VAL:HG12	2.20	0.41
13:O:135:GLN:HE21	13:O:135:GLN:HB3	1.76	0.41
23:a:405:CLA:H62	23:a:405:CLA:H41	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:510:CLA:H2	23:c:510:CLA:H61	1.65	0.41
1:A:232:SER:HB3	1:A:235:TYR:CD1	2.56	0.41
23:B:604:CLA:H61	23:B:604:CLA:H41	1.85	0.41
1:a:298:ASN:ND2	3:c:402:GLY:O	2.53	0.41
1:a:308:ASP:O	6:f:45:ARG:NE	2.53	0.41
2:b:89:GLY:HA2	28:b:602:DGD:HE1	2.02	0.41
2:b:90:PHE:CE2	28:b:602:DGD:HA81	2.56	0.41
23:b:608:CLA:H41	23:b:608:CLA:H62	1.76	0.41
3:c:305:THR:HG22	3:c:308:GLU:CB	2.47	0.41
4:d:55:VAL:HG21	4:d:110:LEU:HD12	2.01	0.41
5:e:20:TRP:HD1	9:j:8:ILE:HD13	1.86	0.41
27:B:617:BCR:H341	27:B:617:BCR:H11C	1.84	0.41
3:C:319:ILE:O	3:C:323:LYS:HG3	2.20	0.41
28:C:517:DGD:HAW2	28:C:517:DGD:HA91	1.78	0.41
27:H:101:BCR:H15C	27:H:101:BCR:H351	1.87	0.41
13:O:206:GLU:CD	13:O:206:GLU:H	2.29	0.41
16:V:68:VAL:O	16:V:71:ILE:HG12	2.20	0.41
3:C:425:TRP:CZ2	23:C:504:CLA:HBA1	2.56	0.41
19:Z:5:PHE:CE1	19:Z:54:VAL:HG13	2.56	0.41
19:Z:33:TRP:O	19:Z:33:TRP:HD1	2.04	0.41
23:a:405:CLA:H92	23:a:405:CLA:H61	1.79	0.41
3:c:55:ALA:HB2	3:c:129:GLY:HA3	2.01	0.41
4:d:43:LEU:HD23	4:d:117:HIS:CE1	2.55	0.41
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.20	0.41
2:B:133:LEU:HB3	2:B:138:MET:HE2	2.03	0.41
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.50	0.41
23:B:606:CLA:H62	23:B:606:CLA:H41	1.79	0.41
3:C:224:ILE:O	3:C:227:VAL:HG23	2.20	0.41
3:C:286:ALA:HB2	23:C:502:CLA:HMD1	2.02	0.41
4:D:43:LEU:HD21	23:D:403:CLA:C3C	2.51	0.41
4:D:205:LEU:HD12	4:D:205:LEU:HA	1.91	0.41
4:D:346:LEU:HD12	4:D:346:LEU:HA	1.90	0.41
24:D:402:PHO:H62	24:D:402:PHO:H41	1.32	0.41
12:M:16:LEU:O	12:M:20:VAL:HG23	2.20	0.41
14:T:29:ILE:O	14:T:31:LYS:N	2.53	0.41
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.56	0.41
1:a:111:PRO:O	1:a:115:ILE:HG13	2.20	0.41
2:b:6:TYR:OH	31:b:623:LMG:HC5	2.21	0.41
23:b:612:CLA:HMD1	7:h:27:THR:HB	2.01	0.41
27:b:620:BCR:H341	27:b:620:BCR:H11C	1.84	0.41
3:c:53:HIS:HB3	23:c:512:CLA:OBD	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:504:CLA:H142	23:c:504:CLA:H112	1.82	0.41
4:d:155:SER:HA	4:d:159:ILE:HB	2.02	0.41
4:d:205:LEU:HD12	4:d:205:LEU:HA	1.89	0.41
4:d:294:ARG:H	4:d:294:ARG:HG2	1.61	0.41
30:d:407:SQD:H441	30:d:407:SQD:H3	2.01	0.41
1:A:337:HIS:CD2	3:C:354:GLU:OE1	2.74	0.41
2:B:12:LEU:HD13	2:B:19:LEU:HA	2.03	0.41
2:B:334:ASP:OD1	2:B:334:ASP:N	2.53	0.41
23:B:602:CLA:H152	28:B:621:DGD:HAW2	2.03	0.41
23:B:610:CLA:H41	23:B:610:CLA:H62	1.78	0.41
4:D:62:GLY:HA3	5:E:63:ILE:HD13	2.03	0.41
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.02	0.41
5:E:56:TYR:O	16:V:27:ALA:HB2	2.20	0.41
12:M:20:VAL:HG13	12:m:20:VAL:HG13	2.02	0.41
15:U:75:LEU:HD21	15:U:101:GLN:HB3	2.02	0.41
18:X:12:ILE:HA	18:X:16:LEU:HD12	2.03	0.41
2:b:221:PRO:HA	2:b:222:PRO:HD3	1.95	0.41
4:d:53:THR:HG22	4:d:67:TYR:CD2	2.56	0.41
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.03	0.41
2:B:18:ARG:NH1	2:B:115:TRP:O	2.47	0.40
23:B:606:CLA:H3A	23:B:606:CLA:HBA2	1.30	0.40
3:C:67:MET:HE1	23:C:504:CLA:ND	2.36	0.40
3:C:305:THR:HG22	3:C:308:GLU:CB	2.51	0.40
23:c:501:CLA:H52	23:c:503:CLA:H92	2.03	0.40
13:o:178:ARG:HD2	13:o:182:PHE:CD1	2.55	0.40
18:x:12:ILE:HG12	18:x:16:LEU:HD12	2.02	0.40
2:B:33:TRP:CD1	27:B:618:BCR:H391	2.56	0.40
2:B:86:ILE:H	2:B:86:ILE:HG13	1.78	0.40
3:C:77:PRO:HG2	3:C:78:GLU:OE2	2.21	0.40
18:X:12:ILE:HG23	18:X:12:ILE:O	2.21	0.40
1:a:177:SER:HA	1:a:180:PHE:CD2	2.56	0.40
2:b:41:GLU:O	2:b:45:PHE:N	2.51	0.40
2:b:153:PHE:O	2:b:157:HIS:HB3	2.20	0.40
23:b:608:CLA:H161	23:b:608:CLA:H141	1.81	0.40
23:b:609:CLA:H3A	23:b:609:CLA:HBA2	1.28	0.40
3:c:122:SER:OG	27:c:514:BCR:H14C	2.20	0.40
23:c:501:CLA:H162	23:c:501:CLA:H141	1.80	0.40
4:d:218:VAL:HA	4:d:221:THR:HG22	2.04	0.40
12:m:3:VAL:HG11	14:t:2:GLU:HG2	2.02	0.40
23:A:403:CLA:H162	23:A:404:CLA:C9	2.51	0.40
23:A:407:CLA:HBC1	31:I:101:LMG:H341	2.01	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.02	0.40
23:B:612:CLA:H122	23:B:612:CLA:H8	1.85	0.40
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.56	0.40
17:y:24:MET:O	17:y:28:ILE:HG23	2.21	0.40
1:a:283:VAL:O	1:a:286:THR:HG22	2.21	0.40
23:a:404:CLA:H3A	23:a:404:CLA:HBA1	1.67	0.40
27:b:621:BCR:H11C	27:b:621:BCR:H341	1.75	0.40
3:c:264:PHE:HE1	23:c:507:CLA:HAB	1.87	0.40
4:d:18:LEU:O	4:d:22:LEU:HG	2.22	0.40
5:e:36:LEU:HA	5:e:39:SER:OG	2.22	0.40
7:h:12:ARG:N	7:h:13:PRO:HD2	2.37	0.40
10:k:24:VAL:O	10:k:27:VAL:HG12	2.22	0.40
18:x:12:ILE:O	18:x:12:ILE:HG23	2.21	0.40
30:A:417:SQD:H61	23:b:619:CLA:H2	2.03	0.40
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.03	0.40
23:B:603:CLA:H192	23:B:603:CLA:H162	1.77	0.40
23:B:610:CLA:H152	23:B:615:CLA:HBD	2.04	0.40
23:B:614:CLA:H112	23:B:614:CLA:H152	1.85	0.40
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.56	0.40
1:a:157:VAL:HG21	23:a:405:CLA:HMC2	2.03	0.40
1:a:182:PHE:O	1:a:186:PHE:HB2	2.21	0.40
1:a:307:ILE:HD11	6:f:45:ARG:NH2	2.36	0.40
25:a:410:PL9:H523	25:a:410:PL9:H531	1.90	0.40
2:b:91:TRP:NE1	33:b:625:LMT:H12	2.35	0.40
2:b:187:PRO:HB3	23:b:604:CLA:HMB1	2.03	0.40
2:b:356:VAL:HG21	2:b:424:ALA:HB3	2.03	0.40
23:b:609:CLA:H41	23:b:609:CLA:H62	1.82	0.40
23:b:610:CLA:H102	31:b:624:LMG:H392	2.03	0.40
3:c:107:ASP:O	3:c:110:PRO:HD2	2.20	0.40
3:c:284:PHE:CZ	28:c:517:DGD:HA91	2.56	0.40
4:d:18:LEU:HD13	18:x:38:ILE:HD13	2.04	0.40
23:d:402:CLA:H92	23:d:402:CLA:H62	1.81	0.40
14:t:29:ILE:O	14:t:31:LYS:N	2.54	0.40
19:z:5:PHE:HB2	19:z:57:LEU:HG	2.03	0.40
20:G:23:UNK:O	20:G:24:UNK:C	2.70	0.40
2:B:134:ASP:OD2	2:B:137:LYS:HE3	2.21	0.40
3:C:75:PHE:CD1	3:C:86:LEU:HD21	2.55	0.40
3:C:264:PHE:HE1	23:C:507:CLA:HAB	1.87	0.40
3:C:399:ALA:O	3:C:401:LEU:N	2.51	0.40
28:D:410:DGD:HG32	28:D:410:DGD:O2D	2.21	0.40
23:a:409:CLA:H162	23:a:409:CLA:H141	1.66	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:416:LMG:H292	11:l:20:GLY:HA2	2.03	0.40
23:b:616:CLA:H171	31:b:623:LMG:H401	2.04	0.40
27:b:620:BCR:H15C	27:b:620:BCR:H351	1.78	0.40
4:d:110:LEU:HD23	4:d:110:LEU:HA	1.84	0.40
31:d:406:LMG:O5	31:d:406:LMG:O4	2.26	0.40
6:f:21:VAL:O	6:f:25:THR:HG23	2.22	0.40
13:o:59:ASP:C	13:o:61:SER:H	2.29	0.40
15:u:83:ALA:HB1	15:u:84:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/360 (92%)	311 (93%)	18 (5%)	4 (1%)	10 43
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	10 43
2	B	488/510 (96%)	448 (92%)	35 (7%)	5 (1%)	12 48
2	b	488/510 (96%)	448 (92%)	36 (7%)	4 (1%)	16 53
3	C	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	9 41
3	c	445/461 (96%)	405 (91%)	33 (7%)	7 (2%)	7 37
4	D	338/352 (96%)	315 (93%)	20 (6%)	3 (1%)	14 50
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	21 59
5	E	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	9 41
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9 41
6	F	33/45 (73%)	30 (91%)	3 (9%)	0	100 100
6	f	33/45 (73%)	30 (91%)	3 (9%)	0	100 100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2 16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2 16
8	I	33/38 (87%)	27 (82%)	5 (15%)	1 (3%)	3 22
8	i	33/38 (87%)	27 (82%)	5 (15%)	1 (3%)	3 22
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3 21
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3 21
10	K	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1 13
10	k	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1 13
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
13	O	241/272 (89%)	207 (86%)	30 (12%)	4 (2%)	7 35
13	o	241/272 (89%)	209 (87%)	29 (12%)	3 (1%)	10 43
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3 20
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3 20
15	U	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	3 21
15	u	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	3 21
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100 100
16	v	135/163 (83%)	126 (93%)	9 (7%)	0	100 100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	2 19
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2 19
18	X	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1 13
18	x	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1 13
19	Z	60/62 (97%)	54 (90%)	4 (7%)	2 (3%)	3 20
19	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7 35
All	All	5138/5650 (91%)	4681 (91%)	382 (7%)	75 (2%)	8 39

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	H	18	TYR
13	O	52	ALA
14	T	30	THR
18	X	45	LYS
1	a	12	ASN
1	a	142	TRP
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
13	o	52	ALA
14	t	30	THR
18	x	45	LYS
1	A	141	PRO
1	A	142	TRP
2	B	489	GLU
3	C	32	GLY
3	C	144	SER
3	C	257	PHE
3	C	416	SER
4	D	239	GLN
7	H	26	GLY
17	y	43	ARG
19	Z	32	ASP
1	a	141	PRO
2	b	489	GLU
3	c	32	GLY
3	c	144	SER
3	c	257	PHE
3	c	416	SER
4	d	239	GLN
7	h	26	GLY
17	g	43	ARG
19	z	32	ASP
2	B	176	GLY
4	D	262	SER
5	E	82	GLN
9	J	38	SER
13	O	88	GLU
1	a	334	ARG
2	b	176	GLY
3	c	194	GLY
5	e	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	j	38	SER
13	o	88	GLU
3	C	194	GLY
13	O	271	PRO
15	U	72	TYR
15	U	83	ALA
4	d	262	SER
7	h	16	SER
13	o	271	PRO
15	u	72	TYR
15	u	83	ALA
1	A	334	ARG
2	B	230	ARG
7	H	16	SER
10	K	13	GLU
13	O	158	ASN
18	X	12	ILE
10	k	13	GLU
10	k	45	PHE
18	x	12	ILE
4	D	234	ALA
10	K	45	PHE
19	Z	28	ALA
3	c	462	GLU
15	u	73	PRO
15	U	73	PRO
8	I	32	PRO
3	c	209	ILE
3	C	209	ILE
8	i	32	PRO

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	271/291 (93%)	262 (97%)	9 (3%)	33 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	271/291 (93%)	262 (97%)	9 (3%)	33	54
2	B	390/407 (96%)	377 (97%)	13 (3%)	33	54
2	b	390/407 (96%)	379 (97%)	11 (3%)	38	59
3	C	347/362 (96%)	334 (96%)	13 (4%)	30	51
3	c	347/362 (96%)	335 (96%)	12 (4%)	32	53
4	D	275/283 (97%)	261 (95%)	14 (5%)	21	42
4	d	275/283 (97%)	260 (94%)	15 (6%)	19	41
5	E	72/73 (99%)	67 (93%)	5 (7%)	14	36
5	e	72/73 (99%)	67 (93%)	5 (7%)	14	36
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	50 (94%)	3 (6%)	18	40
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	40
8	I	32/35 (91%)	31 (97%)	1 (3%)	35	56
8	i	32/35 (91%)	31 (97%)	1 (3%)	35	56
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	48
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	48
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	57
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	57
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	199 (98%)	3 (2%)	57	71
13	o	202/228 (89%)	200 (99%)	2 (1%)	68	77
14	T	29/29 (100%)	28 (97%)	1 (3%)	32	54
14	t	29/29 (100%)	28 (97%)	1 (3%)	32	54
15	U	84/112 (75%)	81 (96%)	3 (4%)	31	52
15	u	84/112 (75%)	80 (95%)	4 (5%)	23	44
16	V	116/138 (84%)	113 (97%)	3 (3%)	40	61
16	v	116/138 (84%)	113 (97%)	3 (3%)	40	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	g	20/37 (54%)	16 (80%)	4 (20%)	1 7
17	y	20/37 (54%)	16 (80%)	4 (20%)	1 7
18	X	30/34 (88%)	27 (90%)	3 (10%)	7 24
18	x	30/34 (88%)	27 (90%)	3 (10%)	7 24
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18 39
19	z	52/52 (100%)	49 (94%)	3 (6%)	18 39
All	All	4244/4616 (92%)	4086 (96%)	158 (4%)	30 51

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	VAL
1	A	202	VAL
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	275	LEU
1	A	286	THR
1	A	292	THR
1	A	306	VAL
2	B	18	ARG
2	B	223	GLN
2	B	262	THR
2	B	308	LYS
2	B	309	LEU
2	B	354	LEU
2	B	362	PHE
2	B	422	ARG
2	B	467	ILE
2	B	485	GLU
2	B	486	LEU
2	B	488	PRO
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	104	GLU
3	C	165	LEU
3	C	174	LEU
3	C	244	CYS
3	C	254	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	417	VAL
3	C	469	MET
3	C	472	LEU
4	D	43	LEU
4	D	84	SER
4	D	91	LEU
4	D	180	ARG
4	D	201	VAL
4	D	205	LEU
4	D	241	GLU
4	D	256	ILE
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	323	GLU
4	D	345	VAL
4	D	346	LEU
5	E	18	ARG
5	E	77	GLU
5	E	80	LEU
5	E	82	GLN
5	E	84	LYS
7	H	27	THR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
11	L	11	GLU
13	O	31	LEU
13	O	97	VAL
13	O	230	VAL
14	T	29	ILE
15	U	88	VAL
15	U	114	VAL
15	U	132	LEU
16	V	63	CYS
16	V	68	VAL
16	V	116	GLU
17	y	25	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	y	28	ILE
17	y	36	ILE
17	y	46	LEU
18	X	11	THR
18	X	12	ILE
18	X	42	GLN
19	Z	14	ILE
19	Z	33	TRP
19	Z	62	VAL
1	a	157	VAL
1	a	202	VAL
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	275	LEU
1	a	286	THR
1	a	292	THR
1	a	306	VAL
2	b	223	GLN
2	b	262	THR
2	b	308	LYS
2	b	309	LEU
2	b	354	LEU
2	b	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
2	b	488	PRO
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	165	LEU
3	c	174	LEU
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	305	THR
3	c	355	THR
3	c	417	VAL
3	c	469	MET
3	c	472	LEU
4	d	20	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	d	43	LEU
4	d	84	SER
4	d	91	LEU
4	d	180	ARG
4	d	201	VAL
4	d	205	LEU
4	d	241	GLU
4	d	256	ILE
4	d	259	ILE
4	d	279	LEU
4	d	291	LEU
4	d	323	GLU
4	d	345	VAL
4	d	346	LEU
5	e	18	ARG
5	e	77	GLU
5	e	80	LEU
5	e	82	GLN
5	e	84	LYS
7	h	27	THR
7	h	56	ASP
7	h	60	VAL
8	i	33	LYS
9	j	7	ARG
11	l	11	GLU
13	o	31	LEU
13	o	97	VAL
14	t	29	ILE
15	u	88	VAL
15	u	103	GLN
15	u	114	VAL
15	u	132	LEU
16	v	63	CYS
16	v	68	VAL
16	v	116	GLU
17	g	25	ILE
17	g	28	ILE
17	g	36	ILE
17	g	46	LEU
18	x	11	THR
18	x	12	ILE
18	x	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	z	14	ILE
19	z	33	TRP
19	z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	261	GLN
1	A	303	ASN
1	A	337	HIS
2	B	26	HIS
2	B	194	ASN
2	B	201	HIS
2	B	409	GLN
3	C	44	ASN
3	C	56	HIS
3	C	229	ASN
4	D	186	GLN
4	D	197	HIS
4	D	250	ASN
4	D	255	GLN
4	D	301	GLN
4	D	322	ASN
4	D	332	GLN
12	M	32	GLN
13	O	150	ASN
13	O	173	ASN
15	U	93	ASN
15	U	111	HIS
16	V	112	GLN
1	a	303	ASN
2	b	26	HIS
2	b	53	ASN
2	b	201	HIS
2	b	331	ASN
2	b	343	HIS
2	b	374	ASN
3	c	44	ASN
3	c	56	HIS
3	c	118	HIS
3	c	229	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	d	98	GLN
4	d	117	HIS
4	d	142	ASN
4	d	186	GLN
4	d	255	GLN
4	d	301	GLN
4	d	322	ASN
12	m	32	GLN
13	o	150	ASN
13	o	173	ASN
15	u	111	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CLA	B	615	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	6 (7%)
33	LMT	b	626	-	36,36,36	0.44	0	47,47,47	0.68	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	615	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	5 (6%)
27	BCR	c	516	-	41,41,41	0.69	0	56,56,56	1.95	15 (26%)
24	PHO	D	402	-	58,69,69	2.21	11 (18%)	55,99,99	1.49	5 (9%)
28	DGD	c	519	-	67,67,67	1.16	7 (10%)	81,81,81	1.43	10 (12%)
34	HEM	F	101	6,5	50,50,50	1.85	9 (18%)	67,82,82	1.33	7 (10%)
25	PL9	A	408	-	45,45,55	1.30	7 (15%)	56,57,69	1.57	13 (23%)
28	DGD	d	408	-	64,64,67	1.14	7 (10%)	78,78,81	1.40	9 (11%)
27	BCR	J	102	-	41,41,41	0.72	0	56,56,56	3.43	24 (42%)
33	LMT	D	411	-	32,32,36	0.49	1 (3%)	43,43,47	0.72	1 (2%)
31	LMG	c	520	-	45,45,55	1.22	7 (15%)	53,53,63	1.40	8 (15%)
31	LMG	C	520	-	45,45,55	1.21	7 (15%)	53,53,63	1.44	8 (15%)
23	CLA	B	606	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
33	LMT	b	625	-	36,36,36	0.41	0	47,47,47	0.76	1 (2%)
30	SQD	A	413	-	49,51,54	0.99	4 (8%)	59,62,65	1.48	10 (16%)
27	BCR	a	412	-	41,41,41	0.71	0	56,56,56	1.91	15 (26%)
27	BCR	b	621	-	41,41,41	0.72	0	56,56,56	2.19	18 (32%)
23	CLA	d	403	-	69,73,73	1.20	6 (8%)	82,113,113	1.26	5 (6%)
31	LMG	d	406	-	48,48,55	1.17	7 (14%)	56,56,63	1.38	7 (12%)
33	LMT	m	101	-	36,36,36	0.39	0	47,47,47	0.72	1 (2%)
27	BCR	f	102	-	41,41,41	0.69	0	56,56,56	2.19	17 (30%)
34	HEM	V	201	16	50,50,50	1.83	8 (16%)	67,82,82	1.14	2 (2%)
23	CLA	C	509	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
28	DGD	D	410	-	64,64,67	1.15	7 (10%)	78,78,81	1.38	8 (10%)
23	CLA	C	501	-	69,73,73	1.20	7 (10%)	82,113,113	1.25	5 (6%)
33	LMT	i	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.65	0
31	LMG	M	101	-	42,42,55	1.33	7 (16%)	50,50,63	1.50	8 (16%)
25	PL9	a	410	-	45,45,55	1.25	7 (15%)	56,57,69	1.66	13 (23%)
27	BCR	k	102	-	41,41,41	0.71	0	56,56,56	1.90	13 (23%)
23	CLA	B	601	-	69,73,73	1.23	8 (11%)	82,113,113	1.26	6 (7%)
23	CLA	B	603	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
23	CLA	B	611	-	69,73,73	1.18	8 (11%)	82,113,113	1.34	5 (6%)
25	PL9	d	404	-	55,55,55	1.28	8 (14%)	68,69,69	1.68	15 (22%)
29	LHG	A	415	-	36,36,48	1.09	2 (5%)	39,42,54	1.08	2 (5%)
27	BCR	B	620	-	41,41,41	0.72	1 (2%)	56,56,56	2.14	17 (30%)
23	CLA	c	501	-	69,73,73	1.17	7 (10%)	82,113,113	1.32	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	616	-	69,73,73	1.19	9 (13%)	82,113,113	1.25	4 (4%)
23	CLA	c	510	-	69,73,73	1.19	8 (11%)	82,113,113	1.21	4 (4%)
23	CLA	b	606	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	6 (7%)
31	LMG	e	101	-	44,44,55	1.23	7 (15%)	52,52,63	1.30	8 (15%)
23	CLA	c	512	-	69,73,73	1.18	6 (8%)	82,113,113	1.29	5 (6%)
23	CLA	b	607	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	7 (8%)
28	DGD	B	621	-	59,59,67	1.29	9 (15%)	73,73,81	1.14	6 (8%)
23	CLA	D	403	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
30	SQD	a	401	-	52,54,54	0.98	4 (7%)	62,65,65	1.56	10 (16%)
23	CLA	a	406	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	7 (8%)
23	CLA	b	618	-	69,73,73	1.18	5 (7%)	82,113,113	1.31	6 (7%)
23	CLA	C	507	-	69,73,73	1.17	6 (8%)	82,113,113	1.31	6 (7%)
27	BCR	K	102	-	41,41,41	0.74	0	56,56,56	1.86	11 (19%)
27	BCR	H	101	-	41,41,41	0.72	0	56,56,56	1.73	15 (26%)
27	BCR	A	410	-	41,41,41	0.75	1 (2%)	56,56,56	1.99	14 (25%)
23	CLA	C	505	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)
30	SQD	D	409	-	41,43,54	1.12	4 (9%)	51,54,65	1.96	10 (19%)
22	BCT	A	402	21	3,3,3	0.66	0	2,3,3	0.04	0
25	PL9	D	404	-	55,55,55	1.25	8 (14%)	68,69,69	1.70	19 (27%)
23	CLA	B	613	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	7 (8%)
25	PL9	j	101	-	35,35,55	1.20	5 (14%)	44,45,69	1.61	8 (18%)
28	DGD	c	518	-	63,63,67	1.23	9 (14%)	77,77,81	1.25	7 (9%)
23	CLA	B	612	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	6 (7%)
28	DGD	C	518	-	67,67,67	1.16	7 (10%)	81,81,81	1.45	9 (11%)
23	CLA	b	619	-	69,73,73	1.19	8 (11%)	82,113,113	1.21	6 (7%)
24	PHO	a	408	-	58,69,69	2.17	9 (15%)	55,99,99	1.34	5 (9%)
27	BCR	C	514	-	41,41,41	0.77	0	56,56,56	2.42	20 (35%)
23	CLA	a	409	-	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
28	DGD	b	602	-	53,53,67	1.26	6 (11%)	67,67,81	1.38	9 (13%)
23	CLA	b	605	-	69,73,73	1.20	7 (10%)	82,113,113	1.26	4 (4%)
31	LMG	k	103	-	48,48,55	1.16	6 (12%)	56,56,63	1.29	6 (10%)
24	PHO	a	407	-	58,69,69	2.11	11 (18%)	55,99,99	1.43	7 (12%)
23	CLA	B	608	-	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
33	LMT	M	103	-	36,36,36	0.41	0	47,47,47	0.69	1 (2%)
23	CLA	B	610	-	69,73,73	1.20	7 (10%)	82,113,113	1.33	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	616	-	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
22	BCT	d	401	21	3,3,3	0.67	0	2,3,3	0.17	0
23	CLA	b	610	-	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
31	LMG	M	102	-	42,42,55	1.30	7 (16%)	50,50,63	1.48	8 (16%)
23	CLA	B	602	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
29	LHG	a	417	-	36,36,48	1.08	2 (5%)	39,42,54	1.08	2 (5%)
33	LMT	I	102	-	36,36,36	0.42	0	47,47,47	0.69	1 (2%)
31	LMG	C	519	-	48,48,55	1.15	6 (12%)	56,56,63	1.35	7 (12%)
23	CLA	c	508	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
27	BCR	j	102	-	41,41,41	0.74	0	56,56,56	3.44	23 (41%)
23	CLA	c	509	-	69,73,73	1.19	5 (7%)	82,113,113	1.31	5 (6%)
27	BCR	c	514	-	41,41,41	0.71	0	56,56,56	2.46	19 (33%)
28	DGD	A	411	-	57,57,67	1.25	8 (14%)	71,71,81	1.60	12 (16%)
27	BCR	Z	101	-	41,41,41	0.64	0	56,56,56	1.89	16 (28%)
23	CLA	c	513	-	69,73,73	1.18	6 (8%)	82,113,113	1.34	6 (7%)
27	BCR	T	102	-	41,41,41	0.76	0	56,56,56	1.93	14 (25%)
23	CLA	B	604	-	69,73,73	1.19	6 (8%)	82,113,113	1.30	7 (8%)
28	DGD	b	622	-	59,59,67	1.26	9 (15%)	73,73,81	1.16	6 (8%)
31	LMG	d	405	-	46,46,55	1.20	7 (15%)	54,54,63	1.36	6 (11%)
33	LMT	B	624	-	36,36,36	0.44	0	47,47,47	0.71	1 (2%)
23	CLA	C	510	-	69,73,73	1.22	8 (11%)	82,113,113	1.27	4 (4%)
27	BCR	B	617	-	41,41,41	0.74	0	56,56,56	1.95	12 (21%)
23	CLA	C	506	-	69,73,73	1.20	5 (7%)	82,113,113	1.36	6 (7%)
23	CLA	b	613	-	69,73,73	1.20	7 (10%)	82,113,113	1.26	5 (6%)
23	CLA	c	503	-	69,73,73	1.21	6 (8%)	82,113,113	1.25	5 (6%)
23	CLA	A	405	-	69,73,73	1.19	8 (11%)	82,113,113	1.21	5 (6%)
31	LMG	i	101	-	43,43,55	1.29	7 (16%)	51,51,63	1.31	7 (13%)
23	CLA	c	502	-	69,73,73	1.19	7 (10%)	82,113,113	1.33	5 (6%)
23	CLA	a	404	-	69,73,73	1.20	7 (10%)	82,113,113	1.32	6 (7%)
28	DGD	a	413	-	57,57,67	1.23	7 (12%)	71,71,81	1.57	12 (16%)
23	CLA	B	605	-	69,73,73	1.15	7 (10%)	82,113,113	1.28	5 (6%)
29	LHG	A	412	-	38,38,48	1.07	2 (5%)	41,44,54	0.99	2 (4%)
23	CLA	C	511	3	69,73,73	1.18	7 (10%)	82,113,113	1.36	6 (7%)
33	LMT	b	603	-	36,36,36	0.40	0	47,47,47	0.62	0
30	SQD	a	415	-	49,51,54	1.01	3 (6%)	59,62,65	1.51	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	609	-	69,73,73	1.19	6 (8%)	82,113,113	1.30	6 (7%)
23	CLA	b	604	-	69,73,73	1.22	7 (10%)	82,113,113	1.29	6 (7%)
31	LMG	b	624	-	49,49,55	1.18	7 (14%)	57,57,63	1.39	8 (14%)
27	BCR	C	515	-	41,41,41	0.69	0	56,56,56	1.99	15 (26%)
23	CLA	A	404	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	6 (7%)
30	SQD	B	625	-	45,47,54	1.04	4 (8%)	55,58,65	1.50	8 (14%)
25	PL9	J	101	-	35,35,55	1.21	5 (14%)	44,45,69	1.59	7 (15%)
23	CLA	A	403	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	5 (6%)
23	CLA	b	617	-	69,73,73	1.16	7 (10%)	82,113,113	1.27	4 (4%)
23	CLA	C	512	-	69,73,73	1.19	7 (10%)	82,113,113	1.32	5 (6%)
30	SQD	A	417	-	52,54,54	1.02	4 (7%)	62,65,65	1.55	10 (16%)
28	DGD	C	517	-	63,63,67	1.23	10 (15%)	77,77,81	1.22	7 (9%)
27	BCR	c	515	-	41,41,41	0.64	0	56,56,56	1.81	15 (26%)
27	BCR	b	620	-	41,41,41	0.66	0	56,56,56	1.95	14 (25%)
24	PHO	A	406	-	58,69,69	2.21	9 (15%)	55,99,99	1.66	8 (14%)
23	CLA	c	506	-	69,73,73	1.21	7 (10%)	82,113,113	1.33	7 (8%)
23	CLA	d	402	-	69,73,73	1.17	6 (8%)	82,113,113	1.32	5 (6%)
33	LMT	T	101	-	36,36,36	0.41	0	47,47,47	0.86	1 (2%)
33	LMT	B	623	-	36,36,36	0.41	0	47,47,47	0.74	1 (2%)
27	BCR	B	619	-	41,41,41	0.65	0	56,56,56	1.89	15 (26%)
31	LMG	a	402	-	42,42,55	1.25	6 (14%)	50,50,63	1.48	8 (16%)
23	CLA	B	614	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	4 (4%)
30	SQD	d	407	-	41,43,54	1.14	3 (7%)	51,54,65	1.97	9 (17%)
23	CLA	a	405	-	69,73,73	1.17	8 (11%)	82,113,113	1.35	7 (8%)
27	BCR	D	405	-	41,41,41	0.67	0	56,56,56	2.24	18 (32%)
23	CLA	C	513	-	69,73,73	1.19	6 (8%)	82,113,113	1.31	6 (7%)
23	CLA	C	502	-	69,73,73	1.18	8 (11%)	82,113,113	1.32	5 (6%)
23	CLA	C	503	-	69,73,73	1.20	6 (8%)	82,113,113	1.24	6 (7%)
30	SQD	b	601	-	45,47,54	1.04	3 (6%)	55,58,65	1.53	9 (16%)
31	LMG	E	101	-	44,44,55	1.23	7 (15%)	52,52,63	1.36	8 (15%)
31	LMG	a	416	-	51,51,55	1.15	6 (11%)	59,59,63	1.41	5 (8%)
23	CLA	b	608	-	69,73,73	1.17	7 (10%)	82,113,113	1.28	4 (4%)
31	LMG	b	623	-	49,49,55	1.22	7 (14%)	57,57,63	1.35	7 (12%)
33	LMT	B	628	-	36,36,36	0.47	0	47,47,47	0.64	0
27	BCR	B	618	-	41,41,41	0.73	0	56,56,56	2.29	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	614	-	69,73,73	1.21	8 (11%)	82,113,113	1.29	6 (7%)
28	DGD	C	516	-	54,54,67	1.26	7 (12%)	68,68,81	1.28	9 (13%)
27	BCR	T	103	-	41,41,41	0.71	0	56,56,56	2.29	17 (30%)
23	CLA	c	504	-	69,73,73	1.21	7 (10%)	82,113,113	1.38	6 (7%)
23	CLA	c	505	-	69,73,73	1.18	6 (8%)	82,113,113	1.40	7 (8%)
23	CLA	D	401	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
31	LMG	D	407	-	49,49,55	1.20	7 (14%)	57,57,63	1.26	8 (14%)
34	HEM	v	201	16	50,50,50	2.02	11 (22%)	67,82,82	1.37	6 (8%)
30	SQD	F	102	-	43,45,54	1.05	2 (4%)	53,56,65	1.62	9 (16%)
27	BCR	x	101	-	41,41,41	0.71	0	56,56,56	1.73	17 (30%)
23	CLA	b	612	-	69,73,73	1.20	6 (8%)	82,113,113	1.21	5 (6%)
23	CLA	b	609	-	69,73,73	1.20	6 (8%)	82,113,113	1.29	5 (6%)
23	CLA	c	511	-	69,73,73	1.22	6 (8%)	82,113,113	1.32	4 (4%)
31	LMG	B	622	-	49,49,55	1.20	7 (14%)	57,57,63	1.38	8 (14%)
31	LMG	D	406	-	46,46,55	1.18	6 (13%)	54,54,63	1.36	6 (11%)
23	CLA	B	607	-	69,73,73	1.16	6 (8%)	82,113,113	1.35	6 (7%)
23	CLA	c	507	-	69,73,73	1.18	6 (8%)	82,113,113	1.30	6 (7%)
34	HEM	f	101	6,5	50,50,50	1.85	10 (20%)	67,82,82	1.35	4 (5%)
31	LMG	A	418	-	42,42,55	1.25	6 (14%)	50,50,63	1.53	11 (22%)
31	LMG	I	101	-	43,43,55	1.28	8 (18%)	51,51,63	1.34	8 (15%)
29	LHG	a	414	-	38,38,48	1.09	2 (5%)	41,44,54	0.97	3 (7%)
28	DGD	c	517	-	54,54,67	1.28	7 (12%)	68,68,81	1.28	8 (11%)
28	DGD	B	626	-	53,53,67	1.26	7 (13%)	67,67,81	1.39	9 (13%)
31	LMG	D	408	-	48,48,55	1.22	7 (14%)	56,56,63	1.38	7 (12%)
23	CLA	A	407	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	4 (4%)
30	SQD	f	103	-	43,45,54	1.04	2 (4%)	53,56,65	1.59	11 (20%)
33	LMT	x	102	-	32,32,36	0.49	1 (3%)	43,43,47	0.67	1 (2%)
23	CLA	b	611	-	69,73,73	1.20	7 (10%)	82,113,113	1.35	9 (10%)
31	LMG	A	414	-	51,51,55	1.18	6 (11%)	59,59,63	1.35	5 (8%)
33	LMT	B	627	-	36,36,36	0.45	0	47,47,47	0.80	1 (2%)
23	CLA	C	504	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
23	CLA	C	508	-	69,73,73	1.20	8 (11%)	82,113,113	1.28	4 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	615	-	1/1/15/20	10/39/115/115	-
33	LMT	b	626	-	-	2/21/61/61	0/2/2/2
23	CLA	b	615	-	1/1/15/20	9/39/115/115	-
27	BCR	c	516	-	-	8/29/63/63	0/2/2/2
24	PHO	D	402	-	-	8/37/103/103	0/5/6/6
28	DGD	c	519	-	-	21/55/95/95	0/2/2/2
34	HEM	F	101	6,5	-	2/14/54/54	-
25	PL9	A	408	-	-	22/41/61/73	0/1/1/1
28	DGD	d	408	-	-	29/52/92/95	0/2/2/2
27	BCR	J	102	-	-	2/29/63/63	0/2/2/2
33	LMT	D	411	-	-	0/17/57/61	0/2/2/2
31	LMG	c	520	-	-	21/40/60/70	0/1/1/1
31	LMG	C	520	-	-	19/40/60/70	0/1/1/1
23	CLA	B	606	-	1/1/15/20	13/39/115/115	-
33	LMT	b	625	-	-	2/21/61/61	0/2/2/2
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
27	BCR	a	412	-	-	3/29/63/63	0/2/2/2
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
23	CLA	d	403	-	1/1/15/20	10/39/115/115	-
31	LMG	d	406	-	-	20/43/63/70	0/1/1/1
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
27	BCR	f	102	-	-	6/29/63/63	0/2/2/2
34	HEM	V	201	16	-	4/14/54/54	-
23	CLA	C	509	-	1/1/15/20	18/39/115/115	-
28	DGD	D	410	-	-	31/52/92/95	0/2/2/2
23	CLA	C	501	-	1/1/15/20	14/39/115/115	-
33	LMT	i	102	-	-	3/21/61/61	0/2/2/2
31	LMG	M	101	-	-	15/37/57/70	0/1/1/1
25	PL9	a	410	-	-	23/41/61/73	0/1/1/1
27	BCR	k	102	-	-	8/29/63/63	0/2/2/2
23	CLA	B	601	-	1/1/15/20	14/39/115/115	-
23	CLA	B	603	-	1/1/15/20	15/39/115/115	-
23	CLA	B	611	-	1/1/15/20	12/39/115/115	-
25	PL9	d	404	-	-	13/53/73/73	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	A	415	-	-	12/41/41/53	-
27	BCR	B	620	-	-	2/29/63/63	0/2/2/2
23	CLA	c	501	-	1/1/15/20	15/39/115/115	-
23	CLA	B	616	-	1/1/15/20	19/39/115/115	-
23	CLA	c	510	-	1/1/15/20	17/39/115/115	-
23	CLA	b	606	-	1/1/15/20	15/39/115/115	-
31	LMG	e	101	-	-	18/39/59/70	0/1/1/1
23	CLA	c	512	-	1/1/15/20	19/39/115/115	-
23	CLA	b	607	-	1/1/15/20	9/39/115/115	-
28	DGD	B	621	-	-	19/47/87/95	0/2/2/2
23	CLA	D	403	-	1/1/15/20	9/39/115/115	-
30	SQD	a	401	-	-	15/49/69/69	0/1/1/1
23	CLA	a	406	-	1/1/15/20	10/39/115/115	-
23	CLA	b	618	-	1/1/15/20	8/39/115/115	-
23	CLA	C	507	-	1/1/15/20	13/39/115/115	-
27	BCR	K	102	-	-	8/29/63/63	0/2/2/2
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	BCR	A	410	-	-	0/29/63/63	0/2/2/2
23	CLA	C	505	-	1/1/15/20	20/39/115/115	-
30	SQD	D	409	-	-	11/38/58/69	0/1/1/1
25	PL9	D	404	-	-	12/53/73/73	0/1/1/1
23	CLA	B	613	-	1/1/15/20	15/39/115/115	-
25	PL9	j	101	-	-	13/29/49/73	0/1/1/1
28	DGD	c	518	-	-	22/51/91/95	0/2/2/2
23	CLA	B	612	-	1/1/15/20	10/39/115/115	-
28	DGD	C	518	-	-	24/55/95/95	0/2/2/2
23	CLA	b	619	-	1/1/15/20	19/39/115/115	-
24	PHO	a	408	-	-	10/37/103/103	0/5/6/6
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
23	CLA	a	409	-	1/1/15/20	8/39/115/115	-
28	DGD	b	602	-	-	18/41/81/95	0/2/2/2
23	CLA	b	605	-	1/1/15/20	18/39/115/115	-
31	LMG	k	103	-	-	17/43/63/70	0/1/1/1
24	PHO	a	407	-	-	11/37/103/103	0/5/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	608	-	1/1/15/20	15/39/115/115	-
33	LMT	M	103	-	-	0/21/61/61	0/2/2/2
23	CLA	B	610	-	1/1/15/20	18/39/115/115	-
23	CLA	b	616	-	1/1/15/20	15/39/115/115	-
23	CLA	b	610	-	1/1/15/20	9/39/115/115	-
31	LMG	M	102	-	-	17/37/57/70	0/1/1/1
23	CLA	B	602	-	1/1/15/20	13/39/115/115	-
29	LHG	a	417	-	-	13/41/41/53	-
33	LMT	I	102	-	-	3/21/61/61	0/2/2/2
31	LMG	C	519	-	-	16/43/63/70	0/1/1/1
23	CLA	c	508	-	1/1/15/20	13/39/115/115	-
27	BCR	j	102	-	-	6/29/63/63	0/2/2/2
23	CLA	c	509	-	1/1/15/20	18/39/115/115	-
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
28	DGD	A	411	-	-	11/45/85/95	0/2/2/2
27	BCR	Z	101	-	-	2/29/63/63	0/2/2/2
23	CLA	c	513	-	1/1/15/20	21/39/115/115	-
27	BCR	T	102	-	-	2/29/63/63	0/2/2/2
23	CLA	B	604	-	1/1/15/20	10/39/115/115	-
28	DGD	b	622	-	-	19/47/87/95	0/2/2/2
31	LMG	d	405	-	-	10/41/61/70	0/1/1/1
33	LMT	B	624	-	-	2/21/61/61	0/2/2/2
23	CLA	C	510	-	1/1/15/20	16/39/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	C	506	-	1/1/15/20	18/39/115/115	-
23	CLA	b	613	-	1/1/15/20	17/39/115/115	-
23	CLA	c	503	-	1/1/15/20	13/39/115/115	-
23	CLA	A	405	-	1/1/15/20	10/39/115/115	-
31	LMG	i	101	-	-	19/38/58/70	0/1/1/1
23	CLA	c	502	-	1/1/15/20	12/39/115/115	-
23	CLA	a	404	-	1/1/15/20	8/39/115/115	-
28	DGD	a	413	-	-	11/45/85/95	0/2/2/2
23	CLA	B	605	-	1/1/15/20	15/39/115/115	-
29	LHG	A	412	-	-	17/43/43/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	511	3	1/1/15/20	13/39/115/115	-
33	LMT	b	603	-	-	3/21/61/61	0/2/2/2
30	SQD	a	415	-	-	17/46/66/69	0/1/1/1
23	CLA	B	609	-	1/1/15/20	9/39/115/115	-
23	CLA	b	604	-	1/1/15/20	13/39/115/115	-
31	LMG	b	624	-	-	15/44/64/70	0/1/1/1
27	BCR	C	515	-	-	7/29/63/63	0/2/2/2
23	CLA	A	404	-	1/1/15/20	15/39/115/115	-
30	SQD	B	625	-	-	14/42/62/69	0/1/1/1
25	PL9	J	101	-	-	11/29/49/73	0/1/1/1
23	CLA	A	403	-	1/1/15/20	9/39/115/115	-
23	CLA	b	617	-	1/1/15/20	14/39/115/115	-
23	CLA	C	512	-	1/1/15/20	19/39/115/115	-
30	SQD	A	417	-	-	15/49/69/69	0/1/1/1
28	DGD	C	517	-	-	21/51/91/95	0/2/2/2
27	BCR	c	515	-	-	4/29/63/63	0/2/2/2
27	BCR	b	620	-	-	0/29/63/63	0/2/2/2
24	PHO	A	406	-	-	11/37/103/103	0/5/6/6
23	CLA	c	506	-	1/1/15/20	15/39/115/115	-
23	CLA	d	402	-	1/1/15/20	13/39/115/115	-
33	LMT	T	101	-	-	3/21/61/61	0/2/2/2
33	LMT	B	623	-	-	2/21/61/61	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
31	LMG	a	402	-	-	16/37/57/70	0/1/1/1
23	CLA	B	614	-	1/1/15/20	14/39/115/115	-
30	SQD	d	407	-	-	11/38/58/69	0/1/1/1
23	CLA	a	405	-	1/1/15/20	15/39/115/115	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
23	CLA	C	513	-	1/1/15/20	18/39/115/115	-
23	CLA	C	502	-	1/1/15/20	10/39/115/115	-
23	CLA	C	503	-	1/1/15/20	14/39/115/115	-
30	SQD	b	601	-	-	13/42/62/69	0/1/1/1
31	LMG	E	101	-	-	18/39/59/70	0/1/1/1
31	LMG	a	416	-	-	22/46/66/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	608	-	1/1/15/20	17/39/115/115	-
31	LMG	b	623	-	-	22/44/64/70	0/1/1/1
33	LMT	B	628	-	-	3/21/61/61	0/2/2/2
27	BCR	B	618	-	-	9/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/15/20	11/39/115/115	-
28	DGD	C	516	-	-	18/42/82/95	0/2/2/2
27	BCR	T	103	-	-	9/29/63/63	0/2/2/2
23	CLA	c	504	-	1/1/15/20	13/39/115/115	-
23	CLA	c	505	-	1/1/15/20	19/39/115/115	-
23	CLA	D	401	-	1/1/15/20	14/39/115/115	-
31	LMG	D	407	-	-	24/44/64/70	0/1/1/1
34	HEM	v	201	16	-	4/14/54/54	-
30	SQD	F	102	-	-	17/40/60/69	0/1/1/1
27	BCR	x	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	612	-	-	9/39/115/115	-
23	CLA	b	609	-	1/1/15/20	14/39/115/115	-
23	CLA	c	511	-	1/1/15/20	13/39/115/115	-
31	LMG	B	622	-	-	15/44/64/70	0/1/1/1
31	LMG	D	406	-	-	10/41/61/70	0/1/1/1
23	CLA	B	607	-	1/1/15/20	9/39/115/115	-
23	CLA	c	507	-	1/1/15/20	14/39/115/115	-
34	HEM	f	101	6,5	-	2/14/54/54	-
31	LMG	A	418	-	-	15/37/57/70	0/1/1/1
31	LMG	I	101	-	-	21/38/58/70	0/1/1/1
29	LHG	a	414	-	-	17/43/43/53	-
28	DGD	c	517	-	-	20/42/82/95	0/2/2/2
28	DGD	B	626	-	-	18/41/81/95	0/2/2/2
31	LMG	D	408	-	-	21/43/63/70	0/1/1/1
23	CLA	A	407	-	1/1/15/20	8/39/115/115	-
30	SQD	f	103	-	-	15/40/60/69	0/1/1/1
33	LMT	x	102	-	-	0/17/57/61	0/2/2/2
23	CLA	b	611	-	1/1/15/20	18/39/115/115	-
31	LMG	A	414	-	-	20/46/66/70	0/1/1/1
33	LMT	B	627	-	-	3/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	504	-	1/1/15/20	11/39/115/115	-
23	CLA	C	508	-	1/1/15/20	13/39/115/115	-

All (908) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	PHO	C1B-C2B	10.10	1.50	1.39
24	a	407	PHO	C1B-C2B	9.66	1.50	1.39
24	A	406	PHO	C1B-C2B	9.61	1.50	1.39
24	a	408	PHO	C1B-C2B	9.51	1.49	1.39
24	A	406	PHO	C3B-C4B	8.88	1.50	1.41
24	a	408	PHO	C3B-C4B	8.71	1.50	1.41
24	D	402	PHO	C3B-C4B	8.33	1.49	1.41
34	v	201	HEM	C3D-C2D	8.32	1.54	1.36
34	F	101	HEM	C3D-C2D	8.02	1.54	1.36
34	V	201	HEM	C3D-C2D	7.94	1.53	1.36
24	a	407	PHO	C3B-C4B	7.81	1.49	1.41
34	f	101	HEM	C3D-C2D	7.75	1.53	1.36
34	v	201	HEM	FE-ND	4.85	2.09	1.94
34	f	101	HEM	FE-ND	4.73	2.09	1.94
34	V	201	HEM	FE-ND	4.69	2.09	1.94
24	a	408	PHO	C1D-C2D	4.60	1.44	1.39
24	D	402	PHO	C1D-C2D	4.45	1.44	1.39
34	v	201	HEM	FE-NA	4.40	2.09	1.95
29	a	414	LHG	O7-C7	4.38	1.46	1.34
29	a	414	LHG	O8-C23	4.37	1.46	1.33
29	A	412	LHG	O7-C7	4.32	1.46	1.34
34	F	101	HEM	FE-ND	4.29	2.08	1.94
24	A	406	PHO	C4D-CHA	4.26	1.45	1.39
29	A	415	LHG	O8-C23	4.25	1.45	1.33
29	A	415	LHG	O7-C7	4.19	1.46	1.34
29	a	417	LHG	O8-C23	4.18	1.45	1.33
29	A	412	LHG	O8-C23	4.17	1.45	1.33
29	a	417	LHG	O7-C7	4.13	1.45	1.34
24	a	407	PHO	C1D-C2D	4.10	1.44	1.39
34	v	201	HEM	FE-NB	4.08	2.07	1.94
24	A	406	PHO	C1D-C2D	4.07	1.44	1.39
23	B	601	CLA	C1D-ND	3.97	1.43	1.37
23	c	506	CLA	C1D-ND	3.92	1.43	1.37
23	b	611	CLA	C1D-ND	3.90	1.43	1.37
23	b	604	CLA	C1D-ND	3.87	1.42	1.37
23	c	509	CLA	C1D-ND	3.83	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C1D-ND	3.82	1.42	1.37
23	C	506	CLA	C1D-ND	3.81	1.42	1.37
23	c	511	CLA	C1D-ND	3.81	1.42	1.37
23	c	503	CLA	C1D-ND	3.80	1.42	1.37
23	b	605	CLA	C1D-ND	3.79	1.42	1.37
23	b	618	CLA	C1D-ND	3.79	1.42	1.37
23	b	613	CLA	C1D-ND	3.79	1.42	1.37
34	v	201	HEM	FE-NC	3.77	2.07	1.95
23	A	404	CLA	C1D-ND	3.77	1.42	1.37
23	C	511	CLA	C1D-ND	3.73	1.42	1.37
23	b	608	CLA	C1D-ND	3.72	1.42	1.37
23	c	502	CLA	C1D-ND	3.72	1.42	1.37
23	B	608	CLA	C1D-ND	3.72	1.42	1.37
23	c	513	CLA	C1D-ND	3.72	1.42	1.37
23	d	403	CLA	C1D-ND	3.72	1.42	1.37
23	C	510	CLA	C1D-ND	3.70	1.42	1.37
23	B	609	CLA	C1D-ND	3.70	1.42	1.37
23	C	507	CLA	C1D-ND	3.70	1.42	1.37
23	C	501	CLA	C1D-ND	3.69	1.42	1.37
23	B	610	CLA	C1D-ND	3.68	1.42	1.37
31	D	406	LMG	O7-C8	-3.67	1.38	1.46
23	a	404	CLA	C1D-ND	3.66	1.42	1.37
23	C	513	CLA	C1D-ND	3.65	1.42	1.37
23	c	504	CLA	C1D-ND	3.64	1.42	1.37
23	b	612	CLA	C1D-ND	3.64	1.42	1.37
23	C	503	CLA	C1D-ND	3.64	1.42	1.37
23	a	409	CLA	C1D-ND	3.63	1.42	1.37
23	C	512	CLA	C1D-ND	3.63	1.42	1.37
23	B	606	CLA	C1D-ND	3.62	1.42	1.37
23	A	407	CLA	C1D-ND	3.62	1.42	1.37
23	B	616	CLA	C1D-ND	3.61	1.42	1.37
34	F	101	HEM	FE-NA	3.61	2.07	1.95
24	D	402	PHO	C4D-CHA	3.61	1.44	1.39
28	C	516	DGD	O2G-C2G	-3.60	1.38	1.46
31	D	407	LMG	O7-C8	-3.59	1.38	1.46
23	B	602	CLA	C1D-ND	3.58	1.42	1.37
23	c	504	CLA	C4B-NB	3.58	1.42	1.37
23	A	403	CLA	C1D-ND	3.58	1.42	1.37
23	c	512	CLA	C1D-ND	3.57	1.42	1.37
34	f	101	HEM	FE-NB	3.57	2.05	1.94
23	c	505	CLA	C1D-ND	3.57	1.42	1.37
23	b	616	CLA	C1D-ND	3.57	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	C1D-ND	3.55	1.42	1.37
23	c	510	CLA	C1D-ND	3.55	1.42	1.37
23	b	610	CLA	C1D-ND	3.54	1.42	1.37
23	c	501	CLA	C1D-ND	3.54	1.42	1.37
23	B	604	CLA	C1D-ND	3.54	1.42	1.37
23	C	502	CLA	C1D-ND	3.53	1.42	1.37
23	C	504	CLA	C1D-ND	3.53	1.42	1.37
28	B	621	DGD	O2G-C2G	-3.53	1.38	1.46
23	c	508	CLA	C1D-ND	3.52	1.42	1.37
23	B	603	CLA	C1D-ND	3.52	1.42	1.37
23	d	402	CLA	C1D-ND	3.52	1.42	1.37
23	C	508	CLA	C1D-ND	3.52	1.42	1.37
23	D	403	CLA	C1D-ND	3.51	1.42	1.37
23	B	607	CLA	C1D-ND	3.51	1.42	1.37
23	c	507	CLA	C1D-ND	3.50	1.42	1.37
23	a	405	CLA	C1D-ND	3.50	1.42	1.37
25	A	408	PL9	C33-C34	3.49	1.41	1.33
24	a	408	PHO	C4D-CHA	3.49	1.44	1.39
23	b	607	CLA	C1D-ND	3.45	1.42	1.37
28	b	622	DGD	O2G-C2G	-3.45	1.38	1.46
24	a	407	PHO	C4D-CHA	3.45	1.44	1.39
23	B	611	CLA	C1D-ND	3.45	1.42	1.37
31	d	405	LMG	O7-C8	-3.44	1.38	1.46
23	B	613	CLA	C1D-ND	3.44	1.42	1.37
23	D	401	CLA	C1D-ND	3.44	1.42	1.37
23	b	619	CLA	C1D-ND	3.42	1.42	1.37
23	C	505	CLA	C1D-ND	3.42	1.42	1.37
34	V	201	HEM	FE-NA	3.41	2.06	1.95
23	B	615	CLA	C1D-ND	3.41	1.42	1.37
23	a	404	CLA	C4B-NB	3.40	1.42	1.37
25	D	404	PL9	C38-C39	3.39	1.40	1.33
34	F	101	HEM	FE-NB	3.38	2.05	1.94
25	d	404	PL9	C38-C39	3.38	1.40	1.33
28	c	517	DGD	O2G-C2G	-3.36	1.38	1.46
25	a	410	PL9	C33-C34	3.35	1.40	1.33
23	b	614	CLA	C1D-ND	3.35	1.42	1.37
23	c	505	CLA	C4B-NB	3.35	1.42	1.37
23	A	403	CLA	C4B-NB	3.35	1.42	1.37
25	D	404	PL9	C33-C34	3.34	1.40	1.33
31	b	624	LMG	O7-C8	-3.34	1.38	1.46
31	b	623	LMG	O7-C8	-3.34	1.38	1.46
23	c	511	CLA	C4B-NB	3.34	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C1D-ND	3.33	1.42	1.37
31	k	103	LMG	O7-C8	-3.33	1.38	1.46
23	b	615	CLA	C1D-ND	3.32	1.42	1.37
23	C	509	CLA	C1D-ND	3.32	1.42	1.37
23	B	612	CLA	C1D-ND	3.31	1.42	1.37
31	C	519	LMG	O7-C8	-3.31	1.38	1.46
31	I	101	LMG	O7-C8	-3.31	1.38	1.46
31	M	102	LMG	O1-C7	-3.31	1.38	1.43
25	d	404	PL9	C43-C44	3.30	1.40	1.33
23	C	503	CLA	C4B-NB	3.30	1.42	1.37
30	d	407	SQD	O48-C23	3.30	1.43	1.33
23	a	406	CLA	C1D-ND	3.30	1.42	1.37
31	A	418	LMG	O7-C8	-3.29	1.38	1.46
25	d	404	PL9	C33-C34	3.29	1.40	1.33
23	B	601	CLA	C4B-NB	3.28	1.42	1.37
23	B	614	CLA	C4B-NB	3.28	1.42	1.37
31	D	408	LMG	O7-C8	-3.27	1.38	1.46
31	M	101	LMG	O1-C7	-3.27	1.38	1.43
23	b	614	CLA	C4B-NB	3.27	1.42	1.37
31	M	102	LMG	O7-C8	-3.24	1.39	1.46
31	a	402	LMG	O7-C8	-3.23	1.39	1.46
23	b	612	CLA	C4B-NB	3.22	1.42	1.37
28	b	602	DGD	O1G-C1A	3.21	1.42	1.33
31	a	416	LMG	O7-C10	3.21	1.43	1.34
28	C	517	DGD	O2G-C2G	-3.21	1.39	1.46
30	B	625	SQD	O48-C23	3.20	1.42	1.33
23	C	512	CLA	C4B-NB	3.20	1.42	1.37
31	i	101	LMG	O7-C8	-3.20	1.39	1.46
30	b	601	SQD	O48-C23	3.20	1.42	1.33
23	c	506	CLA	C4B-NB	3.19	1.42	1.37
23	B	614	CLA	C1D-ND	3.19	1.42	1.37
23	B	602	CLA	C4B-NB	3.19	1.42	1.37
30	A	413	SQD	O48-C23	3.18	1.42	1.33
23	B	607	CLA	C4B-NB	3.18	1.42	1.37
23	d	403	CLA	C4B-NB	3.17	1.42	1.37
31	M	101	LMG	O7-C8	-3.17	1.39	1.46
34	f	101	HEM	CAC-C3C	3.16	1.55	1.47
23	A	407	CLA	C4B-NB	3.16	1.42	1.37
23	D	401	CLA	C4B-NB	3.16	1.42	1.37
23	C	505	CLA	C4B-NB	3.15	1.42	1.37
30	F	102	SQD	O48-C23	3.15	1.42	1.33
23	b	610	CLA	C4B-NB	3.15	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	415	SQD	O48-C23	3.15	1.42	1.33
30	a	401	SQD	O48-C23	3.14	1.42	1.33
31	C	520	LMG	O7-C10	3.14	1.43	1.34
23	B	603	CLA	C4B-NB	3.14	1.42	1.37
23	c	503	CLA	C4B-NB	3.14	1.42	1.37
23	C	506	CLA	C4B-NB	3.14	1.42	1.37
23	b	611	CLA	C4B-NB	3.14	1.42	1.37
23	b	617	CLA	C1D-ND	3.13	1.42	1.37
23	C	508	CLA	C4B-NB	3.13	1.42	1.37
28	c	519	DGD	O2G-C1B	3.12	1.43	1.34
28	D	410	DGD	O2G-C2G	-3.12	1.39	1.46
23	c	509	CLA	C4B-NB	3.12	1.42	1.37
23	b	619	CLA	C4B-NB	3.12	1.42	1.37
30	A	417	SQD	O48-C23	3.11	1.42	1.33
23	B	605	CLA	C1D-ND	3.11	1.41	1.37
30	f	103	SQD	O48-C23	3.10	1.42	1.33
23	d	402	CLA	C4B-NB	3.10	1.41	1.37
23	C	503	CLA	C1B-C2B	3.10	1.50	1.43
23	C	501	CLA	C4B-NB	3.09	1.41	1.37
23	C	511	CLA	C4B-NB	3.09	1.41	1.37
28	c	517	DGD	O1G-C1A	3.09	1.42	1.33
23	c	505	CLA	C1B-C2B	3.09	1.50	1.43
23	C	510	CLA	C4B-NB	3.09	1.41	1.37
28	C	518	DGD	O2G-C1B	3.08	1.43	1.34
31	d	406	LMG	O7-C8	-3.08	1.39	1.46
23	b	608	CLA	C4B-NB	3.07	1.41	1.37
30	D	409	SQD	O48-C23	3.07	1.42	1.33
23	a	409	CLA	C4B-NB	3.07	1.41	1.37
30	d	407	SQD	O47-C7	3.07	1.42	1.34
23	B	610	CLA	C4B-NB	3.07	1.41	1.37
28	d	408	DGD	O2G-C2G	-3.06	1.39	1.46
25	D	404	PL9	C43-C44	3.06	1.40	1.33
23	C	502	CLA	C4B-NB	3.06	1.41	1.37
23	b	604	CLA	C4B-NB	3.06	1.41	1.37
23	B	611	CLA	C4B-NB	3.05	1.41	1.37
23	B	615	CLA	C4B-NB	3.05	1.41	1.37
31	c	520	LMG	O7-C10	3.05	1.42	1.34
28	B	626	DGD	O2G-C1B	3.05	1.42	1.34
34	v	201	HEM	CAC-C3C	3.04	1.55	1.47
28	b	602	DGD	O2G-C2G	-3.04	1.39	1.46
28	c	518	DGD	O2G-C2G	-3.04	1.39	1.46
23	c	504	CLA	C1B-C2B	3.04	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C4B-NB	3.03	1.41	1.37
23	b	607	CLA	C4B-NB	3.03	1.41	1.37
23	C	509	CLA	C4B-NB	3.03	1.41	1.37
28	a	413	DGD	O2G-C2G	-3.03	1.39	1.46
31	A	414	LMG	O7-C8	-3.02	1.39	1.46
23	b	616	CLA	C4B-NB	3.02	1.41	1.37
31	A	414	LMG	O7-C10	3.02	1.42	1.34
23	c	512	CLA	C4B-NB	3.02	1.41	1.37
28	C	518	DGD	O2G-C2G	-3.02	1.39	1.46
23	B	609	CLA	C4B-NB	3.01	1.41	1.37
30	b	601	SQD	O47-C7	3.01	1.42	1.34
23	a	406	CLA	C4B-NB	3.01	1.41	1.37
31	B	622	LMG	O7-C8	-3.01	1.39	1.46
34	V	201	HEM	CAC-C3C	3.00	1.55	1.47
23	a	405	CLA	C4B-NB	3.00	1.41	1.37
23	c	511	CLA	C1B-C2B	3.00	1.50	1.43
23	b	605	CLA	C4B-NB	3.00	1.41	1.37
23	C	513	CLA	C4B-NB	3.00	1.41	1.37
34	F	101	HEM	CAB-C3B	3.00	1.55	1.47
23	b	609	CLA	C4B-NB	2.99	1.41	1.37
31	E	101	LMG	O7-C10	2.99	1.42	1.34
31	M	101	LMG	O7-C10	2.99	1.42	1.34
23	c	501	CLA	C4B-NB	2.98	1.41	1.37
23	B	601	CLA	C1B-C2B	2.98	1.50	1.43
23	b	613	CLA	C4B-NB	2.98	1.41	1.37
23	c	508	CLA	C4B-NB	2.98	1.41	1.37
23	b	617	CLA	C4B-NB	2.98	1.41	1.37
23	B	605	CLA	C4B-NB	2.98	1.41	1.37
23	C	501	CLA	C1B-C2B	2.98	1.50	1.43
31	B	622	LMG	O7-C10	2.97	1.42	1.34
30	A	417	SQD	O47-C7	2.97	1.42	1.34
30	F	102	SQD	O47-C7	2.96	1.42	1.34
23	A	405	CLA	C4B-NB	2.96	1.41	1.37
28	D	410	DGD	O1G-C1A	2.96	1.42	1.33
34	f	101	HEM	CAB-C3B	2.96	1.55	1.47
23	c	510	CLA	C4B-NB	2.95	1.41	1.37
23	b	615	CLA	C4B-NB	2.95	1.41	1.37
23	b	619	CLA	C1B-C2B	2.95	1.50	1.43
31	i	101	LMG	O1-C7	-2.95	1.38	1.43
34	v	201	HEM	CAB-C3B	2.95	1.55	1.47
34	F	101	HEM	CAC-C3C	2.94	1.55	1.47
23	B	616	CLA	C4B-NB	2.94	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	CLA	C4B-NB	2.93	1.41	1.37
23	d	402	CLA	C1B-C2B	2.93	1.50	1.43
23	C	511	CLA	C1B-C2B	2.92	1.50	1.43
23	C	505	CLA	C1B-C2B	2.92	1.50	1.43
23	B	612	CLA	C4B-NB	2.92	1.41	1.37
23	b	606	CLA	C4B-NB	2.92	1.41	1.37
31	a	416	LMG	O7-C8	-2.92	1.39	1.46
23	B	608	CLA	C4B-NB	2.92	1.41	1.37
25	J	101	PL9	C23-C24	2.92	1.39	1.33
31	M	102	LMG	O7-C10	2.92	1.42	1.34
28	B	626	DGD	O1G-C1A	2.92	1.41	1.33
23	B	613	CLA	C4B-NB	2.91	1.41	1.37
30	D	409	SQD	O47-C7	2.91	1.42	1.34
23	D	403	CLA	C4B-NB	2.91	1.41	1.37
28	A	411	DGD	O2G-C1B	2.91	1.42	1.34
23	a	406	CLA	C1B-C2B	2.91	1.50	1.43
25	A	408	PL9	C13-C14	2.90	1.39	1.33
23	C	512	CLA	C1B-C2B	2.90	1.49	1.43
28	c	519	DGD	O2G-C2G	-2.90	1.39	1.46
23	A	404	CLA	C4B-NB	2.89	1.41	1.37
23	B	602	CLA	C1B-C2B	2.88	1.49	1.43
25	j	101	PL9	C23-C24	2.88	1.39	1.33
23	c	507	CLA	C4B-NB	2.88	1.41	1.37
31	e	101	LMG	O7-C8	-2.87	1.39	1.46
23	b	604	CLA	C1B-C2B	2.87	1.49	1.43
23	b	607	CLA	C1B-C2B	2.87	1.49	1.43
23	c	502	CLA	C4B-NB	2.87	1.41	1.37
28	A	411	DGD	O2G-C2G	-2.86	1.39	1.46
25	J	101	PL9	C8-C9	2.86	1.39	1.33
25	d	404	PL9	C18-C19	2.86	1.39	1.33
23	B	604	CLA	C4B-NB	2.86	1.41	1.37
23	C	504	CLA	C4B-NB	2.86	1.41	1.37
28	d	408	DGD	O1G-C1A	2.86	1.41	1.33
28	C	516	DGD	O1G-C1A	2.86	1.41	1.33
28	C	517	DGD	O1G-C1A	2.85	1.41	1.33
23	c	503	CLA	C1B-C2B	2.85	1.49	1.43
28	c	518	DGD	O2G-C1B	2.85	1.42	1.34
31	E	101	LMG	O8-C28	2.85	1.41	1.33
25	j	101	PL9	C13-C14	2.85	1.39	1.33
31	i	101	LMG	O7-C10	2.85	1.42	1.34
25	a	410	PL9	C38-C39	2.85	1.41	1.32
23	c	506	CLA	C1B-C2B	2.85	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PL9	C38-C39	2.84	1.41	1.32
28	c	519	DGD	O1G-C1A	2.84	1.41	1.33
28	B	626	DGD	O2G-C2G	-2.84	1.39	1.46
31	c	520	LMG	O8-C28	2.83	1.41	1.33
23	B	615	CLA	C1B-C2B	2.83	1.49	1.43
30	a	401	SQD	O47-C7	2.83	1.42	1.34
23	B	614	CLA	C1B-C2B	2.83	1.49	1.43
30	a	415	SQD	O47-C7	2.83	1.42	1.34
23	B	606	CLA	C4B-NB	2.83	1.41	1.37
28	b	622	DGD	O1G-C1A	2.82	1.41	1.33
30	B	625	SQD	O47-C7	2.82	1.42	1.34
23	C	510	CLA	C1B-C2B	2.82	1.49	1.43
28	b	602	DGD	O2G-C1B	2.82	1.42	1.34
28	c	517	DGD	O2G-C1B	2.82	1.42	1.34
23	c	502	CLA	C1B-C2B	2.82	1.49	1.43
25	d	404	PL9	C23-C24	2.82	1.39	1.33
23	b	615	CLA	C1B-C2B	2.82	1.49	1.43
28	B	621	DGD	O3G-C3G	-2.82	1.38	1.43
25	a	410	PL9	C23-C24	2.81	1.39	1.33
28	C	518	DGD	O1G-C1A	2.81	1.41	1.33
25	J	101	PL9	C18-C19	2.81	1.39	1.33
23	A	403	CLA	C1B-C2B	2.81	1.49	1.43
23	C	502	CLA	C1B-C2B	2.81	1.49	1.43
30	f	103	SQD	O47-C7	2.81	1.42	1.34
34	f	101	HEM	FE-NA	2.81	2.04	1.95
31	M	101	LMG	O8-C9	-2.80	1.38	1.45
31	e	101	LMG	O7-C10	2.80	1.42	1.34
23	c	513	CLA	C1B-C2B	2.80	1.49	1.43
31	a	402	LMG	O7-C10	2.80	1.42	1.34
31	d	406	LMG	O7-C10	2.80	1.42	1.34
23	c	501	CLA	C1B-C2B	2.80	1.49	1.43
25	j	101	PL9	C18-C19	2.79	1.39	1.33
31	A	414	LMG	O1-C7	-2.79	1.38	1.43
23	A	405	CLA	C1B-C2B	2.79	1.49	1.43
23	B	604	CLA	C1B-C2B	2.79	1.49	1.43
23	C	507	CLA	C4B-NB	2.79	1.41	1.37
28	b	622	DGD	O3G-C3G	-2.79	1.38	1.43
25	D	404	PL9	C18-C19	2.79	1.39	1.33
25	j	101	PL9	C8-C9	2.79	1.39	1.33
23	b	612	CLA	C1B-C2B	2.79	1.49	1.43
28	a	413	DGD	O2G-C1B	2.79	1.42	1.34
31	C	520	LMG	O8-C28	2.79	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	406	LMG	O8-C28	2.79	1.41	1.33
25	A	408	PL9	C23-C24	2.79	1.39	1.33
23	c	509	CLA	C1B-C2B	2.79	1.49	1.43
28	B	621	DGD	O1G-C1A	2.78	1.41	1.33
28	c	518	DGD	O1G-C1A	2.77	1.41	1.33
31	C	519	LMG	O8-C28	2.77	1.41	1.33
23	B	607	CLA	C1B-C2B	2.77	1.49	1.43
31	D	407	LMG	O8-C9	-2.77	1.39	1.45
34	f	101	HEM	FE-NC	2.76	2.04	1.95
31	D	408	LMG	O3-C3	-2.76	1.36	1.43
23	d	403	CLA	C1B-C2B	2.76	1.49	1.43
23	a	404	CLA	C1B-C2B	2.76	1.49	1.43
25	J	101	PL9	C13-C14	2.76	1.39	1.33
31	a	416	LMG	O8-C28	2.75	1.41	1.33
31	c	520	LMG	O7-C8	-2.75	1.40	1.46
23	D	401	CLA	C1B-C2B	2.75	1.49	1.43
31	d	406	LMG	O3-C3	-2.75	1.36	1.43
23	c	512	CLA	C1B-C2B	2.75	1.49	1.43
31	B	622	LMG	O1-C7	-2.75	1.39	1.43
25	A	408	PL9	C18-C19	2.75	1.39	1.33
31	D	407	LMG	O1-C7	-2.74	1.39	1.43
25	A	408	PL9	C8-C9	2.74	1.39	1.33
31	b	623	LMG	O6-C5	-2.74	1.37	1.44
28	a	413	DGD	O1G-C1A	2.73	1.41	1.33
23	C	508	CLA	C1B-C2B	2.73	1.49	1.43
31	b	624	LMG	O8-C9	-2.73	1.39	1.45
31	A	418	LMG	O7-C10	2.72	1.42	1.34
31	a	416	LMG	O3-C3	-2.72	1.36	1.43
31	k	103	LMG	O8-C28	2.72	1.41	1.33
23	C	513	CLA	C1B-C2B	2.72	1.49	1.43
23	b	605	CLA	C1B-C2B	2.72	1.49	1.43
23	b	610	CLA	C1B-C2B	2.72	1.49	1.43
24	a	407	PHO	CAC-C3C	-2.71	1.46	1.51
31	M	102	LMG	O8-C28	2.71	1.41	1.33
23	b	614	CLA	C1B-C2B	2.71	1.49	1.43
31	b	624	LMG	O7-C10	2.71	1.41	1.34
23	C	509	CLA	C1B-C2B	2.71	1.49	1.43
23	c	510	CLA	C1B-C2B	2.71	1.49	1.43
23	B	609	CLA	C1B-C2B	2.71	1.49	1.43
34	V	201	HEM	CAB-C3B	2.71	1.54	1.47
31	C	520	LMG	O7-C8	-2.70	1.40	1.46
23	b	617	CLA	C1B-C2B	2.70	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	CLA	C1B-C2B	2.70	1.49	1.43
25	D	404	PL9	C13-C14	2.70	1.39	1.33
25	D	404	PL9	C23-C24	2.70	1.39	1.33
23	A	403	CLA	C3B-C4B	2.70	1.50	1.42
23	B	608	CLA	C1B-C2B	2.69	1.49	1.43
23	B	612	CLA	C1B-C2B	2.69	1.49	1.43
31	A	414	LMG	O8-C28	2.69	1.41	1.33
25	d	404	PL9	C13-C14	2.69	1.39	1.33
31	d	405	LMG	O7-C10	2.69	1.41	1.34
31	a	402	LMG	O8-C28	2.69	1.41	1.33
23	c	507	CLA	C1B-C2B	2.69	1.49	1.43
23	A	407	CLA	C1B-C2B	2.69	1.49	1.43
31	D	408	LMG	O7-C10	2.69	1.41	1.34
23	b	616	CLA	C1B-C2B	2.69	1.49	1.43
25	a	410	PL9	C18-C19	2.68	1.39	1.33
31	E	101	LMG	O7-C8	-2.68	1.40	1.46
31	b	623	LMG	O7-C10	2.68	1.41	1.34
23	a	409	CLA	C1B-C2B	2.68	1.49	1.43
30	A	413	SQD	O47-C7	2.68	1.41	1.34
28	b	602	DGD	O6E-C5E	-2.68	1.37	1.44
23	B	610	CLA	C1B-C2B	2.67	1.49	1.43
23	a	409	CLA	CHC-C1C	2.67	1.43	1.38
23	D	403	CLA	C1B-C2B	2.67	1.49	1.43
23	B	605	CLA	C1B-C2B	2.67	1.49	1.43
31	e	101	LMG	O8-C9	-2.66	1.39	1.45
31	A	418	LMG	O8-C9	-2.66	1.39	1.45
25	d	404	PL9	C8-C9	2.66	1.39	1.33
28	d	408	DGD	O2G-C1B	2.66	1.41	1.34
23	B	611	CLA	C1B-C2B	2.66	1.49	1.43
23	B	616	CLA	C1B-C2B	2.66	1.49	1.43
31	I	101	LMG	O7-C10	2.66	1.41	1.34
31	A	414	LMG	O3-C3	-2.65	1.36	1.43
23	B	613	CLA	C1B-C2B	2.65	1.49	1.43
31	k	103	LMG	O7-C10	2.65	1.41	1.34
31	M	102	LMG	O8-C9	-2.65	1.39	1.45
28	B	626	DGD	O5D-C6D	-2.65	1.39	1.43
31	k	103	LMG	O1-C7	-2.65	1.39	1.43
31	e	101	LMG	O8-C28	2.65	1.41	1.33
31	C	519	LMG	O7-C10	2.65	1.41	1.34
31	i	101	LMG	O8-C9	-2.64	1.39	1.45
23	B	603	CLA	C1B-C2B	2.64	1.49	1.43
31	I	101	LMG	O8-C28	2.64	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	626	DGD	O6E-C5E	-2.63	1.37	1.44
23	C	507	CLA	C1B-C2B	2.63	1.49	1.43
28	C	517	DGD	O2G-C1B	2.63	1.41	1.34
31	b	624	LMG	O1-C7	-2.63	1.39	1.43
28	A	411	DGD	O1G-C1A	2.63	1.41	1.33
31	M	101	LMG	O8-C28	2.63	1.41	1.33
31	B	622	LMG	O3-C3	-2.63	1.36	1.43
24	a	407	PHO	CMC-C2C	-2.63	1.46	1.50
31	d	405	LMG	O1-C7	-2.63	1.39	1.43
31	B	622	LMG	O8-C28	2.63	1.41	1.33
24	D	402	PHO	CMC-C2C	-2.62	1.46	1.50
24	a	407	PHO	CMD-C2D	-2.62	1.46	1.51
31	D	408	LMG	O8-C28	2.62	1.41	1.33
25	a	410	PL9	C13-C14	2.62	1.39	1.33
31	i	101	LMG	O3-C3	-2.61	1.36	1.43
31	a	402	LMG	O1-C7	-2.61	1.39	1.43
31	I	101	LMG	O3-C3	-2.61	1.36	1.43
31	b	623	LMG	O8-C28	2.60	1.40	1.33
31	b	623	LMG	O8-C9	-2.60	1.39	1.45
24	A	406	PHO	C3D-C4D	2.60	1.44	1.41
23	b	608	CLA	C1B-C2B	2.60	1.49	1.43
23	a	404	CLA	C3B-C4B	2.60	1.50	1.42
31	D	408	LMG	O8-C9	-2.60	1.39	1.45
31	A	414	LMG	O8-C9	-2.60	1.39	1.45
23	C	506	CLA	C1B-C2B	2.60	1.49	1.43
31	D	406	LMG	O8-C9	-2.60	1.39	1.45
31	D	406	LMG	O3-C3	-2.60	1.36	1.43
31	b	623	LMG	O3-C3	-2.60	1.36	1.43
25	a	410	PL9	C28-C29	2.60	1.39	1.33
31	b	623	LMG	O1-C7	-2.59	1.39	1.43
31	d	405	LMG	O8-C28	2.59	1.40	1.33
31	b	624	LMG	O3-C3	-2.58	1.36	1.43
25	a	410	PL9	C8-C9	2.58	1.39	1.33
31	D	407	LMG	O8-C28	2.58	1.40	1.33
23	B	606	CLA	C1B-C2B	2.58	1.49	1.43
31	d	405	LMG	O3-C3	-2.58	1.36	1.43
28	C	516	DGD	O6E-C5E	-2.58	1.38	1.44
31	b	624	LMG	O8-C28	2.58	1.40	1.33
31	I	101	LMG	O8-C9	-2.58	1.39	1.45
23	C	504	CLA	C1B-C2B	2.57	1.49	1.43
23	b	608	CLA	C3B-C4B	2.57	1.50	1.42
23	b	605	CLA	CHC-C1C	2.57	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	416	LMG	O8-C9	-2.57	1.39	1.45
31	i	101	LMG	O8-C28	2.57	1.40	1.33
23	A	404	CLA	CHC-C1C	2.56	1.43	1.38
31	I	101	LMG	O1-C7	-2.56	1.39	1.43
31	D	407	LMG	O7-C10	2.56	1.41	1.34
23	B	602	CLA	CHC-C1C	2.56	1.43	1.38
31	E	101	LMG	O8-C9	-2.56	1.39	1.45
23	b	606	CLA	C1B-C2B	2.55	1.49	1.43
31	A	418	LMG	O8-C28	2.55	1.40	1.33
23	b	614	CLA	CMB-C2B	-2.55	1.45	1.50
31	k	103	LMG	O8-C9	-2.55	1.39	1.45
28	A	411	DGD	O1G-C1G	-2.54	1.39	1.45
23	b	613	CLA	C1B-C2B	2.54	1.49	1.43
28	C	516	DGD	O2G-C1B	2.54	1.41	1.34
31	M	101	LMG	O3-C3	-2.54	1.36	1.43
24	D	402	PHO	CMD-C2D	-2.54	1.46	1.51
23	b	609	CLA	C1B-C2B	2.54	1.49	1.43
23	b	611	CLA	CHC-C1C	2.54	1.43	1.38
31	E	101	LMG	O3-C3	-2.53	1.36	1.43
23	c	508	CLA	C1B-C2B	2.53	1.49	1.43
23	a	409	CLA	C3B-C4B	2.53	1.50	1.42
28	C	518	DGD	O3G-C3G	-2.53	1.39	1.43
31	B	622	LMG	O8-C9	-2.53	1.39	1.45
24	a	408	PHO	CMC-C2C	-2.53	1.46	1.50
31	a	402	LMG	O3-C3	-2.52	1.36	1.43
31	A	418	LMG	O1-C7	-2.52	1.39	1.43
31	a	402	LMG	O8-C9	-2.52	1.39	1.45
24	A	406	PHO	CMB-C2B	-2.52	1.46	1.51
24	a	407	PHO	CMB-C2B	-2.52	1.46	1.51
31	c	520	LMG	O8-C9	-2.51	1.39	1.45
28	c	518	DGD	O5D-C6D	-2.51	1.39	1.43
31	c	520	LMG	O3-C3	-2.51	1.36	1.43
28	B	621	DGD	O5D-C6D	-2.51	1.39	1.43
28	c	517	DGD	O6E-C5E	-2.51	1.38	1.44
28	c	519	DGD	O3G-C3G	-2.50	1.39	1.43
31	D	408	LMG	O1-C7	-2.50	1.39	1.43
23	c	511	CLA	C3B-C4B	2.50	1.50	1.42
28	B	621	DGD	O6D-C5D	-2.50	1.38	1.44
25	A	408	PL9	C28-C29	2.50	1.38	1.33
24	a	408	PHO	CMD-C2D	-2.50	1.46	1.51
31	C	519	LMG	O3-C3	-2.49	1.36	1.43
31	A	418	LMG	O3-C3	-2.49	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405	CLA	C3B-C4B	2.49	1.50	1.42
31	C	520	LMG	O3-C3	-2.49	1.36	1.43
23	C	503	CLA	C3B-C4B	2.49	1.50	1.42
30	A	417	SQD	C4-C5	-2.49	1.47	1.53
24	A	406	PHO	CMD-C2D	-2.49	1.46	1.51
31	C	520	LMG	O8-C9	-2.49	1.39	1.45
25	d	404	PL9	C28-C29	2.48	1.38	1.33
24	A	406	PHO	CMC-C2C	-2.48	1.46	1.50
31	d	405	LMG	O8-C9	-2.48	1.39	1.45
28	b	622	DGD	O2G-C1B	2.48	1.41	1.34
28	c	518	DGD	O6E-C5E	-2.48	1.38	1.44
25	D	404	PL9	C8-C9	2.48	1.38	1.33
31	D	406	LMG	O8-C28	2.47	1.40	1.33
28	c	518	DGD	O4D-C4D	-2.47	1.36	1.43
23	b	611	CLA	C1B-C2B	2.47	1.48	1.43
31	e	101	LMG	O3-C3	-2.46	1.36	1.43
23	C	506	CLA	C3B-C4B	2.46	1.49	1.42
31	D	407	LMG	O3-C3	-2.46	1.36	1.43
24	A	406	PHO	CAC-C3C	-2.45	1.47	1.51
31	C	519	LMG	O8-C9	-2.45	1.39	1.45
23	b	608	CLA	CHC-C1C	2.45	1.43	1.38
23	c	506	CLA	C3B-C4B	2.45	1.49	1.42
24	D	402	PHO	CMB-C2B	-2.45	1.46	1.51
28	D	410	DGD	O5D-C6D	-2.45	1.39	1.43
23	b	612	CLA	C3B-C4B	2.45	1.49	1.42
24	D	402	PHO	C3D-C4D	2.45	1.44	1.41
31	k	103	LMG	O3-C3	-2.45	1.36	1.43
28	D	410	DGD	O2G-C1B	2.44	1.41	1.34
31	a	416	LMG	O1-C7	-2.44	1.39	1.43
23	a	405	CLA	C1B-C2B	2.44	1.48	1.43
23	b	611	CLA	C3B-C4B	2.44	1.49	1.42
24	D	402	PHO	CAC-C3C	-2.44	1.47	1.51
31	M	102	LMG	O3-C3	-2.44	1.36	1.43
23	A	404	CLA	C1B-C2B	2.44	1.48	1.43
23	C	506	CLA	CHC-C1C	2.43	1.43	1.38
23	c	504	CLA	C3B-C4B	2.43	1.49	1.42
28	b	622	DGD	O6D-C5D	-2.43	1.38	1.44
23	c	508	CLA	CHC-C1C	2.43	1.43	1.38
28	C	517	DGD	O6E-C5E	-2.42	1.38	1.44
31	d	406	LMG	O1-C7	-2.42	1.39	1.43
23	b	618	CLA	CHC-C1C	2.42	1.43	1.38
23	A	404	CLA	C3B-C4B	2.42	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	602	DGD	O5D-C6D	-2.41	1.39	1.43
25	D	404	PL9	C28-C29	2.41	1.38	1.33
23	c	509	CLA	C3B-C4B	2.41	1.49	1.42
23	b	613	CLA	CHC-C1C	2.41	1.43	1.38
31	D	406	LMG	O7-C10	2.41	1.41	1.34
23	C	511	CLA	C3B-C4B	2.41	1.49	1.42
24	a	408	PHO	CAC-C3C	-2.41	1.47	1.51
23	B	607	CLA	C3B-C4B	2.40	1.49	1.42
28	c	518	DGD	O6D-C5D	-2.40	1.38	1.44
31	C	519	LMG	O1-C7	-2.40	1.39	1.43
23	D	401	CLA	C3B-C4B	2.39	1.49	1.42
28	a	413	DGD	O1G-C1G	-2.39	1.39	1.45
28	C	517	DGD	C4D-C5D	-2.39	1.47	1.53
23	B	604	CLA	MG-NB	-2.38	2.01	2.05
23	b	617	CLA	CHC-C1C	2.38	1.43	1.38
23	c	506	CLA	CHC-C1C	2.38	1.43	1.38
24	a	408	PHO	CMB-C2B	-2.38	1.46	1.51
23	C	504	CLA	CHC-C1C	2.38	1.43	1.38
23	b	614	CLA	C3B-C4B	2.37	1.49	1.42
23	c	508	CLA	C3B-C4B	2.37	1.49	1.42
34	V	201	HEM	FE-NB	2.37	2.02	1.94
23	B	612	CLA	MG-NB	-2.37	2.01	2.05
28	C	517	DGD	O4D-C4D	-2.37	1.37	1.43
23	C	509	CLA	C3B-C4B	2.37	1.49	1.42
23	B	602	CLA	C3B-C4B	2.36	1.49	1.42
23	b	618	CLA	C3B-C4B	2.36	1.49	1.42
30	A	417	SQD	O2-C2	-2.36	1.37	1.43
23	B	610	CLA	CHC-C1C	2.36	1.43	1.38
23	C	504	CLA	C3B-C4B	2.36	1.49	1.42
23	c	507	CLA	MG-NB	-2.36	2.01	2.05
23	B	611	CLA	CMB-C2B	-2.36	1.45	1.50
23	d	403	CLA	CHC-C1C	2.35	1.43	1.38
23	c	505	CLA	C3B-C4B	2.35	1.49	1.42
31	D	407	LMG	O6-C5	-2.35	1.38	1.44
31	c	520	LMG	O1-C7	-2.35	1.39	1.43
23	B	613	CLA	MG-NB	-2.35	2.01	2.05
23	B	608	CLA	MG-NB	-2.35	2.01	2.05
23	C	503	CLA	CHC-C1C	2.35	1.43	1.38
23	b	606	CLA	C3B-C4B	2.34	1.49	1.42
28	C	517	DGD	O5D-C6D	-2.34	1.39	1.43
23	B	615	CLA	CHC-C1C	2.34	1.43	1.38
23	b	605	CLA	C3B-C4B	2.34	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C3B-C4B	2.34	1.49	1.42
23	c	502	CLA	CHC-C1C	2.34	1.43	1.38
23	b	615	CLA	C3B-C4B	2.34	1.49	1.42
23	b	613	CLA	C3B-C4B	2.33	1.49	1.42
23	B	615	CLA	C3B-C4B	2.33	1.49	1.42
23	c	502	CLA	C3B-C4B	2.33	1.49	1.42
23	B	606	CLA	CHC-C1C	2.33	1.43	1.38
28	B	621	DGD	O2G-C1B	2.32	1.40	1.34
28	A	411	DGD	O3G-C3G	-2.32	1.39	1.43
23	C	502	CLA	C3B-C4B	2.32	1.49	1.42
23	B	605	CLA	C3B-C4B	2.32	1.49	1.42
23	C	502	CLA	CHC-C1C	2.32	1.43	1.38
23	b	614	CLA	CHC-C1C	2.32	1.43	1.38
23	c	504	CLA	CHC-C1C	2.31	1.43	1.38
23	b	606	CLA	CHC-C1C	2.31	1.43	1.38
23	B	607	CLA	CHC-C1C	2.31	1.43	1.38
23	b	612	CLA	CHC-C1C	2.31	1.43	1.38
24	a	408	PHO	C3D-C4D	2.31	1.44	1.41
23	B	610	CLA	C3B-C4B	2.31	1.49	1.42
28	a	413	DGD	O3G-C3G	-2.30	1.39	1.43
23	b	617	CLA	MG-NB	-2.30	2.01	2.05
31	D	408	LMG	O6-C5	-2.30	1.38	1.44
23	A	407	CLA	C3B-C4B	2.30	1.49	1.42
28	C	516	DGD	C4E-C5E	-2.30	1.48	1.53
23	A	405	CLA	C3B-C4B	2.30	1.49	1.42
31	d	406	LMG	O8-C9	-2.30	1.40	1.45
23	C	508	CLA	C3B-C4B	2.30	1.49	1.42
23	c	509	CLA	CHC-C1C	2.30	1.43	1.38
23	b	616	CLA	C3B-C4B	2.29	1.49	1.42
23	C	513	CLA	CHC-C1C	2.29	1.43	1.38
23	D	403	CLA	C3B-C4B	2.29	1.49	1.42
23	a	406	CLA	C3B-C4B	2.29	1.49	1.42
23	a	404	CLA	CHC-C1C	2.29	1.43	1.38
23	d	403	CLA	C3B-C4B	2.29	1.49	1.42
23	c	510	CLA	MG-NB	-2.28	2.01	2.05
23	b	615	CLA	CHC-C1C	2.28	1.43	1.38
23	B	606	CLA	C3B-C4B	2.28	1.49	1.42
23	B	608	CLA	C3B-C4B	2.28	1.49	1.42
23	B	603	CLA	C3B-C4B	2.28	1.49	1.42
31	e	101	LMG	O1-C7	-2.27	1.39	1.43
31	B	622	LMG	O6-C5	-2.27	1.38	1.44
31	I	101	LMG	O6-C5	-2.27	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	CHC-C1C	2.27	1.43	1.38
28	b	622	DGD	O5D-C6D	-2.27	1.39	1.43
24	a	407	PHO	C3D-C4D	2.27	1.44	1.41
23	C	512	CLA	CHC-C1C	2.27	1.43	1.38
23	C	512	CLA	C3B-C4B	2.27	1.49	1.42
28	C	517	DGD	O6D-C5D	-2.27	1.38	1.44
23	b	609	CLA	CHC-C1C	2.27	1.43	1.38
28	c	518	DGD	C4D-C5D	-2.26	1.48	1.53
31	e	101	LMG	O6-C5	-2.26	1.38	1.44
23	C	507	CLA	MG-NB	-2.25	2.01	2.05
28	C	518	DGD	O6E-C5E	-2.25	1.38	1.44
23	b	616	CLA	CHC-C1C	2.25	1.43	1.38
23	c	510	CLA	CHC-C1C	2.25	1.43	1.38
23	B	608	CLA	CHC-C1C	2.25	1.43	1.38
23	c	510	CLA	C3B-C4B	2.25	1.49	1.42
28	B	621	DGD	O6E-C5E	-2.25	1.38	1.44
23	b	610	CLA	C3B-C4B	2.25	1.49	1.42
23	B	601	CLA	CHC-C1C	2.25	1.43	1.38
23	C	511	CLA	CHC-C1C	2.25	1.43	1.38
28	b	622	DGD	O6E-C5E	-2.25	1.38	1.44
23	b	617	CLA	C3B-C4B	2.25	1.49	1.42
23	c	512	CLA	C3B-C4B	2.24	1.49	1.42
23	B	611	CLA	MG-NB	-2.24	2.01	2.05
33	i	102	LMT	O1'-C1'	2.24	1.43	1.40
31	D	406	LMG	O1-C7	-2.24	1.39	1.43
23	c	505	CLA	CHC-C1C	2.24	1.43	1.38
23	c	513	CLA	C3B-C4B	2.24	1.49	1.42
23	a	406	CLA	CHC-C1C	2.24	1.43	1.38
23	B	612	CLA	CMD-C2D	-2.24	1.46	1.50
23	c	505	CLA	CMD-C2D	-2.24	1.46	1.50
23	B	614	CLA	MG-NB	-2.24	2.01	2.05
23	C	501	CLA	C3B-C4B	2.23	1.49	1.42
28	c	518	DGD	O1G-C1G	-2.23	1.40	1.45
28	c	517	DGD	O4D-C4D	-2.23	1.37	1.43
23	c	503	CLA	C3B-C4B	2.23	1.49	1.42
23	B	609	CLA	C3B-C4B	2.23	1.49	1.42
23	C	510	CLA	CMB-C2B	-2.22	1.46	1.50
23	B	616	CLA	MG-NB	-2.22	2.01	2.05
23	b	606	CLA	MG-NB	-2.22	2.01	2.05
23	B	611	CLA	C3B-C4B	2.22	1.49	1.42
23	B	601	CLA	C3B-C4B	2.22	1.49	1.42
28	c	519	DGD	O6E-C5E	-2.22	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	MG-NB	-2.22	2.01	2.05
28	a	413	DGD	O6E-C5E	-2.22	1.39	1.44
23	B	612	CLA	C3B-C4B	2.21	1.49	1.42
23	b	607	CLA	MG-NB	-2.21	2.01	2.05
23	C	507	CLA	C3B-C4B	2.21	1.49	1.42
23	c	510	CLA	CMD-C2D	-2.21	1.46	1.50
23	a	405	CLA	MG-NB	-2.21	2.01	2.05
23	B	606	CLA	MG-NB	-2.21	2.01	2.05
24	a	407	PHO	C4D-ND	-2.21	1.35	1.38
23	C	513	CLA	C3B-C4B	2.21	1.49	1.42
25	J	101	PL9	C28-C29	2.20	1.39	1.32
23	B	613	CLA	C3B-C4B	2.20	1.49	1.42
34	v	201	HEM	CMB-C2B	2.20	1.55	1.50
23	b	614	CLA	MG-NB	-2.20	2.01	2.05
23	C	507	CLA	CHC-C1C	2.20	1.42	1.38
23	b	604	CLA	CMB-C2B	-2.20	1.46	1.50
23	c	511	CLA	CHC-C1C	2.20	1.42	1.38
23	D	401	CLA	CHC-C1C	2.20	1.42	1.38
23	a	404	CLA	CMD-C2D	-2.20	1.46	1.50
23	b	617	CLA	CMD-C2D	-2.20	1.46	1.50
28	C	518	DGD	O1G-C1G	-2.20	1.40	1.45
23	B	605	CLA	CHC-C1C	2.20	1.42	1.38
23	C	505	CLA	CMD-C2D	-2.20	1.46	1.50
23	C	510	CLA	C3B-C4B	2.20	1.49	1.42
28	d	408	DGD	O5D-C6D	-2.20	1.39	1.43
23	B	609	CLA	CHC-C1C	2.19	1.42	1.38
23	B	604	CLA	CMB-C2B	-2.19	1.46	1.50
23	c	508	CLA	CMB-C2B	-2.19	1.46	1.50
23	c	513	CLA	CHC-C1C	2.19	1.42	1.38
23	C	505	CLA	CHC-C1C	2.19	1.42	1.38
23	C	510	CLA	CHC-C1C	2.19	1.42	1.38
28	a	413	DGD	O4D-C4D	-2.18	1.37	1.43
34	f	101	HEM	CMC-C2C	2.18	1.55	1.50
28	A	411	DGD	O6E-C5E	-2.18	1.39	1.44
31	c	520	LMG	O6-C5	-2.18	1.39	1.44
28	D	410	DGD	O6E-C5E	-2.18	1.39	1.44
23	A	403	CLA	CHC-C1C	2.17	1.42	1.38
23	B	612	CLA	CHC-C1C	2.17	1.42	1.38
23	B	614	CLA	CHC-C1C	2.17	1.42	1.38
31	C	520	LMG	O6-C5	-2.17	1.39	1.44
23	C	505	CLA	C3B-C4B	2.17	1.49	1.42
23	B	613	CLA	CHC-C1C	2.17	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	401	SQD	O2-C2	-2.17	1.37	1.43
23	d	402	CLA	C3B-C4B	2.17	1.49	1.42
23	B	605	CLA	MG-NB	-2.17	2.01	2.05
23	B	604	CLA	CMD-C2D	-2.17	1.46	1.50
23	B	608	CLA	CMB-C2B	-2.16	1.46	1.50
23	D	403	CLA	MG-NB	-2.16	2.01	2.05
23	b	615	CLA	CMD-C2D	-2.16	1.46	1.50
31	E	101	LMG	O1-C7	-2.16	1.40	1.43
28	c	519	DGD	O4D-C4D	-2.16	1.37	1.43
23	b	614	CLA	CMD-C2D	-2.16	1.46	1.50
23	c	512	CLA	MG-NB	-2.16	2.01	2.05
23	D	403	CLA	CHC-C1C	2.16	1.42	1.38
23	b	619	CLA	MG-NB	-2.16	2.01	2.05
25	j	101	PL9	C28-C29	2.16	1.38	1.32
23	A	404	CLA	CMB-C2B	-2.15	1.46	1.50
23	B	616	CLA	C3B-C4B	2.15	1.49	1.42
30	A	413	SQD	O47-C45	-2.15	1.41	1.46
23	b	607	CLA	C3B-C4B	2.15	1.49	1.42
23	B	611	CLA	CHC-C1C	2.15	1.42	1.38
23	a	406	CLA	MG-NB	-2.15	2.01	2.05
23	c	512	CLA	CHC-C1C	2.14	1.42	1.38
30	B	625	SQD	O2-C2	-2.14	1.37	1.43
23	B	616	CLA	CMC-C2C	-2.14	1.46	1.50
23	a	406	CLA	CMD-C2D	-2.14	1.46	1.50
31	i	101	LMG	O6-C5	-2.14	1.39	1.44
23	B	616	CLA	CHC-C1C	2.14	1.42	1.38
23	c	504	CLA	CMD-C2D	-2.14	1.46	1.50
23	b	619	CLA	C3B-C4B	2.14	1.49	1.42
23	B	608	CLA	CMD-C2D	-2.14	1.46	1.50
23	A	405	CLA	CHC-C1C	2.13	1.42	1.38
23	b	611	CLA	CMB-C2B	-2.13	1.46	1.50
34	V	201	HEM	CMB-C2B	2.13	1.55	1.50
23	b	613	CLA	MG-NB	-2.13	2.01	2.05
23	C	508	CLA	CHC-C1C	2.13	1.42	1.38
23	b	609	CLA	C3B-C4B	2.13	1.48	1.42
23	C	508	CLA	CMB-C2B	-2.13	1.46	1.50
23	A	403	CLA	CMD-C2D	-2.13	1.46	1.50
23	b	616	CLA	CMB-C2B	-2.13	1.46	1.50
23	B	601	CLA	CMB-C2B	-2.13	1.46	1.50
23	B	610	CLA	CMB-C2B	-2.13	1.46	1.50
28	C	518	DGD	O4D-C4D	-2.13	1.37	1.43
28	A	411	DGD	O4D-C4D	-2.13	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I	101	LMG	C4-C5	-2.12	1.48	1.53
23	C	501	CLA	CHC-C1C	2.12	1.42	1.38
23	B	605	CLA	CMD-C2D	-2.12	1.46	1.50
23	A	407	CLA	CHC-C1C	2.12	1.42	1.38
31	C	520	LMG	O1-C7	-2.12	1.40	1.43
23	C	510	CLA	CMD-C2D	-2.12	1.46	1.50
23	b	605	CLA	CMB-C2B	-2.12	1.46	1.50
31	E	101	LMG	O6-C5	-2.12	1.39	1.44
31	M	101	LMG	O6-C5	-2.12	1.39	1.44
23	c	501	CLA	C3B-C4B	2.11	1.48	1.42
23	C	509	CLA	CHC-C1C	2.11	1.42	1.38
23	b	608	CLA	CMC-C2C	-2.11	1.46	1.50
23	b	610	CLA	CHC-C1C	2.11	1.42	1.38
28	B	621	DGD	O1G-C1G	-2.11	1.40	1.45
23	c	503	CLA	CHC-C1C	2.11	1.42	1.38
28	A	411	DGD	C4D-C5D	-2.11	1.48	1.53
30	b	601	SQD	O2-C2	-2.11	1.37	1.43
23	C	502	CLA	CMD-C2D	-2.11	1.46	1.50
23	B	606	CLA	CMB-C2B	-2.11	1.46	1.50
23	C	504	CLA	MG-NB	-2.11	2.01	2.05
28	c	519	DGD	O1G-C1G	-2.11	1.40	1.45
28	B	626	DGD	O1G-C1G	-2.10	1.40	1.45
23	C	508	CLA	MG-NB	-2.10	2.01	2.05
23	b	604	CLA	C3B-C4B	2.10	1.48	1.42
23	A	405	CLA	CMB-C2B	-2.10	1.46	1.50
23	B	603	CLA	MG-NB	-2.10	2.01	2.05
23	b	609	CLA	CMB-C2B	-2.10	1.46	1.50
23	c	501	CLA	CMB-C2B	-2.10	1.46	1.50
28	b	622	DGD	O1G-C1G	-2.10	1.40	1.45
23	c	508	CLA	MG-NB	-2.10	2.01	2.05
28	d	408	DGD	O6E-C5E	-2.09	1.39	1.44
23	C	510	CLA	MG-NB	-2.09	2.01	2.05
34	F	101	HEM	FE-NC	2.09	2.02	1.95
23	b	607	CLA	CHC-C1C	2.09	1.42	1.38
23	c	510	CLA	CMB-C2B	-2.09	1.46	1.50
23	B	607	CLA	CMD-C2D	-2.09	1.46	1.50
28	C	517	DGD	O1G-C1G	-2.09	1.40	1.45
23	a	406	CLA	CMB-C2B	-2.09	1.46	1.50
23	D	401	CLA	MG-NB	-2.09	2.01	2.05
23	C	513	CLA	CMB-C2B	-2.09	1.46	1.50
23	C	509	CLA	MG-NB	-2.08	2.01	2.05
34	F	101	HEM	CMC-C2C	2.08	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	602	DGD	O4D-C4D	-2.08	1.37	1.43
31	b	624	LMG	O6-C5	-2.08	1.39	1.44
24	D	402	PHO	C3B-C2B	-2.08	1.37	1.40
23	C	505	CLA	MG-NB	-2.08	2.01	2.05
23	c	501	CLA	CHC-C1C	2.08	1.42	1.38
23	C	503	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	607	CLA	CMD-C2D	-2.08	1.46	1.50
23	C	508	CLA	CMD-C2D	-2.08	1.46	1.50
34	v	201	HEM	CMD-C2D	2.08	1.55	1.50
23	a	404	CLA	CMB-C2B	-2.08	1.46	1.50
23	C	501	CLA	C1D-C2D	2.08	1.49	1.45
23	C	502	CLA	CMC-C2C	-2.08	1.46	1.50
23	C	505	CLA	CMB-C2B	-2.07	1.46	1.50
23	d	402	CLA	CHC-C1C	2.07	1.42	1.38
23	B	603	CLA	CMD-C2D	-2.07	1.46	1.50
23	c	502	CLA	CMD-C2D	-2.07	1.46	1.50
28	C	517	DGD	O5D-C1E	-2.07	1.36	1.40
23	B	616	CLA	CMB-C2B	-2.07	1.46	1.50
23	B	615	CLA	CMD-C2D	-2.07	1.46	1.50
23	b	604	CLA	CMC-C2C	-2.07	1.46	1.50
23	b	604	CLA	MG-NB	-2.07	2.01	2.05
23	c	502	CLA	CMB-C2B	-2.07	1.46	1.50
23	B	611	CLA	CMD-C2D	-2.07	1.46	1.50
28	B	621	DGD	O4D-C4D	-2.07	1.37	1.43
23	b	607	CLA	CMB-C2B	-2.06	1.46	1.50
23	c	506	CLA	C3D-C4D	2.06	1.48	1.44
23	b	608	CLA	CMD-C2D	-2.06	1.46	1.50
23	D	401	CLA	CMD-C2D	-2.06	1.46	1.50
23	B	601	CLA	C3D-C4D	2.06	1.48	1.44
23	A	407	CLA	MG-NB	-2.06	2.01	2.05
34	f	101	HEM	CMA-C3A	2.06	1.55	1.50
23	B	602	CLA	CMD-C2D	-2.06	1.46	1.50
23	B	613	CLA	CMB-C2B	-2.06	1.46	1.50
30	a	401	SQD	C4-C5	-2.06	1.48	1.53
23	b	611	CLA	CMD-C2D	-2.06	1.46	1.50
23	b	619	CLA	CMC-C2C	-2.05	1.46	1.50
23	c	503	CLA	MG-NB	-2.05	2.01	2.05
23	C	509	CLA	CMD-C2D	-2.05	1.46	1.50
23	B	615	CLA	MG-NB	-2.05	2.01	2.05
23	b	610	CLA	CMD-C2D	-2.05	1.46	1.50
28	C	516	DGD	O1G-C1G	-2.05	1.40	1.45
27	B	620	BCR	C1-C6	-2.05	1.51	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	CMD-C2D	-2.05	1.46	1.50
23	d	403	CLA	MG-NB	-2.04	2.01	2.05
28	B	626	DGD	C4E-C5E	-2.04	1.48	1.53
23	B	601	CLA	CMC-C2C	-2.04	1.46	1.50
23	d	402	CLA	CMD-C2D	-2.04	1.46	1.50
23	a	405	CLA	CMD-C2D	-2.04	1.46	1.50
33	x	102	LMT	O1'-C1'	2.04	1.43	1.40
23	B	609	CLA	MG-NB	-2.04	2.01	2.05
23	A	407	CLA	CMD-C2D	-2.04	1.46	1.50
23	C	511	CLA	CMB-C2B	-2.04	1.46	1.50
23	b	605	CLA	CMD-C2D	-2.04	1.46	1.50
28	d	408	DGD	O6D-C5D	-2.04	1.39	1.44
23	C	512	CLA	C3D-C4D	2.04	1.48	1.44
23	B	613	CLA	CMD-C2D	-2.04	1.46	1.50
23	b	610	CLA	MG-NB	-2.04	2.01	2.05
28	C	516	DGD	O4D-C4D	-2.04	1.37	1.43
24	a	407	PHO	C3B-C2B	-2.04	1.37	1.40
31	d	406	LMG	O6-C5	-2.04	1.39	1.44
23	C	501	CLA	CMB-C2B	-2.03	1.46	1.50
23	a	405	CLA	CMC-C2C	-2.03	1.46	1.50
33	D	411	LMT	O1'-C1'	2.03	1.43	1.40
23	a	409	CLA	CMD-C2D	-2.03	1.46	1.50
28	d	408	DGD	O1G-C1G	-2.03	1.40	1.45
23	a	409	CLA	CMB-C2B	-2.03	1.46	1.50
30	D	409	SQD	O3-C3	-2.03	1.37	1.43
23	b	615	CLA	MG-NB	-2.03	2.01	2.05
23	a	405	CLA	CMB-C2B	-2.03	1.46	1.50
34	v	201	HEM	CMA-C3A	2.03	1.54	1.50
23	A	403	CLA	CMC-C2C	-2.03	1.46	1.50
34	F	101	HEM	CMA-C3A	2.03	1.54	1.50
23	b	619	CLA	CMB-C2B	-2.03	1.46	1.50
30	D	409	SQD	O6-C1	2.03	1.43	1.40
23	c	507	CLA	CMB-C2B	-2.03	1.46	1.50
23	b	613	CLA	CMB-C2B	-2.03	1.46	1.50
23	B	602	CLA	CMB-C2B	-2.03	1.46	1.50
30	A	413	SQD	O2-C2	-2.02	1.37	1.43
23	b	619	CLA	CHC-C1C	2.02	1.42	1.38
23	B	616	CLA	CMD-C2D	-2.02	1.46	1.50
24	D	402	PHO	C4D-ND	-2.02	1.35	1.38
23	C	502	CLA	CMB-C2B	-2.02	1.46	1.50
23	B	615	CLA	CMC-C2C	-2.02	1.46	1.50
23	c	501	CLA	MG-NB	-2.02	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	517	DGD	C4D-C5D	-2.02	1.48	1.53
23	A	403	CLA	CMB-C2B	-2.02	1.46	1.50
23	C	512	CLA	CMB-C2B	-2.02	1.46	1.50
23	D	403	CLA	CMC-C2C	-2.02	1.46	1.50
23	C	504	CLA	CMB-C2B	-2.02	1.46	1.50
34	V	201	HEM	CMA-C3A	2.02	1.54	1.50
27	A	410	BCR	C1-C6	-2.02	1.51	1.53
31	d	405	LMG	O6-C5	-2.02	1.39	1.44
34	v	201	HEM	CMC-C2C	2.02	1.54	1.50
23	b	606	CLA	CMB-C2B	-2.02	1.46	1.50
23	A	405	CLA	CMC-C2C	-2.02	1.46	1.50
23	c	513	CLA	CMB-C2B	-2.02	1.46	1.50
23	C	509	CLA	CMB-C2B	-2.01	1.46	1.50
23	c	507	CLA	C3B-C4B	2.01	1.48	1.42
28	c	517	DGD	C4E-C5E	-2.01	1.48	1.53
28	D	410	DGD	O6D-C5D	-2.01	1.39	1.44
23	B	610	CLA	MG-NB	-2.01	2.01	2.05
30	B	625	SQD	O4-C4	-2.01	1.38	1.43
23	c	511	CLA	CMC-C2C	-2.01	1.46	1.50
23	C	504	CLA	CMD-C2D	-2.01	1.46	1.50
31	M	102	LMG	O6-C5	-2.01	1.39	1.44
23	B	603	CLA	CMB-C2B	-2.01	1.46	1.50
23	c	506	CLA	CMB-C2B	-2.01	1.46	1.50
23	b	612	CLA	CMD-C2D	-2.01	1.46	1.50
23	C	511	CLA	CMC-C2C	-2.01	1.46	1.50
23	A	404	CLA	CMD-C2D	-2.00	1.46	1.50
23	c	504	CLA	CMB-C2B	-2.00	1.46	1.50
30	d	407	SQD	O6-C1	2.00	1.43	1.40
30	a	415	SQD	O3-C3	-2.00	1.38	1.43
28	D	410	DGD	C4D-C5D	-2.00	1.48	1.53
28	b	622	DGD	O4D-C4D	-2.00	1.38	1.43
34	f	101	HEM	CMD-C2D	2.00	1.54	1.50

