Full wwPDB X-ray Structure Validation Report (i)

Apr 25, 2026 – 01:21 PM EDT

PDB ID	:	4IXR / pdb_00004ixr
Title	:	RT fs X-ray diffraction of Photosystem II, first illuminated 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	:	5.90 Å(reported)

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

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

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

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

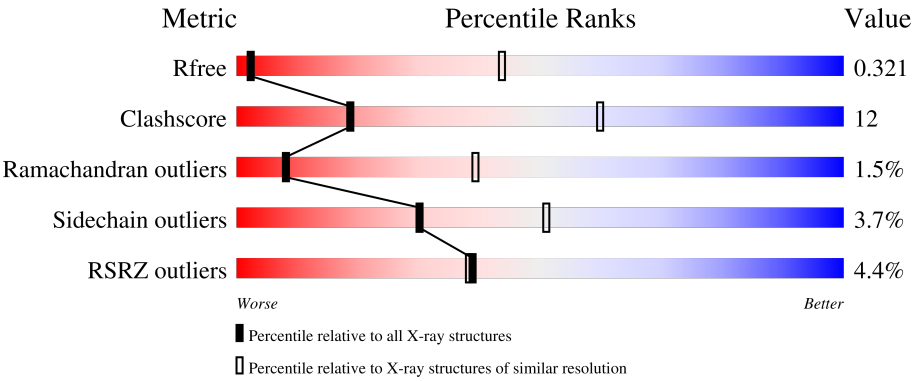
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)

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 5.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1135 (7.80-4.00)
Clashscore	190562	1201 (7.80-4.00)
Ramachandran outliers	187476	1026 (7.80-4.00)
Sidechain outliers	187428	1017 (7.82-3.98)
RSRZ outliers	180081	1128 (7.80-4.00)

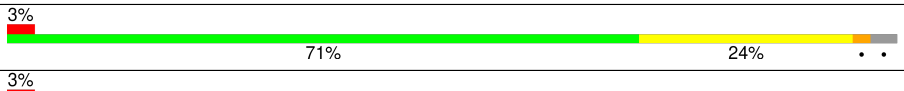
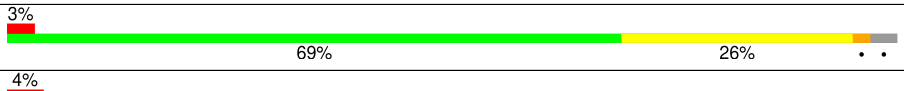
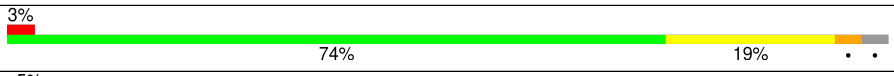
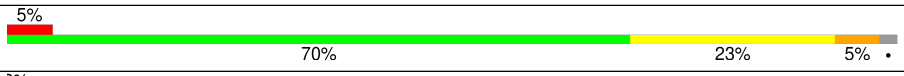
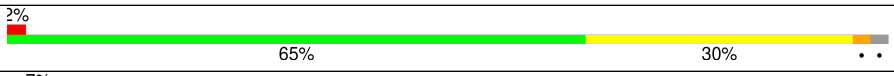
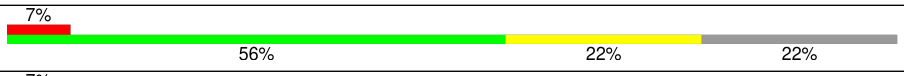
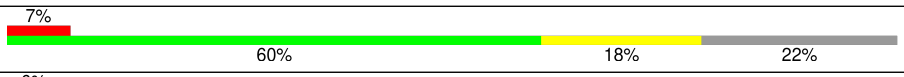
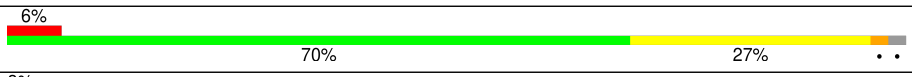
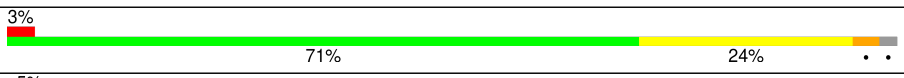
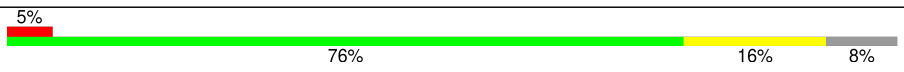
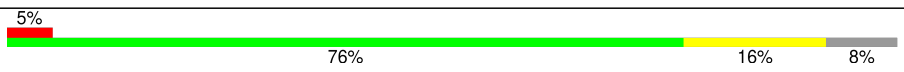
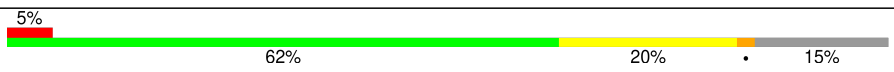
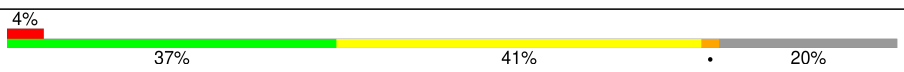
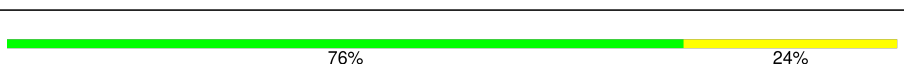
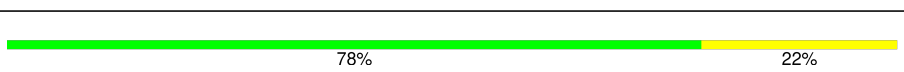
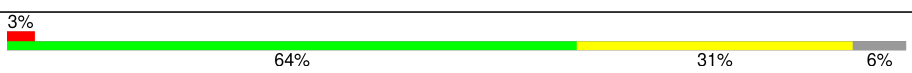
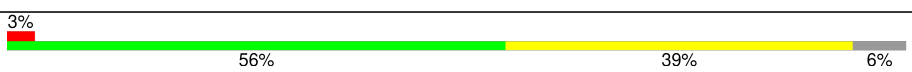
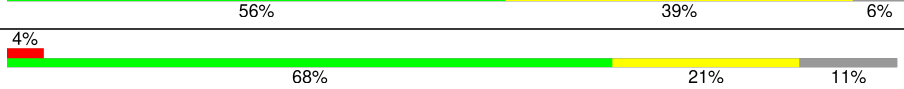
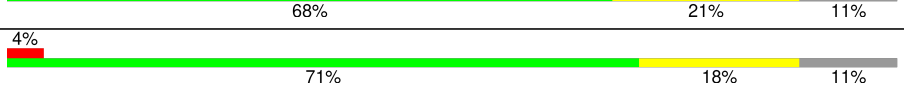
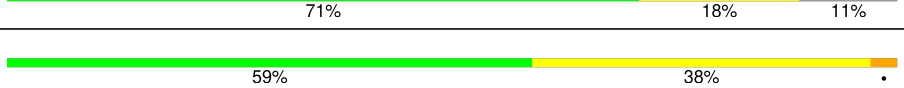
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% 63% 28% · 7%
1	a	360	3% 63% 28% · 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	3% 59% 41%
15	U	134	4% 61% 8% 28%
15	u	134	2% 56% 13% 28%
16	V	163	6% 71% 11% 16%
16	v	163	2% 73% 10% 16%
17	g	46	7% 41% 17% 39%
17	y	46	7% 41% 15% 39%
18	X	41	5% 59% 24% 5% 10%
18	x	41	12% 66% 22% 10%
19	Z	62	3% 79% 18%
19	z	62	3% 77% 19%
20	G	28	93% 7%
20	Y	28	93% 7%

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	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	612	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	b	620	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	PL9	J	101	-	-	-	X
27	BCR	j	102	-	-	-	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			

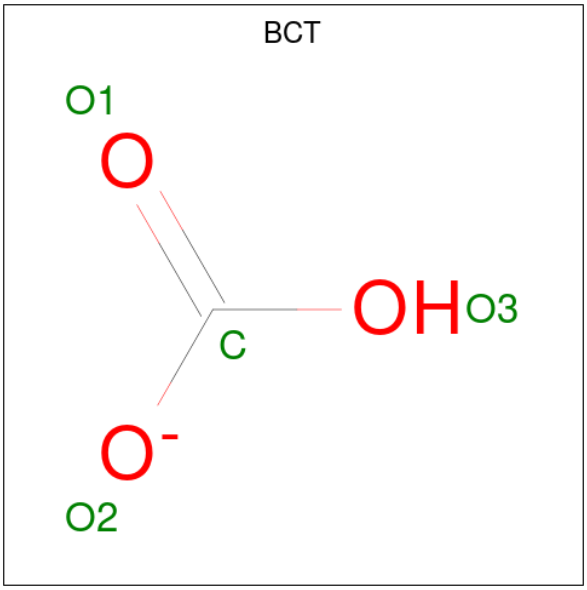
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

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

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

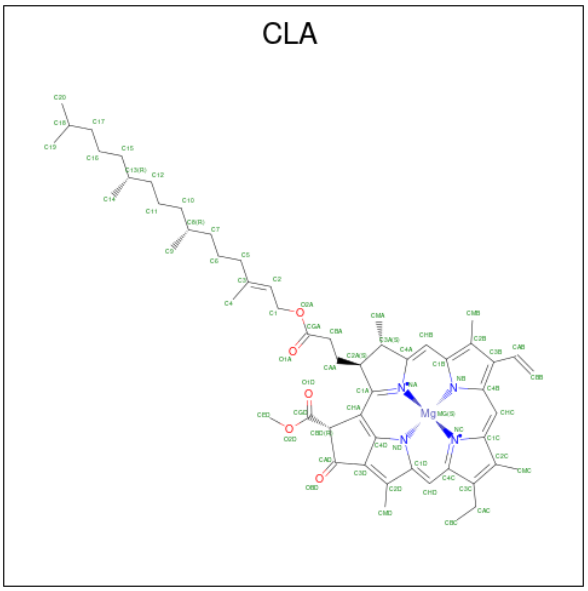
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total Fe 1 1	0	0
21	a	1	Total Fe 1 1	0	0

- 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	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...

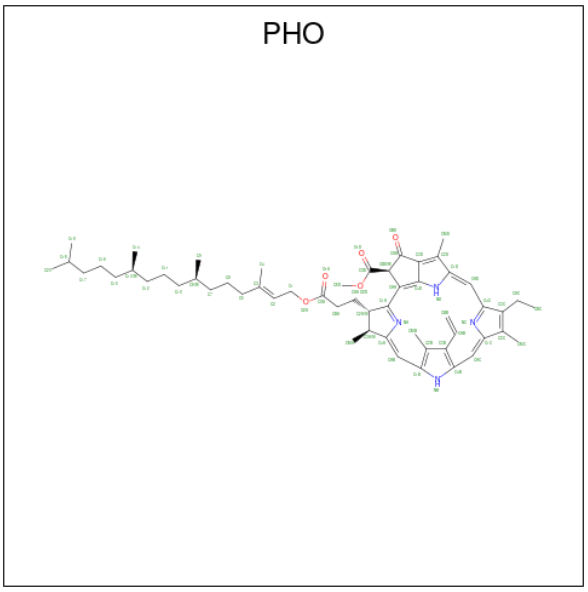
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

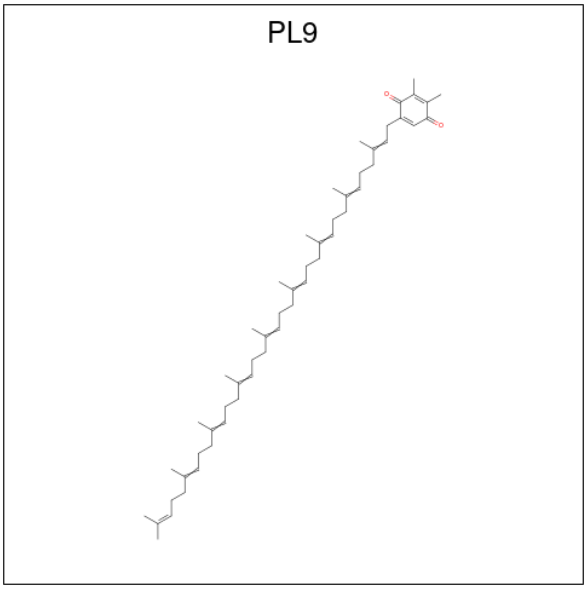
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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



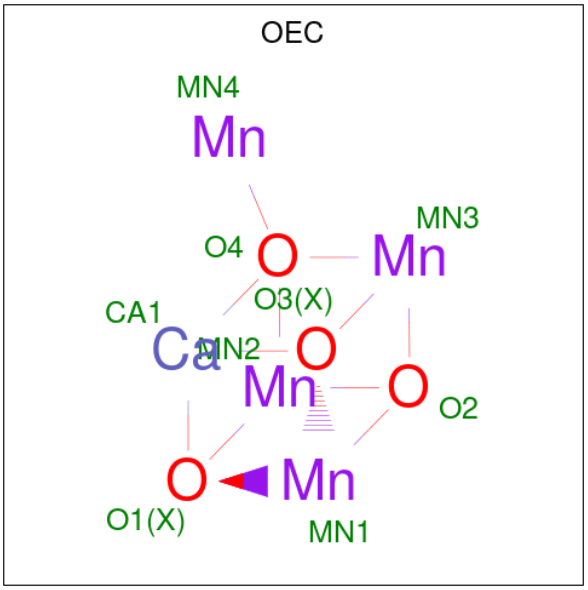
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



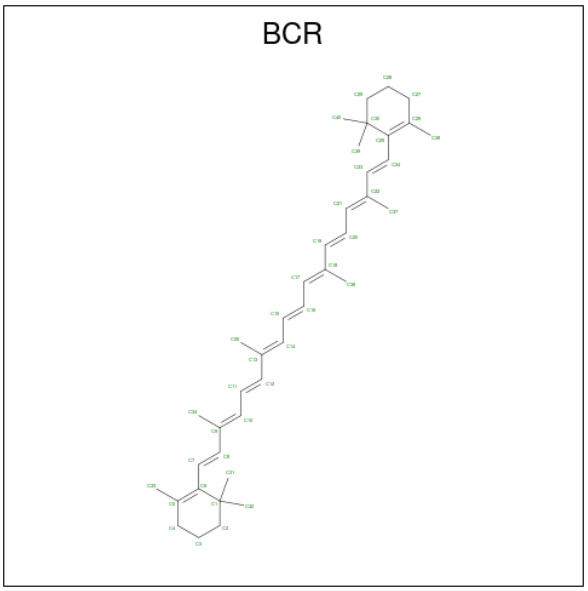
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 45 43 2	0	0
25	D	1	Total C O 55 53 2	0	0
25	J	1	Total C O 35 33 2	0	0
25	a	1	Total C O 45 43 2	0	0
25	d	1	Total C O 55 53 2	0	0
25	j	1	Total C O 35 33 2	0	0

- 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: $C_{40}H_{56}$).



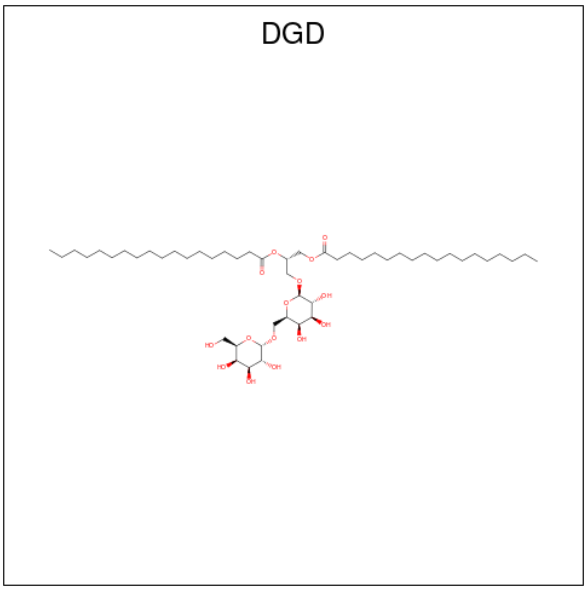
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total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

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



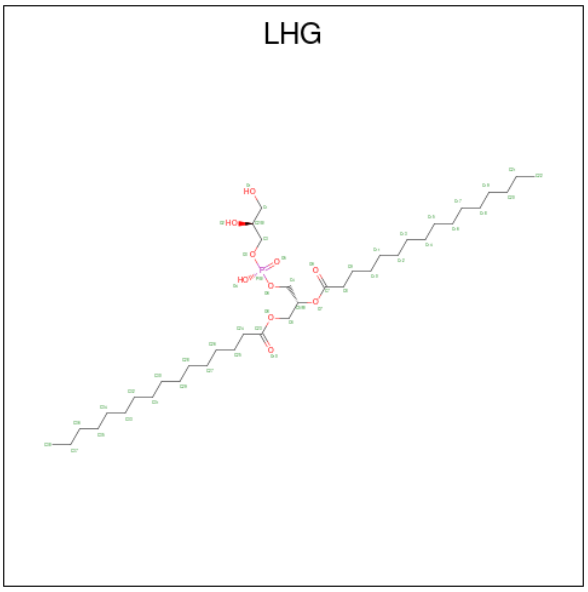
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 56 41 15	0	0

Continued on next page...

Continued from previous page...

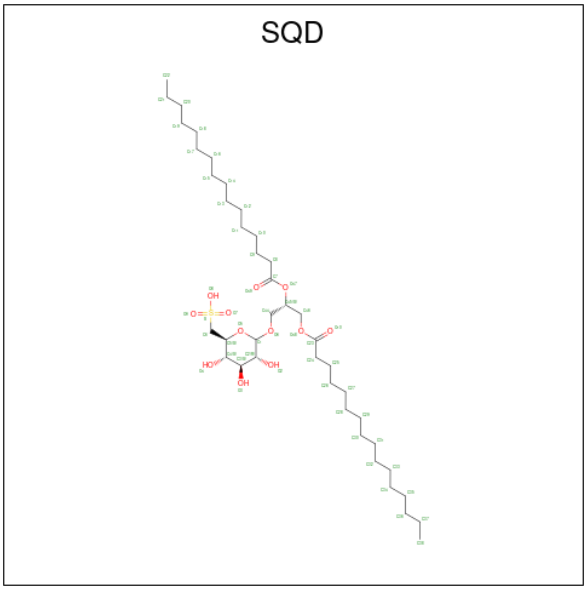
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	B	1	Total C O 58 43 15	0	0
28	B	1	Total C O 52 37 15	0	0
28	C	1	Total C O 53 38 15	0	0
28	C	1	Total C O 62 47 15	0	0
28	C	1	Total C O 66 51 15	0	0
28	D	1	Total C O 63 48 15	0	0
28	a	1	Total C O 56 41 15	0	0
28	b	1	Total C O 52 37 15	0	0
28	b	1	Total C O 58 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: $C_{38}H_{75}O_{10}P$).



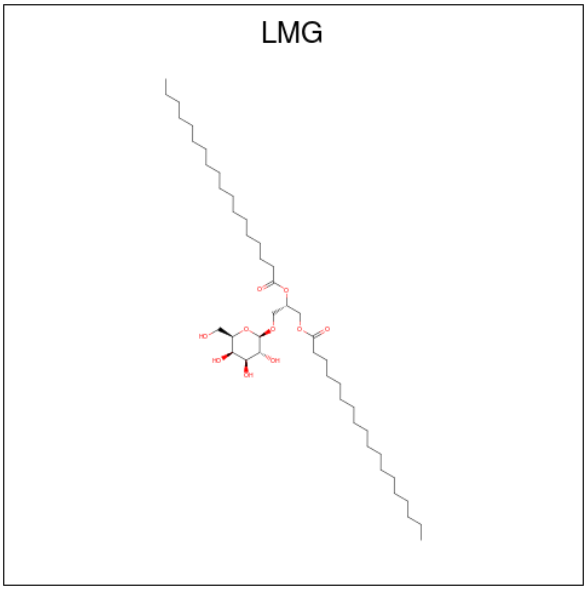
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			39	28	10	1		
29	A	1	Total	C	O	P	0	0
			37	26	10	1		
29	a	1	Total	C	O	P	0	0
			39	28	10	1		
29	a	1	Total	C	O	P	0	0
			37	26	10	1		

- 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...

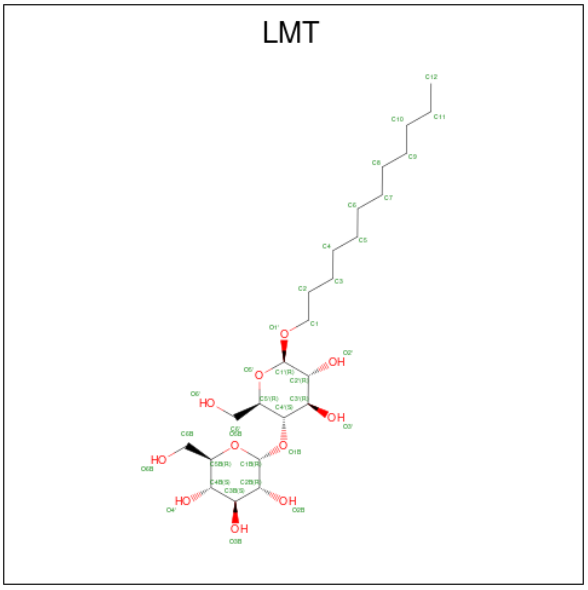
Continued from previous page...

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	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 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	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
31	m	1	Total C O 42 32 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	a	1	Total Cl 1 1	0	0

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



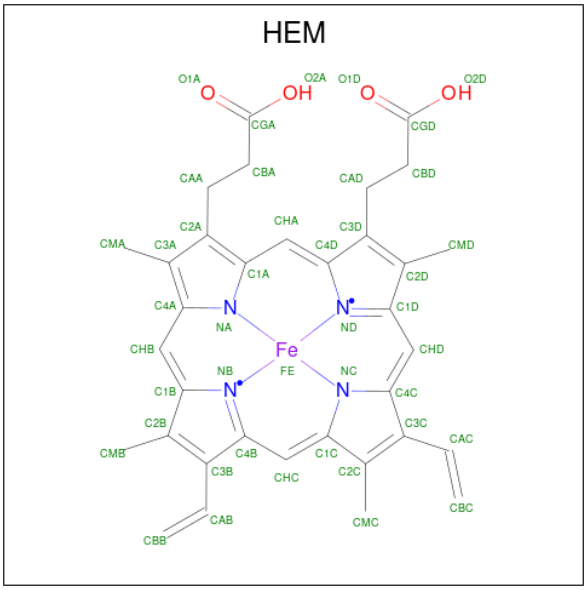
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	D	1	Total C O 31 20 11	0	0
33	I	1	Total C O 35 24 11	0	0
33	M	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35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

- 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).

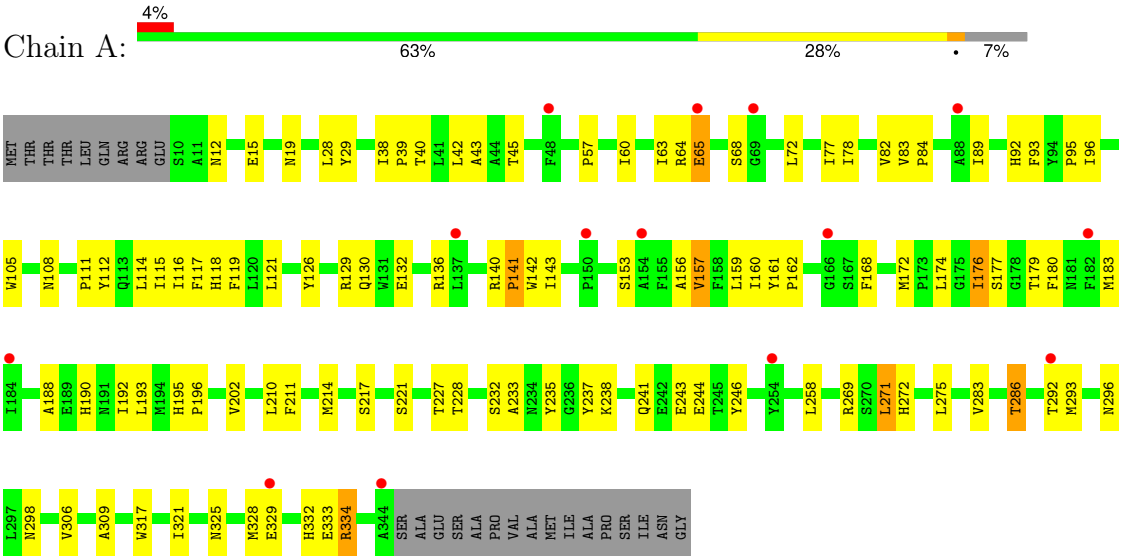
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	K	1	Total Ca 1 1	0	0
35	O	1	Total Ca 1 1	0	0
35	k	1	Total Ca 1 1	0	0
35	o	1	Total Ca 1 1	0	0

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.

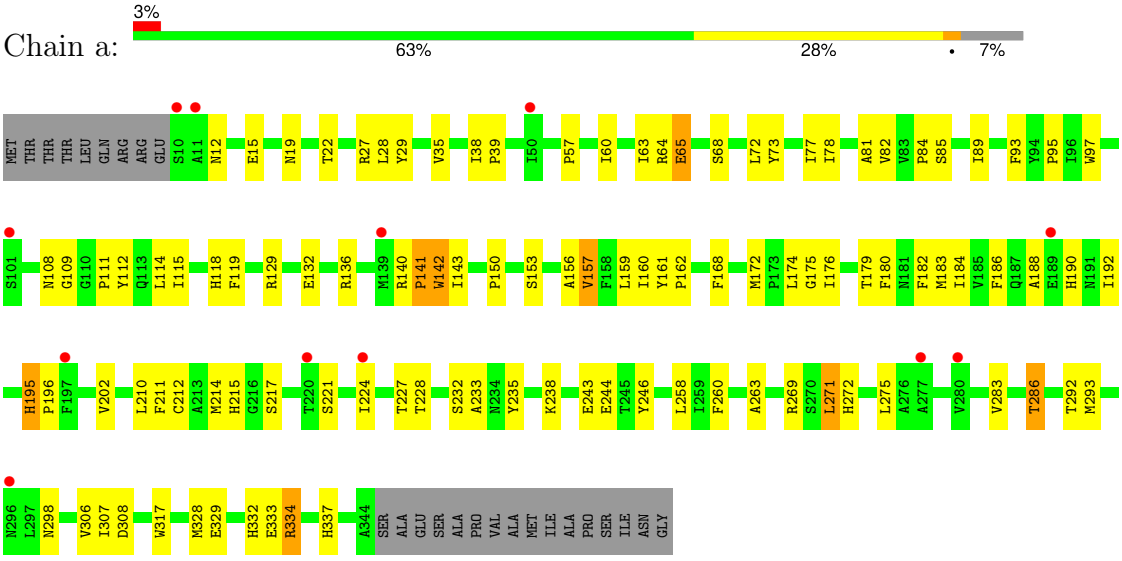
• Molecule 1: Photosystem Q(B) protein 1

Chain A:



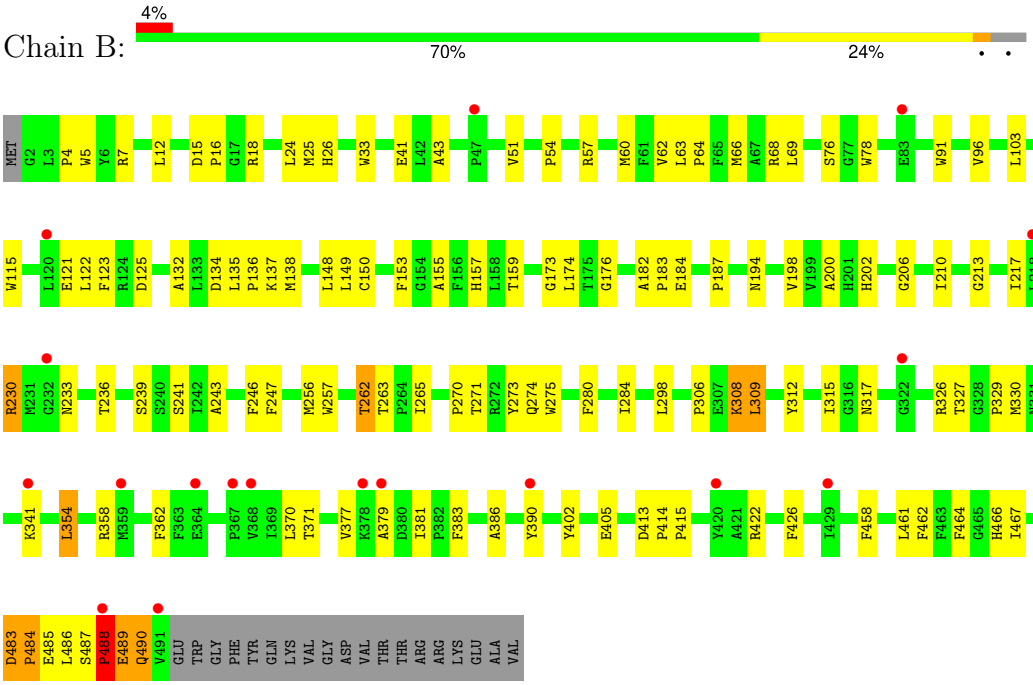
• Molecule 1: Photosystem Q(B) protein 1

Chain a:



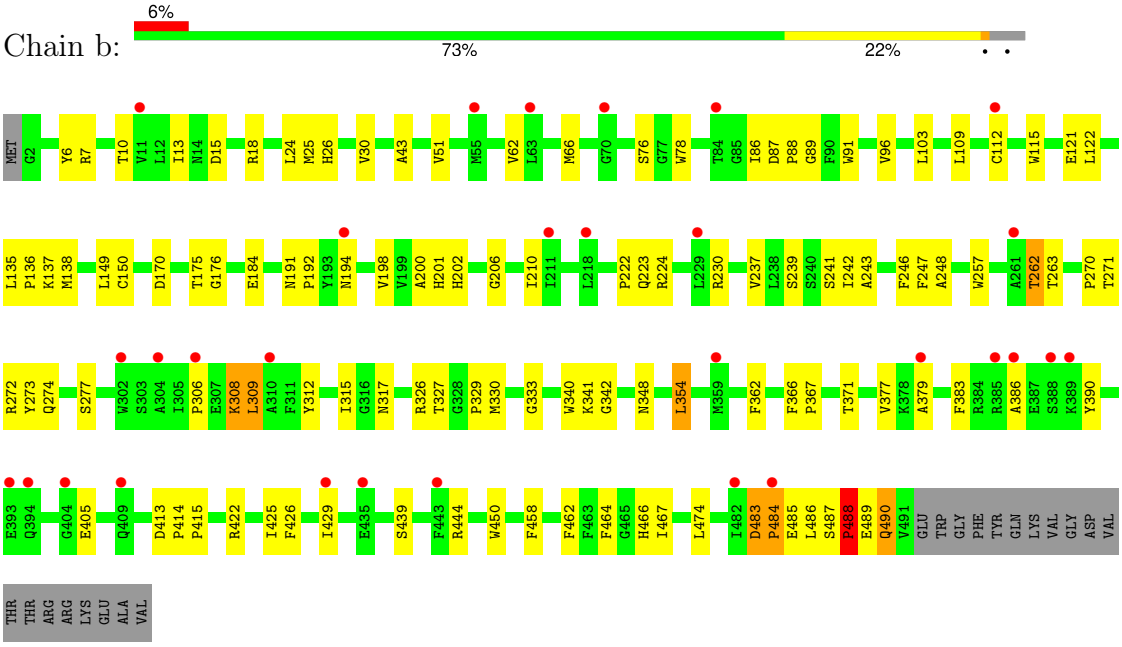
• Molecule 2: Photosystem II core light harvesting protein

Chain B:



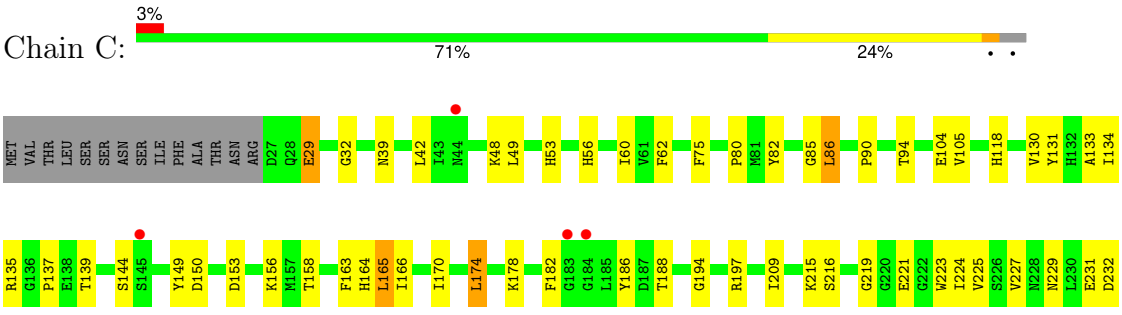
• Molecule 2: Photosystem II core light harvesting protein

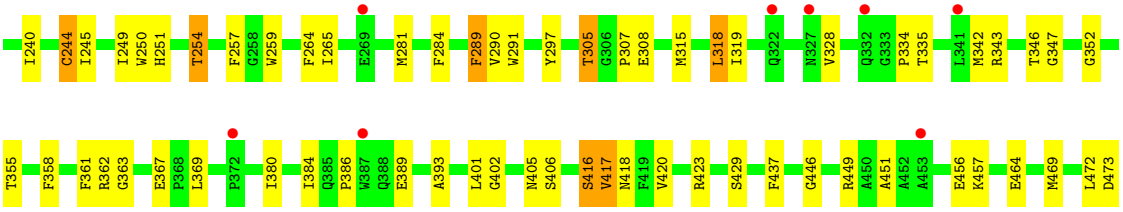
Chain b:



• Molecule 3: Photosystem II CP43 protein

Chain C:

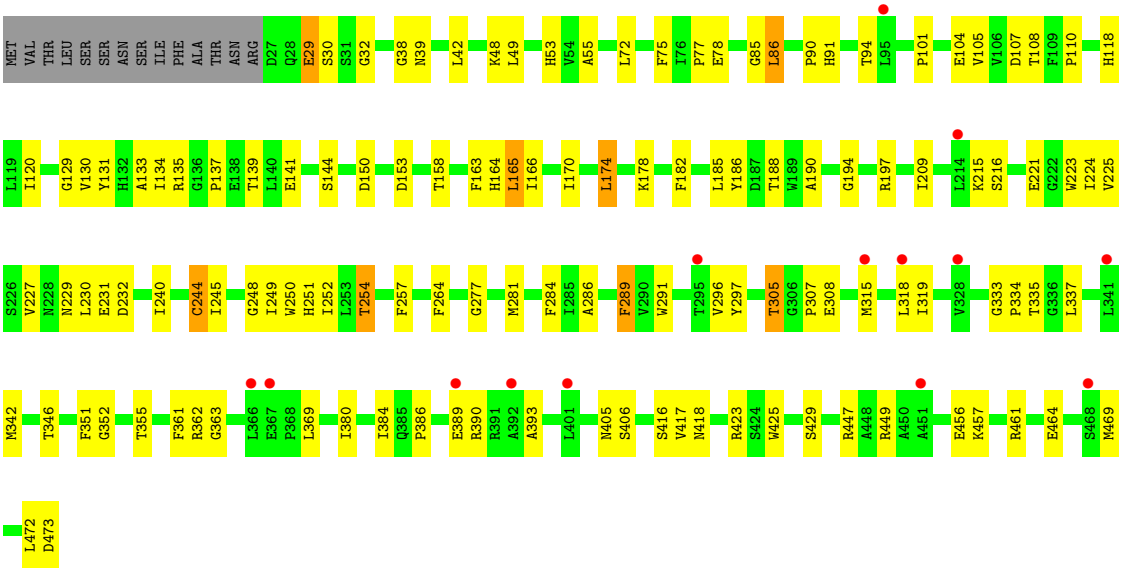




• Molecule 3: Photosystem II CP43 protein

Chain c:

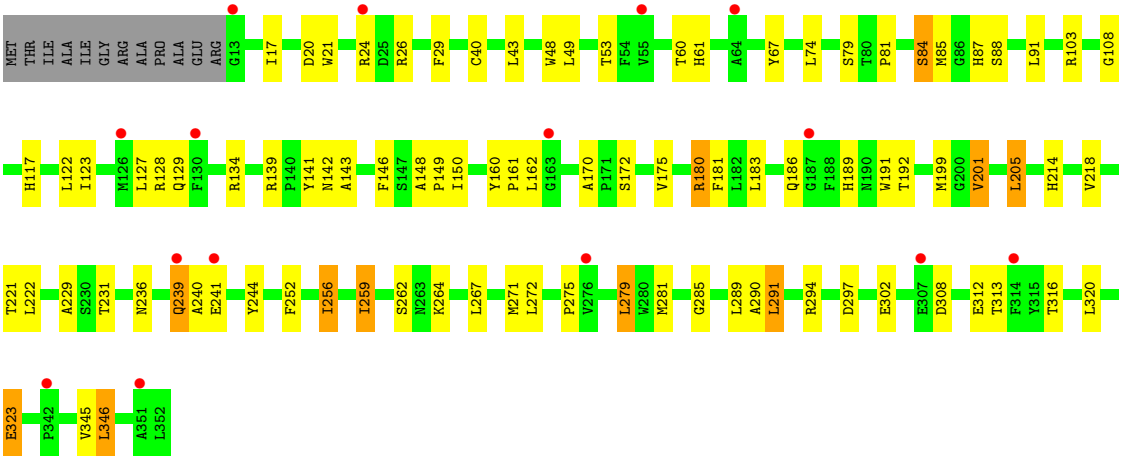




• Molecule 4: Photosystem II D2 protein

Chain D:

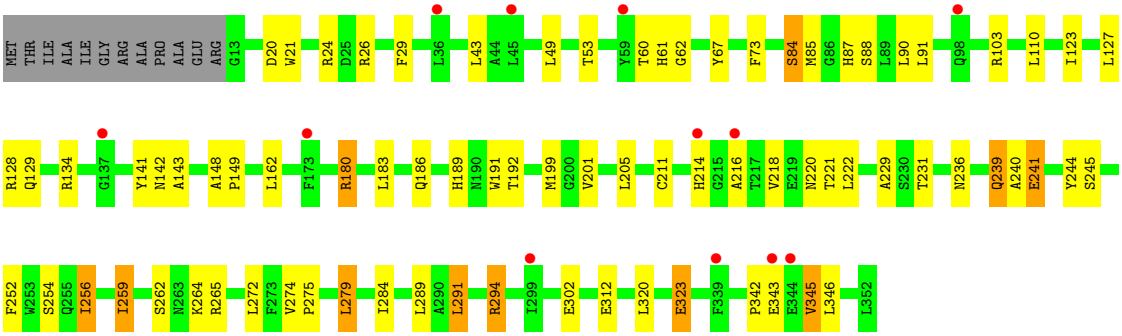




• Molecule 4: Photosystem II D2 protein

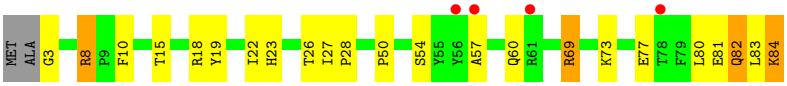
Chain d:





• Molecule 5: Cytochrome b559 subunit alpha





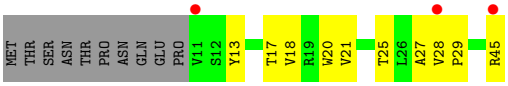
• Molecule 5: Cytochrome b559 subunit alpha





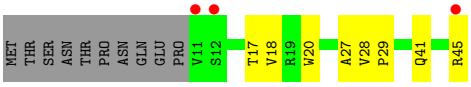
• Molecule 6: Cytochrome b559 subunit beta





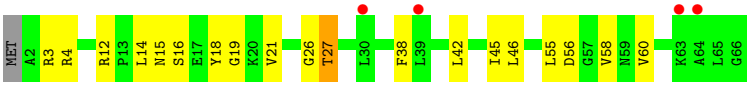
• Molecule 6: Cytochrome b559 subunit beta





• Molecule 7: Photosystem II reaction center protein H

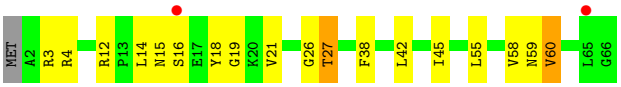




• Molecule 7: Photosystem II reaction center protein H

Chain h:

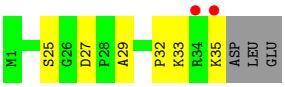




• Molecule 8: Photosystem II reaction center protein I

Chain I:

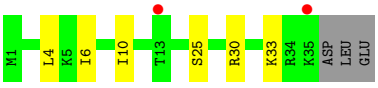




• Molecule 8: Photosystem II reaction center protein I

Chain i:





• Molecule 9: Photosystem II reaction center protein J

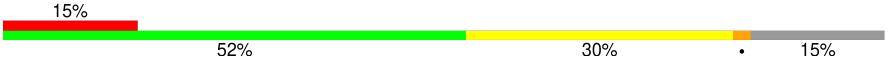
Chain J:

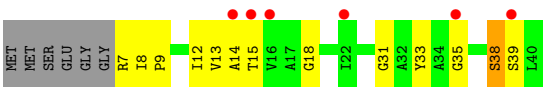




• Molecule 9: Photosystem II reaction center protein J

Chain j:

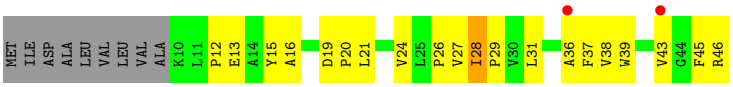




• Molecule 10: Photosystem II reaction center protein K

Chain K:

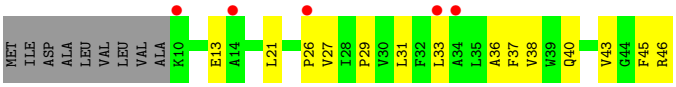




• Molecule 10: Photosystem II reaction center protein K

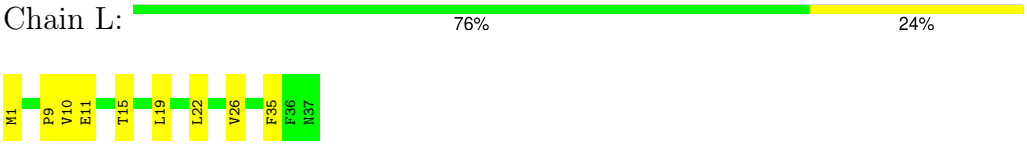
Chain k:





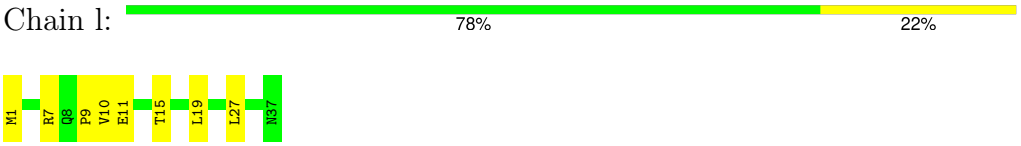
• Molecule 11: Photosystem II reaction center protein L

Chain L:



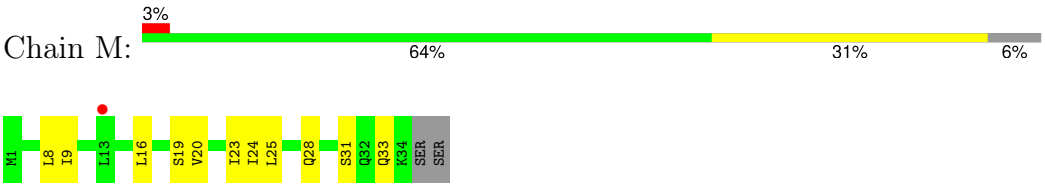
• Molecule 11: Photosystem II reaction center protein L

Chain l:



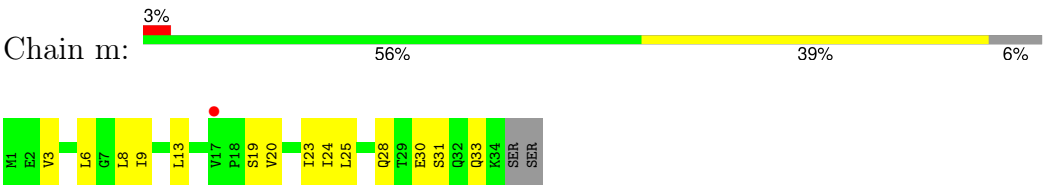
• Molecule 12: Photosystem II reaction center protein M

Chain M:



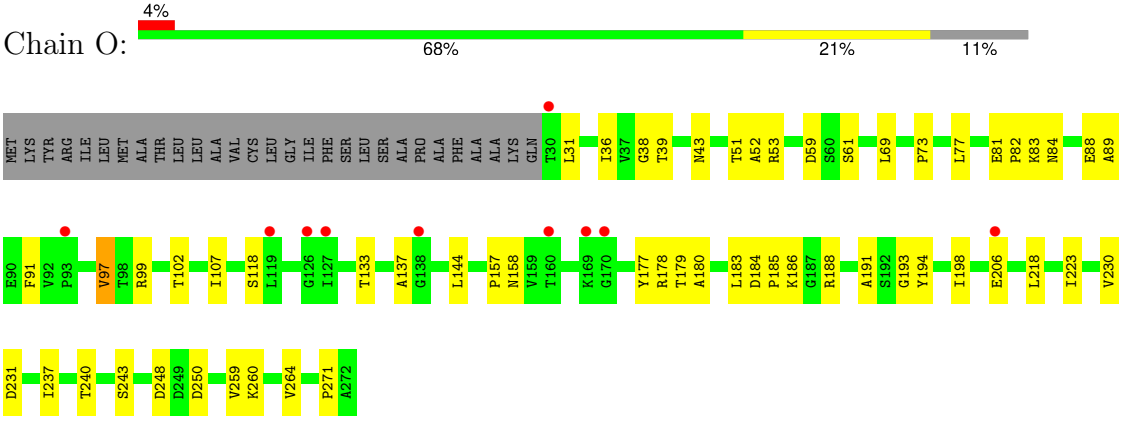
• Molecule 12: Photosystem II reaction center protein M

Chain m:



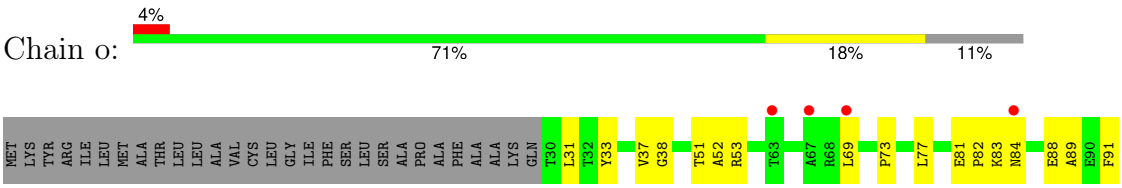
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

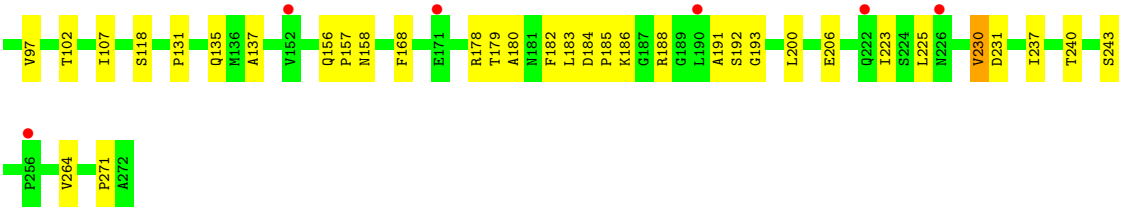
Chain O:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:





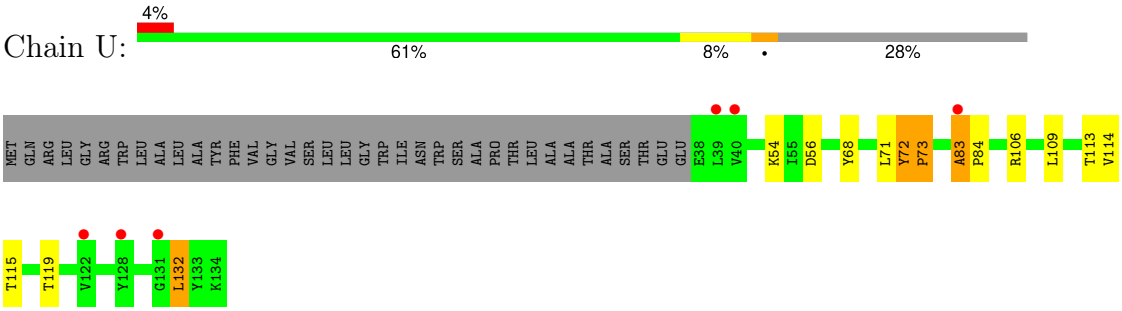
• Molecule 14: Photosystem II reaction center protein T



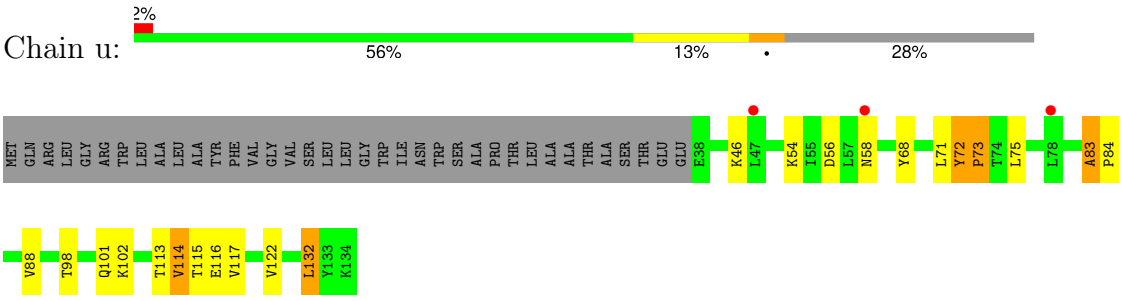
• Molecule 14: Photosystem II reaction center protein T



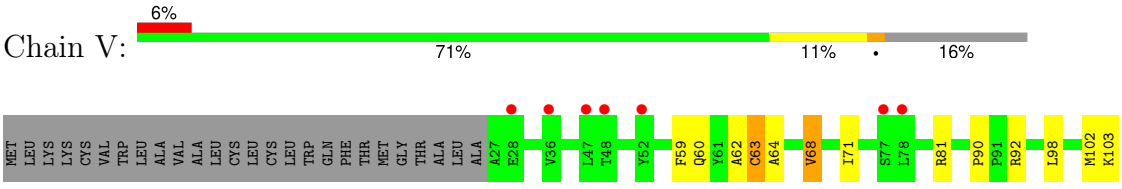
• Molecule 15: Photosystem II 12 kDa extrinsic protein

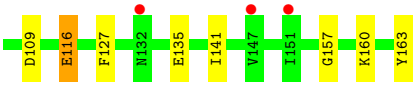


• Molecule 15: Photosystem II 12 kDa extrinsic protein



• Molecule 16: Cytochrome c-550



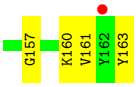


• Molecule 16: Cytochrome c-550

Chain v:

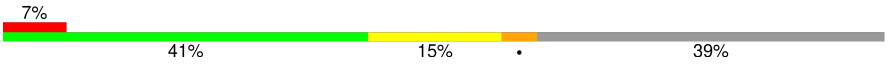


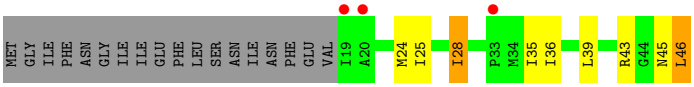




• Molecule 17: Photosystem II reaction center protein ycf12

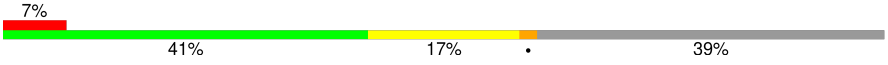
Chain y:

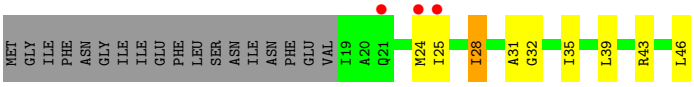




• Molecule 17: Photosystem II reaction center protein ycf12

Chain g:

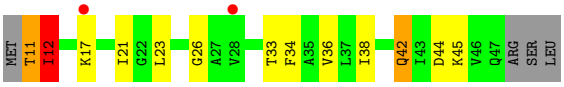




• Molecule 18: Photosystem II reaction center X protein

Chain X:

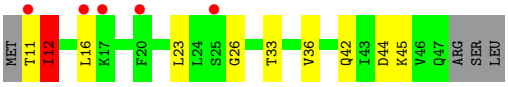




• Molecule 18: Photosystem II reaction center X protein

Chain x:

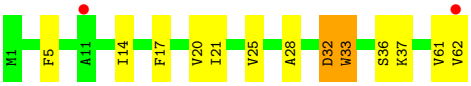




• Molecule 19: Photosystem II reaction center protein Z

Chain Z:

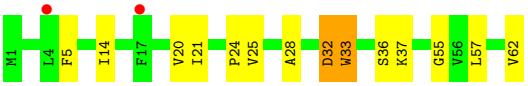




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

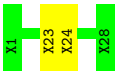




• Molecule 20: Photosystem II reaction center protein Y

Chain G:

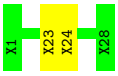




• Molecule 20: Photosystem II reaction center protein Y

Chain Y:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	131.98Å 227.57Å 306.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.97 – 5.90 82.97 – 5.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (82.97-5.90) 98.4 (82.97-5.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.285 , 0.313 0.288 , 0.321	Depositor DCC
R_{free} test set	1200 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	1.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 79.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.74	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 2.55% 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: LMT, PHO, DGD, OEC, CLA, HEM, BCR, LHG, LMG, CL, SQD, BCT, FE2, PL9, CA

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	3/3700 (0.1%)
1	a	0.38	0/2712	0.86	5/3700 (0.1%)
2	B	0.37	0/3986	0.85	12/5433 (0.2%)
2	b	0.37	0/3986	0.86	8/5433 (0.1%)
3	C	0.37	0/3556	0.82	3/4842 (0.1%)
3	c	0.37	0/3556	0.85	6/4842 (0.1%)
4	D	0.35	0/2801	0.81	2/3818 (0.1%)
4	d	0.36	0/2801	0.84	0/3818
5	E	0.37	0/685	0.88	3/933 (0.3%)
5	e	0.37	0/685	0.89	0/933
6	F	0.46	0/291	0.83	0/397
6	f	0.46	0/291	0.85	0/397
7	H	0.38	0/520	0.74	0/709
7	h	0.38	0/520	0.78	0/709
8	I	0.37	0/293	0.83	0/395
8	i	0.37	0/293	0.88	0/395
9	J	0.39	0/255	0.91	0/346
9	j	0.38	0/255	0.90	0/346
10	K	0.51	0/303	0.91	1/416 (0.2%)
10	k	0.44	0/303	0.92	0/416
11	L	0.33	0/311	0.76	0/422
11	l	0.33	0/311	0.78	0/422
12	M	0.55	0/270	1.08	0/367
12	m	0.53	0/270	1.10	0/367
13	O	0.35	0/1876	0.74	0/2548
13	o	0.36	0/1876	0.77	4/2548 (0.2%)
14	T	0.40	0/284	0.83	0/381
14	t	0.37	0/284	0.81	0/381
15	U	0.35	0/785	0.83	0/1064
15	u	0.43	0/785	0.89	0/1064
16	V	0.39	0/1081	0.85	2/1468 (0.1%)
16	v	0.37	0/1081	0.82	4/1468 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	g	0.40	0/202	0.86	0/272
17	y	0.38	0/202	0.84	0/272
18	X	0.47	0/273	0.87	0/370
18	x	0.50	0/273	0.88	0/370
19	Z	0.37	0/490	0.86	0/669
19	z	0.35	0/490	0.88	0/669
All	All	0.38	0/41948	0.84	53/57100 (0.1%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	483	ASP	CA-C-N	10.73	133.25	119.84
2	b	483	ASP	C-N-CA	10.73	133.25	119.84
2	B	483	ASP	CA-C-N	10.40	132.84	119.84
2	B	483	ASP	C-N-CA	10.40	132.84	119.84
2	B	413	ASP	CA-C-N	6.75	127.33	120.38
2	B	413	ASP	C-N-CA	6.75	127.33	120.38
2	b	194	ASN	CA-C-N	6.60	126.37	119.05
2	b	194	ASN	C-N-CA	6.60	126.37	119.05
2	b	413	ASP	CA-C-N	6.51	127.09	120.38
2	b	413	ASP	C-N-CA	6.51	127.09	120.38
2	B	15	ASP	CA-C-N	5.85	125.99	119.32
2	B	15	ASP	C-N-CA	5.85	125.99	119.32
1	a	60	ILE	N-CA-C	5.78	115.97	110.42
16	v	75	ASN	CA-C-N	5.75	125.45	119.82
16	v	75	ASN	C-N-CA	5.75	125.45	119.82
13	o	156	GLN	CA-C-N	5.72	125.67	119.78
13	o	156	GLN	C-N-CA	5.72	125.67	119.78
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
2	B	236	THR	N-CA-C	-5.44	107.01	113.97
3	C	464	GLU	CA-C-N	5.44	126.64	119.84
3	C	464	GLU	C-N-CA	5.44	126.64	119.84
10	K	28	ILE	CB-CA-C	-5.33	108.64	113.70
3	c	190	ALA	CA-C-N	5.33	124.78	119.24
3	c	190	ALA	C-N-CA	5.33	124.78	119.24
4	D	308	ASP	CA-C-N	5.31	126.02	120.12
4	D	308	ASP	C-N-CA	5.31	126.02	120.12
1	A	83	VAL	N-CA-C	5.30	113.19	108.63
2	b	15	ASP	CA-C-N	5.29	125.35	119.32
2	b	15	ASP	C-N-CA	5.29	125.35	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	GLU	CA-C-N	5.28	125.53	119.83
1	A	65	GLU	C-N-CA	5.28	125.53	119.83
5	E	8	ARG	CA-C-N	5.28	126.43	119.84
5	E	8	ARG	C-N-CA	5.28	126.43	119.84
13	o	200	LEU	CA-C-N	5.27	125.33	119.32
13	o	200	LEU	C-N-CA	5.27	125.33	119.32
2	B	332	LYS	N-CA-C	-5.25	106.82	113.18
16	v	127	PHE	CA-C-N	5.22	125.53	119.47
16	v	127	PHE	C-N-CA	5.22	125.53	119.47
3	C	318	LEU	N-CA-C	-5.18	105.71	111.36
1	a	65	GLU	CA-C-N	5.18	125.42	119.83
1	a	65	GLU	C-N-CA	5.18	125.42	119.83
2	B	194	ASN	CA-C-N	5.18	125.22	119.32
2	B	194	ASN	C-N-CA	5.18	125.22	119.32
3	c	363	GLY	CA-C-N	5.09	124.53	119.24
3	c	363	GLY	C-N-CA	5.09	124.53	119.24
1	a	195	HIS	CA-C-N	5.08	124.52	119.24
1	a	195	HIS	C-N-CA	5.08	124.52	119.24
3	c	333	GLY	CA-C-N	5.07	126.18	119.84
3	c	333	GLY	C-N-CA	5.07	126.18	119.84
5	E	69	ARG	N-CA-C	5.05	116.47	111.07
2	B	381	ILE	CA-C-N	5.01	124.91	119.85
2	B	381	ILE	C-N-CA	5.01	124.91	119.85

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	85	0
1	a	2627	0	2524	91	0
2	B	3850	0	3718	95	0
2	b	3850	0	3718	90	0
3	C	3444	0	3365	86	0
3	c	3444	0	3365	90	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2706	0	2608	72	0
4	d	2706	0	2608	71	0
5	E	666	0	651	16	0
5	e	666	0	651	20	0
6	F	282	0	291	8	0
6	f	282	0	291	8	0
7	H	507	0	521	15	0
7	h	507	0	521	15	0
8	I	286	0	308	2	0
8	i	286	0	308	3	0
9	J	249	0	262	6	0
9	j	249	0	262	8	0
10	K	293	0	305	18	0
10	k	293	0	305	11	0
11	L	304	0	316	10	0
11	l	304	0	316	7	0
12	M	267	0	289	13	0
12	m	267	0	289	16	0
13	O	1845	0	1801	36	0
13	o	1845	0	1801	32	0
14	T	275	0	288	11	0
14	t	275	0	288	11	0
15	U	774	0	773	9	0
15	u	774	0	773	13	0
16	V	1060	0	1068	12	0
16	v	1060	0	1068	12	0
17	g	201	0	226	8	0
17	y	201	0	226	6	0
18	X	270	0	299	10	0
18	x	270	0	299	8	0
19	Z	479	0	516	12	0
19	z	479	0	516	11	0
20	G	140	0	32	1	0
20	Y	140	0	32	1	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	25	0
23	B	1040	0	1152	75	0
23	C	845	0	936	46	0
23	D	130	0	144	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	260	0	288	34	0
23	b	1040	0	1152	70	0
23	c	845	0	936	41	0
23	d	130	0	144	9	0
24	A	64	0	74	5	0
24	D	64	0	74	6	0
24	a	128	0	148	13	0
25	A	45	0	61	2	0
25	D	55	0	80	6	0
25	J	35	0	45	0	0
25	a	45	0	61	5	0
25	d	55	0	80	9	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	6	0
27	B	160	0	224	22	0
27	C	120	0	168	14	0
27	D	40	0	56	3	0
27	H	40	0	56	3	0
27	J	40	0	56	3	0
27	T	80	0	112	15	0
27	a	40	0	56	7	0
27	b	80	0	112	8	0
27	c	80	0	112	14	0
27	d	40	0	56	2	0
27	h	40	0	56	4	0
27	j	40	0	56	4	0
27	k	40	0	56	8	0
27	y	40	0	56	6	0
27	z	40	0	56	3	0
28	A	56	0	70	1	0
28	B	110	0	136	2	0
28	C	181	0	245	15	0
28	D	63	0	87	1	0
28	a	56	0	70	2	0
28	b	110	0	136	5	0
28	c	181	0	244	14	0
28	d	63	0	87	1	0
29	A	76	0	95	7	0
29	a	76	0	95	5	0
30	A	105	0	147	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	47	0	61	2	0
30	D	43	0	50	4	0
30	F	45	0	54	2	0
30	a	105	0	147	10	0
30	b	47	0	61	4	0
30	d	43	0	50	4	0
30	f	45	0	54	2	0
31	A	93	0	125	5	0
31	B	98	0	135	8	0
31	C	93	0	126	5	0
31	D	94	0	126	4	0
31	E	44	0	58	1	0
31	I	43	0	55	2	0
31	M	42	0	53	4	0
31	a	93	0	124	6	0
31	b	98	0	135	8	0
31	c	45	0	59	2	0
31	d	94	0	126	8	0
31	e	44	0	58	1	0
31	i	43	0	55	3	0
31	k	48	0	66	3	0
31	m	42	0	53	4	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	B	140	0	184	5	0
33	D	31	0	35	1	0
33	I	35	0	46	2	0
33	M	35	0	46	1	0
33	b	140	0	184	5	0
33	d	31	0	35	1	0
33	i	35	0	46	2	0
33	m	35	0	46	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	5	0
34	v	43	0	30	4	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	51361	1211	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 (1211) 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)
4:d:26:ARG:HD3	6:f:18:VAL:HG11	1.54	0.88
3:C:39:ASN:HB2	23:C:508:CLA:HBA1	1.57	0.86
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.57	0.86
27:T:101:BCR:H383	30:b:601:SQD:H92	1.57	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.58	0.85
13:o:82:PRO:HG3	13:o:89:ALA:HB2	1.60	0.83
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.59	0.83
10:K:21:LEU:HD13	17:y:24:MET:HE2	1.62	0.82
27:B:617:BCR:H383	30:B:626:SQD:H92	1.62	0.82
3:c:39:ASN:HB2	23:c:508:CLA:HBA1	1.62	0.81
30:D:408:SQD:H171	30:D:408:SQD:H301	1.66	0.77
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.66	0.77
23:C:507:CLA:H112	27:C:516:BCR:H362	1.66	0.77
12:M:28:GLN:HA	12:m:28:GLN:HA	1.64	0.77
3:c:297:TYR:O	3:c:423:ARG:NH2	2.18	0.77
10:k:21:LEU:HD13	17:g:24:MET:HE2	1.64	0.77
3:C:250:TRP:O	3:C:254:THR:OG1	2.03	0.76
1:a:192:ILE:HA	1:a:293:MET:HE1	1.66	0.76
3:C:362:ARG:H	28:C:517:DGD:HE4	1.52	0.75
4:D:199:MET:HG2	25:D:404:PL9:H322	1.68	0.75
24:a:408:PHO:H151	23:d:402:CLA:H172	1.66	0.75
4:d:29:PHE:O	4:d:128:ARG:NH2	2.21	0.74
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.67	0.74
23:B:608:CLA:HBA2	30:D:408:SQD:H101	1.70	0.74
24:A:406:PHO:HBC3	4:D:279:LEU:HG	1.70	0.74
23:A:404:CLA:HED1	25:D:404:PL9:H372	1.69	0.73
3:C:291:TRP:O	3:C:305:THR:OG1	2.05	0.73
34:V:201:HEM:HBC2	34:V:201:HEM:HHD	1.70	0.73
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.70	0.73
23:C:508:CLA:HBC3	23:C:510:CLA:H92	1.69	0.73
12:m:25:LEU:O	12:m:28:GLN:HG3	1.88	0.73
3:c:250:TRP:O	3:c:254:THR:OG1	2.07	0.73
23:b:612:CLA:H42	4:d:127:LEU:HD11	1.68	0.73
27:B:618:BCR:H10C	14:t:18:PHE:HB2	1.71	0.73
1:a:183:MET:HB3	23:a:404:CLA:HBC2	1.72	0.72
3:c:362:ARG:H	28:c:516:DGD:HE4	1.54	0.72
13:o:69:LEU:HB3	13:o:107:ILE:HB	1.70	0.72
4:D:29:PHE:O	4:D:128:ARG:NH2	2.23	0.72