All (1292) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J	102	BCR	C32-C1-C6	-14.03	88.24	110.24
27	j	102	BCR	C32-C1-C6	-13.95	88.37	110.24
27	j	102	BCR	C32-C1-C31	-9.26	82.13	108.63
27	J	102	BCR	C32-C1-C31	-9.17	82.39	108.63
27	B	618	BCR	C7-C8-C9	-8.76	113.28	126.23
27	C	514	BCR	C7-C8-C9	8.59	138.94	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	103	BCR	C7-C8-C9	-8.41	113.79	126.23
27	c	514	BCR	C7-C8-C9	8.27	138.47	126.23
23	c	505	CLA	C4A-NA-C1A	8.22	110.43	106.68
23	c	504	CLA	C4A-NA-C1A	7.81	110.24	106.68
23	C	511	CLA	C4A-NA-C1A	7.71	110.20	106.68
23	B	607	CLA	C4A-NA-C1A	7.59	110.14	106.68
23	d	402	CLA	C4A-NA-C1A	7.56	110.13	106.68
23	c	502	CLA	C4A-NA-C1A	7.53	110.12	106.68
24	A	406	PHO	C4D-CHA-CBD	-7.37	104.92	108.45
23	C	512	CLA	C4A-NA-C1A	7.30	110.01	106.68
23	c	513	CLA	C4A-NA-C1A	7.26	109.99	106.68
23	A	403	CLA	C4A-NA-C1A	7.25	109.99	106.68
23	C	505	CLA	C4A-NA-C1A	7.15	109.94	106.68
23	c	509	CLA	C4A-NA-C1A	7.15	109.94	106.68
23	b	615	CLA	C4A-NA-C1A	7.13	109.93	106.68
23	C	502	CLA	C4A-NA-C1A	7.01	109.88	106.68
23	C	513	CLA	C4A-NA-C1A	7.00	109.87	106.68
23	b	616	CLA	C4A-NA-C1A	7.00	109.87	106.68
30	D	409	SQD	O6-C1-C2	6.99	118.89	108.27
23	c	511	CLA	C4A-NA-C1A	6.97	109.86	106.68
23	c	506	CLA	C4A-NA-C1A	6.92	109.84	106.68
23	b	605	CLA	C4A-NA-C1A	6.91	109.83	106.68
23	c	501	CLA	C4A-NA-C1A	6.90	109.83	106.68
27	j	102	BCR	C31-C1-C6	6.84	120.96	110.24
23	b	607	CLA	C4A-NA-C1A	6.82	109.79	106.68
23	B	610	CLA	C4A-NA-C1A	6.78	109.77	106.68
23	B	615	CLA	C4A-NA-C1A	6.77	109.77	106.68
23	B	602	CLA	C4A-NA-C1A	6.77	109.77	106.68
23	B	611	CLA	C4A-NA-C1A	6.76	109.77	106.68
23	C	503	CLA	C4A-NA-C1A	6.75	109.76	106.68
23	b	618	CLA	C4A-NA-C1A	6.75	109.76	106.68
23	b	608	CLA	C4A-NA-C1A	6.74	109.75	106.68
23	C	504	CLA	C4A-NA-C1A	6.72	109.74	106.68
27	J	102	BCR	C31-C1-C6	6.70	120.75	110.24
24	D	402	PHO	C4D-CHA-CBD	-6.69	105.25	108.45
23	b	617	CLA	C4A-NA-C1A	6.66	109.72	106.68
23	a	409	CLA	C4A-NA-C1A	6.65	109.71	106.68
30	d	407	SQD	O6-C1-C2	6.63	118.35	108.27
23	C	501	CLA	C4A-NA-C1A	6.61	109.69	106.68
23	a	404	CLA	C4A-NA-C1A	6.59	109.68	106.68
23	B	605	CLA	C4A-NA-C1A	6.55	109.67	106.68
23	C	507	CLA	C4A-NA-C1A	6.53	109.66	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	C4A-NA-C1A	6.49	109.64	106.68
23	b	610	CLA	C4A-NA-C1A	6.49	109.64	106.68
23	c	512	CLA	C4A-NA-C1A	6.48	109.64	106.68
23	C	508	CLA	C4A-NA-C1A	6.47	109.63	106.68
23	B	609	CLA	C4A-NA-C1A	6.47	109.63	106.68
23	b	611	CLA	C4A-NA-C1A	6.47	109.63	106.68
27	D	405	BCR	C7-C8-C9	-6.45	116.70	126.23
23	C	506	CLA	C4A-NA-C1A	6.44	109.62	106.68
23	C	509	CLA	C4A-NA-C1A	6.43	109.61	106.68
23	d	403	CLA	C4A-NA-C1A	6.43	109.61	106.68
23	D	401	CLA	C4A-NA-C1A	6.38	109.59	106.68
23	B	603	CLA	C4A-NA-C1A	6.35	109.58	106.68
27	f	102	BCR	C7-C8-C9	-6.30	116.92	126.23
23	b	604	CLA	C4A-NA-C1A	6.28	109.55	106.68
27	c	514	BCR	C15-C14-C13	-6.27	118.48	127.28
23	A	407	CLA	C4A-NA-C1A	6.27	109.54	106.68
23	b	609	CLA	C4A-NA-C1A	6.26	109.54	106.68
23	B	604	CLA	C4A-NA-C1A	6.25	109.53	106.68
23	c	508	CLA	C4A-NA-C1A	6.22	109.52	106.68
23	B	606	CLA	C4A-NA-C1A	6.21	109.51	106.68
23	c	503	CLA	C4A-NA-C1A	6.19	109.50	106.68
23	B	613	CLA	C4A-NA-C1A	6.17	109.49	106.68
23	c	507	CLA	C4A-NA-C1A	6.16	109.49	106.68
23	B	614	CLA	C4A-NA-C1A	6.14	109.48	106.68
23	A	404	CLA	C4A-NA-C1A	6.09	109.46	106.68
23	a	406	CLA	C4A-NA-C1A	6.07	109.45	106.68
23	b	619	CLA	C4A-NA-C1A	6.04	109.44	106.68
23	a	405	CLA	C4A-NA-C1A	6.02	109.42	106.68
23	C	510	CLA	C4A-NA-C1A	6.01	109.42	106.68
23	b	606	CLA	C4A-NA-C1A	6.01	109.42	106.68
28	A	411	DGD	C3G-O3G-C1D	6.00	126.66	113.80
23	D	403	CLA	C4A-NA-C1A	5.97	109.40	106.68
23	B	608	CLA	C4A-NA-C1A	5.91	109.37	106.68
23	b	614	CLA	C4A-NA-C1A	5.88	109.36	106.68
23	b	613	CLA	C4A-NA-C1A	5.86	109.35	106.68
27	J	102	BCR	C15-C14-C13	-5.84	119.08	127.28
28	a	413	DGD	C3G-O3G-C1D	5.81	126.26	113.80
23	B	612	CLA	C4A-NA-C1A	5.81	109.33	106.68
27	B	618	BCR	C11-C10-C9	-5.81	119.14	127.28
34	v	201	HEM	C4D-ND-C1D	5.80	112.07	105.21
23	c	510	CLA	C4A-NA-C1A	5.78	109.31	106.68
28	c	519	DGD	C3G-O3G-C1D	5.73	126.08	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	612	CLA	C4A-NA-C1A	5.72	109.29	106.68
23	B	616	CLA	C4A-NA-C1A	5.60	109.23	106.68
27	j	102	BCR	C15-C14-C13	-5.59	119.44	127.28
27	J	102	BCR	C32-C1-C2	-5.57	87.56	108.95
27	j	102	BCR	C32-C1-C2	-5.48	87.91	108.95
27	B	620	BCR	C3-C4-C5	-5.44	104.36	114.06
23	A	405	CLA	C4A-NA-C1A	5.41	109.15	106.68
27	j	102	BCR	C20-C21-C22	-5.38	119.73	127.28
30	D	409	SQD	C44-O6-C1	5.38	125.33	113.80
27	f	102	BCR	C15-C14-C13	-5.36	119.77	127.28
28	C	518	DGD	C3G-O3G-C1D	5.34	125.25	113.80
27	T	103	BCR	C11-C10-C9	-5.32	119.81	127.28
27	c	515	BCR	C15-C14-C13	-5.28	119.88	127.28
24	a	407	PHO	C4D-CHA-CBD	-5.25	105.94	108.45
27	A	410	BCR	C33-C5-C6	-5.20	118.81	124.48
27	D	405	BCR	C11-C10-C9	-5.20	119.99	127.28
27	D	405	BCR	C28-C27-C26	-5.15	104.87	114.06
28	d	408	DGD	O3G-C1D-C2D	5.14	116.08	108.27
27	J	102	BCR	C28-C27-C26	-5.13	104.91	114.06
27	C	514	BCR	C15-C14-C13	-5.11	120.11	127.28
30	d	407	SQD	C44-O6-C1	5.10	124.72	113.80
27	b	621	BCR	C24-C23-C22	-5.09	118.71	126.23
27	j	102	BCR	C28-C27-C26	-5.06	105.03	114.06
27	j	102	BCR	C24-C23-C22	-5.04	118.78	126.23
27	c	514	BCR	C33-C5-C6	-5.03	118.99	124.48
27	B	618	BCR	C3-C4-C5	-5.02	105.11	114.06
34	F	101	HEM	C4D-ND-C1D	5.01	111.14	105.21
27	A	410	BCR	C16-C17-C18	-5.00	120.27	127.28
27	J	102	BCR	C11-C10-C9	-4.98	120.29	127.28
27	J	102	BCR	C20-C21-C22	-4.91	120.40	127.28
24	a	408	PHO	C4D-CHA-CBD	-4.90	106.11	108.45
27	C	514	BCR	C8-C7-C6	4.88	140.04	127.00
27	k	102	BCR	C15-C14-C13	-4.86	120.47	127.28
27	b	621	BCR	C3-C4-C5	-4.84	105.43	114.06
25	j	101	PL9	C7-C3-C4	4.83	120.89	116.91
25	J	101	PL9	C7-C3-C4	4.83	120.89	116.91
27	f	102	BCR	C28-C27-C26	-4.79	105.52	114.06
34	f	101	HEM	C4D-ND-C1D	4.77	110.86	105.21
27	Z	101	BCR	C15-C14-C13	-4.77	120.59	127.28
27	C	514	BCR	C33-C5-C6	-4.73	119.32	124.48
27	B	620	BCR	C24-C23-C22	-4.72	119.25	126.23
27	T	102	BCR	C15-C14-C13	-4.67	120.73	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J	102	BCR	C24-C23-C22	-4.67	119.33	126.23
27	c	514	BCR	C8-C7-C6	4.66	139.45	127.00
27	B	617	BCR	C15-C14-C13	-4.66	120.75	127.28
27	A	410	BCR	C15-C14-C13	-4.66	120.75	127.28
27	b	620	BCR	C7-C8-C9	-4.62	119.40	126.23
27	T	103	BCR	C3-C4-C5	-4.62	105.82	114.06
28	D	410	DGD	O3G-C1D-C2D	4.61	115.28	108.27
27	j	102	BCR	C11-C10-C9	-4.60	120.83	127.28
27	T	102	BCR	C16-C17-C18	-4.59	120.84	127.28
34	V	201	HEM	C4D-ND-C1D	4.55	110.59	105.21
27	f	102	BCR	C16-C17-C18	-4.54	120.91	127.28
28	C	518	DGD	C1D-O6D-C5D	-4.51	104.91	113.72
28	c	519	DGD	C1D-O6D-C5D	-4.51	104.91	113.72
27	B	618	BCR	C28-C27-C26	-4.49	106.05	114.06
27	B	619	BCR	C28-C27-C26	-4.49	106.05	114.06
24	A	406	PHO	C2B-C1B-NB	-4.47	106.20	109.43
27	B	620	BCR	C7-C8-C9	-4.45	119.65	126.23
27	J	102	BCR	C16-C17-C18	-4.45	121.04	127.28
27	j	102	BCR	C7-C8-C9	-4.45	119.66	126.23
28	A	411	DGD	O2G-C1B-C2B	4.44	121.08	111.48
27	C	515	BCR	C7-C8-C9	-4.44	119.67	126.23
31	a	416	LMG	O7-C10-C11	4.41	121.02	111.48
27	C	515	BCR	C15-C14-C13	-4.40	121.11	127.28
27	a	412	BCR	C33-C5-C6	-4.39	119.69	124.48
27	k	102	BCR	C16-C17-C18	-4.37	121.14	127.28
27	b	621	BCR	C11-C10-C9	-4.36	121.16	127.28
27	f	102	BCR	C33-C5-C6	-4.36	119.73	124.48
27	b	621	BCR	C7-C8-C9	-4.35	119.80	126.23
27	B	617	BCR	C16-C17-C18	-4.35	121.18	127.28
25	d	404	PL9	C7-C3-C4	4.32	120.47	116.91
30	b	601	SQD	O7-S-C6	4.31	113.19	106.76
27	b	620	BCR	C15-C14-C13	-4.28	121.28	127.28
27	D	405	BCR	C24-C23-C22	-4.28	119.91	126.23
27	H	101	BCR	C33-C5-C6	-4.26	119.83	124.48
27	T	103	BCR	C28-C27-C26	-4.26	106.46	114.06
27	a	412	BCR	C16-C17-C18	-4.25	121.31	127.28
27	T	102	BCR	C24-C23-C22	-4.25	119.94	126.23
27	k	102	BCR	C38-C26-C25	-4.25	119.85	124.48
27	C	515	BCR	C28-C27-C26	-4.23	106.51	114.06
27	c	514	BCR	C16-C17-C18	-4.23	121.34	127.28
27	c	516	BCR	C7-C8-C9	-4.23	119.98	126.23
24	D	402	PHO	C2B-C1B-NB	-4.22	106.38	109.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	407	SQD	O47-C7-C8	4.22	120.61	111.48
27	B	617	BCR	C7-C8-C9	-4.22	119.99	126.23
27	c	514	BCR	C11-C10-C9	-4.21	121.38	127.28
27	a	412	BCR	C15-C14-C13	-4.20	121.39	127.28
27	C	514	BCR	C3-C4-C5	-4.20	106.57	114.06
27	c	516	BCR	C15-C14-C13	-4.19	121.40	127.28
27	c	516	BCR	C16-C17-C18	-4.18	121.42	127.28
31	A	414	LMG	O7-C10-C11	4.17	120.51	111.48
27	Z	101	BCR	C24-C23-C22	-4.16	120.07	126.23
27	B	619	BCR	C15-C14-C13	-4.15	121.46	127.28
25	a	410	PL9	C7-C3-C4	4.14	120.32	116.91
27	Z	101	BCR	C16-C17-C18	-4.13	121.48	127.28
28	a	413	DGD	O2G-C1B-C2B	4.13	120.41	111.48
27	b	621	BCR	C16-C17-C18	-4.12	121.50	127.28
27	K	102	BCR	C3-C4-C5	-4.12	106.71	114.06
27	B	617	BCR	C24-C23-C22	-4.12	120.14	126.23
27	c	516	BCR	C28-C27-C26	-4.12	106.71	114.06
27	B	620	BCR	C16-C17-C18	-4.11	121.51	127.28
27	b	620	BCR	C28-C27-C26	-4.11	106.73	114.06
27	b	621	BCR	C15-C14-C13	-4.11	121.52	127.28
27	K	102	BCR	C7-C8-C9	-4.11	120.16	126.23
27	b	620	BCR	C24-C23-C22	-4.10	120.17	126.23
27	D	405	BCR	C15-C14-C13	-4.09	121.54	127.28
31	b	624	LMG	O7-C10-C11	4.08	120.31	111.48
27	B	617	BCR	C33-C5-C6	-4.07	120.04	124.48
27	x	101	BCR	C24-C23-C22	-4.07	120.22	126.23
23	a	405	CLA	C1-C2-C3	-4.06	119.55	126.20
27	a	412	BCR	C38-C26-C25	-4.06	120.06	124.48
27	x	101	BCR	C33-C5-C6	-4.06	120.06	124.48
27	B	620	BCR	C38-C26-C25	-4.04	120.08	124.48
27	T	103	BCR	C38-C26-C25	-4.03	120.08	124.48
27	K	102	BCR	C38-C26-C25	-4.03	120.09	124.48
27	A	410	BCR	C3-C4-C5	-4.01	106.91	114.06
31	M	101	LMG	O7-C10-C11	4.01	120.15	111.48
31	d	405	LMG	O7-C10-C11	4.00	120.14	111.48
30	D	409	SQD	O47-C7-C8	4.00	120.14	111.48
30	A	413	SQD	O9-S-O7	-4.00	100.83	113.82
31	D	408	LMG	O1-C1-C2	3.99	114.34	108.27
30	B	625	SQD	O7-S-C6	3.98	112.70	106.76
31	B	622	LMG	O7-C10-C11	3.98	120.10	111.48
31	M	102	LMG	O7-C10-C11	3.98	120.08	111.48
27	b	621	BCR	C38-C26-C25	-3.97	120.15	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	401	SQD	O47-C7-C8	3.97	120.06	111.48
27	b	621	BCR	C20-C21-C22	-3.96	121.72	127.28
30	f	103	SQD	O9-S-O7	-3.96	100.94	113.82
30	F	102	SQD	O9-S-O7	-3.95	100.97	113.82
30	F	102	SQD	O47-C7-C8	3.95	120.03	111.48
27	J	102	BCR	C7-C8-C9	-3.95	120.40	126.23
30	d	407	SQD	O9-S-O7	-3.93	101.03	113.82
30	d	407	SQD	O9-S-C6	3.92	112.61	106.76
27	b	621	BCR	C4-C5-C6	-3.92	117.41	122.70
27	T	102	BCR	C33-C5-C6	-3.92	120.21	124.48
27	B	620	BCR	C4-C5-C6	-3.91	117.42	122.70
31	C	520	LMG	O7-C10-C11	3.91	119.94	111.48
30	A	417	SQD	O47-C7-C8	3.90	119.93	111.48
30	D	409	SQD	O9-S-O7	-3.90	101.13	113.82
28	d	408	DGD	O2D-C2D-C1D	3.90	119.37	110.08
31	c	520	LMG	O7-C10-C11	3.89	119.90	111.48
27	D	405	BCR	C33-C5-C6	-3.87	120.26	124.48
31	a	416	LMG	C7-O1-C1	3.87	122.08	113.80
31	b	623	LMG	O7-C10-C11	3.86	119.83	111.48
27	D	405	BCR	C16-C17-C18	-3.86	121.87	127.28
27	c	516	BCR	C11-C10-C9	-3.85	121.87	127.28
30	F	102	SQD	C1-O5-C5	3.85	121.24	113.72
30	a	415	SQD	O9-S-O7	-3.85	101.31	113.82
29	a	417	LHG	O7-C7-C8	3.83	119.77	111.48
30	f	103	SQD	O47-C7-C8	3.83	119.77	111.48
28	D	410	DGD	O2D-C2D-C1D	3.82	119.18	110.08
27	k	102	BCR	C20-C21-C22	-3.82	121.92	127.28
24	a	407	PHO	C2B-C1B-NB	-3.82	106.67	109.43
27	k	102	BCR	C3-C4-C5	-3.81	107.26	114.06
29	A	415	LHG	O7-C7-C8	3.81	119.72	111.48
27	B	620	BCR	C15-C14-C13	-3.81	121.94	127.28
27	B	618	BCR	C38-C26-C25	-3.80	120.34	124.48
27	C	515	BCR	C38-C26-C25	-3.76	120.38	124.48
30	D	409	SQD	O9-S-C6	3.76	112.37	106.76
28	A	411	DGD	C1D-O6D-C5D	-3.76	106.38	113.72
27	B	620	BCR	C11-C10-C9	-3.75	122.01	127.28
27	K	102	BCR	C16-C17-C18	-3.75	122.02	127.28
30	B	625	SQD	O9-S-O7	-3.75	101.64	113.82
28	c	518	DGD	O2G-C1B-C2B	3.74	119.58	111.48
28	A	411	DGD	O6D-C5D-C6D	3.74	114.11	106.69
30	b	601	SQD	O9-S-O7	-3.74	101.66	113.82
27	A	410	BCR	C38-C26-C25	-3.74	120.40	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J	102	BCR	C2-C1-C6	3.74	115.87	110.44
30	d	407	SQD	C1-O5-C5	3.74	121.02	113.72
28	b	622	DGD	C1D-O6D-C5D	-3.74	106.42	113.72
28	d	408	DGD	O5D-C1E-C2E	3.73	113.93	108.27
31	C	519	LMG	O7-C10-C11	3.72	119.53	111.48
28	B	621	DGD	C1D-O6D-C5D	-3.72	106.46	113.72
30	f	103	SQD	O7-S-C6	3.71	112.29	106.76
28	b	602	DGD	O5D-C1E-C2E	3.70	113.89	108.27
27	B	620	BCR	C20-C21-C22	-3.69	122.10	127.28
27	c	515	BCR	C20-C21-C22	-3.68	122.12	127.28
30	a	401	SQD	O5-C1-C2	3.67	117.92	110.37
27	B	617	BCR	C38-C26-C25	-3.67	120.48	124.48
23	b	611	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
27	j	102	BCR	C16-C17-C18	-3.66	122.15	127.28
27	Z	101	BCR	C3-C4-C5	-3.66	107.53	114.06
25	d	404	PL9	C7-C3-C2	-3.66	119.08	123.39
27	B	619	BCR	C20-C21-C22	-3.65	122.16	127.28
27	C	515	BCR	C20-C21-C22	-3.65	122.16	127.28
30	a	401	SQD	C1-O5-C5	3.64	120.84	113.72
31	A	418	LMG	O7-C10-C11	3.64	119.35	111.48
31	D	406	LMG	O7-C10-C11	3.64	119.35	111.48
27	j	102	BCR	C29-C30-C25	3.64	115.72	110.44
27	c	515	BCR	C3-C4-C5	-3.63	107.59	114.06
31	D	407	LMG	O7-C10-C11	3.61	119.29	111.48
30	f	103	SQD	C1-O5-C5	3.61	120.77	113.72
27	f	102	BCR	C24-C23-C22	-3.60	120.91	126.23
27	a	412	BCR	C24-C23-C22	-3.60	120.91	126.23
30	a	401	SQD	O9-S-O7	-3.60	102.13	113.82
25	D	404	PL9	C22-C23-C24	-3.60	119.39	127.62
27	T	102	BCR	C38-C26-C25	-3.60	120.56	124.48
30	a	415	SQD	O47-C7-C8	3.59	119.25	111.48
27	a	412	BCR	C3-C4-C5	-3.59	107.65	114.06
28	C	518	DGD	O6D-C5D-C6D	3.59	113.81	106.69
27	c	514	BCR	C7-C6-C5	-3.59	113.30	121.56
31	a	402	LMG	O7-C10-C11	3.59	119.24	111.48
30	A	413	SQD	O47-C7-C8	3.58	119.23	111.48
28	C	518	DGD	O5D-C1E-C2E	3.57	113.70	108.27
25	d	404	PL9	C25-C24-C26	3.57	121.43	115.23
25	A	408	PL9	C25-C24-C26	3.57	121.43	115.23
28	d	408	DGD	C3G-O3G-C1D	3.57	121.44	113.80
27	T	102	BCR	C20-C21-C22	-3.56	122.28	127.28
28	c	519	DGD	C2G-O2G-C1B	3.56	126.32	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	517	DGD	O2G-C1B-C2B	3.56	119.17	111.48
29	A	412	LHG	O7-C7-C8	3.55	119.17	111.48
31	k	103	LMG	O7-C10-C11	3.55	119.17	111.48
27	c	515	BCR	C33-C5-C6	-3.55	120.61	124.48
31	d	406	LMG	O1-C1-C2	3.54	113.64	108.27
23	B	606	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
34	F	101	HEM	C3B-C2B-C1B	3.53	109.06	106.41
27	C	515	BCR	C11-C10-C9	-3.53	122.32	127.28
27	c	514	BCR	C3-C4-C5	-3.53	107.76	114.06
25	a	410	PL9	C35-C34-C36	3.53	121.36	115.23
30	A	413	SQD	C1-O5-C5	3.53	120.61	113.72
30	a	401	SQD	O5-C5-C4	3.52	116.04	109.70
30	A	417	SQD	C1-O5-C5	3.51	120.58	113.72
30	A	417	SQD	O9-S-O7	-3.51	102.41	113.82
23	c	504	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
27	B	617	BCR	C20-C21-C22	-3.51	122.36	127.28
27	K	102	BCR	C15-C14-C13	-3.50	122.37	127.28
27	c	514	BCR	C1-C6-C7	3.50	125.14	115.65
27	J	102	BCR	C29-C30-C25	3.50	115.52	110.44
25	A	408	PL9	C7-C3-C4	3.49	119.79	116.91
27	T	102	BCR	C11-C10-C9	-3.49	122.38	127.28
25	D	404	PL9	C7-C3-C4	3.49	119.78	116.91
27	c	516	BCR	C33-C5-C6	-3.49	120.68	124.48
27	C	515	BCR	C16-C17-C18	-3.49	122.39	127.28
27	b	620	BCR	C11-C10-C9	-3.48	122.39	127.28
27	b	620	BCR	C20-C21-C22	-3.48	122.40	127.28
27	j	102	BCR	C2-C1-C6	3.48	115.49	110.44
27	B	617	BCR	C11-C10-C9	-3.47	122.41	127.28
27	k	102	BCR	C7-C8-C9	-3.47	121.10	126.23
25	D	404	PL9	C7-C8-C9	-3.47	120.86	126.83
27	H	101	BCR	C16-C17-C18	-3.47	122.42	127.28
27	B	619	BCR	C16-C17-C18	-3.46	122.42	127.28
24	A	406	PHO	O2D-CGD-O1D	-3.46	117.11	123.85
31	d	405	LMG	C7-O1-C1	3.46	121.22	113.80
27	x	101	BCR	C10-C11-C12	-3.45	113.20	123.20
25	j	101	PL9	C7-C3-C2	-3.45	119.32	123.39
30	A	413	SQD	O7-S-C6	3.45	111.91	106.76
28	B	626	DGD	O2G-C1B-C2B	3.45	118.94	111.48
27	C	514	BCR	C11-C10-C9	-3.44	122.45	127.28
29	a	414	LHG	O7-C7-C8	3.44	118.92	111.48
27	Z	101	BCR	C33-C5-C6	-3.44	120.73	124.48
27	c	515	BCR	C16-C17-C18	-3.43	122.46	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	619	BCR	C24-C23-C22	-3.43	121.16	126.23
27	j	102	BCR	C31-C1-C2	3.43	122.13	108.95
24	a	408	PHO	C2B-C1B-NB	-3.43	106.95	109.43
24	a	408	PHO	O1D-CGD-CBD	3.41	129.90	124.72
23	b	610	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
27	T	103	BCR	C2-C1-C6	3.40	115.38	110.44
28	b	602	DGD	C3D-C4D-C5D	3.40	116.39	110.23
23	c	512	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
28	a	413	DGD	O6D-C5D-C6D	3.39	113.42	106.69
27	B	618	BCR	C4-C5-C6	-3.38	118.13	122.70
28	D	410	DGD	C3G-O3G-C1D	3.38	121.05	113.80
23	b	609	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
27	J	102	BCR	C31-C1-C2	3.38	121.93	108.95
25	J	101	PL9	C7-C3-C2	-3.38	119.41	123.39
31	k	103	LMG	O8-C28-C29	3.38	122.13	111.83
28	C	516	DGD	O2G-C1B-C2B	3.37	118.78	111.48
27	f	102	BCR	C11-C10-C9	-3.37	122.55	127.28
27	A	410	BCR	C24-C23-C22	-3.36	121.27	126.23
23	b	613	CLA	C3B-C4B-NB	-3.36	107.53	110.53
27	j	102	BCR	C27-C26-C25	-3.35	118.17	122.70
31	i	101	LMG	O7-C10-C11	3.35	118.73	111.48
27	C	515	BCR	C33-C5-C6	-3.35	120.83	124.48
27	x	101	BCR	C20-C21-C22	-3.35	122.58	127.28
30	D	409	SQD	C1-O5-C5	3.35	120.26	113.72
31	M	101	LMG	C1-O6-C5	-3.35	107.18	113.72
30	F	102	SQD	O7-S-C6	3.35	111.75	106.76
30	d	407	SQD	O5-C5-C4	3.34	115.73	109.70
28	C	518	DGD	C2G-O2G-C1B	3.34	125.79	117.80
31	A	414	LMG	C1-O6-C5	-3.34	107.20	113.72
27	a	412	BCR	C11-C10-C9	-3.33	122.61	127.28
28	c	518	DGD	O3G-C1D-C2D	3.33	113.33	108.27
27	H	101	BCR	C24-C23-C22	-3.32	121.32	126.23
27	T	102	BCR	C7-C8-C9	-3.32	121.33	126.23
27	B	619	BCR	C3-C4-C5	-3.32	108.14	114.06
23	b	617	CLA	C3B-C4B-NB	-3.32	107.57	110.53
31	D	406	LMG	O8-C28-C29	3.31	121.94	111.83
30	F	102	SQD	O9-S-C6	3.31	111.70	106.76
31	M	101	LMG	C6-C5-C4	-3.31	104.89	113.02
25	a	410	PL9	C7-C3-C2	-3.31	119.49	123.39
23	B	614	CLA	C3B-C4B-NB	-3.31	107.58	110.53
27	x	101	BCR	C15-C14-C13	-3.31	122.64	127.28
25	a	410	PL9	C25-C24-C26	3.30	120.95	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	415	SQD	C1-O5-C5	3.30	120.16	113.72
30	B	625	SQD	C44-O6-C1	3.29	120.86	113.80
25	D	404	PL9	C7-C3-C2	-3.29	119.51	123.39
30	b	601	SQD	C44-O6-C1	3.29	120.85	113.80
25	A	408	PL9	C35-C34-C36	3.29	120.94	115.23
25	d	404	PL9	C37-C38-C39	-3.29	120.09	127.62
27	b	620	BCR	C3-C4-C5	-3.29	108.19	114.06
28	B	626	DGD	C3G-O3G-C1D	3.28	120.84	113.80
23	A	405	CLA	C3B-C4B-NB	-3.28	107.60	110.53
30	A	417	SQD	C44-O6-C1	3.28	120.83	113.80
27	T	103	BCR	C4-C5-C6	-3.28	118.27	122.70
27	C	514	BCR	C1-C6-C7	3.28	124.53	115.65
28	a	413	DGD	C1D-O6D-C5D	-3.27	107.33	113.72
23	b	614	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
27	C	514	BCR	C20-C21-C22	-3.27	122.69	127.28
27	C	515	BCR	C3-C4-C5	-3.27	108.23	114.06
23	B	607	CLA	O2D-CGD-O1D	-3.26	117.49	123.85
30	A	417	SQD	O5-C5-C4	3.26	115.58	109.70
31	C	519	LMG	O8-C28-C29	3.26	121.78	111.83
27	c	516	BCR	C38-C26-C25	-3.26	120.93	124.48
31	C	519	LMG	C1-O6-C5	-3.25	107.36	113.72
23	C	504	CLA	C3B-C4B-NB	-3.25	107.63	110.53
27	C	514	BCR	C28-C27-C26	-3.25	108.27	114.06
30	A	413	SQD	O9-S-C6	3.25	111.60	106.76
27	Z	101	BCR	C20-C21-C22	-3.24	122.73	127.28
27	b	620	BCR	C16-C17-C18	-3.24	122.73	127.28
28	c	517	DGD	O5D-C1E-C2E	3.24	113.19	108.27
27	b	620	BCR	C33-C5-C6	-3.24	120.95	124.48
34	f	101	HEM	C3B-C2B-C1B	3.23	108.84	106.41
23	C	506	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
31	C	520	LMG	O8-C28-C29	3.23	121.68	111.83
28	b	602	DGD	C3G-O3G-C1D	3.23	120.71	113.80
27	b	621	BCR	C2-C1-C6	3.23	115.12	110.44
31	D	408	LMG	C1-O6-C5	-3.22	107.42	113.72
27	B	619	BCR	C11-C10-C9	-3.22	122.76	127.28
31	C	520	LMG	O1-C1-C2	3.22	113.16	108.27
23	b	604	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
23	b	608	CLA	C3B-C4B-NB	-3.21	107.66	110.53
25	J	101	PL9	C25-C24-C26	3.21	120.80	115.23
23	b	609	CLA	C3B-C4B-NB	-3.21	107.67	110.53
23	C	510	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
23	c	503	CLA	O2D-CGD-O1D	-3.20	117.62	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	C3B-C4B-NB	-3.20	107.67	110.53
25	j	101	PL9	C25-C24-C26	3.20	120.78	115.23
27	C	514	BCR	C7-C6-C5	-3.19	114.21	121.56
31	M	102	LMG	C1-O6-C5	-3.19	107.50	113.72
31	M	102	LMG	C3-C4-C5	3.19	116.01	110.23
30	F	102	SQD	O5-C5-C4	3.18	115.42	109.70
23	a	406	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
27	a	412	BCR	C20-C21-C22	-3.16	122.84	127.28
31	c	520	LMG	C1-O6-C5	-3.16	107.55	113.72
31	c	520	LMG	O8-C28-C29	3.16	121.46	111.83
25	D	404	PL9	C35-C34-C36	3.15	120.69	115.23
23	B	616	CLA	C3B-C4B-NB	-3.14	107.72	110.53
23	B	612	CLA	C3B-C4B-NB	-3.14	107.73	110.53
24	a	407	PHO	O1D-CGD-CBD	3.14	129.48	124.72
27	J	102	BCR	C27-C26-C25	-3.13	118.47	122.70
27	f	102	BCR	C29-C30-C25	3.13	114.98	110.44
25	d	404	PL9	C7-C8-C9	-3.13	121.44	126.83
23	B	609	CLA	C1-C2-C3	-3.12	121.08	126.20
27	K	102	BCR	C24-C23-C22	-3.12	121.62	126.23
28	a	413	DGD	C4D-C3D-C2D	-3.12	105.36	110.83
27	c	516	BCR	C3-C4-C5	-3.12	108.50	114.06
31	b	623	LMG	O1-C1-C2	3.11	113.00	108.27
31	A	418	LMG	C7-O1-C1	3.11	120.47	113.80
31	B	622	LMG	O8-C28-C29	3.11	121.31	111.83
23	B	614	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
30	a	415	SQD	O5-C5-C4	3.11	115.30	109.70
23	c	506	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
30	A	417	SQD	O5-C1-C2	3.10	116.74	110.37
23	b	616	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
23	c	508	CLA	C3B-C4B-NB	-3.10	107.77	110.53
23	B	604	CLA	C3B-C4B-NB	-3.09	107.77	110.53
28	A	411	DGD	C3G-C2G-C1G	-3.09	104.58	111.78
24	A	406	PHO	O1D-CGD-CBD	3.09	129.40	124.72
31	A	414	LMG	O8-C28-C29	3.09	121.25	111.83
28	c	519	DGD	O1G-C1A-C2A	3.08	121.24	111.83
30	D	409	SQD	O5-C5-C4	3.08	115.26	109.70
28	c	517	DGD	O2G-C1B-C2B	3.08	118.15	111.48
23	D	403	CLA	C3B-C4B-NB	-3.08	107.78	110.53
27	Z	101	BCR	C11-C10-C9	-3.08	122.96	127.28
25	d	404	PL9	C35-C34-C36	3.08	120.57	115.23
23	C	503	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
27	B	619	BCR	C7-C8-C9	-3.07	121.69	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	501	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
31	A	418	LMG	C6-C5-C4	-3.07	105.48	113.02
25	a	410	PL9	C22-C23-C24	-3.07	120.60	127.62
31	d	406	LMG	O7-C10-C11	3.07	118.12	111.48
23	C	506	CLA	CHB-C4A-NA	3.07	128.83	124.40
31	D	406	LMG	C7-O1-C1	3.07	120.37	113.80
27	C	514	BCR	C24-C23-C22	-3.06	121.70	126.23
30	a	415	SQD	O7-S-C6	3.06	111.32	106.76
23	b	619	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
27	C	514	BCR	C16-C17-C18	-3.05	122.99	127.28
23	d	403	CLA	C3B-C4B-NB	-3.05	107.81	110.53
31	b	624	LMG	O8-C28-C29	3.05	121.13	111.83
23	C	511	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
27	D	405	BCR	C16-C15-C14	-3.04	117.29	123.52
31	C	520	LMG	C7-O1-C1	3.04	120.32	113.80
23	b	611	CLA	C3B-C4B-NB	-3.04	107.82	110.53
23	A	404	CLA	C3B-C4B-NB	-3.04	107.82	110.53
31	M	101	LMG	C3-C4-C5	3.04	115.74	110.23
27	b	620	BCR	C29-C30-C25	3.03	114.84	110.44
31	M	102	LMG	C6-C5-C4	-3.03	105.58	113.02
27	b	621	BCR	C33-C5-C4	3.03	120.05	113.60
23	c	505	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
31	E	101	LMG	O8-C28-C29	3.02	121.05	111.83
31	D	407	LMG	O8-C28-C29	3.02	121.05	111.83
31	a	416	LMG	O8-C28-C29	3.02	121.04	111.83
27	B	618	BCR	C2-C1-C6	3.02	114.82	110.44
23	B	613	CLA	C3B-C4B-NB	-3.01	107.84	110.53
31	b	624	LMG	O1-C1-C2	3.01	112.85	108.27
23	B	607	CLA	CHB-C4A-NA	3.01	128.75	124.40
23	b	614	CLA	C3B-C4B-NB	-3.01	107.84	110.53
24	a	408	PHO	O2D-CGD-O1D	-3.01	118.00	123.85
27	B	620	BCR	C33-C5-C4	3.01	120.01	113.60
31	d	406	LMG	C1-O6-C5	-3.00	107.86	113.72
27	c	514	BCR	C28-C27-C26	-3.00	108.71	114.06
27	K	102	BCR	C33-C5-C6	-2.99	121.22	124.48
28	B	626	DGD	C3D-C4D-C5D	2.99	115.66	110.23
23	b	613	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
23	b	606	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
24	a	407	PHO	O2D-CGD-O1D	-2.98	118.04	123.85
23	B	610	CLA	C3B-C4B-NB	-2.98	107.87	110.53
23	C	502	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
31	d	405	LMG	O8-C28-C29	2.98	120.91	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
30	f	103	SQD	C44-O6-C1	2.97	120.17	113.80
28	C	516	DGD	O5D-C1E-C2E	2.97	112.78	108.27
27	B	619	BCR	C33-C5-C6	-2.97	121.24	124.48
25	d	404	PL9	C22-C23-C24	-2.97	120.83	127.62
28	C	518	DGD	O1G-C1A-C2A	2.96	120.87	111.83
27	D	405	BCR	C3-C4-C5	-2.96	108.78	114.06
31	A	414	LMG	C7-O1-C1	2.96	120.14	113.80
24	D	402	PHO	O2D-CGD-O1D	-2.96	118.08	123.85
28	B	626	DGD	O5D-C1E-C2E	2.96	112.77	108.27
28	a	413	DGD	C3G-C2G-C1G	-2.96	104.89	111.78
28	D	410	DGD	O5D-C1E-C2E	2.96	112.77	108.27
23	B	605	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
31	D	408	LMG	C7-O1-C1	2.96	120.14	113.80
28	B	626	DGD	C6D-C5D-C4D	-2.96	105.86	112.07
27	c	514	BCR	C20-C21-C22	-2.95	123.14	127.28
27	C	514	BCR	C38-C26-C25	-2.95	121.27	124.48
30	f	103	SQD	O5-C5-C4	2.94	114.99	109.70
31	D	408	LMG	O7-C10-C11	2.94	117.83	111.48
23	D	401	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
27	c	514	BCR	C35-C13-C14	-2.93	118.06	122.82
23	B	608	CLA	C1-C2-C3	-2.93	121.39	126.20
30	a	401	SQD	C44-O6-C1	2.93	120.08	113.80
23	A	407	CLA	CHB-C4A-NA	2.93	128.63	124.40
23	b	606	CLA	C3B-C4B-NB	-2.93	107.91	110.53
23	B	611	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
23	D	403	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
28	A	411	DGD	O4D-C4D-C5D	-2.93	102.11	109.32
31	k	103	LMG	C1-O6-C5	-2.93	108.00	113.72
23	b	608	CLA	CHB-C4A-NA	2.93	128.62	124.40
23	c	513	CLA	CHB-C4A-NA	2.93	128.62	124.40
27	j	102	BCR	C33-C5-C6	-2.92	121.29	124.48
27	c	516	BCR	C20-C21-C22	-2.92	123.18	127.28
31	A	418	LMG	O8-C28-C29	2.92	120.75	111.83
31	a	402	LMG	C6-C5-C4	-2.92	105.85	113.02
31	D	406	LMG	O8-C28-O10	-2.92	116.33	123.63
30	F	102	SQD	C44-O6-C1	2.92	120.05	113.80
23	B	604	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
23	B	603	CLA	C3B-C4B-NB	-2.92	107.93	110.53
28	C	517	DGD	O1G-C1A-C2A	2.91	120.72	111.83
31	I	101	LMG	O7-C10-C11	2.91	117.78	111.48
31	E	101	LMG	C8-O7-C10	2.91	124.75	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
27	B	618	BCR	C29-C30-C25	2.91	114.66	110.44
31	b	623	LMG	O4-C4-C3	-2.91	103.53	110.38
30	a	415	SQD	O6-C1-C2	2.90	112.68	108.27
23	c	502	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
25	A	408	PL9	C22-C23-C24	-2.90	120.99	127.62
30	b	601	SQD	O9-S-C6	2.90	111.08	106.76
27	K	102	BCR	C11-C10-C9	-2.89	123.22	127.28
23	a	404	CLA	C1-C2-C3	-2.89	121.45	126.20
31	a	416	LMG	C1-O6-C5	-2.89	108.07	113.72
24	D	402	PHO	O1D-CGD-CBD	2.89	129.11	124.72
23	c	511	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
27	H	101	BCR	C15-C14-C13	-2.88	123.23	127.28
27	H	101	BCR	C10-C11-C12	-2.88	114.85	123.20
23	c	513	CLA	C3B-C4B-NB	-2.88	107.96	110.53
31	a	402	LMG	C3-C4-C5	2.88	115.45	110.23
27	T	103	BCR	C23-C24-C25	-2.87	119.32	127.00
27	B	618	BCR	C21-C20-C19	-2.87	114.87	123.20
28	b	602	DGD	O2G-C1B-C2B	2.87	117.70	111.48
28	C	517	DGD	O5D-C6D-C5D	-2.87	102.95	109.42
27	T	103	BCR	C29-C30-C25	2.87	114.61	110.44
31	a	402	LMG	O8-C28-C29	2.86	120.57	111.83
24	a	408	PHO	CMB-C2B-C3B	2.86	130.40	124.68
23	b	615	CLA	C3B-C4B-NB	-2.86	107.98	110.53
23	d	402	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
31	B	622	LMG	O1-C1-C2	2.86	112.61	108.27
23	B	615	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
31	I	101	LMG	O8-C28-C29	2.85	120.53	111.83
27	c	515	BCR	C24-C23-C22	-2.85	122.02	126.23
23	c	509	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	C	513	CLA	C3B-C4B-NB	-2.85	107.99	110.53
23	b	607	CLA	C1-C2-C3	-2.84	121.54	126.20
27	J	102	BCR	C33-C5-C6	-2.84	121.38	124.48
28	c	517	DGD	C1D-O6D-C5D	-2.84	108.17	113.72
23	B	606	CLA	C3B-C4B-NB	-2.84	107.99	110.53
23	c	509	CLA	CHB-C4A-NA	2.84	128.50	124.40
31	b	623	LMG	C1-O6-C5	-2.84	108.18	113.72
28	c	519	DGD	O6D-C5D-C6D	2.84	112.32	106.69
23	a	405	CLA	C3B-C4B-NB	-2.83	108.00	110.53
23	A	404	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
23	a	409	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
30	B	625	SQD	O9-S-C6	2.83	110.98	106.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	f	102	BCR	C38-C26-C25	-2.83	121.40	124.48
23	C	506	CLA	C3B-C4B-NB	-2.83	108.01	110.53
27	K	102	BCR	C20-C21-C22	-2.83	123.31	127.28
30	a	401	SQD	C1-C2-C3	2.83	115.95	110.01
27	A	410	BCR	C11-C10-C9	-2.82	123.32	127.28
23	c	507	CLA	C3B-C4B-NB	-2.82	108.01	110.53
23	c	504	CLA	CHB-C4A-NA	2.82	128.47	124.40
27	c	516	BCR	C29-C30-C25	2.82	114.53	110.44
23	C	507	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
23	c	503	CLA	C3B-C4B-NB	-2.82	108.02	110.53
27	B	620	BCR	C2-C1-C6	2.81	114.53	110.44
25	D	404	PL9	C25-C24-C26	2.81	120.11	115.23
23	C	501	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
23	b	607	CLA	C3B-C4B-NB	-2.81	108.02	110.53
27	B	617	BCR	C3-C4-C5	-2.81	109.05	114.06
30	a	415	SQD	C44-O6-C1	2.81	119.82	113.80
33	B	627	LMT	O1B-C4'-C3'	2.81	114.37	107.23
23	c	509	CLA	C3B-C4B-NB	-2.81	108.02	110.53
27	H	101	BCR	C38-C26-C25	-2.81	121.42	124.48
31	b	624	LMG	C1-O6-C5	-2.81	108.24	113.72
28	B	621	DGD	O3D-C3D-C4D	2.80	116.99	110.38
23	c	508	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
33	D	411	LMT	C1B-O1B-C4'	-2.80	111.33	117.98
28	c	519	DGD	C4D-C3D-C2D	-2.80	105.91	110.83
23	c	512	CLA	C3B-C4B-NB	-2.80	108.03	110.53
34	f	101	HEM	C3B-C4B-NB	-2.80	107.46	109.47
27	D	405	BCR	C23-C24-C25	-2.80	119.52	127.00
31	b	623	LMG	O8-C28-C29	2.80	120.37	111.83
23	b	617	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
23	B	608	CLA	C3B-C4B-NB	-2.79	108.03	110.53
31	A	418	LMG	C3-C4-C5	2.79	115.30	110.23
25	a	410	PL9	C12-C13-C14	-2.79	121.24	127.62
28	d	408	DGD	O1G-C1A-C2A	2.79	120.34	111.83
23	A	403	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	B	602	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
23	c	513	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
27	H	101	BCR	C20-C21-C22	-2.78	123.38	127.28
23	c	507	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
31	e	101	LMG	C7-O1-C1	2.78	119.75	113.80
31	i	101	LMG	O8-C28-C29	2.78	120.30	111.83
31	d	406	LMG	C7-O1-C1	2.78	119.75	113.80
27	k	102	BCR	C33-C5-C6	-2.78	121.46	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	103	BCR	C21-C20-C19	-2.77	115.16	123.20
28	C	518	DGD	C4D-C3D-C2D	-2.77	105.96	110.83
23	c	510	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
27	x	101	BCR	C16-C17-C18	-2.77	123.39	127.28
27	T	103	BCR	C38-C26-C27	2.77	119.50	113.60
23	b	611	CLA	CHB-C4A-NA	2.77	128.39	124.40
23	A	404	CLA	C1-C2-C3	-2.77	121.67	126.20
27	A	410	BCR	C20-C21-C22	-2.77	123.40	127.28
28	a	413	DGD	O4D-C4D-C5D	-2.76	102.52	109.32
23	C	513	CLA	CHB-C4A-NA	2.76	128.39	124.40
31	D	408	LMG	O8-C28-C29	2.76	120.26	111.83
25	D	404	PL9	C37-C38-C39	-2.76	121.30	127.62
23	a	409	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	D	404	PL9	C12-C13-C14	-2.76	121.31	127.62
23	B	610	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
30	a	401	SQD	O7-S-C6	2.75	110.87	106.76
31	C	520	LMG	C1-O6-C5	-2.75	108.34	113.72
27	D	405	BCR	C29-C30-C25	2.75	114.44	110.44
23	C	509	CLA	CHB-C4A-NA	2.75	128.37	124.40
30	B	625	SQD	O5-C5-C4	2.75	114.66	109.70
31	d	405	LMG	O8-C28-O10	-2.75	116.75	123.63
27	H	101	BCR	C8-C7-C6	-2.75	119.66	127.00
23	b	612	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
31	A	418	LMG	C1-O6-C5	-2.75	108.36	113.72
31	e	101	LMG	O8-C28-C29	2.75	120.21	111.83
28	b	622	DGD	O3D-C3D-C4D	2.74	116.84	110.38
30	b	601	SQD	O47-C7-C8	2.74	117.42	111.48
30	b	601	SQD	O5-C5-C4	2.74	114.64	109.70
23	b	605	CLA	CHB-C4A-NA	2.74	128.35	124.40
23	c	502	CLA	CHB-C4A-NA	2.73	128.35	124.40
23	C	502	CLA	C3B-C4B-NB	-2.73	108.09	110.53
31	c	520	LMG	C7-O1-C1	2.73	119.64	113.80
33	T	101	LMT	O1B-C4'-C3'	2.73	114.16	107.23
27	f	102	BCR	C16-C15-C14	-2.72	117.95	123.52
23	C	508	CLA	C3B-C4B-NB	-2.72	108.10	110.53
30	A	417	SQD	C1-C2-C3	2.72	115.73	110.01
28	c	518	DGD	O5D-C6D-C5D	-2.72	103.29	109.42
28	c	518	DGD	C4D-C3D-C2D	-2.72	106.06	110.83
27	J	102	BCR	C1-C6-C5	-2.72	118.92	122.64
23	a	404	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
27	T	103	BCR	C33-C5-C4	2.72	119.39	113.60
23	B	615	CLA	C3B-C4B-NB	-2.71	108.11	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	CHB-C4A-NA	2.71	128.32	124.40
27	D	405	BCR	C27-C26-C25	-2.71	119.04	122.70
23	b	618	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
30	f	103	SQD	O9-S-C6	2.71	110.80	106.76
23	b	618	CLA	C3B-C4B-NB	-2.71	108.11	110.53
23	C	507	CLA	C3B-C4B-NB	-2.71	108.11	110.53
28	b	602	DGD	O1G-C1A-C2A	2.71	120.09	111.83
28	D	410	DGD	O1G-C1A-C2A	2.71	120.09	111.83
25	d	404	PL9	C40-C39-C41	2.70	119.92	115.23
23	B	616	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
31	a	402	LMG	C1-O6-C5	-2.70	108.45	113.72
23	b	612	CLA	C3B-C4B-NB	-2.70	108.12	110.53
23	a	406	CLA	C1-C2-C3	-2.69	121.78	126.20
23	c	502	CLA	C3B-C4B-NB	-2.69	108.12	110.53
23	B	609	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
27	D	405	BCR	C21-C20-C19	-2.69	115.39	123.20
27	B	619	BCR	C29-C30-C25	2.69	114.35	110.44
27	Z	101	BCR	C28-C27-C26	-2.69	109.26	114.06
23	d	403	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
23	C	512	CLA	CHB-C4A-NA	2.69	128.28	124.40
23	c	505	CLA	CHB-C4A-NA	2.69	128.28	124.40
23	b	610	CLA	CHB-C4A-NA	2.69	128.28	124.40
31	d	406	LMG	O8-C28-C29	2.68	120.02	111.83
23	B	604	CLA	C1-C2-C3	-2.68	121.80	126.20
30	a	415	SQD	O9-S-C6	2.68	110.76	106.76
23	D	401	CLA	C3B-C4B-NB	-2.68	108.14	110.53
23	b	605	CLA	C3B-C4B-NB	-2.68	108.14	110.53
27	j	102	BCR	C39-C30-C25	-2.67	106.05	110.24
24	A	406	PHO	CMB-C2B-C3B	2.67	130.02	124.68
27	j	102	BCR	C38-C26-C27	2.67	119.29	113.60
27	B	617	BCR	C23-C24-C25	-2.66	119.88	127.00
27	C	514	BCR	C34-C9-C10	-2.66	118.50	122.82
23	B	605	CLA	C3B-C4B-NB	-2.66	108.15	110.53
24	A	406	PHO	C3B-C4B-NB	-2.66	105.73	107.46
27	Z	101	BCR	C8-C7-C6	-2.66	119.89	127.00
23	B	611	CLA	C3B-C4B-NB	-2.66	108.16	110.53
23	C	509	CLA	C3B-C4B-NB	-2.66	108.16	110.53
25	J	101	PL9	C12-C13-C14	-2.66	121.54	127.62
23	a	409	CLA	CHB-C4A-NA	2.66	128.23	124.40
23	C	513	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
27	C	515	BCR	C29-C30-C25	2.65	114.30	110.44
23	C	505	CLA	C3B-C4B-NB	-2.65	108.16	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	625	SQD	O48-C23-C24	2.65	119.92	111.83
25	D	404	PL9	C42-C43-C44	-2.65	121.56	127.62
27	C	514	BCR	C35-C13-C14	-2.65	118.52	122.82
23	b	618	CLA	CHB-C4A-NA	2.65	128.22	124.40
23	B	609	CLA	CHB-C4A-NA	2.65	128.22	124.40
28	A	411	DGD	O1G-C1A-C2A	2.65	119.90	111.83
23	c	509	CLA	C1-C2-C3	-2.65	121.86	126.20
23	C	502	CLA	CHB-C4A-NA	2.65	128.22	124.40
30	A	413	SQD	O5-C5-C4	2.64	114.46	109.70
23	c	507	CLA	C1-C2-C3	-2.64	121.86	126.20
23	C	504	CLA	CHB-C4A-NA	2.64	128.21	124.40
27	c	514	BCR	C34-C9-C10	-2.64	118.54	122.82
23	A	407	CLA	C3B-C4B-NB	-2.64	108.17	110.53
31	E	101	LMG	O7-C10-C11	2.64	117.18	111.48
27	H	101	BCR	C35-C13-C12	2.64	122.11	118.09
23	c	506	CLA	CHB-C4A-NA	2.64	128.20	124.40
31	M	102	LMG	O8-C28-C29	2.63	119.87	111.83
23	a	405	CLA	CHB-C4A-NA	2.63	128.20	124.40
27	B	619	BCR	C27-C26-C25	-2.63	119.15	122.70
31	M	101	LMG	O8-C28-C29	2.63	119.86	111.83
23	a	404	CLA	C3B-C4B-NB	-2.63	108.18	110.53
23	B	611	CLA	C1-C2-C3	-2.63	121.89	126.20
27	f	102	BCR	C38-C26-C27	2.63	119.20	113.60
31	d	406	LMG	C1-C2-C3	-2.63	104.48	110.01
23	C	510	CLA	C3B-C4B-NB	-2.62	108.19	110.53
23	a	406	CLA	C3B-C4B-NB	-2.62	108.19	110.53
30	A	417	SQD	O7-S-C6	2.62	110.67	106.76
29	A	415	LHG	O8-C23-C24	2.62	119.82	111.83
27	c	515	BCR	C8-C7-C6	-2.62	120.01	127.00
25	J	101	PL9	C15-C14-C16	2.62	119.77	115.23
27	D	405	BCR	C38-C26-C27	2.61	119.17	113.60
23	c	508	CLA	CHB-C4A-NA	2.61	128.17	124.40
27	c	515	BCR	C7-C8-C9	-2.61	122.38	126.23
30	B	625	SQD	O47-C7-C8	2.61	117.12	111.48
23	B	611	CLA	CHB-C4A-NA	2.61	128.16	124.40
23	C	507	CLA	CHB-C4A-NA	2.61	128.16	124.40
28	b	622	DGD	O2G-C1B-C2B	2.61	117.12	111.48
28	A	411	DGD	C4D-C3D-C2D	-2.61	106.25	110.83
23	A	405	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
31	C	520	LMG	C6-C5-C4	-2.60	106.64	113.02
31	e	101	LMG	O1-C1-C2	2.59	112.21	108.27
23	B	607	CLA	C3B-C4B-NB	-2.59	108.22	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	E	101	LMG	C7-O1-C1	2.59	119.34	113.80
31	a	402	LMG	C7-O1-C1	2.59	119.34	113.80
28	a	413	DGD	O1G-C1A-C2A	2.59	119.72	111.83
31	c	520	LMG	O1-C1-C2	2.58	112.20	108.27
27	B	618	BCR	C23-C24-C25	-2.58	120.10	127.00
23	C	512	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
23	b	608	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
27	T	102	BCR	C36-C18-C19	2.58	122.03	118.09
23	c	501	CLA	C3B-C4B-NB	-2.58	108.23	110.53
30	A	413	SQD	O8-S-C6	2.58	110.95	105.97
25	d	404	PL9	C32-C33-C34	-2.57	121.73	127.62
27	j	102	BCR	C11-C12-C13	-2.57	119.31	126.36
27	c	514	BCR	C24-C23-C22	-2.57	122.43	126.23
27	x	101	BCR	C3-C4-C5	-2.57	109.47	114.06
28	b	622	DGD	O1G-C1A-C2A	2.57	119.68	111.83
23	b	618	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
31	A	418	LMG	O3-C3-C4	-2.57	104.31	110.38
28	A	411	DGD	C6D-C5D-C4D	-2.57	106.67	112.07
23	C	512	CLA	C3B-C4B-NB	-2.57	108.24	110.53
27	T	102	BCR	C3-C4-C5	-2.57	109.47	114.06
23	c	513	CLA	C1-C2-C3	-2.56	122.00	126.20
31	C	519	LMG	C7-O1-C1	2.56	119.29	113.80
27	B	618	BCR	C33-C5-C4	2.56	119.06	113.60
23	C	501	CLA	C3B-C4B-NB	-2.56	108.24	110.53
25	j	101	PL9	C12-C13-C14	-2.56	121.76	127.62
23	A	404	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
34	f	101	HEM	C1B-NB-C4B	2.55	108.23	105.21
23	c	512	CLA	CHB-C4A-NA	2.55	128.08	124.40
23	a	404	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
27	b	620	BCR	C27-C26-C25	-2.55	119.26	122.70
23	C	501	CLA	CHB-C4A-NA	2.55	128.08	124.40
31	D	408	LMG	C1-C2-C3	-2.55	104.65	110.01
31	I	101	LMG	C1-O6-C5	-2.55	108.75	113.72
23	B	606	CLA	CHB-C4A-NA	2.55	128.07	124.40
31	I	101	LMG	O1-C1-C2	2.55	112.14	108.27
23	C	508	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
23	B	605	CLA	CHB-C4A-NA	2.55	128.07	124.40
23	a	404	CLA	CHB-C4A-NA	2.54	128.07	124.40
23	B	609	CLA	C3B-C4B-NB	-2.54	108.26	110.53
33	b	625	LMT	C1B-O1B-C4'	-2.54	111.96	117.98
23	b	616	CLA	CHB-C4A-NA	2.54	128.06	124.40
29	a	417	LHG	O8-C23-C24	2.54	119.57	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
23	b	607	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
23	b	616	CLA	C3B-C4B-NB	-2.53	108.27	110.53
28	c	517	DGD	O1G-C1A-C2A	2.53	119.55	111.83
23	C	512	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
27	j	102	BCR	C1-C6-C5	-2.53	119.18	122.64
31	e	101	LMG	C8-O7-C10	2.53	123.84	117.80
23	b	610	CLA	C3B-C4B-NB	-2.53	108.28	110.53
23	C	504	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
23	b	606	CLA	CHB-C4A-NA	2.53	128.04	124.40
33	B	624	LMT	C1B-O1B-C4'	-2.52	111.99	117.98
23	d	403	CLA	CHB-C4A-NA	2.52	128.04	124.40
31	k	103	LMG	O8-C28-O10	-2.52	117.31	123.63
23	A	403	CLA	CHB-C4A-NA	2.52	128.04	124.40
25	D	404	PL9	C32-C33-C34	-2.52	121.85	127.62
23	c	511	CLA	C3B-C4B-NB	-2.52	108.28	110.53
28	c	518	DGD	O1G-C1A-C2A	2.52	119.52	111.83
31	D	406	LMG	C3-C4-C5	2.52	114.80	110.23
30	b	601	SQD	O48-C23-C24	2.52	119.51	111.83
28	c	519	DGD	O5D-C1E-C2E	2.52	112.09	108.27
23	C	511	CLA	CHB-C4A-NA	2.51	128.03	124.40
23	b	605	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
23	b	612	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	C	506	CLA	CAA-CBA-CGA	-2.51	106.08	113.21
30	A	413	SQD	O48-C23-C24	2.51	119.47	111.83
25	a	410	PL9	C20-C19-C21	2.50	119.57	115.23
25	j	101	PL9	C22-C23-C24	-2.50	121.91	127.62
28	a	413	DGD	C6E-C5E-C4E	-2.50	106.89	113.02
31	B	622	LMG	C1-O6-C5	-2.49	108.85	113.72
27	T	103	BCR	C24-C23-C22	-2.49	122.55	126.23
23	C	503	CLA	C3B-C4B-NB	-2.49	108.31	110.53
23	B	602	CLA	C3B-C4B-NB	-2.49	108.31	110.53
27	D	405	BCR	C38-C26-C25	-2.48	121.77	124.48
34	F	101	HEM	C1B-NB-C4B	2.48	108.15	105.21
23	B	613	CLA	CHB-C4A-NA	2.48	127.98	124.40
25	d	404	PL9	C15-C14-C16	2.48	119.53	115.23
27	B	618	BCR	C38-C26-C27	2.48	118.88	113.60
23	A	404	CLA	CHB-C4A-NA	2.48	127.98	124.40
27	J	102	BCR	C11-C12-C13	-2.48	119.57	126.36
23	B	615	CLA	CHB-C4A-NA	2.48	127.97	124.40
25	a	410	PL9	C32-C33-C34	-2.48	121.96	127.62
23	c	512	CLA	O2A-CGA-O1A	-2.47	117.44	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	CHB-C4A-NA	2.47	127.97	124.40
31	D	407	LMG	C4-C3-C2	2.47	115.17	110.83
23	b	617	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	B	612	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
23	B	602	CLA	CHB-C4A-NA	2.46	127.96	124.40
27	f	102	BCR	C21-C20-C19	-2.46	116.06	123.20
23	b	619	CLA	C3B-C4B-NB	-2.46	108.33	110.53
23	b	609	CLA	CHB-C4A-NA	2.46	127.95	124.40
28	C	517	DGD	O3G-C1D-C2D	2.46	112.01	108.27
23	C	507	CLA	C1-C2-C3	-2.46	122.17	126.20
30	D	409	SQD	O48-C23-C24	2.46	119.34	111.83
23	A	403	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
31	I	101	LMG	C7-O1-C1	2.46	119.06	113.80
27	f	102	BCR	C27-C26-C25	-2.46	119.38	122.70
28	C	517	DGD	O6E-C1E-C2E	2.46	115.42	110.37
23	a	409	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
27	H	101	BCR	C3-C4-C5	-2.46	109.68	114.06
27	x	101	BCR	C34-C9-C8	2.45	121.84	118.09
27	C	515	BCR	C23-C24-C25	-2.45	120.44	127.00
23	c	501	CLA	CHB-C4A-NA	2.45	127.94	124.40
27	Z	101	BCR	C15-C16-C17	-2.45	118.51	123.52
31	D	408	LMG	O8-C28-O10	-2.45	117.51	123.63
31	e	101	LMG	O7-C10-O9	-2.45	117.99	123.70
23	b	611	CLA	C1-C2-C3	-2.45	122.19	126.20
31	i	101	LMG	C1-O6-C5	-2.45	108.94	113.72
23	c	511	CLA	CHB-C4A-NA	2.44	127.93	124.40
28	B	621	DGD	O2G-C1B-C2B	2.44	116.77	111.48
27	k	102	BCR	C24-C23-C22	-2.44	122.63	126.23
23	B	603	CLA	CHB-C4A-NA	2.44	127.92	124.40
27	C	514	BCR	C23-C24-C25	-2.44	120.49	127.00
28	B	621	DGD	O1G-C1A-C2A	2.44	119.27	111.83
23	B	610	CLA	CHB-C4A-NA	2.44	127.91	124.40
27	c	516	BCR	C23-C24-C25	-2.43	120.50	127.00
30	F	102	SQD	O5-C1-C2	2.43	115.37	110.37
23	B	605	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
23	C	506	CLA	C1-C2-C3	-2.43	122.21	126.20
23	C	502	CLA	C1-C2-C3	-2.43	122.21	126.20
30	F	102	SQD	O48-C23-C24	2.43	119.24	111.83
23	D	403	CLA	CHB-C4A-NA	2.43	127.90	124.40
27	H	101	BCR	C16-C15-C14	-2.43	118.56	123.52
23	B	613	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
23	c	502	CLA	C1-C2-C3	-2.42	122.23	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	x	101	BCR	C35-C13-C12	2.42	121.79	118.09
23	c	506	CLA	C3B-C4B-NB	-2.42	108.37	110.53
31	i	101	LMG	C7-O1-C1	2.42	118.99	113.80
23	C	508	CLA	CHB-C4A-NA	2.42	127.89	124.40
25	A	408	PL9	C7-C3-C2	-2.42	120.54	123.39
28	a	413	DGD	C3D-C4D-C5D	2.42	114.61	110.23
31	D	407	LMG	C7-O1-C1	2.41	118.97	113.80
34	F	101	HEM	C3B-C4B-NB	-2.41	107.73	109.47
28	B	626	DGD	O1G-C1A-C2A	2.41	119.19	111.83
25	d	404	PL9	C12-C13-C14	-2.41	122.10	127.62
23	b	618	CLA	C1-C2-C3	-2.41	122.24	126.20
31	C	519	LMG	O8-C28-O10	-2.41	117.60	123.63
27	J	102	BCR	C38-C26-C27	2.41	118.73	113.60
28	B	626	DGD	O6D-C1D-O3G	2.41	115.73	110.04
27	c	514	BCR	C38-C26-C25	-2.41	121.86	124.48
23	b	604	CLA	C3B-C4B-NB	-2.41	108.38	110.53
27	T	103	BCR	C15-C16-C17	-2.40	118.60	123.52
27	f	102	BCR	C3-C4-C5	-2.40	109.77	114.06
27	f	102	BCR	C23-C24-C25	-2.40	120.58	127.00
27	C	514	BCR	C39-C30-C25	-2.40	106.47	110.24
34	v	201	HEM	C1B-NB-C4B	2.40	108.05	105.21
23	A	405	CLA	C1-C2-C3	-2.40	122.26	126.20
23	b	606	CLA	C1-C2-C3	-2.40	122.26	126.20
27	c	516	BCR	C15-C16-C17	-2.40	118.61	123.52
27	c	515	BCR	C38-C26-C25	-2.40	121.87	124.48
27	C	515	BCR	C15-C16-C17	-2.40	118.61	123.52
23	C	510	CLA	C1-C2-C3	-2.40	122.27	126.20
31	C	519	LMG	C6-C5-C4	-2.39	107.14	113.02
30	a	401	SQD	O48-C23-C24	2.39	119.13	111.83
23	B	603	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
23	B	610	CLA	C1-C2-C3	-2.39	122.28	126.20
28	C	516	DGD	O1G-C1A-C2A	2.39	119.12	111.83
31	D	407	LMG	C1-O6-C5	-2.39	109.06	113.72
31	E	101	LMG	O9-C10-C11	-2.39	114.45	123.78
27	D	405	BCR	C36-C18-C19	2.39	121.73	118.09
27	J	102	BCR	C39-C30-C25	-2.38	106.50	110.24
34	F	101	HEM	CHB-C1B-NB	2.38	127.31	124.37
31	i	101	LMG	O8-C28-O10	-2.38	117.67	123.63
30	f	103	SQD	O8-S-C6	2.38	110.57	105.97
23	B	615	CLA	C1-C2-C3	-2.38	122.30	126.20
30	a	415	SQD	O48-C23-C24	2.38	119.08	111.83
28	C	516	DGD	C6E-C5E-C4E	-2.38	107.19	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	619	BCR	C2-C1-C6	2.37	113.89	110.44
30	d	407	SQD	O7-S-C6	2.37	110.30	106.76
23	B	608	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
31	D	407	LMG	O1-C1-C2	2.37	111.87	108.27
27	C	515	BCR	C21-C20-C19	-2.37	116.33	123.20
30	B	625	SQD	C1-O5-C5	2.37	118.35	113.72
27	Z	101	BCR	C23-C24-C25	-2.37	120.67	127.00
25	A	408	PL9	C20-C19-C21	2.37	119.34	115.23
23	C	511	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
28	d	408	DGD	O2G-C1B-C2B	2.37	116.60	111.48
23	B	607	CLA	O2D-CGD-CBD	2.37	115.36	111.23
33	M	103	LMT	C1B-O1B-C4'	-2.36	112.37	117.98
27	B	620	BCR	C32-C1-C6	-2.36	106.53	110.24
28	d	408	DGD	O2G-C1B-O1B	-2.36	118.18	123.70
27	x	101	BCR	C38-C26-C25	-2.36	121.91	124.48
27	Z	101	BCR	C7-C8-C9	-2.36	122.75	126.23
28	A	411	DGD	O3D-C3D-C4D	2.36	115.94	110.38
27	k	102	BCR	C15-C16-C17	-2.36	118.69	123.52
23	C	507	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
23	B	601	CLA	C1-C2-C3	-2.36	122.34	126.20
23	c	506	CLA	C1-C2-C3	-2.36	122.34	126.20
23	C	511	CLA	C3B-C4B-NB	-2.36	108.43	110.53
25	D	404	PL9	C40-C39-C41	2.35	119.31	115.23
30	A	413	SQD	C44-O6-C1	2.35	118.84	113.80
27	f	102	BCR	C36-C18-C19	2.35	121.68	118.09
27	T	102	BCR	C23-C24-C25	-2.35	120.71	127.00
28	D	410	DGD	O2G-C1B-C2B	2.35	116.57	111.48
28	b	602	DGD	O6D-C1D-O3G	2.35	115.60	110.04
23	d	402	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
23	b	613	CLA	CHB-C4A-NA	2.35	127.79	124.40
23	a	405	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
30	f	103	SQD	O48-C23-C24	2.35	118.99	111.83
23	a	409	CLA	C1-C2-C3	-2.35	122.35	126.20
23	B	604	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
23	b	607	CLA	CHB-C4A-NA	2.34	127.78	124.40
27	a	412	BCR	C28-C27-C26	-2.34	109.88	114.06
25	D	404	PL9	C15-C14-C16	2.34	119.30	115.23
28	b	622	DGD	C3G-O3G-C1D	2.34	118.82	113.80
28	C	517	DGD	C1D-O6D-C5D	-2.34	109.15	113.72
23	B	601	CLA	C3B-C4B-NB	-2.33	108.45	110.53
23	b	611	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
23	c	507	CLA	CHB-C4A-NA	2.33	127.77	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	624	LMG	C3-C4-C5	2.33	114.46	110.23
27	x	101	BCR	C8-C7-C6	-2.33	120.77	127.00
27	C	515	BCR	C2-C1-C6	2.33	113.82	110.44
27	H	101	BCR	C33-C5-C4	2.33	118.56	113.60
23	B	601	CLA	CHB-C4A-NA	2.32	127.75	124.40
27	T	102	BCR	C28-C27-C26	-2.32	109.92	114.06
23	C	511	CLA	C1-C2-C3	-2.32	122.40	126.20
25	A	408	PL9	C12-C13-C14	-2.32	122.32	127.62
28	D	410	DGD	O2G-C1B-O1B	-2.32	118.28	123.70
23	b	613	CLA	O2D-CGD-CBD	2.32	115.28	111.23
31	e	101	LMG	O7-C10-C11	2.32	116.50	111.48
31	c	520	LMG	C6-C5-C4	-2.32	107.33	113.02
23	c	504	CLA	C1-C2-C3	-2.32	122.40	126.20
23	b	604	CLA	C1-C2-C3	-2.32	122.40	126.20
30	A	417	SQD	O48-C23-C24	2.31	118.89	111.83
25	j	101	PL9	C15-C14-C16	2.31	119.24	115.23
33	m	101	LMT	C1B-O1B-C4'	-2.31	112.50	117.98
23	b	607	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
27	Z	101	BCR	C10-C11-C12	-2.31	116.50	123.20
27	b	621	BCR	C28-C27-C26	-2.31	109.93	114.06
27	J	102	BCR	C35-C13-C14	-2.31	119.08	122.82
23	C	505	CLA	CBA-CAA-C2A	2.31	120.66	113.79
23	B	609	CLA	CAA-CBA-CGA	-2.31	106.66	113.21
28	C	516	DGD	C3G-O3G-C1D	2.31	118.74	113.80
27	C	514	BCR	C29-C30-C25	2.30	113.79	110.44
28	c	519	DGD	O1G-C1A-O1A	-2.30	117.86	123.63
25	A	408	PL9	C32-C33-C34	-2.30	122.35	127.62
23	B	608	CLA	CHB-C4A-NA	2.30	127.72	124.40
27	a	412	BCR	C23-C24-C25	-2.30	120.85	127.00
24	A	406	PHO	O2D-CGD-CBD	2.30	113.48	110.95
23	D	401	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
27	A	410	BCR	C32-C1-C6	-2.30	106.64	110.24
31	a	402	LMG	O1-C1-C2	2.30	111.77	108.27
25	A	408	PL9	C10-C9-C11	2.30	119.22	115.23
31	d	405	LMG	C3-C4-C5	2.30	114.40	110.23
28	d	408	DGD	C2G-O2G-C1B	2.30	123.30	117.80
31	A	418	LMG	O8-C28-O10	-2.30	117.88	123.63
27	c	515	BCR	C28-C27-C26	-2.30	109.96	114.06
29	A	412	LHG	O8-C23-C24	2.30	118.83	111.83
28	d	408	DGD	O5D-C6D-C5D	2.29	114.59	109.42
23	C	509	CLA	C1-C2-C3	-2.29	122.44	126.20
25	J	101	PL9	C22-C23-C24	-2.29	122.38	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	CHB-C4A-NA	2.29	127.70	124.40
27	K	102	BCR	C33-C5-C4	2.29	118.47	113.60
23	b	607	CLA	CAA-CBA-CGA	-2.29	106.71	113.21
28	B	621	DGD	C3G-O3G-C1D	2.29	118.70	113.80
27	T	103	BCR	C16-C17-C18	-2.29	124.07	127.28
23	c	505	CLA	C3B-C4B-NB	-2.29	108.49	110.53
28	b	602	DGD	C6D-C5D-C4D	-2.28	107.27	112.07
23	B	601	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
23	B	612	CLA	CHB-C4A-NA	2.28	127.69	124.40
27	a	412	BCR	C8-C7-C6	-2.28	120.92	127.00
25	j	101	PL9	C20-C19-C21	2.28	119.18	115.23
28	a	413	DGD	O3D-C3D-C4D	2.27	115.73	110.38
25	D	404	PL9	C10-C9-C11	2.27	119.17	115.23
34	F	101	HEM	CHD-C4C-NC	2.27	126.93	124.45
30	D	409	SQD	O7-S-C6	2.27	110.15	106.76
30	a	415	SQD	O8-S-C6	2.27	110.36	105.97
31	a	416	LMG	O1-C7-C8	2.27	116.33	110.82
33	x	102	LMT	C1B-O1B-C4'	-2.26	112.61	117.98
25	J	101	PL9	C20-C19-C21	2.26	119.16	115.23
28	c	517	DGD	C6E-C5E-C4E	-2.26	107.46	113.02
27	B	619	BCR	C15-C16-C17	-2.26	118.89	123.52
27	B	620	BCR	C8-C7-C6	-2.26	120.97	127.00
23	c	504	CLA	C3B-C4B-NB	-2.26	108.52	110.53
28	C	516	DGD	O3G-C3G-C2G	2.25	116.30	110.82
31	E	101	LMG	O1-C1-C2	2.25	111.69	108.27
25	a	410	PL9	C15-C14-C16	2.25	119.13	115.23
23	C	513	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
23	B	604	CLA	CHB-C4A-NA	2.24	127.64	124.40
31	I	101	LMG	C6-C5-C4	-2.24	107.52	113.02
27	Z	101	BCR	C38-C26-C25	-2.24	122.04	124.48
33	b	626	LMT	C1B-O1B-C4'	-2.24	112.67	117.98
27	C	515	BCR	C38-C26-C27	2.24	118.36	113.60
23	D	403	CLA	C1-C2-C3	-2.23	122.54	126.20
23	c	503	CLA	O2D-CGD-CBD	2.23	115.14	111.23
28	C	518	DGD	O1G-C1A-O1A	-2.23	118.04	123.63
27	c	516	BCR	C21-C20-C19	-2.23	116.73	123.20
27	H	101	BCR	C21-C20-C19	-2.23	116.73	123.20
23	c	501	CLA	C1-C2-C3	-2.23	122.54	126.20
25	D	404	PL9	C27-C28-C29	-2.23	122.52	127.62
31	M	102	LMG	O6-C5-C4	2.23	113.72	109.70
27	a	412	BCR	C16-C15-C14	-2.23	118.96	123.52
31	A	418	LMG	O1-C1-C2	2.23	111.66	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	612	CLA	C1-C2-C3	-2.23	122.55	126.20
27	b	621	BCR	C40-C30-C25	-2.23	106.75	110.24
30	f	103	SQD	O6-C1-C2	2.22	111.65	108.27
31	e	101	LMG	C1-O6-C5	-2.22	109.38	113.72
27	A	410	BCR	C23-C24-C25	-2.22	121.06	127.00
28	C	516	DGD	C1D-O6D-C5D	-2.22	109.38	113.72
31	b	623	LMG	C7-O1-C1	2.22	118.56	113.80
23	b	604	CLA	CHB-C4A-NA	2.22	127.60	124.40
27	a	412	BCR	C21-C20-C19	-2.22	116.77	123.20
33	I	102	LMT	O1B-C4'-C3'	2.22	112.87	107.23
31	k	103	LMG	C6-C5-C4	-2.22	107.57	113.02
23	B	603	CLA	C1-C2-C3	-2.22	122.56	126.20
23	C	503	CLA	CHB-C4A-NA	2.22	127.60	124.40
27	K	102	BCR	C32-C1-C6	-2.22	106.77	110.24
27	T	102	BCR	C36-C18-C17	-2.22	119.23	122.82
28	c	518	DGD	O6E-C1E-C2E	2.22	114.92	110.37
28	c	517	DGD	C1G-O1G-C1A	2.21	125.21	117.12
31	A	414	LMG	O8-C28-O10	-2.21	118.09	123.63
24	D	402	PHO	O2A-CGA-O1A	-2.21	118.10	123.63
27	c	515	BCR	C15-C16-C17	-2.21	119.00	123.52
23	B	613	CLA	C1-C2-C3	-2.21	122.58	126.20
23	b	614	CLA	C1-C2-C3	-2.21	122.58	126.20
28	B	626	DGD	O4D-C4D-C5D	-2.21	103.88	109.32
23	A	405	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
30	d	407	SQD	O48-C23-C24	2.21	118.56	111.83
31	b	624	LMG	O8-C28-O10	-2.20	118.11	123.63
31	b	623	LMG	C4-C3-C2	2.20	114.70	110.83
27	B	617	BCR	C8-C7-C6	-2.20	121.12	127.00
23	c	504	CLA	O2D-CGD-CBD	2.20	115.08	111.23
25	a	410	PL9	C7-C8-C9	-2.20	123.04	126.83
28	C	517	DGD	O4D-C4D-C5D	-2.20	103.91	109.32
27	H	101	BCR	C36-C18-C19	2.20	121.45	118.09
25	j	101	PL9	C10-C9-C11	2.19	119.04	115.23
27	c	514	BCR	C29-C30-C25	2.19	113.63	110.44
23	b	614	CLA	O2D-CGD-CBD	2.19	115.06	111.23
25	D	404	PL9	C51-C49-C50	2.19	119.64	114.59
28	B	621	DGD	C4D-C3D-C2D	-2.19	106.98	110.83
23	d	402	CLA	CHB-C4A-NA	2.19	127.56	124.40
23	D	403	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
23	b	615	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
24	A	406	PHO	C2D-C1D-ND	-2.19	107.85	109.43
28	c	518	DGD	C1D-O6D-C5D	-2.19	109.45	113.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	411	DGD	C3D-C4D-C5D	2.19	114.20	110.23
27	B	617	BCR	C28-C27-C26	-2.19	110.16	114.06
27	b	620	BCR	C2-C1-C6	2.19	113.61	110.44
25	d	404	PL9	C20-C19-C21	2.19	119.02	115.23
30	a	401	SQD	O6-C1-C2	2.18	111.59	108.27
23	b	610	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
23	c	513	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
24	a	407	PHO	CMB-C2B-C3B	2.18	129.04	124.68
31	a	402	LMG	O3-C3-C4	-2.18	105.24	110.38
25	A	408	PL9	C30-C29-C31	2.18	119.01	115.23
27	x	101	BCR	C15-C16-C17	-2.18	119.07	123.52
30	A	417	SQD	O2-C2-C3	-2.18	105.25	110.38
25	D	404	PL9	C45-C44-C43	-2.17	118.04	123.63
27	B	619	BCR	C23-C24-C25	-2.17	121.19	127.00
23	C	505	CLA	CHB-C4A-NA	2.17	127.53	124.40
30	f	103	SQD	O5-C1-C2	2.17	114.83	110.37
28	a	413	DGD	C6D-C5D-C4D	-2.17	107.51	112.07
27	A	410	BCR	C21-C20-C19	-2.17	116.91	123.20
24	a	407	PHO	O2A-CGA-O1A	-2.17	118.20	123.63
31	C	519	LMG	O1-C1-C2	2.17	111.57	108.27
27	c	516	BCR	C2-C1-C6	2.17	113.59	110.44
23	B	604	CLA	CHC-C4B-NB	2.17	127.30	124.05
23	B	613	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
27	B	620	BCR	C40-C30-C25	-2.16	106.85	110.24
31	E	101	LMG	C1-O6-C5	-2.16	109.50	113.72
23	c	507	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
31	d	406	LMG	O8-C28-O10	-2.16	118.23	123.63
31	I	101	LMG	O3-C3-C4	-2.15	105.30	110.38
31	E	101	LMG	O7-C10-O9	-2.15	118.68	123.70
23	b	610	CLA	O2D-CGD-CBD	2.15	114.99	111.23
31	B	622	LMG	O8-C28-O10	-2.15	118.26	123.63
31	e	101	LMG	O9-C10-C11	-2.15	115.39	123.78
27	j	102	BCR	C20-C19-C18	-2.14	120.48	126.36
27	H	101	BCR	C15-C16-C17	-2.14	119.13	123.52
23	a	406	CLA	CHB-C4A-NA	2.14	127.49	124.40
23	B	612	CLA	CAA-CBA-CGA	-2.14	107.13	113.21
23	b	606	CLA	O2D-CGD-CBD	2.13	114.96	111.23
34	v	201	HEM	C2A-C1A-NA	-2.13	107.78	110.15
23	B	607	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
28	c	519	DGD	O3D-C3D-C4D	2.13	115.40	110.38
28	c	519	DGD	O2G-C1B-C2B	2.13	116.09	111.48
34	V	201	HEM	CHC-C1C-NC	2.13	126.77	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	614	CLA	CHB-C4A-NA	2.13	127.47	124.40
31	D	407	LMG	O8-C28-O10	-2.13	118.31	123.63
23	B	602	CLA	C1-C2-C3	-2.13	122.71	126.20
27	D	405	BCR	C35-C13-C12	2.12	121.33	118.09
28	C	516	DGD	O2G-C1B-O1B	-2.12	118.74	123.70
23	d	402	CLA	O1D-CGD-CBD	2.12	128.71	124.52
27	A	410	BCR	C8-C7-C6	-2.12	121.33	127.00
28	A	411	DGD	C6E-C5E-C4E	-2.12	107.81	113.02
27	A	410	BCR	C10-C11-C12	-2.12	117.05	123.20
28	C	516	DGD	O3D-C3D-C4D	2.12	115.38	110.38
27	Z	101	BCR	C21-C20-C19	-2.12	117.05	123.20
23	a	406	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
31	i	101	LMG	C3-C4-C5	2.12	114.08	110.23
27	b	620	BCR	C38-C26-C27	2.12	118.12	113.60
25	d	404	PL9	C36-C34-C33	-2.12	116.41	121.17
31	M	101	LMG	O8-C9-C8	-2.12	102.30	108.40
27	c	516	BCR	C38-C26-C27	2.11	118.10	113.60
31	b	624	LMG	C7-O1-C1	2.11	118.32	113.80
31	M	101	LMG	O1-C1-C2	2.11	111.47	108.27
27	j	102	BCR	C37-C22-C21	-2.11	119.40	122.82
27	A	410	BCR	C34-C9-C8	2.11	121.31	118.09
27	k	102	BCR	C36-C18-C19	2.11	121.30	118.09
25	D	404	PL9	C20-C19-C21	2.10	118.88	115.23
23	C	513	CLA	C1-C2-C3	-2.10	122.75	126.20
23	B	615	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
23	B	614	CLA	CHB-C4A-NA	2.10	127.44	124.40
27	f	102	BCR	C33-C5-C4	2.10	118.08	113.60
30	b	601	SQD	O6-C1-C2	2.10	111.47	108.27
28	b	622	DGD	C4D-C3D-C2D	-2.10	107.14	110.83
31	C	520	LMG	O3-C3-C4	-2.10	105.42	110.38
31	M	101	LMG	O4-C4-C3	-2.10	105.42	110.38
23	A	407	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
27	J	102	BCR	C15-C16-C17	-2.10	119.22	123.52
23	A	403	CLA	C1-C2-C3	-2.10	122.76	126.20
31	c	520	LMG	O3-C3-C4	-2.10	105.43	110.38
31	C	520	LMG	O8-C28-O10	-2.10	118.38	123.63
23	c	510	CLA	CHB-C4A-NA	2.10	127.43	124.40
31	i	101	LMG	C8-O7-C10	2.10	122.81	117.80
23	B	603	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
23	C	503	CLA	O2D-CGD-CBD	2.09	114.89	111.23
23	D	403	CLA	O2D-CGD-CBD	2.09	114.89	111.23
27	c	514	BCR	C34-C9-C8	2.09	121.28	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	404	PL9	C51-C49-C50	2.09	119.39	114.59
28	b	602	DGD	C1E-C2E-C3E	2.09	114.40	110.01
34	v	201	HEM	CAC-C3C-C4C	2.09	129.80	124.82
34	F	101	HEM	C2B-C1B-NB	-2.09	107.44	109.84
27	B	618	BCR	C35-C13-C12	2.08	121.27	118.09
27	c	514	BCR	C33-C5-C4	2.08	118.04	113.60
25	a	410	PL9	C53-C6-C1	2.08	119.54	115.28
25	d	404	PL9	C27-C28-C29	-2.08	122.86	127.62
23	b	616	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
27	x	101	BCR	C36-C18-C19	2.08	121.26	118.09
25	a	410	PL9	C17-C18-C19	-2.08	122.87	127.62
23	c	501	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
31	B	622	LMG	C3-C4-C5	2.07	113.99	110.23
27	k	102	BCR	C23-C24-C25	-2.07	121.46	127.00
28	c	517	DGD	C4D-C3D-C2D	-2.07	107.19	110.83
23	b	615	CLA	C1-C2-C3	-2.07	122.80	126.20
31	b	624	LMG	O6-C5-C4	2.07	113.43	109.70
31	d	405	LMG	O6-C5-C4	2.07	113.43	109.70
23	C	504	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
28	D	410	DGD	O5D-C6D-C5D	2.07	114.08	109.42
31	A	418	LMG	O7-C10-O9	-2.07	118.87	123.70
27	T	103	BCR	C32-C1-C6	-2.07	107.00	110.24
25	A	408	PL9	C53-C6-C1	2.07	119.51	115.28
28	b	602	DGD	O4D-C4D-C5D	-2.06	104.24	109.32
23	C	509	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
27	b	621	BCR	C16-C15-C14	-2.06	119.30	123.52
25	A	408	PL9	C41-C39-C40	2.06	119.33	114.59
23	B	613	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
28	C	518	DGD	O2G-C1B-C2B	2.06	115.94	111.48
27	C	514	BCR	C2-C3-C4	-2.06	106.75	111.28
27	k	102	BCR	C11-C10-C9	-2.06	124.39	127.28
27	b	621	BCR	C21-C20-C19	-2.06	117.23	123.20
27	j	102	BCR	C15-C16-C17	-2.06	119.31	123.52
27	J	102	BCR	C30-C25-C26	-2.06	119.82	122.64
27	b	621	BCR	C35-C13-C12	2.06	121.23	118.09
27	J	102	BCR	C36-C18-C17	-2.06	119.48	122.82
27	x	101	BCR	C16-C15-C14	-2.06	119.31	123.52
23	C	503	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
23	C	501	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
27	a	412	BCR	C36-C18-C19	2.06	121.23	118.09
23	a	405	CLA	CHB-C1B-NB	2.06	127.13	124.05
23	c	508	CLA	O2A-CGA-O1A	-2.05	118.49	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	620	BCR	C16-C15-C14	-2.05	119.32	123.52
23	a	405	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
27	c	514	BCR	C2-C1-C6	2.05	113.42	110.44
25	a	410	PL9	C41-C39-C40	2.05	119.31	114.59
23	b	611	CLA	O2D-CGD-CBD	2.05	114.81	111.23
31	B	622	LMG	C6-C5-C4	-2.05	107.99	113.02
31	c	520	LMG	O8-C28-O10	-2.05	118.50	123.63
34	v	201	HEM	CHC-C4B-NB	2.05	126.63	124.42
27	D	405	BCR	C20-C21-C22	-2.05	124.41	127.28
27	k	102	BCR	C35-C13-C12	2.04	121.21	118.09
27	x	101	BCR	C11-C10-C9	-2.04	124.41	127.28
31	B	622	LMG	O6-C5-C4	2.04	113.38	109.70
30	A	413	SQD	O5-C1-C2	2.04	114.56	110.37
27	b	620	BCR	C39-C30-C25	-2.04	107.05	110.24
23	d	403	CLA	C1-C2-C3	-2.04	122.86	126.20
29	a	414	LHG	O8-C23-C24	2.04	118.05	111.83
27	b	621	BCR	C32-C1-C6	-2.03	107.05	110.24
27	c	515	BCR	C23-C24-C25	-2.03	121.57	127.00
27	B	620	BCR	C37-C22-C23	2.03	121.19	118.09
31	D	406	LMG	C6-C5-C4	-2.03	108.03	113.02
23	b	619	CLA	CHB-C4A-NA	2.03	127.33	124.40
23	b	604	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
23	c	505	CLA	CBA-CAA-C2A	2.03	119.84	113.79
23	b	619	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
28	B	626	DGD	C1E-C2E-C3E	2.03	114.28	110.01
29	a	414	LHG	C6-O8-C23	2.03	124.53	117.12
27	c	515	BCR	C11-C10-C9	-2.03	124.43	127.28
31	I	101	LMG	C8-O7-C10	2.03	122.65	117.80
27	C	514	BCR	C2-C1-C6	2.03	113.38	110.44
23	a	406	CLA	O2D-CGD-CBD	2.03	114.77	111.23
23	c	505	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
31	A	418	LMG	O6-C5-C4	2.03	113.35	109.70
25	D	404	PL9	C36-C34-C33	-2.03	116.62	121.17
27	x	101	BCR	C33-C5-C4	2.02	117.91	113.60
23	B	612	CLA	C1-C2-C3	-2.02	122.88	126.20
25	A	408	PL9	C11-C9-C8	-2.02	116.62	121.17
27	c	515	BCR	C21-C20-C19	-2.02	117.34	123.20
30	b	601	SQD	C1-O5-C5	2.02	117.67	113.72
27	B	618	BCR	C15-C14-C13	-2.02	124.44	127.28
23	D	401	CLA	CHB-C4A-NA	2.02	127.32	124.40
23	c	506	CLA	O2D-CGD-CBD	2.02	114.76	111.23
27	T	103	BCR	C36-C18-C19	2.02	121.17	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D	407	LMG	O4-C4-C3	-2.02	105.62	110.38
24	a	407	PHO	C1-C2-C3	-2.02	122.89	126.20
31	k	103	LMG	C7-O1-C1	2.02	118.12	113.80
33	B	623	LMT	C1B-O1B-C4'	-2.02	113.19	117.98
27	b	621	BCR	C37-C22-C23	2.02	121.17	118.09
23	b	611	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
27	T	102	BCR	C15-C16-C17	-2.01	119.40	123.52
23	b	609	CLA	O1D-CGD-CBD	2.01	128.49	124.52
27	c	515	BCR	C10-C11-C12	-2.01	117.38	123.20
23	c	505	CLA	C3A-C2A-C1A	2.01	104.35	101.34
23	B	606	CLA	O2D-CGD-CBD	2.01	114.74	111.23
31	M	102	LMG	O1-C1-C2	2.01	111.32	108.27
23	B	610	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
28	c	517	DGD	O4D-C4D-C5D	-2.01	104.38	109.32
27	x	101	BCR	C40-C30-C25	-2.01	107.10	110.24
27	B	619	BCR	C38-C26-C27	2.01	117.87	113.60
25	D	404	PL9	C45-C44-C46	2.01	118.71	115.23
23	b	619	CLA	O1D-CGD-CBD	2.00	128.47	124.52
23	b	611	CLA	O1D-CGD-CBD	2.00	128.47	124.52
31	M	102	LMG	O4-C4-C3	-2.00	105.65	110.38
27	Z	101	BCR	C34-C9-C8	2.00	121.15	118.09
27	B	620	BCR	C21-C20-C19	-2.00	117.40	123.20
27	a	412	BCR	C40-C30-C25	-2.00	107.10	110.24
34	v	201	HEM	CAA-CBA-CGA	-2.00	108.36	113.67
30	D	409	SQD	O8-S-C6	2.00	109.83	105.97
23	c	506	CLA	C3A-C2A-C1A	2.00	104.33	101.34

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	403	CLA	ND
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	608	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	501	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	401	CLA	ND
23	D	403	CLA	ND
23	a	404	CLA	ND
23	a	405	CLA	ND
23	a	406	CLA	ND
23	a	409	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	b	617	CLA	ND
23	b	618	CLA	ND
23	b	619	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	c	501	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND