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:407:LMG:H292	1.72	0.72
30:a:415:SQD:H311	23:c:508:CLA:H71	1.72	0.71
31:a:416:LMG:H231	25:d:404:PL9:H352	1.72	0.71
23:B:608:CLA:H42	4:D:127:LEU:HD11	1.72	0.71
2:b:262:THR:HG22	2:b:263:THR:HG23	1.70	0.71
1:A:63:ILE:HB	3:C:335:THR:HG21	1.70	0.71
23:b:609:CLA:HBB1	23:b:610:CLA:H51	1.71	0.71
14:T:18:PHE:HB2	27:T:102:BCR:H10C	1.72	0.71
1:a:129:ARG:HH21	4:d:256:ILE:HD12	1.54	0.71
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.24	0.71
4:d:199:MET:HG2	25:d:404:PL9:H322	1.72	0.71
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.71	0.71
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.73	0.71
24:a:408:PHO:HBC3	4:d:279:LEU:HG	1.72	0.70
27:T:101:BCR:H23C	2:b:25:MET:HE3	1.74	0.70
23:a:405:CLA:HED1	25:d:404:PL9:H372	1.72	0.70
23:b:610:CLA:H72	27:b:622:BCR:H311	1.74	0.70
27:T:102:BCR:H19C	27:b:621:BCR:H363	1.73	0.70
30:d:408:SQD:H171	30:d:408:SQD:H301	1.74	0.70
23:c:508:CLA:HBC3	23:c:510:CLA:H92	1.73	0.70
1:a:63:ILE:HB	3:c:335:THR:HG21	1.73	0.69
34:v:201:HEM:HBC2	34:v:201:HEM:HHD	1.72	0.69
1:a:190:HIS:HB3	1:a:293:MET:HE2	1.73	0.69
23:A:403:CLA:H71	23:A:404:CLA:HAB	1.75	0.69
7:H:38:PHE:HB2	27:H:101:BCR:H10C	1.73	0.69
31:M:101:LMG:HC61	11:l:9:PRO:HB3	1.74	0.69
9:j:15:THR:HG21	10:k:38:VAL:HG13	1.75	0.69
23:B:606:CLA:H72	27:B:620:BCR:H311	1.74	0.69
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.74	0.69
4:d:236:ASN:ND2	4:d:239:GLN:O	2.26	0.69
3:C:48:LYS:NZ	3:C:133:ALA:O	2.25	0.69
4:D:236:ASN:ND2	4:D:239:GLN:O	2.25	0.69
5:e:60:GLN:OE1	5:e:84:LYS:NZ	2.26	0.69
23:D:403:CLA:H42	18:X:26:GLY:HA3	1.76	0.68
28:b:602:DGD:HB22	33:b:604:LMT:H72	1.75	0.68
1:A:15:GLU:O	1:A:19:ASN:ND2	2.25	0.68
12:M:25:LEU:O	12:M:28:GLN:HG3	1.93	0.68
29:A:415:LHG:H271	29:A:415:LHG:H101	1.76	0.67
12:M:20:VAL:O	12:M:24:ILE:HG13	1.94	0.67
3:C:449:ARG:HE	23:C:505:CLA:HED1	1.59	0.67
17:y:35:ILE:HG22	19:Z:21:ILE:HG23	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:29:TYR:O	1:a:129:ARG:NH1	2.28	0.67
23:c:513:CLA:HAB	27:z:101:BCR:H24C	1.77	0.67
4:D:21:TRP:O	4:D:26:ARG:NH2	2.25	0.67
1:a:57:PRO:HG3	1:a:68:SER:HB3	1.77	0.67
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.77	0.66
2:b:149:LEU:HG	23:b:607:CLA:HBC1	1.76	0.66
2:B:43:ALA:HA	31:a:402:LMG:H112	1.75	0.66
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.60	0.66
1:a:174:LEU:HD22	24:a:407:PHO:H151	1.76	0.66
3:c:405:ASN:HB2	28:c:518:DGD:HG31	1.78	0.66
17:g:35:ILE:HG22	19:z:21:ILE:HG23	1.76	0.66
2:B:262:THR:HG22	2:B:263:THR:HG23	1.77	0.66
1:a:214:MET:HE2	1:a:214:MET:HA	1.76	0.66
3:c:216:SER:HB3	3:c:221:GLU:HB2	1.76	0.66
27:B:618:BCR:H19C	27:B:619:BCR:H363	1.75	0.66
2:b:271:THR:HG22	2:b:273:TYR:H	1.60	0.66
23:d:403:CLA:H42	18:x:26:GLY:HA3	1.78	0.66
2:B:149:LEU:HG	23:B:603:CLA:HBC1	1.76	0.65
2:b:317:ASN:HA	2:b:330:MET:HE1	1.76	0.65
23:b:607:CLA:H193	7:h:42:LEU:HD12	1.77	0.65
12:m:20:VAL:O	12:m:24:ILE:HG13	1.95	0.65
23:B:605:CLA:HBB1	23:B:606:CLA:H51	1.77	0.65
4:D:186:GLN:HB2	23:D:401:CLA:HBC1	1.76	0.65
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.77	0.65
4:D:24:ARG:NH2	18:X:44:ASP:O	2.29	0.65
1:a:329:GLU:O	1:a:332:HIS:ND1	2.28	0.65
23:C:511:CLA:H171	19:Z:20:VAL:HA	1.78	0.65
1:A:29:TYR:O	1:A:129:ARG:NH1	2.29	0.65
2:b:24:LEU:HD21	23:b:620:CLA:HAB	1.77	0.65
29:a:417:LHG:H271	29:a:417:LHG:H101	1.78	0.65
31:A:418:LMG:H112	2:b:43:ALA:HA	1.79	0.64
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.32	0.64
3:C:118:HIS:CE1	31:C:521:LMG:H192	2.33	0.64
16:V:62:ALA:O	34:V:201:HEM:HAB	1.98	0.64
23:B:603:CLA:H193	7:H:42:LEU:HD12	1.80	0.63
6:F:17:THR:HG23	6:F:20:TRP:H	1.63	0.63
7:h:55:LEU:HB2	7:h:58:VAL:HG12	1.78	0.63
3:C:297:TYR:O	3:C:423:ARG:NH2	2.31	0.63
15:u:56:ASP:OD2	15:u:115:THR:OG1	2.16	0.63
2:B:271:THR:HG22	2:B:273:TYR:H	1.63	0.63
23:C:503:CLA:H172	23:C:510:CLA:HBB2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:405:ASN:HB2	28:C:519:DGD:HG31	1.80	0.63
23:c:507:CLA:H112	27:c:515:BCR:H362	1.81	0.63
31:A:414:LMG:H231	25:D:404:PL9:H352	1.81	0.63
2:B:24:LEU:HD21	23:B:616:CLA:HAB	1.81	0.63
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.80	0.63
1:A:140:ARG:HH22	29:A:412:LHG:P	2.22	0.63
10:k:26:PRO:O	10:k:29:PRO:HD2	1.99	0.63
4:d:24:ARG:NH2	18:x:44:ASP:O	2.32	0.62
1:a:221:SER:HB3	4:d:141:TYR:HB2	1.81	0.62
6:f:17:THR:HG23	6:f:20:TRP:H	1.65	0.62
1:A:183:MET:HB3	23:A:403:CLA:HBC2	1.80	0.62
30:A:413:SQD:H241	29:A:415:LHG:HC81	1.82	0.62
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.62
31:d:407:LMG:H111	11:l:19:LEU:HD21	1.82	0.62
2:B:25:MET:HE3	27:B:617:BCR:H23C	1.81	0.61
1:a:72:LEU:HD13	31:a:402:LMG:H111	1.82	0.61
2:B:5:TRP:HZ3	23:B:611:CLA:H51	1.64	0.61
23:D:403:CLA:H43	18:X:23:LEU:HA	1.83	0.61
4:d:186:GLN:HB2	23:d:402:CLA:HBC1	1.83	0.61
31:D:407:LMG:H111	11:L:19:LEU:HD21	1.81	0.61
11:L:9:PRO:HB3	31:m:102:LMG:HC61	1.82	0.61
3:c:406:SER:O	3:c:418:ASN:ND2	2.32	0.61
16:v:62:ALA:O	34:v:201:HEM:HAB	2.00	0.61
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.83	0.61
1:A:192:ILE:HA	1:A:293:MET:HE1	1.82	0.61
13:o:77:LEU:HB3	13:o:91:PHE:HB3	1.81	0.61
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.83	0.61
3:C:342:MET:HE3	3:C:352:GLY:HA2	1.82	0.61
23:c:509:CLA:H121	23:c:509:CLA:HBD	1.81	0.61
4:D:192:THR:HG23	23:D:401:CLA:HBC2	1.82	0.61
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.83	0.60
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.30	0.60
3:c:118:HIS:CE1	31:c:519:LMG:H192	2.36	0.60
23:a:405:CLA:H42	25:d:404:PL9:H162	1.84	0.60
2:b:458:PHE:HB3	23:b:608:CLA:HBC2	1.82	0.60
13:o:178:ARG:HG3	13:o:178:ARG:HH11	1.67	0.60
1:A:72:LEU:HD13	31:A:418:LMG:H111	1.84	0.60
2:B:327:THR:HG21	31:B:623:LMG:H111	1.85	0.59
23:C:509:CLA:H121	23:C:509:CLA:HBD	1.84	0.59
1:A:28:LEU:HB2	30:A:417:SQD:H91	1.83	0.59
3:c:164:HIS:ND1	23:c:507:CLA:OBD	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:403:CLA:H43	18:x:23:LEU:HA	1.85	0.59
23:b:612:CLA:H151	23:b:613:CLA:H203	1.85	0.59
1:A:64:ARG:O	13:O:178:ARG:NH2	2.36	0.59
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.85	0.59
1:a:28:LEU:HB2	30:a:401:SQD:H91	1.85	0.59
12:m:31:SER:HA	31:m:102:LMG:HC1	1.84	0.59
1:A:214:MET:HA	1:A:214:MET:HE2	1.83	0.59
3:C:49:LEU:O	3:C:53:HIS:ND1	2.34	0.59
2:b:270:PRO:HG3	2:b:312:TYR:HD2	1.67	0.59
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.68	0.58
1:a:317:TRP:CZ3	4:d:180:ARG:HD3	2.37	0.58
4:d:21:TRP:O	4:d:26:ARG:NH2	2.32	0.58
30:a:415:SQD:H241	29:a:417:LHG:HC81	1.83	0.58
1:a:217:SER:HA	4:d:272:LEU:HD12	1.84	0.58
2:b:383:PHE:CZ	13:o:193:GLY:HA2	2.38	0.58
16:v:59:PHE:HA	16:v:63:CYS:SG	2.42	0.58
1:a:64:ARG:O	13:o:178:ARG:NH2	2.36	0.58
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.84	0.58
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.86	0.58
13:o:180:ALA:HB1	13:o:191:ALA:HB2	1.86	0.58
3:C:165:LEU:HD21	23:C:506:CLA:HAB	1.85	0.58
30:a:401:SQD:H311	27:a:412:BCR:H342	1.85	0.58
23:b:606:CLA:HBD	23:b:606:CLA:H2	1.85	0.58
1:A:132:GLU:O	1:A:136:ARG:HG2	2.04	0.58
23:A:405:CLA:H142	23:D:401:CLA:H151	1.85	0.58
14:T:21:ILE:HD12	27:T:102:BCR:H332	1.85	0.58
30:A:413:SQD:H223	28:C:519:DGD:HAE1	1.86	0.57
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.69	0.57
15:u:72:TYR:HB3	15:u:73:PRO:HD3	1.85	0.57
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.85	0.57
1:a:334:ARG:NH1	13:o:183:LEU:O	2.38	0.57
4:D:259:ILE:HG12	31:D:407:LMG:H292	1.87	0.57
3:c:215:LYS:HB3	3:c:223:TRP:HA	1.86	0.57
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.69	0.57
34:F:101:HEM:HBC2	34:F:101:HEM:HMC2	1.87	0.57
23:a:404:CLA:H122	24:a:407:PHO:H3A	1.86	0.57
3:c:48:LYS:NZ	3:c:133:ALA:O	2.37	0.57
13:o:73:PRO:HG2	13:o:102:THR:HB	1.86	0.57
1:a:65:GLU:OE2	1:a:334:ARG:NH2	2.38	0.56
3:c:229:ASN:ND2	3:c:232:ASP:OD1	2.32	0.56
7:h:38:PHE:HB2	27:h:101:BCR:H10C	1.85	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:603:CLA:C2D	23:B:605:CLA:H2	2.35	0.56
1:a:15:GLU:O	1:a:19:ASN:ND2	2.35	0.56
3:c:49:LEU:O	3:c:53:HIS:ND1	2.37	0.56
3:c:165:LEU:HD21	23:c:506:CLA:HAB	1.87	0.56
3:c:229:ASN:HD22	3:c:231:GLU:HB2	1.69	0.56
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.88	0.56
23:a:405:CLA:H203	24:a:407:PHO:H71	1.88	0.56
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.40	0.56
3:c:305:THR:HG23	3:c:307:PRO:HD2	1.86	0.56
30:d:408:SQD:H241	30:d:408:SQD:H111	1.88	0.56
19:z:32:ASP:CG	19:z:33:TRP:H	2.13	0.56
30:D:408:SQD:H241	30:D:408:SQD:H111	1.85	0.56
19:Z:33:TRP:O	19:Z:37:LYS:HB2	2.05	0.56
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.86	0.56
1:a:153:SER:HB3	23:a:404:CLA:HED1	1.88	0.56
2:b:150:CYS:HA	23:b:607:CLA:HBC2	1.85	0.56
3:c:131:TYR:HE1	3:c:135:ARG:HD2	1.69	0.56
15:u:54:LYS:HD2	15:u:113:THR:HG23	1.87	0.56
1:a:317:TRP:HZ3	4:d:180:ARG:HD3	1.71	0.56
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.86	0.56
23:c:505:CLA:H11	27:c:515:BCR:H312	1.87	0.56
2:B:150:CYS:HA	23:B:603:CLA:HBC2	1.87	0.56
1:a:190:HIS:O	1:a:298:ASN:HB3	2.06	0.55
3:C:406:SER:O	3:C:418:ASN:ND2	2.39	0.55
23:b:610:CLA:H71	27:b:622:BCR:H342	1.88	0.55
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.40	0.55
3:c:449:ARG:HE	23:c:505:CLA:HED1	1.70	0.55
23:b:609:CLA:H202	23:b:613:CLA:HBB2	1.88	0.55
1:a:132:GLU:O	1:a:136:ARG:HG2	2.06	0.55
2:b:121:GLU:O	7:h:12:ARG:NH2	2.39	0.55
23:b:612:CLA:HBA2	30:d:408:SQD:H101	1.87	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.89	0.55
1:a:232:SER:OG	31:a:416:LMG:O3	2.20	0.55
30:A:413:SQD:H311	23:C:508:CLA:H71	1.89	0.55
23:C:513:CLA:HAB	27:C:515:BCR:H24C	1.89	0.55
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.88	0.55
2:B:239:SER:O	2:B:466:HIS:ND1	2.39	0.55
23:B:608:CLA:H151	23:B:609:CLA:H203	1.89	0.55
3:C:284:PHE:HB3	28:C:517:DGD:HA51	1.89	0.55
13:O:73:PRO:HG2	13:O:102:THR:HB	1.89	0.55
24:A:406:PHO:H151	23:D:401:CLA:H172	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:501:CLA:C2D	23:C:503:CLA:H2	2.37	0.55
23:a:404:CLA:H172	24:a:407:PHO:H43	1.88	0.55
23:b:611:CLA:HBB1	31:b:625:LMG:H341	1.89	0.55
3:c:342:MET:HE3	3:c:352:GLY:HA2	1.89	0.55
27:c:514:BCR:H391	10:k:36:ALA:HB2	1.90	0.55
2:B:78:TRP:HB3	13:o:137:ALA:HB1	1.89	0.54
23:a:406:CLA:H142	23:d:402:CLA:H151	1.89	0.54
13:o:83:LYS:HG2	13:o:84:ASN:H	1.72	0.54
1:A:84:PRO:HA	1:A:112:TYR:CG	2.42	0.54
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.90	0.54
13:o:240:THR:HG22	13:o:264:VAL:HG12	1.90	0.54
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.88	0.54
23:a:405:CLA:HAA1	25:d:404:PL9:H362	1.89	0.54
3:c:291:TRP:O	3:c:305:THR:OG1	2.25	0.54
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.07	0.54
23:c:505:CLA:HBD	23:c:505:CLA:HBA1	1.90	0.54
2:B:121:GLU:O	7:H:12:ARG:NH2	2.41	0.54
16:V:59:PHE:HA	16:V:63:CYS:SG	2.48	0.54
2:b:18:ARG:NH2	30:b:601:SQD:O9	2.41	0.54
4:d:84:SER:HB2	4:d:85:MET:HE2	1.90	0.54
31:D:407:LMG:O5	31:D:407:LMG:O4	2.23	0.54
2:b:201:HIS:HD2	2:b:202:HIS:CE1	2.26	0.54
2:b:371:THR:HG22	2:b:377:VAL:HA	1.89	0.54
23:b:608:CLA:HBD	23:b:609:CLA:H43	1.89	0.54
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.43	0.54
23:B:615:CLA:H172	23:B:615:CLA:H111	1.90	0.54
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.89	0.54
28:C:518:DGD:HA41	31:C:520:LMG:H391	1.89	0.54
31:C:520:LMG:HC62	27:J:102:BCR:H271	1.90	0.54
12:M:31:SER:HA	31:M:101:LMG:HC1	1.90	0.54
19:z:33:TRP:O	19:z:37:LYS:HB2	2.07	0.54
23:b:615:CLA:H41	23:b:618:CLA:HBC3	1.88	0.54
1:A:111:PRO:O	1:A:115:ILE:HG13	2.08	0.53
2:B:41:GLU:HB3	2:B:60:MET:SD	2.48	0.53
2:b:96:VAL:HG22	23:b:610:CLA:HBA1	1.89	0.53
3:c:461:ARG:NH1	4:d:241:GLU:OE1	2.41	0.53
15:u:98:THR:O	15:u:102:LYS:HG3	2.08	0.53
1:A:183:MET:HE1	23:A:404:CLA:HMD2	1.89	0.53
1:A:211:PHE:HA	1:A:214:MET:HB2	1.89	0.53
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.89	0.53
1:A:214:MET:HE1	4:D:142:ASN:HD21	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.89	0.53
33:B:628:LMT:H122	14:t:7:VAL:HG12	1.89	0.53
2:b:315:ILE:HG22	2:b:426:PHE:HB3	1.90	0.53
2:B:271:THR:HB	2:B:274:GLN:HG3	1.90	0.53
23:a:404:CLA:HHC	23:a:404:CLA:HBB1	1.89	0.53
16:v:81:ARG:CZ	16:v:157:GLY:HA3	2.37	0.53
5:e:15:THR:HG23	9:j:8:ILE:O	2.08	0.53
23:B:603:CLA:C3D	23:B:605:CLA:H2	2.39	0.53
23:B:604:CLA:HBB1	23:B:607:CLA:CBB	2.38	0.53
4:D:214:HIS:ND1	25:D:404:PL9:O2	2.27	0.53
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.90	0.53
1:A:210:LEU:HG	24:A:406:PHO:NC	2.24	0.53
2:B:198:VAL:O	2:B:202:HIS:ND1	2.35	0.53
4:D:49:LEU:O	4:D:53:THR:HG23	2.09	0.53
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.91	0.53
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.91	0.53
1:a:244:GLU:HG3	1:a:246:TYR:H	1.73	0.53
2:B:125:ASP:HB2	2:B:132:ALA:HB3	1.91	0.53
28:B:627:DGD:HB22	33:B:629:LMT:H72	1.91	0.53
1:a:210:LEU:HG	24:a:408:PHO:NC	2.24	0.53
23:a:406:CLA:HAB	23:d:402:CLA:H72	1.90	0.53
1:A:78:ILE:O	1:A:176:ILE:HB	2.09	0.52
1:A:140:ARG:NH2	29:A:412:LHG:O5	2.36	0.52
23:B:602:CLA:H42	7:H:45:ILE:HD11	1.90	0.52
1:a:141:PRO:O	1:a:143:ILE:N	2.41	0.52
1:a:214:MET:HE1	4:d:142:ASN:HD21	1.74	0.52
23:A:403:CLA:H122	24:D:402:PHO:H3A	1.91	0.52
34:f:101:HEM:HBC2	34:f:101:HEM:HMC2	1.91	0.52
23:B:606:CLA:H203	30:a:401:SQD:H332	1.92	0.52
10:k:31:LEU:HB3	27:k:102:BCR:C15	2.40	0.52
23:A:404:CLA:H203	24:D:402:PHO:H71	1.92	0.52
2:b:26:HIS:CE1	23:b:616:CLA:HMA2	2.44	0.52
27:A:410:BCR:H311	30:A:417:SQD:H351	1.92	0.52
2:B:241:SER:HB3	23:B:612:CLA:HED3	1.91	0.52
13:O:83:LYS:HG2	13:O:84:ASN:H	1.75	0.52
1:a:153:SER:HB2	23:a:404:CLA:H43	1.92	0.52
23:A:405:CLA:H93	23:D:401:CLA:H152	1.92	0.52
31:D:407:LMG:O6	11:L:15:THR:HG21	2.10	0.52
3:c:29:GLU:HB3	10:k:46:ARG:HH11	1.74	0.52
3:c:305:THR:HG22	3:c:308:GLU:HB2	1.91	0.52
3:c:334:PRO:HA	13:o:179:THR:OG1	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:33:TRP:HA	19:z:36:SER:HB3	1.92	0.52
1:A:244:GLU:HG3	1:A:246:TYR:H	1.73	0.52
2:b:327:THR:HG21	31:b:625:LMG:H111	1.92	0.52
28:b:602:DGD:O1B	28:b:602:DGD:O2D	2.28	0.52
2:B:317:ASN:HA	2:B:330:MET:HE1	1.92	0.51
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.44	0.51
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.74	0.51
27:A:410:BCR:H342	30:A:417:SQD:H342	1.92	0.51
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.45	0.51
2:b:222:PRO:HG3	7:h:27:THR:H	1.75	0.51
3:c:393:ALA:HB1	34:v:201:HEM:HBC1	1.93	0.51
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.46	0.51
2:B:122:LEU:O	7:H:15:ASN:ND2	2.40	0.51
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.75	0.51
3:C:158:THR:O	3:C:251:HIS:HB3	2.09	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.45	0.51
23:b:619:CLA:H172	23:b:619:CLA:H111	1.92	0.51
23:c:512:CLA:H143	23:c:513:CLA:H162	1.92	0.51
10:k:40:GLN:HA	10:k:43:VAL:HG12	1.91	0.51
30:A:417:SQD:H332	23:b:610:CLA:H203	1.93	0.51
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.93	0.51
5:E:15:THR:HG23	9:J:8:ILE:O	2.10	0.51
19:Z:32:ASP:CG	19:Z:33:TRP:H	2.18	0.51
23:a:404:CLA:H71	23:a:405:CLA:HAB	1.91	0.51
2:b:76:SER:HG	2:b:78:TRP:CD1	2.28	0.51
23:c:508:CLA:H172	28:c:517:DGD:HBW2	1.93	0.51
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.43	0.51
1:A:183:MET:HA	23:A:403:CLA:HMD1	1.91	0.51
2:B:371:THR:HG22	2:B:377:VAL:HA	1.93	0.51
4:d:302:GLU:OE1	13:o:186:LYS:NZ	2.37	0.51
13:o:230:VAL:HG13	13:o:237:ILE:HG22	1.93	0.51
23:A:404:CLA:HAA1	25:D:404:PL9:H362	1.91	0.51
23:B:603:CLA:CBB	23:B:605:CLA:H152	2.41	0.51
13:O:230:VAL:HG12	13:O:231:ASP:H	1.74	0.51
30:a:415:SQD:H223	28:c:518:DGD:HAE1	1.91	0.51
2:b:474:LEU:O	4:d:134:ARG:NH1	2.44	0.51
3:c:380:ILE:HA	3:c:384:ILE:HD11	1.93	0.51
2:b:243:ALA:HB2	2:b:466:HIS:CE1	2.46	0.51
2:b:271:THR:HB	2:b:274:GLN:HG3	1.92	0.51
3:c:75:PHE:HD1	3:c:86:LEU:HD21	1.76	0.51
3:c:315:MET:HE1	3:c:369:LEU:HD12	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLY:O	2:B:217:ILE:HG13	2.10	0.51
3:C:85:GLY:N	28:C:518:DGD:HE4	2.25	0.51
23:b:606:CLA:H42	7:h:45:ILE:HD11	1.93	0.51
23:b:611:CLA:HBC3	27:b:621:BCR:HC8	1.92	0.51
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.91	0.51
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.93	0.51
1:A:238:LYS:HD2	14:T:32:LYS:HB3	1.93	0.51
4:D:146:PHE:C	4:D:149:PRO:HD2	2.36	0.51
33:D:410:LMT:H72	18:X:26:GLY:HA2	1.92	0.51
5:E:81:GLU:C	5:E:83:LEU:H	2.19	0.51
3:c:130:VAL:O	3:c:134:ILE:HG12	2.11	0.51
31:d:407:LMG:O6	11:l:15:THR:HG21	2.11	0.51
5:e:81:GLU:C	5:e:83:LEU:H	2.19	0.51
2:B:222:PRO:HG3	7:H:27:THR:H	1.75	0.50
3:C:315:MET:HE1	3:C:369:LEU:HD12	1.93	0.50
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.93	0.50
2:b:62:VAL:HG12	2:b:66:MET:HE2	1.93	0.50
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.92	0.50
23:B:602:CLA:HBD	23:B:602:CLA:H2	1.92	0.50
30:F:102:SQD:H131	18:X:36:VAL:HG11	1.93	0.50
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.76	0.50
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.26	0.50
2:b:241:SER:HB3	23:b:616:CLA:HED3	1.93	0.50
3:c:425:TRP:CE2	23:c:504:CLA:HBA1	2.46	0.50
23:B:611:CLA:H171	23:B:613:CLA:ND	2.26	0.50
4:d:49:LEU:HD13	27:d:405:BCR:C15	2.42	0.50
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.41	0.50
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.94	0.50
1:a:183:MET:HE1	23:a:405:CLA:HMD2	1.92	0.50
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.93	0.50
27:B:618:BCR:H332	14:t:21:ILE:HD12	1.94	0.50
11:L:10:VAL:O	12:M:28:GLN:NE2	2.34	0.50
27:T:101:BCR:H23C	2:b:25:MET:HG2	1.94	0.50
1:a:78:ILE:O	1:a:176:ILE:HB	2.11	0.50
3:c:473:ASP:HB2	14:t:26:PRO:HB3	1.93	0.50
27:c:514:BCR:H311	27:c:514:BCR:H343	1.93	0.50
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.92	0.50
2:B:184:GLU:H	2:B:200:ALA:HB2	1.77	0.50
3:c:361:PHE:HA	28:c:516:DGD:HE62	1.94	0.50
4:d:221:THR:HG23	4:d:244:TYR:HB2	1.93	0.50
1:A:119:PHE:HZ	23:A:403:CLA:H8	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ALA:O	2:B:159:THR:OG1	2.26	0.50
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.46	0.50
16:V:102:MET:HE1	16:V:141:ILE:HD12	1.93	0.50
23:b:611:CLA:H102	31:b:625:LMG:H392	1.94	0.50
1:A:190:HIS:O	1:A:298:ASN:HB3	2.12	0.50
27:B:617:BCR:H341	27:B:618:BCR:H24C	1.93	0.50
9:J:14:ALA:O	9:J:18:GLY:N	2.42	0.50
23:b:607:CLA:C3D	23:b:609:CLA:H2	2.41	0.50
3:c:150:ASP:HB3	3:c:153:ASP:HB2	1.94	0.50
5:e:55:TYR:O	5:e:84:LYS:HE3	2.12	0.50
9:j:14:ALA:O	9:j:18:GLY:N	2.42	0.50
13:O:36:ILE:O	13:O:39:THR:OG1	2.28	0.50
23:b:611:CLA:H122	31:b:625:LMG:H412	1.93	0.50
3:c:186:TYR:HE2	3:c:188:THR:HG22	1.76	0.50
3:c:429:SER:HB3	28:c:517:DGD:HA81	1.94	0.50
3:C:361:PHE:HA	28:C:517:DGD:HE62	1.92	0.49
30:F:102:SQD:H162	18:X:33:THR:HA	1.93	0.49
13:o:118:SER:HB3	13:o:157:PRO:HA	1.93	0.49
2:B:7:ARG:HH21	31:B:622:LMG:HC3	1.76	0.49
2:B:329:PRO:HB3	23:B:607:CLA:HED1	1.94	0.49
23:B:604:CLA:HBB1	23:B:607:CLA:HBB2	1.93	0.49
14:T:7:VAL:HG12	33:b:603:LMT:H122	1.94	0.49
1:a:159:LEU:C	1:a:162:PRO:HD2	2.37	0.49
1:a:238:LYS:HD2	14:t:32:LYS:HB3	1.93	0.49
23:b:612:CLA:H51	23:b:613:CLA:H101	1.94	0.49
29:A:412:LHG:HC32	4:D:229:ALA:O	2.12	0.49
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.93	0.49
17:y:39:LEU:HD21	19:Z:25:VAL:HA	1.94	0.49
18:X:34:PHE:O	18:X:38:ILE:HG12	2.12	0.49
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.47	0.49
23:C:511:CLA:HMB1	27:C:514:BCR:H382	1.95	0.49
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.94	0.49
4:d:222:LEU:HD23	4:d:244:TYR:HB3	1.94	0.49
1:A:244:GLU:CD	4:D:264:LYS:HZ3	2.20	0.49
1:A:334:ARG:NH1	13:O:183:LEU:O	2.46	0.49
23:A:404:CLA:HBA1	23:A:404:CLA:CHA	2.42	0.49
3:C:56:HIS:HE1	3:C:60:ILE:HD11	1.78	0.49
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.76	0.49
7:H:3:ARG:NH2	11:L:1:MET:HE1	2.27	0.49
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.95	0.49
2:b:6:TYR:OH	31:b:624:LMG:HC5	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:286:ALA:HB2	23:c:502:CLA:HMD1	1.93	0.49
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.93	0.49
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.48	0.49
13:O:77:LEU:HB2	13:O:260:LYS:HB3	1.95	0.49
23:b:607:CLA:C2D	23:b:609:CLA:H2	2.43	0.49
3:c:248:GLY:O	3:c:252:ILE:HG12	2.12	0.49
3:c:319:ILE:HG21	3:c:389:GLU:HG3	1.94	0.49
1:A:217:SER:HA	4:D:272:LEU:HD12	1.94	0.49
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.95	0.49
1:a:283:VAL:O	1:a:286:THR:HG22	2.13	0.49
1:a:328:MET:HE1	4:d:183:LEU:HD22	1.93	0.49
4:d:60:THR:HG23	4:d:61:HIS:CD2	2.48	0.49
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.48	0.49
1:A:116:ILE:HG13	1:A:117:PHE:N	2.27	0.49
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.94	0.49
12:M:31:SER:OG	12:m:28:GLN:O	2.19	0.49
27:T:101:BCR:C23	2:b:25:MET:HG2	2.43	0.49
1:a:85:SER:HA	1:a:109:GLY:HA3	1.93	0.49
2:b:122:LEU:O	7:h:15:ASN:ND2	2.44	0.49
3:c:405:ASN:CB	28:c:518:DGD:HG31	2.41	0.49
13:o:230:VAL:HG12	13:o:231:ASP:H	1.78	0.49
3:C:62:PHE:HZ	10:K:28:ILE:HD12	1.77	0.49
3:C:405:ASN:CB	28:C:519:DGD:HG31	2.43	0.49
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.94	0.48
23:C:508:CLA:H172	28:C:518:DGD:HBW2	1.95	0.48
19:Z:33:TRP:HA	19:Z:36:SER:HB3	1.95	0.48
3:c:131:TYR:CE1	3:c:135:ARG:HD2	2.48	0.48
23:c:504:CLA:H202	28:c:518:DGD:HAF2	1.93	0.48
23:B:611:CLA:H41	23:B:614:CLA:HBC3	1.95	0.48
27:B:618:BCR:H352	27:B:619:BCR:H382	1.95	0.48
3:C:90:PRO:O	3:C:94:THR:HG23	2.12	0.48
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.13	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.48
17:g:39:LEU:HD21	19:z:25:VAL:HA	1.95	0.48
3:C:437:PHE:HA	23:C:508:CLA:HMC2	1.95	0.48
23:b:606:CLA:HAA2	7:h:45:ILE:HD12	1.94	0.48
23:c:511:CLA:H171	19:z:20:VAL:HA	1.95	0.48
12:m:19:SER:O	12:m:23:ILE:HG13	2.13	0.48
2:B:458:PHE:HB3	23:B:604:CLA:HBC2	1.95	0.48
3:C:343:ARG:NH1	3:C:347:GLY:O	2.46	0.48
23:b:607:CLA:H2	23:b:609:CLA:H93	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:53:HIS:HB3	23:c:512:CLA:OBD	2.12	0.48
30:f:102:SQD:H131	18:x:36:VAL:HG11	1.94	0.48
23:A:405:CLA:HAB	23:D:401:CLA:H72	1.96	0.48
2:B:327:THR:HG22	23:B:607:CLA:H12	1.94	0.48
3:C:429:SER:HB3	28:C:518:DGD:HA81	1.95	0.48
23:A:403:CLA:H51	24:D:402:PHO:C3B	2.43	0.48
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.48	0.48
23:a:405:CLA:CHA	23:a:405:CLA:HBA1	2.43	0.48
4:d:73:PHE:CZ	31:d:406:LMG:H172	2.48	0.48
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.94	0.48
23:A:403:CLA:HHC	23:A:403:CLA:HBB1	1.95	0.48
23:B:616:CLA:H12	23:B:616:CLA:H72	1.96	0.48
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.95	0.48
1:a:111:PRO:O	1:a:115:ILE:HG13	2.13	0.48
1:A:329:GLU:O	1:A:332:HIS:ND1	2.43	0.48
14:T:4:ILE:HD13	27:T:102:BCR:H381	1.94	0.48
1:a:232:SER:HB3	1:a:235:TYR:HD1	1.78	0.48
2:b:488:PRO:O	2:b:490:GLN:N	2.44	0.48
3:c:158:THR:O	3:c:251:HIS:HB3	2.13	0.48
9:j:9:PRO:HB2	9:j:12:ILE:HG13	1.94	0.48
27:j:102:BCR:H271	31:k:103:LMG:HC62	1.96	0.48
13:O:118:SER:HB3	13:O:157:PRO:HA	1.95	0.48
3:c:91:HIS:O	3:c:94:THR:OG1	2.32	0.48
31:d:407:LMG:O5	31:d:407:LMG:O4	2.21	0.48
9:j:38:SER:OG	9:j:39:SER:N	2.47	0.48
1:A:283:VAL:O	1:A:286:THR:HG22	2.14	0.48
27:A:410:BCR:H342	30:A:417:SQD:H311	1.95	0.48
2:B:135:LEU:HA	2:B:138:MET:HE3	1.96	0.48
4:D:146:PHE:O	4:D:149:PRO:HD2	2.13	0.48
1:a:57:PRO:HG3	1:a:68:SER:CB	2.44	0.48
2:b:191:ASN:HD21	7:h:59:ASN:C	2.22	0.48
2:b:239:SER:O	2:b:466:HIS:ND1	2.43	0.48
15:u:117:VAL:HG13	15:u:122:VAL:HG21	1.94	0.48
23:A:404:CLA:H42	25:D:404:PL9:H162	1.96	0.47
3:C:363:GLY:O	3:C:367:GLU:HG2	2.13	0.47
23:b:606:CLA:H162	23:b:606:CLA:H122	1.47	0.47
23:b:607:CLA:H61	23:b:607:CLA:H41	1.70	0.47
3:c:277:GLY:C	23:c:505:CLA:HBC2	2.39	0.47
3:c:337:LEU:HA	13:o:131:PRO:HG3	1.96	0.47
1:A:157:VAL:HG13	1:A:172:MET:HB3	1.95	0.47
27:B:620:BCR:H15C	27:B:620:BCR:H351	1.75	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:135:LEU:HA	2:b:138:MET:HE3	1.96	0.47
10:k:27:VAL:HG23	31:k:103:LMG:H322	1.95	0.47
1:A:43:ALA:HB1	27:A:410:BCR:H362	1.96	0.47
23:B:602:CLA:H122	23:B:602:CLA:H162	1.54	0.47
3:C:130:VAL:O	3:C:134:ILE:HG12	2.14	0.47
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.43	0.47
12:M:19:SER:O	12:M:23:ILE:HG13	2.14	0.47
2:b:257:TRP:CE2	4:d:291:LEU:HD12	2.49	0.47
23:b:611:CLA:H193	11:l:27:LEU:HD11	1.96	0.47
2:B:25:MET:HG2	27:B:617:BCR:C23	2.45	0.47
1:a:35:VAL:HG13	27:a:412:BCR:HC31	1.97	0.47
1:A:141:PRO:O	1:A:143:ILE:N	2.47	0.47
2:B:474:LEU:O	4:D:134:ARG:NH1	2.47	0.47
27:B:618:BCR:HC32	31:d:407:LMG:H392	1.96	0.47
4:D:60:THR:HG23	4:D:61:HIS:CD2	2.49	0.47
1:a:269:ARG:NH1	4:d:231:THR:HB	2.29	0.47
23:a:409:CLA:HBC1	31:i:101:LMG:H341	1.97	0.47
23:c:501:CLA:H193	23:c:507:CLA:H111	1.96	0.47
1:A:174:LEU:HD22	24:D:402:PHO:H151	1.97	0.47
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.96	0.47
27:k:102:BCR:H333	17:g:28:ILE:HG22	1.96	0.47
27:A:410:BCR:H11C	27:A:410:BCR:H341	1.79	0.47
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.50	0.47
2:B:487:SER:N	2:B:488:PRO:HD2	2.30	0.47
27:T:102:BCR:H352	27:b:621:BCR:H382	1.97	0.47
1:a:271:LEU:HD11	25:a:410:PL9:C4	2.44	0.47
28:a:413:DGD:HAT2	3:c:281:MET:HG3	1.95	0.47
2:b:184:GLU:H	2:b:200:ALA:HB2	1.80	0.47
3:c:425:TRP:CZ2	23:c:504:CLA:HBA1	2.50	0.47
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.30	0.47
2:B:33:TRP:CD1	27:B:618:BCR:H391	2.50	0.47
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.96	0.47
16:V:90:PRO:O	16:V:92:ARG:HD3	2.15	0.47
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.96	0.47
1:a:114:LEU:O	1:a:118:HIS:ND1	2.46	0.47
3:c:240:ILE:O	3:c:244:CYS:HB2	2.14	0.47
4:d:343:GLU:HG2	16:v:161:VAL:HG11	1.97	0.47
1:A:221:SER:HB2	4:D:139:ARG:O	2.15	0.47
1:A:232:SER:OG	31:A:414:LMG:O3	2.21	0.47
4:D:49:LEU:HD13	27:D:405:BCR:C15	2.45	0.47
10:K:16:ALA:O	10:K:19:ASP:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:404:CLA:HBA1	23:a:404:CLA:H3A	1.70	0.47
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.97	0.47
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.97	0.47
3:c:284:PHE:HB3	28:c:516:DGD:HA51	1.96	0.47
3:c:386:PRO:HB3	16:v:116:GLU:HG2	1.97	0.47
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.95	0.47
13:o:223:ILE:HG13	13:o:243:SER:HB3	1.96	0.47
23:B:602:CLA:H62	23:B:602:CLA:H41	1.50	0.47
23:B:608:CLA:CHA	23:B:608:CLA:HBA1	2.45	0.47
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.97	0.47
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.96	0.47
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.96	0.47
2:b:198:VAL:O	2:b:202:HIS:ND1	2.44	0.47
27:c:514:BCR:H331	27:c:514:BCR:HC7	1.57	0.47
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.50	0.46
2:b:326:ARG:HB3	2:b:444:ARG:HG2	1.96	0.46
23:b:612:CLA:HBA1	23:b:612:CLA:CHA	2.45	0.46
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.97	0.46
3:C:451:ALA:HA	3:C:456:GLU:CD	2.40	0.46
4:D:312:GLU:HB2	13:O:185:PRO:CG	2.45	0.46
16:V:98:LEU:O	16:V:102:MET:HG3	2.15	0.46
2:b:348:ASN:HB3	2:b:354:LEU:HD21	1.97	0.46
2:B:25:MET:HG2	27:B:617:BCR:H23C	1.97	0.46
23:C:502:CLA:HBB2	23:C:510:CLA:H152	1.97	0.46
23:C:505:CLA:H11	27:C:516:BCR:H312	1.96	0.46
27:C:516:BCR:H15C	27:C:516:BCR:H351	1.78	0.46
23:a:404:CLA:HBD	23:a:405:CLA:HAC2	1.98	0.46
23:C:511:CLA:H151	19:Z:20:VAL:O	2.15	0.46
8:I:29:ALA:HA	8:I:35:LYS:HB2	1.97	0.46
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.50	0.46
4:d:214:HIS:ND1	25:d:404:PL9:O2	2.36	0.46
2:B:256:MET:HA	2:B:263:THR:HG21	1.97	0.46
33:B:629:LMT:H62	8:i:4:LEU:HD22	1.97	0.46
1:a:156:ALA:HA	1:a:160:ILE:HB	1.98	0.46
24:a:408:PHO:CHB	23:d:402:CLA:H101	2.45	0.46
23:c:509:CLA:H11	23:c:509:CLA:H51	1.68	0.46
15:u:75:LEU:HD21	15:u:101:GLN:HB3	1.98	0.46
3:C:319:ILE:HG21	3:C:389:GLU:HG3	1.98	0.46
12:M:28:GLN:O	12:m:31:SER:OG	2.30	0.46
1:a:129:ARG:NH2	4:d:256:ILE:HD12	2.26	0.46
1:a:215:HIS:ND1	25:a:410:PL9:O1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:501:CLA:C2D	23:c:503:CLA:H2	2.46	0.46
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.51	0.46
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.51	0.46
2:B:18:ARG:NH2	30:B:626:SQD:O9	2.49	0.46
27:B:620:BCR:H11C	27:B:620:BCR:H341	1.82	0.46
23:C:506:CLA:H202	23:C:506:CLA:H161	1.79	0.46
23:a:404:CLA:H191	31:d:407:LMG:H352	1.98	0.46
23:b:608:CLA:HBB1	23:b:611:CLA:CBB	2.45	0.46
23:b:619:CLA:H52	23:b:619:CLA:H12	1.78	0.46
3:c:85:GLY:N	28:c:517:DGD:HE4	2.31	0.46
4:d:189:HIS:HA	4:d:294:ARG:HD2	1.98	0.46
5:e:19:TYR:O	5:e:23:HIS:ND1	2.41	0.46
11:l:10:VAL:O	12:m:28:GLN:NE2	2.33	0.46
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.98	0.46
30:A:417:SQD:H61	23:b:620:CLA:H2	1.97	0.46
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.98	0.46
23:B:612:CLA:H171	23:B:613:CLA:HBB2	1.98	0.46
3:C:245:ILE:O	3:C:249:ILE:HG12	2.15	0.46
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.98	0.46
1:a:211:PHE:HA	1:a:214:MET:HB2	1.97	0.46
2:b:464:PHE:HD2	23:b:615:CLA:HAC2	1.80	0.46
3:c:90:PRO:O	3:c:94:THR:HG23	2.15	0.46
18:x:12:ILE:HA	18:x:16:LEU:HD12	1.98	0.46
2:B:137:LYS:HD2	7:H:14:LEU:O	2.16	0.46
23:B:613:CLA:H191	27:B:619:BCR:H333	1.98	0.46
27:C:514:BCR:H343	27:C:514:BCR:H311	1.98	0.46
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.98	0.46
24:D:402:PHO:H62	24:D:402:PHO:H41	1.38	0.46
10:K:21:LEU:HD21	27:y:101:BCR:HC31	1.98	0.46
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.46	0.46
23:c:511:CLA:H93	27:c:514:BCR:H272	1.97	0.46
31:i:101:LMG:H221	33:i:102:LMT:H81	1.98	0.46
10:k:21:LEU:HD21	27:k:102:BCR:HC31	1.98	0.46
24:A:406:PHO:HMA2	25:A:408:PL9:H222	1.98	0.45
3:C:56:HIS:CE1	3:C:60:ILE:HD11	2.51	0.45
10:K:31:LEU:HB3	27:y:101:BCR:C15	2.46	0.45
2:b:201:HIS:HD2	2:b:202:HIS:ND1	2.14	0.45
3:c:223:TRP:CG	3:c:224:ILE:H	2.32	0.45
4:d:252:PHE:O	4:d:256:ILE:HG22	2.16	0.45
17:g:24:MET:O	17:g:28:ILE:HG23	2.16	0.45
1:A:153:SER:HB3	23:A:403:CLA:HED1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:PHE:HB2	23:B:608:CLA:HBC1	1.98	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.16	0.45
3:C:224:ILE:O	3:C:227:VAL:HG23	2.16	0.45
12:M:9:ILE:HD12	12:m:8:LEU:HG	1.99	0.45
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.98	0.45
1:a:227:THR:HG21	1:a:233:ALA:HA	1.98	0.45
23:c:504:CLA:H2	28:c:517:DGD:HA22	1.98	0.45
27:c:514:BCR:H15C	27:c:514:BCR:H351	1.66	0.45
5:e:26:THR:HB	34:f:101:HEM:CAB	2.46	0.45
13:o:240:THR:HA	13:o:264:VAL:HA	1.97	0.45
23:B:609:CLA:HMD1	7:H:27:THR:HB	1.98	0.45
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.80	0.45
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.80	0.45
23:C:507:CLA:H62	23:C:507:CLA:H92	1.72	0.45
2:b:341:LYS:HA	2:b:405:GLU:HB2	1.99	0.45
23:c:503:CLA:H172	23:c:510:CLA:HBB2	1.98	0.45
33:d:410:LMT:H72	18:x:26:GLY:HA2	1.98	0.45
23:A:407:CLA:H162	23:A:407:CLA:H141	1.63	0.45
2:B:464:PHE:HD2	23:B:611:CLA:HAC2	1.80	0.45
23:B:603:CLA:H192	23:B:603:CLA:H162	1.78	0.45
5:E:50:PRO:HB3	5:E:54:SER:O	2.16	0.45
2:b:91:TRP:HE1	33:b:626:LMT:H12	1.81	0.45
23:A:403:CLA:H172	24:D:402:PHO:H43	1.97	0.45
23:B:603:CLA:H2	23:B:605:CLA:H93	1.97	0.45
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.32	0.45
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.99	0.45
10:K:37:PHE:HB3	27:y:101:BCR:C40	2.47	0.45
13:O:177:TYR:HD2	13:O:178:ARG:HG2	1.81	0.45
1:a:161:TYR:HB3	1:a:162:PRO:HD3	1.99	0.45
2:b:329:PRO:HB3	23:b:611:CLA:HED1	1.97	0.45
3:c:166:ILE:O	3:c:170:ILE:HG13	2.17	0.45
3:c:229:ASN:ND2	3:c:231:GLU:HB2	2.32	0.45
3:c:346:THR:HG21	13:o:38:GLY:HA2	1.98	0.45
4:d:274:VAL:HG13	25:d:404:PL9:C23	2.47	0.45
13:o:178:ARG:HD2	13:o:182:PHE:CD1	2.51	0.45
13:o:192:SER:OG	13:o:193:GLY:N	2.49	0.45
2:b:270:PRO:HG3	2:b:312:TYR:CD2	2.50	0.45
30:f:102:SQD:H162	18:x:33:THR:HA	1.98	0.45
15:u:68:TYR:HB2	15:u:71:LEU:HD12	1.97	0.45
23:A:403:CLA:HBA1	23:A:403:CLA:H3A	1.61	0.45
5:e:10:PHE:N	31:e:101:LMG:O3	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ALA:HA	1:A:160:ILE:HB	1.98	0.45
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.82	0.45
12:M:8:LEU:HG	12:m:9:ILE:HD12	1.99	0.45
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.99	0.45
15:U:106:ARG:HA	15:U:109:LEU:HG	1.98	0.45
27:y:101:BCR:H332	19:Z:17:PHE:CD1	2.51	0.45
27:b:621:BCR:H351	27:b:621:BCR:H15C	1.75	0.45
4:d:85:MET:HA	5:e:69:ARG:HB3	1.98	0.45
6:f:27:ALA:HB1	34:f:101:HEM:CAC	2.47	0.45
1:A:159:LEU:C	1:A:162:PRO:HD2	2.42	0.45
28:A:411:DGD:HAT2	3:C:281:MET:HG3	1.98	0.45
23:B:601:CLA:HMB2	27:H:101:BCR:H281	1.98	0.45
33:B:628:LMT:H1B	33:B:628:LMT:H3'	1.56	0.45
3:C:223:TRP:CG	3:C:224:ILE:H	2.34	0.45
23:C:509:CLA:H51	23:C:509:CLA:H11	1.71	0.45
5:E:19:TYR:O	5:E:23:HIS:ND1	2.40	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
27:T:101:BCR:H341	27:T:102:BCR:H24C	1.98	0.45
1:a:73:TYR:CE2	31:a:402:LMG:HC5	2.52	0.45
1:a:180:PHE:HA	1:a:183:MET:HE3	1.99	0.45
3:c:29:GLU:HB2	3:c:30:SER:H	1.63	0.45
3:c:296:VAL:HG23	3:c:297:TYR:CD2	2.52	0.45
5:e:60:GLN:HG2	5:e:62:SER:H	1.81	0.45
23:A:404:CLA:H202	23:A:404:CLA:H162	1.75	0.45
23:B:603:CLA:H61	23:B:603:CLA:H41	1.80	0.45
31:C:521:LMG:H111	31:C:521:LMG:H292	1.99	0.45
23:a:405:CLA:H162	23:a:405:CLA:H202	1.71	0.45
29:a:414:LHG:HC12	23:c:508:CLA:O1D	2.17	0.45
2:b:462:PHE:HA	23:b:615:CLA:HMC2	1.99	0.45
27:h:101:BCR:H15C	27:h:101:BCR:H351	1.82	0.45
31:i:101:LMG:H181	33:i:102:LMT:H42	1.99	0.45
2:B:315:ILE:HG22	2:B:426:PHE:HB3	2.00	0.44
23:D:401:CLA:H61	23:D:401:CLA:H41	1.65	0.44
1:a:333:GLU:HB2	1:a:337:HIS:HE1	1.82	0.44
23:a:405:CLA:HMA2	25:d:404:PL9:H411	1.99	0.44
23:b:620:CLA:H72	23:b:620:CLA:H12	1.99	0.44
3:c:55:ALA:HB2	3:c:129:GLY:HA3	1.98	0.44
23:c:511:CLA:H141	19:z:20:VAL:HG13	2.00	0.44
27:c:514:BCR:H353	27:k:102:BCR:H321	2.00	0.44
30:d:408:SQD:H3	30:d:408:SQD:H441	1.98	0.44
2:B:96:VAL:HG22	23:B:606:CLA:HBA1	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:614:CLA:H91	23:B:614:CLA:H112	1.76	0.44
27:D:405:BCR:H15C	27:D:405:BCR:H351	1.82	0.44
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.99	0.44
3:c:361:PHE:HD1	28:c:516:DGD:HE61	1.82	0.44
4:d:216:ALA:O	4:d:220:ASN:ND2	2.45	0.44
4:d:294:ARG:H	4:d:294:ARG:HG2	1.61	0.44
2:B:12:LEU:HB2	23:B:612:CLA:HMC1	1.99	0.44
2:B:247:PHE:HE1	23:B:602:CLA:H101	1.82	0.44
4:D:40:CYS:HB3	4:D:117:HIS:O	2.18	0.44
17:y:45:ASN:HD22	19:Z:28:ALA:HA	1.81	0.44
1:a:232:SER:HB3	1:a:235:TYR:CD1	2.51	0.44
2:b:89:GLY:HA2	28:b:602:DGD:HD61	2.00	0.44
27:c:515:BCR:H15C	27:c:515:BCR:H351	1.75	0.44
4:d:129:GLN:OE1	4:d:143:ALA:HA	2.18	0.44
2:B:26:HIS:CE1	23:B:612:CLA:HMA2	2.52	0.44
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	1.99	0.44
23:C:511:CLA:H93	23:C:511:CLA:H61	1.81	0.44
2:b:277:SER:OG	28:b:623:DGD:O5E	2.33	0.44
1:A:298:ASN:ND2	3:C:402:GLY:O	2.50	0.44
2:B:187:PRO:HB3	23:B:601:CLA:HMB1	2.00	0.44
3:C:240:ILE:HD11	27:C:516:BCR:H372	1.99	0.44
3:C:456:GLU:HG2	3:C:457:LYS:HG3	1.99	0.44
23:C:501:CLA:C1D	23:C:503:CLA:H2	2.47	0.44
23:C:505:CLA:HBA1	23:C:505:CLA:HBD	2.00	0.44
4:D:84:SER:HB2	4:D:85:MET:HE2	1.99	0.44
6:F:27:ALA:HB1	34:F:101:HEM:CAC	2.47	0.44
27:a:412:BCR:H24C	27:a:412:BCR:H371	1.76	0.44
2:b:18:ARG:NH2	30:b:601:SQD:S	2.84	0.44
2:b:327:THR:HG22	23:b:611:CLA:H12	2.00	0.44
23:b:618:CLA:H112	23:b:618:CLA:H91	1.73	0.44
5:e:50:PRO:HB3	5:e:54:SER:O	2.18	0.44
2:B:68:ARG:HH22	23:B:604:CLA:HED1	1.82	0.44
3:C:361:PHE:HD1	28:C:517:DGD:HE61	1.83	0.44
23:C:504:CLA:H121	28:C:518:DGD:HBE2	1.99	0.44
13:O:240:THR:HA	13:O:264:VAL:HA	1.98	0.44
2:b:135:LEU:HB2	2:b:136:PRO:HD3	1.99	0.44
2:b:341:LYS:HD2	2:b:429:ILE:HG22	1.98	0.44
23:b:608:CLA:H161	23:b:608:CLA:H202	1.81	0.44
1:A:29:TYR:O	1:A:129:ARG:HD2	2.18	0.44
1:A:57:PRO:HA	1:A:68:SER:HA	2.00	0.44
23:A:403:CLA:H202	23:A:404:CLA:H93	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:LEU:HA	2:B:210:ILE:HD11	2.00	0.44
2:B:338:GLN:HB3	13:o:84:ASN:HB3	1.99	0.44
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.00	0.44
27:B:619:BCR:H341	27:B:619:BCR:H11C	1.84	0.44
23:C:510:CLA:H2	23:C:510:CLA:H61	1.73	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.81	0.44
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.18	0.44
1:a:271:LEU:HD21	25:a:410:PL9:HC71	1.99	0.44
23:b:617:CLA:H51	31:b:624:LMG:H231	2.00	0.44
23:c:507:CLA:H92	23:c:507:CLA:H62	1.74	0.44
27:A:410:BCR:H15C	27:A:410:BCR:H351	1.80	0.44
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.99	0.44
23:B:606:CLA:H3A	23:B:606:CLA:HBA2	1.30	0.44
3:C:164:HIS:ND1	23:C:507:CLA:OBD	2.42	0.44
13:O:59:ASP:C	13:O:61:SER:H	2.26	0.44
1:a:141:PRO:HB2	1:a:142:TRP:H	1.64	0.44
23:a:409:CLA:H162	23:a:409:CLA:H141	1.69	0.44
2:b:414:PRO:HB2	2:b:415:PRO:HD3	1.99	0.44
23:b:610:CLA:H3A	23:b:610:CLA:HBA2	1.28	0.44
3:c:163:PHE:CG	23:c:512:CLA:HAB	2.53	0.44
23:d:403:CLA:H61	23:d:403:CLA:H41	1.77	0.44
6:f:17:THR:OG1	6:f:18:VAL:N	2.51	0.44
15:u:58:ASN:ND2	15:u:114:VAL:HG13	2.32	0.44
16:v:160:LYS:HA	16:v:163:TYR:CD2	2.53	0.44
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.53	0.44
2:b:333:GLY:O	2:b:439:SER:HB3	2.18	0.44
2:b:340:TRP:CD1	2:b:342:GLY:H	2.36	0.44
4:d:320:LEU:HD23	4:d:323:GLU:OE1	2.17	0.44
27:h:101:BCR:H24C	27:h:101:BCR:H371	1.81	0.44
1:A:193:LEU:HD11	23:A:403:CLA:HMC2	2.00	0.43
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
2:B:76:SER:HG	2:B:78:TRP:CD1	2.36	0.43
2:B:134:ASP:OD2	2:B:137:LYS:HE3	2.18	0.43
2:B:174:LEU:HD23	2:B:308:LYS:HG2	1.99	0.43
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.00	0.43
2:b:135:LEU:HD22	2:b:237:VAL:HG21	1.99	0.43
8:i:6:ILE:O	8:i:10:ILE:HG12	2.18	0.43
16:v:102:MET:HE3	34:v:201:HEM:HBB2	1.99	0.43
24:A:406:PHO:H161	4:D:48:TRP:CE2	2.53	0.43
23:B:604:CLA:HBD	23:B:605:CLA:H43	2.00	0.43
3:C:265:ILE:HG12	23:C:505:CLA:HED1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:511:CLA:H93	27:C:514:BCR:H272	1.99	0.43
4:D:285:GLY:O	4:D:289:LEU:HG	2.18	0.43
27:T:102:BCR:H11C	27:T:102:BCR:H341	1.79	0.43
1:a:150:PRO:HB2	23:a:404:CLA:H61	1.99	0.43
3:c:386:PRO:O	3:c:390:ARG:HG2	2.18	0.43
27:c:514:BCR:H11C	27:c:514:BCR:H341	1.78	0.43
4:d:110:LEU:HD23	4:d:110:LEU:HA	1.83	0.43
9:j:33:TYR:HB3	27:j:102:BCR:H383	2.00	0.43
1:A:238:LYS:O	1:A:241:GLN:HG3	2.18	0.43
23:B:607:CLA:H202	4:D:281:MET:SD	2.57	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
10:K:43:VAL:CG2	10:K:46:ARG:HE	2.32	0.43
19:Z:5:PHE:CG	19:Z:61:VAL:HG21	2.53	0.43
3:c:185:LEU:HB2	3:c:230:LEU:HD13	1.99	0.43
3:c:318:LEU:HD13	3:c:351:PHE:HE1	1.82	0.43
5:e:81:GLU:O	5:e:83:LEU:N	2.42	0.43
31:A:414:LMG:H211	11:L:26:VAL:HG21	2.00	0.43
23:B:606:CLA:H62	23:B:606:CLA:H41	1.80	0.43
23:B:608:CLA:HAB	4:D:123:ILE:HG23	2.01	0.43
23:B:614:CLA:OBD	11:L:10:VAL:HG21	2.18	0.43
27:B:618:BCR:H381	14:t:4:ILE:HD13	2.00	0.43
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.53	0.43
4:D:148:ALA:HB1	4:D:279:LEU:HB2	2.00	0.43
4:D:320:LEU:HD23	4:D:323:GLU:OE1	2.18	0.43
30:a:401:SQD:H342	27:a:412:BCR:H342	2.01	0.43
23:a:404:CLA:H151	24:a:407:PHO:H72	2.00	0.43
30:a:415:SQD:H172	29:a:417:LHG:H172	2.00	0.43
2:b:18:ARG:HD2	2:b:115:TRP:CE3	2.54	0.43
3:c:137:PRO:HB2	3:c:139:THR:O	2.18	0.43
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.53	0.43
23:B:602:CLA:H72	7:H:46:LEU:HD13	2.01	0.43
31:I:101:LMG:H181	33:I:102:LMT:H42	2.01	0.43
13:O:218:LEU:HD22	15:U:119:THR:HG21	2.01	0.43
2:b:306:PRO:HG2	2:b:309:LEU:HB2	2.00	0.43
3:c:224:ILE:O	3:c:227:VAL:HG23	2.18	0.43
4:d:275:PRO:O	4:d:279:LEU:HD23	2.19	0.43
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.18	0.43
7:h:12:ARG:O	7:h:12:ARG:HD3	2.18	0.43
15:u:83:ALA:HB1	15:u:84:PRO:HD2	1.99	0.43
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.00	0.43
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:313:THR:OG1	4:D:316:THR:HG23	2.18	0.43
13:O:137:ALA:HB1	2:b:78:TRP:HB3	2.00	0.43
1:a:35:VAL:HG13	27:a:412:BCR:C3	2.49	0.43
1:a:97:TRP:HE1	28:a:413:DGD:HO3D	1.58	0.43
23:a:405:CLA:H11	23:a:405:CLA:H51	1.67	0.43
2:b:247:PHE:HB2	23:b:612:CLA:HBC1	1.99	0.43
23:A:403:CLA:H62	23:A:403:CLA:H102	1.80	0.43
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.01	0.43
2:B:275:TRP:CH2	2:B:358:ARG:HD3	2.54	0.43
2:B:326:ARG:NH2	4:D:297:ASP:OD2	2.52	0.43
23:B:607:CLA:C4A	23:B:607:CLA:HBA2	2.48	0.43
27:C:514:BCR:H391	10:K:36:ALA:HB2	2.00	0.43
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.01	0.43
5:E:10:PHE:N	31:E:101:LMG:O3	2.52	0.43
16:V:103:LYS:NZ	16:V:135:GLU:OE1	2.34	0.43
1:a:308:ASP:O	6:f:45:ARG:NE	2.52	0.43
7:h:19:GLY:O	7:h:21:VAL:HG13	2.18	0.43
27:j:102:BCR:H351	27:j:102:BCR:H15C	1.66	0.43
13:o:184:ASP:OD2	13:o:188:ARG:HB2	2.18	0.43
13:o:206:GLU:H	13:o:206:GLU:CD	2.27	0.43
23:B:607:CLA:H192	31:B:622:LMG:H342	2.01	0.43
27:B:618:BCR:C10	14:t:18:PHE:HB2	2.46	0.43
3:C:137:PRO:HG3	23:C:513:CLA:HED2	2.00	0.43
4:D:275:PRO:O	4:D:279:LEU:HD23	2.17	0.43
15:U:73:PRO:HD2	16:V:109:ASP:CG	2.43	0.43
1:a:153:SER:CB	23:a:404:CLA:H11	2.49	0.43
23:b:612:CLA:HAB	4:d:123:ILE:HG23	2.00	0.43
27:j:102:BCR:H24C	27:j:102:BCR:H371	1.85	0.43
2:B:69:LEU:HD21	23:B:603:CLA:HED3	2.01	0.43
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.43
3:C:386:PRO:HB3	16:V:116:GLU:HG2	2.01	0.43
13:O:248:ASP:CG	13:O:250:ASP:H	2.26	0.43
1:a:157:VAL:HG13	1:a:172:MET:HB3	2.01	0.43
3:c:38:GLY:HA3	23:c:511:CLA:HMD2	2.01	0.43
4:d:244:TYR:OH	4:d:264:LYS:HE3	2.19	0.43
10:k:37:PHE:HB3	27:k:102:BCR:C40	2.47	0.43
13:o:135:GLN:HE21	13:o:135:GLN:HB3	1.68	0.43
2:B:354:LEU:HB3	2:B:370:LEU:HB3	2.00	0.43
23:B:604:CLA:H11	23:B:605:CLA:H11	2.00	0.43
23:C:504:CLA:H202	28:C:519:DGD:HAF2	2.01	0.43
27:C:514:BCR:H331	27:C:514:BCR:HC7	1.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:79:SER:HA	4:D:172:SER:HB3	2.01	0.43
9:J:14:ALA:HB3	27:y:101:BCR:H393	2.00	0.43
15:U:54:LYS:HD2	15:U:113:THR:HG23	2.01	0.43
2:b:7:ARG:HH21	31:b:624:LMG:HC3	1.83	0.43
2:b:103:LEU:HD21	23:b:609:CLA:HMC2	2.01	0.43
2:b:248:ALA:HA	23:b:607:CLA:H42	2.00	0.43
2:b:487:SER:N	2:b:488:PRO:HD2	2.33	0.43
23:b:612:CLA:H18	23:b:613:CLA:H192	2.01	0.43
23:b:615:CLA:H52	23:b:618:CLA:HBC3	2.00	0.43
31:c:519:LMG:H111	31:c:519:LMG:H292	2.01	0.43
4:d:53:THR:HG22	4:d:67:TYR:CD2	2.53	0.43
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.01	0.42
2:B:461:LEU:HD23	2:B:461:LEU:HA	1.90	0.42
14:T:1:MET:HE2	12:m:6:LEU:HD21	2.00	0.42
24:a:408:PHO:HMC3	4:d:279:LEU:HD21	2.00	0.42
4:d:90:LEU:HD23	4:d:90:LEU:HA	1.82	0.42
31:m:102:LMG:H142	31:m:102:LMG:H311	2.01	0.42
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.49	0.42
23:C:509:CLA:H142	23:C:509:CLA:H112	1.88	0.42
5:E:22:ILE:O	5:E:26:THR:HG23	2.19	0.42
1:a:27:ARG:NH1	4:d:254:SER:O	2.49	0.42
2:b:109:LEU:O	27:b:622:BCR:H21C	2.19	0.42
2:b:170:ASP:OD1	2:b:175:THR:N	2.51	0.42
2:b:206:GLY:O	2:b:210:ILE:HG13	2.19	0.42
4:d:312:GLU:HB2	13:o:185:PRO:CG	2.49	0.42
27:k:102:BCR:H351	27:k:102:BCR:H15C	1.73	0.42
27:z:101:BCR:H24C	27:z:101:BCR:H371	1.78	0.42
2:B:230:ARG:O	2:B:233:ASN:HB3	2.19	0.42
23:B:608:CLA:H51	23:B:609:CLA:H101	2.01	0.42
28:B:627:DGD:O1B	28:B:627:DGD:O2D	2.37	0.42
12:M:16:LEU:O	12:M:20:VAL:HG23	2.20	0.42
13:O:144:LEU:HD13	13:O:259:VAL:HG11	2.01	0.42
27:T:101:BCR:H15C	27:T:101:BCR:H351	1.80	0.42
2:b:112:CYS:HB3	27:b:622:BCR:H393	2.01	0.42
3:c:464:GLU:OE2	4:d:245:SER:OG	2.24	0.42
13:o:51:THR:O	13:o:53:ARG:N	2.52	0.42
23:B:612:CLA:H8	23:B:612:CLA:H122	1.87	0.42
1:a:141:PRO:C	1:a:143:ILE:H	2.28	0.42
1:a:212:CYS:HB2	4:d:211:CYS:HB2	2.01	0.42
1:a:334:ARG:NH2	4:d:312:GLU:OE2	2.53	0.42
27:a:412:BCR:H15C	27:a:412:BCR:H351	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:366:PHE:CD1	2:b:367:PRO:HD2	2.54	0.42
2:b:450:TRP:NE1	23:b:611:CLA:HBA1	2.33	0.42
13:o:168:PHE:HB2	13:o:225:LEU:HB2	2.00	0.42
16:v:98:LEU:O	16:v:102:MET:HG3	2.20	0.42
1:A:114:LEU:O	1:A:118:HIS:ND1	2.53	0.42
2:B:206:GLY:O	2:B:210:ILE:HG13	2.19	0.42
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.55	0.42
6:F:17:THR:OG1	6:F:18:VAL:N	2.52	0.42
1:a:119:PHE:HZ	23:a:404:CLA:H8	1.84	0.42
1:a:224:ILE:O	4:d:265:ARG:NH2	2.52	0.42
4:d:49:LEU:O	4:d:53:THR:HG23	2.19	0.42
4:d:239:GLN:HB3	4:d:240:ALA:H	1.54	0.42
4:d:342:PRO:O	4:d:345:VAL:HG12	2.19	0.42
2:B:386:ALA:HB3	15:U:132:LEU:HD11	2.01	0.42
27:B:618:BCR:H11C	27:B:618:BCR:H341	1.69	0.42
31:C:520:LMG:H322	10:K:27:VAL:HG23	2.02	0.42
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.55	0.42
1:a:81:ALA:HB2	1:a:175:GLY:HA3	2.02	0.42
4:d:274:VAL:HA	25:d:404:PL9:H253	2.02	0.42
12:m:3:VAL:HG11	14:t:2:GLU:HG2	2.02	0.42
19:z:33:TRP:O	19:z:33:TRP:CD1	2.72	0.42
1:A:40:THR:HG21	1:A:121:LEU:HD23	2.01	0.42
2:B:18:ARG:NH1	2:B:115:TRP:O	2.43	0.42
2:B:103:LEU:HD21	23:B:605:CLA:HMC2	2.01	0.42
2:B:280:PHE:O	2:B:284:ILE:HG13	2.19	0.42
2:B:483:ASP:OD2	2:B:484:PRO:HD2	2.20	0.42
23:B:605:CLA:H62	23:B:605:CLA:H41	1.75	0.42
3:C:163:PHE:CG	23:C:512:CLA:HAB	2.54	0.42
3:C:174:LEU:HG	23:C:512:CLA:H92	2.02	0.42
18:X:17:LYS:O	18:X:21:ILE:HG13	2.20	0.42
3:c:72:LEU:HD11	3:c:108:THR:HB	2.00	0.42
27:c:514:BCR:H24C	27:c:514:BCR:H371	1.89	0.42
2:B:489:GLU:HB2	5:E:3:GLY:N	2.35	0.42
3:C:418:ASN:HB2	28:C:519:DGD:O4E	2.20	0.42
23:C:512:CLA:H61	23:C:512:CLA:H13	2.02	0.42
27:C:515:BCR:H20C	27:C:515:BCR:H361	1.93	0.42
27:C:515:BCR:H351	27:C:515:BCR:H15C	1.76	0.42
4:D:201:VAL:O	4:D:205:LEU:HB2	2.20	0.42
7:H:3:ARG:HH21	11:L:1:MET:HE1	1.84	0.42
1:a:176:ILE:HD12	23:a:405:CLA:HED3	2.02	0.42
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:456:GLU:HG2	3:c:457:LYS:HG3	2.02	0.42
23:c:503:CLA:H193	23:c:503:CLA:H161	1.81	0.42
27:c:514:BCR:H353	27:k:102:BCR:C32	2.50	0.42
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.01	0.42
23:C:504:CLA:H2	28:C:518:DGD:HA22	2.01	0.42
4:D:252:PHE:O	4:D:256:ILE:HG22	2.19	0.42
27:J:102:BCR:H351	27:J:102:BCR:H15C	1.60	0.42
10:K:24:VAL:O	10:K:27:VAL:HG12	2.20	0.42
18:X:11:THR:HG23	18:X:12:ILE:HG22	2.01	0.42
1:a:172:MET:SD	1:a:179:THR:HG23	2.60	0.42
24:a:407:PHO:H41	24:a:407:PHO:H62	1.36	0.42
4:d:62:GLY:HA3	5:e:63:ILE:HD13	2.02	0.42
4:d:148:ALA:HB1	4:d:279:LEU:HB2	2.02	0.42
4:D:81:PRO:HG3	4:D:108:GLY:O	2.19	0.42
4:D:346:LEU:HA	4:D:346:LEU:HD12	1.85	0.42
30:D:408:SQD:H3	30:D:408:SQD:H441	2.01	0.42
28:D:409:DGD:O5E	28:D:409:DGD:O4E	2.31	0.42
17:y:28:ILE:O	27:y:101:BCR:H14C	2.20	0.42
23:a:404:CLA:HHC	23:a:404:CLA:CBB	2.50	0.42
23:b:614:CLA:H12	23:b:614:CLA:H51	1.86	0.42
4:d:67:TYR:CD1	31:d:406:LMG:HC72	2.55	0.42
2:B:7:ARG:NH2	31:B:622:LMG:HC3	2.35	0.41
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.41
27:J:102:BCR:H24C	27:J:102:BCR:H371	1.87	0.41
1:a:57:PRO:HA	1:a:68:SER:HA	2.02	0.41
2:b:386:ALA:HB3	15:u:132:LEU:HD11	2.02	0.41
3:c:457:LYS:HG2	4:d:229:ALA:HA	2.02	0.41
1:A:176:ILE:HD12	23:A:404:CLA:HED3	2.02	0.41
1:A:179:THR:HG22	1:A:183:MET:HE2	2.01	0.41
1:A:235:TYR:C	1:A:237:TYR:H	2.27	0.41
1:A:321:ILE:HG22	1:A:325:ASN:ND2	2.35	0.41
23:B:603:CLA:H92	23:B:603:CLA:HBB2	2.02	0.41
23:B:610:CLA:H12	23:B:610:CLA:H51	1.78	0.41
27:B:619:BCR:H351	27:B:619:BCR:H15C	1.81	0.41
3:C:259:TRP:H	3:C:259:TRP:CD1	2.38	0.41
23:C:511:CLA:H141	19:Z:20:VAL:HG13	2.02	0.41
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.50	0.41
1:a:260:PHE:CZ	1:a:263:ALA:HB2	2.55	0.41
23:a:405:CLA:O1A	24:a:407:PHO:HMB1	2.20	0.41
23:b:605:CLA:HMB2	27:h:101:BCR:H281	2.02	0.41
3:c:86:LEU:HB3	3:c:90:PRO:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:141:GLU:CD	3:c:141:GLU:H	2.28	0.41
3:c:197:ARG:NH2	3:c:231:GLU:OE2	2.52	0.41
23:c:504:CLA:H141	23:c:504:CLA:H161	1.76	0.41
13:o:33:TYR:O	13:o:37:VAL:HG23	2.20	0.41
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.02	0.41
23:C:509:CLA:H141	23:C:512:CLA:HMD2	2.02	0.41
23:C:513:CLA:H3A	23:C:513:CLA:HBA2	1.80	0.41
27:H:101:BCR:H371	27:H:101:BCR:H24C	1.81	0.41
14:T:8:PHE:CD1	27:T:102:BCR:H373	2.55	0.41
30:b:601:SQD:H202	30:b:601:SQD:H171	1.91	0.41
3:c:215:LYS:HG2	3:c:221:GLU:HB3	2.01	0.41
3:c:264:PHE:HE1	23:c:507:CLA:HAB	1.84	0.41
23:c:506:CLA:HBB2	23:c:507:CLA:H52	2.03	0.41
28:d:409:DGD:O2D	28:d:409:DGD:HG32	2.20	0.41
14:t:3:THR:O	14:t:7:VAL:HG23	2.19	0.41
15:u:46:LYS:NZ	15:u:116:GLU:O	2.48	0.41
23:B:606:CLA:C3D	33:B:624:LMT:H11	2.50	0.41
23:B:616:CLA:H111	23:B:616:CLA:H143	1.83	0.41
31:B:623:LMG:H142	11:L:35:PHE:CE1	2.56	0.41
27:T:101:BCR:H333	12:m:13:LEU:HD12	2.02	0.41
30:a:401:SQD:H311	30:a:401:SQD:H342	1.84	0.41
23:a:404:CLA:H152	24:a:407:PHO:H51	2.01	0.41
2:b:86:ILE:H	2:b:86:ILE:HG13	1.74	0.41
23:b:614:CLA:H41	23:b:614:CLA:H62	1.84	0.41
3:c:223:TRP:CD2	3:c:224:ILE:HG13	2.54	0.41
4:d:88:SER:HB2	5:e:69:ARG:NH2	2.35	0.41
5:e:14:ILE:HG22	9:j:13:VAL:HG11	2.02	0.41
16:v:147:VAL:O	16:v:150:LYS:HB2	2.21	0.41
17:g:31:ALA:O	17:g:35:ILE:HG23	2.19	0.41
3:C:380:ILE:HA	3:C:384:ILE:HD11	2.03	0.41
4:D:294:ARG:H	4:D:294:ARG:HG2	1.65	0.41
6:F:21:VAL:O	6:F:25:THR:HG23	2.20	0.41
14:T:3:THR:O	14:T:7:VAL:HG23	2.21	0.41
27:T:101:BCR:H341	27:T:101:BCR:H11C	1.86	0.41
2:b:247:PHE:HE1	23:b:606:CLA:H101	1.85	0.41
23:b:606:CLA:H193	28:b:623:DGD:HA71	2.03	0.41
23:b:619:CLA:H92	23:b:619:CLA:H62	1.83	0.41
5:e:49:THR:HA	5:e:50:PRO:HD3	1.92	0.41
13:o:81:GLU:HA	13:o:82:PRO:HD3	1.85	0.41
29:A:412:LHG:H382	23:C:510:CLA:H93	2.02	0.41
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.50	0.41
7:H:12:ARG:HD3	7:H:12:ARG:O	2.21	0.41
31:I:101:LMG:H221	33:I:102:LMT:H81	2.01	0.41
9:J:38:SER:OG	9:J:39:SER:N	2.49	0.41
11:L:22:LEU:O	11:L:26:VAL:HG22	2.20	0.41
12:M:20:VAL:HG13	12:m:20:VAL:HG13	2.02	0.41
1:a:195:HIS:HA	1:a:196:PRO:HD3	1.93	0.41
1:a:215:HIS:HA	25:a:410:PL9:O1	2.20	0.41
2:b:24:LEU:HD21	23:b:620:CLA:CAB	2.49	0.41
2:b:242:ILE:HG22	2:b:466:HIS:HB2	2.03	0.41
2:b:272:ARG:HG3	2:b:273:TYR:N	2.35	0.41
23:c:511:CLA:H151	19:z:20:VAL:O	2.20	0.41
5:e:10:PHE:CE1	34:f:101:HEM:HBD2	2.56	0.41
16:v:81:ARG:NE	16:v:157:GLY:HA3	2.36	0.41
17:g:32:GLY:O	17:g:35:ILE:HG12	2.21	0.41
30:A:413:SQD:H172	29:A:415:LHG:H172	2.03	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
2:B:153:PHE:O	2:B:157:HIS:HB3	2.20	0.41
2:B:462:PHE:HA	23:B:611:CLA:HMC2	2.02	0.41
2:B:488:PRO:O	2:B:490:GLN:N	2.47	0.41
3:C:290:VAL:O	3:C:423:ARG:NH1	2.53	0.41
23:C:503:CLA:H193	23:C:503:CLA:H161	1.80	0.41
4:D:239:GLN:HB3	4:D:240:ALA:H	1.57	0.41
4:D:267:LEU:O	4:D:271:MET:HG3	2.20	0.41
13:O:194:TYR:CE1	13:O:198:ILE:HD13	2.56	0.41
1:a:22:THR:HG21	8:i:30:ARG:HD3	2.03	0.41
1:a:307:ILE:HD11	6:f:45:ARG:NH2	2.35	0.41
2:b:224:ARG:CZ	33:b:627:LMT:H2'	2.51	0.41
3:c:186:TYR:CE2	3:c:188:THR:HG22	2.53	0.41
23:c:506:CLA:H202	23:c:506:CLA:H161	1.81	0.41
1:A:126:TYR:O	1:A:130:GLN:HG3	2.20	0.41
30:A:417:SQD:H342	30:A:417:SQD:H311	1.86	0.41
2:B:182:ALA:HA	2:B:183:PRO:HD3	1.93	0.41
23:B:603:CLA:HBB2	23:B:605:CLA:H152	2.03	0.41
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.52	0.41
3:C:318:LEU:HG	3:C:328:VAL:HG11	2.03	0.41
19:Z:33:TRP:O	19:Z:33:TRP:CD1	2.73	0.41
1:a:140:ARG:HH22	29:a:414:LHG:P	2.44	0.41
2:b:30:VAL:HG12	23:b:609:CLA:HHD	2.03	0.41
23:b:619:CLA:H72	23:b:620:CLA:HBB1	2.02	0.41
7:h:3:ARG:NH2	11:l:1:MET:HE1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:5:PHE:HB2	19:z:57:LEU:HG	2.02	0.41
19:z:55:GLY:HA2	27:z:101:BCR:H312	2.01	0.41
23:B:604:CLA:H61	23:B:604:CLA:H41	1.91	0.41
27:B:619:BCR:H24C	27:B:619:BCR:H371	1.89	0.41
31:B:623:LMG:HC3	33:M:102:LMT:O2'	2.21	0.41
3:C:264:PHE:HE1	23:C:507:CLA:HAB	1.86	0.41
4:D:74:LEU:O	4:D:175:VAL:HB	2.20	0.41
4:D:180:ARG:HG3	4:D:181:PHE:N	2.34	0.41
5:E:8:ARG:HB2	6:F:13:TYR:HB3	2.02	0.41
31:M:101:LMG:H201	23:b:618:CLA:H101	2.02	0.41
14:T:29:ILE:O	14:T:31:LYS:N	2.54	0.41
1:a:129:ARG:NH2	4:d:256:ILE:HA	2.36	0.41
1:a:180:PHE:O	1:a:184:ILE:HG13	2.21	0.41
23:a:406:CLA:H143	23:a:406:CLA:H161	1.77	0.41
2:b:10:THR:O	2:b:13:ILE:HG13	2.21	0.41
2:b:87:ASP:HA	2:b:88:PRO:HD2	1.98	0.41
2:b:137:LYS:HD2	7:h:14:LEU:O	2.21	0.41
2:b:257:TRP:CD2	4:d:291:LEU:HD12	2.56	0.41
2:b:366:PHE:CG	2:b:367:PRO:HD2	2.56	0.41
23:b:606:CLA:H41	23:b:606:CLA:H62	1.50	0.41
23:b:616:CLA:H8	23:b:616:CLA:H122	1.93	0.41
3:c:120:ILE:HD11	27:c:514:BCR:HC8	2.02	0.41
3:c:447:ARG:HH11	3:c:447:ARG:HG2	1.86	0.41
5:e:42:LEU:O	5:e:46:VAL:HG23	2.21	0.41
12:m:30:GLU:O	31:m:102:LMG:HC3	2.20	0.41
20:Y:23:UNK:O	20:Y:24:UNK:C	2.68	0.41
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.03	0.41
2:B:91:TRP:CH2	23:B:606:CLA:H12	2.56	0.41
2:B:150:CYS:HB2	23:B:603:CLA:CMC	2.51	0.41
3:C:281:MET:HE3	23:C:505:CLA:HAC2	2.03	0.41
27:D:405:BCR:H341	27:D:405:BCR:H11C	1.75	0.41
31:M:101:LMG:H352	23:b:618:CLA:H72	2.03	0.41
2:b:192:PRO:HD2	7:h:60:VAL:HG12	2.03	0.41
23:b:616:CLA:H171	23:b:617:CLA:HBB2	2.02	0.41
3:c:101:PRO:O	3:c:104:GLU:HB2	2.21	0.41
3:c:174:LEU:HD13	23:c:502:CLA:H111	2.03	0.41
3:c:245:ILE:O	3:c:249:ILE:HG12	2.21	0.41
27:c:515:BCR:H11C	27:c:515:BCR:H341	1.82	0.41
18:x:12:ILE:O	18:x:12:ILE:HG23	2.21	0.41
1:A:271:LEU:HD11	25:A:408:PL9:C4	2.51	0.40
2:B:109:LEU:O	27:B:620:BCR:H21C	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:603:CLA:CGA	23:B:603:CLA:H3A	2.51	0.40
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.02	0.40
3:C:406:SER:HA	3:C:420:VAL:HG23	2.02	0.40
5:E:81:GLU:O	5:E:83:LEU:N	2.46	0.40
20:G:23:UNK:O	20:G:24:UNK:C	2.68	0.40
1:a:258:LEU:O	4:d:128:ARG:NH1	2.54	0.40
23:a:405:CLA:H62	23:a:405:CLA:H41	1.73	0.40
33:b:603:LMT:H3'	33:b:603:LMT:H1B	1.55	0.40
23:c:510:CLA:OBD	10:k:33:LEU:HD23	2.21	0.40
15:u:73:PRO:HD2	16:v:109:ASP:CG	2.45	0.40
1:A:141:PRO:HG3	3:C:446:GLY:C	2.46	0.40
23:B:604:CLA:H161	23:B:604:CLA:H202	1.79	0.40
23:B:605:CLA:H202	23:B:605:CLA:H162	1.96	0.40
27:C:514:BCR:H24C	27:C:514:BCR:H371	1.88	0.40
27:C:515:BCR:H24C	27:C:515:BCR:H371	1.79	0.40
5:E:26:THR:HB	34:F:101:HEM:CAB	2.51	0.40
10:K:19:ASP:N	10:K:20:PRO:HD2	2.36	0.40
13:O:51:THR:O	13:O:53:ARG:N	2.53	0.40
13:O:97:VAL:HG12	13:O:133:THR:O	2.21	0.40
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.56	0.40
30:a:401:SQD:H351	27:a:412:BCR:H311	2.03	0.40
23:a:406:CLA:H161	25:a:410:PL9:H253	2.02	0.40
2:b:483:ASP:CB	2:b:484:PRO:HD2	2.52	0.40
3:c:77:PRO:HG2	3:c:78:GLU:OE2	2.21	0.40
3:c:107:ASP:O	3:c:110:PRO:HD2	2.21	0.40
23:c:501:CLA:H52	23:c:503:CLA:H92	2.02	0.40
28:c:517:DGD:HA41	31:k:103:LMG:H391	2.03	0.40
27:k:102:BCR:H14C	17:g:28:ILE:O	2.21	0.40
1:A:177:SER:HA	1:A:180:PHE:CD2	2.56	0.40
1:A:258:LEU:O	4:D:128:ARG:NH1	2.55	0.40
23:B:607:CLA:H122	31:B:623:LMG:H412	2.03	0.40
23:B:608:CLA:H18	23:B:609:CLA:H192	2.03	0.40
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.04	0.40
3:C:334:PRO:HA	13:O:179:THR:OG1	2.22	0.40
23:C:501:CLA:H193	23:C:507:CLA:H111	2.03	0.40
23:C:512:CLA:H143	23:C:513:CLA:H162	2.03	0.40
10:K:43:VAL:HG22	10:K:46:ARG:HE	1.87	0.40
16:V:68:VAL:O	16:V:71:ILE:HG12	2.20	0.40
28:c:517:DGD:HA91	28:c:517:DGD:HAW2	1.92	0.40
14:t:9:ILE:O	14:t:13:ILE:HG13	2.21	0.40
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.94	0.40

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	2.36	0.40
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.56	0.40
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.87	0.40
23:B:607:CLA:HBB1	31:B:623:LMG:H341	2.03	0.40
3:C:166:ILE:O	3:C:170:ILE:HG13	2.20	0.40
3:C:240:ILE:O	3:C:244:CYS:HB2	2.22	0.40
3:C:416:SER:OG	3:C:417:VAL:N	2.54	0.40
13:O:206:GLU:H	13:O:206:GLU:CD	2.28	0.40
16:V:60:GLN:HA	16:V:64:ALA:HB2	2.02	0.40
1:a:182:PHE:O	1:a:186:PHE:HB2	2.22	0.40
31:b:625:LMG:H421	4:d:284:ILE:HD13	2.02	0.40
27:d:405:BCR:H11C	27:d:405:BCR:H341	1.83	0.40
1:A:42:LEU:HA	1:A:45:THR:HG22	2.03	0.40
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.04	0.40
23:C:511:CLA:H42	10:K:39:TRP:CD1	2.56	0.40
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.04	0.40
17:y:39:LEU:HB3	17:y:46:LEU:HD21	2.03	0.40
1:a:238:LYS:HD3	1:a:238:LYS:HA	1.90	0.40
31:a:416:LMG:H382	23:b:618:CLA:HBC1	2.02	0.40
23:b:607:CLA:HBB2	23:b:607:CLA:H92	2.03	0.40
23:b:609:CLA:H161	23:b:609:CLA:H141	1.82	0.40
5:e:22:ILE:O	5:e:26:THR:HG23	2.21	0.40
5:e:27:ILE:HB	5:e:28:PRO:HD3	2.04	0.40
11:l:7:ARG:H	11:l:7:ARG:HG3	1.66	0.40
15:u:73:PRO:HG2	16:v:107:THR:HB	2.02	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%)	17 (5%)	5 (2%)	8 39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	10	43
2	B	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	12	48
2	b	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	12	48
3	C	445/461 (96%)	406 (91%)	33 (7%)	6 (1%)	9	42
3	c	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	9	42
4	D	338/352 (96%)	316 (94%)	20 (6%)	2 (1%)	21	59
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	21	59
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	42
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	42
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
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	16
8	I	33/38 (87%)	27 (82%)	4 (12%)	2 (6%)	1	12
8	i	33/38 (87%)	28 (85%)	4 (12%)	1 (3%)	3	22
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3	22
9	j	32/40 (80%)	28 (88%)	2 (6%)	2 (6%)	1	12
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%)	34 (97%)	1 (3%)	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%)	206 (86%)	31 (13%)	4 (2%)	7	36
13	o	241/272 (89%)	208 (86%)	29 (12%)	4 (2%)	7	36
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	21
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	21
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%)	125 (93%)	10 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2 19
17	y	26/46 (56%)	19 (73%)	6 (23%)	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%)	5 (8%)	1 (2%)	7 36
19	z	60/62 (97%)	54 (90%)	3 (5%)	3 (5%)	1 15
All	All	5138/5650 (91%)	4681 (91%)	378 (7%)	79 (2%)	8 39

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
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	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	c	257	PHE
3	c	416	SER
4	d	239	GLN
5	e	82	GLN
7	h	26	GLY
9	j	38	SER
17	g	43	ARG
19	z	32	ASP
1	A	142	TRP
3	C	194	GLY
5	E	82	GLN
9	J	38	SER
13	O	88	GLU
15	U	83	ALA
1	a	334	ARG
3	c	194	GLY
13	o	88	GLU
13	o	271	PRO
15	u	72	TYR
1	A	334	ARG
4	D	262	SER
13	O	271	PRO
15	U	72	TYR
4	d	262	SER
7	h	16	SER
8	i	25	SER
10	k	45	PHE
13	o	158	ASN
15	u	83	ALA
2	B	176	GLY
2	B	230	ARG
7	H	16	SER
10	K	13	GLU
10	K	45	PHE
15	U	73	PRO
2	b	176	GLY
10	k	13	GLU
18	x	12	ILE
8	I	25	SER
13	O	158	ASN
18	X	12	ILE
2	b	230	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	z	28	ALA
15	u	73	PRO
8	I	32	PRO
3	C	209	ILE
1	A	176	ILE
3	c	209	ILE
19	z	24	PRO
9	j	35	GLY

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	55
1	a	271/291 (93%)	262 (97%)	9 (3%)	33	55
2	B	390/407 (96%)	378 (97%)	12 (3%)	35	56
2	b	390/407 (96%)	377 (97%)	13 (3%)	33	55
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%)	260 (94%)	15 (6%)	19	41
4	d	275/283 (97%)	259 (94%)	16 (6%)	18	39
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%)	51 (96%)	2 (4%)	29	50
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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 58
11	l	35/35 (100%)	34 (97%)	1 (3%)	37 58
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%)	200 (99%)	2 (1%)	68 77
13	o	202/228 (89%)	199 (98%)	3 (2%)	57 71
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%)	82 (98%)	2 (2%)	43 63
15	u	84/112 (75%)	81 (96%)	3 (4%)	31 52
16	V	116/138 (84%)	113 (97%)	3 (3%)	40 61
16	v	116/138 (84%)	113 (97%)	3 (3%)	40 61
17	g	20/37 (54%)	17 (85%)	3 (15%)	3 12
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%)	4087 (96%)	157 (4%)	30 51

All (157) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	114	VAL
15	U	132	LEU
16	V	63	CYS
16	V	68	VAL
16	V	116	GLU
17	y	25	ILE
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	422	ARG
2	b	425	ILE
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	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
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	294	ARG
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	60	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	g	25	ILE
17	g	28	ILE
17	g	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	A	303	ASN
2	B	26	HIS
2	B	201	HIS
2	B	281	GLN
2	B	374	ASN
2	B	409	GLN
3	C	44	ASN
3	C	56	HIS
3	C	229	ASN
4	D	142	ASN
4	D	186	GLN
4	D	322	ASN
12	M	32	GLN
13	O	150	ASN
13	O	173	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	U	93	ASN
15	U	111	HIS
16	V	112	GLN
17	y	45	ASN
1	a	303	ASN
1	a	337	HIS
2	b	26	HIS
2	b	194	ASN
2	b	201	HIS
2	b	282	GLN
2	b	343	HIS
2	b	374	ASN
2	b	409	GLN
3	c	44	ASN
3	c	56	HIS
3	c	118	HIS
3	c	229	ASN
4	d	98	GLN
4	d	142	ASN
4	d	250	ASN
4	d	255	GLN
4	d	301	GLN
12	m	32	GLN
12	m	33	GLN
15	u	93	ASN
15	u	111	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
25	PL9	j	101	-	35,35,55	1.21	5 (14%)	44,45,69	1.55	8 (18%)
24	PHO	a	408	-	58,69,69	2.16	9 (15%)	55,99,99	1.41	6 (10%)
27	BCR	J	102	-	41,41,41	0.75	0	56,56,56	3.44	25 (44%)
33	LMT	m	101	-	36,36,36	0.42	0	47,47,47	0.66	0
23	CLA	A	404	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	6 (7%)
23	CLA	c	504	-	69,73,73	1.17	6 (8%)	82,113,113	1.32	4 (4%)
23	CLA	D	403	-	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
23	CLA	C	511	3	69,73,73	1.19	6 (8%)	82,113,113	1.37	6 (7%)
23	CLA	B	605	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	5 (6%)
23	CLA	c	506	-	69,73,73	1.19	5 (7%)	82,113,113	1.33	6 (7%)
31	LMG	B	622	-	49,49,55	1.14	7 (14%)	57,57,63	1.30	6 (10%)
28	DGD	d	409	-	64,64,67	1.14	6 (9%)	78,78,81	1.41	10 (12%)
28	DGD	c	518	-	67,67,67	1.11	6 (8%)	81,81,81	1.45	13 (16%)
23	CLA	C	505	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	5 (6%)
28	DGD	C	517	-	54,54,67	1.22	6 (11%)	68,68,81	1.24	5 (7%)
30	SQD	B	626	-	45,47,54	1.03	3 (6%)	55,58,65	1.49	9 (16%)
31	LMG	A	414	-	51,51,55	1.15	6 (11%)	59,59,63	1.34	5 (8%)
28	DGD	D	409	-	64,64,67	1.15	6 (9%)	78,78,81	1.40	8 (10%)
33	LMT	b	627	-	36,36,36	0.44	0	47,47,47	0.66	1 (2%)
27	BCR	C	516	-	41,41,41	0.70	0	56,56,56	1.96	15 (26%)
27	BCR	T	102	-	41,41,41	0.71	0	56,56,56	2.27	17 (30%)
23	CLA	B	616	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
23	CLA	b	611	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
23	CLA	B	614	-	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
30	SQD	F	102	-	43,45,54	1.04	2 (4%)	53,56,65	1.60	10 (18%)
23	CLA	a	404	-	69,73,73	1.21	7 (10%)	82,113,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LHG	a	417	-	36,36,48	1.09	2 (5%)	39,42,54	1.02	2 (5%)
27	BCR	y	101	-	41,41,41	0.74	0	56,56,56	1.95	13 (23%)
31	LMG	d	406	-	46,46,55	1.19	7 (15%)	54,54,63	1.32	6 (11%)
28	DGD	B	627	-	53,53,67	1.22	6 (11%)	67,67,81	1.42	9 (13%)
23	CLA	b	608	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	6 (7%)
23	CLA	A	405	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	7 (8%)
23	CLA	b	616	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	4 (4%)
33	LMT	D	410	-	32,32,36	0.51	1 (3%)	43,43,47	0.71	1 (2%)
33	LMT	B	629	-	36,36,36	0.46	0	47,47,47	0.66	0
27	BCR	B	619	-	41,41,41	0.67	0	56,56,56	1.87	15 (26%)
27	BCR	c	514	-	41,41,41	0.71	0	56,56,56	2.39	20 (35%)
23	CLA	B	607	-	69,73,73	1.16	6 (8%)	82,113,113	1.38	7 (8%)
33	LMT	B	628	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
23	CLA	c	502	-	69,73,73	1.19	10 (14%)	82,113,113	1.31	7 (8%)
23	CLA	c	510	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
27	BCR	A	410	-	41,41,41	0.73	0	56,56,56	1.89	11 (19%)
31	LMG	a	416	-	51,51,55	1.12	6 (11%)	59,59,63	1.38	6 (10%)
30	SQD	A	417	-	52,54,54	1.01	5 (9%)	62,65,65	1.60	11 (17%)
22	BCT	d	401	21	3,3,3	0.62	0	2,3,3	0.26	0
27	BCR	C	514	-	41,41,41	0.75	0	56,56,56	2.37	22 (39%)
23	CLA	B	603	-	69,73,73	1.19	8 (11%)	82,113,113	1.27	4 (4%)
33	LMT	b	604	-	36,36,36	0.40	0	47,47,47	0.64	0
30	SQD	b	601	-	45,47,54	1.02	3 (6%)	55,58,65	1.53	9 (16%)
23	CLA	C	506	-	69,73,73	1.19	6 (8%)	82,113,113	1.30	5 (6%)
28	DGD	C	519	-	67,67,67	1.12	7 (10%)	81,81,81	1.41	9 (11%)
30	SQD	a	401	-	52,54,54	1.00	5 (9%)	62,65,65	1.63	10 (16%)
23	CLA	B	611	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
23	CLA	D	401	-	69,73,73	1.17	7 (10%)	82,113,113	1.24	6 (7%)
27	BCR	k	102	-	41,41,41	0.74	0	56,56,56	1.97	16 (28%)
25	PL9	d	404	-	55,55,55	1.27	8 (14%)	68,69,69	1.72	19 (27%)
27	BCR	z	101	-	41,41,41	0.63	0	56,56,56	1.85	13 (23%)
23	CLA	c	501	-	69,73,73	1.17	6 (8%)	82,113,113	1.30	6 (7%)
27	BCR	d	405	-	41,41,41	0.67	0	56,56,56	2.17	17 (30%)
25	PL9	J	101	-	35,35,55	1.22	5 (14%)	44,45,69	1.56	7 (15%)
31	LMG	d	407	-	48,48,55	1.17	8 (16%)	56,56,63	1.48	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	a	409	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
31	LMG	C	520	-	48,48,55	1.13	6 (12%)	56,56,63	1.30	5 (8%)
25	PL9	D	404	-	55,55,55	1.28	8 (14%)	68,69,69	1.64	16 (23%)
24	PHO	D	402	-	58,69,69	2.18	10 (17%)	55,99,99	1.48	6 (10%)
30	SQD	D	408	-	41,43,54	1.12	4 (9%)	51,54,65	1.93	10 (19%)
31	LMG	m	102	-	42,42,55	1.34	7 (16%)	50,50,63	1.56	7 (14%)
28	DGD	c	516	-	54,54,67	1.24	5 (9%)	68,68,81	1.26	8 (11%)
23	CLA	b	619	-	69,73,73	1.17	6 (8%)	82,113,113	1.29	6 (7%)
23	CLA	B	610	-	69,73,73	1.19	7 (10%)	82,113,113	1.28	7 (8%)
30	SQD	A	413	-	49,51,54	0.98	4 (8%)	59,62,65	1.47	10 (16%)
23	CLA	C	513	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	6 (7%)
23	CLA	a	406	-	69,73,73	1.18	6 (8%)	82,113,113	1.36	7 (8%)
28	DGD	a	413	-	57,57,67	1.20	7 (12%)	71,71,81	1.49	12 (16%)
23	CLA	C	503	-	69,73,73	1.18	6 (8%)	82,113,113	1.25	5 (6%)
23	CLA	C	502	-	69,73,73	1.19	7 (10%)	82,113,113	1.27	5 (6%)
31	LMG	i	101	-	43,43,55	1.27	7 (16%)	51,51,63	1.30	7 (13%)
27	BCR	H	101	-	41,41,41	0.70	0	56,56,56	1.76	16 (28%)
31	LMG	a	402	-	42,42,55	1.23	6 (14%)	50,50,63	1.51	9 (18%)
33	LMT	b	626	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
28	DGD	C	518	-	63,63,67	1.22	10 (15%)	77,77,81	1.26	7 (9%)
28	DGD	B	621	-	59,59,67	1.23	9 (15%)	73,73,81	1.09	5 (6%)
23	CLA	C	508	-	69,73,73	1.19	8 (11%)	82,113,113	1.27	5 (6%)
31	LMG	E	101	-	44,44,55	1.19	6 (13%)	52,52,63	1.33	8 (15%)
23	CLA	b	620	-	69,73,73	1.19	9 (13%)	82,113,113	1.21	5 (6%)
23	CLA	B	613	-	69,73,73	1.19	7 (10%)	82,113,113	1.19	4 (4%)
27	BCR	b	621	-	41,41,41	0.64	0	56,56,56	1.97	16 (28%)
31	LMG	b	624	-	49,49,55	1.17	7 (14%)	57,57,63	1.30	7 (12%)
31	LMG	B	623	-	49,49,55	1.19	7 (14%)	57,57,63	1.38	8 (14%)
33	LMT	i	102	-	36,36,36	0.48	1 (2%)	47,47,47	0.68	1 (2%)
31	LMG	D	407	-	48,48,55	1.18	8 (16%)	56,56,63	1.41	7 (12%)
24	PHO	a	407	-	58,69,69	2.14	11 (18%)	55,99,99	1.49	5 (9%)
28	DGD	b	623	-	59,59,67	1.21	9 (15%)	73,73,81	1.13	6 (8%)
23	CLA	B	615	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	6 (7%)
33	LMT	B	624	-	36,36,36	0.42	0	47,47,47	0.70	0
23	CLA	b	609	-	69,73,73	1.17	6 (8%)	82,113,113	1.24	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	d	403	-	69,73,73	1.20	6 (8%)	82,113,113	1.27	5 (6%)
23	CLA	A	403	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	6 (7%)
23	CLA	c	507	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	6 (7%)
34	HEM	v	201	16	50,50,50	2.01	11 (22%)	67,82,82	1.39	5 (7%)
23	CLA	b	607	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
24	PHO	A	406	-	58,69,69	2.20	9 (15%)	55,99,99	1.55	8 (14%)
29	LHG	A	412	-	38,38,48	1.05	2 (5%)	41,44,54	1.00	2 (4%)
23	CLA	B	606	-	69,73,73	1.18	9 (13%)	82,113,113	1.22	5 (6%)
34	HEM	V	201	16	50,50,50	1.92	11 (22%)	67,82,82	1.27	1 (1%)
23	CLA	C	501	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	6 (7%)
23	CLA	c	513	-	69,73,73	1.19	7 (10%)	82,113,113	1.29	6 (7%)
27	BCR	B	617	-	41,41,41	0.71	0	56,56,56	1.86	13 (23%)
23	CLA	c	509	-	69,73,73	1.21	5 (7%)	82,113,113	1.29	5 (6%)
27	BCR	D	405	-	41,41,41	0.65	0	56,56,56	2.20	16 (28%)
23	CLA	A	407	-	69,73,73	1.18	9 (13%)	82,113,113	1.23	5 (6%)
23	CLA	c	512	-	69,73,73	1.19	6 (8%)	82,113,113	1.32	5 (6%)
30	SQD	f	102	-	43,45,54	1.02	2 (4%)	53,56,65	1.61	11 (20%)
29	LHG	A	415	-	36,36,48	1.08	2 (5%)	39,42,54	1.10	2 (5%)
23	CLA	C	510	-	69,73,73	1.21	8 (11%)	82,113,113	1.26	5 (6%)
31	LMG	b	625	-	49,49,55	1.18	7 (14%)	57,57,63	1.41	9 (15%)
33	LMT	M	102	-	36,36,36	0.44	0	47,47,47	0.68	0
31	LMG	I	101	-	43,43,55	1.26	8 (18%)	51,51,63	1.31	8 (15%)
33	LMT	d	410	-	32,32,36	0.49	1 (3%)	43,43,47	0.70	1 (2%)
23	CLA	b	617	-	69,73,73	1.18	7 (10%)	82,113,113	1.36	6 (7%)
31	LMG	e	101	-	44,44,55	1.21	7 (15%)	52,52,63	1.35	9 (17%)
23	CLA	b	605	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	6 (7%)
23	CLA	C	509	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
23	CLA	b	612	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	7 (8%)
33	LMT	I	102	-	36,36,36	0.43	0	47,47,47	0.68	1 (2%)
23	CLA	c	503	-	69,73,73	1.20	6 (8%)	82,113,113	1.22	5 (6%)
23	CLA	b	606	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	5 (6%)
28	DGD	b	602	-	53,53,67	1.23	6 (11%)	67,67,81	1.36	8 (11%)
23	CLA	c	508	-	69,73,73	1.19	7 (10%)	82,113,113	1.31	6 (7%)
23	CLA	B	608	-	69,73,73	1.20	8 (11%)	82,113,113	1.28	6 (7%)
23	CLA	a	405	-	69,73,73	1.19	8 (11%)	82,113,113	1.35	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	BCR	T	101	-	41,41,41	0.71	0	56,56,56	1.79	12 (21%)
23	CLA	c	505	-	69,73,73	1.18	8 (11%)	82,113,113	1.35	6 (7%)
27	BCR	C	515	-	41,41,41	0.63	0	56,56,56	1.92	16 (28%)
23	CLA	c	511	-	69,73,73	1.22	5 (7%)	82,113,113	1.28	6 (7%)
31	LMG	c	519	-	45,45,55	1.21	7 (15%)	53,53,63	1.32	6 (11%)
23	CLA	C	504	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
33	LMT	B	625	-	36,36,36	0.40	0	47,47,47	0.71	1 (2%)
23	CLA	B	612	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
23	CLA	b	613	-	69,73,73	1.18	6 (8%)	82,113,113	1.22	7 (8%)
31	LMG	A	418	-	42,42,55	1.23	6 (14%)	50,50,63	1.50	9 (18%)
34	HEM	f	101	6,5	50,50,50	1.96	10 (20%)	67,82,82	1.45	9 (13%)
23	CLA	B	609	-	69,73,73	1.18	5 (7%)	82,113,113	1.28	5 (6%)
33	LMT	b	603	-	36,36,36	0.44	0	47,47,47	0.76	1 (2%)
27	BCR	a	412	-	41,41,41	0.75	0	56,56,56	1.90	12 (21%)
23	CLA	B	601	-	69,73,73	1.21	9 (13%)	82,113,113	1.31	5 (6%)
31	LMG	D	406	-	46,46,55	1.17	7 (15%)	54,54,63	1.38	6 (11%)
23	CLA	b	610	-	69,73,73	1.20	7 (10%)	82,113,113	1.27	5 (6%)
25	PL9	a	410	-	45,45,55	1.27	7 (15%)	56,57,69	1.65	14 (25%)
29	LHG	a	414	-	38,38,48	1.07	2 (5%)	41,44,54	1.01	3 (7%)
23	CLA	b	618	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	4 (4%)
23	CLA	C	507	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
23	CLA	B	604	-	69,73,73	1.19	8 (11%)	82,113,113	1.30	6 (7%)
31	LMG	C	521	-	45,45,55	1.19	7 (15%)	53,53,63	1.36	8 (15%)
30	SQD	d	408	-	41,43,54	1.12	2 (4%)	51,54,65	1.91	10 (19%)
23	CLA	b	615	-	69,73,73	1.20	9 (13%)	82,113,113	1.30	5 (6%)
31	LMG	k	103	-	48,48,55	1.13	6 (12%)	56,56,63	1.27	6 (10%)
27	BCR	c	515	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)
28	DGD	c	517	-	63,63,67	1.21	11 (17%)	77,77,81	1.29	7 (9%)
23	CLA	B	602	-	69,73,73	1.18	5 (7%)	82,113,113	1.24	5 (6%)
27	BCR	B	620	-	41,41,41	0.71	0	56,56,56	2.15	17 (30%)
34	HEM	F	101	6,5	50,50,50	1.87	8 (16%)	67,82,82	1.38	6 (8%)
28	DGD	A	411	-	57,57,67	1.23	7 (12%)	71,71,81	1.56	12 (16%)
23	CLA	d	402	-	69,73,73	1.18	5 (7%)	82,113,113	1.35	5 (6%)
22	BCT	A	402	21	3,3,3	0.61	0	2,3,3	0.26	0
27	BCR	b	622	-	41,41,41	0.70	0	56,56,56	2.22	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	PL9	A	408	-	45,45,55	1.30	7 (15%)	56,57,69	1.58	13 (23%)
30	SQD	a	415	-	49,51,54	0.97	2 (4%)	59,62,65	1.50	10 (16%)
23	CLA	b	614	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	7 (8%)
31	LMG	M	101	-	42,42,55	1.28	7 (16%)	50,50,63	1.50	6 (12%)
23	CLA	C	512	-	69,73,73	1.17	5 (7%)	82,113,113	1.33	5 (6%)
27	BCR	B	618	-	41,41,41	0.68	0	56,56,56	2.29	18 (32%)
27	BCR	h	101	-	41,41,41	0.72	0	56,56,56	1.77	14 (25%)
27	BCR	j	102	-	41,41,41	0.72	0	56,56,56	3.44	22 (39%)

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
25	PL9	j	101	-	-	13/29/49/73	0/1/1/1
24	PHO	a	408	-	-	13/37/103/103	0/5/6/6
27	BCR	J	102	-	-	6/29/63/63	0/2/2/2
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
23	CLA	A	404	-	1/1/15/20	17/39/115/115	-
23	CLA	c	504	-	1/1/15/20	12/39/115/115	-
23	CLA	D	403	-	1/1/15/20	9/39/115/115	-
23	CLA	C	511	3	1/1/15/20	14/39/115/115	-
23	CLA	B	605	-	1/1/15/20	16/39/115/115	-
23	CLA	c	506	-	1/1/15/20	16/39/115/115	-
31	LMG	B	622	-	-	21/44/64/70	0/1/1/1
28	DGD	d	409	-	-	31/52/92/95	0/2/2/2
28	DGD	c	518	-	-	21/55/95/95	0/2/2/2
23	CLA	C	505	-	1/1/15/20	18/39/115/115	-
28	DGD	C	517	-	-	19/42/82/95	0/2/2/2
30	SQD	B	626	-	-	14/42/62/69	0/1/1/1
31	LMG	A	414	-	-	20/46/66/70	0/1/1/1
28	DGD	D	409	-	-	30/52/92/95	0/2/2/2
33	LMT	b	627	-	-	2/21/61/61	0/2/2/2
27	BCR	C	516	-	-	8/29/63/63	0/2/2/2
27	BCR	T	102	-	-	7/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	616	-	1/1/15/20	19/39/115/115	-
23	CLA	b	611	-	1/1/15/20	9/39/115/115	-
23	CLA	B	614	-	1/1/15/20	14/39/115/115	-
30	SQD	F	102	-	-	17/40/60/69	0/1/1/1
23	CLA	a	404	-	1/1/15/20	8/39/115/115	-
29	LHG	a	417	-	-	13/41/41/53	-
27	BCR	y	101	-	-	8/29/63/63	0/2/2/2
31	LMG	d	406	-	-	10/41/61/70	0/1/1/1
28	DGD	B	627	-	-	17/41/81/95	0/2/2/2
23	CLA	b	608	-	1/1/15/20	9/39/115/115	-
23	CLA	A	405	-	1/1/15/20	12/39/115/115	-
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
33	LMT	D	410	-	-	0/17/57/61	0/2/2/2
33	LMT	B	629	-	-	3/21/61/61	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
23	CLA	B	607	-	1/1/15/20	9/39/115/115	-
33	LMT	B	628	-	-	3/21/61/61	0/2/2/2
23	CLA	c	502	-	1/1/15/20	10/39/115/115	-
23	CLA	c	510	-	1/1/15/20	17/39/115/115	-
27	BCR	A	410	-	-	1/29/63/63	0/2/2/2
31	LMG	a	416	-	-	19/46/66/70	0/1/1/1
30	SQD	A	417	-	-	14/49/69/69	0/1/1/1
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
23	CLA	B	603	-	1/1/15/20	16/39/115/115	-
33	LMT	b	604	-	-	3/21/61/61	0/2/2/2
30	SQD	b	601	-	-	13/42/62/69	0/1/1/1
23	CLA	C	506	-	1/1/15/20	18/39/115/115	-
28	DGD	C	519	-	-	22/55/95/95	0/2/2/2
30	SQD	a	401	-	-	17/49/69/69	0/1/1/1
23	CLA	B	611	-	1/1/15/20	11/39/115/115	-
23	CLA	D	401	-	1/1/15/20	13/39/115/115	-
27	BCR	k	102	-	-	8/29/63/63	0/2/2/2
25	PL9	d	404	-	-	13/53/73/73	0/1/1/1
27	BCR	z	101	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	501	-	1/1/15/20	14/39/115/115	-
27	BCR	d	405	-	-	6/29/63/63	0/2/2/2
25	PL9	J	101	-	-	12/29/49/73	0/1/1/1
31	LMG	d	407	-	-	19/43/63/70	0/1/1/1
23	CLA	a	409	-	1/1/15/20	7/39/115/115	-
31	LMG	C	520	-	-	18/43/63/70	0/1/1/1
25	PL9	D	404	-	-	13/53/73/73	0/1/1/1
24	PHO	D	402	-	-	8/37/103/103	0/5/6/6
30	SQD	D	408	-	-	11/38/58/69	0/1/1/1
31	LMG	m	102	-	-	15/37/57/70	0/1/1/1
28	DGD	c	516	-	-	19/42/82/95	0/2/2/2
23	CLA	b	619	-	1/1/15/20	8/39/115/115	-
23	CLA	B	610	-	1/1/15/20	18/39/115/115	-
30	SQD	A	413	-	-	19/46/66/69	0/1/1/1
23	CLA	C	513	-	1/1/15/20	17/39/115/115	-
23	CLA	a	406	-	1/1/15/20	11/39/115/115	-
28	DGD	a	413	-	-	12/45/85/95	0/2/2/2
23	CLA	C	503	-	1/1/15/20	14/39/115/115	-
23	CLA	C	502	-	1/1/15/20	11/39/115/115	-
31	LMG	i	101	-	-	20/38/58/70	0/1/1/1
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
31	LMG	a	402	-	-	18/37/57/70	0/1/1/1
33	LMT	b	626	-	-	2/21/61/61	0/2/2/2
28	DGD	C	518	-	-	22/51/91/95	0/2/2/2
28	DGD	B	621	-	-	19/47/87/95	0/2/2/2
23	CLA	C	508	-	1/1/15/20	13/39/115/115	-
31	LMG	E	101	-	-	18/39/59/70	0/1/1/1
23	CLA	b	620	-	1/1/15/20	19/39/115/115	-
23	CLA	B	613	-	1/1/15/20	15/39/115/115	-
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
31	LMG	b	624	-	-	22/44/64/70	0/1/1/1
31	LMG	B	623	-	-	15/44/64/70	0/1/1/1
33	LMT	i	102	-	-	3/21/61/61	0/2/2/2
31	LMG	D	407	-	-	20/43/63/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	a	407	-	-	11/37/103/103	0/5/6/6
28	DGD	b	623	-	-	19/47/87/95	0/2/2/2
23	CLA	B	615	-	1/1/15/20	10/39/115/115	-
33	LMT	B	624	-	-	2/21/61/61	0/2/2/2
23	CLA	b	609	-	1/1/15/20	16/39/115/115	-
23	CLA	d	403	-	1/1/15/20	10/39/115/115	-
23	CLA	A	403	-	1/1/15/20	8/39/115/115	-
23	CLA	c	507	-	1/1/15/20	13/39/115/115	-
34	HEM	v	201	16	-	4/14/54/54	-
23	CLA	b	607	-	1/1/15/20	14/39/115/115	-
24	PHO	A	406	-	-	11/37/103/103	0/5/6/6
29	LHG	A	412	-	-	16/43/43/53	-
23	CLA	B	606	-	1/1/15/20	12/39/115/115	-
34	HEM	V	201	16	-	4/14/54/54	-
23	CLA	C	501	-	1/1/15/20	14/39/115/115	-
23	CLA	c	513	-	1/1/15/20	19/39/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	c	509	-	1/1/15/20	18/39/115/115	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
23	CLA	A	407	-	1/1/15/20	7/39/115/115	-
23	CLA	c	512	-	1/1/15/20	19/39/115/115	-
30	SQD	f	102	-	-	16/40/60/69	0/1/1/1
29	LHG	A	415	-	-	13/41/41/53	-
23	CLA	C	510	-	1/1/15/20	15/39/115/115	-
31	LMG	b	625	-	-	16/44/64/70	0/1/1/1
33	LMT	M	102	-	-	0/21/61/61	0/2/2/2
31	LMG	I	101	-	-	20/38/58/70	0/1/1/1
33	LMT	d	410	-	-	0/17/57/61	0/2/2/2
23	CLA	b	617	-	1/1/15/20	15/39/115/115	-
31	LMG	e	101	-	-	18/39/59/70	0/1/1/1
23	CLA	b	605	-	1/1/15/20	14/39/115/115	-
23	CLA	C	509	-	1/1/15/20	18/39/115/115	-
23	CLA	b	612	-	1/1/15/20	17/39/115/115	-
33	LMT	I	102	-	-	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	503	-	1/1/15/20	14/39/115/115	-
23	CLA	b	606	-	1/1/15/20	15/39/115/115	-
28	DGD	b	602	-	-	18/41/81/95	0/2/2/2
23	CLA	c	508	-	1/1/15/20	13/39/115/115	-
23	CLA	B	608	-	1/1/15/20	17/39/115/115	-
23	CLA	a	405	-	1/1/15/20	16/39/115/115	-
27	BCR	T	101	-	-	2/29/63/63	0/2/2/2
23	CLA	c	505	-	1/1/15/20	18/39/115/115	-
27	BCR	C	515	-	-	2/29/63/63	0/2/2/2
23	CLA	c	511	-	1/1/15/20	13/39/115/115	-
31	LMG	c	519	-	-	21/40/60/70	0/1/1/1
23	CLA	C	504	-	1/1/15/20	12/39/115/115	-
33	LMT	B	625	-	-	2/21/61/61	0/2/2/2
23	CLA	B	612	-	1/1/15/20	9/39/115/115	-
23	CLA	b	613	-	1/1/15/20	9/39/115/115	-
31	LMG	A	418	-	-	16/37/57/70	0/1/1/1
34	HEM	f	101	6,5	-	3/14/54/54	-
23	CLA	B	609	-	1/1/15/20	8/39/115/115	-
33	LMT	b	603	-	-	3/21/61/61	0/2/2/2
27	BCR	a	412	-	-	1/29/63/63	0/2/2/2
23	CLA	B	601	-	1/1/15/20	16/39/115/115	-
31	LMG	D	406	-	-	12/41/61/70	0/1/1/1
23	CLA	b	610	-	1/1/15/20	15/39/115/115	-
25	PL9	a	410	-	-	22/41/61/73	0/1/1/1
29	LHG	a	414	-	-	17/43/43/53	-
23	CLA	b	618	-	1/1/15/20	14/39/115/115	-
23	CLA	C	507	-	1/1/15/20	9/39/115/115	-
23	CLA	B	604	-	1/1/15/20	11/39/115/115	-
31	LMG	C	521	-	-	20/40/60/70	0/1/1/1
30	SQD	d	408	-	-	12/38/58/69	0/1/1/1
23	CLA	b	615	-	1/1/15/20	12/39/115/115	-
31	LMG	k	103	-	-	18/43/63/70	0/1/1/1
27	BCR	c	515	-	-	8/29/63/63	0/2/2/2
28	DGD	c	517	-	-	23/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	602	-	1/1/15/20	13/39/115/115	-
27	BCR	B	620	-	-	2/29/63/63	0/2/2/2
34	HEM	F	101	6,5	-	3/14/54/54	-
28	DGD	A	411	-	-	10/45/85/95	0/2/2/2
23	CLA	d	402	-	1/1/15/20	12/39/115/115	-
27	BCR	b	622	-	-	2/29/63/63	0/2/2/2
25	PL9	A	408	-	-	22/41/61/73	0/1/1/1
30	SQD	a	415	-	-	18/46/66/69	0/1/1/1
23	CLA	b	614	-	1/1/15/20	18/39/115/115	-
31	LMG	M	101	-	-	15/37/57/70	0/1/1/1
23	CLA	C	512	-	1/1/15/20	19/39/115/115	-
27	BCR	B	618	-	-	9/29/63/63	0/2/2/2
27	BCR	h	101	-	-	2/29/63/63	0/2/2/2
27	BCR	j	102	-	-	6/29/63/63	0/2/2/2