All (2107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C1A-C2A-CAA-CBA
23	A	404	CLA	C3A-C2A-CAA-CBA
23	A	405	CLA	C2B-C3B-CAB-CBB
23	A	405	CLA	C4B-C3B-CAB-CBB
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C1A-C2A-CAA-CBA
23	B	602	CLA	C6-C7-C8-C9
23	B	604	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C1A-C2A-CAA-CBA
23	B	606	CLA	C3A-C2A-CAA-CBA
23	B	606	CLA	C2B-C3B-CAB-CBB
23	B	606	CLA	C4B-C3B-CAB-CBB
23	B	607	CLA	C1A-C2A-CAA-CBA
23	B	607	CLA	C4B-C3B-CAB-CBB
23	B	608	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	C2B-C3B-CAB-CBB
23	B	609	CLA	C4B-C3B-CAB-CBB
23	B	610	CLA	C2B-C3B-CAB-CBB
23	B	610	CLA	C4B-C3B-CAB-CBB
23	B	610	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	616	CLA	C2B-C3B-CAB-CBB
23	B	616	CLA	C4B-C3B-CAB-CBB
23	B	616	CLA	CBD-CGD-O2D-CED
23	C	501	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	CBD-CGD-O2D-CED
23	C	505	CLA	C1A-C2A-CAA-CBA
23	C	505	CLA	C3A-C2A-CAA-CBA
23	C	505	CLA	C4B-C3B-CAB-CBB
23	C	505	CLA	CBD-CGD-O2D-CED
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	C2B-C3B-CAB-CBB
23	C	510	CLA	C4B-C3B-CAB-CBB
23	C	511	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C3A-C2A-CAA-CBA
23	a	405	CLA	C1A-C2A-CAA-CBA
23	a	406	CLA	C2B-C3B-CAB-CBB
23	a	406	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	CBD-CGD-O2D-CED
23	b	605	CLA	C1A-C2A-CAA-CBA
23	b	605	CLA	C3A-C2A-CAA-CBA
23	b	605	CLA	C6-C7-C8-C9
23	b	606	CLA	CBD-CGD-O2D-CED
23	b	607	CLA	CBD-CGD-O2D-CED
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	609	CLA	C1A-C2A-CAA-CBA
23	b	609	CLA	C3A-C2A-CAA-CBA
23	b	609	CLA	C2B-C3B-CAB-CBB
23	b	609	CLA	C4B-C3B-CAB-CBB
23	b	610	CLA	C1A-C2A-CAA-CBA
23	b	610	CLA	C3A-C2A-CAA-CBA
23	b	610	CLA	C4B-C3B-CAB-CBB
23	b	611	CLA	C1A-C2A-CAA-CBA
23	b	611	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C2B-C3B-CAB-CBB
23	b	612	CLA	C4B-C3B-CAB-CBB
23	b	613	CLA	C2B-C3B-CAB-CBB
23	b	613	CLA	C4B-C3B-CAB-CBB
23	b	613	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	617	CLA	CAD-CBD-CGD-O2D
23	b	619	CLA	C3A-C2A-CAA-CBA
23	b	619	CLA	C2B-C3B-CAB-CBB
23	b	619	CLA	C4B-C3B-CAB-CBB
23	b	619	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	C2B-C3B-CAB-CBB
23	c	501	CLA	C4B-C3B-CAB-CBB
23	c	504	CLA	C4B-C3B-CAB-CBB
23	c	504	CLA	CBD-CGD-O2D-CED
23	c	505	CLA	C1A-C2A-CAA-CBA
23	c	505	CLA	C2B-C3B-CAB-CBB
23	c	505	CLA	C4B-C3B-CAB-CBB
23	c	505	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2B-C3B-CAB-CBB
23	c	510	CLA	C4B-C3B-CAB-CBB
23	d	402	CLA	C4-C3-C5-C6
25	A	408	PL9	C7-C8-C9-C11
25	A	408	PL9	C12-C13-C14-C16
25	A	408	PL9	C17-C18-C19-C20
25	A	408	PL9	C17-C18-C19-C21
25	A	408	PL9	C22-C23-C24-C25
25	A	408	PL9	C27-C28-C29-C30
25	A	408	PL9	C27-C28-C29-C31
25	A	408	PL9	C28-C29-C31-C32
25	A	408	PL9	C30-C29-C31-C32
25	A	408	PL9	C35-C34-C36-C37
25	A	408	PL9	C37-C38-C39-C41
25	D	404	PL9	C27-C28-C29-C30
25	D	404	PL9	C27-C28-C29-C31
25	J	101	PL9	C7-C8-C9-C10
25	J	101	PL9	C7-C8-C9-C11
25	J	101	PL9	C22-C23-C24-C25
25	J	101	PL9	C22-C23-C24-C26
25	a	410	PL9	C7-C8-C9-C11
25	a	410	PL9	C12-C13-C14-C16
25	a	410	PL9	C17-C18-C19-C20
25	a	410	PL9	C17-C18-C19-C21
25	a	410	PL9	C22-C23-C24-C25
25	a	410	PL9	C27-C28-C29-C30
25	a	410	PL9	C27-C28-C29-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	a	410	PL9	C28-C29-C31-C32
25	a	410	PL9	C30-C29-C31-C32
25	d	404	PL9	C22-C23-C24-C25
25	d	404	PL9	C27-C28-C29-C30
25	d	404	PL9	C27-C28-C29-C31
25	j	101	PL9	C7-C8-C9-C10
25	j	101	PL9	C7-C8-C9-C11
25	j	101	PL9	C22-C23-C24-C25
25	j	101	PL9	C22-C23-C24-C26
27	B	618	BCR	C21-C22-C23-C24
27	B	618	BCR	C37-C22-C23-C24
27	B	618	BCR	C23-C24-C25-C26
27	C	514	BCR	C11-C12-C13-C14
27	C	514	BCR	C11-C12-C13-C35
27	C	515	BCR	C7-C8-C9-C10
27	D	405	BCR	C7-C8-C9-C10
27	D	405	BCR	C7-C8-C9-C34
27	K	102	BCR	C7-C8-C9-C10
27	K	102	BCR	C21-C22-C23-C24
27	K	102	BCR	C37-C22-C23-C24
27	T	103	BCR	C21-C22-C23-C24
27	T	103	BCR	C37-C22-C23-C24
27	T	103	BCR	C23-C24-C25-C26
27	c	514	BCR	C11-C12-C13-C14
27	c	514	BCR	C11-C12-C13-C35
27	f	102	BCR	C7-C8-C9-C10
27	f	102	BCR	C7-C8-C9-C34
27	k	102	BCR	C7-C8-C9-C10
27	k	102	BCR	C7-C8-C9-C34
27	k	102	BCR	C21-C22-C23-C24
27	x	101	BCR	C1-C6-C7-C8
27	x	101	BCR	C5-C6-C7-C8
28	A	411	DGD	C2D-C1D-O3G-C3G
28	A	411	DGD	O6D-C1D-O3G-C3G
28	B	626	DGD	C2B-C1B-O2G-C2G
28	B	626	DGD	O1B-C1B-O2G-C2G
28	B	626	DGD	O2G-C2G-C3G-O3G
28	C	516	DGD	C2E-C1E-O5D-C6D
28	C	517	DGD	C2B-C1B-O2G-C2G
28	C	517	DGD	O1B-C1B-O2G-C2G
28	C	517	DGD	O2G-C2G-C3G-O3G
28	C	518	DGD	O6D-C1D-O3G-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	410	DGD	C2B-C1B-O2G-C2G
28	D	410	DGD	O6D-C1D-O3G-C3G
28	a	413	DGD	C2D-C1D-O3G-C3G
28	a	413	DGD	O6D-C1D-O3G-C3G
28	b	602	DGD	C2B-C1B-O2G-C2G
28	b	602	DGD	O1B-C1B-O2G-C2G
28	c	518	DGD	C2B-C1B-O2G-C2G
28	c	518	DGD	O1B-C1B-O2G-C2G
28	c	518	DGD	O2G-C2G-C3G-O3G
28	c	519	DGD	O6D-C1D-O3G-C3G
28	d	408	DGD	C2B-C1B-O2G-C2G
28	d	408	DGD	O6D-C1D-O3G-C3G
29	A	412	LHG	C3-O3-P-O5
29	A	412	LHG	C4-O6-P-O3
29	A	412	LHG	C4-O6-P-O4
29	A	415	LHG	C3-O3-P-O6
29	A	415	LHG	C4-O6-P-O3
29	A	415	LHG	C4-O6-P-O4
29	A	415	LHG	C4-O6-P-O5
29	a	414	LHG	C3-O3-P-O5
29	a	414	LHG	C4-O6-P-O3
29	a	414	LHG	C4-O6-P-O4
29	a	414	LHG	C4-O6-P-O5
29	a	417	LHG	C3-O3-P-O6
29	a	417	LHG	C4-O6-P-O3
29	a	417	LHG	C4-O6-P-O4
29	a	417	LHG	C4-O6-P-O5
30	A	413	SQD	O5-C1-O6-C44
30	A	417	SQD	O6-C44-C45-O47
30	A	417	SQD	C24-C23-O48-C46
30	B	625	SQD	O5-C5-C6-S
30	D	409	SQD	C2-C1-O6-C44
30	D	409	SQD	O6-C44-C45-O47
30	D	409	SQD	O49-C7-O47-C45
30	D	409	SQD	C8-C7-O47-C45
30	F	102	SQD	O5-C1-O6-C44
30	F	102	SQD	C8-C7-O47-C45
30	a	401	SQD	O6-C44-C45-O47
30	a	401	SQD	C24-C23-O48-C46
30	a	415	SQD	O5-C1-O6-C44
30	b	601	SQD	O5-C5-C6-S
30	d	407	SQD	C2-C1-O6-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	d	407	SQD	O6-C44-C45-O47
30	d	407	SQD	O49-C7-O47-C45
30	d	407	SQD	C8-C7-O47-C45
30	f	103	SQD	O5-C1-O6-C44
30	f	103	SQD	C8-C7-O47-C45
30	f	103	SQD	O10-C23-O48-C46
31	B	622	LMG	O9-C10-O7-C8
31	B	622	LMG	C11-C10-O7-C8
31	C	520	LMG	C8-C9-O8-C28
31	C	520	LMG	O9-C10-O7-C8
31	C	520	LMG	C11-C10-O7-C8
31	D	406	LMG	C11-C10-O7-C8
31	D	407	LMG	O1-C7-C8-O7
31	D	407	LMG	O9-C10-O7-C8
31	D	407	LMG	C11-C10-O7-C8
31	D	408	LMG	C2-C1-O1-C7
31	D	408	LMG	O6-C1-O1-C7
31	M	101	LMG	O9-C10-O7-C8
31	M	102	LMG	O9-C10-O7-C8
31	b	623	LMG	O1-C7-C8-O7
31	b	623	LMG	O9-C10-O7-C8
31	b	623	LMG	C11-C10-O7-C8
31	b	624	LMG	O9-C10-O7-C8
31	b	624	LMG	C11-C10-O7-C8
31	c	520	LMG	C8-C9-O8-C28
31	c	520	LMG	O9-C10-O7-C8
31	c	520	LMG	C11-C10-O7-C8
31	d	405	LMG	C11-C10-O7-C8
31	d	406	LMG	C2-C1-O1-C7
31	d	406	LMG	O6-C1-O1-C7
31	d	406	LMG	O10-C28-O8-C9
31	k	103	LMG	C11-C10-O7-C8
34	v	201	HEM	C3D-CAD-CBD-CGD
23	A	403	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	O1D-CGD-O2D-CED
23	C	505	CLA	O1D-CGD-O2D-CED
23	a	404	CLA	O1D-CGD-O2D-CED
23	c	505	CLA	O1D-CGD-O2D-CED
33	B	627	LMT	C3'-C4'-O1B-C1B
33	T	101	LMT	C3'-C4'-O1B-C1B
23	C	503	CLA	O1D-CGD-O2D-CED
23	b	607	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	503	CLA	O1D-CGD-O2D-CED
23	A	403	CLA	CBD-CGD-O2D-CED
23	B	603	CLA	CBD-CGD-O2D-CED
23	B	611	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	CBD-CGD-O2D-CED
23	C	501	CLA	CBD-CGD-O2D-CED
23	C	503	CLA	CBD-CGD-O2D-CED
23	C	506	CLA	CBD-CGD-O2D-CED
23	C	508	CLA	CBD-CGD-O2D-CED
23	a	404	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	CBD-CGD-O2D-CED
23	c	503	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
30	A	417	SQD	O10-C23-O48-C46
30	a	401	SQD	O10-C23-O48-C46
31	D	407	LMG	O10-C28-O8-C9
31	D	408	LMG	O10-C28-O8-C9
31	b	623	LMG	O10-C28-O8-C9
23	B	616	CLA	O1D-CGD-O2D-CED
23	b	619	CLA	O1D-CGD-O2D-CED
28	b	622	DGD	C4D-C5D-C6D-O5D
25	A	408	PL9	C37-C38-C39-C40
25	a	410	PL9	C37-C38-C39-C40
25	a	410	PL9	C37-C38-C39-C41
23	c	511	CLA	O1D-CGD-O2D-CED
31	A	414	LMG	C29-C28-O8-C9
31	D	408	LMG	C29-C28-O8-C9
31	d	406	LMG	C29-C28-O8-C9
23	C	509	CLA	CBD-CGD-O2D-CED
28	D	410	DGD	O1A-C1A-O1G-C1G
28	d	408	DGD	O1A-C1A-O1G-C1G
30	F	102	SQD	O10-C23-O48-C46
31	A	414	LMG	O10-C28-O8-C9
31	C	520	LMG	O10-C28-O8-C9
31	E	101	LMG	O10-C28-O8-C9
31	a	416	LMG	O10-C28-O8-C9
31	c	520	LMG	O10-C28-O8-C9
31	e	101	LMG	O10-C28-O8-C9
23	B	601	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	511	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	O1D-CGD-O2D-CED
23	B	610	CLA	O1D-CGD-O2D-CED
23	C	504	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	O1D-CGD-O2D-CED
28	a	413	DGD	O6E-C5E-C6E-O5E
28	C	517	DGD	C4E-C5E-C6E-O5E
28	c	518	DGD	C4E-C5E-C6E-O5E
28	D	410	DGD	O6D-C5D-C6D-O5D
28	d	408	DGD	O6D-C5D-C6D-O5D
23	B	614	CLA	CBD-CGD-O2D-CED
23	b	616	CLA	CBD-CGD-O2D-CED
28	C	516	DGD	O1B-C1B-O2G-C2G
28	C	518	DGD	O1B-C1B-O2G-C2G
28	D	410	DGD	O1B-C1B-O2G-C2G
28	c	517	DGD	O1B-C1B-O2G-C2G
28	d	408	DGD	O1B-C1B-O2G-C2G
31	A	418	LMG	O9-C10-O7-C8
31	D	406	LMG	O9-C10-O7-C8
31	E	101	LMG	O9-C10-O7-C8
31	I	101	LMG	O9-C10-O7-C8
31	d	405	LMG	O9-C10-O7-C8
31	e	101	LMG	O9-C10-O7-C8
31	i	101	LMG	O9-C10-O7-C8
23	A	405	CLA	C3-C5-C6-C7
23	B	614	CLA	C3-C5-C6-C7
23	a	406	CLA	C3-C5-C6-C7
24	D	402	PHO	C3-C5-C6-C7
24	a	407	PHO	C3-C5-C6-C7
23	b	604	CLA	O1D-CGD-O2D-CED
28	D	410	DGD	C2A-C1A-O1G-C1G
30	F	102	SQD	C24-C23-O48-C46
30	f	103	SQD	C24-C23-O48-C46
31	C	519	LMG	C29-C28-O8-C9
31	C	520	LMG	C29-C28-O8-C9
31	D	407	LMG	C29-C28-O8-C9
31	E	101	LMG	C29-C28-O8-C9
31	b	623	LMG	C29-C28-O8-C9
31	c	520	LMG	C29-C28-O8-C9
31	e	101	LMG	C29-C28-O8-C9
33	b	603	LMT	C3'-C4'-O1B-C1B
23	B	606	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	607	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	CBD-CGD-O2D-CED
23	b	609	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	CBD-CGD-O2D-CED
23	b	614	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
24	A	406	PHO	CBD-CGD-O2D-CED
28	C	516	DGD	C2B-C1B-O2G-C2G
28	c	517	DGD	C2B-C1B-O2G-C2G
31	C	519	LMG	C11-C10-O7-C8
31	M	101	LMG	C11-C10-O7-C8
31	M	102	LMG	C11-C10-O7-C8
23	B	603	CLA	O1D-CGD-O2D-CED
23	b	606	CLA	O1D-CGD-O2D-CED
23	c	504	CLA	O1D-CGD-O2D-CED
23	b	613	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C4-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	D	401	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	606	CLA	C4-C3-C5-C6
25	D	404	PL9	C35-C34-C36-C37
25	a	410	PL9	C35-C34-C36-C37
25	d	404	PL9	C35-C34-C36-C37
23	B	602	CLA	C2-C3-C5-C6
23	B	603	CLA	C2-C3-C5-C6
23	D	401	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	606	CLA	C2-C3-C5-C6
23	d	402	CLA	C2-C3-C5-C6
25	A	408	PL9	C33-C34-C36-C37
25	a	410	PL9	C33-C34-C36-C37
33	B	628	LMT	C3'-C4'-O1B-C1B
23	c	513	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	O1D-CGD-O2D-CED
28	A	411	DGD	O6E-C5E-C6E-O5E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C2A-CAA-CBA-CGA
23	b	613	CLA	C2A-CAA-CBA-CGA
23	B	608	CLA	C3-C5-C6-C7
23	b	611	CLA	C3-C5-C6-C7
23	b	617	CLA	C3-C5-C6-C7
28	d	408	DGD	C2A-C1A-O1G-C1G
31	a	416	LMG	C29-C28-O8-C9
31	i	101	LMG	C29-C28-O8-C9
31	k	103	LMG	C29-C28-O8-C9
25	A	408	PL9	C12-C13-C14-C15
25	a	410	PL9	C12-C13-C14-C15
28	B	621	DGD	C4D-C5D-C6D-O5D
25	A	408	PL9	C22-C23-C24-C26
25	a	410	PL9	C22-C23-C24-C26
31	k	103	LMG	O6-C5-C6-O5
30	F	102	SQD	O49-C7-O47-C45
31	a	402	LMG	O9-C10-O7-C8
33	I	102	LMT	C3'-C4'-O1B-C1B
33	i	102	LMT	C3'-C4'-O1B-C1B
23	c	508	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	C3-C5-C6-C7
23	B	612	CLA	CBD-CGD-O2D-CED
29	A	412	LHG	O2-C2-C3-O3
29	a	414	LHG	O2-C2-C3-O3
23	C	508	CLA	O1D-CGD-O2D-CED
31	I	101	LMG	C29-C28-O8-C9
31	C	519	LMG	O6-C5-C6-O5
23	C	506	CLA	O1D-CGD-O2D-CED
28	C	517	DGD	O6E-C5E-C6E-O5E
23	b	615	CLA	CBD-CGD-O2D-CED
31	A	418	LMG	C11-C10-O7-C8
31	I	101	LMG	C11-C10-O7-C8
31	a	402	LMG	C11-C10-O7-C8
31	d	406	LMG	C11-C10-O7-C8
31	i	101	LMG	C11-C10-O7-C8
31	C	519	LMG	O10-C28-O8-C9
28	C	516	DGD	O6E-C5E-C6E-O5E
31	A	418	LMG	O6-C5-C6-O5
31	D	407	LMG	O6-C5-C6-O5
31	M	101	LMG	O6-C5-C6-O5
31	a	402	LMG	O6-C5-C6-O5
28	A	411	DGD	C4E-C5E-C6E-O5E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	B	621	DGD	C4E-C5E-C6E-O5E
23	b	610	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	C3-C5-C6-C7
28	c	518	DGD	O6E-C5E-C6E-O5E
28	a	413	DGD	C4E-C5E-C6E-O5E
23	C	501	CLA	O1D-CGD-O2D-CED
23	A	404	CLA	C4-C3-C5-C6
24	D	402	PHO	C4-C3-C5-C6
24	a	407	PHO	C4-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
24	D	402	PHO	C2-C3-C5-C6
24	a	407	PHO	C2-C3-C5-C6
31	k	103	LMG	O10-C28-O8-C9
25	A	408	PL9	C24-C26-C27-C28
25	D	404	PL9	C34-C36-C37-C38
25	a	410	PL9	C24-C26-C27-C28
25	a	410	PL9	C29-C31-C32-C33
28	b	622	DGD	C4E-C5E-C6E-O5E
23	B	609	CLA	CBD-CGD-O2D-CED
28	B	621	DGD	O6E-C5E-C6E-O5E
34	V	201	HEM	C3D-CAD-CBD-CGD
23	B	611	CLA	O1D-CGD-O2D-CED
28	B	621	DGD	O6E-C1E-O5D-C6D
28	B	626	DGD	O6E-C1E-O5D-C6D
28	b	622	DGD	O6D-C1D-O3G-C3G
28	b	622	DGD	O6E-C1E-O5D-C6D
28	c	517	DGD	O6D-C1D-O3G-C3G
28	c	517	DGD	O6E-C1E-O5D-C6D
31	C	519	LMG	O6-C1-O1-C7
31	C	520	LMG	O6-C1-O1-C7
31	E	101	LMG	O6-C1-O1-C7
31	M	101	LMG	O6-C1-O1-C7
31	M	102	LMG	O6-C1-O1-C7
31	c	520	LMG	O6-C1-O1-C7
31	e	101	LMG	O6-C1-O1-C7
31	k	103	LMG	O6-C1-O1-C7
28	c	517	DGD	O6E-C5E-C6E-O5E
31	M	102	LMG	O6-C5-C6-O5
31	c	520	LMG	O6-C5-C6-O5
23	b	611	CLA	CBD-CGD-O2D-CED
24	a	408	PHO	CBD-CGD-O2D-CED
28	b	622	DGD	O6E-C5E-C6E-O5E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	C	520	LMG	O6-C5-C6-O5
31	a	416	LMG	O6-C5-C6-O5
31	b	623	LMG	O6-C5-C6-O5
28	D	410	DGD	C4D-C5D-C6D-O5D
28	d	408	DGD	C4D-C5D-C6D-O5D
23	C	509	CLA	O1D-CGD-O2D-CED
31	b	623	LMG	C4-C5-C6-O5
30	b	601	SQD	C8-C7-O47-C45
31	A	414	LMG	O6-C5-C6-O5
31	k	103	LMG	C4-C5-C6-O5
29	A	412	LHG	C1-C2-C3-O3
29	a	414	LHG	C1-C2-C3-O3
23	B	616	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CBA-CGA-O2A-C1
23	b	619	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
24	D	402	PHO	CBA-CGA-O2A-C1
24	a	407	PHO	CBA-CGA-O2A-C1
30	b	601	SQD	C24-C23-O48-C46
23	B	608	CLA	CBD-CGD-O2D-CED
31	C	520	LMG	C4-C5-C6-O5
31	a	416	LMG	C4-C5-C6-O5
23	B	614	CLA	O1D-CGD-O2D-CED
23	C	513	CLA	O1D-CGD-O2D-CED
23	b	616	CLA	O1D-CGD-O2D-CED
28	C	516	DGD	C4E-C5E-C6E-O5E
31	C	519	LMG	C4-C5-C6-O5
23	A	404	CLA	C2-C3-C5-C6
23	B	602	CLA	C3-C5-C6-C7
23	B	608	CLA	C6-C7-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	C	509	CLA	C6-C7-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	b	611	CLA	C6-C7-C8-C9
23	b	613	CLA	C14-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C9
23	c	511	CLA	C6-C7-C8-C9
31	D	407	LMG	C4-C5-C6-O5
23	b	614	CLA	O1D-CGD-O2D-CED
28	B	621	DGD	C2E-C1E-O5D-C6D
28	B	626	DGD	C2E-C1E-O5D-C6D
28	C	516	DGD	C2D-C1D-O3G-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	518	DGD	C2D-C1D-O3G-C3G
28	b	602	DGD	C2E-C1E-O5D-C6D
28	b	622	DGD	C2E-C1E-O5D-C6D
28	c	517	DGD	C2D-C1D-O3G-C3G
28	c	517	DGD	C2E-C1E-O5D-C6D
28	c	519	DGD	C2D-C1D-O3G-C3G
30	A	413	SQD	C2-C1-O6-C44
30	a	415	SQD	C2-C1-O6-C44
31	C	519	LMG	C2-C1-O1-C7
31	C	520	LMG	C2-C1-O1-C7
31	E	101	LMG	C2-C1-O1-C7
31	M	101	LMG	C2-C1-O1-C7
31	M	102	LMG	C2-C1-O1-C7
31	c	520	LMG	C2-C1-O1-C7
31	e	101	LMG	C2-C1-O1-C7
31	k	103	LMG	C2-C1-O1-C7
31	D	406	LMG	C10-C11-C12-C13
23	B	606	CLA	O1D-CGD-O2D-CED
24	a	407	PHO	O1A-CGA-O2A-C1
31	I	101	LMG	O10-C28-O8-C9
31	A	414	LMG	C4-C5-C6-O5
23	b	612	CLA	O1D-CGD-O2D-CED
27	B	618	BCR	C7-C8-C9-C34
27	C	515	BCR	C7-C8-C9-C34
27	K	102	BCR	C7-C8-C9-C34
27	T	103	BCR	C7-C8-C9-C34
27	c	516	BCR	C7-C8-C9-C34
27	f	102	BCR	C37-C22-C23-C24
27	k	102	BCR	C37-C22-C23-C24
27	B	618	BCR	C7-C8-C9-C10
27	C	514	BCR	C7-C8-C9-C10
27	T	103	BCR	C7-C8-C9-C10
27	c	514	BCR	C7-C8-C9-C10
28	c	517	DGD	C4E-C5E-C6E-O5E
31	c	520	LMG	C4-C5-C6-O5
23	B	607	CLA	C2A-CAA-CBA-CGA
23	B	610	CLA	C2A-CAA-CBA-CGA
23	C	508	CLA	C2A-CAA-CBA-CGA
31	E	101	LMG	C28-C29-C30-C31
31	e	101	LMG	C28-C29-C30-C31
23	B	616	CLA	O1A-CGA-O2A-C1
23	b	619	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	513	CLA	O1A-CGA-O2A-C1
24	D	402	PHO	O1A-CGA-O2A-C1
30	B	625	SQD	C8-C7-O47-C45
28	b	602	DGD	O2G-C2G-C3G-O3G
23	B	607	CLA	C15-C16-C17-C18
23	b	617	CLA	O1D-CGD-O2D-CED
23	c	501	CLA	O1D-CGD-O2D-CED
25	D	404	PL9	C22-C23-C24-C25
25	J	101	PL9	C12-C13-C14-C15
23	b	610	CLA	C15-C16-C17-C18
23	b	615	CLA	C5-C6-C7-C8
23	b	605	CLA	C3-C5-C6-C7
23	C	512	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	C13-C15-C16-C17
23	B	605	CLA	CBA-CGA-O2A-C1
23	B	612	CLA	C5-C6-C7-C8
23	B	616	CLA	C10-C11-C12-C13
23	c	509	CLA	C5-C6-C7-C8
28	c	517	DGD	C1B-C2B-C3B-C4B
31	c	520	LMG	C28-C29-C30-C31
31	d	405	LMG	C10-C11-C12-C13
28	c	519	DGD	O1B-C1B-O2G-C2G
30	f	103	SQD	O49-C7-O47-C45
31	k	103	LMG	O9-C10-O7-C8
23	B	607	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	O1D-CGD-O2D-CED
25	D	404	PL9	C29-C31-C32-C33
25	d	404	PL9	C29-C31-C32-C33
23	A	404	CLA	C3-C5-C6-C7
23	B	616	CLA	C5-C6-C7-C8
23	a	406	CLA	C10-C11-C12-C13
23	b	615	CLA	C13-C15-C16-C17
23	c	506	CLA	C15-C16-C17-C18
31	I	101	LMG	O6-C5-C6-O5
28	C	516	DGD	C1B-C2B-C3B-C4B
28	b	602	DGD	C1A-C2A-C3A-C4A
28	d	408	DGD	C1B-C2B-C3B-C4B
31	C	520	LMG	C10-C11-C12-C13
31	C	520	LMG	C28-C29-C30-C31
23	C	513	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
23	B	601	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	604	CLA	C13-C15-C16-C17
23	D	401	CLA	C15-C16-C17-C18
23	b	619	CLA	C10-C11-C12-C13
23	c	506	CLA	C5-C6-C7-C8
23	c	508	CLA	C15-C16-C17-C18
23	d	402	CLA	C15-C16-C17-C18
24	A	406	PHO	C15-C16-C17-C18
23	B	601	CLA	C2A-CAA-CBA-CGA
23	C	512	CLA	C2A-CAA-CBA-CGA
23	b	604	CLA	C2A-CAA-CBA-CGA
23	c	508	CLA	C2A-CAA-CBA-CGA
23	c	512	CLA	C2A-CAA-CBA-CGA
23	A	404	CLA	C15-C16-C17-C18
23	B	610	CLA	C8-C10-C11-C12
23	C	501	CLA	C15-C16-C17-C18
23	C	503	CLA	C10-C11-C12-C13
23	C	506	CLA	C15-C16-C17-C18
23	C	508	CLA	C10-C11-C12-C13
23	b	610	CLA	C13-C15-C16-C17
23	b	612	CLA	C13-C15-C16-C17
23	b	619	CLA	C5-C6-C7-C8
23	c	504	CLA	C13-C15-C16-C17
28	A	411	DGD	C1B-C2B-C3B-C4B
28	B	626	DGD	C1A-C2A-C3A-C4A
28	D	410	DGD	C1B-C2B-C3B-C4B
28	a	413	DGD	C1B-C2B-C3B-C4B
31	B	622	LMG	C10-C11-C12-C13
31	b	624	LMG	C10-C11-C12-C13
23	b	609	CLA	O1D-CGD-O2D-CED
31	i	101	LMG	O10-C28-O8-C9
28	B	621	DGD	O6D-C1D-O3G-C3G
28	C	516	DGD	O6D-C1D-O3G-C3G
28	C	516	DGD	O6E-C1E-O5D-C6D
28	b	602	DGD	O6E-C1E-O5D-C6D
31	A	418	LMG	O6-C1-O1-C7
23	A	405	CLA	C10-C11-C12-C13
23	B	607	CLA	C13-C15-C16-C17
23	B	608	CLA	C15-C16-C17-C18
23	B	611	CLA	C15-C16-C17-C18
23	B	612	CLA	C13-C15-C16-C17
23	C	504	CLA	C13-C15-C16-C17
23	C	504	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	509	CLA	C5-C6-C7-C8
23	a	405	CLA	C15-C16-C17-C18
23	b	604	CLA	C13-C15-C16-C17
23	b	607	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
23	b	613	CLA	C8-C10-C11-C12
23	b	614	CLA	C15-C16-C17-C18
23	c	503	CLA	C10-C11-C12-C13
24	a	408	PHO	C15-C16-C17-C18
31	c	520	LMG	C10-C11-C12-C13
23	C	508	CLA	C15-C16-C17-C18
23	c	501	CLA	C15-C16-C17-C18
23	c	504	CLA	C15-C16-C17-C18
23	c	507	CLA	C5-C6-C7-C8
23	c	508	CLA	C10-C11-C12-C13
31	C	519	LMG	O9-C10-O7-C8
31	i	101	LMG	O6-C5-C6-O5
23	A	403	CLA	C3-C5-C6-C7
23	b	619	CLA	C3-C5-C6-C7
23	B	612	CLA	O1D-CGD-O2D-CED
23	B	613	CLA	C5-C6-C7-C8
23	C	501	CLA	C8-C10-C11-C12
23	C	506	CLA	C13-C15-C16-C17
23	C	507	CLA	C5-C6-C7-C8
23	c	501	CLA	C8-C10-C11-C12
23	c	505	CLA	C10-C11-C12-C13
30	a	415	SQD	C7-C8-C9-C10
23	c	513	CLA	O1D-CGD-O2D-CED
24	A	406	PHO	O1D-CGD-O2D-CED
23	C	504	CLA	C10-C11-C12-C13
23	C	510	CLA	C15-C16-C17-C18
23	c	506	CLA	C13-C15-C16-C17
23	d	402	CLA	C13-C15-C16-C17
31	M	101	LMG	C29-C28-O8-C9
31	M	102	LMG	C29-C28-O8-C9
31	D	408	LMG	C11-C10-O7-C8
30	b	601	SQD	O10-C23-O48-C46
31	C	519	LMG	C10-C11-C12-C13
23	C	513	CLA	C15-C16-C17-C18
23	c	501	CLA	C10-C11-C12-C13
28	C	516	DGD	C1A-C2A-C3A-C4A
28	b	622	DGD	C1B-C2B-C3B-C4B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	625	SQD	C24-C23-O48-C46
23	A	405	CLA	C15-C16-C17-C18
23	B	615	CLA	C13-C15-C16-C17
23	C	505	CLA	C10-C11-C12-C13
23	b	619	CLA	C13-C15-C16-C17
23	c	504	CLA	C10-C11-C12-C13
23	c	511	CLA	C5-C6-C7-C8
23	c	513	CLA	C15-C16-C17-C18
28	c	518	DGD	O6D-C5D-C6D-O5D
30	B	625	SQD	O10-C23-O48-C46
23	B	616	CLA	C3-C5-C6-C7
23	b	615	CLA	O1D-CGD-O2D-CED
28	c	517	DGD	C1A-C2A-C3A-C4A
23	b	616	CLA	C5-C6-C7-C8
31	M	101	LMG	C4-C5-C6-O5
23	B	616	CLA	C13-C15-C16-C17
23	C	506	CLA	C5-C6-C7-C8
23	C	511	CLA	C5-C6-C7-C8
23	D	401	CLA	C13-C15-C16-C17
23	c	510	CLA	C15-C16-C17-C18
28	C	517	DGD	O6D-C5D-C6D-O5D
28	c	518	DGD	C4D-C5D-C6D-O5D
23	B	608	CLA	C5-C6-C7-C8
23	b	618	CLA	C13-C15-C16-C17
25	A	408	PL9	C7-C8-C9-C10
28	C	517	DGD	C2D-C1D-O3G-C3G
28	C	517	DGD	C2E-C1E-O5D-C6D
28	c	518	DGD	C2E-C1E-O5D-C6D
31	B	622	LMG	C2-C1-O1-C7
31	I	101	LMG	C2-C1-O1-C7
28	B	621	DGD	C1B-C2B-C3B-C4B
25	d	404	PL9	C34-C36-C37-C38
23	C	501	CLA	C10-C11-C12-C13
30	A	413	SQD	C7-C8-C9-C10
31	a	402	LMG	C4-C5-C6-O5
27	B	618	BCR	C11-C12-C13-C35
27	C	514	BCR	C7-C8-C9-C34
27	D	405	BCR	C37-C22-C23-C24
27	c	514	BCR	C7-C8-C9-C34
27	c	516	BCR	C37-C22-C23-C24
27	j	102	BCR	C7-C8-C9-C34
27	c	516	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	f	102	BCR	C21-C22-C23-C24
28	b	622	DGD	O6D-C5D-C6D-O5D
34	f	101	HEM	C3D-CAD-CBD-CGD
23	B	605	CLA	O1A-CGA-O2A-C1
23	b	609	CLA	C2A-CAA-CBA-CGA
28	C	517	DGD	C4D-C5D-C6D-O5D
28	D	410	DGD	C1G-C2G-O2G-C1B
28	d	408	DGD	C1G-C2G-O2G-C1B
31	E	101	LMG	C7-C8-O7-C10
31	e	101	LMG	C7-C8-O7-C10
23	c	512	CLA	O1A-CGA-O2A-C1
23	C	502	CLA	C3-C5-C6-C7
23	a	404	CLA	C3-C5-C6-C7
23	a	405	CLA	C3-C5-C6-C7
23	a	406	CLA	C15-C16-C17-C18
30	D	409	SQD	O5-C1-O6-C44
31	a	402	LMG	O6-C1-O1-C7
28	C	518	DGD	C2B-C1B-O2G-C2G
23	a	409	CLA	C10-C11-C12-C13
23	B	609	CLA	O1D-CGD-O2D-CED
31	A	418	LMG	C4-C5-C6-O5
23	C	512	CLA	CBA-CGA-O2A-C1
23	C	503	CLA	C5-C6-C7-C8
23	C	509	CLA	C2-C1-O2A-CGA
23	b	611	CLA	C5-C6-C7-C8
28	d	408	DGD	C3A-C4A-C5A-C6A
29	a	417	LHG	C11-C10-C9-C8
31	A	418	LMG	C11-C12-C13-C14
31	D	408	LMG	C36-C37-C38-C39
28	C	516	DGD	C3A-C4A-C5A-C6A
28	d	408	DGD	C7B-C8B-C9B-CAB
30	B	625	SQD	C11-C10-C9-C8
31	A	414	LMG	C34-C35-C36-C37
31	B	622	LMG	C31-C32-C33-C34
31	a	416	LMG	C14-C15-C16-C17
31	b	623	LMG	C31-C32-C33-C34
30	b	601	SQD	C11-C10-C9-C8
31	A	414	LMG	C29-C30-C31-C32
28	A	411	DGD	C5B-C6B-C7B-C8B
28	C	518	DGD	C9B-CAB-CBB-CCB
28	D	410	DGD	C3A-C4A-C5A-C6A
28	D	410	DGD	C7B-C8B-C9B-CAB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	A	413	SQD	C14-C15-C16-C17
31	A	414	LMG	C14-C15-C16-C17
31	D	407	LMG	C31-C32-C33-C34
31	b	623	LMG	C30-C31-C32-C33
31	d	406	LMG	C36-C37-C38-C39
28	B	626	DGD	C2A-C3A-C4A-C5A
28	b	602	DGD	C2A-C3A-C4A-C5A
28	c	519	DGD	C9B-CAB-CBB-CCB
29	A	415	LHG	C11-C10-C9-C8
31	a	416	LMG	C29-C30-C31-C32
31	a	416	LMG	C34-C35-C36-C37
23	B	601	CLA	C4B-C3B-CAB-CBB
23	B	604	CLA	C4B-C3B-CAB-CBB
23	B	605	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	b	607	CLA	C4B-C3B-CAB-CBB
23	b	608	CLA	C4B-C3B-CAB-CBB
23	d	403	CLA	C4B-C3B-CAB-CBB
28	B	621	DGD	C6B-C7B-C8B-C9B
28	c	517	DGD	C3A-C4A-C5A-C6A
31	M	102	LMG	C29-C30-C31-C32
28	b	622	DGD	C6B-C7B-C8B-C9B
30	f	103	SQD	C12-C13-C14-C15
31	M	101	LMG	C29-C30-C31-C32
29	a	414	LHG	C25-C26-C27-C28
31	b	624	LMG	C31-C32-C33-C34
31	k	103	LMG	C10-C11-C12-C13
23	A	407	CLA	C10-C11-C12-C13
28	d	408	DGD	CCB-CDB-CEB-CFB
29	A	412	LHG	C25-C26-C27-C28
23	B	602	CLA	C3A-C2A-CAA-CBA
23	B	607	CLA	C3A-C2A-CAA-CBA
23	B	608	CLA	C3A-C2A-CAA-CBA
23	B	616	CLA	C3A-C2A-CAA-CBA
23	C	507	CLA	C3A-C2A-CAA-CBA
23	a	405	CLA	C3A-C2A-CAA-CBA
23	c	505	CLA	C3A-C2A-CAA-CBA
23	c	507	CLA	C3A-C2A-CAA-CBA
23	c	512	CLA	C3A-C2A-CAA-CBA
28	a	413	DGD	C5B-C6B-C7B-C8B
31	B	622	LMG	C34-C35-C36-C37
31	a	402	LMG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C10-C11-C12-C13
23	c	503	CLA	C5-C6-C7-C8
23	B	613	CLA	C16-C17-C18-C19
23	b	611	CLA	O1D-CGD-O2D-CED
31	D	408	LMG	C19-C20-C21-C22
29	A	415	LHG	C24-C25-C26-C27
30	F	102	SQD	C12-C13-C14-C15
31	I	101	LMG	C14-C15-C16-C17
31	b	624	LMG	C34-C35-C36-C37
28	C	518	DGD	O1G-C1G-C2G-C3G
28	c	519	DGD	O1G-C1G-C2G-C3G
28	C	517	DGD	C2A-C3A-C4A-C5A
28	c	517	DGD	C3B-C4B-C5B-C6B
29	a	417	LHG	C24-C25-C26-C27
31	i	101	LMG	C14-C15-C16-C17
28	C	517	DGD	C1A-C2A-C3A-C4A
31	b	623	LMG	C28-C29-C30-C31
28	C	516	DGD	C3B-C4B-C5B-C6B
28	D	410	DGD	CCB-CDB-CEB-CFB
28	D	410	DGD	CEB-CFB-CGB-CHB
28	c	519	DGD	C3B-C4B-C5B-C6B
30	a	415	SQD	C14-C15-C16-C17
31	C	520	LMG	C29-C30-C31-C32
31	D	407	LMG	C30-C31-C32-C33
31	a	402	LMG	C18-C19-C20-C21
31	d	406	LMG	C15-C16-C17-C18
31	d	406	LMG	C19-C20-C21-C22
33	I	102	LMT	C6-C7-C8-C9
33	i	102	LMT	C6-C7-C8-C9
33	b	625	LMT	C1-C2-C3-C4
31	C	520	LMG	C12-C13-C14-C15
31	c	520	LMG	C12-C13-C14-C15
33	B	623	LMT	C1-C2-C3-C4
28	B	626	DGD	C5B-C6B-C7B-C8B
31	c	520	LMG	C29-C30-C31-C32
31	D	407	LMG	C28-C29-C30-C31
23	B	601	CLA	C2B-C3B-CAB-CBB
23	B	604	CLA	C2B-C3B-CAB-CBB
23	B	607	CLA	C2B-C3B-CAB-CBB
23	C	501	CLA	C2B-C3B-CAB-CBB
23	C	504	CLA	C2B-C3B-CAB-CBB
23	C	505	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C2B-C3B-CAB-CBB
23	b	610	CLA	C2B-C3B-CAB-CBB
23	c	504	CLA	C2B-C3B-CAB-CBB
27	B	618	BCR	C23-C24-C25-C30
27	C	514	BCR	C1-C6-C7-C8
27	C	515	BCR	C23-C24-C25-C30
27	D	405	BCR	C1-C6-C7-C8
27	D	405	BCR	C5-C6-C7-C8
27	H	101	BCR	C1-C6-C7-C8
27	H	101	BCR	C5-C6-C7-C8
27	T	103	BCR	C23-C24-C25-C30
27	f	102	BCR	C1-C6-C7-C8
27	f	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C30
28	d	408	DGD	CEB-CFB-CGB-CHB
28	c	519	DGD	C2B-C1B-O2G-C2G
23	b	608	CLA	CBA-CGA-O2A-C1
31	I	101	LMG	C16-C17-C18-C19
31	b	623	LMG	C18-C19-C20-C21
34	F	101	HEM	C3D-CAD-CBD-CGD
28	C	518	DGD	C3B-C4B-C5B-C6B
28	d	408	DGD	CAB-CBB-CCB-CDB
30	f	103	SQD	C11-C12-C13-C14
31	D	408	LMG	C13-C14-C15-C16
23	B	606	CLA	C2A-CAA-CBA-CGA
31	d	406	LMG	C13-C14-C15-C16
23	C	512	CLA	O1A-CGA-O2A-C1
28	d	408	DGD	C2A-C3A-C4A-C5A
28	d	408	DGD	CDB-CEB-CFB-CGB
30	A	413	SQD	C27-C28-C29-C30
30	F	102	SQD	C11-C12-C13-C14
31	D	408	LMG	C14-C15-C16-C17
31	D	408	LMG	C15-C16-C17-C18
31	i	101	LMG	C16-C17-C18-C19
31	d	406	LMG	O9-C10-O7-C8
23	b	608	CLA	C4-C3-C5-C6
28	b	602	DGD	C9B-CAB-CBB-CCB
31	I	101	LMG	C12-C13-C14-C15
25	J	101	PL9	C27-C28-C29-C31
31	A	418	LMG	C18-C19-C20-C21
31	i	101	LMG	C12-C13-C14-C15
28	c	518	DGD	C1A-C2A-C3A-C4A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	509	CLA	CBA-CGA-O2A-C1
31	b	624	LMG	C29-C28-O8-C9
23	a	405	CLA	C6-C7-C8-C9
28	D	410	DGD	C2A-C3A-C4A-C5A
30	f	103	SQD	C10-C11-C12-C13
33	B	627	LMT	C2-C3-C4-C5
28	D	410	DGD	CDB-CEB-CFB-CGB
28	c	518	DGD	C2A-C3A-C4A-C5A
28	d	408	DGD	C4B-C5B-C6B-C7B
33	B	627	LMT	C7-C8-C9-C10
28	c	518	DGD	O6E-C1E-O5D-C6D
31	B	622	LMG	O6-C1-O1-C7
31	I	101	LMG	O6-C1-O1-C7
31	d	406	LMG	C14-C15-C16-C17
31	M	102	LMG	O10-C28-O8-C9
28	C	518	DGD	CAB-CBB-CCB-CDB
28	D	410	DGD	CAB-CBB-CCB-CDB
28	D	410	DGD	C4B-C5B-C6B-C7B
30	a	415	SQD	C27-C28-C29-C30
28	B	621	DGD	O6D-C5D-C6D-O5D
23	b	614	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	C16-C17-C18-C19
31	A	414	LMG	C11-C10-O7-C8
31	E	101	LMG	C11-C10-O7-C8
31	e	101	LMG	C11-C10-O7-C8
23	b	604	CLA	C10-C11-C12-C13
23	c	506	CLA	C10-C11-C12-C13
28	d	408	DGD	C6B-C7B-C8B-C9B
30	B	625	SQD	C11-C12-C13-C14
31	a	416	LMG	C30-C31-C32-C33
31	D	407	LMG	C18-C19-C20-C21
23	C	512	CLA	C13-C15-C16-C17
23	D	403	CLA	C15-C16-C17-C18
31	D	408	LMG	C8-C7-O1-C1
31	a	416	LMG	C8-C7-O1-C1
31	A	414	LMG	C30-C31-C32-C33
23	b	613	CLA	C16-C17-C18-C19
24	a	408	PHO	O1D-CGD-O2D-CED
28	b	602	DGD	C5B-C6B-C7B-C8B
31	i	101	LMG	C13-C14-C15-C16
31	b	624	LMG	C13-C14-C15-C16
33	T	101	LMT	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	503	CLA	C8-C10-C11-C12
30	A	417	SQD	C18-C19-C20-C21
33	T	101	LMT	C2-C3-C4-C5
30	B	625	SQD	C9-C10-C11-C12
23	C	513	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
28	D	410	DGD	C6B-C7B-C8B-C9B
30	b	601	SQD	C11-C12-C13-C14
30	F	102	SQD	C10-C11-C12-C13
31	E	101	LMG	C15-C16-C17-C18
25	A	408	PL9	C29-C31-C32-C33
23	B	604	CLA	C8-C10-C11-C12
23	b	605	CLA	C13-C15-C16-C17
23	c	512	CLA	C13-C15-C16-C17
23	d	403	CLA	C15-C16-C17-C18
23	B	613	CLA	C16-C17-C18-C20
23	b	613	CLA	C16-C17-C18-C20
28	c	517	DGD	C4A-C5A-C6A-C7A
31	I	101	LMG	C13-C14-C15-C16
31	e	101	LMG	C15-C16-C17-C18
23	b	608	CLA	O1A-CGA-O2A-C1
31	D	406	LMG	O6-C5-C6-O5
25	j	101	PL9	C27-C28-C29-C31
28	B	626	DGD	C9B-CAB-CBB-CCB
28	C	516	DGD	C4A-C5A-C6A-C7A
29	a	414	LHG	C30-C31-C32-C33
23	B	602	CLA	C13-C15-C16-C17
23	c	513	CLA	C13-C15-C16-C17
23	B	608	CLA	O1D-CGD-O2D-CED
31	A	418	LMG	C32-C33-C34-C35
31	E	101	LMG	O6-C5-C6-O5
28	C	518	DGD	O1G-C1G-C2G-O2G
28	c	519	DGD	O1G-C1G-C2G-O2G
30	A	413	SQD	O6-C44-C45-O47
28	c	518	DGD	CCB-CDB-CEB-CFB
28	c	519	DGD	CAB-CBB-CCB-CDB
31	B	622	LMG	C13-C14-C15-C16
23	D	403	CLA	CBA-CGA-O2A-C1
23	c	504	CLA	CBA-CGA-O2A-C1
28	C	516	DGD	C4B-C5B-C6B-C7B
28	b	622	DGD	C5B-C6B-C7B-C8B
30	A	417	SQD	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	a	402	LMG	C31-C32-C33-C34
28	c	517	DGD	C4B-C5B-C6B-C7B
23	c	509	CLA	C2-C1-O2A-CGA
23	c	503	CLA	C8-C10-C11-C12
28	d	408	DGD	C3B-C4B-C5B-C6B
31	b	623	LMG	C19-C20-C21-C22
28	D	410	DGD	C5B-C6B-C7B-C8B
23	c	510	CLA	C2-C3-C5-C6
31	D	408	LMG	O9-C10-O7-C8
23	a	409	CLA	C5-C6-C7-C8
31	A	418	LMG	C31-C32-C33-C34
23	C	501	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
23	d	403	CLA	CBA-CGA-O2A-C1
28	d	408	DGD	C5B-C6B-C7B-C8B
29	A	412	LHG	C30-C31-C32-C33
31	a	402	LMG	C32-C33-C34-C35
31	b	623	LMG	C36-C37-C38-C39
23	A	407	CLA	C5-C6-C7-C8
31	e	101	LMG	O6-C5-C6-O5
28	C	517	DGD	CCB-CDB-CEB-CFB
28	D	410	DGD	C5A-C6A-C7A-C8A
23	c	509	CLA	O1A-CGA-O2A-C1
23	c	502	CLA	C3-C5-C6-C7
28	b	602	DGD	C2B-C3B-C4B-C5B
23	B	616	CLA	C1A-C2A-CAA-CBA
23	C	501	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C1A-C2A-CAA-CBA
23	b	619	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
30	A	413	SQD	C11-C10-C9-C8
31	b	623	LMG	C13-C14-C15-C16
28	B	621	DGD	C3B-C4B-C5B-C6B
25	d	404	PL9	C47-C48-C49-C51
28	b	602	DGD	C3A-C4A-C5A-C6A
30	a	415	SQD	C17-C18-C19-C20
28	B	621	DGD	C5B-C6B-C7B-C8B
23	B	601	CLA	C6-C7-C8-C10
23	B	613	CLA	C11-C10-C8-C7
23	B	615	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C12-C13-C15-C16
23	C	502	CLA	C11-C12-C13-C15
23	C	503	CLA	C11-C12-C13-C15
23	C	505	CLA	C6-C7-C8-C10
23	C	505	CLA	C12-C13-C15-C16
23	C	511	CLA	C12-C13-C15-C16
23	b	605	CLA	C6-C7-C8-C10
23	b	606	CLA	C6-C7-C8-C10
23	b	616	CLA	C11-C10-C8-C7
23	b	618	CLA	C12-C13-C15-C16
23	c	502	CLA	C11-C12-C13-C15
23	c	503	CLA	C11-C12-C13-C15
23	c	508	CLA	C11-C10-C8-C7
23	d	402	CLA	C12-C13-C15-C16
24	a	408	PHO	C12-C13-C15-C16
28	D	410	DGD	C3B-C4B-C5B-C6B
30	b	601	SQD	C9-C10-C11-C12
23	b	604	CLA	C16-C17-C18-C20
23	b	616	CLA	C16-C17-C18-C20
23	c	512	CLA	C16-C17-C18-C20
23	B	614	CLA	C15-C16-C17-C18
23	C	512	CLA	C5-C6-C7-C8
23	b	614	CLA	O1A-CGA-O2A-C1
31	B	622	LMG	O10-C28-O8-C9
31	D	407	LMG	C36-C37-C38-C39
23	c	510	CLA	CBD-CGD-O2D-CED
23	B	601	CLA	C10-C11-C12-C13
23	C	510	CLA	C4-C3-C5-C6
25	j	101	PL9	C15-C14-C16-C17
31	I	101	LMG	C4-C5-C6-O5
23	C	510	CLA	C2-C3-C5-C6
30	A	413	SQD	C17-C18-C19-C20
23	b	607	CLA	C8-C10-C11-C12
23	C	513	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C2A-CAA-CBA-CGA
23	B	603	CLA	C6-C7-C8-C9
23	B	606	CLA	C14-C13-C15-C16
23	B	615	CLA	C11-C10-C8-C9
23	C	502	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	401	CLA	C14-C13-C15-C16
23	b	609	CLA	C14-C13-C15-C16
23	b	612	CLA	C6-C7-C8-C9
23	b	618	CLA	C11-C10-C8-C9
23	c	502	CLA	C14-C13-C15-C16
23	c	505	CLA	C6-C7-C8-C9
23	c	505	CLA	C14-C13-C15-C16
23	c	506	CLA	C14-C13-C15-C16
23	c	508	CLA	C11-C10-C8-C9
23	c	512	CLA	C11-C12-C13-C14
28	C	517	DGD	CAB-CBB-CCB-CDB
23	B	611	CLA	CBA-CGA-O2A-C1
23	C	511	CLA	CBA-CGA-O2A-C1
25	j	101	PL9	C12-C13-C14-C15
28	b	622	DGD	C3B-C4B-C5B-C6B
28	c	518	DGD	C2D-C1D-O3G-C3G
31	b	624	LMG	C2-C1-O1-C7
23	c	505	CLA	C15-C16-C17-C18
31	D	408	LMG	C32-C33-C34-C35
31	D	408	LMG	C28-C29-C30-C31
31	d	406	LMG	C10-C11-C12-C13
31	d	406	LMG	C28-C29-C30-C31
25	A	408	PL9	C14-C16-C17-C18
28	D	410	DGD	C1G-C2G-C3G-O3G
28	b	602	DGD	C1G-C2G-C3G-O3G
28	b	622	DGD	O1G-C1G-C2G-C3G
28	d	408	DGD	C1G-C2G-C3G-O3G
30	A	417	SQD	O6-C44-C45-C46
30	B	625	SQD	C44-C45-C46-O48
30	a	401	SQD	O6-C44-C45-C46
30	b	601	SQD	C44-C45-C46-O48
31	C	519	LMG	C7-C8-C9-O8
31	D	407	LMG	O1-C7-C8-C9
31	D	408	LMG	O1-C7-C8-C9
31	I	101	LMG	O1-C7-C8-C9
31	d	406	LMG	O1-C7-C8-C9
31	k	103	LMG	C7-C8-C9-O8
28	C	516	DGD	C5A-C6A-C7A-C8A
30	a	415	SQD	C11-C10-C9-C8
23	C	505	CLA	C15-C16-C17-C18
31	M	102	LMG	C4-C5-C6-O5
23	C	505	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	622	LMG	C29-C28-O8-C9
23	B	610	CLA	C16-C17-C18-C20
28	B	626	DGD	C2B-C3B-C4B-C5B
28	d	408	DGD	C8B-C9B-CAB-CBB
23	B	602	CLA	C5-C6-C7-C8
30	D	409	SQD	C9-C10-C11-C12
23	c	510	CLA	C4-C3-C5-C6
27	c	515	BCR	C7-C8-C9-C34
28	d	408	DGD	C5A-C6A-C7A-C8A
31	d	405	LMG	O6-C5-C6-O5
23	D	403	CLA	O1A-CGA-O2A-C1
23	c	504	CLA	O1A-CGA-O2A-C1
23	B	604	CLA	C15-C16-C17-C18
31	D	407	LMG	C20-C21-C22-C23
31	E	101	LMG	C17-C18-C19-C20
28	c	517	DGD	C5A-C6A-C7A-C8A
23	C	504	CLA	CBA-CGA-O2A-C1
30	d	407	SQD	C9-C10-C11-C12
23	c	502	CLA	C13-C15-C16-C17
31	d	406	LMG	C32-C33-C34-C35
23	B	610	CLA	C16-C17-C18-C19
28	c	519	DGD	C1A-C2A-C3A-C4A
28	B	626	DGD	C3A-C4A-C5A-C6A
31	D	407	LMG	C19-C20-C21-C22
29	a	417	LHG	O6-C4-C5-O7
29	A	415	LHG	C24-C23-O8-C6
31	a	416	LMG	C11-C10-O7-C8
23	d	403	CLA	O1A-CGA-O2A-C1
31	a	416	LMG	C15-C16-C17-C18
31	e	101	LMG	C19-C20-C21-C22
31	A	414	LMG	C15-C16-C17-C18
23	C	512	CLA	C16-C17-C18-C20
23	b	604	CLA	C16-C17-C18-C19
23	c	512	CLA	C16-C17-C18-C19
31	A	414	LMG	C20-C21-C22-C23
31	d	406	LMG	C11-C12-C13-C14
31	d	405	LMG	C38-C39-C40-C41
31	a	402	LMG	C28-C29-C30-C31
31	D	407	LMG	C17-C18-C19-C20
30	a	415	SQD	O6-C44-C45-O47
31	I	101	LMG	O1-C7-C8-O7
31	E	101	LMG	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	a	416	LMG	C20-C21-C22-C23
31	e	101	LMG	C17-C18-C19-C20
23	A	403	CLA	C2A-CAA-CBA-CGA
23	a	404	CLA	C2A-CAA-CBA-CGA
23	C	512	CLA	C3-C5-C6-C7
31	D	406	LMG	C38-C39-C40-C41
23	b	607	CLA	C15-C16-C17-C18
30	a	401	SQD	C32-C33-C34-C35
31	D	408	LMG	C10-C11-C12-C13
23	B	610	CLA	CBA-CGA-O2A-C1
23	C	509	CLA	CBA-CGA-O2A-C1
23	b	613	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
23	C	507	CLA	CBD-CGD-O2D-CED
23	C	510	CLA	CBD-CGD-O2D-CED
31	D	408	LMG	C11-C12-C13-C14
23	b	619	CLA	C8-C10-C11-C12
33	B	624	LMT	C2B-C1B-O1B-C4'
23	C	510	CLA	C3-C5-C6-C7
28	C	518	DGD	C1A-C2A-C3A-C4A
29	a	414	LHG	C23-C24-C25-C26
28	D	410	DGD	C8B-C9B-CAB-CBB
23	C	502	CLA	C13-C15-C16-C17
23	a	409	CLA	C13-C15-C16-C17
23	B	601	CLA	C16-C17-C18-C20
23	C	505	CLA	C4-C3-C5-C6
33	i	102	LMT	C5'-C4'-O1B-C1B
25	D	404	PL9	C47-C48-C49-C51
30	A	417	SQD	C30-C31-C32-C33
31	d	405	LMG	C31-C32-C33-C34
34	V	201	HEM	C4D-C3D-CAD-CBD
30	A	417	SQD	C12-C13-C14-C15
23	A	403	CLA	C11-C12-C13-C14
23	B	609	CLA	C6-C7-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	C	502	CLA	C11-C12-C13-C14
23	C	503	CLA	C11-C12-C13-C14
23	C	505	CLA	C6-C7-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	C	512	CLA	C11-C12-C13-C14
23	b	606	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	618	CLA	C14-C13-C15-C16
23	c	502	CLA	C11-C12-C13-C14
23	c	503	CLA	C11-C12-C13-C14
23	c	511	CLA	C14-C13-C15-C16
23	d	402	CLA	C14-C13-C15-C16
24	A	406	PHO	C14-C13-C15-C16
24	a	407	PHO	C6-C7-C8-C9
24	a	408	PHO	C14-C13-C15-C16
28	c	518	DGD	CAB-CBB-CCB-CDB
23	B	605	CLA	C15-C16-C17-C18
23	b	617	CLA	C15-C16-C17-C18
23	B	608	CLA	C4B-C3B-CAB-CBB
23	B	615	CLA	C4B-C3B-CAB-CBB
23	C	502	CLA	C4B-C3B-CAB-CBB
23	C	512	CLA	C4B-C3B-CAB-CBB
23	C	513	CLA	C4B-C3B-CAB-CBB
23	D	403	CLA	C4B-C3B-CAB-CBB
23	b	611	CLA	C4B-C3B-CAB-CBB
23	b	618	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
23	c	512	CLA	C4B-C3B-CAB-CBB
23	c	513	CLA	C4B-C3B-CAB-CBB
30	A	417	SQD	C10-C11-C12-C13
31	a	402	LMG	C15-C16-C17-C18
31	D	406	LMG	C31-C32-C33-C34
28	B	621	DGD	CAB-CBB-CCB-CDB
23	c	504	CLA	C2A-CAA-CBA-CGA
28	D	410	DGD	C2D-C1D-O3G-C3G
28	d	408	DGD	C2D-C1D-O3G-C3G
28	C	516	DGD	C2A-C3A-C4A-C5A
31	D	407	LMG	C15-C16-C17-C18
31	k	103	LMG	C16-C17-C18-C19
23	c	510	CLA	C3-C5-C6-C7
28	b	622	DGD	CAB-CBB-CCB-CDB
29	A	412	LHG	O6-C4-C5-C6
29	a	417	LHG	O6-C4-C5-C6
30	A	413	SQD	C10-C11-C12-C13
31	b	623	LMG	C20-C21-C22-C23
31	e	101	LMG	C18-C19-C20-C21
23	B	602	CLA	C6-C7-C8-C10
23	B	603	CLA	C6-C7-C8-C10
23	B	606	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	610	CLA	C11-C12-C13-C15
23	B	611	CLA	C11-C10-C8-C7
23	B	613	CLA	C11-C12-C13-C15
23	C	502	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C7
23	C	510	CLA	C6-C7-C8-C10
23	C	511	CLA	C6-C7-C8-C10
23	C	512	CLA	C11-C12-C13-C15
23	C	512	CLA	C12-C13-C15-C16
23	D	401	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C10-C8-C7
23	a	405	CLA	C12-C13-C15-C16
23	b	609	CLA	C12-C13-C15-C16
23	b	612	CLA	C12-C13-C15-C16
23	b	613	CLA	C11-C12-C13-C15
23	b	614	CLA	C11-C10-C8-C7
23	b	618	CLA	C11-C10-C8-C7
23	b	619	CLA	C11-C10-C8-C7
23	b	619	CLA	C12-C13-C15-C16
23	c	502	CLA	C12-C13-C15-C16
23	c	505	CLA	C6-C7-C8-C10
23	c	505	CLA	C12-C13-C15-C16
23	c	506	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	c	511	CLA	C6-C7-C8-C10
23	c	511	CLA	C12-C13-C15-C16
23	c	512	CLA	C11-C12-C13-C15
24	A	406	PHO	C12-C13-C15-C16
28	B	626	DGD	CAB-CBB-CCB-CDB
23	B	616	CLA	C8-C10-C11-C12
31	b	624	LMG	O10-C28-O8-C9
23	C	513	CLA	C4-C3-C5-C6
23	c	513	CLA	C4-C3-C5-C6
23	b	608	CLA	C15-C16-C17-C18
23	c	509	CLA	C15-C16-C17-C18
23	b	608	CLA	C2-C3-C5-C6
33	b	626	LMT	C2B-C1B-O1B-C4'
23	B	611	CLA	O1A-CGA-O2A-C1
23	C	511	CLA	O1A-CGA-O2A-C1
31	M	101	LMG	O10-C28-O8-C9
23	a	405	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	505	CLA	O1A-CGA-O2A-C1
31	C	519	LMG	C12-C13-C14-C15
27	D	405	BCR	C21-C22-C23-C24
34	V	201	HEM	C2D-C3D-CAD-CBD
31	A	414	LMG	C31-C32-C33-C34
33	I	102	LMT	C5'-C4'-O1B-C1B
28	c	517	DGD	C2A-C3A-C4A-C5A
28	B	621	DGD	O1G-C1G-C2G-C3G
28	B	626	DGD	C1G-C2G-C3G-O3G
28	C	517	DGD	C1G-C2G-C3G-O3G
28	c	518	DGD	C1G-C2G-C3G-O3G
30	A	413	SQD	O6-C44-C45-C46
30	a	415	SQD	O6-C44-C45-C46
31	A	414	LMG	O1-C7-C8-C9
31	B	622	LMG	C7-C8-C9-O8
31	M	101	LMG	C7-C8-C9-O8
31	M	102	LMG	C7-C8-C9-O8
31	b	624	LMG	C7-C8-C9-O8
28	D	410	DGD	CBA-CCA-CDA-CEA
31	A	418	LMG	C12-C13-C14-C15
23	C	512	CLA	C16-C17-C18-C19
23	A	407	CLA	C13-C15-C16-C17
28	c	519	DGD	CFA-CGA-CHA-CIA
30	a	401	SQD	C12-C13-C14-C15
31	D	407	LMG	C13-C14-C15-C16
31	i	101	LMG	C18-C19-C20-C21
23	c	505	CLA	C4-C3-C5-C6
31	C	519	LMG	C16-C17-C18-C19
23	C	513	CLA	C2-C3-C5-C6
23	c	513	CLA	C2-C3-C5-C6
23	c	507	CLA	C3-C5-C6-C7
29	a	414	LHG	O6-C4-C5-O7
23	C	504	CLA	O1A-CGA-O2A-C1
27	B	617	BCR	C1-C6-C7-C8
27	C	514	BCR	C5-C6-C7-C8
27	C	515	BCR	C1-C6-C7-C8
27	K	102	BCR	C1-C6-C7-C8
27	K	102	BCR	C23-C24-C25-C30
27	Z	101	BCR	C1-C6-C7-C8
27	c	515	BCR	C1-C6-C7-C8
27	c	516	BCR	C1-C6-C7-C8
27	c	516	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	k	102	BCR	C1-C6-C7-C8
29	A	412	LHG	C8-C7-O7-C5
24	a	407	PHO	C5-C6-C7-C8
23	b	619	CLA	C15-C16-C17-C18
31	E	101	LMG	C18-C19-C20-C21
23	b	608	CLA	C5-C6-C7-C8
30	A	413	SQD	O47-C45-C46-O48
30	B	625	SQD	O47-C45-C46-O48
30	a	415	SQD	O47-C45-C46-O48
30	b	601	SQD	O47-C45-C46-O48
30	f	103	SQD	O47-C45-C46-O48
31	A	414	LMG	O1-C7-C8-O7
31	B	622	LMG	O7-C8-C9-O8
31	b	624	LMG	O7-C8-C9-O8
31	e	101	LMG	O1-C7-C8-O7
31	i	101	LMG	O1-C7-C8-O7
31	k	103	LMG	O7-C8-C9-O8
31	A	418	LMG	C15-C16-C17-C18
31	k	103	LMG	C30-C31-C32-C33
28	D	410	DGD	C1A-C2A-C3A-C4A
31	I	101	LMG	C18-C19-C20-C21
23	c	505	CLA	C8-C10-C11-C12
23	c	505	CLA	C2-C3-C5-C6
30	A	413	SQD	C15-C16-C17-C18
31	b	623	LMG	C17-C18-C19-C20
23	B	601	CLA	C16-C17-C18-C19
30	A	413	SQD	C31-C32-C33-C34
30	a	415	SQD	C10-C11-C12-C13
30	D	409	SQD	C7-C8-C9-C10
31	C	520	LMG	C13-C14-C15-C16
23	c	512	CLA	C3-C5-C6-C7
23	B	601	CLA	C6-C7-C8-C9
23	B	609	CLA	C14-C13-C15-C16
23	B	613	CLA	C11-C10-C8-C9
23	D	401	CLA	C6-C7-C8-C9
23	a	405	CLA	C14-C13-C15-C16
23	b	612	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C10-C8-C9
31	M	101	LMG	C11-C12-C13-C14
23	B	610	CLA	C10-C11-C12-C13
30	d	407	SQD	O5-C1-O6-C44
31	b	624	LMG	O6-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	d	408	DGD	CBA-CCA-CDA-CEA
33	B	624	LMT	O5B-C1B-O1B-C4'
31	a	416	LMG	C31-C32-C33-C34
34	v	201	HEM	C2D-C3D-CAD-CBD
25	a	410	PL9	C14-C16-C17-C18
31	i	101	LMG	C4-C5-C6-O5
28	d	408	DGD	C1A-C2A-C3A-C4A
23	C	505	CLA	C2-C3-C5-C6
23	B	614	CLA	C16-C17-C18-C19
23	B	616	CLA	C15-C16-C17-C18
23	C	508	CLA	C5-C6-C7-C8
28	c	519	DGD	C8B-C9B-CAB-CBB
31	a	402	LMG	C12-C13-C14-C15
31	a	402	LMG	C30-C31-C32-C33
23	C	509	CLA	O1A-CGA-O2A-C1
29	a	417	LHG	C24-C23-O8-C6
28	C	518	DGD	CDB-CEB-CFB-CGB
23	b	608	CLA	C10-C11-C12-C13
23	c	508	CLA	C5-C6-C7-C8
30	a	415	SQD	C31-C32-C33-C34
31	b	624	LMG	C15-C16-C17-C18
29	a	414	LHG	O6-C4-C5-C6
27	B	620	BCR	C37-C22-C23-C24
30	a	415	SQD	C15-C16-C17-C18
31	c	520	LMG	C13-C14-C15-C16
23	A	404	CLA	C12-C13-C15-C16
23	B	605	CLA	C11-C10-C8-C7
23	B	608	CLA	C6-C7-C8-C10
23	B	609	CLA	C12-C13-C15-C16
23	B	616	CLA	C11-C10-C8-C7
23	C	501	CLA	C11-C12-C13-C15
23	C	508	CLA	C12-C13-C15-C16
23	C	509	CLA	C11-C10-C8-C7
23	b	608	CLA	C11-C10-C8-C7
23	b	611	CLA	C6-C7-C8-C10
23	b	616	CLA	C11-C12-C13-C15
23	c	501	CLA	C11-C12-C13-C15
23	c	503	CLA	C11-C10-C8-C7
23	c	508	CLA	C12-C13-C15-C16
23	c	509	CLA	C11-C10-C8-C7
23	c	512	CLA	C12-C13-C15-C16
31	A	418	LMG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	A	417	SQD	C33-C34-C35-C36
30	B	625	SQD	C12-C13-C14-C15
23	C	507	CLA	C3-C5-C6-C7
27	B	618	BCR	C11-C12-C13-C14
27	c	516	BCR	C21-C22-C23-C24
27	j	102	BCR	C7-C8-C9-C10
23	b	605	CLA	CBA-CGA-O2A-C1
23	B	610	CLA	O1A-CGA-O2A-C1
31	A	414	LMG	C8-C7-O1-C1
31	d	406	LMG	C8-C7-O1-C1
28	B	621	DGD	C7A-C8A-C9A-CAA
23	b	617	CLA	C16-C17-C18-C20
30	b	601	SQD	O49-C7-O47-C45
23	b	615	CLA	C4-C3-C5-C6
25	D	404	PL9	C15-C14-C16-C17
23	b	613	CLA	O1A-CGA-O2A-C1
23	c	505	CLA	O1A-CGA-O2A-C1
33	b	626	LMT	O5B-C1B-O1B-C4'
28	b	602	DGD	CAB-CBB-CCB-CDB
23	c	501	CLA	C13-C15-C16-C17
28	C	518	DGD	C3G-C2G-O2G-C1B
31	C	520	LMG	C9-C8-O7-C10
29	A	415	LHG	O10-C23-O8-C6
28	C	516	DGD	C2B-C3B-C4B-C5B
31	b	623	LMG	C15-C16-C17-C18
31	A	418	LMG	C17-C18-C19-C20
23	c	511	CLA	O1A-CGA-O2A-C1
30	b	601	SQD	C12-C13-C14-C15
31	B	622	LMG	C15-C16-C17-C18
29	A	412	LHG	O9-C7-O7-C5
31	D	406	LMG	C11-C12-C13-C14
28	C	517	DGD	O6E-C1E-O5D-C6D
31	i	101	LMG	O6-C1-O1-C7
28	A	411	DGD	C3B-C4B-C5B-C6B
30	D	409	SQD	O6-C44-C45-C46
30	d	407	SQD	O6-C44-C45-C46
31	b	623	LMG	O1-C7-C8-C9
31	i	101	LMG	O1-C7-C8-C9
23	b	613	CLA	C5-C6-C7-C8
34	F	101	HEM	C4B-C3B-CAB-CBB
34	V	201	HEM	C4C-C3C-CAC-CBC
34	f	101	HEM	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	v	201	HEM	C4C-C3C-CAC-CBC
25	a	410	PL9	C7-C8-C9-C10
25	J	101	PL9	C15-C14-C16-C17
29	a	417	LHG	C25-C26-C27-C28
28	D	410	DGD	O2G-C2G-C3G-O3G
28	b	602	DGD	O1G-C1G-C2G-O2G
30	F	102	SQD	O47-C45-C46-O48
31	E	101	LMG	O1-C7-C8-O7
31	M	102	LMG	O7-C8-C9-O8
23	A	404	CLA	C6-C7-C8-C9
23	A	404	CLA	C14-C13-C15-C16
23	B	613	CLA	C11-C12-C13-C14
23	B	615	CLA	C6-C7-C8-C9
23	C	512	CLA	C14-C13-C15-C16
23	a	404	CLA	C11-C12-C13-C14
23	b	606	CLA	C11-C12-C13-C14
23	b	618	CLA	C6-C7-C8-C9
23	d	402	CLA	C6-C7-C8-C9
23	B	614	CLA	C16-C17-C18-C20
30	a	401	SQD	C10-C11-C12-C13
28	C	517	DGD	C4B-C5B-C6B-C7B
28	C	517	DGD	C7B-C8B-C9B-CAB
28	c	519	DGD	CDB-CEB-CFB-CGB
24	a	408	PHO	C10-C11-C12-C13
30	d	407	SQD	C7-C8-C9-C10
31	M	102	LMG	C30-C31-C32-C33
23	A	404	CLA	C5-C6-C7-C8
23	c	509	CLA	C10-C11-C12-C13
31	M	102	LMG	C11-C12-C13-C14
30	F	102	SQD	C2-C1-O6-C44
31	i	101	LMG	C2-C1-O1-C7
23	C	509	CLA	C15-C16-C17-C18
31	A	418	LMG	C13-C14-C15-C16
28	a	413	DGD	C8B-C9B-CAB-CBB
23	B	605	CLA	C5-C6-C7-C8
33	B	628	LMT	C5'-C4'-O1B-C1B
23	A	407	CLA	C16-C17-C18-C19
23	B	605	CLA	C10-C11-C12-C13
31	C	519	LMG	C30-C31-C32-C33
30	a	401	SQD	C23-C24-C25-C26
31	D	407	LMG	C10-C11-C12-C13
23	b	605	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	b	622	DGD	C4B-C5B-C6B-C7B
23	c	507	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	C16-C17-C18-C19
23	C	507	CLA	O1D-CGD-O2D-CED
25	J	101	PL9	C19-C21-C22-C23
25	j	101	PL9	C19-C21-C22-C23
23	A	404	CLA	C4B-C3B-CAB-CBB
23	C	509	CLA	C4B-C3B-CAB-CBB
23	c	509	CLA	C4B-C3B-CAB-CBB
23	b	607	CLA	CBA-CGA-O2A-C1
25	d	404	PL9	C15-C14-C16-C17
23	A	405	CLA	C5-C6-C7-C8
23	B	608	CLA	C13-C15-C16-C17
31	B	622	LMG	C35-C36-C37-C38
28	C	518	DGD	C8B-C9B-CAB-CBB
30	B	625	SQD	O49-C7-O47-C45
28	c	518	DGD	C7B-C8B-C9B-CAB
31	b	624	LMG	C35-C36-C37-C38
23	B	606	CLA	C13-C15-C16-C17
23	b	605	CLA	O1D-CGD-O2D-CED
23	A	407	CLA	C11-C10-C8-C7
23	B	608	CLA	C11-C12-C13-C15
23	B	610	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	C	503	CLA	C11-C10-C8-C7
23	C	506	CLA	C11-C12-C13-C15
23	a	409	CLA	C11-C10-C8-C7
23	b	611	CLA	C11-C12-C13-C15
23	b	613	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C15
23	d	403	CLA	C11-C10-C8-C7
23	B	603	CLA	C16-C17-C18-C19
23	B	604	CLA	CBA-CGA-O2A-C1
23	b	611	CLA	CBA-CGA-O2A-C1
23	B	612	CLA	C10-C11-C12-C13
31	k	103	LMG	C12-C13-C14-C15
23	b	605	CLA	CBD-CGD-O2D-CED
31	A	418	LMG	C30-C31-C32-C33
23	b	611	CLA	O1A-CGA-O2A-C1
29	A	412	LHG	C2-C3-O3-P
31	i	101	LMG	C29-C30-C31-C32
23	c	510	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	401	SQD	C26-C27-C28-C29
29	A	412	LHG	O6-C4-C5-O7
29	A	415	LHG	O6-C4-C5-O7
30	A	413	SQD	C8-C7-O47-C45
23	B	605	CLA	C11-C10-C8-C9
23	B	610	CLA	C11-C12-C13-C14
23	B	611	CLA	C11-C10-C8-C9
23	B	616	CLA	C11-C10-C8-C9
23	C	501	CLA	C11-C12-C13-C14
23	C	503	CLA	C11-C10-C8-C9
23	C	508	CLA	C14-C13-C15-C16
23	C	509	CLA	C11-C10-C8-C9
23	C	510	CLA	C6-C7-C8-C9
23	b	608	CLA	C11-C10-C8-C9
23	b	616	CLA	C11-C10-C8-C9
23	b	616	CLA	C11-C12-C13-C14
23	b	619	CLA	C11-C10-C8-C9
23	c	501	CLA	C11-C12-C13-C14
23	c	508	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C10-C8-C9
23	c	512	CLA	C14-C13-C15-C16
28	B	626	DGD	C8B-C9B-CAB-CBB
30	a	415	SQD	C16-C17-C18-C19
31	a	402	LMG	C17-C18-C19-C20
23	c	507	CLA	O1D-CGD-O2D-CED
23	b	609	CLA	C13-C15-C16-C17
33	B	623	LMT	C4-C5-C6-C7
30	D	409	SQD	O5-C5-C6-S
28	C	518	DGD	CDA-CEA-CFA-CGA
33	b	625	LMT	C4-C5-C6-C7
29	a	417	LHG	O10-C23-O8-C6
28	B	621	DGD	O1G-C1G-C2G-O2G
28	b	622	DGD	O1G-C1G-C2G-O2G
28	d	408	DGD	O2G-C2G-C3G-O3G
31	D	408	LMG	O1-C7-C8-O7
31	M	101	LMG	O7-C8-C9-O8
31	a	416	LMG	O1-C7-C8-O7
31	c	520	LMG	O1-C7-C8-O7
31	c	520	LMG	O7-C8-C9-O8
28	C	518	DGD	CEA-CFA-CGA-CHA
23	b	615	CLA	C10-C11-C12-C13
30	f	103	SQD	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	I	101	LMG	C29-C30-C31-C32
30	F	102	SQD	C44-C45-C46-O48
30	f	103	SQD	C44-C45-C46-O48
31	e	101	LMG	O1-C7-C8-C9
23	B	611	CLA	C4-C3-C5-C6
28	B	621	DGD	C7B-C8B-C9B-CAB
30	b	601	SQD	C15-C16-C17-C18
31	b	623	LMG	C29-C30-C31-C32
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C5-C6-C7-C8
23	b	606	CLA	C16-C17-C18-C19
23	C	504	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C10-C11-C12-C13
24	D	402	PHO	C5-C6-C7-C8
31	D	406	LMG	O10-C28-O8-C9
28	A	411	DGD	C8B-C9B-CAB-CBB
28	a	413	DGD	C3B-C4B-C5B-C6B
28	c	517	DGD	C2B-C3B-C4B-C5B
29	A	415	LHG	C25-C26-C27-C28
25	J	101	PL9	C12-C13-C14-C16
25	d	404	PL9	C32-C33-C34-C36
28	C	518	DGD	CBA-CCA-CDA-CEA
33	b	603	LMT	C5'-C4'-O1B-C1B
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
27	B	618	BCR	C13-C14-C15-C16
29	A	412	LHG	C4-O6-P-O5
29	A	415	LHG	C3-O3-P-O5
29	a	417	LHG	C3-O3-P-O5
28	b	622	DGD	C7A-C8A-C9A-CAA
28	B	621	DGD	C4B-C5B-C6B-C7B
28	b	602	DGD	C8B-C9B-CAB-CBB
28	c	519	DGD	CEA-CFA-CGA-CHA
31	D	406	LMG	C17-C18-C19-C20
23	a	405	CLA	C4-C3-C5-C6
23	B	605	CLA	C2B-C3B-CAB-CBB
23	b	607	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	608	CLA	C2B-C3B-CAB-CBB
23	d	403	CLA	C2B-C3B-CAB-CBB
27	c	514	BCR	C5-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C26
23	b	615	CLA	C2-C3-C5-C6
30	f	103	SQD	C24-C25-C26-C27
34	v	201	HEM	C4D-C3D-CAD-CBD
23	b	606	CLA	C8-C10-C11-C12
23	b	617	CLA	C5-C6-C7-C8
27	j	102	BCR	C37-C22-C23-C24
29	a	414	LHG	C2-C3-O3-P
28	a	413	DGD	C2A-C3A-C4A-C5A
23	C	510	CLA	C16-C17-C18-C19
31	b	623	LMG	C10-C11-C12-C13
23	B	604	CLA	O1A-CGA-O2A-C1
23	b	607	CLA	O1A-CGA-O2A-C1
28	c	518	DGD	C3A-C4A-C5A-C6A
25	A	408	PL9	C4-C3-C7-C8
25	a	410	PL9	C4-C3-C7-C8
28	c	518	DGD	C4B-C5B-C6B-C7B
28	c	519	DGD	C3G-C2G-O2G-C1B
31	c	520	LMG	C9-C8-O7-C10
25	A	408	PL9	C19-C21-C22-C23
25	j	101	PL9	C24-C26-C27-C28
30	F	102	SQD	C29-C30-C31-C32
23	c	510	CLA	O1D-CGD-O2D-CED
28	c	519	DGD	CDA-CEA-CFA-CGA
23	B	603	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C19
23	c	512	CLA	C5-C6-C7-C8
29	A	415	LHG	O6-C4-C5-C6
23	B	603	CLA	C11-C12-C13-C14
23	C	511	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	b	613	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	d	403	CLA	C11-C10-C8-C9
23	B	603	CLA	C11-C10-C8-C7
23	C	509	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C11-C12-C13-C15
24	A	406	PHO	C13-C15-C16-C17
23	A	407	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C20
23	B	610	CLA	C5-C6-C7-C8
30	a	401	SQD	C17-C18-C19-C20
31	D	407	LMG	C2-C1-O1-C7
23	B	612	CLA	C4-C3-C5-C6
31	C	519	LMG	O7-C8-C9-O8
31	C	520	LMG	O1-C7-C8-O7
31	d	406	LMG	O1-C7-C8-O7
23	c	512	CLA	CAA-CBA-CGA-O2A
23	C	510	CLA	O1D-CGD-O2D-CED
30	B	625	SQD	C15-C16-C17-C18
29	a	414	LHG	O9-C7-O7-C5
30	A	413	SQD	C44-C45-C46-O48
30	a	415	SQD	C44-C45-C46-O48
28	C	518	DGD	CFA-CGA-CHA-CIA
30	A	417	SQD	C23-C24-C25-C26
23	b	616	CLA	C13-C15-C16-C17
27	T	103	BCR	C11-C12-C13-C35
27	a	412	BCR	C7-C8-C9-C34
23	B	606	CLA	C16-C17-C18-C20
29	a	414	LHG	C8-C7-O7-C5
25	j	101	PL9	C17-C18-C19-C21
30	A	413	SQD	C16-C17-C18-C19
27	B	620	BCR	C21-C22-C23-C24
28	C	517	DGD	C5D-C6D-O5D-C1E
23	B	614	CLA	C2A-CAA-CBA-CGA
27	T	103	BCR	C13-C14-C15-C16
23	b	609	CLA	C16-C17-C18-C20
31	a	416	LMG	C38-C39-C40-C41
23	b	613	CLA	C10-C11-C12-C13
31	i	101	LMG	C17-C18-C19-C20
23	A	405	CLA	C2C-C3C-CAC-CBC
28	A	411	DGD	C2A-C3A-C4A-C5A
23	C	509	CLA	C10-C11-C12-C13
23	b	617	CLA	C4C-C3C-CAC-CBC
24	A	406	PHO	C10-C11-C12-C13
23	C	512	CLA	CAA-CBA-CGA-O2A
23	A	405	CLA	C6-C7-C8-C9
23	C	506	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	409	CLA	C11-C10-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	619	CLA	C14-C13-C15-C16
24	D	402	PHO	C6-C7-C8-C9
29	A	412	LHG	C24-C25-C26-C27
30	D	409	SQD	C10-C11-C12-C13
23	B	611	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	b	614	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
23	a	406	CLA	C2C-C3C-CAC-CBC
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	611	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	B	611	CLA	C2-C3-C5-C6
23	B	612	CLA	C2-C3-C5-C6
25	D	404	PL9	C13-C14-C16-C17
23	b	606	CLA	C15-C16-C17-C18
28	c	518	DGD	C7A-C8A-C9A-CAA
23	C	510	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
28	C	518	DGD	O6E-C5E-C6E-O5E
23	A	405	CLA	C6-C7-C8-C10
23	C	506	CLA	C6-C7-C8-C10
23	C	507	CLA	C11-C10-C8-C7
23	C	513	CLA	C11-C10-C8-C7
23	a	406	CLA	C6-C7-C8-C10
23	C	501	CLA	C13-C15-C16-C17
31	d	405	LMG	C17-C18-C19-C20
31	d	406	LMG	C34-C35-C36-C37
31	d	405	LMG	O10-C28-O8-C9
33	B	628	LMT	C1-C2-C3-C4
29	A	412	LHG	C23-C24-C25-C26
31	d	405	LMG	C11-C12-C13-C14
23	A	403	CLA	C3A-C2A-CAA-CBA
23	C	513	CLA	C3A-C2A-CAA-CBA
23	a	404	CLA	C3A-C2A-CAA-CBA
23	c	513	CLA	C3A-C2A-CAA-CBA
30	F	102	SQD	C26-C27-C28-C29
30	a	401	SQD	C33-C34-C35-C36
25	d	404	PL9	C13-C14-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	a	416	LMG	C35-C36-C37-C38
24	a	408	PHO	C13-C15-C16-C17
23	b	617	CLA	C2C-C3C-CAC-CBC
28	D	410	DGD	CAA-CBA-CCA-CDA
23	b	616	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C8-C10-C11-C12
27	C	515	BCR	C37-C22-C23-C24
28	D	410	DGD	CBB-CCB-CDB-CEB
23	b	616	CLA	C8-C10-C11-C12
30	a	401	SQD	C18-C19-C20-C21
31	D	408	LMG	C34-C35-C36-C37
23	B	603	CLA	C15-C16-C17-C18
25	D	404	PL9	C9-C11-C12-C13
25	J	101	PL9	C24-C26-C27-C28
25	a	410	PL9	C19-C21-C22-C23
28	D	410	DGD	O1G-C1G-C2G-C3G
28	b	602	DGD	C5A-C6A-C7A-C8A
23	B	613	CLA	C10-C11-C12-C13
23	a	406	CLA	C5-C6-C7-C8
23	b	611	CLA	C13-C15-C16-C17
31	D	407	LMG	C16-C17-C18-C19
25	D	404	PL9	C47-C48-C49-C50
23	B	616	CLA	C11-C12-C13-C14
23	C	506	CLA	C11-C10-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	C	513	CLA	C14-C13-C15-C16
23	a	406	CLA	C6-C7-C8-C9
23	b	619	CLA	C11-C12-C13-C14
23	c	506	CLA	C11-C10-C8-C9
23	c	513	CLA	C11-C10-C8-C9
28	C	517	DGD	C7A-C8A-C9A-CAA
29	a	414	LHG	C4-C5-O7-C7
25	d	404	PL9	C47-C48-C49-C50
31	c	520	LMG	C34-C35-C36-C37
31	D	407	LMG	C29-C30-C31-C32
23	A	404	CLA	C2A-CAA-CBA-CGA
31	A	414	LMG	C38-C39-C40-C41
23	A	403	CLA	C1A-C2A-CAA-CBA
23	D	401	CLA	C1A-C2A-CAA-CBA
23	a	404	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	A	417	SQD	C26-C27-C28-C29
28	c	519	DGD	C7A-C8A-C9A-CAA
23	A	404	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	509	CLA	C2B-C3B-CAB-CBB
23	C	512	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C2B-C3B-CAB-CBB
23	D	403	CLA	C2B-C3B-CAB-CBB
23	b	605	CLA	C2B-C3B-CAB-CBB
23	b	611	CLA	C2B-C3B-CAB-CBB
23	b	614	CLA	C2B-C3B-CAB-CBB
23	b	618	CLA	C2B-C3B-CAB-CBB
23	c	509	CLA	C2B-C3B-CAB-CBB
23	c	512	CLA	C2B-C3B-CAB-CBB
23	c	513	CLA	C2B-C3B-CAB-CBB
23	d	402	CLA	C2B-C3B-CAB-CBB
27	B	617	BCR	C5-C6-C7-C8
27	C	515	BCR	C5-C6-C7-C8
27	C	515	BCR	C23-C24-C25-C26
27	K	102	BCR	C23-C24-C25-C26
27	T	102	BCR	C1-C6-C7-C8
27	Z	101	BCR	C5-C6-C7-C8
27	a	412	BCR	C23-C24-C25-C30
27	c	514	BCR	C1-C6-C7-C8
27	c	515	BCR	C5-C6-C7-C8
27	c	516	BCR	C5-C6-C7-C8
27	c	516	BCR	C23-C24-C25-C26
27	j	102	BCR	C1-C6-C7-C8
27	j	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C5-C6-C7-C8
31	I	101	LMG	C17-C18-C19-C20
25	A	408	PL9	C15-C14-C16-C17
28	A	411	DGD	C4B-C5B-C6B-C7B
31	a	402	LMG	C13-C14-C15-C16
23	B	603	CLA	C11-C12-C13-C15
23	B	605	CLA	C11-C12-C13-C15
23	C	511	CLA	C11-C10-C8-C7
23	D	401	CLA	C11-C10-C8-C7
23	b	604	CLA	C6-C7-C8-C10
23	b	605	CLA	C11-C10-C8-C7
23	b	608	CLA	C11-C12-C13-C15
23	c	506	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	507	CLA	C11-C12-C13-C15
23	c	508	CLA	C11-C12-C13-C15
23	c	509	CLA	C6-C7-C8-C10
23	c	511	CLA	C11-C10-C8-C7
23	c	513	CLA	C11-C10-C8-C7
31	i	101	LMG	C19-C20-C21-C22
23	B	606	CLA	C16-C17-C18-C19
31	C	520	LMG	O7-C8-C9-O8
28	c	518	DGD	C4A-C5A-C6A-C7A
28	C	518	DGD	O1A-C1A-O1G-C1G
23	D	403	CLA	C8-C10-C11-C12
23	b	614	CLA	C2-C3-C5-C6
23	A	403	CLA	C2-C1-O2A-CGA
23	B	610	CLA	C2-C1-O2A-CGA
31	b	624	LMG	C28-C29-C30-C31
23	c	511	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C14-C13-C15-C16
24	a	408	PHO	C11-C10-C8-C9
28	C	517	DGD	C3A-C4A-C5A-C6A
23	B	613	CLA	C13-C15-C16-C17
23	C	511	CLA	C4-C3-C5-C6
33	b	603	LMT	C1-C2-C3-C4
25	J	101	PL9	C13-C14-C16-C17
25	j	101	PL9	C13-C14-C16-C17
28	C	518	DGD	C7A-C8A-C9A-CAA
30	a	401	SQD	C25-C26-C27-C28
28	C	518	DGD	C1G-C2G-C3G-O3G
28	b	602	DGD	O1G-C1G-C2G-C3G
30	a	415	SQD	C29-C30-C31-C32
23	C	509	CLA	C2A-CAA-CBA-CGA
31	M	101	LMG	C30-C31-C32-C33
23	C	505	CLA	C8-C10-C11-C12
23	d	403	CLA	C8-C10-C11-C12
23	b	609	CLA	C4-C3-C5-C6
23	c	511	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
28	d	408	DGD	CAA-CBA-CCA-CDA
23	b	605	CLA	C4B-C3B-CAB-CBB
23	d	402	CLA	C4B-C3B-CAB-CBB
31	a	402	LMG	O10-C28-O8-C9
31	e	101	LMG	C31-C32-C33-C34
31	A	414	LMG	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	a	408	PHO	CHA-CBD-CGD-O1D
23	c	513	CLA	C16-C17-C18-C20
28	B	626	DGD	O1G-C1G-C2G-O2G
30	d	407	SQD	C10-C11-C12-C13
23	b	615	CLA	C3-C5-C6-C7
23	B	610	CLA	C13-C15-C16-C17
23	d	402	CLA	C11-C10-C8-C7
23	B	614	CLA	C4C-C3C-CAC-CBC
28	c	519	DGD	CBB-CCB-CDB-CEB
30	F	102	SQD	C24-C25-C26-C27
30	f	103	SQD	C26-C27-C28-C29
31	B	622	LMG	C12-C13-C14-C15
23	b	609	CLA	C16-C17-C18-C19
23	a	406	CLA	C4C-C3C-CAC-CBC
31	I	101	LMG	C19-C20-C21-C22
27	T	103	BCR	C11-C12-C13-C14
27	c	515	BCR	C7-C8-C9-C10
23	B	601	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C10-C8-C9
23	b	604	CLA	C11-C12-C13-C14
23	c	505	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C10-C8-C9
23	c	510	CLA	C11-C10-C8-C9
24	A	406	PHO	C11-C10-C8-C9
28	b	602	DGD	C2G-C3G-O3G-C1D
28	c	518	DGD	C5D-C6D-O5D-C1E
30	f	103	SQD	C45-C44-O6-C1
31	i	101	LMG	C8-C7-O1-C1
23	B	614	CLA	C2C-C3C-CAC-CBC
23	a	405	CLA	C2A-CAA-CBA-CGA
23	d	403	CLA	C2A-CAA-CBA-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	b	617	CLA	C2-C1-O2A-CGA
25	j	101	PL9	C12-C13-C14-C16
23	b	609	CLA	C15-C16-C17-C18
23	c	504	CLA	C3A-C2A-CAA-CBA
31	E	101	LMG	O9-C10-C11-C12
28	c	517	DGD	C2A-C1A-O1G-C1G
28	a	413	DGD	C2E-C1E-O5D-C6D
31	d	406	LMG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	414	LHG	C6-C5-O7-C7
31	M	102	LMG	C9-C8-O7-C10
30	A	413	SQD	C29-C30-C31-C32
28	C	518	DGD	CBB-CCB-CDB-CEB
30	F	102	SQD	C9-C10-C11-C12
31	C	519	LMG	C29-C30-C31-C32
31	b	623	LMG	C14-C15-C16-C17
23	c	502	CLA	C16-C17-C18-C20
28	a	413	DGD	C4B-C5B-C6B-C7B
23	b	617	CLA	C2A-CAA-CBA-CGA
23	a	405	CLA	C2-C3-C5-C6
23	B	603	CLA	C8-C10-C11-C12
23	B	605	CLA	C8-C10-C11-C12
31	C	520	LMG	O1-C7-C8-C9
31	C	520	LMG	C7-C8-C9-O8
31	E	101	LMG	O1-C7-C8-C9
31	a	416	LMG	O1-C7-C8-C9
31	c	520	LMG	C7-C8-C9-O8
30	A	417	SQD	C17-C18-C19-C20
30	B	625	SQD	C10-C11-C12-C13
31	a	416	LMG	C12-C13-C14-C15
30	a	401	SQD	C30-C31-C32-C33
23	b	608	CLA	C8-C10-C11-C12
24	a	407	PHO	C15-C16-C17-C18
28	d	408	DGD	CBB-CCB-CDB-CEB
30	f	103	SQD	C15-C16-C17-C18
31	k	103	LMG	C34-C35-C36-C37
23	A	407	CLA	C11-C10-C8-C9
23	B	603	CLA	C11-C10-C8-C9
23	B	608	CLA	C11-C12-C13-C14
23	B	612	CLA	C6-C7-C8-C9
23	b	611	CLA	C11-C12-C13-C14
30	B	625	SQD	C19-C20-C21-C22
28	b	622	DGD	C7B-C8B-C9B-CAB
23	A	405	CLA	C4C-C3C-CAC-CBC
23	C	507	CLA	CAA-CBA-CGA-O2A
23	C	511	CLA	C2A-CAA-CBA-CGA
23	D	403	CLA	C2A-CAA-CBA-CGA
23	B	601	CLA	C11-C12-C13-C15
23	B	601	CLA	C12-C13-C15-C16
23	B	612	CLA	C6-C7-C8-C10
23	C	505	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C11-C10-C8-C7
23	C	507	CLA	C11-C12-C13-C15
23	C	508	CLA	C11-C12-C13-C15
23	C	510	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16
23	b	605	CLA	C12-C13-C15-C16
23	c	504	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C10-C8-C7
23	c	506	CLA	C6-C7-C8-C10
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
24	A	406	PHO	C11-C10-C8-C7
24	a	408	PHO	C11-C10-C8-C7
28	C	518	DGD	C4B-C5B-C6B-C7B
23	B	604	CLA	C4C-C3C-CAC-CBC
23	a	405	CLA	C2C-C3C-CAC-CBC
23	B	602	CLA	C2B-C3B-CAB-CBB
23	B	608	CLA	C2B-C3B-CAB-CBB
23	B	611	CLA	C2B-C3B-CAB-CBB
23	B	615	CLA	C2B-C3B-CAB-CBB
23	C	502	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
27	J	102	BCR	C1-C6-C7-C8
27	J	102	BCR	C5-C6-C7-C8
27	K	102	BCR	C5-C6-C7-C8
27	T	102	BCR	C5-C6-C7-C8
27	a	412	BCR	C23-C24-C25-C26
30	a	415	SQD	C8-C7-O47-C45
23	B	613	CLA	CAA-CBA-CGA-O2A
23	b	616	CLA	CAA-CBA-CGA-O2A
28	c	519	DGD	C4B-C5B-C6B-C7B
23	A	404	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	a	404	CLA	C2-C1-O2A-CGA
23	a	405	CLA	C2-C1-O2A-CGA
31	e	101	LMG	O9-C10-C11-C12
23	D	401	CLA	CAA-CBA-CGA-O2A
31	k	103	LMG	O8-C28-C29-C30
31	b	623	LMG	O6-C1-O1-C7
31	D	408	LMG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	501	CLA	CAA-CBA-CGA-O2A
23	A	404	CLA	C2C-C3C-CAC-CBC
23	B	603	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C16-C17-C18-C19
29	A	412	LHG	C28-C29-C30-C31
23	C	503	CLA	C15-C16-C17-C18
23	d	402	CLA	CAA-CBA-CGA-O2A
31	A	414	LMG	O7-C10-C11-C12
31	a	416	LMG	O7-C10-C11-C12
27	x	101	BCR	C9-C10-C11-C12
29	a	417	LHG	C7-C8-C9-C10
23	c	501	CLA	CAA-CBA-CGA-O2A
23	b	611	CLA	C2-C3-C5-C6
31	E	101	LMG	C31-C32-C33-C34
28	B	626	DGD	C5A-C6A-C7A-C8A
23	b	608	CLA	C11-C12-C13-C14
23	c	507	CLA	C11-C12-C13-C14
23	d	402	CLA	C11-C10-C8-C9
23	c	510	CLA	CAA-CBA-CGA-O2A
28	B	621	DGD	O2G-C1B-C2B-C3B
28	b	622	DGD	O2G-C1B-C2B-C3B
31	M	102	LMG	O1-C7-C8-C9
31	c	520	LMG	O1-C7-C8-C9
23	B	602	CLA	C4B-C3B-CAB-CBB
23	C	506	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	C	513	CLA	C1A-C2A-CAA-CBA
23	D	401	CLA	C4B-C3B-CAB-CBB
23	a	405	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
31	D	406	LMG	C19-C20-C21-C22
31	I	101	LMG	C20-C21-C22-C23
23	B	606	CLA	C4-C3-C5-C6
23	D	401	CLA	C5-C6-C7-C8
28	C	517	DGD	O6D-C1D-O3G-C3G
31	D	407	LMG	O6-C1-O1-C7
30	a	401	SQD	O47-C7-C8-C9
31	I	101	LMG	C15-C16-C17-C18
31	M	102	LMG	O1-C7-C8-O7
31	d	405	LMG	O1-C7-C8-O7
25	d	404	PL9	C21-C22-C23-C24
31	c	520	LMG	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	j	102	BCR	C21-C22-C23-C24
23	b	617	CLA	CAA-CBA-CGA-O2A
23	c	509	CLA	C2A-CAA-CBA-CGA
29	a	414	LHG	C24-C25-C26-C27
23	C	510	CLA	C13-C15-C16-C17
23	c	502	CLA	O1A-CGA-O2A-C1
23	C	510	CLA	CAA-CBA-CGA-O2A
30	D	409	SQD	O47-C7-C8-C9
30	d	407	SQD	O47-C7-C8-C9
23	B	608	CLA	C4-C3-C5-C6
30	F	102	SQD	C15-C16-C17-C18
23	C	508	CLA	C2-C1-O2A-CGA
23	c	508	CLA	C2-C1-O2A-CGA
24	a	407	PHO	C2-C1-O2A-CGA
23	c	507	CLA	CAA-CBA-CGA-O2A
28	c	517	DGD	O1G-C1A-C2A-C3A
23	B	602	CLA	C11-C10-C8-C7
23	B	611	CLA	C6-C7-C8-C10
23	C	504	CLA	C6-C7-C8-C10
23	C	513	CLA	C11-C12-C13-C15
23	b	604	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C7
23	c	513	CLA	C11-C12-C13-C15
24	a	407	PHO	C12-C13-C15-C16
23	c	502	CLA	CBA-CGA-O2A-C1
28	c	519	DGD	CBA-CCA-CDA-CEA
29	A	412	LHG	C4-C5-O7-C7
31	M	101	LMG	C9-C8-O7-C10
31	C	519	LMG	O8-C28-C29-C30
23	a	405	CLA	C4C-C3C-CAC-CBC
30	b	601	SQD	C19-C20-C21-C22
24	a	407	PHO	C13-C15-C16-C17
31	M	101	LMG	O8-C28-C29-C30
31	M	102	LMG	O8-C28-C29-C30
23	A	407	CLA	C4-C3-C5-C6
23	a	409	CLA	C4-C3-C5-C6
23	B	612	CLA	CAA-CBA-CGA-O2A
25	D	404	PL9	C46-C47-C48-C49
25	a	410	PL9	C16-C17-C18-C19
23	d	402	CLA	CAA-CBA-CGA-O1A
28	B	621	DGD	O1B-C1B-C2B-C3B
23	B	602	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	406	PHO	CBA-CGA-O2A-C1
23	C	506	CLA	C6-C7-C8-C9
23	C	508	CLA	C11-C12-C13-C14
23	D	401	CLA	C11-C10-C8-C9
23	b	605	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	c	504	CLA	C6-C7-C8-C9
23	c	508	CLA	C11-C12-C13-C14
23	c	513	CLA	C11-C12-C13-C14
31	E	101	LMG	O7-C10-C11-C12
23	b	616	CLA	CAA-CBA-CGA-O1A
28	c	518	DGD	CBB-CCB-CDB-CEB
23	c	502	CLA	C5-C6-C7-C8
23	D	401	CLA	CAA-CBA-CGA-O1A
28	b	622	DGD	O1B-C1B-C2B-C3B
23	B	615	CLA	CBA-CGA-O2A-C1
31	e	101	LMG	O7-C10-C11-C12
30	d	407	SQD	O5-C5-C6-S
24	A	406	PHO	O1A-CGA-O2A-C1
31	a	416	LMG	C16-C17-C18-C19
28	D	410	DGD	C8A-C9A-CAA-CBA
23	c	507	CLA	CAA-CBA-CGA-O1A
28	c	517	DGD	O1A-C1A-C2A-C3A
28	B	626	DGD	C2G-C3G-O3G-C1D
28	B	626	DGD	C5D-C6D-O5D-C1E
28	C	518	DGD	C2G-C3G-O3G-C1D
30	F	102	SQD	C45-C44-O6-C1
31	D	407	LMG	C8-C7-O1-C1
31	I	101	LMG	C8-C7-O1-C1
23	B	615	CLA	O1A-CGA-O2A-C1
23	C	502	CLA	O1A-CGA-O2A-C1
30	A	413	SQD	O49-C7-O47-C45
31	a	416	LMG	O7-C8-C9-O8
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	507	CLA	CAA-CBA-CGA-O1A
31	k	103	LMG	O10-C28-C29-C30
28	A	411	DGD	C7A-C8A-C9A-CAA
31	A	414	LMG	C19-C20-C21-C22
25	d	404	PL9	C9-C11-C12-C13
25	a	410	PL9	C15-C14-C16-C17
23	C	506	CLA	C8-C10-C11-C12
23	c	510	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAA-CBA-CGA-O2A
31	a	416	LMG	O9-C10-C11-C12
28	c	519	DGD	CCB-CDB-CEB-CFB
23	A	403	CLA	CAD-CBD-CGD-O2D
23	B	609	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	b	608	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C2-C1-O2A-CGA
24	D	402	PHO	C2-C1-O2A-CGA
30	A	417	SQD	C25-C26-C27-C28
23	c	501	CLA	CAA-CBA-CGA-O1A
28	C	516	DGD	O1A-C1A-C2A-C3A
30	A	413	SQD	O49-C7-C8-C9
30	A	417	SQD	O47-C7-C8-C9
31	D	408	LMG	C31-C32-C33-C34
25	j	101	PL9	C21-C22-C23-C24
23	c	510	CLA	CAA-CBA-CGA-O1A
23	C	505	CLA	CAA-CBA-CGA-O2A
23	b	615	CLA	CAA-CBA-CGA-O2A
23	C	501	CLA	CAA-CBA-CGA-O1A
31	A	414	LMG	C12-C13-C14-C15
30	A	413	SQD	O47-C7-C8-C9
23	C	502	CLA	CBA-CGA-O2A-C1

There are no ring outliers.

163 monomers are involved in 556 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	615	CLA	4	0
33	b	626	LMT	1	0
23	b	615	CLA	5	0
27	c	516	BCR	2	0
24	D	402	PHO	7	0
28	c	519	DGD	4	0
34	F	101	HEM	4	0
25	A	408	PL9	2	0
27	J	102	BCR	5	0
33	D	411	LMT	1	0
31	c	520	LMG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	C	520	LMG	2	0
23	B	606	CLA	8	0
33	b	625	LMT	4	0
30	A	413	SQD	6	0
27	a	412	BCR	2	0
27	b	621	BCR	5	0
23	d	403	CLA	3	0
31	d	406	LMG	6	0
27	f	102	BCR	3	0
34	V	201	HEM	3	0
23	C	509	CLA	1	0
28	D	410	DGD	3	0
23	C	501	CLA	3	0
33	i	102	LMT	1	0
31	M	101	LMG	2	0
25	a	410	PL9	5	0
27	k	102	BCR	7	0
23	B	603	CLA	11	0
23	B	611	CLA	6	0
25	d	404	PL9	7	0
29	A	415	LHG	3	0
27	B	620	BCR	5	0
23	c	501	CLA	5	0
23	B	616	CLA	4	0
23	c	510	CLA	3	0
23	b	606	CLA	10	0
23	c	512	CLA	3	0
23	b	607	CLA	4	0
28	B	621	DGD	1	0
23	D	403	CLA	4	0
30	a	401	SQD	2	0
23	a	406	CLA	3	0
23	b	618	CLA	2	0
23	C	507	CLA	4	0
27	K	102	BCR	9	0
27	H	101	BCR	2	0
27	A	410	BCR	5	0
23	C	505	CLA	4	0
30	D	409	SQD	3	0
25	D	404	PL9	5	0
23	B	613	CLA	1	0
28	c	518	DGD	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	612	CLA	4	0
28	C	518	DGD	4	0
23	b	619	CLA	4	0
24	a	408	PHO	5	0
27	C	514	BCR	10	0
23	a	409	CLA	2	0
28	b	602	DGD	6	0
23	b	605	CLA	9	0
31	k	103	LMG	2	0
24	a	407	PHO	9	0
23	B	608	CLA	8	0
23	B	610	CLA	3	0
23	b	616	CLA	3	0
23	b	610	CLA	9	0
31	M	102	LMG	4	0
23	B	602	CLA	8	0
29	a	417	LHG	3	0
33	I	102	LMT	2	0
31	C	519	LMG	2	0
23	c	508	CLA	3	0
27	j	102	BCR	4	0
23	c	509	CLA	4	0
27	c	514	BCR	9	0
28	A	411	DGD	1	0
27	Z	101	BCR	4	0
23	c	513	CLA	2	0
27	T	102	BCR	7	0
23	B	604	CLA	6	0
28	b	622	DGD	2	0
31	d	405	LMG	3	0
23	C	510	CLA	3	0
27	B	617	BCR	8	0
23	C	506	CLA	1	0
23	b	613	CLA	1	0
23	c	503	CLA	4	0
23	A	405	CLA	4	0
31	i	101	LMG	2	0
23	c	502	CLA	2	0
23	a	404	CLA	14	0
23	B	605	CLA	9	0
29	A	412	LHG	3	0
23	C	511	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	b	603	LMT	1	0
30	a	415	SQD	4	0
23	B	609	CLA	5	0
23	b	604	CLA	2	0
31	b	624	LMG	4	0
27	C	515	BCR	6	0
23	A	404	CLA	14	0
30	B	625	SQD	1	0
25	J	101	PL9	2	0
23	A	403	CLA	13	0
23	b	617	CLA	2	0
23	C	512	CLA	3	0
30	A	417	SQD	6	0
28	C	517	DGD	6	0
27	c	515	BCR	3	0
27	b	620	BCR	7	0
24	A	406	PHO	5	0
23	c	506	CLA	2	0
23	d	402	CLA	9	0
33	T	101	LMT	2	0
33	B	623	LMT	1	0
27	B	619	BCR	5	0
31	a	402	LMG	2	0
23	B	614	CLA	6	0
30	d	407	SQD	4	0
23	a	405	CLA	15	0
27	D	405	BCR	3	0
23	C	513	CLA	3	0
23	C	502	CLA	2	0
23	C	503	CLA	3	0
30	b	601	SQD	2	0
31	E	101	LMG	1	0
31	a	416	LMG	5	0
23	b	608	CLA	11	0
31	b	623	LMG	3	0
33	B	628	LMT	2	0
27	B	618	BCR	9	0
23	b	614	CLA	5	0
28	C	516	DGD	4	0
27	T	103	BCR	7	0
23	c	504	CLA	5	0
23	c	505	CLA	4	0

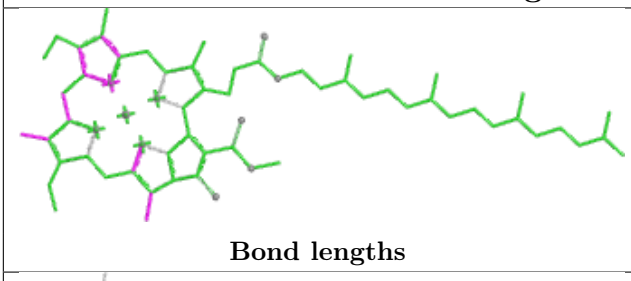
Continued on next page...

Continued from previous page...

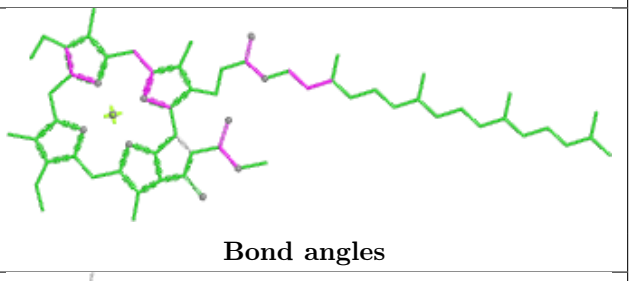
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	401	CLA	7	0
31	D	407	LMG	2	0
34	v	201	HEM	5	0
30	F	102	SQD	2	0
27	x	101	BCR	4	0
23	b	612	CLA	4	0
23	b	609	CLA	8	0
23	c	511	CLA	4	0
31	B	622	LMG	4	0
31	D	406	LMG	1	0
23	B	607	CLA	8	0
23	c	507	CLA	5	0
34	f	101	HEM	4	0
31	A	418	LMG	2	0
31	I	101	LMG	3	0
29	a	414	LHG	4	0
28	c	517	DGD	5	0
28	B	626	DGD	4	0
31	D	408	LMG	7	0
23	A	407	CLA	1	0
30	f	103	SQD	2	0
23	b	611	CLA	7	0
31	A	414	LMG	4	0
33	B	627	LMT	1	0
23	C	504	CLA	6	0
23	C	508	CLA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