All (903) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	C1B-C2B	9.99	1.50	1.39
24	D	402	PHO	C1B-C2B	9.98	1.50	1.39
24	a	408	PHO	C1B-C2B	9.46	1.49	1.39
24	A	406	PHO	C1B-C2B	9.28	1.49	1.39
24	A	406	PHO	C3B-C4B	9.01	1.50	1.41
24	a	408	PHO	C3B-C4B	8.53	1.50	1.41
34	v	201	HEM	C3D-C2D	8.25	1.54	1.36
24	D	402	PHO	C3B-C4B	8.19	1.49	1.41
34	V	201	HEM	C3D-C2D	8.03	1.54	1.36
34	f	101	HEM	C3D-C2D	7.98	1.54	1.36
24	a	407	PHO	C3B-C4B	7.95	1.49	1.41
34	F	101	HEM	C3D-C2D	7.95	1.53	1.36
34	f	101	HEM	FE-ND	5.57	2.12	1.94
34	v	201	HEM	FE-NA	5.24	2.12	1.95
34	V	201	HEM	FE-ND	4.93	2.10	1.94
24	a	408	PHO	C1D-C2D	4.59	1.44	1.39
29	a	414	LHG	O8-C23	4.36	1.46	1.33
34	V	201	HEM	FE-NA	4.31	2.09	1.95
29	a	417	LHG	O8-C23	4.30	1.45	1.33
29	A	415	LHG	O8-C23	4.28	1.45	1.33
34	v	201	HEM	FE-ND	4.27	2.08	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	PHO	C1D-C2D	4.25	1.44	1.39
29	A	412	LHG	O8-C23	4.25	1.45	1.33
29	a	417	LHG	O7-C7	4.21	1.46	1.34
29	a	414	LHG	O7-C7	4.17	1.46	1.34
29	A	412	LHG	O7-C7	4.17	1.46	1.34
29	A	415	LHG	O7-C7	4.15	1.46	1.34
23	B	601	CLA	C1D-ND	4.10	1.43	1.37
34	F	101	HEM	FE-ND	4.05	2.07	1.94
24	D	402	PHO	C1D-C2D	4.05	1.44	1.39
34	f	101	HEM	FE-NB	4.04	2.07	1.94
24	A	406	PHO	C4D-CHA	4.03	1.45	1.39
34	v	201	HEM	FE-NB	4.02	2.07	1.94
34	f	101	HEM	FE-NA	3.98	2.08	1.95
23	c	511	CLA	C1D-ND	3.93	1.43	1.37
23	c	509	CLA	C1D-ND	3.85	1.42	1.37
23	C	511	CLA	C1D-ND	3.83	1.42	1.37
34	F	101	HEM	FE-NB	3.82	2.06	1.94
24	a	407	PHO	C1D-C2D	3.81	1.43	1.39
23	B	608	CLA	C1D-ND	3.80	1.42	1.37
23	c	506	CLA	C1D-ND	3.80	1.42	1.37
23	C	506	CLA	C1D-ND	3.79	1.42	1.37
23	B	609	CLA	C1D-ND	3.79	1.42	1.37
23	b	605	CLA	C1D-ND	3.77	1.42	1.37
23	b	614	CLA	C1D-ND	3.77	1.42	1.37
23	C	501	CLA	C1D-ND	3.76	1.42	1.37
23	B	613	CLA	C1D-ND	3.76	1.42	1.37
23	a	404	CLA	C1D-ND	3.75	1.42	1.37
23	b	606	CLA	C1D-ND	3.75	1.42	1.37
23	b	610	CLA	C1D-ND	3.74	1.42	1.37
23	c	502	CLA	C1D-ND	3.73	1.42	1.37
23	a	409	CLA	C1D-ND	3.72	1.42	1.37
23	b	619	CLA	C1D-ND	3.72	1.42	1.37
23	c	513	CLA	C1D-ND	3.71	1.42	1.37
23	a	405	CLA	C1D-ND	3.70	1.42	1.37
23	d	403	CLA	C1D-ND	3.70	1.42	1.37
23	c	505	CLA	C1D-ND	3.68	1.42	1.37
23	b	617	CLA	C1D-ND	3.67	1.42	1.37
23	C	507	CLA	C1D-ND	3.66	1.42	1.37
23	c	503	CLA	C1D-ND	3.65	1.42	1.37
23	C	513	CLA	C1D-ND	3.65	1.42	1.37
24	a	408	PHO	C4D-CHA	3.65	1.45	1.39
23	A	407	CLA	C1D-ND	3.63	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C1D-ND	3.63	1.42	1.37
23	B	607	CLA	C1D-ND	3.63	1.42	1.37
23	c	512	CLA	C1D-ND	3.62	1.42	1.37
23	C	503	CLA	C1D-ND	3.62	1.42	1.37
23	C	504	CLA	C1D-ND	3.60	1.42	1.37
23	A	404	CLA	C1D-ND	3.60	1.42	1.37
23	b	611	CLA	C1D-ND	3.60	1.42	1.37
23	B	610	CLA	C1D-ND	3.57	1.42	1.37
23	C	509	CLA	C1D-ND	3.57	1.42	1.37
25	A	408	PL9	C33-C34	3.57	1.41	1.33
24	D	402	PHO	C4D-CHA	3.56	1.44	1.39
23	d	402	CLA	C1D-ND	3.56	1.42	1.37
23	b	613	CLA	C1D-ND	3.55	1.42	1.37
23	A	405	CLA	C1D-ND	3.55	1.42	1.37
23	C	505	CLA	C1D-ND	3.55	1.42	1.37
23	C	512	CLA	C1D-ND	3.54	1.42	1.37
23	B	616	CLA	C1D-ND	3.53	1.42	1.37
23	c	501	CLA	C1D-ND	3.52	1.42	1.37
23	a	406	CLA	C1D-ND	3.52	1.42	1.37
23	c	508	CLA	C1D-ND	3.52	1.42	1.37
23	C	510	CLA	C1D-ND	3.52	1.42	1.37
24	a	407	PHO	C4D-CHA	3.52	1.44	1.39
23	b	607	CLA	C1D-ND	3.52	1.42	1.37
23	B	615	CLA	C1D-ND	3.51	1.42	1.37
23	c	504	CLA	C1D-ND	3.51	1.42	1.37
23	B	603	CLA	C1D-ND	3.50	1.42	1.37
25	D	404	PL9	C38-C39	3.48	1.41	1.33
23	A	403	CLA	C4B-NB	3.48	1.42	1.37
23	B	604	CLA	C1D-ND	3.47	1.42	1.37
23	B	606	CLA	C1D-ND	3.45	1.42	1.37
23	a	404	CLA	C4B-NB	3.45	1.42	1.37
34	F	101	HEM	FE-NA	3.44	2.06	1.95
23	b	609	CLA	C1D-ND	3.44	1.42	1.37
23	C	508	CLA	C1D-ND	3.43	1.42	1.37
23	D	401	CLA	C1D-ND	3.43	1.42	1.37
23	C	502	CLA	C1D-ND	3.42	1.42	1.37
34	v	201	HEM	FE-NC	3.42	2.06	1.95
23	D	403	CLA	C1D-ND	3.42	1.42	1.37
23	b	612	CLA	C1D-ND	3.42	1.42	1.37
23	b	608	CLA	C1D-ND	3.42	1.42	1.37
23	b	615	CLA	C1D-ND	3.40	1.42	1.37
23	B	605	CLA	C1D-ND	3.40	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	406	LMG	O7-C8	-3.39	1.38	1.46
23	A	403	CLA	C1D-ND	3.39	1.42	1.37
23	c	507	CLA	C1D-ND	3.39	1.42	1.37
28	C	517	DGD	O2G-C2G	-3.39	1.38	1.46
23	c	510	CLA	C1D-ND	3.39	1.42	1.37
25	d	404	PL9	C38-C39	3.38	1.40	1.33
25	a	410	PL9	C33-C34	3.38	1.40	1.33
23	c	509	CLA	C4B-NB	3.38	1.42	1.37
25	D	404	PL9	C33-C34	3.37	1.40	1.33
28	B	621	DGD	O2G-C2G	-3.36	1.38	1.46
23	C	508	CLA	C4B-NB	3.34	1.42	1.37
25	d	404	PL9	C33-C34	3.32	1.40	1.33
23	b	615	CLA	C4B-NB	3.32	1.42	1.37
23	b	618	CLA	C1D-ND	3.32	1.42	1.37
31	i	101	LMG	O7-C8	-3.32	1.38	1.46
23	a	406	CLA	C4B-NB	3.32	1.42	1.37
23	d	403	CLA	C4B-NB	3.32	1.42	1.37
23	b	620	CLA	C1D-ND	3.31	1.42	1.37
31	d	406	LMG	O7-C8	-3.31	1.38	1.46
31	D	407	LMG	O7-C8	-3.30	1.38	1.46
23	B	611	CLA	C1D-ND	3.30	1.42	1.37
23	d	402	CLA	C4B-NB	3.29	1.42	1.37
25	D	404	PL9	C43-C44	3.29	1.40	1.33
23	c	511	CLA	C4B-NB	3.28	1.42	1.37
31	B	622	LMG	O7-C8	-3.27	1.38	1.46
30	d	408	SQD	O48-C23	3.26	1.42	1.33
23	B	614	CLA	C1D-ND	3.25	1.42	1.37
30	a	401	SQD	O48-C23	3.25	1.42	1.33
23	b	611	CLA	C4B-NB	3.24	1.42	1.37
23	c	506	CLA	C4B-NB	3.22	1.42	1.37
28	b	623	DGD	O2G-C2G	-3.22	1.39	1.46
30	D	408	SQD	O48-C23	3.21	1.42	1.33
31	C	520	LMG	O7-C8	-3.21	1.39	1.46
23	c	504	CLA	C4B-NB	3.21	1.42	1.37
23	a	409	CLA	C4B-NB	3.20	1.42	1.37
30	A	413	SQD	O48-C23	3.20	1.42	1.33
30	a	415	SQD	O48-C23	3.20	1.42	1.33
23	b	616	CLA	C1D-ND	3.19	1.42	1.37
31	m	102	LMG	O1-C7	-3.19	1.38	1.43
31	I	101	LMG	O7-C8	-3.19	1.39	1.46
23	c	512	CLA	C4B-NB	3.18	1.42	1.37
23	a	405	CLA	C4B-NB	3.18	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	FE-NB	3.17	2.04	1.94
28	c	516	DGD	O2G-C2G	-3.16	1.39	1.46
23	C	502	CLA	C4B-NB	3.16	1.42	1.37
31	k	103	LMG	O7-C8	-3.16	1.39	1.46
28	b	602	DGD	O1G-C1A	3.16	1.42	1.33
23	c	501	CLA	C4B-NB	3.15	1.42	1.37
30	b	601	SQD	O48-C23	3.15	1.42	1.33
28	C	519	DGD	O2G-C1B	3.14	1.43	1.34
23	B	611	CLA	C4B-NB	3.14	1.42	1.37
31	m	102	LMG	O7-C8	-3.13	1.39	1.46
23	B	607	CLA	C4B-NB	3.13	1.42	1.37
23	B	612	CLA	C4B-NB	3.12	1.42	1.37
23	B	604	CLA	C4B-NB	3.12	1.42	1.37
28	c	518	DGD	O2G-C1B	3.12	1.43	1.34
31	A	418	LMG	O7-C8	-3.12	1.39	1.46
31	b	625	LMG	O7-C8	-3.12	1.39	1.46
23	B	608	CLA	C4B-NB	3.12	1.42	1.37
23	c	503	CLA	C4B-NB	3.12	1.42	1.37
23	c	508	CLA	C4B-NB	3.11	1.42	1.37
23	c	505	CLA	C4B-NB	3.11	1.41	1.37
23	b	618	CLA	C4B-NB	3.11	1.41	1.37
23	B	605	CLA	C4B-NB	3.11	1.41	1.37
30	A	417	SQD	O48-C23	3.10	1.42	1.33
23	C	506	CLA	C4B-NB	3.10	1.41	1.37
23	b	609	CLA	C4B-NB	3.10	1.41	1.37
30	B	626	SQD	O48-C23	3.09	1.42	1.33
31	b	624	LMG	O7-C8	-3.09	1.39	1.46
28	c	516	DGD	O1G-C1A	3.09	1.42	1.33
23	C	510	CLA	C4B-NB	3.09	1.41	1.37
28	a	413	DGD	O2G-C2G	-3.08	1.39	1.46
34	F	101	HEM	CAC-C3C	3.08	1.55	1.47
23	C	512	CLA	C4B-NB	3.08	1.41	1.37
23	c	507	CLA	C4B-NB	3.08	1.41	1.37
31	d	407	LMG	O7-C8	-3.08	1.39	1.46
23	D	401	CLA	C4B-NB	3.08	1.41	1.37
31	a	416	LMG	O7-C8	-3.08	1.39	1.46
23	B	612	CLA	C1D-ND	3.07	1.41	1.37
23	B	615	CLA	C4B-NB	3.07	1.41	1.37
23	B	603	CLA	C4B-NB	3.07	1.41	1.37
25	d	404	PL9	C43-C44	3.07	1.40	1.33
23	b	608	CLA	C4B-NB	3.07	1.41	1.37
30	f	102	SQD	O48-C23	3.06	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	402	LMG	O7-C8	-3.06	1.39	1.46
23	b	620	CLA	C4B-NB	3.06	1.41	1.37
28	c	517	DGD	O2G-C2G	-3.05	1.39	1.46
23	B	601	CLA	C4B-NB	3.05	1.41	1.37
23	b	610	CLA	C4B-NB	3.05	1.41	1.37
34	f	101	HEM	CAC-C3C	3.05	1.55	1.47
25	J	101	PL9	C23-C24	3.04	1.40	1.33
23	c	513	CLA	C4B-NB	3.04	1.41	1.37
23	C	505	CLA	C4B-NB	3.04	1.41	1.37
23	C	501	CLA	C4B-NB	3.03	1.41	1.37
28	C	518	DGD	O2G-C2G	-3.02	1.39	1.46
30	F	102	SQD	O48-C23	3.02	1.42	1.33
31	B	623	LMG	O7-C8	-3.02	1.39	1.46
28	D	409	DGD	O2G-C2G	-3.01	1.39	1.46
30	d	408	SQD	O47-C7	3.01	1.42	1.34
23	b	613	CLA	C4B-NB	3.01	1.41	1.37
23	d	403	CLA	C1B-C2B	3.01	1.50	1.43
31	C	521	LMG	O7-C10	3.00	1.42	1.34
34	F	101	HEM	CAB-C3B	3.00	1.55	1.47
34	v	201	HEM	CAC-C3C	3.00	1.55	1.47
23	a	406	CLA	C1B-C2B	3.00	1.50	1.43
23	C	502	CLA	C1B-C2B	3.00	1.50	1.43
23	b	605	CLA	C4B-NB	3.00	1.41	1.37
25	a	410	PL9	C38-C39	3.00	1.41	1.32
23	C	509	CLA	C4B-NB	3.00	1.41	1.37
30	D	408	SQD	O47-C7	2.99	1.42	1.34
23	d	402	CLA	C1B-C2B	2.99	1.50	1.43
23	c	509	CLA	C1B-C2B	2.99	1.50	1.43
23	C	503	CLA	C4B-NB	2.98	1.41	1.37
31	B	623	LMG	O7-C10	2.98	1.42	1.34
31	M	101	LMG	O7-C8	-2.97	1.39	1.46
31	M	101	LMG	O7-C10	2.97	1.42	1.34
25	A	408	PL9	C38-C39	2.97	1.41	1.32
28	D	409	DGD	O1G-C1A	2.97	1.42	1.33
31	A	414	LMG	O7-C8	-2.97	1.39	1.46
28	A	411	DGD	O2G-C1B	2.97	1.42	1.34
23	c	511	CLA	C1B-C2B	2.97	1.50	1.43
34	f	101	HEM	CAB-C3B	2.96	1.55	1.47
34	F	101	HEM	FE-NC	2.96	2.04	1.95
30	F	102	SQD	O47-C7	2.96	1.42	1.34
23	c	503	CLA	C1B-C2B	2.96	1.50	1.43
34	V	201	HEM	CAC-C3C	2.96	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C4B-NB	2.95	1.41	1.37
31	e	101	LMG	O7-C8	-2.95	1.39	1.46
31	c	519	LMG	O7-C10	2.95	1.42	1.34
28	B	627	DGD	O1G-C1A	2.95	1.42	1.33
31	A	414	LMG	O7-C10	2.95	1.42	1.34
23	D	403	CLA	C4B-NB	2.95	1.41	1.37
23	b	607	CLA	C4B-NB	2.95	1.41	1.37
23	b	608	CLA	C1B-C2B	2.95	1.50	1.43
28	B	627	DGD	O2G-C1B	2.94	1.42	1.34
23	B	610	CLA	C4B-NB	2.94	1.41	1.37
23	b	620	CLA	C1B-C2B	2.94	1.50	1.43
23	c	510	CLA	C4B-NB	2.94	1.41	1.37
23	B	616	CLA	C4B-NB	2.93	1.41	1.37
28	C	517	DGD	O1G-C1A	2.93	1.41	1.33
23	B	602	CLA	C4B-NB	2.93	1.41	1.37
30	A	417	SQD	O47-C7	2.93	1.42	1.34
23	B	609	CLA	C4B-NB	2.93	1.41	1.37
23	B	614	CLA	C4B-NB	2.93	1.41	1.37
23	B	604	CLA	C1B-C2B	2.92	1.50	1.43
31	M	101	LMG	O1-C7	-2.92	1.38	1.43
28	d	409	DGD	O1G-C1A	2.92	1.41	1.33
28	d	409	DGD	O2G-C2G	-2.92	1.39	1.46
23	C	501	CLA	C1B-C2B	2.91	1.50	1.43
25	j	101	PL9	C13-C14	2.91	1.39	1.33
31	a	416	LMG	O7-C10	2.91	1.42	1.34
23	c	501	CLA	C1B-C2B	2.91	1.50	1.43
23	C	511	CLA	C4B-NB	2.91	1.41	1.37
23	b	612	CLA	C4B-NB	2.91	1.41	1.37
23	A	404	CLA	C4B-NB	2.90	1.41	1.37
23	B	615	CLA	C1B-C2B	2.90	1.49	1.43
28	B	627	DGD	O2G-C2G	-2.90	1.39	1.46
23	B	606	CLA	C4B-NB	2.90	1.41	1.37
28	b	602	DGD	O2G-C1B	2.90	1.42	1.34
28	C	518	DGD	O1G-C1A	2.89	1.41	1.33
23	C	511	CLA	C1B-C2B	2.89	1.49	1.43
23	b	617	CLA	C4B-NB	2.88	1.41	1.37
23	C	508	CLA	C1B-C2B	2.88	1.49	1.43
31	c	519	LMG	O7-C8	-2.88	1.39	1.46
23	c	505	CLA	C1B-C2B	2.87	1.49	1.43
23	a	404	CLA	C1B-C2B	2.87	1.49	1.43
30	b	601	SQD	O47-C7	2.87	1.42	1.34
23	B	602	CLA	C1B-C2B	2.87	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	407	CLA	C4B-NB	2.86	1.41	1.37
31	m	102	LMG	O7-C10	2.86	1.42	1.34
23	b	606	CLA	C4B-NB	2.86	1.41	1.37
25	j	101	PL9	C18-C19	2.86	1.39	1.33
31	E	101	LMG	O7-C10	2.86	1.42	1.34
28	c	516	DGD	O2G-C1B	2.86	1.42	1.34
23	C	513	CLA	C4B-NB	2.84	1.41	1.37
25	j	101	PL9	C23-C24	2.84	1.39	1.33
25	J	101	PL9	C8-C9	2.84	1.39	1.33
30	a	401	SQD	O47-C7	2.84	1.42	1.34
34	v	201	HEM	CAB-C3B	2.84	1.55	1.47
23	A	405	CLA	C4B-NB	2.83	1.41	1.37
25	A	408	PL9	C18-C19	2.83	1.39	1.33
23	C	505	CLA	C1B-C2B	2.83	1.49	1.43
23	b	613	CLA	C1B-C2B	2.83	1.49	1.43
28	b	623	DGD	O1G-C1A	2.83	1.41	1.33
23	b	618	CLA	C1B-C2B	2.83	1.49	1.43
23	b	614	CLA	C4B-NB	2.83	1.41	1.37
23	b	619	CLA	C4B-NB	2.82	1.41	1.37
23	C	503	CLA	C1B-C2B	2.82	1.49	1.43
23	b	615	CLA	C1B-C2B	2.82	1.49	1.43
28	b	602	DGD	O2G-C2G	-2.81	1.40	1.46
28	c	518	DGD	O1G-C1A	2.81	1.41	1.33
31	D	407	LMG	O3-C3	-2.80	1.36	1.43
23	C	512	CLA	C1B-C2B	2.80	1.49	1.43
25	j	101	PL9	C8-C9	2.80	1.39	1.33
30	f	102	SQD	O47-C7	2.80	1.42	1.34
31	b	625	LMG	O7-C10	2.80	1.42	1.34
28	C	519	DGD	O2G-C2G	-2.80	1.40	1.46
23	a	409	CLA	C1B-C2B	2.80	1.49	1.43
25	J	101	PL9	C13-C14	2.79	1.39	1.33
23	c	512	CLA	C1B-C2B	2.79	1.49	1.43
23	A	403	CLA	C1B-C2B	2.79	1.49	1.43
28	B	621	DGD	O3G-C3G	-2.79	1.38	1.43
25	d	404	PL9	C23-C24	2.79	1.39	1.33
25	J	101	PL9	C18-C19	2.79	1.39	1.33
23	B	612	CLA	C1B-C2B	2.79	1.49	1.43
28	A	411	DGD	O2G-C2G	-2.79	1.40	1.46
25	D	404	PL9	C18-C19	2.79	1.39	1.33
31	A	418	LMG	O7-C10	2.79	1.42	1.34
31	k	103	LMG	O8-C28	2.79	1.41	1.33
31	a	402	LMG	O7-C10	2.78	1.42	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C1B-C2B	2.78	1.49	1.43
23	C	507	CLA	C4B-NB	2.78	1.41	1.37
23	b	609	CLA	C1B-C2B	2.78	1.49	1.43
25	A	408	PL9	C13-C14	2.78	1.39	1.33
30	A	413	SQD	O47-C7	2.78	1.42	1.34
31	C	521	LMG	O8-C28	2.77	1.41	1.33
23	b	616	CLA	C4B-NB	2.77	1.41	1.37
28	C	519	DGD	O1G-C1A	2.77	1.41	1.33
25	a	410	PL9	C13-C14	2.77	1.39	1.33
31	C	521	LMG	O7-C8	-2.77	1.40	1.46
31	e	101	LMG	O7-C10	2.76	1.42	1.34
31	I	101	LMG	O7-C10	2.76	1.42	1.34
31	E	101	LMG	O7-C8	-2.76	1.40	1.46
23	b	611	CLA	C1B-C2B	2.76	1.49	1.43
23	c	502	CLA	C4B-NB	2.76	1.41	1.37
23	B	613	CLA	C1B-C2B	2.76	1.49	1.43
31	b	624	LMG	O7-C10	2.76	1.42	1.34
25	A	408	PL9	C23-C24	2.76	1.39	1.33
30	B	626	SQD	O47-C7	2.76	1.42	1.34
23	b	610	CLA	C1B-C2B	2.75	1.49	1.43
23	D	401	CLA	C1B-C2B	2.75	1.49	1.43
31	m	102	LMG	O8-C28	2.75	1.41	1.33
23	b	605	CLA	C1B-C2B	2.75	1.49	1.43
23	A	407	CLA	C1B-C2B	2.75	1.49	1.43
28	c	517	DGD	O2G-C1B	2.75	1.42	1.34
23	C	510	CLA	C1B-C2B	2.74	1.49	1.43
23	c	508	CLA	C1B-C2B	2.74	1.49	1.43
25	a	410	PL9	C23-C24	2.74	1.39	1.33
28	A	411	DGD	O1G-C1A	2.74	1.41	1.33
23	B	601	CLA	C1B-C2B	2.74	1.49	1.43
23	c	507	CLA	C1B-C2B	2.74	1.49	1.43
30	a	415	SQD	O47-C7	2.74	1.42	1.34
25	D	404	PL9	C23-C24	2.73	1.39	1.33
34	V	201	HEM	CAB-C3B	2.73	1.54	1.47
25	A	408	PL9	C8-C9	2.73	1.39	1.33
28	B	621	DGD	O1G-C1A	2.73	1.41	1.33
28	c	518	DGD	O2G-C2G	-2.73	1.40	1.46
23	c	506	CLA	C1B-C2B	2.72	1.49	1.43
28	a	413	DGD	O1G-C1A	2.72	1.41	1.33
23	B	614	CLA	C1B-C2B	2.72	1.49	1.43
23	B	605	CLA	C1B-C2B	2.72	1.49	1.43
23	c	504	CLA	C1B-C2B	2.72	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	418	LMG	O8-C9	-2.72	1.39	1.45
28	C	518	DGD	O2G-C1B	2.71	1.41	1.34
31	d	407	LMG	O7-C10	2.71	1.41	1.34
25	d	404	PL9	C13-C14	2.71	1.39	1.33
31	c	519	LMG	O8-C28	2.71	1.41	1.33
23	b	607	CLA	C1B-C2B	2.71	1.49	1.43
31	M	101	LMG	O8-C28	2.71	1.41	1.33
31	m	102	LMG	O8-C9	-2.70	1.39	1.45
23	B	606	CLA	C1B-C2B	2.70	1.49	1.43
23	B	608	CLA	C1B-C2B	2.70	1.49	1.43
31	b	624	LMG	O8-C28	2.69	1.41	1.33
31	B	622	LMG	O7-C10	2.69	1.41	1.34
31	A	414	LMG	O3-C3	-2.69	1.36	1.43
25	d	404	PL9	C18-C19	2.69	1.39	1.33
23	B	616	CLA	C1B-C2B	2.68	1.49	1.43
23	C	513	CLA	C1B-C2B	2.68	1.49	1.43
31	E	101	LMG	O8-C28	2.68	1.41	1.33
23	A	405	CLA	C1B-C2B	2.68	1.49	1.43
31	a	402	LMG	O8-C28	2.67	1.41	1.33
31	b	625	LMG	O3-C3	-2.67	1.36	1.43
28	c	517	DGD	O1G-C1A	2.67	1.41	1.33
25	d	404	PL9	C8-C9	2.67	1.39	1.33
23	b	617	CLA	C1B-C2B	2.67	1.49	1.43
28	C	517	DGD	O2G-C1B	2.67	1.41	1.34
31	C	520	LMG	O8-C28	2.67	1.41	1.33
23	C	506	CLA	C1B-C2B	2.67	1.49	1.43
23	b	619	CLA	C1B-C2B	2.67	1.49	1.43
31	e	101	LMG	O8-C28	2.67	1.41	1.33
31	i	101	LMG	O8-C9	-2.66	1.39	1.45
23	c	502	CLA	C1B-C2B	2.66	1.49	1.43
23	B	607	CLA	C1B-C2B	2.66	1.49	1.43
23	B	609	CLA	C1B-C2B	2.66	1.49	1.43
28	a	413	DGD	O2G-C1B	2.66	1.41	1.34
23	B	611	CLA	C1B-C2B	2.66	1.49	1.43
31	d	407	LMG	O8-C28	2.66	1.41	1.33
31	i	101	LMG	O7-C10	2.65	1.41	1.34
31	a	416	LMG	O8-C28	2.65	1.41	1.33
31	B	623	LMG	O3-C3	-2.65	1.36	1.43
31	d	406	LMG	O7-C10	2.65	1.41	1.34
23	b	616	CLA	C1B-C2B	2.64	1.49	1.43
23	C	509	CLA	C1B-C2B	2.64	1.49	1.43
31	A	414	LMG	O8-C28	2.63	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M	101	LMG	O8-C9	-2.63	1.39	1.45
23	D	403	CLA	C1B-C2B	2.63	1.49	1.43
31	C	520	LMG	O7-C10	2.63	1.41	1.34
31	D	407	LMG	O8-C28	2.62	1.41	1.33
23	A	403	CLA	C3B-C4B	2.62	1.50	1.42
31	B	622	LMG	O8-C28	2.62	1.41	1.33
31	d	407	LMG	O3-C3	-2.62	1.36	1.43
23	a	409	CLA	C3B-C4B	2.61	1.50	1.42
31	I	101	LMG	O8-C28	2.61	1.41	1.33
28	b	623	DGD	O3G-C3G	-2.61	1.39	1.43
23	c	510	CLA	C1B-C2B	2.61	1.49	1.43
31	e	101	LMG	O8-C9	-2.61	1.39	1.45
28	B	627	DGD	O6E-C5E	-2.60	1.38	1.44
34	f	101	HEM	FE-NC	2.60	2.03	1.95
28	c	517	DGD	O5D-C6D	-2.60	1.39	1.43
28	C	519	DGD	O3G-C3G	-2.60	1.39	1.43
31	k	103	LMG	O7-C10	2.60	1.41	1.34
31	a	416	LMG	O3-C3	-2.60	1.36	1.43
23	C	504	CLA	C4B-NB	2.60	1.41	1.37
25	a	410	PL9	C8-C9	2.60	1.39	1.33
31	D	406	LMG	O7-C10	2.59	1.41	1.34
25	a	410	PL9	C18-C19	2.59	1.39	1.33
31	D	407	LMG	O7-C10	2.59	1.41	1.34
23	b	606	CLA	CHC-C1C	2.58	1.43	1.38
25	D	404	PL9	C8-C9	2.58	1.39	1.33
24	a	407	PHO	CMB-C2B	-2.58	1.46	1.51
28	d	409	DGD	O2G-C1B	2.58	1.41	1.34
31	B	623	LMG	O8-C28	2.58	1.40	1.33
23	B	603	CLA	C1B-C2B	2.58	1.49	1.43
31	E	101	LMG	O8-C9	-2.57	1.39	1.45
25	d	404	PL9	C28-C29	2.57	1.39	1.33
24	D	402	PHO	CMD-C2D	-2.57	1.46	1.51
24	A	406	PHO	C3D-C4D	2.57	1.44	1.41
25	D	404	PL9	C13-C14	2.57	1.39	1.33
23	b	606	CLA	C1B-C2B	2.56	1.49	1.43
24	D	402	PHO	CMC-C2C	-2.56	1.46	1.50
31	A	418	LMG	O1-C7	-2.56	1.39	1.43
24	a	407	PHO	CMD-C2D	-2.55	1.46	1.51
31	b	625	LMG	O8-C28	2.55	1.40	1.33
23	C	508	CLA	C3B-C4B	2.55	1.50	1.42
31	c	519	LMG	O8-C9	-2.55	1.39	1.45
24	A	406	PHO	CMC-C2C	-2.55	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	CLA	C3B-C4B	2.55	1.50	1.42
23	C	507	CLA	C1B-C2B	2.54	1.49	1.43
28	b	623	DGD	O2G-C1B	2.54	1.41	1.34
31	B	623	LMG	O8-C9	-2.54	1.39	1.45
31	i	101	LMG	O1-C7	-2.54	1.39	1.43
31	I	101	LMG	O8-C9	-2.54	1.39	1.45
31	d	406	LMG	O8-C28	2.54	1.40	1.33
23	c	511	CLA	C3B-C4B	2.54	1.50	1.42
23	a	405	CLA	C1B-C2B	2.53	1.49	1.43
31	b	625	LMG	O8-C9	-2.53	1.39	1.45
23	a	409	CLA	CHC-C1C	2.53	1.43	1.38
31	m	102	LMG	O3-C3	-2.53	1.36	1.43
28	b	602	DGD	O6E-C5E	-2.53	1.38	1.44
31	a	416	LMG	O8-C9	-2.53	1.39	1.45
31	b	624	LMG	O6-C5	-2.53	1.38	1.44
28	A	411	DGD	O3G-C3G	-2.53	1.39	1.43
25	A	408	PL9	C28-C29	2.52	1.38	1.33
23	a	405	CLA	C3B-C4B	2.52	1.50	1.42
23	A	404	CLA	C3B-C4B	2.52	1.50	1.42
31	D	406	LMG	O3-C3	-2.52	1.36	1.43
31	i	101	LMG	O3-C3	-2.51	1.36	1.43
23	A	404	CLA	CHC-C1C	2.51	1.43	1.38
31	d	406	LMG	O8-C9	-2.51	1.39	1.45
23	c	509	CLA	C3B-C4B	2.51	1.50	1.42
31	D	406	LMG	O8-C28	2.51	1.40	1.33
31	c	519	LMG	O3-C3	-2.51	1.36	1.43
23	c	511	CLA	CHC-C1C	2.51	1.43	1.38
31	d	406	LMG	O3-C3	-2.50	1.36	1.43
24	A	406	PHO	CAC-C3C	-2.50	1.47	1.51
28	a	413	DGD	O3G-C3G	-2.50	1.39	1.43
24	a	408	PHO	CMC-C2C	-2.50	1.46	1.50
23	b	612	CLA	C1B-C2B	2.50	1.49	1.43
28	D	409	DGD	O2G-C1B	2.50	1.41	1.34
31	M	101	LMG	O3-C3	-2.49	1.36	1.43
31	A	414	LMG	O1-C7	-2.49	1.39	1.43
24	a	407	PHO	CMC-C2C	-2.49	1.46	1.50
31	B	622	LMG	O8-C9	-2.49	1.39	1.45
31	a	402	LMG	O3-C3	-2.49	1.36	1.43
31	I	101	LMG	O3-C3	-2.49	1.36	1.43
23	c	508	CLA	C3B-C4B	2.49	1.50	1.42
28	C	518	DGD	O5D-C6D	-2.49	1.39	1.43
23	a	406	CLA	C3B-C4B	2.48	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	C3D-C4D	2.48	1.44	1.41
24	A	406	PHO	CMD-C2D	-2.48	1.46	1.51
31	I	101	LMG	O1-C7	-2.47	1.39	1.43
28	c	518	DGD	O4D-C4D	-2.47	1.36	1.43
28	B	621	DGD	O2G-C1B	2.47	1.41	1.34
24	A	406	PHO	CMB-C2B	-2.47	1.46	1.51
24	a	408	PHO	CMD-C2D	-2.47	1.46	1.51
23	B	614	CLA	MG-NB	-2.47	2.00	2.05
31	b	624	LMG	O1-C7	-2.47	1.39	1.43
31	A	414	LMG	O8-C9	-2.46	1.39	1.45
23	c	506	CLA	C3B-C4B	2.46	1.49	1.42
31	i	101	LMG	O8-C28	2.46	1.40	1.33
31	D	407	LMG	O8-C9	-2.46	1.39	1.45
23	b	619	CLA	CHC-C1C	2.46	1.43	1.38
23	B	610	CLA	C1B-C2B	2.46	1.48	1.43
31	B	623	LMG	O1-C7	-2.46	1.39	1.43
23	C	509	CLA	C3B-C4B	2.46	1.49	1.42
28	C	519	DGD	O4D-C4D	-2.45	1.36	1.43
31	d	406	LMG	O1-C7	-2.45	1.39	1.43
24	D	402	PHO	CMB-C2B	-2.45	1.46	1.51
31	b	624	LMG	O8-C9	-2.45	1.39	1.45
24	a	408	PHO	CAC-C3C	-2.44	1.47	1.51
23	B	609	CLA	CHC-C1C	2.44	1.43	1.38
23	b	609	CLA	C3B-C4B	2.44	1.49	1.42
24	a	407	PHO	CAC-C3C	-2.44	1.47	1.51
31	d	407	LMG	O8-C9	-2.44	1.39	1.45
31	C	520	LMG	O3-C3	-2.43	1.36	1.43
25	a	410	PL9	C28-C29	2.43	1.38	1.33
23	B	608	CLA	CHC-C1C	2.43	1.43	1.38
31	D	406	LMG	O8-C9	-2.43	1.39	1.45
31	b	624	LMG	O3-C3	-2.43	1.36	1.43
24	D	402	PHO	CAC-C3C	-2.43	1.47	1.51
23	c	510	CLA	CHC-C1C	2.43	1.43	1.38
31	e	101	LMG	O3-C3	-2.43	1.36	1.43
28	A	411	DGD	O4D-C4D	-2.43	1.36	1.43
23	c	509	CLA	CHC-C1C	2.42	1.43	1.38
23	B	602	CLA	CHC-C1C	2.42	1.43	1.38
23	c	512	CLA	C3B-C4B	2.42	1.49	1.42
28	C	517	DGD	O6E-C5E	-2.42	1.38	1.44
31	C	521	LMG	O8-C9	-2.42	1.39	1.45
31	C	521	LMG	O3-C3	-2.42	1.37	1.43
23	B	607	CLA	C3B-C4B	2.41	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	418	LMG	O8-C28	2.41	1.40	1.33
23	b	615	CLA	CMB-C2B	-2.41	1.45	1.50
31	C	520	LMG	O8-C9	-2.41	1.39	1.45
24	a	408	PHO	CMB-C2B	-2.41	1.46	1.51
28	c	516	DGD	O6E-C5E	-2.41	1.38	1.44
23	B	605	CLA	C3B-C4B	2.40	1.49	1.42
31	A	418	LMG	O3-C3	-2.40	1.37	1.43
23	b	614	CLA	C1B-C2B	2.40	1.48	1.43
24	a	408	PHO	C3D-C4D	2.40	1.44	1.41
28	c	517	DGD	O6E-C5E	-2.40	1.38	1.44
23	A	405	CLA	MG-NB	-2.39	2.01	2.05
31	k	103	LMG	O3-C3	-2.39	1.37	1.43
23	B	607	CLA	CHC-C1C	2.39	1.43	1.38
23	B	613	CLA	C3B-C4B	2.39	1.49	1.42
23	c	503	CLA	C3B-C4B	2.39	1.49	1.42
23	b	606	CLA	C3B-C4B	2.39	1.49	1.42
23	b	609	CLA	CHC-C1C	2.39	1.43	1.38
23	B	606	CLA	MG-NB	-2.39	2.01	2.05
25	D	404	PL9	C28-C29	2.39	1.38	1.33
23	b	613	CLA	C3B-C4B	2.39	1.49	1.42
23	b	612	CLA	MG-NB	-2.39	2.01	2.05
23	B	609	CLA	C3B-C4B	2.38	1.49	1.42
31	E	101	LMG	O3-C3	-2.38	1.37	1.43
31	a	402	LMG	O1-C7	-2.38	1.39	1.43
23	A	404	CLA	C1B-C2B	2.38	1.48	1.43
31	k	103	LMG	O1-C7	-2.38	1.39	1.43
23	a	406	CLA	CHC-C1C	2.38	1.43	1.38
31	B	622	LMG	O3-C3	-2.38	1.37	1.43
23	C	504	CLA	C1B-C2B	2.38	1.48	1.43
31	B	622	LMG	O6-C5	-2.37	1.38	1.44
28	C	518	DGD	O6E-C5E	-2.37	1.38	1.44
23	B	610	CLA	CHC-C1C	2.37	1.43	1.38
23	B	603	CLA	CHC-C1C	2.37	1.43	1.38
31	a	416	LMG	O1-C7	-2.37	1.39	1.43
23	C	513	CLA	CHC-C1C	2.37	1.43	1.38
23	B	612	CLA	C3B-C4B	2.37	1.49	1.42
23	D	401	CLA	C3B-C4B	2.37	1.49	1.42
23	c	510	CLA	C3B-C4B	2.37	1.49	1.42
23	c	506	CLA	CHC-C1C	2.37	1.43	1.38
23	B	602	CLA	C3B-C4B	2.36	1.49	1.42
23	d	403	CLA	C3B-C4B	2.36	1.49	1.42
23	b	618	CLA	CHC-C1C	2.36	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C3B-C4B	2.36	1.49	1.42
23	b	616	CLA	MG-NB	-2.35	2.01	2.05
23	C	504	CLA	CHC-C1C	2.35	1.43	1.38
28	C	518	DGD	O4D-C4D	-2.35	1.37	1.43
23	C	503	CLA	C3B-C4B	2.35	1.49	1.42
28	C	518	DGD	O5D-C1E	-2.35	1.36	1.40
23	c	510	CLA	CMD-C2D	-2.34	1.46	1.50
23	A	405	CLA	C3B-C4B	2.34	1.49	1.42
23	b	611	CLA	C3B-C4B	2.34	1.49	1.42
28	c	518	DGD	O3G-C3G	-2.34	1.39	1.43
23	C	509	CLA	CHC-C1C	2.34	1.43	1.38
28	c	517	DGD	O4D-C4D	-2.34	1.37	1.43
23	c	508	CLA	CHC-C1C	2.33	1.43	1.38
24	D	402	PHO	C3D-C4D	2.33	1.44	1.41
23	b	614	CLA	C3B-C4B	2.33	1.49	1.42
23	C	506	CLA	CHC-C1C	2.33	1.43	1.38
23	D	403	CLA	CHC-C1C	2.33	1.43	1.38
31	a	402	LMG	O8-C9	-2.33	1.40	1.45
23	B	605	CLA	CHC-C1C	2.33	1.43	1.38
23	b	619	CLA	C3B-C4B	2.33	1.49	1.42
23	B	616	CLA	MG-NB	-2.33	2.01	2.05
23	C	508	CLA	CHC-C1C	2.33	1.43	1.38
23	B	603	CLA	C3B-C4B	2.32	1.49	1.42
23	B	610	CLA	MG-NB	-2.32	2.01	2.05
28	A	411	DGD	O1G-C1G	-2.32	1.40	1.45
23	B	608	CLA	C3B-C4B	2.32	1.49	1.42
23	D	403	CLA	C3B-C4B	2.31	1.49	1.42
23	C	504	CLA	C3B-C4B	2.31	1.49	1.42
23	C	512	CLA	C3B-C4B	2.31	1.49	1.42
23	B	614	CLA	CHC-C1C	2.30	1.43	1.38
23	B	612	CLA	CHC-C1C	2.30	1.43	1.38
28	a	413	DGD	O4D-C4D	-2.30	1.37	1.43
23	B	611	CLA	CMB-C2B	-2.30	1.46	1.50
23	b	614	CLA	MG-NB	-2.30	2.01	2.05
31	d	407	LMG	O1-C7	-2.30	1.39	1.43
23	C	501	CLA	C3B-C4B	2.29	1.49	1.42
23	c	502	CLA	CHC-C1C	2.29	1.43	1.38
28	c	516	DGD	O4D-C4D	-2.29	1.37	1.43
30	A	417	SQD	O2-C2	-2.28	1.37	1.43
23	b	614	CLA	CHC-C1C	2.28	1.43	1.38
23	c	501	CLA	C3B-C4B	2.28	1.49	1.42
23	C	511	CLA	C3B-C4B	2.28	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	k	103	LMG	O8-C9	-2.28	1.40	1.45
23	C	506	CLA	C3B-C4B	2.28	1.49	1.42
23	C	507	CLA	C3B-C4B	2.28	1.49	1.42
23	c	507	CLA	MG-NB	-2.28	2.01	2.05
23	B	611	CLA	MG-NB	-2.27	2.01	2.05
31	i	101	LMG	O6-C5	-2.27	1.38	1.44
23	c	505	CLA	C3B-C4B	2.27	1.49	1.42
23	C	512	CLA	CHC-C1C	2.27	1.43	1.38
23	b	615	CLA	C3B-C4B	2.26	1.49	1.42
23	C	513	CLA	C3B-C4B	2.26	1.49	1.42
23	B	612	CLA	CMD-C2D	-2.26	1.46	1.50
28	c	517	DGD	O5D-C1E	-2.26	1.36	1.40
23	B	601	CLA	CHC-C1C	2.26	1.43	1.38
23	C	507	CLA	MG-NB	-2.26	2.01	2.05
28	b	602	DGD	O4D-C4D	-2.26	1.37	1.43
23	C	510	CLA	C3B-C4B	2.25	1.49	1.42
23	A	403	CLA	CHC-C1C	2.25	1.43	1.38
31	I	101	LMG	O6-C5	-2.25	1.38	1.44
23	B	611	CLA	C3B-C4B	2.25	1.49	1.42
23	d	403	CLA	CHC-C1C	2.25	1.43	1.38
23	c	502	CLA	MG-NB	-2.25	2.01	2.05
30	A	417	SQD	C4-C5	-2.25	1.48	1.53
23	C	505	CLA	C3B-C4B	2.25	1.49	1.42
23	B	612	CLA	MG-NB	-2.24	2.01	2.05
23	b	618	CLA	C3B-C4B	2.24	1.49	1.42
28	C	518	DGD	C4D-C5D	-2.24	1.48	1.53
23	C	510	CLA	CMB-C2B	-2.23	1.46	1.50
23	c	510	CLA	MG-NB	-2.23	2.01	2.05
31	m	102	LMG	O6-C5	-2.23	1.38	1.44
23	C	511	CLA	CHC-C1C	2.23	1.43	1.38
23	B	610	CLA	C3B-C4B	2.23	1.49	1.42
23	b	607	CLA	C3B-C4B	2.23	1.49	1.42
28	c	517	DGD	O1G-C1G	-2.23	1.40	1.45
28	D	409	DGD	O5D-C6D	-2.23	1.39	1.43
31	D	407	LMG	O6-C5	-2.23	1.38	1.44
23	c	502	CLA	C3B-C4B	2.23	1.49	1.42
23	b	613	CLA	CHC-C1C	2.23	1.42	1.38
23	A	403	CLA	CMD-C2D	-2.23	1.46	1.50
23	B	604	CLA	CHC-C1C	2.22	1.42	1.38
31	C	520	LMG	O1-C7	-2.22	1.39	1.43
28	B	621	DGD	O6D-C5D	-2.22	1.38	1.44
23	B	613	CLA	CHC-C1C	2.22	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	621	DGD	O4D-C4D	-2.22	1.37	1.43
28	b	623	DGD	O6E-C5E	-2.22	1.39	1.44
23	c	501	CLA	CHC-C1C	2.22	1.42	1.38
23	b	610	CLA	CHC-C1C	2.22	1.42	1.38
23	c	512	CLA	CHC-C1C	2.21	1.42	1.38
23	D	403	CLA	MG-NB	-2.21	2.01	2.05
23	C	510	CLA	MG-NB	-2.21	2.01	2.05
23	c	503	CLA	CHC-C1C	2.21	1.42	1.38
31	B	623	LMG	O6-C5	-2.21	1.39	1.44
23	D	401	CLA	CHC-C1C	2.21	1.42	1.38
23	C	504	CLA	MG-NB	-2.21	2.01	2.05
23	a	404	CLA	CMD-C2D	-2.21	1.46	1.50
23	B	615	CLA	MG-NB	-2.21	2.01	2.05
28	B	627	DGD	O4D-C4D	-2.21	1.37	1.43
23	B	611	CLA	CHC-C1C	2.20	1.42	1.38
28	c	517	DGD	O6D-C5D	-2.20	1.39	1.44
23	C	507	CLA	CHC-C1C	2.20	1.42	1.38
23	a	405	CLA	CHC-C1C	2.20	1.42	1.38
23	b	611	CLA	CHC-C1C	2.20	1.42	1.38
23	C	503	CLA	CHC-C1C	2.20	1.42	1.38
23	C	501	CLA	CHC-C1C	2.20	1.42	1.38
23	C	505	CLA	CMD-C2D	-2.20	1.46	1.50
23	b	607	CLA	MG-NB	-2.20	2.01	2.05
31	c	519	LMG	O6-C5	-2.20	1.39	1.44
23	A	407	CLA	C3B-C4B	2.20	1.49	1.42
31	b	625	LMG	O1-C7	-2.19	1.40	1.43
23	d	402	CLA	CMD-C2D	-2.19	1.46	1.50
24	D	402	PHO	CBD-CGD	-2.19	1.49	1.52
23	B	604	CLA	C3B-C4B	2.19	1.49	1.42
23	c	505	CLA	CHC-C1C	2.19	1.42	1.38
23	c	513	CLA	C3B-C4B	2.19	1.49	1.42
23	B	608	CLA	CMD-C2D	-2.19	1.46	1.50
31	D	407	LMG	O1-C7	-2.19	1.40	1.43
23	b	616	CLA	C3B-C4B	2.19	1.49	1.42
23	A	407	CLA	MG-NB	-2.19	2.01	2.05
23	b	616	CLA	CMD-C2D	-2.19	1.46	1.50
23	B	615	CLA	C3B-C4B	2.18	1.49	1.42
23	b	608	CLA	MG-NB	-2.18	2.01	2.05
28	a	413	DGD	O1G-C1G	-2.18	1.40	1.45
34	v	201	HEM	CMB-C2B	2.18	1.55	1.50
23	b	607	CLA	CHC-C1C	2.18	1.42	1.38
23	b	612	CLA	CMB-C2B	-2.18	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	CHC-C1C	2.17	1.42	1.38
23	B	614	CLA	CMD-C2D	-2.17	1.46	1.50
25	J	101	PL9	C28-C29	2.17	1.39	1.32
31	E	101	LMG	O6-C5	-2.17	1.39	1.44
23	B	606	CLA	C3B-C4B	2.17	1.49	1.42
23	A	405	CLA	CHC-C1C	2.17	1.42	1.38
23	C	502	CLA	C3B-C4B	2.17	1.49	1.42
23	B	601	CLA	C3B-C4B	2.17	1.49	1.42
31	d	407	LMG	O6-C5	-2.17	1.39	1.44
25	j	101	PL9	C28-C29	2.17	1.38	1.32
31	b	625	LMG	O6-C5	-2.17	1.39	1.44
23	b	605	CLA	CMB-C2B	-2.17	1.46	1.50
30	a	401	SQD	O2-C2	-2.16	1.37	1.43
31	B	622	LMG	O1-C7	-2.16	1.40	1.43
23	B	604	CLA	CMD-C2D	-2.16	1.46	1.50
23	C	505	CLA	MG-NB	-2.16	2.01	2.05
23	b	612	CLA	C3B-C4B	2.16	1.49	1.42
23	c	505	CLA	CMD-C2D	-2.16	1.46	1.50
23	B	615	CLA	CHC-C1C	2.15	1.42	1.38
31	e	101	LMG	O6-C5	-2.15	1.39	1.44
34	F	101	HEM	CMC-C2C	2.15	1.55	1.50
23	b	613	CLA	MG-NB	-2.15	2.01	2.05
23	B	616	CLA	C3B-C4B	2.15	1.49	1.42
23	B	613	CLA	MG-NB	-2.15	2.01	2.05
31	c	519	LMG	O1-C7	-2.15	1.40	1.43
23	b	610	CLA	CMB-C2B	-2.15	1.46	1.50
23	C	510	CLA	CMD-C2D	-2.15	1.46	1.50
28	D	409	DGD	O6E-C5E	-2.15	1.39	1.44
23	b	618	CLA	CMD-C2D	-2.14	1.46	1.50
23	a	406	CLA	CMD-C2D	-2.14	1.46	1.50
23	B	604	CLA	MG-NB	-2.14	2.01	2.05
23	B	601	CLA	CMB-C2B	-2.14	1.46	1.50
23	b	608	CLA	CMD-C2D	-2.14	1.46	1.50
33	i	102	LMT	O1'-C1'	2.14	1.43	1.40
28	b	602	DGD	O5D-C6D	-2.13	1.40	1.43
34	f	101	HEM	CMA-C3A	2.13	1.55	1.50
34	V	201	HEM	FE-NC	2.13	2.02	1.95
23	b	617	CLA	C3B-C4B	2.13	1.48	1.42
23	b	620	CLA	CMB-C2B	-2.13	1.46	1.50
23	b	608	CLA	C3B-C4B	2.13	1.48	1.42
23	C	510	CLA	CHC-C1C	2.13	1.42	1.38
23	b	610	CLA	C3B-C4B	2.13	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	CMD-C2D	-2.13	1.46	1.50
23	B	614	CLA	C3B-C4B	2.12	1.48	1.42
23	b	605	CLA	C3B-C4B	2.12	1.48	1.42
31	C	521	LMG	O6-C5	-2.12	1.39	1.44
23	b	606	CLA	MG-NB	-2.12	2.01	2.05
23	c	502	CLA	CMD-C2D	-2.12	1.46	1.50
28	a	413	DGD	O6E-C5E	-2.12	1.39	1.44
23	B	604	CLA	CMB-C2B	-2.12	1.46	1.50
23	c	508	CLA	CMB-C2B	-2.12	1.46	1.50
23	c	504	CLA	CHC-C1C	2.12	1.42	1.38
23	d	402	CLA	C3B-C4B	2.12	1.48	1.42
30	B	626	SQD	O2-C2	-2.12	1.37	1.43
34	V	201	HEM	CMD-C2D	2.12	1.55	1.50
33	D	410	LMT	O1'-C1'	2.12	1.43	1.40
23	C	502	CLA	MG-NB	-2.12	2.01	2.05
23	C	503	CLA	MG-NB	-2.12	2.01	2.05
34	V	201	HEM	CMB-C2B	2.12	1.55	1.50
31	D	407	LMG	O2-C2	-2.11	1.37	1.43
23	b	617	CLA	CHC-C1C	2.11	1.42	1.38
24	a	407	PHO	C4D-ND	-2.11	1.35	1.38
23	b	612	CLA	CMD-C2D	-2.11	1.46	1.50
23	C	508	CLA	CMD-C2D	-2.11	1.46	1.50
28	B	621	DGD	O6E-C5E	-2.11	1.39	1.44
23	b	620	CLA	MG-NB	-2.11	2.01	2.05
23	C	508	CLA	CMB-C2B	-2.11	1.46	1.50
24	a	407	PHO	C3B-C2B	-2.11	1.37	1.40
28	C	517	DGD	O4D-C4D	-2.11	1.37	1.43
23	D	401	CLA	CMD-C2D	-2.11	1.46	1.50
23	B	610	CLA	CMB-C2B	-2.11	1.46	1.50
23	A	407	CLA	CHC-C1C	2.11	1.42	1.38
23	b	609	CLA	CMD-C2D	-2.11	1.46	1.50
23	d	403	CLA	CMD-C2D	-2.10	1.46	1.50
28	C	518	DGD	O6D-C5D	-2.10	1.39	1.44
23	D	401	CLA	MG-NB	-2.10	2.01	2.05
28	C	519	DGD	O1G-C1G	-2.10	1.40	1.45
23	b	617	CLA	CMB-C2B	-2.10	1.46	1.50
28	B	621	DGD	O1G-C1G	-2.10	1.40	1.45
23	B	616	CLA	CMB-C2B	-2.10	1.46	1.50
23	B	603	CLA	CMB-C2B	-2.10	1.46	1.50
31	d	407	LMG	O2-C2	-2.10	1.37	1.43
23	b	616	CLA	CMC-C2C	-2.10	1.46	1.50
23	B	606	CLA	CMB-C2B	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	CMB-C2B	-2.09	1.46	1.50
23	C	513	CLA	MG-NB	-2.09	2.01	2.05
31	M	101	LMG	O6-C5	-2.09	1.39	1.44
28	d	409	DGD	O6E-C5E	-2.09	1.39	1.44
23	a	404	CLA	CHC-C1C	2.09	1.42	1.38
30	A	417	SQD	O47-C45	-2.09	1.41	1.46
28	b	623	DGD	O6D-C5D	-2.09	1.39	1.44
31	C	521	LMG	O1-C7	-2.09	1.40	1.43
34	f	101	HEM	CMC-C2C	2.09	1.55	1.50
34	V	201	HEM	CMA-C3A	2.09	1.55	1.50
23	B	611	CLA	CMD-C2D	-2.09	1.46	1.50
23	B	616	CLA	CMC-C2C	-2.09	1.46	1.50
23	A	404	CLA	MG-NB	-2.09	2.01	2.05
23	C	502	CLA	CMD-C2D	-2.09	1.46	1.50
23	C	507	CLA	CMB-C2B	-2.08	1.46	1.50
28	c	518	DGD	O6E-C5E	-2.08	1.39	1.44
23	C	502	CLA	CMC-C2C	-2.08	1.46	1.50
23	b	619	CLA	MG-NB	-2.08	2.01	2.05
23	A	404	CLA	CMB-C2B	-2.08	1.46	1.50
28	B	621	DGD	O5D-C6D	-2.08	1.40	1.43
23	c	507	CLA	C3B-C4B	2.08	1.48	1.42
23	b	611	CLA	CMD-C2D	-2.08	1.46	1.50
31	D	406	LMG	O1-C7	-2.08	1.40	1.43
30	A	413	SQD	O47-C45	-2.08	1.41	1.46
23	b	618	CLA	CMB-C2B	-2.08	1.46	1.50
23	b	612	CLA	CHC-C1C	2.08	1.42	1.38
23	b	605	CLA	CMC-C2C	-2.08	1.46	1.50
28	b	623	DGD	O5D-C6D	-2.08	1.40	1.43
23	B	616	CLA	CHC-C1C	2.07	1.42	1.38
28	A	411	DGD	O6E-C5E	-2.07	1.39	1.44
23	b	615	CLA	MG-NB	-2.07	2.01	2.05
23	b	620	CLA	C3B-C4B	2.07	1.48	1.42
30	a	401	SQD	C4-C5	-2.07	1.48	1.53
23	c	502	CLA	CMB-C2B	-2.07	1.46	1.50
23	D	403	CLA	CMD-C2D	-2.07	1.46	1.50
23	B	608	CLA	CMB-C2B	-2.07	1.46	1.50
33	d	410	LMT	O1'-C1'	2.07	1.43	1.40
31	d	406	LMG	O6-C5	-2.07	1.39	1.44
23	c	513	CLA	MG-NB	-2.07	2.01	2.05
34	v	201	HEM	CMA-C3A	2.07	1.55	1.50
23	b	617	CLA	CMD-C2D	-2.07	1.46	1.50
23	b	606	CLA	CMB-C2B	-2.06	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	CHC-C1C	2.06	1.42	1.38
23	b	620	CLA	CHC-C1C	2.06	1.42	1.38
30	a	401	SQD	O47-C45	-2.06	1.41	1.46
23	C	504	CLA	CMB-C2B	-2.06	1.46	1.50
28	d	409	DGD	O4D-C4D	-2.06	1.37	1.43
23	a	409	CLA	CMC-C2C	-2.06	1.46	1.50
23	c	507	CLA	CMD-C2D	-2.06	1.46	1.50
23	C	508	CLA	CMC-C2C	-2.06	1.46	1.50
31	D	406	LMG	O6-C5	-2.06	1.39	1.44
30	b	601	SQD	O2-C2	-2.06	1.37	1.43
23	a	405	CLA	CMB-C2B	-2.06	1.46	1.50
23	b	620	CLA	CMC-C2C	-2.06	1.46	1.50
23	B	605	CLA	CMD-C2D	-2.05	1.46	1.50
23	b	615	CLA	CMD-C2D	-2.05	1.46	1.50
34	f	101	HEM	CMD-C2D	2.05	1.55	1.50
23	b	618	CLA	MG-NB	-2.05	2.01	2.05
23	c	501	CLA	CMD-C2D	-2.05	1.46	1.50
23	c	505	CLA	CMB-C2B	-2.05	1.46	1.50
23	C	505	CLA	CMB-C2B	-2.05	1.46	1.50
28	B	627	DGD	C4E-C5E	-2.05	1.48	1.53
23	B	606	CLA	CMC-C2C	-2.05	1.46	1.50
28	C	517	DGD	C4E-C5E	-2.05	1.48	1.53
23	c	502	CLA	CMC-C2C	-2.04	1.46	1.50
30	A	413	SQD	O2-C2	-2.04	1.37	1.43
31	I	101	LMG	C4-C5	-2.04	1.48	1.53
23	A	407	CLA	CMC-C2C	-2.04	1.46	1.50
23	b	614	CLA	CMB-C2B	-2.04	1.46	1.50
28	c	517	DGD	O3G-C3G	-2.04	1.40	1.43
28	C	518	DGD	C4E-C5E	-2.04	1.48	1.53
23	B	606	CLA	CMD-C2D	-2.04	1.46	1.50
23	B	603	CLA	MG-NB	-2.04	2.01	2.05
23	c	510	CLA	CMB-C2B	-2.03	1.46	1.50
34	v	201	HEM	CMD-C2D	2.03	1.54	1.50
23	B	615	CLA	CMB-C2B	-2.03	1.46	1.50
23	a	405	CLA	MG-NB	-2.03	2.01	2.05
28	D	409	DGD	O4D-C4D	-2.03	1.37	1.43
23	b	608	CLA	CMB-C2B	-2.03	1.46	1.50
23	b	610	CLA	CMD-C2D	-2.03	1.46	1.50
28	d	409	DGD	O5D-C6D	-2.03	1.40	1.43
28	c	517	DGD	C4D-C5D	-2.03	1.48	1.53
23	c	503	CLA	MG-NB	-2.03	2.01	2.05
31	e	101	LMG	C4-C5	-2.03	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	MG-NB	-2.03	2.01	2.05
23	C	513	CLA	CMB-C2B	-2.03	1.46	1.50
23	b	607	CLA	CMB-C2B	-2.03	1.46	1.50
23	b	605	CLA	CMD-C2D	-2.02	1.46	1.50
23	c	504	CLA	CMB-C2B	-2.02	1.46	1.50
28	b	623	DGD	O4D-C4D	-2.02	1.37	1.43
23	B	613	CLA	CMB-C2B	-2.02	1.46	1.50
23	A	407	CLA	CMD-C2D	-2.02	1.46	1.50
23	B	601	CLA	CMC-C2C	-2.02	1.46	1.50
23	B	601	CLA	MG-NB	-2.02	2.01	2.05
23	b	611	CLA	CMB-C2B	-2.02	1.46	1.50
23	b	605	CLA	MG-NB	-2.02	2.01	2.05
23	C	501	CLA	CMB-C2B	-2.02	1.46	1.50
23	B	601	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	615	CLA	CHC-C1C	2.02	1.42	1.38
23	A	405	CLA	CMB-C2B	-2.02	1.46	1.50
28	b	623	DGD	O1G-C1G	-2.02	1.40	1.45
23	B	607	CLA	CMB-C2B	-2.02	1.46	1.50
23	A	407	CLA	CMB-C2B	-2.01	1.46	1.50
23	B	605	CLA	CMB-C2B	-2.01	1.46	1.50
23	C	511	CLA	CMB-C2B	-2.01	1.46	1.50
34	v	201	HEM	CMC-C2C	2.01	1.54	1.50
23	A	403	CLA	CMB-C2B	-2.01	1.46	1.50
23	c	513	CLA	CMB-C2B	-2.01	1.46	1.50
23	C	509	CLA	CMB-C2B	-2.01	1.46	1.50
23	a	405	CLA	CMD-C2D	-2.01	1.46	1.50
23	c	505	CLA	CMC-C2C	-2.01	1.46	1.50
23	C	506	CLA	CMD-C2D	-2.01	1.46	1.50
23	b	620	CLA	CMD-C2D	-2.01	1.46	1.50
23	B	606	CLA	CHC-C1C	2.01	1.42	1.38
23	C	504	CLA	CMD-C2D	-2.01	1.46	1.50
23	b	615	CLA	CMC-C2C	-2.01	1.46	1.50
30	D	408	SQD	O6-C1	2.01	1.43	1.40
23	B	608	CLA	MG-NB	-2.01	2.01	2.05
34	V	201	HEM	CMC-C2C	2.00	1.54	1.50
23	B	611	CLA	CMC-C2C	-2.00	1.46	1.50
23	c	508	CLA	C3D-C4D	2.00	1.48	1.44
23	a	404	CLA	CMB-C2B	-2.00	1.46	1.50
30	D	408	SQD	O3-C3	-2.00	1.38	1.43
28	C	519	DGD	O6E-C5E	-2.00	1.39	1.44
23	c	502	CLA	C3D-C4D	2.00	1.48	1.44
23	c	512	CLA	C3D-C4D	2.00	1.48	1.44

All (1294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	j	102	BCR	C32-C1-C6	-14.09	88.14	110.24
27	J	102	BCR	C32-C1-C6	-13.79	88.62	110.24
27	J	102	BCR	C32-C1-C31	-9.11	82.55	108.63
27	j	102	BCR	C32-C1-C31	-9.08	82.62	108.63
27	T	102	BCR	C7-C8-C9	-8.97	112.96	126.23
27	B	618	BCR	C7-C8-C9	-8.83	113.18	126.23
27	C	514	BCR	C7-C8-C9	8.49	138.79	126.23
27	c	514	BCR	C7-C8-C9	8.27	138.47	126.23
23	B	607	CLA	C4A-NA-C1A	7.83	110.25	106.68
23	d	402	CLA	C4A-NA-C1A	7.81	110.24	106.68
23	C	511	CLA	C4A-NA-C1A	7.79	110.23	106.68
23	c	505	CLA	C4A-NA-C1A	7.69	110.19	106.68
23	c	509	CLA	C4A-NA-C1A	7.47	110.09	106.68
23	b	618	CLA	C4A-NA-C1A	7.40	110.06	106.68
23	a	406	CLA	C4A-NA-C1A	7.39	110.05	106.68
23	b	617	CLA	C4A-NA-C1A	7.28	110.00	106.68
23	C	512	CLA	C4A-NA-C1A	7.16	109.94	106.68
23	c	504	CLA	C4A-NA-C1A	7.14	109.94	106.68
23	B	605	CLA	C4A-NA-C1A	7.10	109.92	106.68
23	a	404	CLA	C4A-NA-C1A	7.09	109.91	106.68
23	B	601	CLA	C4A-NA-C1A	7.02	109.88	106.68
23	C	505	CLA	C4A-NA-C1A	6.99	109.87	106.68
23	B	603	CLA	C4A-NA-C1A	6.94	109.84	106.68
27	d	405	BCR	C7-C8-C9	-6.89	116.04	126.23
23	c	512	CLA	C4A-NA-C1A	6.88	109.82	106.68
23	B	608	CLA	C4A-NA-C1A	6.87	109.81	106.68
23	b	611	CLA	C4A-NA-C1A	6.86	109.81	106.68
23	c	502	CLA	C4A-NA-C1A	6.82	109.79	106.68
23	b	619	CLA	C4A-NA-C1A	6.77	109.77	106.68
23	b	616	CLA	C4A-NA-C1A	6.76	109.76	106.68
23	c	511	CLA	C4A-NA-C1A	6.75	109.76	106.68
23	b	610	CLA	C4A-NA-C1A	6.75	109.76	106.68
23	B	602	CLA	C4A-NA-C1A	6.74	109.76	106.68
23	B	604	CLA	C4A-NA-C1A	6.73	109.75	106.68
23	b	608	CLA	C4A-NA-C1A	6.71	109.74	106.68
23	C	504	CLA	C4A-NA-C1A	6.70	109.74	106.68
23	C	506	CLA	C4A-NA-C1A	6.70	109.74	106.68
23	B	609	CLA	C4A-NA-C1A	6.70	109.73	106.68
23	c	513	CLA	C4A-NA-C1A	6.69	109.73	106.68
23	C	509	CLA	C4A-NA-C1A	6.67	109.72	106.68
23	c	506	CLA	C4A-NA-C1A	6.67	109.72	106.68
23	a	409	CLA	C4A-NA-C1A	6.65	109.71	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	501	CLA	C4A-NA-C1A	6.65	109.71	106.68
27	j	102	BCR	C31-C1-C6	6.64	120.66	110.24
23	C	503	CLA	C4A-NA-C1A	6.64	109.71	106.68
23	b	606	CLA	C4A-NA-C1A	6.64	109.71	106.68
23	C	513	CLA	C4A-NA-C1A	6.63	109.70	106.68
23	d	403	CLA	C4A-NA-C1A	6.62	109.70	106.68
27	D	405	BCR	C7-C8-C9	-6.59	116.49	126.23
23	C	508	CLA	C4A-NA-C1A	6.58	109.68	106.68
23	C	501	CLA	C4A-NA-C1A	6.57	109.68	106.68
27	J	102	BCR	C31-C1-C6	6.57	120.55	110.24
23	C	502	CLA	C4A-NA-C1A	6.57	109.68	106.68
23	c	508	CLA	C4A-NA-C1A	6.57	109.68	106.68
24	D	402	PHO	C4D-CHA-CBD	-6.54	105.32	108.45
23	b	609	CLA	C4A-NA-C1A	6.48	109.63	106.68
24	A	406	PHO	C4D-CHA-CBD	-6.48	105.35	108.45
23	b	607	CLA	C4A-NA-C1A	6.45	109.62	106.68
23	b	620	CLA	C4A-NA-C1A	6.43	109.61	106.68
23	c	507	CLA	C4A-NA-C1A	6.39	109.59	106.68
23	b	615	CLA	C4A-NA-C1A	6.37	109.59	106.68
23	A	407	CLA	C4A-NA-C1A	6.35	109.58	106.68
23	B	615	CLA	C4A-NA-C1A	6.33	109.57	106.68
23	B	612	CLA	C4A-NA-C1A	6.33	109.56	106.68
23	B	614	CLA	C4A-NA-C1A	6.30	109.55	106.68
23	A	403	CLA	C4A-NA-C1A	6.28	109.55	106.68
30	D	408	SQD	O6-C1-C2	6.28	117.82	108.27
27	J	102	BCR	C15-C14-C13	-6.27	118.48	127.28
23	b	605	CLA	C4A-NA-C1A	6.22	109.52	106.68
23	C	507	CLA	C4A-NA-C1A	6.22	109.52	106.68
23	B	613	CLA	C4A-NA-C1A	6.17	109.50	106.68
23	c	503	CLA	C4A-NA-C1A	6.17	109.50	106.68
27	b	622	BCR	C24-C23-C22	-6.17	117.11	126.23
23	B	611	CLA	C4A-NA-C1A	6.16	109.49	106.68
23	D	403	CLA	C4A-NA-C1A	6.15	109.48	106.68
23	A	404	CLA	C4A-NA-C1A	6.11	109.47	106.68
23	D	401	CLA	C4A-NA-C1A	6.08	109.45	106.68
30	d	408	SQD	O6-C1-C2	6.03	117.43	108.27
23	b	614	CLA	C4A-NA-C1A	6.03	109.43	106.68
34	v	201	HEM	C4D-ND-C1D	5.99	112.30	105.21
24	a	407	PHO	C4D-CHA-CBD	-5.96	105.60	108.45
23	B	610	CLA	C4A-NA-C1A	5.90	109.37	106.68
23	B	616	CLA	C4A-NA-C1A	5.83	109.34	106.68
23	b	613	CLA	C4A-NA-C1A	5.82	109.33	106.68

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	5.81	109.33	106.68
23	B	606	CLA	C4A-NA-C1A	5.68	109.27	106.68
27	B	618	BCR	C11-C10-C9	-5.68	119.32	127.28
27	J	102	BCR	C32-C1-C2	-5.66	87.22	108.95
23	c	510	CLA	C4A-NA-C1A	5.64	109.25	106.68
27	c	514	BCR	C15-C14-C13	-5.62	119.40	127.28
23	a	405	CLA	C4A-NA-C1A	5.61	109.24	106.68
27	j	102	BCR	C32-C1-C2	-5.59	87.49	108.95
28	c	518	DGD	C3G-O3G-C1D	5.54	125.67	113.80
27	j	102	BCR	C15-C14-C13	-5.52	119.54	127.28
27	J	102	BCR	C28-C27-C26	-5.51	104.23	114.06
27	B	620	BCR	C24-C23-C22	-5.49	118.12	126.23
27	z	101	BCR	C15-C14-C13	-5.46	119.62	127.28
28	D	409	DGD	O3G-C1D-C2D	5.46	116.57	108.27
28	A	411	DGD	C3G-O3G-C1D	5.43	125.44	113.80
24	a	408	PHO	C4D-CHA-CBD	-5.39	105.87	108.45
23	A	405	CLA	C4A-NA-C1A	5.39	109.14	106.68
34	f	101	HEM	C4D-ND-C1D	5.35	111.54	105.21
27	b	622	BCR	C3-C4-C5	-5.34	104.54	114.06
34	V	201	HEM	C4D-ND-C1D	5.33	111.51	105.21
28	a	413	DGD	C3G-O3G-C1D	5.27	125.08	113.80
28	d	409	DGD	O3G-C1D-C2D	5.26	116.26	108.27
27	j	102	BCR	C28-C27-C26	-5.24	104.72	114.06
27	D	405	BCR	C11-C10-C9	-5.16	120.04	127.28
27	j	102	BCR	C20-C21-C22	-5.14	120.07	127.28
27	a	412	BCR	C33-C5-C6	-5.13	118.88	124.48
34	F	101	HEM	C4D-ND-C1D	5.13	111.28	105.21
30	D	408	SQD	C44-O6-C1	5.12	124.76	113.80
23	C	510	CLA	C4A-NA-C1A	5.09	109.00	106.68
27	D	405	BCR	C28-C27-C26	-5.08	105.00	114.06
27	C	516	BCR	C7-C8-C9	-5.05	118.76	126.23
27	j	102	BCR	C24-C23-C22	-5.03	118.79	126.23
27	j	102	BCR	C11-C10-C9	-5.03	120.22	127.28
27	J	102	BCR	C20-C21-C22	-5.03	120.23	127.28
28	C	519	DGD	C3G-O3G-C1D	5.02	124.56	113.80
27	c	514	BCR	C33-C5-C6	-4.97	119.07	124.48
27	y	101	BCR	C15-C14-C13	-4.96	120.32	127.28
27	d	405	BCR	C28-C27-C26	-4.94	105.24	114.06
27	C	515	BCR	C15-C14-C13	-4.86	120.47	127.28
30	d	408	SQD	C44-O6-C1	4.84	124.17	113.80
27	C	514	BCR	C33-C5-C6	-4.83	119.21	124.48
27	C	514	BCR	C8-C7-C6	4.82	139.88	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	618	BCR	C3-C4-C5	-4.82	105.46	114.06
27	B	620	BCR	C3-C4-C5	-4.79	105.51	114.06
27	B	620	BCR	C16-C17-C18	-4.77	120.59	127.28
27	T	102	BCR	C28-C27-C26	-4.76	105.58	114.06
27	J	102	BCR	C24-C23-C22	-4.73	119.23	126.23
27	c	515	BCR	C7-C8-C9	-4.73	119.24	126.23
27	A	410	BCR	C33-C5-C6	-4.72	119.33	124.48
25	J	101	PL9	C7-C3-C4	4.72	120.80	116.91
27	T	102	BCR	C11-C10-C9	-4.70	120.68	127.28
27	k	102	BCR	C15-C14-C13	-4.69	120.70	127.28
27	T	102	BCR	C3-C4-C5	-4.69	105.70	114.06
27	b	622	BCR	C16-C17-C18	-4.62	120.80	127.28
27	J	102	BCR	C11-C10-C9	-4.60	120.82	127.28
27	c	514	BCR	C8-C7-C6	4.56	139.18	127.00
27	C	514	BCR	C15-C14-C13	-4.53	120.93	127.28
27	k	102	BCR	C24-C23-C22	-4.53	119.54	126.23
27	b	621	BCR	C15-C14-C13	-4.51	120.96	127.28
27	y	101	BCR	C7-C8-C9	-4.49	119.59	126.23
27	c	515	BCR	C15-C14-C13	-4.49	120.99	127.28
27	y	101	BCR	C16-C17-C18	-4.47	121.01	127.28
24	a	407	PHO	C2B-C1B-NB	-4.47	106.20	109.43
27	J	102	BCR	C16-C17-C18	-4.46	121.02	127.28
27	B	619	BCR	C20-C21-C22	-4.46	121.03	127.28
31	d	407	LMG	O1-C1-C2	4.45	115.04	108.27
27	B	617	BCR	C16-C17-C18	-4.45	121.03	127.28
25	j	101	PL9	C7-C3-C4	4.45	120.58	116.91
27	B	620	BCR	C15-C14-C13	-4.44	121.06	127.28
27	B	619	BCR	C28-C27-C26	-4.36	106.29	114.06
27	C	516	BCR	C15-C14-C13	-4.34	121.19	127.28
27	j	102	BCR	C7-C8-C9	-4.34	119.81	126.23
27	k	102	BCR	C38-C26-C25	-4.32	119.77	124.48
30	d	408	SQD	O47-C7-C8	4.32	120.83	111.48
27	H	101	BCR	C33-C5-C6	-4.31	119.78	124.48
27	b	621	BCR	C7-C8-C9	-4.30	119.87	126.23
27	B	620	BCR	C38-C26-C25	-4.29	119.80	124.48
27	b	621	BCR	C28-C27-C26	-4.27	106.44	114.06
27	b	622	BCR	C7-C8-C9	-4.26	119.94	126.23
27	a	412	BCR	C16-C17-C18	-4.25	121.31	127.28
27	d	405	BCR	C33-C5-C6	-4.25	119.85	124.48
27	B	618	BCR	C28-C27-C26	-4.25	106.48	114.06
27	D	405	BCR	C33-C5-C6	-4.24	119.86	124.48
27	C	515	BCR	C16-C17-C18	-4.23	121.34	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	405	BCR	C16-C17-C18	-4.23	121.34	127.28
28	C	519	DGD	C1D-O6D-C5D	-4.22	105.49	113.72
27	d	405	BCR	C15-C14-C13	-4.21	121.37	127.28
27	d	405	BCR	C11-C10-C9	-4.21	121.37	127.28
28	c	518	DGD	C1D-O6D-C5D	-4.21	105.50	113.72
24	D	402	PHO	C2B-C1B-NB	-4.20	106.39	109.43
31	a	416	LMG	C7-O1-C1	4.19	122.77	113.80
27	c	515	BCR	C16-C17-C18	-4.18	121.41	127.28
27	A	410	BCR	C15-C14-C13	-4.17	121.42	127.28
27	T	101	BCR	C24-C23-C22	-4.15	120.10	126.23
30	b	601	SQD	O7-S-C6	4.14	112.94	106.76
27	z	101	BCR	C16-C17-C18	-4.14	121.47	127.28
27	b	621	BCR	C20-C21-C22	-4.13	121.48	127.28
27	C	514	BCR	C3-C4-C5	-4.12	106.70	114.06
27	a	412	BCR	C24-C23-C22	-4.12	120.14	126.23
27	B	617	BCR	C7-C8-C9	-4.12	120.14	126.23
28	B	627	DGD	O5D-C1E-C2E	4.12	114.53	108.27
31	D	407	LMG	O1-C1-C2	4.09	114.49	108.27
27	B	617	BCR	C15-C14-C13	-4.09	121.55	127.28
27	a	412	BCR	C38-C26-C25	-4.08	120.03	124.48
27	k	102	BCR	C7-C8-C9	-4.08	120.20	126.23
28	A	411	DGD	O2G-C1B-C2B	4.07	120.29	111.48
27	c	515	BCR	C28-C27-C26	-4.07	106.80	114.06
27	b	622	BCR	C38-C26-C25	-4.07	120.04	124.48
27	B	617	BCR	C24-C23-C22	-4.07	120.22	126.23
27	b	622	BCR	C15-C14-C13	-4.07	121.58	127.28
27	D	405	BCR	C15-C14-C13	-4.06	121.59	127.28
30	f	102	SQD	O9-S-O7	-4.05	100.65	113.82
25	d	404	PL9	C7-C3-C4	4.05	120.24	116.91
27	a	412	BCR	C15-C14-C13	-4.05	121.61	127.28
31	B	623	LMG	O7-C10-C11	4.04	120.22	111.48
30	a	415	SQD	O9-S-O7	-4.03	100.72	113.82
27	T	101	BCR	C15-C14-C13	-4.02	121.64	127.28
30	A	413	SQD	O9-S-O7	-4.02	100.74	113.82
30	F	102	SQD	O9-S-O7	-4.02	100.75	113.82
30	D	408	SQD	O47-C7-C8	4.02	120.18	111.48
27	T	101	BCR	C33-C5-C6	-4.02	120.10	124.48
27	c	514	BCR	C11-C10-C9	-4.01	121.66	127.28
27	h	101	BCR	C33-C5-C6	-4.01	120.11	124.48
27	B	620	BCR	C20-C21-C22	-4.00	121.67	127.28
28	a	413	DGD	O2G-C1B-C2B	4.00	120.13	111.48
30	F	102	SQD	O47-C7-C8	4.00	120.12	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	624	LMG	O7-C10-C11	3.99	120.12	111.48
30	f	102	SQD	O7-S-C6	3.99	112.71	106.76
31	m	102	LMG	O7-C10-C11	3.98	120.10	111.48
30	D	408	SQD	O9-S-O7	-3.98	100.87	113.82
27	T	101	BCR	C20-C21-C22	-3.98	121.69	127.28
31	M	101	LMG	O7-C10-C11	3.98	120.09	111.48
27	C	515	BCR	C24-C23-C22	-3.98	120.35	126.23
27	k	102	BCR	C16-C17-C18	-3.98	121.70	127.28
27	B	619	BCR	C15-C14-C13	-3.97	121.70	127.28
27	y	101	BCR	C3-C4-C5	-3.96	106.99	114.06
31	B	622	LMG	O7-C10-C11	3.95	120.03	111.48
30	d	408	SQD	O9-S-O7	-3.95	100.99	113.82
27	h	101	BCR	C16-C17-C18	-3.94	121.75	127.28
27	J	102	BCR	C7-C8-C9	-3.92	120.44	126.23
27	b	622	BCR	C11-C10-C9	-3.92	121.79	127.28
27	d	405	BCR	C16-C17-C18	-3.92	121.79	127.28
23	a	405	CLA	C1-C2-C3	-3.91	119.79	126.20
27	b	621	BCR	C24-C23-C22	-3.91	120.45	126.23
27	D	405	BCR	C24-C23-C22	-3.88	120.49	126.23
28	A	411	DGD	C1D-O6D-C5D	-3.88	106.15	113.72
31	A	414	LMG	O7-C10-C11	3.87	119.86	111.48
28	d	409	DGD	O2D-C2D-C1D	3.87	119.30	110.08
30	f	102	SQD	O47-C7-C8	3.87	119.85	111.48
27	y	101	BCR	C38-C26-C25	-3.86	120.27	124.48
27	j	102	BCR	C16-C17-C18	-3.86	121.86	127.28
31	a	416	LMG	O7-C10-C11	3.86	119.82	111.48
25	A	408	PL9	C7-C3-C4	3.85	120.08	116.91
27	B	617	BCR	C33-C5-C6	-3.85	120.28	124.48
30	B	626	SQD	O7-S-C6	3.85	112.50	106.76
30	d	408	SQD	O9-S-C6	3.84	112.49	106.76
27	C	516	BCR	C28-C27-C26	-3.84	107.21	114.06
27	J	102	BCR	C2-C1-C6	3.84	116.01	110.44
27	b	622	BCR	C4-C5-C6	-3.83	117.53	122.70
25	a	410	PL9	C7-C3-C4	3.82	120.06	116.91
31	m	102	LMG	C3-C4-C5	3.82	117.16	110.23
31	d	406	LMG	O7-C10-C11	3.82	119.74	111.48
30	b	601	SQD	O9-S-O7	-3.81	101.43	113.82
29	A	415	LHG	O7-C7-C8	3.81	119.72	111.48
27	C	515	BCR	C33-C5-C6	-3.81	120.33	124.48
30	F	102	SQD	C1-O5-C5	3.81	121.16	113.72
31	C	521	LMG	O7-C10-C11	3.80	119.70	111.48
28	C	519	DGD	C2G-O2G-C1B	3.80	126.89	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	517	DGD	O5D-C6D-C5D	-3.79	100.87	109.42
27	a	412	BCR	C3-C4-C5	-3.79	107.30	114.06
30	A	417	SQD	O47-C7-C8	3.78	119.67	111.48
27	z	101	BCR	C24-C23-C22	-3.78	120.65	126.23
27	j	102	BCR	C2-C1-C6	3.77	115.92	110.44
30	A	417	SQD	O5-C5-C4	3.76	116.47	109.70
27	A	410	BCR	C16-C17-C18	-3.76	122.01	127.28
27	h	101	BCR	C15-C14-C13	-3.75	122.02	127.28
27	c	515	BCR	C11-C10-C9	-3.74	122.03	127.28
27	C	516	BCR	C38-C26-C25	-3.74	120.40	124.48
30	a	401	SQD	O5-C5-C4	3.73	116.43	109.70
27	H	101	BCR	C24-C23-C22	-3.73	120.72	126.23
31	D	406	LMG	O7-C10-C11	3.72	119.54	111.48
24	A	406	PHO	C2B-C1B-NB	-3.72	106.74	109.43
30	B	626	SQD	O9-S-O7	-3.72	101.72	113.82
30	A	413	SQD	C1-O5-C5	3.72	120.98	113.72
30	d	408	SQD	C1-O5-C5	3.71	120.97	113.72
31	b	625	LMG	O7-C10-C11	3.71	119.51	111.48
30	D	408	SQD	C1-O5-C5	3.71	120.97	113.72
27	A	410	BCR	C3-C4-C5	-3.71	107.44	114.06
27	c	514	BCR	C3-C4-C5	-3.71	107.44	114.06
28	B	627	DGD	O2G-C1B-C2B	3.70	119.49	111.48
31	a	402	LMG	O7-C10-C11	3.70	119.49	111.48
29	a	417	LHG	O7-C7-C8	3.69	119.46	111.48
31	A	418	LMG	O7-C10-C11	3.68	119.45	111.48
27	d	405	BCR	C24-C23-C22	-3.68	120.79	126.23
30	a	401	SQD	O47-C7-C8	3.68	119.44	111.48
27	b	621	BCR	C3-C4-C5	-3.68	107.50	114.06
28	c	518	DGD	C2G-O2G-C1B	3.67	126.57	117.80
31	d	407	LMG	C1-O6-C5	-3.66	106.56	113.72
28	c	517	DGD	O2G-C1B-C2B	3.66	119.41	111.48
27	C	516	BCR	C16-C17-C18	-3.64	122.17	127.28
31	c	519	LMG	O7-C10-C11	3.64	119.35	111.48
30	a	401	SQD	O9-S-O7	-3.63	102.02	113.82
28	D	409	DGD	O2D-C2D-C1D	3.62	118.71	110.08
25	a	410	PL9	C35-C34-C36	3.62	121.52	115.23
27	B	620	BCR	C4-C5-C6	-3.62	117.81	122.70
30	a	401	SQD	C1-O5-C5	3.62	120.79	113.72
27	A	410	BCR	C38-C26-C25	-3.61	120.54	124.48
30	f	102	SQD	C1-O5-C5	3.59	120.73	113.72
27	B	620	BCR	C11-C10-C9	-3.58	122.25	127.28
30	a	415	SQD	O47-C7-C8	3.58	119.22	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	CLA	C1-C2-C3	-3.57	120.34	126.20
31	m	102	LMG	C1-O6-C5	-3.57	106.75	113.72
23	A	405	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
28	C	518	DGD	O2G-C1B-C2B	3.56	119.17	111.48
27	k	102	BCR	C3-C4-C5	-3.55	107.72	114.06
27	z	101	BCR	C3-C4-C5	-3.55	107.73	114.06
30	A	417	SQD	C1-O5-C5	3.54	120.64	113.72
31	C	520	LMG	O7-C10-C11	3.54	119.14	111.48
27	C	514	BCR	C11-C10-C9	-3.54	122.32	127.28
27	h	101	BCR	C24-C23-C22	-3.54	121.00	126.23
30	a	401	SQD	O6-C1-C2	3.54	113.64	108.27
27	C	515	BCR	C3-C4-C5	-3.53	107.76	114.06
27	k	102	BCR	C20-C21-C22	-3.53	122.33	127.28
28	C	518	DGD	O5D-C6D-C5D	-3.53	101.47	109.42
25	a	410	PL9	C25-C24-C26	3.53	121.35	115.23
27	c	514	BCR	C16-C17-C18	-3.51	122.35	127.28
27	C	516	BCR	C33-C5-C6	-3.51	120.65	124.48
25	d	404	PL9	C25-C24-C26	3.51	121.31	115.23
25	d	404	PL9	C7-C3-C2	-3.50	119.26	123.39
27	z	101	BCR	C33-C5-C6	-3.50	120.67	124.48
30	A	417	SQD	O9-S-O7	-3.50	102.45	113.82
28	B	627	DGD	C3D-C4D-C5D	3.49	116.57	110.23
23	B	614	CLA	C3B-C4B-NB	-3.48	107.42	110.53
23	c	510	CLA	C3B-C4B-NB	-3.48	107.42	110.53
27	c	515	BCR	C33-C5-C6	-3.48	120.69	124.48
27	j	102	BCR	C29-C30-C25	3.47	115.47	110.44
27	c	514	BCR	C7-C6-C5	-3.46	113.58	121.56
27	B	617	BCR	C11-C10-C9	-3.45	122.44	127.28
27	C	515	BCR	C11-C10-C9	-3.45	122.44	127.28
27	H	101	BCR	C16-C17-C18	-3.45	122.44	127.28
27	A	410	BCR	C20-C21-C22	-3.45	122.44	127.28
30	a	401	SQD	C44-O6-C1	3.45	121.19	113.80
30	D	408	SQD	O9-S-C6	3.45	111.90	106.76
27	B	618	BCR	C38-C26-C25	-3.44	120.73	124.48
28	D	409	DGD	C3G-O3G-C1D	3.44	121.17	113.80
27	c	515	BCR	C38-C26-C25	-3.44	120.73	124.48
24	A	406	PHO	O2D-CGD-O1D	-3.43	117.17	123.85
23	B	606	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
34	f	101	HEM	C3B-C4B-NB	-3.42	107.01	109.47
27	J	102	BCR	C29-C30-C25	3.42	115.40	110.44
28	b	623	DGD	C1D-O6D-C5D	-3.41	107.05	113.72
30	a	415	SQD	C1-O5-C5	3.41	120.39	113.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	622	BCR	C20-C21-C22	-3.41	122.50	127.28
27	J	102	BCR	C31-C1-C2	3.41	122.03	108.95
30	F	102	SQD	O7-S-C6	3.40	111.83	106.76
27	j	102	BCR	C31-C1-C2	3.40	121.99	108.95
30	A	413	SQD	O9-S-C6	3.40	111.83	106.76
23	b	612	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
23	C	504	CLA	C3B-C4B-NB	-3.39	107.50	110.53
27	T	102	BCR	C38-C26-C25	-3.39	120.79	124.48
31	D	406	LMG	O8-C28-C29	3.39	122.16	111.83
29	a	414	LHG	O7-C7-C8	3.38	118.79	111.48
25	A	408	PL9	C25-C24-C26	3.38	121.09	115.23
27	b	621	BCR	C16-C17-C18	-3.37	122.55	127.28
31	k	103	LMG	O7-C10-C11	3.37	118.77	111.48
23	B	607	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
30	A	417	SQD	O5-C1-C2	3.37	117.29	110.37
28	b	602	DGD	O5D-C1E-C2E	3.37	113.39	108.27
30	F	102	SQD	O9-S-C6	3.36	111.77	106.76
27	A	410	BCR	C11-C10-C9	-3.36	122.57	127.28
27	C	514	BCR	C1-C6-C7	3.36	124.76	115.65
27	C	514	BCR	C20-C21-C22	-3.36	122.57	127.28
27	T	101	BCR	C7-C8-C9	-3.35	121.27	126.23
27	j	102	BCR	C27-C26-C25	-3.35	118.17	122.70
29	A	412	LHG	O7-C7-C8	3.35	118.73	111.48
31	M	101	LMG	C3-C4-C5	3.35	116.30	110.23
25	D	404	PL9	C22-C23-C24	-3.35	119.96	127.62
28	b	602	DGD	C3D-C4D-C5D	3.35	116.30	110.23
27	k	102	BCR	C33-C5-C6	-3.33	120.84	124.48
31	b	625	LMG	O1-C1-C2	3.33	113.33	108.27
28	a	413	DGD	O6D-C5D-C6D	3.33	113.29	106.69
27	C	514	BCR	C7-C6-C5	-3.33	113.90	121.56
28	B	621	DGD	C1D-O6D-C5D	-3.32	107.23	113.72
27	c	514	BCR	C20-C21-C22	-3.32	122.62	127.28
31	A	414	LMG	C1-O6-C5	-3.32	107.25	113.72
27	B	619	BCR	C3-C4-C5	-3.31	108.15	114.06
24	a	408	PHO	C2B-C1B-NB	-3.31	107.04	109.43
28	C	517	DGD	O5D-C1E-C2E	3.31	113.29	108.27
30	a	415	SQD	O7-S-C6	3.30	111.68	106.76
25	D	404	PL9	C35-C34-C36	3.29	120.94	115.23
27	c	514	BCR	C1-C6-C7	3.29	124.58	115.65
31	M	101	LMG	C1-O6-C5	-3.29	107.30	113.72
23	D	403	CLA	C3B-C4B-NB	-3.29	107.60	110.53
25	J	101	PL9	C7-C3-C2	-3.28	119.52	123.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	y	101	BCR	C24-C23-C22	-3.28	121.39	126.23
27	T	101	BCR	C11-C10-C9	-3.28	122.69	127.28
31	k	103	LMG	O8-C28-C29	3.27	121.82	111.83
23	b	614	CLA	C3B-C4B-NB	-3.27	107.61	110.53
30	B	626	SQD	C44-O6-C1	3.27	120.81	113.80
25	j	101	PL9	C25-C24-C26	3.27	120.90	115.23
23	B	610	CLA	C3B-C4B-NB	-3.26	107.62	110.53
30	a	401	SQD	O5-C1-C2	3.26	117.07	110.37
27	A	410	BCR	C24-C23-C22	-3.26	121.41	126.23
25	D	404	PL9	C7-C3-C4	3.26	119.60	116.91
30	b	601	SQD	O9-S-C6	3.26	111.62	106.76
34	F	101	HEM	C3B-C2B-C1B	3.26	108.86	106.41
28	d	409	DGD	O5D-C1E-C2E	3.26	113.22	108.27
23	d	403	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
27	c	515	BCR	C3-C4-C5	-3.25	108.26	114.06
30	a	415	SQD	O9-S-C6	3.25	111.61	106.76
28	A	411	DGD	C3G-C2G-C1G	-3.25	104.21	111.78
27	T	101	BCR	C16-C17-C18	-3.25	122.72	127.28
31	C	521	LMG	O8-C28-C29	3.24	121.71	111.83
31	m	102	LMG	C6-C5-C4	-3.24	105.07	113.02
23	b	607	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
28	c	516	DGD	O2G-C1B-C2B	3.24	118.48	111.48
31	a	402	LMG	C3-C4-C5	3.23	116.09	110.23
27	B	619	BCR	C16-C17-C18	-3.23	122.75	127.28
24	A	406	PHO	O1D-CGD-CBD	3.23	129.62	124.72
28	C	519	DGD	O5D-C1E-C2E	3.23	113.17	108.27
23	D	401	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
27	J	102	BCR	C27-C26-C25	-3.22	118.36	122.70
27	C	516	BCR	C20-C21-C22	-3.21	122.77	127.28
23	A	405	CLA	C3B-C4B-NB	-3.21	107.66	110.53
30	A	417	SQD	C44-O6-C1	3.21	120.68	113.80
30	A	413	SQD	O47-C7-C8	3.21	118.42	111.48
27	H	101	BCR	C15-C14-C13	-3.20	122.78	127.28
27	z	101	BCR	C20-C21-C22	-3.20	122.79	127.28
23	b	618	CLA	C3B-C4B-NB	-3.20	107.68	110.53
23	c	512	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
31	B	623	LMG	O1-C1-C2	3.19	113.12	108.27
27	C	516	BCR	C3-C4-C5	-3.19	108.37	114.06
27	B	618	BCR	C4-C5-C6	-3.19	118.40	122.70
24	a	408	PHO	O1D-CGD-CBD	3.19	129.56	124.72
23	A	404	CLA	C3B-C4B-NB	-3.18	107.69	110.53
31	D	407	LMG	C7-O1-C1	3.18	120.62	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	609	CLA	C3B-C4B-NB	-3.18	107.69	110.53
25	d	404	PL9	C37-C38-C39	-3.18	120.35	127.62
24	a	407	PHO	O1D-CGD-CBD	3.18	129.54	124.72
23	c	502	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
27	C	514	BCR	C28-C27-C26	-3.17	108.40	114.06
25	j	101	PL9	C7-C3-C2	-3.17	119.66	123.39
28	B	627	DGD	C3G-O3G-C1D	3.17	120.58	113.80
25	D	404	PL9	C12-C13-C14	-3.16	120.38	127.62
31	M	101	LMG	C6-C5-C4	-3.16	105.25	113.02
30	A	417	SQD	O7-S-C6	3.16	111.47	106.76
25	d	404	PL9	C35-C34-C36	3.16	120.71	115.23
25	A	408	PL9	C35-C34-C36	3.16	120.71	115.23
28	C	517	DGD	O2G-C1B-C2B	3.16	118.31	111.48
30	a	401	SQD	O7-S-C6	3.16	111.47	106.76
23	C	507	CLA	O2D-CGD-O1D	-3.16	117.71	123.85
27	B	618	BCR	C2-C1-C6	3.15	115.02	110.44
30	b	601	SQD	C44-O6-C1	3.15	120.55	113.80
31	A	414	LMG	O8-C28-C29	3.15	121.43	111.83
25	a	410	PL9	C22-C23-C24	-3.15	120.42	127.62
27	B	620	BCR	C2-C1-C6	3.14	115.01	110.44
27	T	102	BCR	C2-C1-C6	3.14	115.00	110.44
23	A	405	CLA	C1-C2-C3	-3.14	121.06	126.20
27	y	101	BCR	C33-C5-C6	-3.14	121.06	124.48
24	D	402	PHO	O1D-CGD-CBD	3.13	129.47	124.72
23	C	513	CLA	C3B-C4B-NB	-3.13	107.73	110.53
23	B	612	CLA	C3B-C4B-NB	-3.13	107.73	110.53
23	c	503	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
31	A	414	LMG	C7-O1-C1	3.12	120.50	113.80
30	d	408	SQD	O5-C5-C4	3.12	115.33	109.70
25	d	404	PL9	C22-C23-C24	-3.12	120.47	127.62
23	a	406	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
23	C	511	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
28	c	517	DGD	O3G-C1D-C2D	3.12	113.01	108.27
31	C	520	LMG	O8-C28-C29	3.11	121.33	111.83
30	D	408	SQD	O5-C5-C4	3.11	115.31	109.70
27	H	101	BCR	C20-C21-C22	-3.11	122.92	127.28
30	a	401	SQD	C1-C2-C3	3.10	116.54	110.01
31	c	519	LMG	C1-O6-C5	-3.10	107.66	113.72
31	d	407	LMG	O7-C10-C11	3.10	118.19	111.48
27	h	101	BCR	C10-C11-C12	-3.10	114.22	123.20
25	d	404	PL9	C7-C8-C9	-3.10	121.49	126.83
23	c	502	CLA	C3B-C4B-NB	-3.10	107.76	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406	CLA	C1-C2-C3	-3.10	121.12	126.20
27	B	620	BCR	C7-C8-C9	-3.09	121.66	126.23
31	B	623	LMG	O8-C28-C29	3.09	121.26	111.83
25	D	404	PL9	C37-C38-C39	-3.09	120.55	127.62
23	b	612	CLA	C3B-C4B-NB	-3.09	107.77	110.53
23	C	510	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
27	b	621	BCR	C11-C10-C9	-3.09	122.95	127.28
23	c	504	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
28	a	413	DGD	C1D-O6D-C5D	-3.08	107.70	113.72
27	H	101	BCR	C8-C7-C6	-3.08	118.77	127.00
27	B	619	BCR	C33-C5-C6	-3.08	121.12	124.48
34	f	101	HEM	C3B-C2B-C1B	3.07	108.72	106.41
23	c	501	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
31	c	519	LMG	O8-C28-C29	3.06	121.18	111.83
23	b	605	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
27	B	617	BCR	C38-C26-C25	-3.06	121.15	124.48
27	C	514	BCR	C38-C26-C25	-3.06	121.15	124.48
28	A	411	DGD	O6D-C5D-C6D	3.05	112.75	106.69
31	D	407	LMG	C1-O6-C5	-3.05	107.77	113.72
23	c	510	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
31	d	406	LMG	O8-C28-C29	3.04	121.12	111.83
23	B	607	CLA	CHB-C4A-NA	3.04	128.78	124.40
31	E	101	LMG	C7-O1-C1	3.03	120.30	113.80
23	B	604	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
23	c	506	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
31	b	625	LMG	O8-C28-C29	3.03	121.07	111.83
25	J	101	PL9	C25-C24-C26	3.03	120.48	115.23
23	C	505	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
28	c	518	DGD	O1G-C1A-C2A	3.02	121.05	111.83
28	B	621	DGD	O3D-C3D-C4D	3.02	117.50	110.38
31	i	101	LMG	O7-C10-C11	3.01	118.00	111.48
31	C	520	LMG	C1-O6-C5	-3.01	107.83	113.72
31	D	407	LMG	O7-C10-C11	3.01	118.00	111.48
25	D	404	PL9	C25-C24-C26	3.01	120.45	115.23
25	A	408	PL9	C22-C23-C24	-3.01	120.74	127.62
27	b	622	BCR	C2-C1-C6	3.00	114.80	110.44
27	d	405	BCR	C29-C30-C25	3.00	114.80	110.44
27	c	514	BCR	C35-C13-C14	-3.00	117.96	122.82
27	B	619	BCR	C11-C10-C9	-3.00	123.07	127.28
23	A	403	CLA	C3B-C4B-NB	-3.00	107.86	110.53
30	A	413	SQD	O7-S-C6	2.99	111.23	106.76
27	C	515	BCR	C20-C21-C22	-2.99	123.08	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	515	BCR	C29-C30-C25	2.99	114.78	110.44
28	d	409	DGD	C3G-O3G-C1D	2.98	120.19	113.80
34	F	101	HEM	C3B-C4B-NB	-2.98	107.33	109.47
23	B	604	CLA	C3B-C4B-NB	-2.98	107.87	110.53
23	B	616	CLA	C3B-C4B-NB	-2.98	107.87	110.53
31	A	418	LMG	C3-C4-C5	2.98	115.63	110.23
24	a	407	PHO	O2D-CGD-O1D	-2.98	118.05	123.85
31	D	406	LMG	C7-O1-C1	2.97	120.17	113.80
31	a	416	LMG	O8-C28-C29	2.97	120.90	111.83
31	a	402	LMG	C6-C5-C4	-2.97	105.72	113.02
23	c	511	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
23	b	610	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
31	d	407	LMG	O8-C28-C29	2.96	120.87	111.83
27	T	102	BCR	C29-C30-C25	2.96	114.74	110.44
27	c	514	BCR	C28-C27-C26	-2.96	108.78	114.06
31	e	101	LMG	C7-O1-C1	2.95	120.13	113.80
23	C	510	CLA	C3B-C4B-NB	-2.95	107.90	110.53
27	C	515	BCR	C15-C16-C17	-2.95	117.49	123.52
23	C	507	CLA	C3B-C4B-NB	-2.95	107.90	110.53
31	a	402	LMG	C7-O1-C1	2.94	120.11	113.80
28	C	519	DGD	O6D-C5D-C6D	2.94	112.53	106.69
31	I	101	LMG	O7-C10-C11	2.94	117.84	111.48
28	C	519	DGD	O1G-C1A-C2A	2.94	120.80	111.83
27	h	101	BCR	C20-C21-C22	-2.93	123.17	127.28
23	b	619	CLA	C3B-C4B-NB	-2.93	107.92	110.53
27	C	516	BCR	C29-C30-C25	2.93	114.69	110.44
27	b	621	BCR	C33-C5-C6	-2.92	121.29	124.48
25	a	410	PL9	C7-C3-C2	-2.92	119.94	123.39
31	A	418	LMG	O8-C28-C29	2.92	120.74	111.83
27	B	619	BCR	C24-C23-C22	-2.92	121.92	126.23
23	c	513	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
31	e	101	LMG	O8-C28-C29	2.91	120.72	111.83
23	b	613	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
24	a	408	PHO	O2D-CGD-O1D	-2.91	118.18	123.85
23	C	510	CLA	C1-C2-C3	-2.90	121.44	126.20
31	A	418	LMG	C7-O1-C1	2.90	120.02	113.80
30	A	417	SQD	C1-C2-C3	2.90	116.12	110.01
23	b	615	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
27	j	102	BCR	C33-C5-C6	-2.90	121.32	124.48
30	f	102	SQD	C44-O6-C1	2.90	120.01	113.80
27	H	101	BCR	C10-C11-C12	-2.90	114.80	123.20
28	A	411	DGD	C4D-C3D-C2D	-2.90	105.74	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	624	LMG	O8-C28-C29	2.89	120.66	111.83
27	c	515	BCR	C20-C21-C22	-2.89	123.22	127.28
23	b	606	CLA	C3B-C4B-NB	-2.89	107.95	110.53
23	B	610	CLA	C1-C2-C3	-2.89	121.46	126.20
31	E	101	LMG	O8-C28-C29	2.89	120.65	111.83
31	d	406	LMG	C7-O1-C1	2.89	119.99	113.80
27	B	618	BCR	C21-C20-C19	-2.89	114.84	123.20
28	c	516	DGD	O5D-C1E-C2E	2.89	112.66	108.27
28	d	409	DGD	O1G-C1A-C2A	2.89	120.63	111.83
23	B	611	CLA	C3B-C4B-NB	-2.88	107.95	110.53
27	T	102	BCR	C4-C5-C6	-2.88	118.81	122.70
23	b	614	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
23	b	617	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
31	a	416	LMG	C1-O6-C5	-2.88	108.10	113.72
31	B	622	LMG	O8-C28-C29	2.87	120.59	111.83
27	B	617	BCR	C20-C21-C22	-2.87	123.25	127.28
33	D	410	LMT	C1B-O1B-C4'	-2.87	111.17	117.98
27	J	102	BCR	C33-C5-C6	-2.87	121.35	124.48
34	f	101	HEM	C1B-NB-C4B	2.87	108.60	105.21
23	c	508	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
23	C	512	CLA	C3B-C4B-NB	-2.87	107.97	110.53
23	B	609	CLA	C3B-C4B-NB	-2.86	107.97	110.53
31	I	101	LMG	O8-C28-C29	2.86	120.57	111.83
23	B	614	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
30	D	408	SQD	O7-S-C6	2.85	111.02	106.76
23	B	603	CLA	C3B-C4B-NB	-2.85	107.98	110.53
23	C	503	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	C	515	BCR	C7-C8-C9	-2.85	122.02	126.23
27	D	405	BCR	C3-C4-C5	-2.85	108.97	114.06
28	A	411	DGD	O4D-C4D-C5D	-2.85	102.31	109.32
27	B	618	BCR	C29-C30-C25	2.85	114.58	110.44
23	b	616	CLA	C3B-C4B-NB	-2.84	107.99	110.53
30	A	417	SQD	O6-C1-C2	2.84	112.59	108.27
25	A	408	PL9	C7-C3-C2	-2.84	120.04	123.39
24	a	408	PHO	CMB-C2B-C3B	2.83	130.35	124.68
31	d	407	LMG	C1-C2-C3	-2.83	104.05	110.01
30	B	626	SQD	O9-S-C6	2.83	110.98	106.76
23	b	617	CLA	CHB-C4A-NA	2.83	128.48	124.40
27	b	622	BCR	C33-C5-C4	2.83	119.63	113.60
28	b	602	DGD	O2G-C1B-C2B	2.83	117.60	111.48
30	F	102	SQD	O5-C5-C4	2.82	114.79	109.70
23	C	502	CLA	O2D-CGD-O1D	-2.82	118.35	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	618	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
23	C	509	CLA	C3B-C4B-NB	-2.82	108.02	110.53
24	A	406	PHO	CMB-C2B-C3B	2.82	130.31	124.68
31	a	402	LMG	O8-C28-C29	2.82	120.42	111.83
23	B	613	CLA	C3B-C4B-NB	-2.81	108.02	110.53
23	B	611	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
27	T	102	BCR	C21-C20-C19	-2.81	115.06	123.20
23	B	608	CLA	C3B-C4B-NB	-2.81	108.02	110.53
23	b	608	CLA	C1-C2-C3	-2.81	121.60	126.20
31	B	622	LMG	O1-C1-C2	2.81	112.53	108.27
31	A	418	LMG	C6-C5-C4	-2.80	106.14	113.02
27	B	619	BCR	C29-C30-C25	2.80	114.51	110.44
23	c	512	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	a	404	CLA	C1-C2-C3	-2.80	121.61	126.20
23	A	403	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
30	a	415	SQD	O5-C5-C4	2.80	114.74	109.70
23	C	509	CLA	CHB-C4A-NA	2.80	128.44	124.40
23	B	606	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	C	501	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	C	512	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	a	406	CLA	CHB-C4A-NA	2.79	128.42	124.40
23	A	404	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
28	C	518	DGD	O3G-C1D-C2D	2.78	112.50	108.27
27	b	621	BCR	C29-C30-C25	2.78	114.48	110.44
23	b	613	CLA	C3B-C4B-NB	-2.78	108.05	110.53
31	D	406	LMG	O8-C28-O10	-2.78	116.67	123.63
28	D	409	DGD	O1G-C1A-C2A	2.78	120.32	111.83
23	b	611	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
23	c	511	CLA	C3B-C4B-NB	-2.78	108.05	110.53
23	C	506	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
31	C	521	LMG	C1-O6-C5	-2.77	108.30	113.72
31	c	519	LMG	O1-C1-C2	2.77	112.48	108.27
28	b	602	DGD	C3G-O3G-C1D	2.77	119.74	113.80
23	b	606	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	c	512	CLA	CHB-C4A-NA	2.77	128.39	124.40
23	c	509	CLA	C1-C2-C3	-2.77	121.67	126.20
23	a	405	CLA	C3B-C4B-NB	-2.77	108.06	110.53
23	c	503	CLA	C3B-C4B-NB	-2.77	108.06	110.53
27	C	514	BCR	C16-C17-C18	-2.76	123.40	127.28
31	m	102	LMG	O8-C28-C29	2.76	120.26	111.83
30	A	413	SQD	O5-C5-C4	2.76	114.68	109.70
30	f	102	SQD	O5-C5-C4	2.76	114.68	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	CHB-C4A-NA	2.76	128.38	124.40
28	b	602	DGD	C6D-C5D-C4D	-2.76	106.28	112.07
31	k	103	LMG	C1-O6-C5	-2.76	108.33	113.72
23	B	605	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
23	b	610	CLA	C3B-C4B-NB	-2.75	108.08	110.53
31	D	407	LMG	O8-C28-C29	2.75	120.22	111.83
28	C	518	DGD	O1G-C1A-C2A	2.75	120.22	111.83
28	C	518	DGD	O6E-C1E-C2E	2.75	116.02	110.37
23	a	409	CLA	C3B-C4B-NB	-2.75	108.08	110.53
28	c	518	DGD	O6D-C5D-C6D	2.74	112.13	106.69
31	B	622	LMG	C7-O1-C1	2.74	119.67	113.80
31	B	623	LMG	C1-O6-C5	-2.74	108.38	113.72
28	C	518	DGD	O4D-C4D-C5D	-2.74	102.58	109.32
31	d	406	LMG	O8-C28-O10	-2.74	116.78	123.63
23	B	609	CLA	CHB-C4A-NA	2.73	128.34	124.40
25	d	404	PL9	C32-C33-C34	-2.73	121.37	127.62
28	c	518	DGD	C4D-C3D-C2D	-2.73	106.04	110.83
31	C	521	LMG	O1-C1-C2	2.73	112.42	108.27
23	b	620	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
23	c	504	CLA	CHB-C4A-NA	2.73	128.34	124.40
30	B	626	SQD	O5-C5-C4	2.72	114.61	109.70
27	B	620	BCR	C33-C5-C4	2.72	119.40	113.60
23	a	405	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
23	B	616	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
23	c	508	CLA	CHB-C4A-NA	2.71	128.32	124.40
23	B	608	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
33	B	628	LMT	O1B-C4'-C3'	2.71	114.12	107.23
28	b	623	DGD	O2G-C1B-C2B	2.71	117.35	111.48
28	D	409	DGD	O5D-C1E-C2E	2.71	112.39	108.27
30	b	601	SQD	O5-C5-C4	2.71	114.58	109.70
23	B	610	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
23	B	605	CLA	CHB-C4A-NA	2.71	128.31	124.40
28	b	623	DGD	O3D-C3D-C4D	2.70	116.75	110.38
23	b	619	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
27	D	405	BCR	C21-C20-C19	-2.70	115.37	123.20
23	b	619	CLA	CHB-C4A-NA	2.70	128.30	124.40
23	B	611	CLA	C1-C2-C3	-2.70	121.77	126.20
23	B	609	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
27	d	405	BCR	C38-C26-C25	-2.70	121.54	124.48
23	C	506	CLA	C3B-C4B-NB	-2.70	108.12	110.53
28	b	602	DGD	O1G-C1A-C2A	2.70	120.06	111.83
27	C	516	BCR	C11-C10-C9	-2.69	123.50	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	608	CLA	C3B-C4B-NB	-2.69	108.13	110.53
23	C	508	CLA	CHB-C4A-NA	2.69	128.28	124.40
27	D	405	BCR	C23-C24-C25	-2.69	119.82	127.00
27	y	101	BCR	C20-C21-C22	-2.69	123.51	127.28
23	C	504	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
27	C	515	BCR	C8-C7-C6	-2.69	119.82	127.00
31	E	101	LMG	C8-O7-C10	2.69	124.22	117.80
23	C	506	CLA	CHB-C4A-NA	2.69	128.28	124.40
23	b	605	CLA	C1-C2-C3	-2.68	121.80	126.20
27	D	405	BCR	C29-C30-C25	2.68	114.34	110.44
23	c	513	CLA	C3B-C4B-NB	-2.68	108.14	110.53
23	b	608	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
23	c	509	CLA	CHB-C4A-NA	2.68	128.27	124.40
31	i	101	LMG	O8-C28-C29	2.68	120.00	111.83
23	b	616	CLA	CHB-C4A-NA	2.68	128.26	124.40
27	c	514	BCR	C38-C26-C25	-2.68	121.56	124.48
23	c	502	CLA	C1-C2-C3	-2.68	121.81	126.20
25	d	404	PL9	C12-C13-C14	-2.67	121.50	127.62
27	J	102	BCR	C1-C6-C5	-2.67	118.98	122.64
30	a	415	SQD	C44-O6-C1	2.67	119.52	113.80
27	H	101	BCR	C38-C26-C25	-2.67	121.57	124.48
31	b	625	LMG	C7-O1-C1	2.67	119.52	113.80
23	c	506	CLA	C1-C2-C3	-2.67	121.83	126.20
23	c	507	CLA	C3B-C4B-NB	-2.66	108.15	110.53
23	b	611	CLA	CHB-C4A-NA	2.66	128.25	124.40
27	h	101	BCR	C38-C26-C25	-2.66	121.58	124.48
30	F	102	SQD	C44-O6-C1	2.66	119.50	113.80
23	a	404	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
23	B	603	CLA	CHB-C4A-NA	2.66	128.24	124.40
30	f	102	SQD	O8-S-C6	2.66	111.11	105.97
23	B	615	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
30	A	413	SQD	O8-S-C6	2.66	111.11	105.97
27	T	102	BCR	C38-C26-C27	2.66	119.26	113.60
23	b	607	CLA	C3B-C4B-NB	-2.66	108.16	110.53
23	B	615	CLA	C3B-C4B-NB	-2.66	108.16	110.53
23	B	601	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
23	A	405	CLA	O2D-CGD-CBD	2.65	115.86	111.23
23	C	513	CLA	CHB-C4A-NA	2.65	128.22	124.40
27	T	101	BCR	C38-C26-C25	-2.65	121.60	124.48
31	I	101	LMG	C1-O6-C5	-2.65	108.55	113.72
23	a	409	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
33	b	626	LMT	C1B-O1B-C4'	-2.65	111.71	117.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	501	CLA	C3B-C4B-NB	-2.64	108.17	110.53
30	b	601	SQD	O48-C23-C24	2.64	119.90	111.83
31	i	101	LMG	C1-O6-C5	-2.64	108.56	113.72
29	A	415	LHG	O8-C23-C24	2.64	119.89	111.83
31	D	406	LMG	C3-C4-C5	2.64	115.02	110.23
28	c	516	DGD	C1D-O6D-C5D	-2.64	108.56	113.72
23	B	608	CLA	CHB-C4A-NA	2.64	128.21	124.40
25	J	101	PL9	C20-C19-C21	2.64	119.81	115.23
24	A	406	PHO	C3B-C4B-NB	-2.64	105.75	107.46
30	B	626	SQD	O48-C23-C24	2.64	119.88	111.83
23	c	505	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
25	D	404	PL9	C7-C3-C2	-2.63	120.28	123.39
27	C	515	BCR	C28-C27-C26	-2.63	109.36	114.06
31	D	407	LMG	C1-C2-C3	-2.63	104.47	110.01
23	C	502	CLA	C1-C2-C3	-2.63	121.88	126.20
27	D	405	BCR	C27-C26-C25	-2.63	119.15	122.70
23	b	607	CLA	CHB-C4A-NA	2.63	128.20	124.40
23	c	502	CLA	CHB-C4A-NA	2.63	128.20	124.40
28	c	518	DGD	O5D-C1E-C2E	2.63	112.27	108.27
27	a	412	BCR	C11-C10-C9	-2.63	123.59	127.28
28	c	517	DGD	O1G-C1A-C2A	2.63	119.84	111.83
23	c	507	CLA	C1-C2-C3	-2.63	121.90	126.20
23	B	604	CLA	O2A-CGA-O1A	-2.62	117.06	123.63
23	B	602	CLA	C3B-C4B-NB	-2.62	108.19	110.53
28	a	413	DGD	C3G-C2G-C1G	-2.62	105.67	111.78
31	E	101	LMG	O7-C10-C11	2.62	117.14	111.48
23	b	615	CLA	C1-C2-C3	-2.62	121.91	126.20
23	C	513	CLA	C1-C2-C3	-2.61	121.91	126.20
23	B	601	CLA	C3B-C4B-NB	-2.61	108.20	110.53
23	c	507	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
31	d	406	LMG	C3-C4-C5	2.61	114.97	110.23
23	a	404	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
25	a	410	PL9	C12-C13-C14	-2.61	121.66	127.62
27	C	514	BCR	C24-C23-C22	-2.61	122.38	126.23
23	C	507	CLA	CHB-C4A-NA	2.61	128.16	124.40
27	z	101	BCR	C8-C7-C6	-2.61	120.04	127.00
27	b	621	BCR	C8-C7-C6	-2.60	120.05	127.00
23	b	606	CLA	C1-C2-C3	-2.60	121.94	126.20
34	F	101	HEM	C1B-NB-C4B	2.60	108.28	105.21
28	a	413	DGD	O1G-C1A-C2A	2.60	119.76	111.83
25	D	404	PL9	C7-C8-C9	-2.60	122.35	126.83
27	d	405	BCR	C16-C15-C14	-2.60	118.21	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	509	CLA	C3B-C4B-NB	-2.60	108.21	110.53
23	C	504	CLA	CHB-C4A-NA	2.60	128.15	124.40
27	T	102	BCR	C23-C24-C25	-2.59	120.08	127.00
31	M	101	LMG	O8-C28-C29	2.59	119.73	111.83
23	b	613	CLA	C1-C2-C3	-2.59	121.95	126.20
23	d	403	CLA	C3B-C4B-NB	-2.59	108.22	110.53
23	C	513	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
23	d	402	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
27	d	405	BCR	C23-C24-C25	-2.58	120.10	127.00
23	b	614	CLA	CHB-C4A-NA	2.58	128.13	124.40
23	a	409	CLA	CHB-C4A-NA	2.58	128.12	124.40
27	d	405	BCR	C38-C26-C27	2.58	119.10	113.60
28	B	621	DGD	O1G-C1A-C2A	2.58	119.69	111.83
23	B	602	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
23	C	503	CLA	C3B-C4B-NB	-2.57	108.23	110.53
23	C	509	CLA	C1-C2-C3	-2.57	121.98	126.20
23	c	504	CLA	C3B-C4B-NB	-2.57	108.23	110.53
31	b	624	LMG	C7-O1-C1	2.57	119.31	113.80
28	C	519	DGD	C4D-C3D-C2D	-2.57	106.32	110.83
23	b	617	CLA	C3B-C4B-NB	-2.57	108.24	110.53
27	h	101	BCR	C8-C7-C6	-2.56	120.15	127.00
23	C	511	CLA	CHB-C4A-NA	2.56	128.09	124.40
23	b	615	CLA	C3B-C4B-NB	-2.56	108.25	110.53
23	c	501	CLA	C1-C2-C3	-2.56	122.01	126.20
23	C	512	CLA	CHB-C4A-NA	2.56	128.09	124.40
27	h	101	BCR	C15-C16-C17	-2.56	118.29	123.52
23	c	506	CLA	CHB-C4A-NA	2.55	128.09	124.40
23	c	508	CLA	C3B-C4B-NB	-2.55	108.25	110.53
27	a	412	BCR	C34-C9-C8	2.55	121.99	118.09
30	b	601	SQD	O47-C7-C8	2.55	117.00	111.48
23	A	404	CLA	CHB-C4A-NA	2.55	128.08	124.40
23	C	508	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
31	a	402	LMG	C1-O6-C5	-2.55	108.75	113.72
23	b	609	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
25	D	404	PL9	C40-C39-C41	2.54	119.64	115.23
25	j	101	PL9	C22-C23-C24	-2.54	121.80	127.62
27	B	618	BCR	C38-C26-C27	2.54	119.02	113.60
23	B	601	CLA	CHB-C4A-NA	2.54	128.07	124.40
23	c	505	CLA	CHB-C4A-NA	2.54	128.06	124.40
33	d	410	LMT	C1B-O1B-C4'	-2.54	111.96	117.98
23	D	403	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
27	d	405	BCR	C21-C20-C19	-2.53	115.86	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	627	DGD	O1G-C1A-C2A	2.53	119.55	111.83
27	h	101	BCR	C34-C9-C8	2.53	121.95	118.09
27	d	405	BCR	C3-C4-C5	-2.53	109.55	114.06
27	B	619	BCR	C2-C1-C6	2.53	114.11	110.44
23	C	503	CLA	CHB-C4A-NA	2.52	128.04	124.40
27	J	102	BCR	C38-C26-C27	2.52	118.98	113.60
28	b	602	DGD	O4D-C4D-C5D	-2.52	103.11	109.32
23	c	506	CLA	C3B-C4B-NB	-2.52	108.28	110.53
28	B	627	DGD	O6D-C1D-O3G	2.52	116.00	110.04
23	c	513	CLA	CHB-C4A-NA	2.52	128.04	124.40
27	B	617	BCR	C3-C4-C5	-2.52	109.57	114.06
31	e	101	LMG	O7-C10-C11	2.52	116.92	111.48
27	H	101	BCR	C35-C13-C12	2.52	121.93	118.09
30	a	401	SQD	O48-C23-C24	2.51	119.50	111.83
27	T	102	BCR	C15-C14-C13	-2.51	123.75	127.28
23	B	607	CLA	C3B-C4B-NB	-2.51	108.29	110.53
30	a	415	SQD	O48-C23-C24	2.51	119.50	111.83
33	b	603	LMT	O1B-C4'-C3'	2.51	113.62	107.23
23	a	404	CLA	C3B-C4B-NB	-2.51	108.29	110.53
29	a	417	LHG	O8-C23-C24	2.51	119.49	111.83
27	j	102	BCR	C1-C6-C5	-2.51	119.21	122.64
23	a	405	CLA	CAA-C2A-C3A	-2.50	106.23	113.00
23	B	613	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	C	508	CLA	C3B-C4B-NB	-2.50	108.30	110.53
23	C	508	CLA	C1-C2-C3	-2.50	122.10	126.20
23	B	611	CLA	CHB-C4A-NA	2.50	128.00	124.40
27	c	514	BCR	C34-C9-C10	-2.49	118.78	122.82
23	b	609	CLA	CHB-C4A-NA	2.49	127.99	124.40
28	B	621	DGD	O2G-C1B-C2B	2.49	116.86	111.48
27	j	102	BCR	C38-C26-C27	2.49	118.90	113.60
27	d	405	BCR	C27-C26-C25	-2.49	119.34	122.70
23	b	612	CLA	C1-C2-C3	-2.49	122.12	126.20
23	c	501	CLA	CHB-C4A-NA	2.48	127.99	124.40
23	B	602	CLA	CHB-C4A-NA	2.48	127.98	124.40
28	C	517	DGD	O1G-C1A-C2A	2.48	119.41	111.83
25	j	101	PL9	C12-C13-C14	-2.48	121.94	127.62
28	A	411	DGD	C3D-C4D-C5D	2.48	114.73	110.23
23	D	401	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
23	C	511	CLA	C1-C2-C3	-2.48	122.13	126.20
27	D	405	BCR	C38-C26-C27	2.48	118.88	113.60
28	a	413	DGD	O4D-C4D-C5D	-2.48	103.22	109.32
27	C	516	BCR	C15-C16-C17	-2.48	118.45	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	501	CLA	CHB-C4A-NA	2.48	127.98	124.40
23	b	618	CLA	CHB-C4A-NA	2.48	127.98	124.40
31	e	101	LMG	O1-C1-C2	2.48	112.04	108.27
28	a	413	DGD	C3D-C4D-C5D	2.48	114.72	110.23
27	T	102	BCR	C15-C16-C17	-2.47	118.46	123.52
23	C	505	CLA	C3B-C4B-NB	-2.47	108.33	110.53
28	A	411	DGD	O1G-C1A-C2A	2.47	119.36	111.83
23	a	405	CLA	CHB-C4A-NA	2.47	127.96	124.40
28	b	602	DGD	O6D-C1D-O3G	2.47	115.87	110.04
27	a	412	BCR	C20-C21-C22	-2.46	123.82	127.28
30	D	408	SQD	O48-C23-C24	2.46	119.35	111.83
27	j	102	BCR	C39-C30-C25	-2.46	106.38	110.24
23	b	611	CLA	C3B-C4B-NB	-2.46	108.33	110.53
27	c	514	BCR	C24-C23-C22	-2.46	122.59	126.23
23	c	501	CLA	C3B-C4B-NB	-2.46	108.33	110.53
25	J	101	PL9	C12-C13-C14	-2.46	122.00	127.62
23	A	407	CLA	CHB-C4A-NA	2.46	127.94	124.40
28	c	518	DGD	O3D-C3D-C4D	2.46	116.16	110.38
27	B	618	BCR	C23-C24-C25	-2.45	120.44	127.00
27	a	412	BCR	C23-C24-C25	-2.45	120.44	127.00
23	b	620	CLA	C3B-C4B-NB	-2.45	108.34	110.53
28	C	517	DGD	O3D-C3D-C4D	2.45	116.16	110.38
23	C	512	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
23	d	403	CLA	O2D-CGD-CBD	2.45	115.52	111.23
23	c	509	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
27	H	101	BCR	C3-C4-C5	-2.44	109.70	114.06
27	B	619	BCR	C15-C16-C17	-2.44	118.52	123.52
27	z	101	BCR	C23-C24-C25	-2.44	120.47	127.00
27	y	101	BCR	C33-C5-C4	2.44	118.80	113.60
28	C	519	DGD	O2G-C1B-C2B	2.44	116.76	111.48
23	a	404	CLA	CHB-C4A-NA	2.44	127.92	124.40
23	D	401	CLA	C3B-C4B-NB	-2.44	108.35	110.53
23	B	612	CLA	CHB-C4A-NA	2.44	127.91	124.40
30	F	102	SQD	O5-C1-C2	2.43	115.37	110.37
31	I	101	LMG	C7-O1-C1	2.43	119.02	113.80
31	D	407	LMG	O8-C28-O10	-2.43	117.55	123.63
23	b	605	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	C	521	LMG	C7-O1-C1	2.43	119.00	113.80
23	B	604	CLA	C1-C2-C3	-2.42	122.22	126.20
25	a	410	PL9	C32-C33-C34	-2.42	122.08	127.62
23	a	405	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
27	B	617	BCR	C23-C24-C25	-2.42	120.53	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
27	z	101	BCR	C11-C10-C9	-2.42	123.88	127.28
27	b	621	BCR	C27-C26-C25	-2.42	119.43	122.70
23	c	510	CLA	CHB-C4A-NA	2.42	127.89	124.40
23	a	409	CLA	O2A-CGA-O1A	-2.42	117.58	123.63
27	B	618	BCR	C33-C5-C4	2.42	118.75	113.60
25	A	408	PL9	C12-C13-C14	-2.42	122.09	127.62
30	d	408	SQD	O48-C23-C24	2.41	119.19	111.83
25	a	410	PL9	C17-C18-C19	-2.41	122.10	127.62
34	f	101	HEM	CHD-C4C-NC	2.41	127.08	124.45
30	d	408	SQD	O7-S-C6	2.41	110.36	106.76
31	b	625	LMG	C1-O6-C5	-2.41	109.02	113.72
27	h	101	BCR	C35-C13-C12	2.41	121.77	118.09
25	D	404	PL9	C32-C33-C34	-2.41	122.11	127.62
28	b	623	DGD	O1G-C1A-C2A	2.41	119.17	111.83
27	J	102	BCR	C35-C13-C14	-2.40	118.92	122.82
23	C	513	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
27	T	102	BCR	C33-C5-C4	2.40	118.71	113.60
27	h	101	BCR	C3-C4-C5	-2.39	109.79	114.06
28	c	517	DGD	O6E-C1E-C2E	2.39	115.28	110.37
25	d	404	PL9	C40-C39-C41	2.39	119.38	115.23
23	C	501	CLA	C1-C2-C3	-2.39	122.28	126.20
31	e	101	LMG	O7-C10-O9	-2.39	118.12	123.70
30	f	102	SQD	O9-S-C6	2.39	110.32	106.76
23	B	605	CLA	C3B-C4B-NB	-2.39	108.40	110.53
27	C	514	BCR	C34-C9-C10	-2.39	118.95	122.82
30	a	415	SQD	O8-S-C6	2.38	110.58	105.97
25	A	408	PL9	C20-C19-C21	2.38	119.37	115.23
23	c	508	CLA	C1-C2-C3	-2.38	122.29	126.20
23	b	617	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
23	d	403	CLA	CHB-C4A-NA	2.38	127.84	124.40
27	z	101	BCR	C28-C27-C26	-2.38	109.81	114.06
28	C	518	DGD	C1D-O6D-C5D	-2.38	109.07	113.72
27	T	101	BCR	C3-C4-C5	-2.38	109.81	114.06
31	C	520	LMG	C7-O1-C1	2.38	118.89	113.80
34	v	201	HEM	C1B-NB-C4B	2.38	108.02	105.21
31	A	418	LMG	O8-C28-O10	-2.38	117.69	123.63
28	c	517	DGD	C1D-O6D-C5D	-2.38	109.08	113.72
23	c	512	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
27	B	618	BCR	C35-C13-C12	2.37	121.71	118.09
27	c	515	BCR	C23-C24-C25	-2.37	120.66	127.00
27	H	101	BCR	C33-C5-C4	2.37	118.65	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	516	BCR	C21-C20-C19	-2.37	116.33	123.20
25	d	404	PL9	C20-C19-C21	2.37	119.34	115.23
27	B	618	BCR	C15-C14-C13	-2.37	123.96	127.28
28	c	516	DGD	O1G-C1A-C2A	2.37	119.06	111.83
27	C	515	BCR	C10-C11-C12	-2.37	116.34	123.20
23	b	610	CLA	CHB-C4A-NA	2.37	127.82	124.40
23	c	503	CLA	CHB-C4A-NA	2.37	127.82	124.40
30	A	413	SQD	O48-C23-C24	2.37	119.05	111.83
27	J	102	BCR	C11-C12-C13	-2.37	119.87	126.36
30	B	626	SQD	O47-C7-C8	2.37	116.60	111.48
23	B	609	CLA	C1-C2-C3	-2.36	122.32	126.20
28	d	409	DGD	O2G-C1B-C2B	2.36	116.60	111.48
27	T	102	BCR	C16-C17-C18	-2.36	123.96	127.28
23	B	606	CLA	CHB-C4A-NA	2.36	127.80	124.40
25	D	404	PL9	C15-C14-C16	2.36	119.32	115.23
27	T	102	BCR	C24-C23-C22	-2.36	122.75	126.23
31	e	101	LMG	C1-O6-C5	-2.36	109.12	113.72
31	e	101	LMG	C8-O7-C10	2.35	123.43	117.80
23	C	507	CLA	O2D-CGD-CBD	2.35	115.35	111.23
27	y	101	BCR	C11-C10-C9	-2.35	123.98	127.28
31	b	625	LMG	C6-C5-C4	-2.35	107.25	113.02
23	A	405	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
23	A	403	CLA	C1-C2-C3	-2.35	122.35	126.20
23	A	407	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
23	b	615	CLA	CHB-C4A-NA	2.34	127.78	124.40
31	A	418	LMG	C1-O6-C5	-2.34	109.15	113.72
28	d	409	DGD	C2G-O2G-C1B	2.34	123.40	117.80
31	m	102	LMG	O4-C4-C3	-2.34	104.86	110.38
31	A	418	LMG	O1-C1-C2	2.34	111.83	108.27
28	a	413	DGD	C4D-C3D-C2D	-2.34	106.73	110.83
23	D	403	CLA	CHB-C4A-NA	2.34	127.77	124.40
28	d	409	DGD	O3D-C3D-C4D	2.34	115.88	110.38
23	A	405	CLA	CHB-C4A-NA	2.34	127.77	124.40
28	a	413	DGD	C6E-C5E-C4E	-2.33	107.29	113.02
28	d	409	DGD	O2G-C1B-O1B	-2.33	118.25	123.70
30	f	102	SQD	O48-C23-C24	2.33	118.95	111.83
23	B	604	CLA	CHB-C4A-NA	2.33	127.76	124.40
27	C	515	BCR	C23-C24-C25	-2.33	120.77	127.00
27	D	405	BCR	C38-C26-C25	-2.33	121.94	124.48
24	D	402	PHO	O2A-CGA-O1A	-2.33	117.81	123.63
31	i	101	LMG	C7-O1-C1	2.33	118.79	113.80
31	k	103	LMG	O8-C28-O10	-2.33	117.81	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	CHB-C4A-NA	2.33	127.76	124.40
31	E	101	LMG	O1-C1-C2	2.32	111.79	108.27
23	b	607	CLA	O2D-CGD-CBD	2.32	115.28	111.23
23	B	605	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
27	c	514	BCR	C29-C30-C25	2.31	113.80	110.44
31	b	624	LMG	C4-C3-C2	2.31	114.89	110.83
27	B	618	BCR	C16-C17-C18	-2.31	124.04	127.28
23	B	601	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
23	B	603	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
28	c	517	DGD	O4D-C4D-C5D	-2.31	103.64	109.32
24	D	402	PHO	O2D-CGD-O1D	-2.31	119.35	123.85
30	A	417	SQD	O48-C23-C24	2.31	118.87	111.83
27	C	514	BCR	C29-C30-C25	2.31	113.79	110.44
25	d	404	PL9	C42-C43-C44	-2.30	122.35	127.62
31	i	101	LMG	O8-C28-O10	-2.30	117.86	123.63
31	B	622	LMG	C4-C3-C2	2.30	114.87	110.83
30	a	415	SQD	O6-C1-C2	2.30	111.77	108.27
28	C	519	DGD	O1G-C1A-O1A	-2.30	117.87	123.63
25	a	410	PL9	C20-C19-C21	2.30	119.22	115.23
31	d	407	LMG	C7-O1-C1	2.30	118.73	113.80
31	b	624	LMG	C1-O6-C5	-2.30	109.23	113.72
25	d	404	PL9	C51-C49-C50	2.30	119.88	114.59
27	T	101	BCR	C23-C24-C25	-2.30	120.86	127.00
23	b	608	CLA	CHB-C4A-NA	2.30	127.72	124.40
31	i	101	LMG	C3-C4-C5	2.30	114.40	110.23
27	a	412	BCR	C34-C9-C10	-2.30	119.10	122.82
23	b	617	CLA	C1-C2-C3	-2.29	122.44	126.20
28	c	518	DGD	O2G-C1B-C2B	2.29	116.44	111.48
31	a	416	LMG	O6-C5-C6	2.29	112.12	106.44
23	c	505	CLA	C3B-C4B-NB	-2.29	108.48	110.53
23	C	511	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
31	E	101	LMG	O9-C10-C11	-2.29	114.83	123.78
27	H	101	BCR	C7-C8-C9	-2.28	122.86	126.23
25	j	101	PL9	C15-C14-C16	2.28	119.19	115.23
30	F	102	SQD	O48-C23-C24	2.28	118.79	111.83
25	J	101	PL9	C15-C14-C16	2.28	119.19	115.23
27	C	515	BCR	C38-C26-C25	-2.28	122.00	124.48
23	a	406	CLA	C3B-C4B-NB	-2.28	108.50	110.53
23	b	605	CLA	CHB-C4A-NA	2.27	127.68	124.40
34	F	101	HEM	CHB-C1B-NB	2.27	127.18	124.37
27	c	515	BCR	C21-C20-C19	-2.27	116.61	123.20
34	v	201	HEM	CHC-C4B-NB	2.27	126.87	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	E	101	LMG	O7-C10-O9	-2.27	118.39	123.70
23	b	612	CLA	CHB-C4A-NA	2.27	127.68	124.40
23	A	403	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
23	B	610	CLA	CHB-C4A-NA	2.27	127.68	124.40
25	A	408	PL9	C32-C33-C34	-2.27	122.43	127.62
25	a	410	PL9	C7-C8-C9	-2.27	122.92	126.83
27	k	102	BCR	C35-C13-C12	2.27	121.55	118.09
28	c	518	DGD	O3G-C1D-C2D	2.27	111.71	108.27
27	y	101	BCR	C35-C13-C12	2.26	121.55	118.09
27	j	102	BCR	C15-C16-C17	-2.26	118.89	123.52
23	C	502	CLA	C3B-C4B-NB	-2.26	108.51	110.53
27	z	101	BCR	C38-C26-C25	-2.26	122.02	124.48
27	h	101	BCR	C36-C18-C19	2.26	121.54	118.09
23	b	605	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
23	c	508	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
23	B	612	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
23	b	613	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
23	c	507	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
27	k	102	BCR	C35-C13-C14	-2.25	119.17	122.82
23	c	507	CLA	CHB-C4A-NA	2.25	127.65	124.40
23	b	610	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
23	C	502	CLA	CHB-C4A-NA	2.25	127.64	124.40
23	A	407	CLA	C3B-C4B-NB	-2.25	108.52	110.53
31	C	520	LMG	O8-C28-O10	-2.25	118.01	123.63
28	B	627	DGD	C4D-C3D-C2D	-2.24	106.89	110.83
31	c	519	LMG	C3-C4-C5	2.24	114.30	110.23
31	B	623	LMG	O8-C28-O10	-2.24	118.02	123.63
23	d	402	CLA	O1D-CGD-CBD	2.24	128.94	124.52
30	d	408	SQD	O8-S-C6	2.24	110.30	105.97
23	b	619	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
23	c	501	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
23	D	401	CLA	O1D-CGD-CBD	2.24	128.94	124.52
23	C	504	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
23	b	614	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
27	C	516	BCR	C23-C24-C25	-2.24	121.02	127.00
28	b	623	DGD	C3G-O3G-C1D	2.24	118.59	113.80
27	B	619	BCR	C27-C26-C25	-2.24	119.68	122.70
27	c	515	BCR	C15-C16-C17	-2.24	118.94	123.52
28	a	413	DGD	O3D-C3D-C4D	2.24	115.65	110.38
34	v	201	HEM	C2A-C1A-NA	-2.24	107.67	110.15
23	c	511	CLA	CHB-C4A-NA	2.23	127.62	124.40
27	C	516	BCR	C38-C26-C27	2.23	118.36	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
23	C	511	CLA	C3B-C4B-NB	-2.23	108.54	110.53
23	B	615	CLA	CHB-C4A-NA	2.23	127.62	124.40
31	C	521	LMG	C3-C4-C5	2.23	114.28	110.23
23	c	513	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
28	A	411	DGD	O3D-C3D-C4D	2.23	115.63	110.38
27	b	621	BCR	C2-C1-C6	2.23	113.67	110.44
24	a	408	PHO	C2D-C1D-ND	-2.23	107.82	109.43
28	B	627	DGD	C1E-C2E-C3E	2.23	114.69	110.01
27	B	618	BCR	C31-C1-C6	-2.23	106.75	110.24
23	B	602	CLA	C1-C2-C3	-2.22	122.55	126.20
23	b	607	CLA	C1-C2-C3	-2.22	122.55	126.20
23	D	403	CLA	C1-C2-C3	-2.22	122.56	126.20
31	e	101	LMG	C6-C5-C4	-2.22	107.56	113.02
24	D	402	PHO	CMB-C2B-C3B	2.22	129.12	124.68
31	a	402	LMG	O3-C3-C4	-2.22	105.14	110.38
34	f	101	HEM	C2A-C1A-NA	-2.22	107.69	110.15
28	A	411	DGD	C6D-C5D-C4D	-2.22	107.41	112.07
27	B	618	BCR	C15-C16-C17	-2.22	118.98	123.52
27	B	619	BCR	C7-C8-C9	-2.22	122.95	126.23
25	A	408	PL9	C30-C29-C31	2.22	119.08	115.23
23	B	607	CLA	C1-C2-C3	-2.22	122.57	126.20
27	A	410	BCR	C34-C9-C10	-2.21	119.23	122.82
23	a	409	CLA	C1-C2-C3	-2.21	122.57	126.20
28	B	627	DGD	C6D-C5D-C4D	-2.21	107.42	112.07
27	C	516	BCR	C2-C1-C6	2.21	113.65	110.44
25	d	404	PL9	C15-C14-C16	2.21	119.07	115.23
28	D	409	DGD	O2G-C1B-O1B	-2.21	118.54	123.70
31	B	623	LMG	C3-C4-C5	2.21	114.24	110.23
30	f	102	SQD	O5-C1-C2	2.21	114.90	110.37
25	J	101	PL9	C22-C23-C24	-2.21	122.57	127.62
30	B	626	SQD	C10-C9-C8	-2.21	105.02	113.13
23	A	403	CLA	CHB-C4A-NA	2.20	127.58	124.40
27	H	101	BCR	C36-C18-C19	2.20	121.45	118.09
31	k	103	LMG	C7-O1-C1	2.20	118.51	113.80
27	j	102	BCR	C11-C12-C13	-2.20	120.33	126.36
28	c	516	DGD	C1G-O1G-C1A	2.20	125.15	117.12
30	b	601	SQD	C10-C9-C8	-2.19	105.06	113.13
27	H	101	BCR	C16-C15-C14	-2.19	119.03	123.52
27	c	515	BCR	C38-C26-C27	2.19	118.27	113.60
27	C	514	BCR	C35-C13-C14	-2.19	119.27	122.82
23	B	613	CLA	O2D-CGD-O1D	-2.19	119.59	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	j	101	PL9	C20-C19-C21	2.19	119.03	115.23
23	b	616	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
27	B	617	BCR	C36-C18-C19	2.19	121.43	118.09
23	B	614	CLA	CHB-C4A-NA	2.18	127.55	124.40
27	H	101	BCR	C21-C20-C19	-2.18	116.87	123.20
23	B	610	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
27	D	405	BCR	C16-C15-C14	-2.18	119.05	123.52
27	b	622	BCR	C21-C20-C19	-2.18	116.87	123.20
28	c	516	DGD	C6E-C5E-C4E	-2.18	107.66	113.02
29	a	414	LHG	O8-C23-C24	2.18	118.49	111.83
28	C	517	DGD	O2G-C1B-O1B	-2.18	118.60	123.70
23	b	613	CLA	CHB-C4A-NA	2.18	127.55	124.40
27	J	102	BCR	C36-C18-C17	-2.18	119.28	122.82
27	A	410	BCR	C23-C24-C25	-2.18	121.17	127.00
25	D	404	PL9	C51-C49-C50	2.18	119.60	114.59
23	D	403	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
30	F	102	SQD	O8-S-C6	2.18	110.18	105.97
25	D	404	PL9	C27-C28-C29	-2.18	122.64	127.62
30	D	408	SQD	O8-S-C6	2.18	110.18	105.97
31	c	519	LMG	C6-C5-C4	-2.18	107.67	113.02
27	c	515	BCR	C2-C1-C6	2.18	113.60	110.44
31	b	624	LMG	O4-C4-C3	-2.17	105.25	110.38
31	I	101	LMG	C6-C5-C4	-2.17	107.68	113.02
23	c	513	CLA	C1-C2-C3	-2.17	122.64	126.20
31	b	625	LMG	O8-C28-O10	-2.17	118.19	123.63
27	b	622	BCR	C28-C27-C26	-2.17	110.18	114.06
27	b	622	BCR	C38-C26-C27	2.17	118.22	113.60
23	B	606	CLA	O1D-CGD-CBD	2.17	128.80	124.52
23	C	509	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
31	I	101	LMG	C3-C4-C5	2.17	114.16	110.23
27	y	101	BCR	C32-C1-C6	-2.17	106.85	110.24
23	b	619	CLA	C1-C2-C3	-2.17	122.65	126.20
27	C	514	BCR	C34-C9-C8	2.16	121.39	118.09
30	A	413	SQD	C44-O6-C1	2.16	118.43	113.80
27	k	102	BCR	C23-C24-C25	-2.16	121.23	127.00
28	c	516	DGD	O3D-C3D-C4D	2.16	115.46	110.38
23	c	511	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
27	J	102	BCR	C30-C25-C26	-2.16	119.69	122.64
25	d	404	PL9	C17-C18-C19	-2.16	122.69	127.62
23	A	404	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
34	F	101	HEM	CBA-CAA-C2A	-2.15	106.58	112.53
31	I	101	LMG	C8-O7-C10	2.15	122.95	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	y	101	BCR	C35-C13-C14	-2.15	119.33	122.82
25	j	101	PL9	C10-C9-C11	2.15	118.97	115.23
28	A	411	DGD	C6E-C5E-C4E	-2.15	107.73	113.02
23	b	609	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
23	b	620	CLA	CHB-C4A-NA	2.15	127.51	124.40
30	B	626	SQD	C1-O5-C5	2.15	117.92	113.72
31	e	101	LMG	O9-C10-C11	-2.15	115.37	123.78
23	C	501	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
27	d	405	BCR	C33-C5-C4	2.15	118.18	113.60
28	c	518	DGD	O1G-C1A-O1A	-2.15	118.26	123.63
23	B	608	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
25	d	404	PL9	C53-C6-C1	2.14	119.67	115.28
29	A	412	LHG	O8-C23-C24	2.14	118.36	111.83
31	b	625	LMG	O3-C3-C4	-2.14	105.33	110.38
24	a	407	PHO	O2A-CGA-O1A	-2.14	118.28	123.63
27	z	101	BCR	C10-C11-C12	-2.14	117.01	123.20
30	A	413	SQD	O5-C1-C2	2.14	114.76	110.37
23	B	616	CLA	CHB-C4A-NA	2.13	127.48	124.40
31	E	101	LMG	C1-O6-C5	-2.13	109.56	113.72
27	H	101	BCR	C15-C16-C17	-2.13	119.16	123.52
27	b	621	BCR	C15-C16-C17	-2.13	119.17	123.52
27	c	514	BCR	C23-C24-C25	-2.13	121.32	127.00
23	B	607	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
27	B	620	BCR	C38-C26-C27	2.12	118.12	113.60
23	c	511	CLA	C1-C2-C3	-2.12	122.72	126.20
23	c	505	CLA	CBA-CAA-C2A	2.12	120.10	113.79
27	J	102	BCR	C37-C22-C21	-2.12	119.38	122.82
31	b	624	LMG	C3-C4-C5	2.12	114.08	110.23
27	B	618	BCR	C24-C23-C22	-2.12	123.10	126.23
23	c	505	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
23	b	608	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
23	B	614	CLA	CHC-C4B-NB	2.12	127.22	124.05
23	C	505	CLA	CBA-CAA-C2A	2.12	120.09	113.79
31	b	625	LMG	O6-C5-C4	2.12	113.51	109.70
27	B	620	BCR	C21-C20-C19	-2.11	117.07	123.20
23	d	402	CLA	CHB-C4A-NA	2.11	127.45	124.40
30	A	417	SQD	O2-C2-C3	-2.11	105.39	110.38
27	k	102	BCR	C33-C5-C4	2.11	118.10	113.60
25	a	410	PL9	C27-C28-C29	-2.11	122.79	127.62
30	f	102	SQD	O6-C1-C2	2.11	111.47	108.27
27	k	102	BCR	C32-C1-C6	-2.11	106.94	110.24
31	d	406	LMG	C6-C5-C4	-2.11	107.84	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	515	BCR	C36-C18-C19	2.11	121.31	118.09
23	B	615	CLA	C1-C2-C3	-2.11	122.75	126.20
28	D	409	DGD	O2G-C1B-C2B	2.10	116.03	111.48
34	f	101	HEM	CBA-CAA-C2A	-2.10	106.72	112.53
33	B	625	LMT	C1B-O1B-C4'	-2.10	113.00	117.98
30	b	601	SQD	C1-O5-C5	2.10	117.82	113.72
23	a	406	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
27	z	101	BCR	C15-C16-C17	-2.10	119.23	123.52
23	c	502	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
27	A	410	BCR	C21-C20-C19	-2.09	117.14	123.20
25	d	404	PL9	C36-C34-C33	-2.09	116.47	121.17
27	j	102	BCR	C35-C13-C14	-2.09	119.43	122.82
31	B	623	LMG	O6-C5-C4	2.09	113.47	109.70
28	D	409	DGD	C1D-O6D-C5D	-2.09	109.64	113.72
23	c	503	CLA	O2D-CGD-CBD	2.09	114.88	111.23
23	b	614	CLA	CMB-C2B-C3B	2.09	131.46	126.55
34	v	201	HEM	C3B-C2B-C1B	2.09	107.98	106.41
23	B	612	CLA	C1-C2-C3	-2.09	122.78	126.20
23	B	607	CLA	O2D-CGD-CBD	2.09	114.88	111.23
31	d	407	LMG	O8-C28-O10	-2.09	118.41	123.63
27	B	620	BCR	C32-C1-C6	-2.09	106.97	110.24
31	A	414	LMG	O8-C28-O10	-2.08	118.42	123.63
31	B	622	LMG	O4-C4-C3	-2.08	105.47	110.38
27	B	617	BCR	C8-C7-C6	-2.08	121.44	127.00
25	d	404	PL9	C10-C9-C11	2.08	118.84	115.23
31	k	103	LMG	C3-C4-C5	2.08	114.00	110.23
27	b	622	BCR	C23-C24-C25	-2.08	121.44	127.00
31	D	406	LMG	C1-O6-C5	-2.08	109.66	113.72
25	A	408	PL9	C26-C24-C23	-2.08	116.50	121.17
27	c	514	BCR	C12-C13-C14	2.08	122.28	119.01
27	b	622	BCR	C20-C19-C18	-2.08	120.67	126.36
23	C	510	CLA	CHB-C4A-NA	2.07	127.39	124.40
28	B	621	DGD	C4D-C3D-C2D	-2.07	107.19	110.83
27	C	514	BCR	C23-C24-C25	-2.07	121.47	127.00
27	c	514	BCR	C34-C9-C8	2.07	121.25	118.09
23	C	506	CLA	CAA-CBA-CGA	-2.07	107.33	113.21
28	c	518	DGD	C6E-C5E-C4E	-2.07	107.94	113.02
25	d	404	PL9	C47-C48-C49	-2.07	120.75	127.64
25	A	408	PL9	C15-C14-C16	2.07	118.82	115.23
23	B	611	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
28	a	413	DGD	O6D-C1D-O3G	2.07	114.93	110.04
25	A	408	PL9	C10-C9-C11	2.07	118.81	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	404	PL9	C20-C19-C21	2.07	118.81	115.23
27	c	514	BCR	C33-C5-C4	2.07	118.00	113.60
31	m	102	LMG	O8-C9-C8	-2.06	102.44	108.40
31	C	521	LMG	O8-C28-O10	-2.06	118.46	123.63
27	J	102	BCR	C15-C16-C17	-2.06	119.30	123.52
27	k	102	BCR	C11-C10-C9	-2.06	124.39	127.28
27	B	620	BCR	C1-C6-C5	-2.06	119.82	122.64
28	d	409	DGD	O1G-C1A-O1A	-2.06	118.47	123.63
24	A	406	PHO	O2D-CGD-CBD	2.06	113.21	110.95
27	C	514	BCR	C39-C30-C25	-2.05	107.02	110.24
33	i	102	LMT	O1'-C1'-C2'	2.05	111.39	108.27
31	B	623	LMG	O3-C3-C4	-2.05	105.53	110.38
27	J	102	BCR	C39-C30-C25	-2.05	107.02	110.24
27	C	514	BCR	C2-C3-C4	-2.05	106.76	111.28
27	T	102	BCR	C27-C26-C25	-2.05	119.93	122.70
23	b	613	CLA	O2D-CGD-CBD	2.05	114.81	111.23
23	c	502	CLA	O2D-CGD-CBD	2.05	114.81	111.23
33	I	102	LMT	O1B-C4'-C3'	2.05	112.44	107.23
27	b	622	BCR	C31-C1-C6	-2.05	107.03	110.24
27	C	514	BCR	C2-C1-C6	2.05	113.41	110.44
25	a	410	PL9	C15-C14-C16	2.05	118.78	115.23
27	T	101	BCR	C8-C7-C6	-2.05	121.53	127.00
31	i	101	LMG	O1-C1-C2	2.05	111.38	108.27
24	A	406	PHO	C2D-C1D-ND	-2.04	107.95	109.43
23	b	620	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
23	c	506	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
27	C	514	BCR	C33-C5-C4	2.04	117.95	113.60
27	b	621	BCR	C31-C1-C6	-2.04	107.05	110.24
29	a	414	LHG	C5-O7-C7	-2.04	112.92	117.80
27	k	102	BCR	C38-C26-C27	2.04	117.94	113.60
27	d	405	BCR	C36-C18-C19	2.03	121.20	118.09
23	B	608	CLA	C1-C2-C3	-2.03	122.87	126.20
27	B	619	BCR	C37-C22-C21	-2.03	119.52	122.82
23	D	401	CLA	CHB-C4A-NA	2.03	127.33	124.40
25	a	410	PL9	C10-C9-C11	2.03	118.75	115.23
23	C	503	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
25	A	408	PL9	C11-C9-C8	-2.03	116.62	121.17
23	C	509	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
23	b	611	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
27	C	515	BCR	C33-C5-C4	2.03	117.92	113.60
34	f	101	HEM	C2B-C1B-NB	-2.03	107.51	109.84
27	k	102	BCR	C28-C27-C26	-2.02	110.45	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	h	101	BCR	C16-C15-C14	-2.02	119.38	123.52
23	A	407	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
33	b	627	LMT	C1B-O1B-C4'	-2.02	113.18	117.98
31	I	101	LMG	O8-C28-O10	-2.02	118.58	123.63
23	C	504	CLA	C3A-C2A-C1A	2.02	104.36	101.34
23	b	614	CLA	O2D-CGD-CBD	2.02	114.76	111.23
27	B	620	BCR	C15-C16-C17	-2.02	119.39	123.52
31	a	416	LMG	O8-C28-O10	-2.02	118.58	123.63
23	C	507	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
31	C	521	LMG	C6-C5-C4	-2.02	108.07	113.02
28	c	516	DGD	O4D-C4D-C5D	-2.02	104.36	109.32
25	D	404	PL9	C30-C29-C31	2.02	118.73	115.23
31	a	402	LMG	O7-C10-O9	-2.01	119.00	123.70
34	f	101	HEM	CHB-C1B-NB	2.01	126.86	124.37
25	D	404	PL9	C53-C6-C1	2.01	119.40	115.28
23	a	405	CLA	C16-C15-C13	-2.01	109.28	115.97
31	a	402	LMG	O6-C5-C4	2.01	113.32	109.70
27	B	617	BCR	C40-C30-C25	-2.01	107.09	110.24
23	b	612	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
31	A	418	LMG	O3-C3-C4	-2.01	105.64	110.38
23	B	615	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
27	B	620	BCR	C28-C27-C26	-2.01	110.48	114.06
23	c	510	CLA	C1-C2-C3	-2.01	122.91	126.20
25	a	410	PL9	C53-C6-C1	2.01	119.39	115.28
27	b	621	BCR	C38-C26-C27	2.01	117.87	113.60
27	D	405	BCR	C33-C5-C4	2.01	117.87	113.60
27	T	101	BCR	C28-C27-C26	-2.00	110.48	114.06
23	a	406	CLA	O2D-CGD-CBD	2.00	114.73	111.23
27	a	412	BCR	C21-C20-C19	-2.00	117.40	123.20
31	M	101	LMG	O3-C3-C4	-2.00	105.66	110.38
28	b	623	DGD	C2G-O2G-C1B	2.00	122.59	117.80
23	b	612	CLA	O1D-CGD-CBD	2.00	128.47	124.52
28	c	518	DGD	O6D-C1D-O3G	2.00	114.77	110.04
27	B	619	BCR	C31-C1-C6	-2.00	107.11	110.24

All (70) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
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
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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
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	b	617	CLA	ND
23	b	618	CLA	ND
23	b	619	CLA	ND
23	b	620	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	402	CLA	ND
23	d	403	CLA	ND

All (2110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C1A-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	C3A-C2A-CAA-CBA
23	B	602	CLA	C6-C7-C8-C9
23	B	603	CLA	CBD-CGD-O2D-CED
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	C4B-C3B-CAB-CBB
23	B	607	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	607	CLA	C2B-C3B-CAB-CBB
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
23	B	616	CLA	C3A-C2A-CAA-CBA
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	CBD-CGD-O2D-CED
23	C	505	CLA	C1A-C2A-CAA-CBA
23	C	505	CLA	C3A-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	C	511	CLA	CBD-CGD-O2D-CED
23	C	511	CLA	C6-C7-C8-C9
23	C	512	CLA	C1A-C2A-CAA-CBA
23	D	401	CLA	C2-C3-C5-C6
23	D	401	CLA	C4-C3-C5-C6
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	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	C6-C7-C8-C9
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	609	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	C1A-C2A-CAA-CBA
23	b	610	CLA	C3A-C2A-CAA-CBA
23	b	610	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	611	CLA	C4B-C3B-CAB-CBB
23	b	611	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	C1A-C2A-CAA-CBA
23	b	613	CLA	C2B-C3B-CAB-CBB
23	b	613	CLA	C4B-C3B-CAB-CBB
23	b	614	CLA	C2B-C3B-CAB-CBB
23	b	614	CLA	C4B-C3B-CAB-CBB
23	b	614	CLA	CBD-CGD-O2D-CED
23	b	618	CLA	CAD-CBD-CGD-O1D
23	b	618	CLA	CAD-CBD-CGD-O2D
23	b	620	CLA	C3A-C2A-CAA-CBA
23	b	620	CLA	C2B-C3B-CAB-CBB
23	b	620	CLA	C4B-C3B-CAB-CBB
23	b	620	CLA	CBD-CGD-O2D-CED
23	c	501	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	c	512	CLA	C1A-C2A-CAA-CBA
23	d	402	CLA	C2-C3-C5-C6
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	C30-C29-C31-C32
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	C27-C28-C29-C30
25	a	410	PL9	C27-C28-C29-C31
25	a	410	PL9	C28-C29-C31-C32
25	a	410	PL9	C30-C29-C31-C32
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	C23-C24-C25-C26
27	B	618	BCR	C23-C24-C25-C30
27	C	514	BCR	C11-C12-C13-C14
27	C	514	BCR	C11-C12-C13-C35
27	C	516	BCR	C7-C8-C9-C10
27	D	405	BCR	C5-C6-C7-C8
27	D	405	BCR	C7-C8-C9-C10
27	D	405	BCR	C7-C8-C9-C34
27	T	102	BCR	C21-C22-C23-C24
27	T	102	BCR	C23-C24-C25-C26
27	T	102	BCR	C23-C24-C25-C30
27	y	101	BCR	C7-C8-C9-C10
27	y	101	BCR	C7-C8-C9-C34
27	y	101	BCR	C21-C22-C23-C24
27	y	101	BCR	C37-C22-C23-C24
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	C7-C8-C9-C34
27	k	102	BCR	C21-C22-C23-C24
27	k	102	BCR	C37-C22-C23-C24
28	A	411	DGD	C2D-C1D-O3G-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	A	411	DGD	O6D-C1D-O3G-C3G
28	B	627	DGD	C2B-C1B-O2G-C2G
28	B	627	DGD	O1B-C1B-O2G-C2G
28	C	517	DGD	C2D-C1D-O3G-C3G
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	409	DGD	C2B-C1B-O2G-C2G
28	D	409	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	b	602	DGD	O2G-C2G-C3G-O3G
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	C2D-C1D-O3G-C3G
28	c	518	DGD	O6D-C1D-O3G-C3G
28	d	409	DGD	C2B-C1B-O2G-C2G
28	d	409	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	626	SQD	O5-C5-C6-S
30	D	408	SQD	C2-C1-O6-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	D	408	SQD	O6-C44-C45-O47
30	D	408	SQD	O49-C7-O47-C45
30	D	408	SQD	C8-C7-O47-C45
30	F	102	SQD	O5-C1-O6-C44
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	408	SQD	C2-C1-O6-C44
30	d	408	SQD	O6-C44-C45-O47
30	d	408	SQD	O49-C7-O47-C45
30	d	408	SQD	C8-C7-O47-C45
30	f	102	SQD	O5-C1-O6-C44
31	B	622	LMG	O1-C7-C8-O7
31	B	622	LMG	O9-C10-O7-C8
31	B	622	LMG	C11-C10-O7-C8
31	B	623	LMG	O9-C10-O7-C8
31	B	623	LMG	C11-C10-O7-C8
31	C	520	LMG	C11-C10-O7-C8
31	C	521	LMG	O9-C10-O7-C8
31	C	521	LMG	C11-C10-O7-C8
31	D	406	LMG	C11-C10-O7-C8
31	D	407	LMG	C2-C1-O1-C7
31	D	407	LMG	O6-C1-O1-C7
31	M	101	LMG	O9-C10-O7-C8
31	b	624	LMG	O1-C7-C8-O7
31	b	624	LMG	O9-C10-O7-C8
31	b	624	LMG	C11-C10-O7-C8
31	b	625	LMG	O9-C10-O7-C8
31	b	625	LMG	C11-C10-O7-C8
31	c	519	LMG	C8-C9-O8-C28
31	c	519	LMG	O9-C10-O7-C8
31	c	519	LMG	C11-C10-O7-C8
31	d	406	LMG	O9-C10-O7-C8
31	d	406	LMG	C11-C10-O7-C8
31	d	407	LMG	C2-C1-O1-C7
31	d	407	LMG	O6-C1-O1-C7
31	k	103	LMG	C11-C10-O7-C8
31	m	102	LMG	O9-C10-O7-C8
23	A	403	CLA	O1D-CGD-O2D-CED
23	C	503	CLA	O1D-CGD-O2D-CED
23	C	505	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	404	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	O1D-CGD-O2D-CED
23	c	505	CLA	O1D-CGD-O2D-CED
33	B	628	LMT	C3'-C4'-O1B-C1B
33	b	603	LMT	C3'-C4'-O1B-C1B
23	B	604	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	O1D-CGD-O2D-CED
23	b	620	CLA	O1D-CGD-O2D-CED
23	c	503	CLA	O1D-CGD-O2D-CED
23	A	403	CLA	CBD-CGD-O2D-CED
23	B	611	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	CBD-CGD-O2D-CED
23	B	614	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	a	404	CLA	CBD-CGD-O2D-CED
23	b	607	CLA	CBD-CGD-O2D-CED
23	b	615	CLA	CBD-CGD-O2D-CED
23	b	617	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
23	c	512	CLA	CBD-CGD-O2D-CED
30	A	417	SQD	O10-C23-O48-C46
30	a	401	SQD	O10-C23-O48-C46
30	f	102	SQD	O10-C23-O48-C46
31	B	622	LMG	O10-C28-O8-C9
31	D	407	LMG	O10-C28-O8-C9
31	E	101	LMG	O10-C28-O8-C9
31	a	416	LMG	O10-C28-O8-C9
31	b	624	LMG	O10-C28-O8-C9
31	d	407	LMG	O10-C28-O8-C9
28	B	621	DGD	C4D-C5D-C6D-O5D
25	A	408	PL9	C37-C38-C39-C40
25	A	408	PL9	C37-C38-C39-C41
25	a	410	PL9	C37-C38-C39-C40
25	a	410	PL9	C37-C38-C39-C41
31	C	521	LMG	C8-C9-O8-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	511	CLA	O1D-CGD-O2D-CED
31	d	407	LMG	C29-C28-O8-C9
31	e	101	LMG	C29-C28-O8-C9
23	B	607	CLA	CBD-CGD-O2D-CED
23	C	501	CLA	CBD-CGD-O2D-CED
28	D	409	DGD	O1A-C1A-O1G-C1G
28	d	409	DGD	O1A-C1A-O1G-C1G
30	F	102	SQD	O10-C23-O48-C46
31	A	414	LMG	O10-C28-O8-C9
31	C	521	LMG	O10-C28-O8-C9
31	c	519	LMG	O10-C28-O8-C9
31	e	101	LMG	O10-C28-O8-C9
28	c	517	DGD	C4E-C5E-C6E-O5E
23	C	511	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	O1D-CGD-O2D-CED
23	C	504	CLA	O1D-CGD-O2D-CED
23	b	609	CLA	O1D-CGD-O2D-CED
23	b	614	CLA	O1D-CGD-O2D-CED
23	c	504	CLA	O1D-CGD-O2D-CED
28	D	409	DGD	O6D-C5D-C6D-O5D
28	d	409	DGD	O6D-C5D-C6D-O5D
28	C	517	DGD	O1B-C1B-O2G-C2G
28	D	409	DGD	O1B-C1B-O2G-C2G
28	c	516	DGD	O1B-C1B-O2G-C2G
28	d	409	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	e	101	LMG	O9-C10-O7-C8
31	i	101	LMG	O9-C10-O7-C8
23	B	601	CLA	O1D-CGD-O2D-CED
23	b	605	CLA	O1D-CGD-O2D-CED
28	C	518	DGD	C4E-C5E-C6E-O5E
23	A	405	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
28	D	409	DGD	C2A-C1A-O1G-C1G
28	d	409	DGD	C2A-C1A-O1G-C1G
30	f	102	SQD	C24-C23-O48-C46
31	A	414	LMG	C29-C28-O8-C9
31	C	521	LMG	C29-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	D	407	LMG	C29-C28-O8-C9
31	E	101	LMG	C29-C28-O8-C9
31	a	416	LMG	C29-C28-O8-C9
31	c	519	LMG	C29-C28-O8-C9
28	a	413	DGD	O6E-C5E-C6E-O5E
23	B	606	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	CBD-CGD-O2D-CED
23	b	618	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
24	A	406	PHO	CBD-CGD-O2D-CED
24	a	408	PHO	CBD-CGD-O2D-CED
28	C	517	DGD	C2B-C1B-O2G-C2G
28	c	516	DGD	C2B-C1B-O2G-C2G
30	F	102	SQD	C8-C7-O47-C45
30	f	102	SQD	C8-C7-O47-C45
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	c	508	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	O1D-CGD-O2D-CED
33	b	604	LMT	C3'-C4'-O1B-C1B
23	B	610	CLA	O1D-CGD-O2D-CED
23	b	611	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C4-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	b	606	CLA	C4-C3-C5-C6
23	b	607	CLA	C4-C3-C5-C6
23	b	609	CLA	C4-C3-C5-C6
25	A	408	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	b	606	CLA	C2-C3-C5-C6
23	b	607	CLA	C2-C3-C5-C6
25	A	408	PL9	C28-C29-C31-C32
25	A	408	PL9	C33-C34-C36-C37
25	a	410	PL9	C33-C34-C36-C37
33	B	629	LMT	C3'-C4'-O1B-C1B
23	B	611	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	607	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	O1D-CGD-O2D-CED
28	A	411	DGD	O6E-C5E-C6E-O5E
31	k	103	LMG	O6-C5-C6-O5
23	B	608	CLA	C3-C5-C6-C7
23	B	614	CLA	C3-C5-C6-C7
23	b	612	CLA	C3-C5-C6-C7
23	b	618	CLA	C3-C5-C6-C7
30	F	102	SQD	C24-C23-O48-C46
31	B	622	LMG	C29-C28-O8-C9
31	C	520	LMG	C29-C28-O8-C9
31	b	624	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
25	a	410	PL9	C22-C23-C24-C25
28	b	623	DGD	C4D-C5D-C6D-O5D
25	A	408	PL9	C22-C23-C24-C26
25	a	410	PL9	C22-C23-C24-C26
31	C	520	LMG	O6-C5-C6-O5
31	I	101	LMG	O9-C10-O7-C8
31	a	402	LMG	O9-C10-O7-C8
23	B	613	CLA	O1D-CGD-O2D-CED
23	C	506	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C3-C5-C6-C7
23	C	509	CLA	C3-C5-C6-C7
23	b	606	CLA	C3-C5-C6-C7
23	C	512	CLA	CBD-CGD-O2D-CED
33	i	102	LMT	C3'-C4'-O1B-C1B
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	i	101	LMG	C29-C28-O8-C9
28	c	517	DGD	O6E-C5E-C6E-O5E
31	A	418	LMG	O6-C5-C6-O5
31	k	103	LMG	O10-C28-O8-C9
28	A	411	DGD	C4E-C5E-C6E-O5E
31	b	624	LMG	O6-C5-C6-O5
23	b	613	CLA	CBD-CGD-O2D-CED
31	A	418	LMG	C11-C10-O7-C8
31	I	101	LMG	C11-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	a	402	LMG	C11-C10-O7-C8
31	i	101	LMG	C11-C10-O7-C8
33	I	102	LMT	C3'-C4'-O1B-C1B
28	a	413	DGD	C4E-C5E-C6E-O5E
23	b	617	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	C3-C5-C6-C7
23	B	614	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	C4-C3-C5-C6
24	D	402	PHO	C4-C3-C5-C6
24	a	407	PHO	C4-C3-C5-C6
24	D	402	PHO	C2-C3-C5-C6
24	a	407	PHO	C2-C3-C5-C6
31	C	520	LMG	O10-C28-O8-C9
31	A	414	LMG	O6-C5-C6-O5
31	B	622	LMG	O6-C5-C6-O5
31	M	101	LMG	O6-C5-C6-O5
31	a	402	LMG	O6-C5-C6-O5
25	A	408	PL9	C24-C26-C27-C28
25	A	408	PL9	C29-C31-C32-C33
25	D	404	PL9	C34-C36-C37-C38
25	a	410	PL9	C24-C26-C27-C28
25	a	410	PL9	C29-C31-C32-C33
25	d	404	PL9	C34-C36-C37-C38
28	B	621	DGD	C4E-C5E-C6E-O5E
28	C	518	DGD	O6E-C5E-C6E-O5E
28	c	516	DGD	O6E-C5E-C6E-O5E
34	V	201	HEM	C3D-CAD-CBD-CGD
34	v	201	HEM	C3D-CAD-CBD-CGD
31	k	103	LMG	C4-C5-C6-O5
23	B	607	CLA	C2A-CAA-CBA-CGA
23	b	611	CLA	C2A-CAA-CBA-CGA
23	b	614	CLA	C2A-CAA-CBA-CGA
23	C	501	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	O1D-CGD-O2D-CED
28	B	621	DGD	O6D-C1D-O3G-C3G
28	B	621	DGD	O6E-C1E-O5D-C6D
28	b	623	DGD	O6D-C1D-O3G-C3G
28	b	623	DGD	O6E-C1E-O5D-C6D
31	A	418	LMG	O6-C1-O1-C7
31	C	520	LMG	O6-C1-O1-C7
31	C	521	LMG	O6-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	E	101	LMG	O6-C1-O1-C7
31	M	101	LMG	O6-C1-O1-C7
31	c	519	LMG	O6-C1-O1-C7
31	e	101	LMG	O6-C1-O1-C7
31	k	103	LMG	O6-C1-O1-C7
31	C	521	LMG	O6-C5-C6-O5
31	c	519	LMG	O6-C5-C6-O5
23	b	615	CLA	O1D-CGD-O2D-CED
23	B	608	CLA	CBD-CGD-O2D-CED
23	B	609	CLA	CBD-CGD-O2D-CED
23	B	612	CLA	CBD-CGD-O2D-CED
28	C	517	DGD	O6E-C5E-C6E-O5E
31	a	416	LMG	O6-C5-C6-O5
25	D	404	PL9	C22-C23-C24-C25
25	d	404	PL9	C22-C23-C24-C25
28	D	409	DGD	C4D-C5D-C6D-O5D
28	d	409	DGD	C4D-C5D-C6D-O5D
28	B	621	DGD	O6E-C5E-C6E-O5E
28	b	623	DGD	C4E-C5E-C6E-O5E
31	B	622	LMG	C4-C5-C6-O5
31	a	416	LMG	C4-C5-C6-O5
23	b	612	CLA	CBD-CGD-O2D-CED
31	d	407	LMG	C11-C10-O7-C8
31	A	414	LMG	C4-C5-C6-O5
31	C	520	LMG	C4-C5-C6-O5
31	C	520	LMG	O9-C10-O7-C8
23	B	607	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	CBA-CGA-O2A-C1
23	B	616	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CBA-CGA-O2A-C1
23	b	620	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
28	c	516	DGD	C4E-C5E-C6E-O5E
23	B	605	CLA	C2-C3-C5-C6
23	b	609	CLA	C2-C3-C5-C6
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	a	405	CLA	C6-C7-C8-C9
23	b	612	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C14-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	C	513	CLA	O1D-CGD-O2D-CED
28	B	621	DGD	C2E-C1E-O5D-C6D
28	B	627	DGD	C2E-C1E-O5D-C6D
28	C	517	DGD	C2E-C1E-O5D-C6D
28	C	519	DGD	C2D-C1D-O3G-C3G
28	b	602	DGD	C2E-C1E-O5D-C6D
28	b	623	DGD	C2E-C1E-O5D-C6D
28	c	516	DGD	C2D-C1D-O3G-C3G
28	c	516	DGD	C2E-C1E-O5D-C6D
30	A	413	SQD	C2-C1-O6-C44
30	a	415	SQD	C2-C1-O6-C44
31	C	520	LMG	C2-C1-O1-C7
31	C	521	LMG	C2-C1-O1-C7
31	E	101	LMG	C2-C1-O1-C7
31	M	101	LMG	C2-C1-O1-C7
31	c	519	LMG	C2-C1-O1-C7
31	e	101	LMG	C2-C1-O1-C7
31	k	103	LMG	C2-C1-O1-C7
31	m	102	LMG	C2-C1-O1-C7
31	C	521	LMG	C4-C5-C6-O5
31	b	624	LMG	C4-C5-C6-O5
27	B	618	BCR	C7-C8-C9-C34
27	B	618	BCR	C37-C22-C23-C24
27	C	516	BCR	C7-C8-C9-C34
27	T	102	BCR	C7-C8-C9-C34
27	T	102	BCR	C37-C22-C23-C24
27	c	515	BCR	C7-C8-C9-C34
27	c	515	BCR	C37-C22-C23-C24
27	B	618	BCR	C7-C8-C9-C10
27	C	514	BCR	C7-C8-C9-C10
27	T	102	BCR	C7-C8-C9-C10
23	B	610	CLA	C2A-CAA-CBA-CGA
31	E	101	LMG	C28-C29-C30-C31
31	d	406	LMG	C10-C11-C12-C13
23	B	616	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	O1A-CGA-O2A-C1
24	D	402	PHO	O1A-CGA-O2A-C1
24	a	407	PHO	O1A-CGA-O2A-C1
31	I	101	LMG	O10-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	b	623	DGD	O6E-C5E-C6E-O5E
31	c	519	LMG	C4-C5-C6-O5
23	b	616	CLA	CBD-CGD-O2D-CED
30	B	626	SQD	C8-C7-O47-C45
28	B	627	DGD	O2G-C2G-C3G-O3G
31	m	102	LMG	C29-C28-O8-C9
23	B	607	CLA	C15-C16-C17-C18
31	D	406	LMG	C10-C11-C12-C13
31	e	101	LMG	C28-C29-C30-C31
23	c	501	CLA	O1D-CGD-O2D-CED
24	a	408	PHO	O1D-CGD-O2D-CED
25	A	408	PL9	C7-C8-C9-C10
23	B	609	CLA	C13-C15-C16-C17
23	B	612	CLA	C5-C6-C7-C8
23	c	509	CLA	C5-C6-C7-C8
23	d	402	CLA	C15-C16-C17-C18
23	b	610	CLA	O1D-CGD-O2D-CED
28	C	517	DGD	C4E-C5E-C6E-O5E
23	c	512	CLA	CBA-CGA-O2A-C1
30	b	601	SQD	C24-C23-O48-C46
31	I	101	LMG	O6-C5-C6-O5
28	C	517	DGD	C1B-C2B-C3B-C4B
28	c	516	DGD	C1B-C2B-C3B-C4B
31	C	521	LMG	C28-C29-C30-C31
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	A	405	CLA	C10-C11-C12-C13
23	D	401	CLA	C13-C15-C16-C17
23	a	406	CLA	C10-C11-C12-C13
23	b	612	CLA	C15-C16-C17-C18
23	b	620	CLA	C5-C6-C7-C8
23	c	503	CLA	C10-C11-C12-C13
31	i	101	LMG	O6-C5-C6-O5
28	B	627	DGD	C1A-C2A-C3A-C4A
28	a	413	DGD	C1B-C2B-C3B-C4B
28	d	409	DGD	C1B-C2B-C3B-C4B
31	B	623	LMG	C10-C11-C12-C13
31	c	519	LMG	C28-C29-C30-C31
23	B	605	CLA	O1A-CGA-O2A-C1
23	C	513	CLA	O1A-CGA-O2A-C1
23	b	620	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	b	601	SQD	C8-C7-O47-C45
23	B	606	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	C13-C15-C16-C17
23	C	501	CLA	C15-C16-C17-C18
23	C	503	CLA	C10-C11-C12-C13
23	C	509	CLA	C5-C6-C7-C8
23	b	611	CLA	C15-C16-C17-C18
23	b	615	CLA	C15-C16-C17-C18
23	b	616	CLA	C5-C6-C7-C8
23	b	620	CLA	C10-C11-C12-C13
23	c	501	CLA	C15-C16-C17-C18
23	c	504	CLA	C13-C15-C16-C17
23	B	601	CLA	C2A-CAA-CBA-CGA
23	C	508	CLA	C2A-CAA-CBA-CGA
23	C	512	CLA	C2A-CAA-CBA-CGA
23	b	605	CLA	C2A-CAA-CBA-CGA
23	c	508	CLA	C2A-CAA-CBA-CGA
23	c	512	CLA	C2A-CAA-CBA-CGA
23	B	604	CLA	C13-C15-C16-C17
23	B	616	CLA	C5-C6-C7-C8
23	C	506	CLA	C15-C16-C17-C18
23	D	401	CLA	C15-C16-C17-C18
23	b	605	CLA	C13-C15-C16-C17
23	b	614	CLA	C8-C10-C11-C12
23	b	616	CLA	C13-C15-C16-C17
23	c	506	CLA	C15-C16-C17-C18
23	c	508	CLA	C15-C16-C17-C18
23	c	513	CLA	C15-C16-C17-C18
24	a	408	PHO	C15-C16-C17-C18
31	m	102	LMG	O6-C5-C6-O5
28	A	411	DGD	C1B-C2B-C3B-C4B
28	D	409	DGD	C1B-C2B-C3B-C4B
28	b	602	DGD	C1A-C2A-C3A-C4A
31	C	521	LMG	C10-C11-C12-C13
31	b	625	LMG	C10-C11-C12-C13
23	b	618	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
23	A	403	CLA	C3-C5-C6-C7
28	B	627	DGD	O6E-C1E-O5D-C6D
28	C	517	DGD	O6E-C1E-O5D-C6D
28	b	602	DGD	O6E-C1E-O5D-C6D
28	c	516	DGD	O6D-C1D-O3G-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	c	516	DGD	O6E-C1E-O5D-C6D
31	a	402	LMG	O6-C1-O1-C7
31	m	102	LMG	O6-C1-O1-C7
23	A	404	CLA	C15-C16-C17-C18
23	B	607	CLA	C13-C15-C16-C17
23	B	610	CLA	C8-C10-C11-C12
23	B	611	CLA	C15-C16-C17-C18
23	B	612	CLA	C13-C15-C16-C17
23	B	616	CLA	C10-C11-C12-C13
23	C	504	CLA	C13-C15-C16-C17
23	C	513	CLA	C15-C16-C17-C18
23	b	608	CLA	C13-C15-C16-C17
23	b	611	CLA	C13-C15-C16-C17
23	b	613	CLA	C13-C15-C16-C17
23	c	501	CLA	C8-C10-C11-C12
23	c	504	CLA	C15-C16-C17-C18
23	c	507	CLA	C5-C6-C7-C8
23	c	508	CLA	C10-C11-C12-C13
23	d	402	CLA	C13-C15-C16-C17
24	A	406	PHO	C15-C16-C17-C18
31	i	101	LMG	O10-C28-O8-C9
31	A	418	LMG	C4-C5-C6-O5
31	c	519	LMG	C10-C11-C12-C13
23	B	608	CLA	C15-C16-C17-C18
23	C	501	CLA	C8-C10-C11-C12
23	C	504	CLA	C15-C16-C17-C18
23	a	405	CLA	C15-C16-C17-C18
28	C	519	DGD	O1B-C1B-O2G-C2G
30	F	102	SQD	O49-C7-O47-C45
23	A	404	CLA	C3-C5-C6-C7
24	A	406	PHO	O1D-CGD-O2D-CED
23	C	506	CLA	C13-C15-C16-C17
23	C	508	CLA	C10-C11-C12-C13
23	C	508	CLA	C15-C16-C17-C18
23	a	406	CLA	C15-C16-C17-C18
23	c	504	CLA	C10-C11-C12-C13
23	c	510	CLA	C15-C16-C17-C18
30	b	601	SQD	O10-C23-O48-C46
28	b	623	DGD	C1B-C2B-C3B-C4B
30	a	415	SQD	C7-C8-C9-C10
23	C	512	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	D	407	LMG	C11-C10-O7-C8
28	c	516	DGD	C1A-C2A-C3A-C4A
23	C	504	CLA	C10-C11-C12-C13
23	C	506	CLA	C5-C6-C7-C8
23	C	505	CLA	C10-C11-C12-C13
23	c	505	CLA	C10-C11-C12-C13
28	B	621	DGD	C1B-C2B-C3B-C4B
28	c	518	DGD	O1B-C1B-O2G-C2G
30	f	102	SQD	O49-C7-O47-C45
31	k	103	LMG	O9-C10-O7-C8
29	A	412	LHG	C1-C2-C3-O3
29	a	414	LHG	C1-C2-C3-O3
30	B	626	SQD	C24-C23-O48-C46
31	M	101	LMG	C29-C28-O8-C9
23	B	613	CLA	C5-C6-C7-C8
23	C	507	CLA	C5-C6-C7-C8
23	c	506	CLA	C5-C6-C7-C8
23	c	511	CLA	C5-C6-C7-C8
28	C	518	DGD	O6D-C5D-C6D-O5D
28	c	517	DGD	O6D-C5D-C6D-O5D
23	b	620	CLA	C3-C5-C6-C7
23	b	619	CLA	C13-C15-C16-C17
23	b	613	CLA	O1D-CGD-O2D-CED
23	A	405	CLA	C15-C16-C17-C18
23	B	615	CLA	C13-C15-C16-C17
23	B	616	CLA	C13-C15-C16-C17
23	C	510	CLA	C15-C16-C17-C18
23	C	511	CLA	C5-C6-C7-C8
23	c	501	CLA	C10-C11-C12-C13
23	C	512	CLA	CBA-CGA-O2A-C1
28	B	621	DGD	O6D-C5D-C6D-O5D
25	D	404	PL9	C35-C34-C36-C37
28	C	518	DGD	C4D-C5D-C6D-O5D
28	c	517	DGD	C4D-C5D-C6D-O5D
23	B	616	CLA	C3-C5-C6-C7
25	J	101	PL9	C12-C13-C14-C15
25	j	101	PL9	C12-C13-C14-C15
28	C	518	DGD	C2D-C1D-O3G-C3G
28	C	518	DGD	C2E-C1E-O5D-C6D
28	c	517	DGD	C2D-C1D-O3G-C3G
28	c	517	DGD	C2E-C1E-O5D-C6D
31	B	623	LMG	C2-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	I	101	LMG	C2-C1-O1-C7
31	i	101	LMG	C2-C1-O1-C7
23	B	608	CLA	C5-C6-C7-C8
23	b	612	CLA	C5-C6-C7-C8
30	A	413	SQD	C7-C8-C9-C10
28	C	517	DGD	C1A-C2A-C3A-C4A
31	M	101	LMG	C4-C5-C6-O5
23	b	617	CLA	C5-C6-C7-C8
27	C	514	BCR	C7-C8-C9-C34
27	C	516	BCR	C37-C22-C23-C24
27	D	405	BCR	C37-C22-C23-C24
27	c	514	BCR	C7-C8-C9-C34
27	d	405	BCR	C37-C22-C23-C24
27	c	514	BCR	C7-C8-C9-C10
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	620	CLA	C13-C15-C16-C17
31	C	520	LMG	C10-C11-C12-C13
28	D	409	DGD	C1G-C2G-O2G-C1B
28	d	409	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	a	405	CLA	C3-C5-C6-C7
23	a	409	CLA	C10-C11-C12-C13
28	C	517	DGD	O6D-C1D-O3G-C3G
28	b	623	DGD	O6D-C5D-C6D-O5D
23	C	509	CLA	C2-C1-O2A-CGA
30	B	626	SQD	O10-C23-O48-C46
28	b	623	DGD	C6B-C7B-C8B-C9B
28	d	409	DGD	C7B-C8B-C9B-CAB
29	a	417	LHG	C11-C10-C9-C8
31	b	624	LMG	C31-C32-C33-C34
31	b	625	LMG	C31-C32-C33-C34
28	C	517	DGD	C3A-C4A-C5A-C6A
30	b	601	SQD	C11-C10-C9-C8
31	A	414	LMG	C29-C30-C31-C32
31	B	623	LMG	C31-C32-C33-C34
31	a	416	LMG	C14-C15-C16-C17
31	a	416	LMG	C34-C35-C36-C37
31	m	102	LMG	C29-C30-C31-C32
23	a	409	CLA	C5-C6-C7-C8
28	d	409	DGD	C3A-C4A-C5A-C6A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	M	101	LMG	C29-C30-C31-C32
23	b	609	CLA	CBA-CGA-O2A-C1
29	A	412	LHG	C25-C26-C27-C28
31	A	414	LMG	C34-C35-C36-C37
28	D	409	DGD	C7B-C8B-C9B-CAB
28	c	516	DGD	C3A-C4A-C5A-C6A
28	c	518	DGD	C9B-CAB-CBB-CCB
31	A	414	LMG	C14-C15-C16-C17
31	A	418	LMG	C11-C12-C13-C14
31	B	622	LMG	C31-C32-C33-C34
31	D	407	LMG	C36-C37-C38-C39
23	B	609	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	C4B-C3B-CAB-CBB
23	B	605	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C4B-C3B-CAB-CBB
23	D	403	CLA	C4B-C3B-CAB-CBB
23	b	605	CLA	C4B-C3B-CAB-CBB
23	b	608	CLA	C4B-C3B-CAB-CBB
23	b	609	CLA	C4B-C3B-CAB-CBB
23	c	504	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
28	B	627	DGD	C2A-C3A-C4A-C5A
28	D	409	DGD	C3A-C4A-C5A-C6A
30	A	413	SQD	C14-C15-C16-C17
30	a	415	SQD	C14-C15-C16-C17
31	a	402	LMG	C11-C12-C13-C14
23	A	407	CLA	C10-C11-C12-C13
23	b	605	CLA	C10-C11-C12-C13
28	C	519	DGD	C2B-C1B-O2G-C2G
28	c	518	DGD	C2B-C1B-O2G-C2G
28	b	602	DGD	C2A-C3A-C4A-C5A
30	B	626	SQD	C11-C10-C9-C8
31	d	407	LMG	C36-C37-C38-C39
29	A	415	LHG	C11-C10-C9-C8
30	f	102	SQD	C12-C13-C14-C15
31	a	416	LMG	C29-C30-C31-C32
31	b	625	LMG	C34-C35-C36-C37
28	A	411	DGD	C5B-C6B-C7B-C8B
28	C	519	DGD	C9B-CAB-CBB-CCB
28	a	413	DGD	C5B-C6B-C7B-C8B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	414	LHG	C25-C26-C27-C28
31	b	624	LMG	C30-C31-C32-C33
31	d	407	LMG	C19-C20-C21-C22
23	A	404	CLA	C3A-C2A-CAA-CBA
23	B	607	CLA	C3A-C2A-CAA-CBA
23	B	608	CLA	C3A-C2A-CAA-CBA
23	C	507	CLA	C3A-C2A-CAA-CBA
23	C	512	CLA	C3A-C2A-CAA-CBA
23	a	405	CLA	C3A-C2A-CAA-CBA
23	b	612	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
23	B	608	CLA	O1D-CGD-O2D-CED
30	F	102	SQD	C12-C13-C14-C15
31	B	623	LMG	C34-C35-C36-C37
23	C	501	CLA	C10-C11-C12-C13
23	c	512	CLA	C13-C15-C16-C17
31	i	101	LMG	C14-C15-C16-C17
23	d	403	CLA	C15-C16-C17-C18
23	c	504	CLA	CBA-CGA-O2A-C1
28	c	518	DGD	O1G-C1G-C2G-C3G
28	d	409	DGD	CCB-CDB-CEB-CFB
29	a	417	LHG	C24-C25-C26-C27
31	B	622	LMG	C30-C31-C32-C33
28	c	517	DGD	C1A-C2A-C3A-C4A
31	B	622	LMG	C28-C29-C30-C31
23	C	506	CLA	C10-C11-C12-C13
28	C	517	DGD	C3B-C4B-C5B-C6B
28	C	518	DGD	C2A-C3A-C4A-C5A
28	C	519	DGD	C3B-C4B-C5B-C6B
31	I	101	LMG	C14-C15-C16-C17
33	i	102	LMT	C6-C7-C8-C9
23	C	512	CLA	O1A-CGA-O2A-C1
33	b	626	LMT	C1-C2-C3-C4
28	D	409	DGD	CCB-CDB-CEB-CFB
28	D	409	DGD	CEB-CFB-CGB-CHB
28	c	516	DGD	C3B-C4B-C5B-C6B
29	A	415	LHG	C24-C25-C26-C27
31	D	407	LMG	C19-C20-C21-C22
31	c	519	LMG	C12-C13-C14-C15
23	B	612	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	503	CLA	C5-C6-C7-C8
33	B	624	LMT	C1-C2-C3-C4
28	B	621	DGD	C6B-C7B-C8B-C9B
28	B	627	DGD	C5B-C6B-C7B-C8B
28	c	518	DGD	C3B-C4B-C5B-C6B
28	d	409	DGD	CEB-CFB-CGB-CHB
31	C	521	LMG	C29-C30-C31-C32
31	c	519	LMG	C29-C30-C31-C32
31	d	407	LMG	C13-C14-C15-C16
33	I	102	LMT	C6-C7-C8-C9
25	a	410	PL9	C7-C8-C9-C10
23	B	613	CLA	C16-C17-C18-C19
28	C	518	DGD	C1A-C2A-C3A-C4A
31	b	624	LMG	C28-C29-C30-C31
25	d	404	PL9	C47-C48-C49-C51
23	B	601	CLA	C2B-C3B-CAB-CBB
23	B	604	CLA	C2B-C3B-CAB-CBB
23	B	606	CLA	C2B-C3B-CAB-CBB
23	C	501	CLA	C2B-C3B-CAB-CBB
23	C	504	CLA	C2B-C3B-CAB-CBB
23	b	605	CLA	C2B-C3B-CAB-CBB
23	b	611	CLA	C2B-C3B-CAB-CBB
23	c	501	CLA	C2B-C3B-CAB-CBB
23	c	504	CLA	C2B-C3B-CAB-CBB
27	C	514	BCR	C1-C6-C7-C8
27	C	516	BCR	C1-C6-C7-C8
27	D	405	BCR	C1-C6-C7-C8
27	H	101	BCR	C1-C6-C7-C8
27	H	101	BCR	C5-C6-C7-C8
27	c	514	BCR	C1-C6-C7-C8
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
31	D	407	LMG	C13-C14-C15-C16
31	D	407	LMG	C15-C16-C17-C18
23	C	510	CLA	CBD-CGD-O2D-CED
31	b	625	LMG	C29-C28-O8-C9
34	V	201	HEM	C2D-C3D-CAD-CBD
34	F	101	HEM	C3D-CAD-CBD-CGD
34	f	101	HEM	C3D-CAD-CBD-CGD
28	c	517	DGD	C2A-C3A-C4A-C5A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	d	409	DGD	CAB-CBB-CCB-CDB
30	A	413	SQD	C27-C28-C29-C30
31	b	624	LMG	C18-C19-C20-C21
23	b	610	CLA	C2A-CAA-CBA-CGA
31	A	418	LMG	C18-C19-C20-C21
31	B	622	LMG	C18-C19-C20-C21
31	d	407	LMG	C15-C16-C17-C18
23	b	609	CLA	O1A-CGA-O2A-C1
28	D	409	DGD	C2A-C3A-C4A-C5A
30	F	102	SQD	C11-C12-C13-C14
28	d	409	DGD	CDB-CEB-CFB-CGB
31	I	101	LMG	C16-C17-C18-C19
31	i	101	LMG	C16-C17-C18-C19
31	A	414	LMG	C30-C31-C32-C33
31	k	103	LMG	C10-C11-C12-C13
23	b	615	CLA	CBA-CGA-O2A-C1
23	A	403	CLA	C11-C12-C13-C14
28	D	409	DGD	C6B-C7B-C8B-C9B
31	d	407	LMG	C14-C15-C16-C17
31	i	101	LMG	C12-C13-C14-C15
28	C	519	DGD	CAB-CBB-CCB-CDB
28	D	409	DGD	CAB-CBB-CCB-CDB
28	b	602	DGD	C9B-CAB-CBB-CCB
30	a	415	SQD	C27-C28-C29-C30
30	f	102	SQD	C11-C12-C13-C14
31	C	521	LMG	C12-C13-C14-C15
31	D	407	LMG	C14-C15-C16-C17
31	B	623	LMG	O6-C1-O1-C7
31	I	101	LMG	O6-C1-O1-C7
28	d	409	DGD	C2A-C3A-C4A-C5A
28	d	409	DGD	C4B-C5B-C6B-C7B
31	a	402	LMG	C18-C19-C20-C21
31	d	406	LMG	O6-C5-C6-O5
23	C	512	CLA	C13-C15-C16-C17
33	B	628	LMT	C7-C8-C9-C10
25	j	101	PL9	C27-C28-C29-C31
33	B	628	LMT	C2-C3-C4-C5
33	b	603	LMT	C2-C3-C4-C5
28	D	409	DGD	C4B-C5B-C6B-C7B
28	D	409	DGD	CDB-CEB-CFB-CGB
31	E	101	LMG	C15-C16-C17-C18
31	I	101	LMG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	503	CLA	C5-C6-C7-C8
23	b	605	CLA	C16-C17-C18-C20
31	A	414	LMG	C11-C10-O7-C8
31	E	101	LMG	C11-C10-O7-C8
31	e	101	LMG	C11-C10-O7-C8
31	D	407	LMG	C28-C29-C30-C31
28	d	409	DGD	C6B-C7B-C8B-C9B
23	D	403	CLA	C15-C16-C17-C18
31	d	407	LMG	O9-C10-O7-C8
28	c	518	DGD	CAB-CBB-CCB-CDB
30	B	626	SQD	C11-C12-C13-C14
23	c	506	CLA	C10-C11-C12-C13
23	c	513	CLA	C13-C15-C16-C17
27	J	102	BCR	C37-C22-C23-C24
31	B	623	LMG	C29-C28-O8-C9
31	D	407	LMG	C8-C7-O1-C1
31	a	416	LMG	C8-C7-O1-C1
33	b	603	LMT	C7-C8-C9-C10
23	c	504	CLA	C2A-CAA-CBA-CGA
23	B	613	CLA	C16-C17-C18-C20
23	b	605	CLA	C16-C17-C18-C19
23	A	404	CLA	C4-C3-C5-C6
31	a	402	LMG	C31-C32-C33-C34
31	b	625	LMG	C13-C14-C15-C16
31	i	101	LMG	C13-C14-C15-C16
23	B	601	CLA	C10-C11-C12-C13
23	B	602	CLA	C5-C6-C7-C8
31	d	407	LMG	C28-C29-C30-C31
30	F	102	SQD	C10-C11-C12-C13
31	a	416	LMG	C30-C31-C32-C33
31	e	101	LMG	C15-C16-C17-C18
23	c	504	CLA	O1A-CGA-O2A-C1
25	J	101	PL9	C27-C28-C29-C31
30	f	102	SQD	C10-C11-C12-C13
31	I	101	LMG	C13-C14-C15-C16
23	C	513	CLA	C13-C15-C16-C17
23	b	606	CLA	C5-C6-C7-C8
28	b	623	DGD	C5B-C6B-C7B-C8B
28	c	516	DGD	C4A-C5A-C6A-C7A
28	C	519	DGD	O1G-C1G-C2G-O2G
28	c	518	DGD	O1G-C1G-C2G-O2G
30	B	626	SQD	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	409	DGD	C3B-C4B-C5B-C6B
23	B	614	CLA	C15-C16-C17-C18
23	b	606	CLA	C13-C15-C16-C17
31	I	101	LMG	C4-C5-C6-O5
31	a	402	LMG	C4-C5-C6-O5
28	c	516	DGD	C4B-C5B-C6B-C7B
28	c	517	DGD	CCB-CDB-CEB-CFB
28	d	409	DGD	C5B-C6B-C7B-C8B
31	A	418	LMG	C31-C32-C33-C34
31	b	624	LMG	C19-C20-C21-C22
23	c	509	CLA	C2-C1-O2A-CGA
31	D	406	LMG	O6-C5-C6-O5
31	E	101	LMG	O6-C5-C6-O5
34	V	201	HEM	C4D-C3D-CAD-CBD
23	C	510	CLA	C4-C3-C5-C6
25	j	101	PL9	C15-C14-C16-C17
31	D	407	LMG	O9-C10-O7-C8
23	A	407	CLA	C5-C6-C7-C8
28	C	517	DGD	C4A-C5A-C6A-C7A
28	C	517	DGD	C4B-C5B-C6B-C7B
28	D	409	DGD	C5B-C6B-C7B-C8B
28	d	409	DGD	C3B-C4B-C5B-C6B
23	A	403	CLA	C2A-CAA-CBA-CGA
23	C	501	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
28	d	409	DGD	C5A-C6A-C7A-C8A
23	C	503	CLA	C8-C10-C11-C12
23	C	512	CLA	C5-C6-C7-C8
30	b	601	SQD	C11-C12-C13-C14
23	b	612	CLA	O1D-CGD-O2D-CED
23	C	502	CLA	C3-C5-C6-C7
28	b	602	DGD	C5B-C6B-C7B-C8B
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	620	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
23	b	618	CLA	C15-C16-C17-C18
28	C	518	DGD	CCB-CDB-CEB-CFB
30	b	601	SQD	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	B	627	DGD	C9B-CAB-CBB-CCB
30	D	408	SQD	C9-C10-C11-C12
31	D	407	LMG	C32-C33-C34-C35
31	b	624	LMG	C13-C14-C15-C16
23	C	505	CLA	C15-C16-C17-C18
29	a	414	LHG	O6-C4-C5-C6
23	c	502	CLA	C3-C5-C6-C7
23	B	603	CLA	C6-C7-C8-C10
23	B	615	CLA	C11-C10-C8-C7
23	B	615	CLA	C12-C13-C15-C16
23	C	502	CLA	C11-C12-C13-C15
23	C	503	CLA	C11-C10-C8-C7
23	C	503	CLA	C11-C12-C13-C15
23	C	505	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	D	401	CLA	C12-C13-C15-C16
23	b	607	CLA	C11-C12-C13-C15
23	b	617	CLA	C11-C10-C8-C7
23	b	619	CLA	C12-C13-C15-C16
23	c	502	CLA	C11-C12-C13-C15
23	c	503	CLA	C11-C10-C8-C7
23	c	503	CLA	C11-C12-C13-C15
23	c	505	CLA	C6-C7-C8-C10
23	c	511	CLA	C12-C13-C15-C16
23	d	402	CLA	C12-C13-C15-C16
24	A	406	PHO	C12-C13-C15-C16
24	a	408	PHO	C12-C13-C15-C16
29	A	412	LHG	C30-C31-C32-C33
31	a	402	LMG	C32-C33-C34-C35
23	b	617	CLA	C16-C17-C18-C19
23	b	615	CLA	O1A-CGA-O2A-C1
30	A	417	SQD	C18-C19-C20-C21
23	B	602	CLA	C13-C15-C16-C17
28	b	602	DGD	C3A-C4A-C5A-C6A
23	c	510	CLA	C4-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
31	B	623	LMG	C13-C14-C15-C16
31	a	416	LMG	C11-C10-O7-C8
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	503	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C9
23	a	404	CLA	C11-C12-C13-C14
23	b	607	CLA	C6-C7-C8-C9
23	b	607	CLA	C11-C12-C13-C14
23	b	610	CLA	C14-C13-C15-C16
23	b	613	CLA	C6-C7-C8-C9
23	c	505	CLA	C14-C13-C15-C16
23	c	508	CLA	C11-C10-C8-C9
23	c	512	CLA	C11-C12-C13-C14
23	C	504	CLA	CBA-CGA-O2A-C1
23	D	403	CLA	CBA-CGA-O2A-C1
23	d	403	CLA	CBA-CGA-O2A-C1
30	a	415	SQD	C11-C10-C9-C8
28	B	627	DGD	C2B-C3B-C4B-C5B
30	a	401	SQD	C18-C19-C20-C21
30	a	415	SQD	C17-C18-C19-C20
31	b	624	LMG	C36-C37-C38-C39
28	c	518	DGD	C1A-C2A-C3A-C4A
28	B	621	DGD	O1G-C1G-C2G-C3G
28	C	519	DGD	O1G-C1G-C2G-C3G
28	D	409	DGD	C1G-C2G-C3G-O3G
28	b	602	DGD	C1G-C2G-C3G-O3G
28	b	623	DGD	O1G-C1G-C2G-C3G
28	d	409	DGD	C1G-C2G-C3G-O3G
30	A	417	SQD	O6-C44-C45-C46
30	B	626	SQD	C44-C45-C46-O48
30	a	401	SQD	O6-C44-C45-C46
30	b	601	SQD	C44-C45-C46-O48
31	C	520	LMG	C7-C8-C9-O8
31	D	407	LMG	O1-C7-C8-C9
31	d	407	LMG	O1-C7-C8-C9
31	k	103	LMG	C7-C8-C9-O8
28	b	602	DGD	C2B-C3B-C4B-C5B
31	e	101	LMG	O6-C5-C6-O5
23	C	505	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	CBA-CGA-O2A-C1
28	B	627	DGD	C3A-C4A-C5A-C6A
28	d	409	DGD	C8B-C9B-CAB-CBB
31	E	101	LMG	C17-C18-C19-C20
23	b	616	CLA	O1D-CGD-O2D-CED
23	c	503	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	517	DGD	C5A-C6A-C7A-C8A
28	b	623	DGD	C3B-C4B-C5B-C6B
31	B	622	LMG	C36-C37-C38-C39
30	d	408	SQD	C9-C10-C11-C12
23	C	510	CLA	C2-C3-C5-C6
28	B	621	DGD	C3B-C4B-C5B-C6B
23	B	604	CLA	C8-C10-C11-C12
23	b	608	CLA	C8-C10-C11-C12
30	A	413	SQD	C11-C10-C9-C8
30	A	413	SQD	C17-C18-C19-C20
31	i	101	LMG	C4-C5-C6-O5
31	b	625	LMG	O10-C28-O8-C9
31	m	102	LMG	O10-C28-O8-C9
23	B	604	CLA	C15-C16-C17-C18
23	C	502	CLA	C13-C15-C16-C17
23	c	502	CLA	C13-C15-C16-C17
29	a	414	LHG	C30-C31-C32-C33
23	c	505	CLA	C15-C16-C17-C18
31	B	622	LMG	C10-C11-C12-C13
31	B	623	LMG	O10-C28-O8-C9
28	D	409	DGD	C5A-C6A-C7A-C8A
31	B	622	LMG	C19-C20-C21-C22
23	b	608	CLA	C15-C16-C17-C18
28	B	621	DGD	C5B-C6B-C7B-C8B
30	a	401	SQD	C32-C33-C34-C35
33	I	102	LMT	C5'-C4'-O1B-C1B
29	a	417	LHG	O6-C4-C5-O7
31	i	101	LMG	O6-C1-O1-C7
23	B	611	CLA	CBA-CGA-O2A-C1
23	b	614	CLA	CBA-CGA-O2A-C1
29	A	415	LHG	C24-C23-O8-C6
31	D	406	LMG	C38-C39-C40-C41
28	c	516	DGD	C5A-C6A-C7A-C8A
31	A	414	LMG	C20-C21-C22-C23
31	D	406	LMG	C31-C32-C33-C34
31	a	416	LMG	C15-C16-C17-C18
23	a	405	CLA	C4-C3-C5-C6
25	J	101	PL9	C15-C14-C16-C17
28	B	621	DGD	CAB-CBB-CCB-CDB
30	A	417	SQD	C10-C11-C12-C13
31	e	101	LMG	C17-C18-C19-C20
23	B	610	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	518	DGD	CAB-CBB-CCB-CDB
30	A	417	SQD	C32-C33-C34-C35
31	A	414	LMG	C15-C16-C17-C18
31	a	416	LMG	C20-C21-C22-C23
31	A	418	LMG	C28-C29-C30-C31
30	A	413	SQD	O6-C44-C45-O47
30	a	415	SQD	O6-C44-C45-O47
31	A	414	LMG	O1-C7-C8-O7
31	E	101	LMG	O1-C7-C8-O7
31	d	406	LMG	C38-C39-C40-C41
31	B	622	LMG	C20-C21-C22-C23
23	C	509	CLA	CBA-CGA-O2A-C1
31	A	418	LMG	C15-C16-C17-C18
31	d	406	LMG	C31-C32-C33-C34
23	c	510	CLA	C3-C5-C6-C7
31	e	101	LMG	C19-C20-C21-C22
33	b	627	LMT	C2B-C1B-O1B-C4'
23	B	610	CLA	C16-C17-C18-C19
23	c	512	CLA	C16-C17-C18-C20
31	E	101	LMG	C19-C20-C21-C22
23	c	507	CLA	CBD-CGD-O2D-CED
23	d	403	CLA	O1A-CGA-O2A-C1
23	B	610	CLA	CBA-CGA-O2A-C1
29	a	417	LHG	C24-C23-O8-C6
30	A	417	SQD	C12-C13-C14-C15
30	a	401	SQD	C12-C13-C14-C15
31	d	407	LMG	C11-C12-C13-C14
33	i	102	LMT	C5'-C4'-O1B-C1B
23	B	616	CLA	C8-C10-C11-C12
23	b	620	CLA	C8-C10-C11-C12
23	b	614	CLA	C16-C17-C18-C20
23	b	617	CLA	C16-C17-C18-C20
23	C	505	CLA	C4-C3-C5-C6
23	c	513	CLA	C4-C3-C5-C6
31	d	407	LMG	C10-C11-C12-C13
28	c	517	DGD	CAB-CBB-CCB-CDB
33	B	625	LMT	C2B-C1B-O1B-C4'
30	A	413	SQD	C10-C11-C12-C13
31	d	407	LMG	C32-C33-C34-C35
23	A	404	CLA	C6-C7-C8-C9
23	B	603	CLA	C6-C7-C8-C9
23	B	609	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	505	CLA	C14-C13-C15-C16
23	C	511	CLA	C14-C13-C15-C16
23	C	512	CLA	C11-C12-C13-C14
23	D	401	CLA	C14-C13-C15-C16
23	b	613	CLA	C14-C13-C15-C16
23	b	619	CLA	C11-C10-C8-C9
23	b	619	CLA	C14-C13-C15-C16
23	c	502	CLA	C11-C12-C13-C14
23	c	502	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C10-C8-C9
23	c	503	CLA	C11-C12-C13-C14
23	c	505	CLA	C6-C7-C8-C9
23	c	506	CLA	C14-C13-C15-C16
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
31	B	622	LMG	C15-C16-C17-C18
31	k	103	LMG	C16-C17-C18-C19
23	B	616	CLA	C15-C16-C17-C18
23	b	609	CLA	C15-C16-C17-C18
23	B	601	CLA	C4B-C3B-CAB-CBB
23	B	608	CLA	C4B-C3B-CAB-CBB
23	B	611	CLA	C4B-C3B-CAB-CBB
23	B	615	CLA	C4B-C3B-CAB-CBB
23	C	502	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
23	b	612	CLA	C4B-C3B-CAB-CBB
23	b	615	CLA	C4B-C3B-CAB-CBB
23	b	619	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	C2A-CAA-CBA-CGA
31	B	623	LMG	C15-C16-C17-C18
31	b	624	LMG	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	409	DGD	C2D-C1D-O3G-C3G
28	d	409	DGD	C2D-C1D-O3G-C3G
23	C	510	CLA	C3-C5-C6-C7
29	A	412	LHG	O6-C4-C5-C6
23	A	404	CLA	C12-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C10
23	B	605	CLA	C11-C10-C8-C7
23	B	606	CLA	C12-C13-C15-C16
23	B	609	CLA	C12-C13-C15-C16
23	B	610	CLA	C11-C12-C13-C15
23	B	610	CLA	C12-C13-C15-C16
23	B	611	CLA	C11-C10-C8-C7
23	B	613	CLA	C11-C10-C8-C7
23	B	616	CLA	C11-C10-C8-C7
23	C	502	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	506	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C7
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	403	CLA	C11-C10-C8-C7
23	b	606	CLA	C6-C7-C8-C10
23	b	607	CLA	C6-C7-C8-C10
23	b	610	CLA	C12-C13-C15-C16
23	b	613	CLA	C12-C13-C15-C16
23	b	614	CLA	C11-C12-C13-C15
23	b	614	CLA	C12-C13-C15-C16
23	b	619	CLA	C11-C10-C8-C7
23	b	620	CLA	C11-C10-C8-C7
23	c	502	CLA	C12-C13-C15-C16
23	c	505	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	A	407	CLA	C13-C15-C16-C17
23	D	403	CLA	O1A-CGA-O2A-C1
28	b	623	DGD	CAB-CBB-CCB-CDB
23	b	614	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	i	101	LMG	C18-C19-C20-C21
31	B	622	LMG	C17-C18-C19-C20
23	A	403	CLA	C3A-C2A-CAA-CBA
23	C	513	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
23	a	409	CLA	C13-C15-C16-C17
23	b	620	CLA	C15-C16-C17-C18
23	C	513	CLA	C2-C3-C5-C6
28	C	518	DGD	O6E-C1E-O5D-C6D
28	c	517	DGD	O6E-C1E-O5D-C6D
28	D	409	DGD	CBA-CCA-CDA-CEA
23	C	505	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	C15-C16-C17-C18
27	B	618	BCR	C13-C14-C15-C16
27	j	102	BCR	C7-C8-C9-C34
24	a	407	PHO	C5-C6-C7-C8
31	E	101	LMG	C18-C19-C20-C21
30	a	401	SQD	C10-C11-C12-C13
25	j	101	PL9	C19-C21-C22-C23
28	B	627	DGD	C1G-C2G-C3G-O3G
28	c	517	DGD	C1G-C2G-C3G-O3G
30	A	413	SQD	O6-C44-C45-C46
30	a	415	SQD	O6-C44-C45-C46
30	d	408	SQD	O6-C44-C45-C46
31	A	414	LMG	O1-C7-C8-C9
31	B	623	LMG	C7-C8-C9-O8
31	I	101	LMG	O1-C7-C8-C9
31	M	101	LMG	C7-C8-C9-O8
31	b	625	LMG	C7-C8-C9-O8
31	i	101	LMG	O1-C7-C8-C9
31	m	102	LMG	C7-C8-C9-O8
23	C	512	CLA	C3-C5-C6-C7
23	B	601	CLA	C16-C17-C18-C20
28	d	409	DGD	CBA-CCA-CDA-CEA
28	C	517	DGD	C2A-C3A-C4A-C5A
31	A	418	LMG	C12-C13-C14-C15
28	c	518	DGD	CFA-CGA-CHA-CIA
31	C	520	LMG	C16-C17-C18-C19
31	I	101	LMG	C18-C19-C20-C21
23	c	511	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C2-C3-C5-C6
23	c	512	CLA	C3-C5-C6-C7
23	C	512	CLA	C16-C17-C18-C20
31	D	407	LMG	C10-C11-C12-C13
29	a	414	LHG	O6-C4-C5-O7
28	D	409	DGD	C8B-C9B-CAB-CBB
31	B	622	LMG	C13-C14-C15-C16
27	C	514	BCR	C5-C6-C7-C8
27	C	515	BCR	C1-C6-C7-C8
27	C	516	BCR	C23-C24-C25-C30
27	T	101	BCR	C1-C6-C7-C8
27	y	101	BCR	C1-C6-C7-C8
27	y	101	BCR	C23-C24-C25-C30
27	c	514	BCR	C5-C6-C7-C8
27	c	515	BCR	C1-C6-C7-C8
27	c	515	BCR	C23-C24-C25-C30
27	k	102	BCR	C1-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C30
27	z	101	BCR	C1-C6-C7-C8
29	A	412	LHG	C8-C7-O7-C5
30	A	413	SQD	C15-C16-C17-C18
31	D	407	LMG	C11-C12-C13-C14
31	b	625	LMG	C15-C16-C17-C18
31	e	101	LMG	C18-C19-C20-C21
31	m	102	LMG	C11-C12-C13-C14
23	a	405	CLA	C5-C6-C7-C8
28	b	602	DGD	O1G-C1G-C2G-O2G
30	B	626	SQD	O47-C45-C46-O48
30	a	415	SQD	O47-C45-C46-O48
30	b	601	SQD	O47-C45-C46-O48
30	f	102	SQD	O47-C45-C46-O48
31	B	623	LMG	O7-C8-C9-O8
31	I	101	LMG	O1-C7-C8-O7
31	b	625	LMG	O7-C8-C9-O8
31	i	101	LMG	O1-C7-C8-O7
30	A	413	SQD	C31-C32-C33-C34
31	a	402	LMG	C12-C13-C14-C15
30	D	408	SQD	C7-C8-C9-C10
23	B	611	CLA	O1A-CGA-O2A-C1
28	A	411	DGD	C3B-C4B-C5B-C6B
24	D	402	PHO	C5-C6-C7-C8
23	C	505	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	519	LMG	C13-C14-C15-C16
23	B	601	CLA	C16-C17-C18-C19
23	c	512	CLA	C16-C17-C18-C19
28	C	519	DGD	CDB-CEB-CFB-CGB
31	C	521	LMG	C13-C14-C15-C16
31	a	402	LMG	C28-C29-C30-C31
23	b	608	CLA	CBA-CGA-O2A-C1
23	b	614	CLA	O1A-CGA-O2A-C1
23	A	404	CLA	C14-C13-C15-C16
23	B	609	CLA	C14-C13-C15-C16
23	b	617	CLA	C11-C10-C8-C9
23	c	508	CLA	C5-C6-C7-C8
28	c	516	DGD	C2A-C3A-C4A-C5A
30	a	415	SQD	C10-C11-C12-C13
31	b	624	LMG	C17-C18-C19-C20
25	J	101	PL9	C19-C21-C22-C23
25	J	101	PL9	C24-C26-C27-C28
25	a	410	PL9	C14-C16-C17-C18
25	a	410	PL9	C19-C21-C22-C23
33	B	625	LMT	O5B-C1B-O1B-C4'
28	a	413	DGD	C8B-C9B-CAB-CBB
30	A	417	SQD	C30-C31-C32-C33
30	B	626	SQD	C12-C13-C14-C15
31	A	414	LMG	C31-C32-C33-C34
28	D	409	DGD	C1A-C2A-C3A-C4A
31	A	418	LMG	C32-C33-C34-C35
23	c	505	CLA	CBA-CGA-O2A-C1
33	b	627	LMT	O5B-C1B-O1B-C4'
30	b	601	SQD	C15-C16-C17-C18
23	b	617	CLA	C13-C15-C16-C17
23	c	505	CLA	C8-C10-C11-C12
31	M	101	LMG	C11-C12-C13-C14
23	C	509	CLA	O1A-CGA-O2A-C1
31	M	101	LMG	O10-C28-O8-C9
28	d	409	DGD	C1A-C2A-C3A-C4A
30	a	415	SQD	C31-C32-C33-C34
23	A	404	CLA	C5-C6-C7-C8
29	a	417	LHG	O6-C4-C5-C6
23	C	508	CLA	C5-C6-C7-C8
28	C	519	DGD	CDA-CEA-CFA-CGA
23	B	602	CLA	C11-C10-C8-C7
23	B	608	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	613	CLA	C11-C12-C13-C15
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	C	510	CLA	C6-C7-C8-C10
23	a	405	CLA	C12-C13-C15-C16
23	b	609	CLA	C11-C10-C8-C7
23	b	612	CLA	C6-C7-C8-C10
23	b	615	CLA	C11-C10-C8-C7
23	b	617	CLA	C11-C12-C13-C15
23	b	620	CLA	C12-C13-C15-C16
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	c	512	CLA	C12-C13-C15-C16
30	d	408	SQD	C7-C8-C9-C10
31	C	520	LMG	C30-C31-C32-C33
23	C	507	CLA	C3-C5-C6-C7
23	b	609	CLA	C10-C11-C12-C13
27	D	405	BCR	C21-C22-C23-C24
27	c	515	BCR	C21-C22-C23-C24
27	d	405	BCR	C21-C22-C23-C24
34	v	201	HEM	C2D-C3D-CAD-CBD
23	C	511	CLA	CBA-CGA-O2A-C1
30	a	415	SQD	C15-C16-C17-C18
31	A	414	LMG	C8-C7-O1-C1
31	d	407	LMG	C8-C7-O1-C1
23	C	504	CLA	C2A-CAA-CBA-CGA
28	c	518	DGD	CDB-CEB-CFB-CGB
31	m	102	LMG	C30-C31-C32-C33
23	B	610	CLA	O1A-CGA-O2A-C1
29	A	415	LHG	O10-C23-O8-C6
31	a	402	LMG	C15-C16-C17-C18
31	b	624	LMG	C15-C16-C17-C18
23	b	607	CLA	C8-C10-C11-C12
23	c	512	CLA	C5-C6-C7-C8
28	C	519	DGD	C3G-C2G-O2G-C1B
31	C	521	LMG	C9-C8-O7-C10
31	c	519	LMG	C9-C8-O7-C10
23	c	501	CLA	C13-C15-C16-C17
33	B	624	LMT	C4-C5-C6-C7
23	C	510	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	B	627	DGD	CAB-CBB-CCB-CDB
23	B	610	CLA	C10-C11-C12-C13
28	B	621	DGD	C7A-C8A-C9A-CAA
25	D	404	PL9	C47-C48-C49-C51
29	A	412	LHG	O9-C7-O7-C5
29	A	412	LHG	O6-C4-C5-O7
31	A	418	LMG	C17-C18-C19-C20
30	D	408	SQD	O5-C1-O6-C44
31	b	625	LMG	O6-C1-O1-C7
23	c	507	CLA	O1D-CGD-O2D-CED
28	C	518	DGD	C1G-C2G-C3G-O3G
31	B	622	LMG	O1-C7-C8-C9
31	b	624	LMG	O1-C7-C8-C9
34	F	101	HEM	C4B-C3B-CAB-CBB
34	V	201	HEM	C4C-C3C-CAC-CBC
34	f	101	HEM	C4B-C3B-CAB-CBB
34	v	201	HEM	C4C-C3C-CAC-CBC
23	C	512	CLA	C16-C17-C18-C19
28	b	623	DGD	C4B-C5B-C6B-C7B
29	a	417	LHG	C25-C26-C27-C28
30	A	417	SQD	C33-C34-C35-C36
25	D	404	PL9	C15-C14-C16-C17
25	d	404	PL9	C15-C14-C16-C17
23	A	404	CLA	C2-C3-C5-C6
28	C	519	DGD	CFA-CGA-CHA-CIA
30	a	401	SQD	C23-C24-C25-C26
28	C	517	DGD	C2B-C3B-C4B-C5B
23	B	612	CLA	C10-C11-C12-C13
28	D	409	DGD	O2G-C2G-C3G-O3G
28	b	623	DGD	O1G-C1G-C2G-O2G
28	d	409	DGD	O2G-C2G-C3G-O3G
30	A	413	SQD	O47-C45-C46-O48
31	a	416	LMG	O1-C7-C8-O7
31	e	101	LMG	O1-C7-C8-O7
31	m	102	LMG	O7-C8-C9-O8
23	B	605	CLA	C5-C6-C7-C8
23	b	616	CLA	C10-C11-C12-C13
23	B	613	CLA	C11-C12-C13-C14
23	B	615	CLA	C6-C7-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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C14-C13-C15-C16
23	a	405	CLA	C14-C13-C15-C16
23	b	617	CLA	C11-C12-C13-C14
23	b	619	CLA	C6-C7-C8-C9
24	D	402	PHO	C6-C7-C8-C9
28	C	518	DGD	C7B-C8B-C9B-CAB
28	c	518	DGD	C8B-C9B-CAB-CBB
31	M	101	LMG	C30-C31-C32-C33
23	b	608	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	O1A-CGA-O2A-C1
31	a	402	LMG	O10-C28-O8-C9
23	a	406	CLA	C2C-C3C-CAC-CBC
31	d	406	LMG	C11-C12-C13-C14
23	B	605	CLA	C15-C16-C17-C18
23	C	509	CLA	C15-C16-C17-C18
23	b	609	CLA	C5-C6-C7-C8
33	B	629	LMT	C5'-C4'-O1B-C1B
28	a	413	DGD	C3B-C4B-C5B-C6B
31	I	101	LMG	C29-C30-C31-C32
28	C	519	DGD	C1A-C2A-C3A-C4A
29	A	412	LHG	C23-C24-C25-C26
23	c	505	CLA	O1A-CGA-O2A-C1
29	a	417	LHG	O10-C23-O8-C6
30	b	601	SQD	C12-C13-C14-C15
30	A	413	SQD	C8-C7-O47-C45
27	T	102	BCR	C13-C14-C15-C16
30	F	102	SQD	C2-C1-O6-C44
31	b	625	LMG	C2-C1-O1-C7
23	B	614	CLA	C5-C6-C7-C8
23	c	509	CLA	C10-C11-C12-C13
31	k	103	LMG	C30-C31-C32-C33
30	B	626	SQD	C15-C16-C17-C18
23	a	404	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C16-C17-C18-C20
23	b	607	CLA	C16-C17-C18-C19
23	b	607	CLA	C16-C17-C18-C20
23	C	505	CLA	C8-C10-C11-C12
31	b	625	LMG	C35-C36-C37-C38
30	a	415	SQD	C16-C17-C18-C19
23	b	610	CLA	C13-C15-C16-C17
28	b	602	DGD	CAB-CBB-CCB-CDB
27	b	622	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	518	DGD	C4B-C5B-C6B-C7B
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	604	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	CBA-CGA-O2A-C1
23	B	608	CLA	C13-C15-C16-C17
31	a	416	LMG	C31-C32-C33-C34
30	f	102	SQD	C29-C30-C31-C32
27	b	622	BCR	C21-C22-C23-C24
28	C	519	DGD	C8B-C9B-CAB-CBB
30	a	401	SQD	C30-C31-C32-C33
28	c	518	DGD	O6E-C5E-C6E-O5E
34	v	201	HEM	C4D-C3D-CAD-CBD
29	A	415	LHG	O6-C4-C5-C6
30	a	401	SQD	C33-C34-C35-C36
23	B	610	CLA	C5-C6-C7-C8
23	B	603	CLA	C11-C10-C8-C7
23	B	608	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C10
23	a	409	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
23	d	403	CLA	C11-C10-C8-C7
23	B	603	CLA	C16-C17-C18-C19
33	b	604	LMT	C5'-C4'-O1B-C1B
29	A	415	LHG	C25-C26-C27-C28
31	B	623	LMG	C35-C36-C37-C38
23	C	511	CLA	O1A-CGA-O2A-C1
23	C	510	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	C4-C3-C5-C6
23	b	616	CLA	C4-C3-C5-C6
23	A	407	CLA	C16-C17-C18-C19
28	B	621	DGD	C4B-C5B-C6B-C7B
28	B	621	DGD	C7B-C8B-C9B-CAB
28	b	623	DGD	C7A-C8A-C9A-CAA
30	b	601	SQD	O49-C7-O47-C45
29	A	415	LHG	O6-C4-C5-O7
23	B	610	CLA	C11-C12-C13-C14
23	B	611	CLA	C11-C10-C8-C9
23	B	613	CLA	C11-C10-C8-C9
23	B	616	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C11-C12-C13-C14
23	C	510	CLA	C6-C7-C8-C9
23	b	609	CLA	C11-C10-C8-C9
23	b	614	CLA	C11-C12-C13-C14
23	b	615	CLA	C11-C10-C8-C9
23	b	620	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	510	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16
23	d	403	CLA	C11-C10-C8-C9
23	b	614	CLA	C10-C11-C12-C13
24	A	406	PHO	C10-C11-C12-C13
23	a	409	CLA	C16-C17-C18-C19
23	c	507	CLA	C3-C5-C6-C7
28	B	621	DGD	O1G-C1G-C2G-O2G
31	C	520	LMG	O7-C8-C9-O8
31	D	407	LMG	O1-C7-C8-O7
31	M	101	LMG	O7-C8-C9-O8
31	d	407	LMG	O1-C7-C8-O7
31	k	103	LMG	O7-C8-C9-O8
28	c	517	DGD	C4B-C5B-C6B-C7B
28	c	516	DGD	C2B-C3B-C4B-C5B
23	B	614	CLA	C16-C17-C18-C19
30	A	413	SQD	C16-C17-C18-C19
30	D	408	SQD	O6-C44-C45-C46
30	a	415	SQD	C44-C45-C46-O48
30	f	102	SQD	C44-C45-C46-O48
31	E	101	LMG	O1-C7-C8-C9
31	e	101	LMG	O1-C7-C8-C9
23	b	614	CLA	C5-C6-C7-C8
23	b	617	CLA	C10-C11-C12-C13
23	b	618	CLA	C5-C6-C7-C8
24	a	408	PHO	C13-C15-C16-C17
25	J	101	PL9	C13-C14-C16-C17
24	a	407	PHO	CBD-CGD-O2D-CED
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
30	a	415	SQD	C8-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	604	CLA	O1A-CGA-O2A-C1
28	D	409	DGD	CBB-CCB-CDB-CEB
31	i	101	LMG	C29-C30-C31-C32
30	a	401	SQD	C26-C27-C28-C29
31	a	402	LMG	C17-C18-C19-C20
24	A	406	PHO	C13-C15-C16-C17
23	B	615	CLA	O1A-CGA-O2A-C1
31	a	402	LMG	C30-C31-C32-C33
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
29	A	412	LHG	C4-O6-P-O5
29	A	415	LHG	C3-O3-P-O5
29	a	417	LHG	C3-O3-P-O5
23	B	611	CLA	C4-C3-C5-C6
23	B	605	CLA	C2B-C3B-CAB-CBB
23	D	403	CLA	C2B-C3B-CAB-CBB
23	b	608	CLA	C2B-C3B-CAB-CBB
23	b	609	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
31	B	622	LMG	C29-C30-C31-C32
27	A	410	BCR	C7-C8-C9-C34
27	B	618	BCR	C11-C12-C13-C35
27	J	102	BCR	C7-C8-C9-C34
27	j	102	BCR	C37-C22-C23-C24
27	z	101	BCR	C7-C8-C9-C34
29	A	412	LHG	C2-C3-O3-P
29	a	414	LHG	C2-C3-O3-P
31	D	406	LMG	C11-C12-C13-C14
29	a	414	LHG	O9-C7-O7-C5
23	a	406	CLA	C5-C6-C7-C8
23	B	603	CLA	C16-C17-C18-C20
23	C	510	CLA	C16-C17-C18-C20
23	B	606	CLA	C13-C15-C16-C17
28	A	411	DGD	C8B-C9B-CAB-CBB
28	c	518	DGD	CDA-CEA-CFA-CGA
30	a	401	SQD	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	624	LMG	C29-C30-C31-C32
25	A	408	PL9	C4-C3-C7-C8
25	a	410	PL9	C4-C3-C7-C8
31	b	625	LMG	C28-C29-C30-C31
23	b	606	CLA	O1A-CGA-O2A-C1
29	a	414	LHG	C8-C7-O7-C5
30	F	102	SQD	C29-C30-C31-C32
30	A	417	SQD	C17-C18-C19-C20
28	c	518	DGD	C3G-C2G-O2G-C1B
31	B	622	LMG	C16-C17-C18-C19
23	B	603	CLA	C15-C16-C17-C18
28	D	409	DGD	CAA-CBA-CCA-CDA
31	a	402	LMG	C13-C14-C15-C16
31	i	101	LMG	C17-C18-C19-C20
23	B	613	CLA	C10-C11-C12-C13
23	A	405	CLA	C6-C7-C8-C9
23	B	601	CLA	C6-C7-C8-C9
23	B	603	CLA	C11-C12-C13-C14
23	B	605	CLA	C11-C10-C8-C9
23	D	401	CLA	C6-C7-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	a	406	CLA	C6-C7-C8-C9
23	b	605	CLA	C6-C7-C8-C9
23	c	506	CLA	C11-C12-C13-C14
23	d	402	CLA	C6-C7-C8-C9
23	A	405	CLA	C6-C7-C8-C10
23	B	601	CLA	C6-C7-C8-C10
23	B	603	CLA	C11-C12-C13-C15
23	c	504	CLA	C6-C7-C8-C10
31	A	418	LMG	C13-C14-C15-C16
23	A	407	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C20
31	C	520	LMG	C12-C13-C14-C15
28	C	518	DGD	C7A-C8A-C9A-CAA
28	c	517	DGD	C3A-C4A-C5A-C6A
23	a	405	CLA	C2-C3-C5-C6
25	j	101	PL9	C13-C14-C16-C17
28	c	517	DGD	C7A-C8A-C9A-CAA
31	A	414	LMG	C35-C36-C37-C38
30	B	626	SQD	O49-C7-O47-C45
28	B	627	DGD	O1G-C1G-C2G-O2G
30	F	102	SQD	O47-C45-C46-O48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	C	521	LMG	O1-C7-C8-O7
31	A	418	LMG	C30-C31-C32-C33
23	b	618	CLA	C16-C17-C18-C19
23	b	618	CLA	C16-C17-C18-C20
23	A	405	CLA	C5-C6-C7-C8
31	b	624	LMG	C10-C11-C12-C13
30	f	102	SQD	C24-C25-C26-C27
28	c	517	DGD	C7B-C8B-C9B-CAB
23	b	610	CLA	C16-C17-C18-C20
23	C	512	CLA	CAA-CBA-CGA-O2A
25	A	408	PL9	C14-C16-C17-C18
25	A	408	PL9	C19-C21-C22-C23
25	D	404	PL9	C9-C11-C12-C13
30	A	413	SQD	C44-C45-C46-O48
31	A	414	LMG	C38-C39-C40-C41
29	a	414	LHG	C23-C24-C25-C26
23	b	606	CLA	CBA-CGA-O2A-C1
25	j	101	PL9	C12-C13-C14-C16
27	j	102	BCR	C7-C8-C9-C10
23	c	512	CLA	CAA-CBA-CGA-O2A
28	b	602	DGD	C2G-C3G-O3G-C1D
28	c	517	DGD	C5D-C6D-O5D-C1E
23	B	605	CLA	C10-C11-C12-C13
23	B	613	CLA	C13-C15-C16-C17
28	C	519	DGD	CEA-CFA-CGA-CHA
23	B	614	CLA	C2A-CAA-CBA-CGA
23	B	604	CLA	C2C-C3C-CAC-CBC
30	d	408	SQD	O5-C1-O6-C44
23	b	615	CLA	C4-C3-C5-C6
23	b	612	CLA	C13-C15-C16-C17
33	B	629	LMT	C1-C2-C3-C4
23	C	511	CLA	C11-C10-C8-C9
23	a	409	CLA	C11-C10-C8-C9
23	b	620	CLA	C14-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C9
28	B	627	DGD	C8B-C9B-CAB-CBB
28	C	519	DGD	O1A-C1A-O1G-C1G
28	a	413	DGD	C2A-C3A-C4A-C5A
28	c	518	DGD	CEA-CFA-CGA-CHA
31	d	406	LMG	O10-C28-O8-C9
25	d	404	PL9	C13-C14-C16-C17
28	A	411	DGD	C2A-C3A-C4A-C5A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	D	408	SQD	C10-C11-C12-C13
23	C	511	CLA	C11-C10-C8-C7
23	b	612	CLA	C11-C12-C13-C15
23	c	511	CLA	C11-C10-C8-C7
23	C	510	CLA	C13-C15-C16-C17
31	k	103	LMG	C12-C13-C14-C15
33	b	626	LMT	C4-C5-C6-C7
23	B	608	CLA	O1A-CGA-O2A-C1
31	c	519	LMG	O1-C7-C8-O7
23	C	513	CLA	C3A-C2A-CAA-CBA
23	a	404	CLA	C3A-C2A-CAA-CBA
23	b	610	CLA	C4-C3-C5-C6
23	c	513	CLA	C3A-C2A-CAA-CBA
23	B	612	CLA	C2-C3-C5-C6
23	b	616	CLA	C2-C3-C5-C6
28	b	602	DGD	C8B-C9B-CAB-CBB
25	d	404	PL9	C32-C33-C34-C36
23	A	405	CLA	C2C-C3C-CAC-CBC
31	I	101	LMG	C17-C18-C19-C20
29	A	412	LHG	C24-C25-C26-C27
23	C	509	CLA	C10-C11-C12-C13
30	A	417	SQD	C23-C24-C25-C26
30	b	601	SQD	C19-C20-C21-C22
23	b	617	CLA	C8-C10-C11-C12
23	c	503	CLA	C15-C16-C17-C18
27	C	516	BCR	C21-C22-C23-C24
27	J	102	BCR	C21-C22-C23-C24
23	B	611	CLA	C2-C3-C5-C6
23	D	403	CLA	C2A-CAA-CBA-CGA
25	d	404	PL9	C39-C41-C42-C43
28	b	602	DGD	O1G-C1G-C2G-C3G
23	b	607	CLA	C15-C16-C17-C18
31	I	101	LMG	C19-C20-C21-C22
23	C	513	CLA	C14-C13-C15-C16
23	a	405	CLA	C11-C10-C8-C9
23	b	620	CLA	C11-C12-C13-C14
23	c	506	CLA	C11-C10-C8-C9
23	c	513	CLA	C11-C10-C8-C9
23	c	513	CLA	C14-C13-C15-C16
23	c	510	CLA	C16-C17-C18-C19
31	E	101	LMG	C31-C32-C33-C34
29	a	414	LHG	C4-C5-O7-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	m	102	LMG	C9-C8-O7-C10
23	B	613	CLA	C8-C10-C11-C12
23	b	618	CLA	C4C-C3C-CAC-CBC
31	a	416	LMG	C38-C39-C40-C41
23	b	615	CLA	C2-C3-C5-C6
23	B	602	CLA	O1A-CGA-O2A-C1
23	b	618	CLA	C2A-CAA-CBA-CGA
23	A	403	CLA	C1A-C2A-CAA-CBA
23	C	513	CLA	C1A-C2A-CAA-CBA
23	a	404	CLA	C1A-C2A-CAA-CBA
23	a	406	CLA	C4C-C3C-CAC-CBC
30	A	413	SQD	O49-C7-O47-C45
28	d	409	DGD	CBB-CCB-CDB-CEB
31	D	406	LMG	C17-C18-C19-C20
23	A	404	CLA	C2B-C3B-CAB-CBB
23	B	608	CLA	C2B-C3B-CAB-CBB
23	C	502	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	401	CLA	C2B-C3B-CAB-CBB
23	b	612	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
27	B	617	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	y	101	BCR	C5-C6-C7-C8
27	y	101	BCR	C23-C24-C25-C26
27	c	515	BCR	C5-C6-C7-C8
27	c	515	BCR	C23-C24-C25-C26
27	j	102	BCR	C1-C6-C7-C8
27	k	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C26
27	z	101	BCR	C5-C6-C7-C8
30	B	626	SQD	C19-C20-C21-C22
33	b	604	LMT	C1-C2-C3-C4
31	m	102	LMG	C4-C5-C6-O5
23	B	604	CLA	C4C-C3C-CAC-CBC
28	C	519	DGD	O6E-C5E-C6E-O5E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	a	416	LMG	C35-C36-C37-C38
23	A	407	CLA	C11-C10-C8-C7
23	B	605	CLA	C11-C12-C13-C15
23	C	504	CLA	C6-C7-C8-C10
23	C	508	CLA	C11-C12-C13-C15
23	C	509	CLA	C6-C7-C8-C10
23	a	406	CLA	C6-C7-C8-C10
23	b	605	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C10-C8-C7
23	b	609	CLA	C11-C12-C13-C15
23	c	508	CLA	C11-C12-C13-C15
23	c	509	CLA	C6-C7-C8-C10
23	c	513	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
23	a	405	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C2A-CAA-CBA-CGA
23	B	603	CLA	C8-C10-C11-C12
31	C	521	LMG	O7-C8-C9-O8
23	B	602	CLA	CBA-CGA-O2A-C1
28	c	518	DGD	C7A-C8A-C9A-CAA
23	b	610	CLA	C16-C17-C18-C19
28	b	623	DGD	C7B-C8B-C9B-CAB
27	B	620	BCR	C37-C22-C23-C24
23	b	612	CLA	C4-C3-C5-C6
23	C	501	CLA	C13-C15-C16-C17
23	c	510	CLA	C13-C15-C16-C17
25	D	404	PL9	C13-C14-C16-C17
28	c	517	DGD	C4A-C5A-C6A-C7A
30	f	102	SQD	C26-C27-C28-C29
23	A	403	CLA	C2-C1-O2A-CGA
23	b	617	CLA	C2-C1-O2A-CGA
31	d	407	LMG	C34-C35-C36-C37
29	a	414	LHG	C24-C25-C26-C27
24	a	407	PHO	O1D-CGD-O2D-CED
23	D	401	CLA	C3-C5-C6-C7
23	C	507	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C10-C8-C9
31	c	519	LMG	C34-C35-C36-C37
23	C	511	CLA	C4-C3-C5-C6
23	B	608	CLA	CBA-CGA-O2A-C1
25	j	101	PL9	C24-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	409	DGD	O1G-C1G-C2G-C3G
28	d	409	DGD	O1G-C1G-C2G-C3G
31	a	402	LMG	C7-C8-C9-O8
31	a	416	LMG	O1-C7-C8-C9
23	A	404	CLA	C2A-CAA-CBA-CGA
23	C	509	CLA	C2A-CAA-CBA-CGA
31	b	625	LMG	C12-C13-C14-C15
24	a	408	PHO	C10-C11-C12-C13
25	D	404	PL9	C47-C48-C49-C50
23	c	511	CLA	C4-C3-C5-C6
28	d	409	DGD	CAA-CBA-CCA-CDA
31	C	520	LMG	C29-C30-C31-C32
23	B	603	CLA	C4B-C3B-CAB-CBB
23	C	506	CLA	C4B-C3B-CAB-CBB
23	D	401	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
30	F	102	SQD	C24-C25-C26-C27
24	a	408	PHO	CHA-CBD-CGD-O1D
28	b	602	DGD	C5A-C6A-C7A-C8A
31	A	414	LMG	C12-C13-C14-C15
28	C	518	DGD	C3A-C4A-C5A-C6A
23	B	606	CLA	C16-C17-C18-C20
31	c	519	LMG	O7-C8-C9-O8
23	b	609	CLA	C8-C10-C11-C12
28	C	518	DGD	O6D-C1D-O3G-C3G
23	B	601	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C10-C8-C7
23	c	506	CLA	C6-C7-C8-C10
23	c	506	CLA	C11-C10-C8-C7
23	c	507	CLA	C11-C12-C13-C15
30	F	102	SQD	C26-C27-C28-C29
29	a	417	LHG	C7-C8-C9-C10
30	a	415	SQD	C29-C30-C31-C32
23	B	608	CLA	C11-C12-C13-C14
23	B	616	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C10-C8-C9
23	b	605	CLA	C11-C12-C13-C14
23	c	510	CLA	C11-C10-C8-C9
24	A	406	PHO	C11-C10-C8-C9
24	a	408	PHO	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	D	406	LMG	C19-C20-C21-C22
28	C	518	DGD	C5D-C6D-O5D-C1E
30	f	102	SQD	C45-C44-O6-C1
23	b	618	CLA	C2C-C3C-CAC-CBC
30	a	401	SQD	C25-C26-C27-C28
23	C	511	CLA	C2A-CAA-CBA-CGA
23	c	511	CLA	C2A-CAA-CBA-CGA
23	d	403	CLA	C2A-CAA-CBA-CGA
23	B	610	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	B	614	CLA	C2-C1-O2A-CGA
23	a	404	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	b	618	CLA	C2-C1-O2A-CGA
30	F	102	SQD	C15-C16-C17-C18
23	c	510	CLA	C16-C17-C18-C20
28	C	519	DGD	CBB-CCB-CDB-CEB
31	i	101	LMG	C19-C20-C21-C22
28	a	413	DGD	C2E-C1E-O5D-C6D
31	M	101	LMG	C9-C8-O7-C10
25	d	404	PL9	C47-C48-C49-C50
23	d	403	CLA	C4-C3-C5-C6
23	D	403	CLA	C8-C10-C11-C12
30	d	408	SQD	C10-C11-C12-C13
30	A	417	SQD	C26-C27-C28-C29
31	I	101	LMG	C15-C16-C17-C18
28	A	411	DGD	C4B-C5B-C6B-C7B
28	a	413	DGD	C4B-C5B-C6B-C7B
23	C	503	CLA	C15-C16-C17-C18
30	F	102	SQD	C44-C45-C46-O48
31	C	521	LMG	O1-C7-C8-C9
31	C	521	LMG	C7-C8-C9-O8
31	c	519	LMG	O1-C7-C8-C9
25	A	408	PL9	C15-C14-C16-C17
31	C	521	LMG	C34-C35-C36-C37
31	D	407	LMG	C31-C32-C33-C34
24	D	402	PHO	C15-C16-C17-C18
28	C	518	DGD	CBB-CCB-CDB-CEB
30	f	102	SQD	C15-C16-C17-C18
31	d	406	LMG	C17-C18-C19-C20
31	e	101	LMG	C31-C32-C33-C34
31	d	406	LMG	O1-C7-C8-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	D	406	LMG	O10-C28-O8-C9
23	A	407	CLA	C11-C10-C8-C9
23	B	601	CLA	C11-C12-C13-C14
23	B	603	CLA	C11-C10-C8-C9
23	C	506	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C10-C8-C9
23	C	502	CLA	C16-C17-C18-C20
23	c	502	CLA	C16-C17-C18-C20
31	k	103	LMG	O8-C28-C29-C30
31	B	623	LMG	C12-C13-C14-C15
23	b	610	CLA	C15-C16-C17-C18
31	D	407	LMG	C29-C30-C31-C32
31	E	101	LMG	O7-C10-C11-C12
23	C	506	CLA	C11-C10-C8-C7
23	C	513	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16
23	D	401	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	b	607	CLA	C11-C10-C8-C7
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
24	A	406	PHO	C11-C10-C8-C7
23	B	603	CLA	C2B-C3B-CAB-CBB
23	B	611	CLA	C2B-C3B-CAB-CBB
23	B	615	CLA	C2B-C3B-CAB-CBB
23	C	506	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
23	b	615	CLA	C2B-C3B-CAB-CBB
23	b	619	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
27	B	617	BCR	C5-C6-C7-C8
27	J	102	BCR	C5-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
27	a	412	BCR	C23-C24-C25-C30
27	j	102	BCR	C5-C6-C7-C8
31	e	101	LMG	O7-C10-C11-C12
23	A	404	CLA	C2-C1-O2A-CGA
23	B	601	CLA	C2-C1-O2A-CGA
23	a	405	CLA	C2-C1-O2A-CGA
23	c	508	CLA	C2-C1-O2A-CGA
28	c	517	DGD	CBB-CCB-CDB-CEB
23	b	616	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	613	CLA	CAA-CBA-CGA-O2A
28	c	517	DGD	O6D-C1D-O3G-C3G
23	b	617	CLA	CAA-CBA-CGA-O2A
31	e	101	LMG	O9-C10-C11-C12
30	A	413	SQD	C19-C20-C21-C22
23	b	612	CLA	O1A-CGA-O2A-C1
23	d	403	CLA	C8-C10-C11-C12
31	k	103	LMG	C29-C30-C31-C32
31	C	520	LMG	C35-C36-C37-C38
23	b	614	CLA	C13-C15-C16-C17
23	C	507	CLA	CAA-CBA-CGA-O2A
23	D	401	CLA	CAA-CBA-CGA-O2A
23	d	402	CLA	CAA-CBA-CGA-O2A
31	A	414	LMG	O7-C10-C11-C12
28	C	519	DGD	C7A-C8A-C9A-CAA
23	B	608	CLA	C4-C3-C5-C6
25	a	410	PL9	C15-C14-C16-C17
31	b	624	LMG	C16-C17-C18-C19
25	j	101	PL9	C17-C18-C19-C21
23	c	501	CLA	CAA-CBA-CGA-O2A
23	A	404	CLA	C2C-C3C-CAC-CBC
28	C	519	DGD	CCB-CDB-CEB-CFB
29	A	415	LHG	C9-C10-C11-C12
31	E	101	LMG	O9-C10-C11-C12
24	A	406	PHO	O1A-CGA-O2A-C1
23	A	405	CLA	C4C-C3C-CAC-CBC
23	B	614	CLA	C4C-C3C-CAC-CBC
23	A	404	CLA	C11-C10-C8-C9
23	B	605	CLA	C11-C12-C13-C14
23	C	504	CLA	C6-C7-C8-C9
23	C	508	CLA	C11-C12-C13-C14
23	a	405	CLA	C2C-C3C-CAC-CBC
28	B	621	DGD	O2G-C1B-C2B-C3B
31	a	416	LMG	O7-C10-C11-C12
31	m	102	LMG	O8-C28-C29-C30
28	c	518	DGD	CBA-CCA-CDA-CEA
31	c	519	LMG	C7-C8-C9-O8
23	B	601	CLA	C1A-C2A-CAA-CBA
23	a	405	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	c	513	CLA	C1A-C2A-CAA-CBA
31	C	520	LMG	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAA-CBA-CGA-O2A
30	D	408	SQD	O47-C7-C8-C9
30	a	401	SQD	O47-C7-C8-C9
30	d	408	SQD	O47-C7-C8-C9
31	M	101	LMG	O8-C28-C29-C30
28	a	413	DGD	O2G-C2G-C3G-O3G
31	D	406	LMG	O1-C7-C8-O7
25	d	404	PL9	C21-C22-C23-C24
31	A	414	LMG	C16-C17-C18-C19
27	B	618	BCR	C11-C12-C13-C14
27	B	620	BCR	C21-C22-C23-C24
27	J	102	BCR	C7-C8-C9-C10
27	j	102	BCR	C21-C22-C23-C24
28	c	518	DGD	CBB-CCB-CDB-CEB
25	J	101	PL9	C12-C13-C14-C16
31	a	416	LMG	C12-C13-C14-C15
28	C	517	DGD	O1G-C1A-C2A-C3A
28	c	516	DGD	O1G-C1A-C2A-C3A
30	B	626	SQD	C10-C11-C12-C13
23	C	501	CLA	CAA-CBA-CGA-O2A
28	b	623	DGD	O2G-C1B-C2B-C3B
23	B	605	CLA	C8-C10-C11-C12
24	a	407	PHO	C15-C16-C17-C18
23	b	605	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C11-C12-C13-C15
23	b	605	CLA	C12-C13-C15-C16
23	b	615	CLA	C6-C7-C8-C10
23	c	513	CLA	C11-C12-C13-C15
23	d	402	CLA	C11-C10-C8-C7
24	a	407	PHO	C12-C13-C15-C16
24	a	408	PHO	C6-C7-C8-C10
24	a	408	PHO	C11-C10-C8-C7
23	C	502	CLA	CBA-CGA-O2A-C1
24	A	406	PHO	CBA-CGA-O2A-C1
23	C	511	CLA	C2-C3-C5-C6
23	b	610	CLA	C2-C3-C5-C6
30	F	102	SQD	C9-C10-C11-C12
31	k	103	LMG	C34-C35-C36-C37
28	d	409	DGD	C8A-C9A-CAA-CBA
29	A	412	LHG	C4-C5-O7-C7
29	a	414	LHG	C6-C5-O7-C7
23	A	405	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	507	CLA	CAA-CBA-CGA-O2A
31	C	520	LMG	O8-C28-C29-C30
23	d	402	CLA	C5-C6-C7-C8
31	c	519	LMG	C36-C37-C38-C39
25	D	404	PL9	C21-C22-C23-C24
25	j	101	PL9	C21-C22-C23-C24
30	a	415	SQD	C19-C20-C21-C22
28	B	621	DGD	O1B-C1B-C2B-C3B
23	C	502	CLA	O1A-CGA-O2A-C1
30	f	102	SQD	C27-C28-C29-C30
23	b	612	CLA	C2-C3-C5-C6
23	b	617	CLA	CAA-CBA-CGA-O1A
23	d	402	CLA	CAA-CBA-CGA-O1A
23	b	618	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CAA-CBA-CGA-O2A
25	D	404	PL9	C46-C47-C48-C49
23	D	401	CLA	CAA-CBA-CGA-O1A
23	a	405	CLA	C16-C17-C18-C20
28	C	519	DGD	CBA-CCA-CDA-CEA
23	c	510	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	C2A-CAA-CBA-CGA
34	F	101	HEM	CAA-CBA-CGA-O2A
23	B	601	CLA	C14-C13-C15-C16
23	B	602	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C10-C8-C9
23	b	609	CLA	C11-C12-C13-C14
23	b	612	CLA	C11-C12-C13-C14
23	c	504	CLA	C6-C7-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	c	507	CLA	C11-C12-C13-C14
23	c	508	CLA	C11-C12-C13-C14
23	c	513	CLA	C11-C12-C13-C14
23	d	402	CLA	C11-C10-C8-C9
24	a	408	PHO	C6-C7-C8-C9
23	b	616	CLA	CAA-CBA-CGA-O2A
23	a	406	CLA	O1D-CGD-O2D-CED
23	c	501	CLA	CAA-CBA-CGA-O1A
30	D	408	SQD	O5-C5-C6-S
30	d	408	SQD	O5-C5-C6-S
28	c	518	DGD	O1A-C1A-O1G-C1G
23	C	510	CLA	CAA-CBA-CGA-O2A
27	z	101	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	501	CLA	CAA-CBA-CGA-O1A
28	B	627	DGD	C2G-C3G-O3G-C1D
30	F	102	SQD	C45-C44-O6-C1
31	I	101	LMG	C8-C7-O1-C1
31	b	624	LMG	C8-C7-O1-C1
31	i	101	LMG	C8-C7-O1-C1
31	A	418	LMG	O10-C28-O8-C9
34	f	101	HEM	CAA-CBA-CGA-O2A
31	a	402	LMG	C16-C17-C18-C19
23	C	507	CLA	CAA-CBA-CGA-O1A
28	C	517	DGD	O1A-C1A-C2A-C3A
28	b	623	DGD	O1B-C1B-C2B-C3B
23	A	404	CLA	C4C-C3C-CAC-CBC
28	B	627	DGD	C5A-C6A-C7A-C8A
30	a	401	SQD	C9-C10-C11-C12
23	B	613	CLA	CAA-CBA-CGA-O1A
23	B	612	CLA	C3-C5-C6-C7
23	B	614	CLA	CAA-CBA-CGA-O1A
23	c	507	CLA	CAA-CBA-CGA-O1A
23	b	613	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
24	a	408	PHO	CAD-CBD-CGD-O2D
30	A	417	SQD	O47-C7-C8-C9
23	C	508	CLA	C2-C1-O2A-CGA
31	D	406	LMG	O9-C10-C11-C12
23	B	606	CLA	C16-C17-C18-C19
31	i	101	LMG	C15-C16-C17-C18
30	A	413	SQD	C29-C30-C31-C32
28	c	516	DGD	O1A-C1A-C2A-C3A
30	a	401	SQD	O49-C7-C8-C9
30	d	408	SQD	O49-C7-C8-C9
31	k	103	LMG	O10-C28-C29-C30
23	B	610	CLA	C13-C15-C16-C17
23	B	612	CLA	CAA-CBA-CGA-O2A
23	C	505	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CAA-CBA-CGA-O1A
23	A	405	CLA	CBA-CGA-O2A-C1
25	J	101	PL9	C17-C18-C19-C21