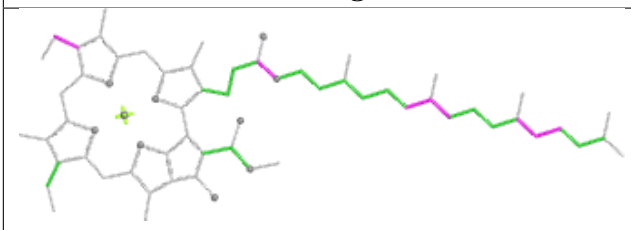
Ligand CLA B 615



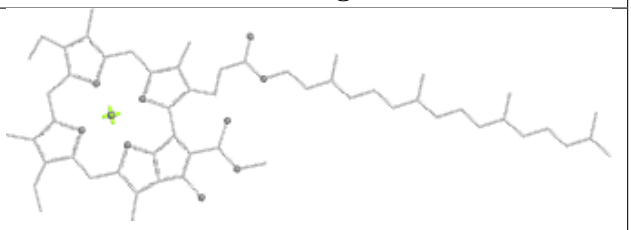
Bond lengths



Bond angles

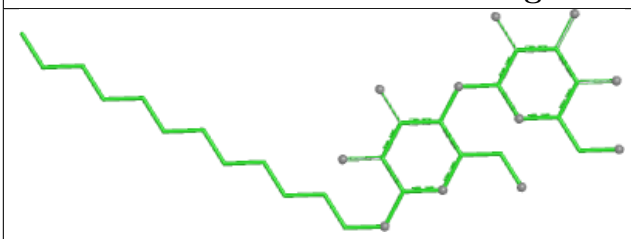


Torsions

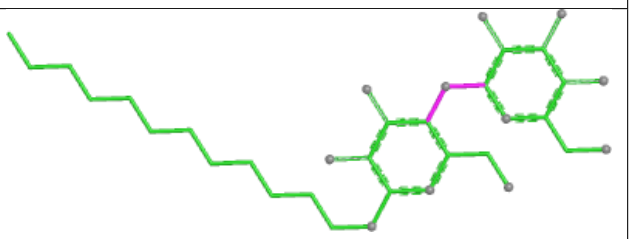


Rings

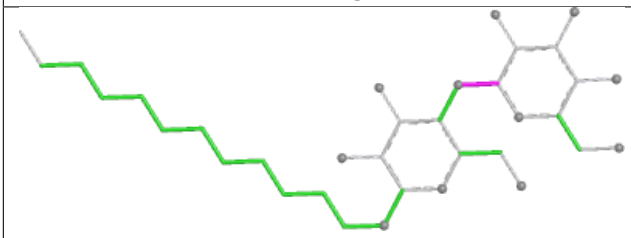
Ligand LMT b 626



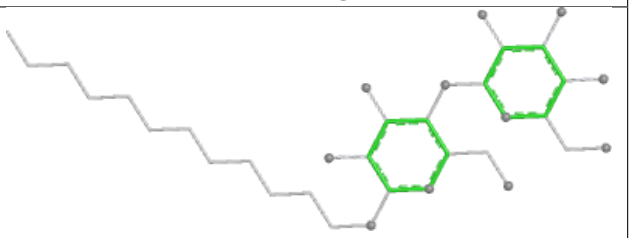
Bond lengths



Bond angles

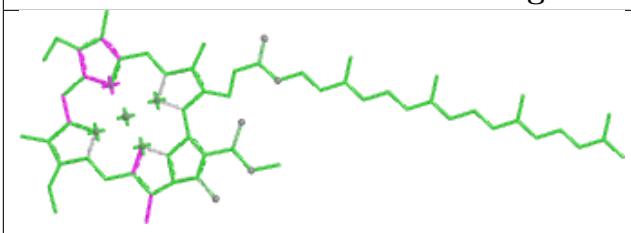


Torsions

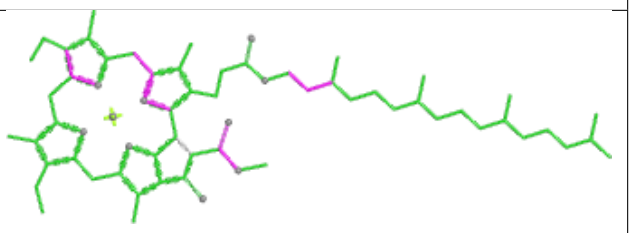


Rings

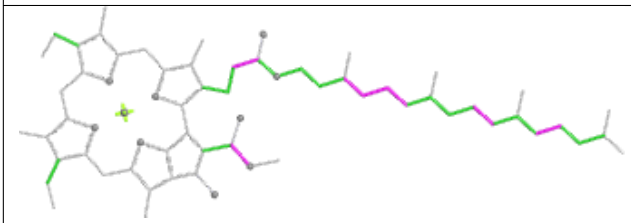
Ligand CLA b 615



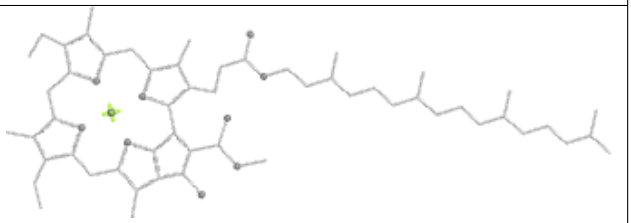
Bond lengths



Bond angles

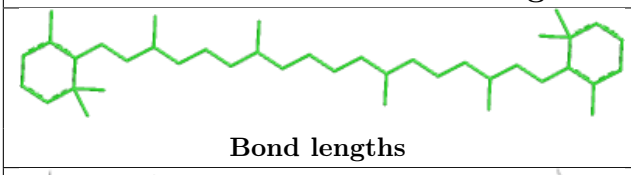


Torsions

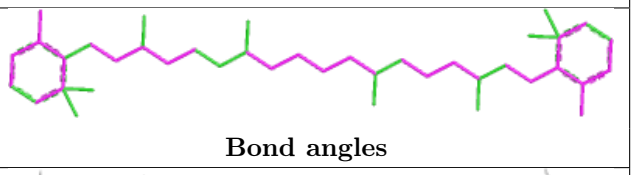


Rings

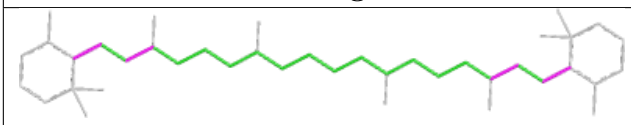
Ligand BCR c 516



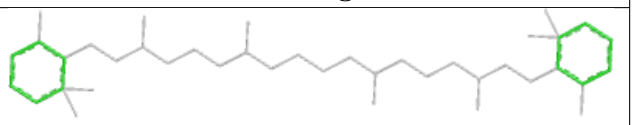
Bond lengths



Bond angles



Torsions

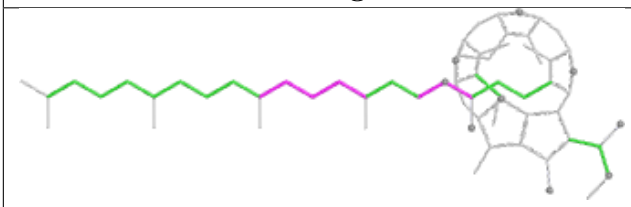


Rings

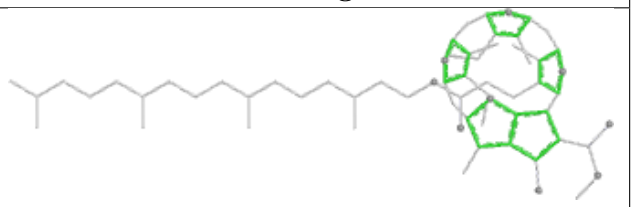
Ligand PHO D 402

Bond lengths

Bond angles

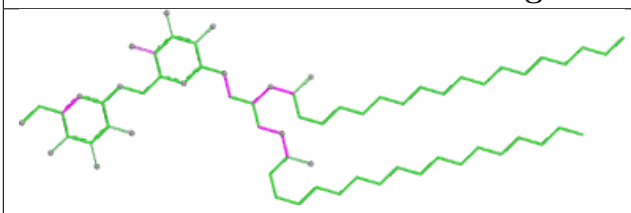


Torsions

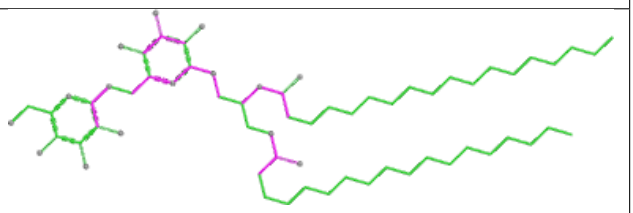


Rings

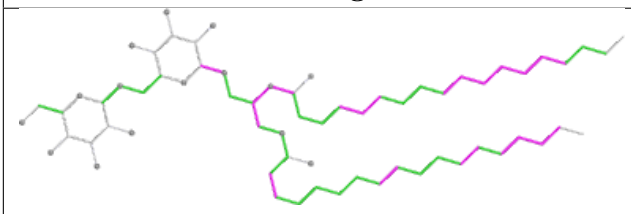
Ligand DGD c 519



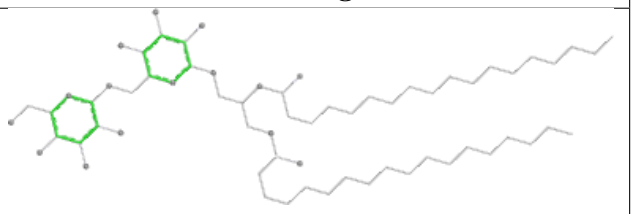
Bond lengths



Bond angles

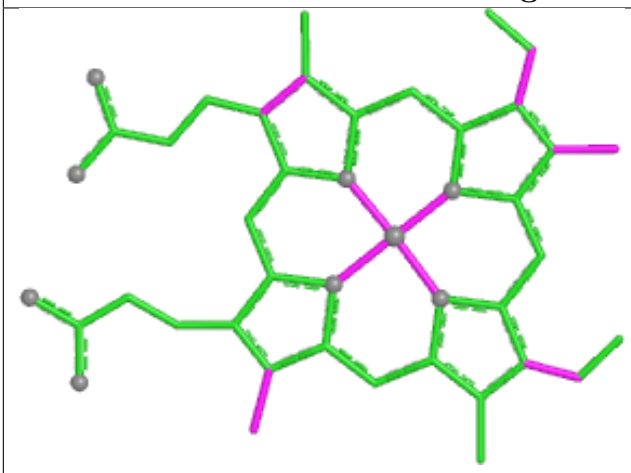


Torsions

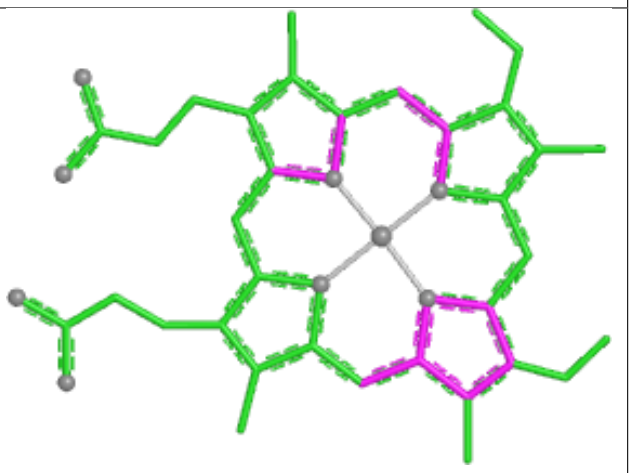


Rings

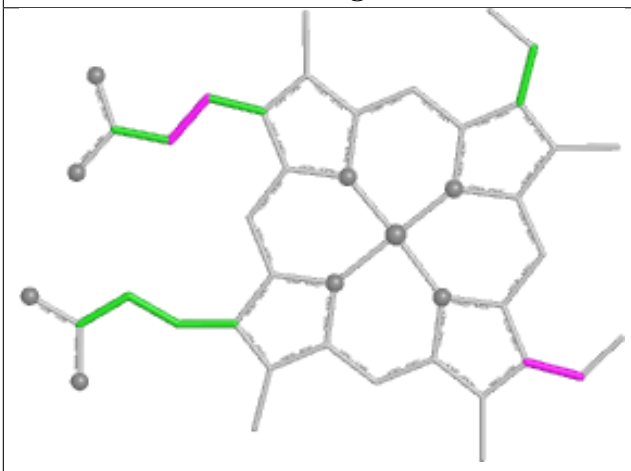
Ligand HEM F 101



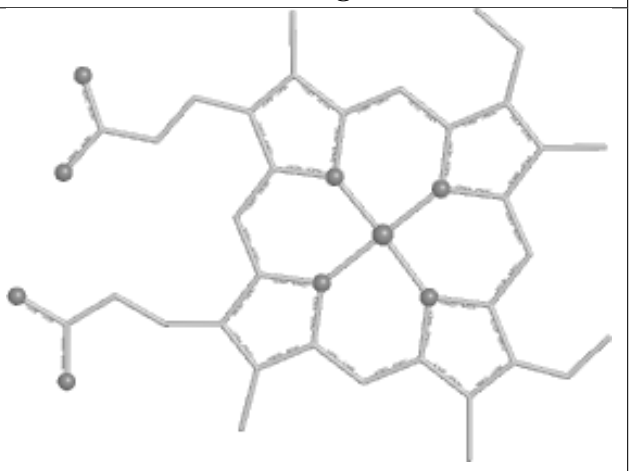
Bond lengths



Bond angles

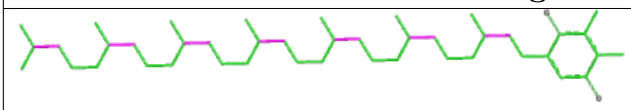


Torsions

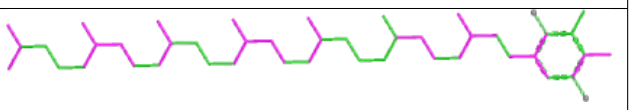


Rings

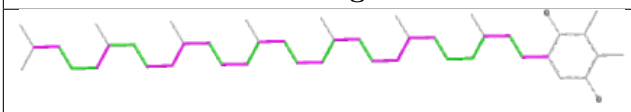
Ligand PL9 A 408



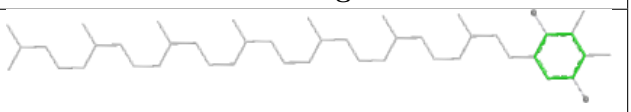
Bond lengths



Bond angles

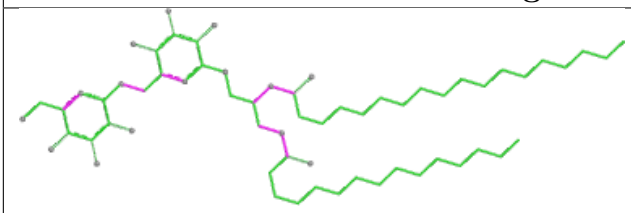


Torsions

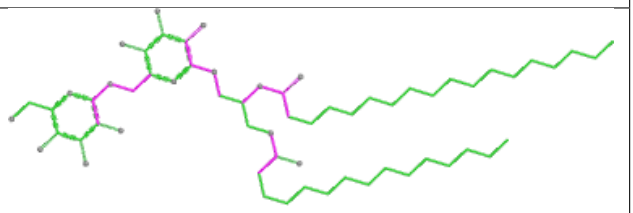


Rings

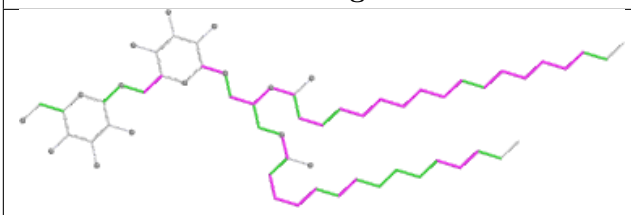
Ligand DGD d 408



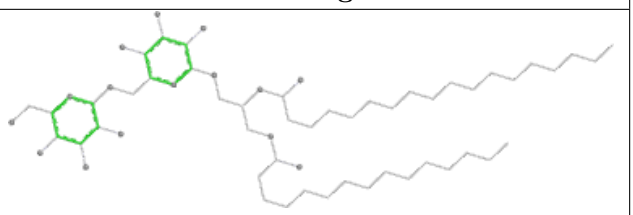
Bond lengths



Bond angles



Torsions

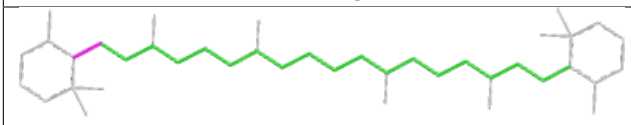


Rings

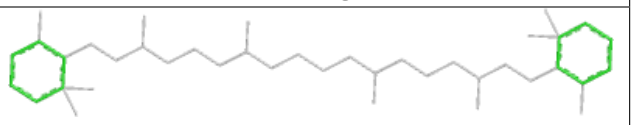
Ligand BCR J 102

Bond lengths

Bond angles

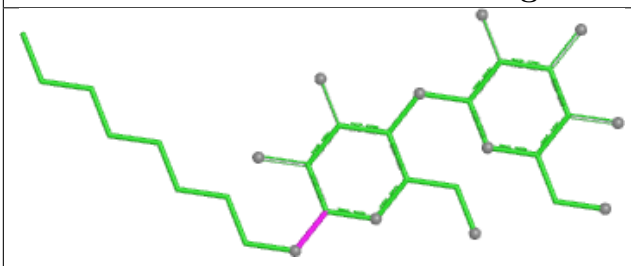


Torsions

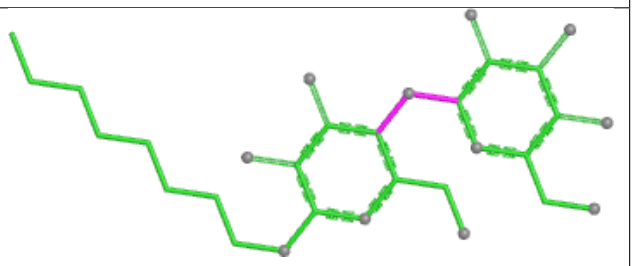


Rings

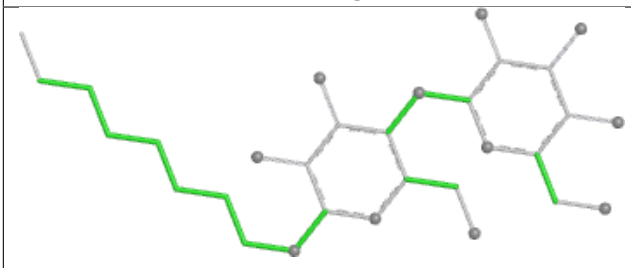
Ligand LMT D 411



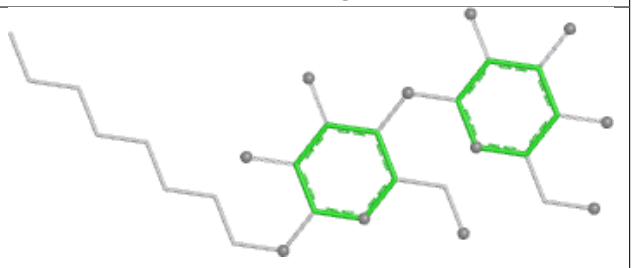
Bond lengths



Bond angles

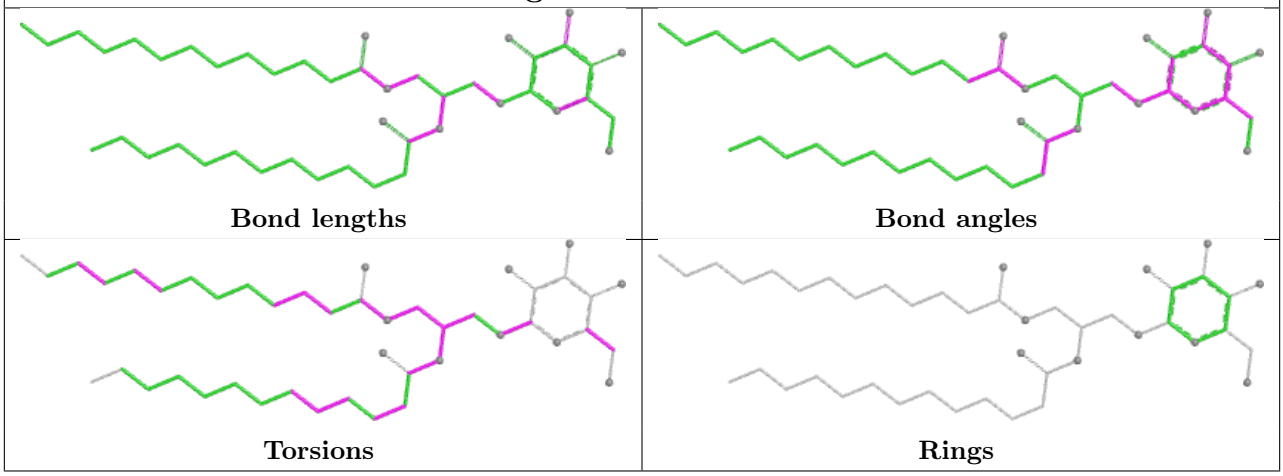


Torsions

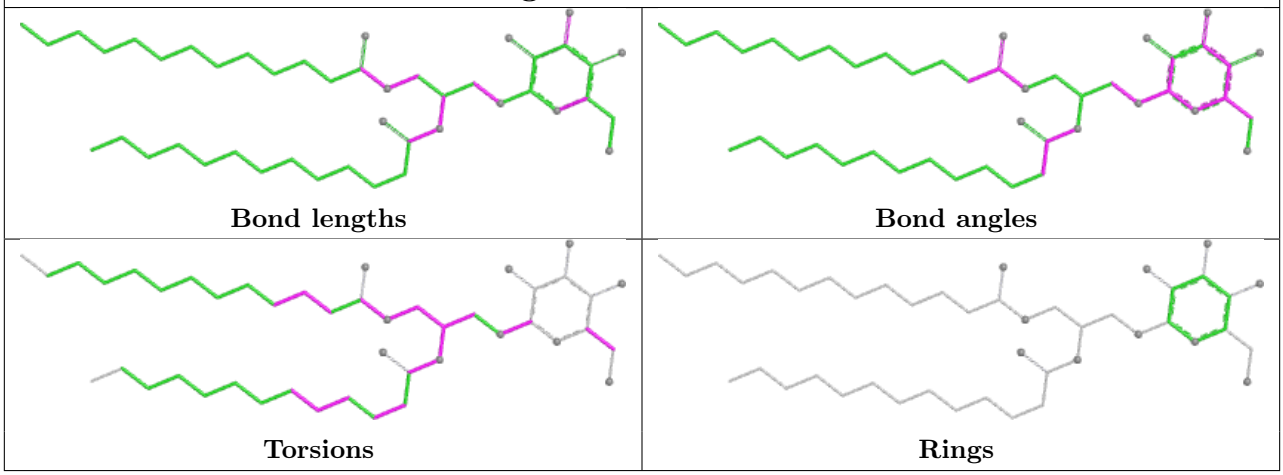


Rings

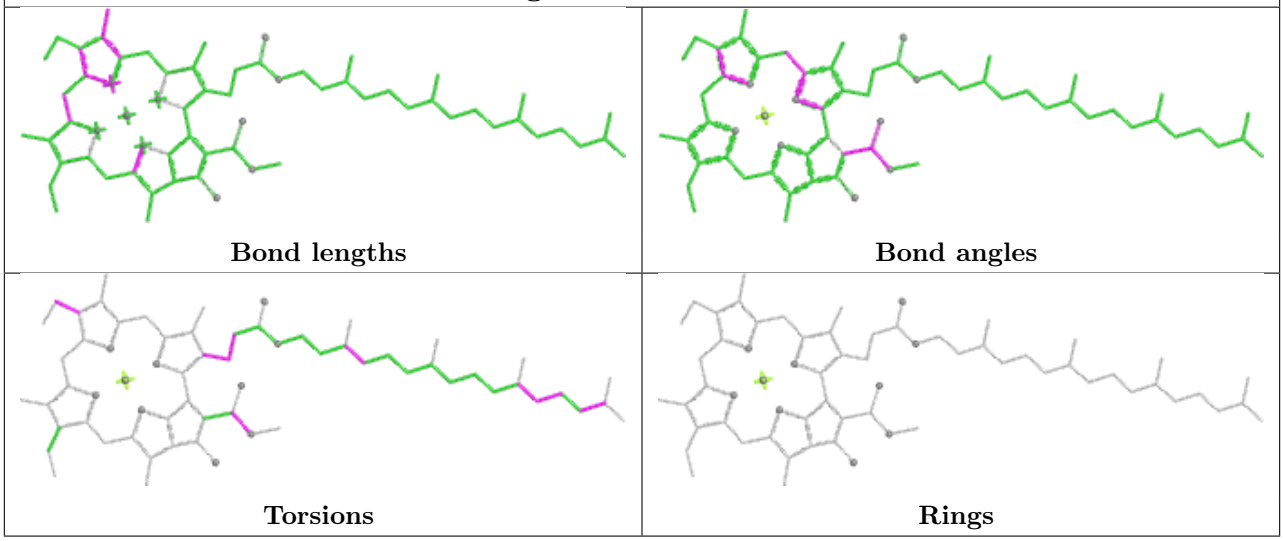
Ligand LMG c 520



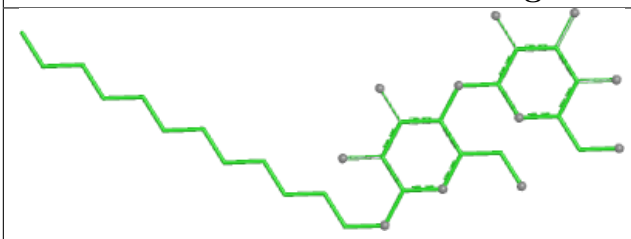
Ligand LMG C 520

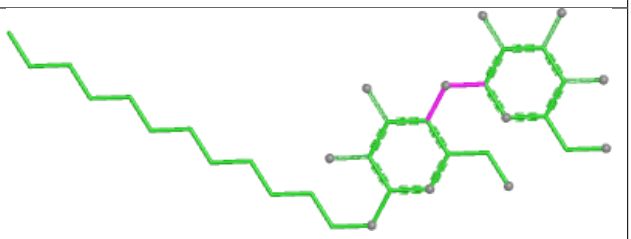


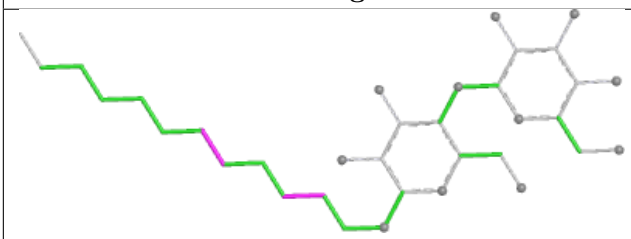
Ligand CLA B 606

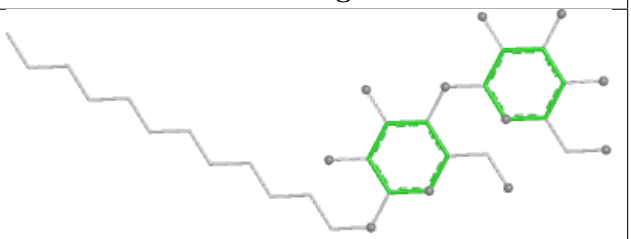


Ligand LMT b 625

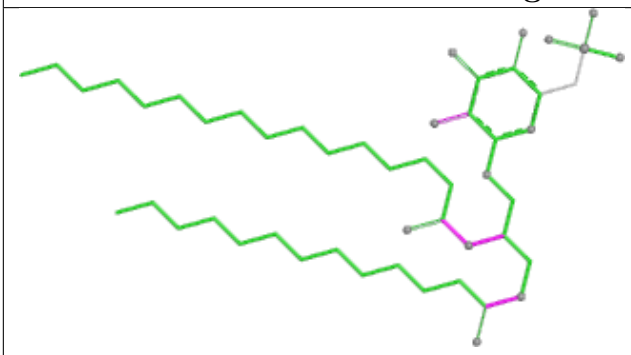

Bond lengths

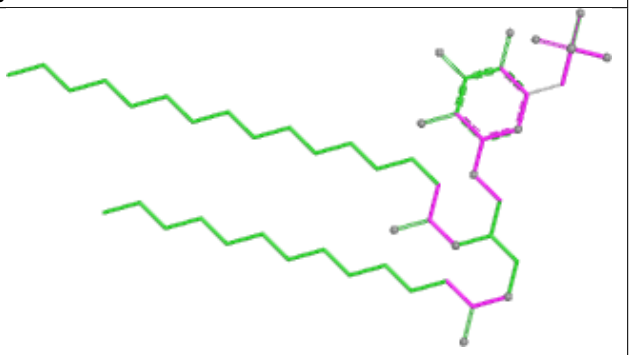

Bond angles

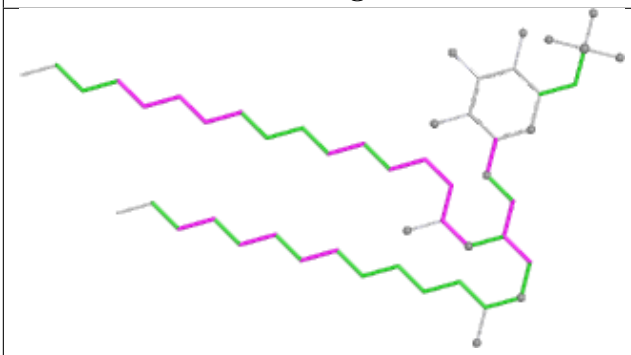

Torsions

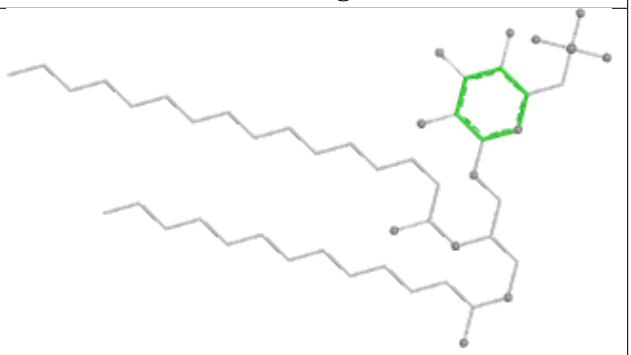

Rings

Ligand SQD A 413

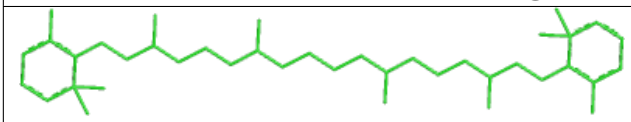

Bond lengths

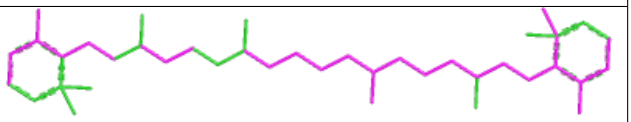

Bond angles

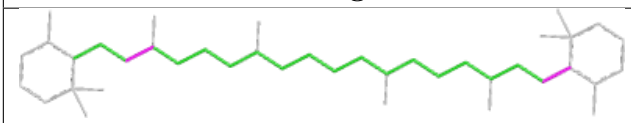

Torsions

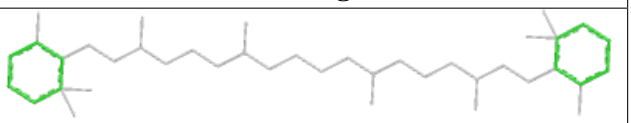

Rings

Ligand BCR a 412

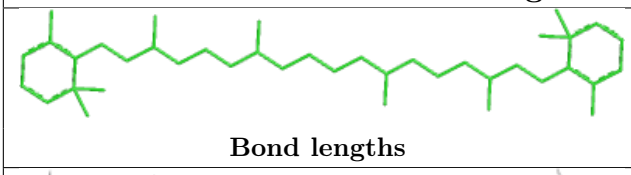

Bond lengths

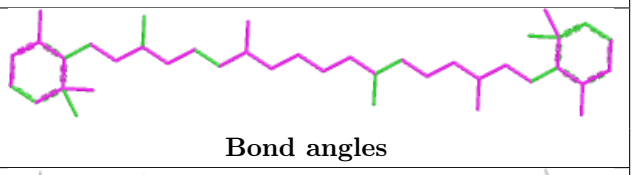

Bond angles

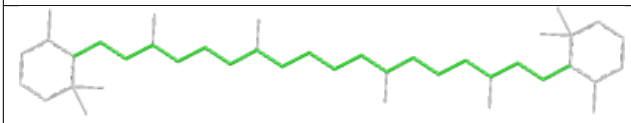

Torsions

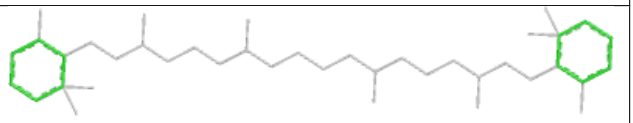

Rings

Ligand BCR b 621

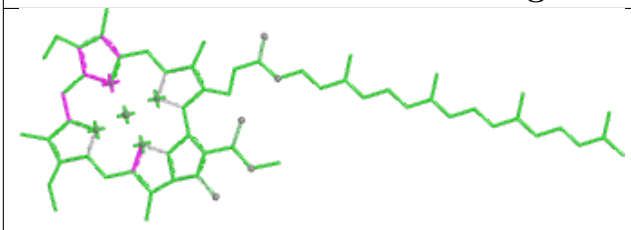

Bond lengths

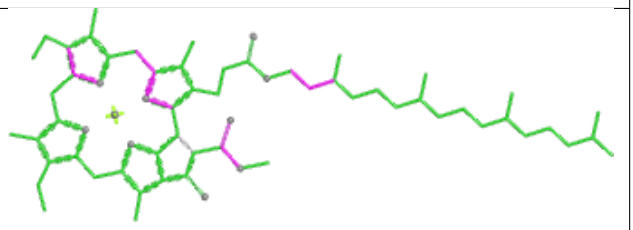

Bond angles

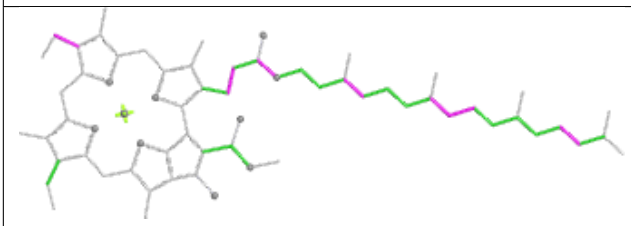

Torsions

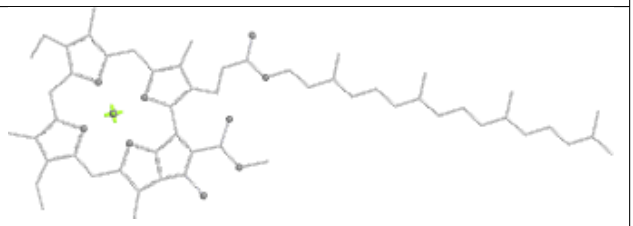

Rings

Ligand CLA d 403

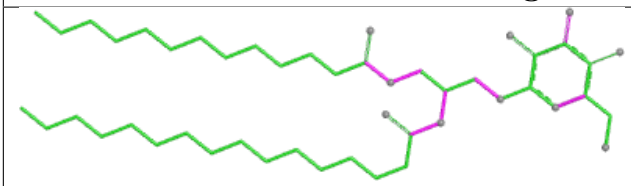

Bond lengths

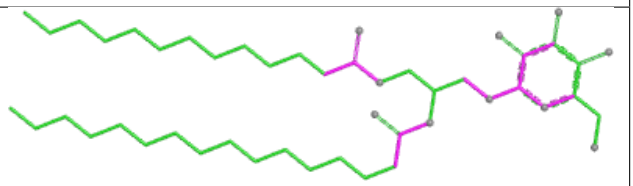

Bond angles

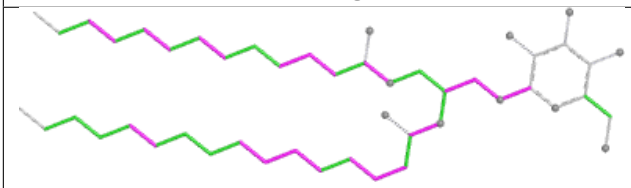

Torsions

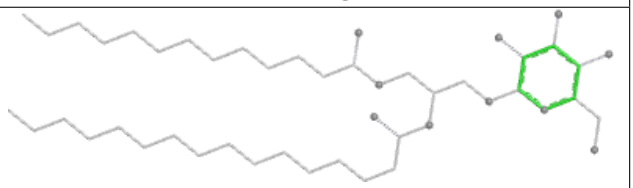

Rings

Ligand LMG d 406

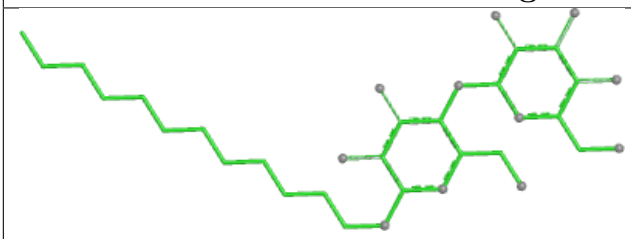

Bond lengths


Bond angles

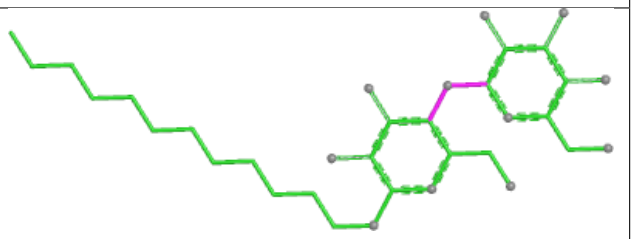

Torsions


Rings

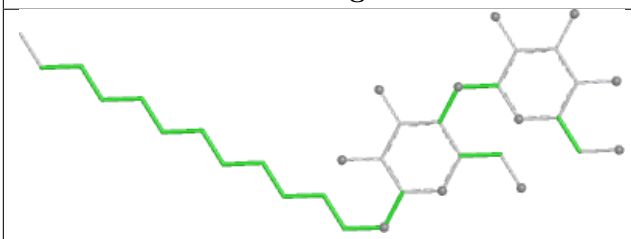
Ligand LMT m 101



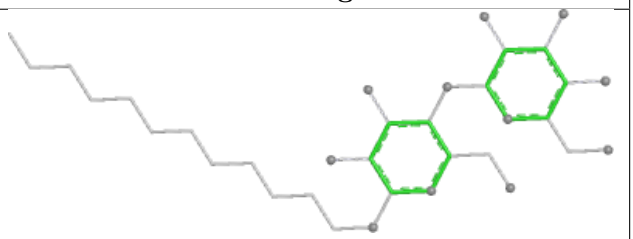
Bond lengths



Bond angles

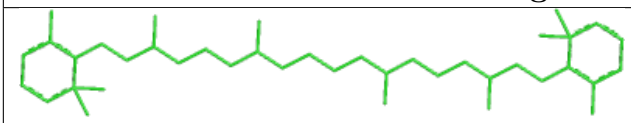


Torsions

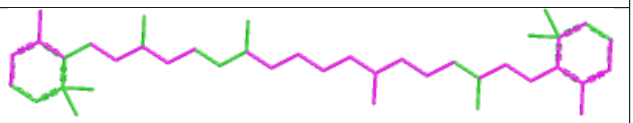


Rings

Ligand BCR f 102

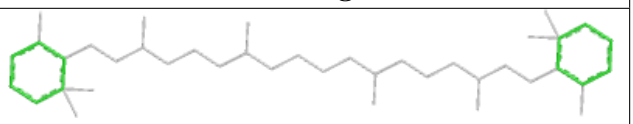


Bond lengths



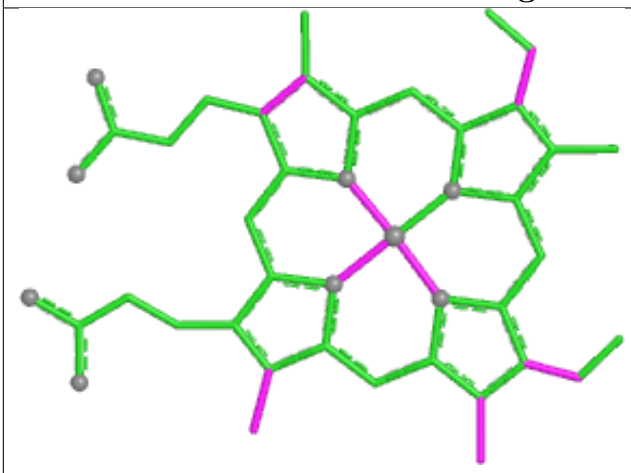
Bond angles

Torsions

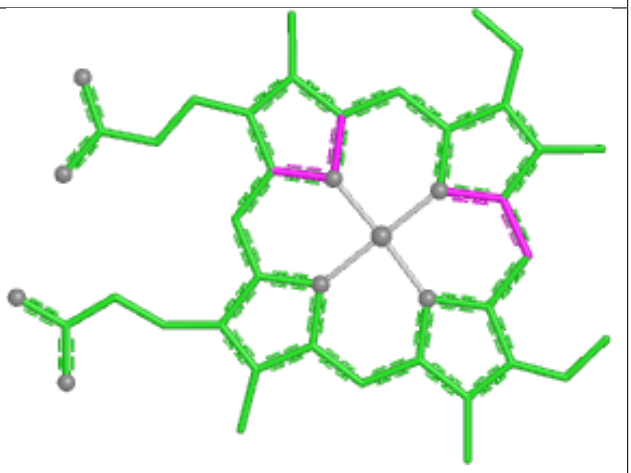


Rings

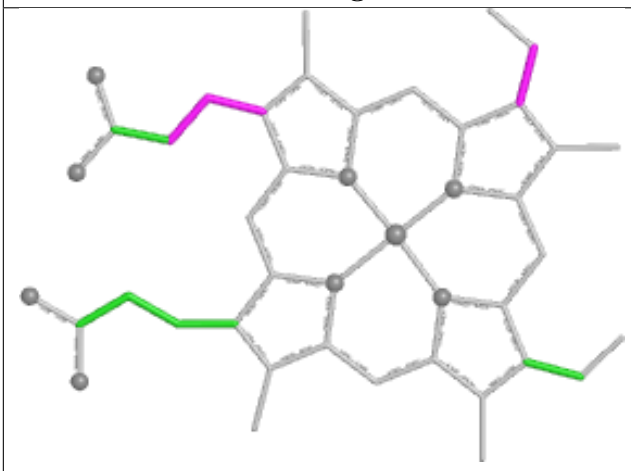
Ligand HEM V 201



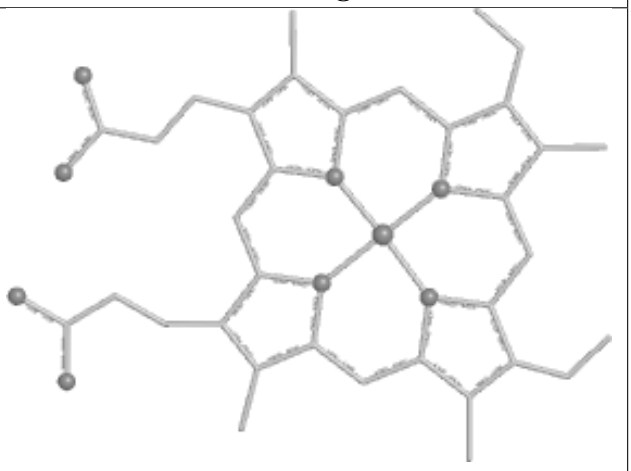
Bond lengths



Bond angles

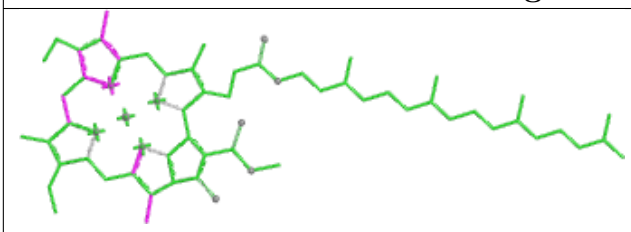


Torsions

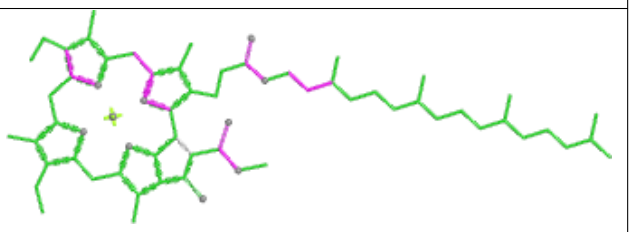


Rings

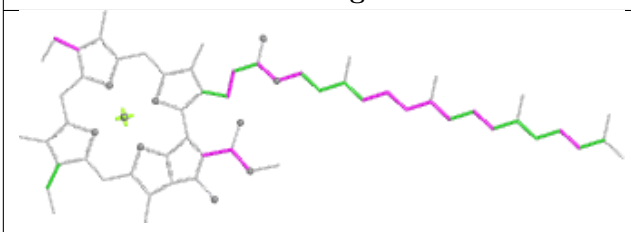
Ligand CLA C 509



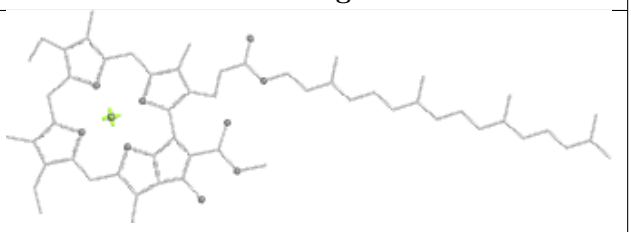
Bond lengths



Bond angles

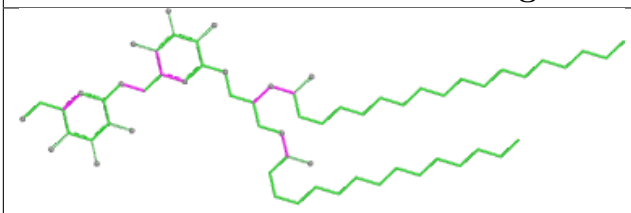


Torsions

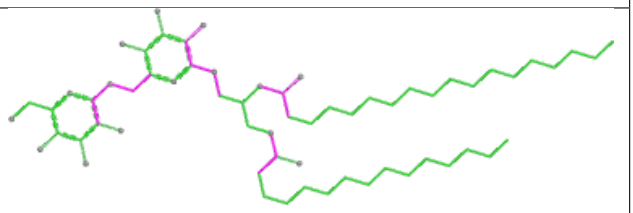


Rings

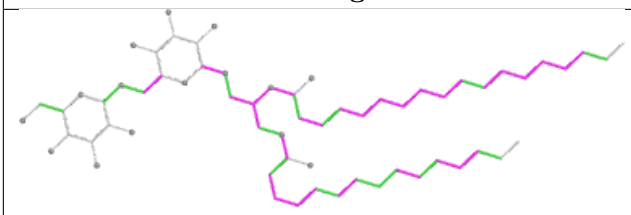
Ligand DGD D 410



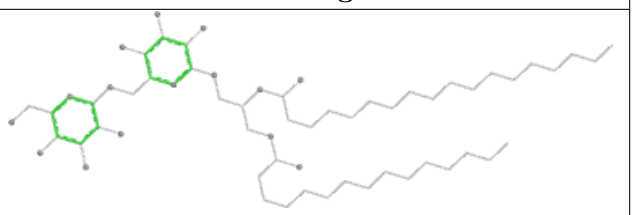
Bond lengths



Bond angles

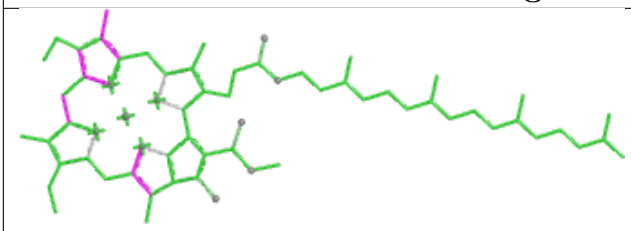


Torsions

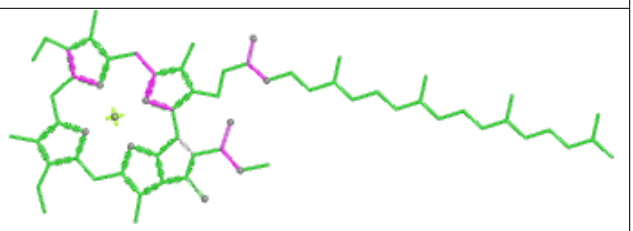


Rings

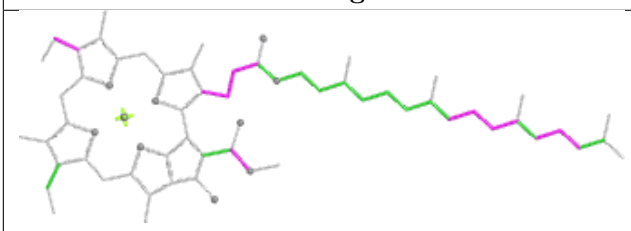
Ligand CLA C 501



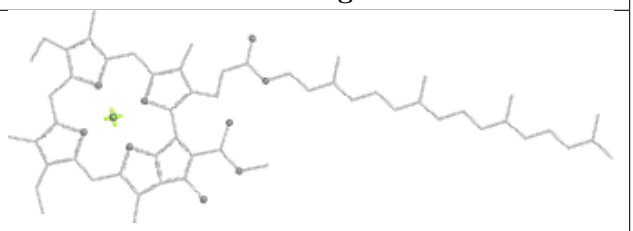
Bond lengths



Bond angles

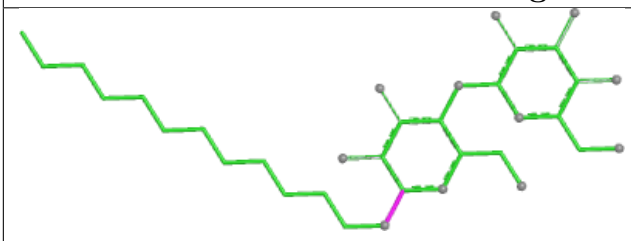


Torsions

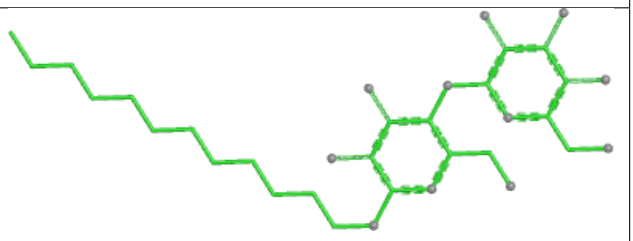


Rings

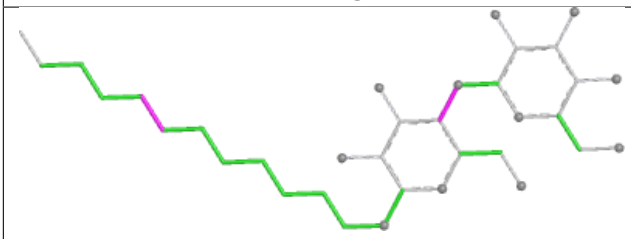
Ligand LMT i 102



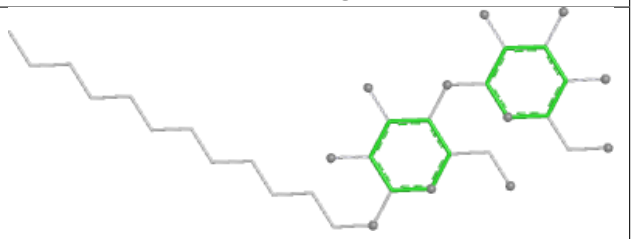
Bond lengths



Bond angles

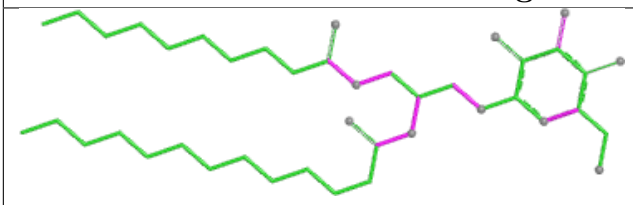


Torsions

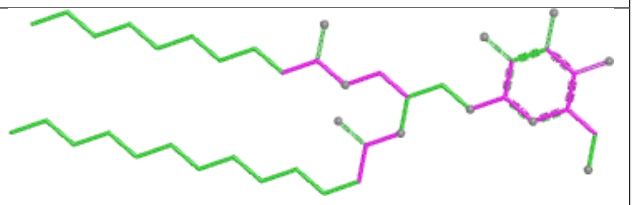


Rings

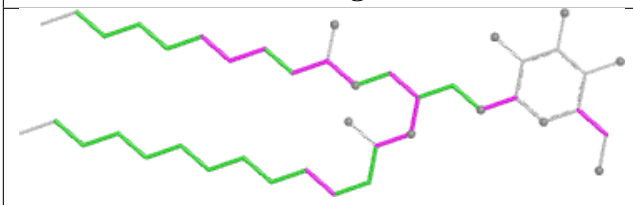
Ligand LMG M 101



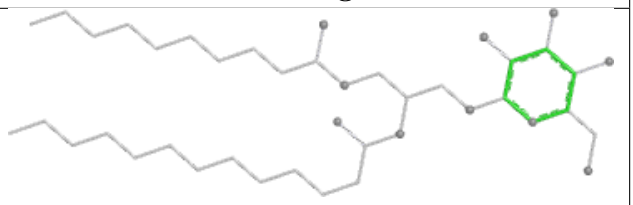
Bond lengths



Bond angles

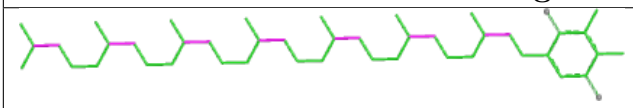


Torsions

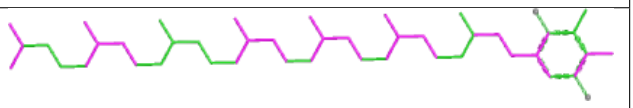


Rings

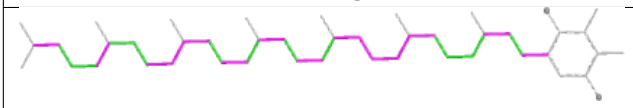
Ligand PL9 a 410



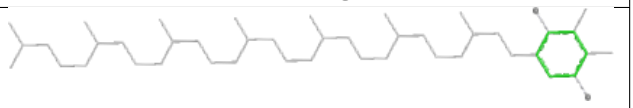
Bond lengths



Bond angles

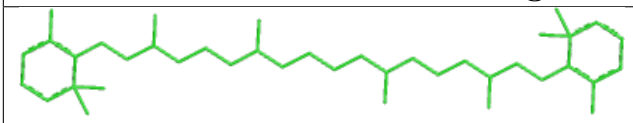


Torsions

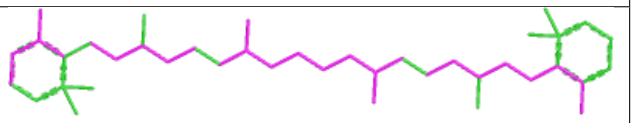


Rings

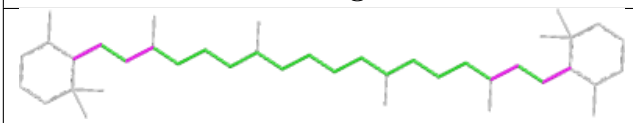
Ligand BCR k 102



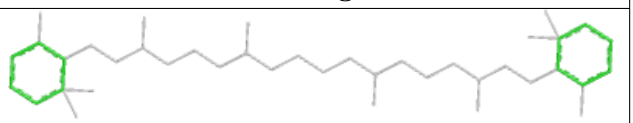
Bond lengths



Bond angles

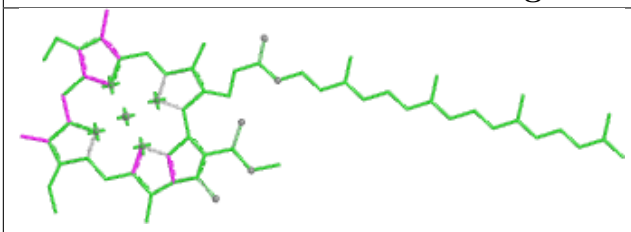


Torsions

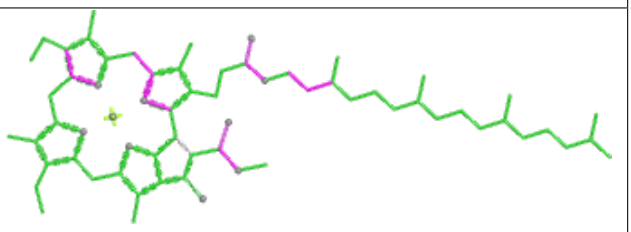


Rings

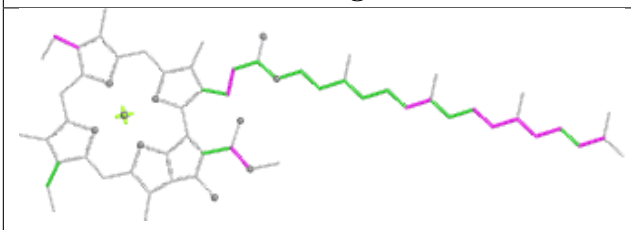
Ligand CLA B 601



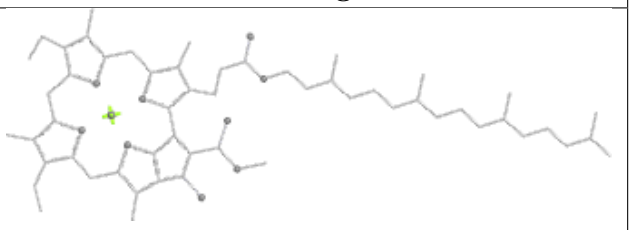
Bond lengths



Bond angles

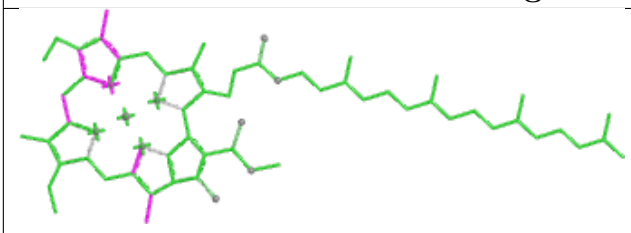


Torsions

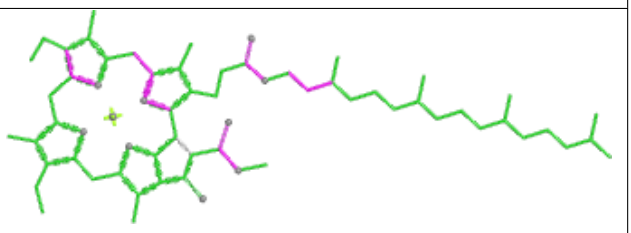


Rings

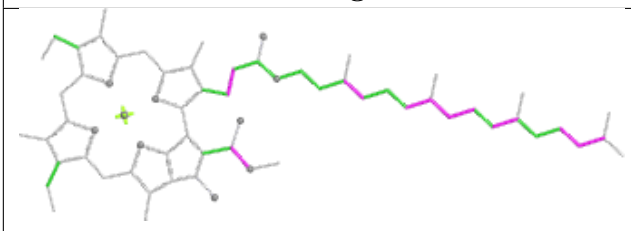
Ligand CLA B 603



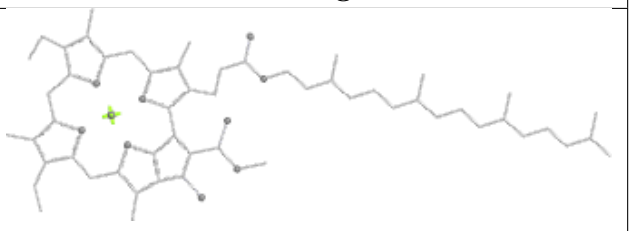
Bond lengths



Bond angles

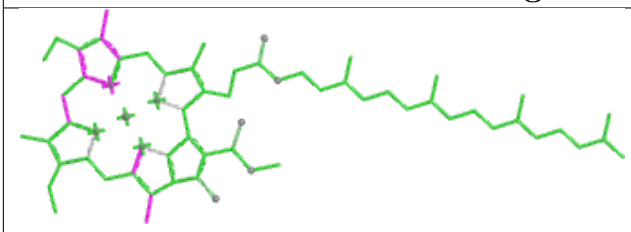


Torsions

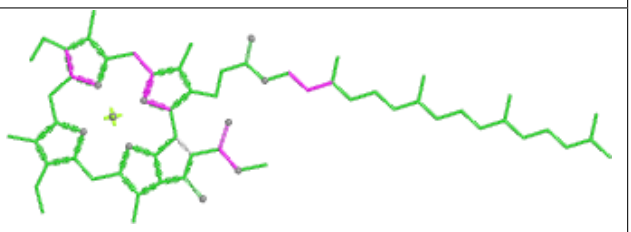


Rings

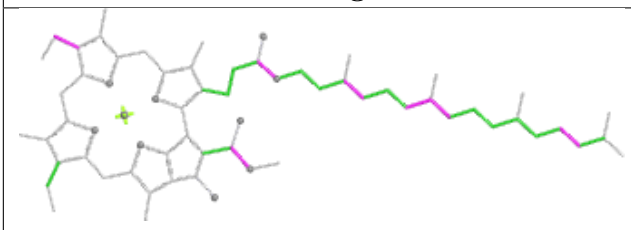
Ligand CLA B 611



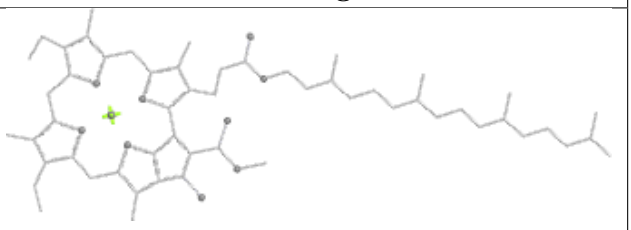
Bond lengths



Bond angles

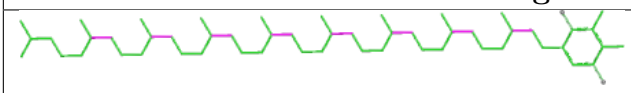


Torsions

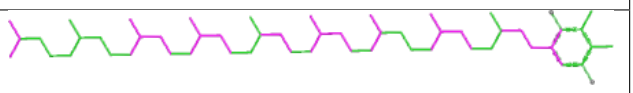


Rings

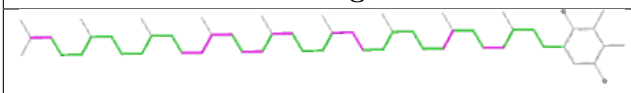
Ligand PL9 d 404



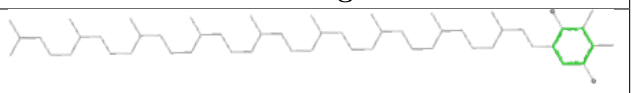
Bond lengths



Bond angles

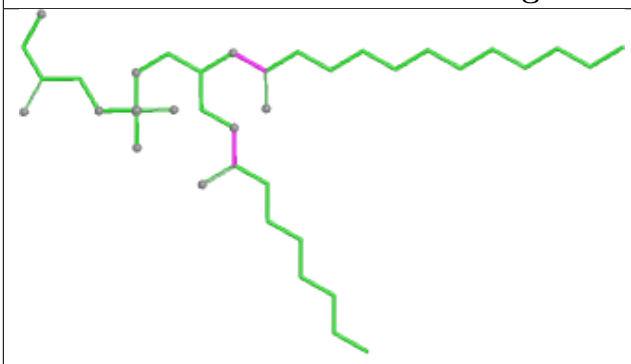


Torsions

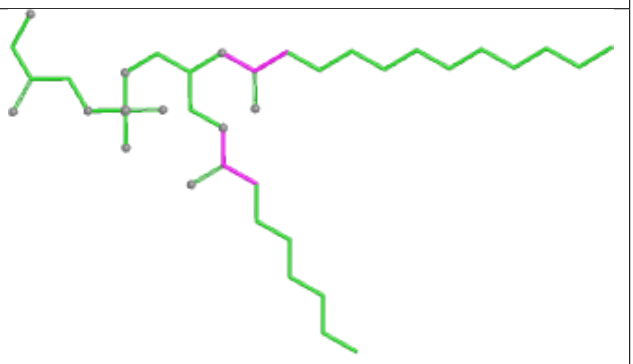


Rings

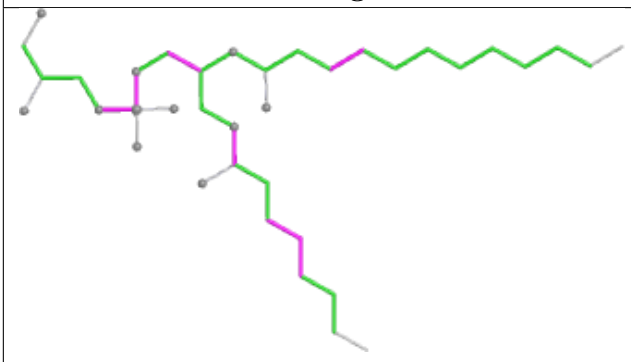
Ligand LHG A 415



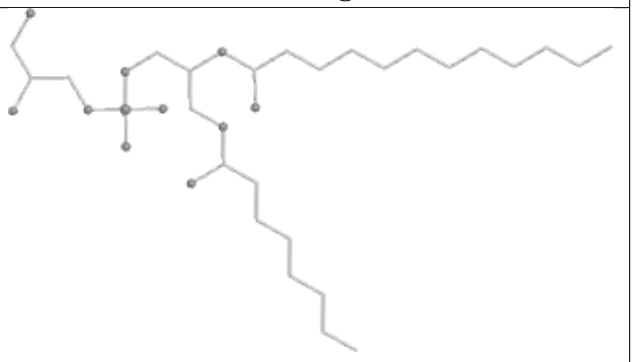
Bond lengths



Bond angles



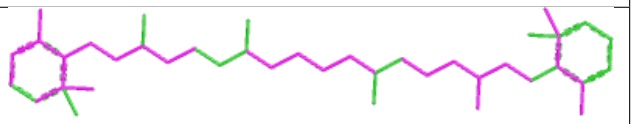
Torsions



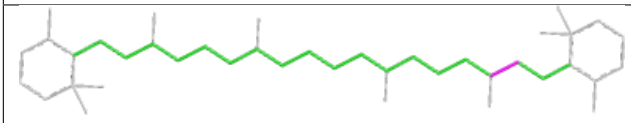
Rings

Ligand BCR B 620

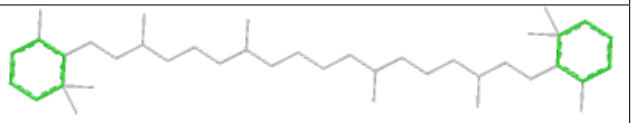
Bond lengths



Bond angles

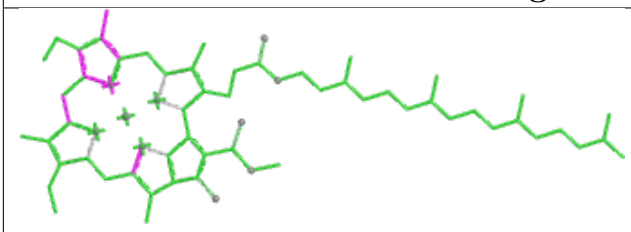


Torsions

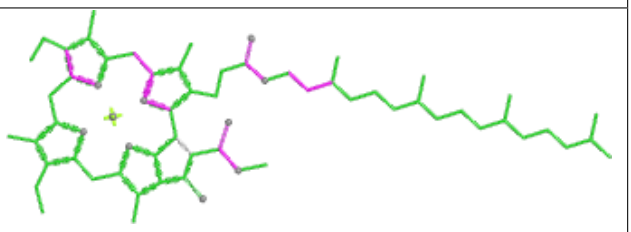


Rings

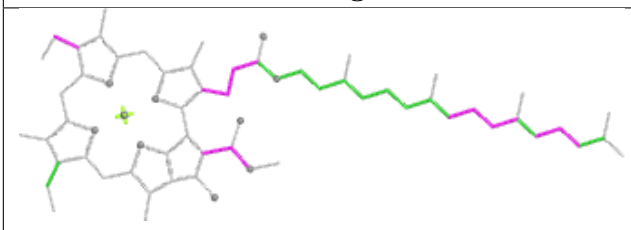
Ligand CLA c 501



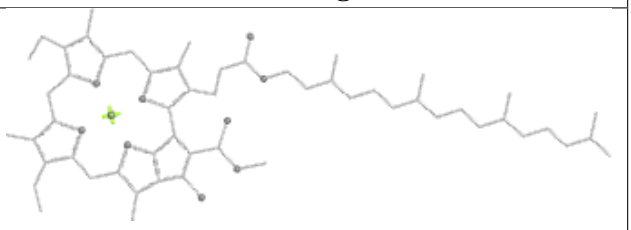
Bond lengths



Bond angles

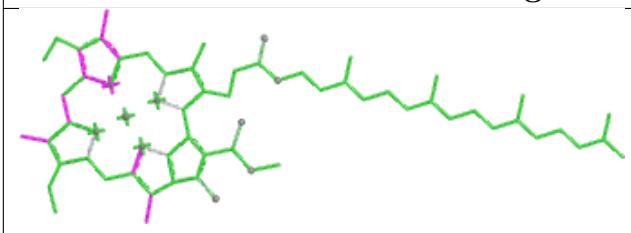


Torsions

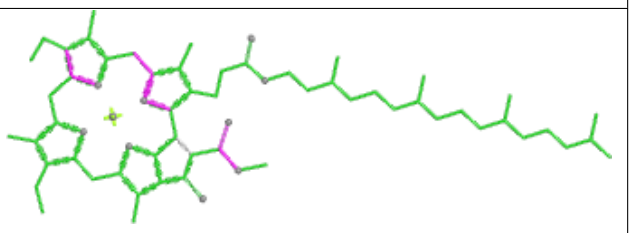


Rings

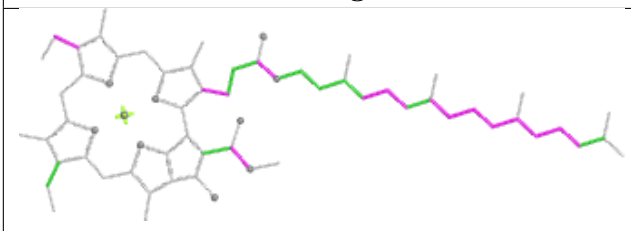
Ligand CLA B 616



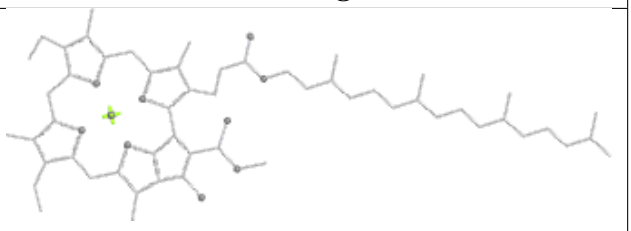
Bond lengths



Bond angles

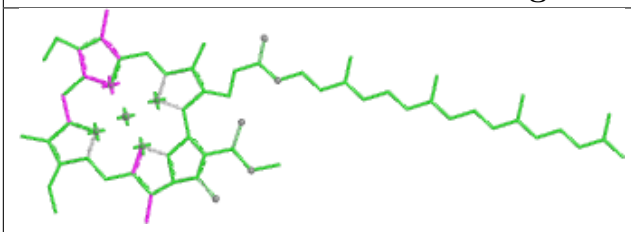


Torsions

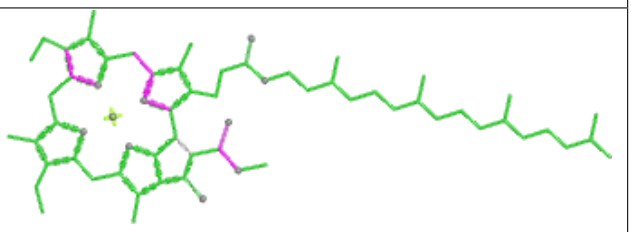


Rings

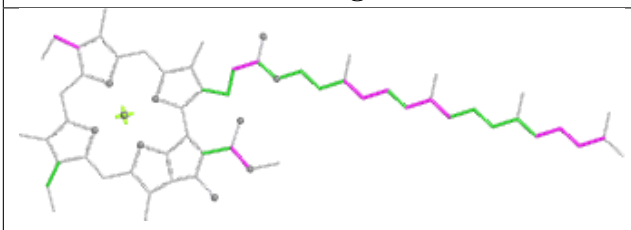
Ligand CLA c 510



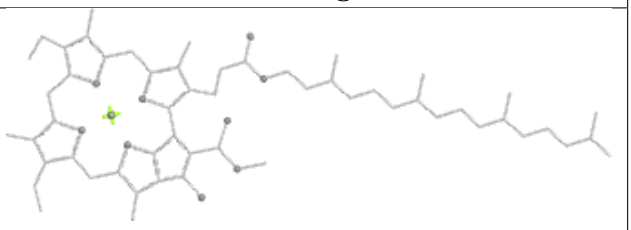
Bond lengths



Bond angles

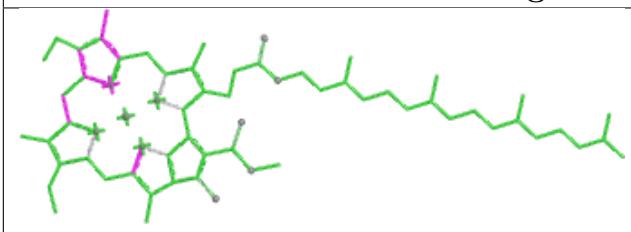


Torsions

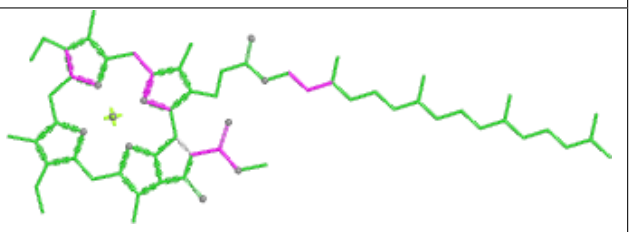


Rings

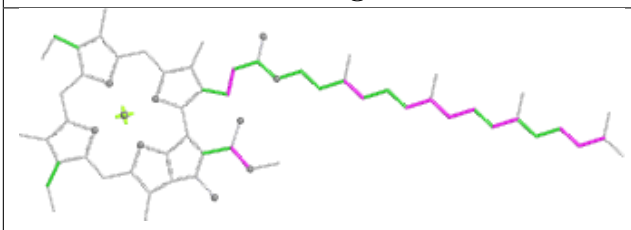
Ligand CLA b 606



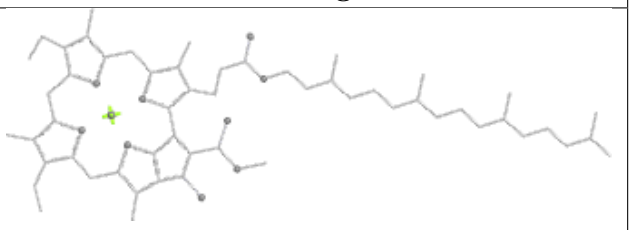
Bond lengths



Bond angles

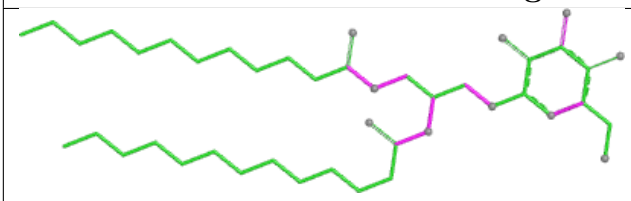


Torsions

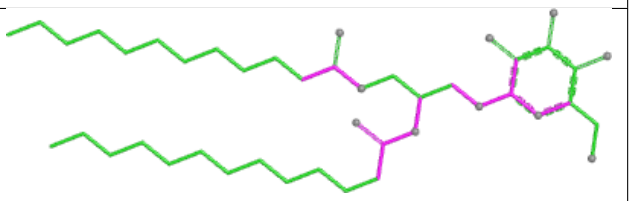


Rings

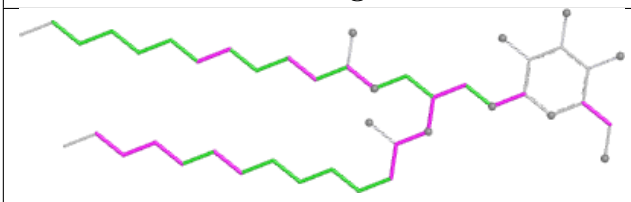
Ligand LMG e 101



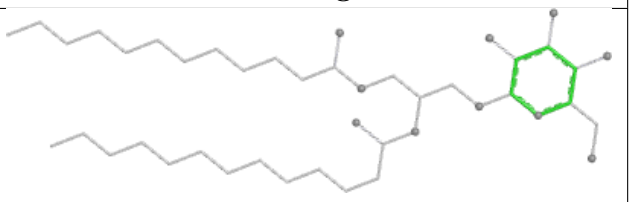
Bond lengths



Bond angles

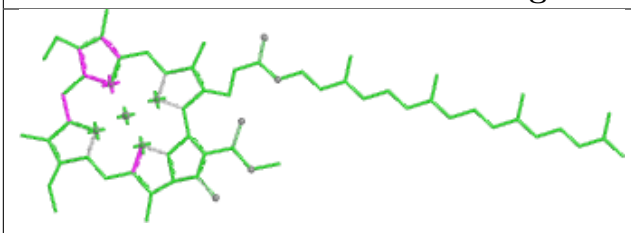


Torsions

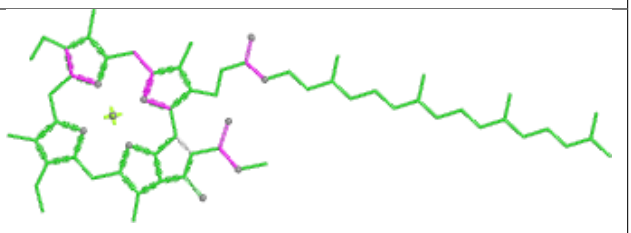


Rings

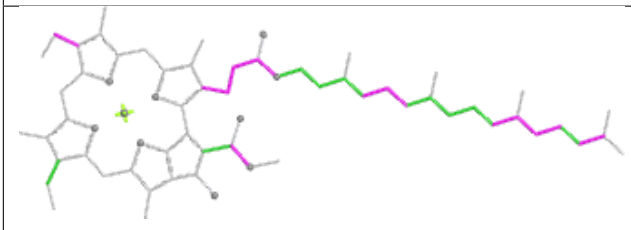
Ligand CLA c 512



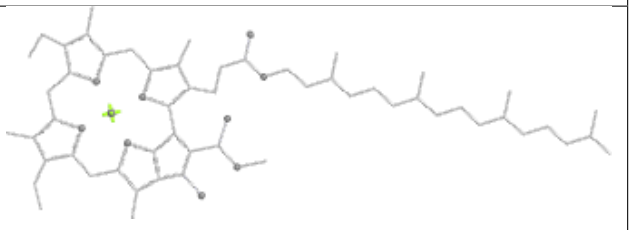
Bond lengths



Bond angles

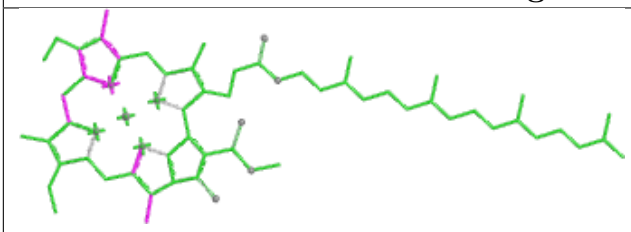


Torsions

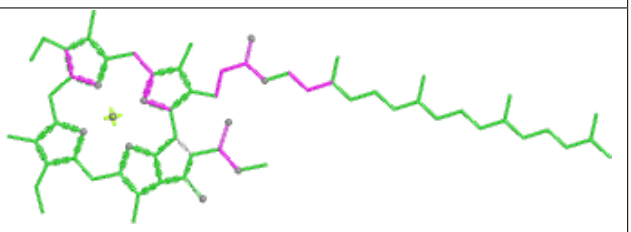


Rings

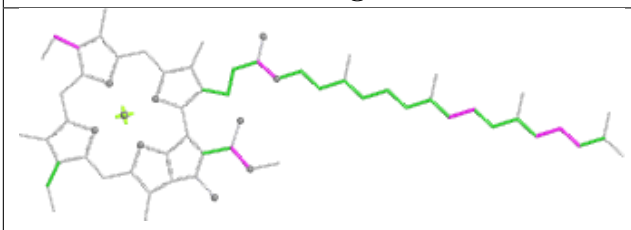
Ligand CLA b 607



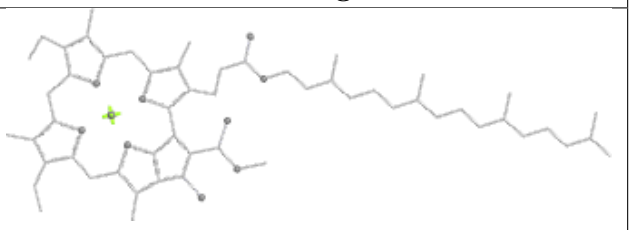
Bond lengths



Bond angles

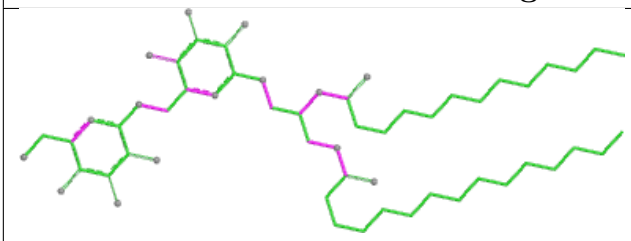


Torsions

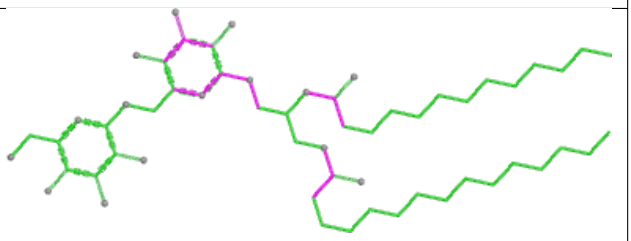


Rings

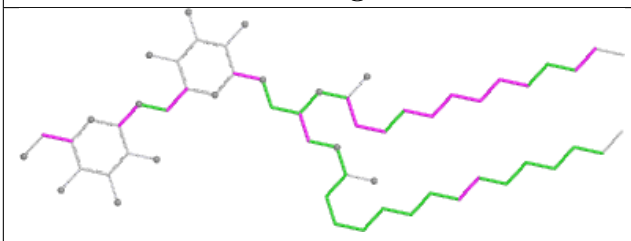
Ligand DGD B 621



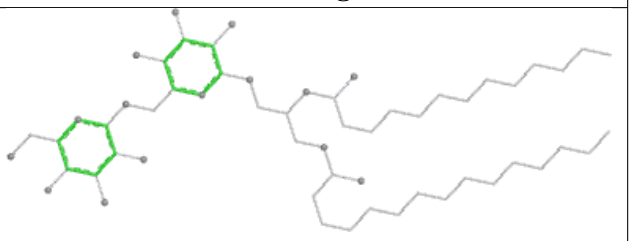
Bond lengths



Bond angles

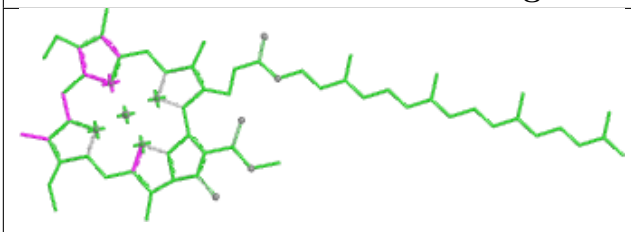


Torsions

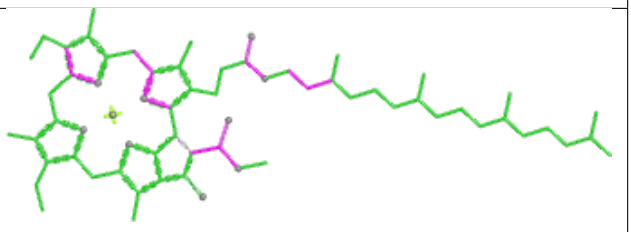


Rings

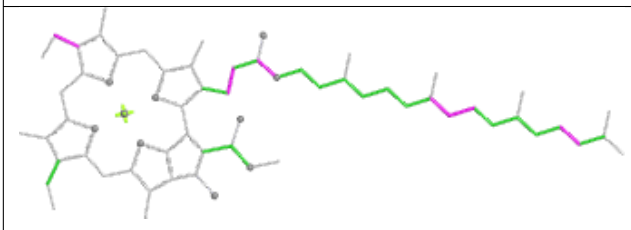
Ligand CLA D 403



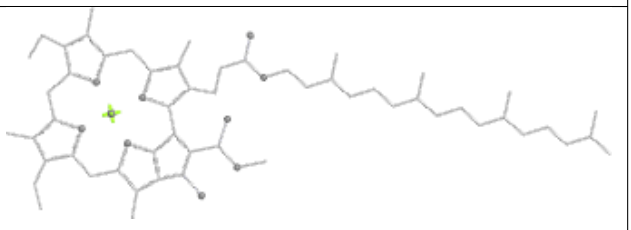
Bond lengths



Bond angles

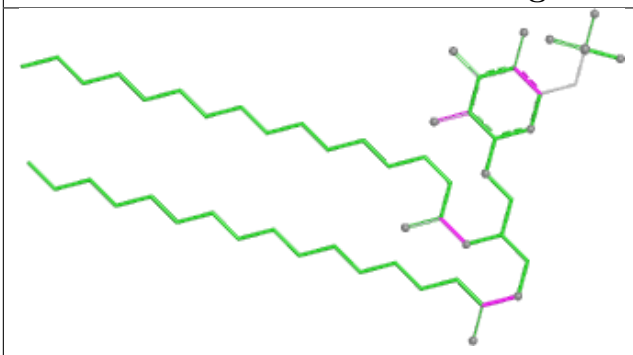


Torsions

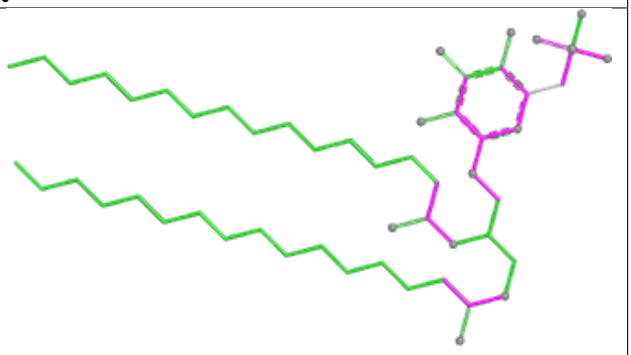


Rings

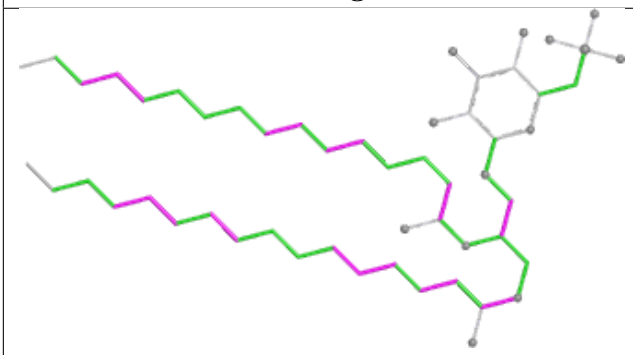
Ligand SQD a 401



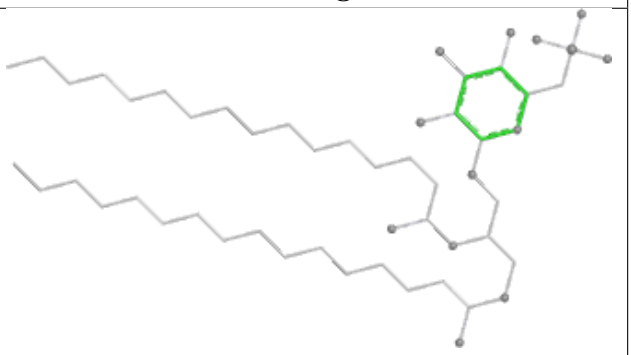
Bond lengths



Bond angles

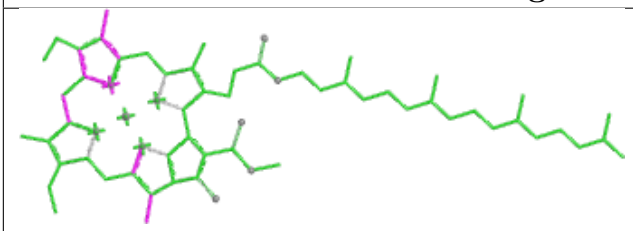


Torsions

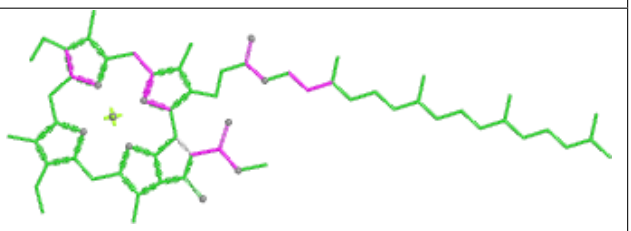


Rings

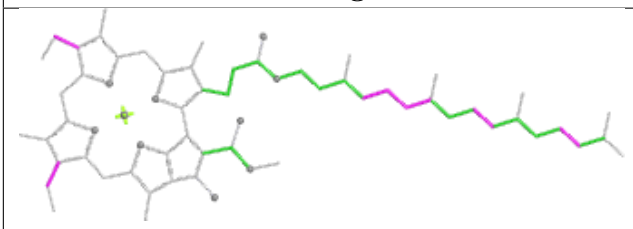
Ligand CLA a 406



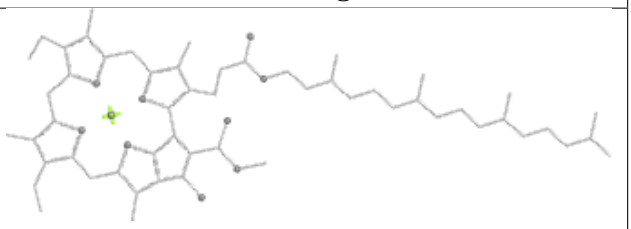
Bond lengths



Bond angles

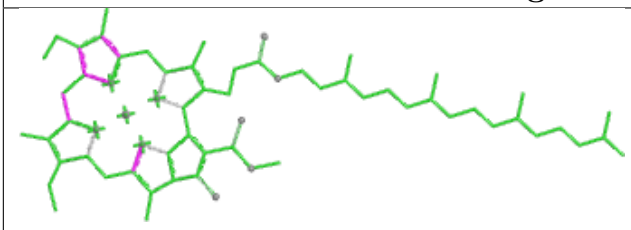


Torsions

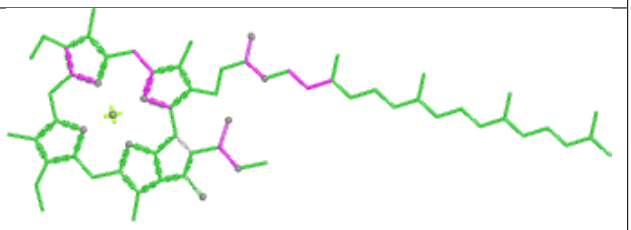


Rings

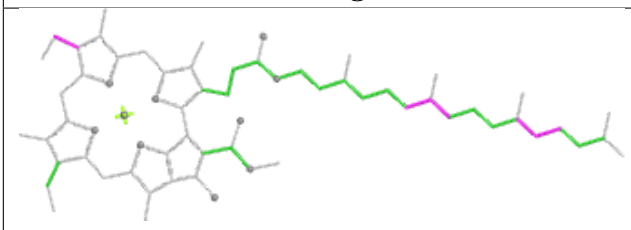
Ligand CLA b 618



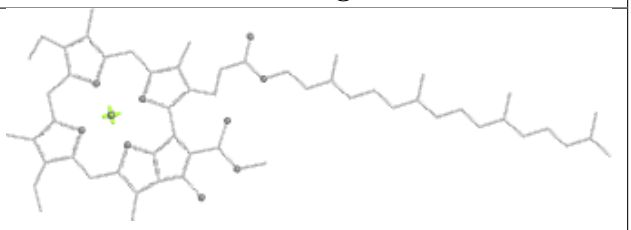
Bond lengths



Bond angles

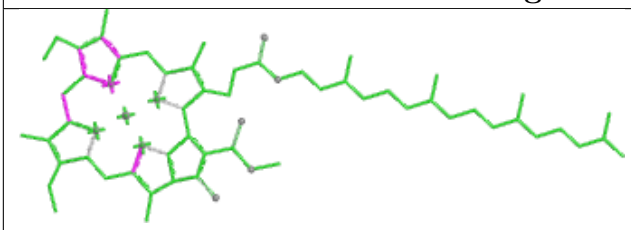


Torsions

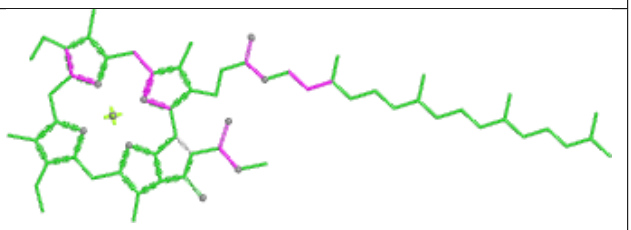


Rings

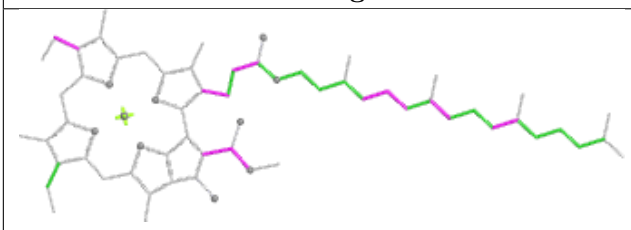
Ligand CLA C 507



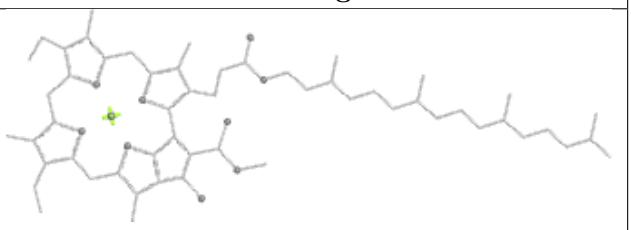
Bond lengths



Bond angles



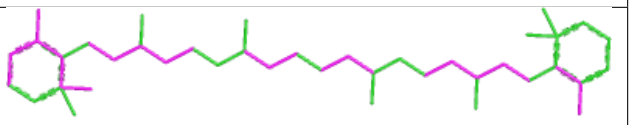
Torsions



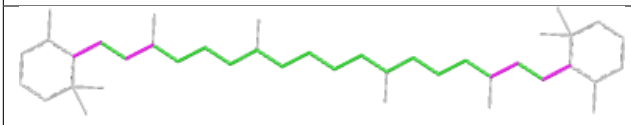
Rings

Ligand BCR K 102

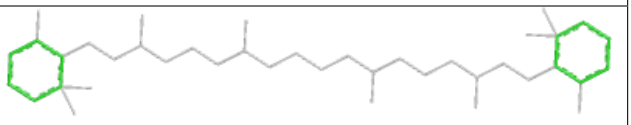
Bond lengths



Bond angles

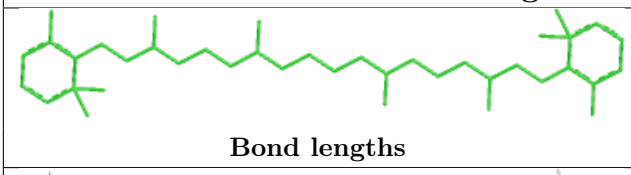


Torsions

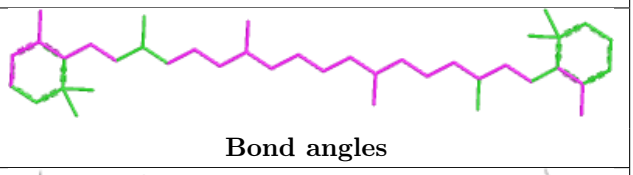


Rings

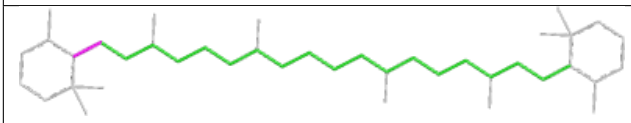
Ligand BCR H 101



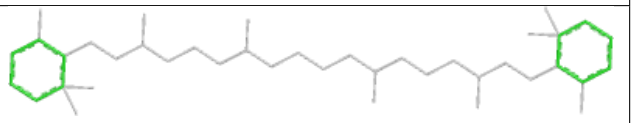
Bond lengths



Bond angles



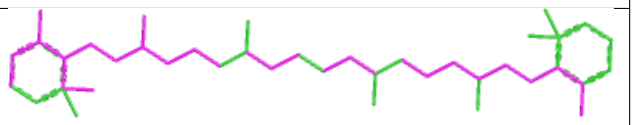
Torsions



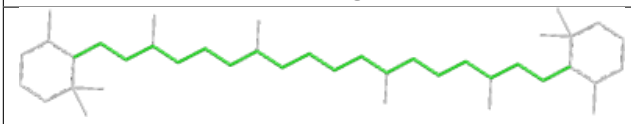
Rings

Ligand BCR A 410

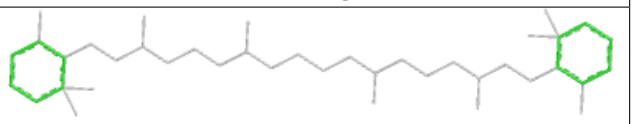
Bond lengths



Bond angles

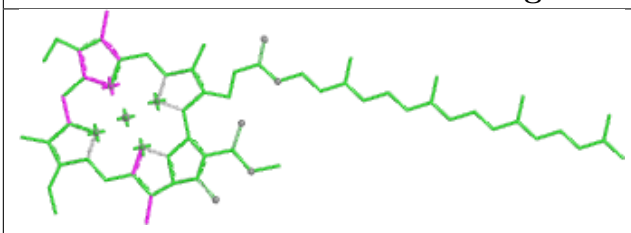


Torsions

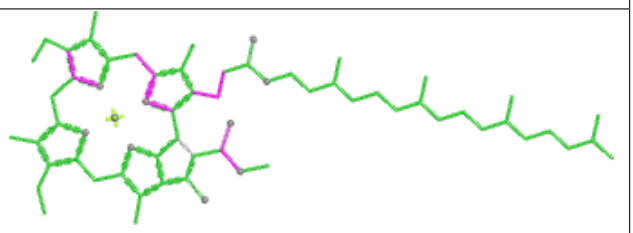


Rings

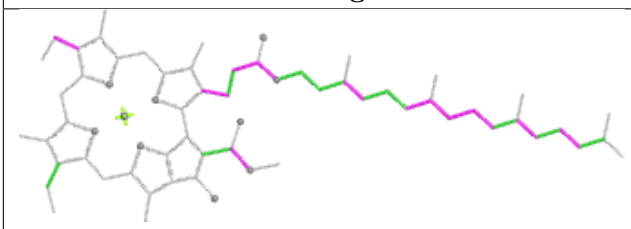
Ligand CLA C 505



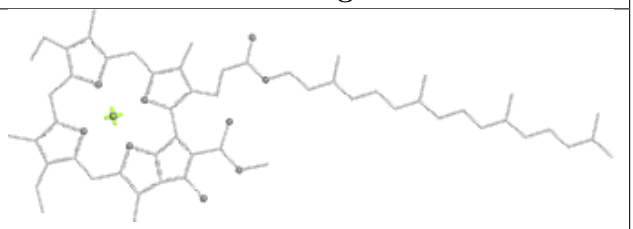
Bond lengths



Bond angles

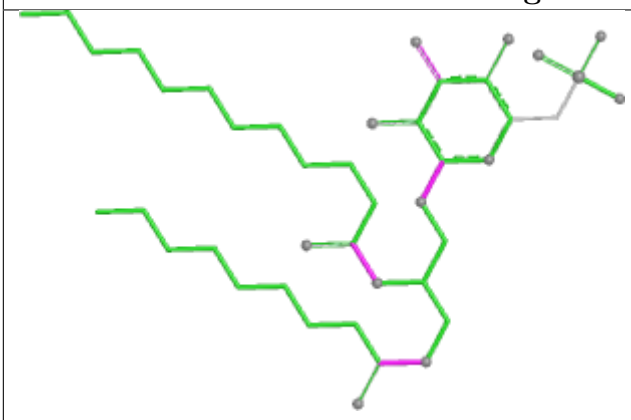


Torsions

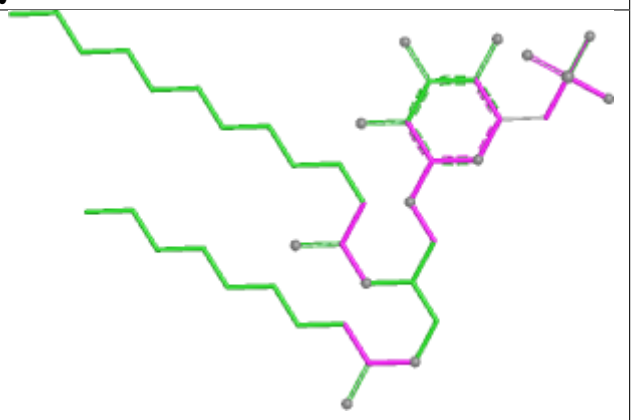


Rings

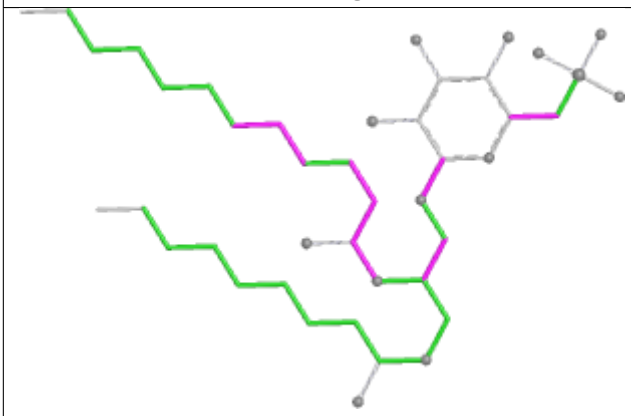
Ligand SQD D 409



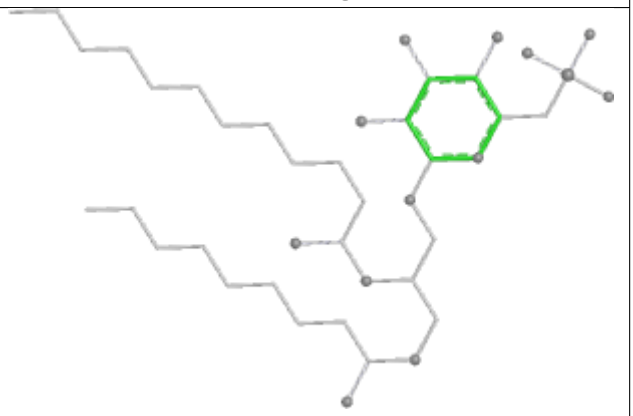
Bond lengths



Bond angles

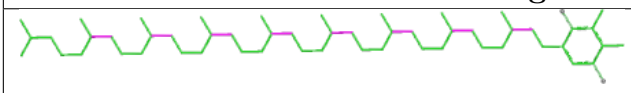


Torsions

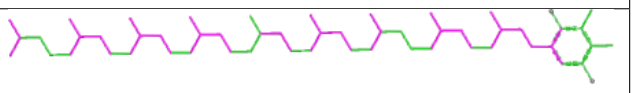


Rings

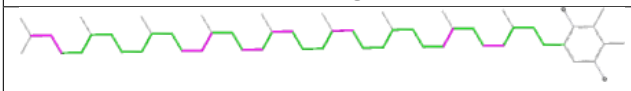
Ligand PL9 D 404



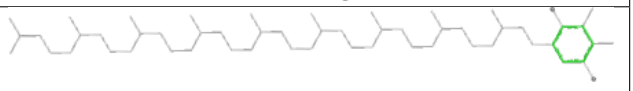
Bond lengths



Bond angles

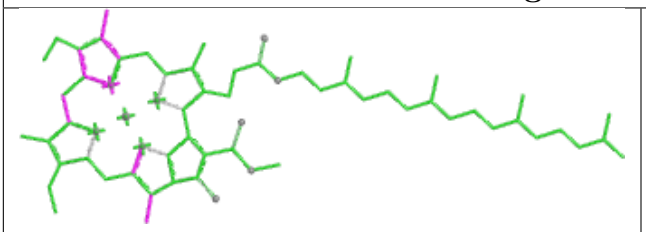


Torsions

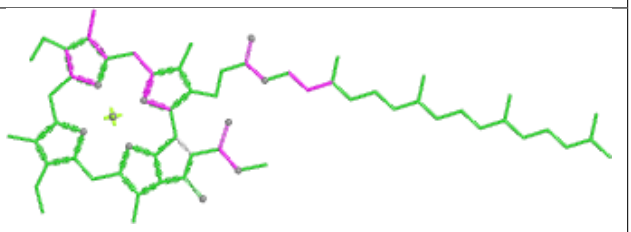


Rings

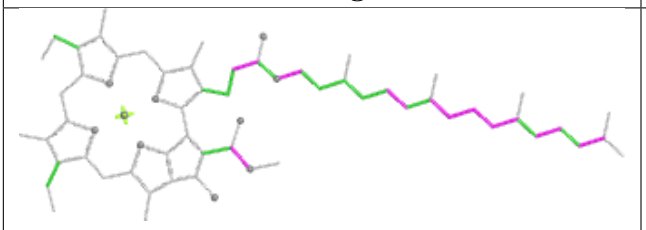
Ligand CLA B 613



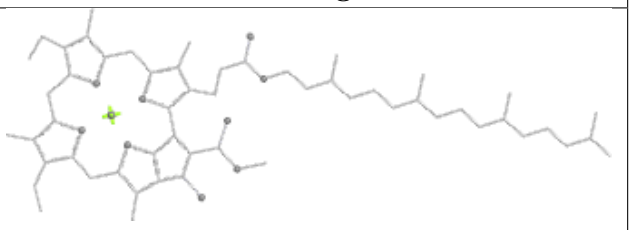
Bond lengths



Bond angles

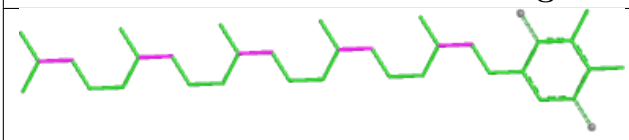


Torsions

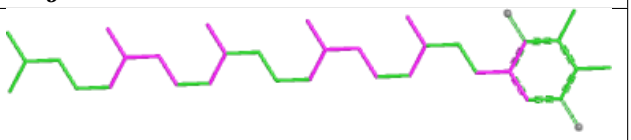


Rings

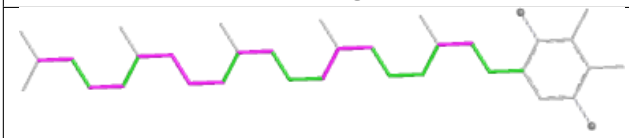
Ligand PL9 j 101



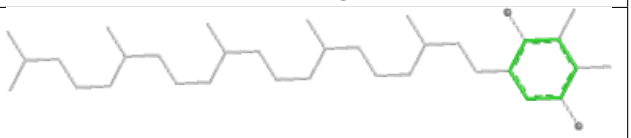
Bond lengths



Bond angles

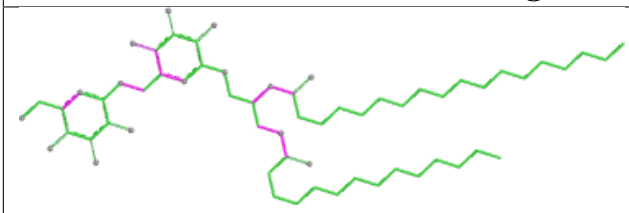


Torsions

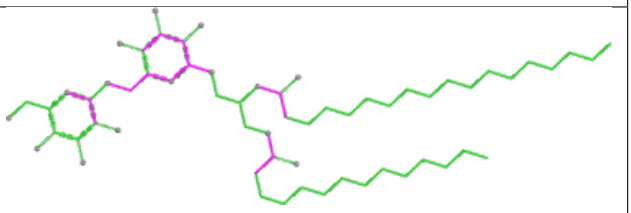


Rings

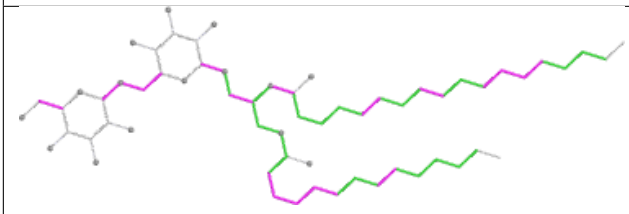
Ligand DGD c 518



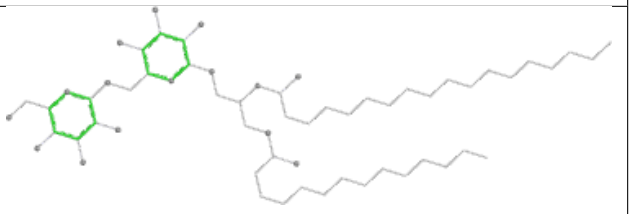
Bond lengths



Bond angles

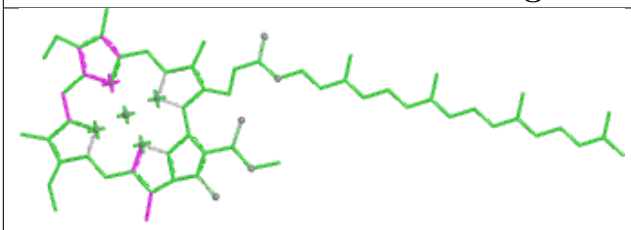


Torsions

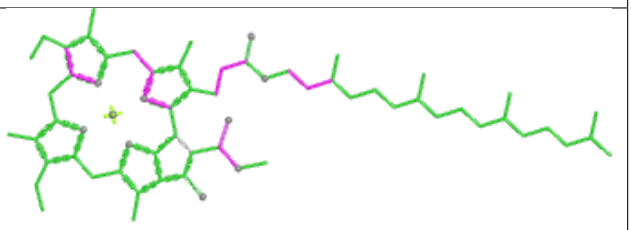


Rings

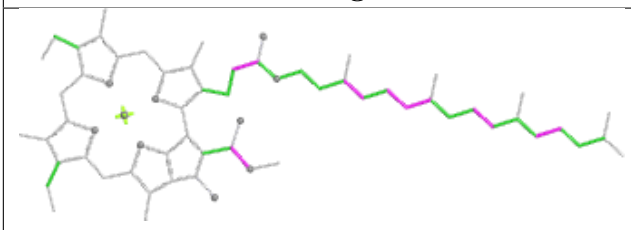
Ligand CLA B 612



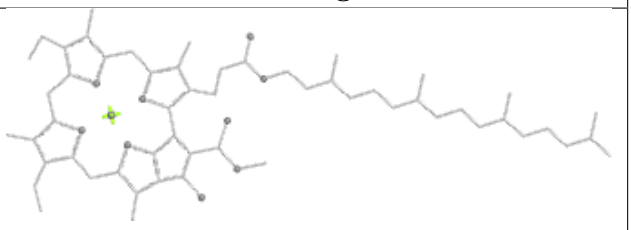
Bond lengths



Bond angles

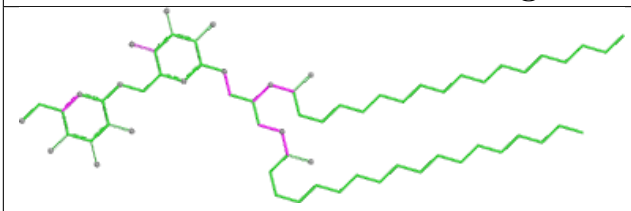


Torsions

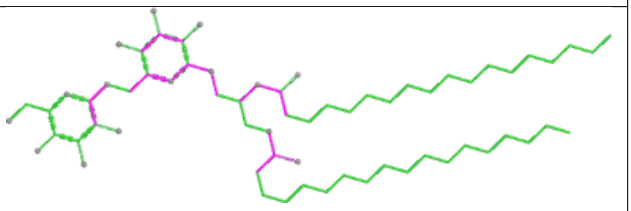


Rings

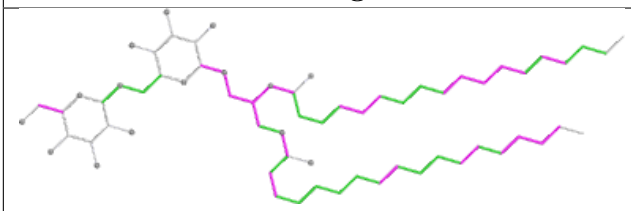
Ligand DGD C 518



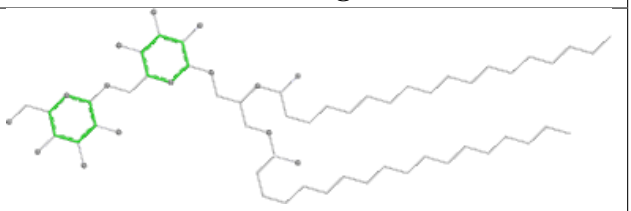
Bond lengths



Bond angles

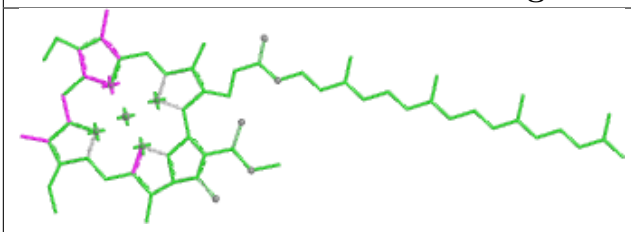


Torsions

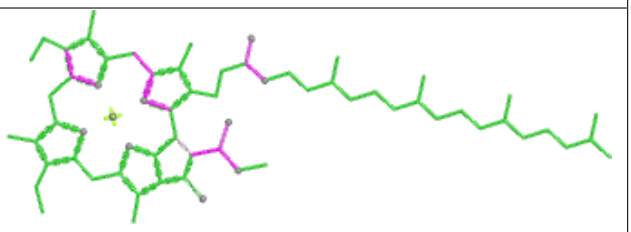


Rings

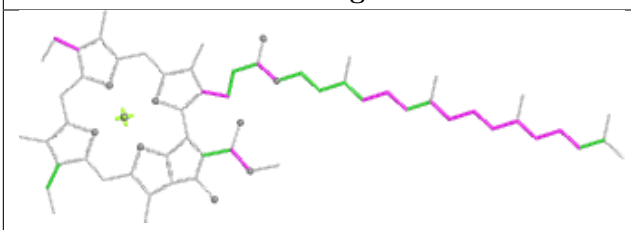
Ligand CLA b 619



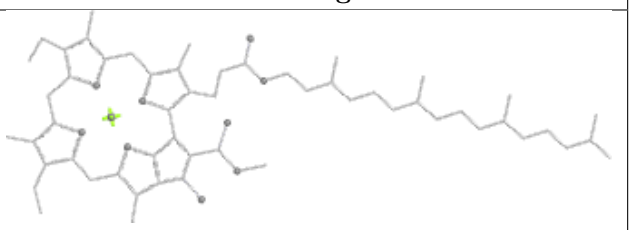
Bond lengths



Bond angles

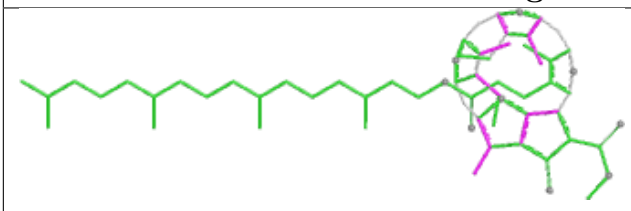


Torsions

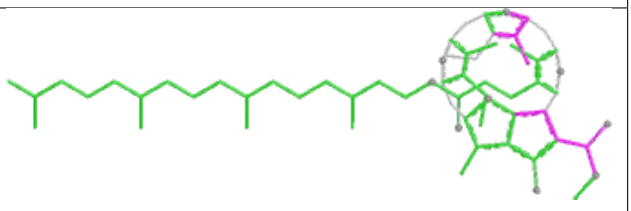


Rings

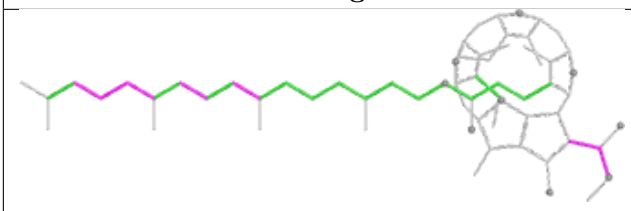
Ligand PHO a 408



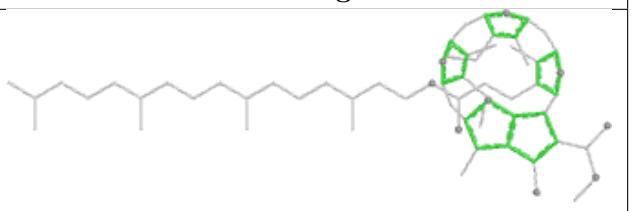
Bond lengths



Bond angles



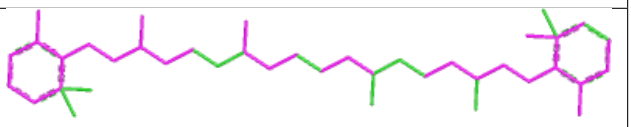
Torsions



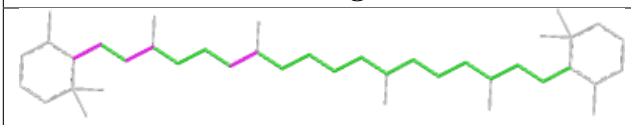
Rings

Ligand BCR C 514

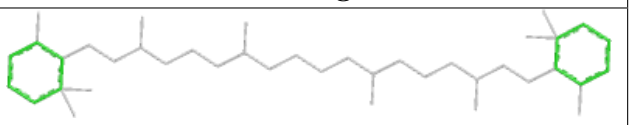
Bond lengths



Bond angles

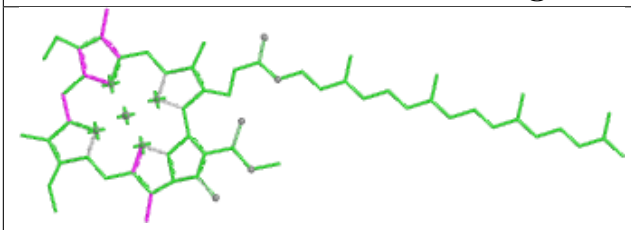


Torsions

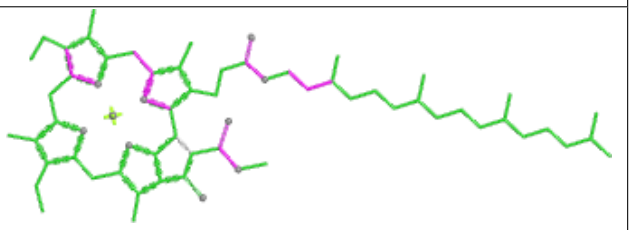


Rings

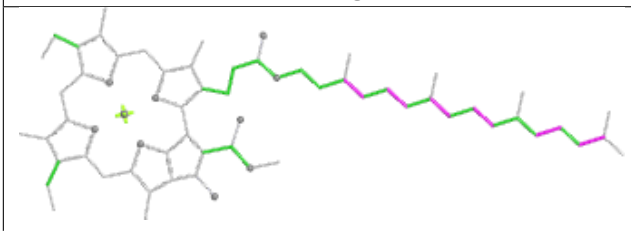
Ligand CLA a 409



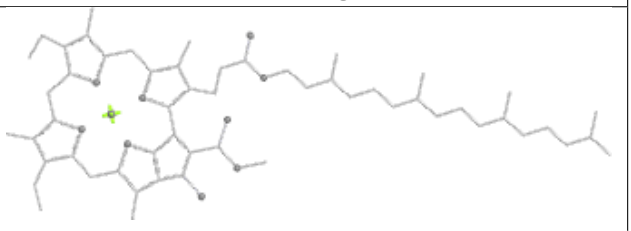
Bond lengths



Bond angles

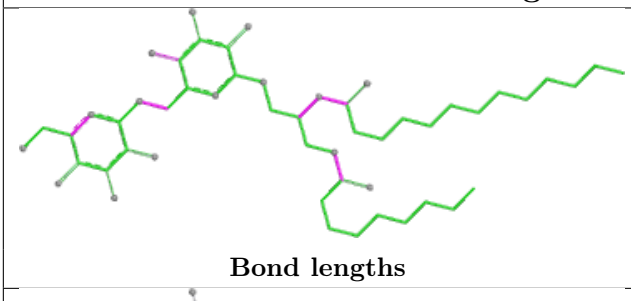


Torsions

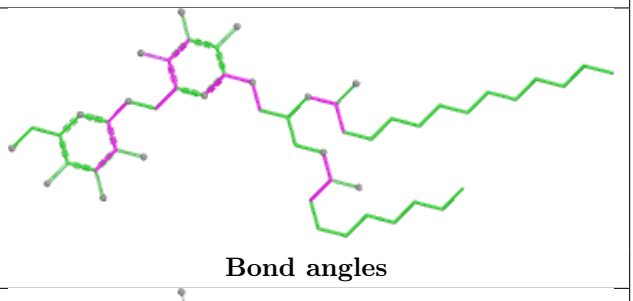


Rings

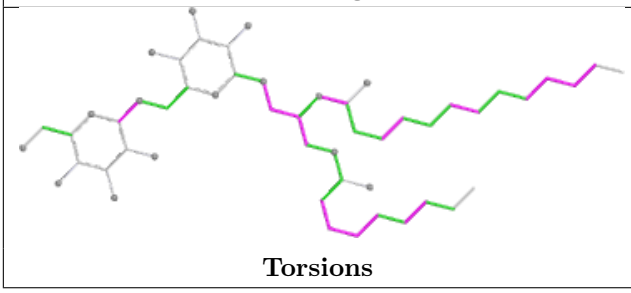
Ligand DGD b 602



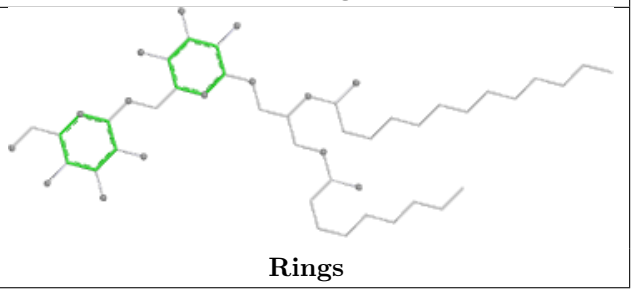
Bond lengths



Bond angles

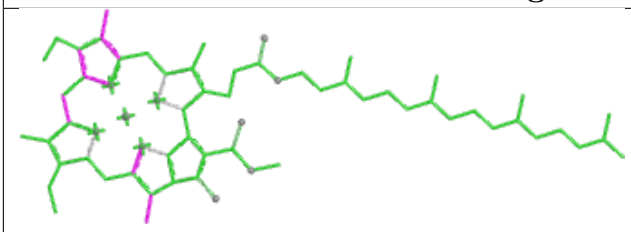


Torsions

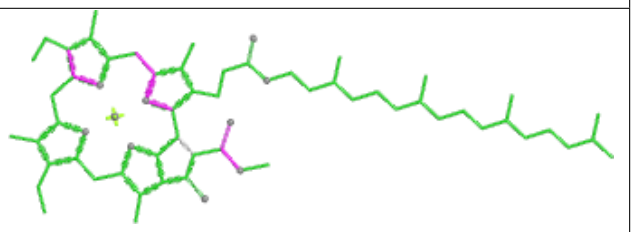


Rings

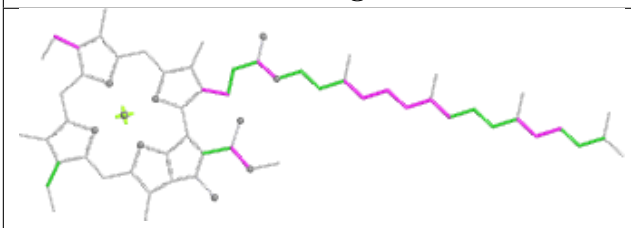
Ligand CLA b 605



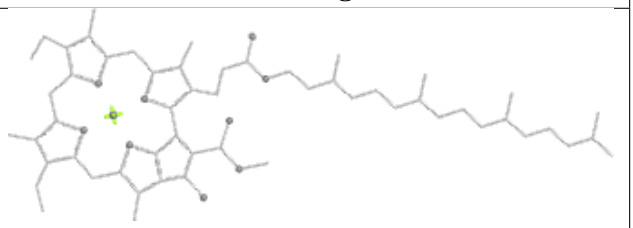
Bond lengths



Bond angles

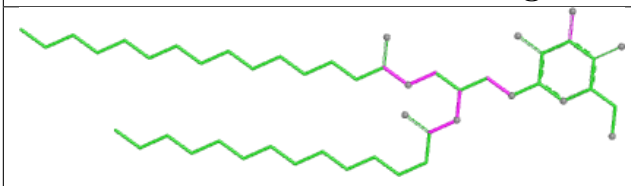


Torsions

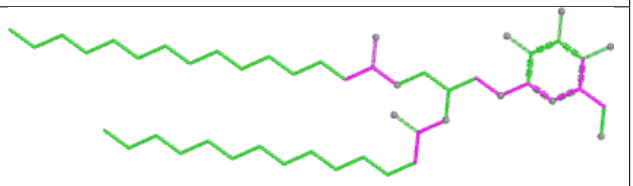


Rings

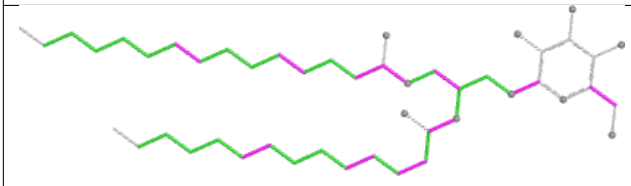
Ligand LMG k 103



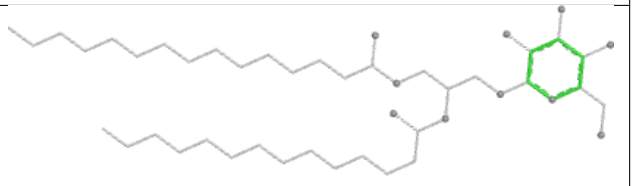
Bond lengths



Bond angles

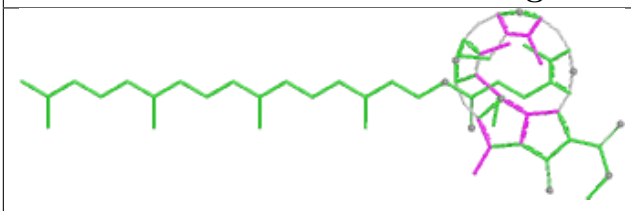


Torsions

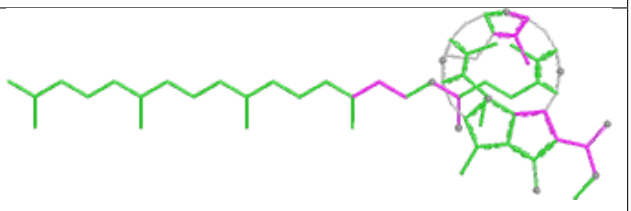


Rings

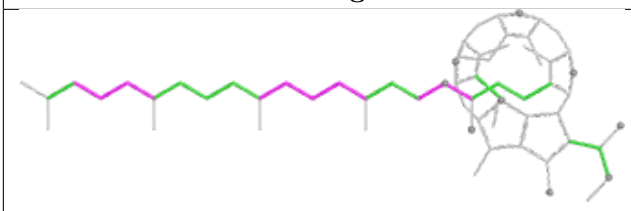
Ligand PHO a 407



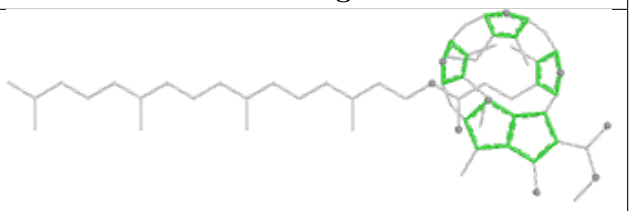
Bond lengths



Bond angles

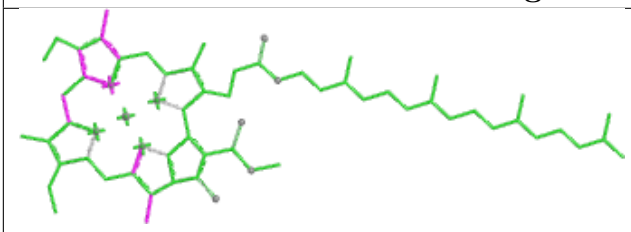


Torsions

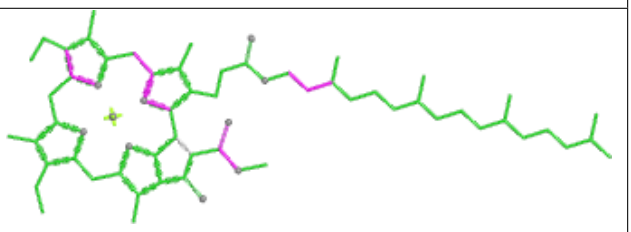


Rings

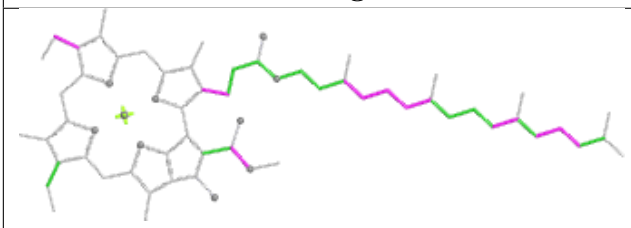
Ligand CLA B 608



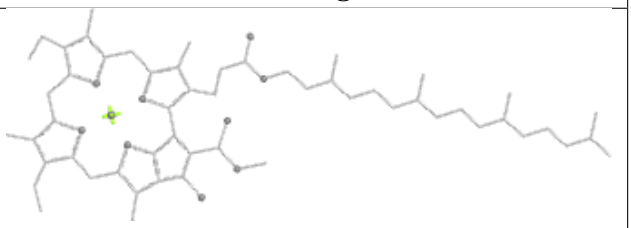
Bond lengths



Bond angles

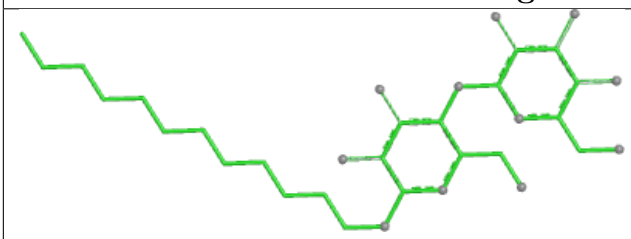


Torsions

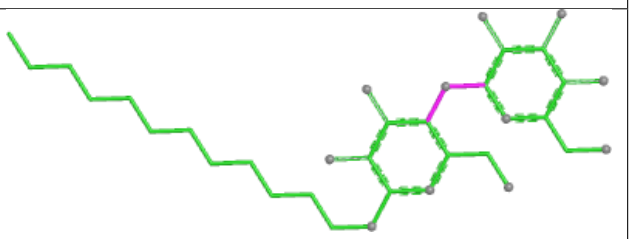


Rings

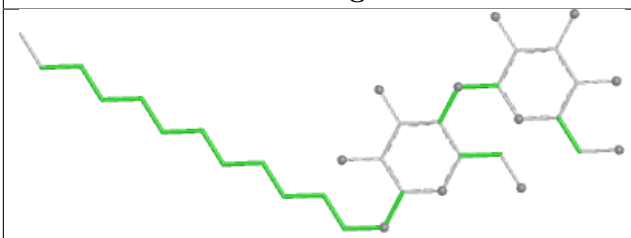
Ligand LMT M 103



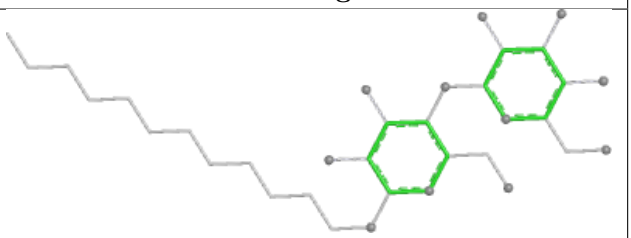
Bond lengths



Bond angles

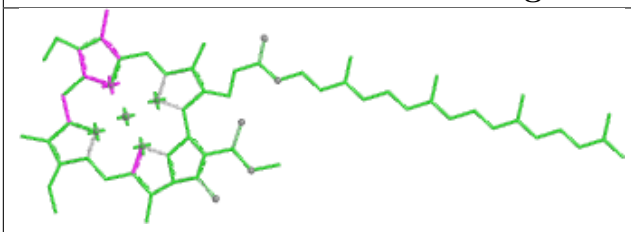


Torsions

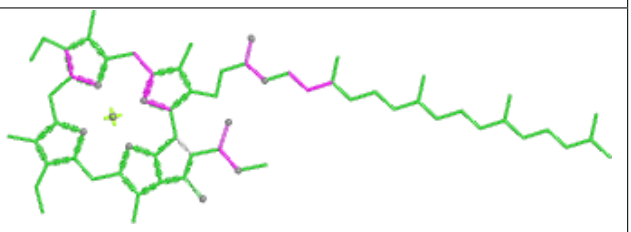


Rings

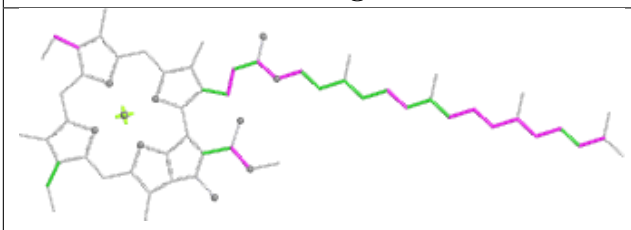
Ligand CLA B 610



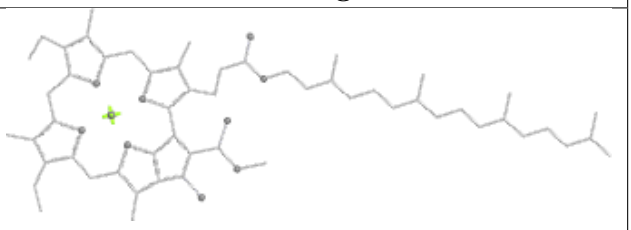
Bond lengths



Bond angles

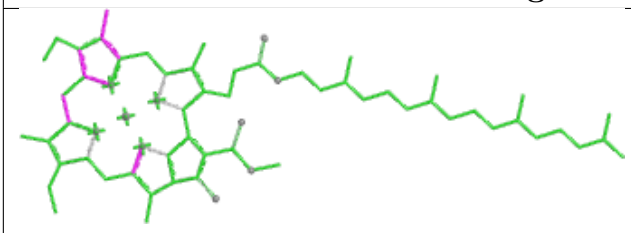


Torsions

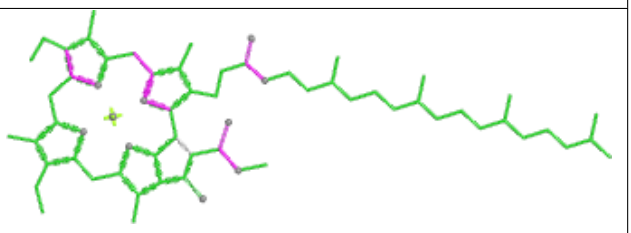


Rings

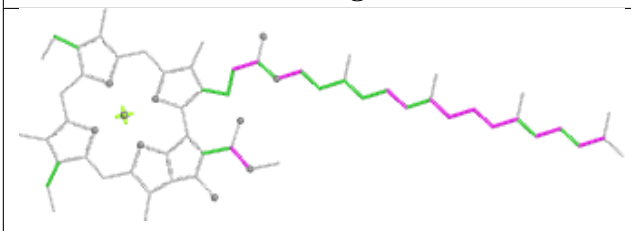
Ligand CLA b 616



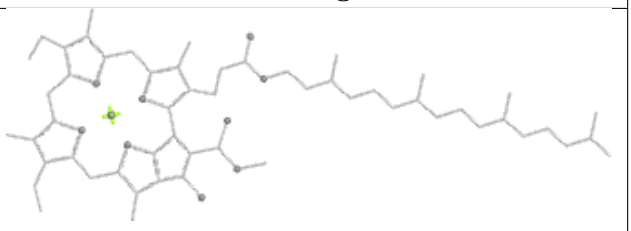
Bond lengths



Bond angles

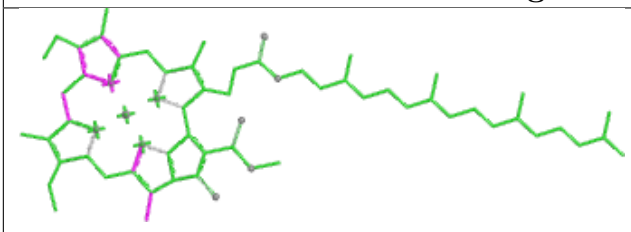


Torsions

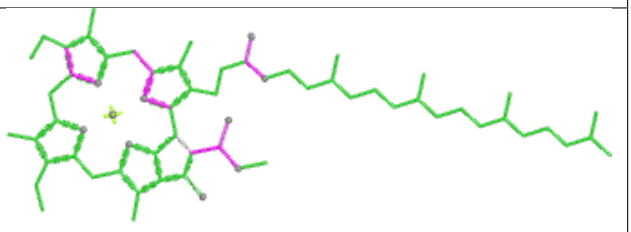


Rings

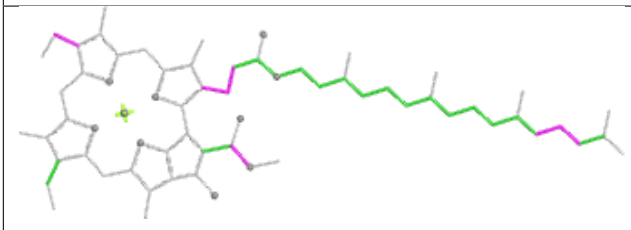
Ligand CLA b 610



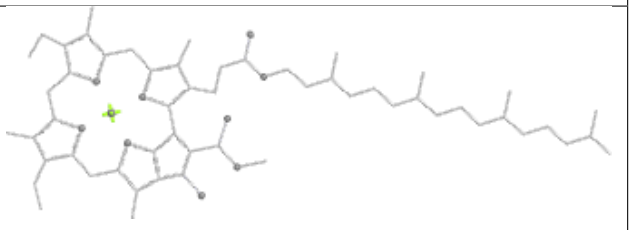
Bond lengths



Bond angles

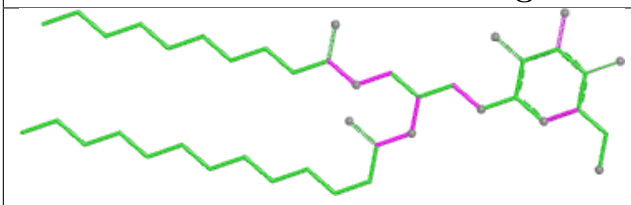


Torsions

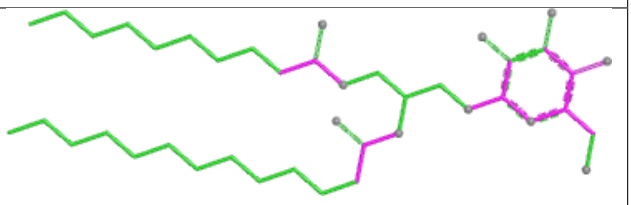


Rings

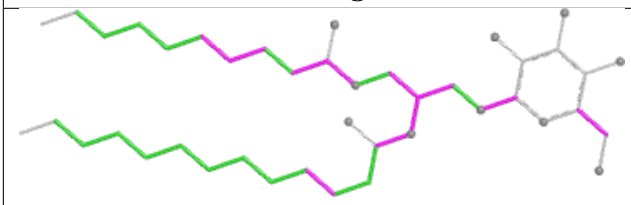
Ligand LMG M 102



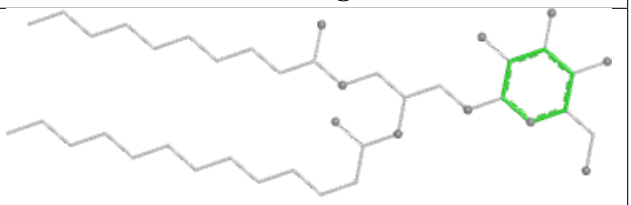
Bond lengths



Bond angles

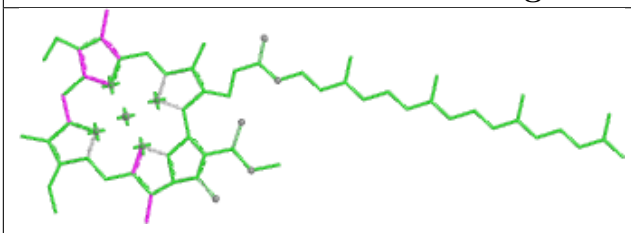


Torsions

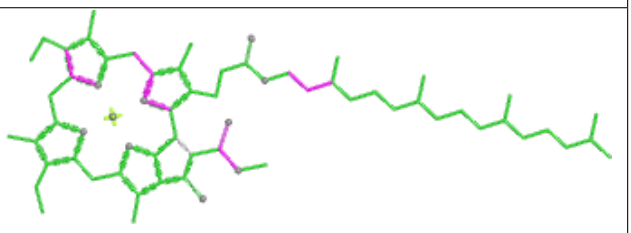


Rings

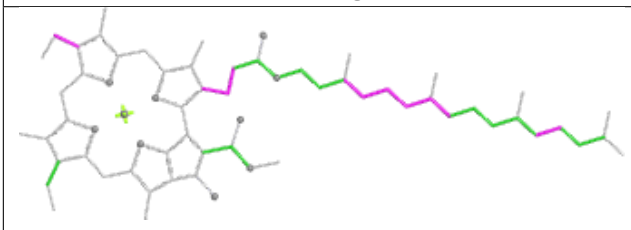
Ligand CLA B 602



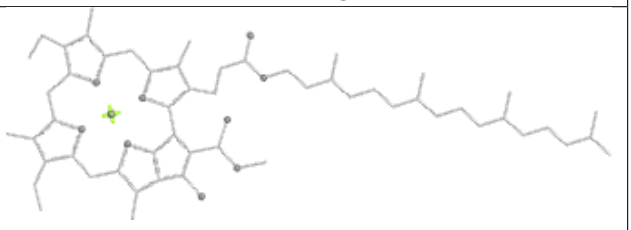
Bond lengths



Bond angles

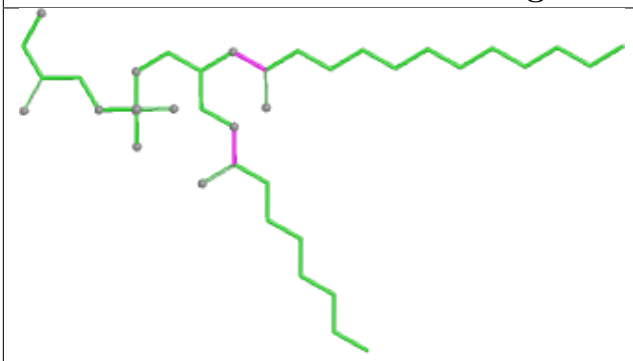


Torsions

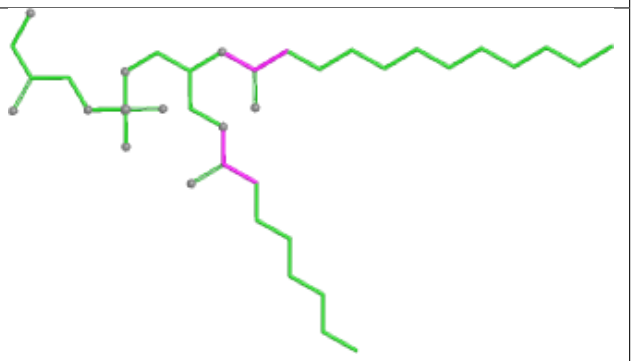


Rings

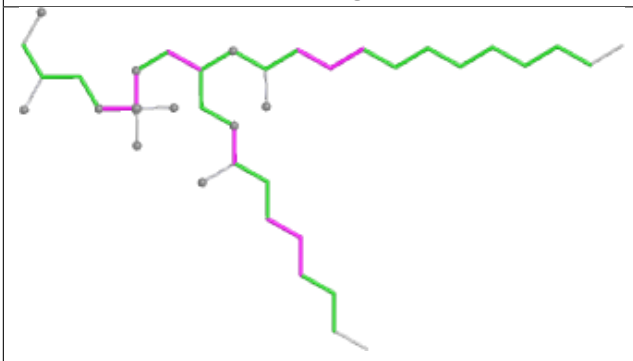
Ligand LHG a 417



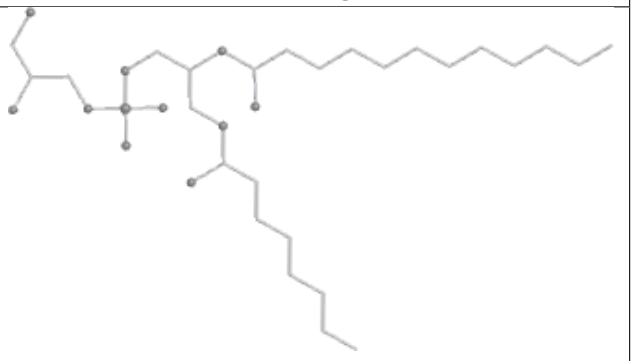
Bond lengths



Bond angles

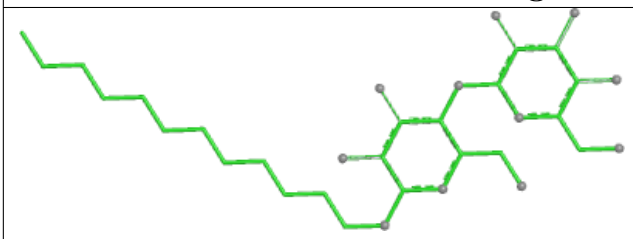


Torsions

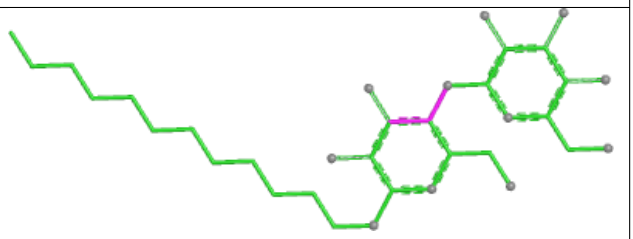


Rings

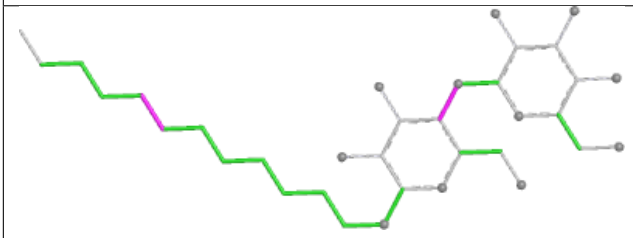
Ligand LMT I 102



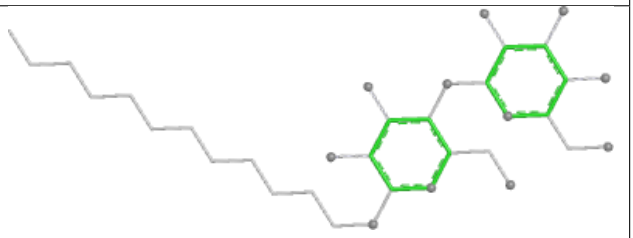
Bond lengths



Bond angles

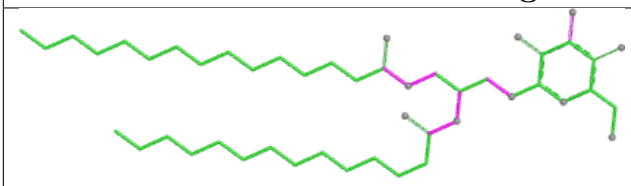


Torsions

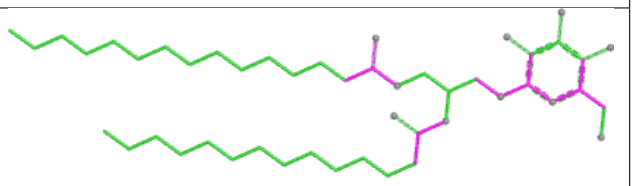


Rings

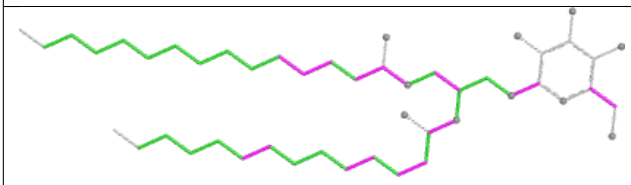
Ligand LMG C 519



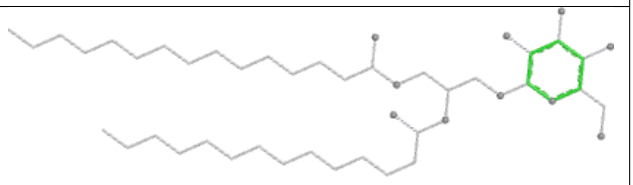
Bond lengths



Bond angles

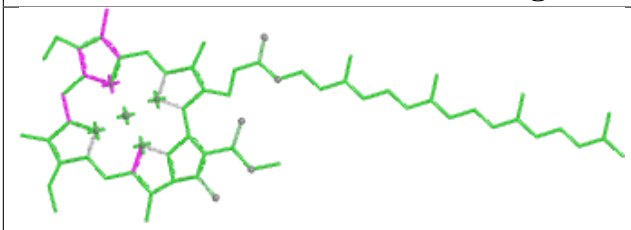


Torsions

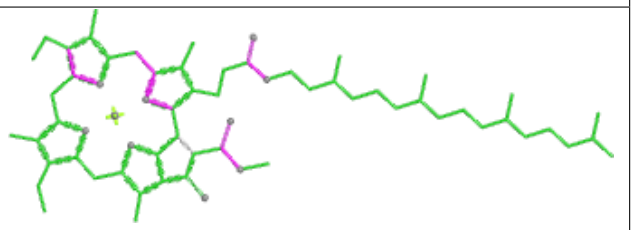


Rings

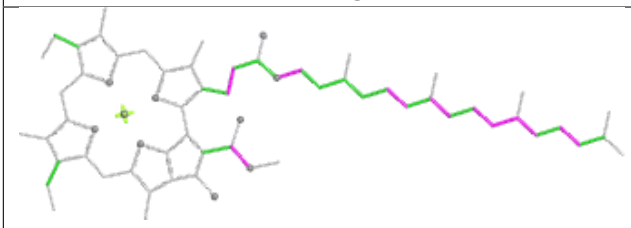
Ligand CLA c 508



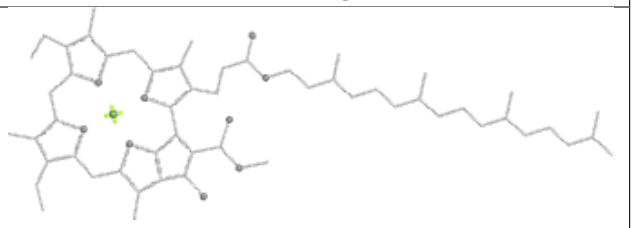
Bond lengths



Bond angles

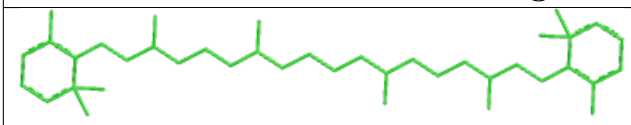


Torsions

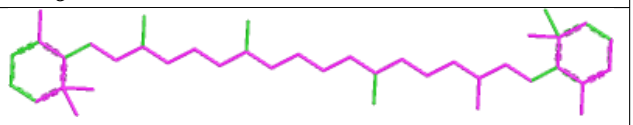


Rings

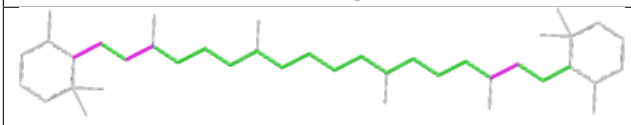
Ligand BCR j 102



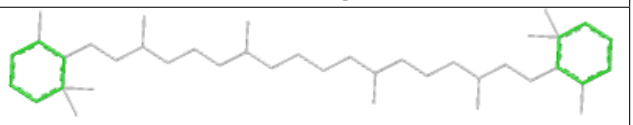
Bond lengths



Bond angles

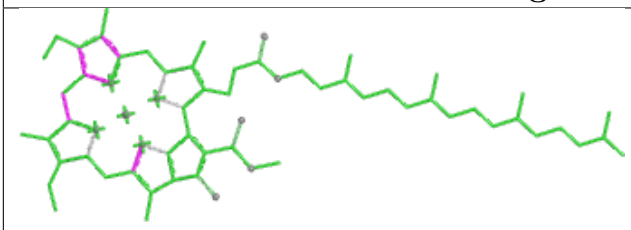


Torsions

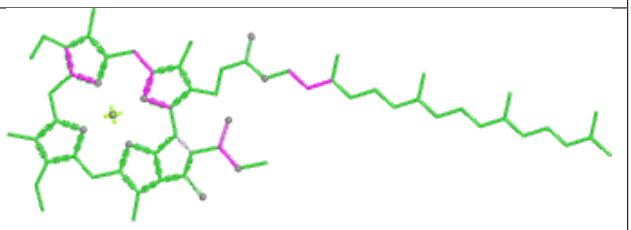


Rings

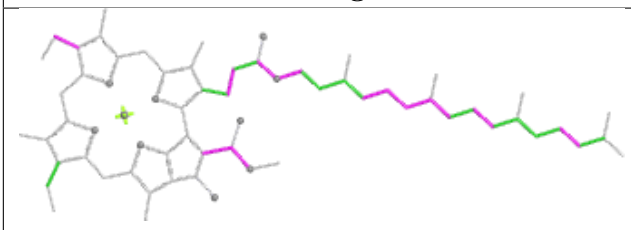
Ligand CLA c 509



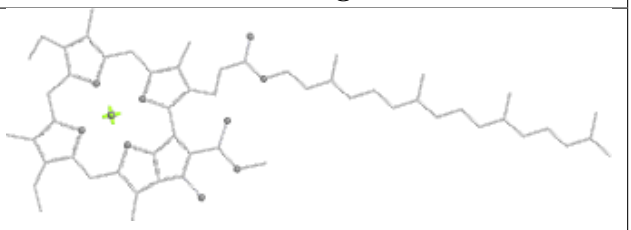
Bond lengths



Bond angles

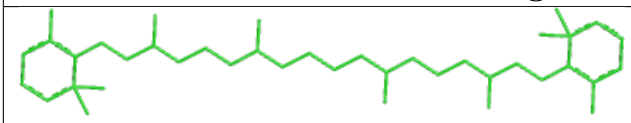


Torsions

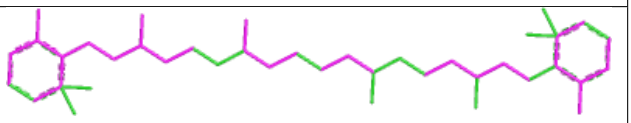


Rings

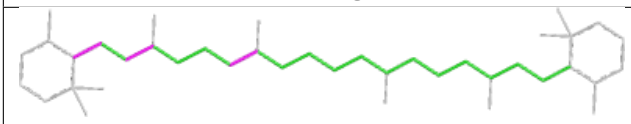
Ligand BCR c 514



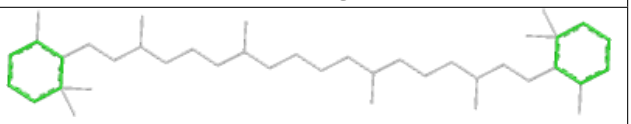
Bond lengths



Bond angles

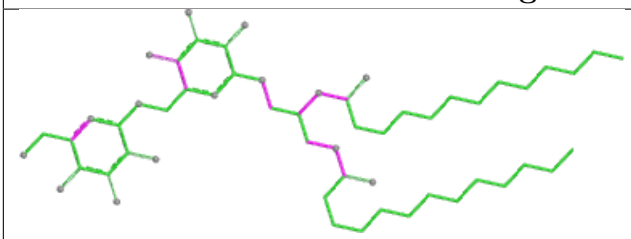


Torsions

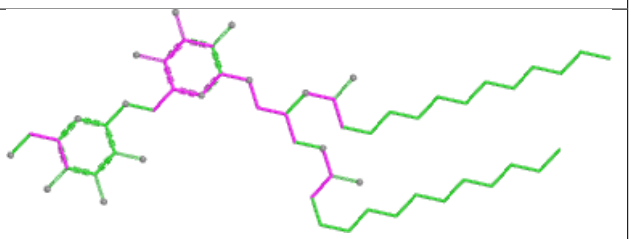


Rings

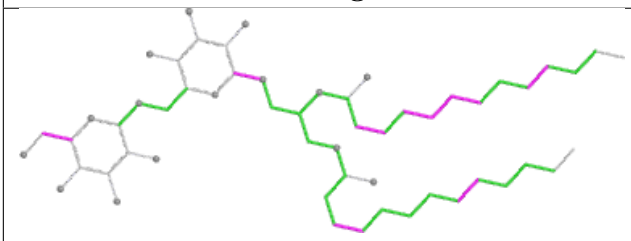
Ligand DGD A 411



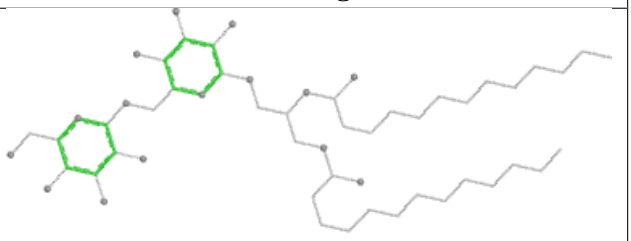
Bond lengths



Bond angles

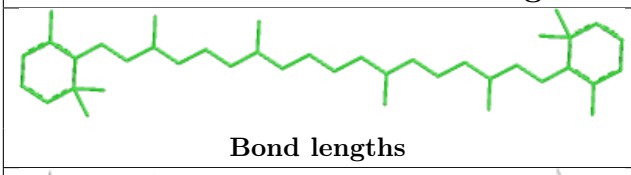


Torsions

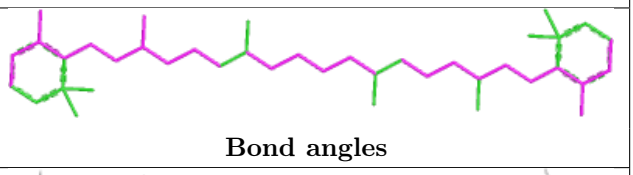


Rings

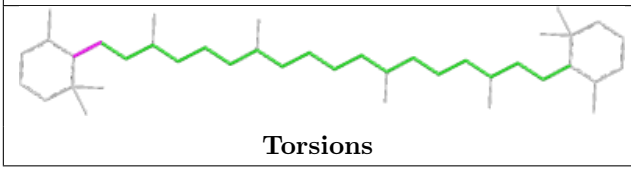
Ligand BCR Z 101



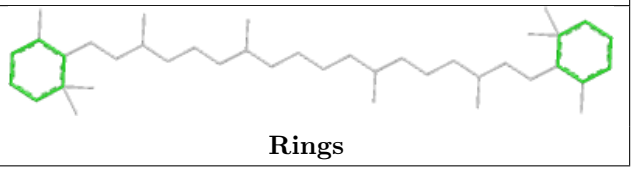
Bond lengths



Bond angles

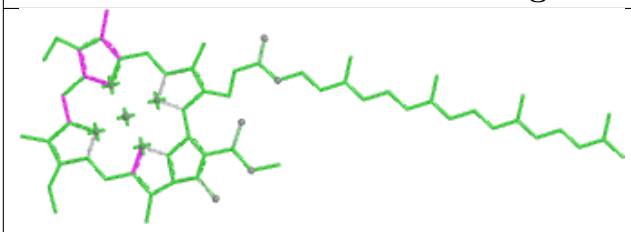


Torsions

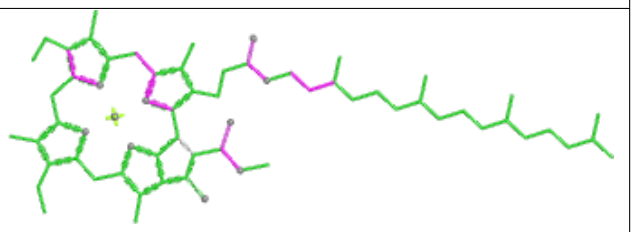


Rings

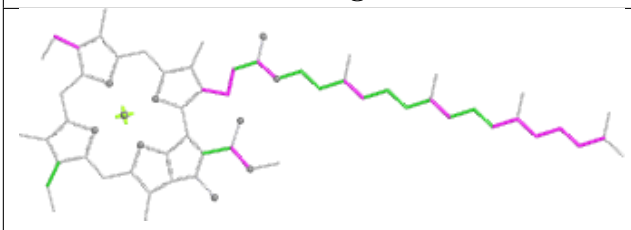
Ligand CLA c 513



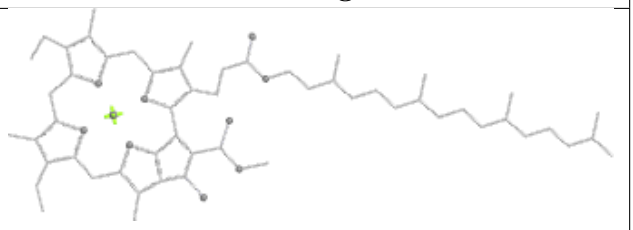
Bond lengths



Bond angles

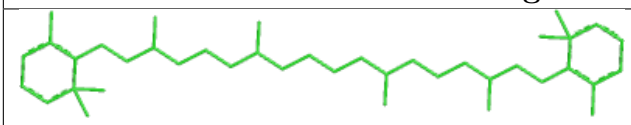


Torsions

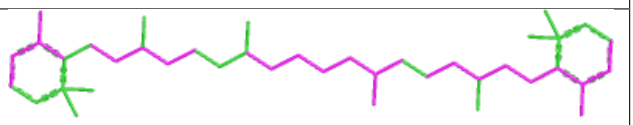


Rings

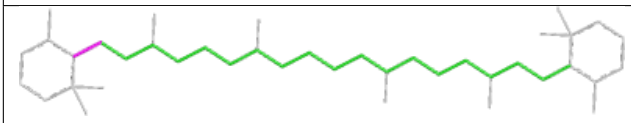
Ligand BCR T 102



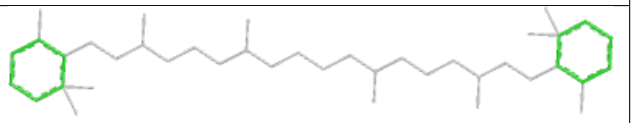
Bond lengths



Bond angles

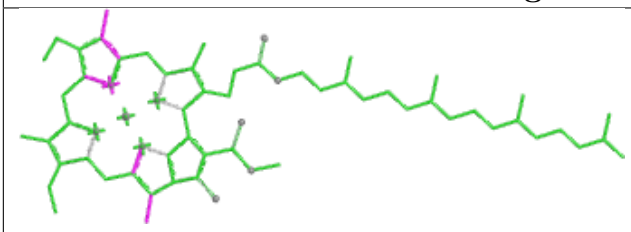


Torsions

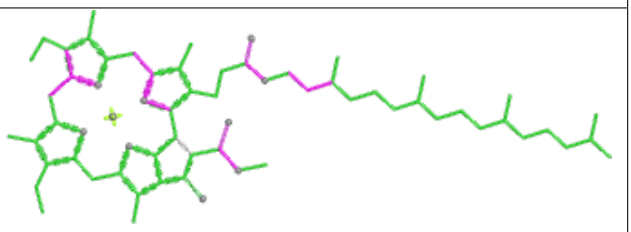


Rings

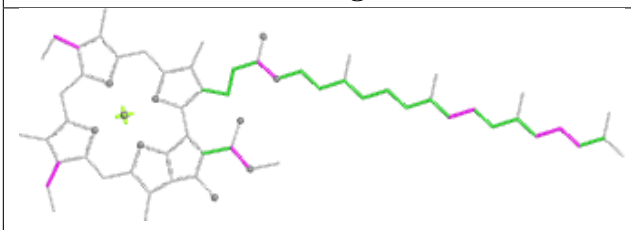
Ligand CLA B 604



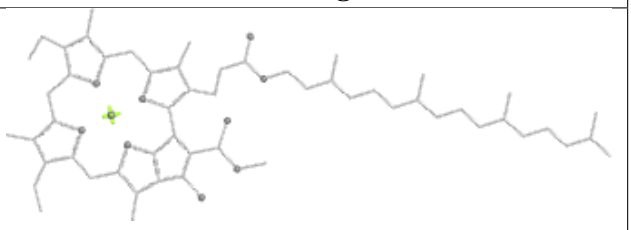
Bond lengths



Bond angles

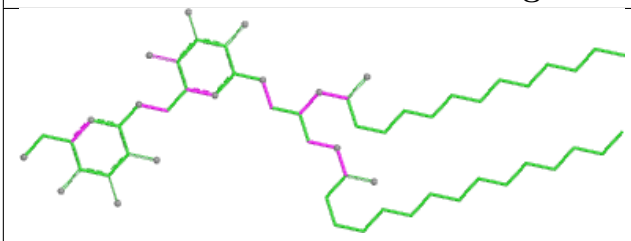


Torsions

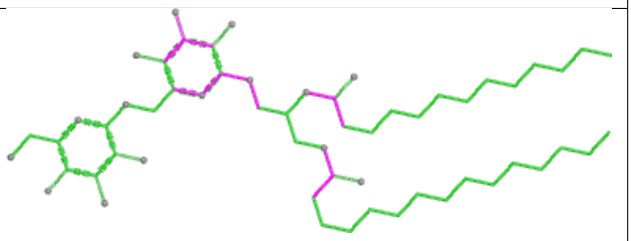


Rings

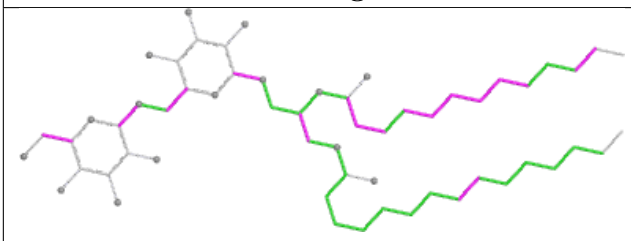
Ligand DGD b 622



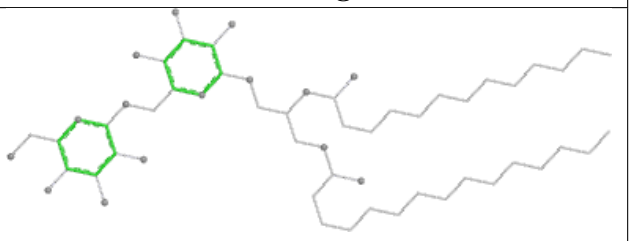
Bond lengths



Bond angles

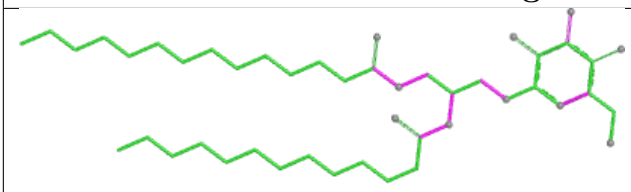


Torsions

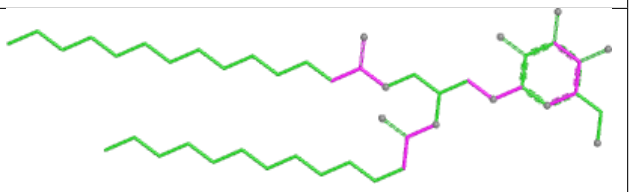


Rings

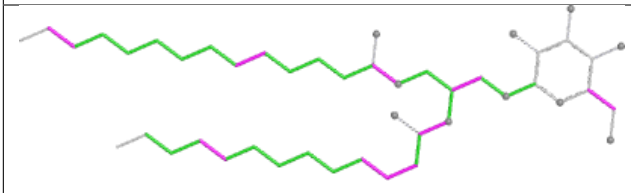
Ligand LMG d 405



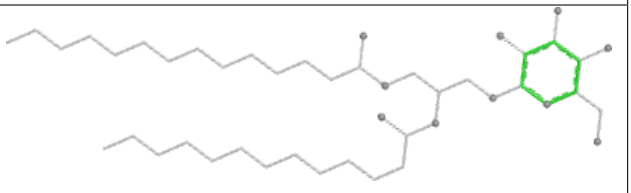
Bond lengths



Bond angles

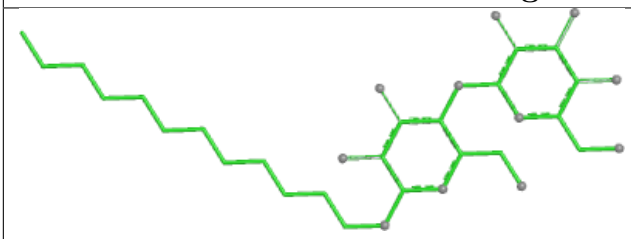


Torsions

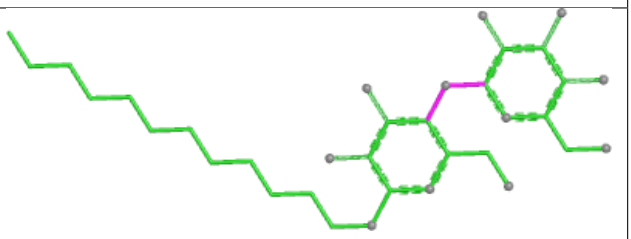


Rings

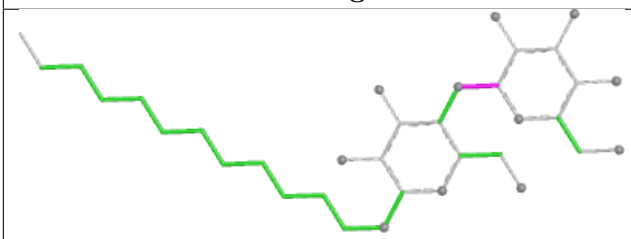
Ligand LMT B 624



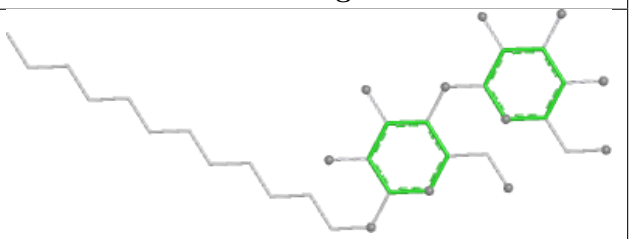
Bond lengths



Bond angles

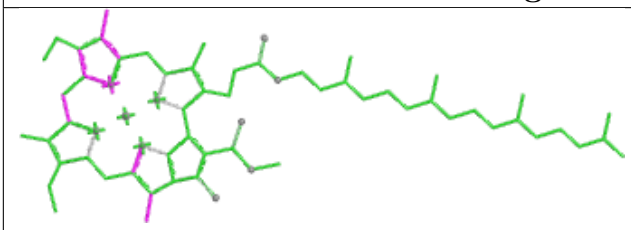


Torsions

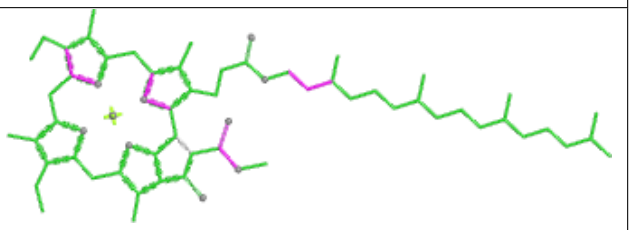


Rings

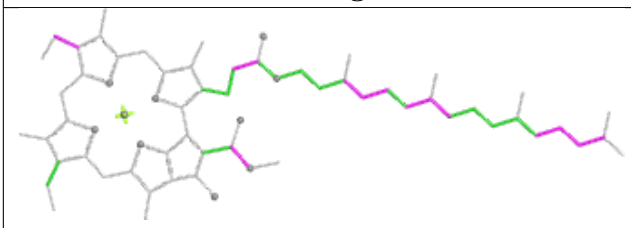
Ligand CLA C 510



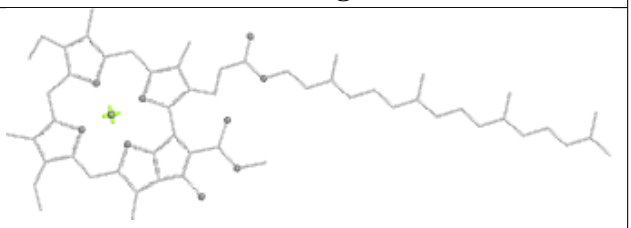
Bond lengths



Bond angles



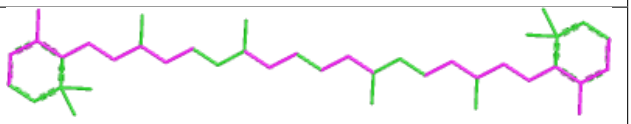
Torsions



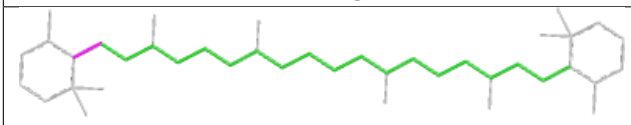
Rings

Ligand BCR B 617

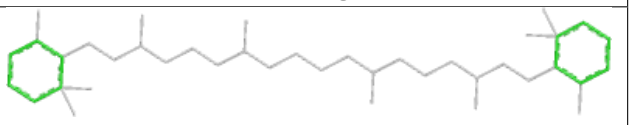
Bond lengths



Bond angles

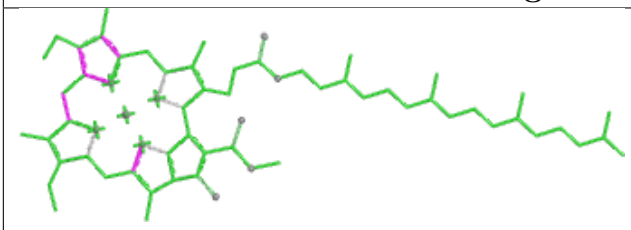


Torsions

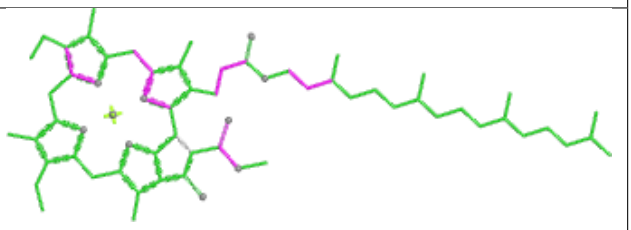


Rings

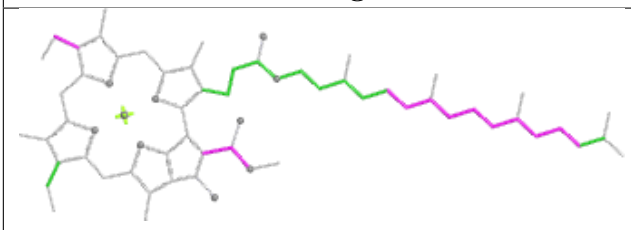
Ligand CLA C 506



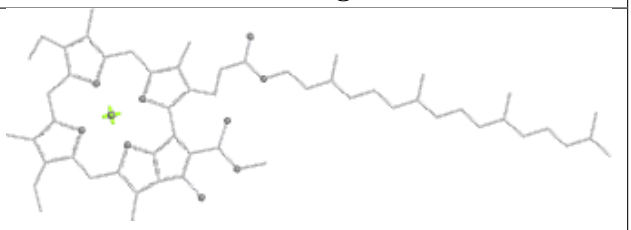
Bond lengths



Bond angles

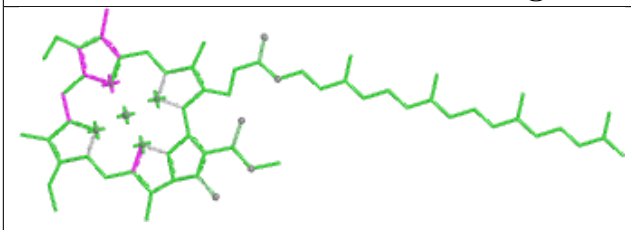


Torsions

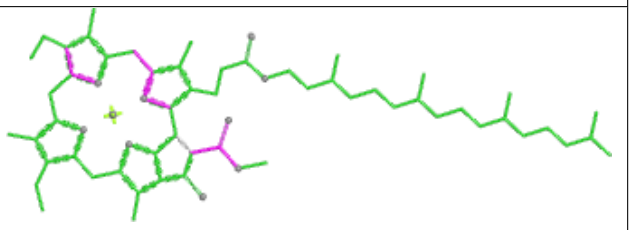


Rings

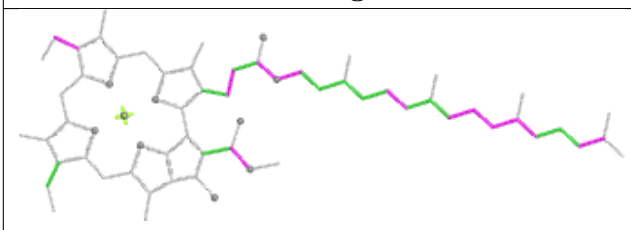
Ligand CLA b 613



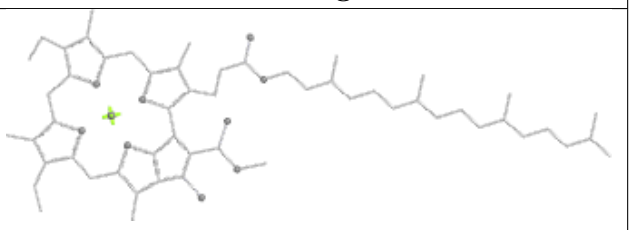
Bond lengths



Bond angles

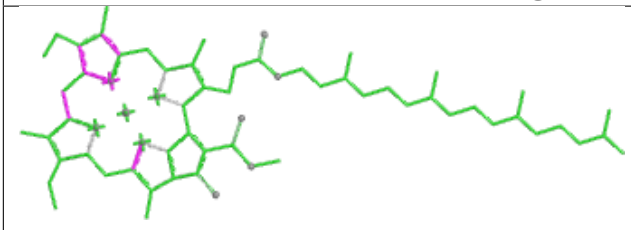


Torsions

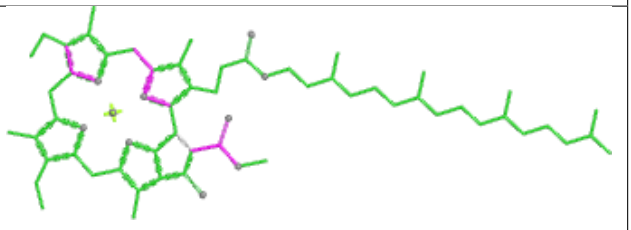


Rings

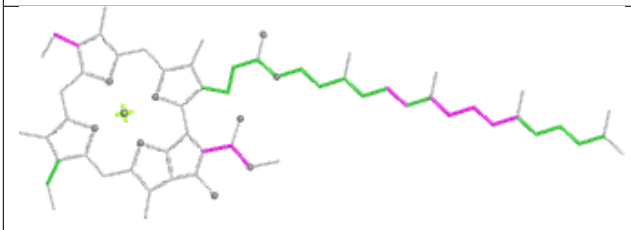
Ligand CLA c 503



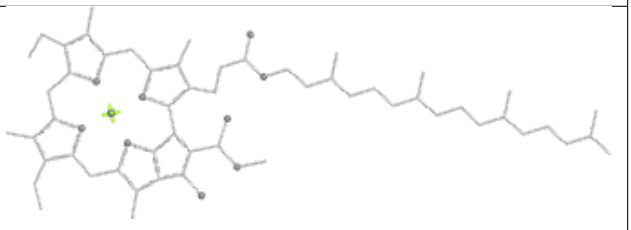
Bond lengths



Bond angles

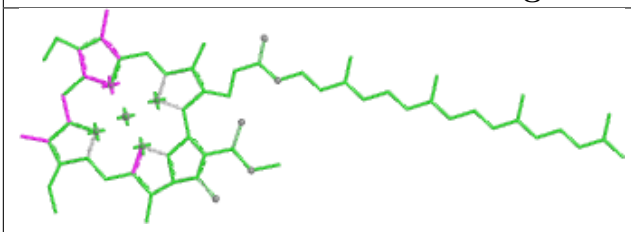


Torsions

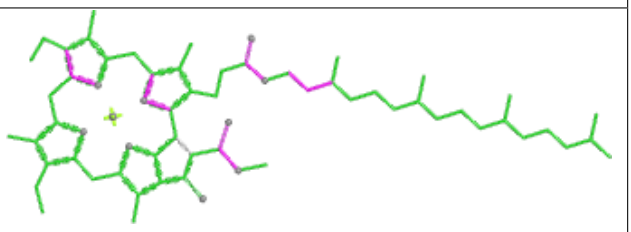


Rings

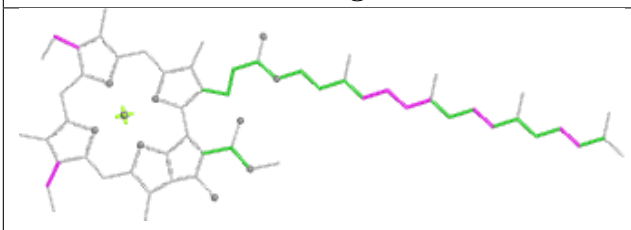
Ligand CLA A 405



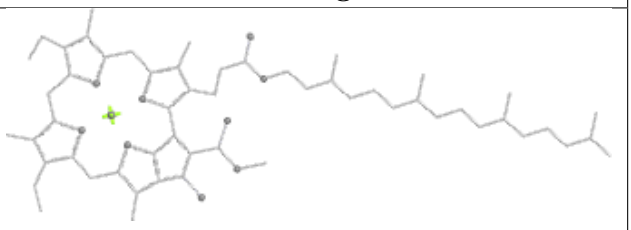
Bond lengths



Bond angles

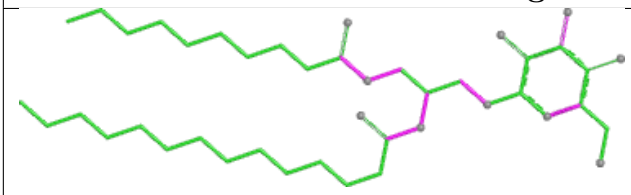


Torsions

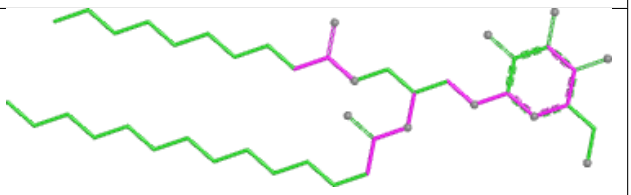


Rings

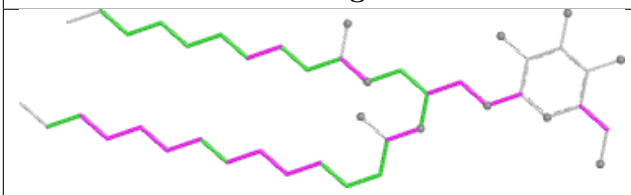
Ligand LMG i 101



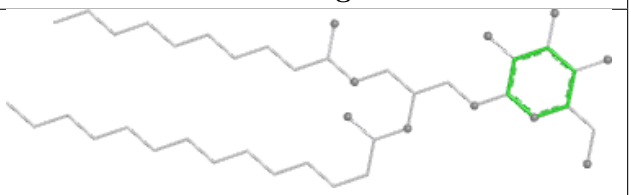
Bond lengths



Bond angles

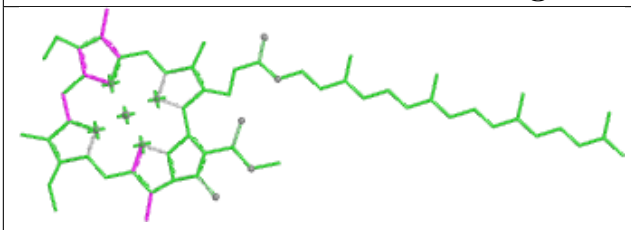


Torsions

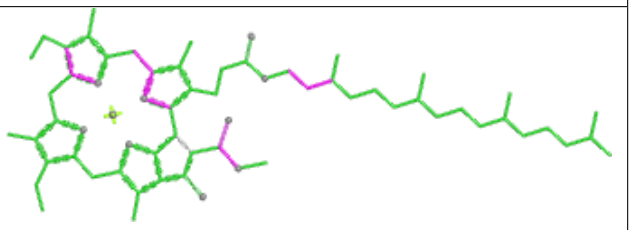


Rings

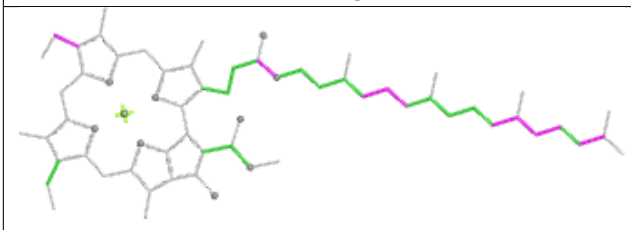
Ligand CLA c 502



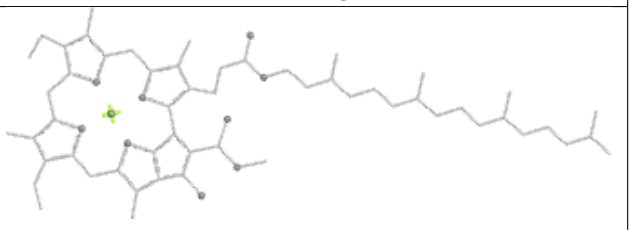
Bond lengths



Bond angles

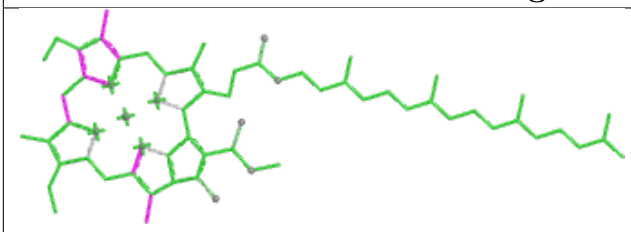


Torsions

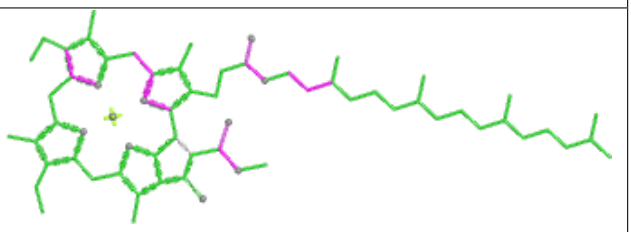


Rings

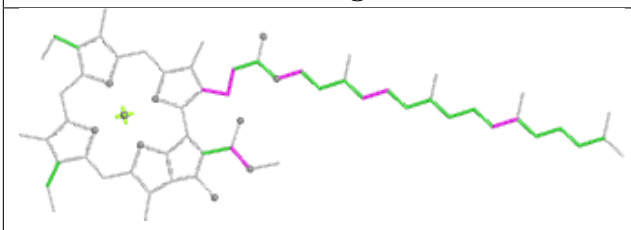
Ligand CLA a 404



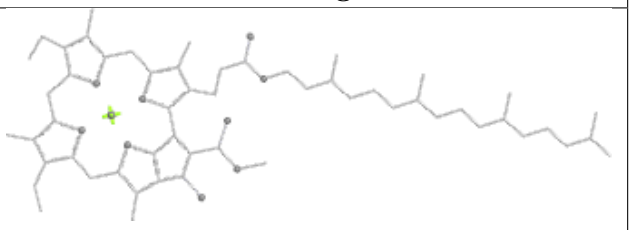
Bond lengths



Bond angles

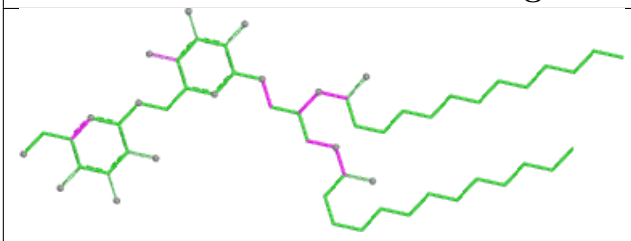


Torsions

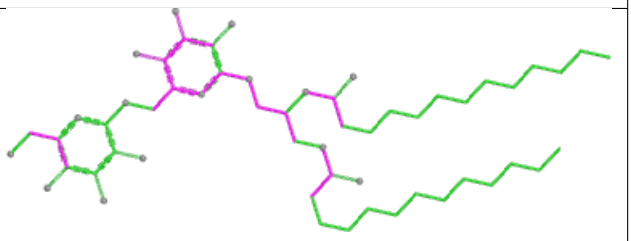


Rings

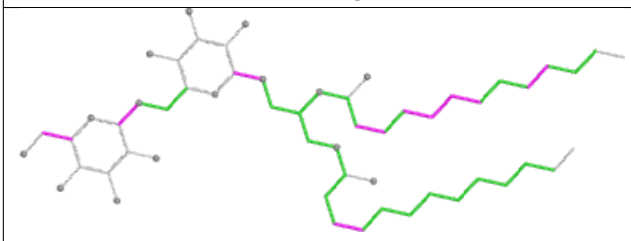
Ligand DGD a 413



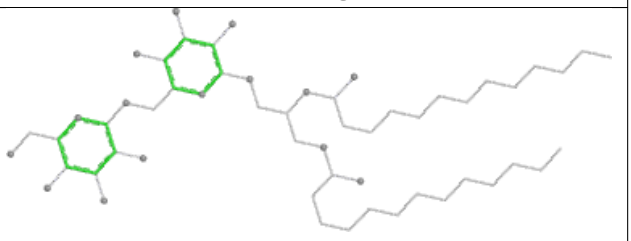
Bond lengths



Bond angles

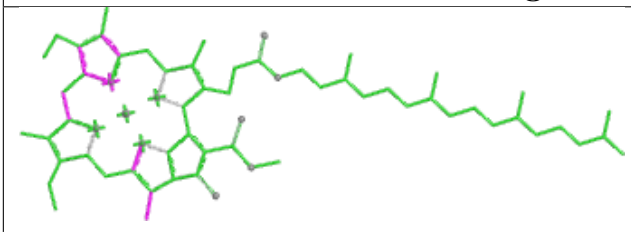


Torsions

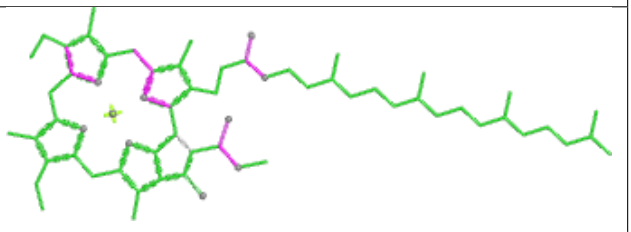


Rings

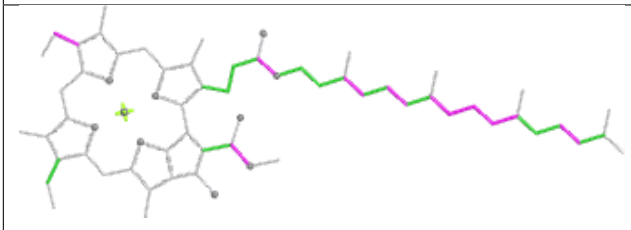
Ligand CLA B 605



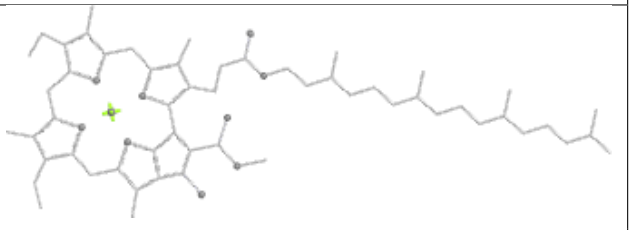
Bond lengths



Bond angles

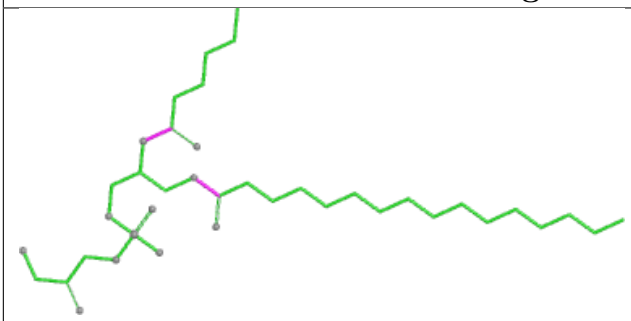


Torsions

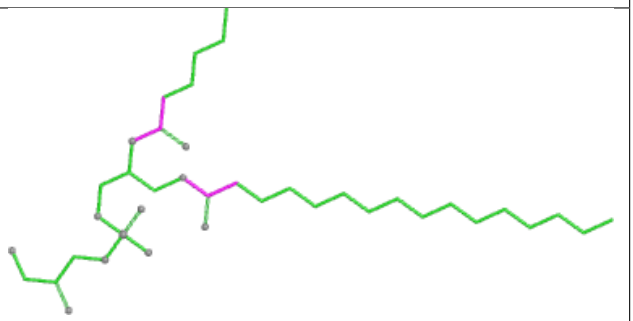


Rings

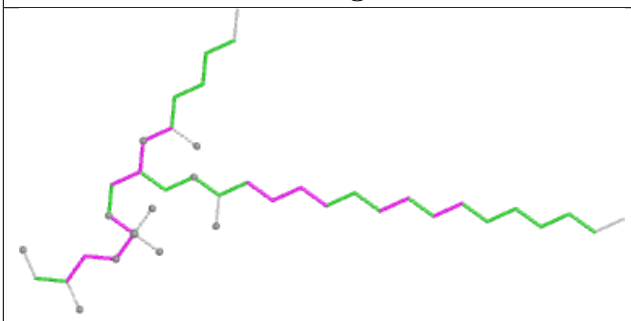
Ligand LHG A 412



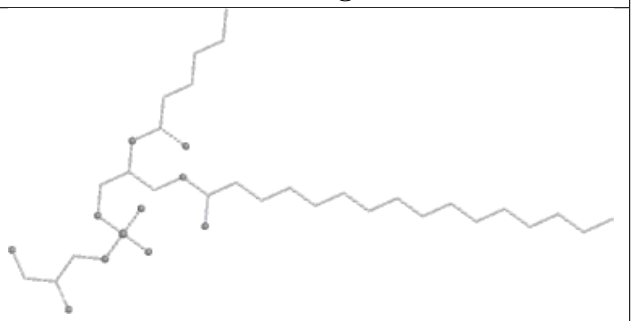
Bond lengths



Bond angles

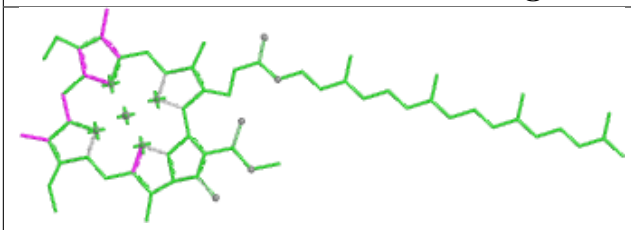


Torsions

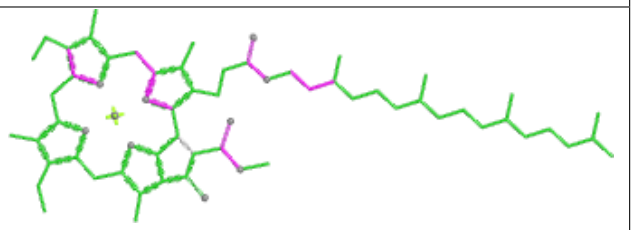


Rings

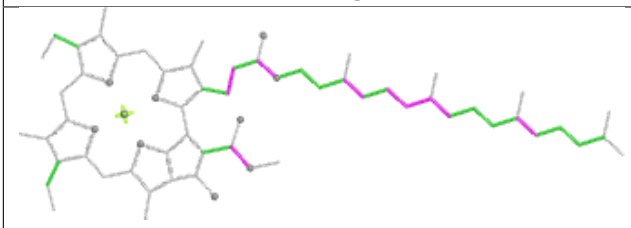
Ligand CLA C 511



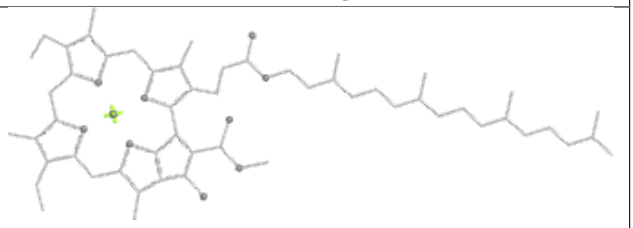
Bond lengths



Bond angles

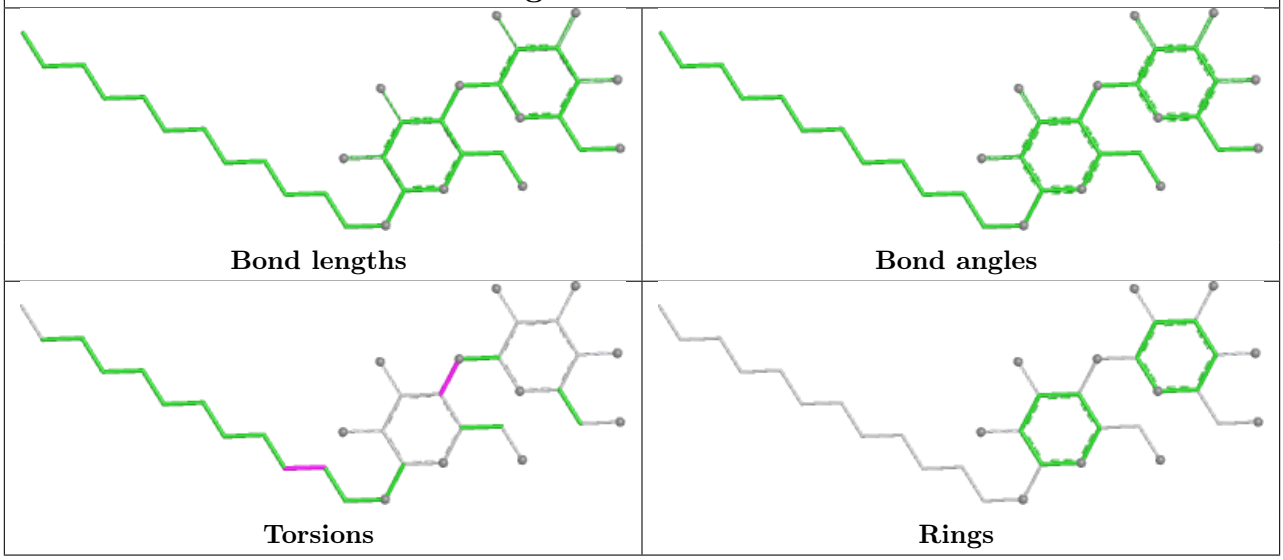


Torsions

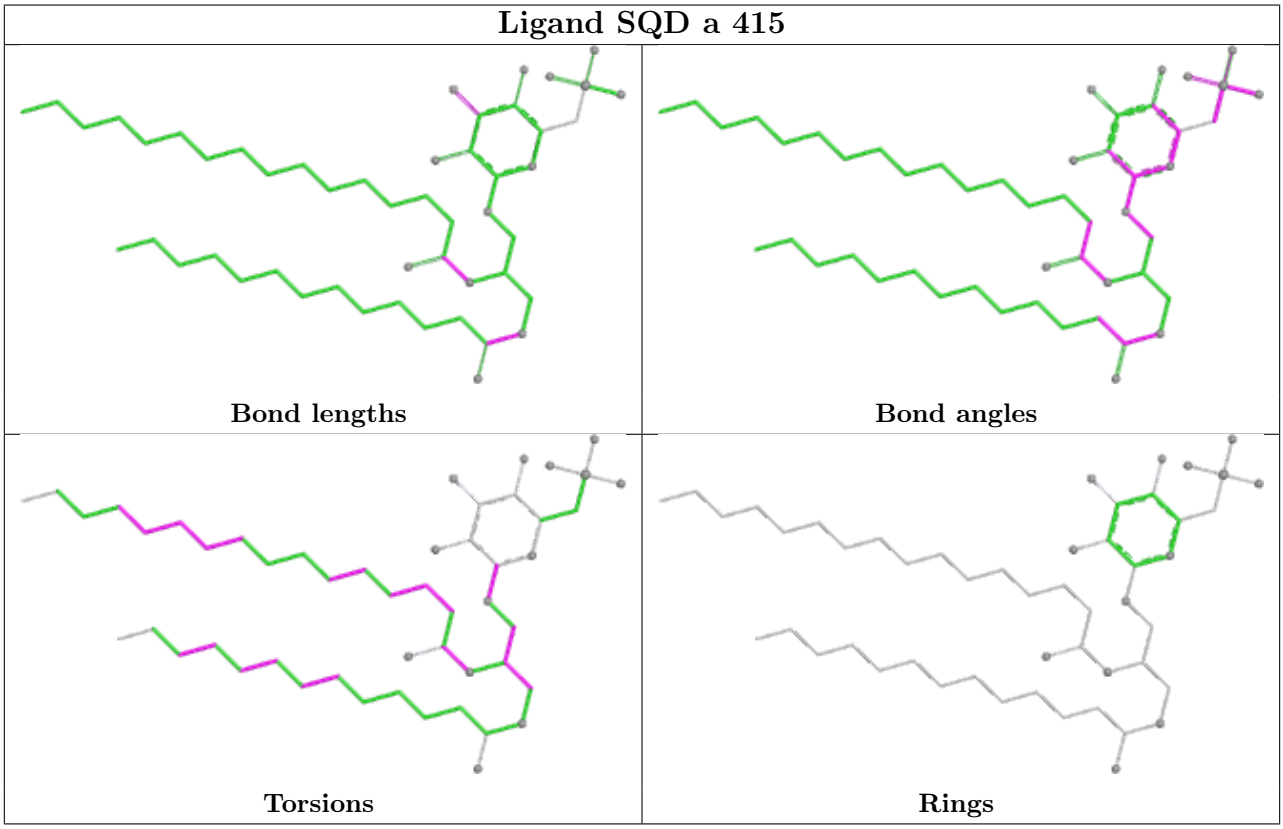


Rings

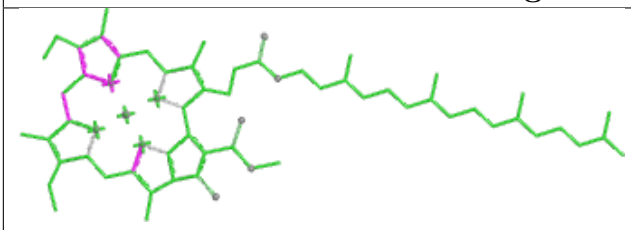
Ligand LMT b 603



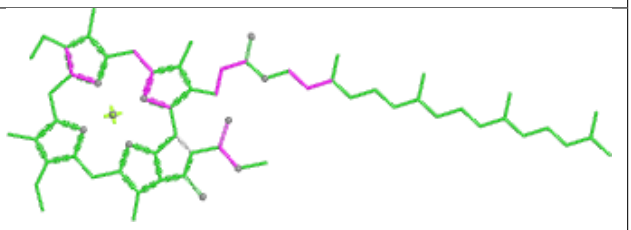
Ligand SQD a 415



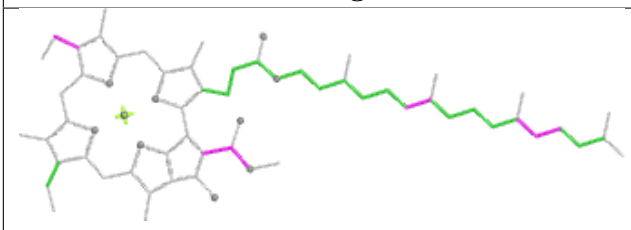
Ligand CLA B 609



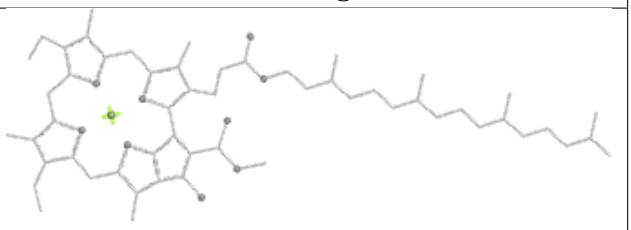
Bond lengths



Bond angles

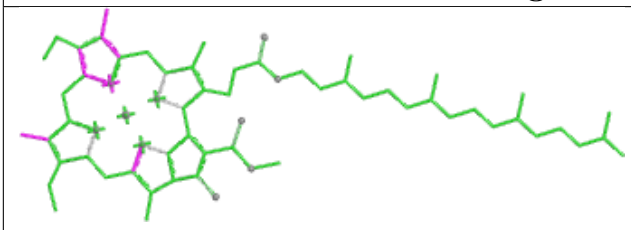


Torsions

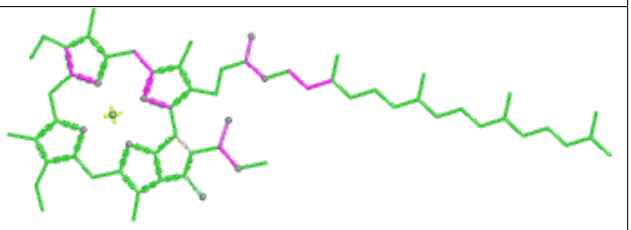


Rings

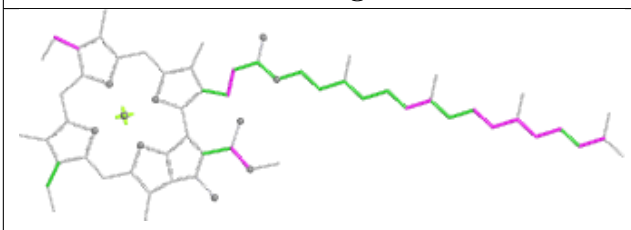
Ligand CLA b 604



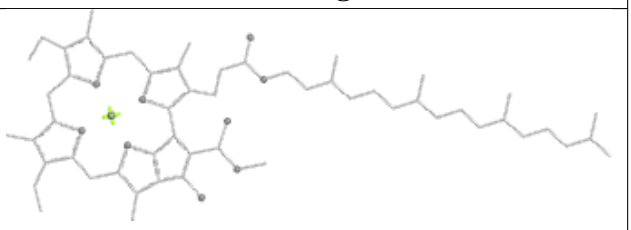
Bond lengths



Bond angles

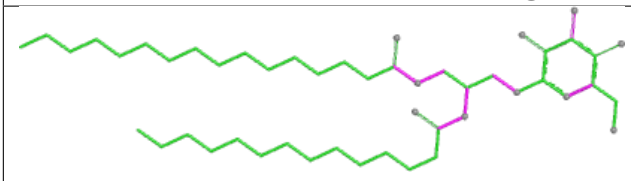


Torsions

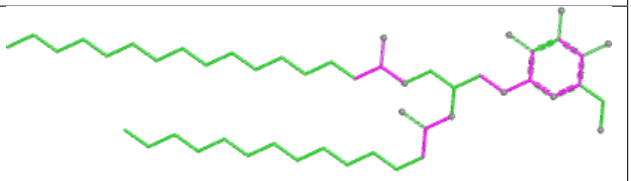


Rings

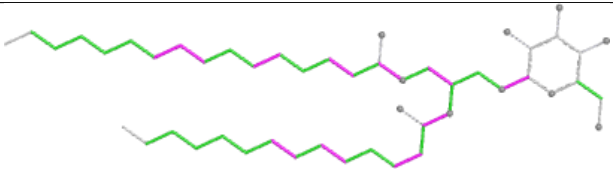
Ligand LMG b 624



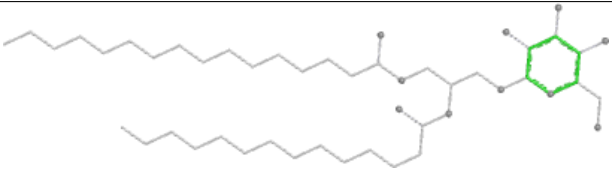
Bond lengths



Bond angles

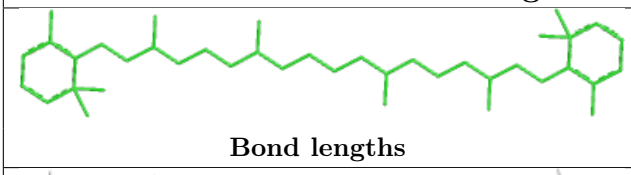


Torsions

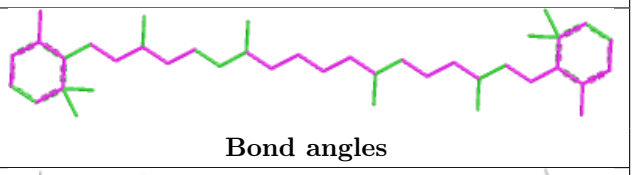


Rings

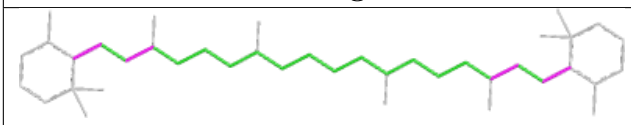
Ligand BCR C 515



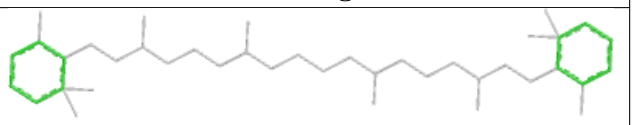
Bond lengths



Bond angles

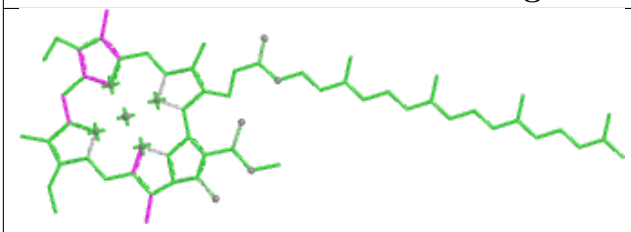


Torsions

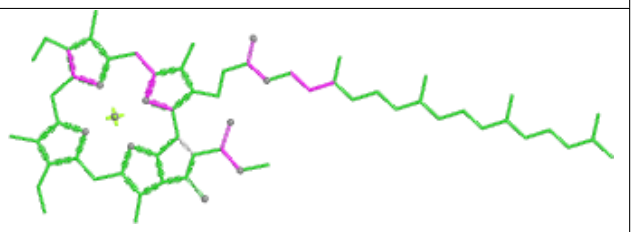


Rings

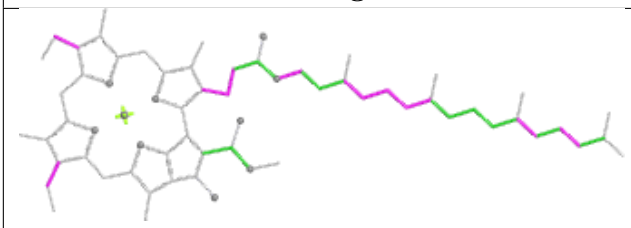
Ligand CLA A 404



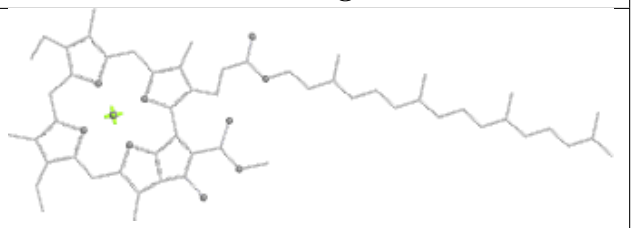
Bond lengths



Bond angles

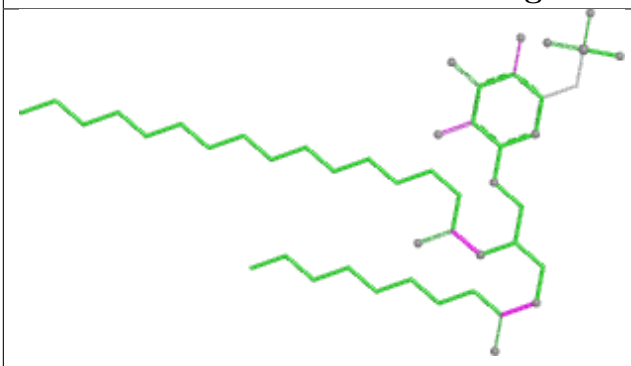


Torsions

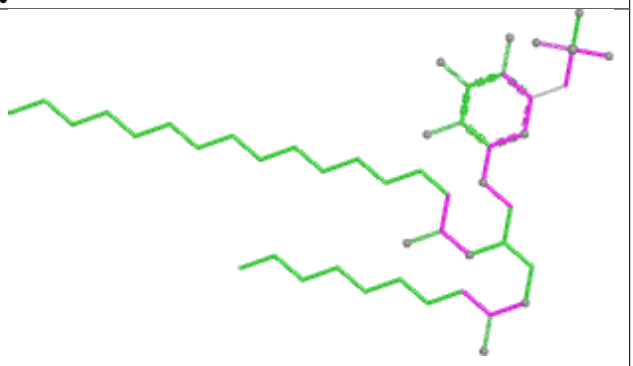


Rings

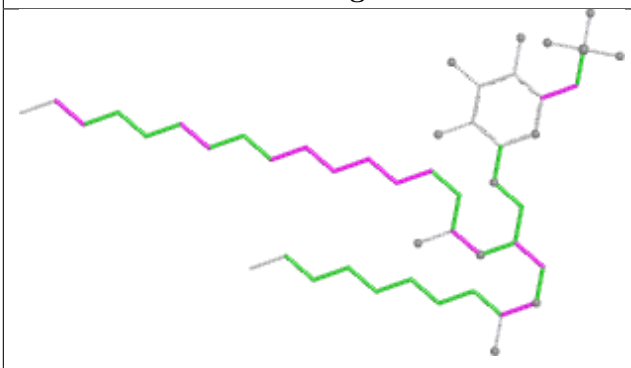
Ligand SQD B 625



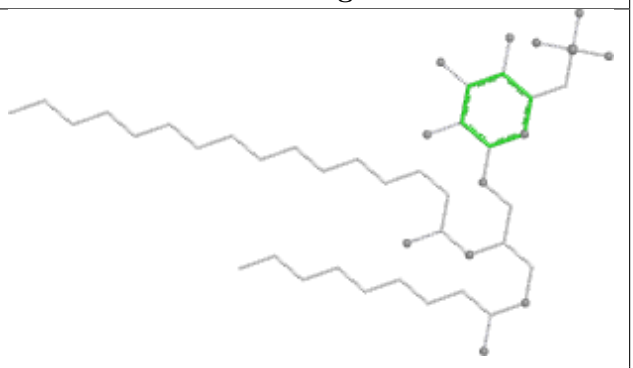
Bond lengths



Bond angles

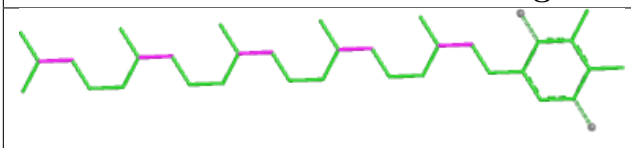


Torsions

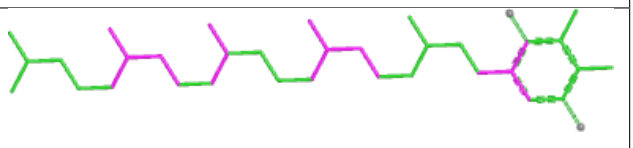


Rings

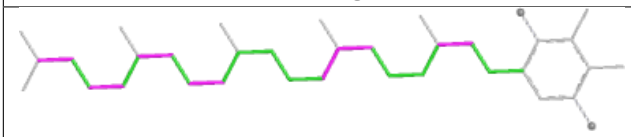
Ligand PL9 J 101



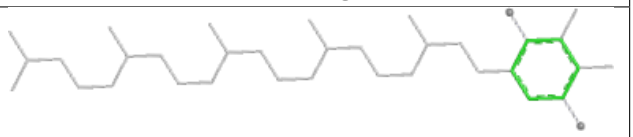
Bond lengths



Bond angles

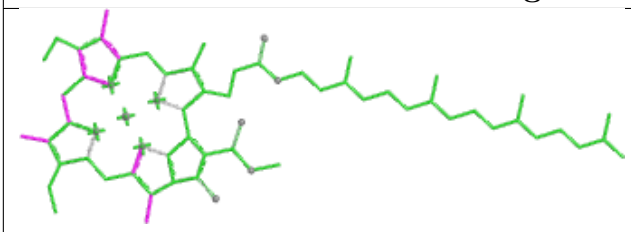


Torsions

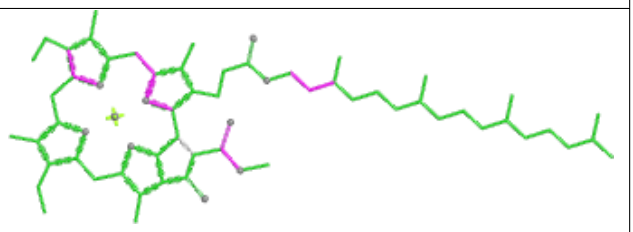


Rings

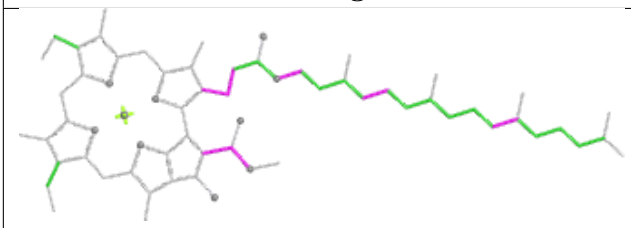
Ligand CLA A 403



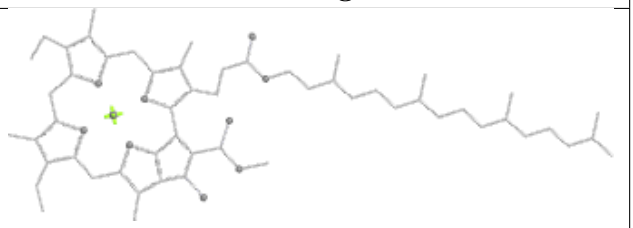
Bond lengths



Bond angles

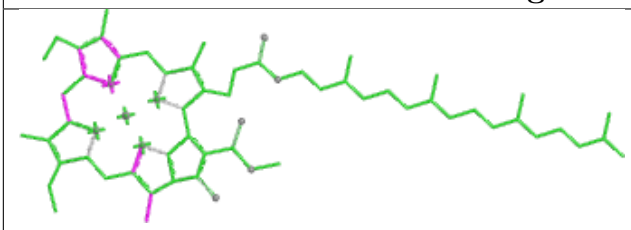


Torsions

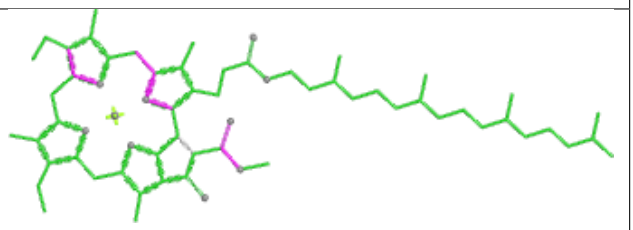


Rings

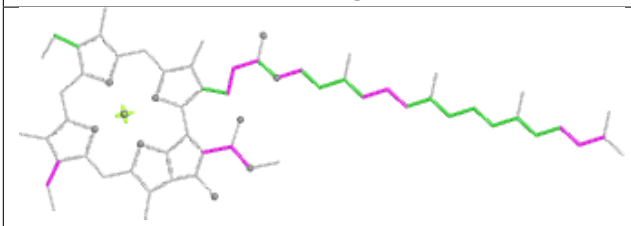
Ligand CLA b 617



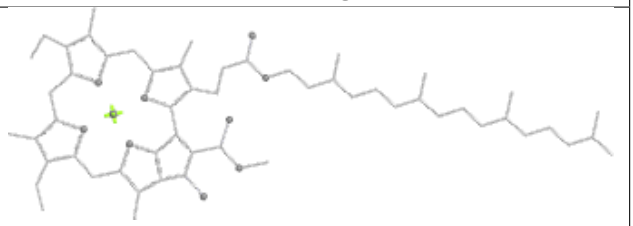
Bond lengths



Bond angles

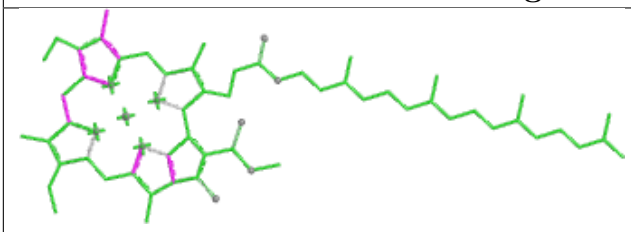


Torsions

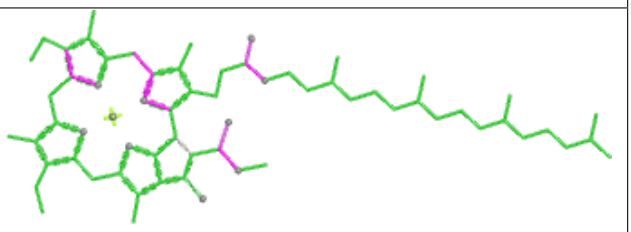


Rings

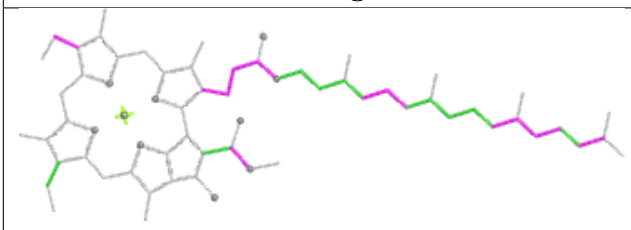
Ligand CLA C 512



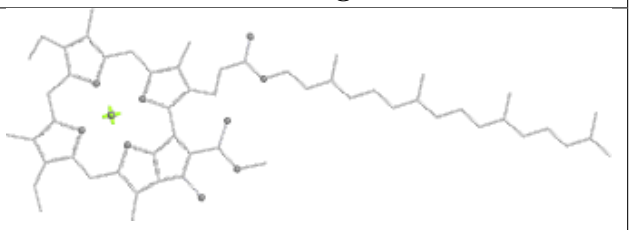
Bond lengths



Bond angles

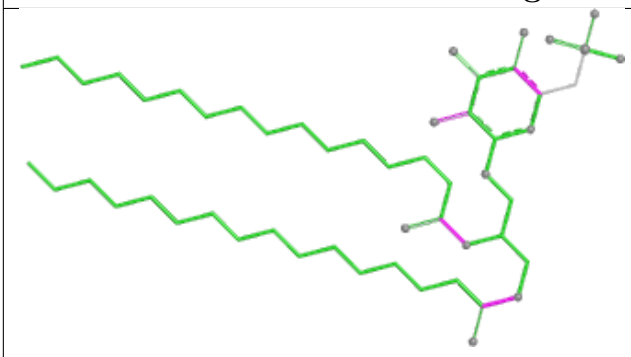


Torsions

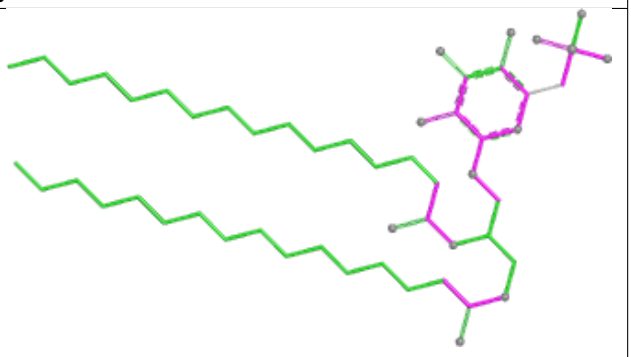


Rings

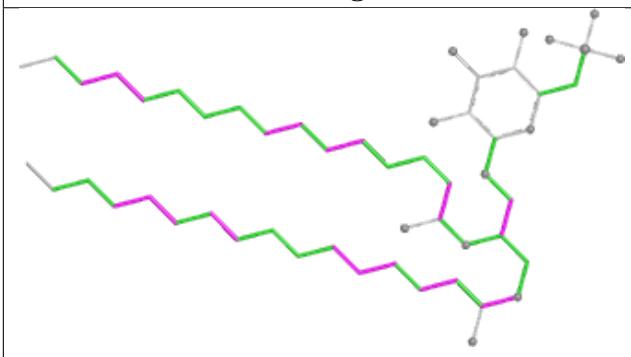
Ligand SQD A 417



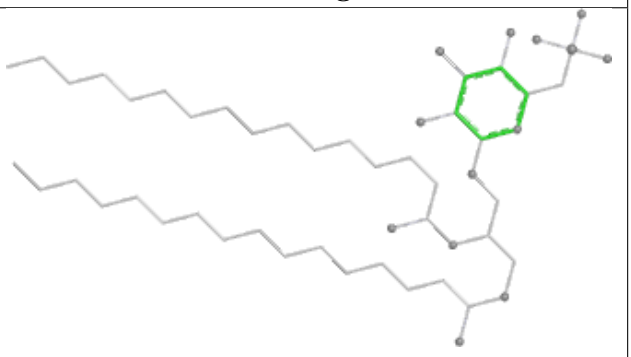
Bond lengths



Bond angles

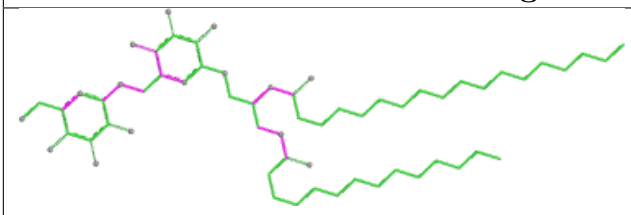


Torsions

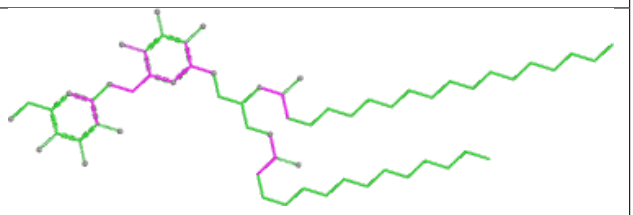


Rings

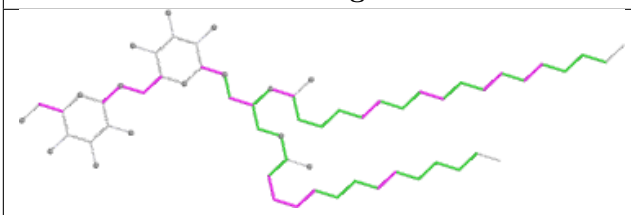
Ligand DGD C 517



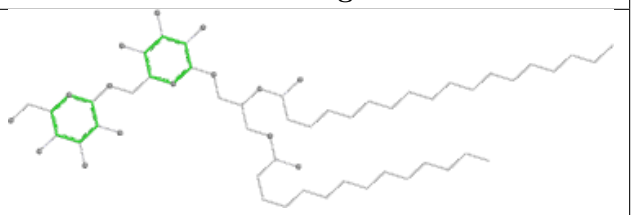
Bond lengths



Bond angles



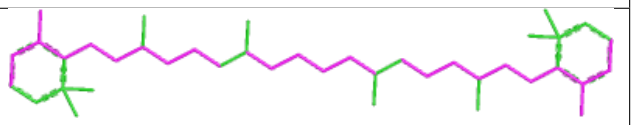
Torsions



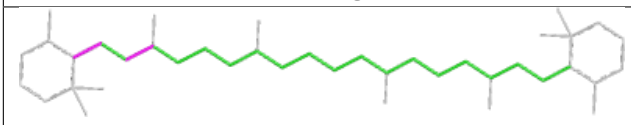
Rings

Ligand BCR c 515

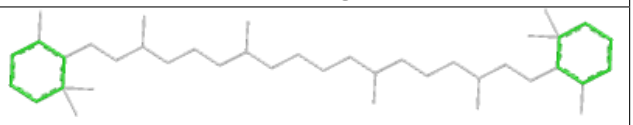
Bond lengths



Bond angles

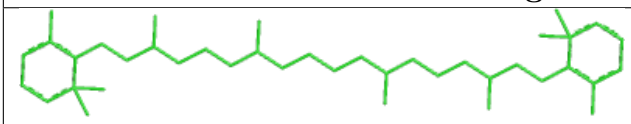


Torsions

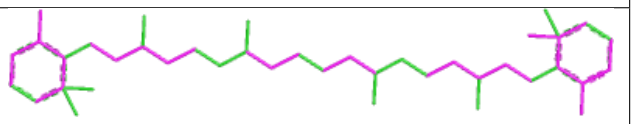


Rings

Ligand BCR b 620

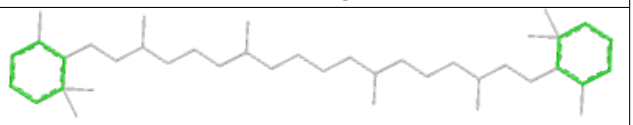


Bond lengths



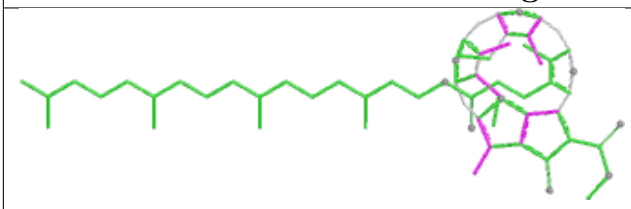
Bond angles

Torsions

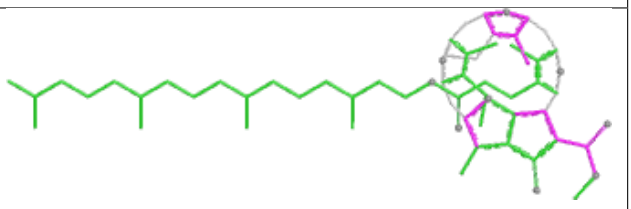


Rings

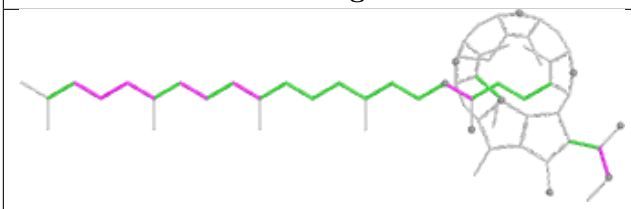
Ligand PHO A 406



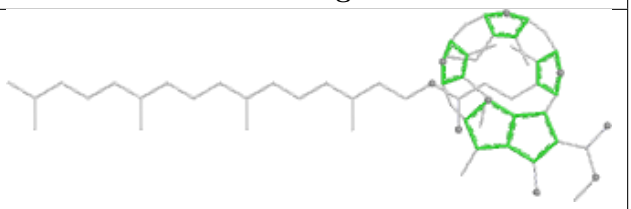
Bond lengths



Bond angles

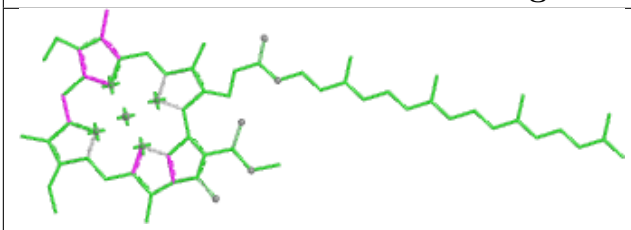


Torsions

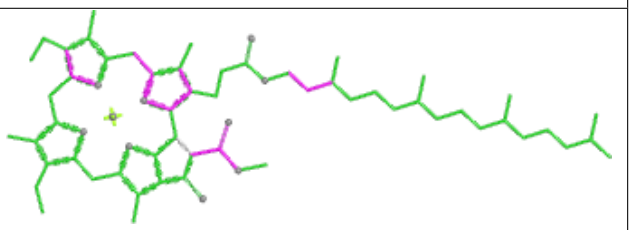


Rings

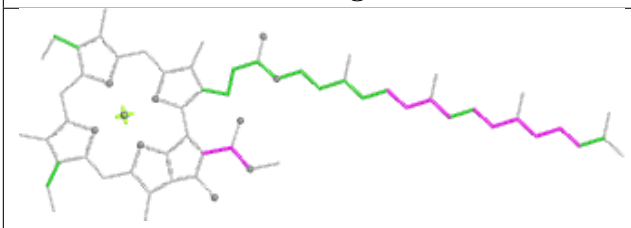
Ligand CLA c 506



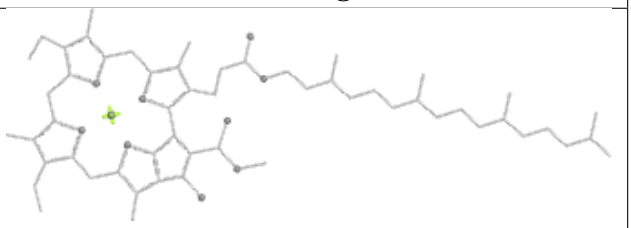
Bond lengths



Bond angles

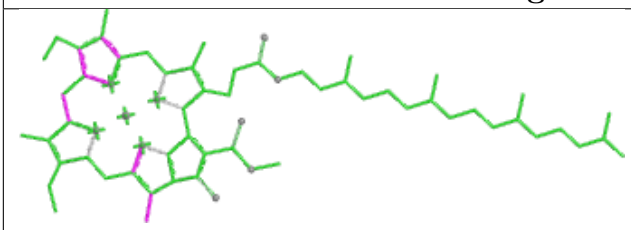


Torsions

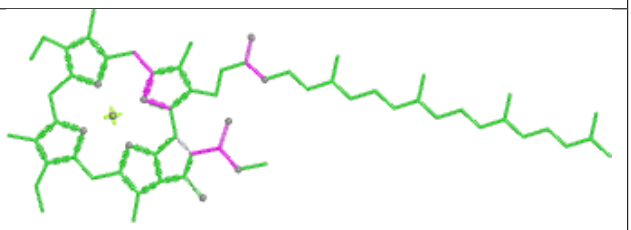


Rings

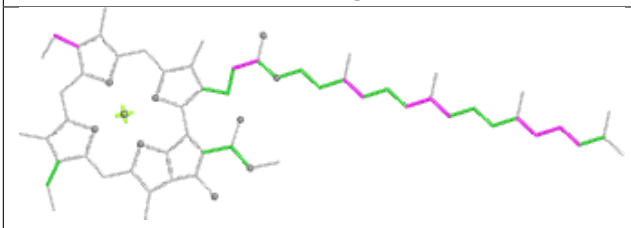
Ligand CLA d 402



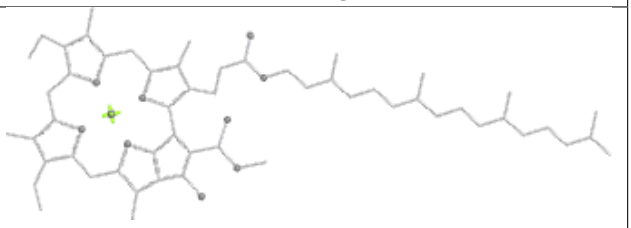
Bond lengths



Bond angles

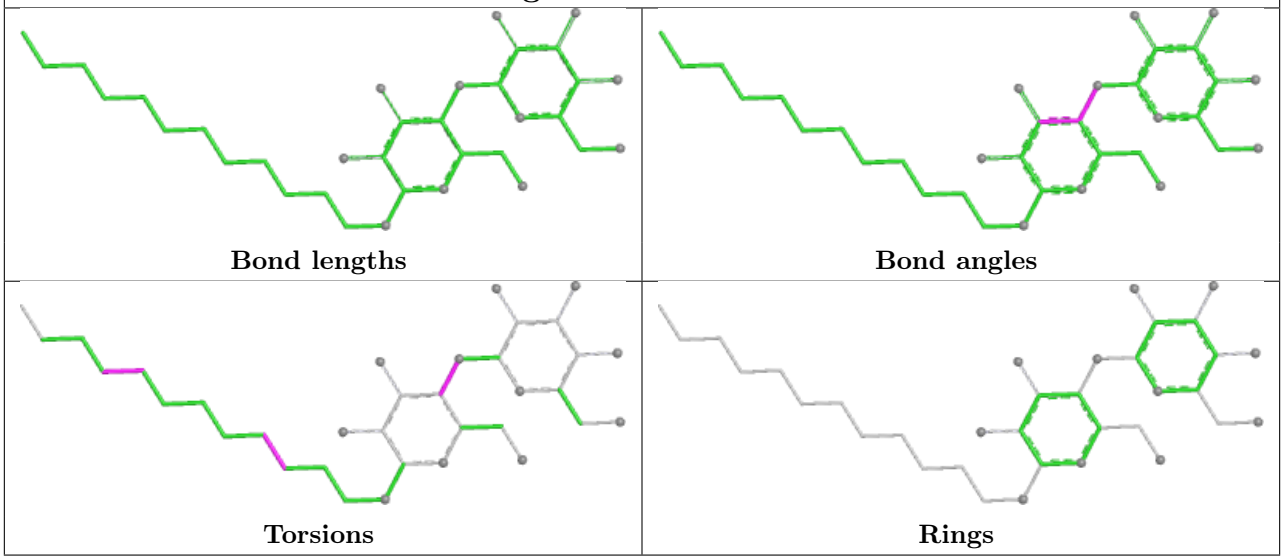


Torsions

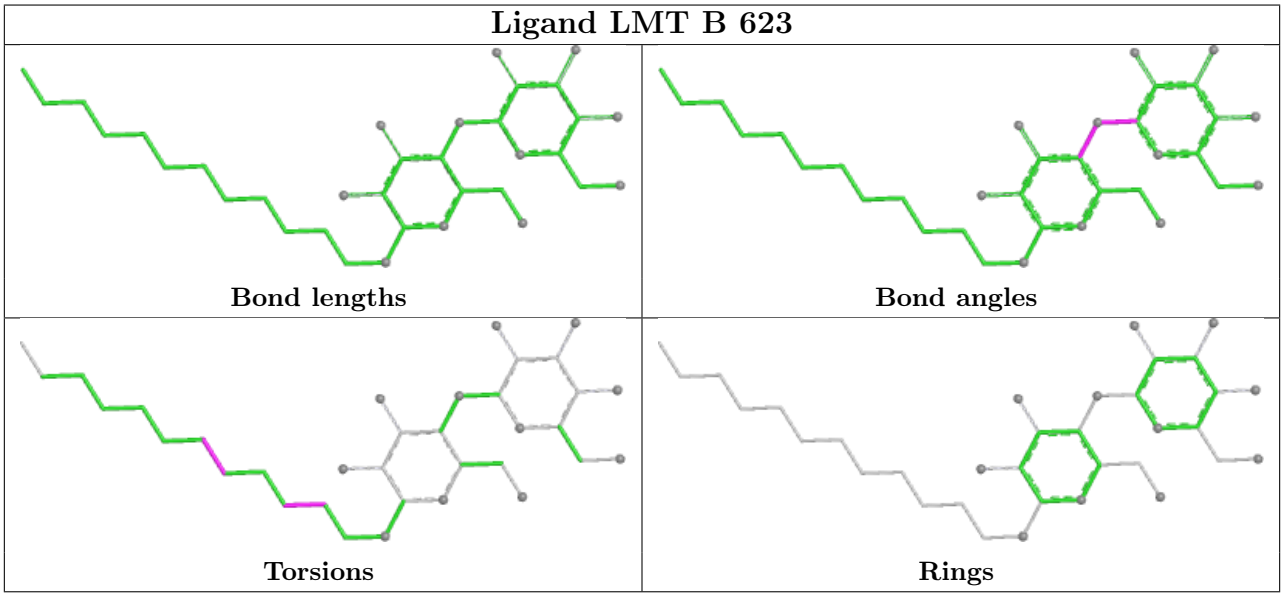


Rings

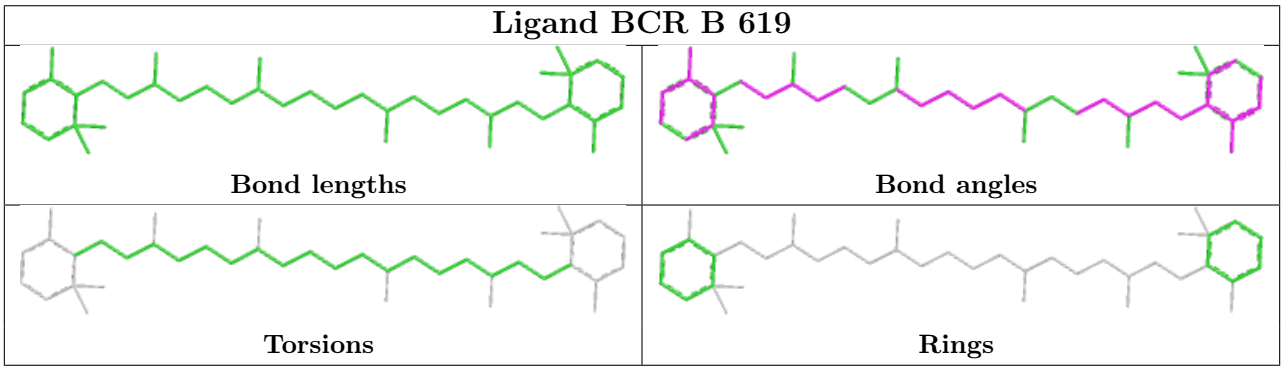
Ligand LMT T 101



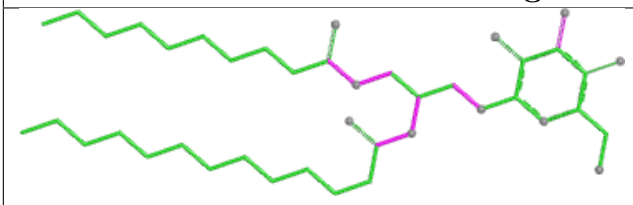
Ligand LMT B 623



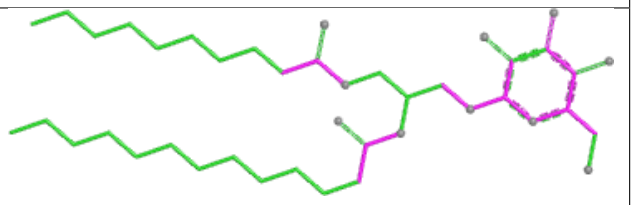
Ligand BCR B 619



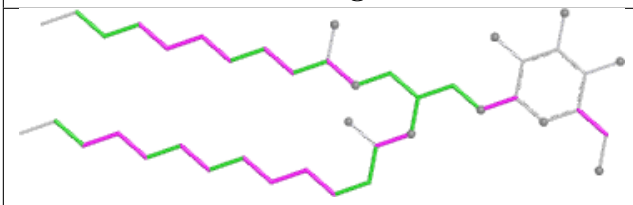
Ligand LMG a 402



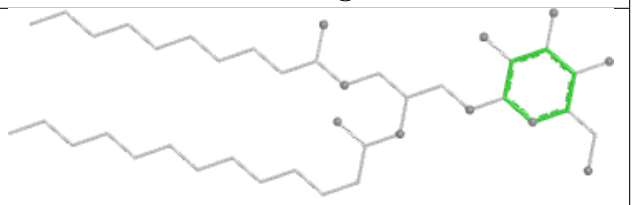
Bond lengths



Bond angles

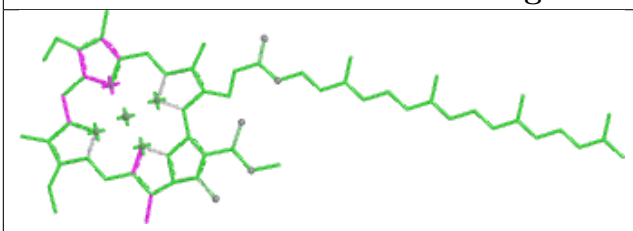


Torsions

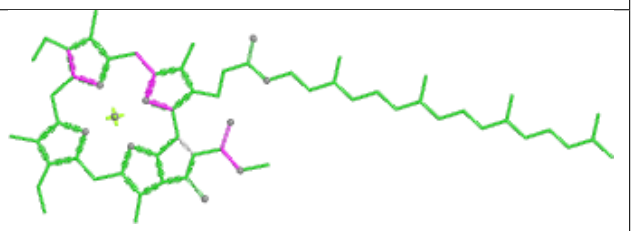


Rings

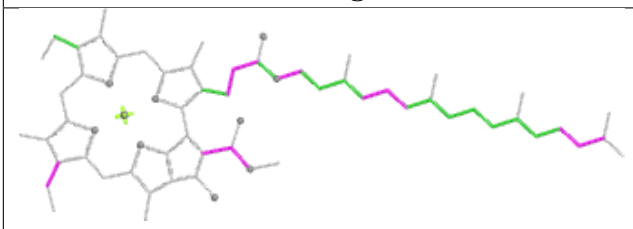
Ligand CLA B 614



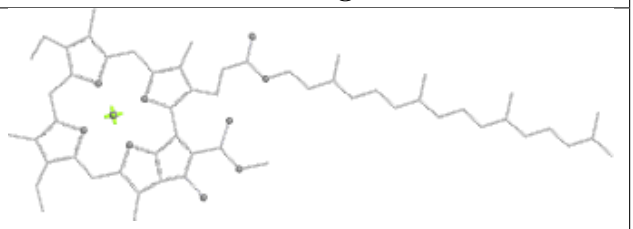
Bond lengths



Bond angles

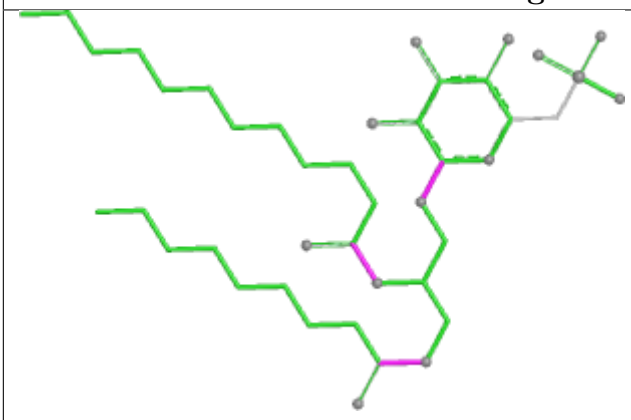


Torsions

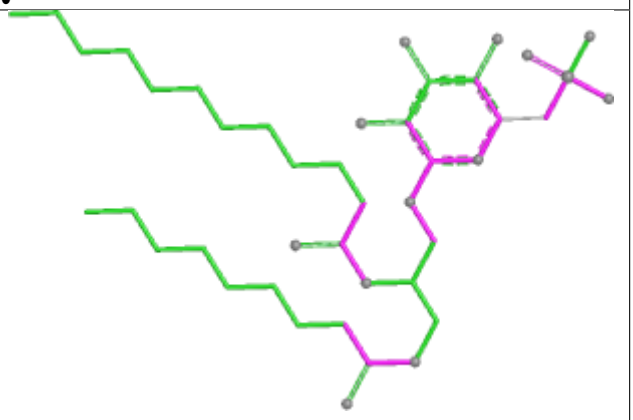


Rings

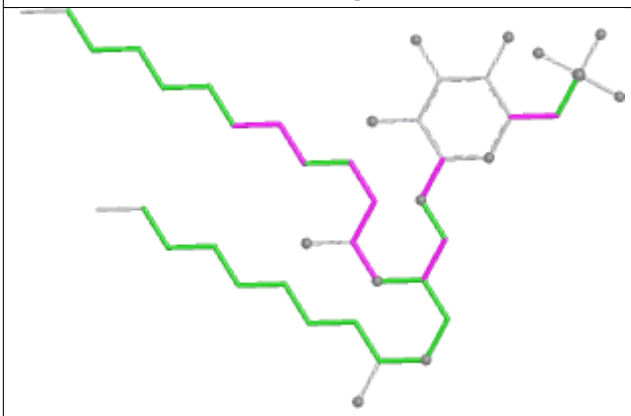
Ligand SQD d 407



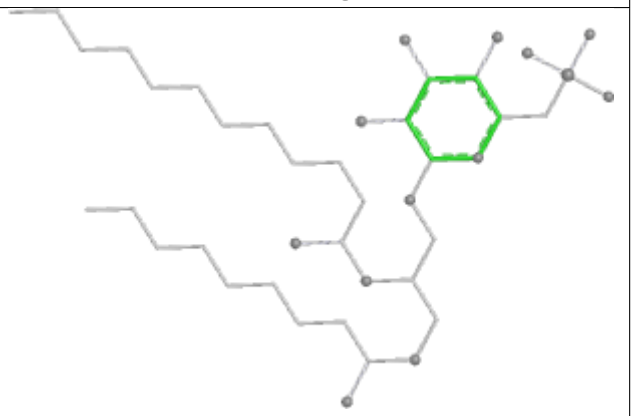
Bond lengths



Bond angles

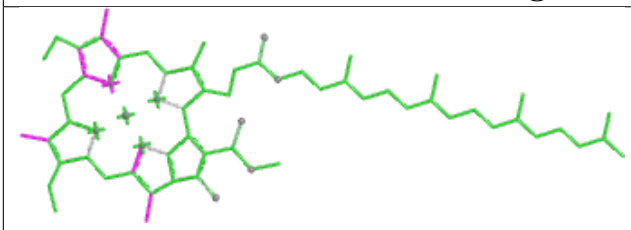


Torsions

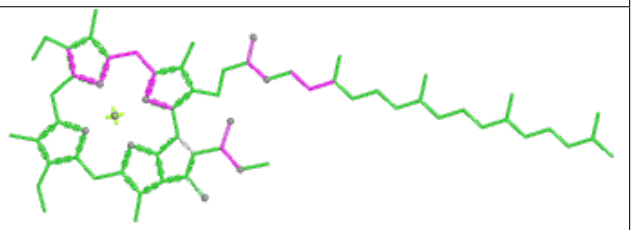


Rings

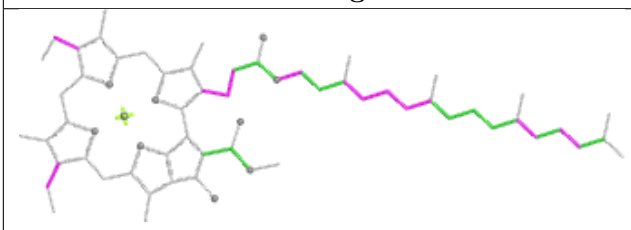
Ligand CLA a 405



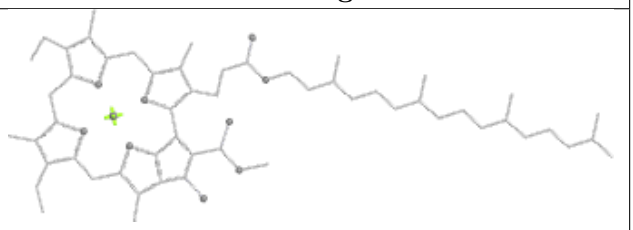
Bond lengths



Bond angles

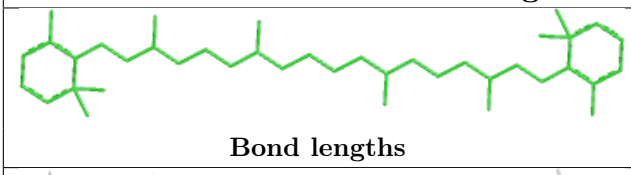


Torsions

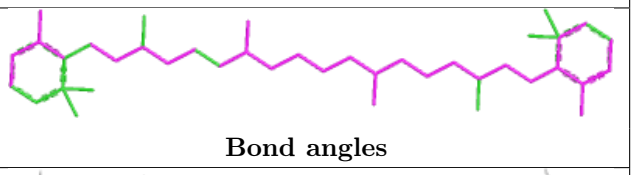


Rings

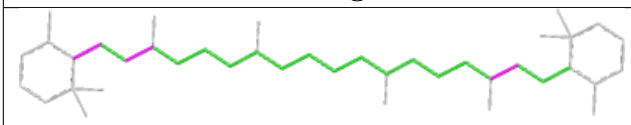
Ligand BCR D 405



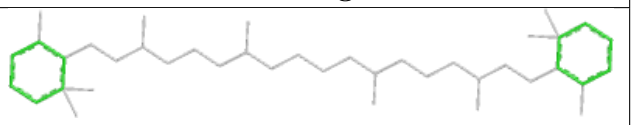
Bond lengths



Bond angles

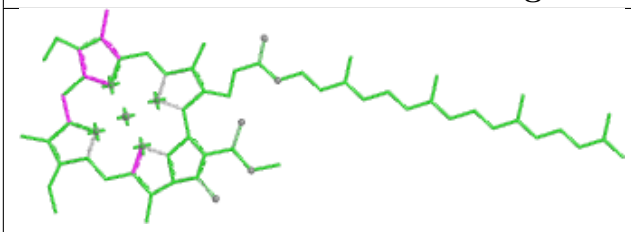


Torsions

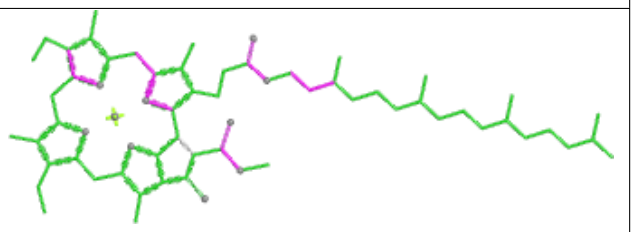


Rings

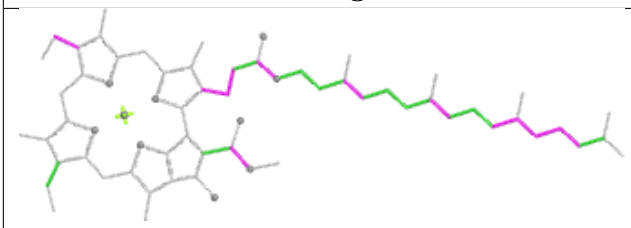
Ligand CLA C 513



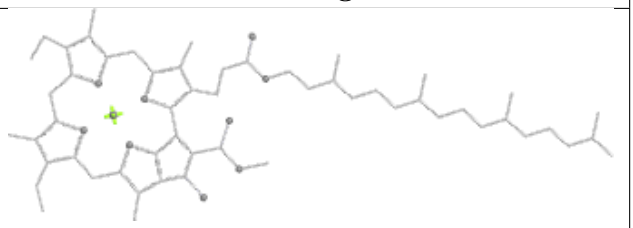
Bond lengths



Bond angles

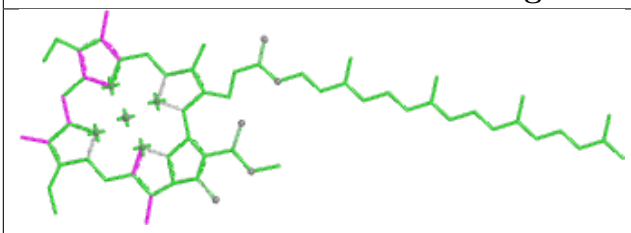


Torsions

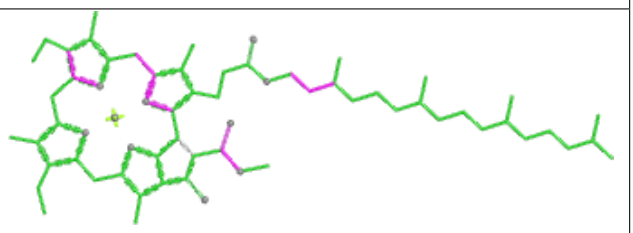


Rings

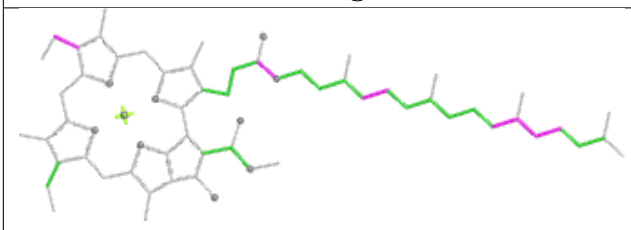
Ligand CLA C 502



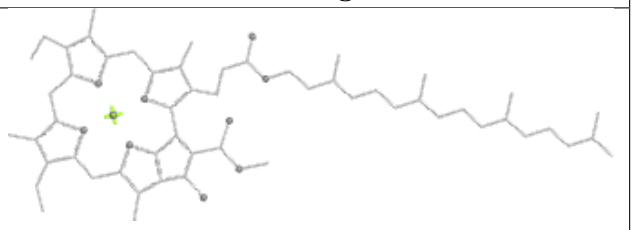
Bond lengths



Bond angles

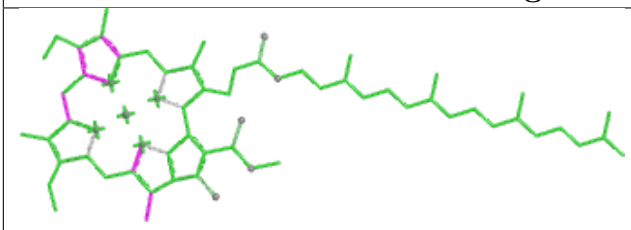


Torsions

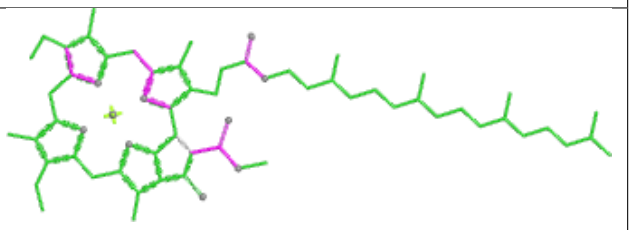


Rings

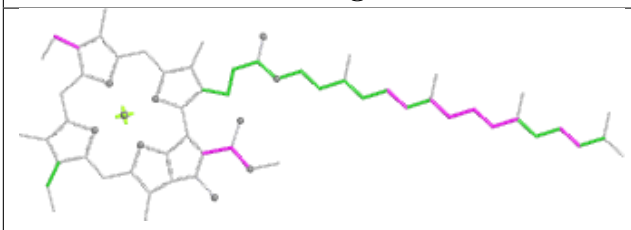
Ligand CLA C 503



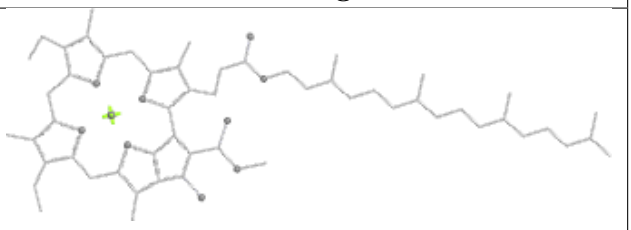
Bond lengths



Bond angles

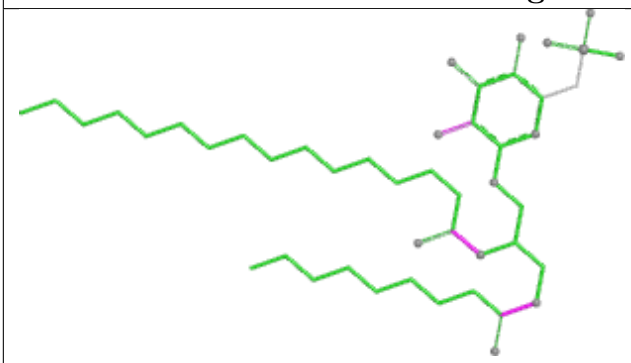


Torsions

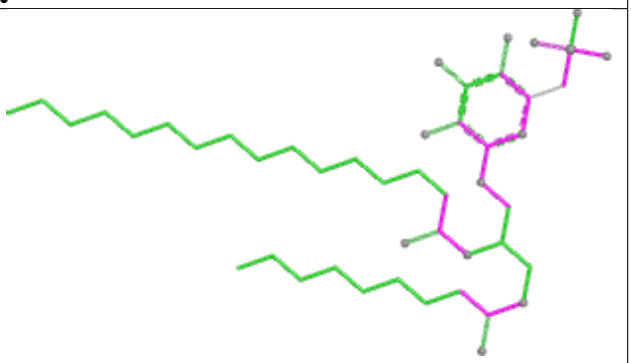


Rings

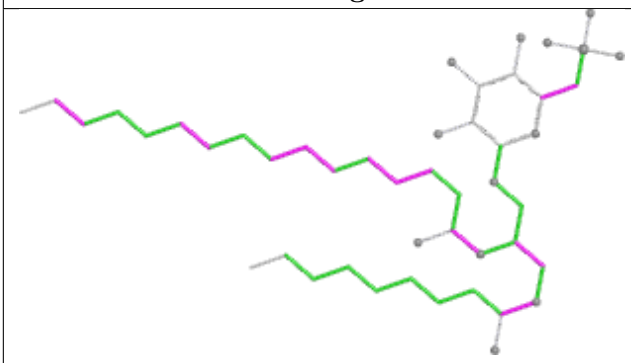
Ligand SQD b 601



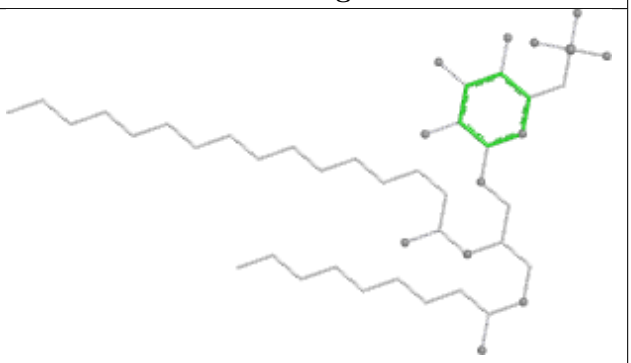
Bond lengths



Bond angles

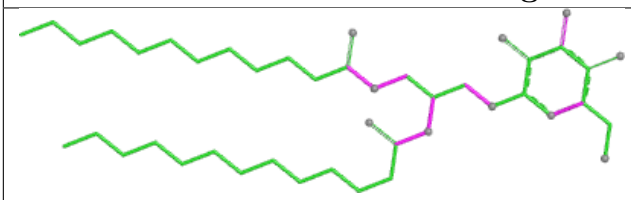


Torsions

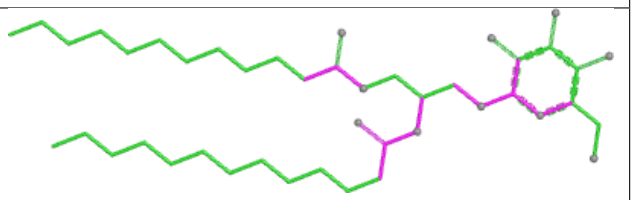


Rings

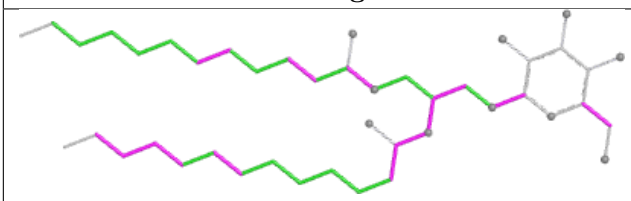
Ligand LMG E 101



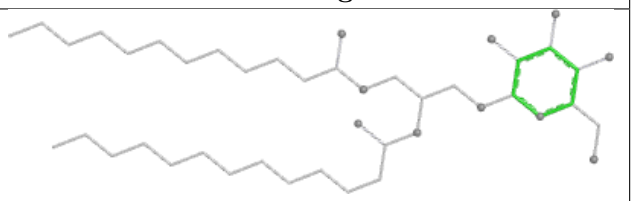
Bond lengths



Bond angles

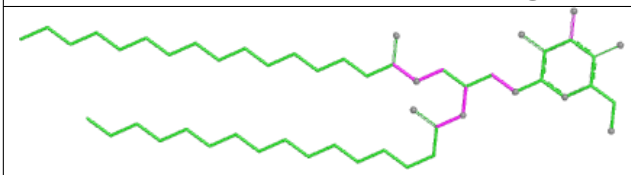


Torsions

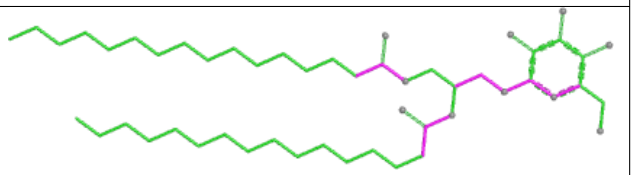


Rings

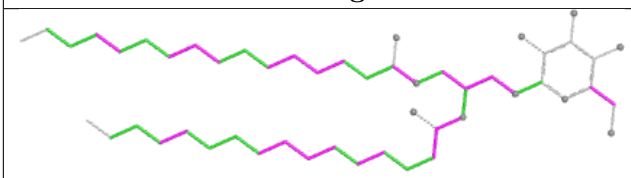
Ligand LMG a 416



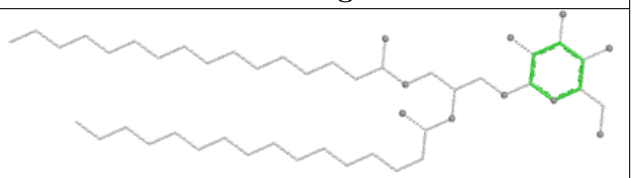
Bond lengths



Bond angles

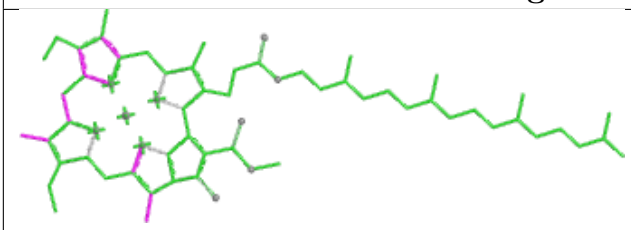


Torsions

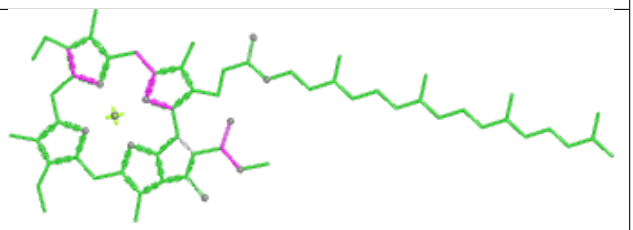


Rings

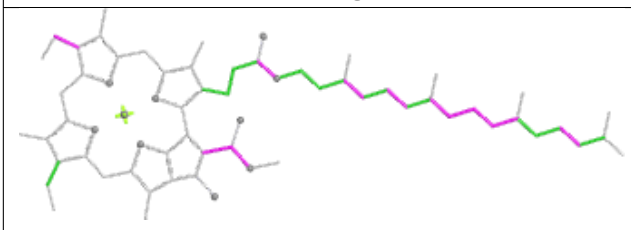
Ligand CLA b 608



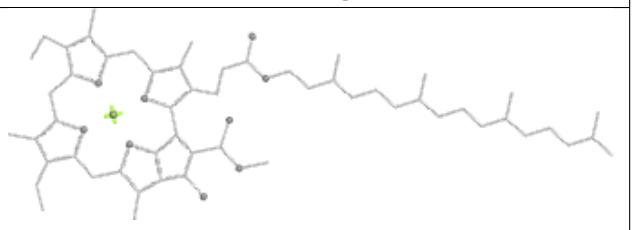
Bond lengths



Bond angles

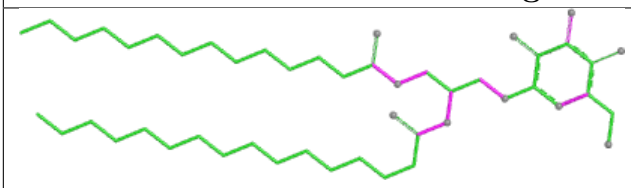


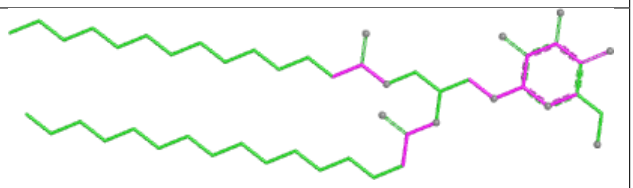
Torsions

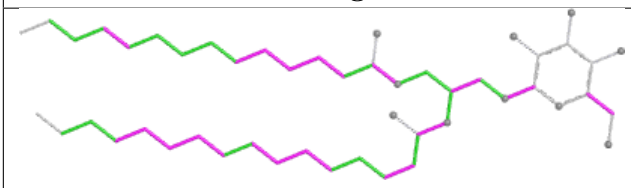


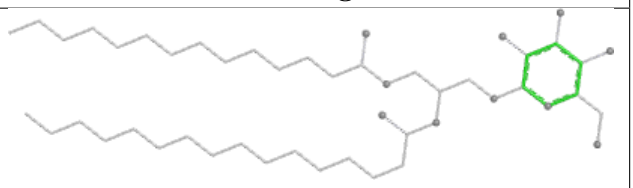
Rings

Ligand LMG b 623

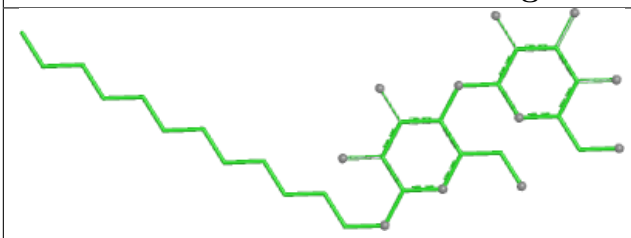

Bond lengths

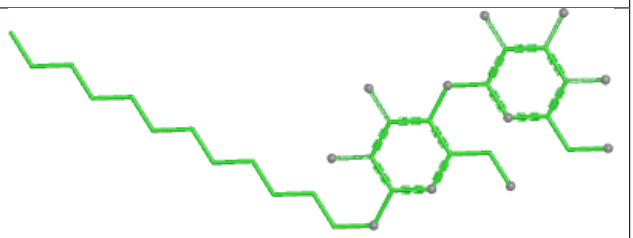

Bond angles

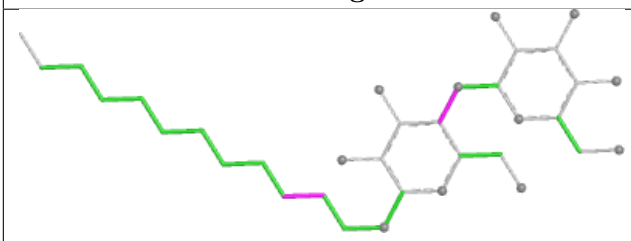

Torsions

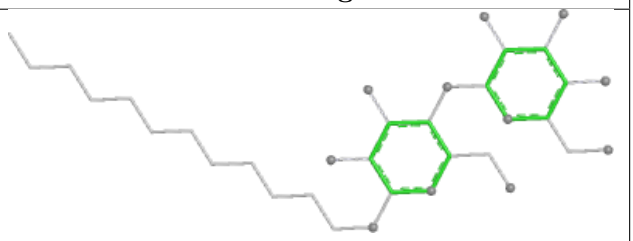

Rings

Ligand LMT B 628

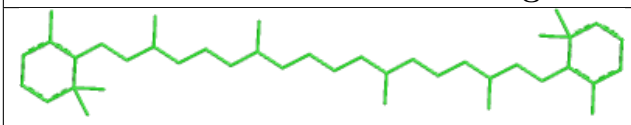

Bond lengths

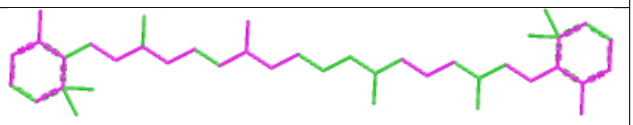

Bond angles

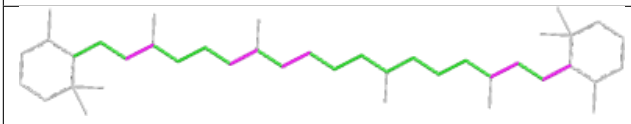

Torsions

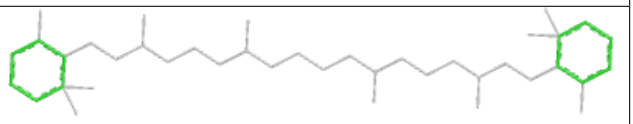

Rings

Ligand BCR B 618

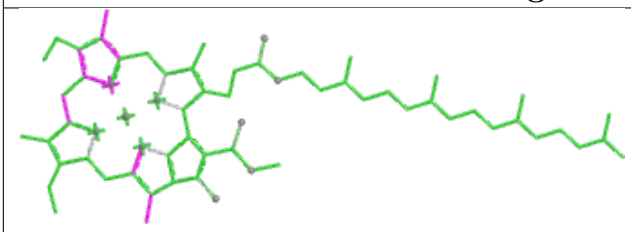

Bond lengths


Bond angles

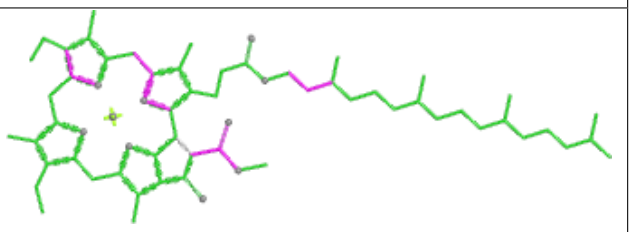

Torsions


Rings

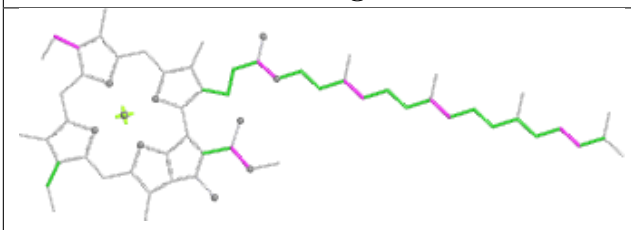
Ligand CLA b 614



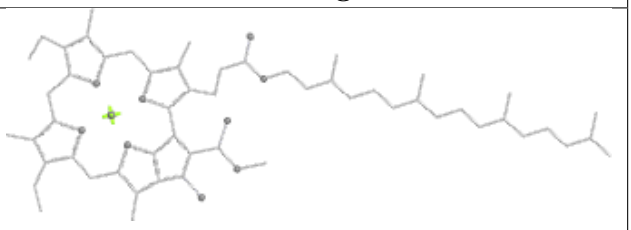
Bond lengths



Bond angles

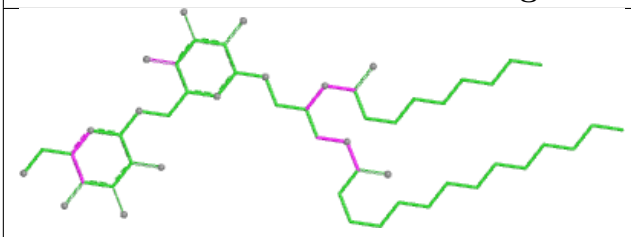


Torsions

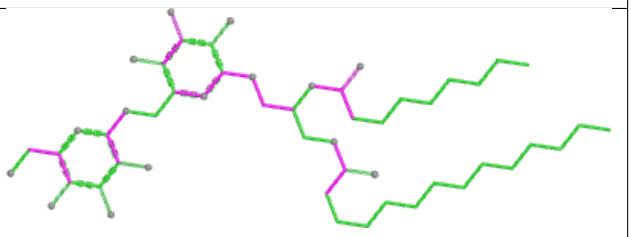


Rings

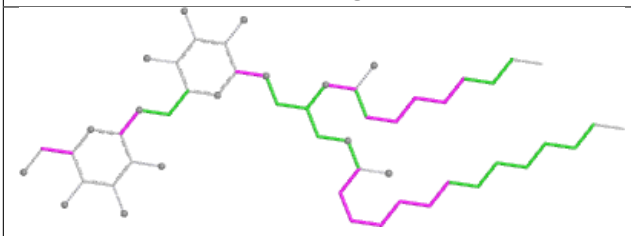
Ligand DGD C 516



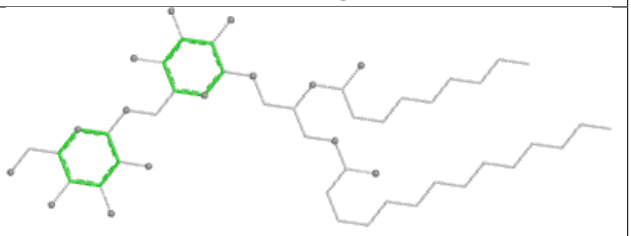
Bond lengths



Bond angles

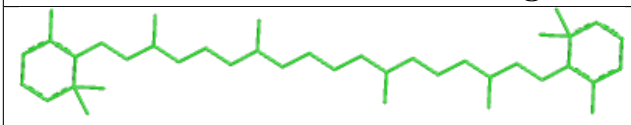


Torsions

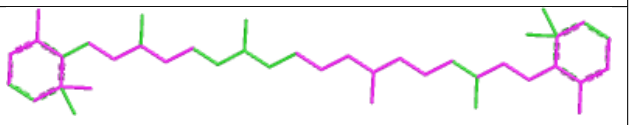


Rings

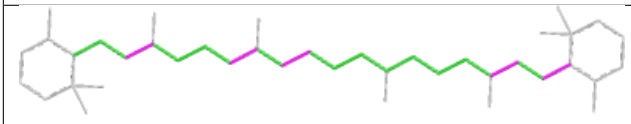
Ligand BCR T 103



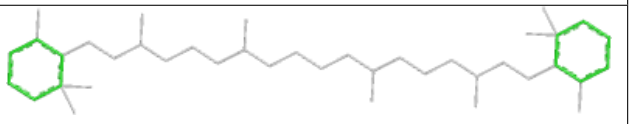
Bond lengths



Bond angles

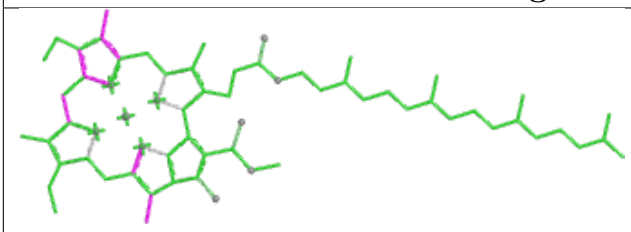


Torsions

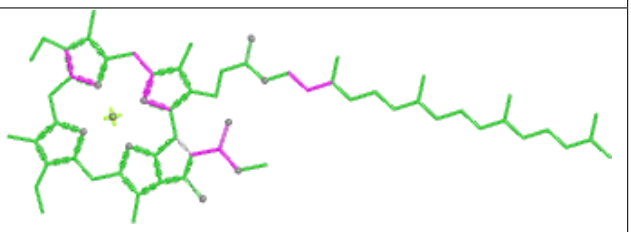


Rings

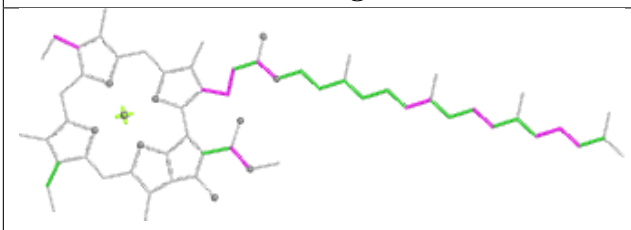
Ligand CLA c 504



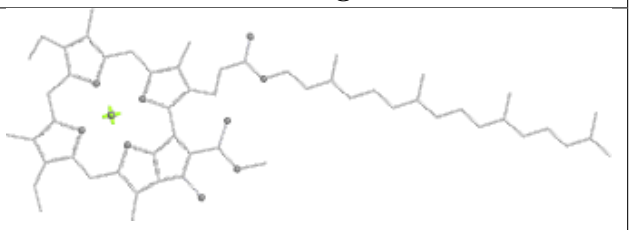
Bond lengths



Bond angles

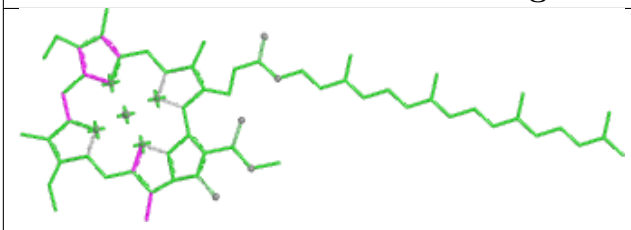


Torsions

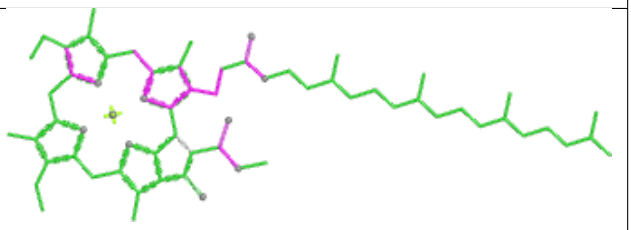


Rings

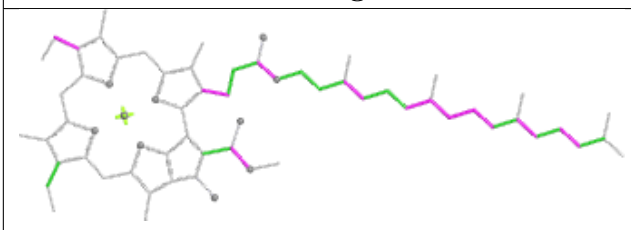
Ligand CLA c 505



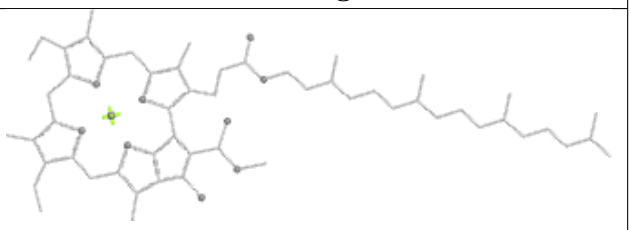
Bond lengths



Bond angles

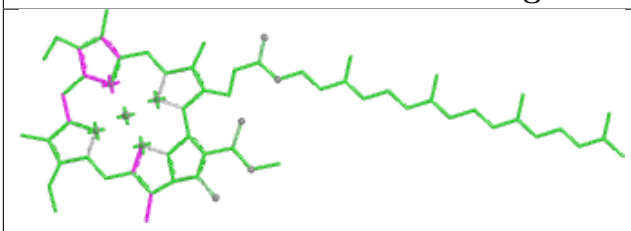


Torsions

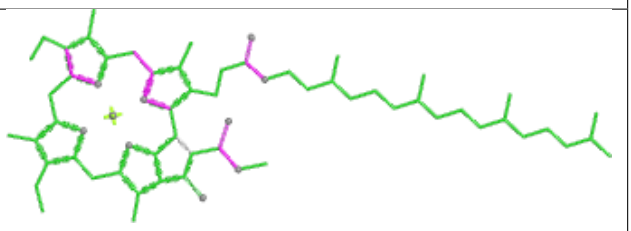


Rings

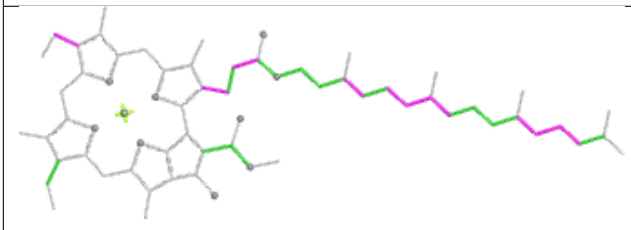
Ligand CLA D 401



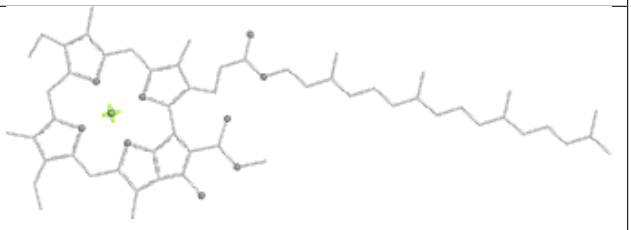
Bond lengths



Bond angles

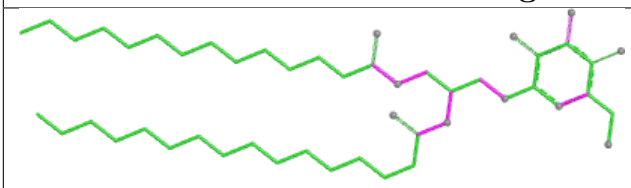


Torsions

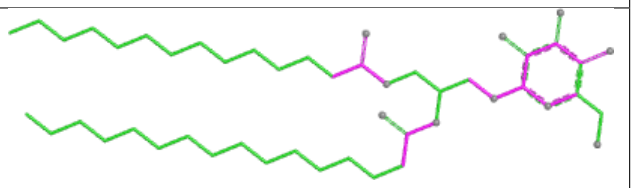


Rings

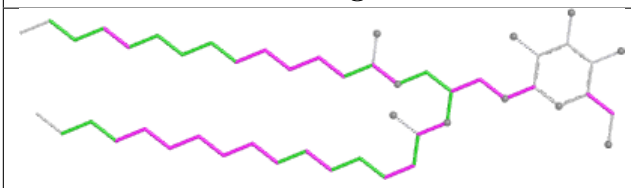
Ligand LMG D 407



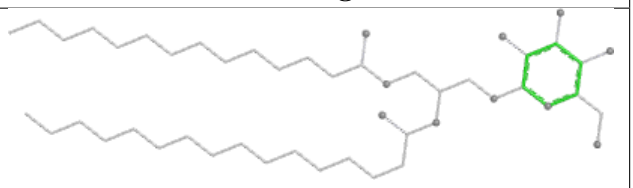
Bond lengths



Bond angles

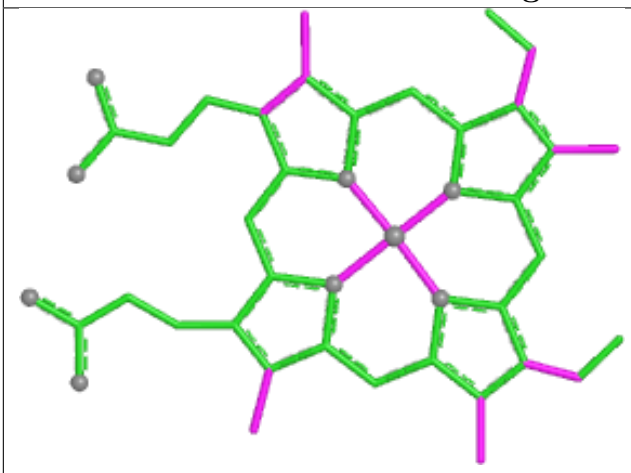


Torsions

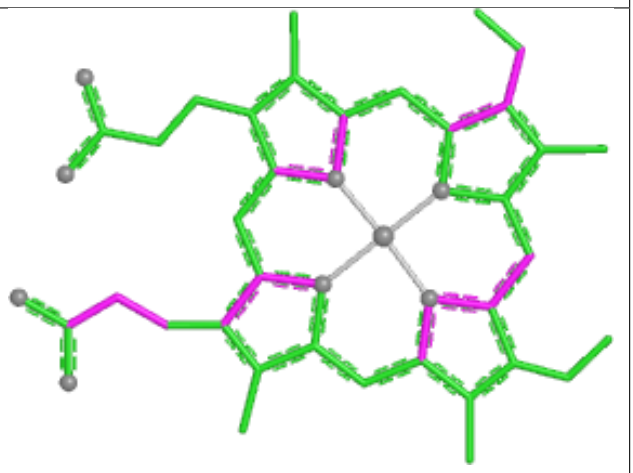


Rings

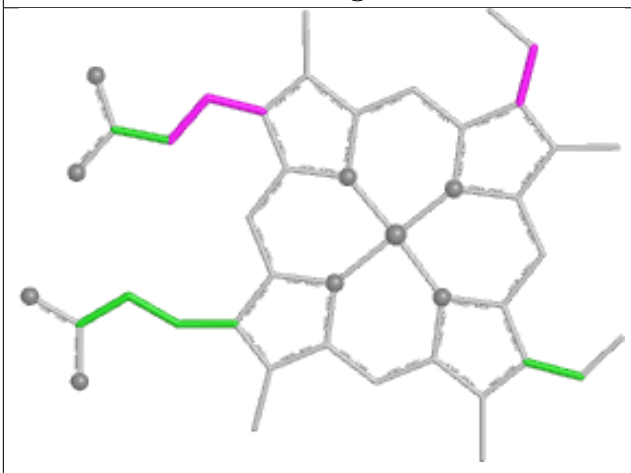
Ligand HEM v 201



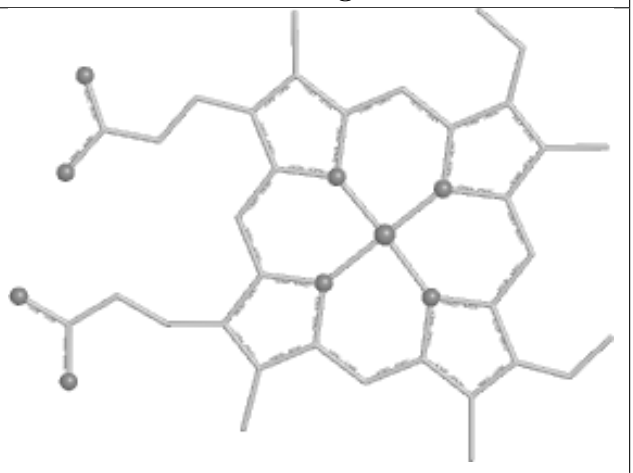
Bond lengths



Bond angles

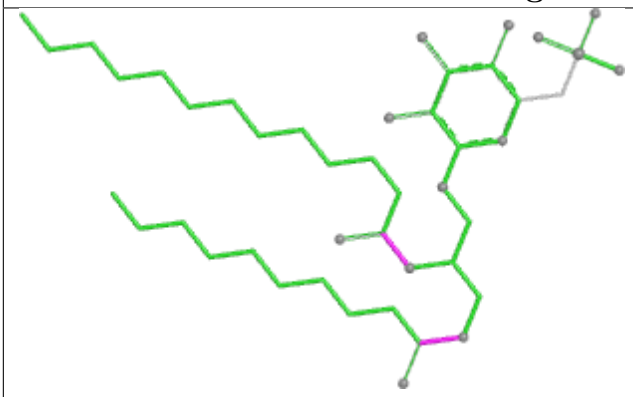


Torsions

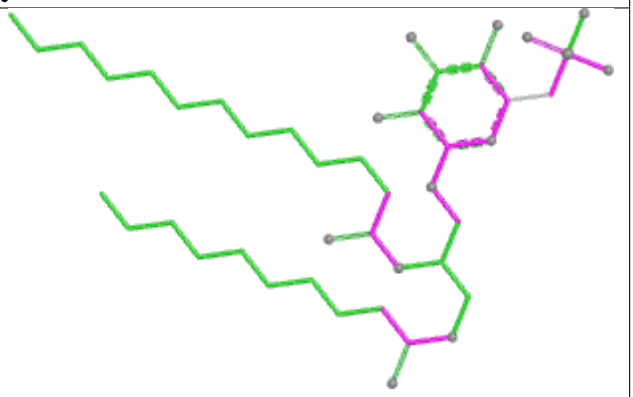


Rings

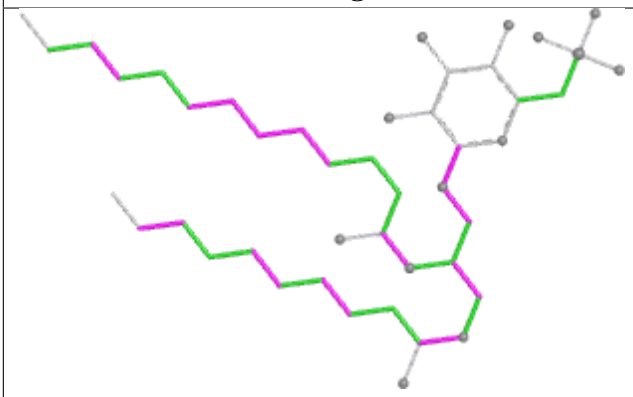
Ligand SQD F 102



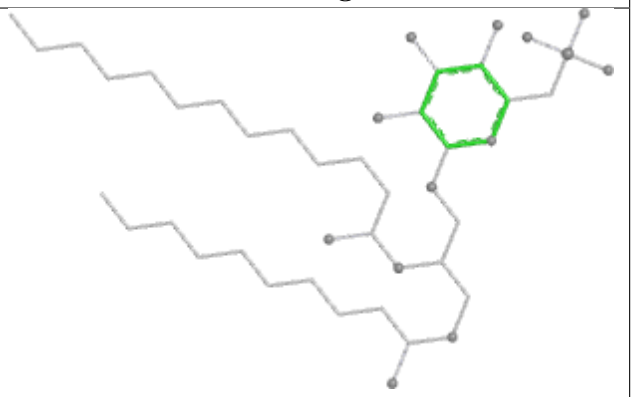
Bond lengths



Bond angles

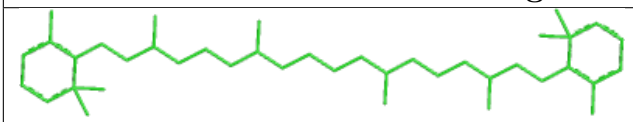


Torsions

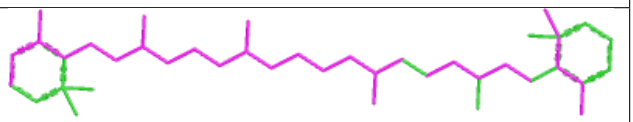


Rings

Ligand BCR x 101

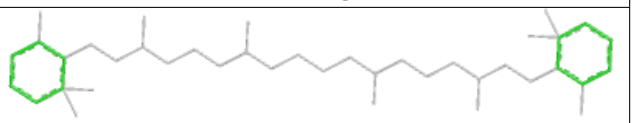


Bond lengths



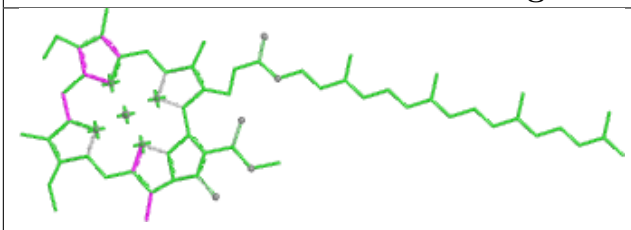
Bond angles

Torsions

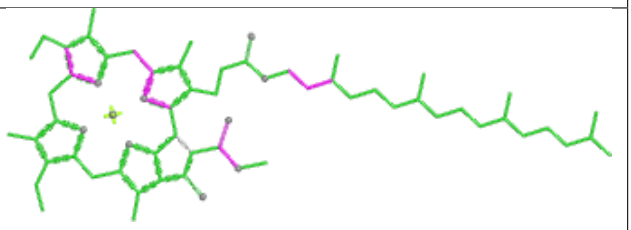


Rings

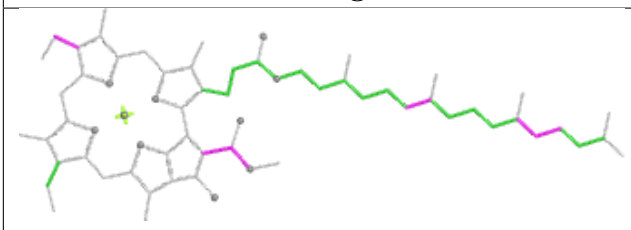
Ligand CLA b 612



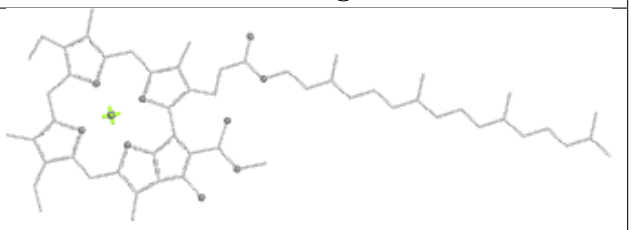
Bond lengths



Bond angles

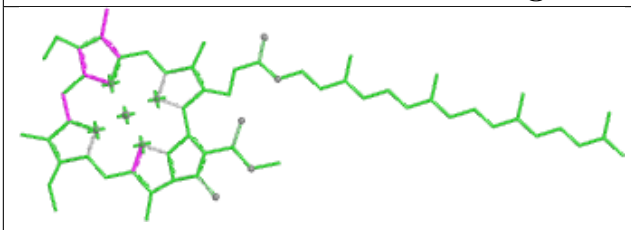


Torsions

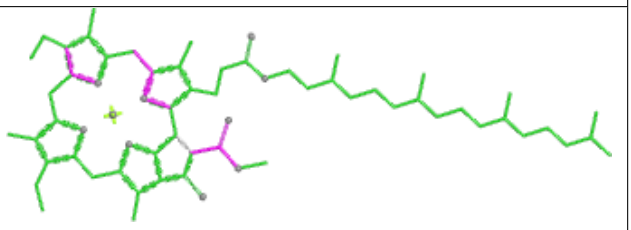


Rings

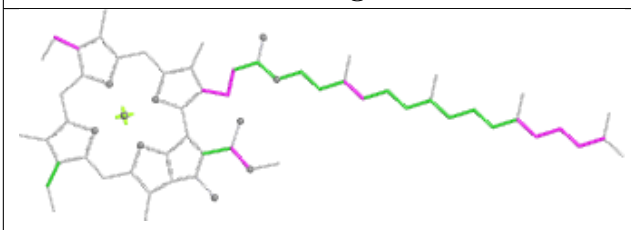
Ligand CLA b 609



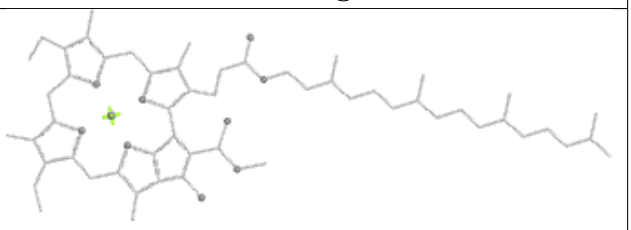
Bond lengths



Bond angles

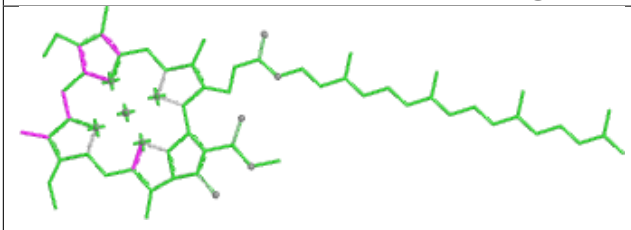


Torsions

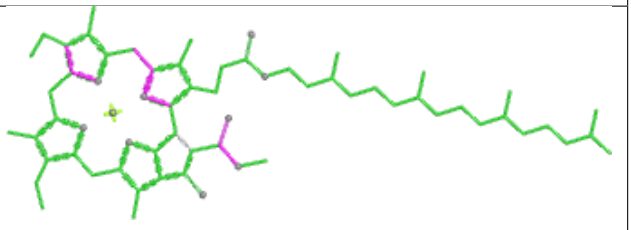


Rings

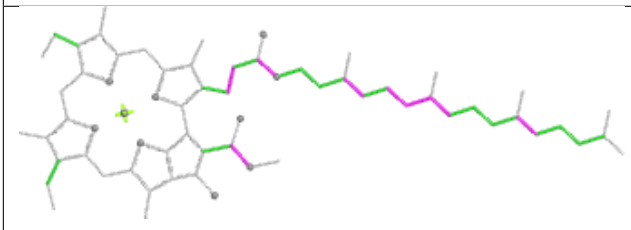
Ligand CLA c 511



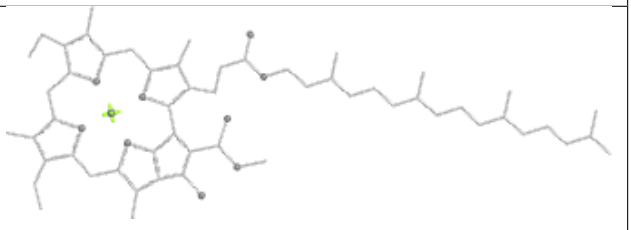
Bond lengths



Bond angles

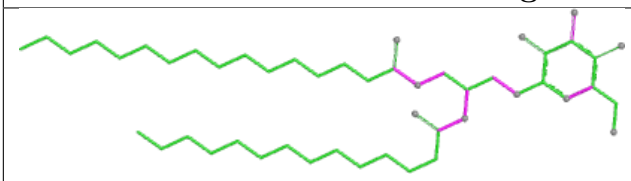


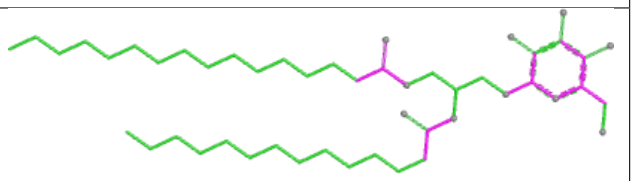
Torsions

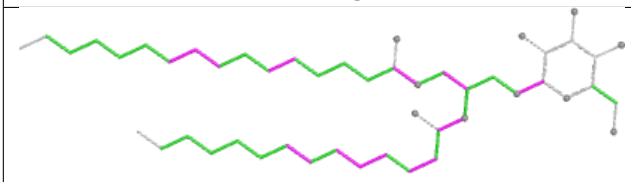


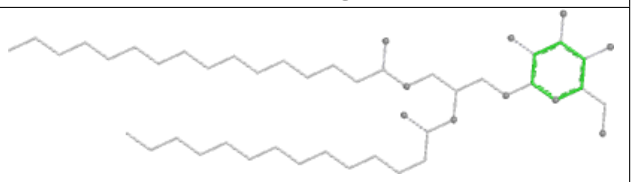
Rings

Ligand LMG B 622

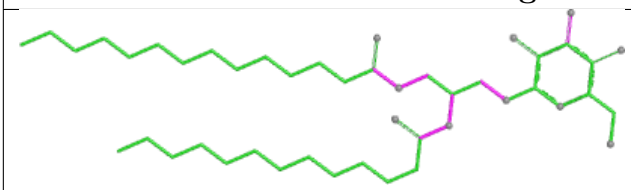

Bond lengths

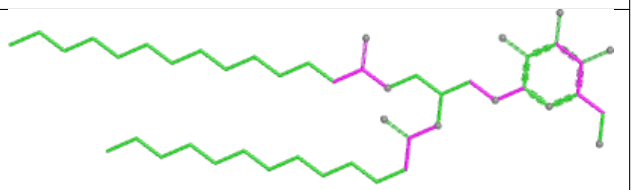

Bond angles

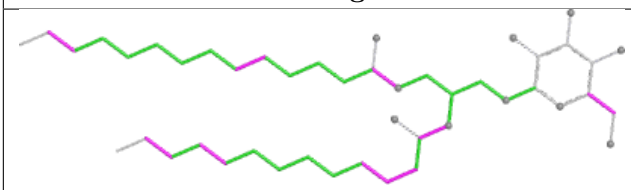