There are no ring outliers.

166 monomers are involved in 561 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	408	PHO	5	0
27	J	102	BCR	3	0
23	A	404	CLA	10	0
23	c	504	CLA	5	0
23	D	403	CLA	2	0
23	C	511	CLA	8	0
23	B	605	CLA	11	0
23	c	506	CLA	3	0
31	B	622	LMG	3	0
28	d	409	DGD	1	0
28	c	518	DGD	4	0
23	C	505	CLA	5	0
28	C	517	DGD	4	0
30	B	626	SQD	2	0
31	A	414	LMG	3	0
28	D	409	DGD	1	0
33	b	627	LMT	1	0
27	C	516	BCR	4	0
27	T	102	BCR	8	0
23	B	616	CLA	3	0
23	b	611	CLA	9	0
23	B	614	CLA	3	0
30	F	102	SQD	2	0
23	a	404	CLA	16	0
29	a	417	LHG	3	0
27	y	101	BCR	6	0
31	d	406	LMG	2	0
28	B	627	DGD	2	0
23	b	608	CLA	4	0
23	A	405	CLA	3	0
23	b	616	CLA	4	0
33	D	410	LMT	1	0
33	B	629	LMT	2	0
27	B	619	BCR	6	0
27	c	514	BCR	10	0
23	B	607	CLA	9	0
33	B	628	LMT	2	0
23	c	502	CLA	2	0
23	c	510	CLA	3	0
27	A	410	BCR	6	0
31	a	416	LMG	3	0
30	A	417	SQD	7	0
27	C	514	BCR	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	603	CLA	14	0
33	b	604	LMT	1	0
30	b	601	SQD	4	0
23	C	506	CLA	2	0
28	C	519	DGD	5	0
30	a	401	SQD	6	0
23	B	611	CLA	5	0
23	D	401	CLA	7	0
27	k	102	BCR	8	0
25	d	404	PL9	9	0
27	z	101	BCR	3	0
23	c	501	CLA	3	0
27	d	405	BCR	2	0
31	d	407	LMG	6	0
23	a	409	CLA	2	0
31	C	520	LMG	3	0
25	D	404	PL9	6	0
24	D	402	PHO	6	0
30	D	408	SQD	4	0
31	m	102	LMG	4	0
28	c	516	DGD	4	0
23	b	619	CLA	4	0
23	B	610	CLA	1	0
30	A	413	SQD	4	0
23	C	513	CLA	4	0
23	a	406	CLA	4	0
28	a	413	DGD	2	0
23	C	503	CLA	4	0
23	C	502	CLA	1	0
31	i	101	LMG	3	0
27	H	101	BCR	3	0
31	a	402	LMG	3	0
33	b	626	LMT	1	0
28	C	518	DGD	6	0
23	C	508	CLA	5	0
31	E	101	LMG	1	0
23	b	620	CLA	5	0
23	B	613	CLA	3	0
27	b	621	BCR	4	0
31	b	624	LMG	3	0
31	B	623	LMG	5	0
33	i	102	LMT	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	407	LMG	4	0
24	a	407	PHO	8	0
28	b	623	DGD	2	0
23	B	615	CLA	1	0
33	B	624	LMT	1	0
23	b	609	CLA	9	0
23	d	403	CLA	3	0
23	A	403	CLA	13	0
23	c	507	CLA	6	0
34	v	201	HEM	4	0
23	b	607	CLA	9	0
24	A	406	PHO	5	0
29	A	412	LHG	4	0
23	B	606	CLA	8	0
34	V	201	HEM	3	0
23	C	501	CLA	3	0
23	c	513	CLA	2	0
27	B	617	BCR	5	0
23	c	509	CLA	2	0
27	D	405	BCR	3	0
23	A	407	CLA	1	0
23	c	512	CLA	3	0
30	f	102	SQD	2	0
29	A	415	LHG	3	0
23	C	510	CLA	5	0
31	b	625	LMG	5	0
33	M	102	LMT	1	0
31	I	101	LMG	2	0
33	d	410	LMT	1	0
23	b	617	CLA	2	0
31	e	101	LMG	1	0
23	b	605	CLA	1	0
23	C	509	CLA	4	0
23	b	612	CLA	8	0
33	I	102	LMT	2	0
23	c	503	CLA	4	0
23	b	606	CLA	7	0
28	b	602	DGD	3	0
23	c	508	CLA	5	0
23	B	608	CLA	8	0
23	a	405	CLA	14	0
27	T	101	BCR	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	505	CLA	4	0
27	C	515	BCR	4	0
23	c	511	CLA	6	0
31	c	519	LMG	2	0
23	C	504	CLA	3	0
23	B	612	CLA	5	0
23	b	613	CLA	4	0
31	A	418	LMG	2	0
34	f	101	HEM	5	0
23	B	609	CLA	4	0
33	b	603	LMT	2	0
27	a	412	BCR	7	0
23	B	601	CLA	2	0
23	b	610	CLA	6	0
25	a	410	PL9	5	0
29	a	414	LHG	2	0
23	b	618	CLA	6	0
23	C	507	CLA	5	0
23	B	604	CLA	8	0
31	C	521	LMG	2	0
30	d	408	SQD	4	0
23	b	615	CLA	4	0
31	k	103	LMG	3	0
27	c	515	BCR	4	0
28	c	517	DGD	6	0
23	B	602	CLA	6	0
27	B	620	BCR	4	0
34	F	101	HEM	4	0
28	A	411	DGD	1	0
23	d	402	CLA	6	0
27	b	622	BCR	4	0
25	A	408	PL9	2	0
30	a	415	SQD	4	0
23	b	614	CLA	2	0
31	M	101	LMG	4	0
23	C	512	CLA	5	0
27	B	618	BCR	10	0
27	h	101	BCR	4	0
27	j	102	BCR	4	0

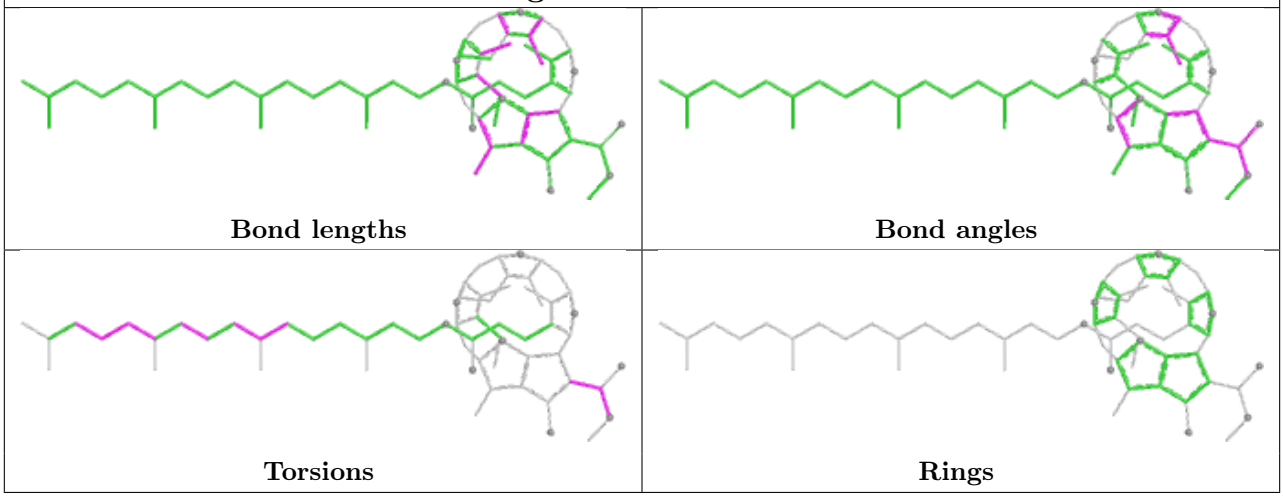
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