Torsions

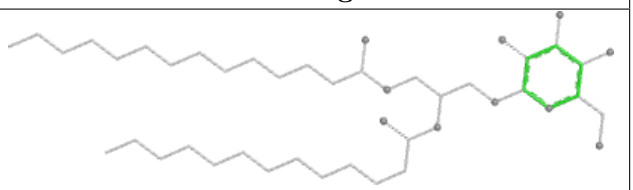

Rings

Ligand LMG D 406

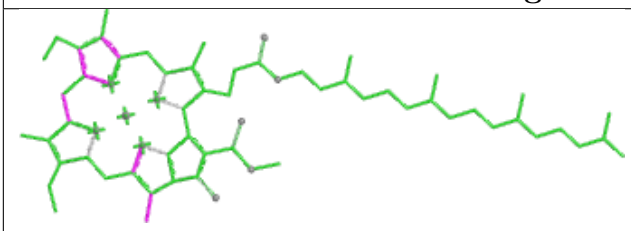

Bond lengths

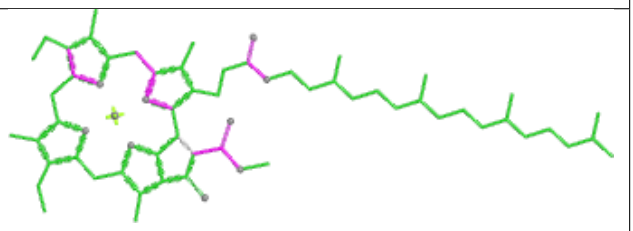

Bond angles

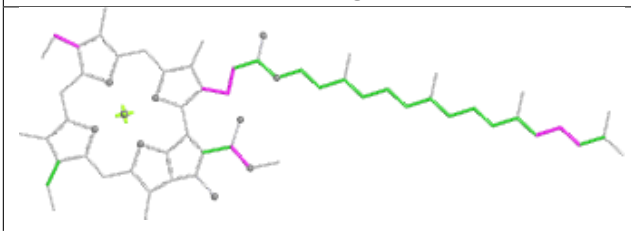

Torsions

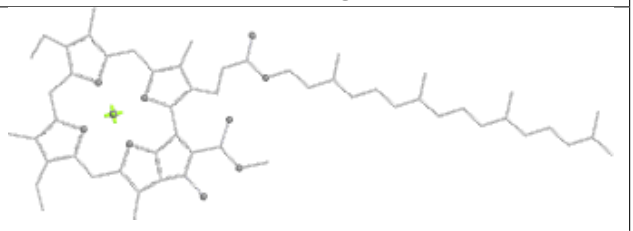

Rings

Ligand CLA B 607

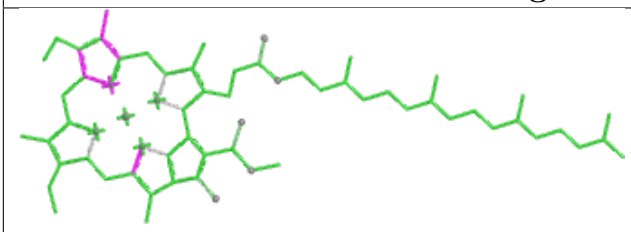

Bond lengths


Bond angles

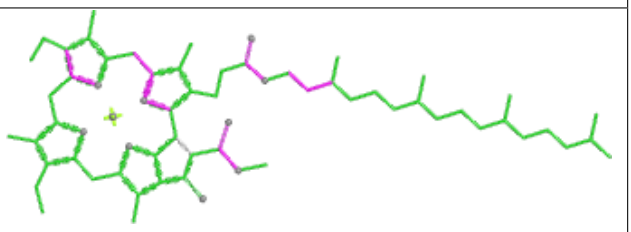

Torsions


Rings

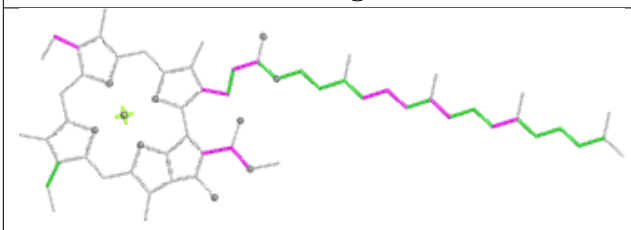
Ligand CLA c 507



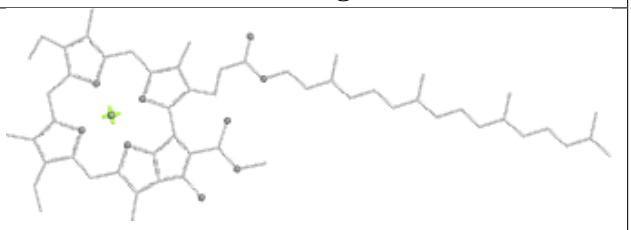
Bond lengths



Bond angles

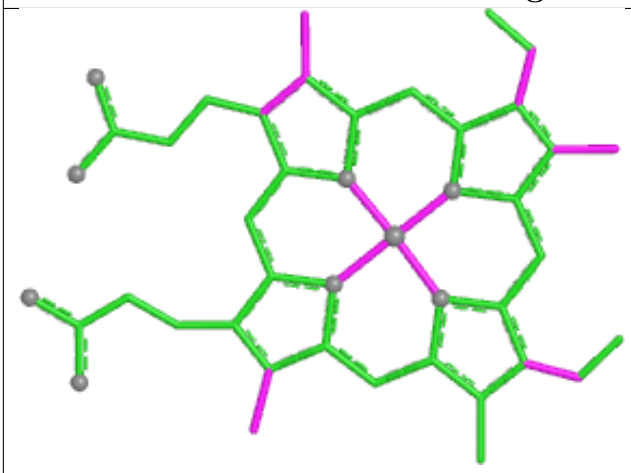


Torsions

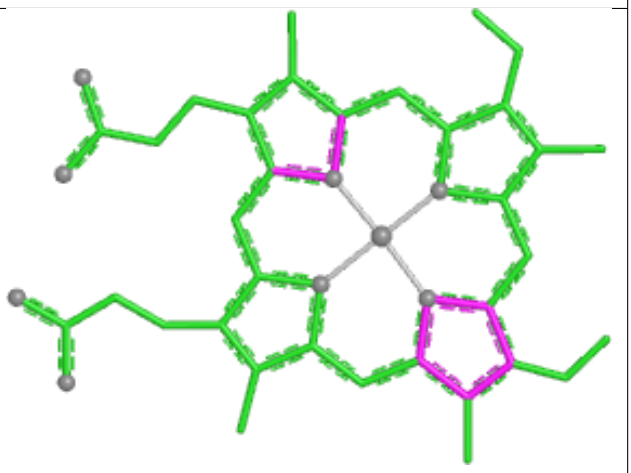


Rings

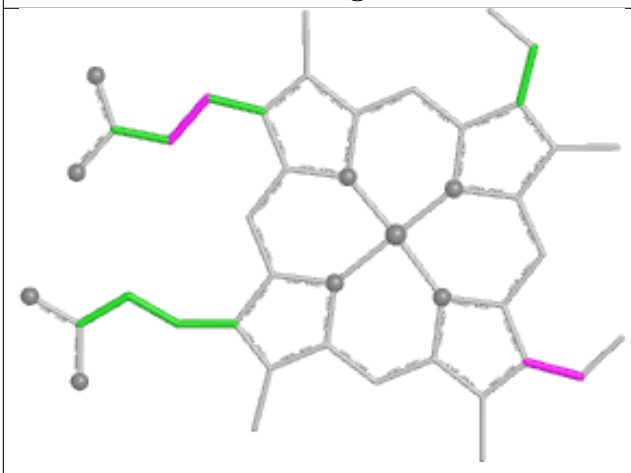
Ligand HEM f 101



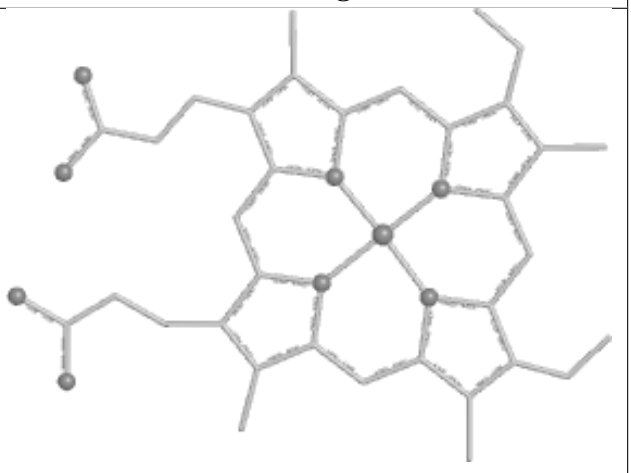
Bond lengths



Bond angles

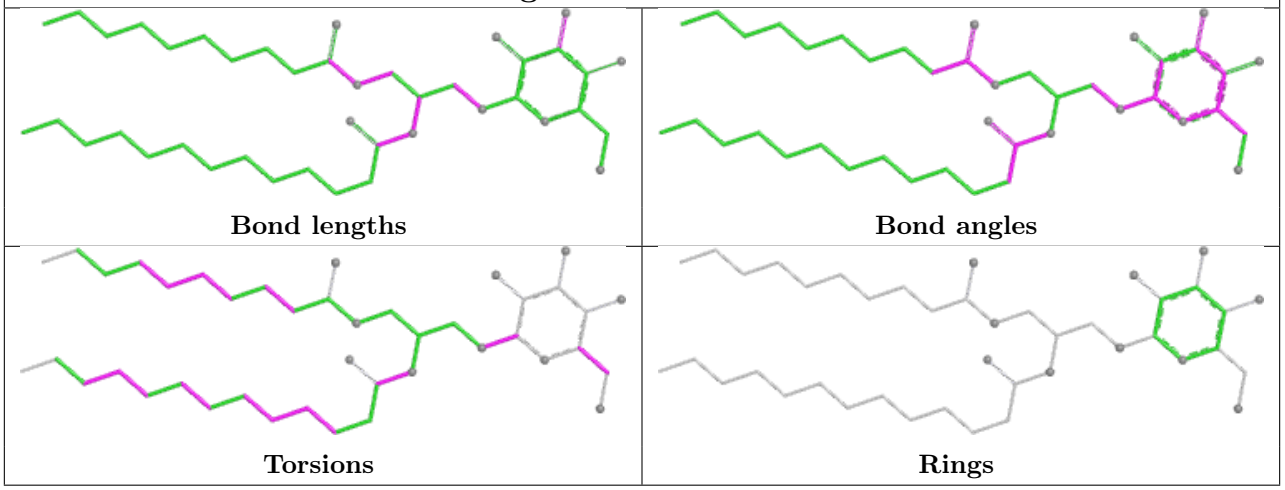


Torsions

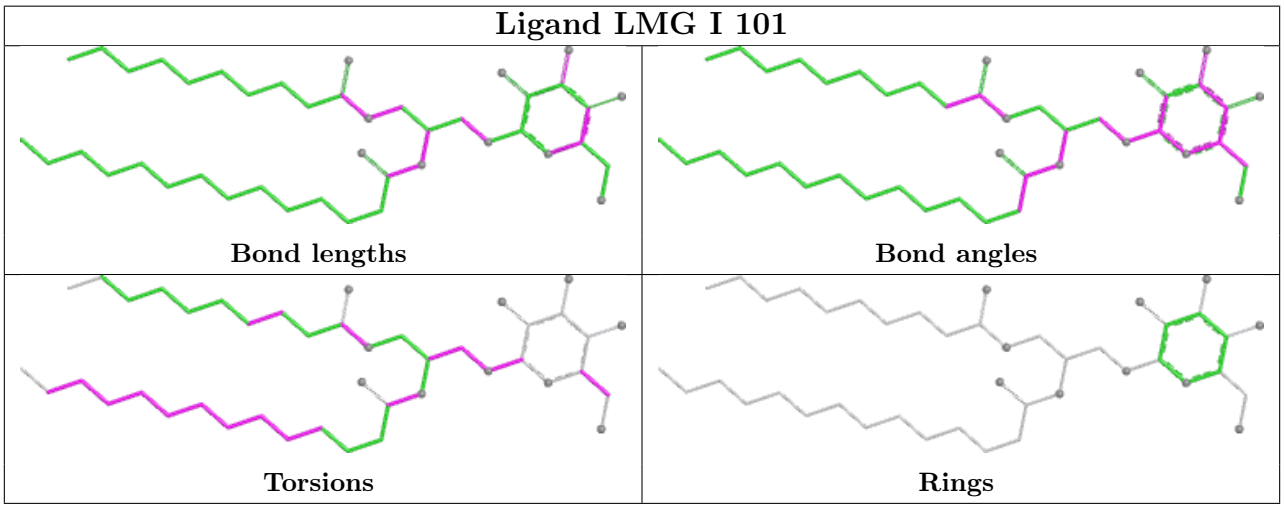


Rings

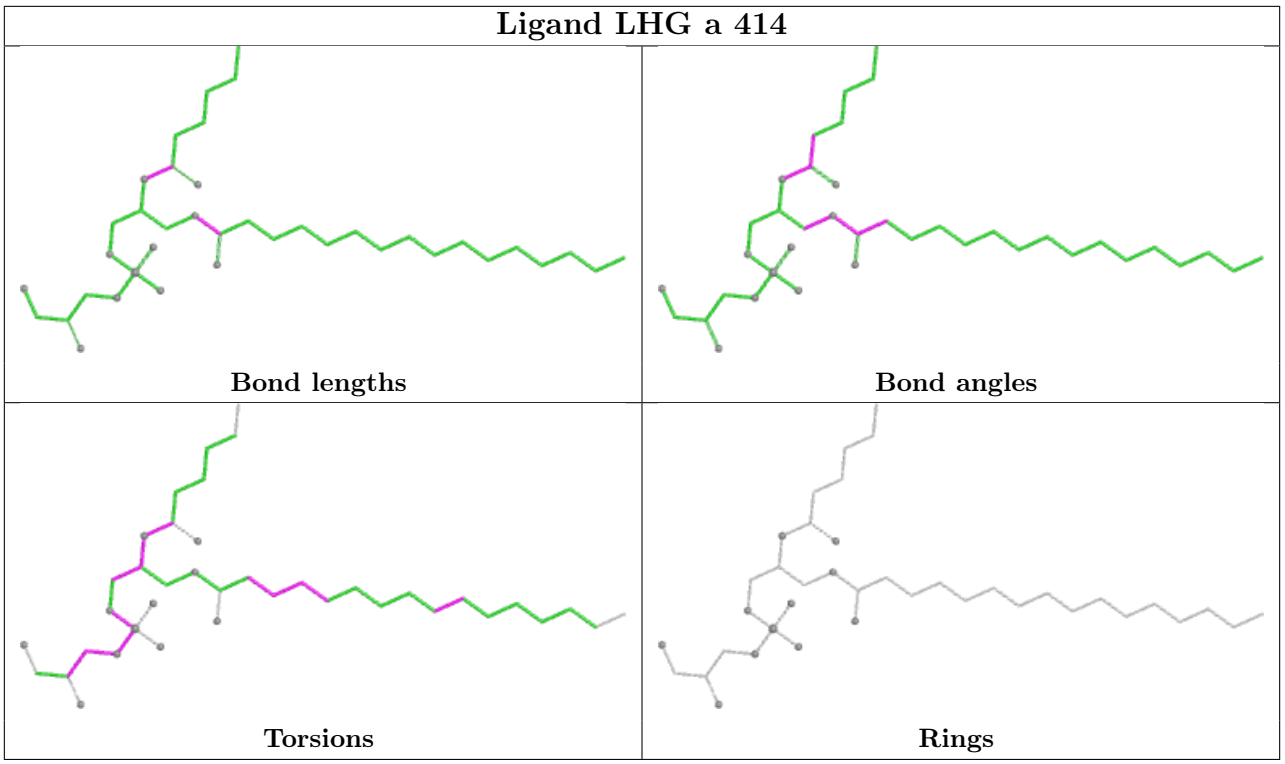
Ligand LMG A 418



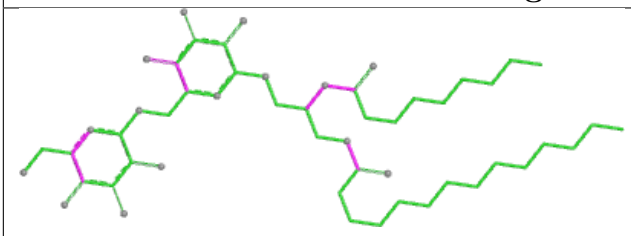
Ligand LMG I 101



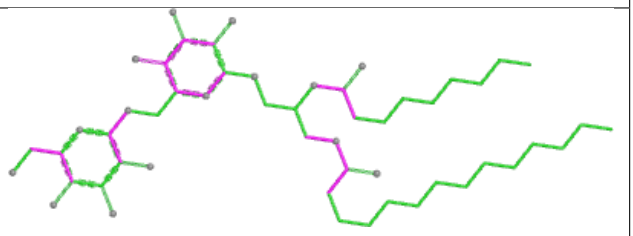
Ligand LHG a 414



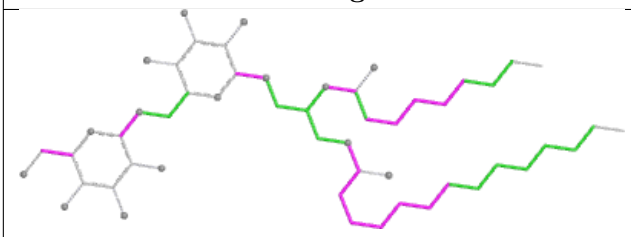
Ligand DGD c 517



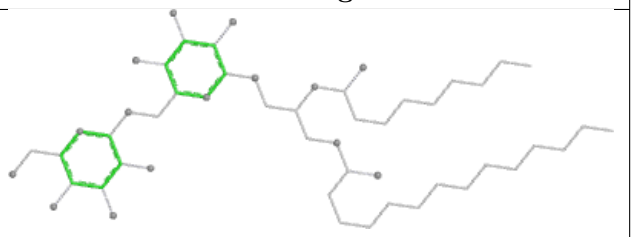
Bond lengths



Bond angles

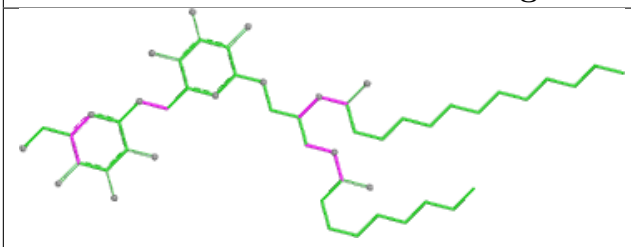


Torsions

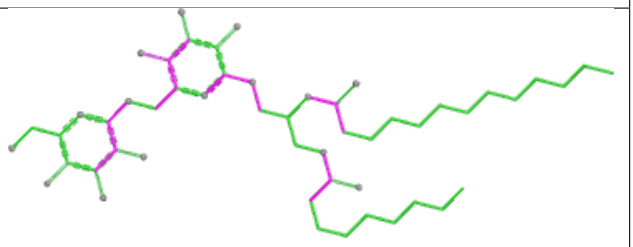


Rings

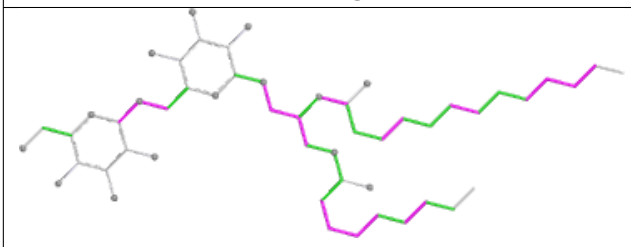
Ligand DGD B 626



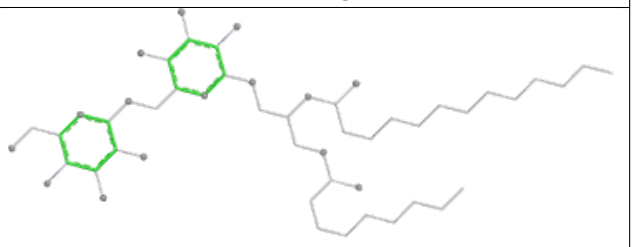
Bond lengths



Bond angles

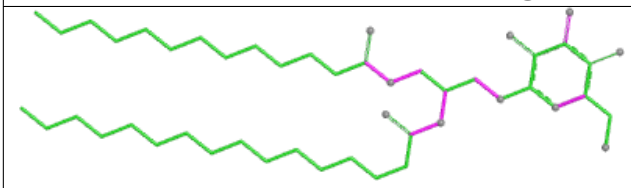


Torsions

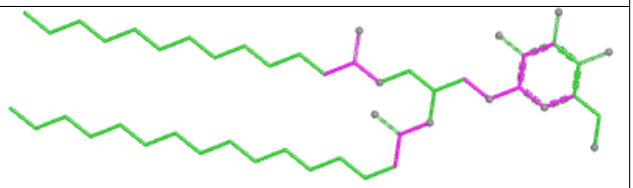


Rings

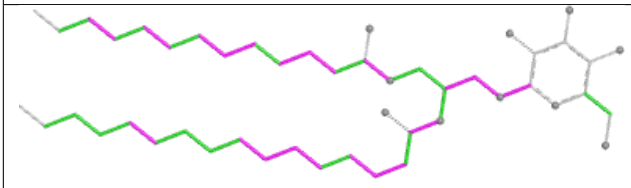
Ligand LMG D 408



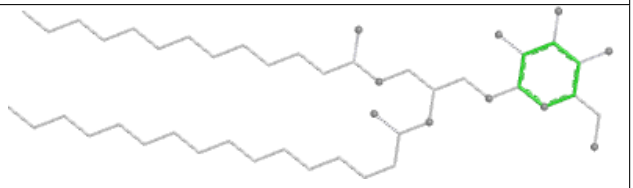
Bond lengths



Bond angles

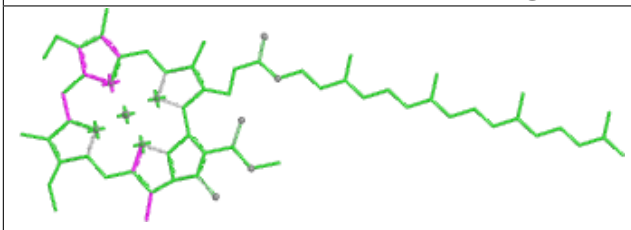


Torsions

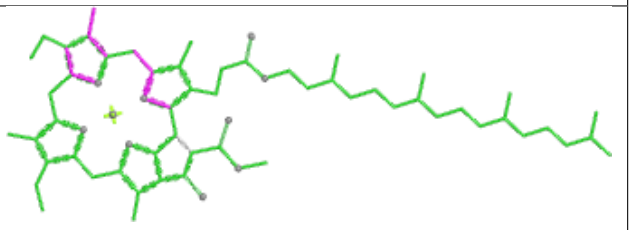


Rings

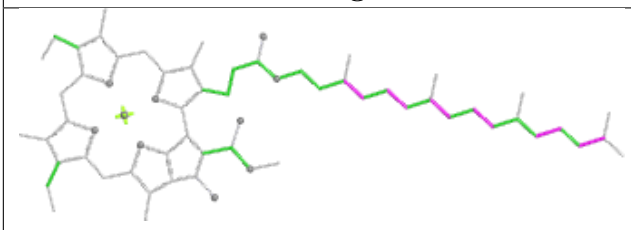
Ligand CLA A 407



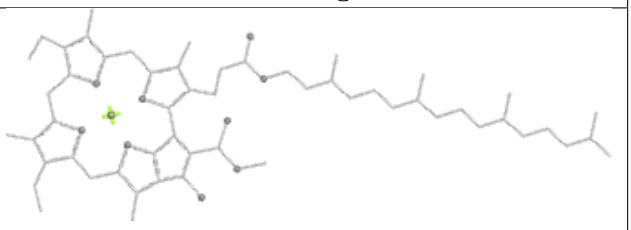
Bond lengths



Bond angles

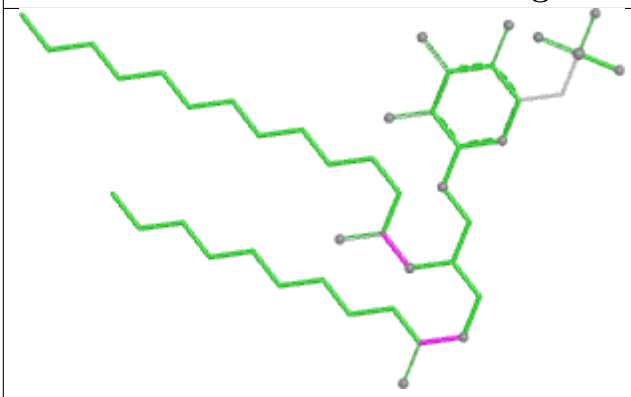


Torsions

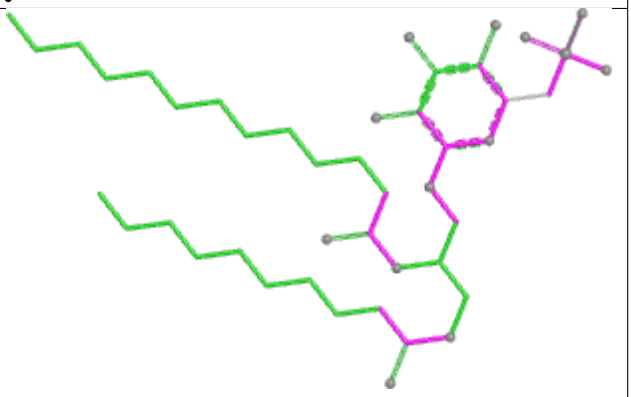


Rings

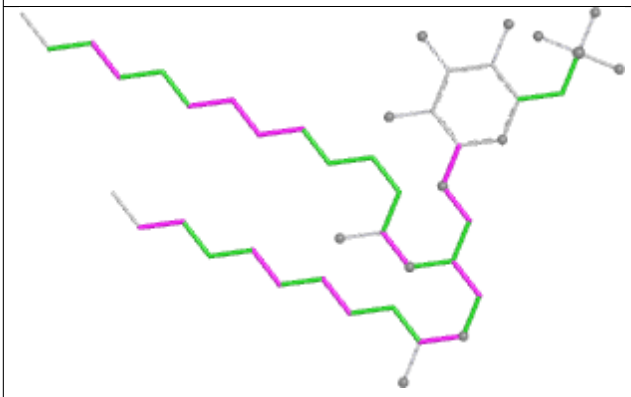
Ligand SQD f 103



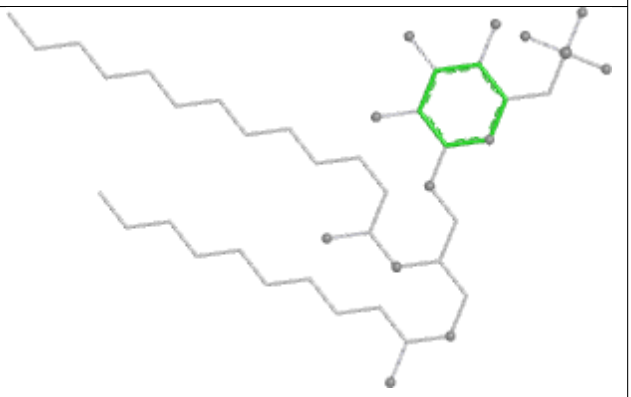
Bond lengths



Bond angles

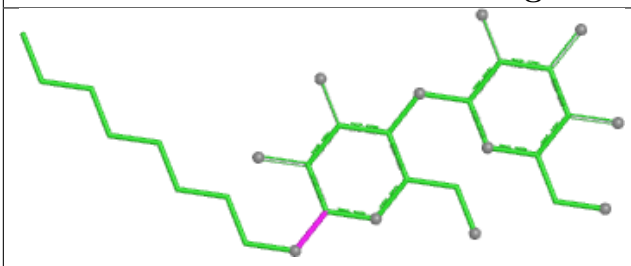


Torsions

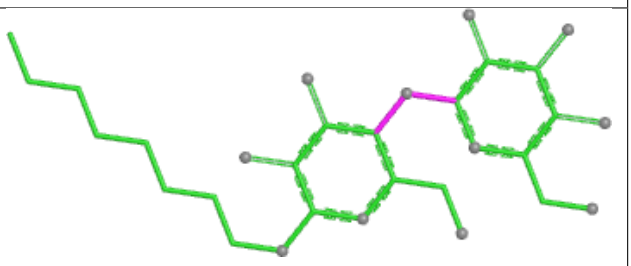


Rings

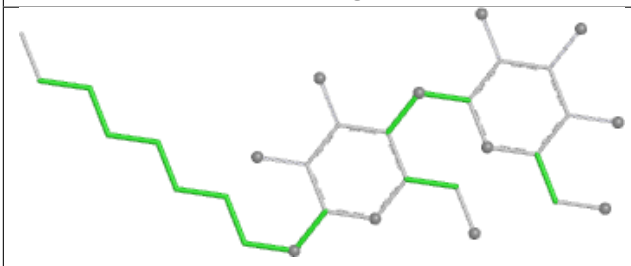
Ligand LMT x 102



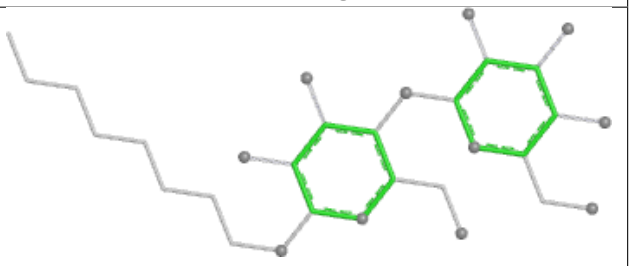
Bond lengths



Bond angles

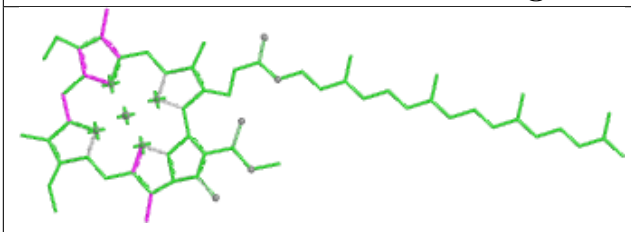


Torsions

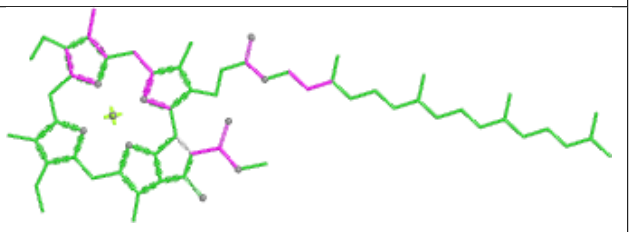


Rings

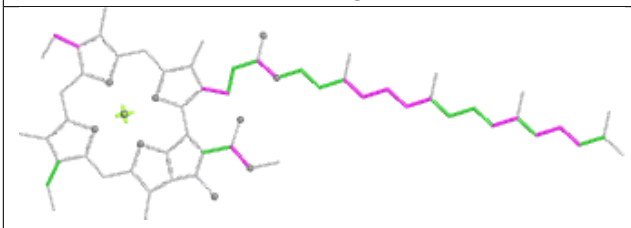
Ligand CLA b 611



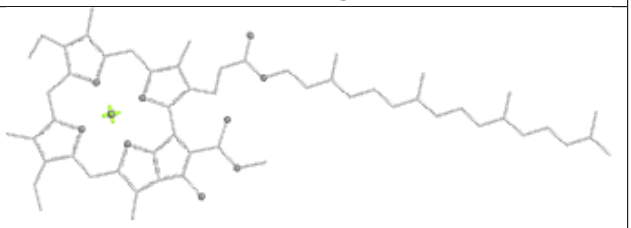
Bond lengths



Bond angles

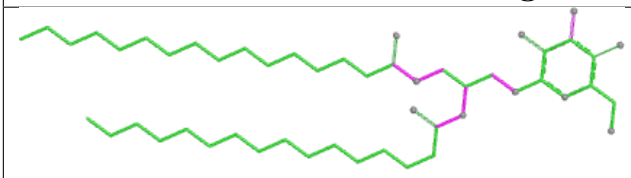


Torsions

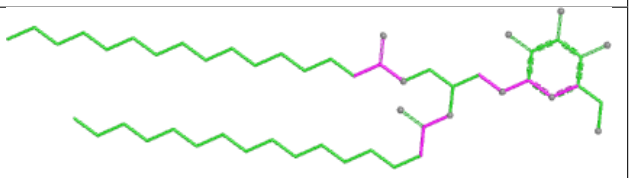


Rings

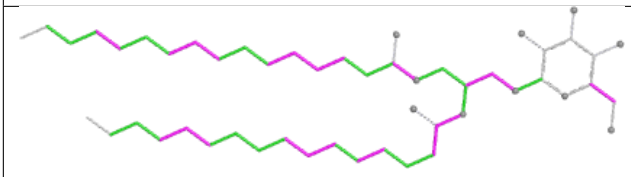
Ligand LMG A 414



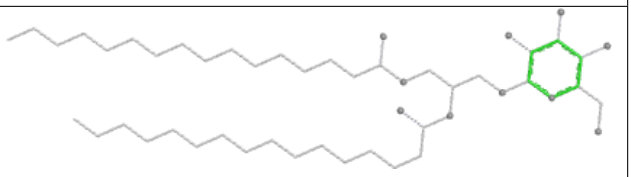
Bond lengths



Bond angles

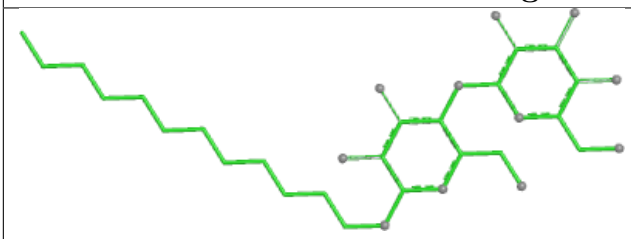


Torsions

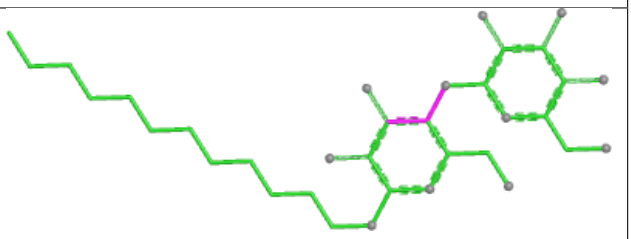


Rings

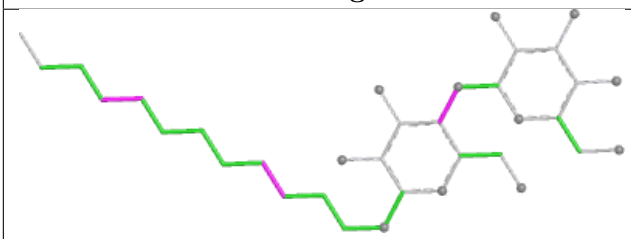
Ligand LMT B 627



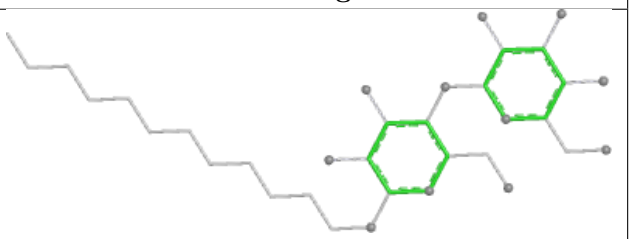
Bond lengths



Bond angles

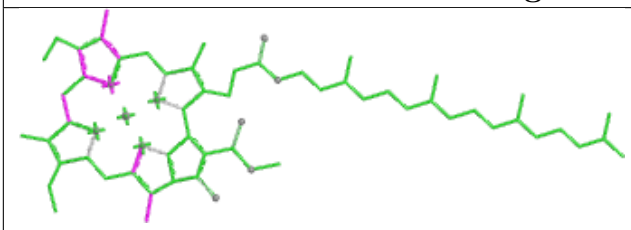


Torsions

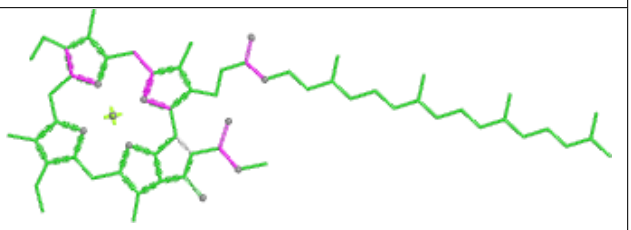


Rings

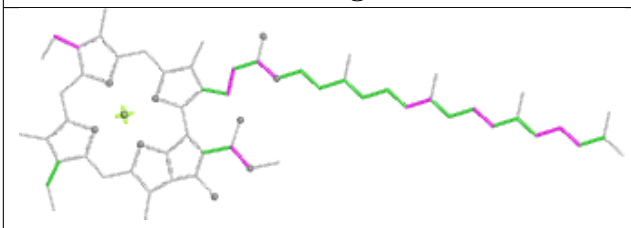
Ligand CLA C 504



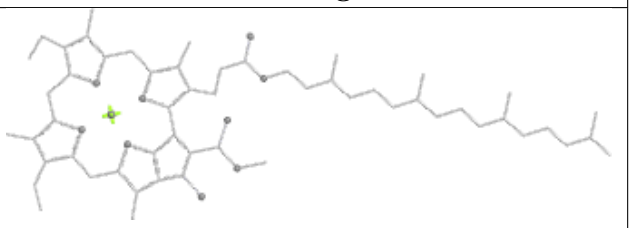
Bond lengths



Bond angles

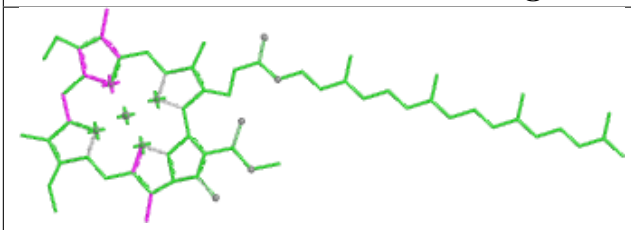


Torsions

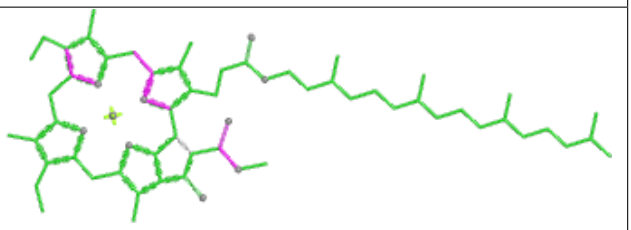


Rings

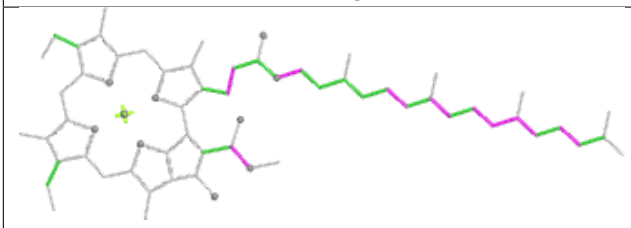
Ligand CLA C 508



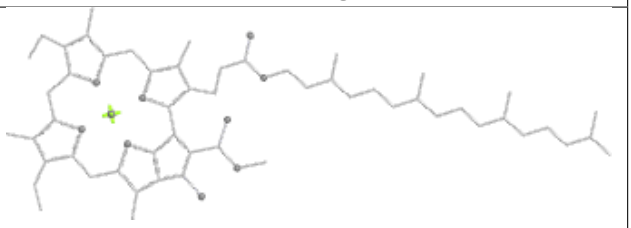
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	335/360 (93%)	0.35	16 (4%)	35	36	44, 65, 104, 152	0
1	a	335/360 (93%)	0.26	10 (2%)	52	45	46, 65, 104, 153	0
2	B	490/510 (96%)	0.38	33 (6%)	24	28	46, 70, 103, 156	0
2	b	490/510 (96%)	0.40	26 (5%)	32	33	43, 70, 103, 160	0
3	C	447/461 (96%)	0.31	12 (2%)	56	47	52, 79, 105, 133	0
3	c	447/461 (96%)	0.25	13 (2%)	53	46	56, 81, 106, 135	0
4	D	340/352 (96%)	0.35	13 (3%)	44	41	44, 66, 102, 139	0
4	d	340/352 (96%)	0.22	11 (3%)	50	44	43, 66, 102, 135	0
5	E	82/84 (97%)	0.36	1 (1%)	76	64	68, 92, 123, 132	0
5	e	82/84 (97%)	0.16	1 (1%)	76	64	70, 92, 123, 127	0
6	F	35/45 (77%)	0.61	4 (11%)	10	17	67, 84, 119, 143	0
6	f	35/45 (77%)	0.21	0	100	100	72, 83, 121, 141	0
7	H	65/66 (98%)	0.72	6 (9%)	14	21	74, 93, 119, 145	0
7	h	65/66 (98%)	0.46	2 (3%)	51	44	73, 94, 119, 148	0
8	I	35/38 (92%)	0.25	0	100	100	65, 80, 106, 120	0
8	i	35/38 (92%)	0.33	2 (5%)	29	32	68, 80, 105, 120	0
9	J	34/40 (85%)	0.40	2 (5%)	28	31	72, 85, 95, 112	0
9	j	34/40 (85%)	0.51	1 (2%)	53	46	77, 87, 96, 115	0
10	K	37/46 (80%)	0.18	0	100	100	76, 88, 99, 125	0
10	k	37/46 (80%)	0.20	0	100	100	73, 89, 104, 126	0
11	L	37/37 (100%)	0.40	1 (2%)	56	47	50, 63, 126, 156	0
11	l	37/37 (100%)	0.46	2 (5%)	31	33	51, 63, 127, 155	0
12	M	34/36 (94%)	0.52	2 (5%)	28	31	53, 69, 107, 165	0
12	m	34/36 (94%)	0.56	3 (8%)	15	21	55, 69, 109, 163	0

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%)	0.26	6 (2%) 58 49	49, 79, 122, 167	0
13	o	243/272 (89%)	0.42	13 (5%) 32 33	49, 79, 121, 167	0
14	T	32/32 (100%)	0.30	0 100 100	57, 69, 159, 169	0
14	t	32/32 (100%)	0.78	3 (9%) 14 20	56, 67, 158, 170	0
15	U	97/134 (72%)	0.43	4 (4%) 41 39	56, 70, 90, 112	0
15	u	97/134 (72%)	0.32	2 (2%) 63 54	56, 70, 89, 111	0
16	V	137/163 (84%)	0.34	9 (6%) 24 28	55, 71, 85, 100	0
16	v	137/163 (84%)	0.25	5 (3%) 46 42	58, 71, 86, 96	0
17	g	28/46 (60%)	0.85	2 (7%) 22 27	96, 108, 125, 129	0
17	y	28/46 (60%)	0.24	0 100 100	92, 108, 128, 129	0
18	X	37/41 (90%)	0.25	1 (2%) 56 47	77, 92, 120, 140	0
18	x	37/41 (90%)	0.43	1 (2%) 56 47	75, 90, 124, 145	0
19	Z	62/62 (100%)	0.51	7 (11%) 10 17	87, 103, 170, 186	0
19	z	62/62 (100%)	0.38	3 (4%) 35 36	88, 104, 169, 184	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.34	217 (4%) 40 39	43, 75, 115, 186	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	393	GLU	7.5
13	O	195	ASP	5.5
1	a	280	VAL	5.4
2	B	214	LEU	5.1
4	D	188	PHE	5.0
2	B	368	VAL	4.9
2	b	385	ARG	4.8
2	B	365	SER	4.7
1	A	251	ALA	4.7
7	H	30	LEU	4.6
4	D	276	VAL	4.4
19	z	17	PHE	4.2
7	H	2	ALA	4.2
2	B	420	TYR	4.2
2	b	443	PHE	4.1
1	A	263	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	211	ILE	4.0
1	A	184	ILE	3.9
2	b	63	LEU	3.9
1	A	222	SER	3.9
16	V	47	LEU	3.9
2	B	417	VAL	3.8
2	B	474	LEU	3.8
7	H	6	TRP	3.8
2	b	386	ALA	3.8
1	A	218	LEU	3.8
2	B	367	PRO	3.8
7	H	10	ILE	3.8
4	D	141	TYR	3.7
2	b	55	MET	3.7
2	B	309	LEU	3.6
2	b	229	LEU	3.6
15	u	58	ASN	3.6
19	Z	14	ILE	3.6
2	B	397	VAL	3.6
3	c	341	LEU	3.5
2	b	218	LEU	3.4
2	B	379	ALA	3.4
12	M	21	PHE	3.4
15	U	42	VAL	3.4
4	d	214	HIS	3.4
16	v	41	GLU	3.4
2	b	119	ASP	3.3
3	C	365	TRP	3.3
16	v	133	LEU	3.3
4	d	344	GLU	3.3
3	C	427	ALA	3.2
2	b	361	ALA	3.2
13	O	93	PRO	3.2
13	o	51	THR	3.2
11	L	18	TYR	3.2
4	D	144	ILE	3.1
4	D	145	ALA	3.1
1	a	224	ILE	3.1
4	d	334	GLN	3.0
1	A	297	LEU	3.0
1	a	50	ILE	3.0
4	D	318	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	t	1	MET	3.0
2	B	443	PHE	3.0
4	d	181	PHE	3.0
13	o	74	THR	2.9
2	b	415	PRO	2.9
19	z	20	VAL	2.9
3	c	401	LEU	2.9
4	d	345	VAL	2.9
7	H	27	THR	2.9
7	h	55	LEU	2.9
2	b	402	TYR	2.9
2	B	69	LEU	2.9
3	C	96	GLY	2.9
6	F	11	VAL	2.9
1	A	206	PHE	2.9
18	x	11	THR	2.8
2	B	475	PHE	2.8
19	Z	17	PHE	2.8
2	b	70	GLY	2.7
1	A	242	GLU	2.7
15	U	39	LEU	2.7
2	b	303	SER	2.7
2	B	478	VAL	2.7
3	c	368	PRO	2.7
2	B	488	PRO	2.7
2	b	207	ILE	2.7
1	a	292	THR	2.7
13	O	30	THR	2.7
4	D	13	GLY	2.7
1	A	202	VAL	2.7
4	d	216	ALA	2.6
13	o	220	LYS	2.6
3	c	315	MET	2.6
16	V	151	ILE	2.6
8	i	11	VAL	2.6
12	m	17	VAL	2.6
4	d	299	ILE	2.6
16	V	48	THR	2.6
13	o	190	LEU	2.6
3	C	332	GLN	2.6
14	t	9	ILE	2.6
17	g	20	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	o	200	LEU	2.6
7	h	13	PRO	2.6
4	D	130	PHE	2.6
12	m	34	LYS	2.6
3	c	329	GLY	2.6
14	t	16	LEU	2.6
1	A	204	GLY	2.5
5	E	6	GLY	2.5
4	d	137	GLY	2.5
9	J	35	GLY	2.5
19	Z	62	VAL	2.5
2	B	386	ALA	2.5
3	C	140	LEU	2.5
4	D	140	PRO	2.5
7	H	55	LEU	2.5
15	U	121	LEU	2.5
18	X	17	LYS	2.5
19	Z	56	VAL	2.5
3	C	268	GLY	2.5
2	B	84	THR	2.5
3	C	134	ILE	2.5
2	B	472	ARG	2.5
3	C	341	LEU	2.4
13	o	216	PHE	2.4
2	B	207	ILE	2.4
2	b	391	SER	2.4
3	C	267	SER	2.4
3	c	388	GLN	2.4
4	d	35	ILE	2.4
2	B	106	LEU	2.4
13	o	152	VAL	2.4
1	A	88	ALA	2.4
1	A	344	ALA	2.4
1	a	277	ALA	2.4
11	l	29	LEU	2.4
1	A	328	MET	2.4
13	o	251	MET	2.4
13	O	186	LYS	2.4
3	C	270	ALA	2.4
2	B	211	ILE	2.4
1	A	61	ASP	2.4
16	V	77	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	c	172	ALA	2.3
6	F	45	ARG	2.3
2	B	370	LEU	2.3
2	B	363	PHE	2.3
1	a	276	ALA	2.3
2	B	477	ASP	2.3
2	B	132	ALA	2.3
13	O	32	THR	2.3
19	Z	4	LEU	2.3
4	D	257	PHE	2.3
6	F	38	ALA	2.3
2	B	218	LEU	2.3
2	B	429	ILE	2.3
2	B	4	PRO	2.3
3	c	372	PRO	2.3
1	A	250	ALA	2.3
2	b	276	ASP	2.3
8	i	35	LYS	2.3
11	l	25	LEU	2.3
13	o	80	GLU	2.3
2	b	228	ALA	2.3
6	F	41	GLN	2.3
16	v	40	SER	2.2
12	M	10	ALA	2.2
16	V	52	TYR	2.2
3	C	69	LEU	2.2
16	V	154	ASP	2.2
19	z	21	ILE	2.2
2	b	195	PRO	2.2
3	c	281	MET	2.2
17	g	30	ILE	2.2
3	c	366	LEU	2.2
1	a	10	SER	2.2
15	U	40	VAL	2.2
3	c	27	ASP	2.2
9	j	35	GLY	2.2
4	D	233	ARG	2.2
13	o	203	ALA	2.1
2	B	464	PHE	2.1
1	a	114	LEU	2.1
9	J	27	LEU	2.1
19	Z	44	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	u	120	ALA	2.1
2	b	13	ILE	2.1
3	c	451	ALA	2.1
2	B	255	THR	2.1
12	m	2	GLU	2.1
3	c	328	VAL	2.1
1	A	68	SER	2.1
1	a	13	LEU	2.1
13	O	202	GLN	2.1
5	e	61	ARG	2.1
19	Z	8	ALA	2.1
2	B	364	GLU	2.1
4	d	165	SER	2.1
1	a	247	ASN	2.1
2	B	144	PHE	2.1
2	b	2	GLY	2.1
2	b	217	ILE	2.1
16	v	39	ASN	2.1
2	B	3	LEU	2.0
2	b	43	ALA	2.0
13	o	158	ASN	2.0
16	V	28	GLU	2.0
4	D	204	VAL	2.0
16	V	65	SER	2.0
3	C	160	ILE	2.0
2	b	282	GLN	2.0
16	v	128	PRO	2.0
2	b	368	VAL	2.0
13	o	217	SER	2.0
13	o	213	VAL	2.0
16	V	147	VAL	2.0
4	D	190	ASN	2.0
4	d	60	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
33	LMT	x	102	31/35	0.53	0.21	79,130,156,157	0
33	LMT	i	102	35/35	0.55	0.21	99,136,146,150	0
23	CLA	b	604	65/65	0.59	0.22	93,108,130,134	0
33	LMT	D	411	31/35	0.60	0.18	82,132,156,156	0
33	LMT	I	102	35/35	0.60	0.24	94,136,147,149	0
31	LMG	C	520	45/55	0.61	0.26	80,119,142,171	0
27	BCR	J	102	40/40	0.63	0.35	109,129,176,177	0
33	LMT	B	623	35/35	0.63	0.17	76,136,170,172	0
32	CL	A	416	1/1	0.64	0.15	49,49,49,49	0
33	LMT	B	628	35/35	0.66	0.23	72,137,162,163	0
23	CLA	B	601	65/65	0.68	0.20	94,108,129,134	0
33	LMT	b	626	35/35	0.69	0.20	99,143,152,153	0
23	CLA	C	507	65/65	0.69	0.23	77,92,101,105	0
27	BCR	j	102	40/40	0.69	0.37	107,125,176,178	0
28	DGD	B	626	52/66	0.72	0.23	77,104,179,183	0
25	PL9	J	101	35/55	0.74	0.45	119,157,183,185	0
31	LMG	c	520	45/55	0.75	0.17	82,119,140,168	0
30	SQD	B	625	47/54	0.76	0.23	73,102,139,146	0
25	PL9	A	408	45/55	0.76	0.30	84,103,119,127	0
33	LMT	b	625	35/35	0.76	0.16	78,139,172,176	0
28	DGD	C	518	66/66	0.78	0.23	58,72,106,121	0
33	LMT	b	603	35/35	0.78	0.20	76,131,155,156	0
27	BCR	k	102	40/40	0.79	0.22	69,85,106,109	0
29	LHG	a	417	37/49	0.79	0.19	111,134,197,206	0
27	BCR	H	101	40/40	0.79	0.24	82,95,131,132	0
31	LMG	b	624	49/55	0.80	0.29	56,76,88,91	0
28	DGD	b	602	52/66	0.80	0.21	81,104,177,178	0
23	CLA	c	513	65/65	0.80	0.17	94,107,138,149	0
29	LHG	A	415	37/49	0.81	0.17	108,137,192,202	0
30	SQD	d	407	43/54	0.81	0.20	73,107,144,149	0
28	DGD	d	408	63/66	0.81	0.26	104,127,184,187	0
33	LMT	B	624	35/35	0.82	0.20	91,142,154,155	0
33	LMT	B	627	35/35	0.82	0.23	71,122,138,140	0
31	LMG	k	103	48/55	0.82	0.29	80,100,118,120	0
28	DGD	D	410	63/66	0.82	0.26	104,127,181,188	0
28	DGD	c	518	62/66	0.82	0.22	65,86,138,143	0
23	CLA	a	409	65/65	0.83	0.23	55,69,129,134	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	SQD	a	415	51/54	0.83	0.22	81,102,128,134	0
30	SQD	b	601	47/54	0.83	0.22	86,99,139,146	0
27	BCR	c	514	40/40	0.83	0.21	66,80,89,91	0
27	BCR	D	405	40/40	0.83	0.24	65,80,101,108	0
31	LMG	M	101	42/55	0.83	0.23	78,110,135,144	0
23	CLA	b	619	65/65	0.83	0.20	78,99,142,147	0
30	SQD	F	102	45/54	0.84	0.25	86,129,153,154	0
29	LHG	A	412	39/49	0.84	0.23	61,80,92,94	0
24	PHO	A	406	64/64	0.84	0.20	57,69,74,76	0
33	LMT	T	101	35/35	0.84	0.25	63,115,136,143	0
25	PL9	j	101	35/55	0.84	0.33	120,159,178,180	0
31	LMG	A	418	42/55	0.84	0.24	76,107,120,142	0
31	LMG	B	622	49/55	0.84	0.24	50,74,85,91	0
28	DGD	A	411	56/66	0.84	0.20	79,100,145,149	0
31	LMG	E	101	44/55	0.84	0.22	85,123,134,138	0
31	LMG	a	402	42/55	0.85	0.23	76,105,121,142	0
31	LMG	a	416	51/55	0.85	0.27	61,80,92,99	0
28	DGD	C	517	62/66	0.85	0.17	61,84,132,147	0
23	CLA	b	618	65/65	0.85	0.16	78,97,109,116	0
23	CLA	C	503	65/65	0.85	0.19	76,88,99,101	0
27	BCR	x	101	40/40	0.85	0.21	81,97,129,130	0
23	CLA	c	509	65/65	0.85	0.17	73,82,91,98	0
30	SQD	a	401	54/54	0.85	0.23	75,116,152,156	0
23	CLA	b	609	65/65	0.85	0.17	71,86,111,121	0
22	BCT	d	401	4/4	0.86	0.13	77,80,82,85	0
23	CLA	b	613	65/65	0.86	0.16	71,81,88,91	0
23	CLA	C	512	65/65	0.86	0.19	83,101,147,151	0
23	CLA	A	407	65/65	0.86	0.21	57,69,128,131	0
27	BCR	c	515	40/40	0.86	0.21	83,95,112,115	0
23	CLA	C	506	65/65	0.86	0.21	75,91,123,134	0
27	BCR	B	618	40/40	0.86	0.25	68,80,90,92	0
33	LMT	m	101	35/35	0.86	0.25	71,95,109,109	0
27	BCR	B	620	40/40	0.86	0.22	77,87,92,92	0
35	CA	o	301	1/1	0.86	0.11	106,106,106,106	0
27	BCR	Z	101	40/40	0.87	0.23	81,93,117,118	0
29	LHG	a	414	39/49	0.87	0.20	62,79,91,94	0
23	CLA	C	511	65/65	0.87	0.18	73,90,100,109	0
23	CLA	c	511	65/65	0.87	0.15	72,91,102,106	0
30	SQD	D	409	43/54	0.87	0.24	72,103,147,151	0
31	LMG	i	101	43/55	0.87	0.21	85,120,158,176	0
31	LMG	C	519	48/55	0.87	0.23	86,99,110,116	0
23	CLA	C	513	65/65	0.87	0.15	93,108,142,149	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	LMG	D	407	49/55	0.87	0.26	59,80,109,117	0
27	BCR	T	103	40/40	0.87	0.23	69,79,87,95	0
35	CA	K	101	1/1	0.87	0.30	72,72,72,72	0
31	LMG	I	101	43/55	0.87	0.20	87,115,159,171	0
27	BCR	a	412	40/40	0.88	0.21	51,71,82,84	0
27	BCR	C	514	40/40	0.88	0.19	70,80,86,90	0
28	DGD	a	413	56/66	0.88	0.18	74,101,145,149	0
31	LMG	M	102	42/55	0.88	0.23	70,109,133,139	0
33	LMT	M	103	35/35	0.88	0.22	68,98,108,115	0
27	BCR	C	515	40/40	0.88	0.20	76,87,95,98	0
23	CLA	c	507	65/65	0.88	0.17	84,94,102,109	0
25	PL9	d	404	55/55	0.88	0.26	48,65,76,86	0
23	CLA	C	504	65/65	0.88	0.20	67,83,133,136	0
27	BCR	K	102	40/40	0.88	0.18	74,85,102,103	0
24	PHO	D	402	64/64	0.88	0.16	48,61,71,77	0
23	CLA	C	501	65/65	0.88	0.18	66,80,90,95	0
30	SQD	A	413	51/54	0.88	0.18	81,95,126,130	0
30	SQD	A	417	54/54	0.88	0.22	81,116,146,153	0
28	DGD	c	519	66/66	0.89	0.18	61,72,104,113	0
27	BCR	T	102	40/40	0.89	0.26	66,73,83,85	0
23	CLA	B	614	65/65	0.89	0.21	64,83,124,132	0
23	CLA	b	611	65/65	0.89	0.17	63,76,96,100	0
23	CLA	c	506	65/65	0.89	0.17	79,94,122,126	0
27	BCR	b	620	40/40	0.89	0.25	59,72,79,80	0
31	LMG	e	101	44/55	0.89	0.18	85,122,133,140	0
27	BCR	b	621	40/40	0.89	0.16	72,83,92,94	0
27	BCR	A	410	40/40	0.89	0.21	53,68,81,91	0
23	CLA	b	612	65/65	0.89	0.17	69,89,104,106	0
31	LMG	D	408	48/55	0.89	0.23	52,73,83,120	0
27	BCR	c	516	40/40	0.89	0.21	76,86,93,103	0
35	CA	k	101	1/1	0.89	0.13	94,94,94,94	0
23	CLA	b	605	65/65	0.89	0.17	73,87,96,98	0
31	LMG	b	623	49/55	0.90	0.23	57,80,96,113	0
27	BCR	f	102	40/40	0.90	0.18	64,83,107,110	0
23	CLA	B	606	65/65	0.90	0.17	68,84,111,123	0
28	DGD	b	622	58/66	0.90	0.19	57,71,97,102	0
23	CLA	a	405	65/65	0.90	0.18	40,54,65,72	0
23	CLA	C	509	65/65	0.90	0.15	65,81,95,98	0
25	PL9	a	410	45/55	0.90	0.21	82,98,119,127	0
23	CLA	B	616	65/65	0.90	0.21	75,93,144,150	0
23	CLA	c	512	65/65	0.90	0.14	90,102,148,154	0
23	CLA	B	610	65/65	0.90	0.16	68,82,87,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	SQD	f	103	45/54	0.90	0.17	88,129,148,155	0
23	CLA	b	607	65/65	0.90	0.17	62,67,112,117	0
23	CLA	b	610	65/65	0.91	0.18	52,64,82,88	0
23	CLA	B	608	65/65	0.91	0.17	62,74,94,97	0
32	CL	d	409	1/1	0.91	0.22	49,49,49,49	0
23	CLA	D	403	65/65	0.91	0.18	73,85,121,124	0
28	DGD	B	621	58/66	0.91	0.17	51,69,99,106	0
23	CLA	B	602	65/65	0.91	0.15	68,87,96,99	0
24	PHO	a	408	64/64	0.91	0.12	58,71,81,87	0
27	BCR	B	619	40/40	0.91	0.24	62,76,82,84	0
23	CLA	c	510	65/65	0.91	0.15	66,74,85,87	0
23	CLA	A	405	65/65	0.91	0.18	48,69,139,145	0
24	PHO	a	407	64/64	0.92	0.17	52,62,71,76	0
31	LMG	D	406	46/55	0.92	0.18	55,74,116,125	0
31	LMG	d	405	46/55	0.92	0.18	65,71,116,128	0
31	LMG	d	406	48/55	0.92	0.18	56,71,86,120	0
23	CLA	c	508	65/65	0.92	0.17	73,84,120,134	0
23	CLA	B	612	65/65	0.92	0.14	56,69,84,87	0
25	PL9	D	404	55/55	0.92	0.21	47,59,70,74	0
23	CLA	B	609	65/65	0.92	0.17	73,89,105,112	0
23	CLA	B	603	65/65	0.92	0.17	65,80,91,105	0
23	CLA	c	503	65/65	0.92	0.11	73,89,97,103	0
34	HEM	f	101	43/43	0.92	0.17	77,103,125,130	0
23	CLA	c	505	65/65	0.92	0.17	66,78,83,86	0
23	CLA	C	510	65/65	0.92	0.14	63,73,85,93	0
23	CLA	b	606	65/65	0.92	0.16	69,79,93,100	0
23	CLA	B	605	65/65	0.93	0.14	58,77,87,92	0
23	CLA	b	614	65/65	0.93	0.16	57,71,79,93	0
23	CLA	b	615	65/65	0.93	0.14	62,72,83,94	0
23	CLA	B	615	65/65	0.93	0.16	82,94,108,116	0
23	CLA	b	608	65/65	0.93	0.15	58,76,85,89	0
27	BCR	B	617	40/40	0.93	0.18	64,73,79,80	0
23	CLA	c	501	65/65	0.93	0.14	68,81,89,95	0
23	CLA	c	502	65/65	0.93	0.11	67,75,101,107	0
23	CLA	a	406	65/65	0.93	0.18	53,70,143,149	0
23	CLA	c	504	65/65	0.93	0.15	69,82,132,136	0
23	CLA	C	508	65/65	0.93	0.16	70,84,123,140	0
28	DGD	c	517	53/66	0.93	0.18	58,75,98,102	0
23	CLA	A	403	65/65	0.93	0.17	47,58,67,68	0
23	CLA	D	401	65/65	0.93	0.14	47,58,85,99	0
23	CLA	d	403	65/65	0.94	0.17	72,88,124,128	0
23	CLA	C	502	65/65	0.94	0.18	62,72,104,112	0

Continued on next page...

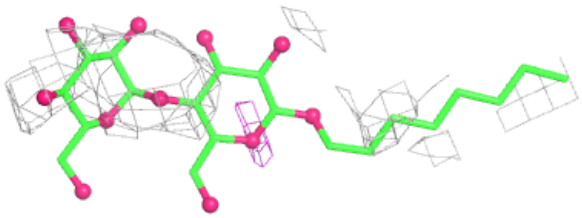
Continued from previous page...