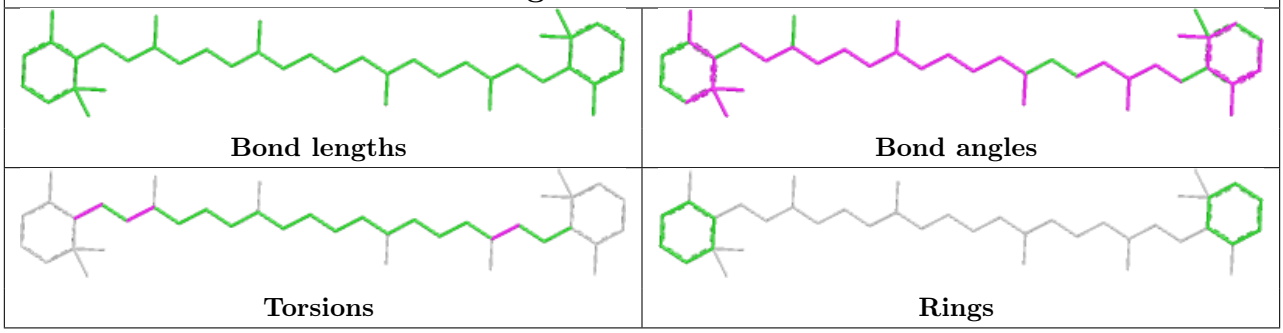
Ligand PL9 j 101



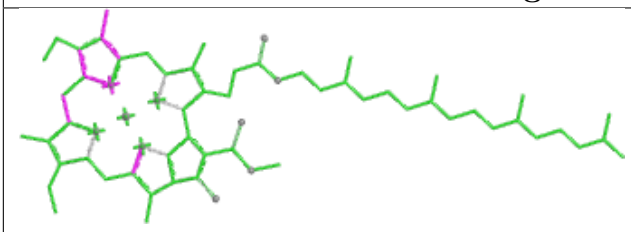
Ligand PHO a 408



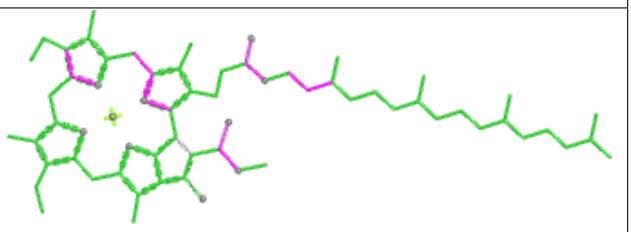
Ligand BCR J 102



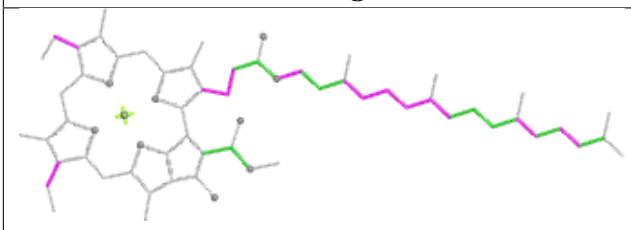
Ligand CLA A 404



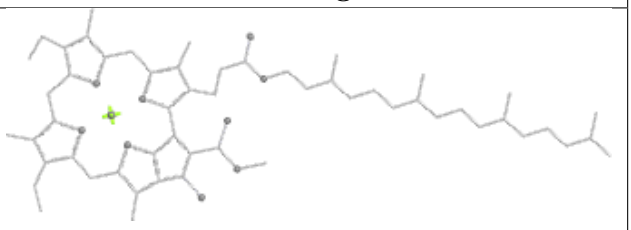
Bond lengths



Bond angles

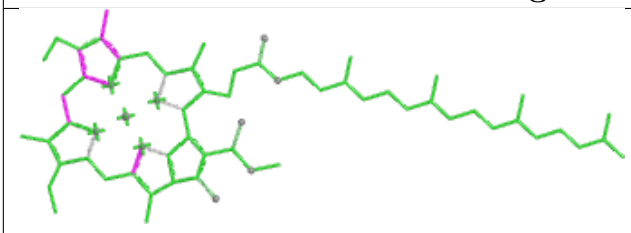


Torsions

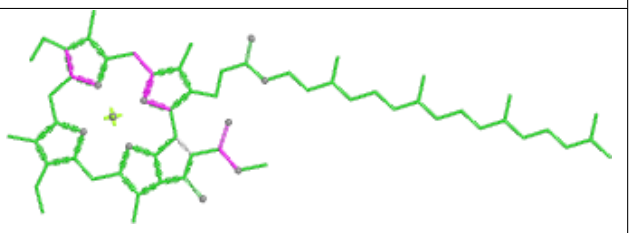


Rings

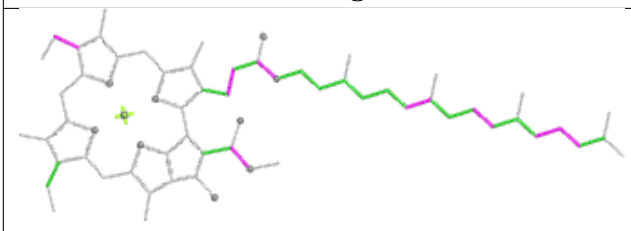
Ligand CLA c 504



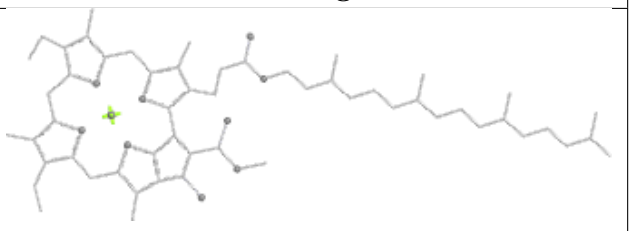
Bond lengths



Bond angles

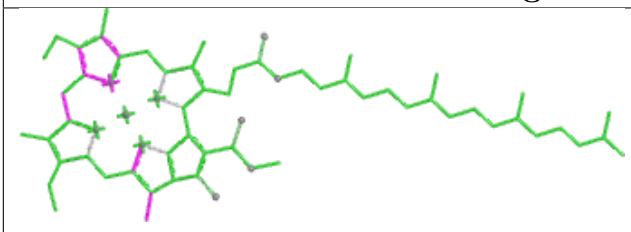


Torsions

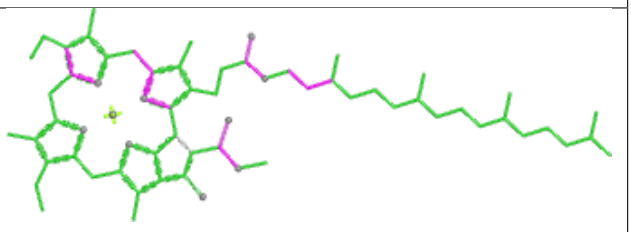


Rings

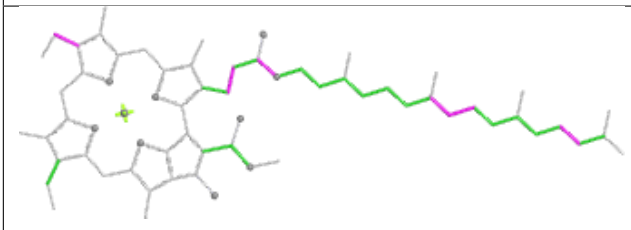
Ligand CLA D 403



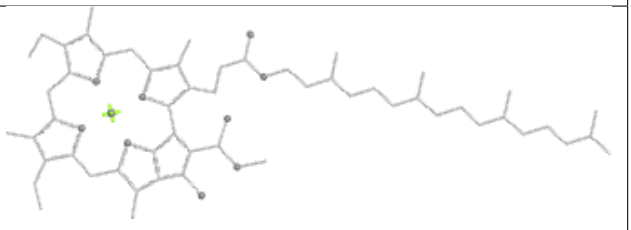
Bond lengths



Bond angles

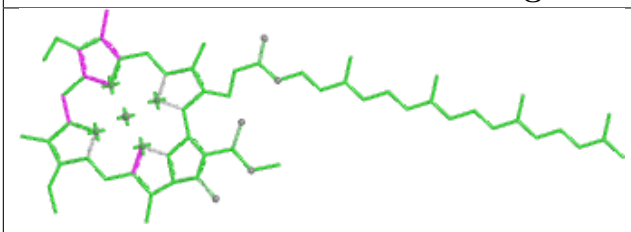


Torsions

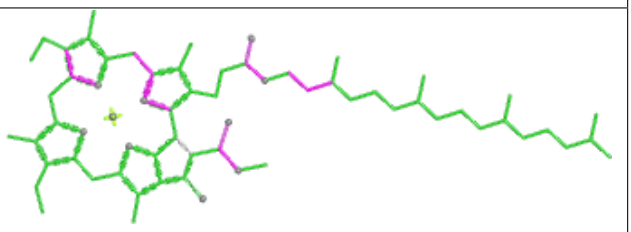


Rings

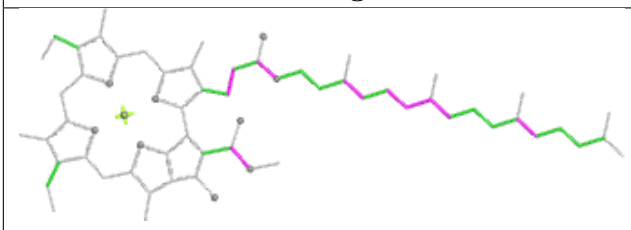
Ligand CLA C 511



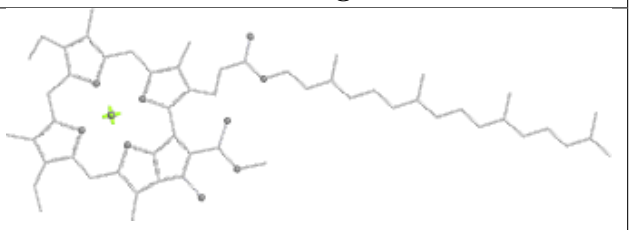
Bond lengths



Bond angles

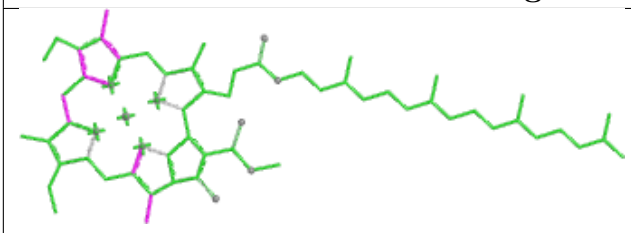


Torsions

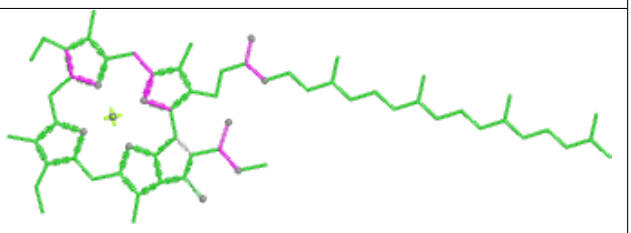


Rings

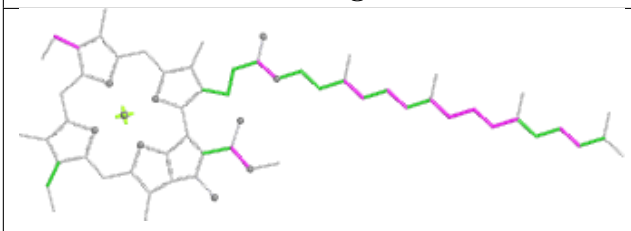
Ligand CLA B 605



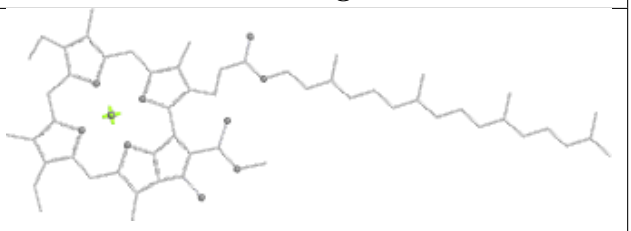
Bond lengths



Bond angles

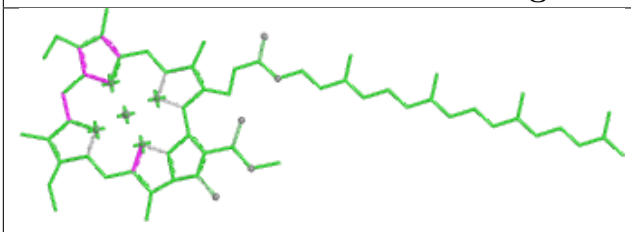


Torsions

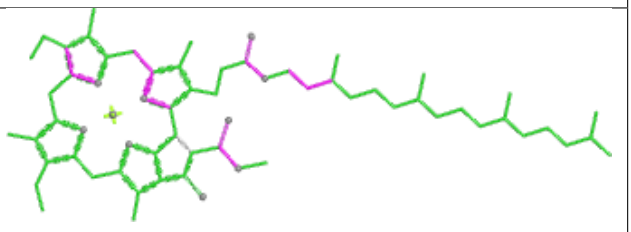


Rings

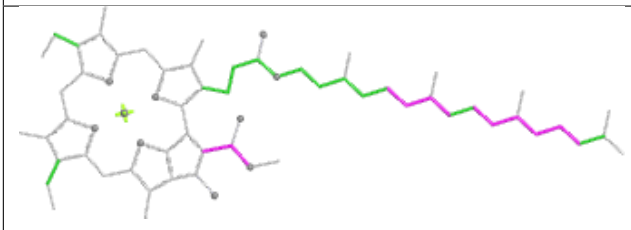
Ligand CLA c 506



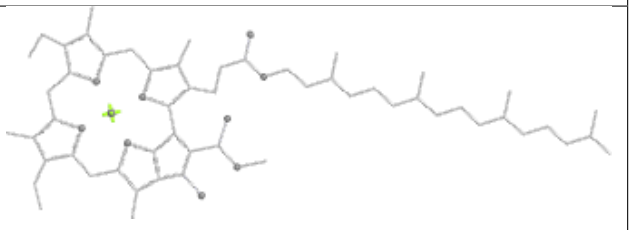
Bond lengths



Bond angles

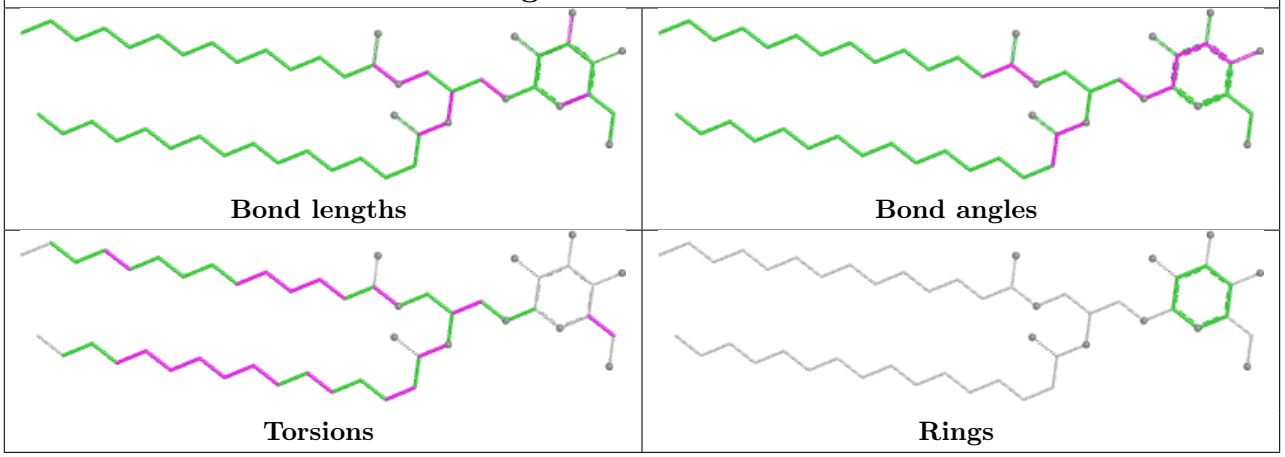


Torsions

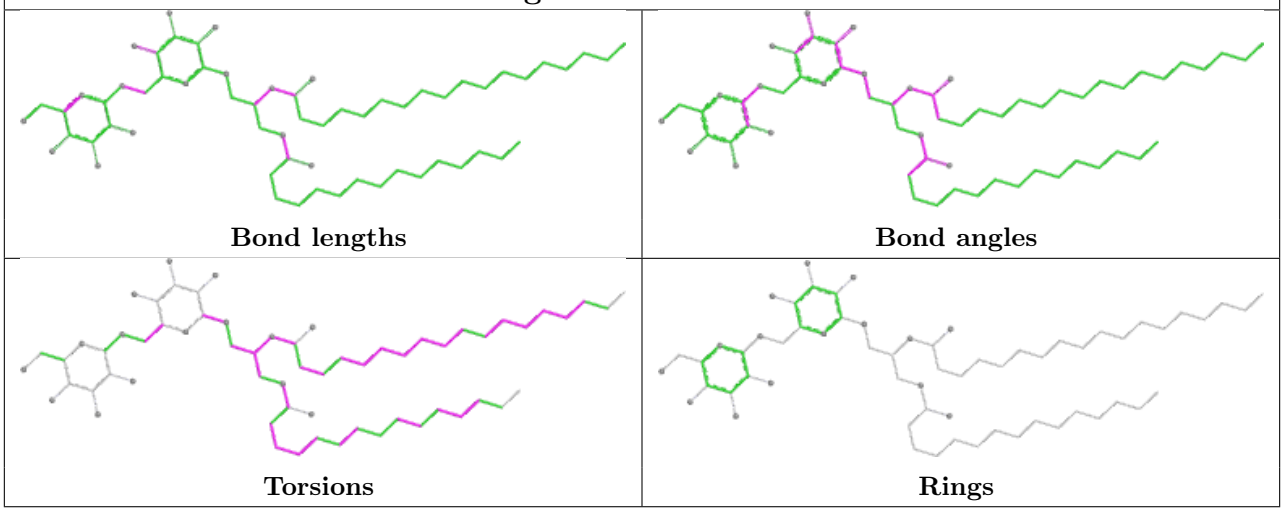


Rings

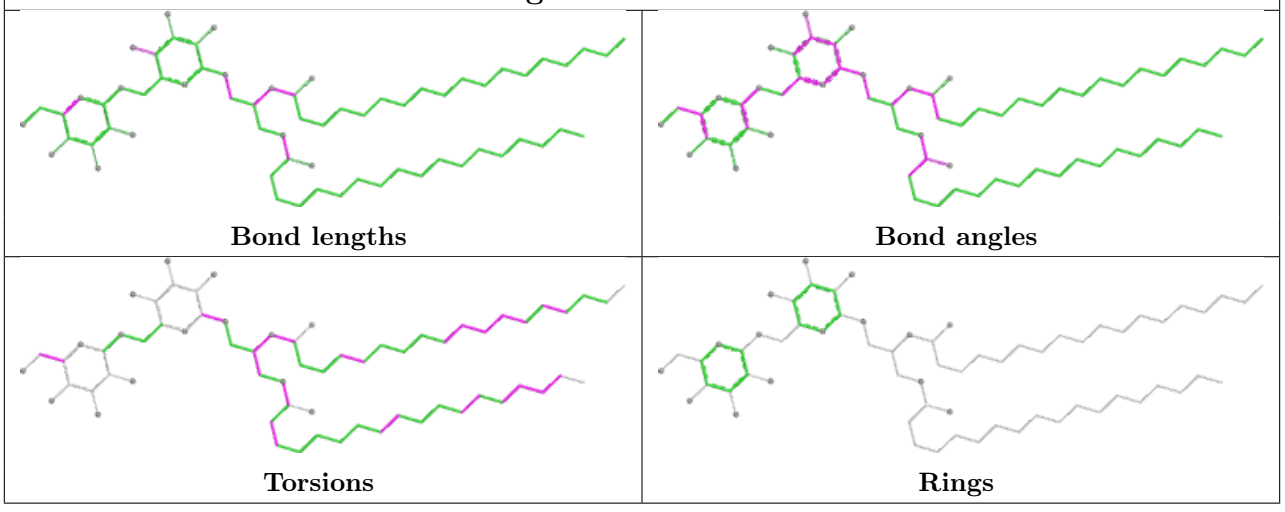
Ligand LMG B 622



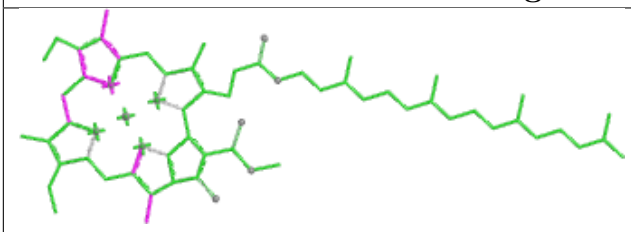
Ligand DGD d 409



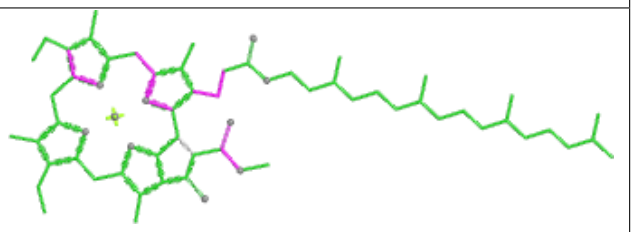
Ligand DGD c 518



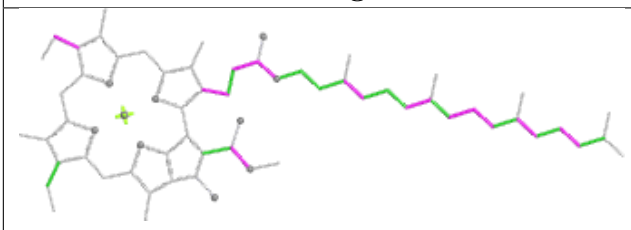
Ligand CLA C 505



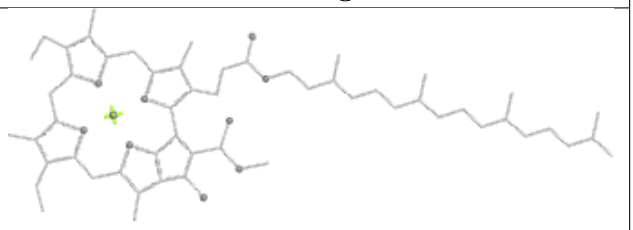
Bond lengths



Bond angles

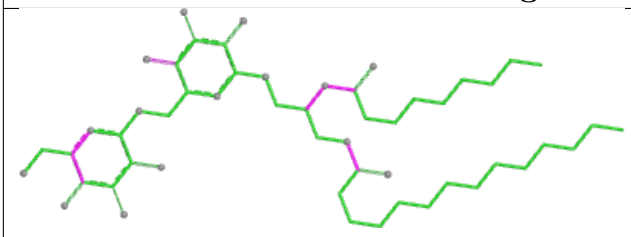


Torsions

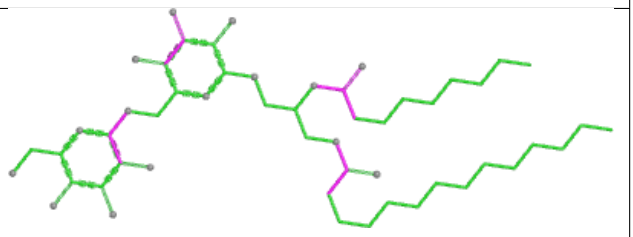


Rings

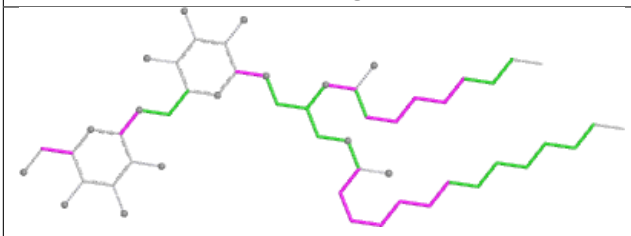
Ligand DGD C 517



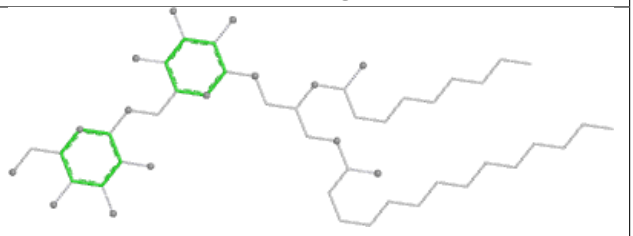
Bond lengths



Bond angles

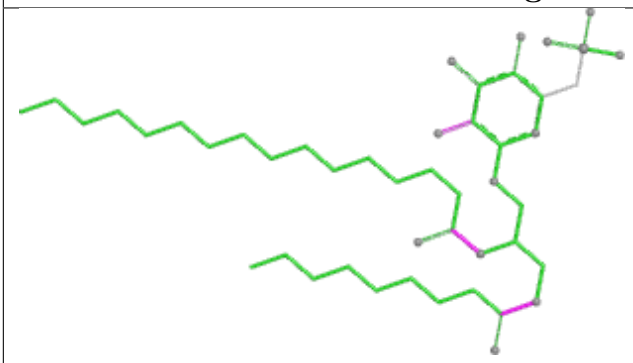


Torsions

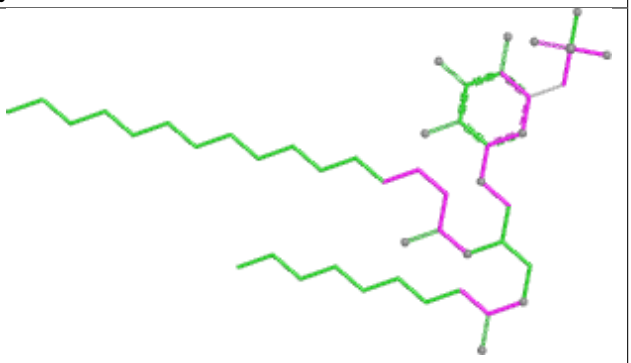


Rings

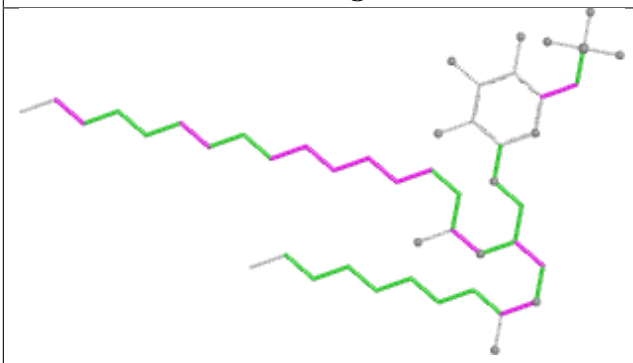
Ligand SQD B 626



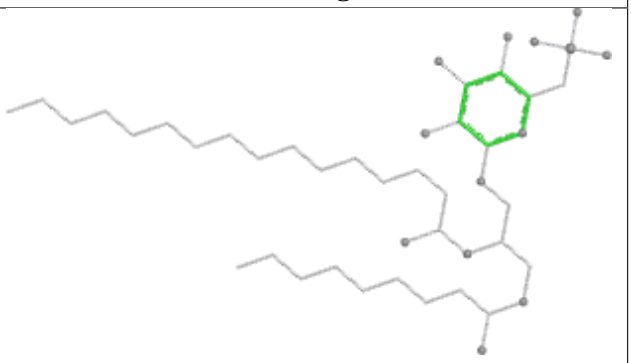
Bond lengths



Bond angles

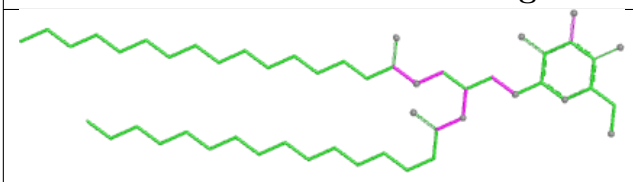


Torsions

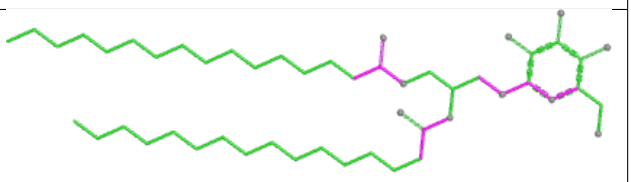


Rings

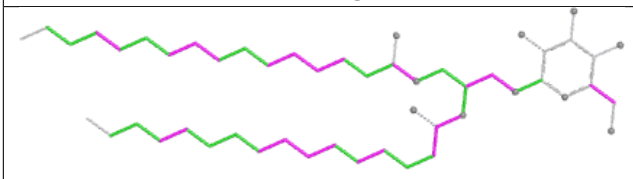
Ligand LMG A 414



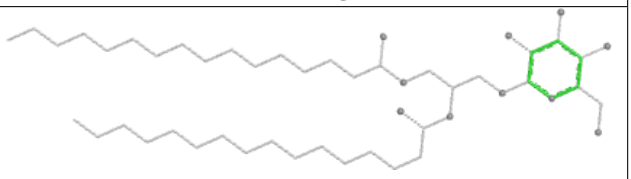
Bond lengths



Bond angles

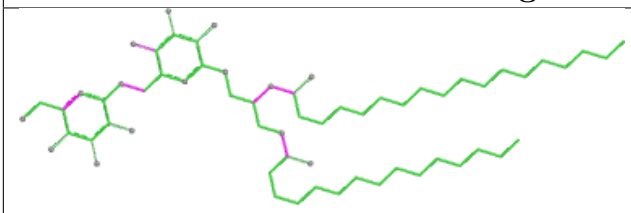


Torsions

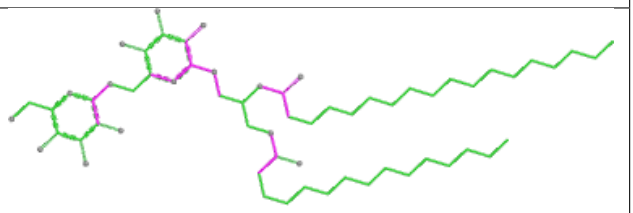


Rings

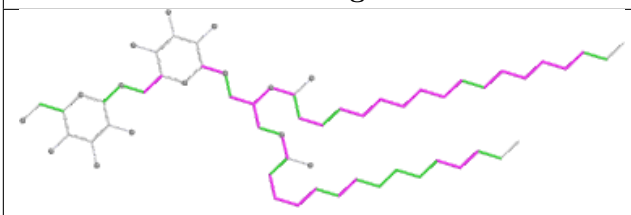
Ligand DGD D 409



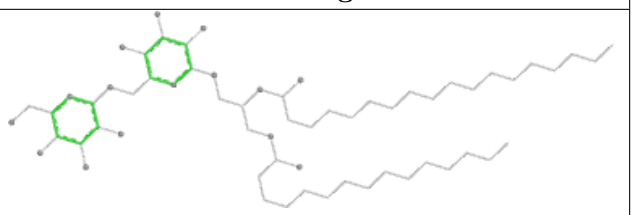
Bond lengths



Bond angles

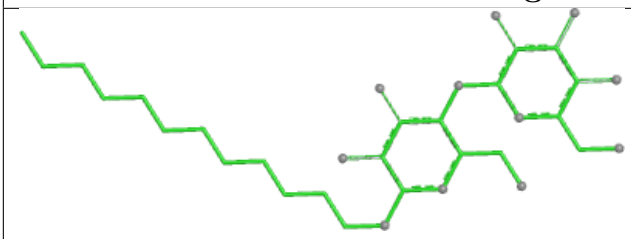


Torsions

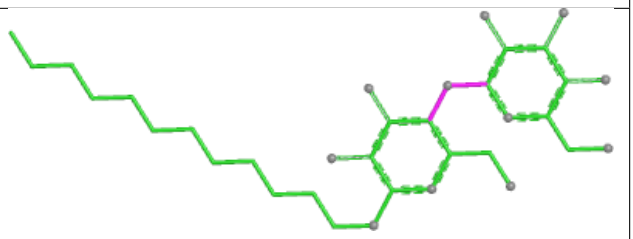


Rings

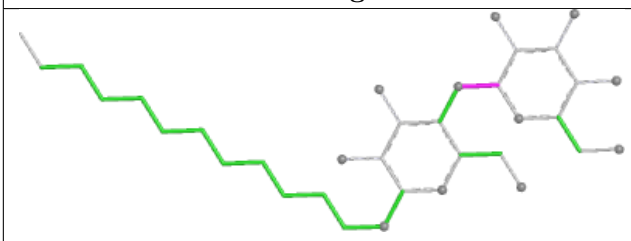
Ligand LMT b 627



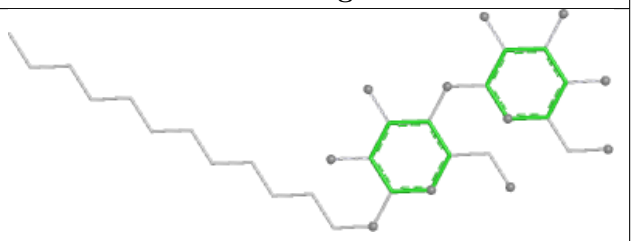
Bond lengths



Bond angles

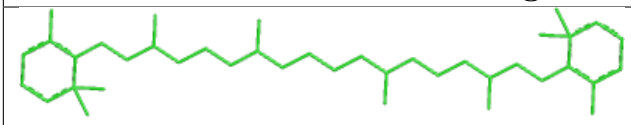


Torsions

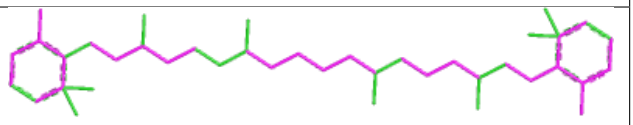


Rings

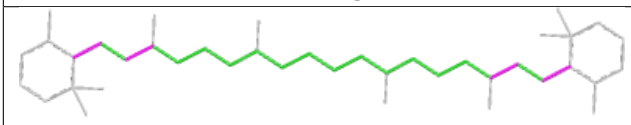
Ligand BCR C 516



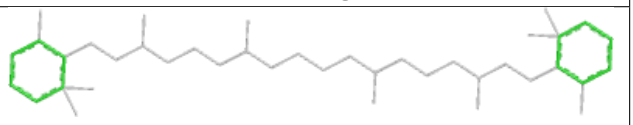
Bond lengths



Bond angles

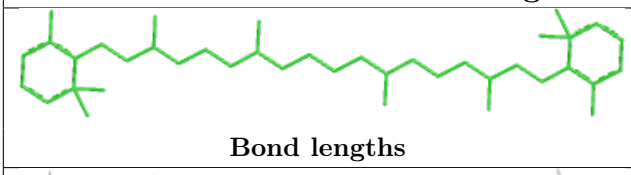


Torsions

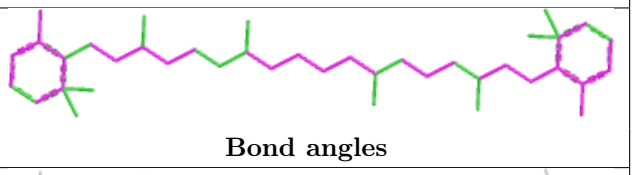


Rings

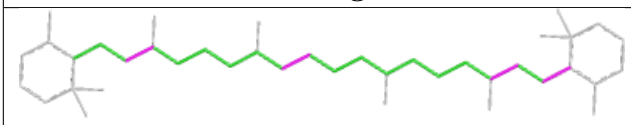
Ligand BCR T 102



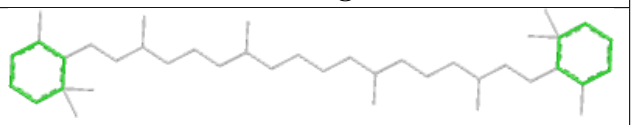
Bond lengths



Bond angles

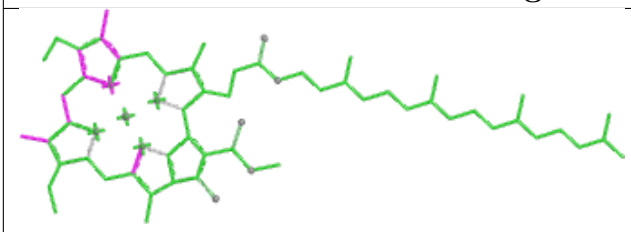


Torsions

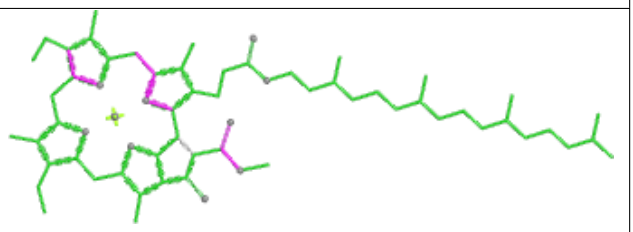


Rings

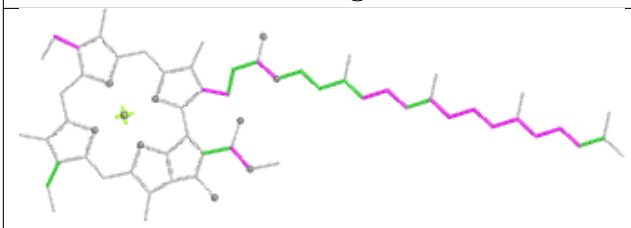
Ligand CLA B 616



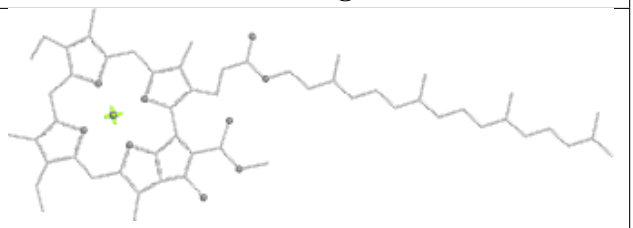
Bond lengths



Bond angles

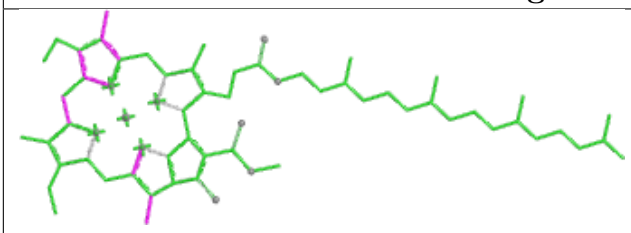


Torsions

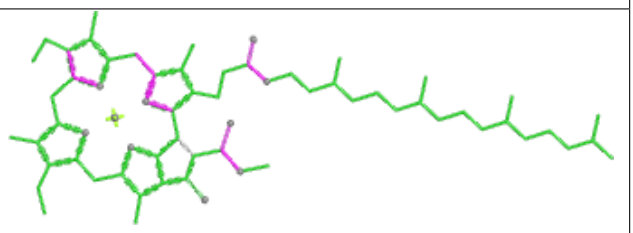


Rings

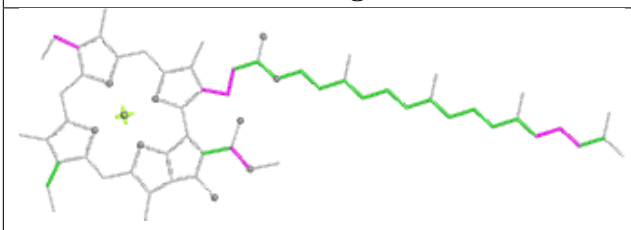
Ligand CLA b 611



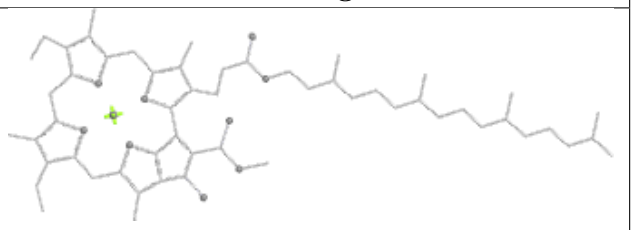
Bond lengths



Bond angles

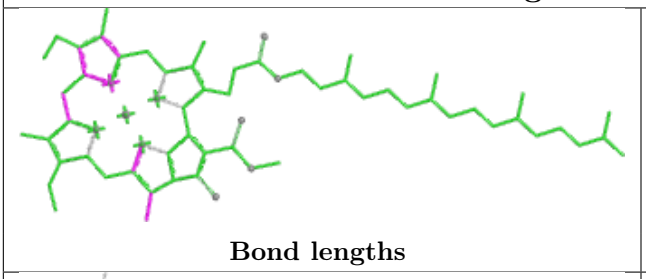


Torsions

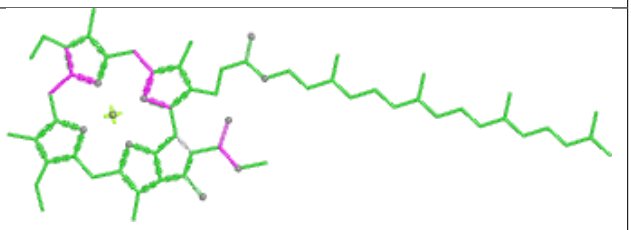


Rings

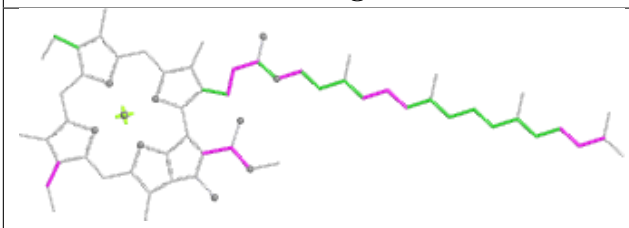
Ligand CLA B 614



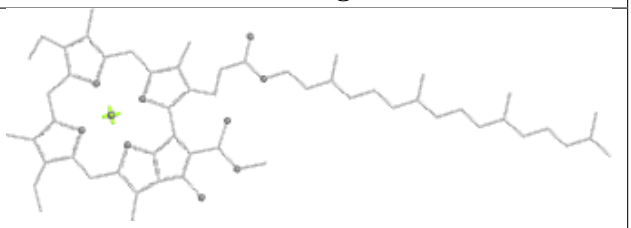
Bond lengths



Bond angles

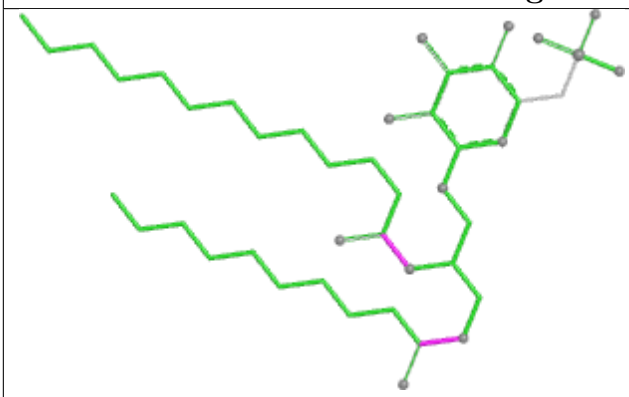


Torsions

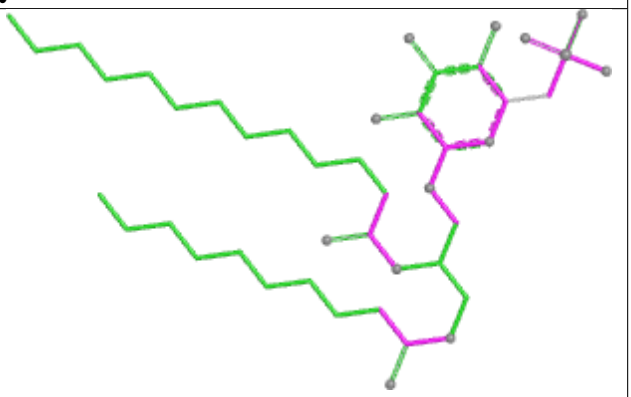


Rings

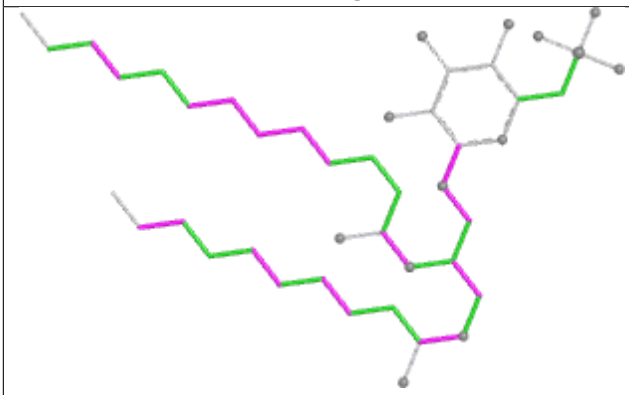
Ligand SQD F 102



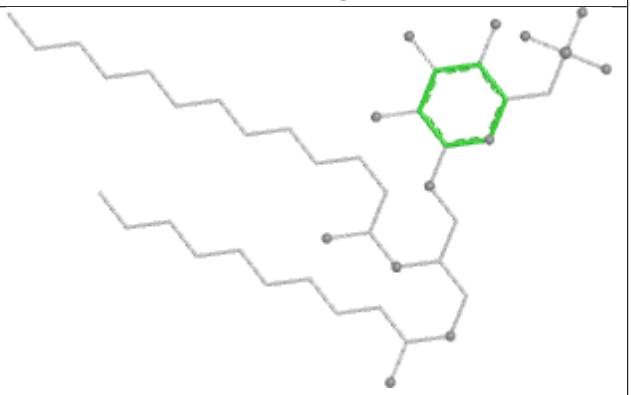
Bond lengths



Bond angles

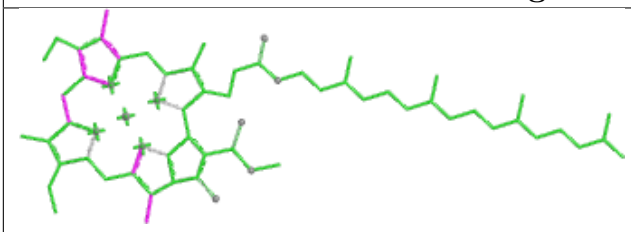


Torsions

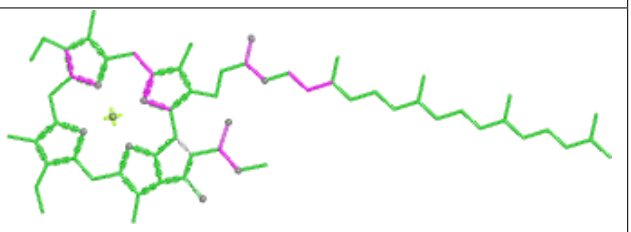


Rings

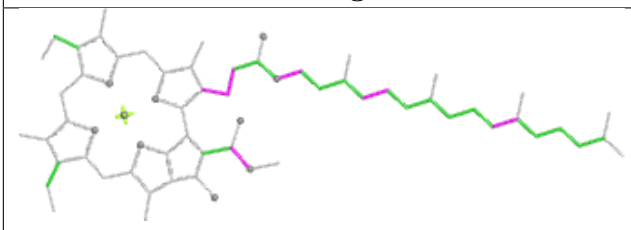
Ligand CLA a 404



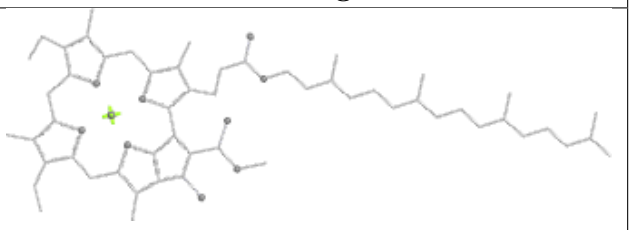
Bond lengths



Bond angles

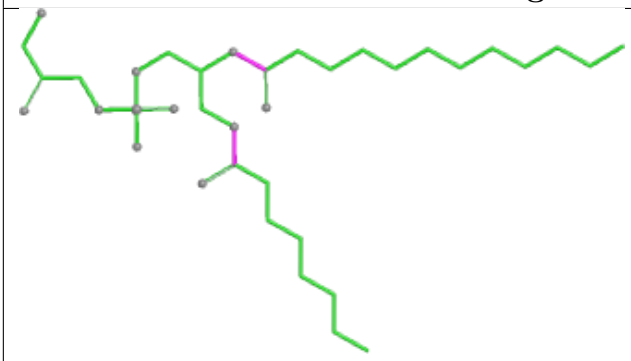


Torsions

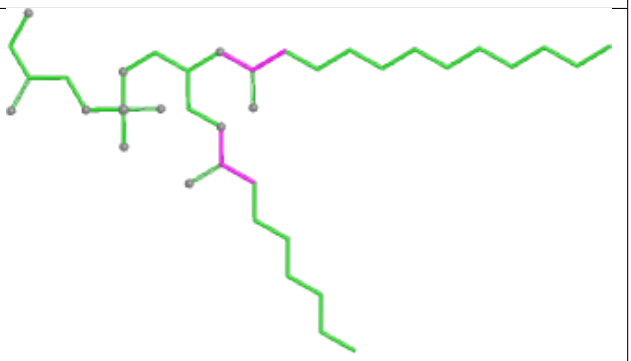


Rings

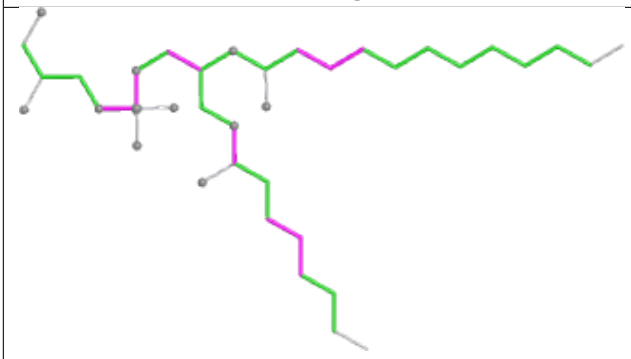
Ligand LHG a 417



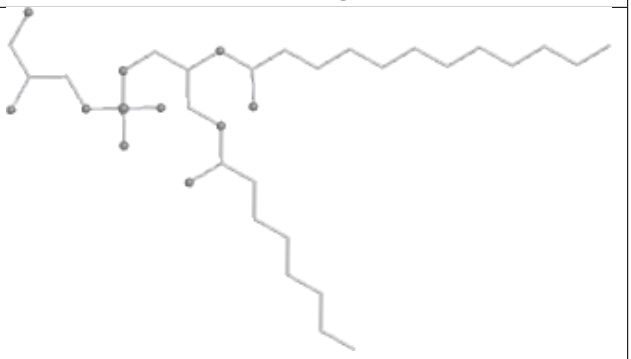
Bond lengths



Bond angles

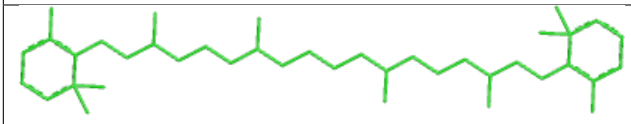


Torsions

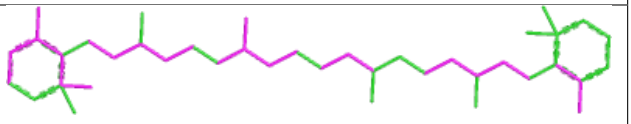


Rings

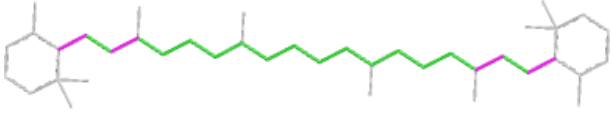
Ligand BCR y 101



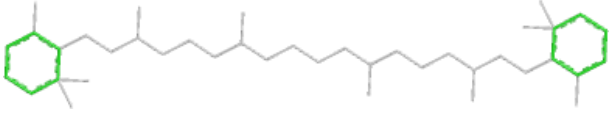
Bond lengths



Bond angles

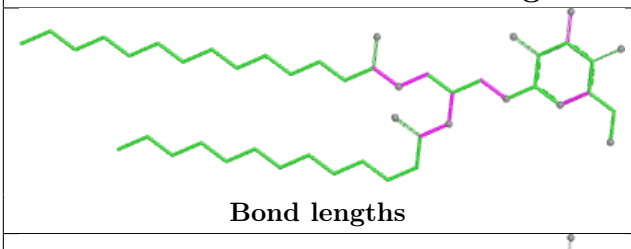


Torsions

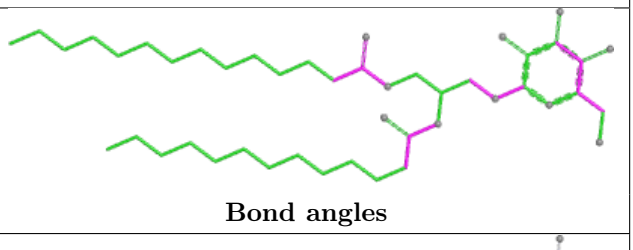


Rings

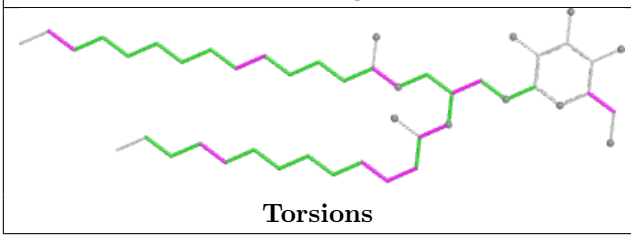
Ligand LMG d 406



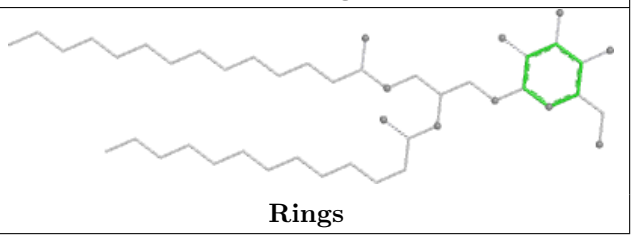
Bond lengths



Bond angles

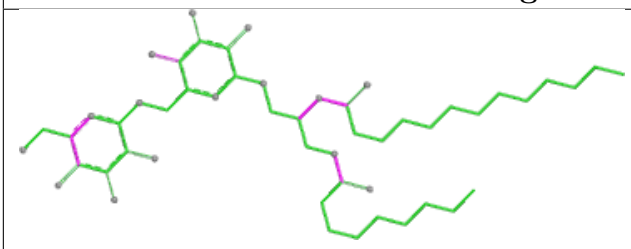


Torsions

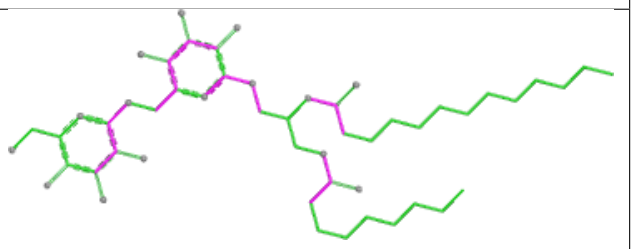


Rings

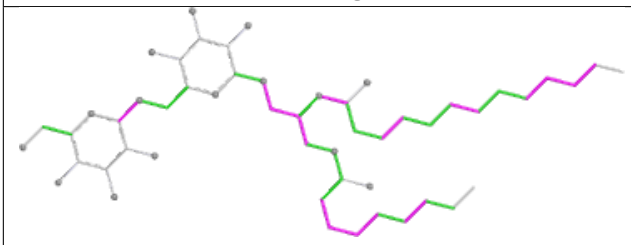
Ligand DGD B 627



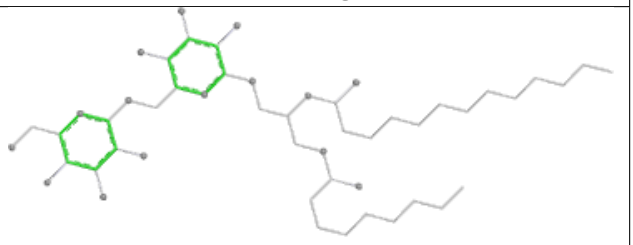
Bond lengths



Bond angles

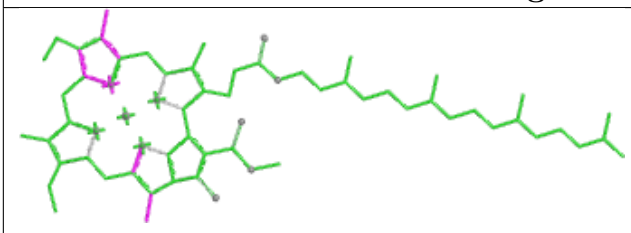


Torsions

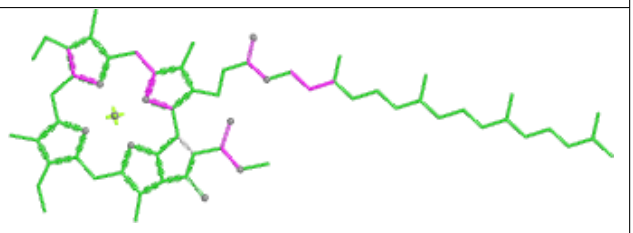


Rings

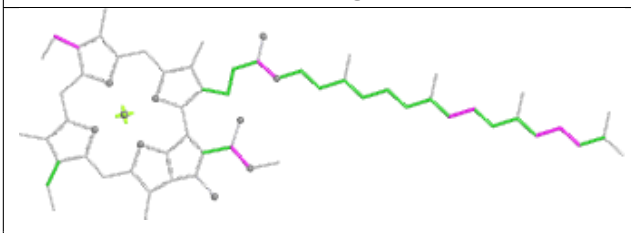
Ligand CLA b 608



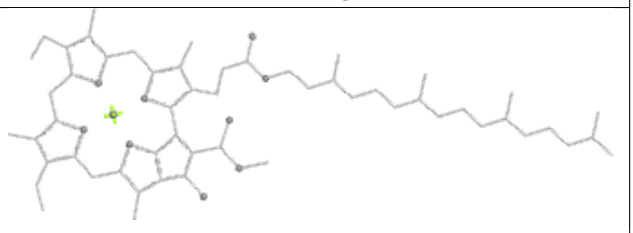
Bond lengths



Bond angles

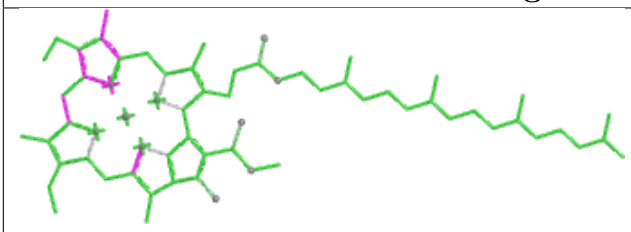


Torsions

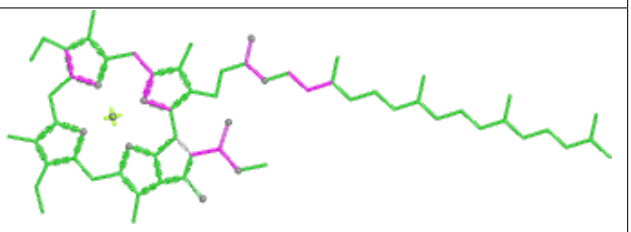


Rings

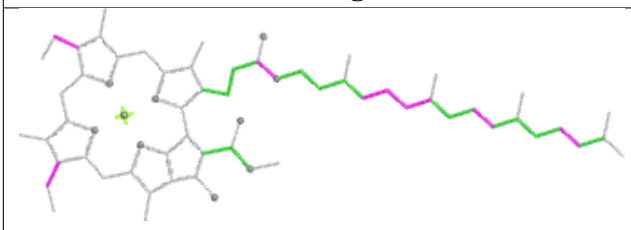
Ligand CLA A 405



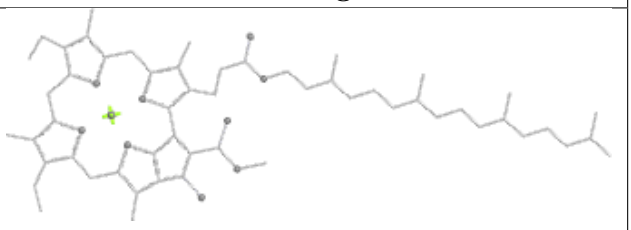
Bond lengths



Bond angles

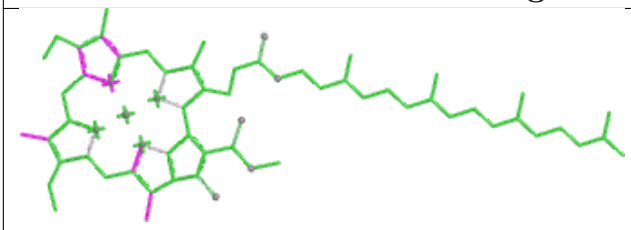


Torsions

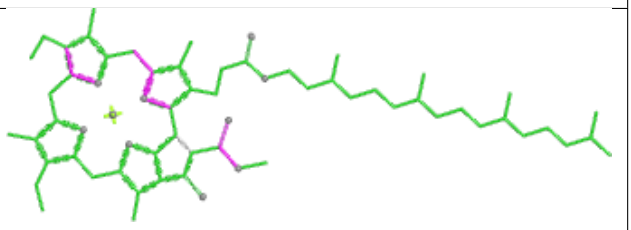


Rings

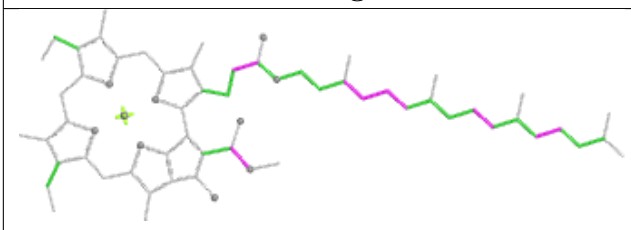
Ligand CLA b 616



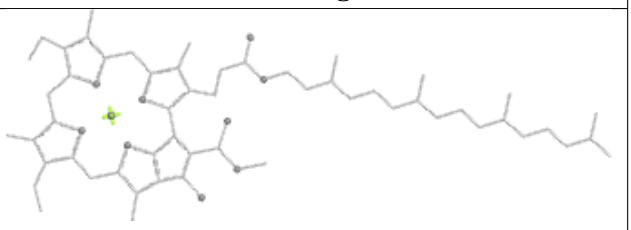
Bond lengths



Bond angles

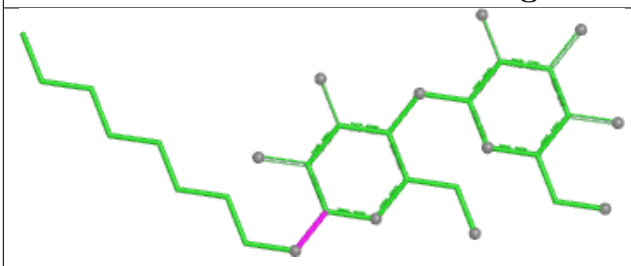


Torsions

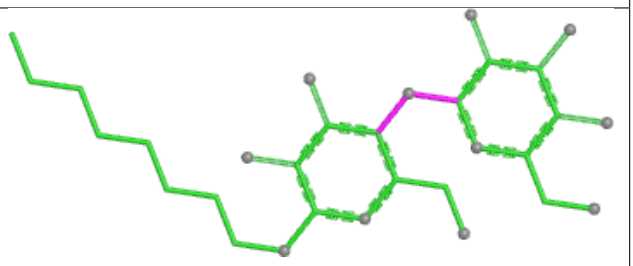


Rings

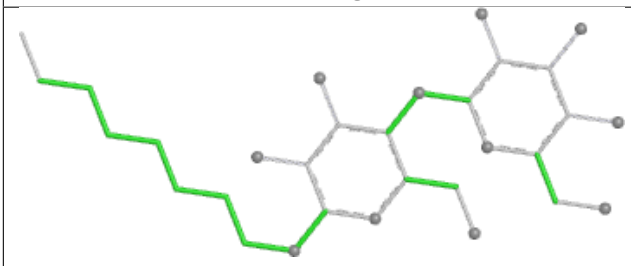
Ligand LMT D 410



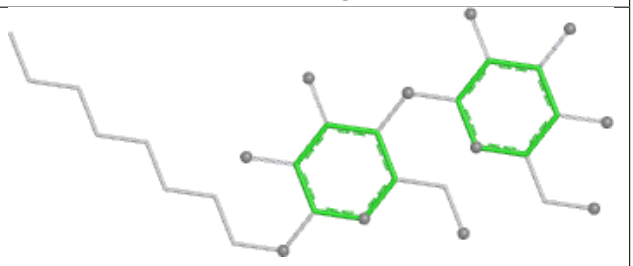
Bond lengths



Bond angles

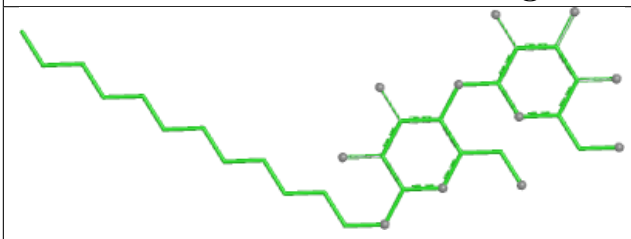


Torsions

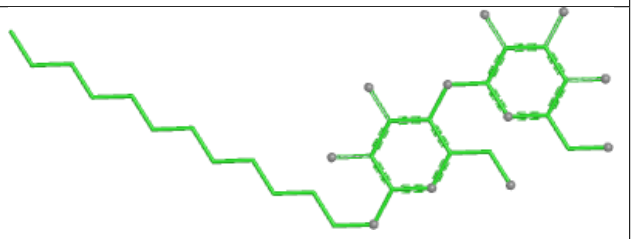


Rings

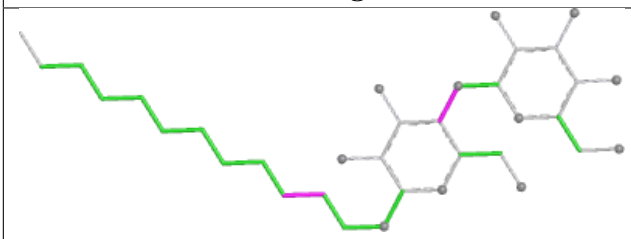
Ligand LMT B 629



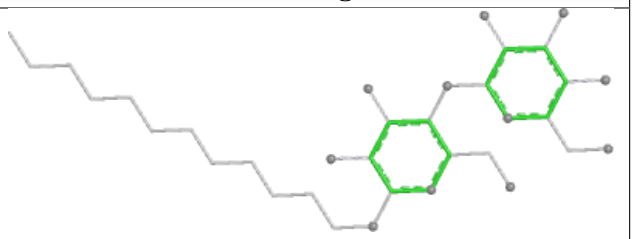
Bond lengths



Bond angles



Torsions

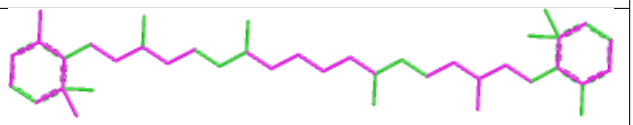


Rings

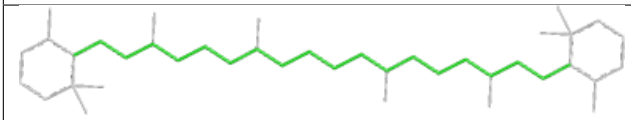
Ligand BCR B 619



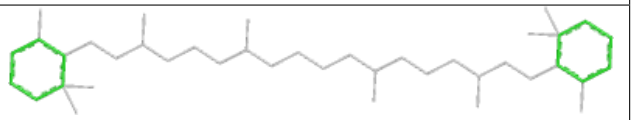
Bond lengths



Bond angles

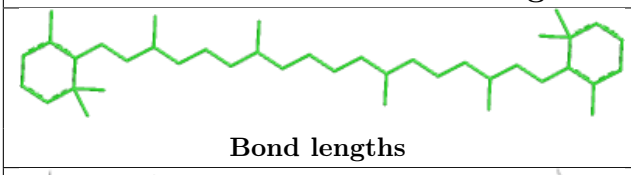


Torsions

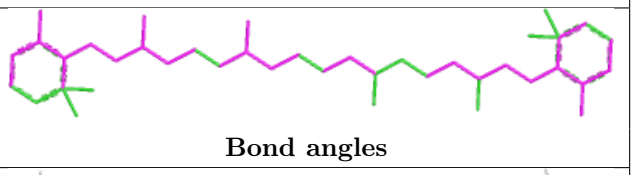


Rings

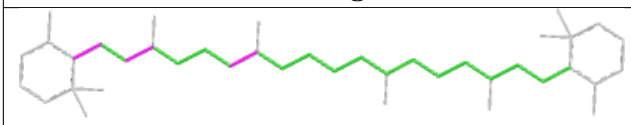
Ligand BCR c 514



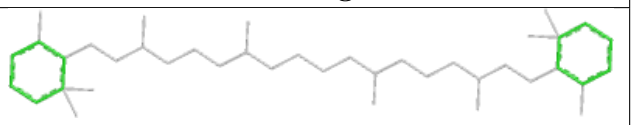
Bond lengths



Bond angles

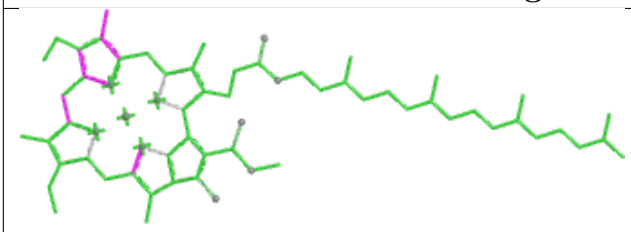


Torsions

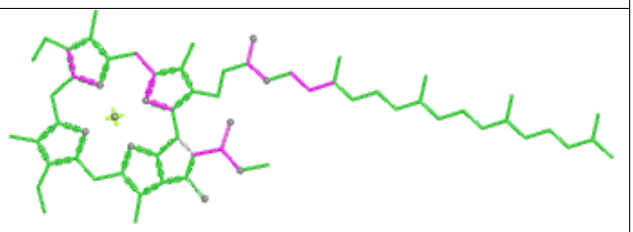


Rings

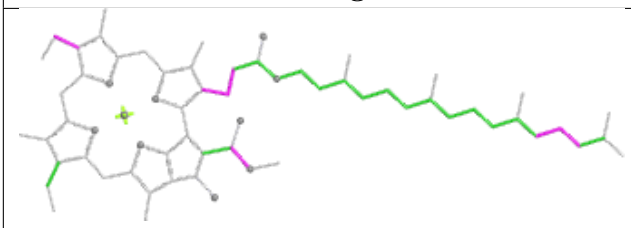
Ligand CLA B 607



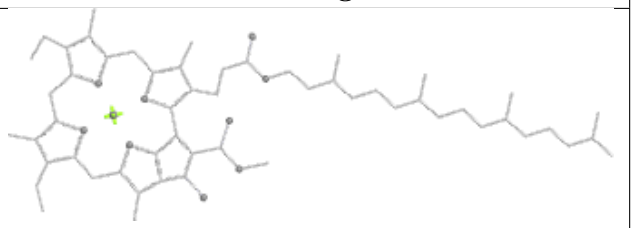
Bond lengths



Bond angles

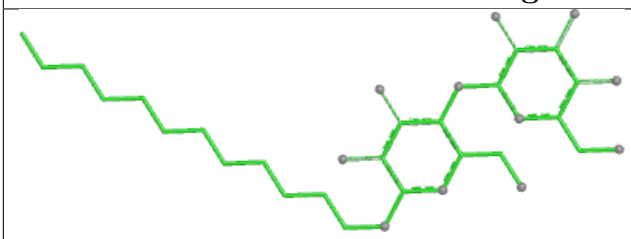


Torsions

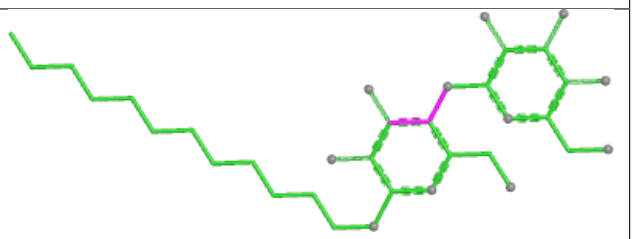


Rings

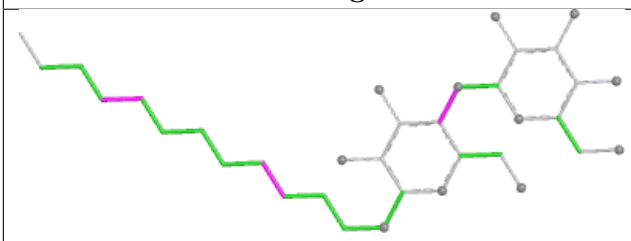
Ligand LMT B 628



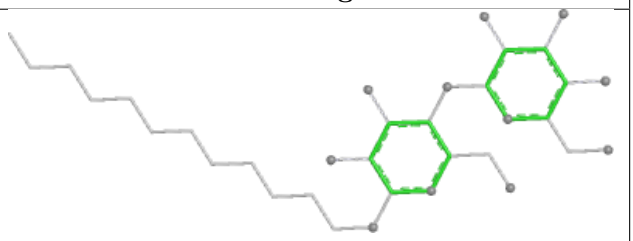
Bond lengths



Bond angles

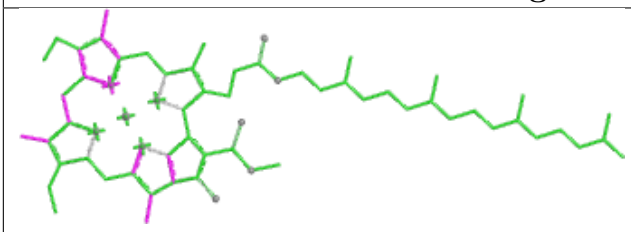


Torsions

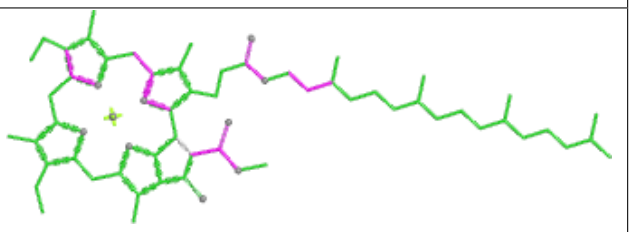


Rings

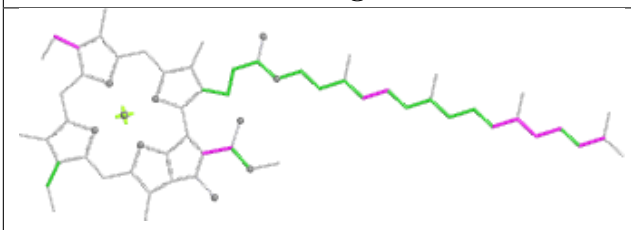
Ligand CLA c 502



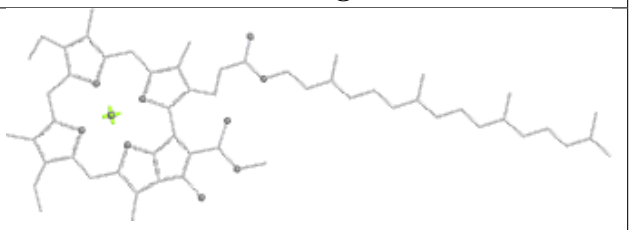
Bond lengths



Bond angles

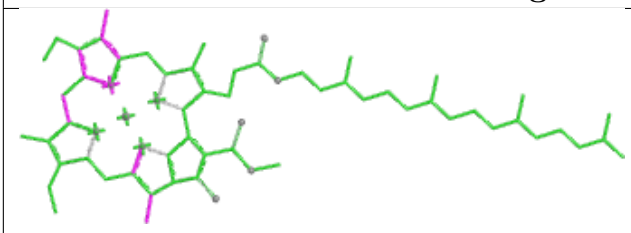


Torsions

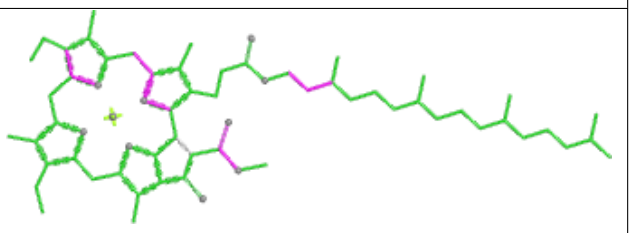


Rings

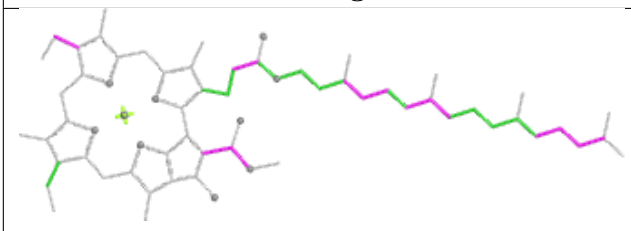
Ligand CLA c 510



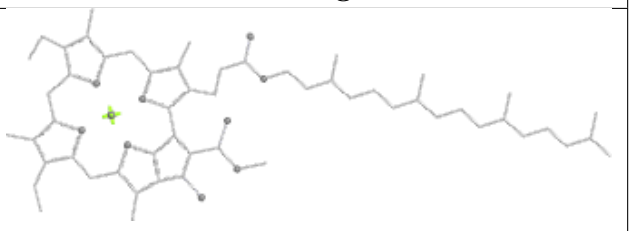
Bond lengths



Bond angles

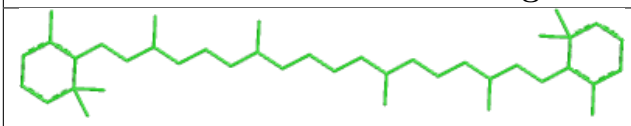


Torsions

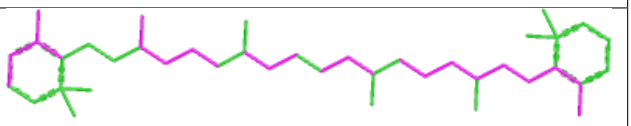


Rings

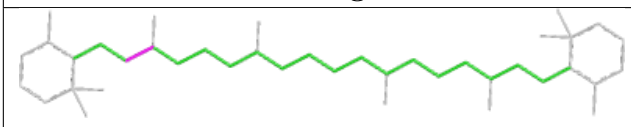
Ligand BCR A 410



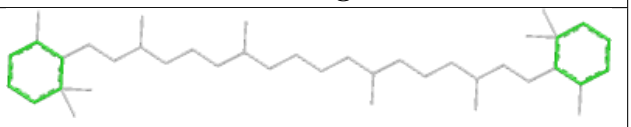
Bond lengths



Bond angles

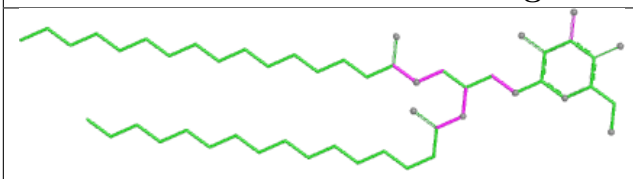


Torsions

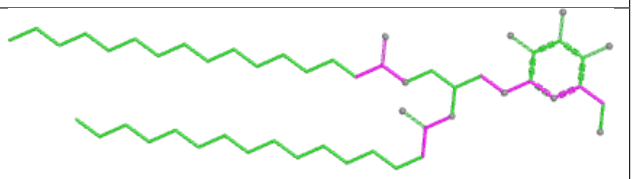


Rings

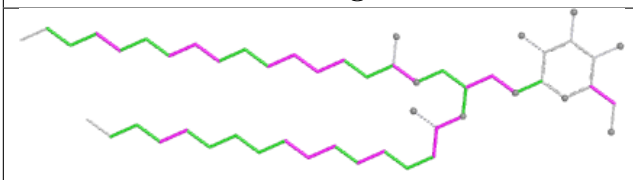
Ligand LMG a 416



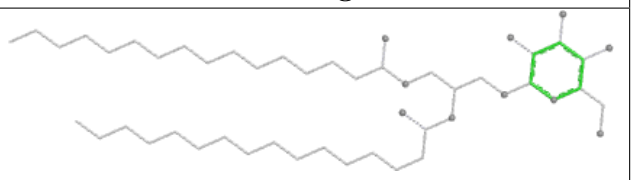
Bond lengths



Bond angles

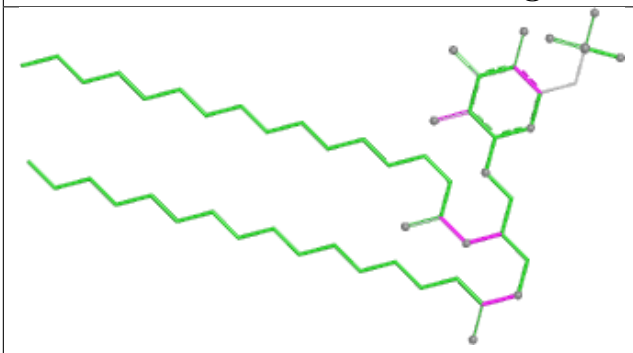


Torsions

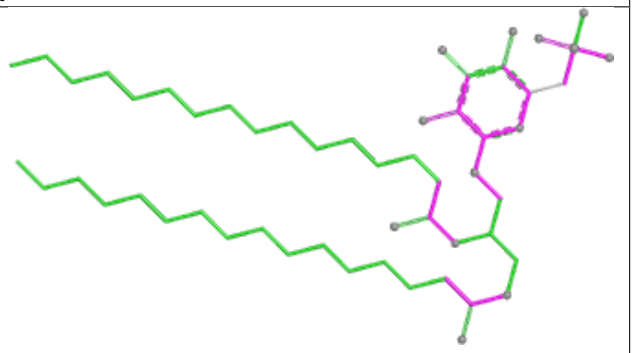


Rings

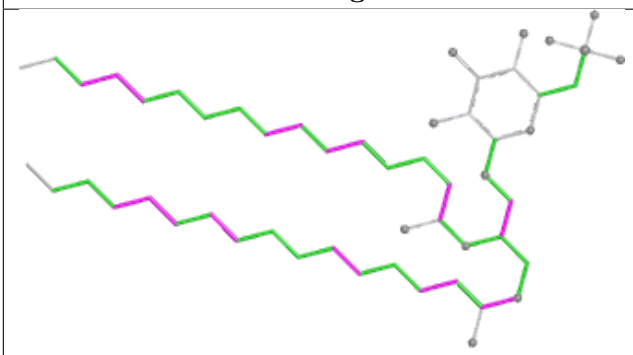
Ligand SQD A 417



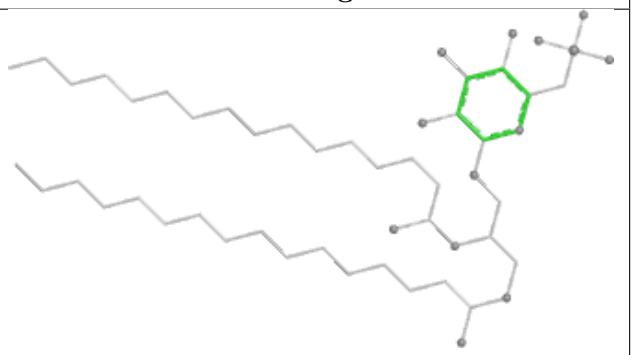
Bond lengths



Bond angles

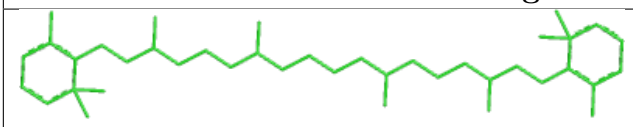


Torsions

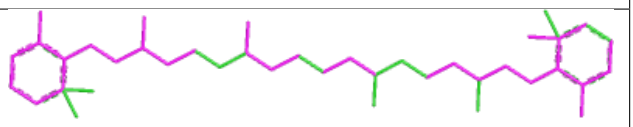


Rings

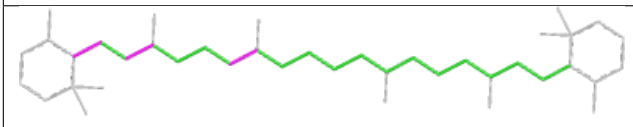
Ligand BCR C 514



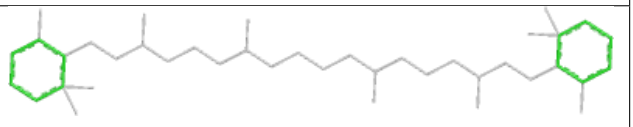
Bond lengths



Bond angles

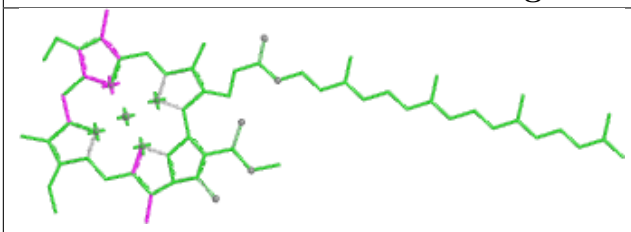


Torsions

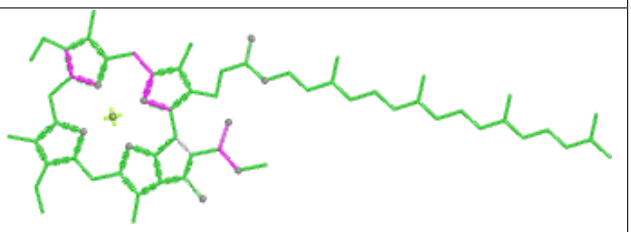


Rings

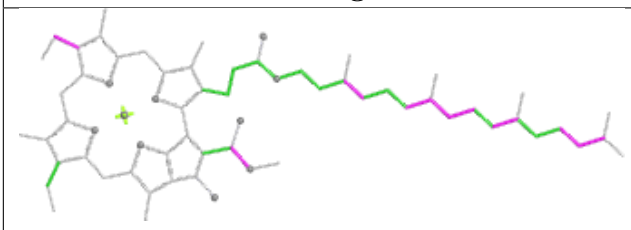
Ligand CLA B 603



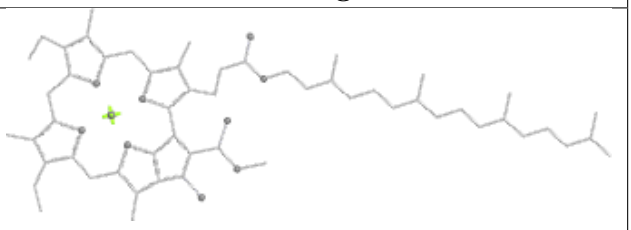
Bond lengths



Bond angles

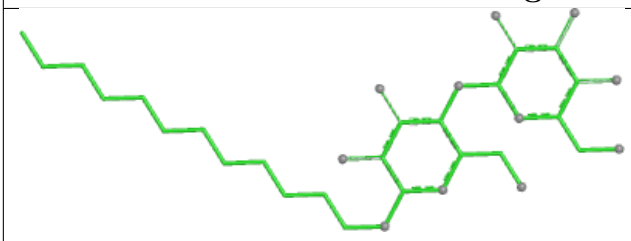


Torsions

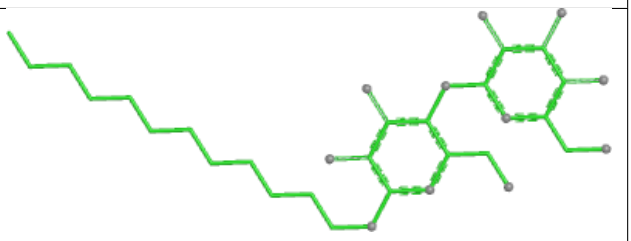


Rings

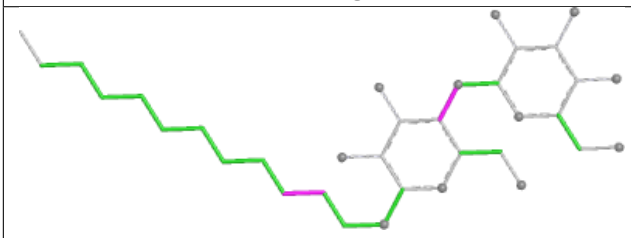
Ligand LMT b 604



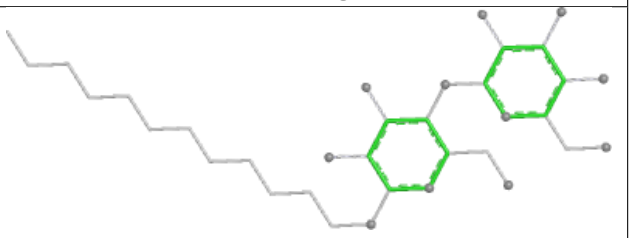
Bond lengths



Bond angles

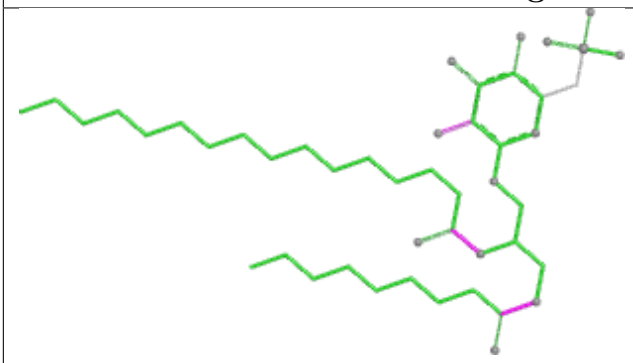


Torsions

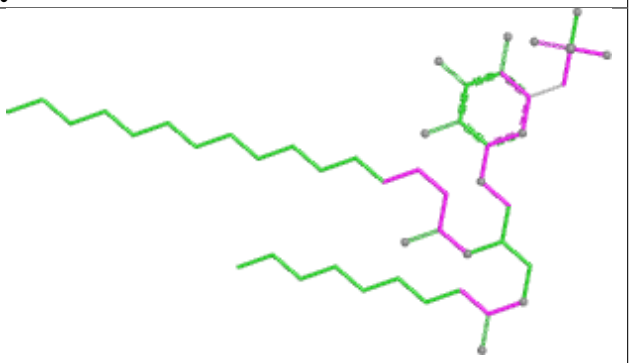


Rings

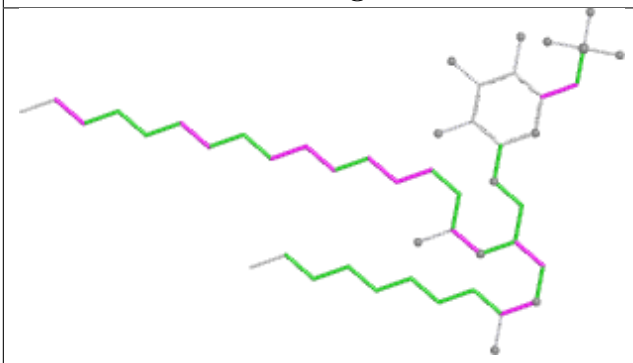
Ligand SQD b 601



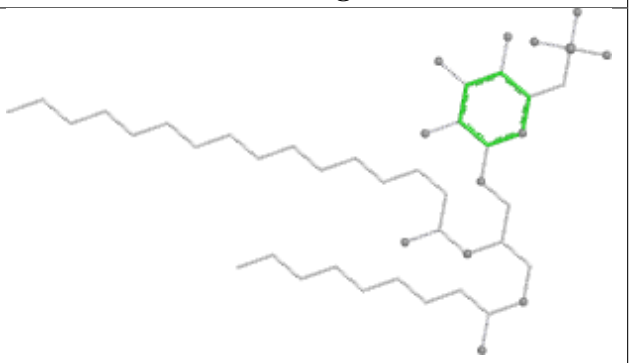
Bond lengths



Bond angles

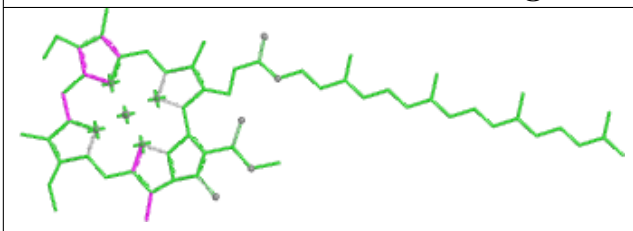


Torsions

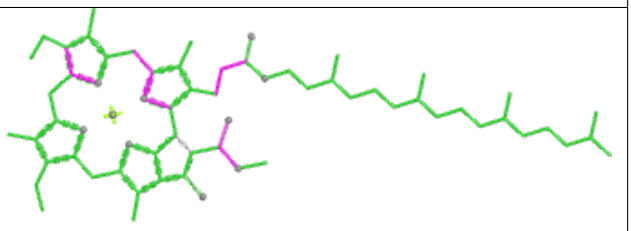


Rings

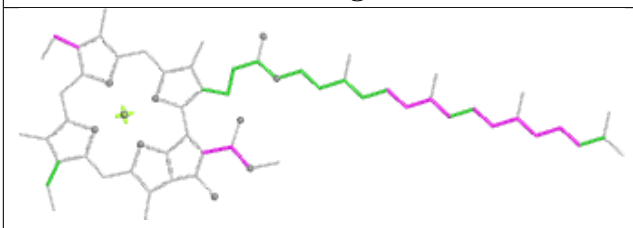
Ligand CLA C 506



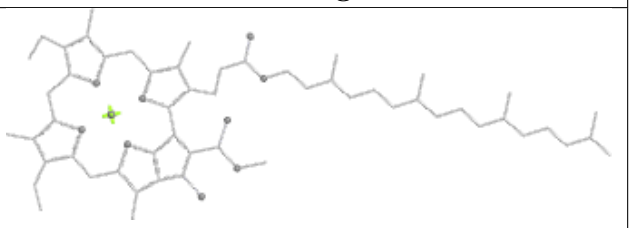
Bond lengths



Bond angles

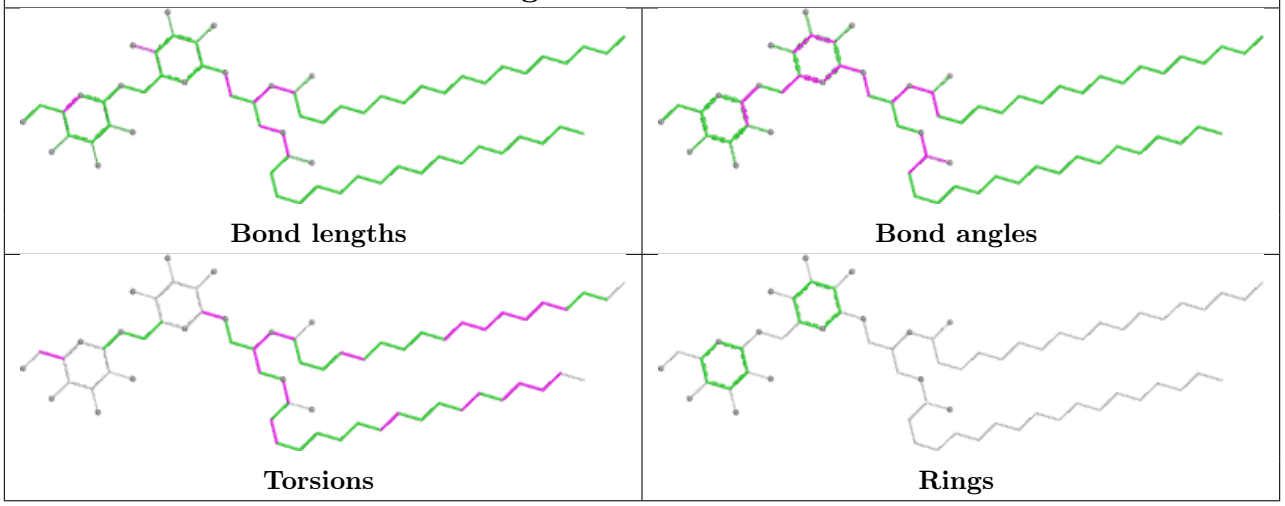


Torsions

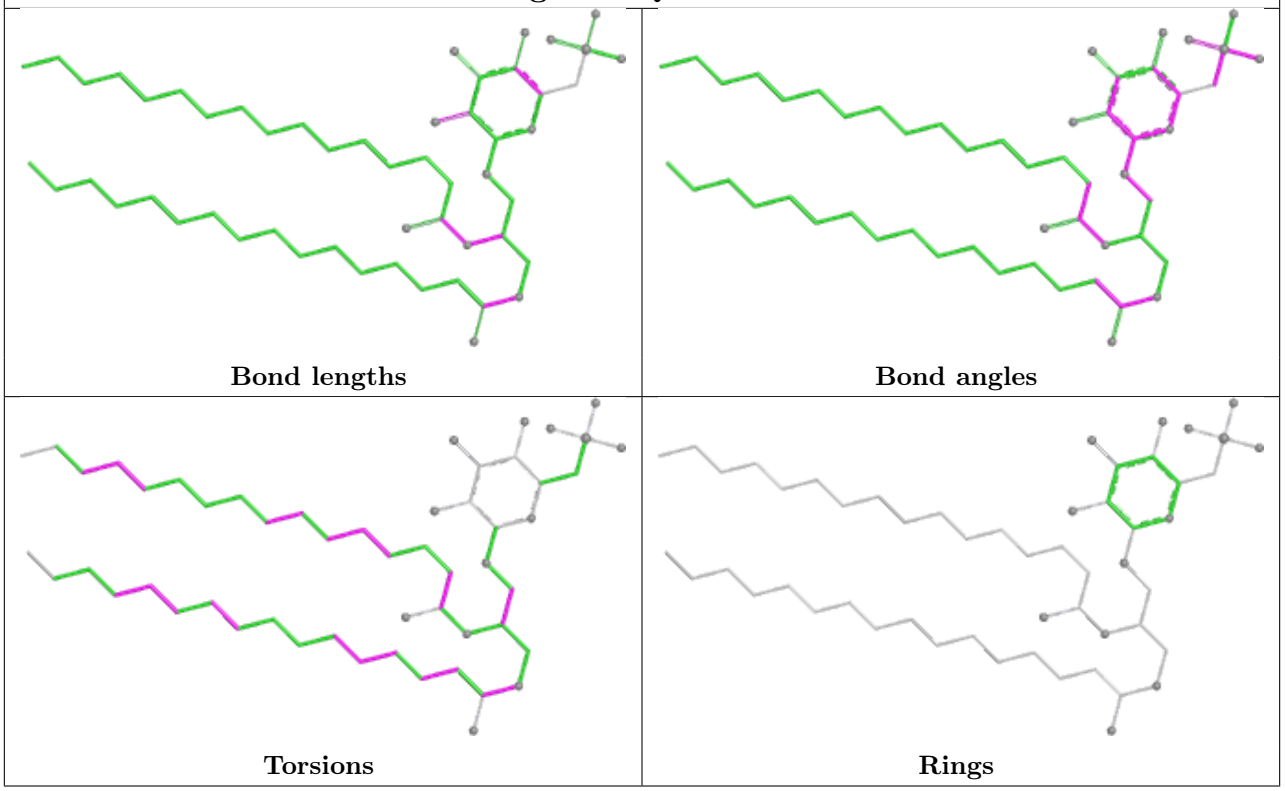


Rings

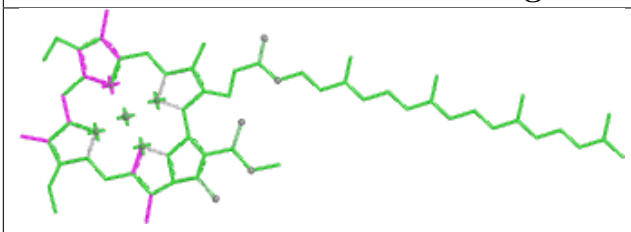
Ligand DGD C 519



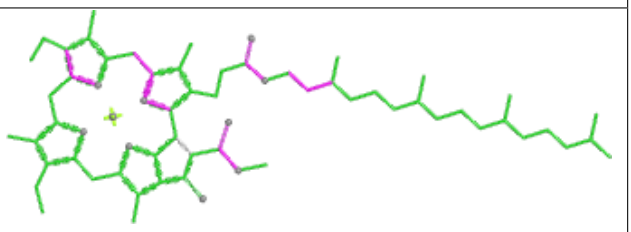
Ligand SQD a 401



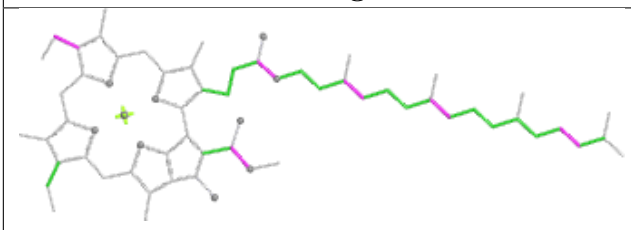
Ligand CLA B 611



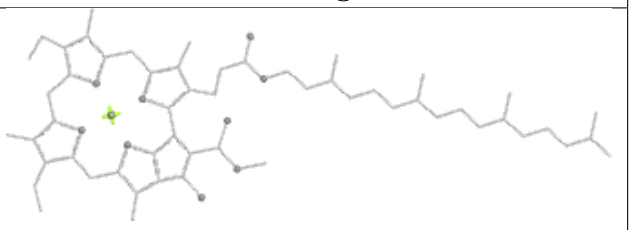
Bond lengths



Bond angles

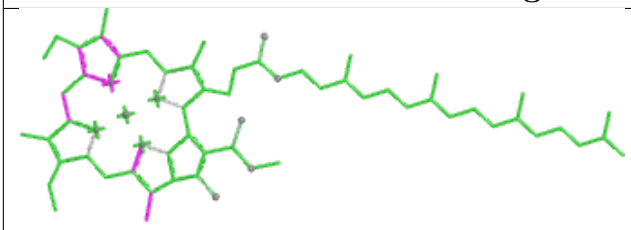


Torsions

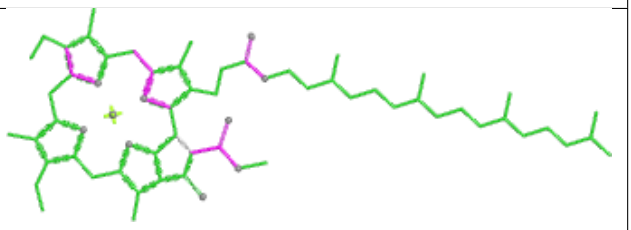


Rings

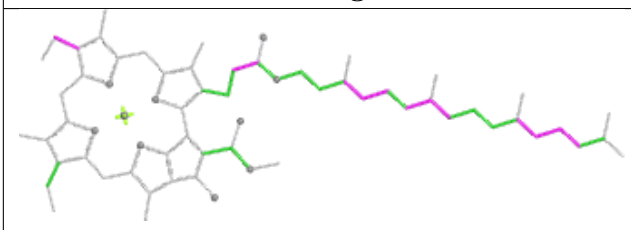
Ligand CLA D 401



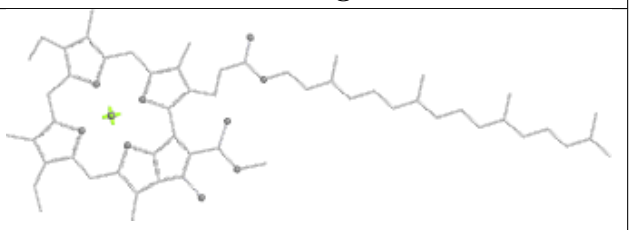
Bond lengths



Bond angles

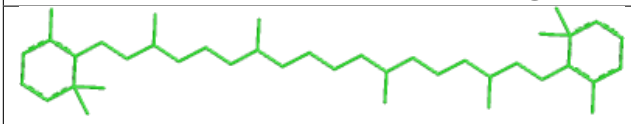


Torsions

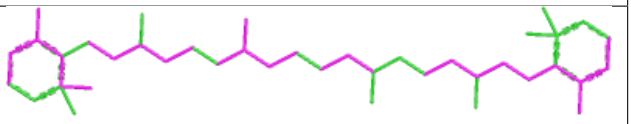


Rings

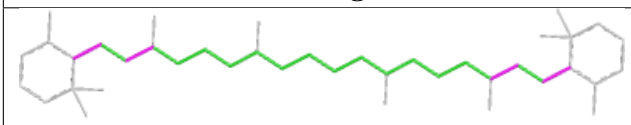
Ligand BCR k 102



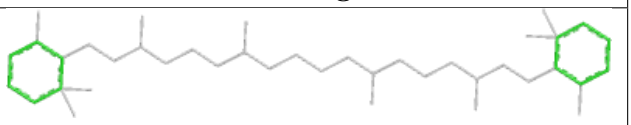
Bond lengths



Bond angles

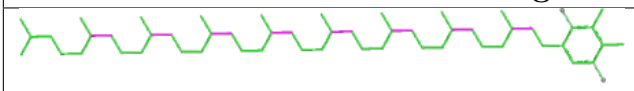


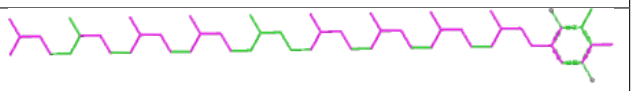
Torsions

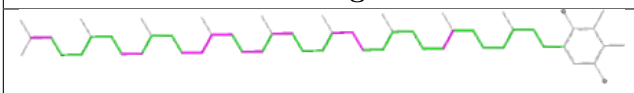


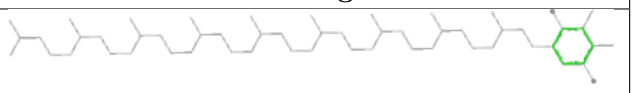
Rings

Ligand PL9 d 404

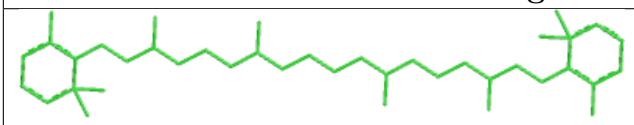

Bond lengths

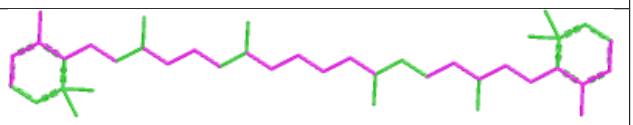

Bond angles


Torsions

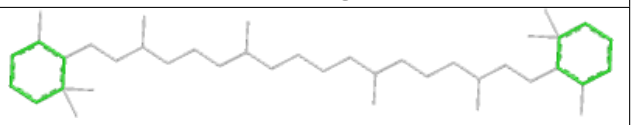

Rings

Ligand BCR z 101

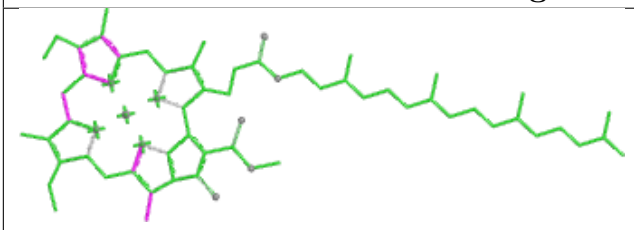

Bond lengths

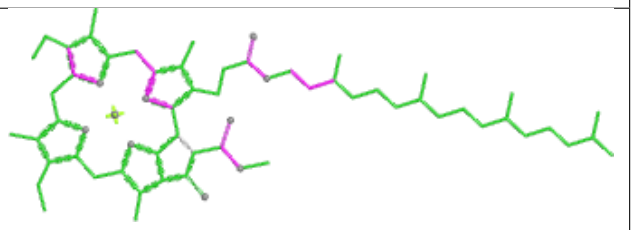

Bond angles

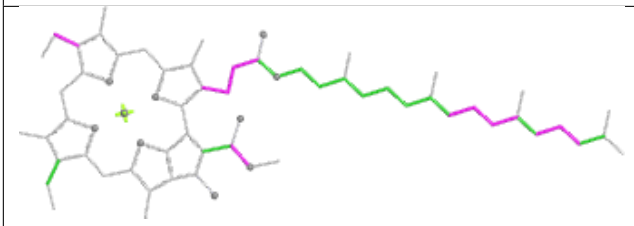

Torsions

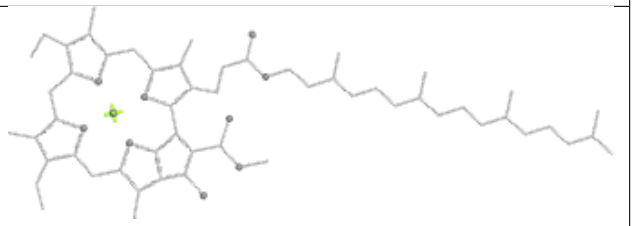

Rings

Ligand CLA c 501

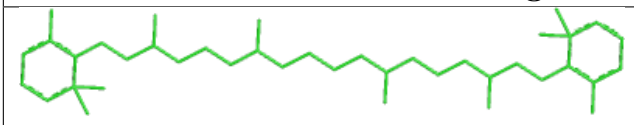

Bond lengths

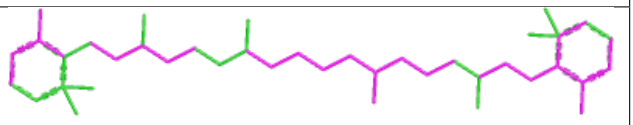

Bond angles

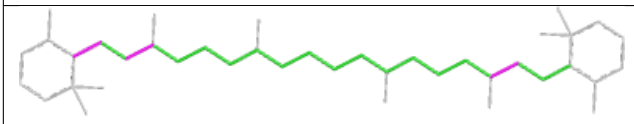

Torsions

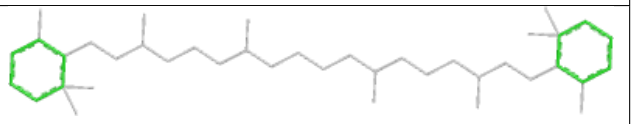

Rings

Ligand BCR d 405

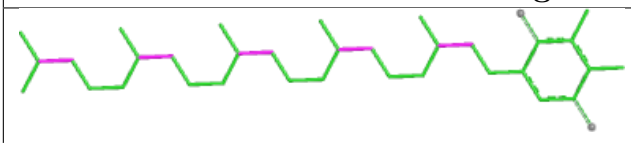

Bond lengths


Bond angles

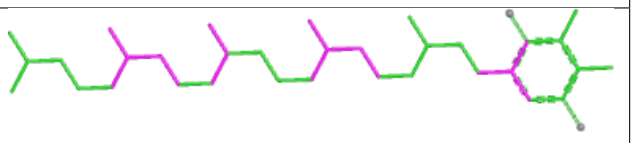

Torsions


Rings

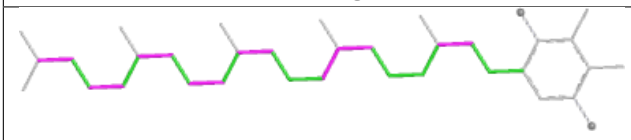
Ligand PL9 J 101



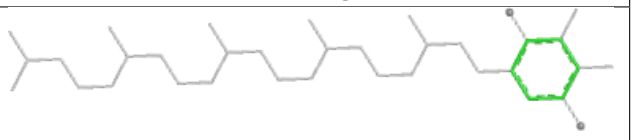
Bond lengths



Bond angles

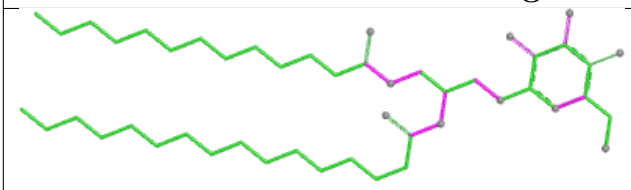


Torsions

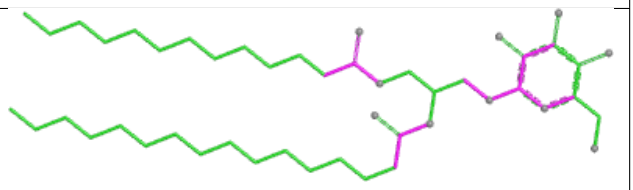


Rings

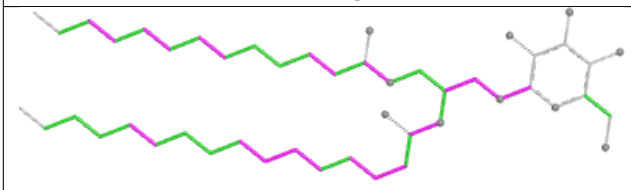
Ligand LMG d 407



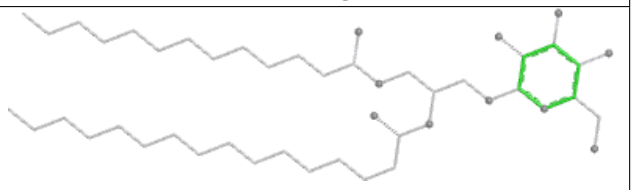
Bond lengths



Bond angles

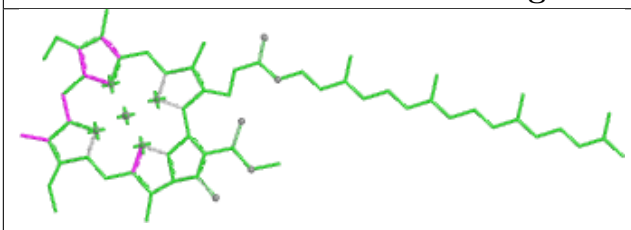


Torsions

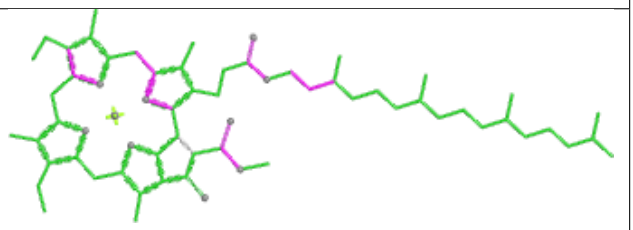


Rings

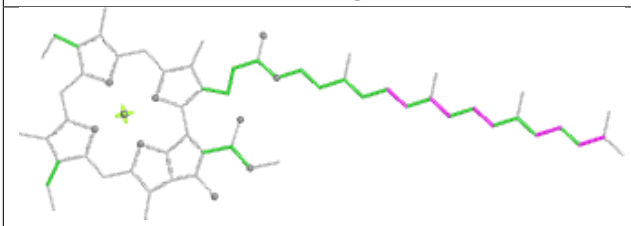
Ligand CLA a 409



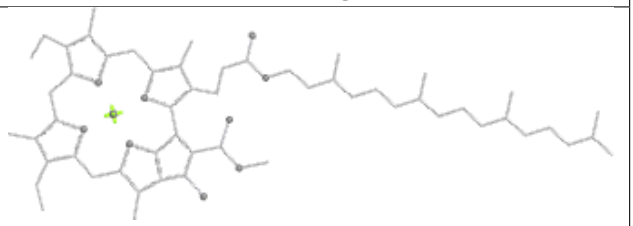
Bond lengths



Bond angles

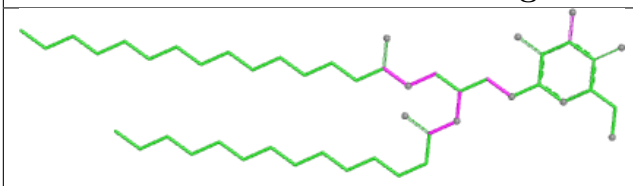


Torsions

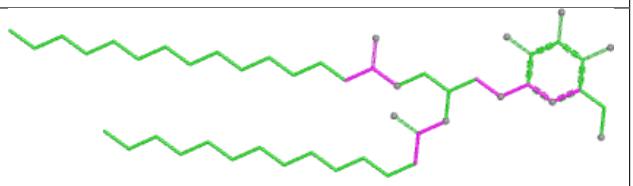


Rings

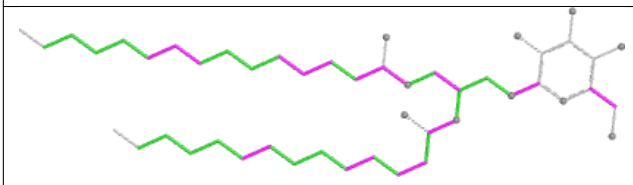
Ligand LMG C 520



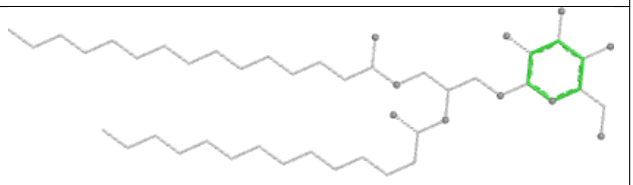
Bond lengths



Bond angles

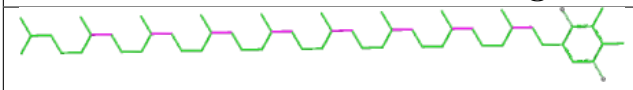


Torsions

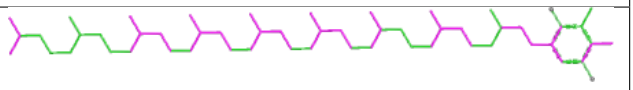


Rings

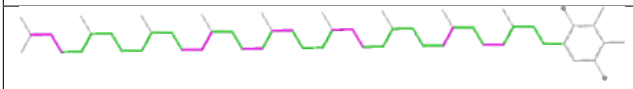
Ligand PL9 D 404



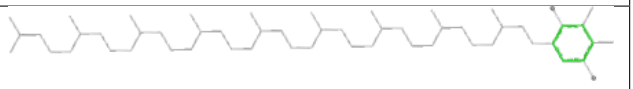
Bond lengths



Bond angles

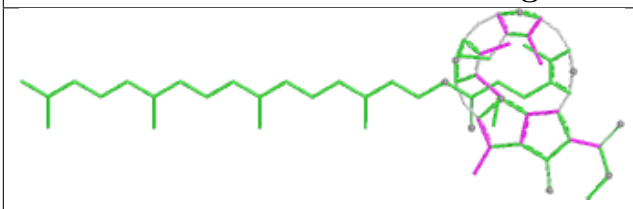


Torsions

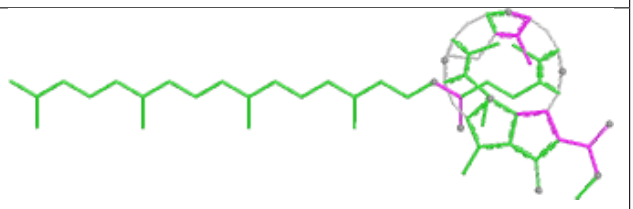


Rings

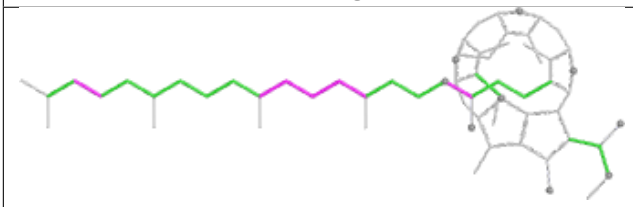
Ligand PHO D 402



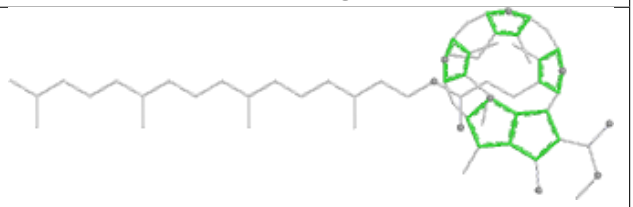
Bond lengths



Bond angles

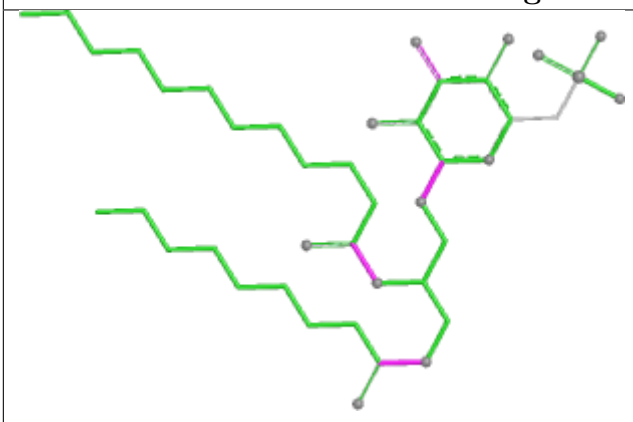


Torsions

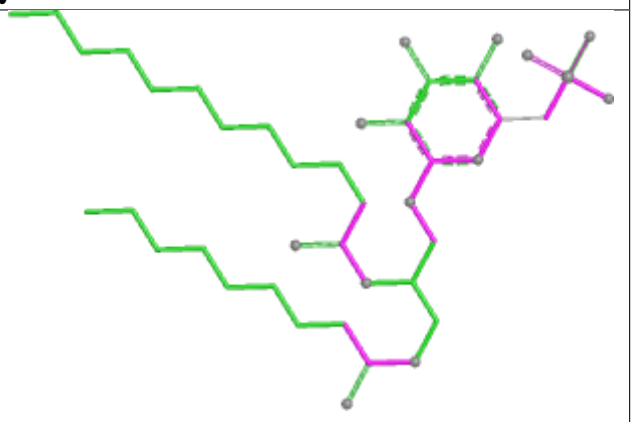


Rings

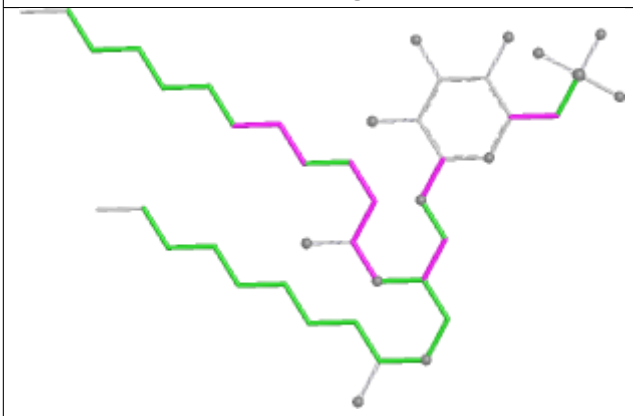
Ligand SQD D 408



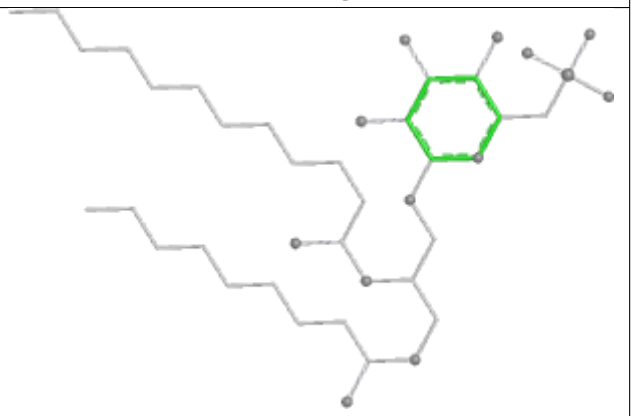
Bond lengths



Bond angles

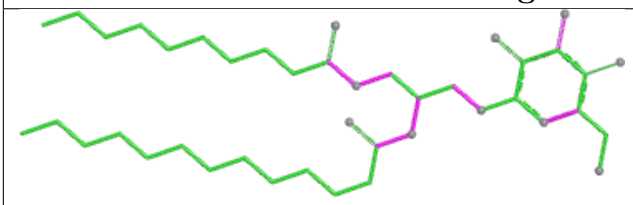


Torsions

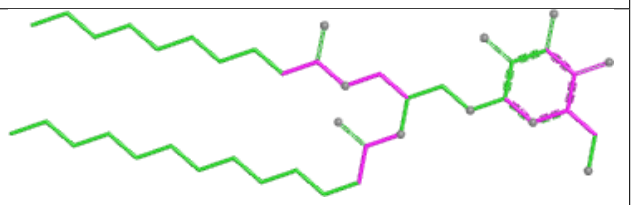


Rings

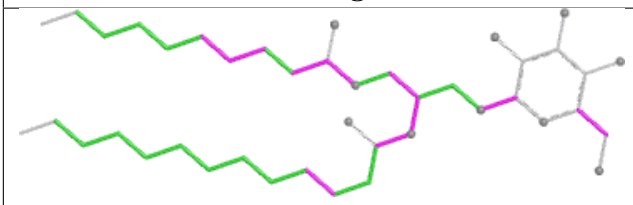
Ligand LMG m 102



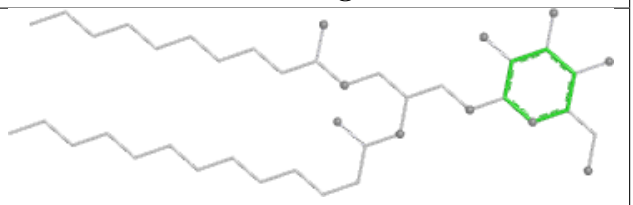
Bond lengths



Bond angles

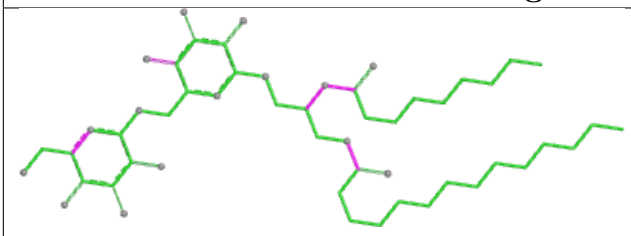


Torsions

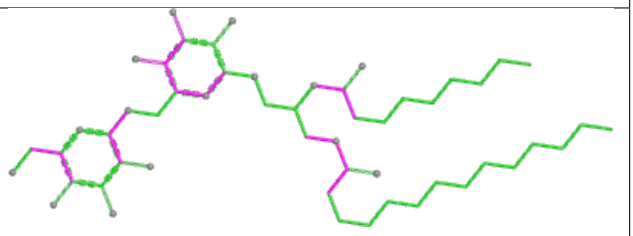


Rings

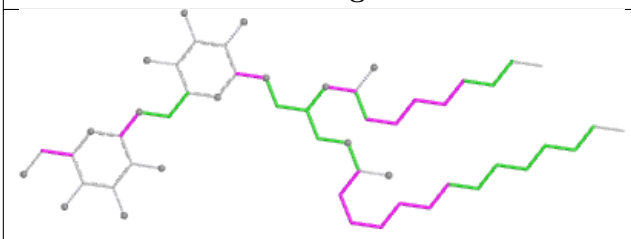
Ligand DGD c 516



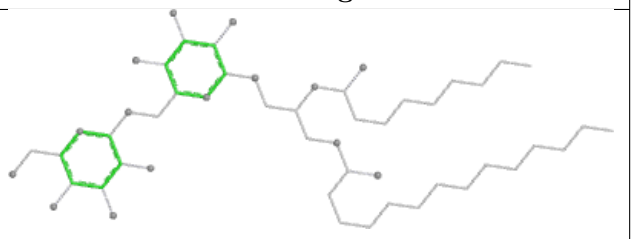
Bond lengths



Bond angles

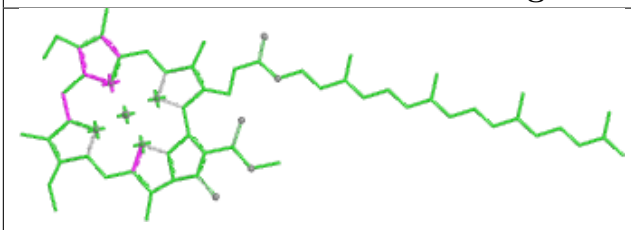


Torsions

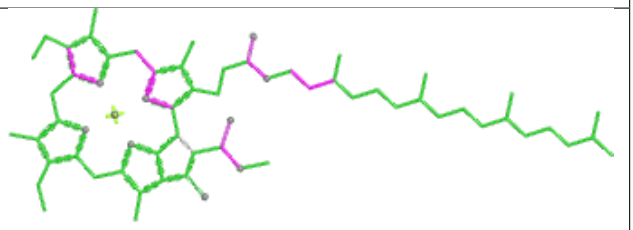


Rings

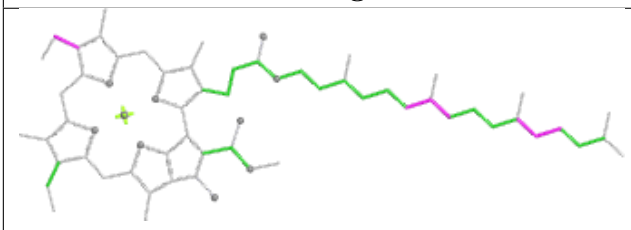
Ligand CLA b 619



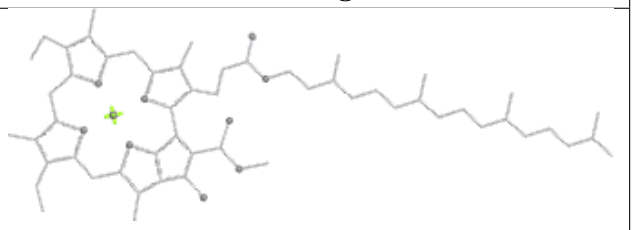
Bond lengths



Bond angles

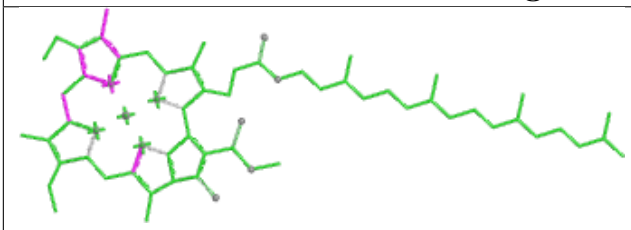


Torsions

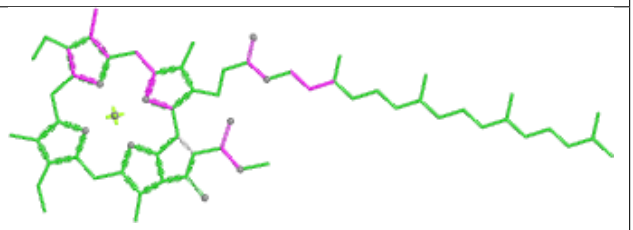


Rings

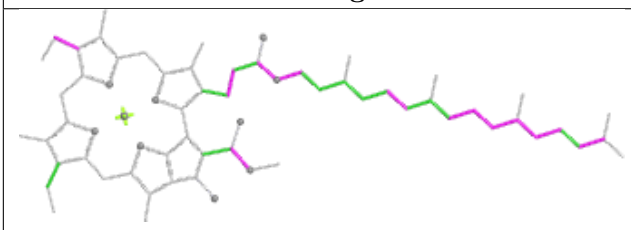
Ligand CLA B 610



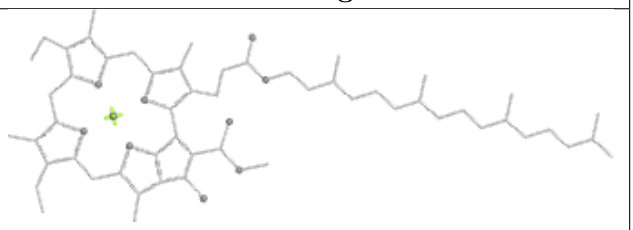
Bond lengths



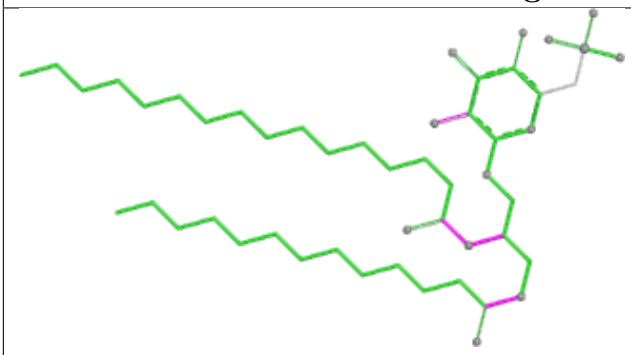
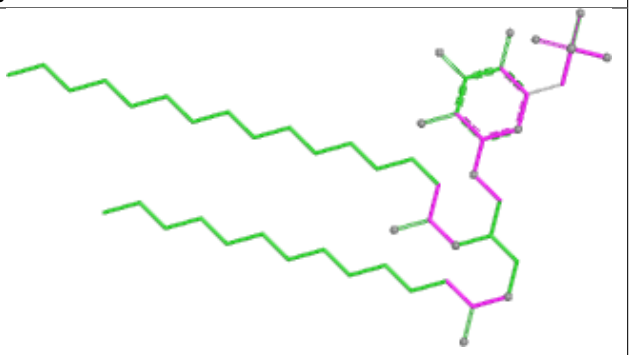
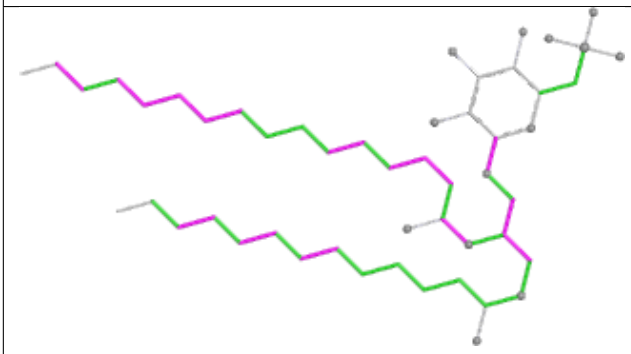
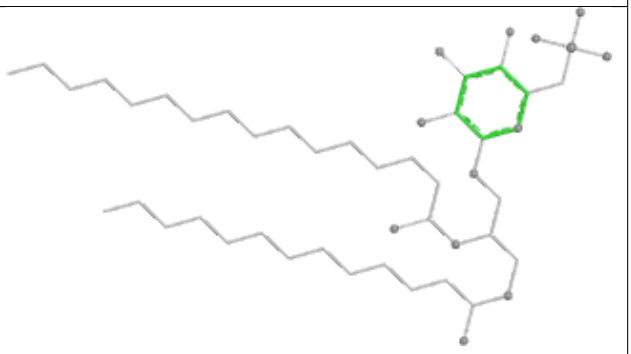
Bond angles

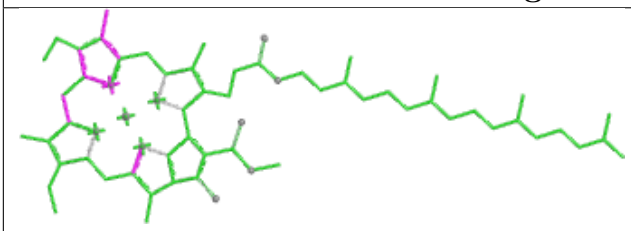
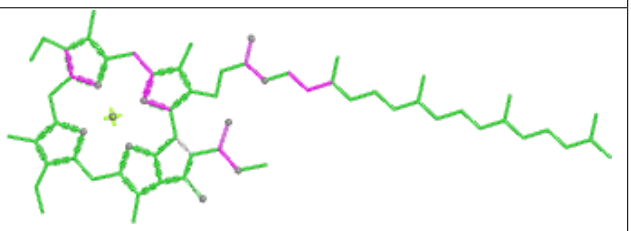
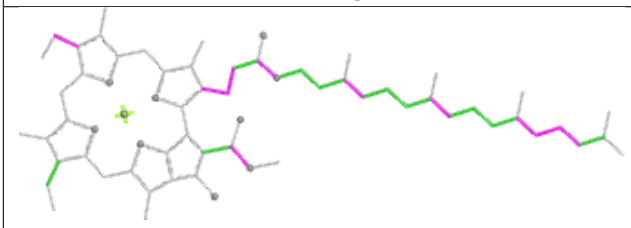
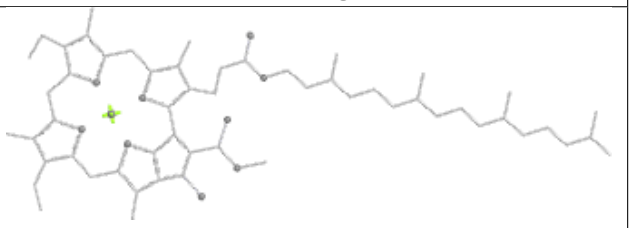


Torsions

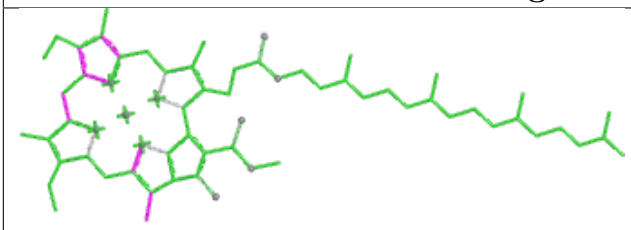


Rings

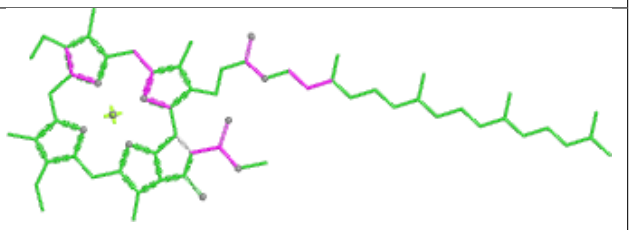
Ligand SQD A 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

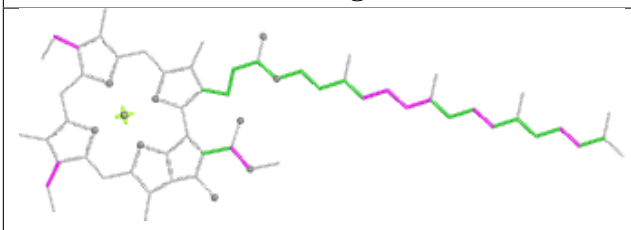
Ligand CLA a 406



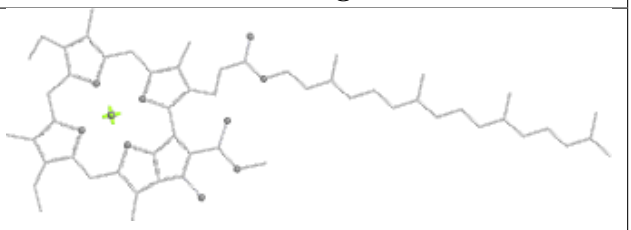
Bond lengths



Bond angles

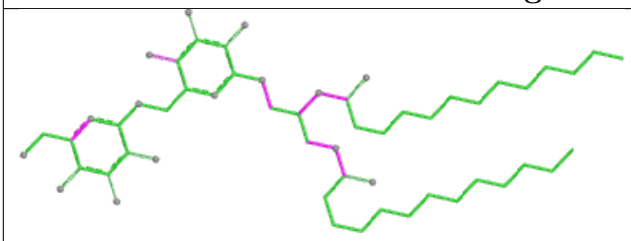


Torsions

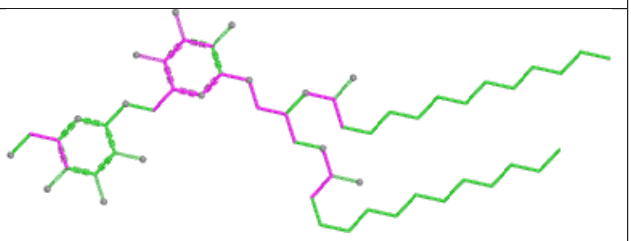


Rings

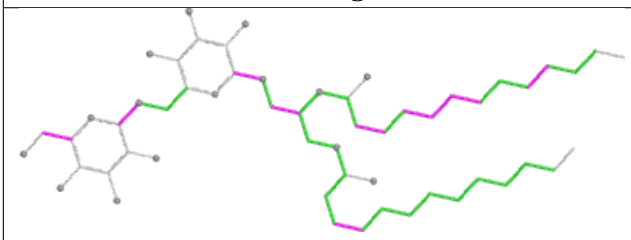
Ligand DGD a 413



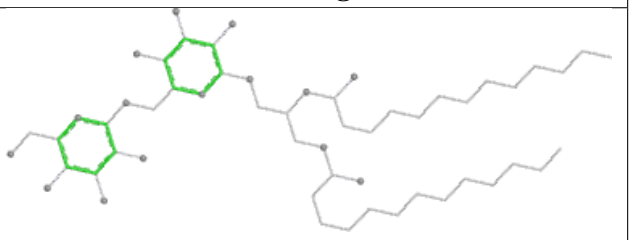
Bond lengths



Bond angles

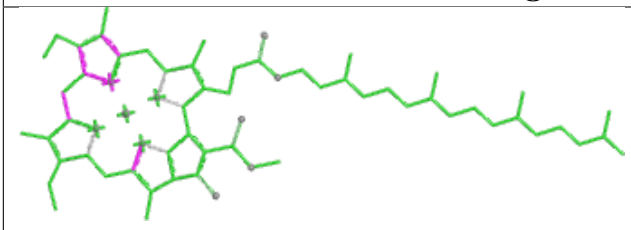


Torsions

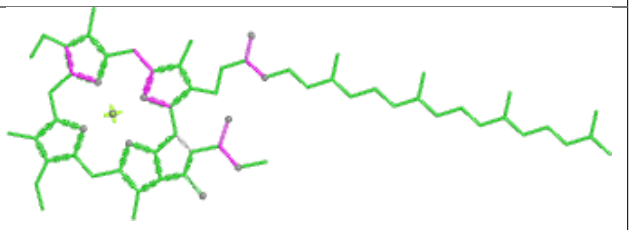


Rings

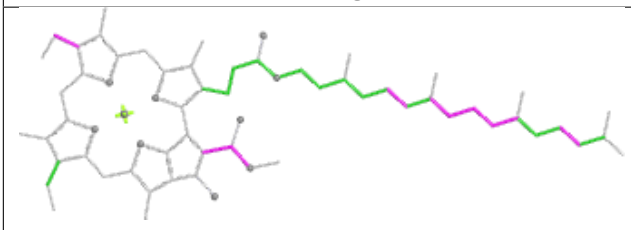
Ligand CLA C 503



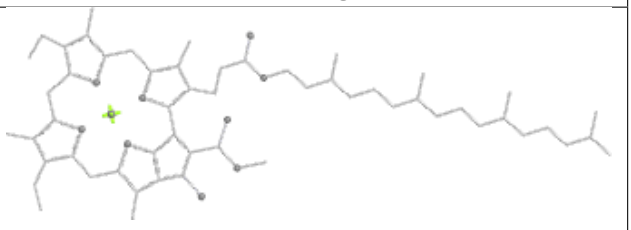
Bond lengths



Bond angles

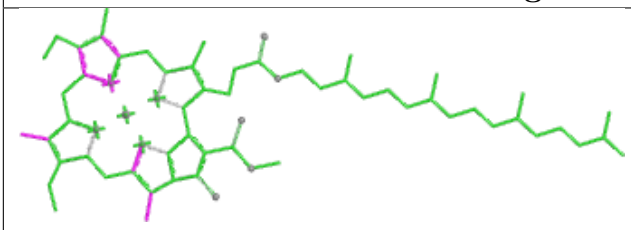


Torsions

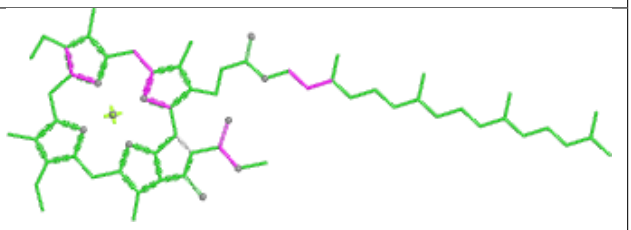


Rings

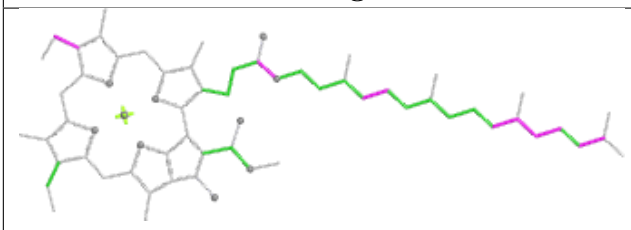
Ligand CLA C 502



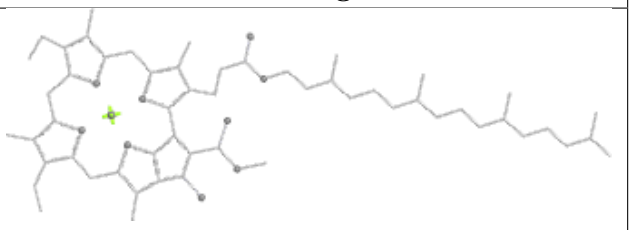
Bond lengths



Bond angles

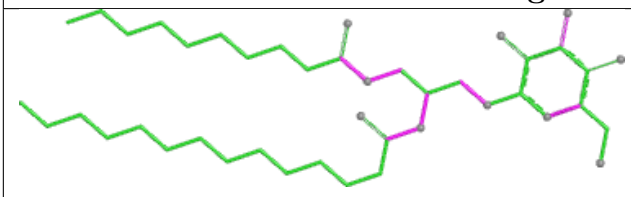


Torsions

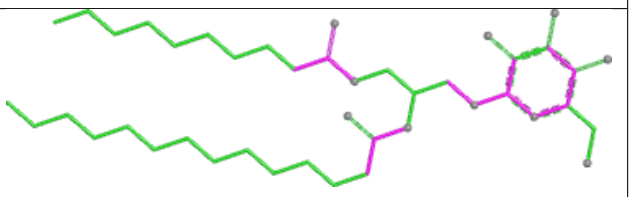


Rings

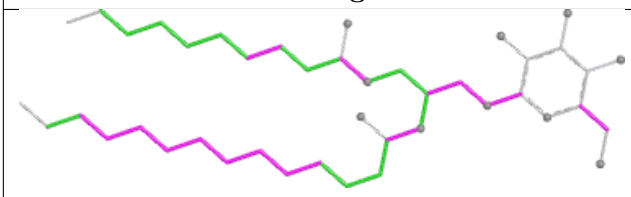
Ligand LMG i 101



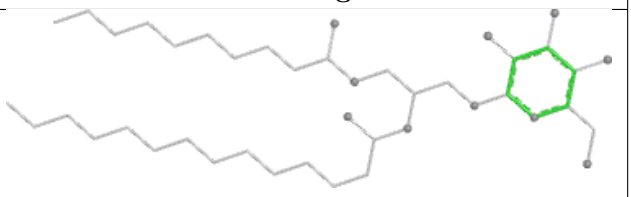
Bond lengths



Bond angles

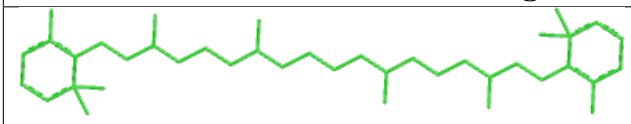


Torsions

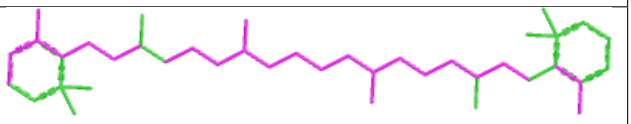


Rings

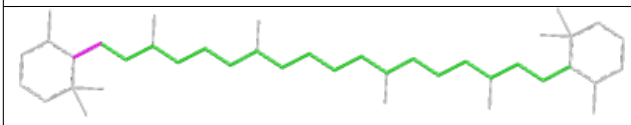
Ligand BCR H 101



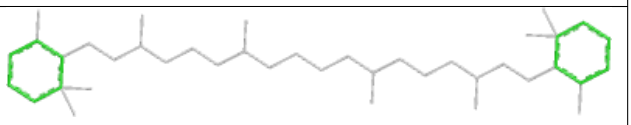
Bond lengths



Bond angles

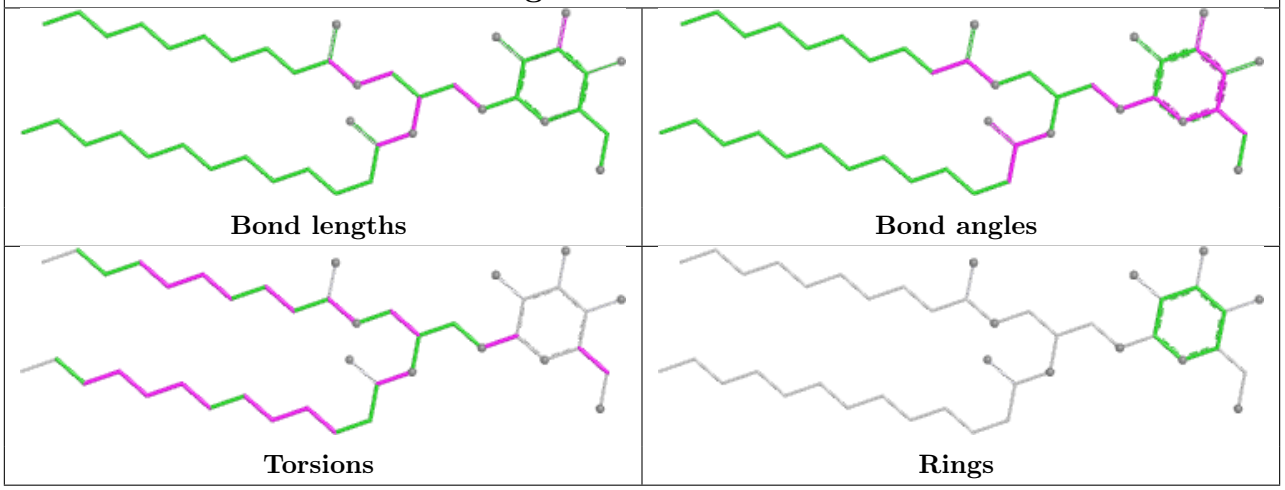


Torsions

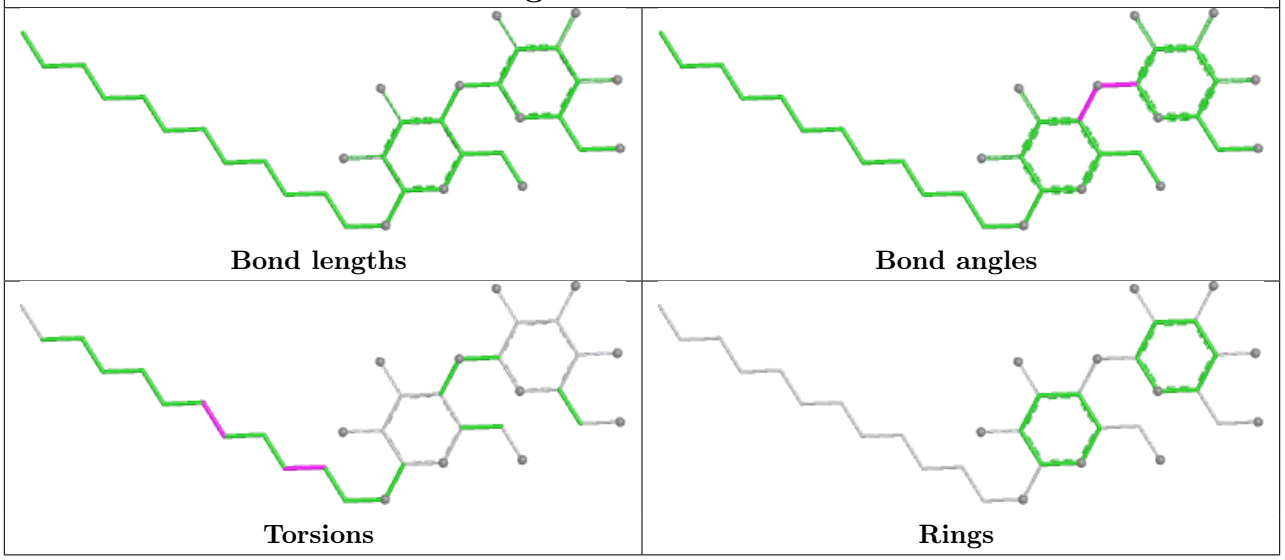


Rings

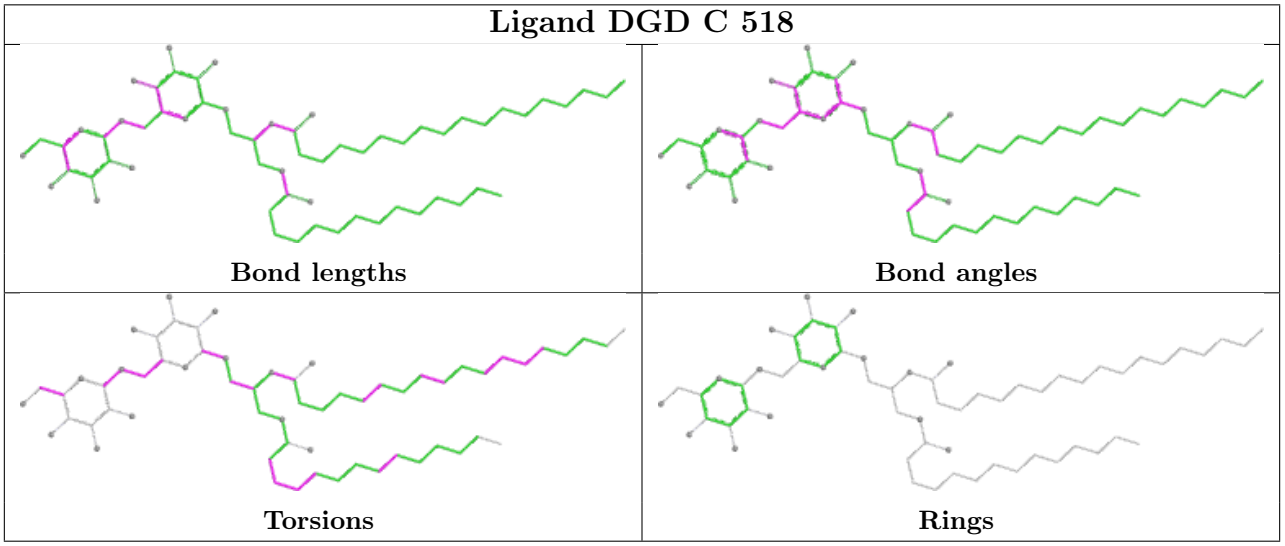
Ligand LMG a 402



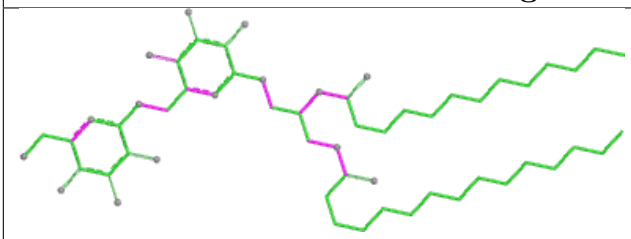
Ligand LMT b 626



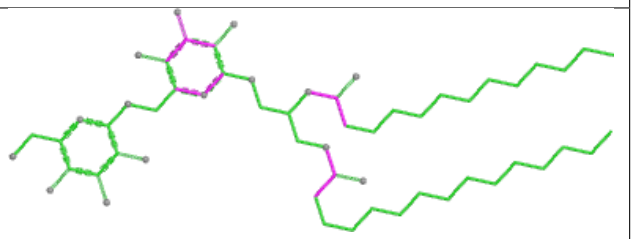
Ligand DGD C 518



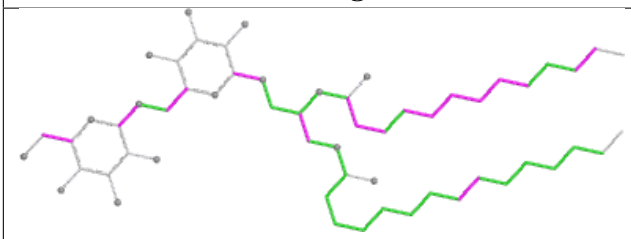
Ligand DGD B 621



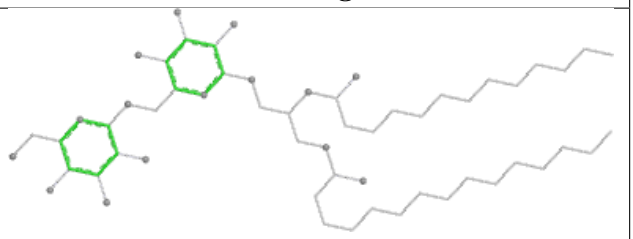
Bond lengths



Bond angles

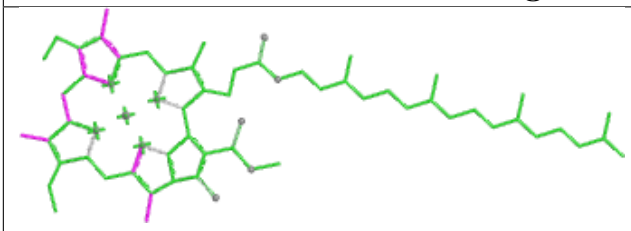


Torsions

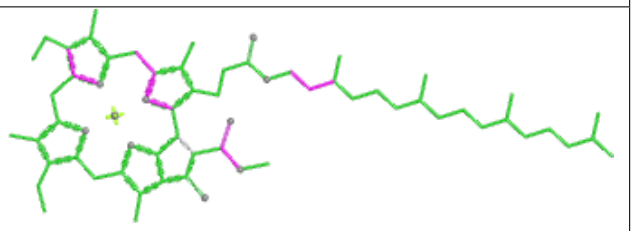


Rings

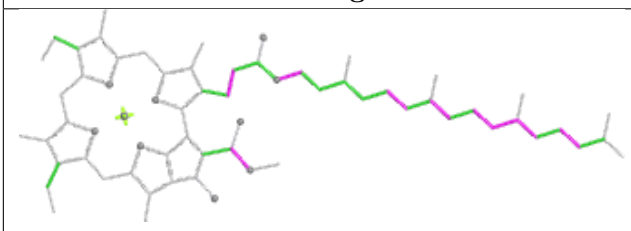
Ligand CLA C 508



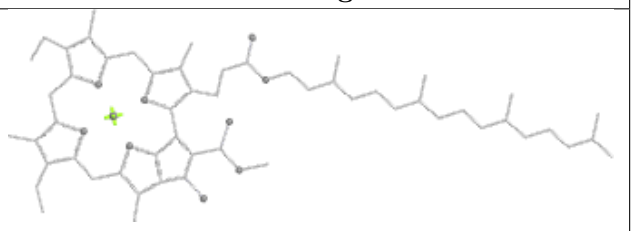
Bond lengths



Bond angles

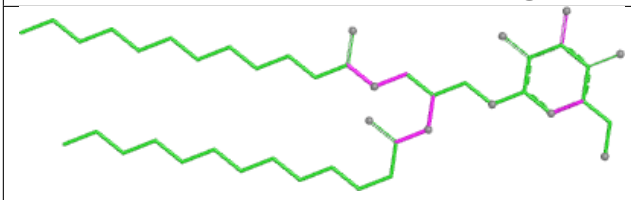


Torsions

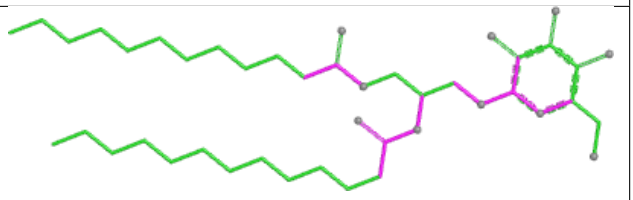


Rings

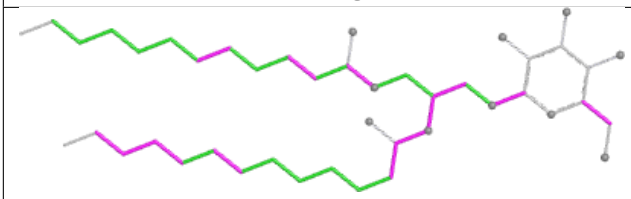
Ligand LMG E 101



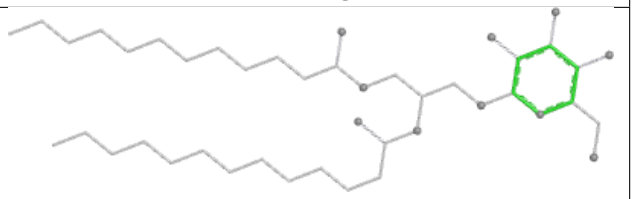
Bond lengths



Bond angles

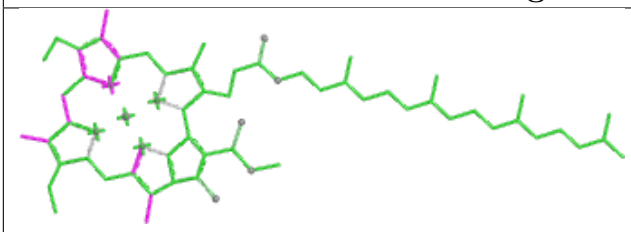


Torsions

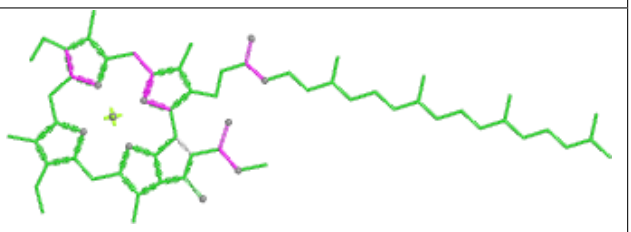


Rings

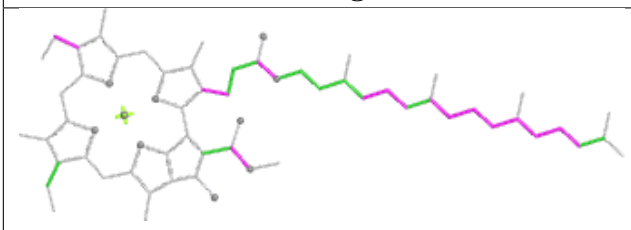
Ligand CLA b 620



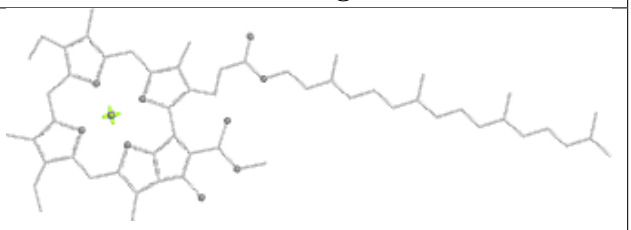
Bond lengths



Bond angles

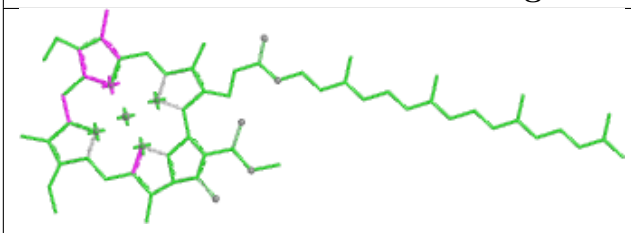


Torsions

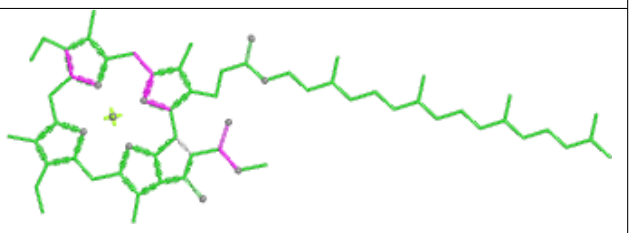


Rings

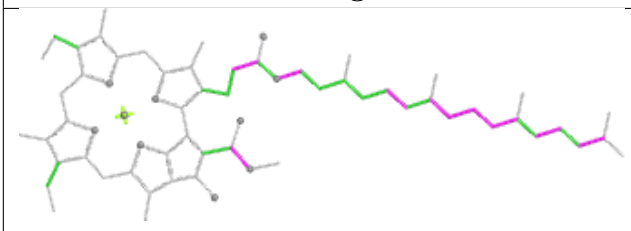
Ligand CLA B 613



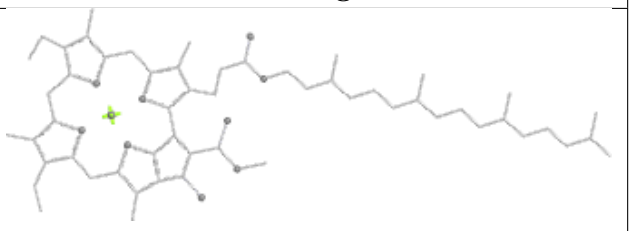
Bond lengths



Bond angles

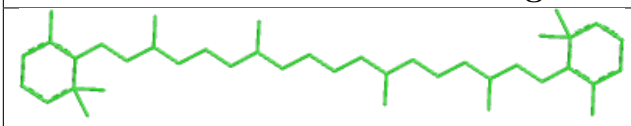


Torsions

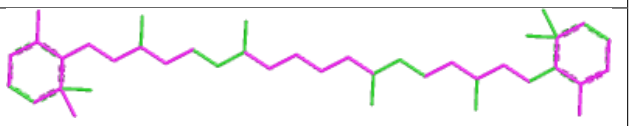


Rings

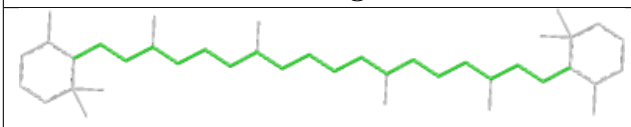
Ligand BCR b 621



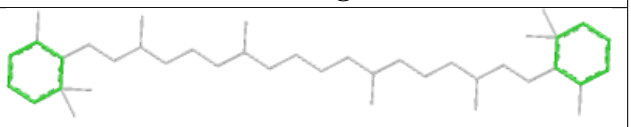
Bond lengths



Bond angles

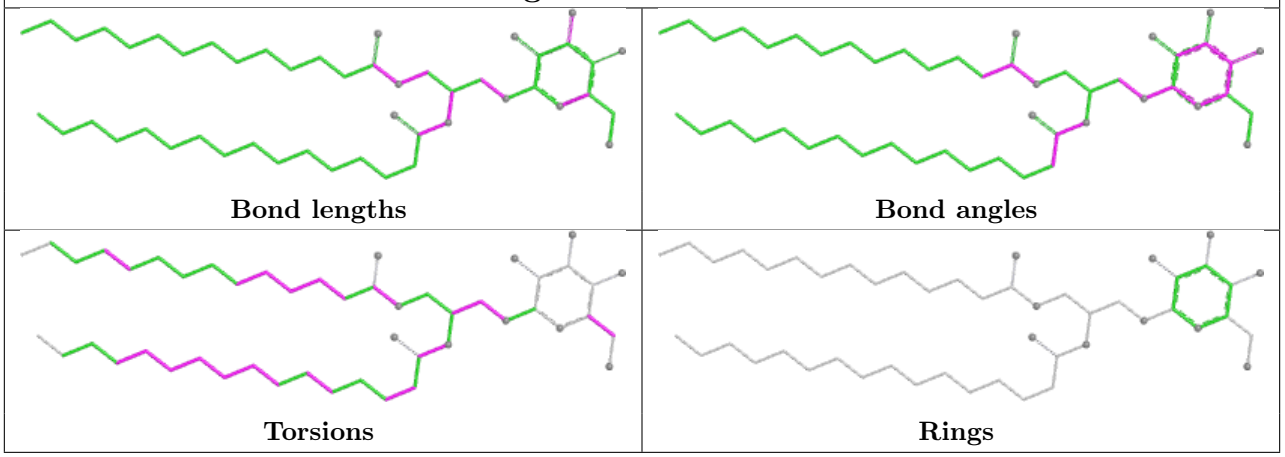


Torsions

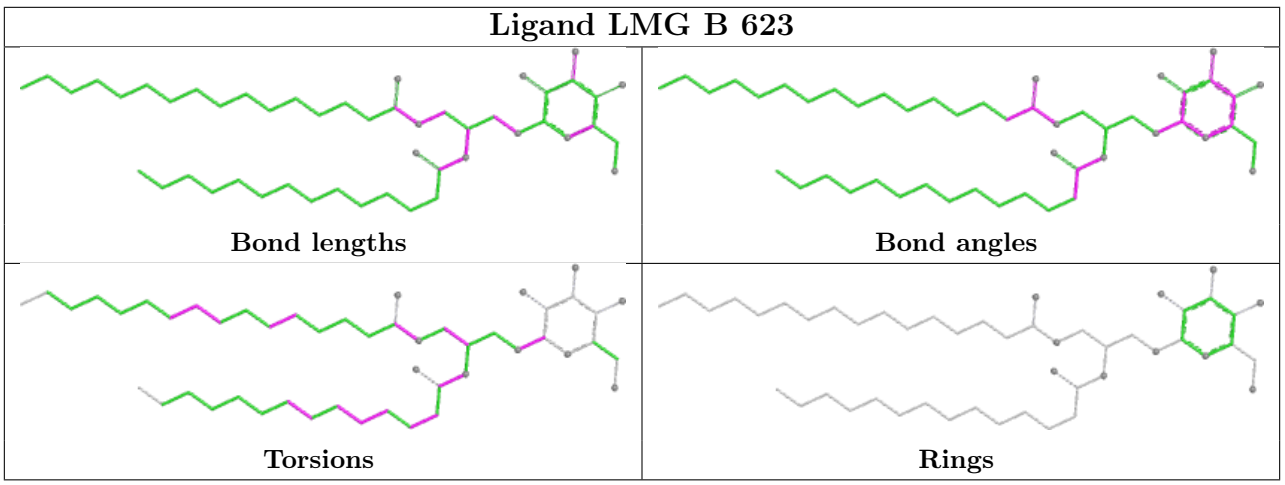


Rings

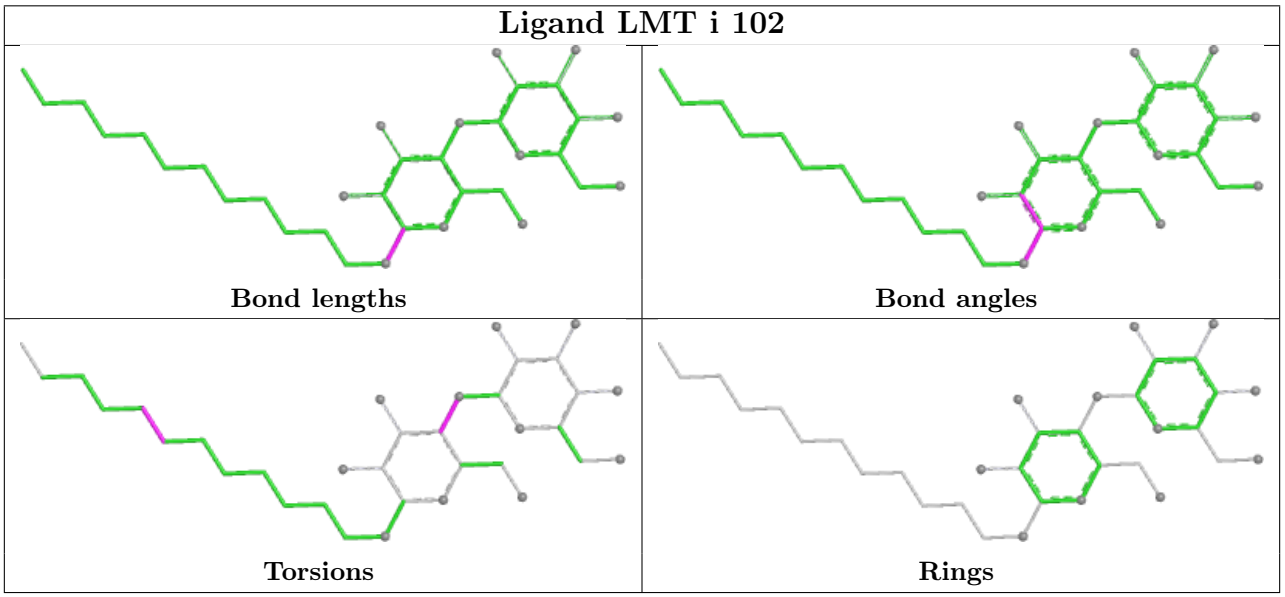
Ligand LMG b 624



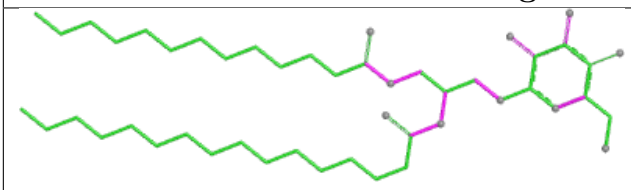
Ligand LMG B 623



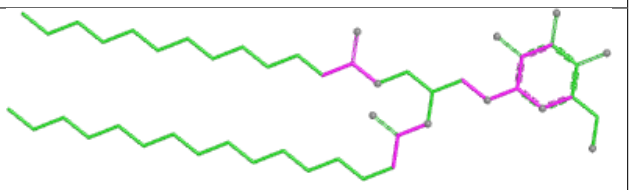
Ligand LMT i 102



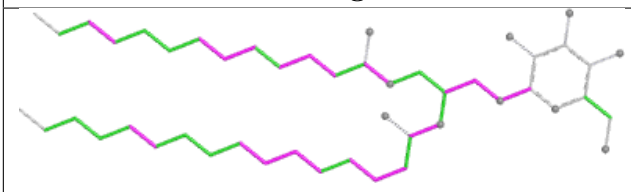
Ligand LMG D 407



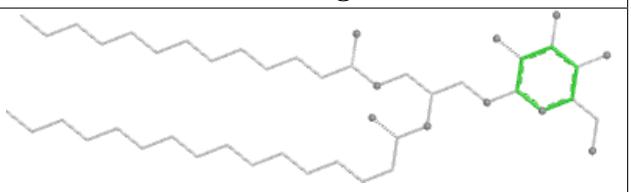
Bond lengths



Bond angles

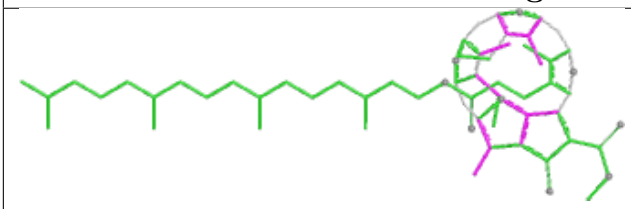


Torsions



Rings

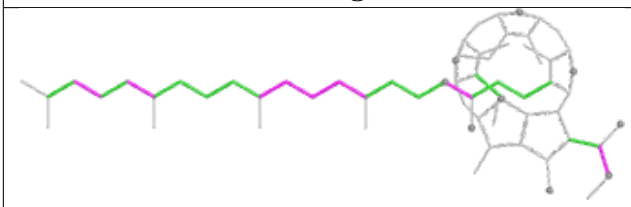
Ligand PHO a 407



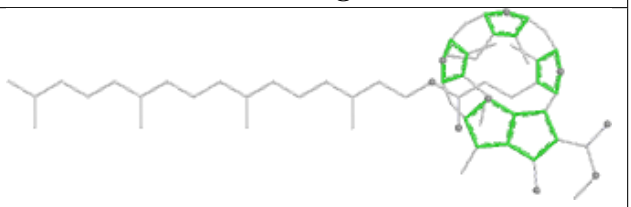
Bond lengths



Bond angles

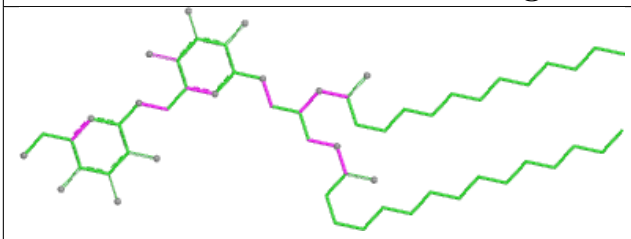


Torsions

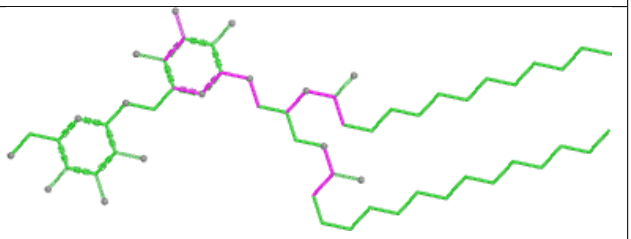


Rings

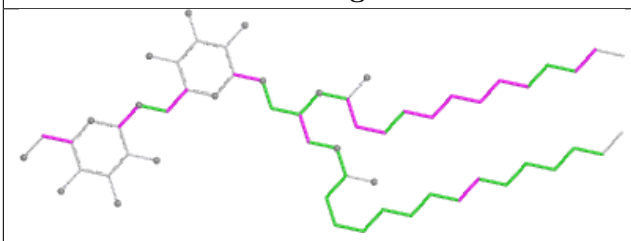
Ligand DGD b 623



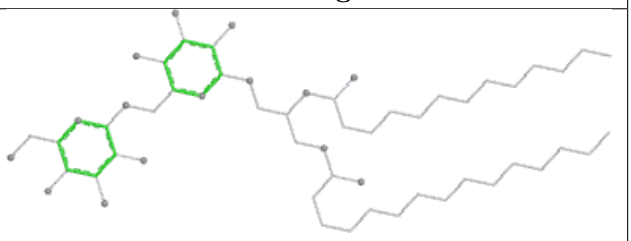
Bond lengths



Bond angles

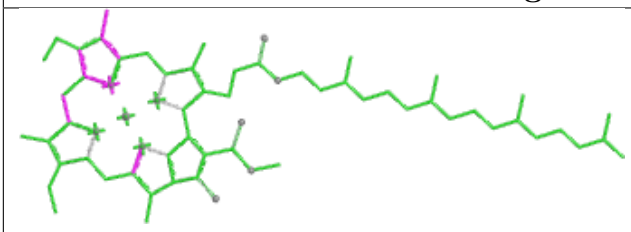


Torsions

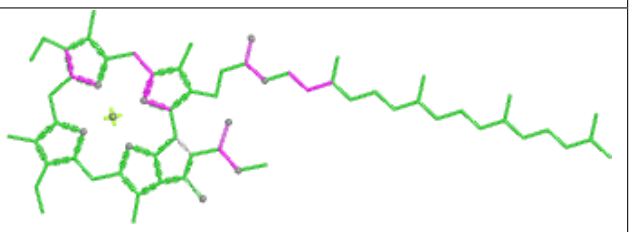


Rings

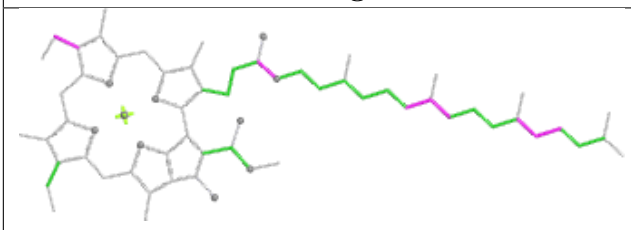
Ligand CLA B 615



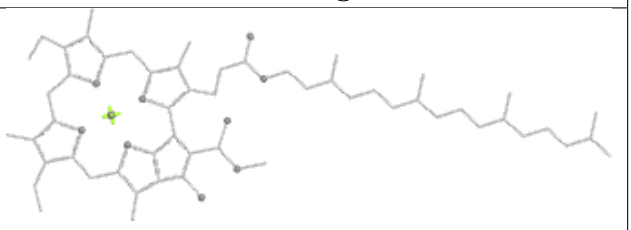
Bond lengths



Bond angles

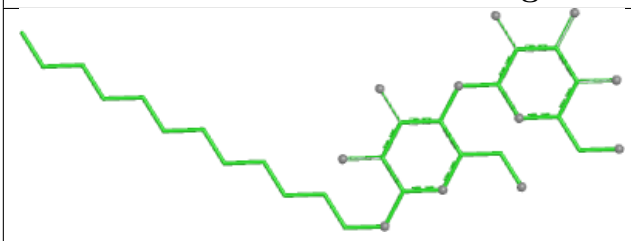


Torsions

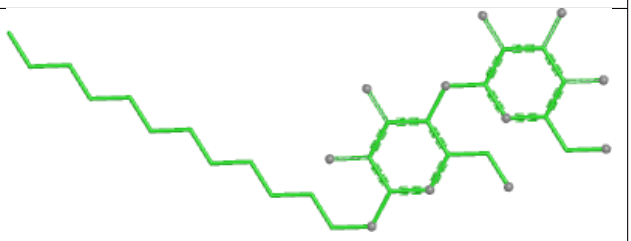


Rings

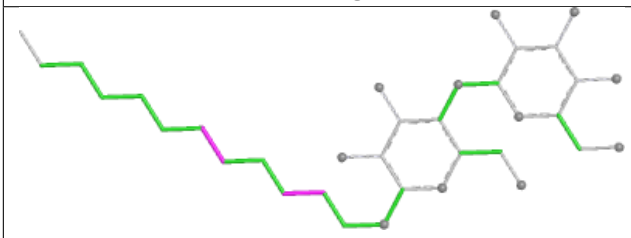
Ligand LMT B 624



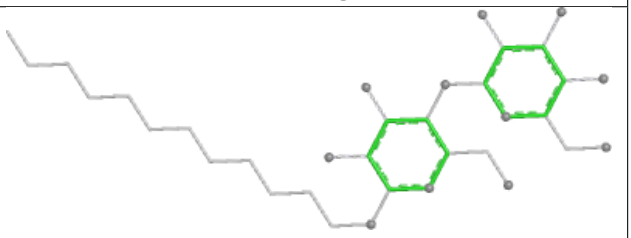
Bond lengths



Bond angles

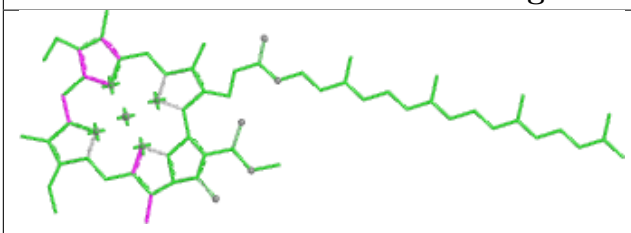


Torsions

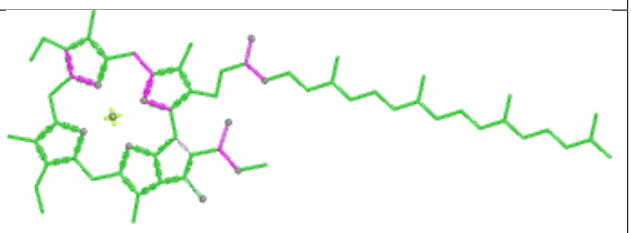


Rings

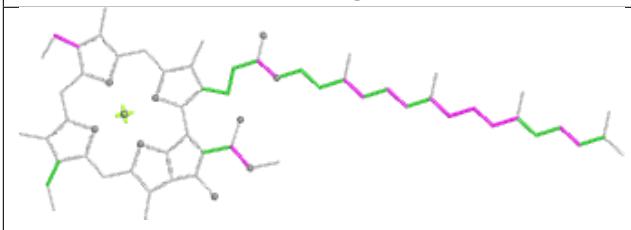
Ligand CLA b 609



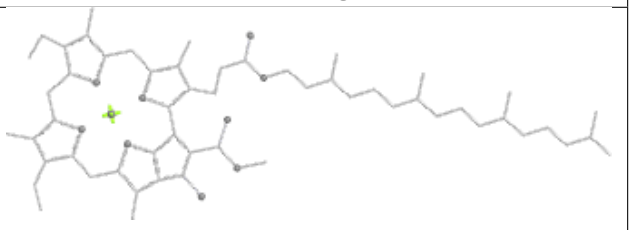
Bond lengths



Bond angles

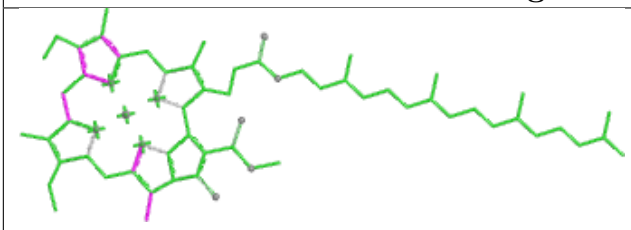


Torsions

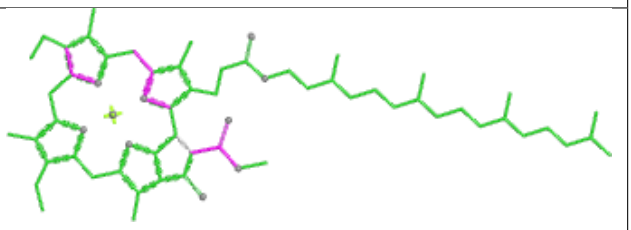


Rings

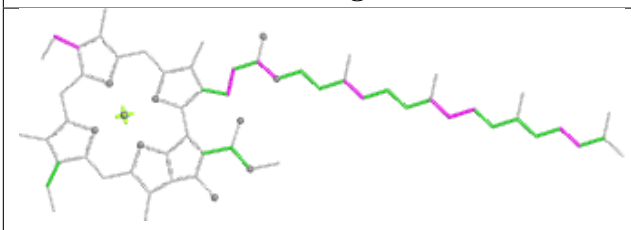
Ligand CLA d 403



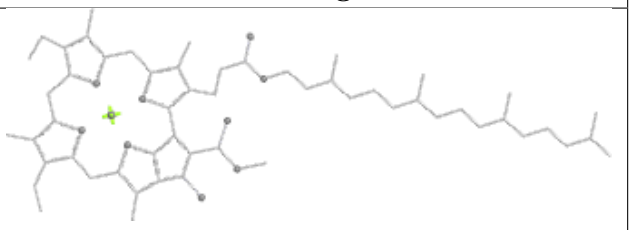
Bond lengths



Bond angles

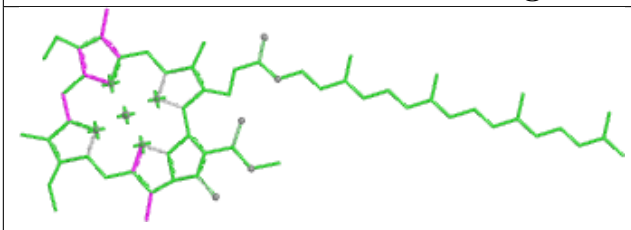


Torsions

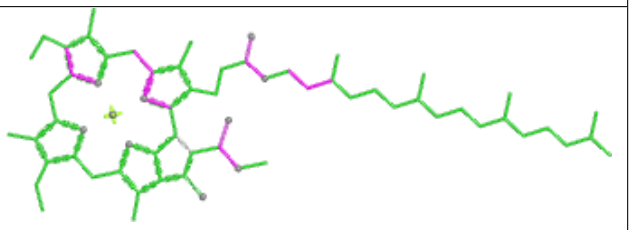


Rings

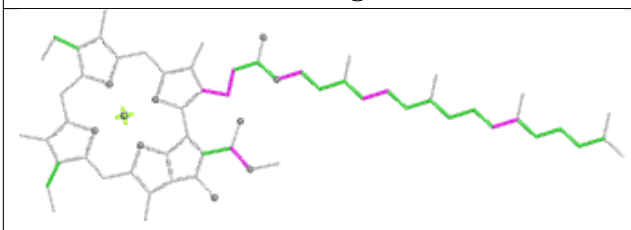
Ligand CLA A 403



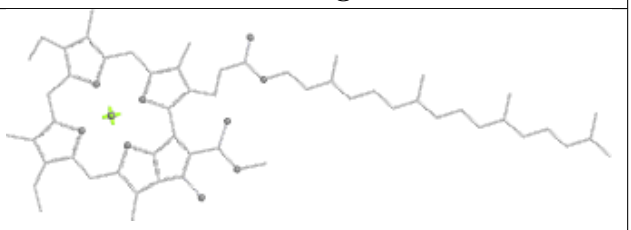
Bond lengths



Bond angles

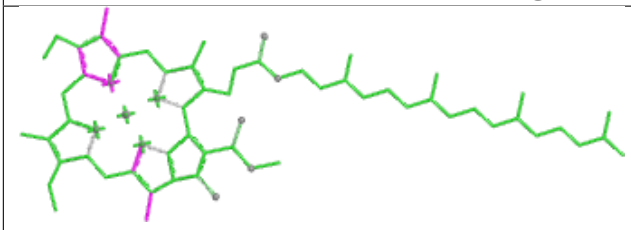


Torsions

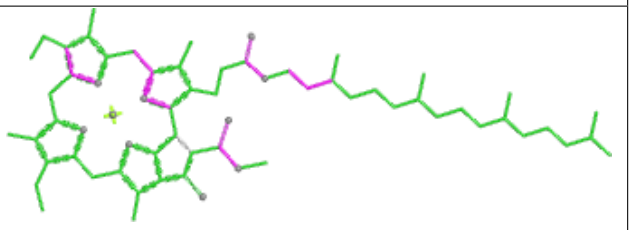


Rings

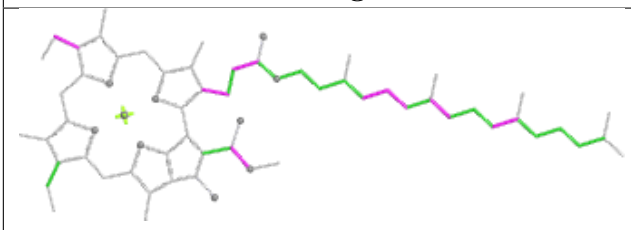
Ligand CLA c 507



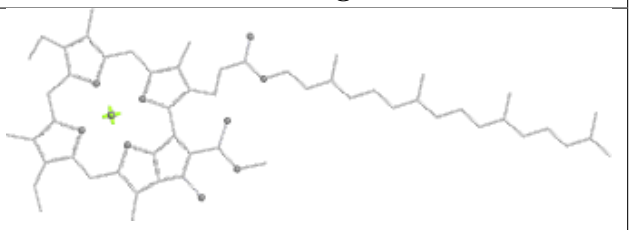
Bond lengths



Bond angles

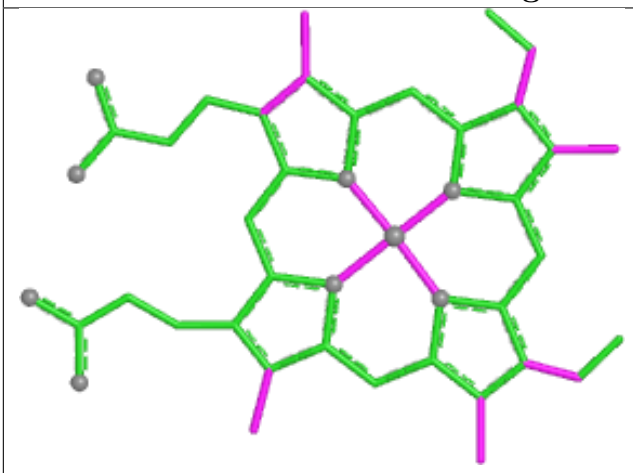


Torsions

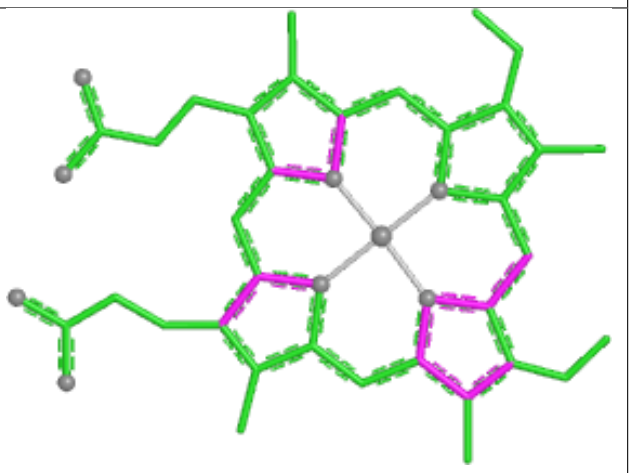


Rings

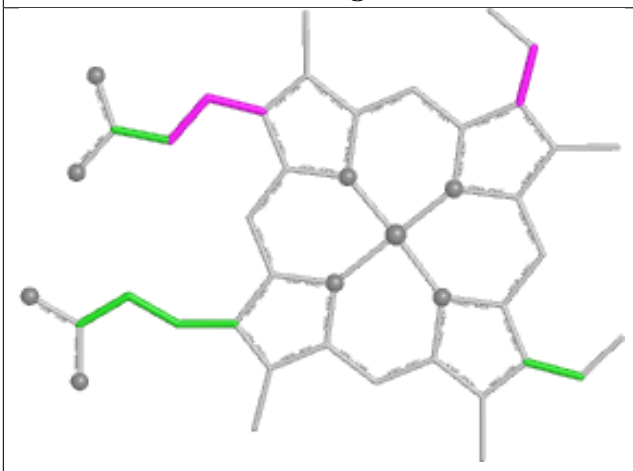
Ligand HEM v 201



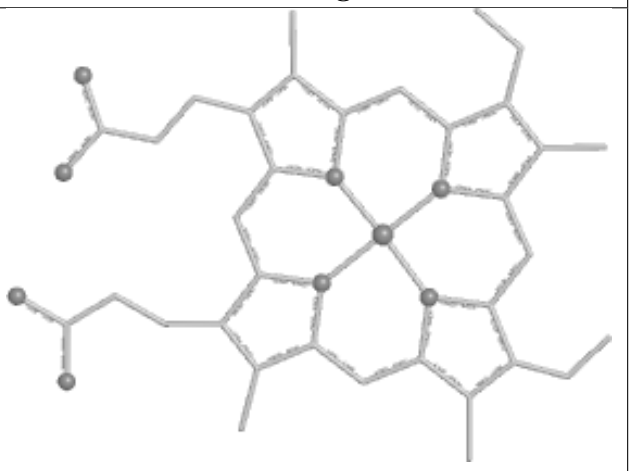
Bond lengths



Bond angles

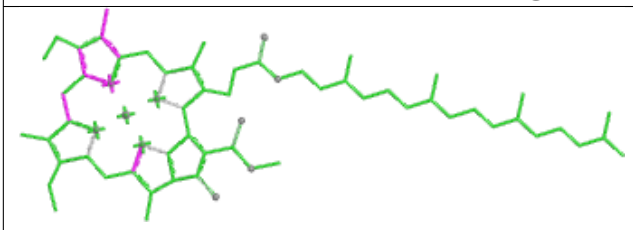


Torsions

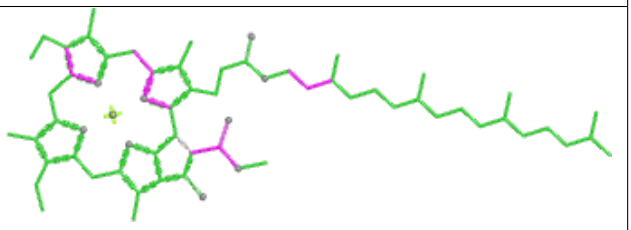


Rings

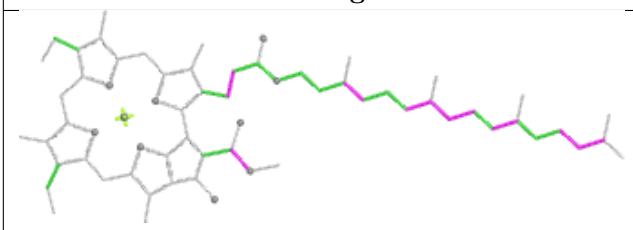
Ligand CLA b 607



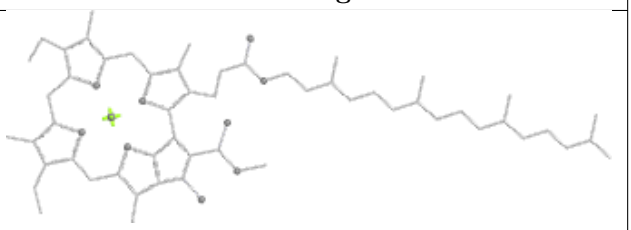
Bond lengths



Bond angles

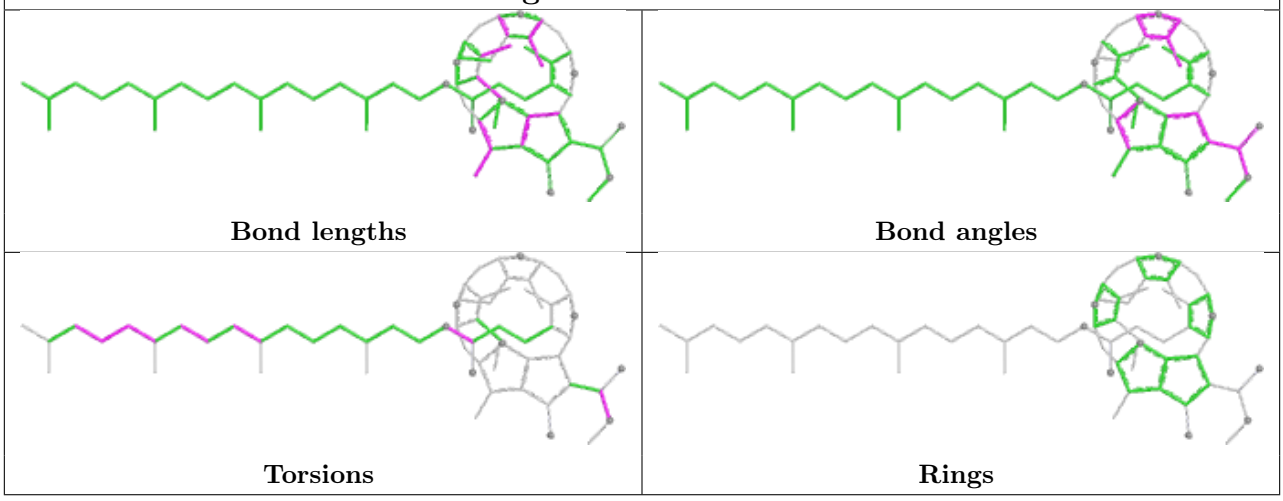


Torsions

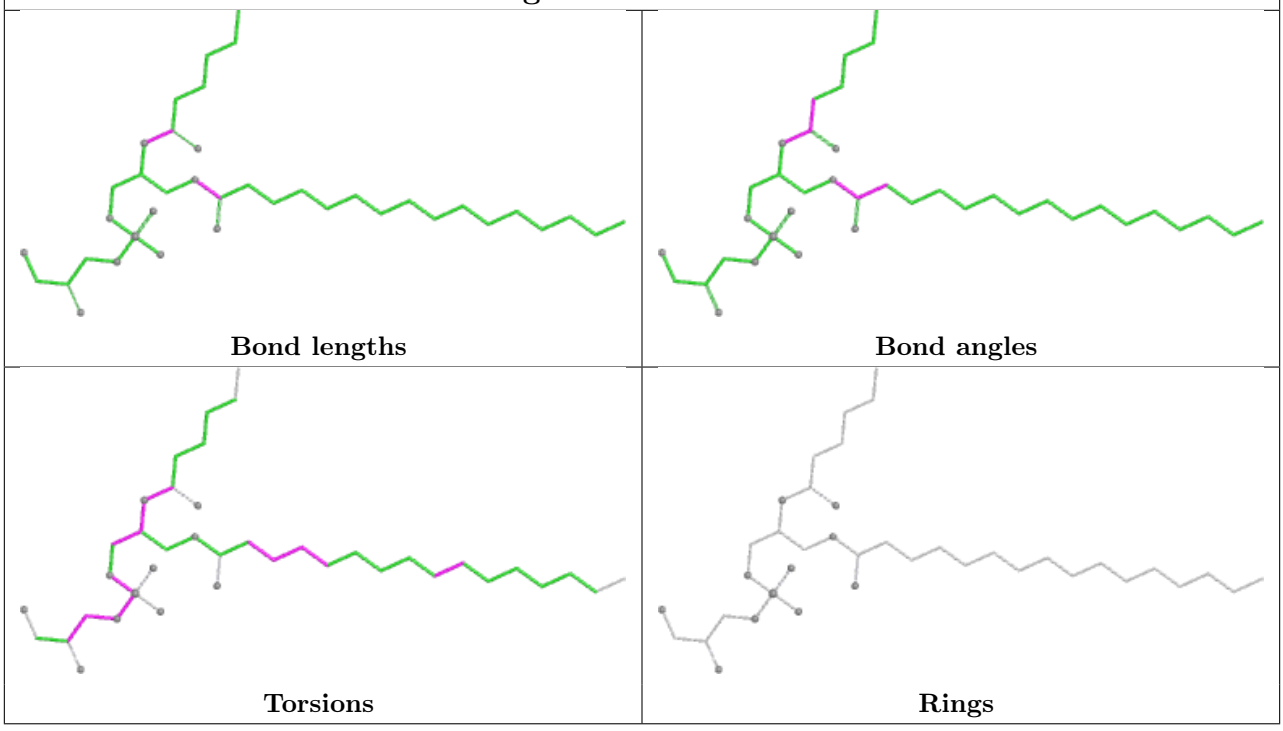


Rings

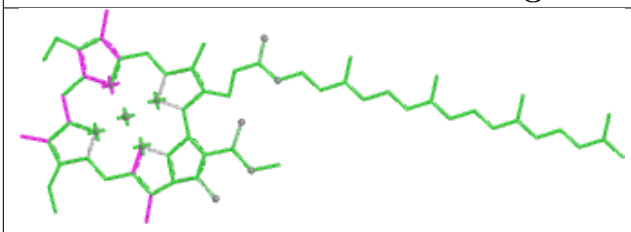
Ligand PHO A 406



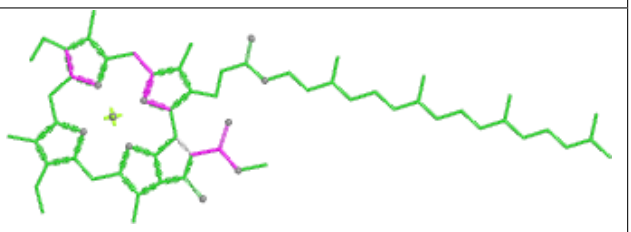
Ligand LHG A 412



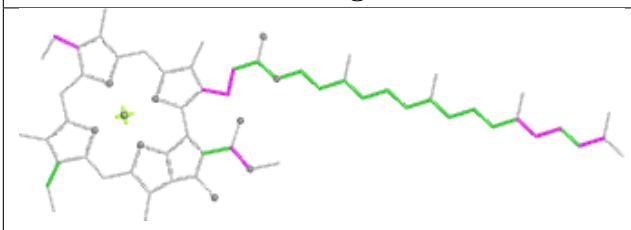
Ligand CLA B 606



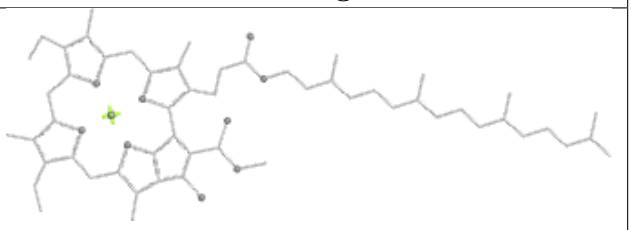
Bond lengths



Bond angles

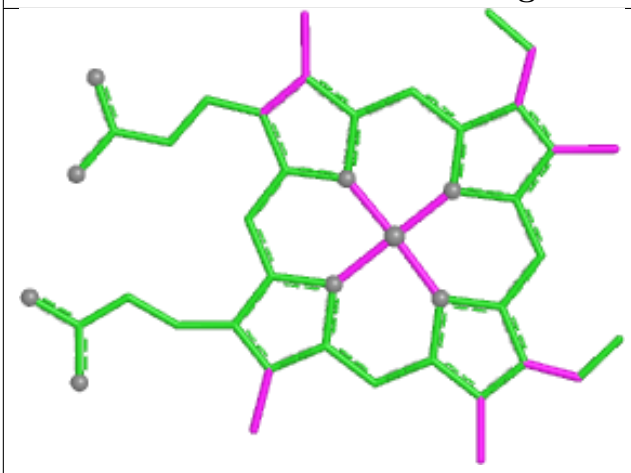


Torsions

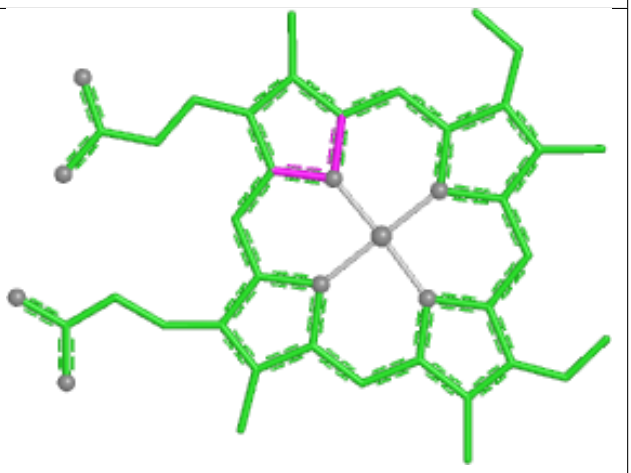


Rings

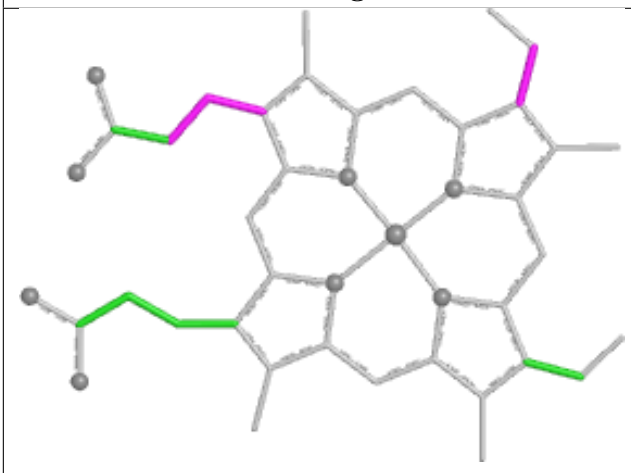
Ligand HEM V 201



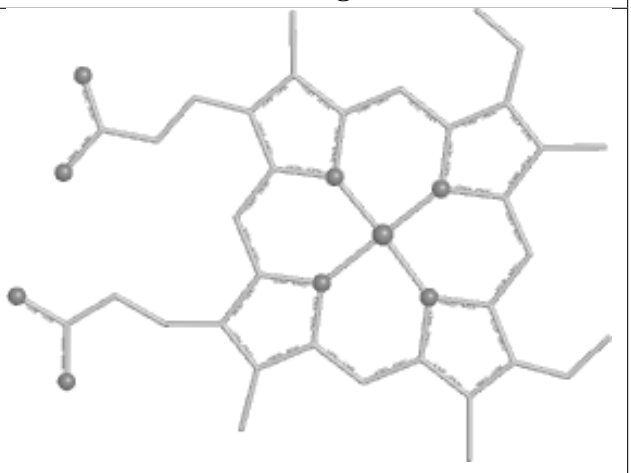
Bond lengths



Bond angles

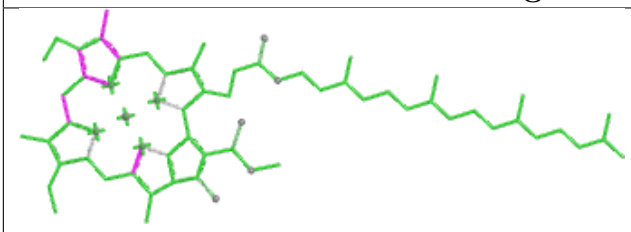


Torsions

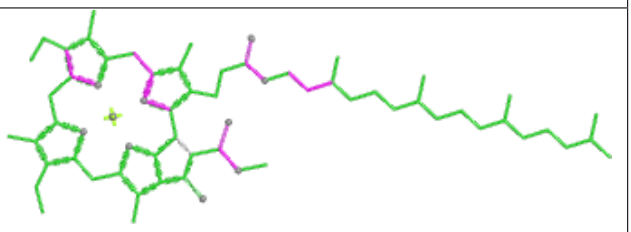


Rings

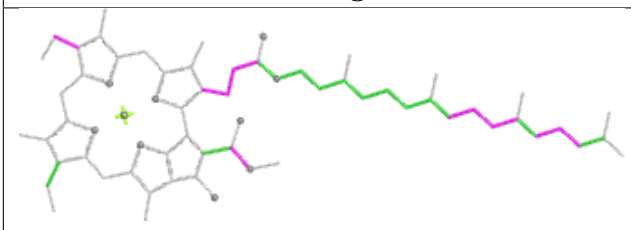
Ligand CLA C 501



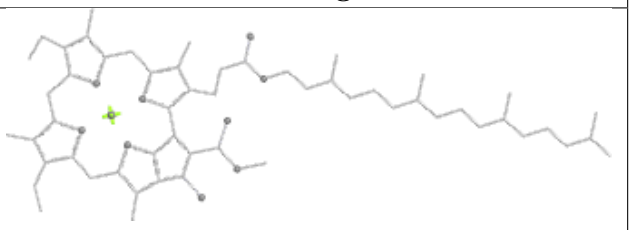
Bond lengths



Bond angles

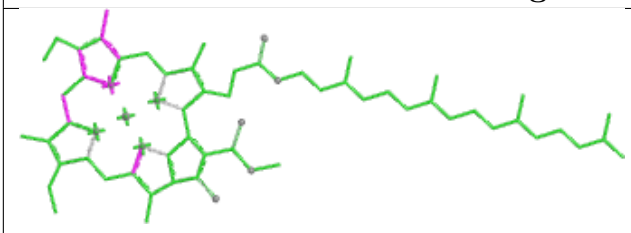


Torsions

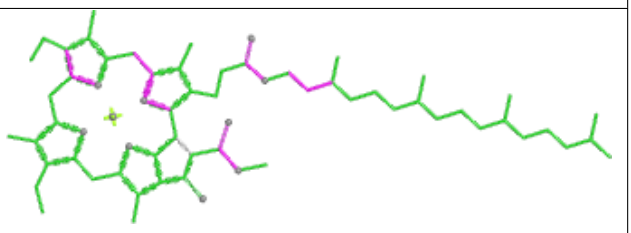


Rings

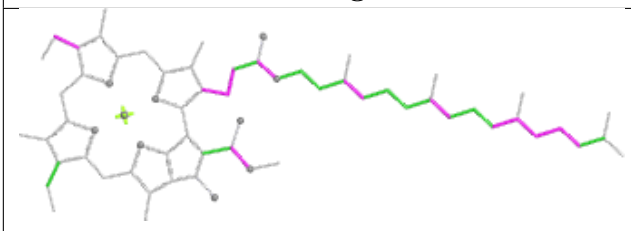
Ligand CLA c 513



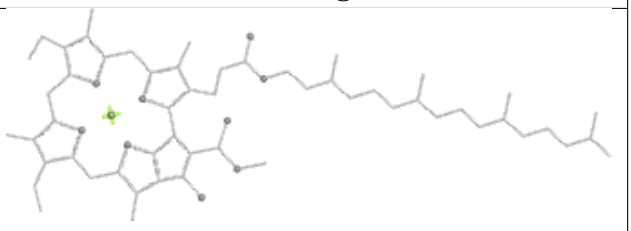
Bond lengths



Bond angles

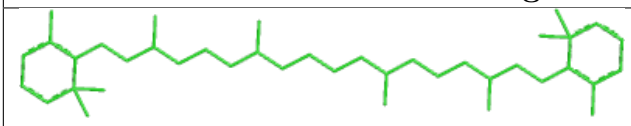


Torsions

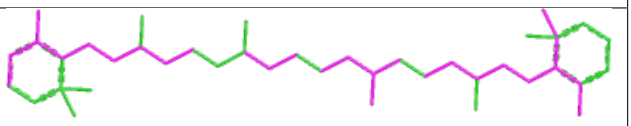


Rings

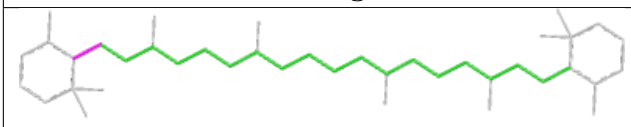
Ligand BCR B 617



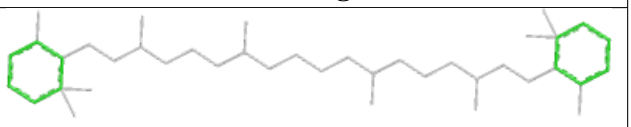
Bond lengths



Bond angles

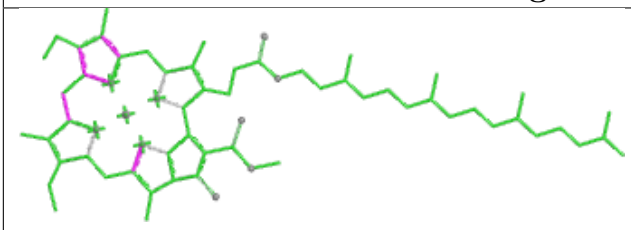


Torsions

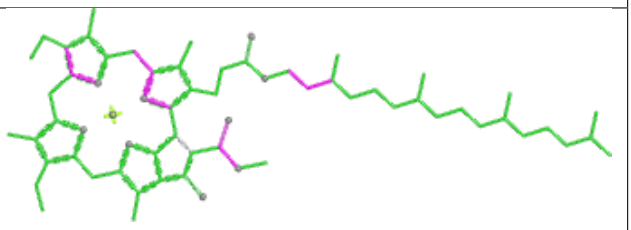


Rings

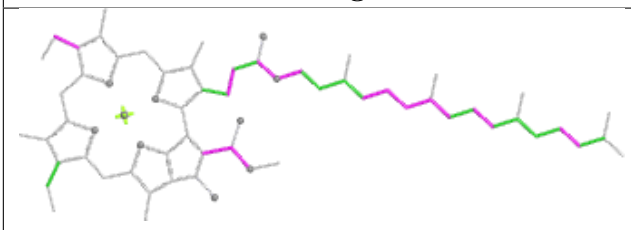
Ligand CLA c 509



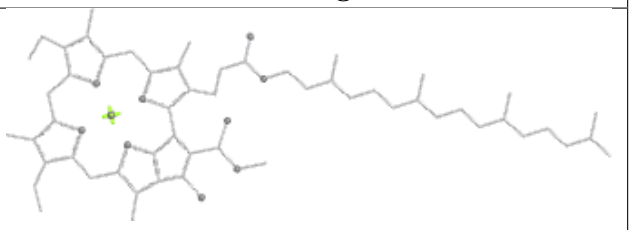
Bond lengths



Bond angles

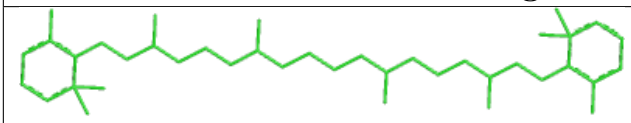


Torsions

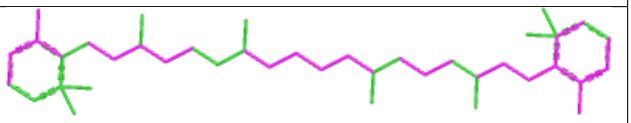


Rings

Ligand BCR D 405



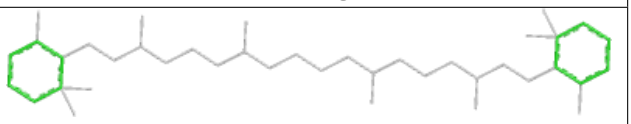
Bond lengths



Bond angles

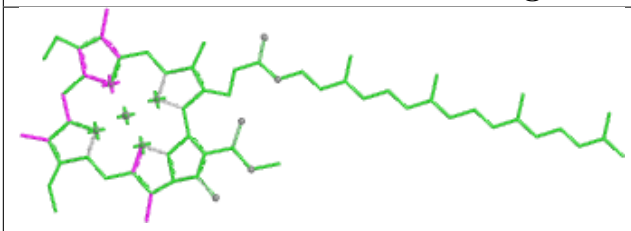


Torsions

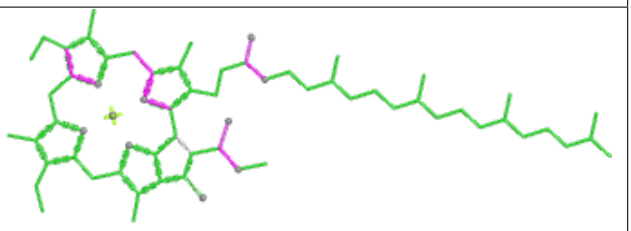


Rings

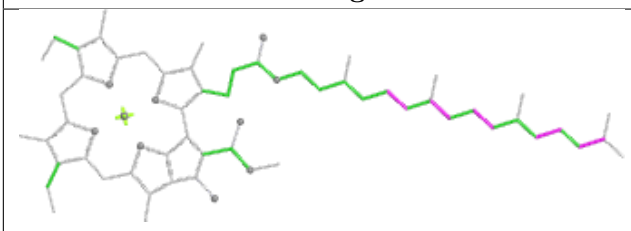
Ligand CLA A 407



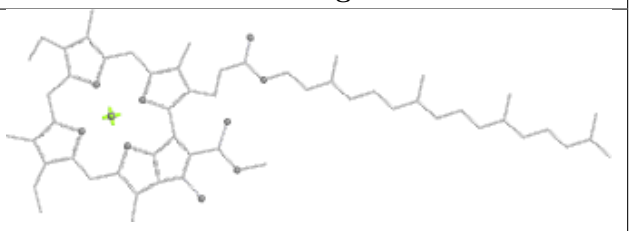
Bond lengths



Bond angles

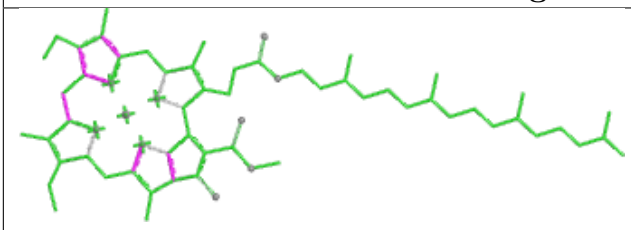


Torsions

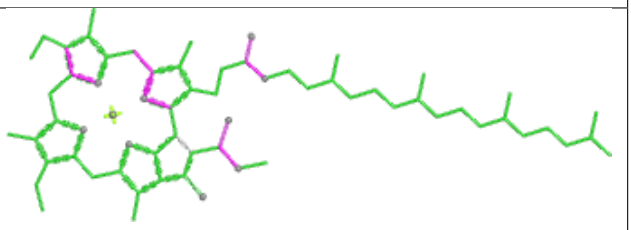


Rings

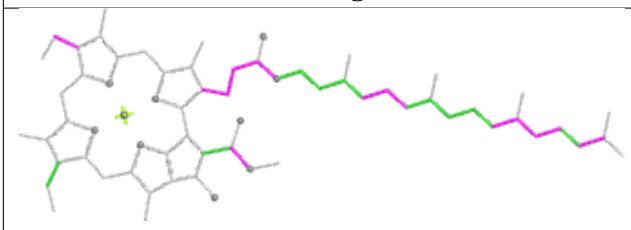
Ligand CLA c 512



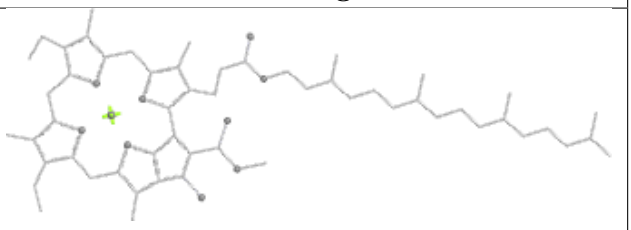
Bond lengths



Bond angles

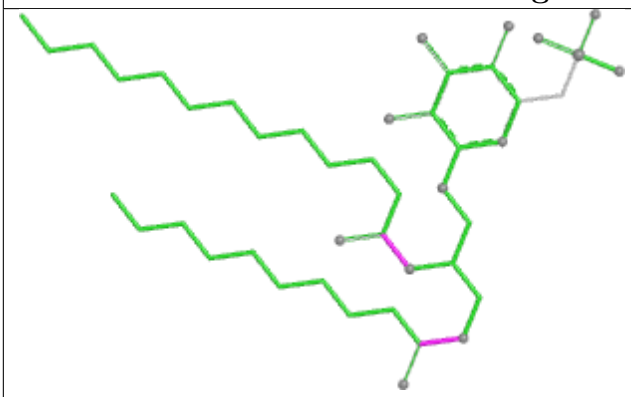


Torsions

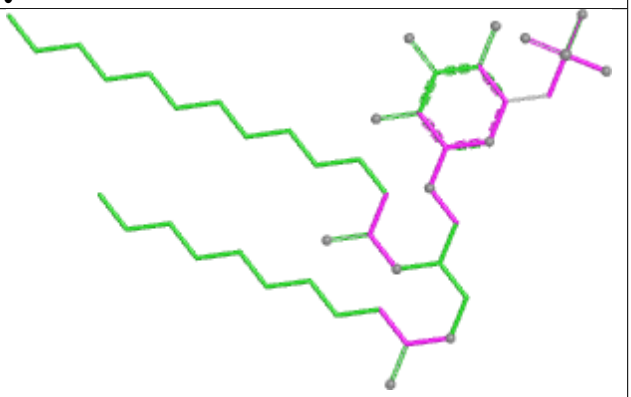


Rings

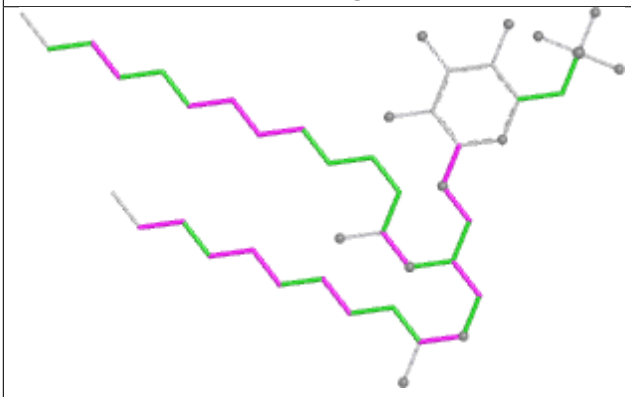
Ligand SQD f 102



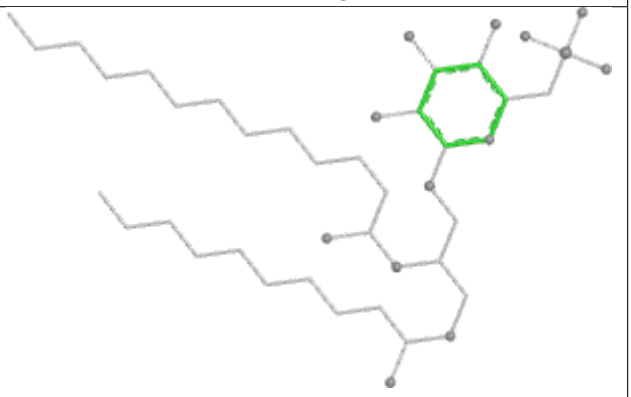
Bond lengths



Bond angles

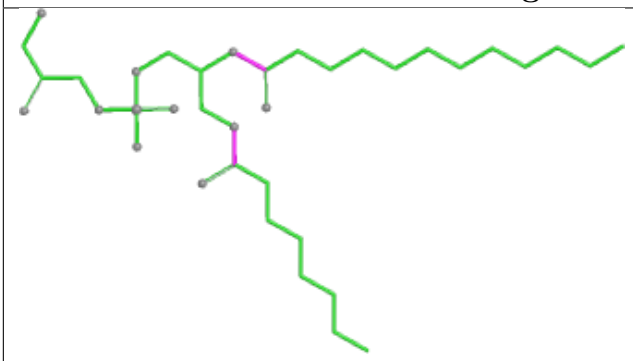


Torsions

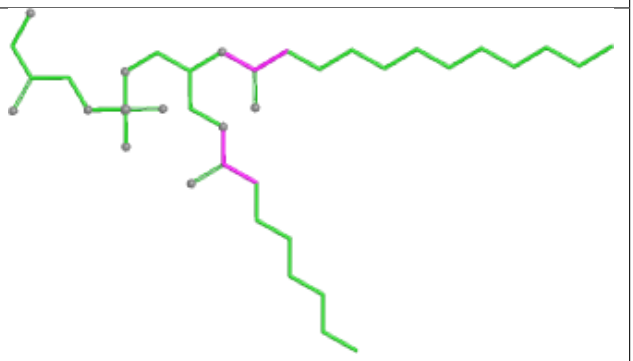


Rings

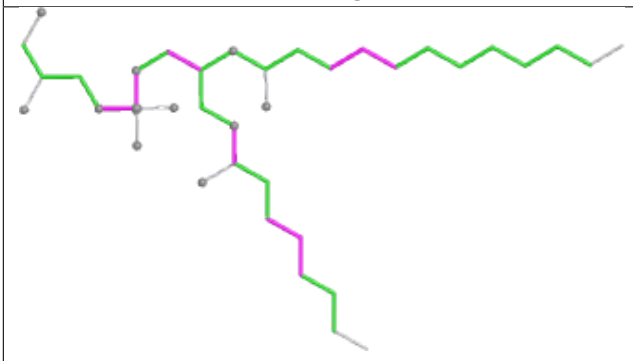
Ligand LHG A 415



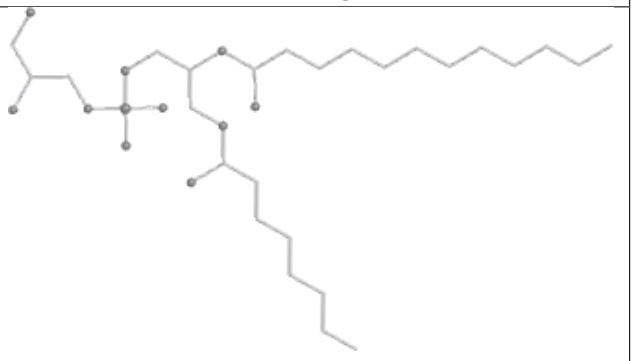
Bond lengths



Bond angles

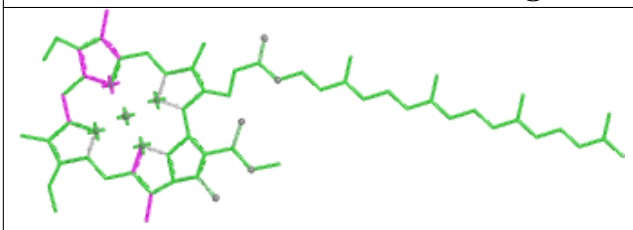


Torsions

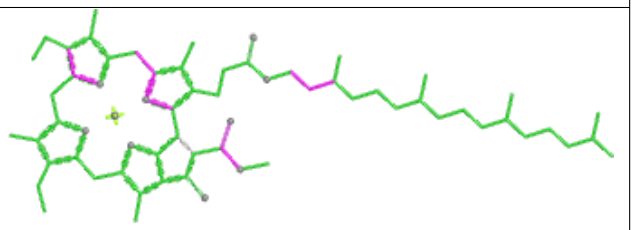


Rings

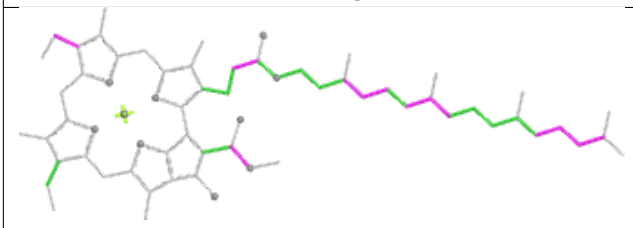
Ligand CLA C 510



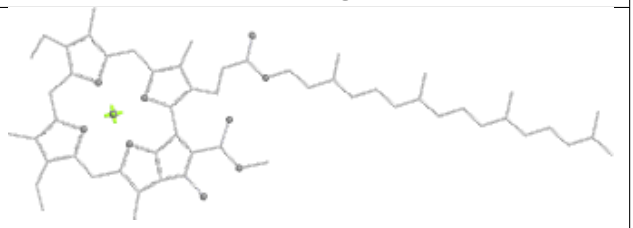
Bond lengths



Bond angles

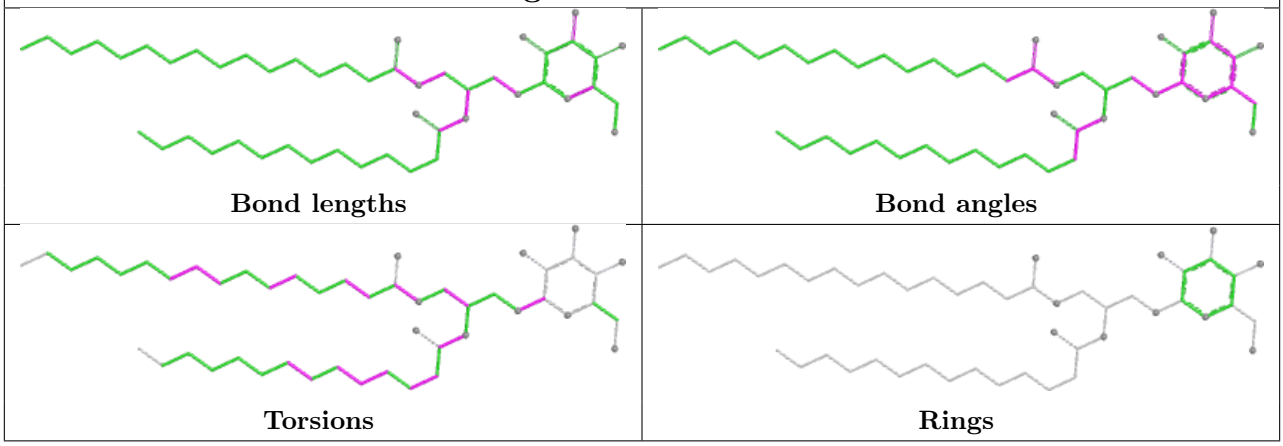


Torsions

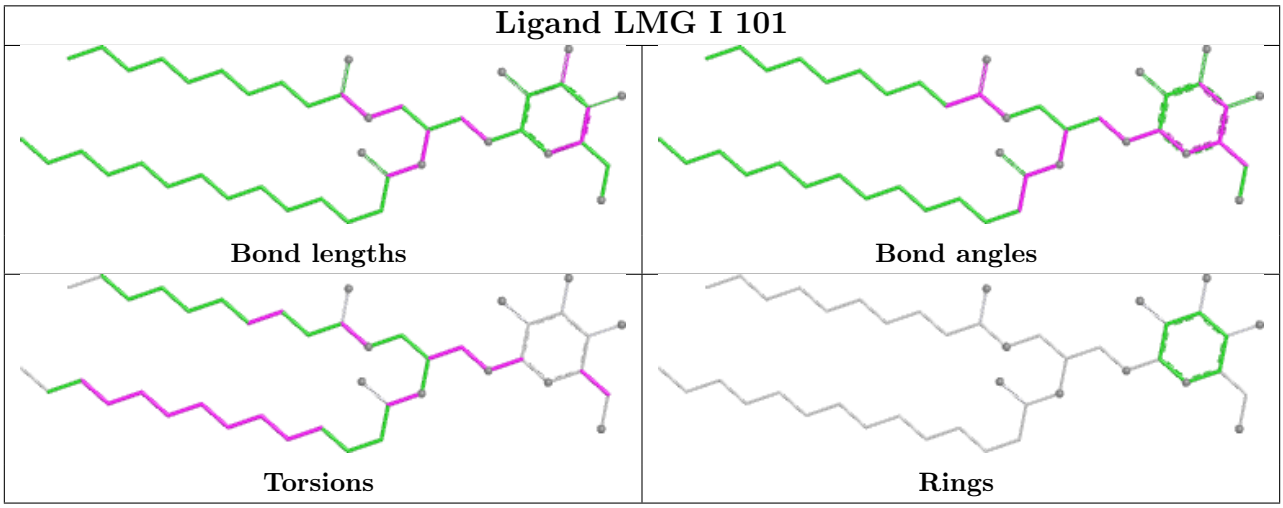


Rings

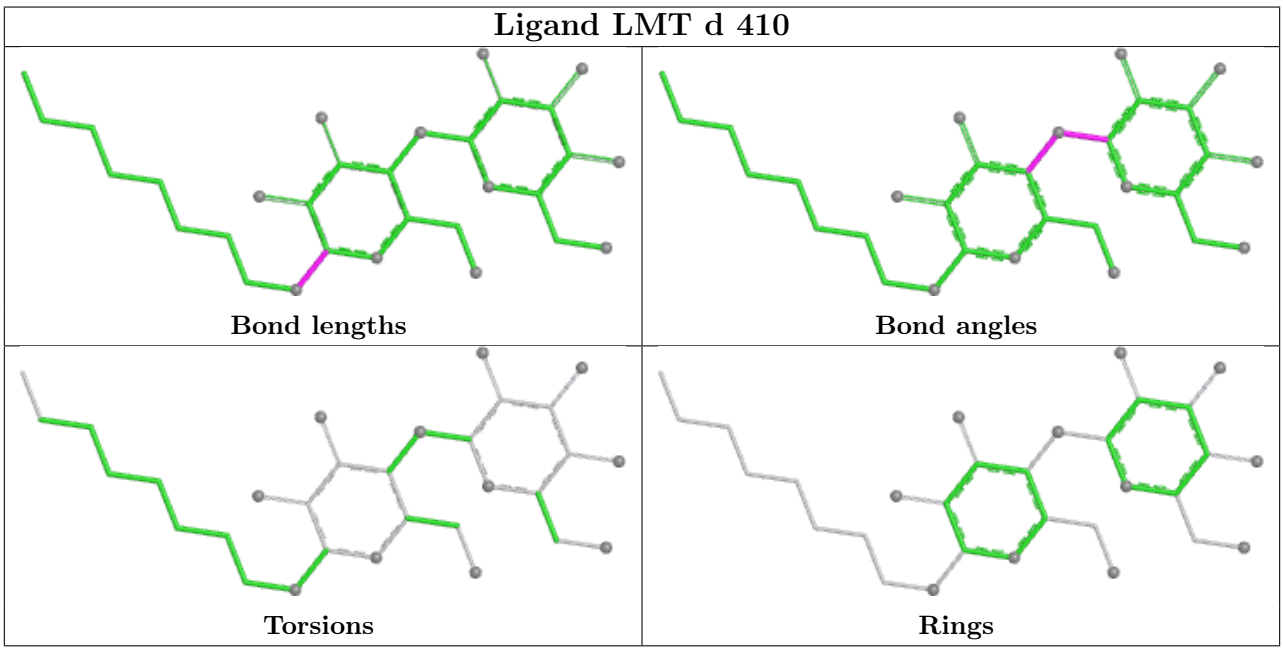
Ligand LMG b 625



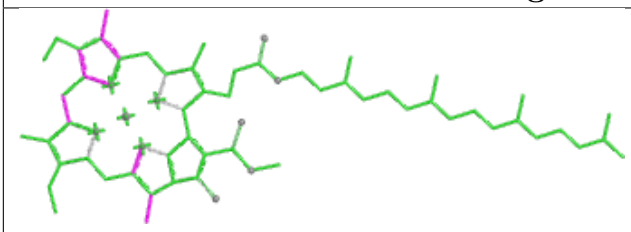
Ligand LMG I 101



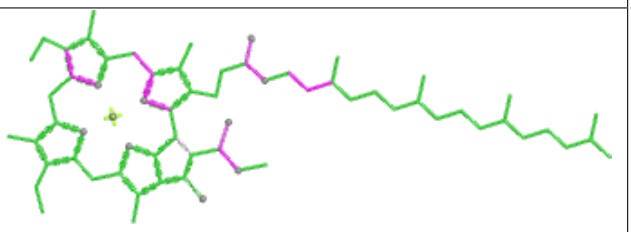
Ligand LMT d 410



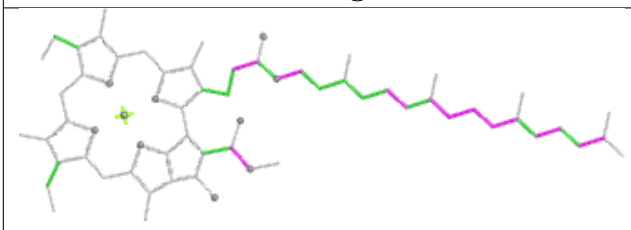
Ligand CLA b 617



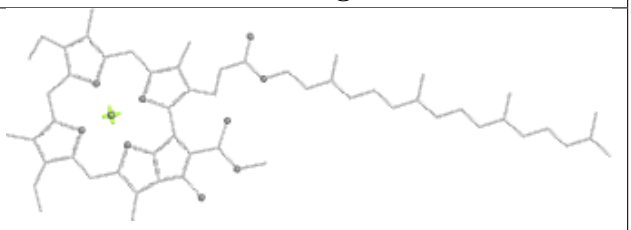
Bond lengths



Bond angles

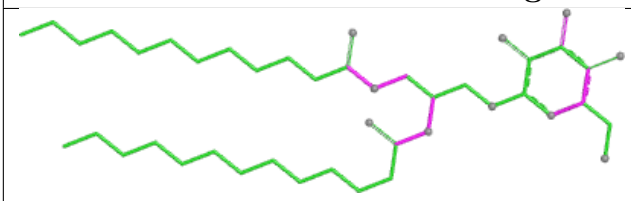


Torsions

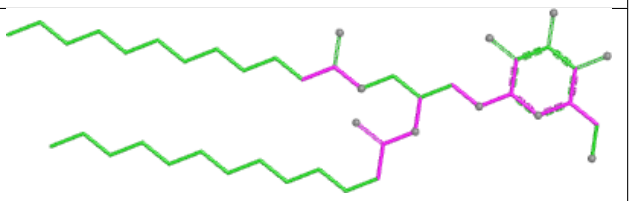


Rings

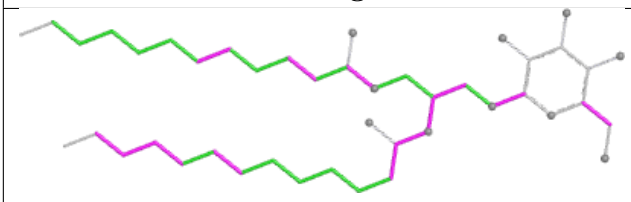
Ligand LMG e 101



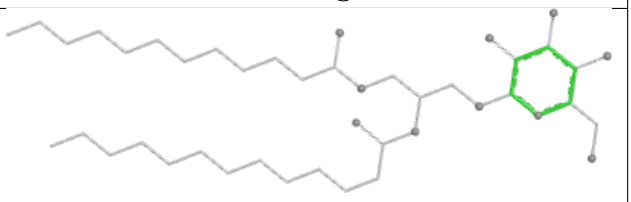
Bond lengths



Bond angles

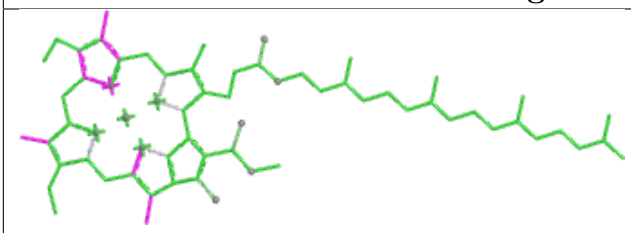


Torsions

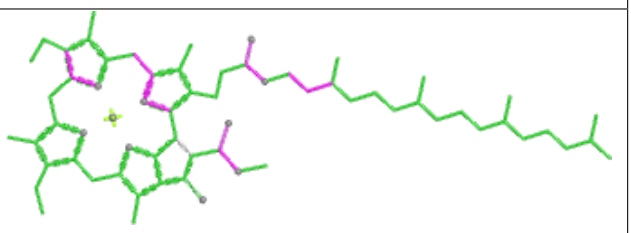


Rings

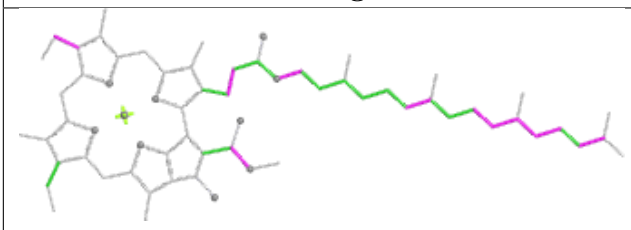
Ligand CLA b 605



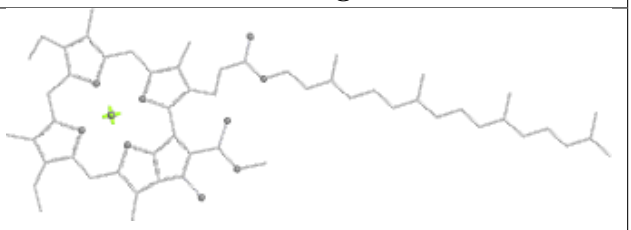
Bond lengths



Bond angles

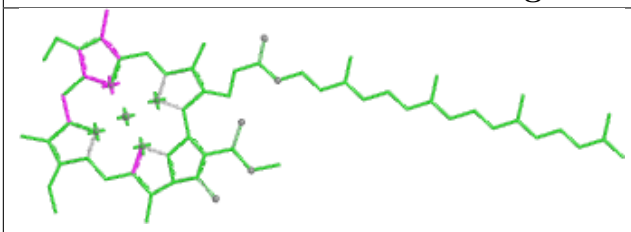


Torsions

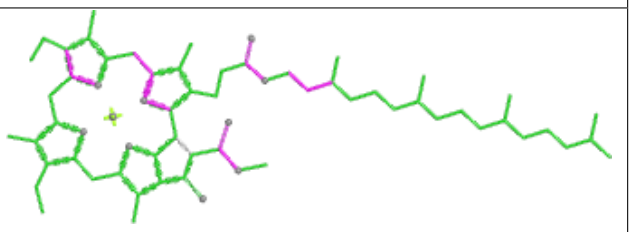


Rings

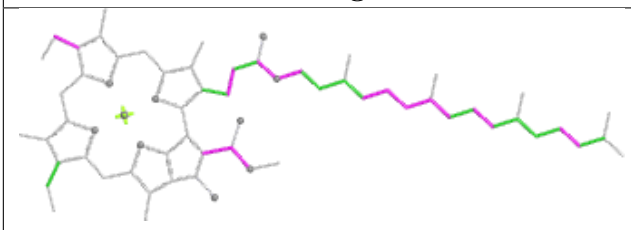
Ligand CLA C 509



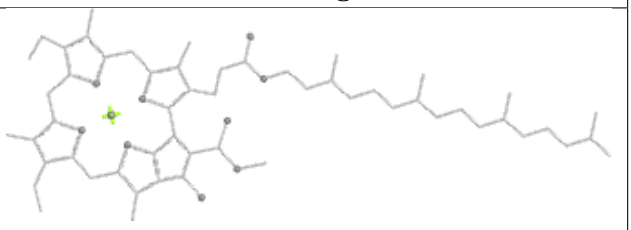
Bond lengths



Bond angles

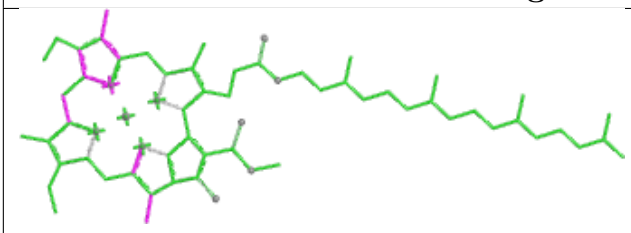


Torsions

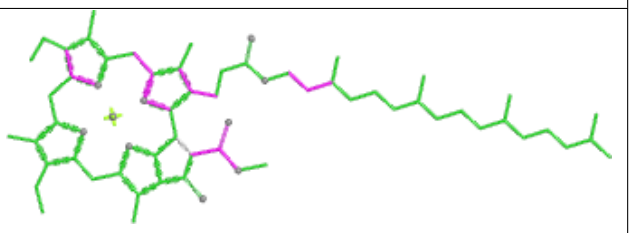


Rings

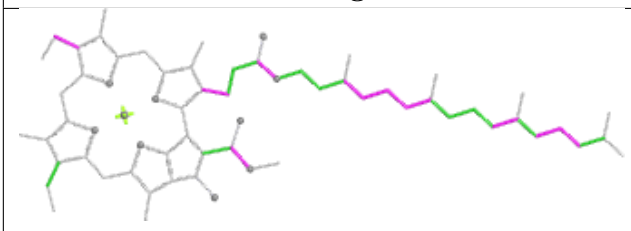
Ligand CLA b 612



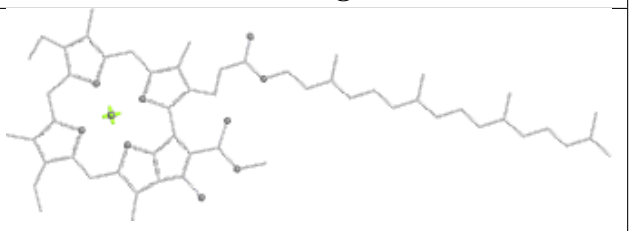
Bond lengths



Bond angles

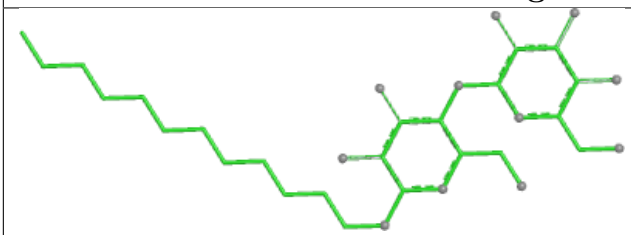


Torsions

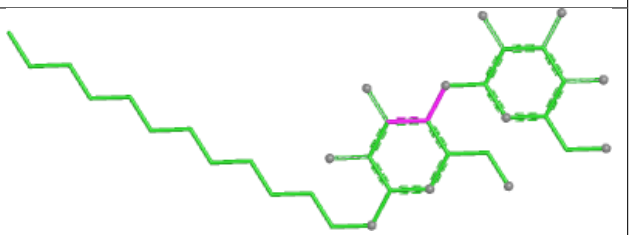


Rings

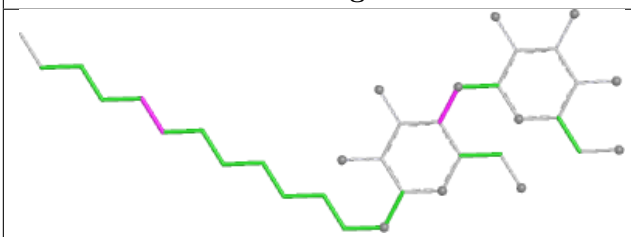
Ligand LMT I 102



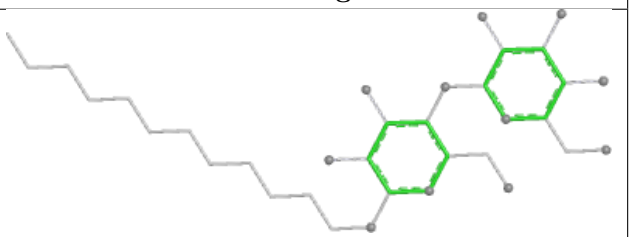
Bond lengths



Bond angles

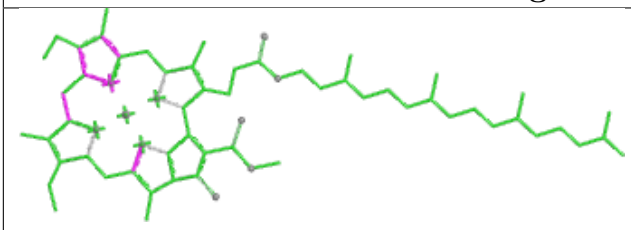


Torsions

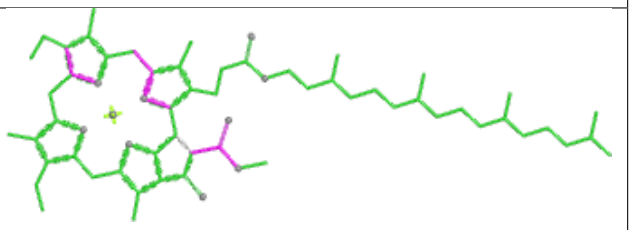


Rings

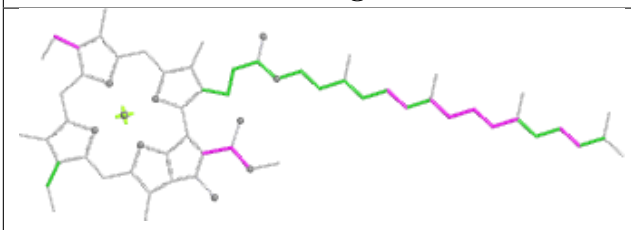
Ligand CLA c 503



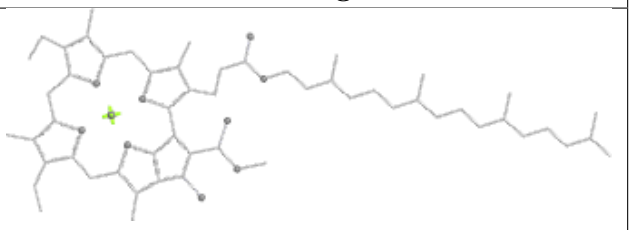
Bond lengths



Bond angles

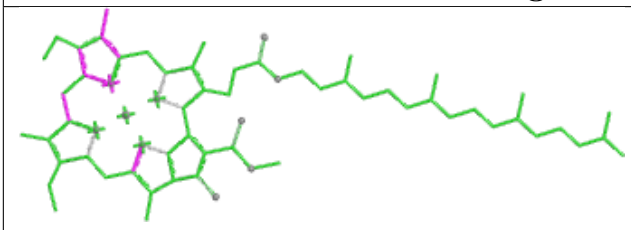


Torsions

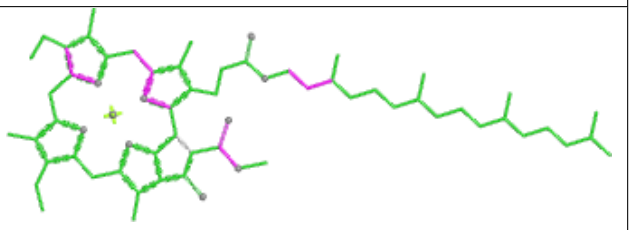


Rings

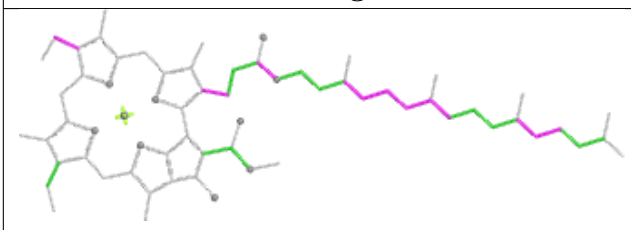
Ligand CLA b 606



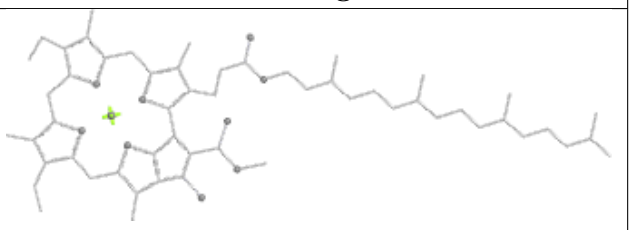
Bond lengths



Bond angles

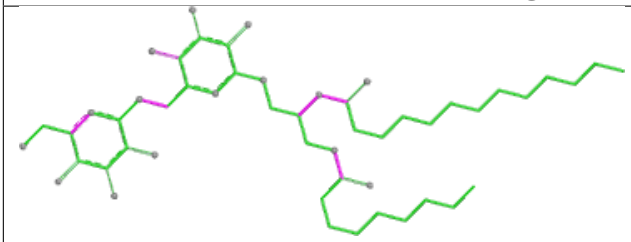


Torsions

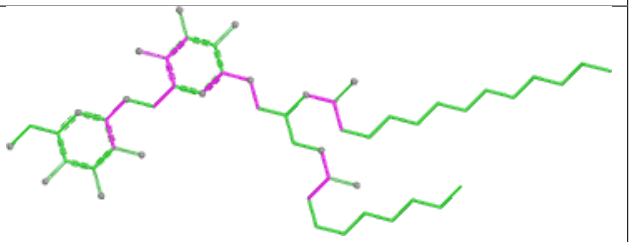


Rings

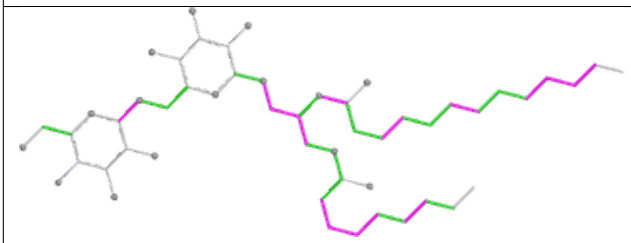
Ligand DGD b 602



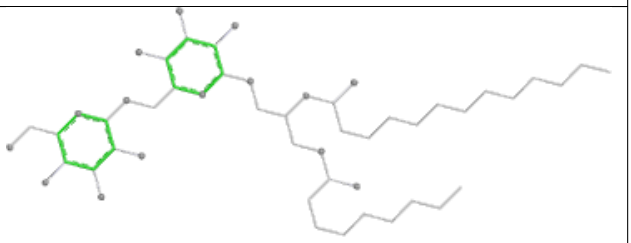
Bond lengths



Bond angles

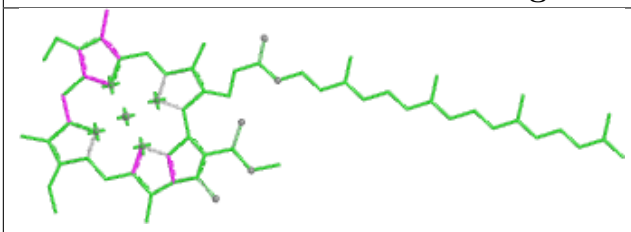


Torsions

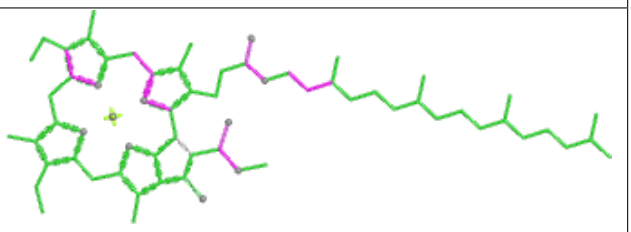


Rings

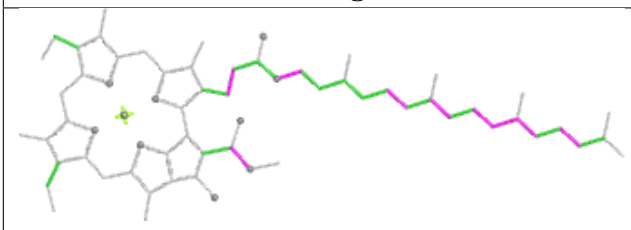
Ligand CLA c 508



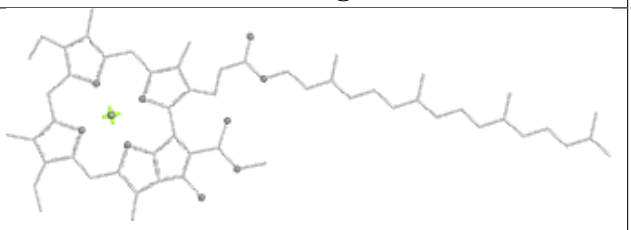
Bond lengths



Bond angles

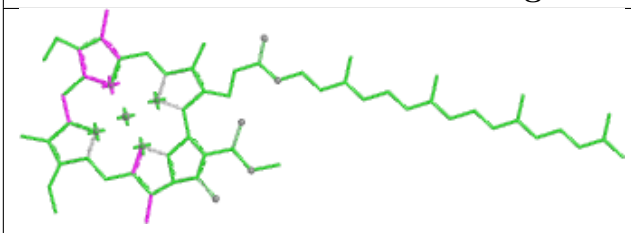


Torsions

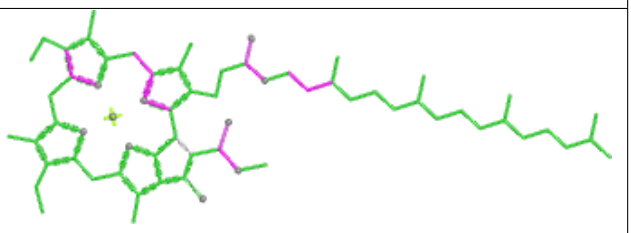


Rings

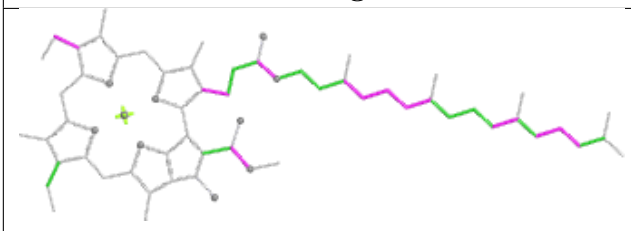
Ligand CLA B 608



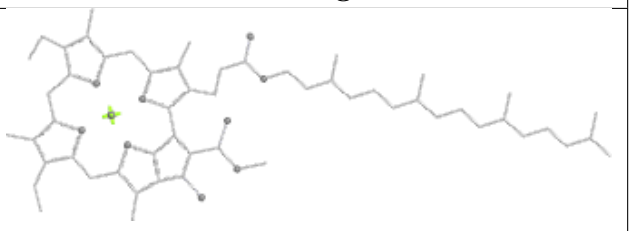
Bond lengths



Bond angles

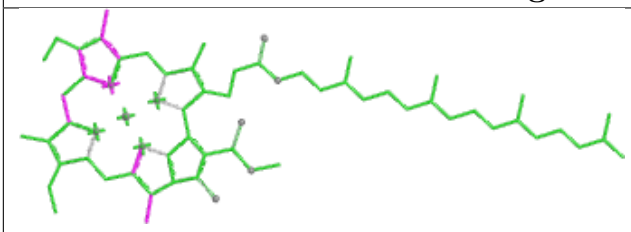


Torsions

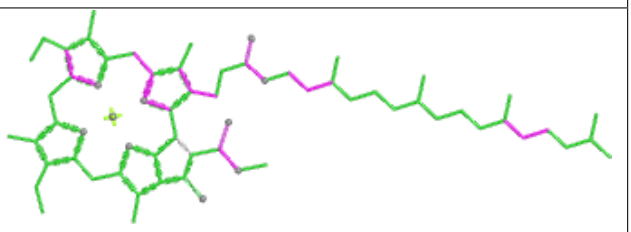


Rings

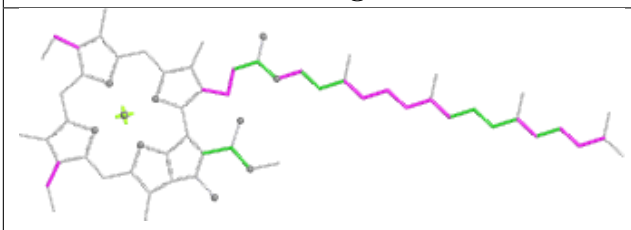
Ligand CLA a 405



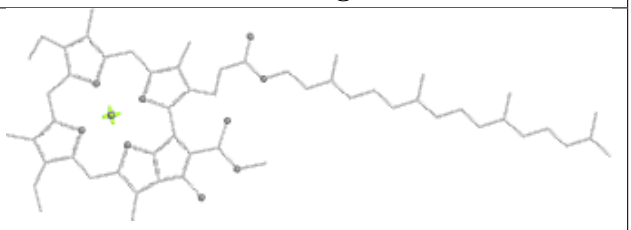
Bond lengths



Bond angles

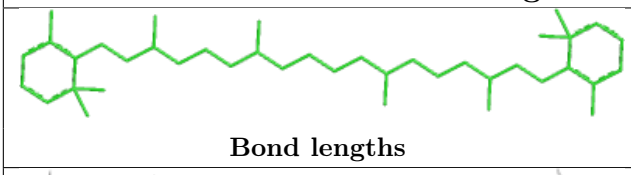


Torsions

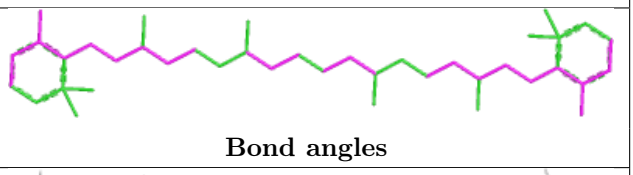


Rings

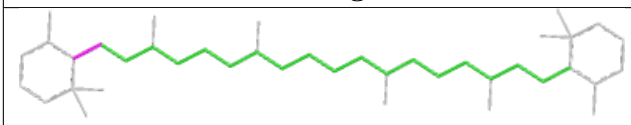
Ligand BCR T 101



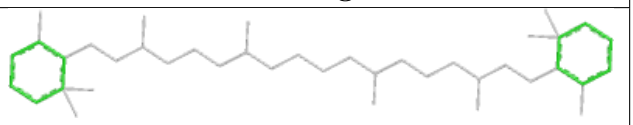
Bond lengths



Bond angles

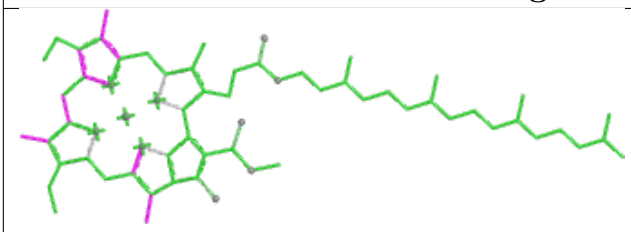


Torsions

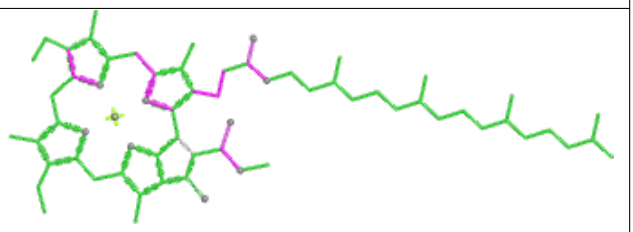


Rings

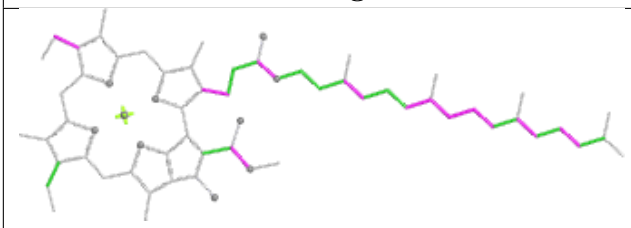
Ligand CLA c 505



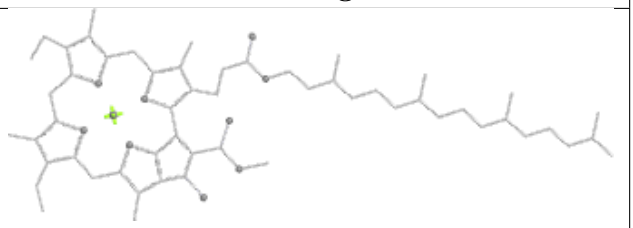
Bond lengths



Bond angles

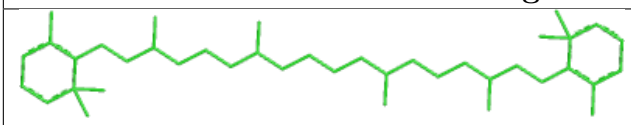


Torsions

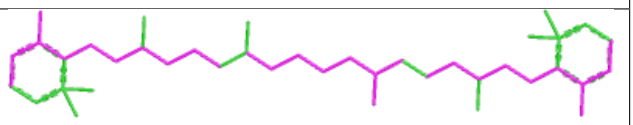


Rings

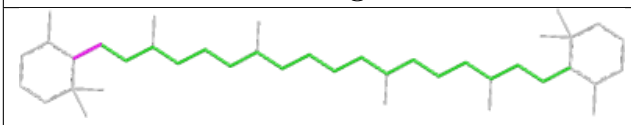
Ligand BCR C 515



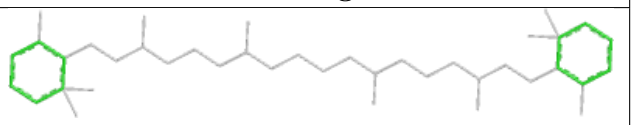
Bond lengths



Bond angles

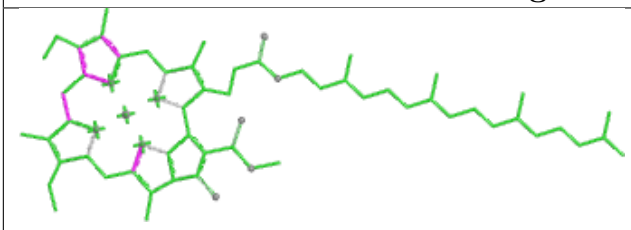


Torsions

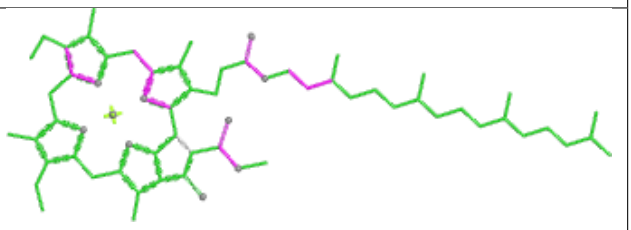


Rings

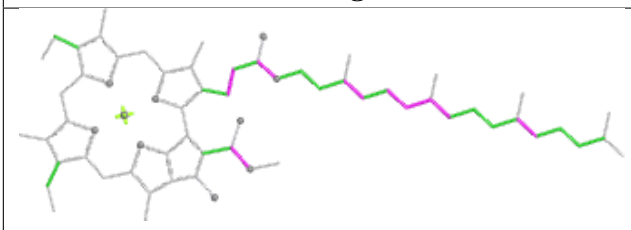
Ligand CLA c 511



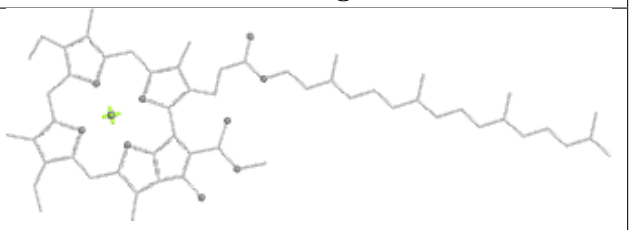
Bond lengths



Bond angles

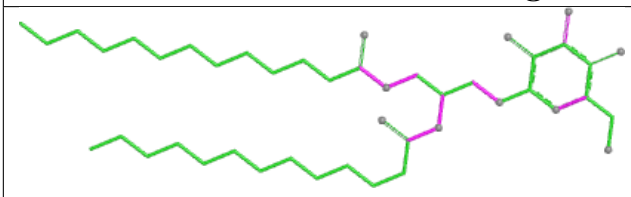


Torsions

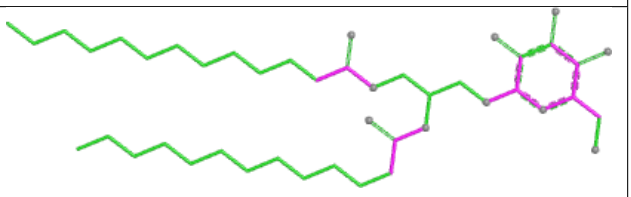


Rings

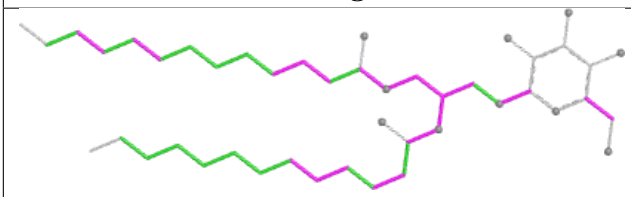
Ligand LMG c 519



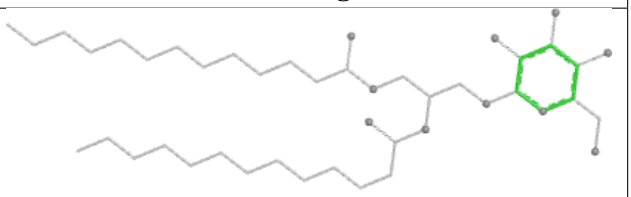
Bond lengths



Bond angles

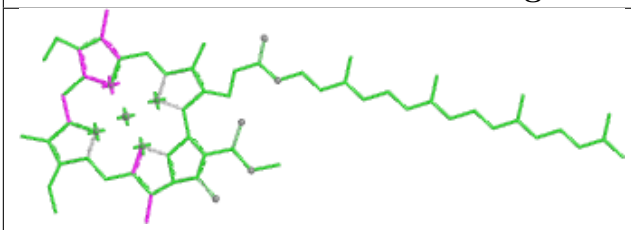


Torsions

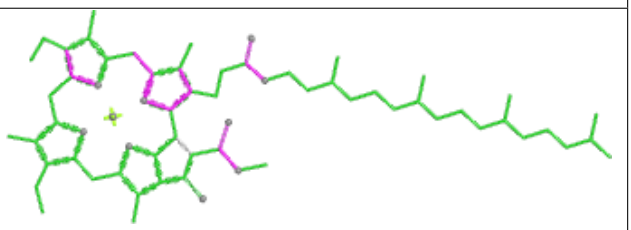


Rings

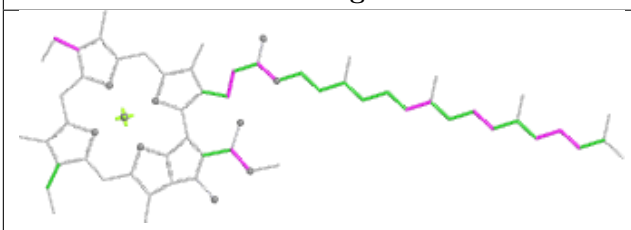
Ligand CLA C 504



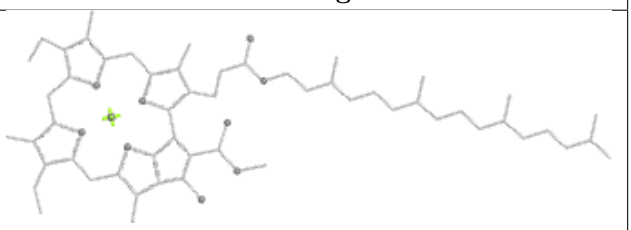
Bond lengths



Bond angles

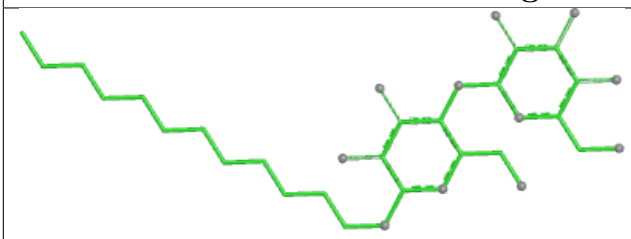


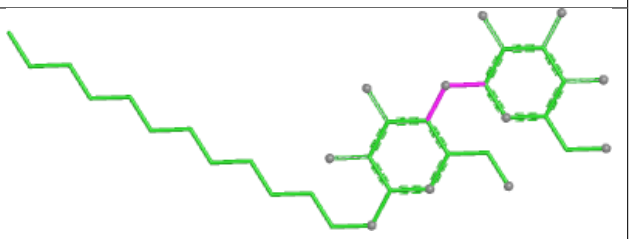
Torsions

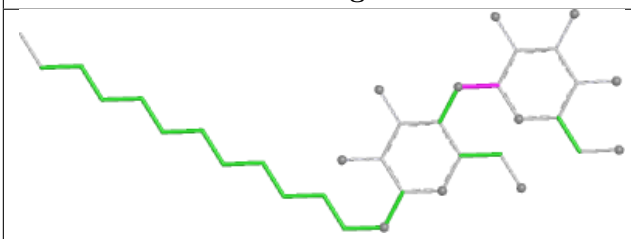


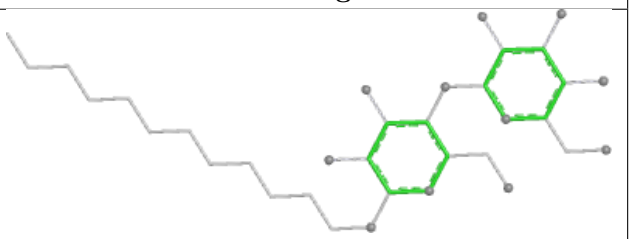
Rings

Ligand LMT B 625

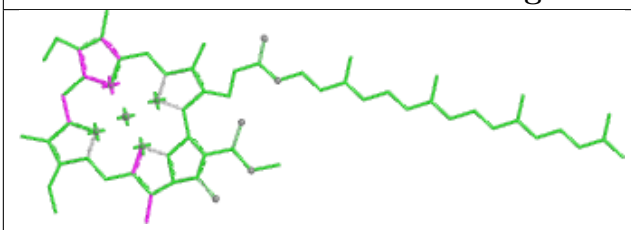

Bond lengths

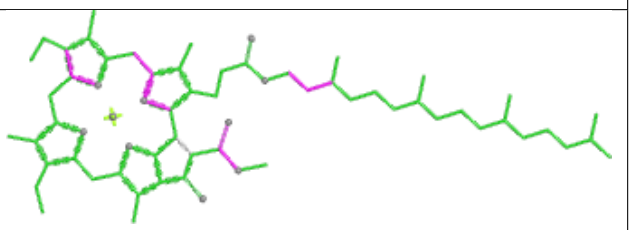

Bond angles

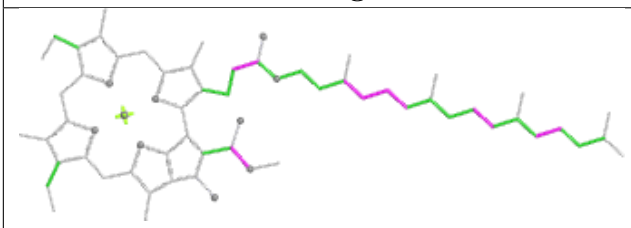

Torsions

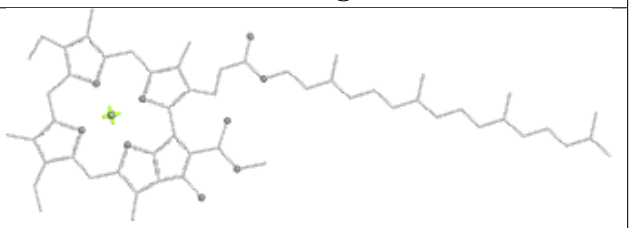

Rings

Ligand CLA B 612

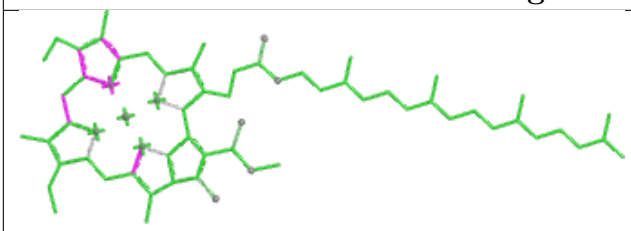

Bond lengths

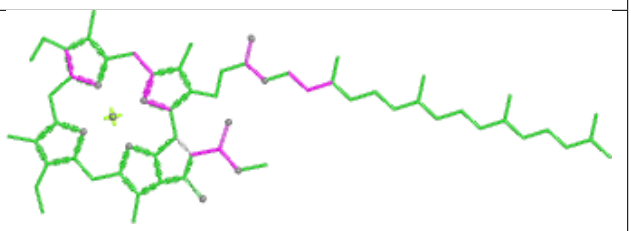

Bond angles

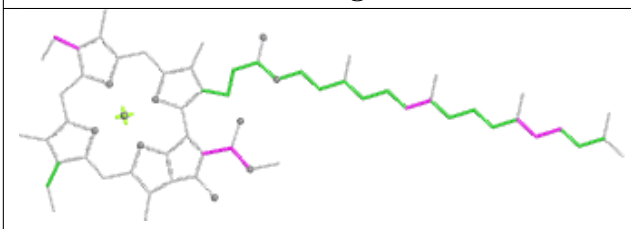

Torsions

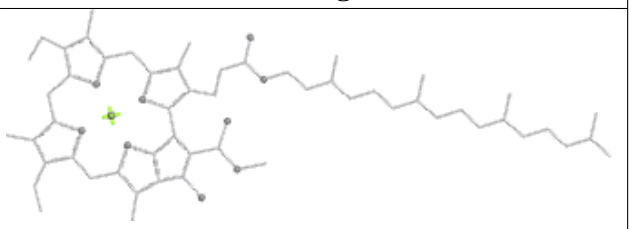

Rings

Ligand CLA b 613

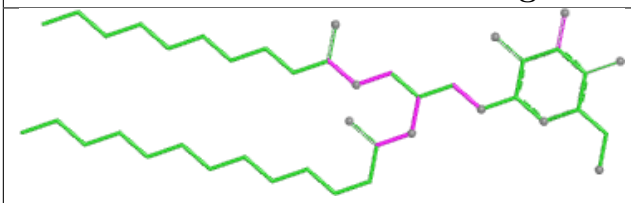

Bond lengths


Bond angles

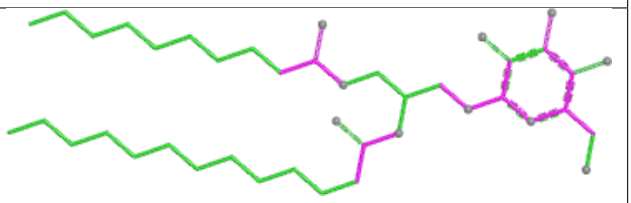