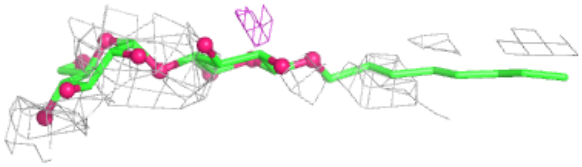
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	LMG	A	414	51/55	0.94	0.18	61,74,88,96	0
23	CLA	b	616	65/65	0.94	0.17	54,68,90,92	0
23	CLA	b	617	65/65	0.94	0.18	67,82,130,135	0
23	CLA	B	613	65/65	0.94	0.16	44,63,88,92	0
23	CLA	B	604	65/65	0.94	0.14	55,66,109,121	0
34	HEM	F	101	43/43	0.94	0.17	92,104,127,128	0
23	CLA	C	505	65/65	0.94	0.14	69,77,84,88	0
34	HEM	v	201	43/43	0.94	0.14	61,68,75,78	0
23	CLA	B	607	65/65	0.94	0.14	56,64,84,91	0
35	CA	O	301	1/1	0.94	0.07	123,123,123,123	0
23	CLA	B	611	65/65	0.94	0.13	65,73,80,81	0
22	BCT	A	402	4/4	0.94	0.10	84,88,89,93	0
23	CLA	A	404	65/65	0.95	0.15	39,54,66,70	0
23	CLA	a	404	65/65	0.95	0.12	44,58,65,73	0
28	DGD	C	516	53/66	0.95	0.17	58,75,97,102	0
23	CLA	d	402	65/65	0.95	0.13	49,59,79,91	0
34	HEM	V	201	43/43	0.96	0.18	46,65,74,79	0
26	OEC	a	411	5/9	0.98	0.18	35,44,62,62	0
21	FE2	A	401	1/1	0.99	0.03	60,60,60,60	0
21	FE2	a	403	1/1	0.99	0.06	70,70,70,70	0
26	OEC	A	409	5/9	0.99	0.15	35,44,46,62	0

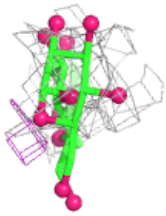
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT x 102:

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

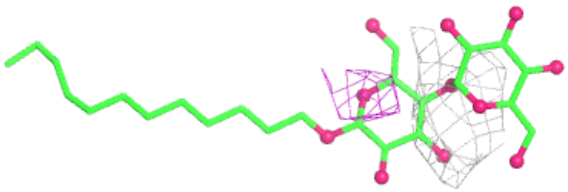


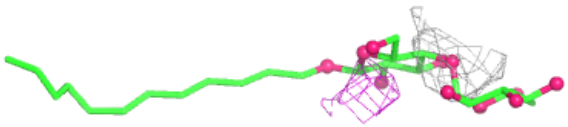


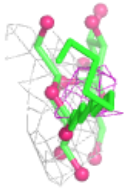


Electron density around LMT i 102:

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

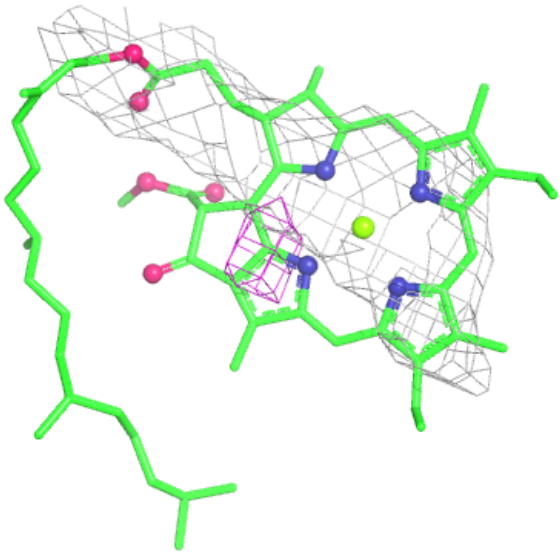


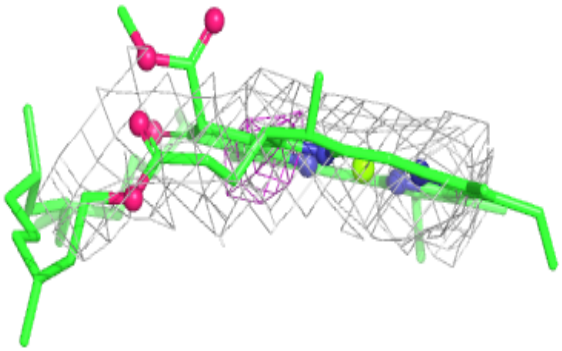


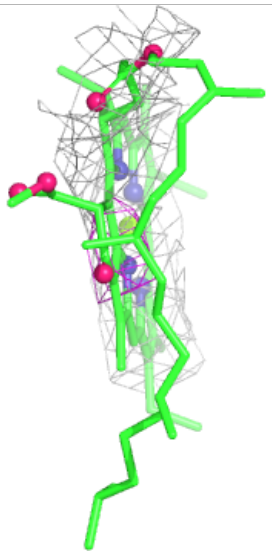


Electron density around CLA b 604:

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

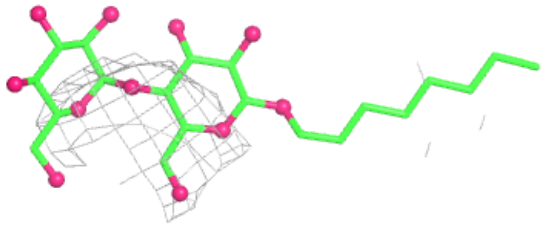


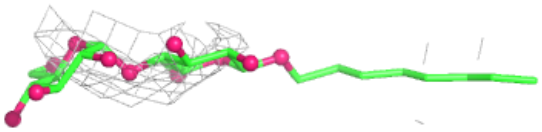


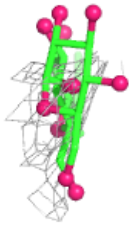


Electron density around LMT D 411:

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

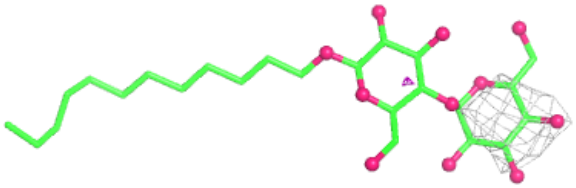


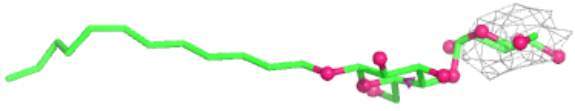




Electron density around LMT I 102:

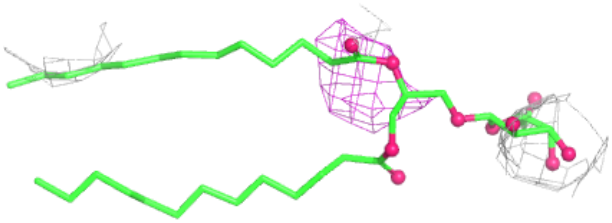
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

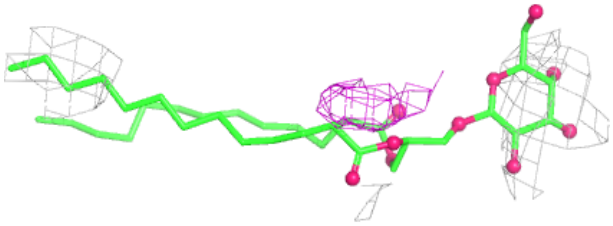


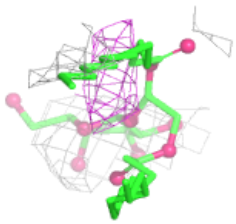


Electron density around LMG C 520:

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

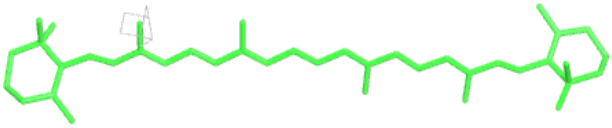


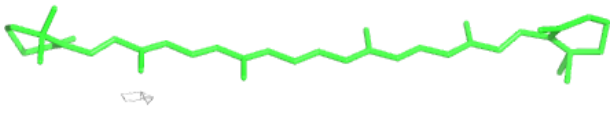




Electron density around BCR J 102:

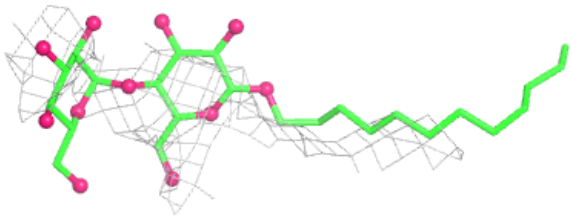
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

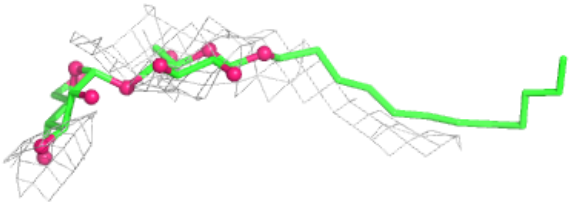


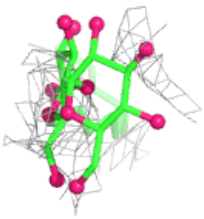


Electron density around LMT B 623:

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

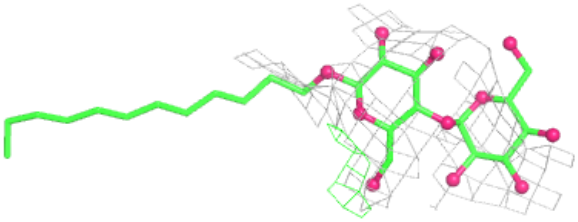


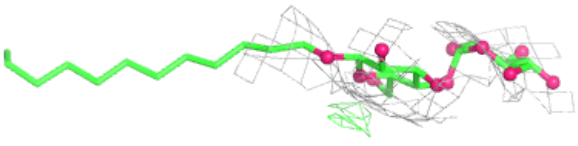




Electron density around LMT B 628:

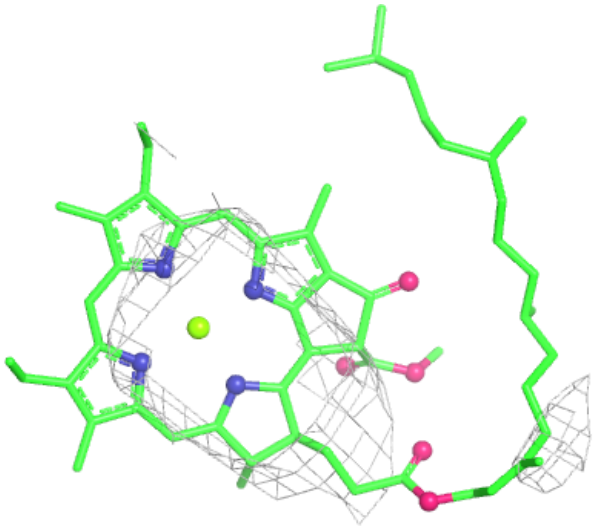
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

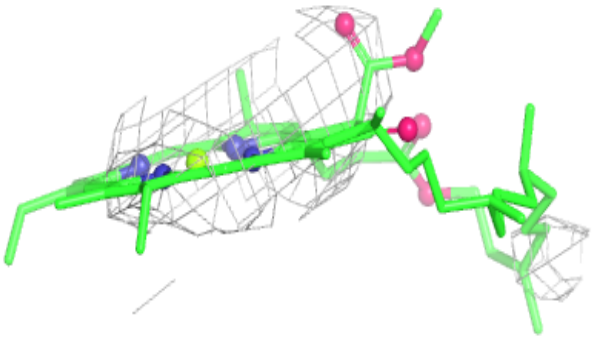


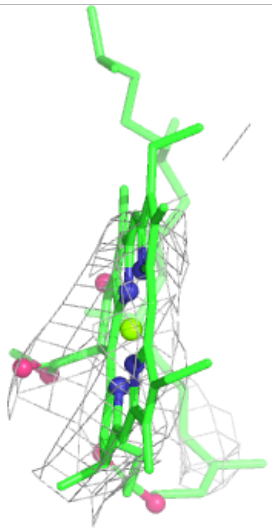


Electron density around CLA B 601:

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

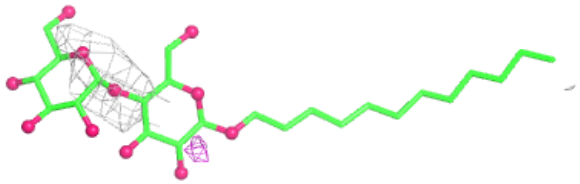


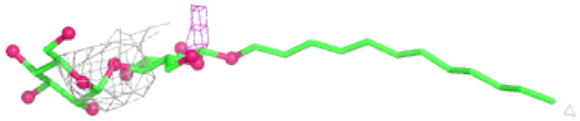




Electron density around LMT b 626:

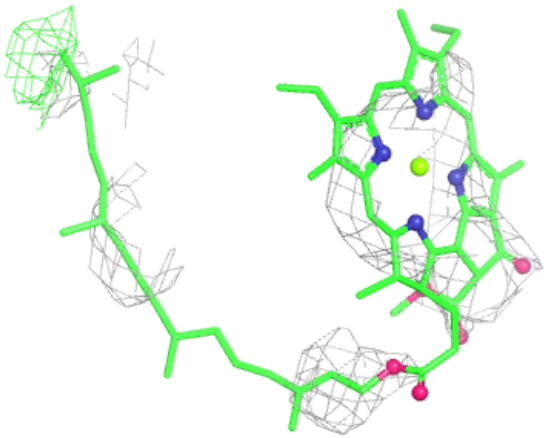
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

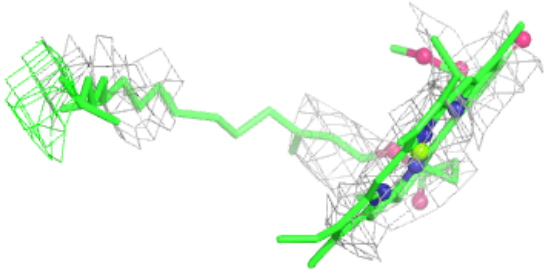




Electron density around CLA C 507:

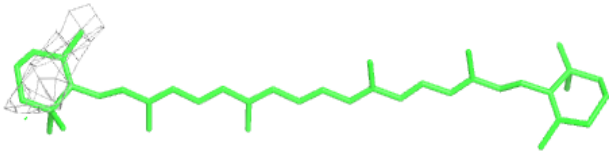
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

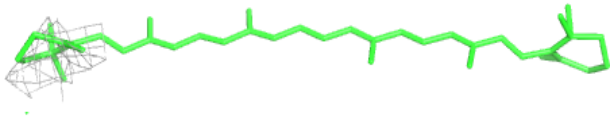


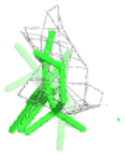


Electron density around BCR j 102:

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

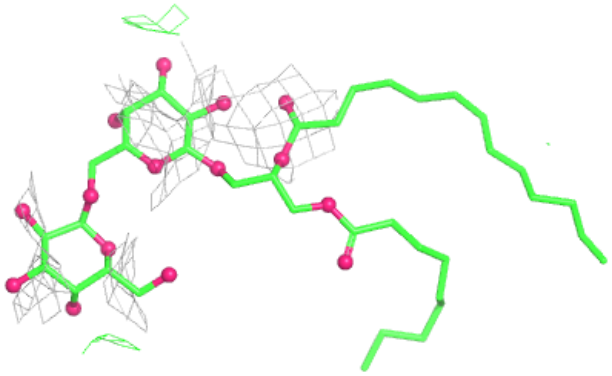


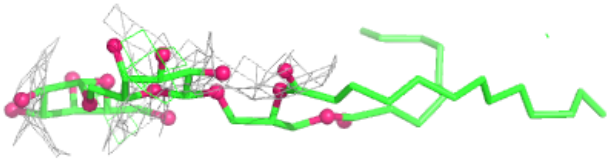




Electron density around DGD B 626:

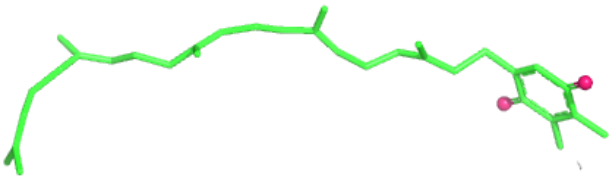
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

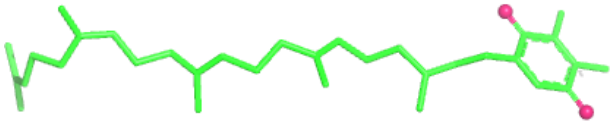


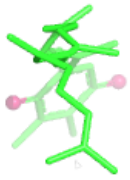


Electron density around PL9 J 101:

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

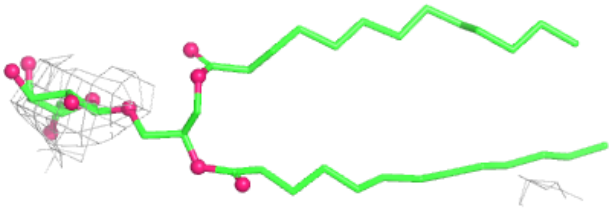


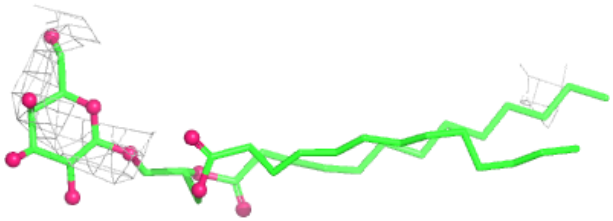


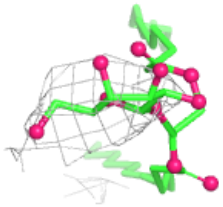


Electron density around LMG c 520:

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

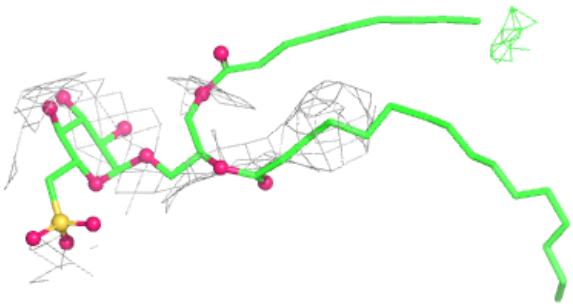


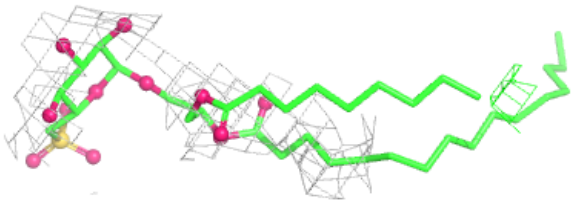


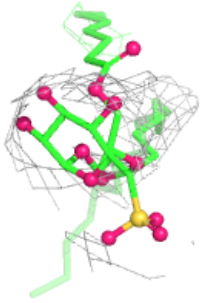


Electron density around SQD B 625:

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

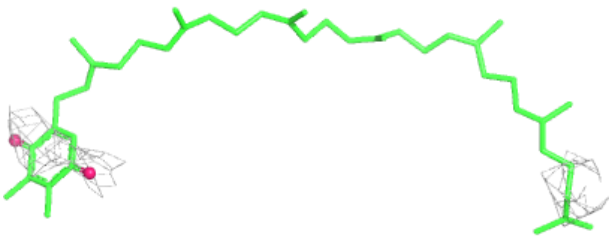


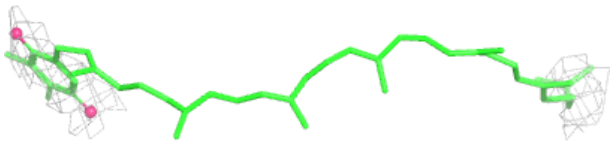




Electron density around PL9 A 408:

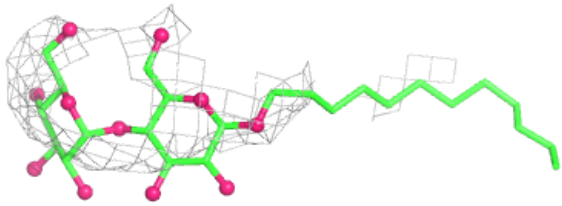
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

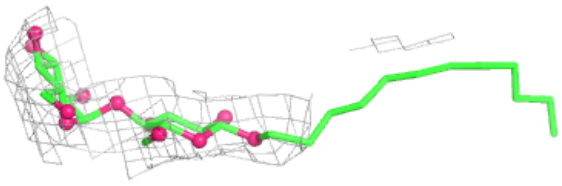


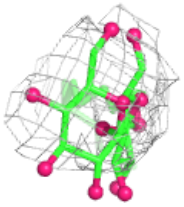


Electron density around LMT b 625:

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

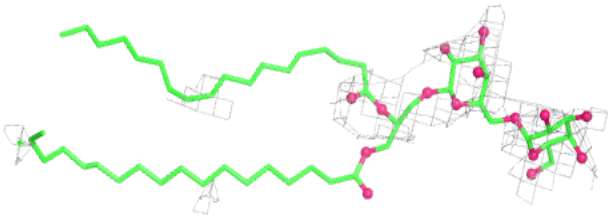


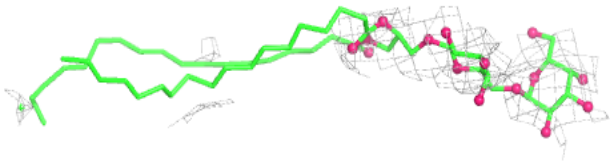


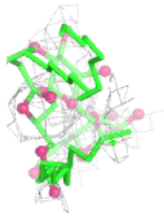


Electron density around DGD C 518:

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

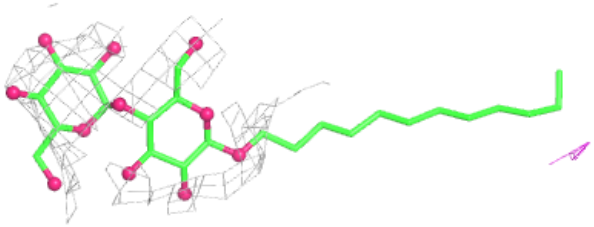


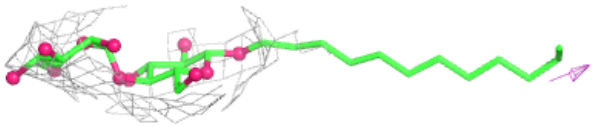


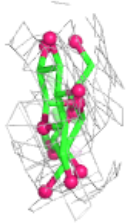


Electron density around LMT b 603:

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

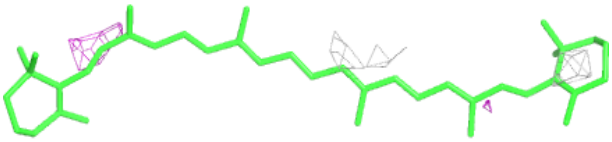


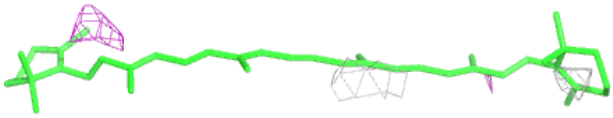


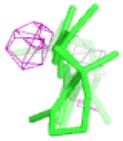


Electron density around BCR k 102:

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

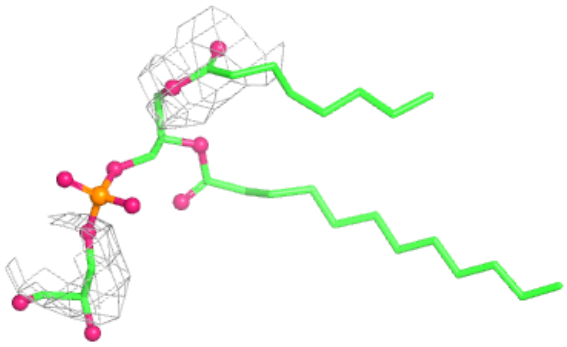


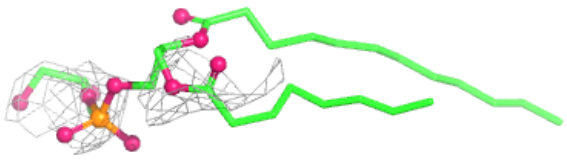


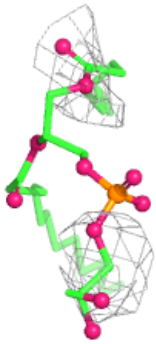


Electron density around LHG a 417:

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

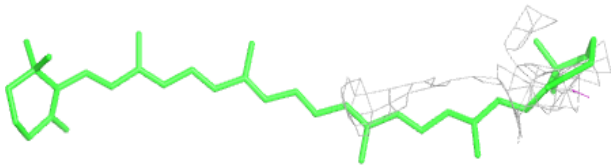


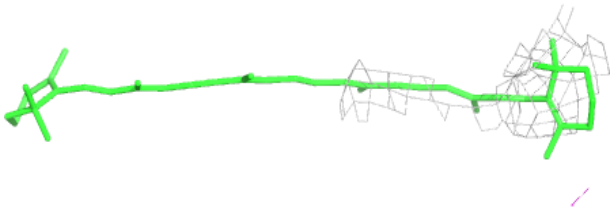


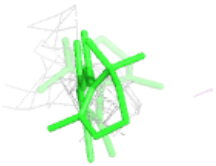


Electron density around BCR H 101:

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

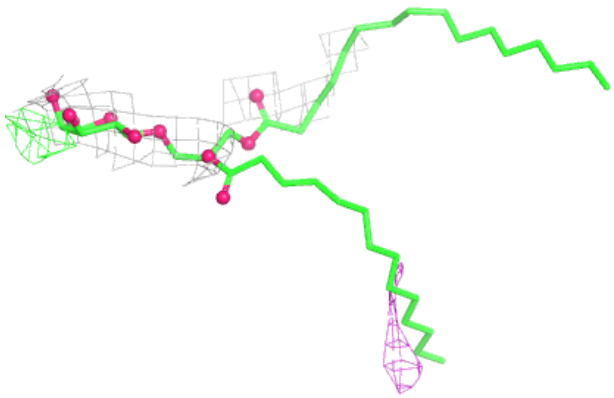


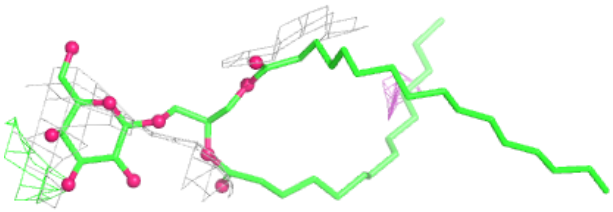




Electron density around LMG b 624:

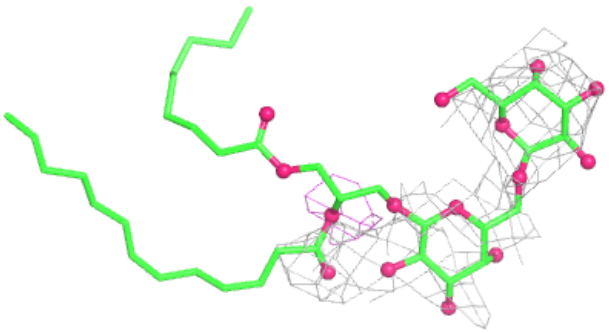
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

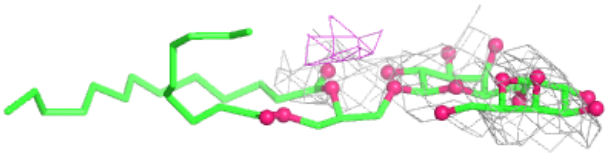




Electron density around DGD b 602:

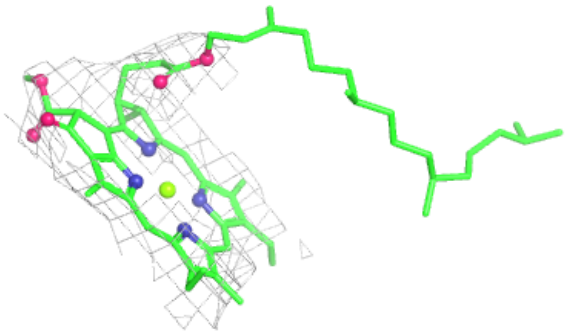
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

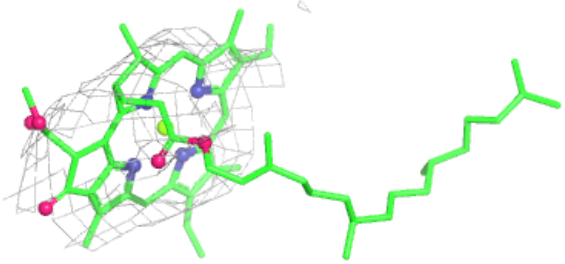


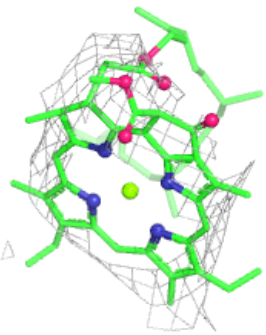


Electron density around CLA c 513:

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

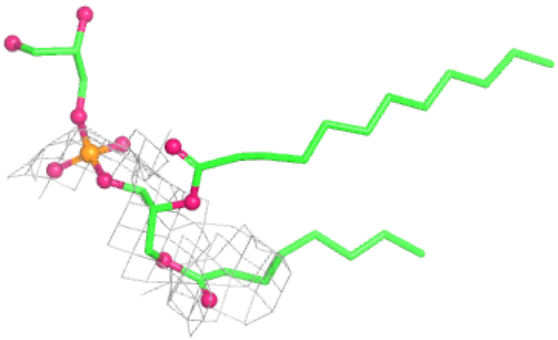


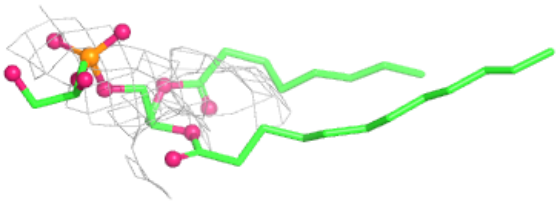


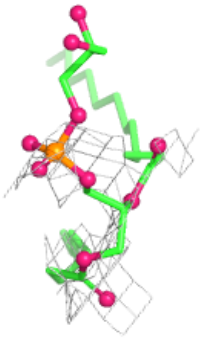


Electron density around LHG A 415:

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

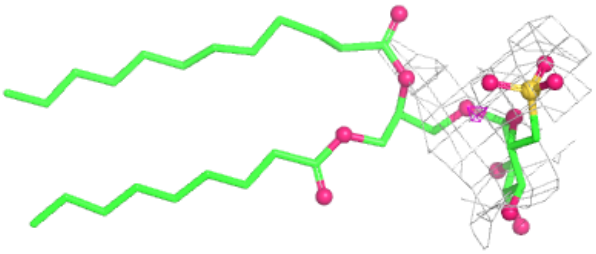


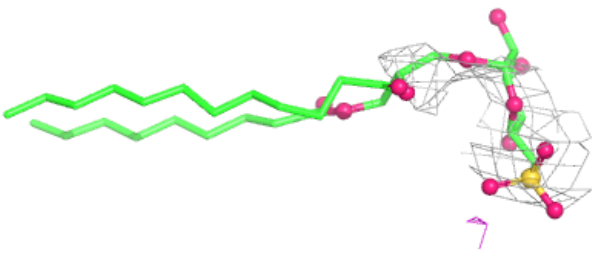


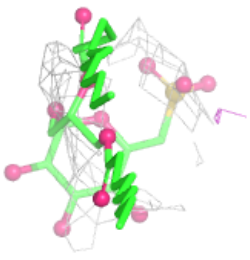


Electron density around SQD d 407:

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

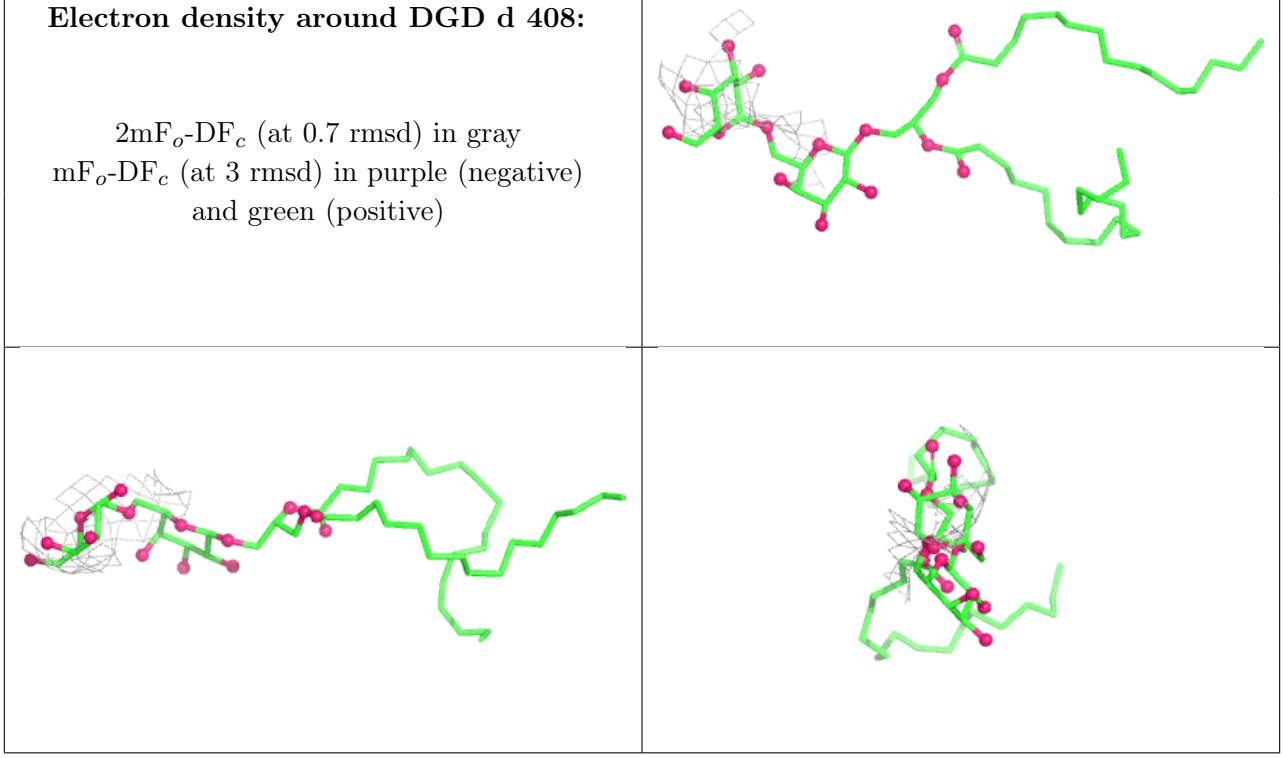






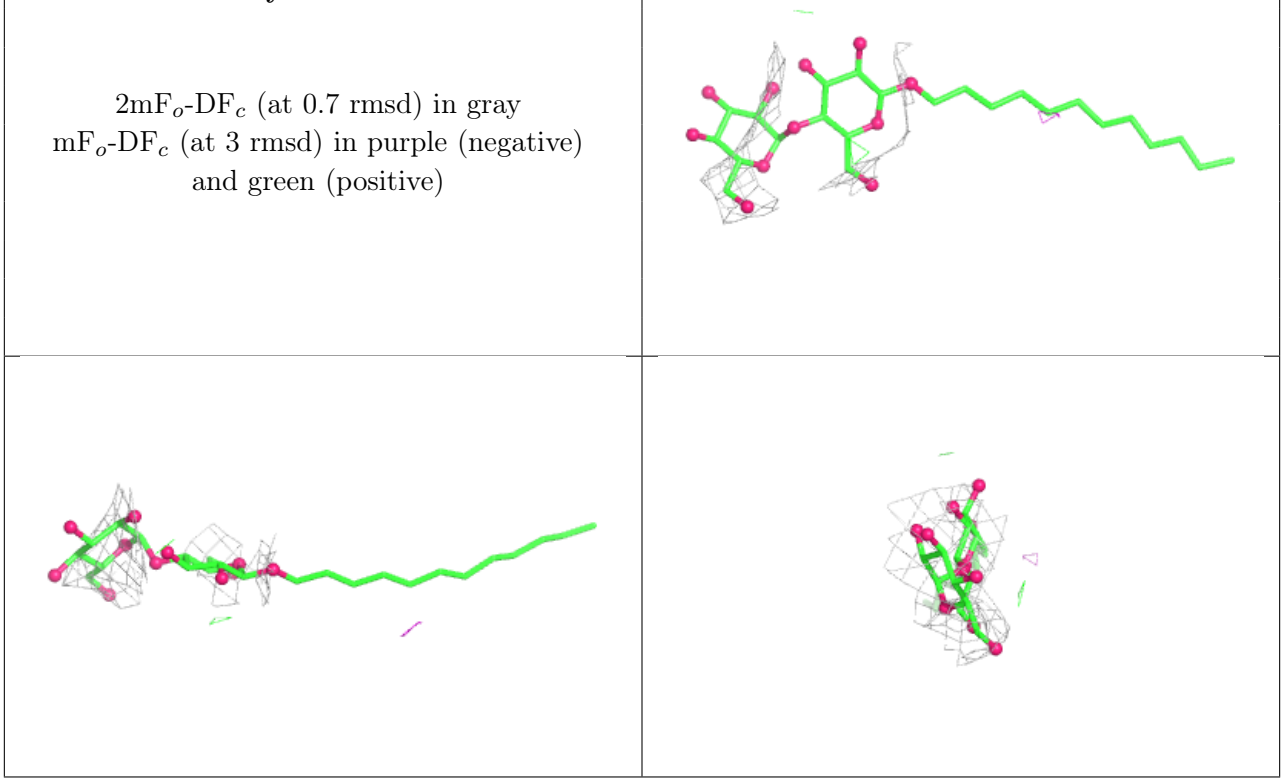
Electron density around DGD d 408:

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



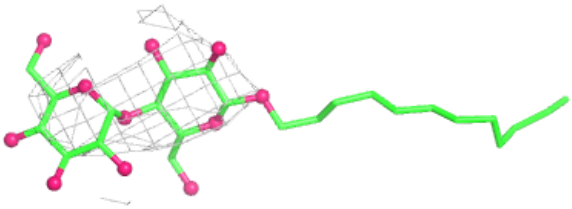
Electron density around LMT B 624:

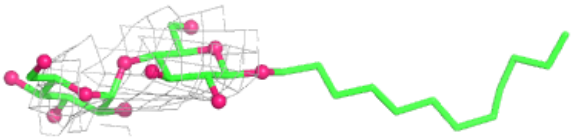
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

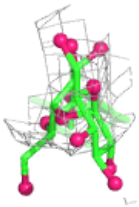


Electron density around LMT B 627:

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

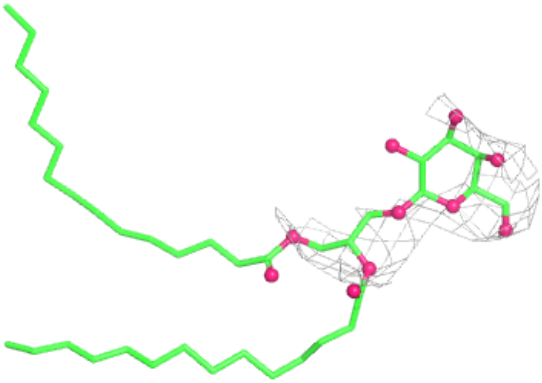


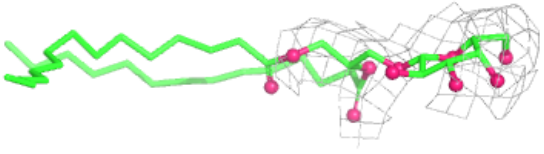




Electron density around LMG k 103:

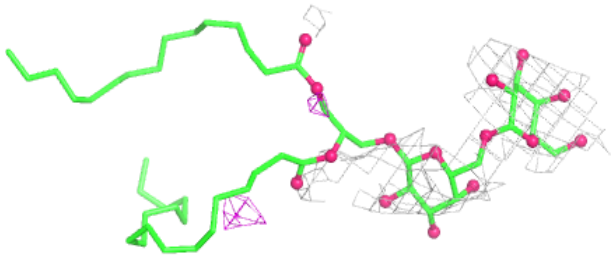
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

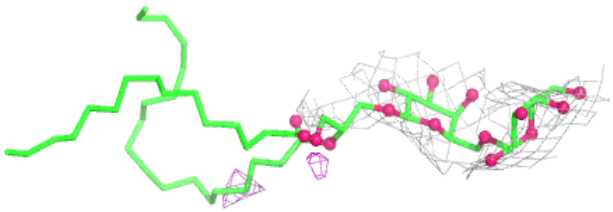




Electron density around DGD D 410:

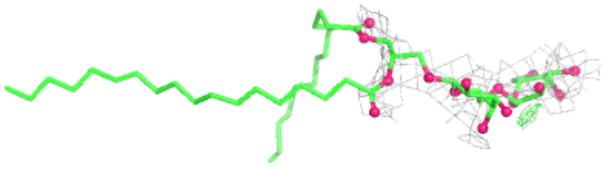
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





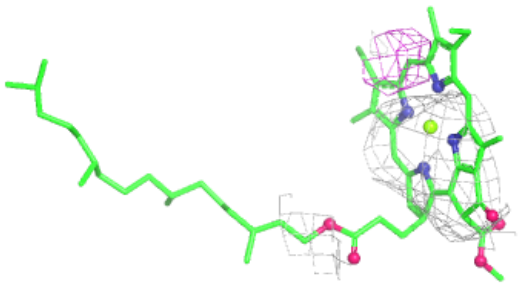
Electron density around DGD c 518:

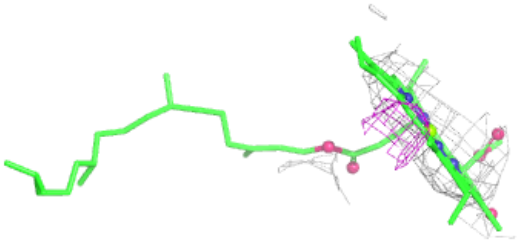
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

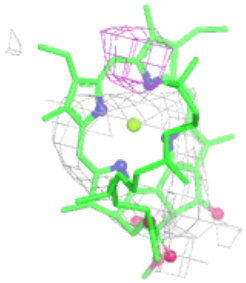


Electron density around CLA a 409:

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

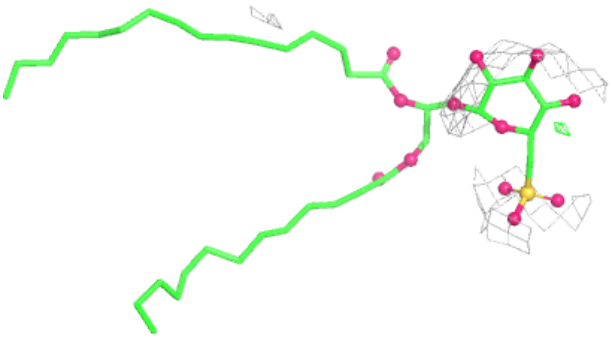


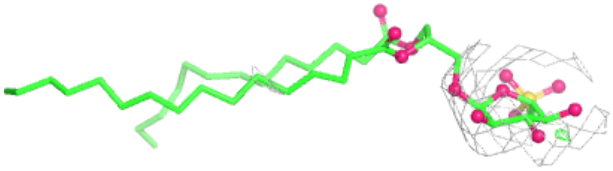


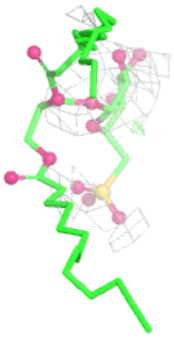


Electron density around SQD a 415:

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

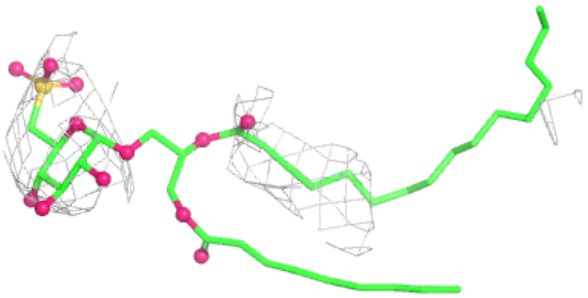


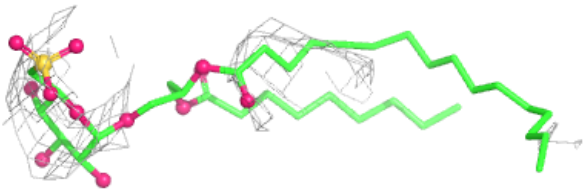


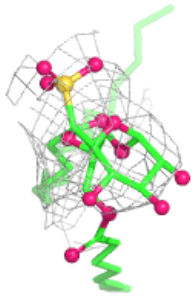


Electron density around SQD b 601:

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

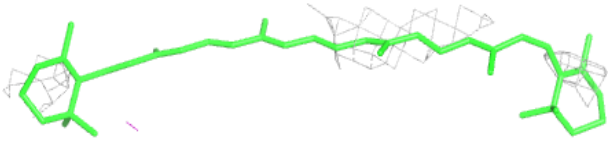


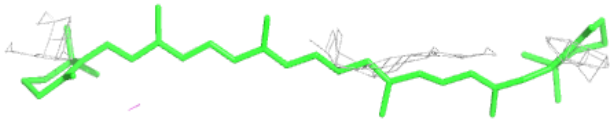




Electron density around BCR c 514:

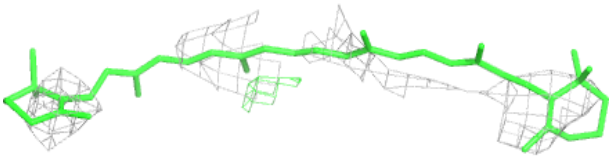
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

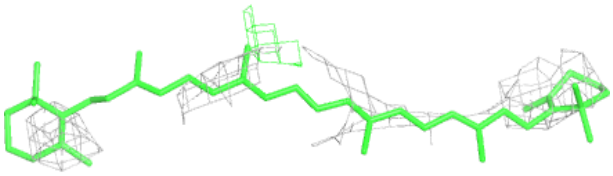


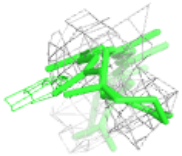


Electron density around BCR D 405:

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

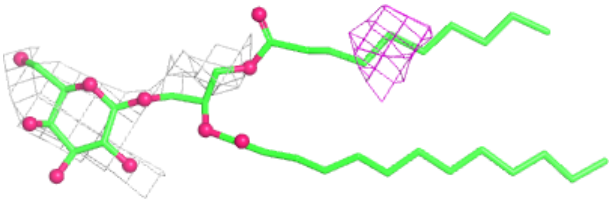


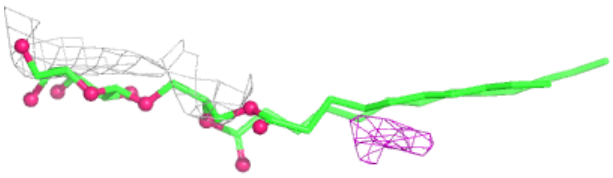


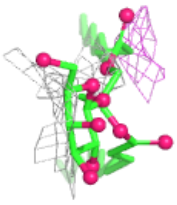


Electron density around LMG M 101:

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

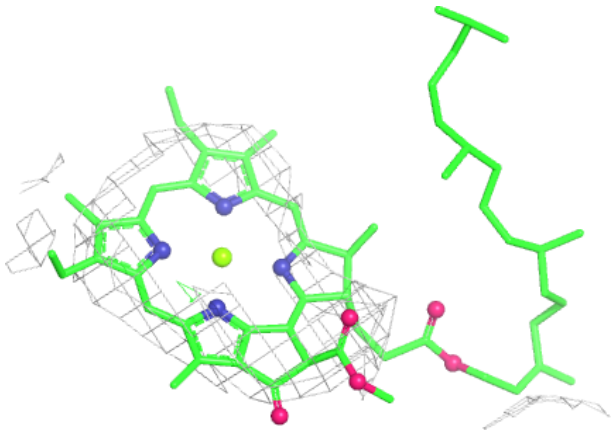


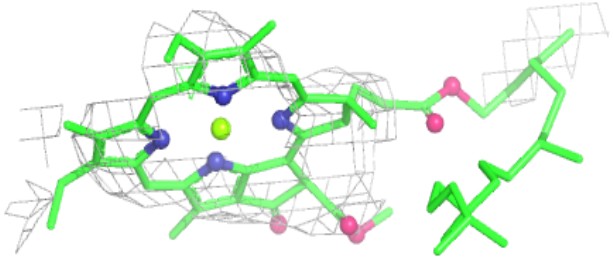


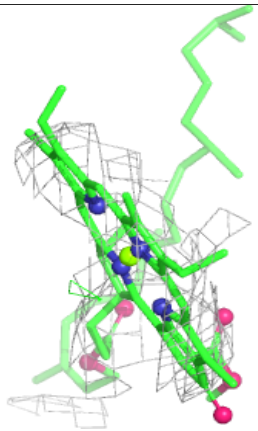


Electron density around CLA b 619:

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

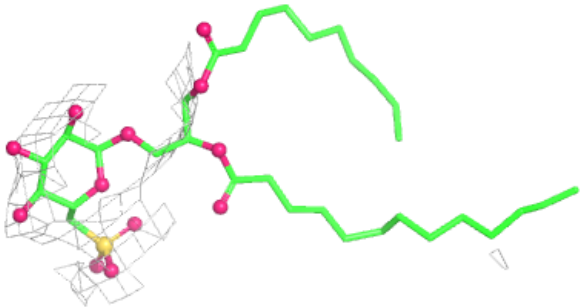


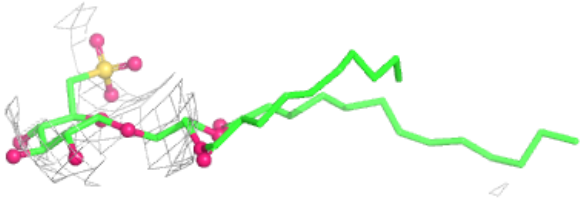


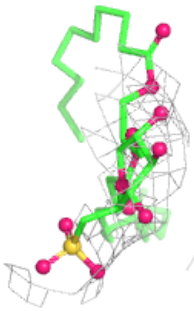


Electron density around SQD F 102:

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

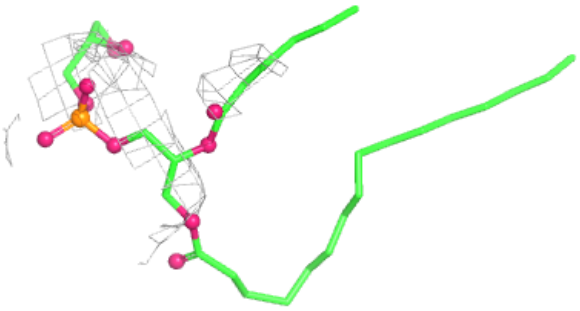


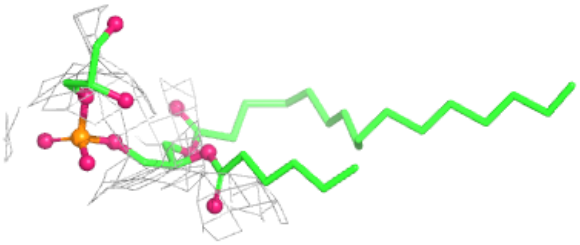


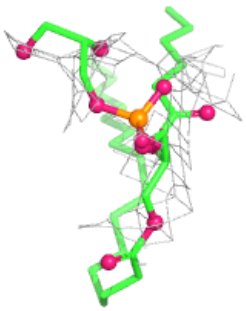


Electron density around LHG A 412:

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

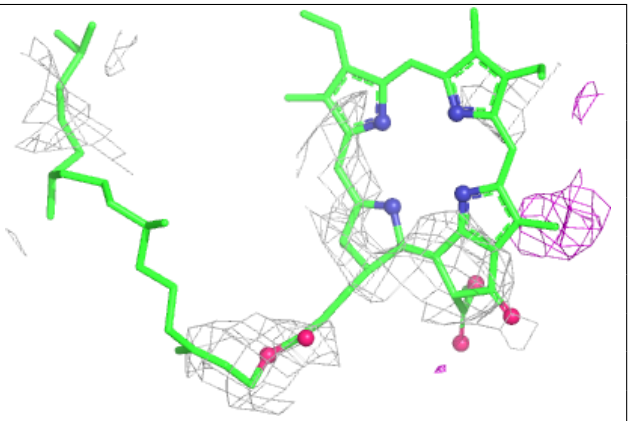


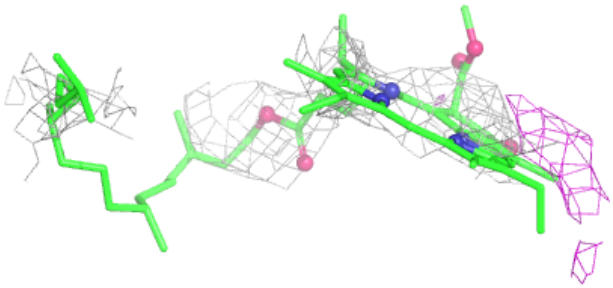


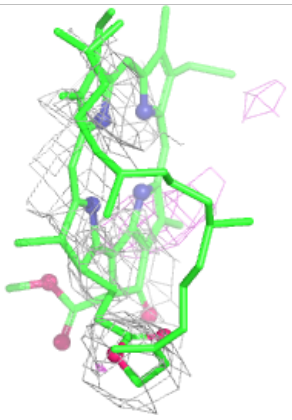


Electron density around PHO A 406:

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

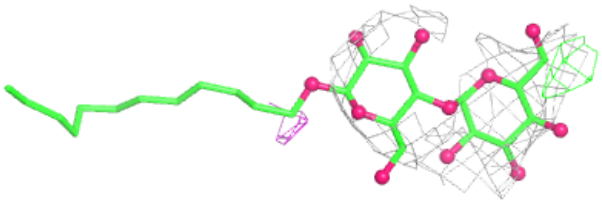


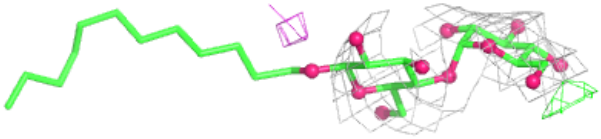




Electron density around LMT T 101:

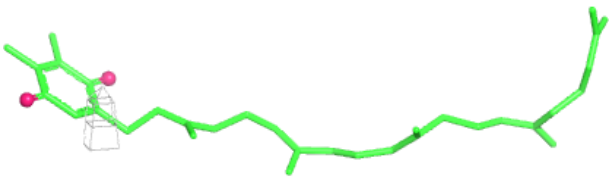
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

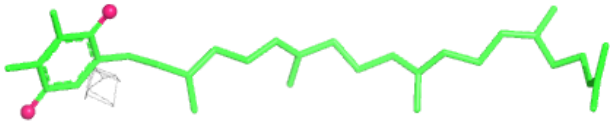


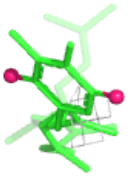


Electron density around PL9 j 101:

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

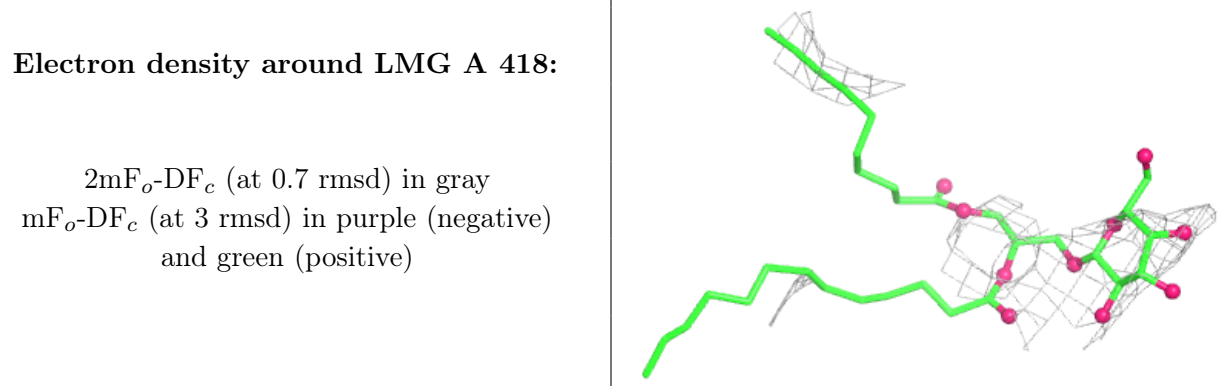


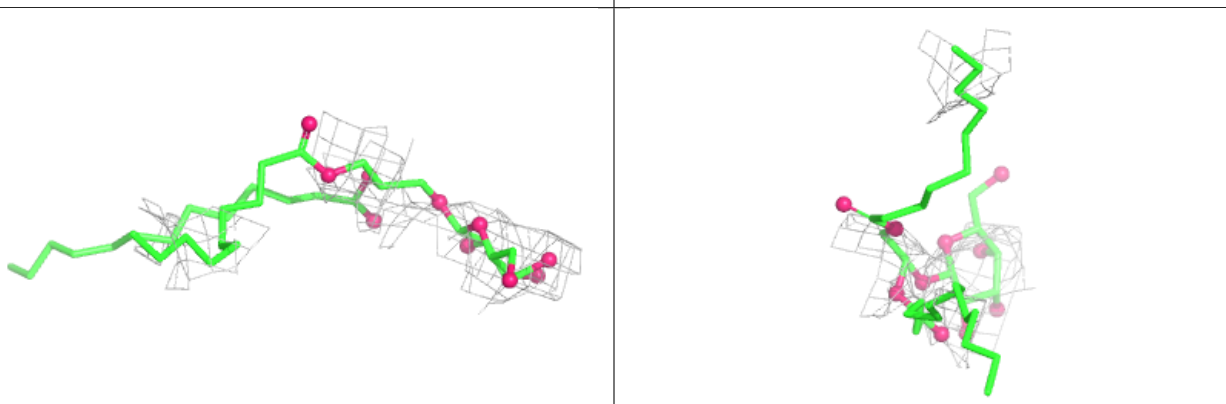




Electron density around LMG A 418:

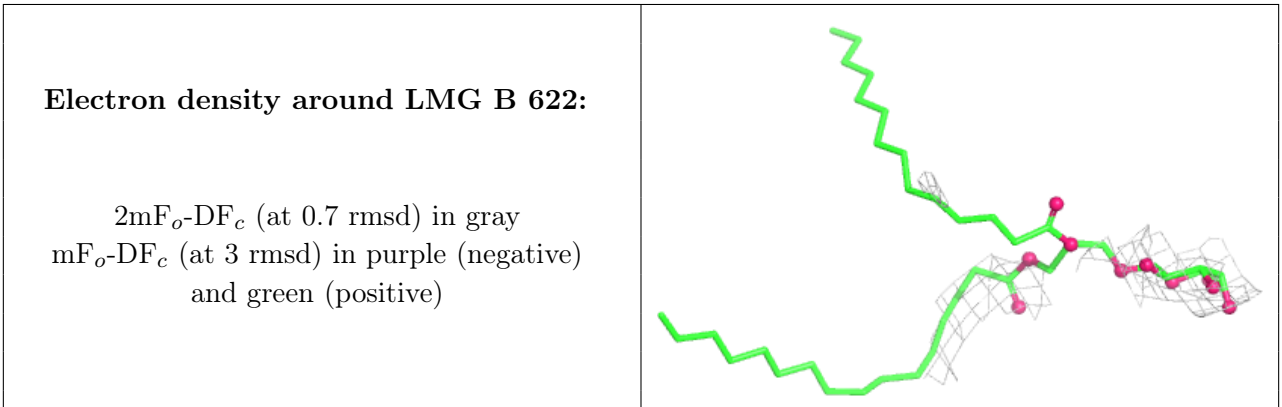
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

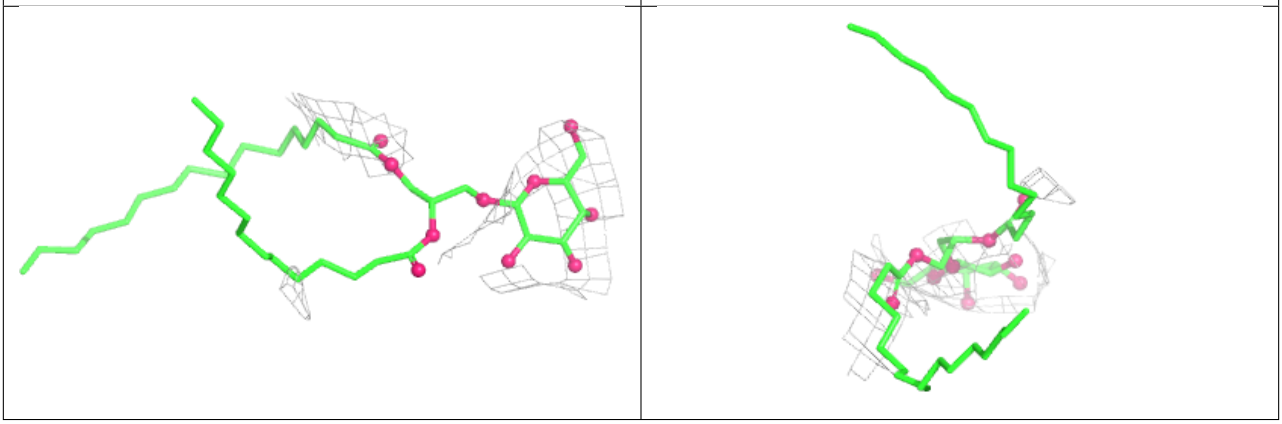




Electron density around LMG B 622:

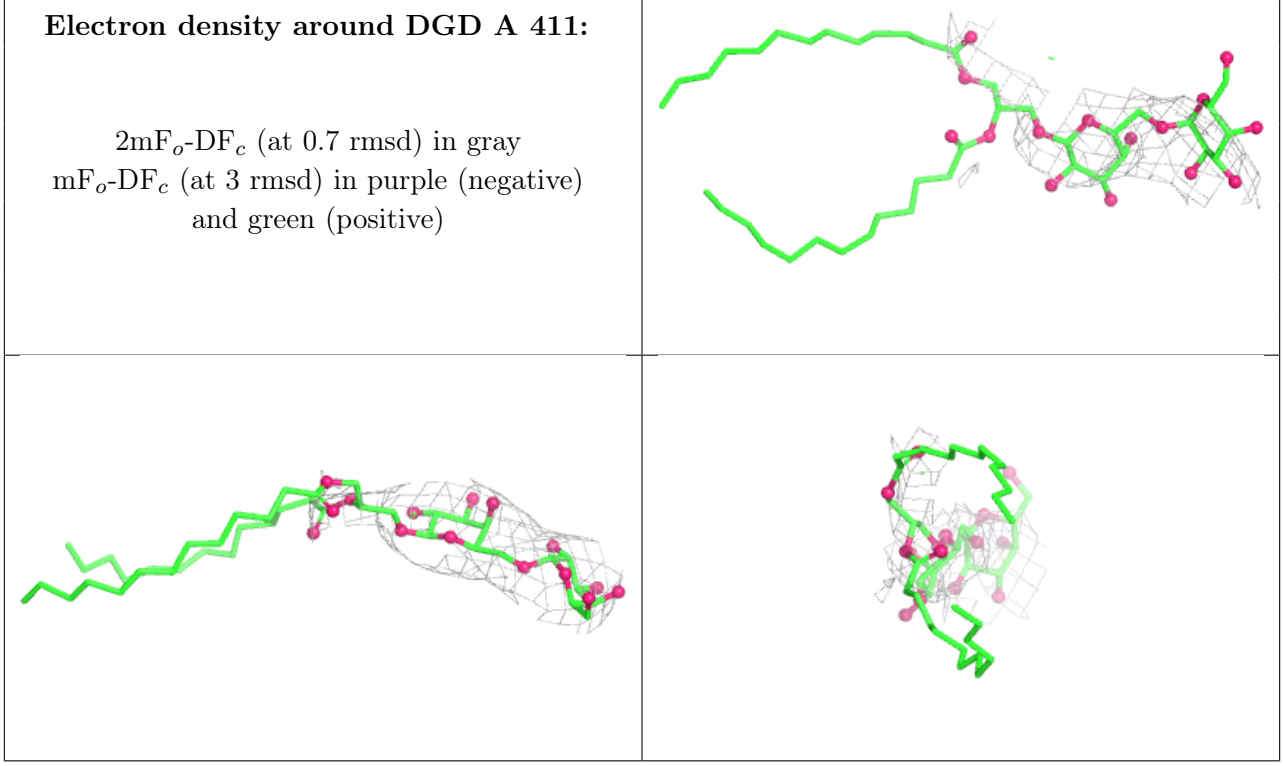
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





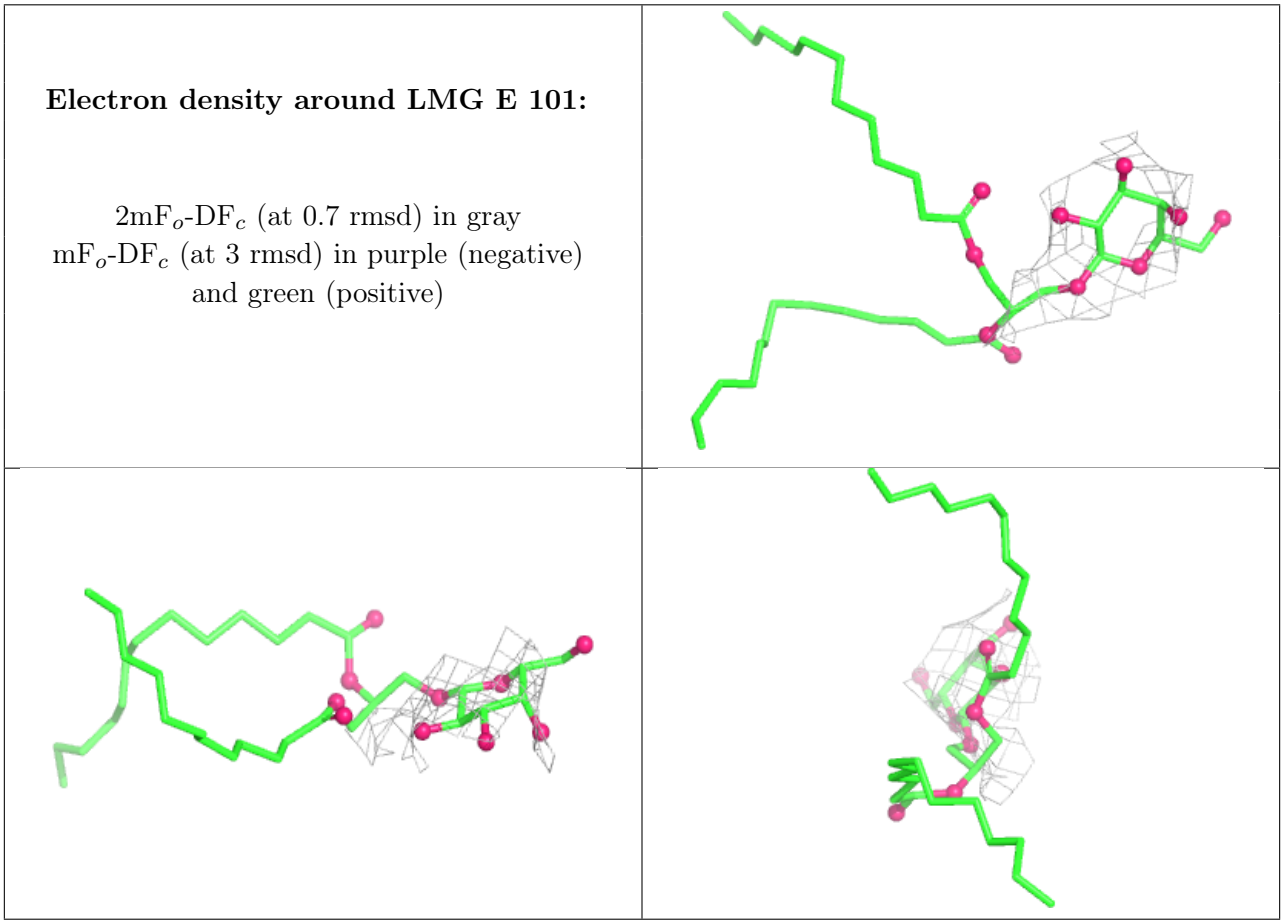
Electron density around DGD A 411:

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



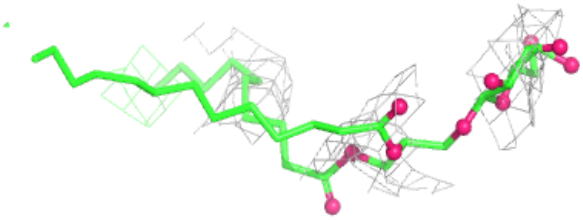
Electron density around LMG E 101:

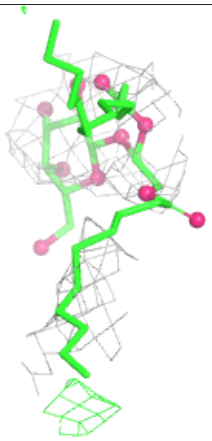
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG a 402:

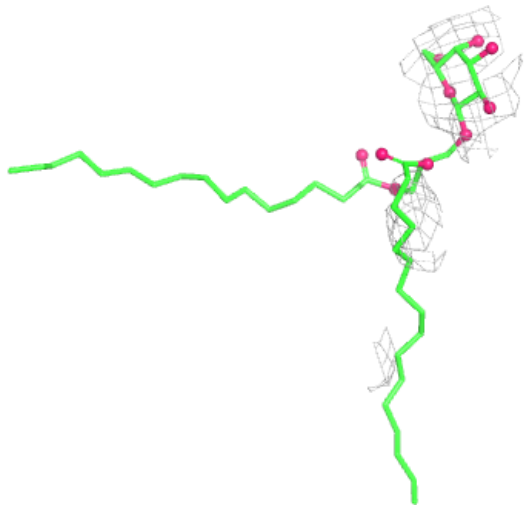
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

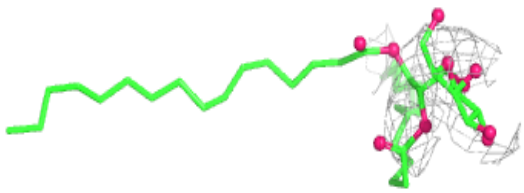




Electron density around LMG a 416:

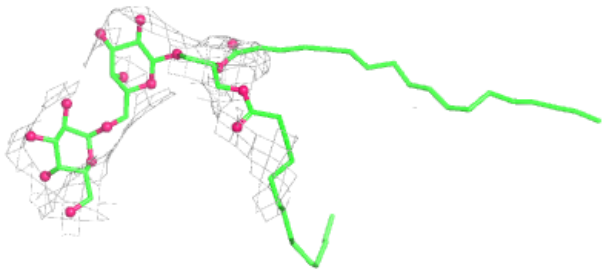
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





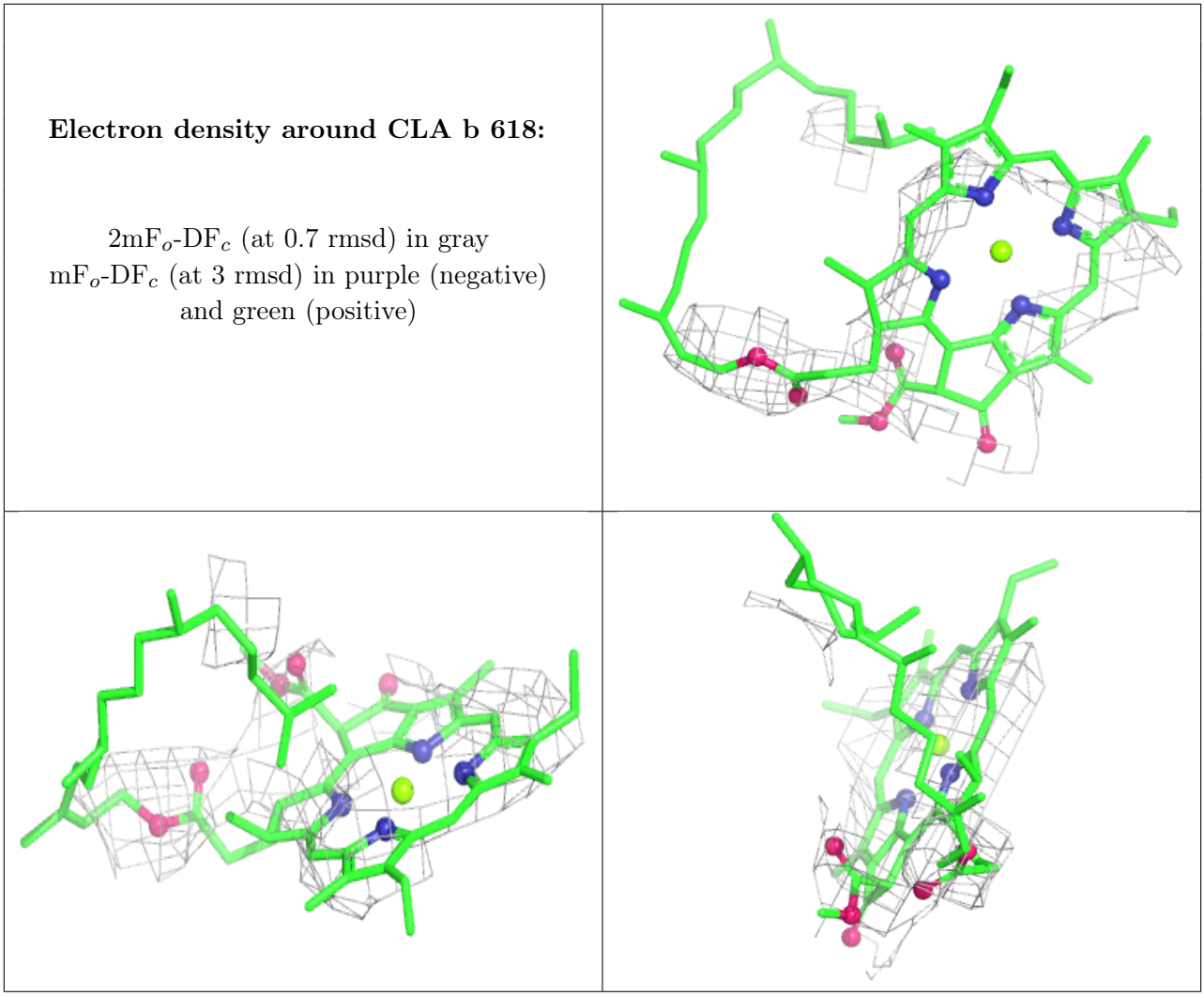
Electron density around DGD C 517:

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



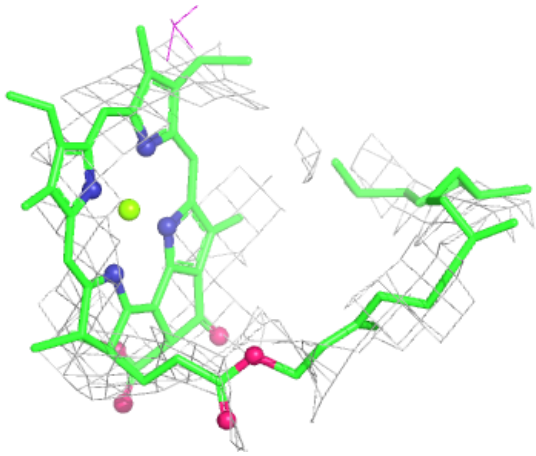
Electron density around CLA b 618:

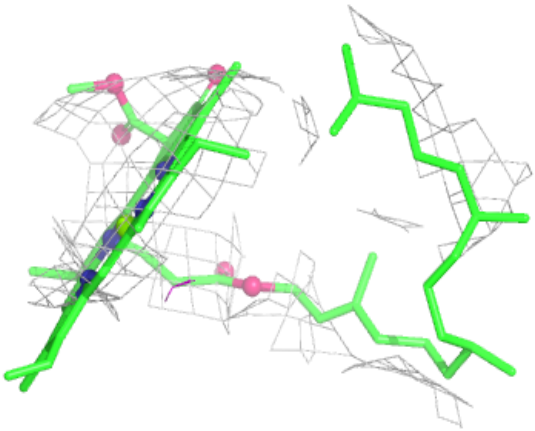
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

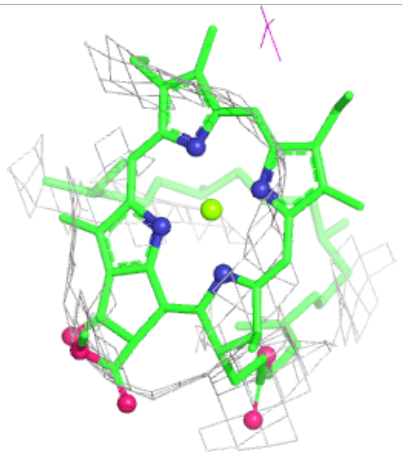


Electron density around CLA C 503:

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

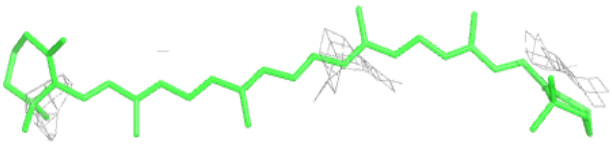


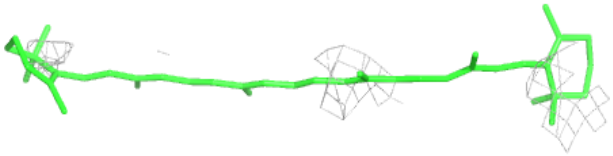


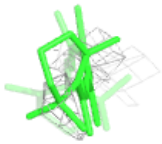


Electron density around BCR x 101:

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

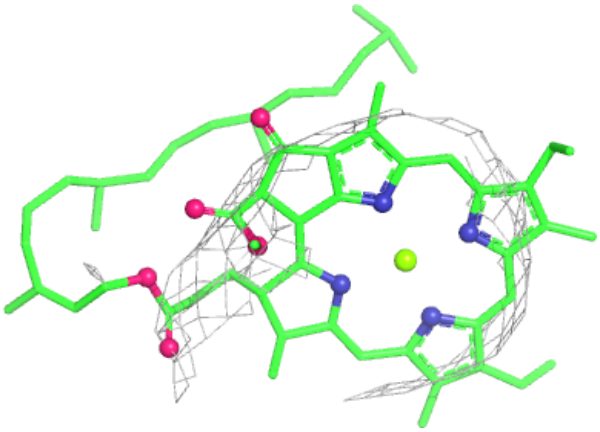


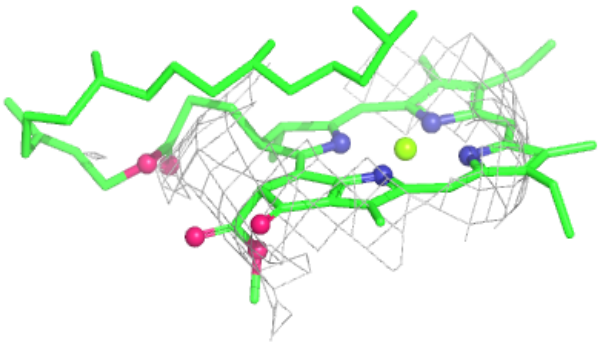


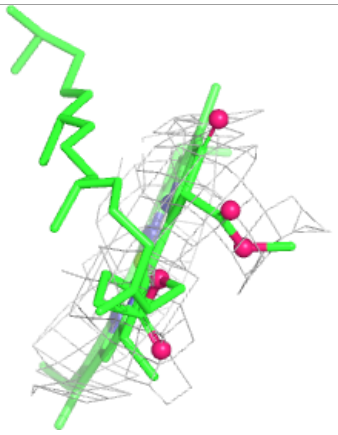


Electron density around CLA c 509:

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

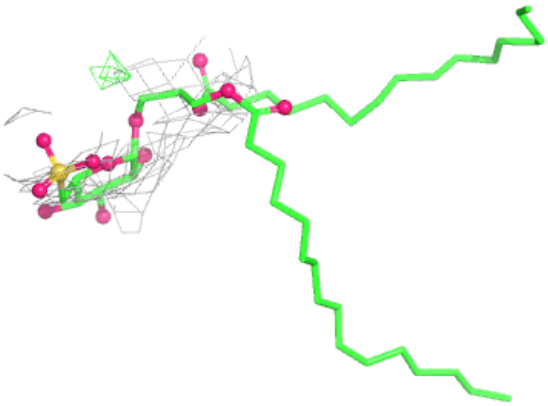


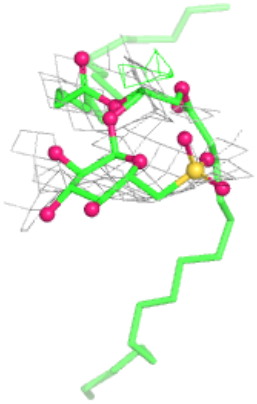




Electron density around SQD a 401:

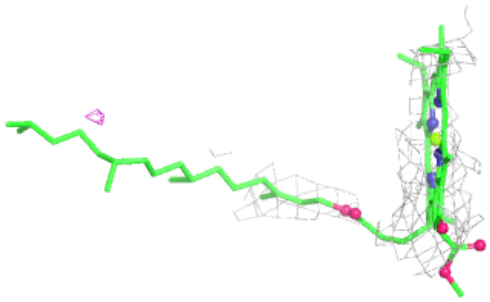
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





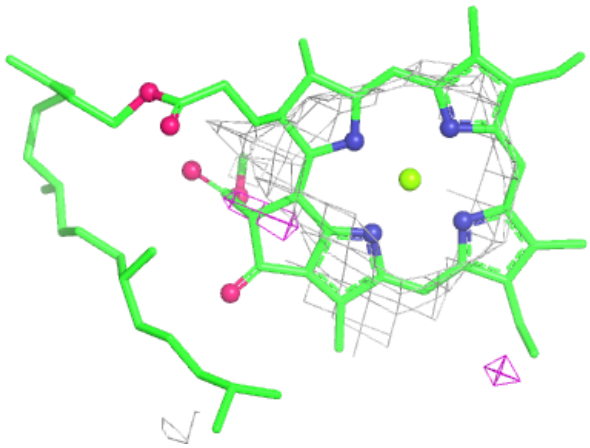
Electron density around CLA b 609:

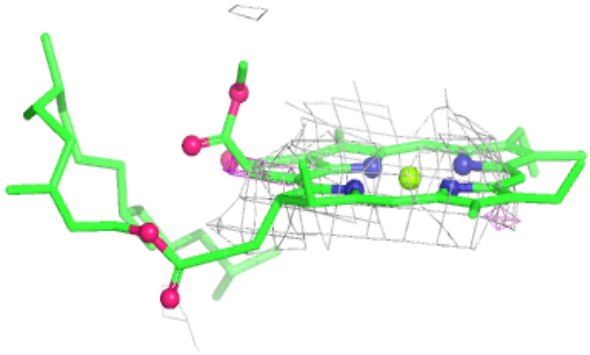
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

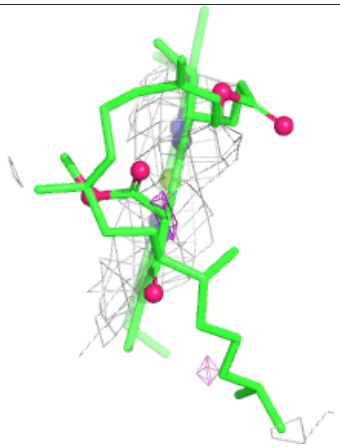


Electron density around CLA b 613:

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

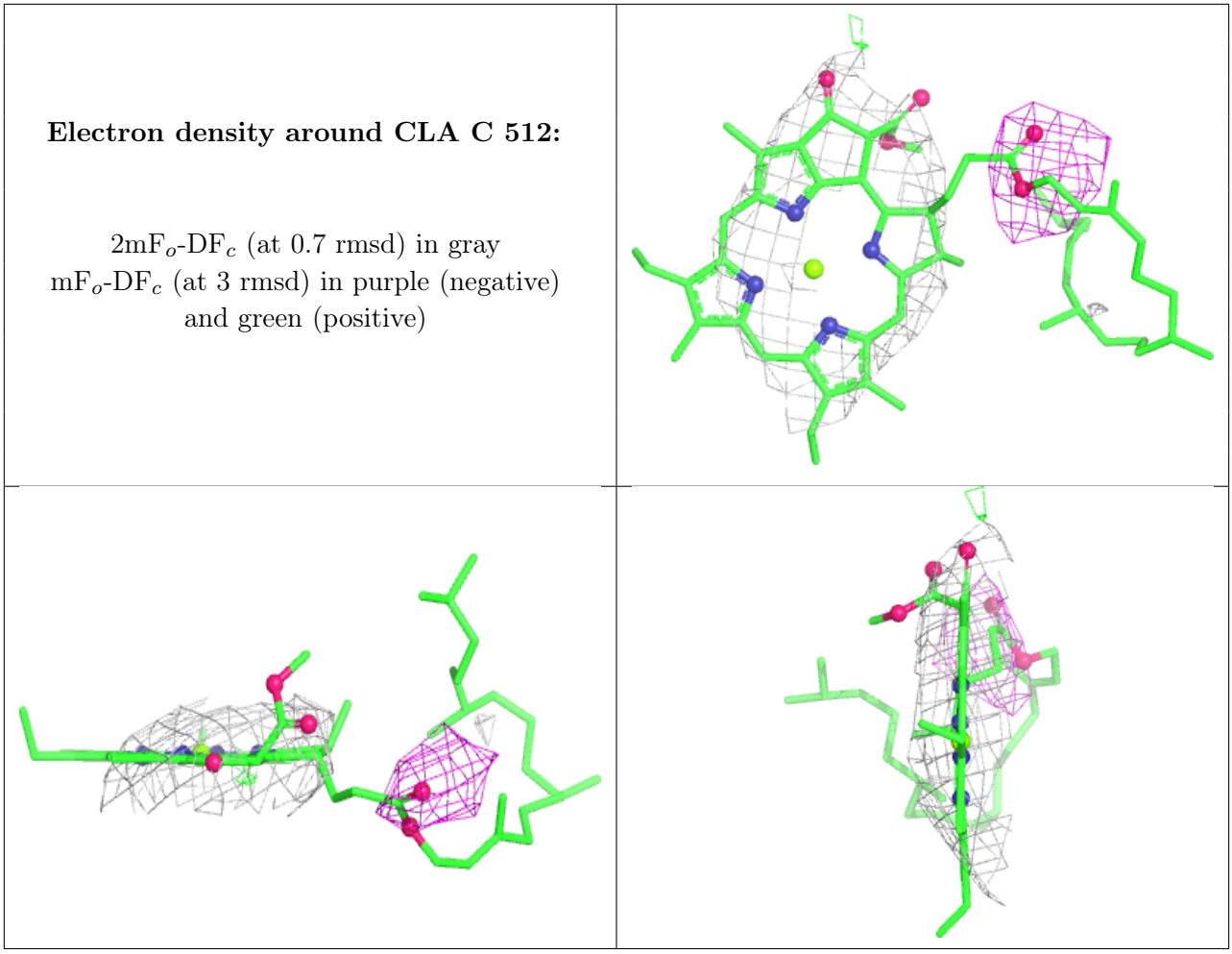






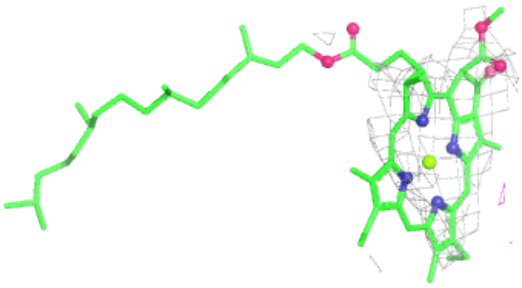
Electron density around CLA C 512:

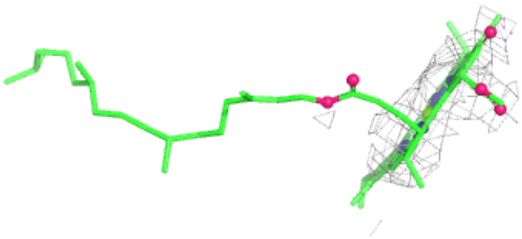
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

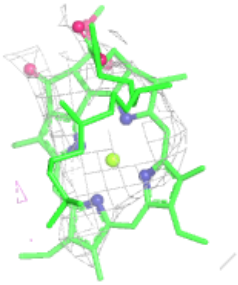


Electron density around CLA A 407:

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

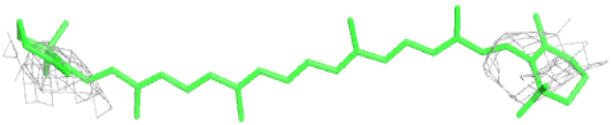


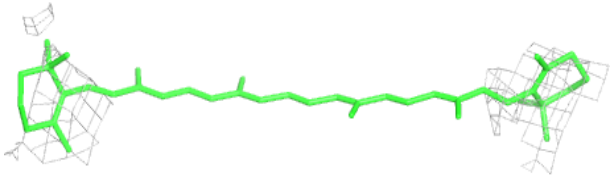


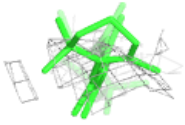


Electron density around BCR c 515:

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

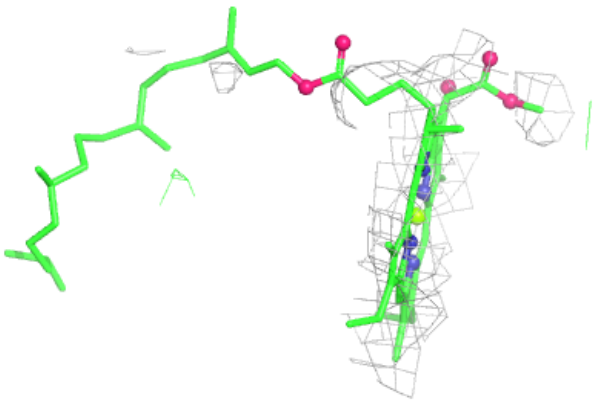


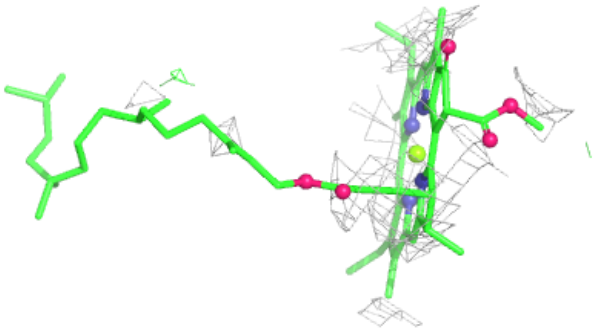


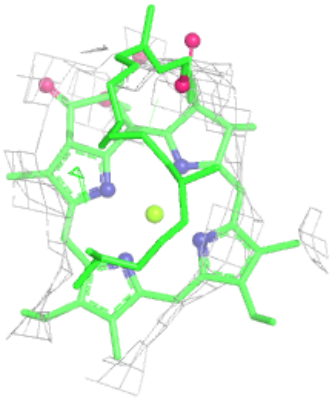


Electron density around CLA C 506:

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

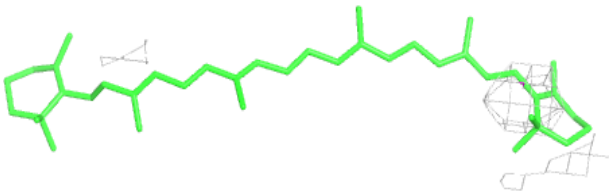


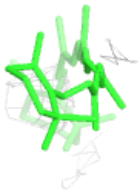




Electron density around BCR B 618:

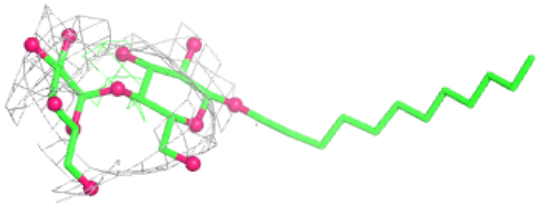
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

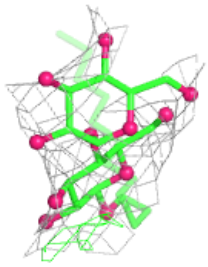




Electron density around LMT m 101:

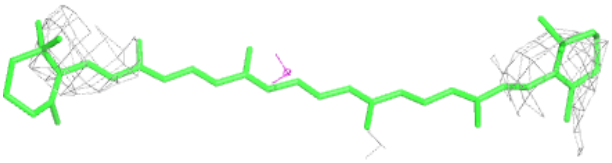
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

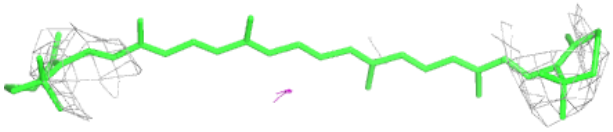


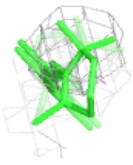


Electron density around BCR B 620:

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

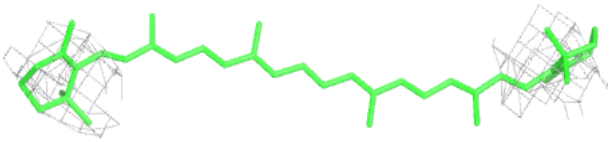


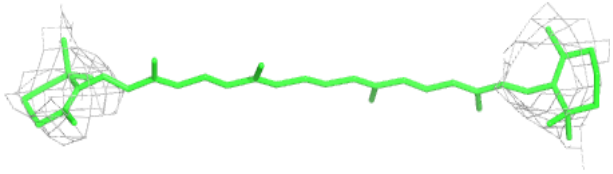


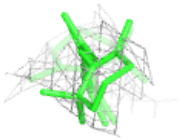


Electron density around BCR Z 101:

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

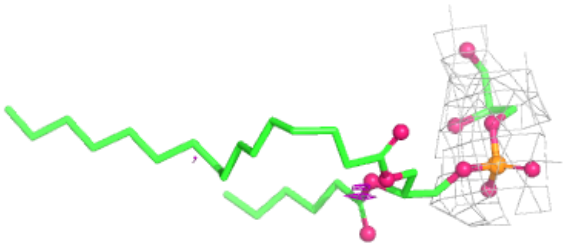






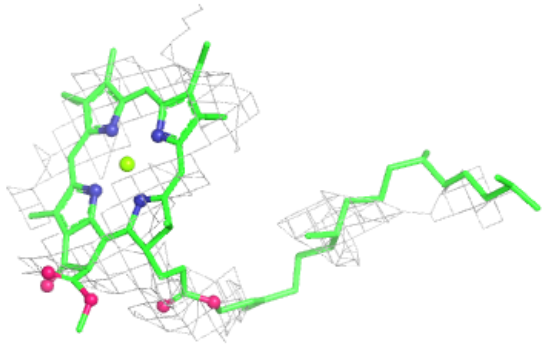
Electron density around LHG a 414:

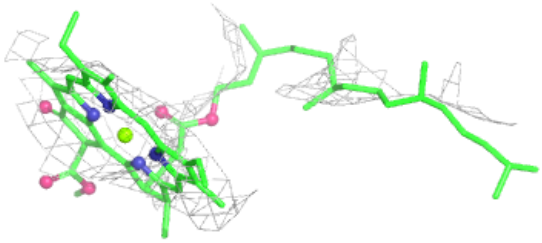
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

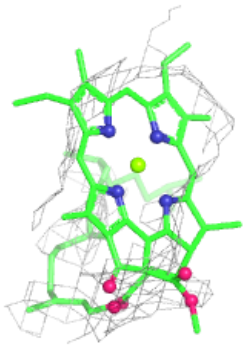


Electron density around CLA C 511:

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

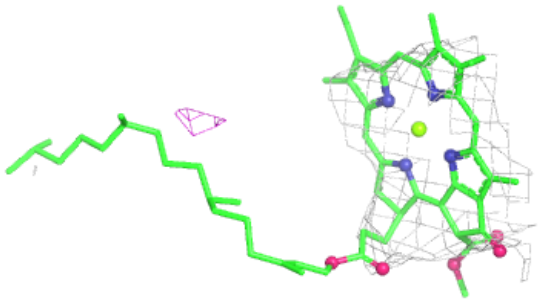


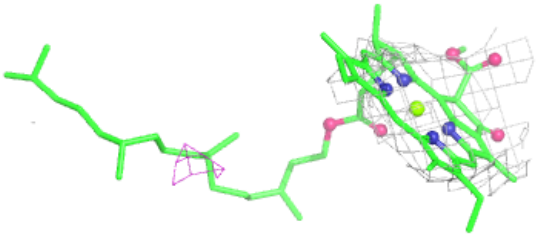


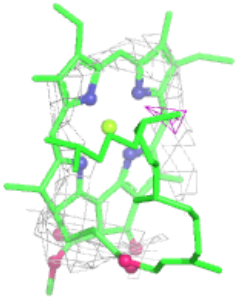


Electron density around CLA c 511:

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

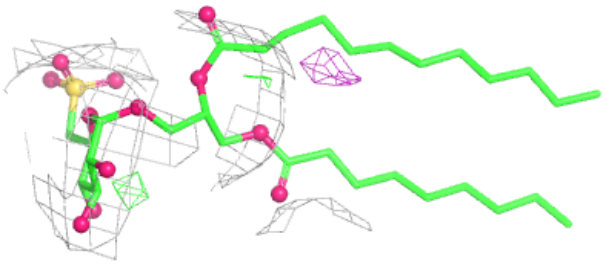


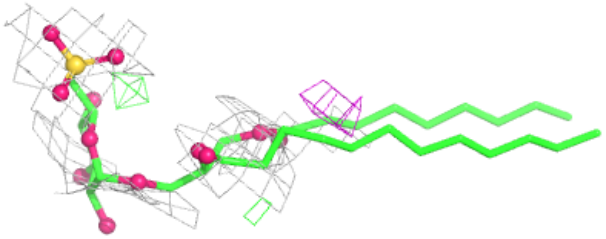


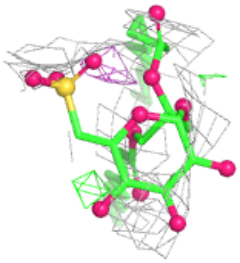


Electron density around SQD D 409:

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

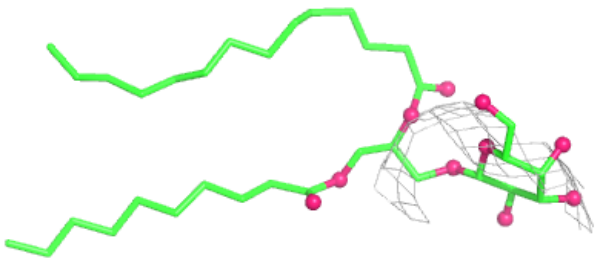


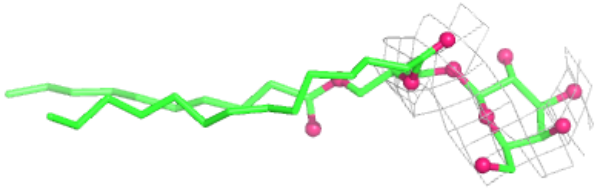


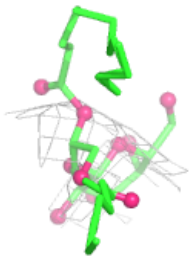


Electron density around LMG i 101:

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

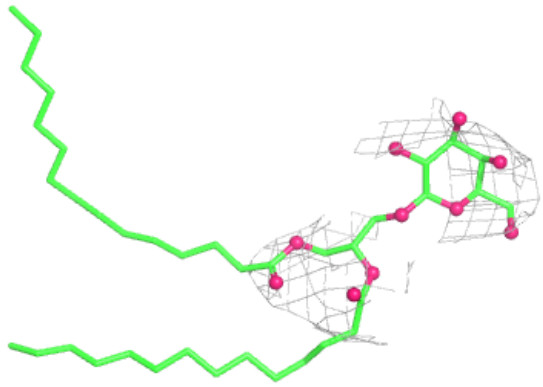


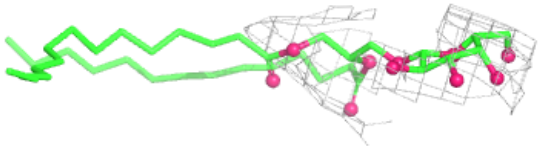




Electron density around LMG C 519:

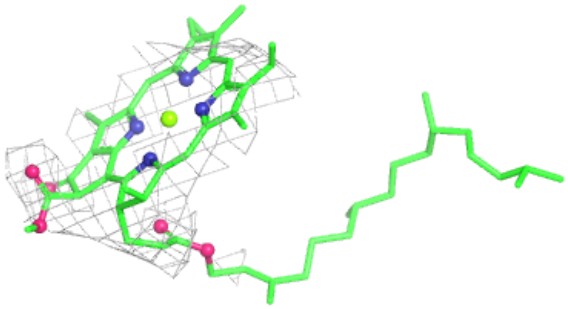
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

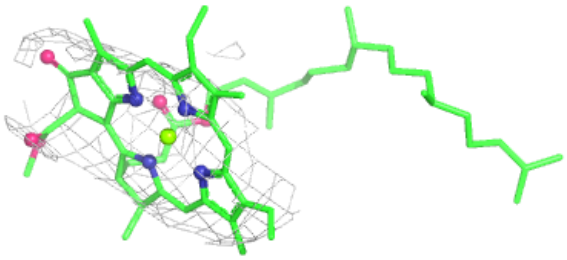


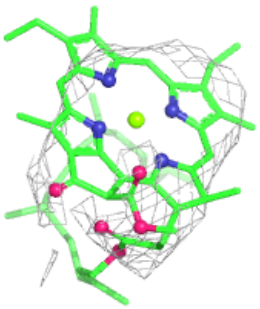


Electron density around CLA C 513:

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

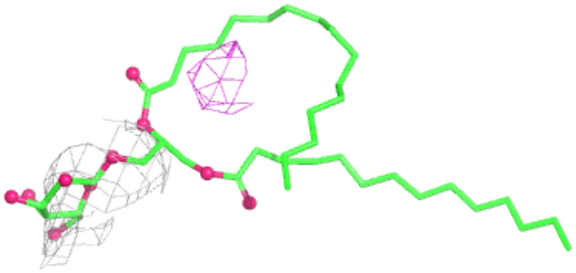






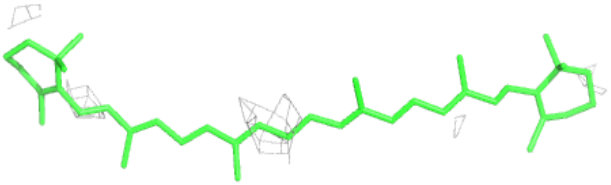
Electron density around LMG D 407:

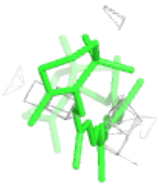
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCR T 103:

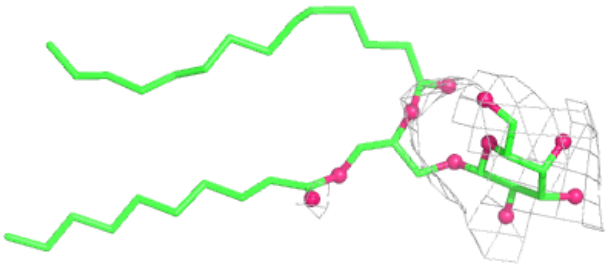
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

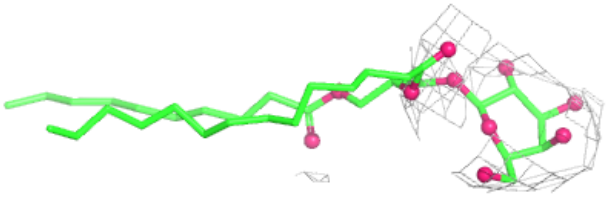


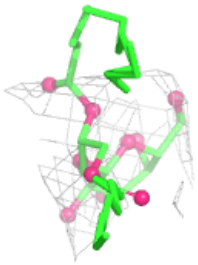


Electron density around LMG I 101:

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

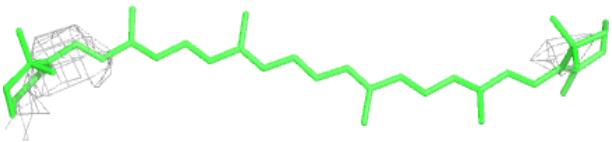


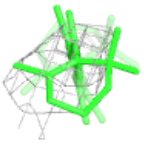




Electron density around BCR a 412:

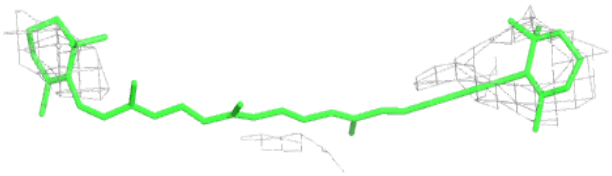
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

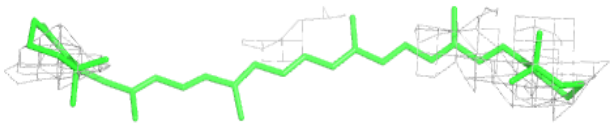


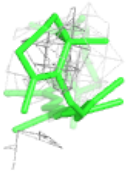


Electron density around BCR C 514:

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

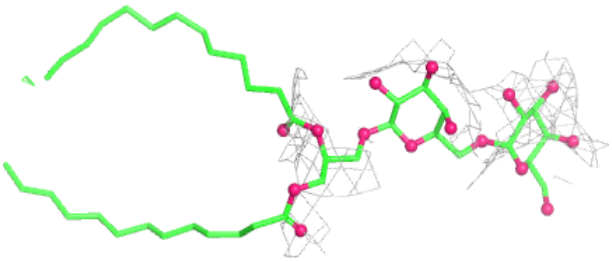


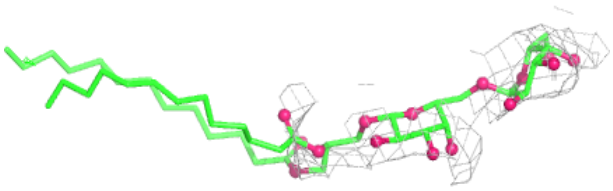




Electron density around DGD a 413:

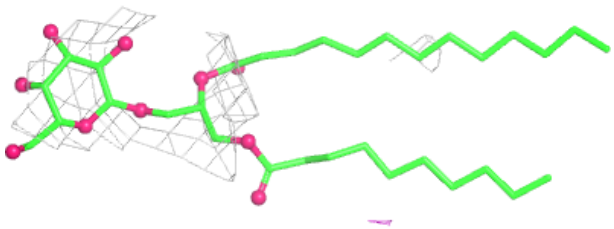
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

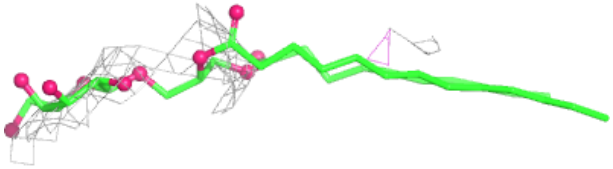


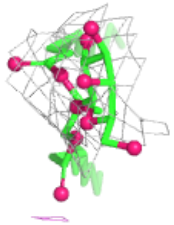


Electron density around LMG M 102:

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

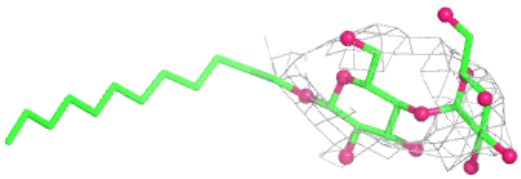


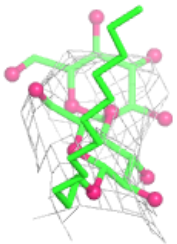




Electron density around LMT M 103:

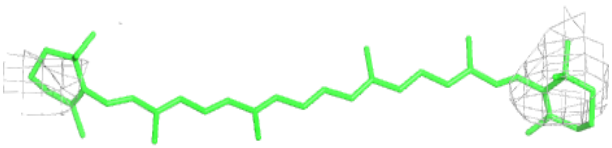
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

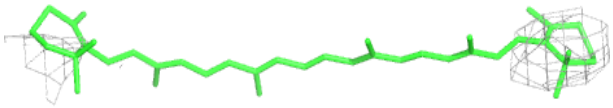


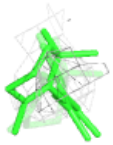


Electron density around BCR C 515:

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

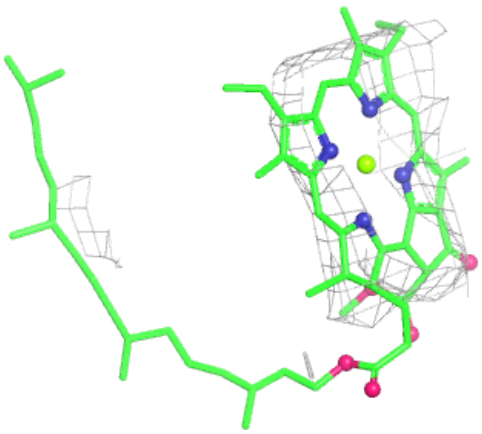


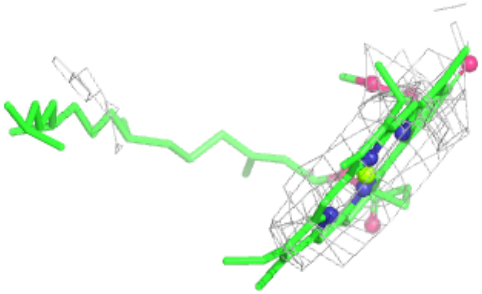


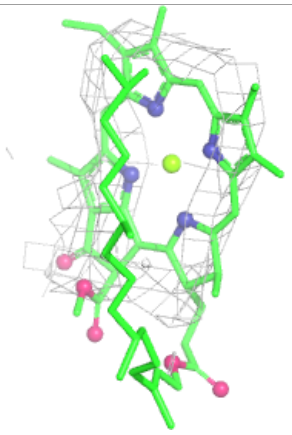


Electron density around CLA c 507:

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

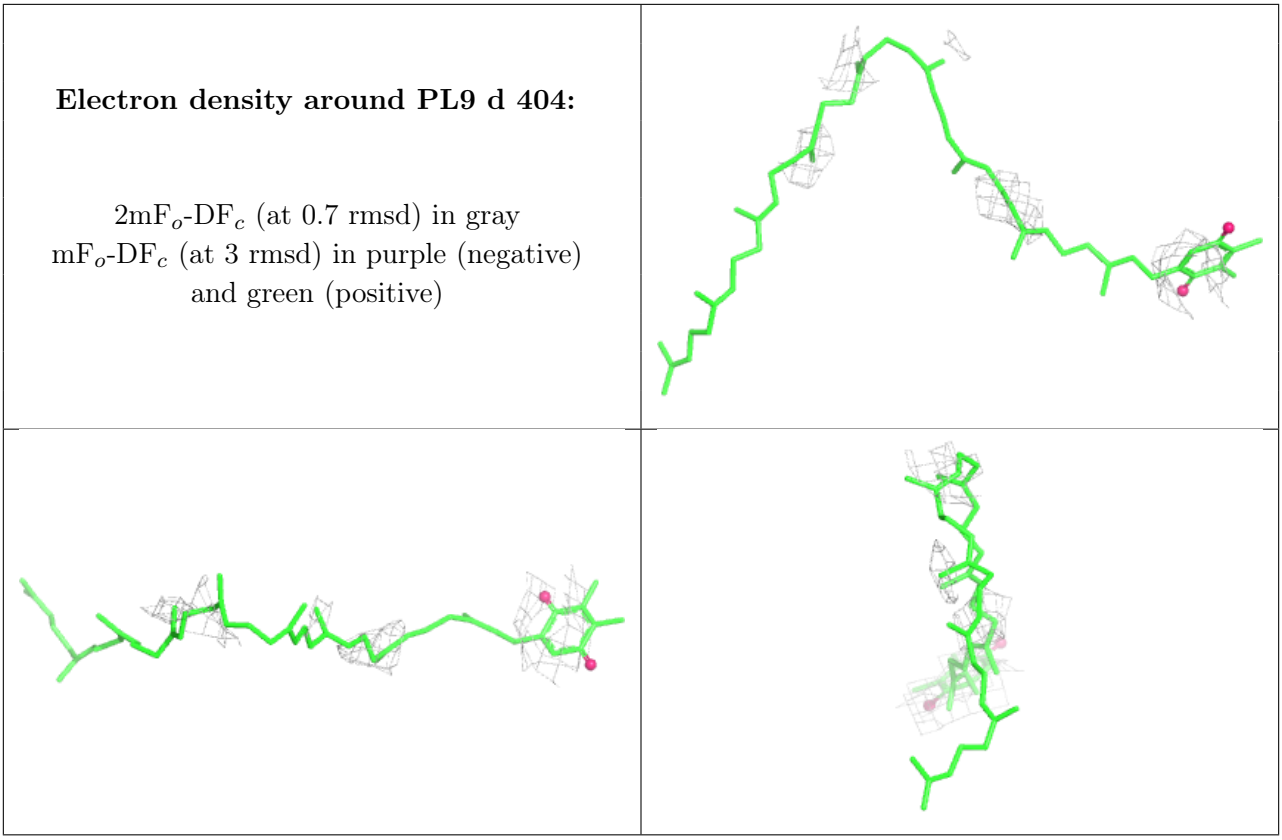






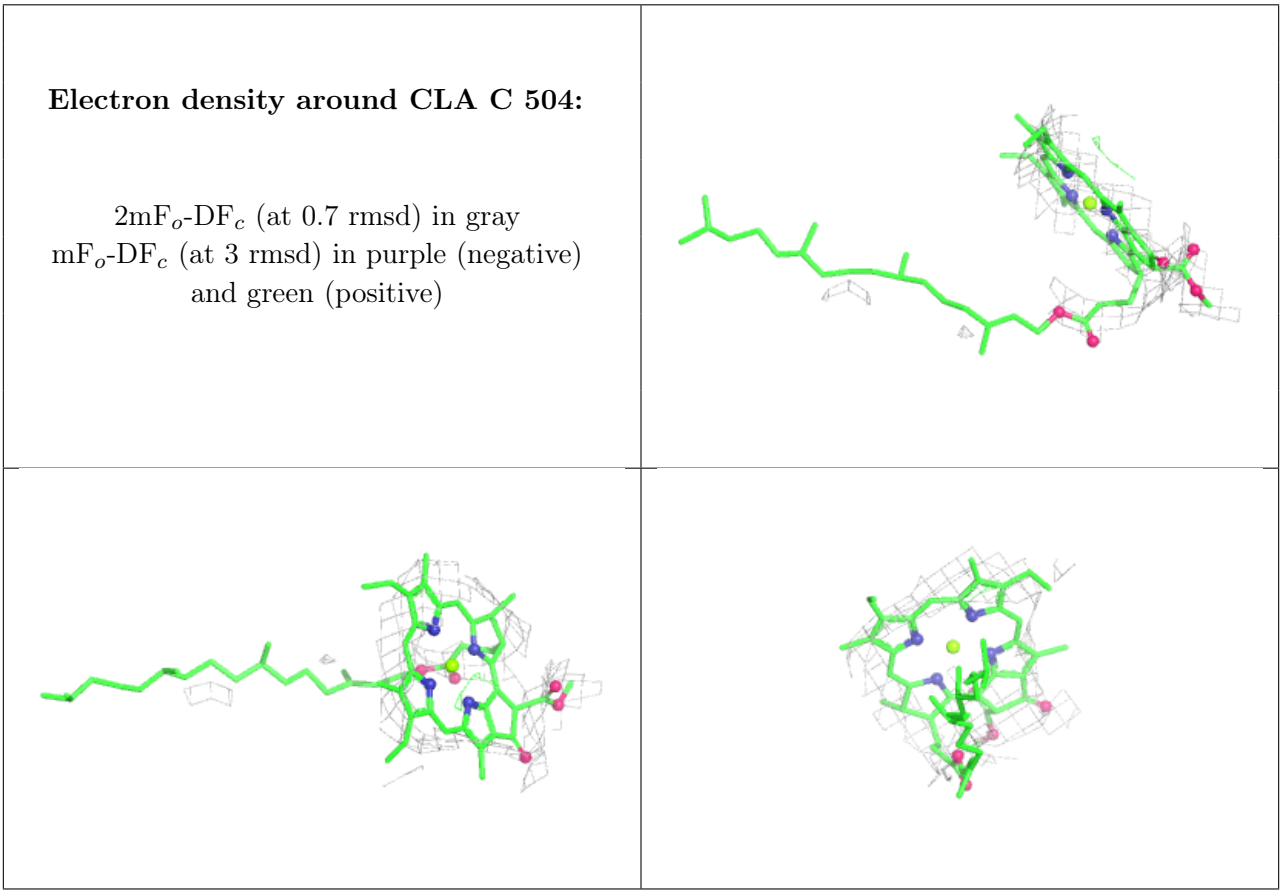
Electron density around PL9 d 404:

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



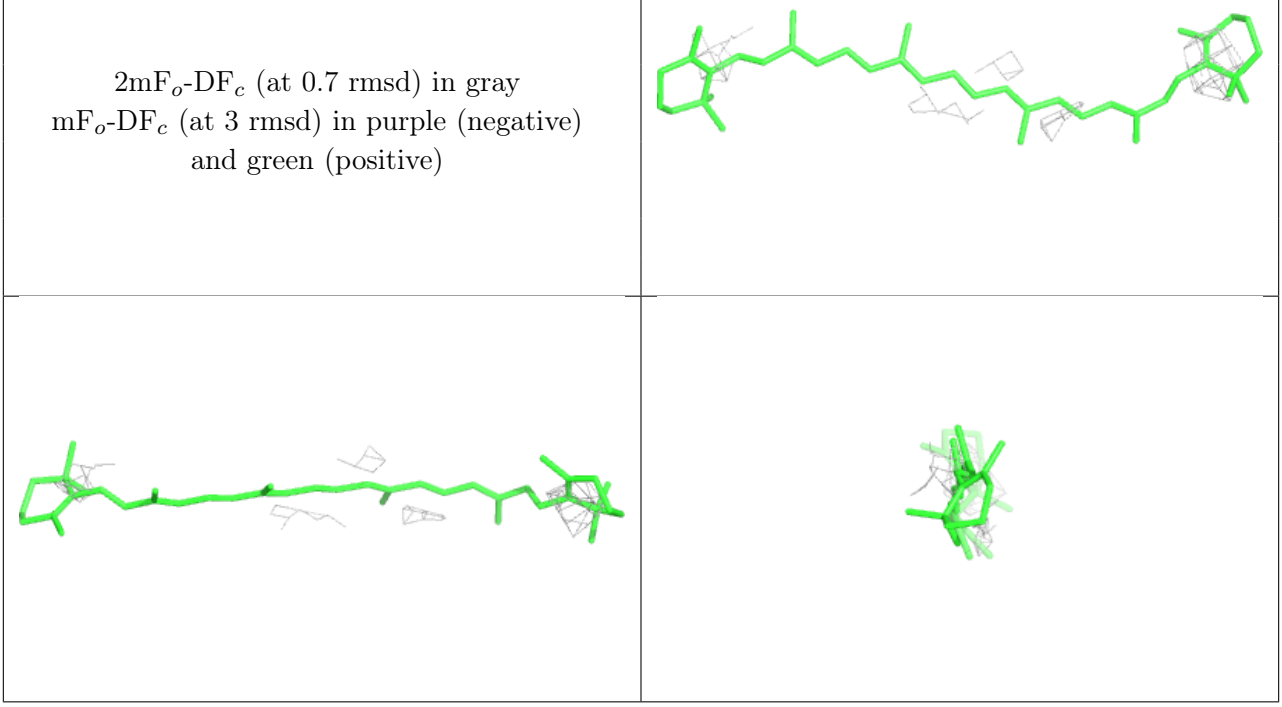
Electron density around CLA C 504:

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



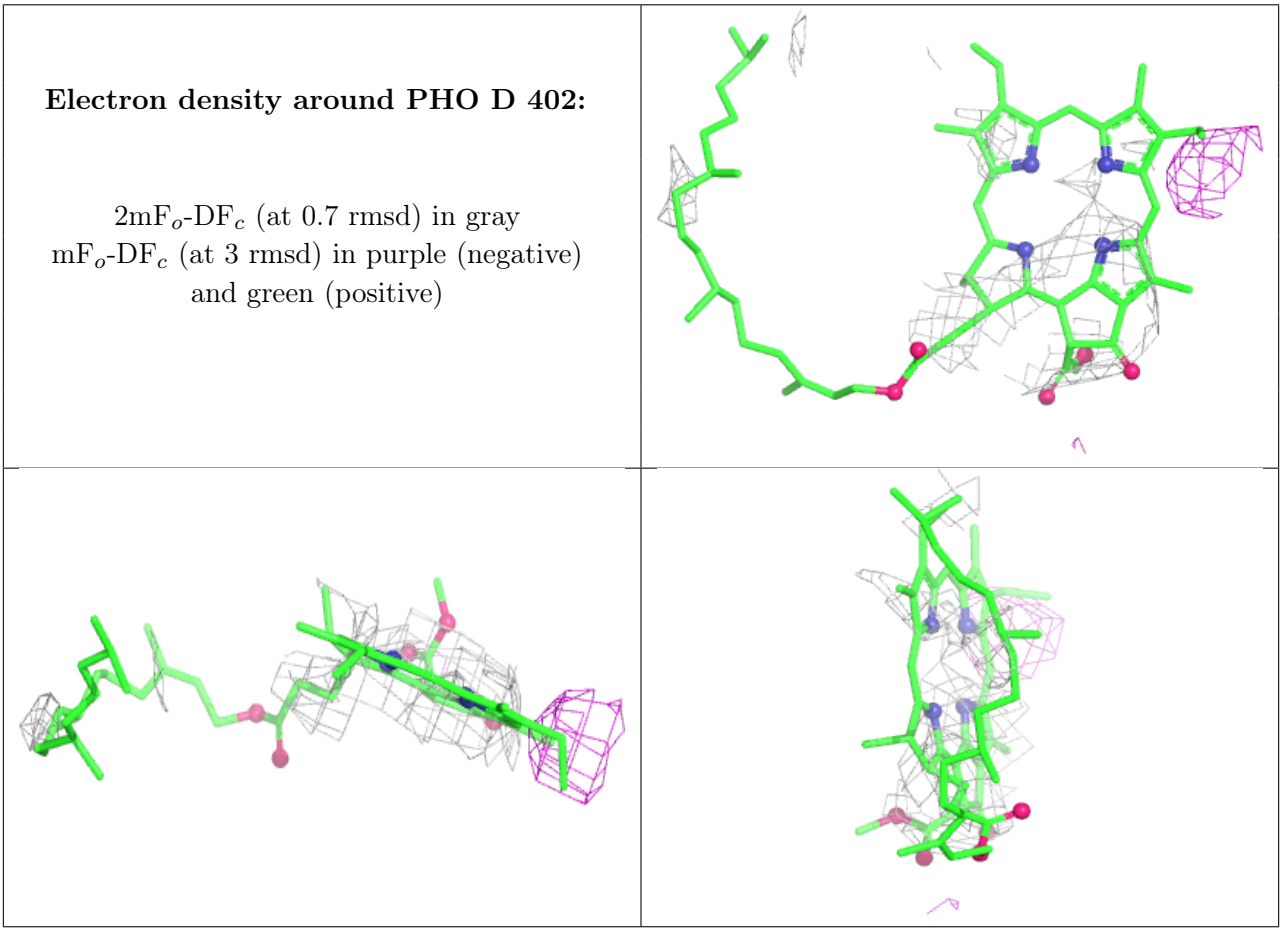
Electron density around BCR K 102:

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



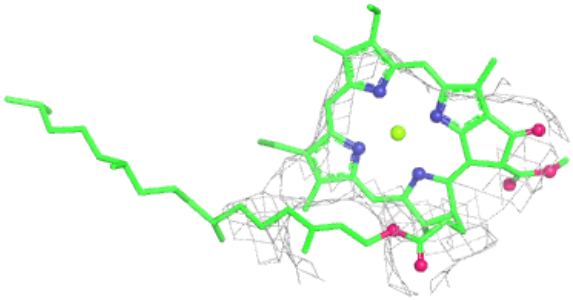
Electron density around PHO D 402:

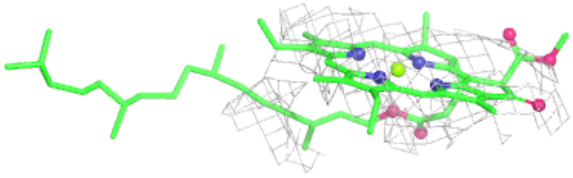
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

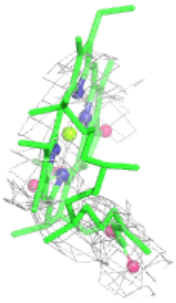


Electron density around CLA C 501:

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

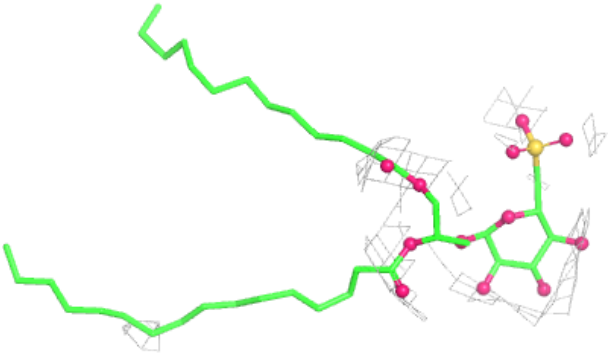


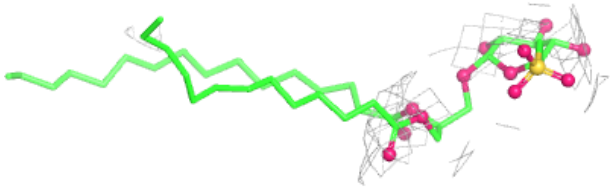




Electron density around SQD A 413:

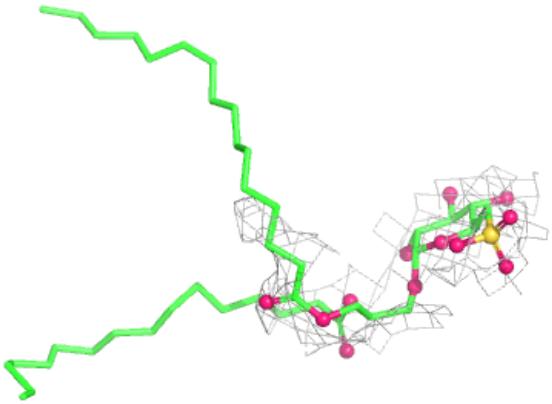
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

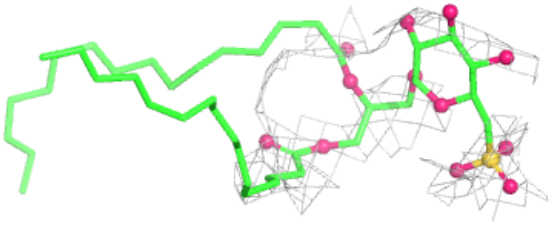


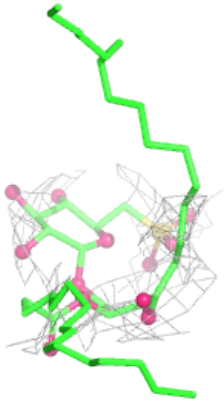


Electron density around SQD A 417:

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

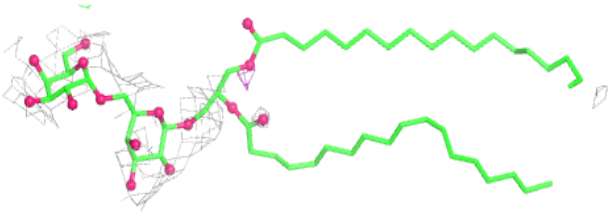


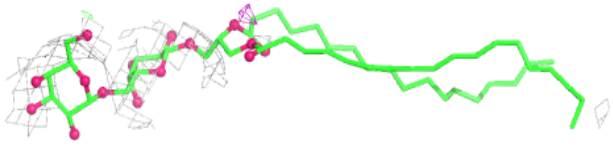


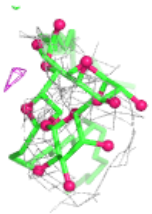


Electron density around DGD c 519:

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

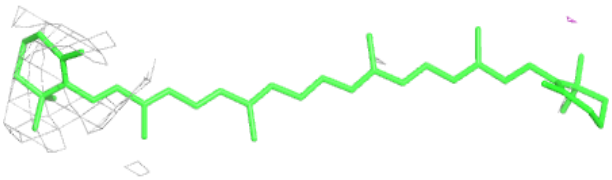


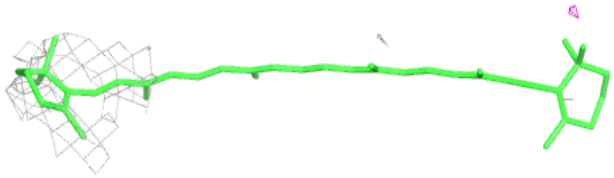


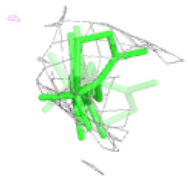


Electron density around BCR T 102:

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

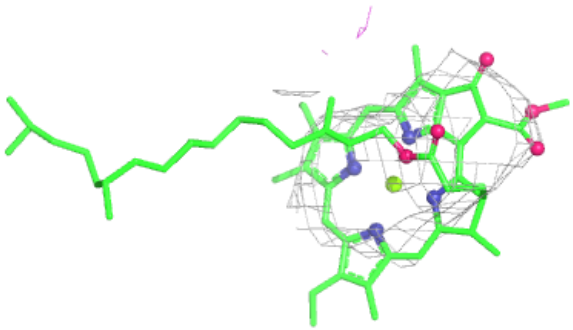


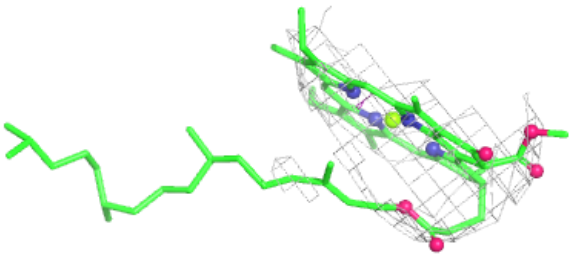




Electron density around CLA B 614:

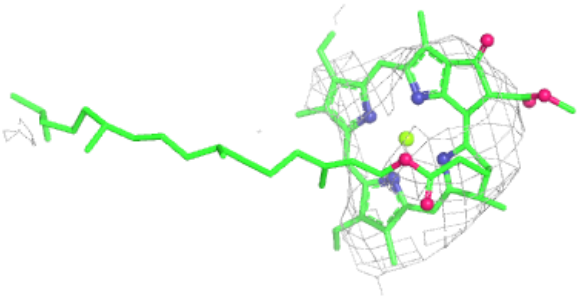
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

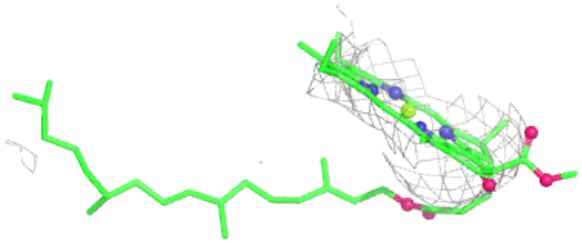


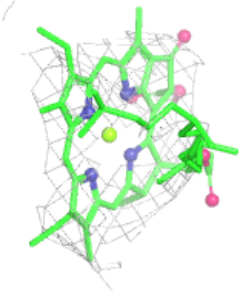


Electron density around CLA b 611:

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

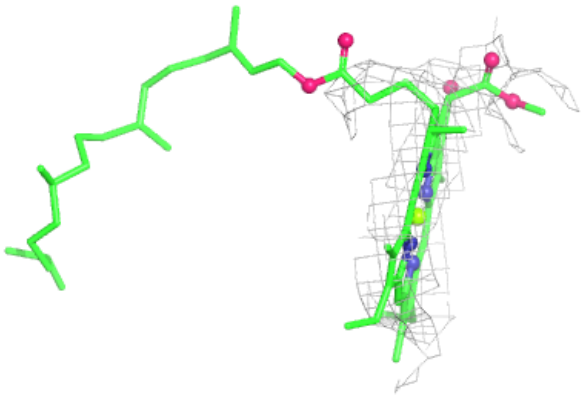


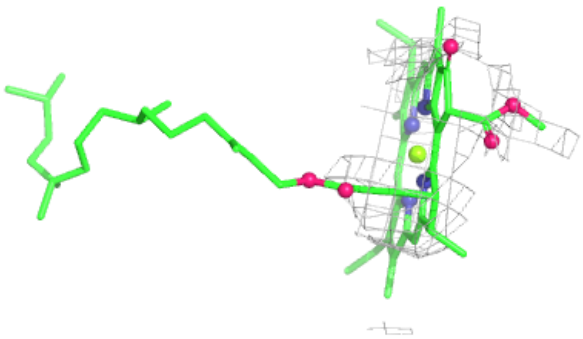


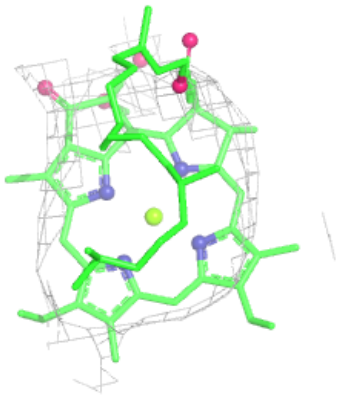


Electron density around CLA c 506:

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

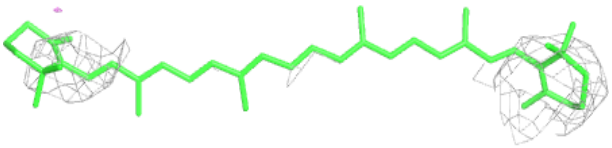


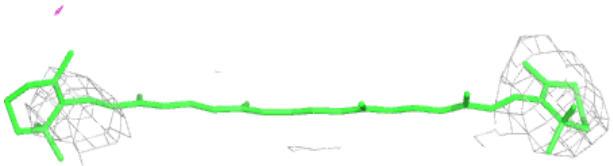


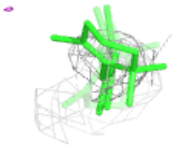


Electron density around BCR b 620:

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

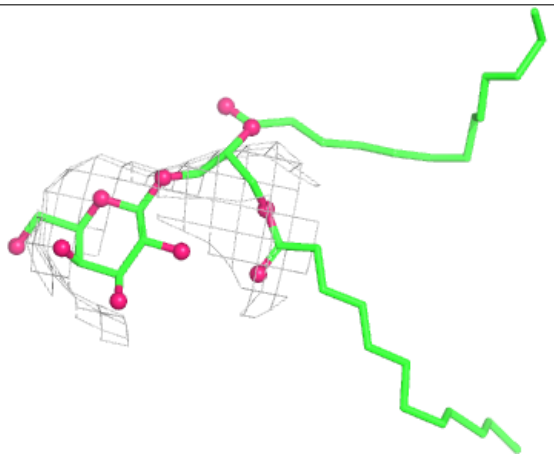


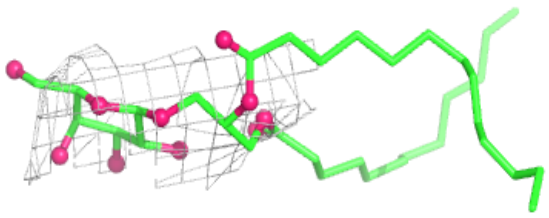


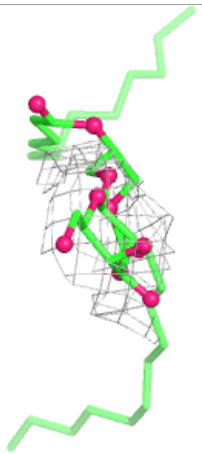


Electron density around LMG e 101:

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

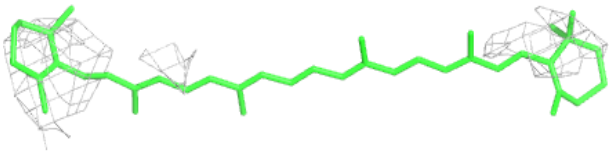


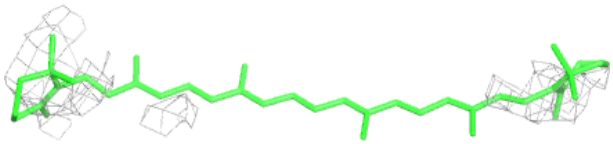


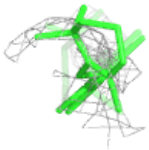


Electron density around BCR b 621:

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

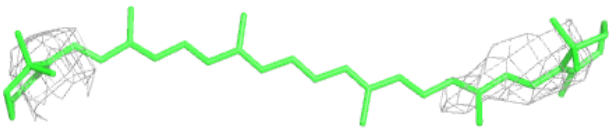


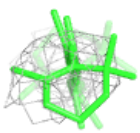




Electron density around BCR A 410:

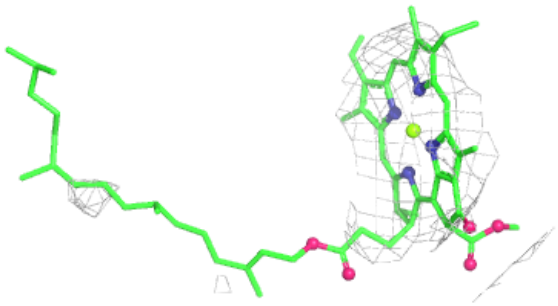
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

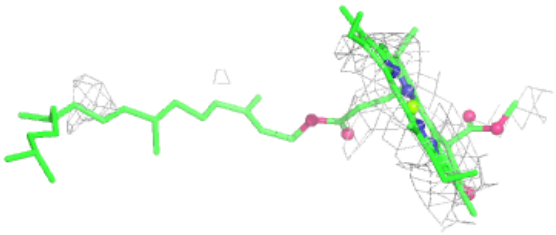


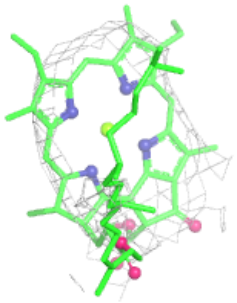


Electron density around CLA b 612:

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

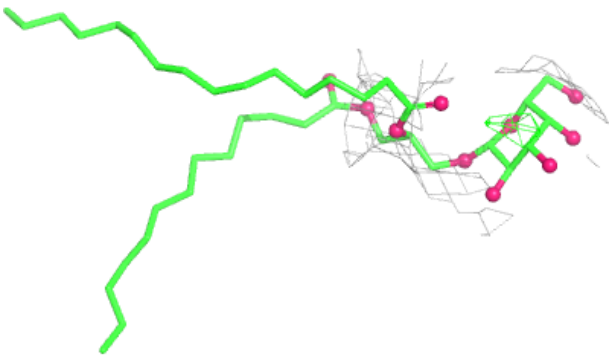


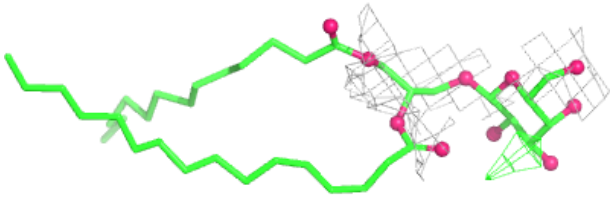


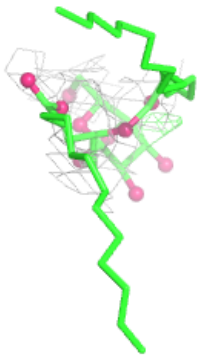


Electron density around LMG D 408:

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

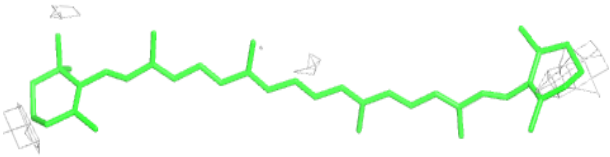


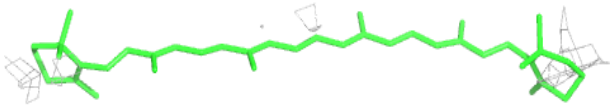




Electron density around BCR c 516:

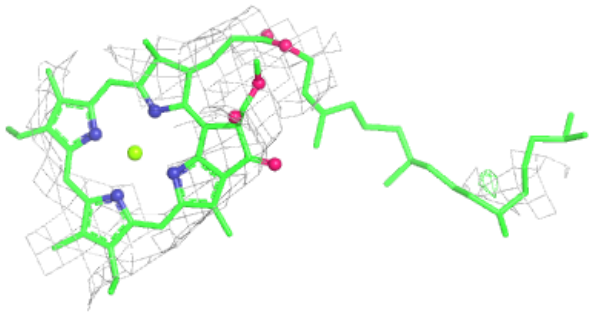
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

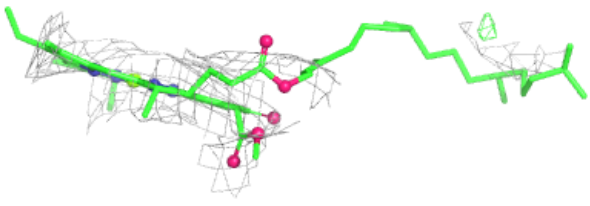


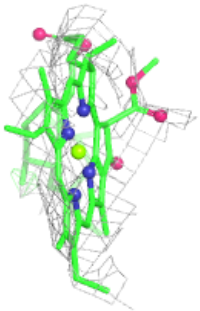


Electron density around CLA b 605:

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

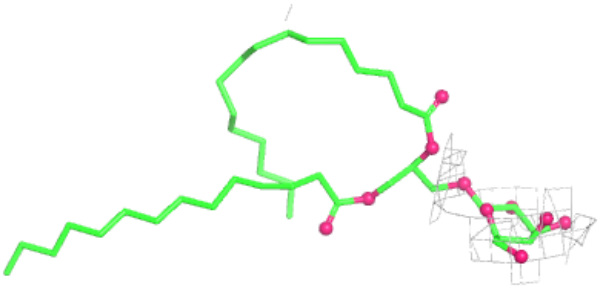


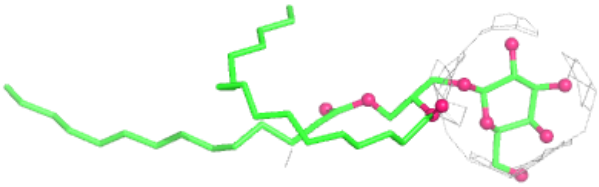




Electron density around LMG b 623:

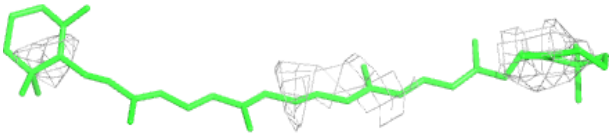
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

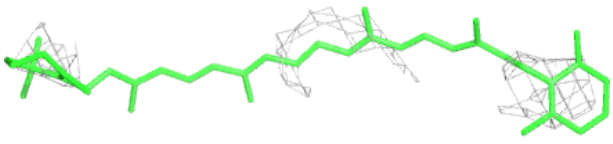


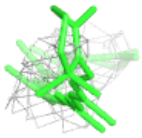


Electron density around BCR f 102:

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

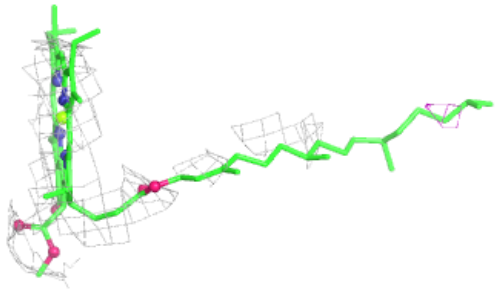


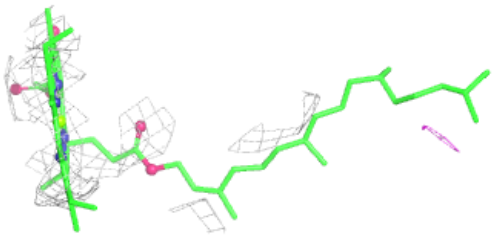


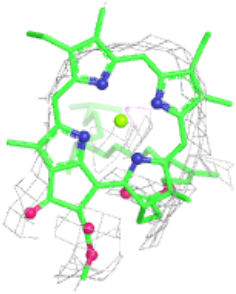


Electron density around CLA B 606:

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

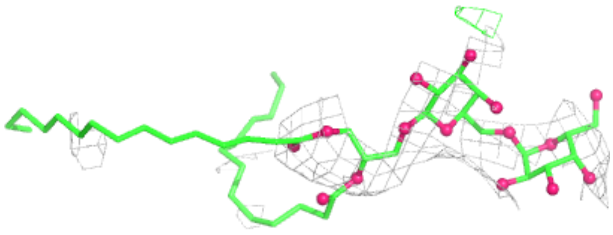






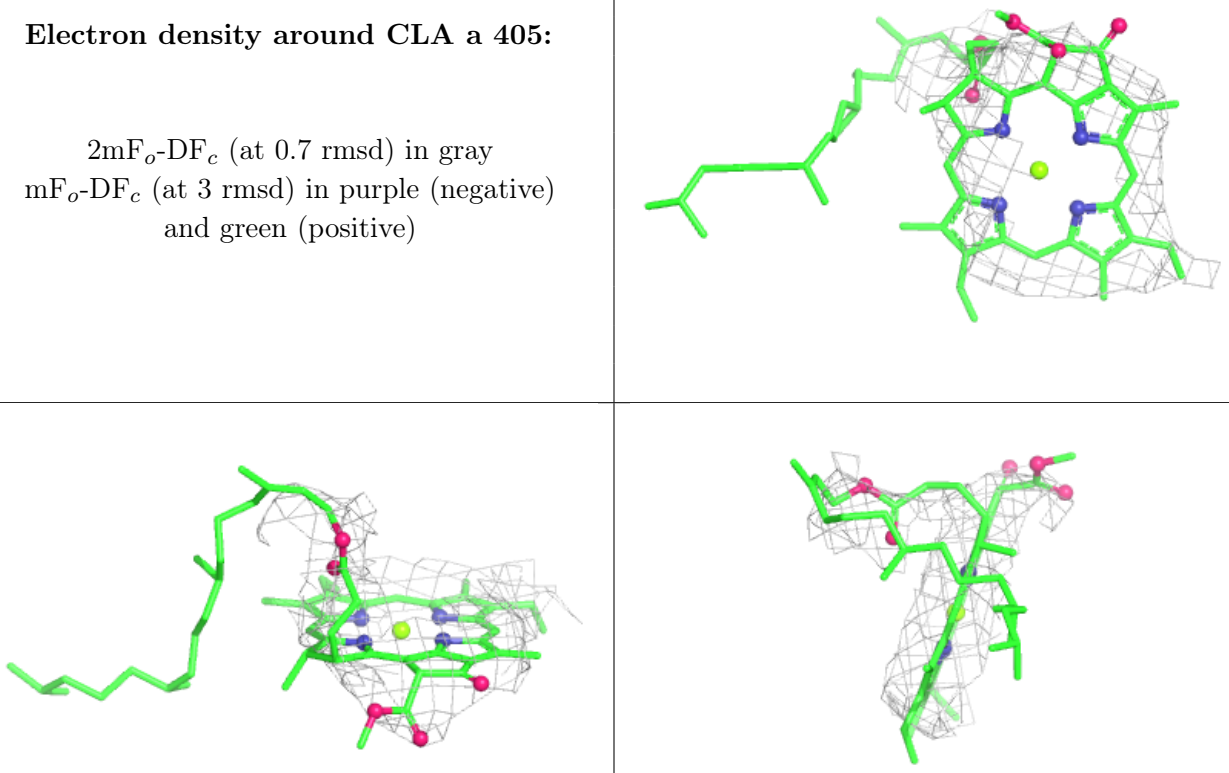
Electron density around DGD b 622:

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



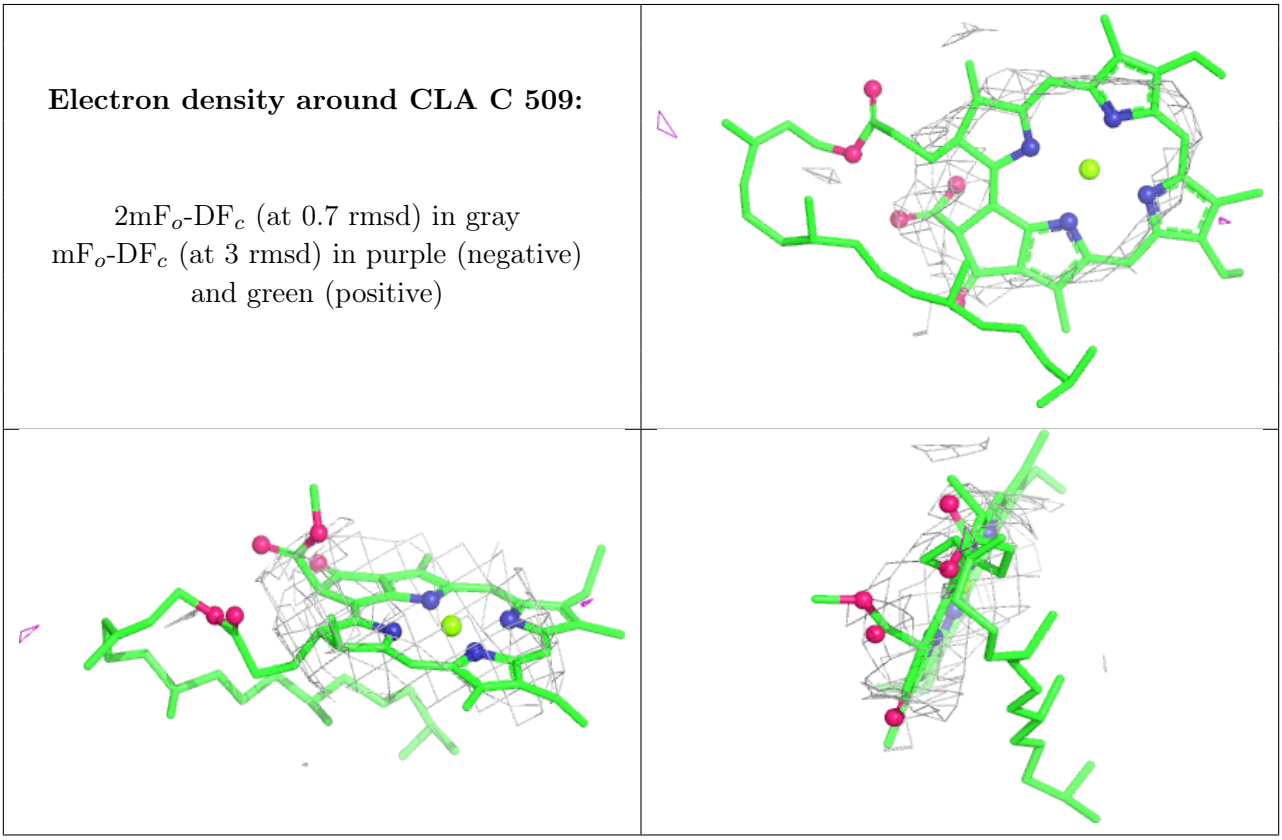
Electron density around CLA a 405:

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



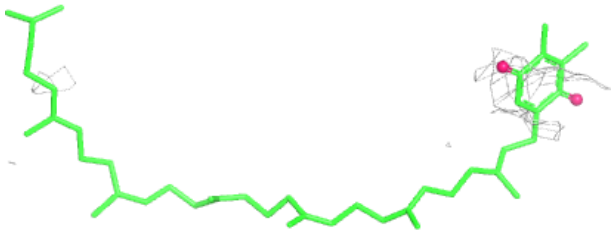
Electron density around CLA C 509:

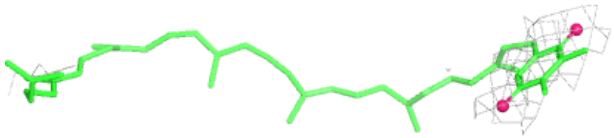
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PL9 a 410:

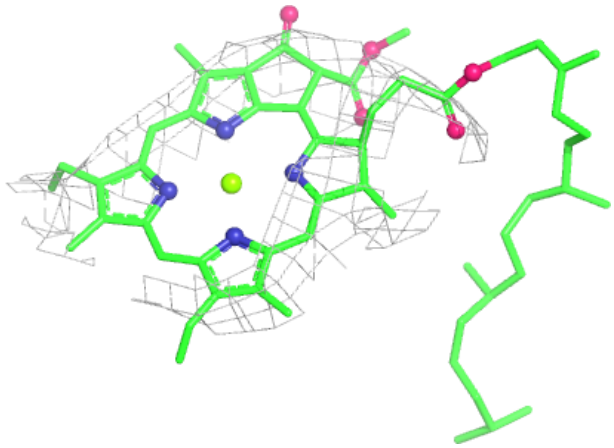
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

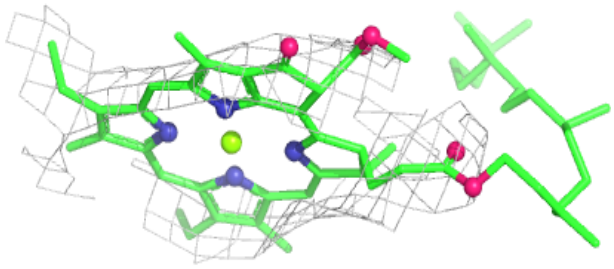


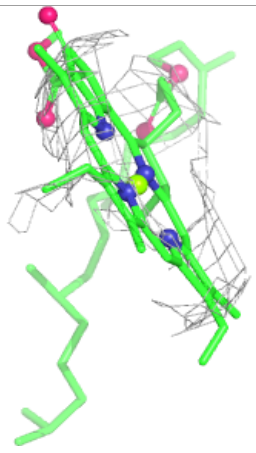


Electron density around CLA B 616:

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

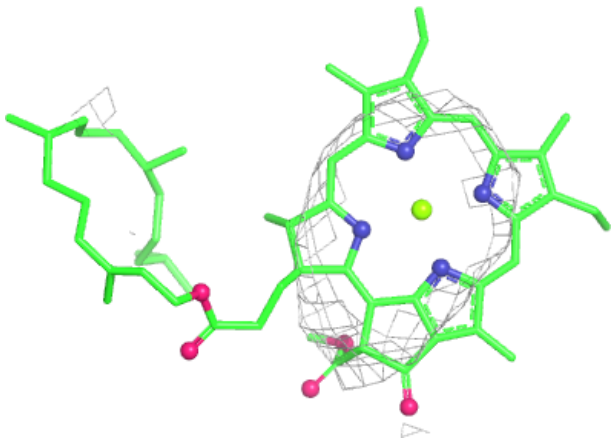


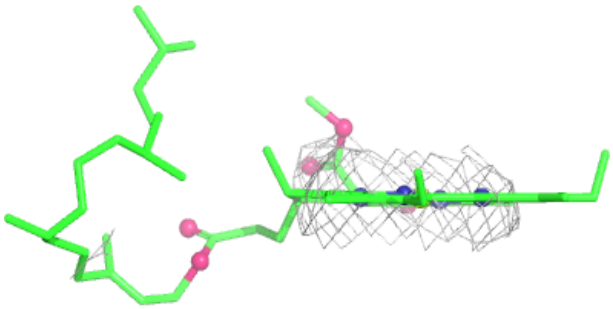


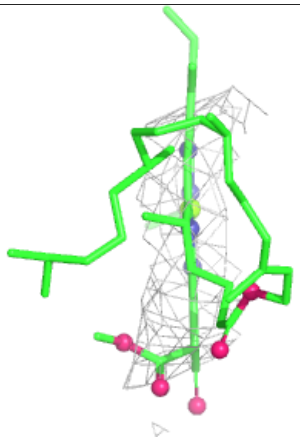


Electron density around CLA c 512:

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

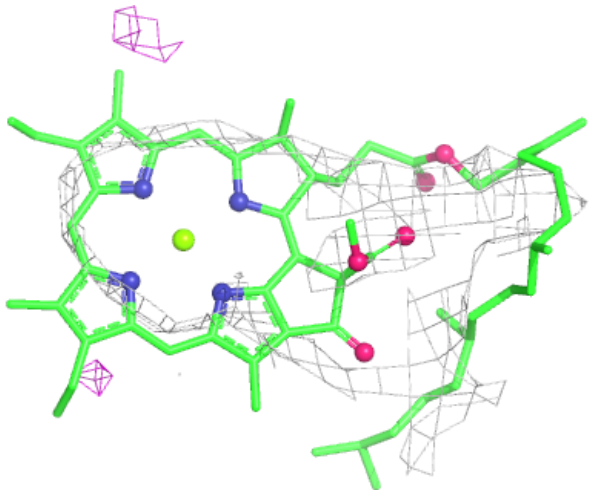


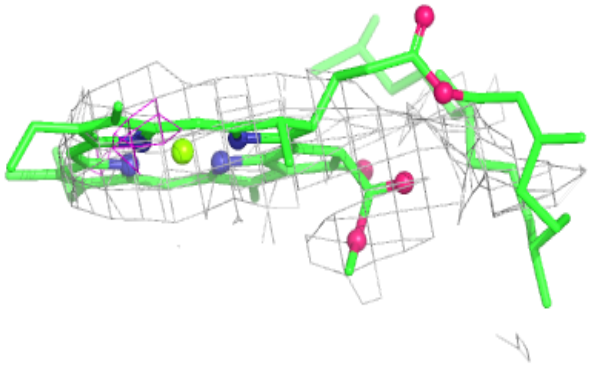




Electron density around CLA B 610:

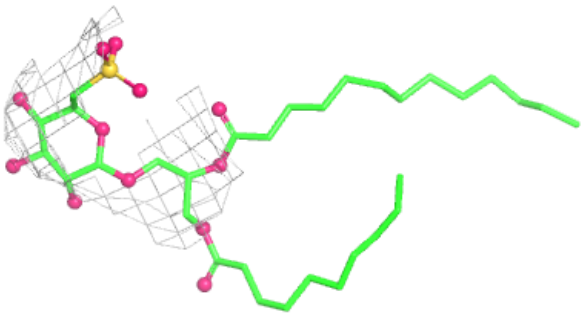
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

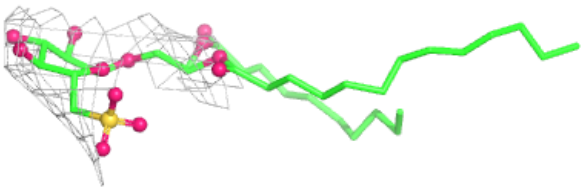




Electron density around SQD f 103:

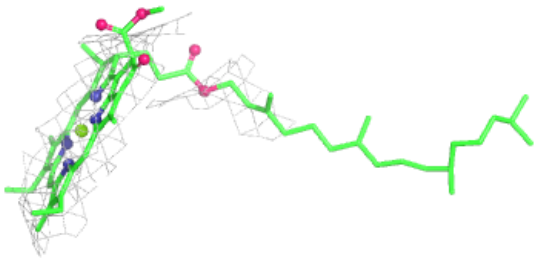
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

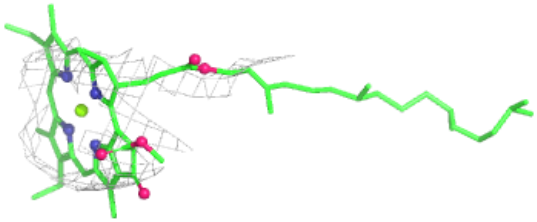


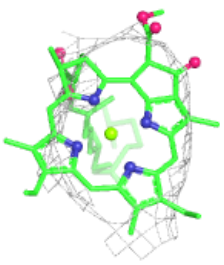


Electron density around CLA b 607:

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

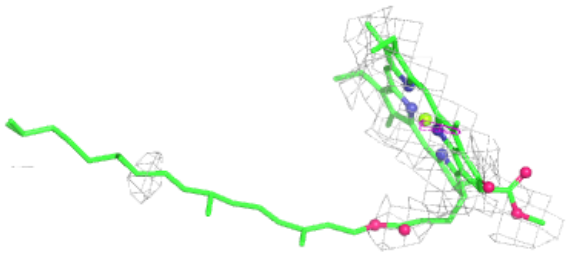


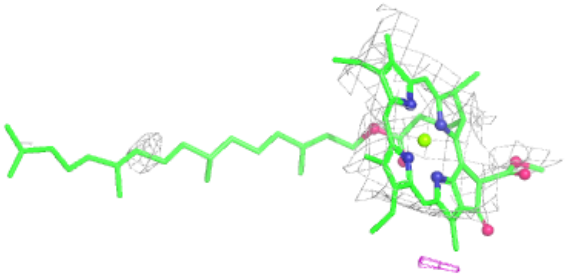




Electron density around CLA b 610:

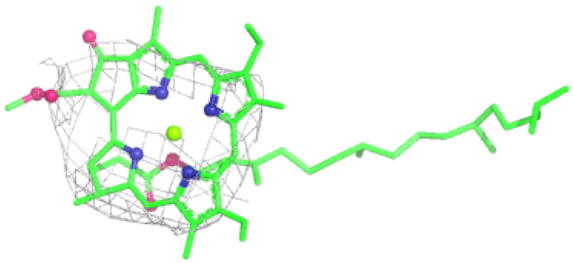
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

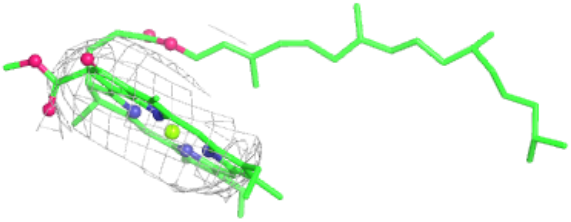


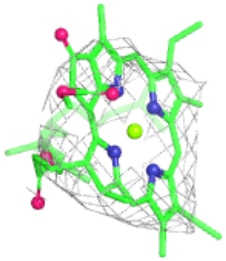


Electron density around CLA B 608:

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

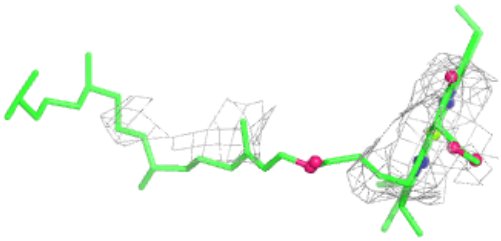


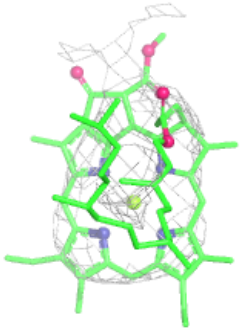




Electron density around CLA D 403:

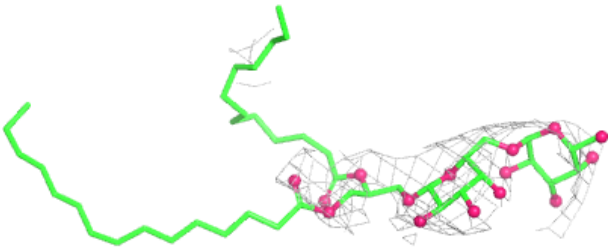
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





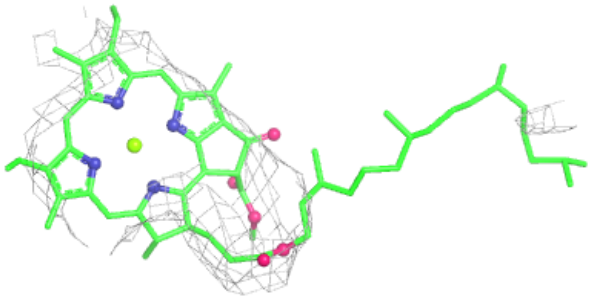
Electron density around DGD B 621:

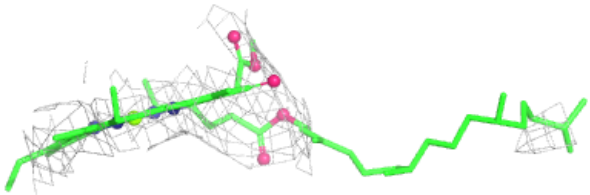
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

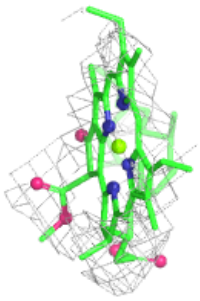


Electron density around CLA B 602:

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

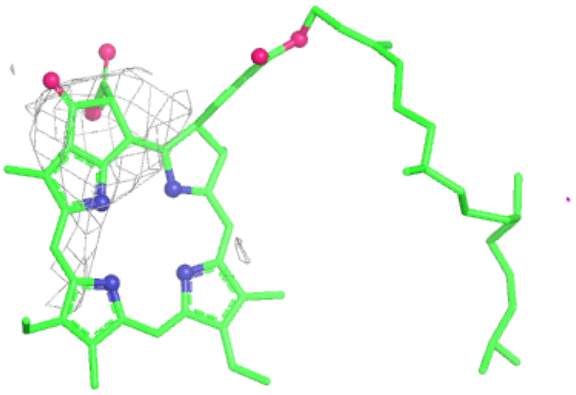


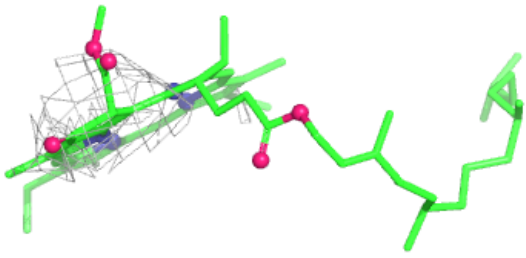


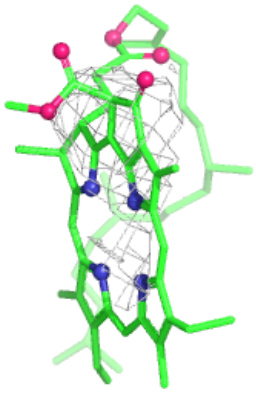


Electron density around PHO a 408:

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

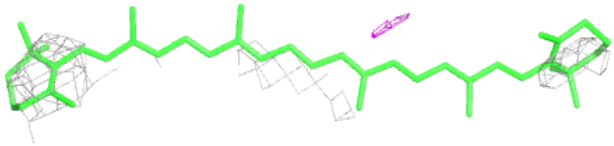


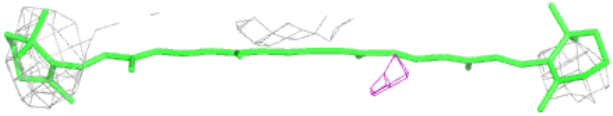


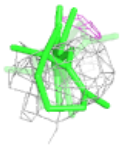


Electron density around BCR B 619:

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

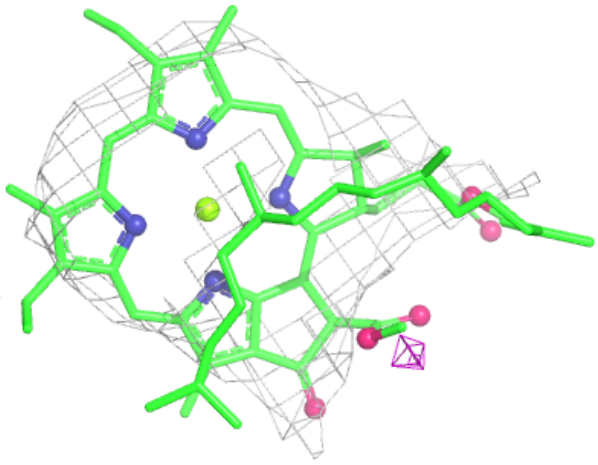


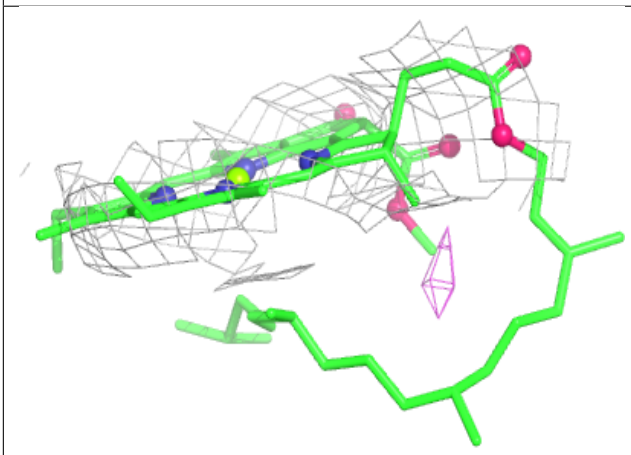


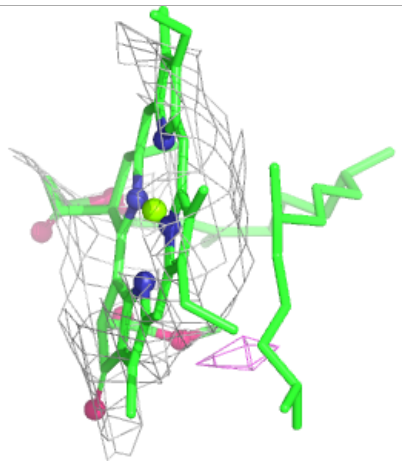


Electron density around CLA c 510:

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

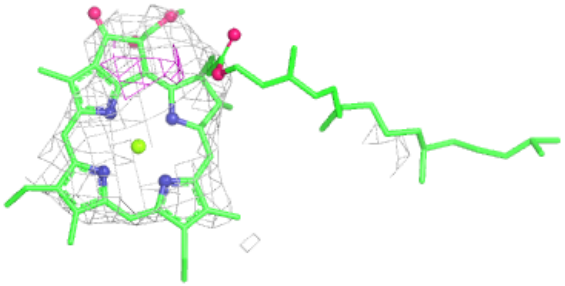


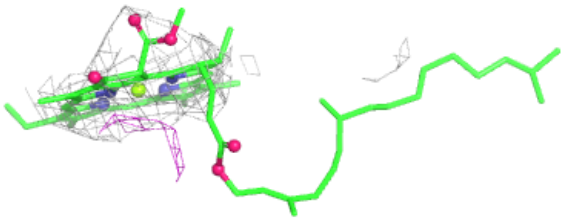


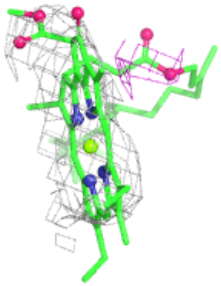


Electron density around CLA A 405:

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

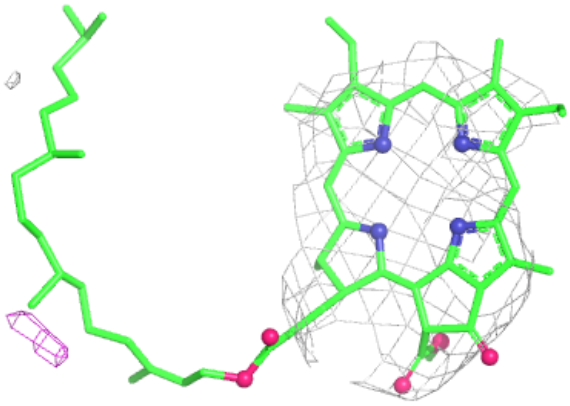


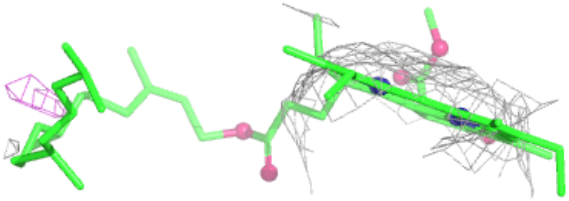


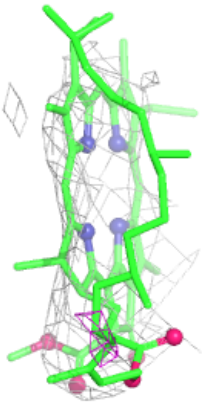


Electron density around PHO a 407:

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

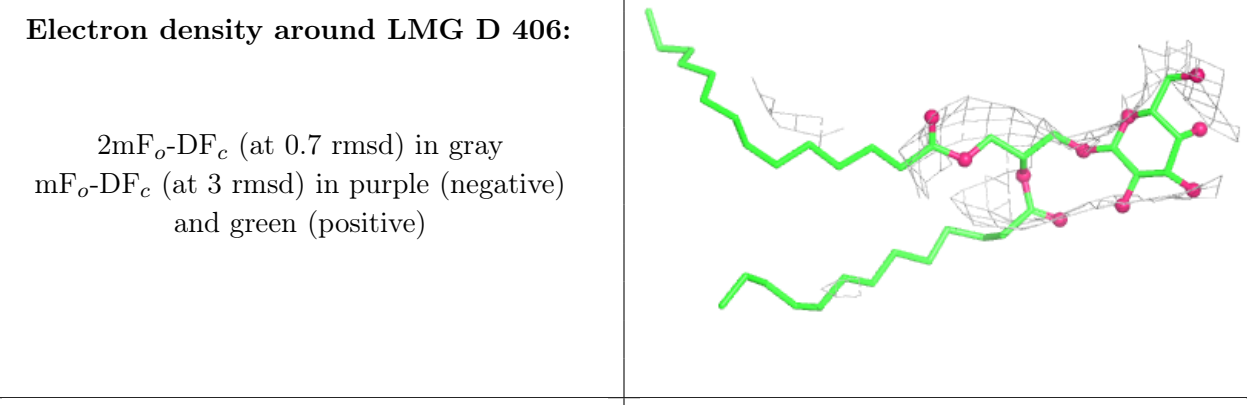


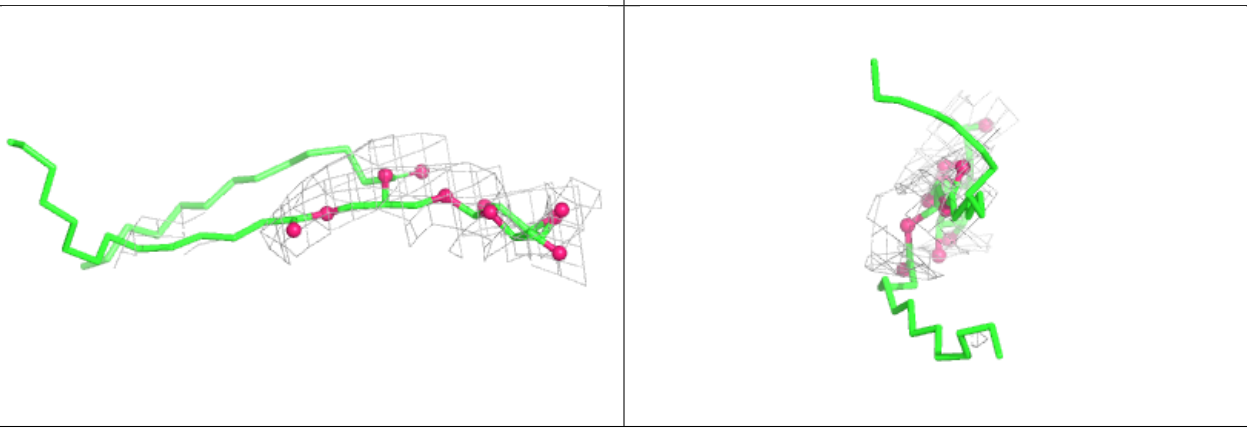




Electron density around LMG D 406:

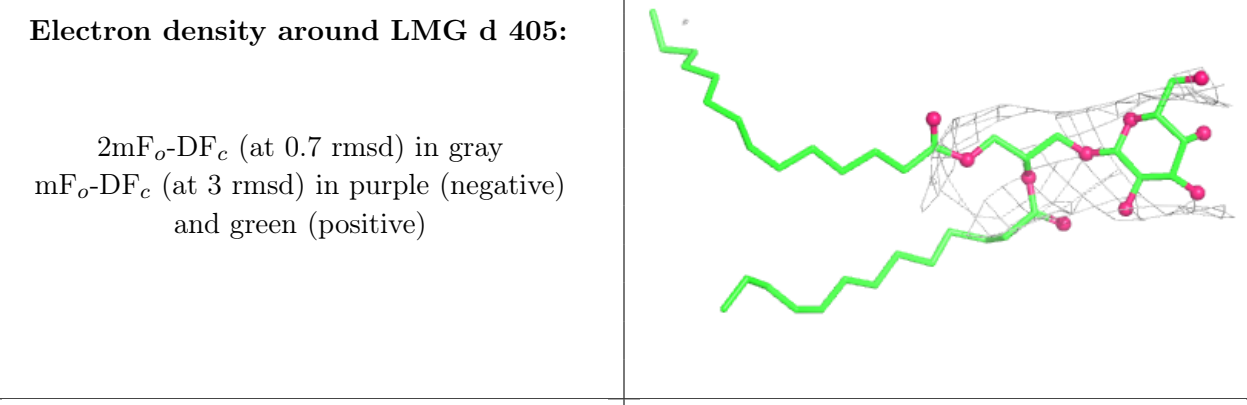
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

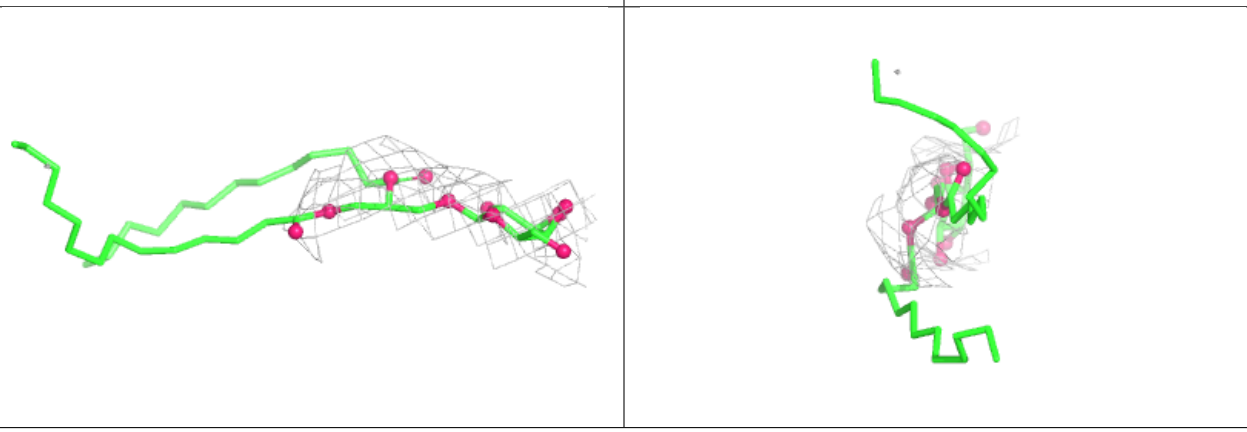




Electron density around LMG d 405:

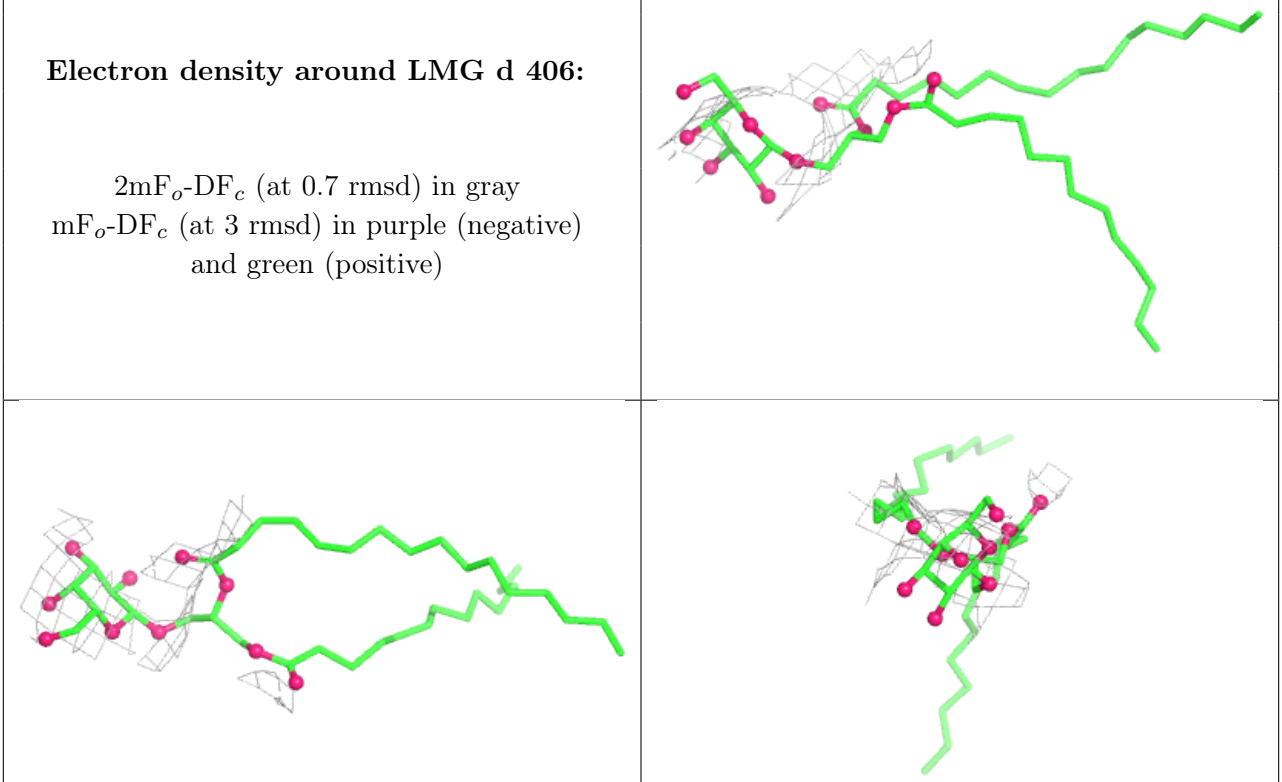
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





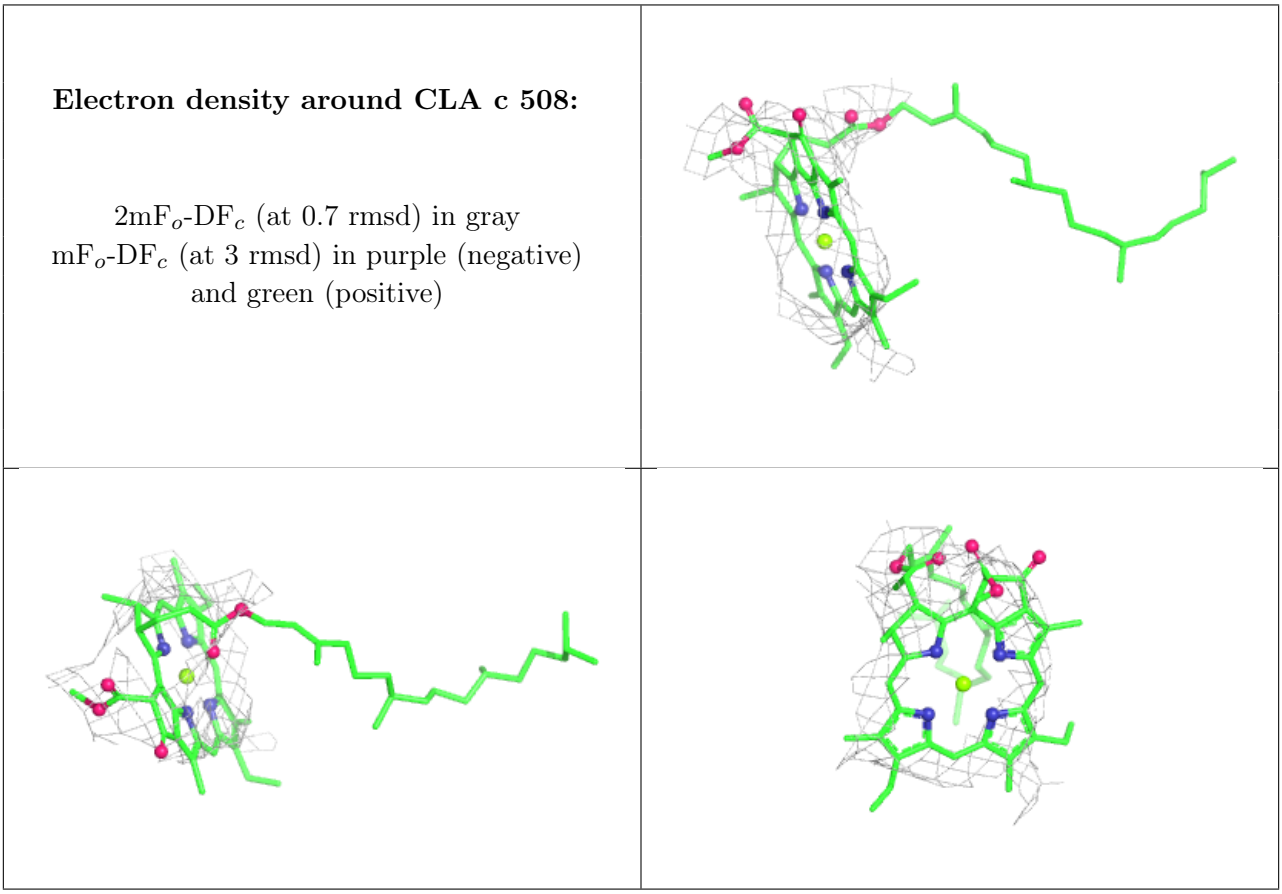
Electron density around LMG d 406:

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



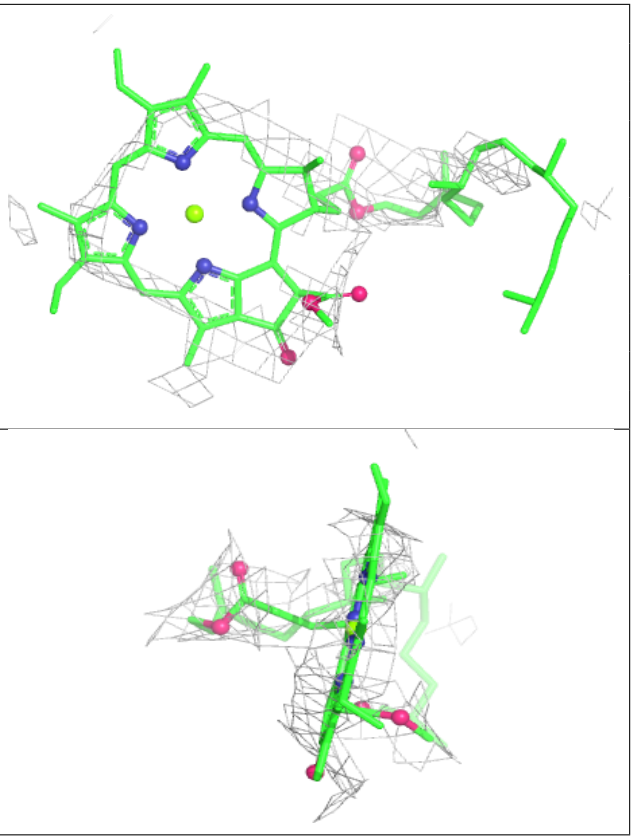
Electron density around CLA c 508:

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



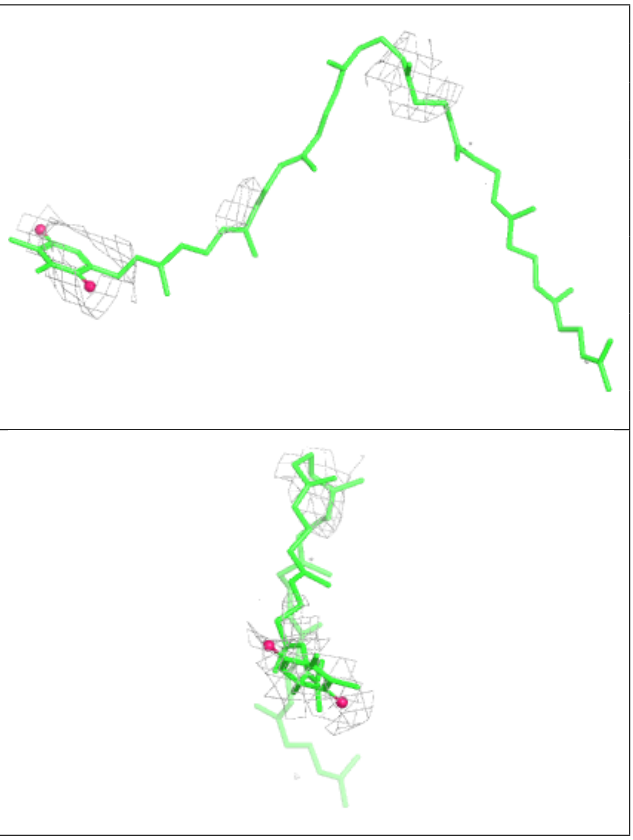
Electron density around CLA B 612:

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



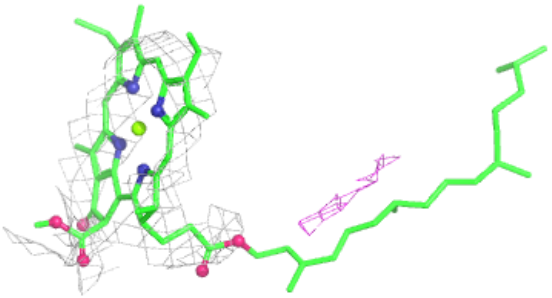
Electron density around PL9 D 404:

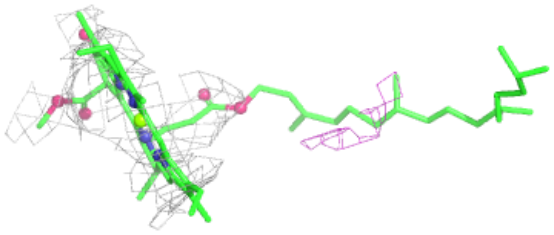
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

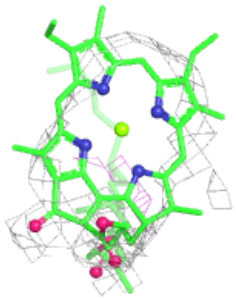


Electron density around CLA B 609:

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

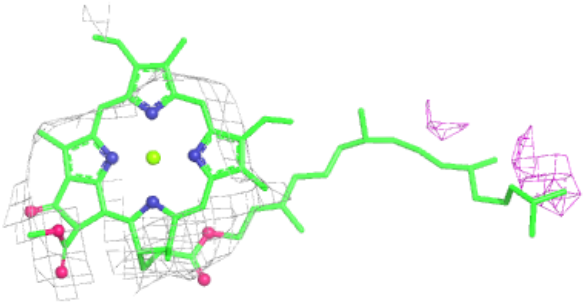


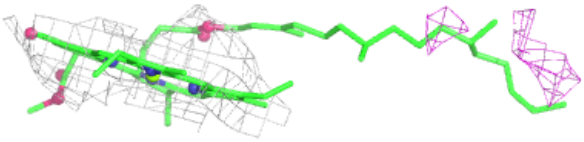


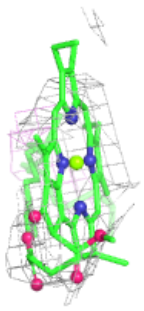


Electron density around CLA B 603:

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

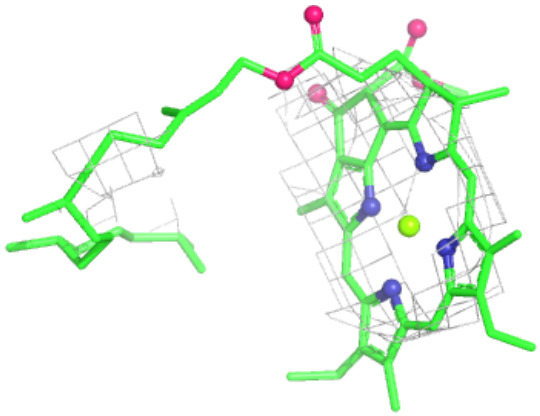


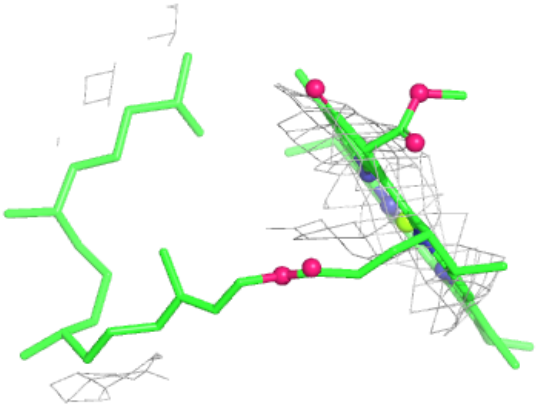


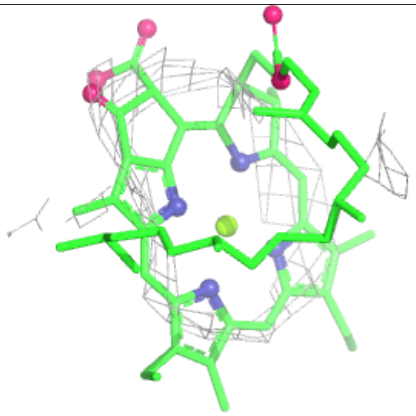


Electron density around CLA c 503:

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

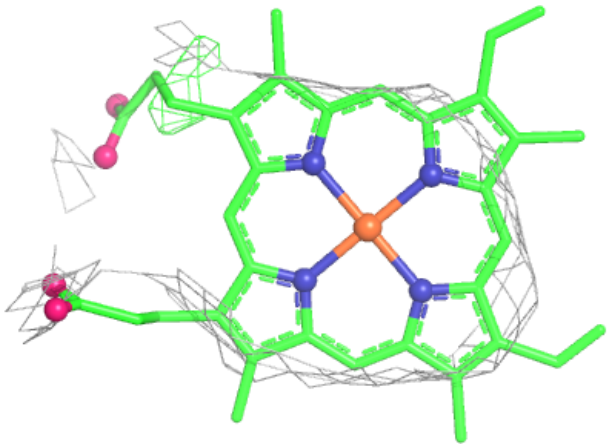


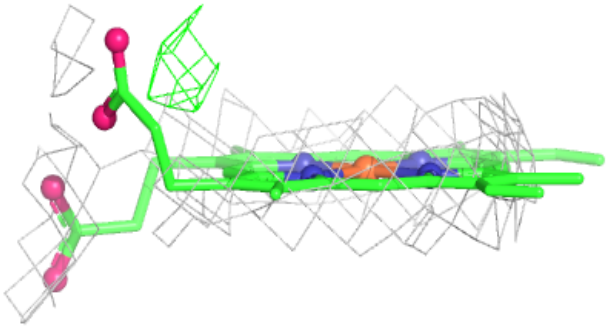


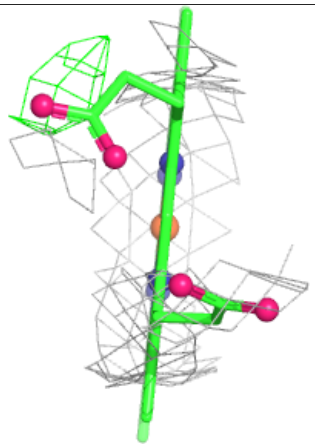


Electron density around HEM f 101:

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

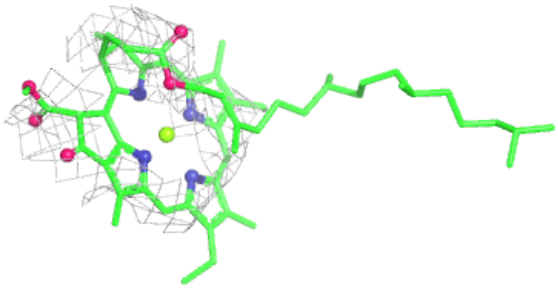


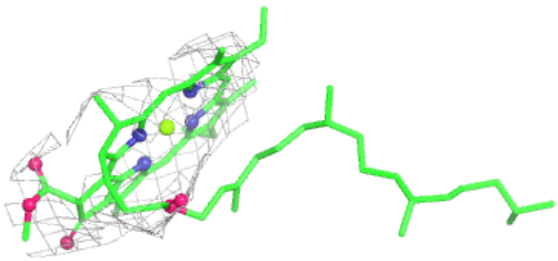


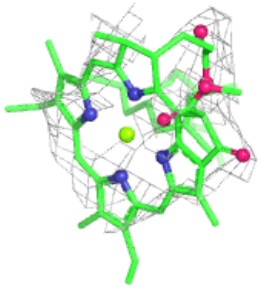


Electron density around CLA c 505:

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

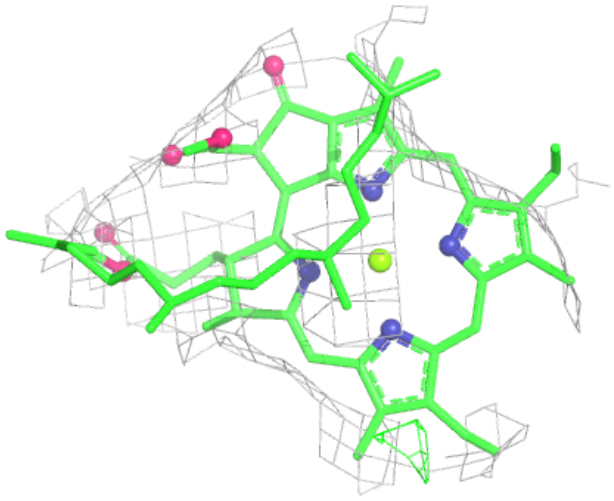


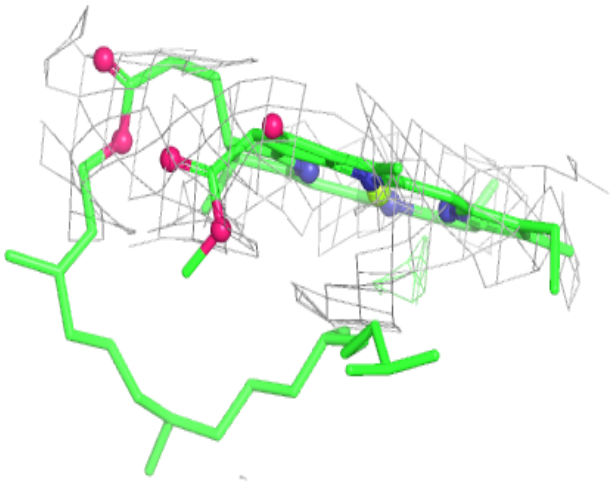


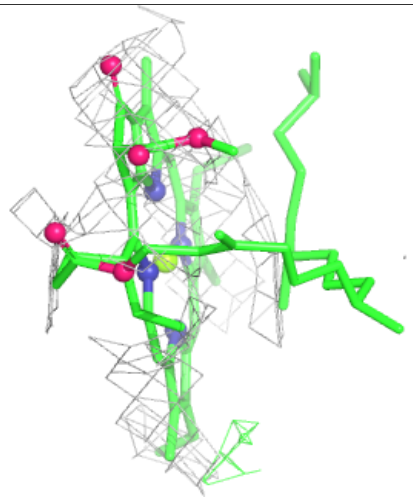


Electron density around CLA C 510:

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

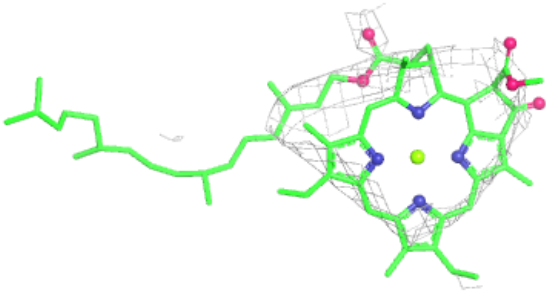


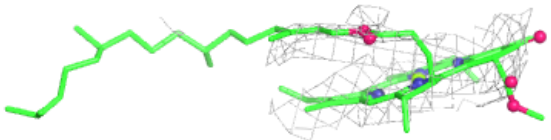


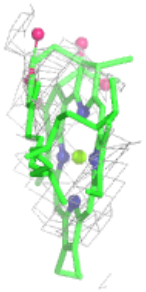


Electron density around CLA b 606:

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

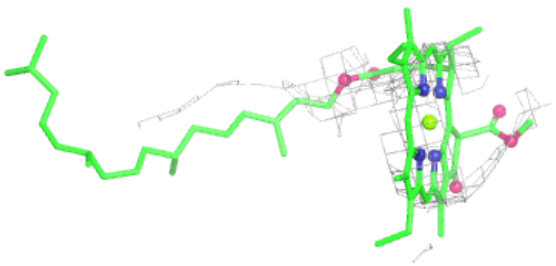


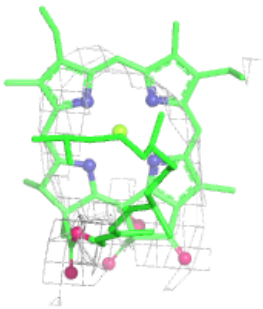




Electron density around CLA B 605:

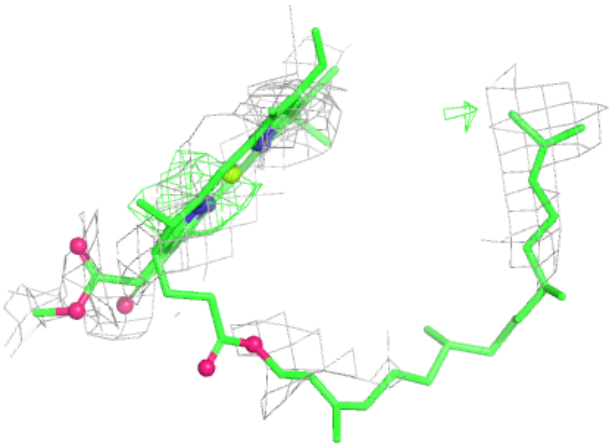
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

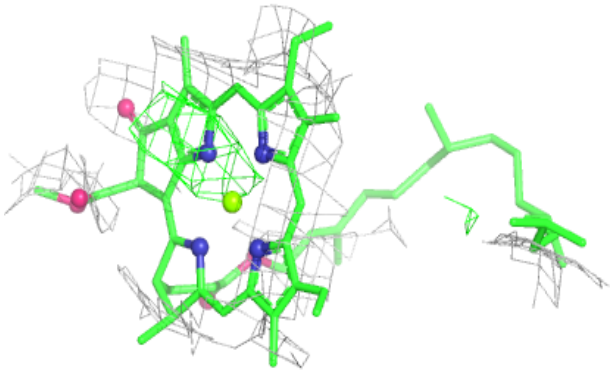


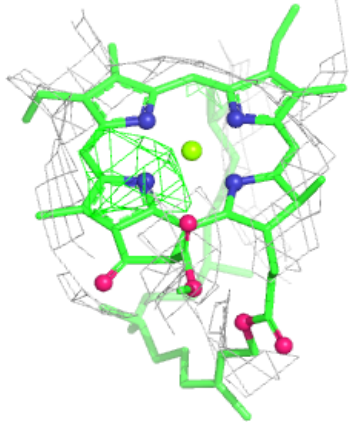


Electron density around CLA b 614:

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

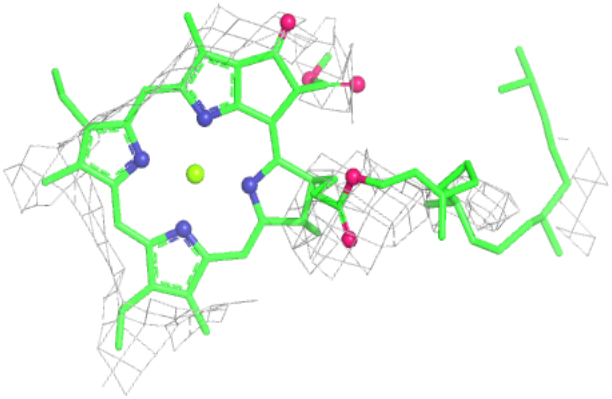


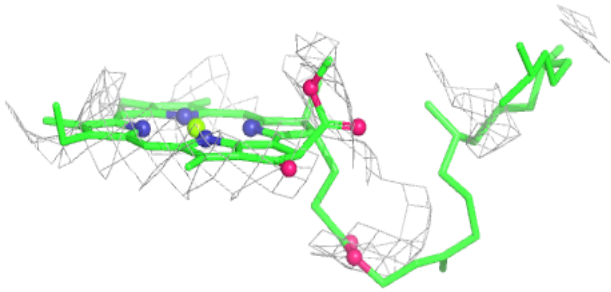


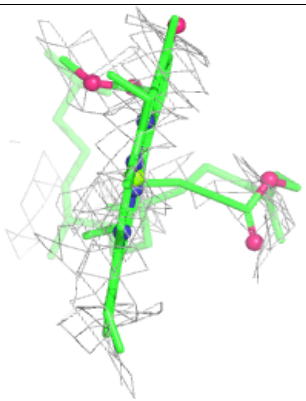


Electron density around CLA b 615:

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

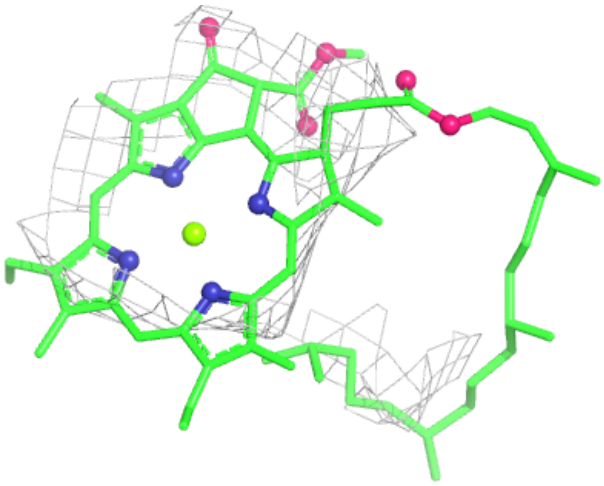


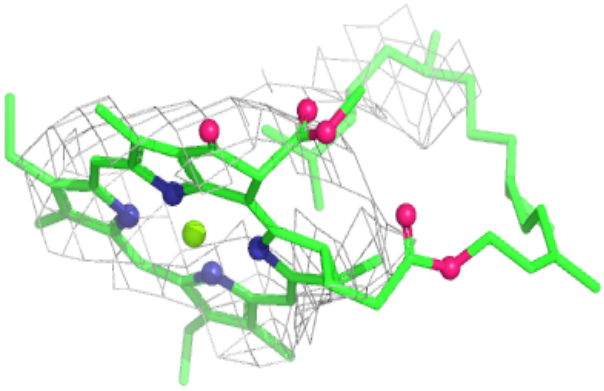




Electron density around CLA B 615:

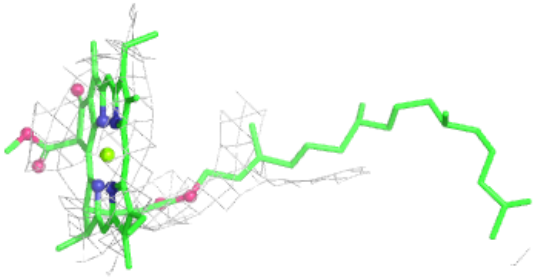
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

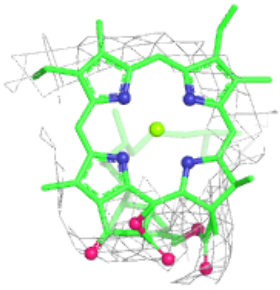




Electron density around CLA b 608:

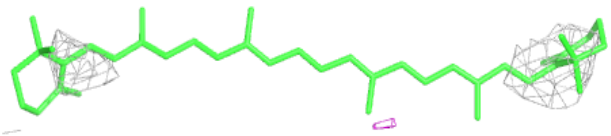
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

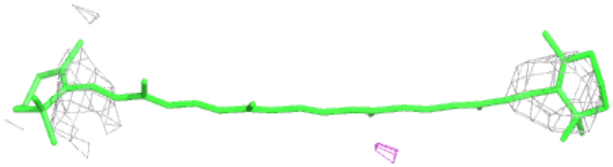


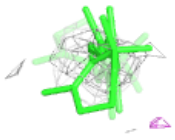


Electron density around BCR B 617:

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

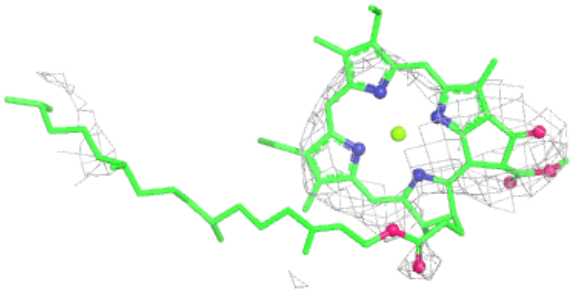


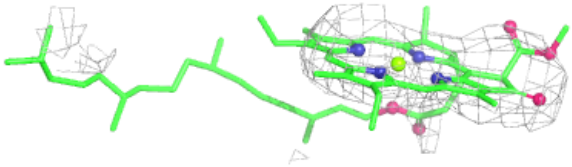


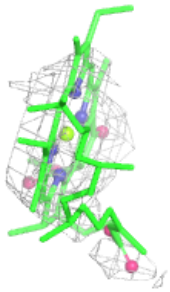


Electron density around CLA c 501:

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

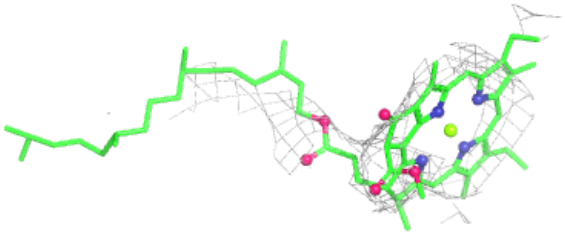


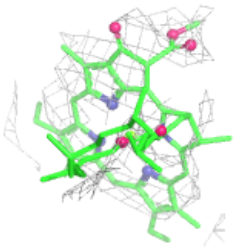




Electron density around CLA c 502:

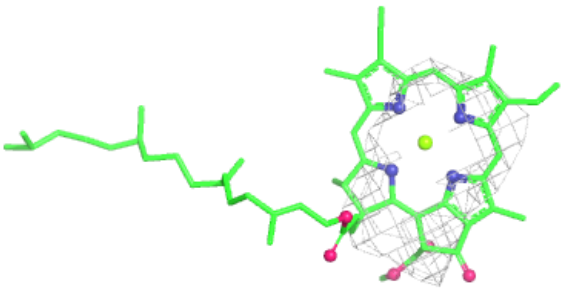
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

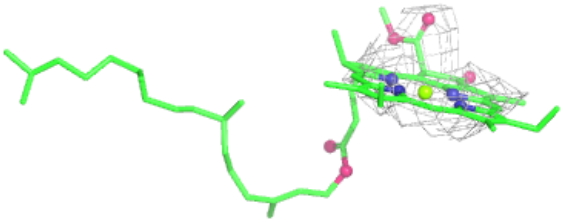




Electron density around CLA a 406:

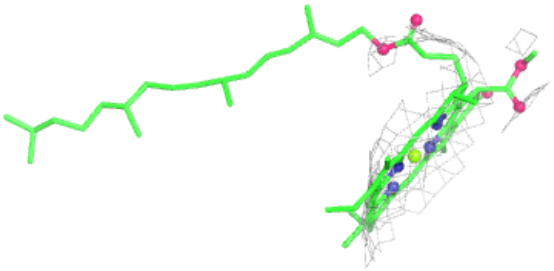
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

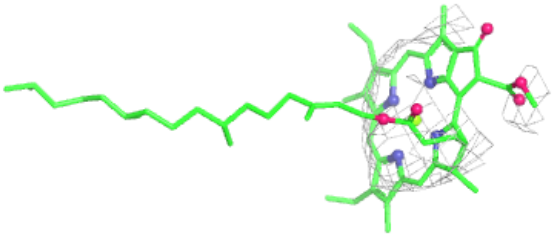




Electron density around CLA c 504:

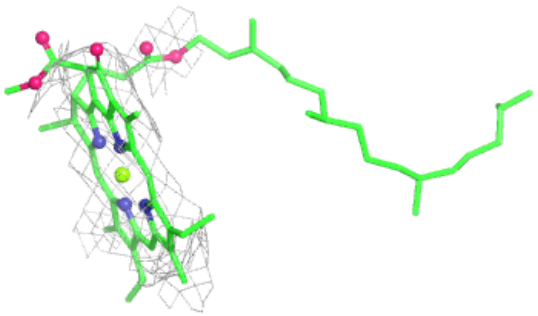
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

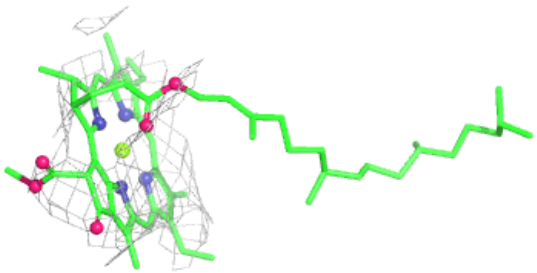


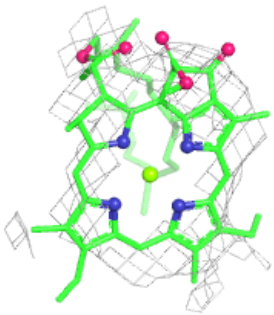


Electron density around CLA C 508:

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

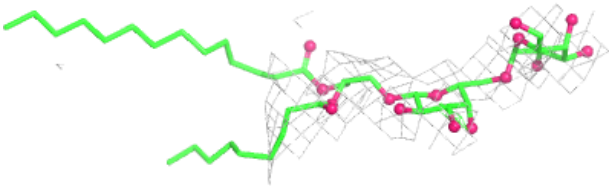


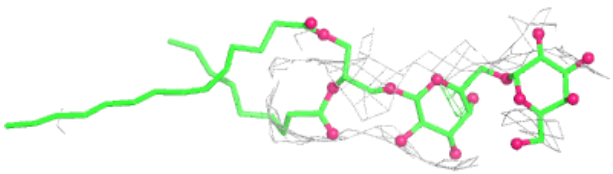


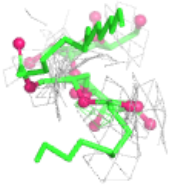


Electron density around DGD c 517:

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

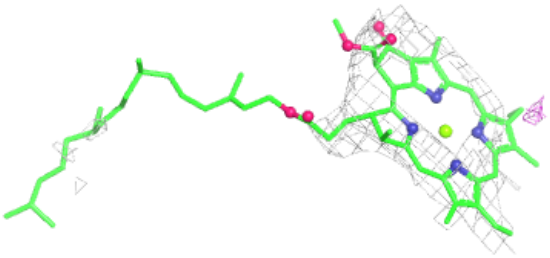


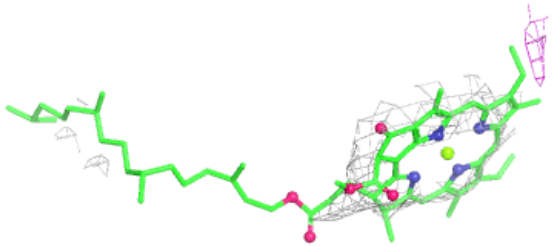


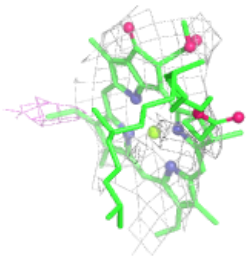


Electron density around CLA A 403:

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

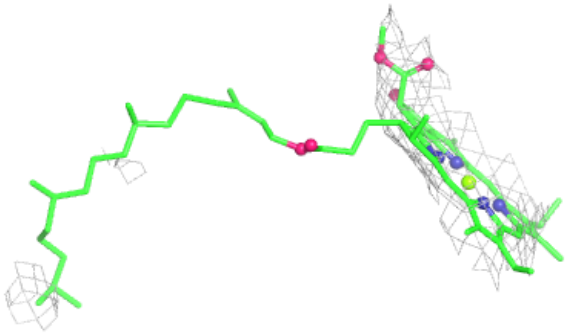


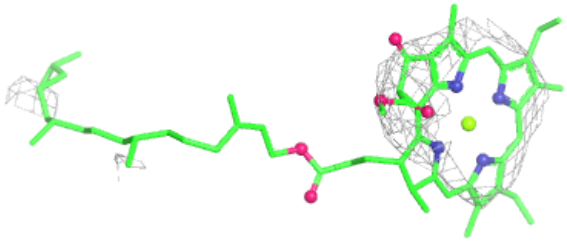


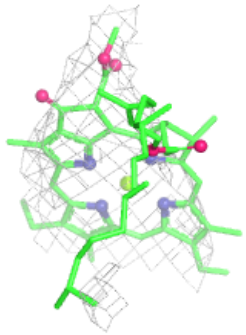


Electron density around CLA D 401:

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

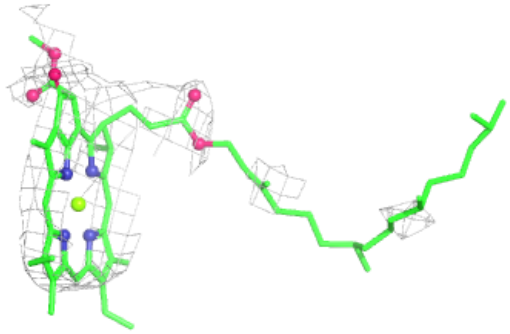


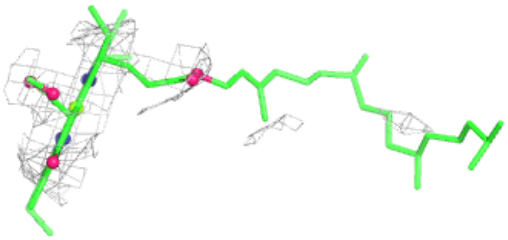


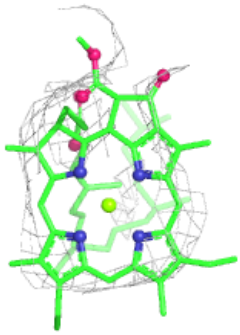


Electron density around CLA d 403:

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

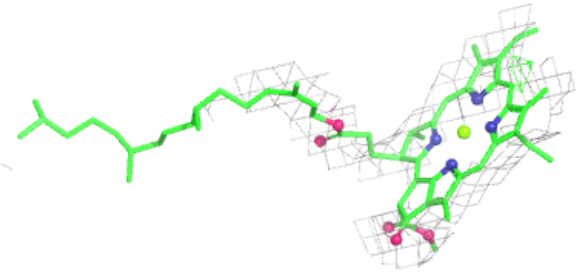


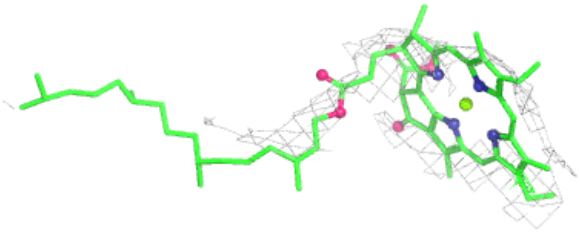


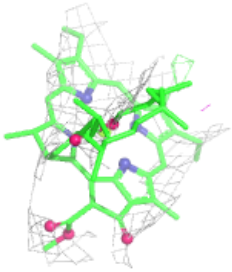


Electron density around CLA C 502:

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

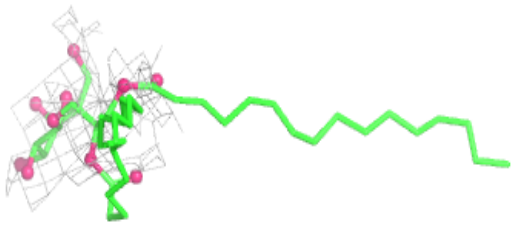






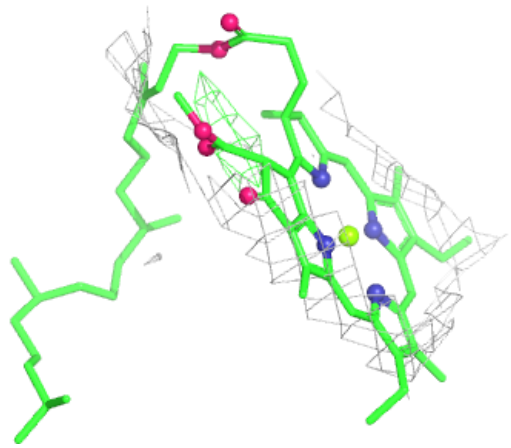
Electron density around LMG A 414:

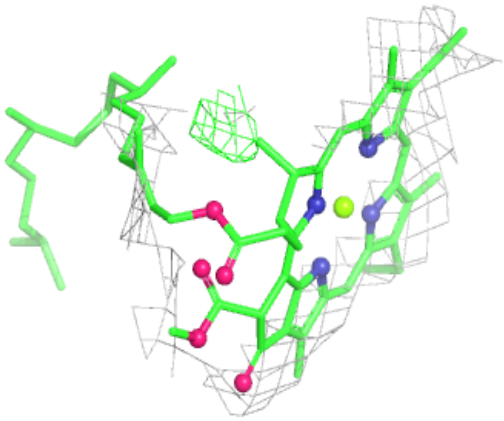
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

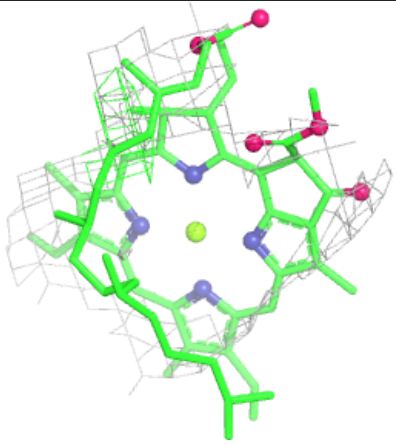


Electron density around CLA b 616:

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

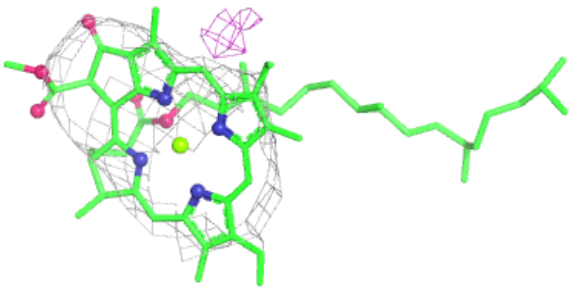


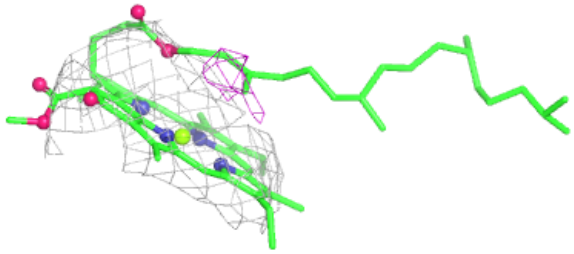


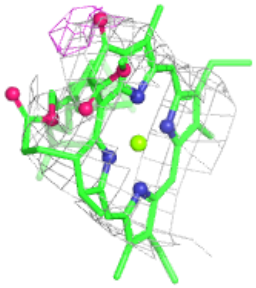


Electron density around CLA b 617:

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

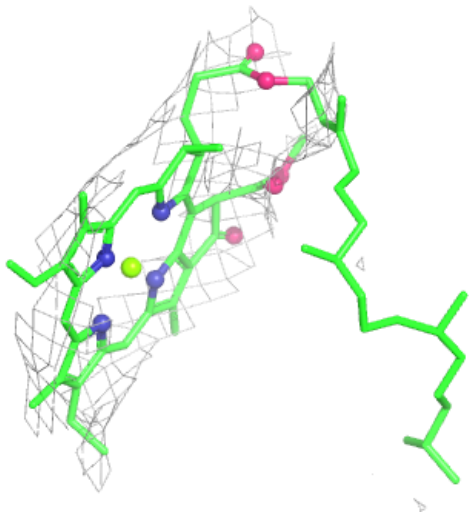


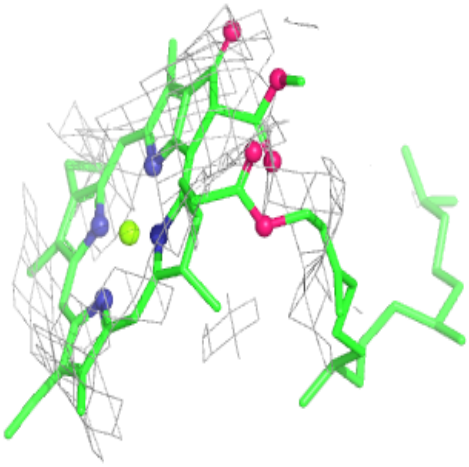


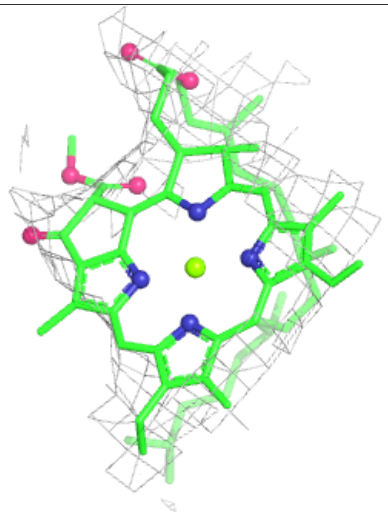


Electron density around CLA B 613:

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

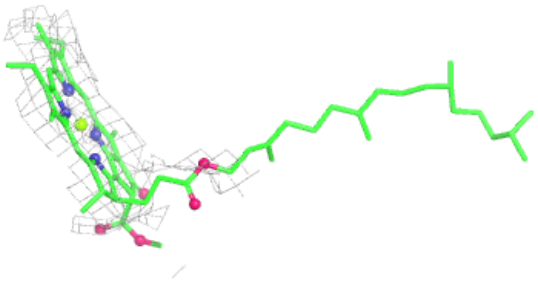


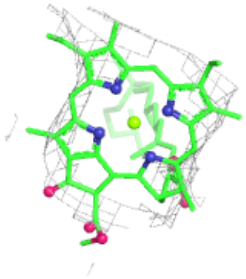




Electron density around CLA B 604:

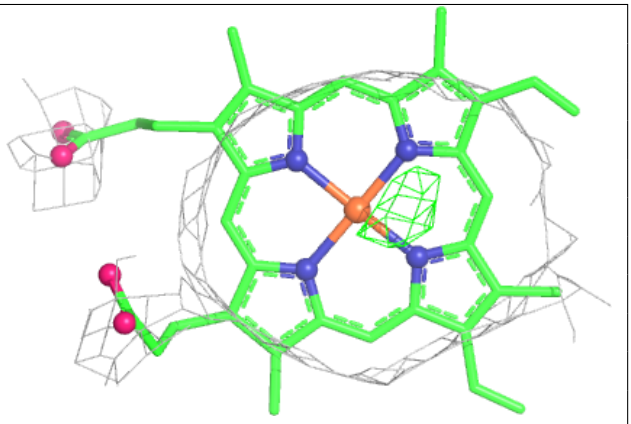
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

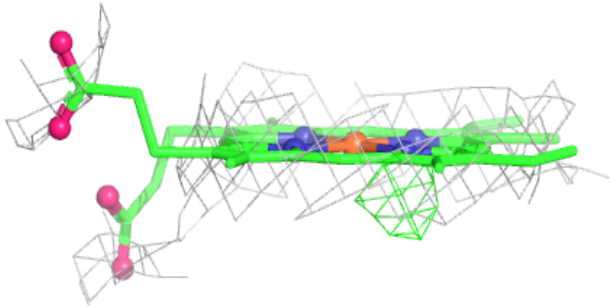


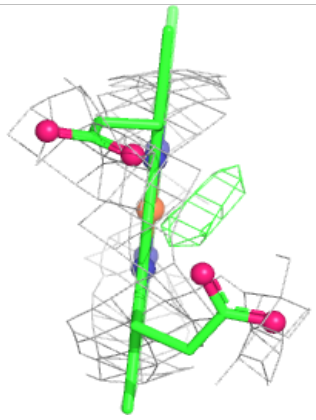


Electron density around HEM F 101:

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

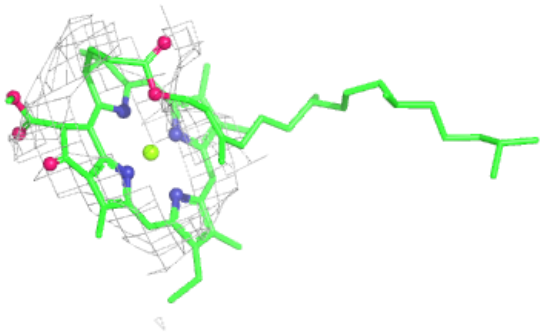


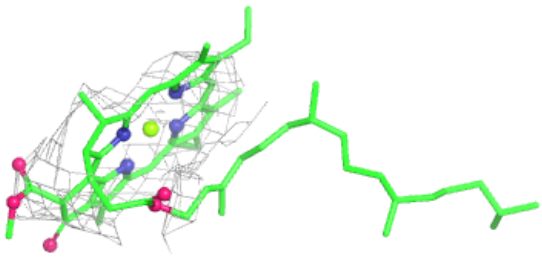


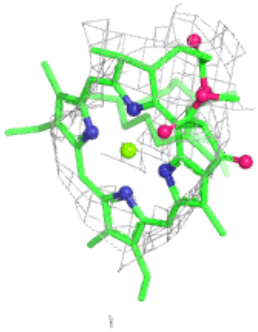


Electron density around CLA C 505:

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

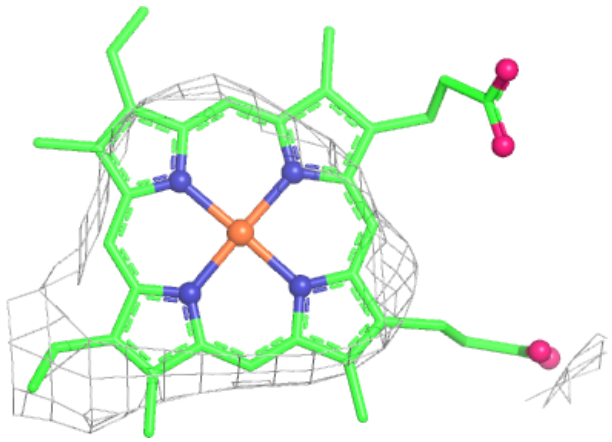


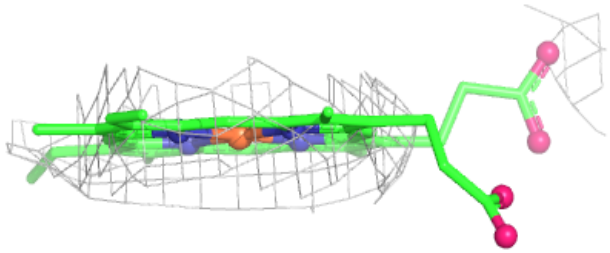


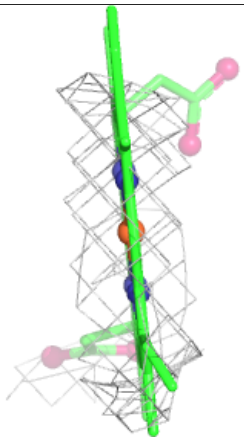


Electron density around HEM v 201:

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

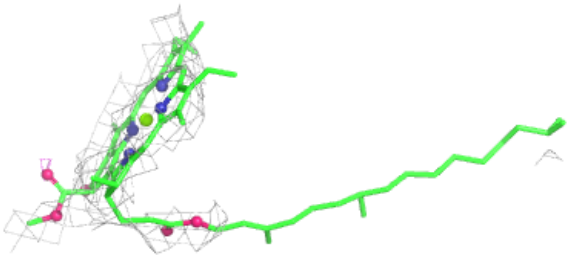


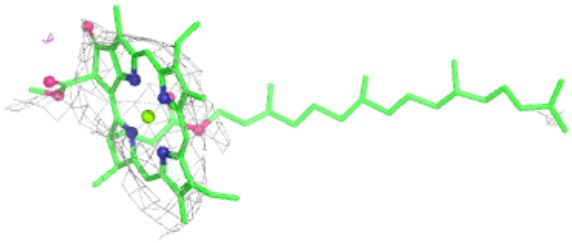


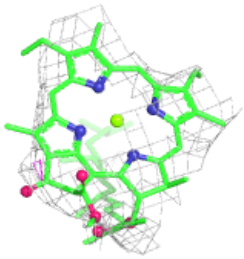


Electron density around CLA B 607:

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

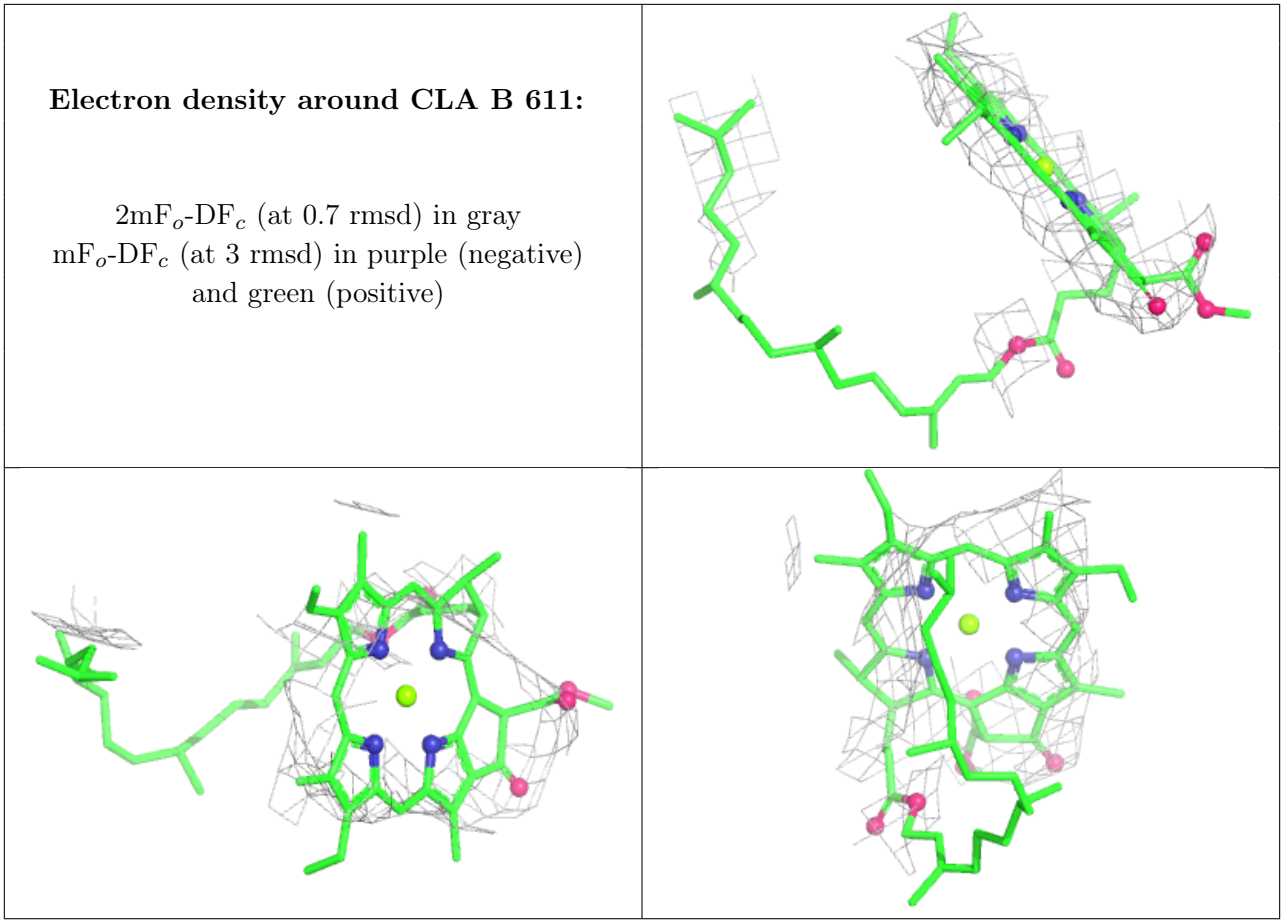






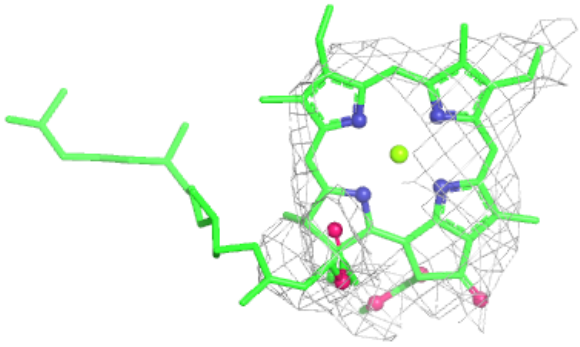
Electron density around CLA B 611:

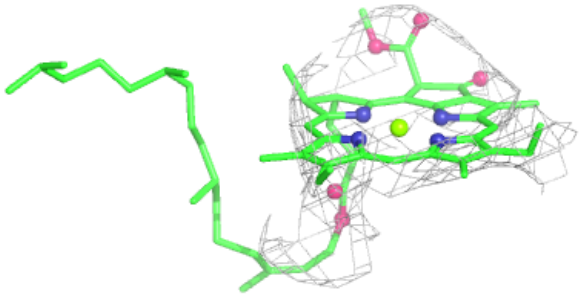
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 404:

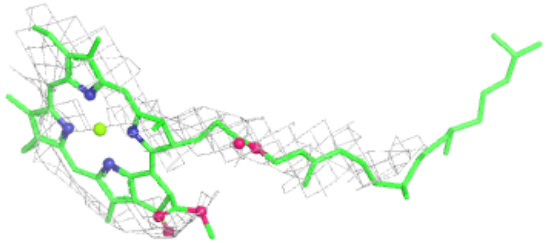
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

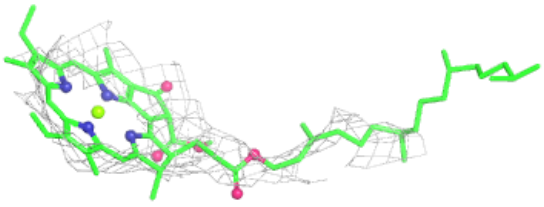


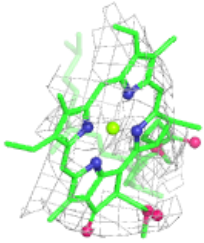


Electron density around CLA a 404:

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

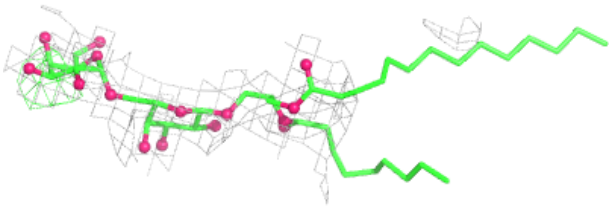


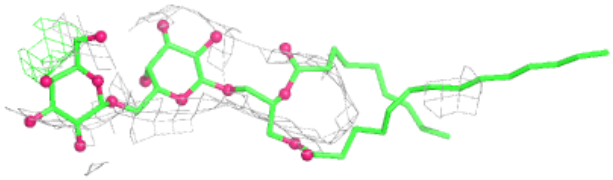


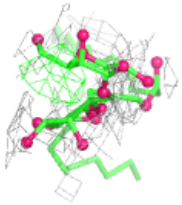


Electron density around DGD C 516:

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

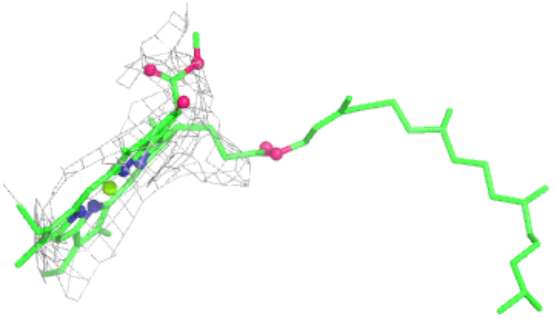


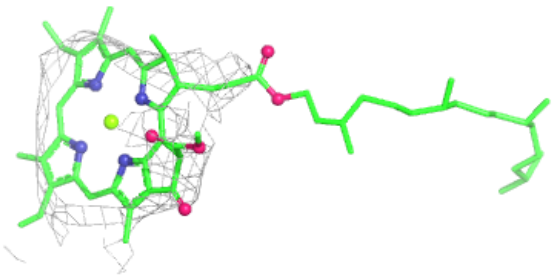


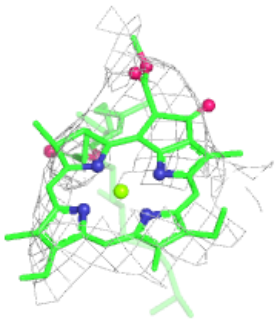


Electron density around CLA d 402:

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

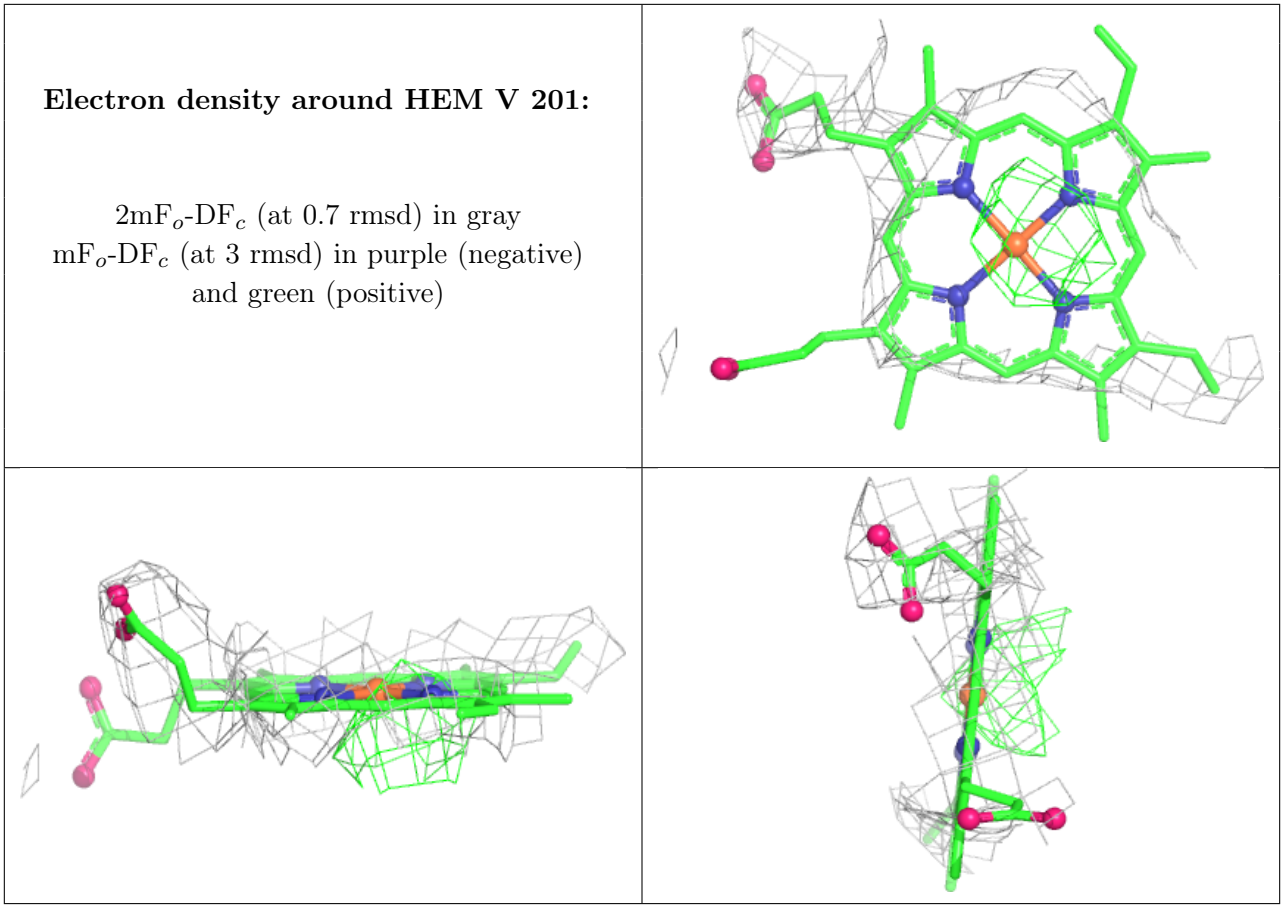






Electron density around HEM V 201:

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



6.5 Other polymers

There are no such residues in this entry.