Torsions


Rings

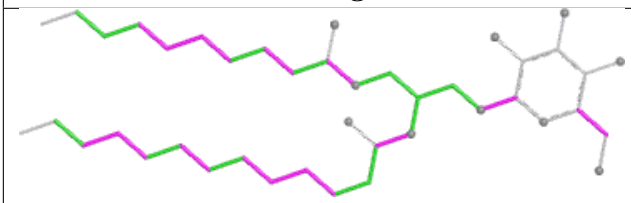
Ligand LMG A 418



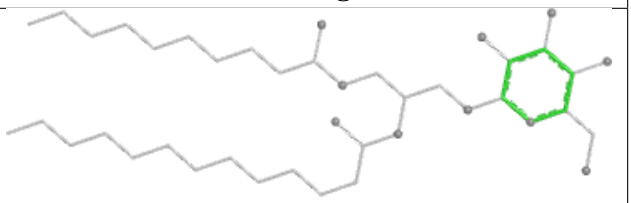
Bond lengths



Bond angles

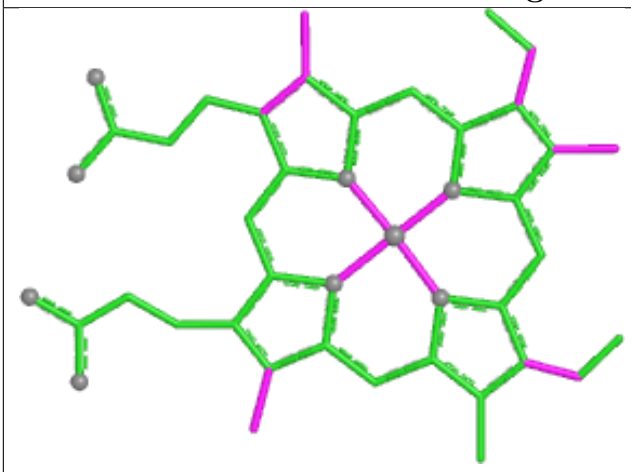


Torsions

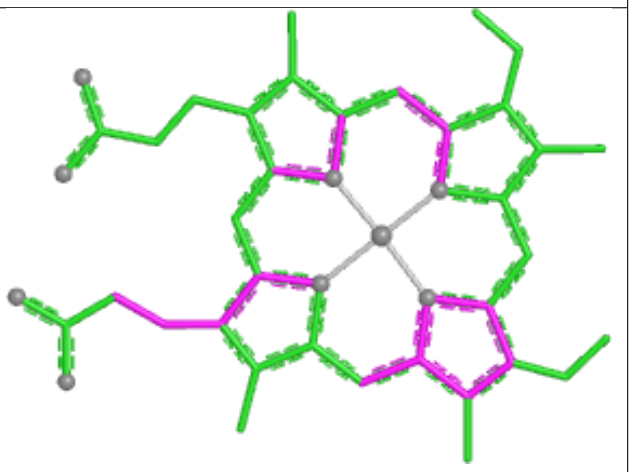


Rings

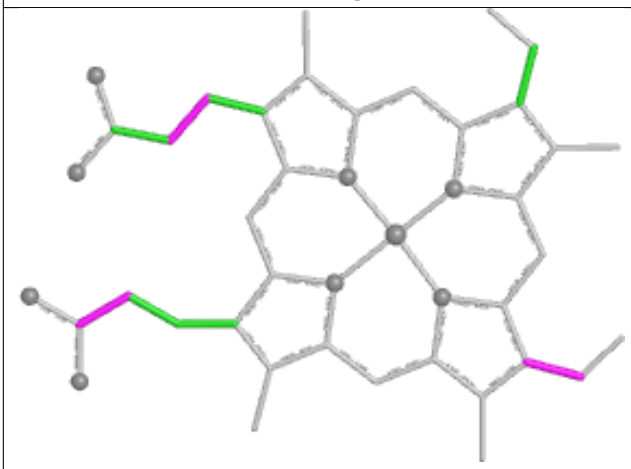
Ligand HEM f 101



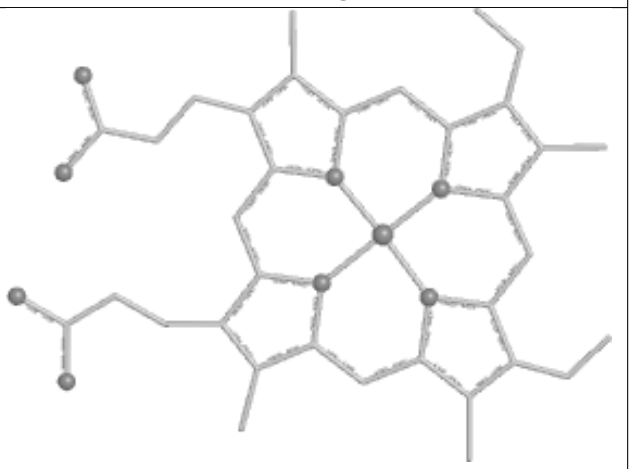
Bond lengths



Bond angles

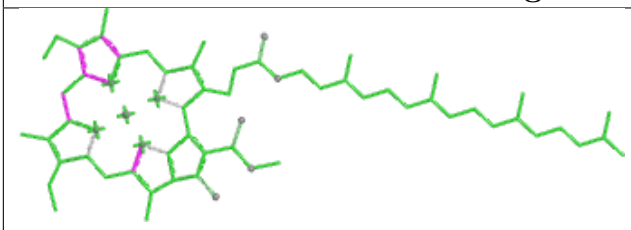


Torsions

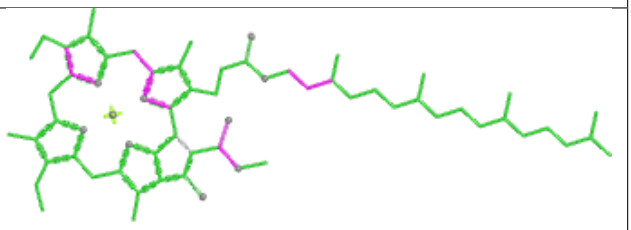


Rings

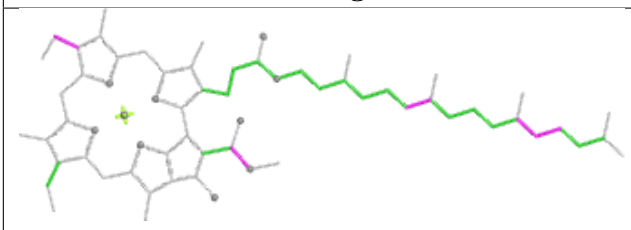
Ligand CLA B 609



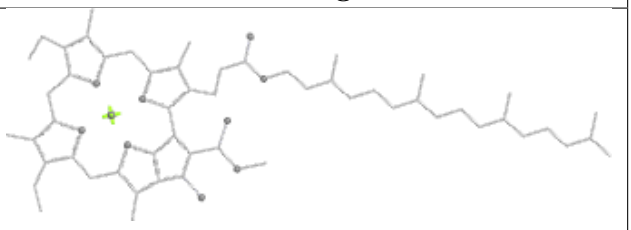
Bond lengths



Bond angles

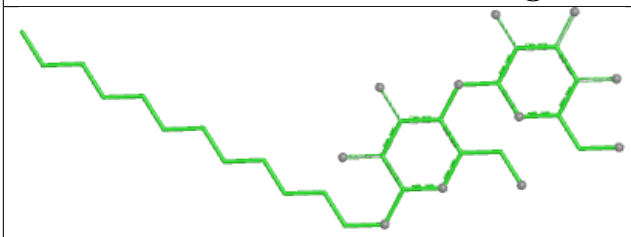


Torsions

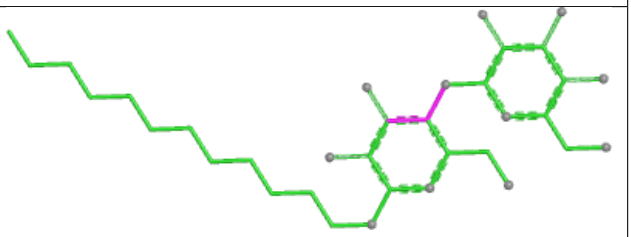


Rings

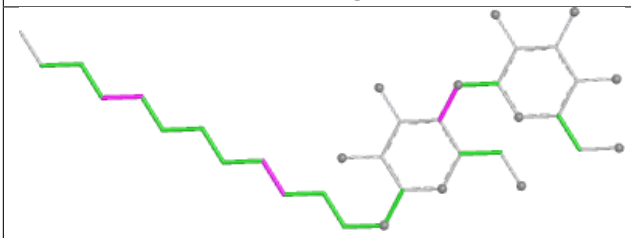
Ligand LMT b 603



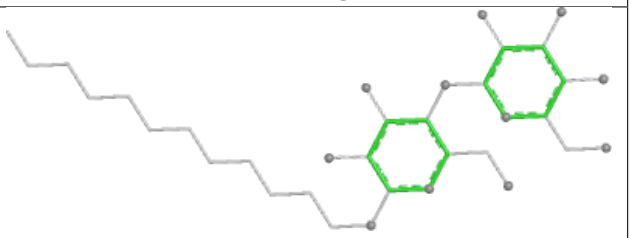
Bond lengths



Bond angles



Torsions

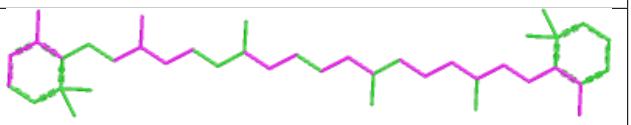


Rings

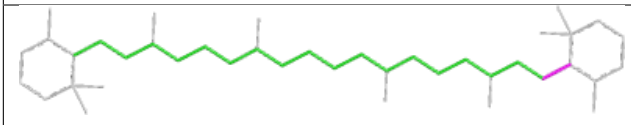
Ligand BCR a 412



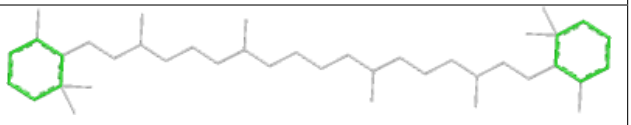
Bond lengths



Bond angles

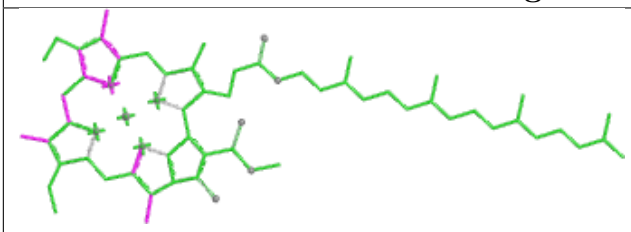


Torsions

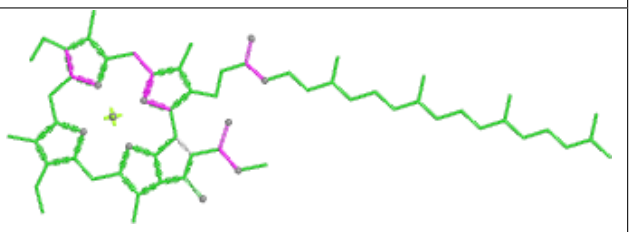


Rings

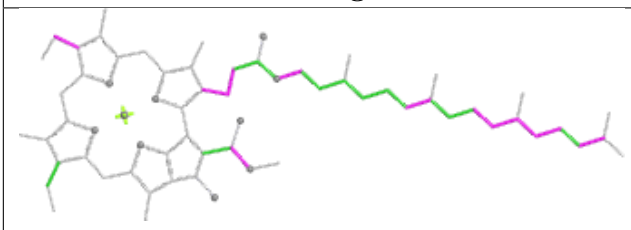
Ligand CLA B 601



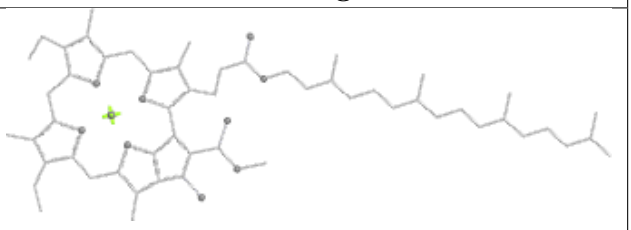
Bond lengths



Bond angles

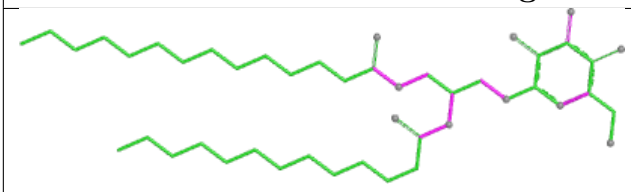


Torsions

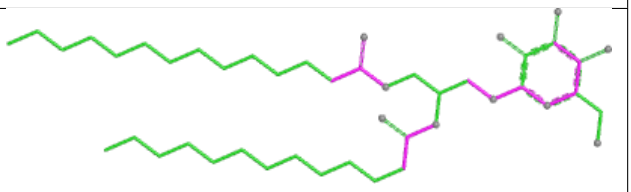


Rings

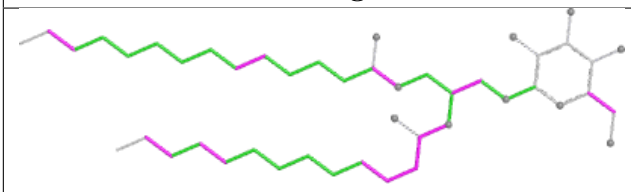
Ligand LMG D 406



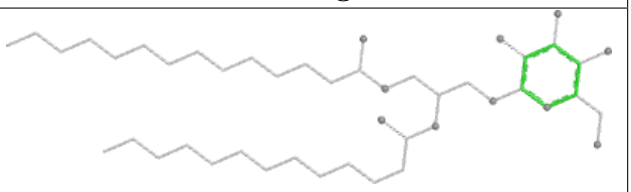
Bond lengths



Bond angles

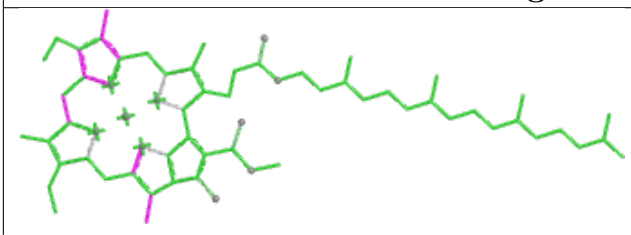


Torsions

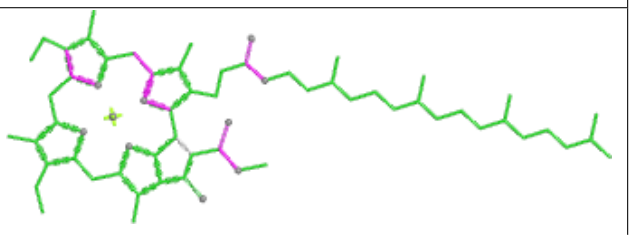


Rings

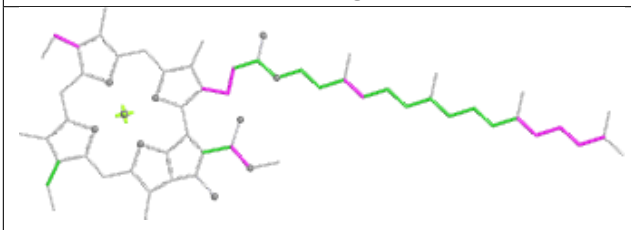
Ligand CLA b 610



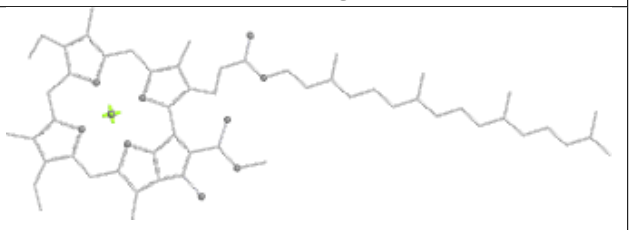
Bond lengths



Bond angles

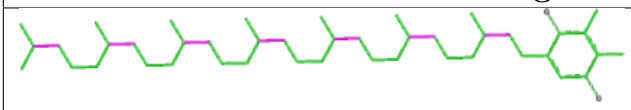


Torsions

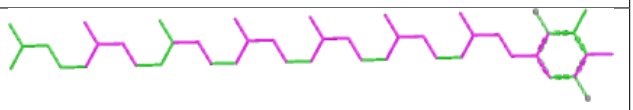


Rings

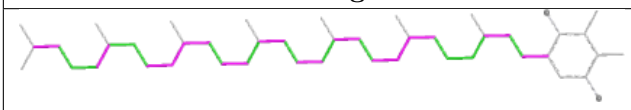
Ligand PL9 a 410



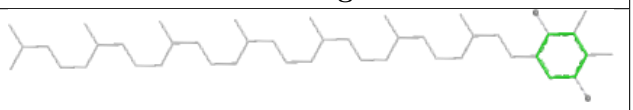
Bond lengths



Bond angles

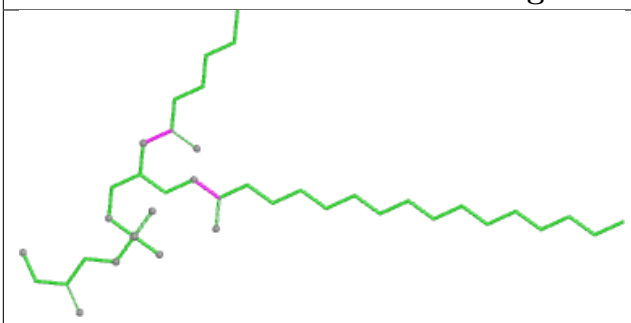


Torsions

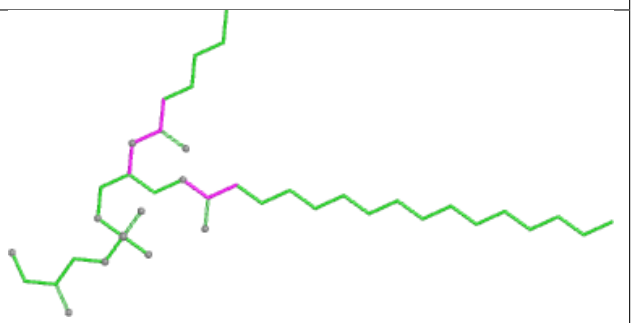


Rings

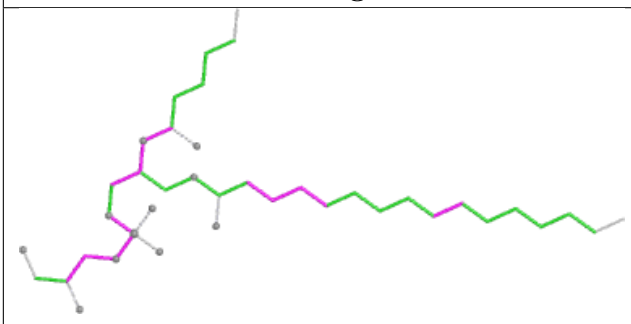
Ligand LHG a 414



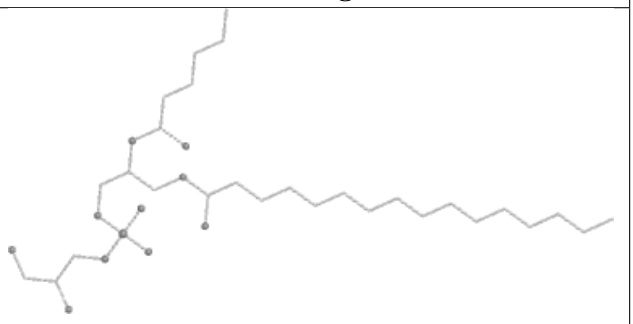
Bond lengths



Bond angles

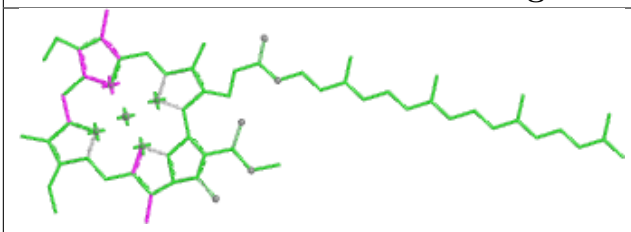


Torsions

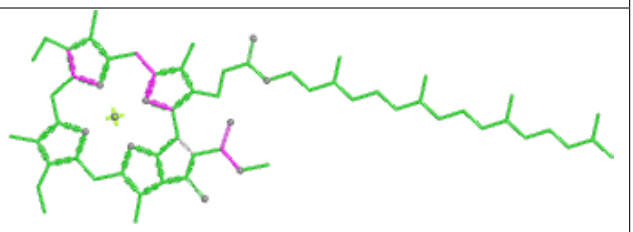


Rings

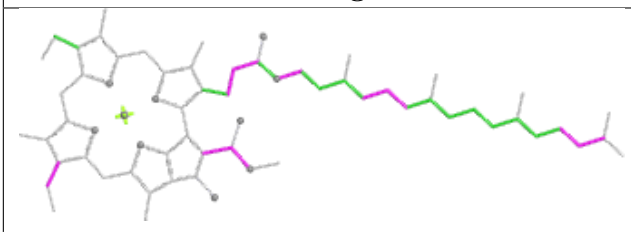
Ligand CLA b 618



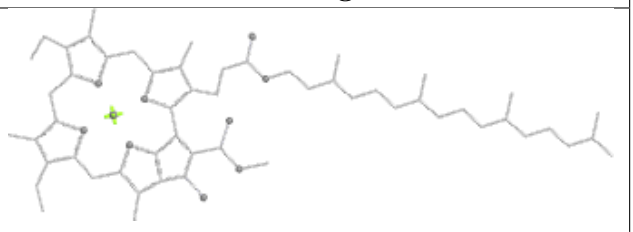
Bond lengths



Bond angles

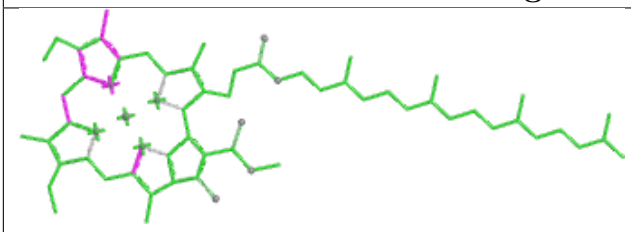


Torsions

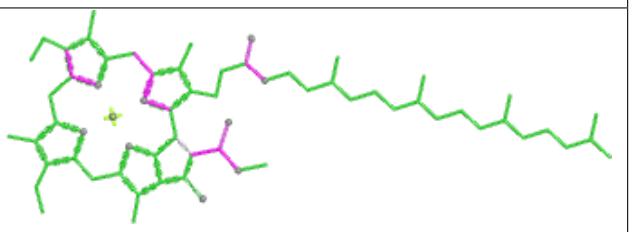


Rings

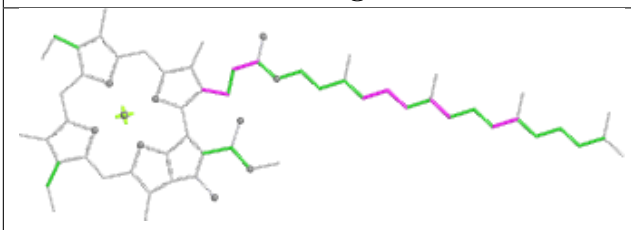
Ligand CLA C 507



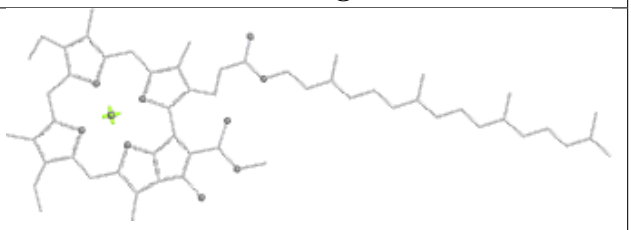
Bond lengths



Bond angles

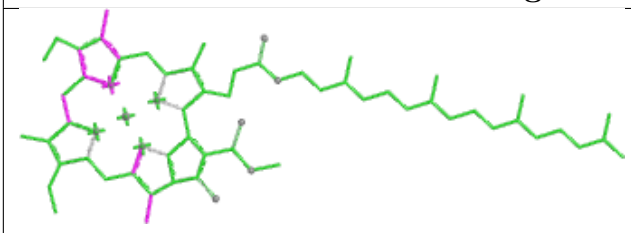


Torsions

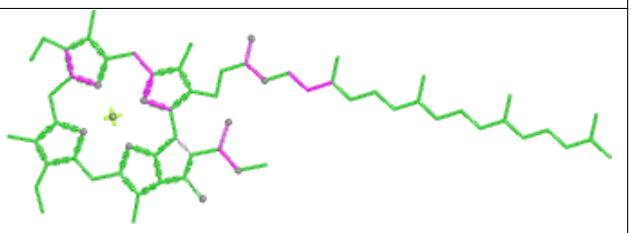


Rings

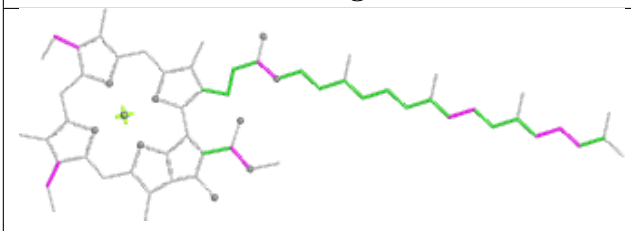
Ligand CLA B 604



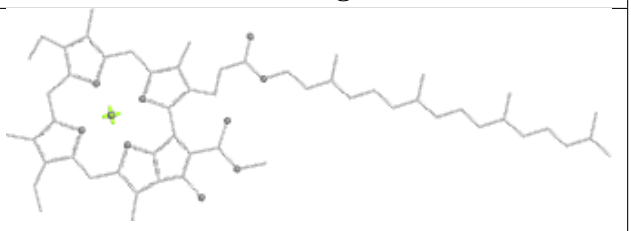
Bond lengths



Bond angles

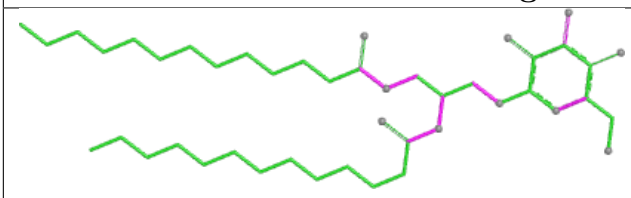


Torsions

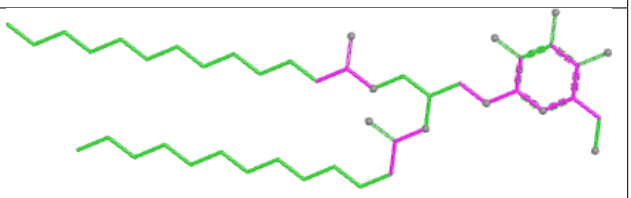


Rings

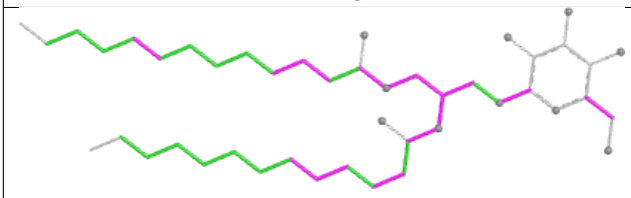
Ligand LMG C 521



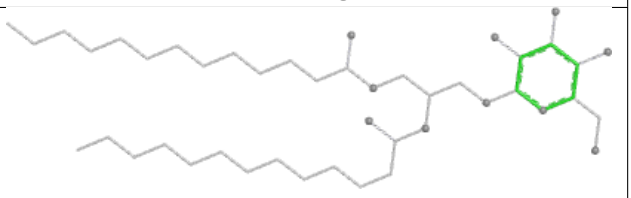
Bond lengths



Bond angles

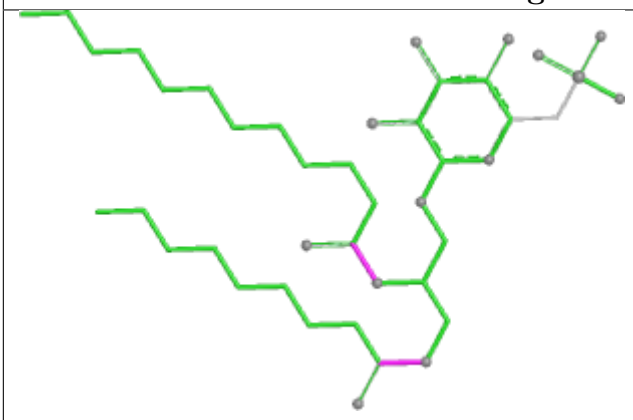


Torsions

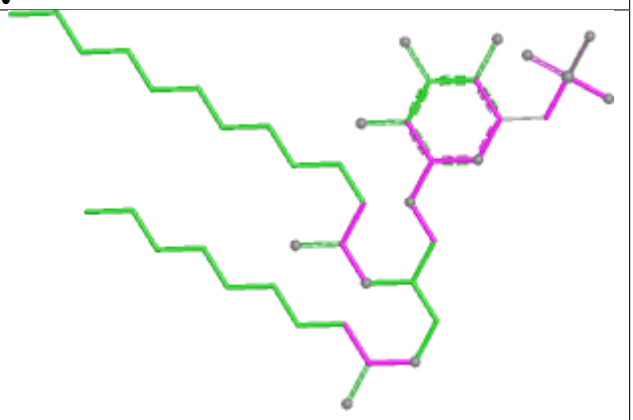


Rings

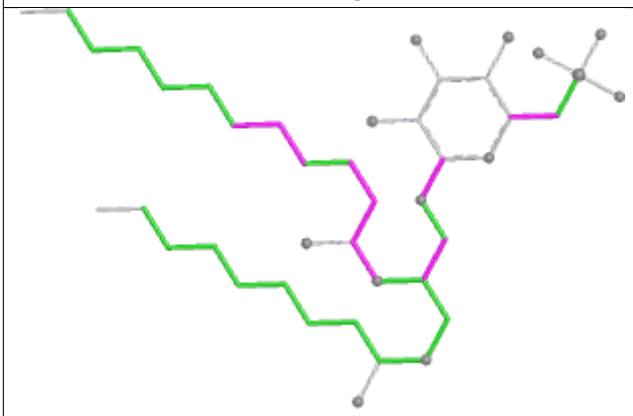
Ligand SQD d 408



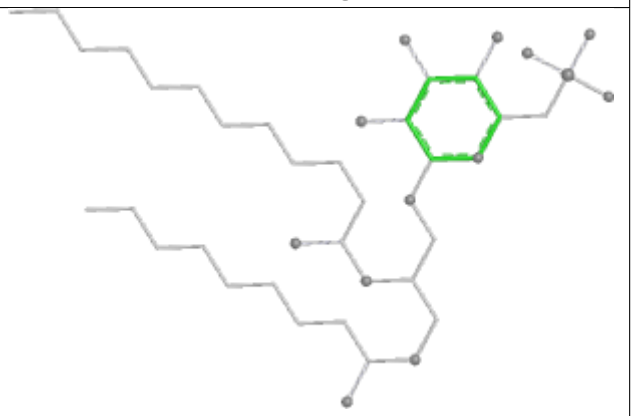
Bond lengths



Bond angles

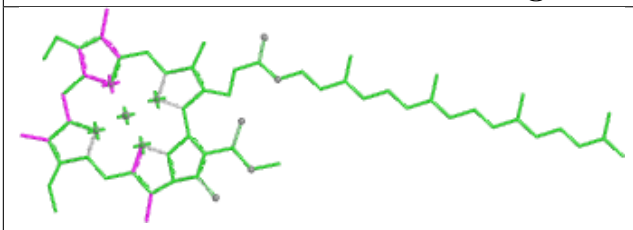


Torsions

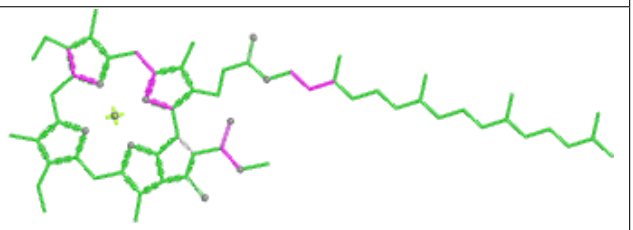


Rings

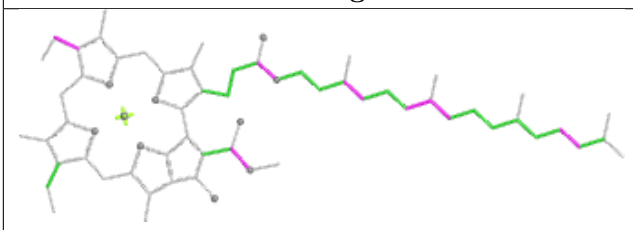
Ligand CLA b 615



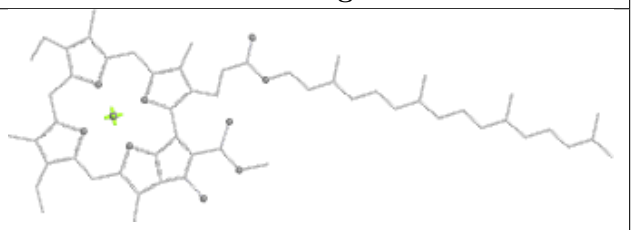
Bond lengths



Bond angles

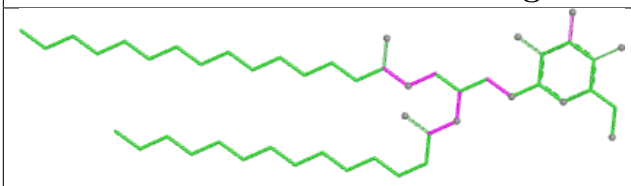


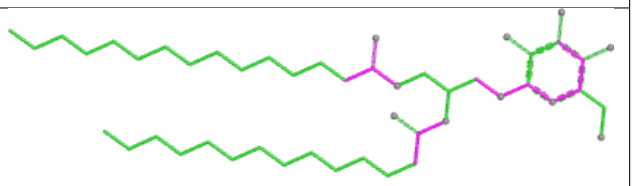
Torsions

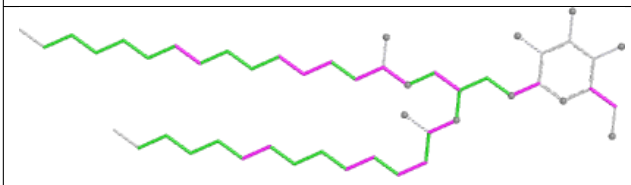


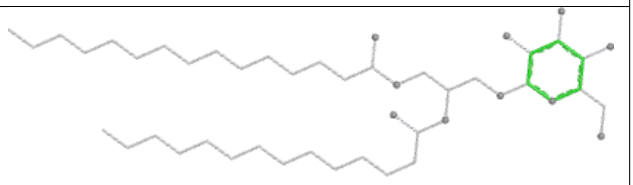
Rings

Ligand LMG k 103


Bond lengths

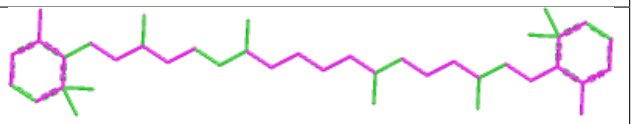

Bond angles

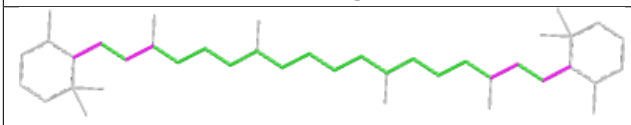

Torsions

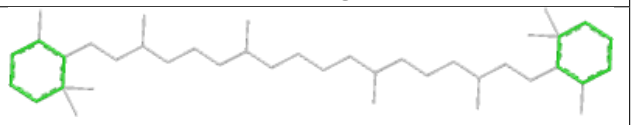

Rings

Ligand BCR c 515

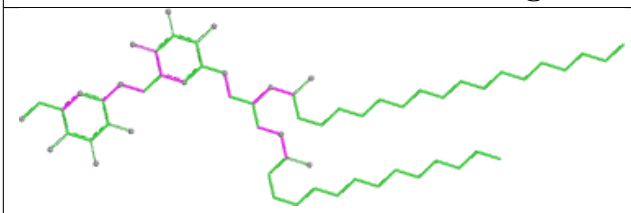

Bond lengths

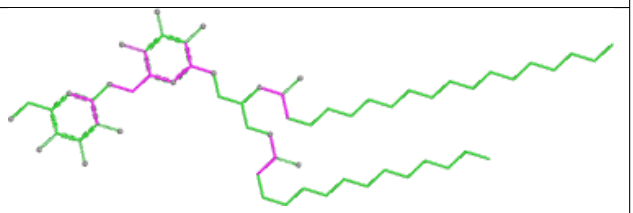

Bond angles

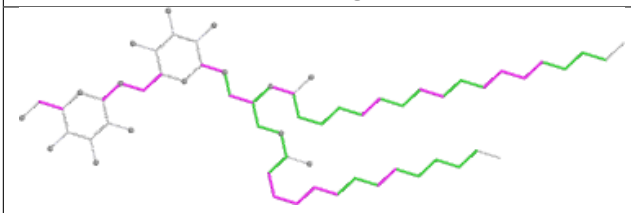

Torsions

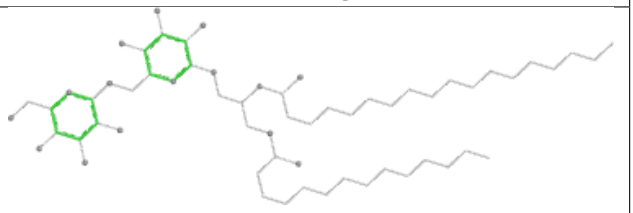

Rings

Ligand DGD c 517

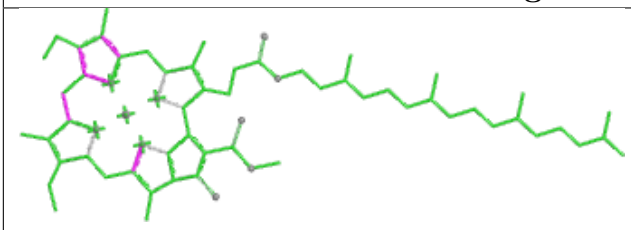

Bond lengths


Bond angles

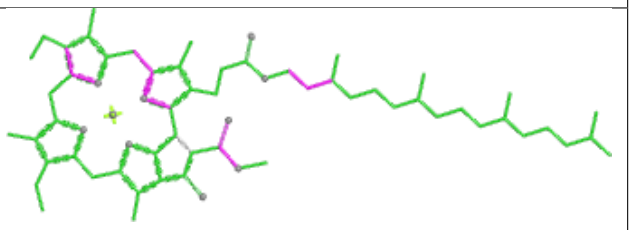

Torsions


Rings

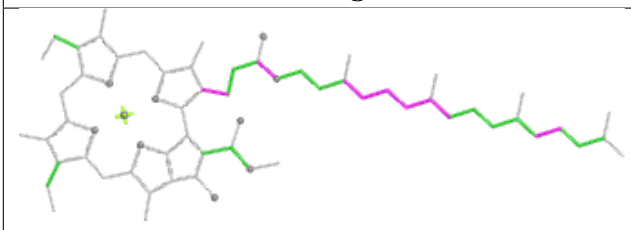
Ligand CLA B 602



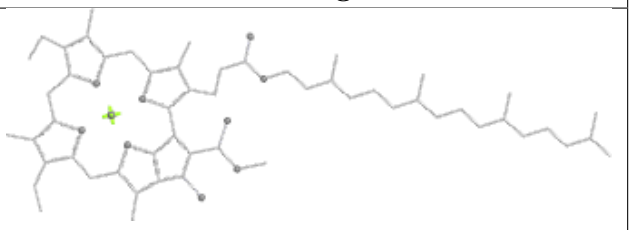
Bond lengths



Bond angles

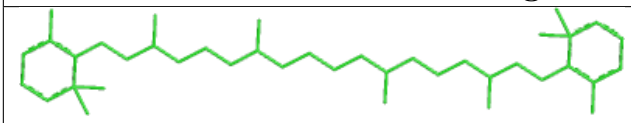


Torsions

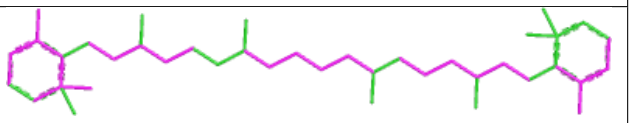


Rings

Ligand BCR B 620



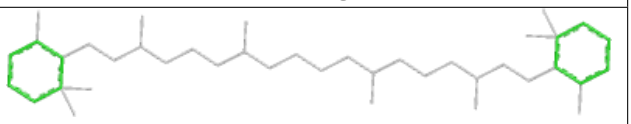
Bond lengths



Bond angles

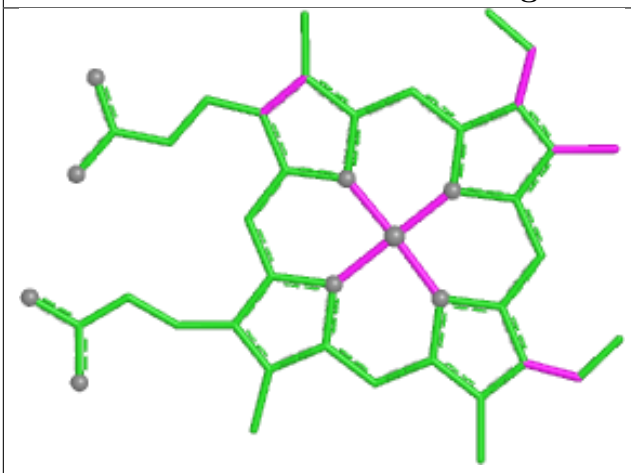


Torsions

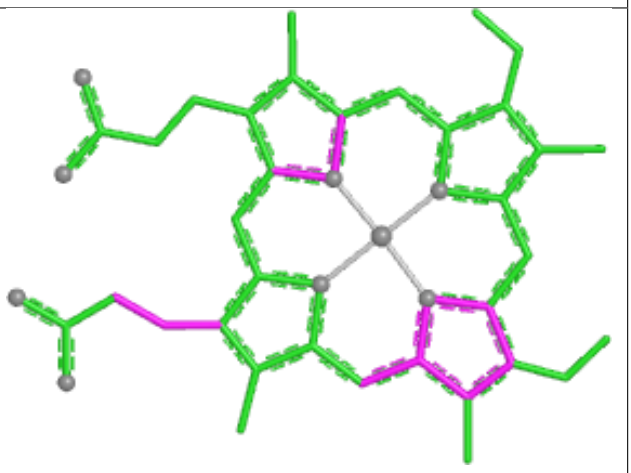


Rings

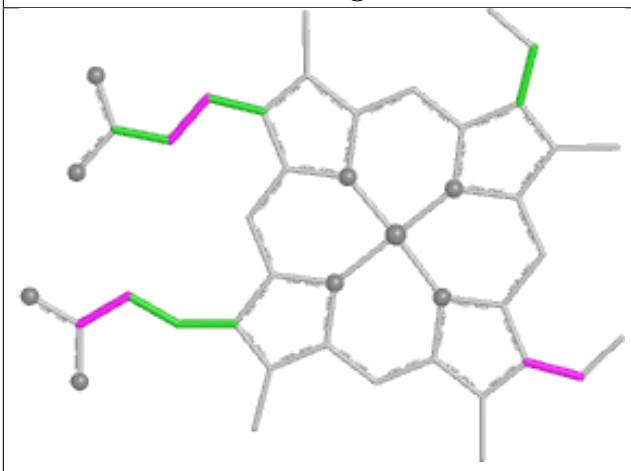
Ligand HEM F 101



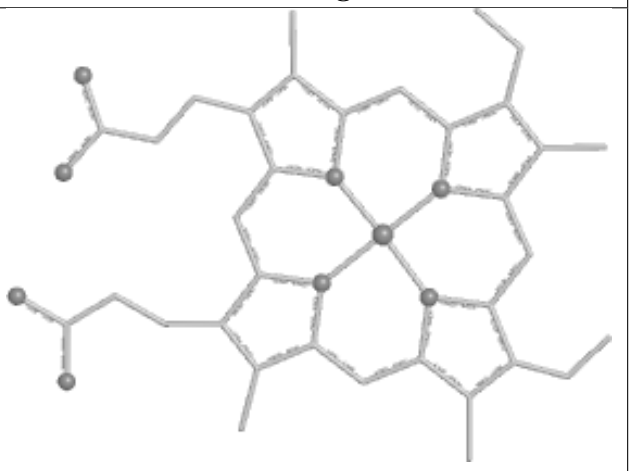
Bond lengths



Bond angles

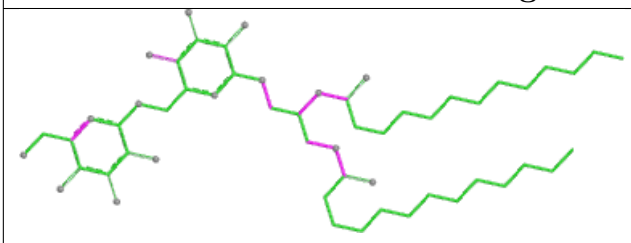


Torsions

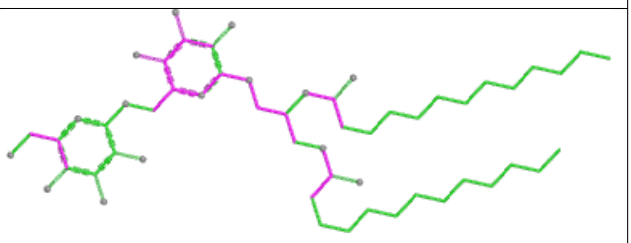


Rings

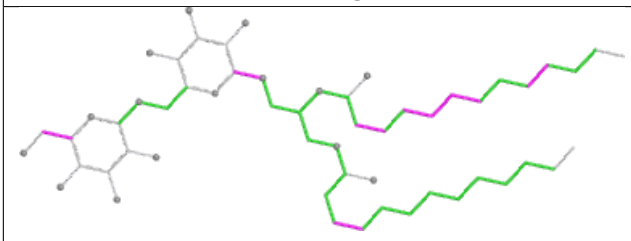
Ligand DGD A 411



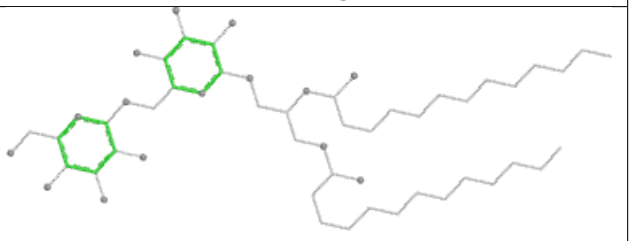
Bond lengths



Bond angles

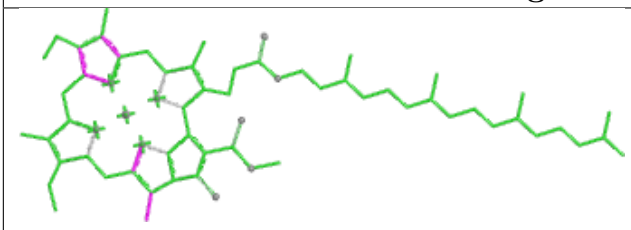


Torsions

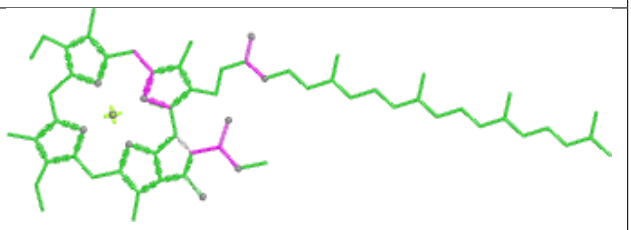


Rings

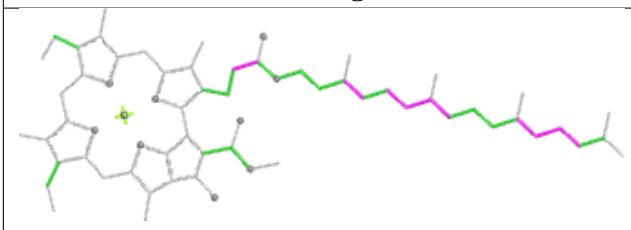
Ligand CLA d 402



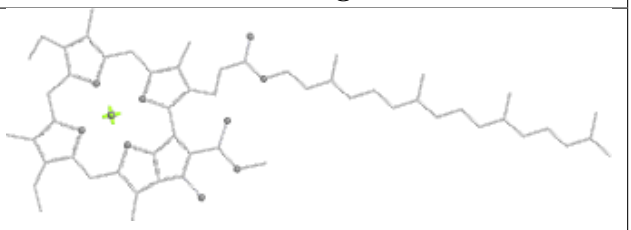
Bond lengths



Bond angles

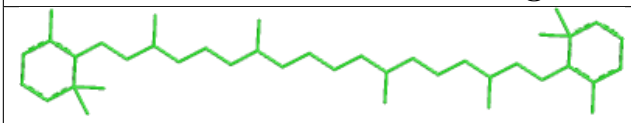


Torsions

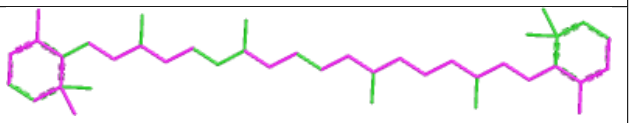


Rings

Ligand BCR b 622



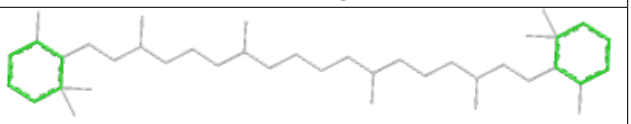
Bond lengths



Bond angles

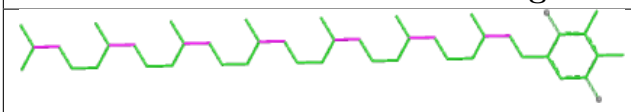


Torsions

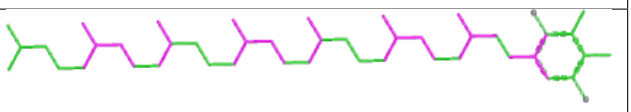


Rings

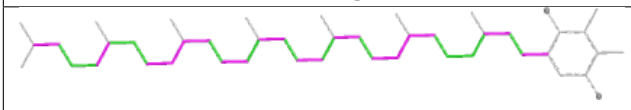
Ligand PL9 A 408



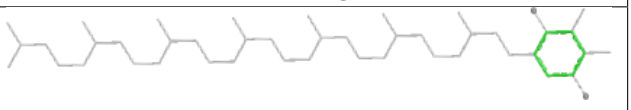
Bond lengths



Bond angles

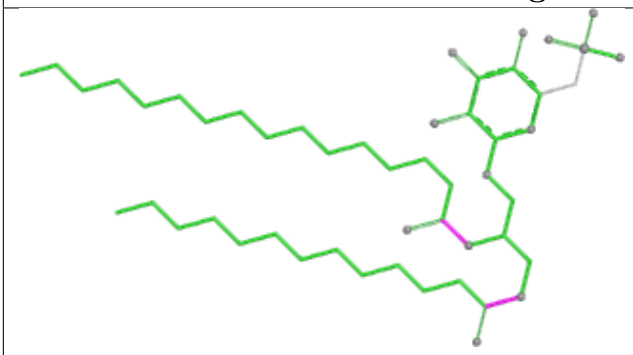


Torsions

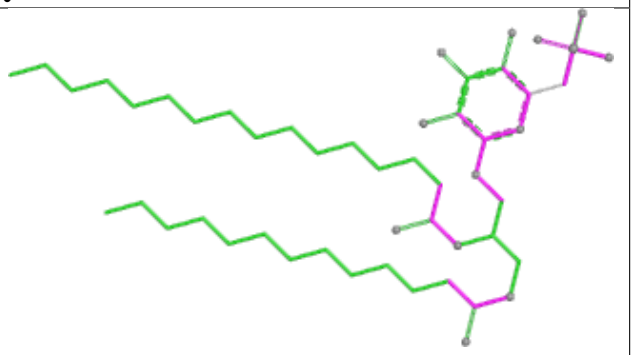


Rings

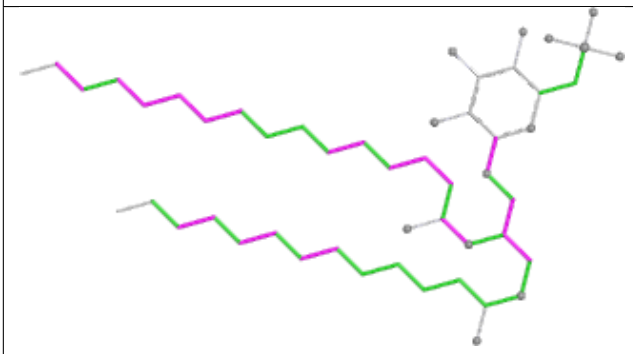
Ligand SQD a 415



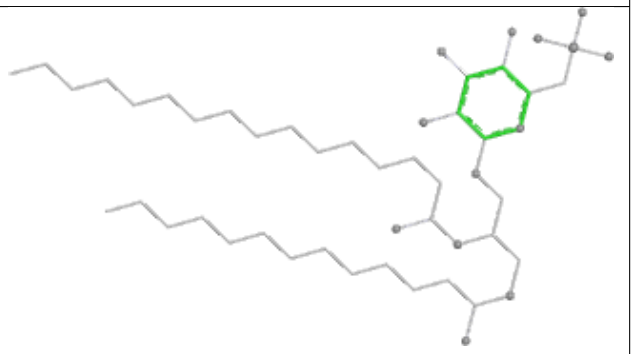
Bond lengths



Bond angles

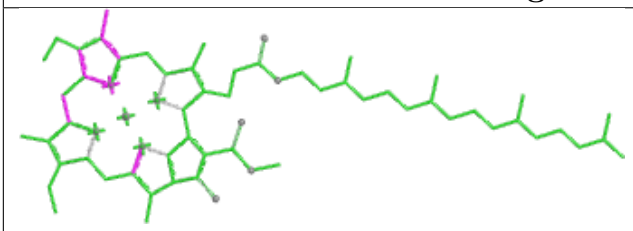


Torsions

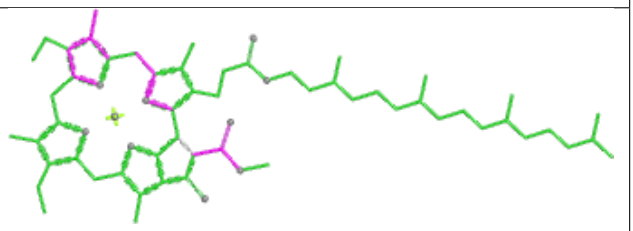


Rings

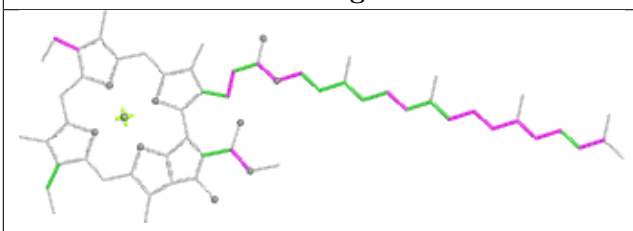
Ligand CLA b 614



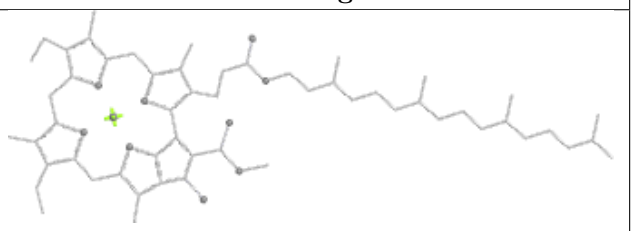
Bond lengths



Bond angles

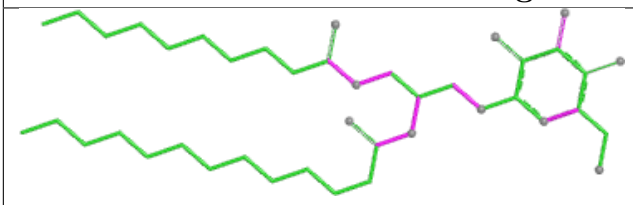


Torsions

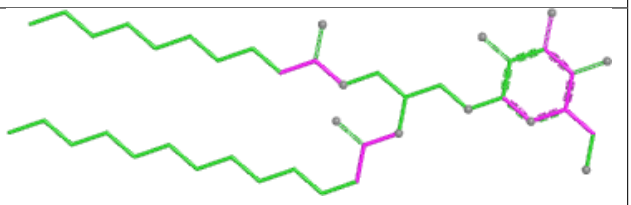


Rings

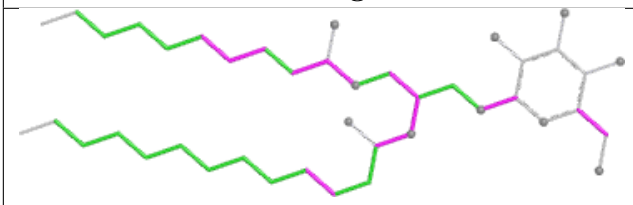
Ligand LMG M 101



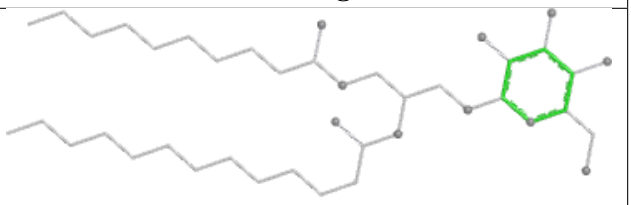
Bond lengths



Bond angles

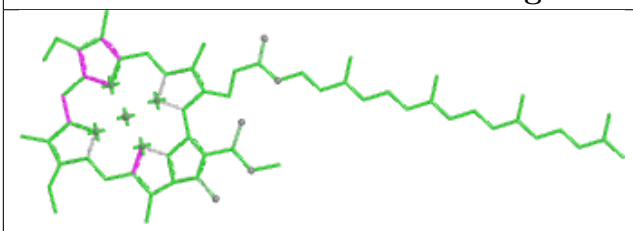


Torsions

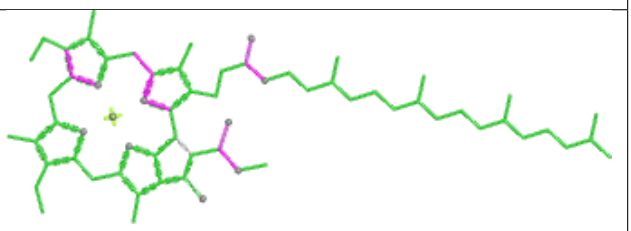


Rings

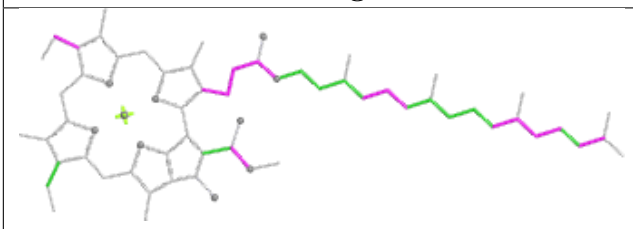
Ligand CLA C 512



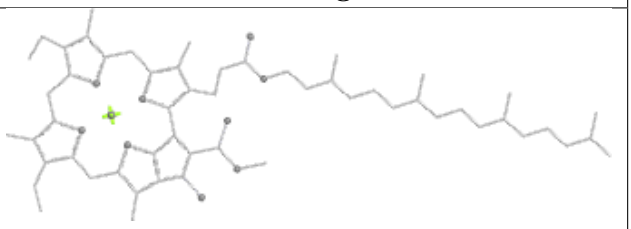
Bond lengths



Bond angles



Torsions

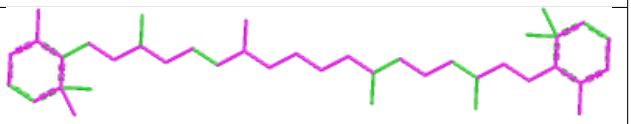


Rings

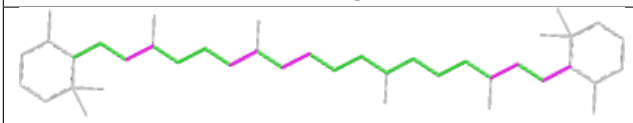
Ligand BCR B 618



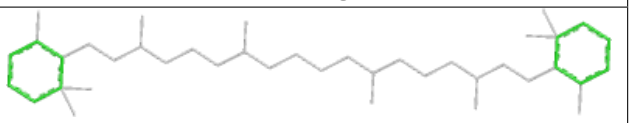
Bond lengths



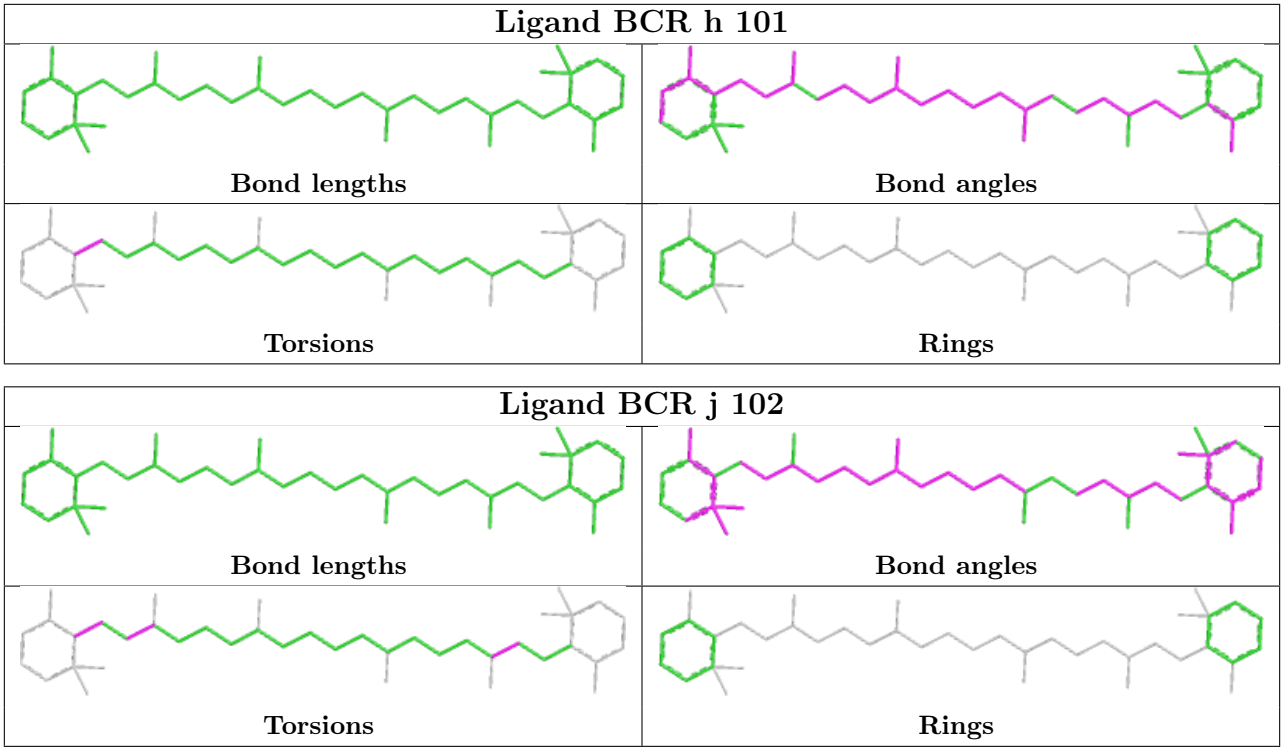
Bond angles



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%)	0.36	14 (4%)	40	39	43, 64, 104, 149	0
1	a	335/360 (93%)	0.25	12 (3%)	46	42	44, 65, 106, 149	0
2	B	490/510 (96%)	0.31	22 (4%)	38	38	46, 69, 103, 159	0
2	b	490/510 (96%)	0.39	30 (6%)	27	31	47, 71, 104, 159	0
3	C	447/461 (96%)	0.31	12 (2%)	56	48	54, 79, 106, 132	0
3	c	447/461 (96%)	0.28	14 (3%)	51	45	56, 81, 105, 135	0
4	D	340/352 (96%)	0.29	15 (4%)	39	38	44, 66, 103, 137	0
4	d	340/352 (96%)	0.22	12 (3%)	47	43	45, 66, 102, 134	0
5	E	82/84 (97%)	0.44	4 (4%)	35	35	68, 92, 125, 130	0
5	e	82/84 (97%)	0.44	2 (2%)	59	51	70, 92, 125, 129	0
6	F	35/45 (77%)	0.47	3 (8%)	16	22	68, 84, 119, 139	0
6	f	35/45 (77%)	0.37	3 (8%)	16	22	73, 85, 120, 141	0
7	H	65/66 (98%)	0.56	4 (6%)	26	31	77, 94, 122, 138	0
7	h	65/66 (98%)	0.52	2 (3%)	51	45	73, 93, 120, 144	0
8	I	35/38 (92%)	0.48	2 (5%)	29	33	65, 79, 107, 118	0
8	i	35/38 (92%)	0.54	2 (5%)	29	33	66, 81, 106, 120	0
9	J	34/40 (85%)	0.52	2 (5%)	28	32	69, 85, 95, 112	0
9	j	34/40 (85%)	0.70	6 (17%)	4	11	74, 88, 95, 116	0
10	K	37/46 (80%)	0.36	2 (5%)	31	33	77, 87, 101, 122	0
10	k	37/46 (80%)	0.59	5 (13%)	7	14	73, 88, 108, 123	0
11	L	37/37 (100%)	0.16	0	100	100	48, 62, 128, 156	0
11	l	37/37 (100%)	0.31	0	100	100	52, 60, 126, 158	0
12	M	34/36 (94%)	0.35	1 (2%)	53	46	56, 71, 110, 164	0
12	m	34/36 (94%)	0.40	1 (2%)	53	46	55, 69, 108, 165	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%)	0.45	10 (4%) 41 40	50, 78, 122, 169	0
13	o	243/272 (89%)	0.38	10 (4%) 41 40	52, 78, 121, 167	0
14	T	32/32 (100%)	0.46	0 100 100	55, 67, 158, 174	0
14	t	32/32 (100%)	0.44	1 (3%) 51 45	54, 69, 159, 168	0
15	U	97/134 (72%)	0.62	6 (6%) 26 31	56, 71, 92, 108	0
15	u	97/134 (72%)	0.42	3 (3%) 51 45	55, 71, 90, 111	0
16	V	137/163 (84%)	0.50	10 (7%) 21 26	53, 71, 86, 101	0
16	v	137/163 (84%)	0.24	4 (2%) 53 46	59, 72, 88, 95	0
17	g	28/46 (60%)	1.02	3 (10%) 11 18	95, 108, 126, 132	0
17	y	28/46 (60%)	0.77	3 (10%) 11 18	89, 107, 126, 131	0
18	X	37/41 (90%)	0.42	2 (5%) 31 33	76, 93, 124, 140	0
18	x	37/41 (90%)	0.56	5 (13%) 7 14	75, 90, 126, 141	0
19	Z	62/62 (100%)	0.44	2 (3%) 50 45	86, 104, 168, 185	0
19	z	62/62 (100%)	0.36	2 (3%) 50 45	88, 105, 172, 187	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.36	231 (4%) 39 38	43, 75, 115, 187	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	482	ILE	8.2
2	b	393	GLU	5.3
5	E	78	THR	4.9
4	D	64	ALA	4.8
3	c	341	LEU	4.8
2	B	478	VAL	4.5
15	U	128	TYR	4.4
13	O	93	PRO	4.3
2	B	218	LEU	4.2
4	d	344	GLU	4.1
3	c	315	MET	3.9
2	b	63	LEU	3.8
4	D	187	GLY	3.8
2	b	304	ALA	3.8
1	a	50	ILE	3.8
2	b	84	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	K	36	ALA	3.7
3	C	387	TRP	3.7
4	d	214	HIS	3.6
19	Z	11	ALA	3.6
4	d	45	LEU	3.6
4	d	173	PHE	3.5
7	H	63	LYS	3.5
2	B	368	VAL	3.5
16	V	47	LEU	3.4
17	g	25	ILE	3.4
16	V	48	THR	3.4
10	k	14	ALA	3.3
13	O	170	GLY	3.3
4	d	216	ALA	3.3
4	D	55	VAL	3.3
2	b	70	GLY	3.3
1	a	10	SER	3.2
8	i	35	LYS	3.2
2	b	211	ILE	3.2
2	B	474	LEU	3.1
9	J	34	ALA	3.1
4	D	241	GLU	3.1
2	b	409	GLN	3.1
2	b	261	ALA	3.1
4	D	314	PHE	3.1
13	O	160	THR	3.0
3	C	322	GLN	3.0
1	A	254	TYR	3.0
1	a	197	PHE	2.9
18	X	28	VAL	2.9
2	B	83	GLU	2.9
4	d	137	GLY	2.9
9	j	14	ALA	2.9
13	O	206	GLU	2.9
4	d	299	ILE	2.8
13	o	171	GLU	2.8
8	I	34	ARG	2.8
17	y	33	PRO	2.8
4	d	343	GLU	2.8
3	c	366	LEU	2.8
1	a	277	ALA	2.8
3	C	269	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	344	ALA	2.8
2	B	106	LEU	2.8
3	C	145	SER	2.8
4	d	59	TYR	2.8
3	C	372	PRO	2.7
1	A	69	GLY	2.7
15	U	131	GLY	2.7
13	O	119	LEU	2.7
2	b	302	TRP	2.7
3	C	184	GLY	2.7
1	A	182	PHE	2.7
16	v	41	GLU	2.7
3	c	392	ALA	2.7
2	b	386	ALA	2.7
2	b	11	VAL	2.7
3	c	95	LEU	2.7
16	V	151	ILE	2.6
2	B	491	VAL	2.6
13	o	152	VAL	2.6
15	u	58	ASN	2.6
15	U	39	LEU	2.6
1	A	184	ILE	2.6
15	u	78	LEU	2.6
16	V	132	ASN	2.6
4	D	130	PHE	2.6
1	a	101	SER	2.6
6	F	28	VAL	2.6
2	b	443	PHE	2.6
17	y	19	ILE	2.6
16	V	147	VAL	2.6
9	j	35	GLY	2.6
19	z	17	PHE	2.6
5	E	57	ALA	2.6
15	u	47	LEU	2.6
8	i	13	THR	2.6
2	b	388	SER	2.6
12	m	17	VAL	2.5
18	x	17	LYS	2.5
5	E	61	ARG	2.5
2	B	367	PRO	2.5
13	O	30	THR	2.5
2	b	389	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	488	PRO	2.5
13	o	84	ASN	2.5
2	b	394	GLN	2.5
3	c	389	GLU	2.5
17	g	21	GLN	2.5
18	x	16	LEU	2.5
9	J	35	GLY	2.5
2	B	341	LYS	2.5
4	d	339	PHE	2.4
7	H	39	LEU	2.4
9	j	15	THR	2.4
18	x	11	THR	2.4
1	a	189	GLU	2.4
5	E	56	TYR	2.4
16	V	52	TYR	2.4
16	v	31	PRO	2.4
2	B	378	LYS	2.4
10	k	34	ALA	2.4
2	B	420	TYR	2.4
9	j	22	ILE	2.4
2	B	364	GLU	2.4
16	V	28	GLU	2.4
1	A	150	PRO	2.4
1	a	280	VAL	2.4
13	o	256	PRO	2.4
15	U	122	VAL	2.4
13	O	126	GLY	2.4
18	X	17	LYS	2.4
1	A	292	THR	2.4
2	b	306	PRO	2.4
2	b	379	ALA	2.4
1	a	224	ILE	2.4
3	C	327	ASN	2.4
2	B	359	MET	2.4
1	A	137	LEU	2.4
4	D	126	MET	2.4
1	a	220	THR	2.4
13	o	190	LEU	2.4
2	B	322	GLY	2.4
16	v	162	TYR	2.4
2	B	232	GLY	2.3
3	C	332	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	379	ALA	2.3
16	V	77	SER	2.3
18	x	25	SER	2.3
1	a	11	ALA	2.3
2	b	112	CYS	2.3
4	d	98	GLN	2.3
4	D	276	VAL	2.3
1	A	88	ALA	2.3
6	f	11	VAL	2.3
3	c	451	ALA	2.3
4	D	307	GLU	2.3
6	f	45	ARG	2.3
10	k	33	LEU	2.3
12	M	13	LEU	2.3
13	o	63	THR	2.3
7	H	64	ALA	2.3
2	b	484	PRO	2.3
7	H	30	LEU	2.3
1	a	139	MET	2.3
1	a	296	ASN	2.2
3	c	295	THR	2.2
2	B	47	PRO	2.2
3	c	468	SER	2.2
5	e	83	LEU	2.2
18	x	20	PHE	2.2
2	b	404	GLY	2.2
4	d	36	LEU	2.2
2	b	385	ARG	2.2
6	f	12	SER	2.2
9	j	39	SER	2.2
13	O	127	ILE	2.2
1	A	166	GLY	2.2
13	O	138	GLY	2.2
16	V	36	VAL	2.2
16	V	78	LEU	2.2
19	z	4	LEU	2.2
10	k	26	PRO	2.2
2	b	429	ILE	2.2
13	O	169	LYS	2.2
3	c	367	GLU	2.2
3	C	183	GLY	2.2
4	D	24	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	U	83	ALA	2.2
17	g	24	MET	2.2
1	A	48	PHE	2.2
6	F	11	VAL	2.2
10	K	43	VAL	2.2
4	D	239	GLN	2.2
15	U	40	VAL	2.2
2	B	337	ALA	2.1
17	y	20	ALA	2.1
2	b	229	LEU	2.1
3	c	401	LEU	2.1
1	A	65	GLU	2.1
3	C	341	LEU	2.1
3	c	328	VAL	2.1
7	h	65	LEU	2.1
1	A	154	ALA	2.1
2	b	218	LEU	2.1
3	c	214	LEU	2.1
2	B	390	TYR	2.1
1	A	329	GLU	2.1
2	B	120	LEU	2.1
3	C	453	ALA	2.1
2	b	435	GLU	2.1
3	c	318	LEU	2.1
13	o	222	GLN	2.1
2	B	429	ILE	2.1
9	j	16	VAL	2.1
2	b	359	MET	2.1
3	C	44	ASN	2.1
7	h	16	SER	2.1
16	v	77	SER	2.1
13	o	69	LEU	2.1
2	b	194	ASN	2.1
14	t	30	THR	2.1
4	D	342	PRO	2.1
6	F	45	ARG	2.0
5	e	56	TYR	2.0
2	b	310	ALA	2.0
4	D	13	GLY	2.0
4	D	351	ALA	2.0
2	b	55	MET	2.0
8	I	35	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	163	GLY	2.0
13	o	67	ALA	2.0
19	Z	62	VAL	2.0
10	k	10	LYS	2.0
13	o	226	ASN	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	d	410	31/35	0.32	0.28	83,134,157,157	0
27	BCR	j	102	40/40	0.56	0.44	110,128,180,184	0
33	LMT	D	410	31/35	0.57	0.18	83,133,154,159	0
33	LMT	B	624	35/35	0.58	0.21	80,142,170,171	0
33	LMT	B	629	35/35	0.58	0.21	70,137,165,168	0
33	LMT	i	102	35/35	0.59	0.18	99,137,146,152	0
31	LMG	C	521	45/55	0.60	0.23	84,119,143,175	0
23	CLA	b	605	65/65	0.62	0.24	88,108,124,137	0
27	BCR	J	102	40/40	0.63	0.37	108,125,177,180	0
25	PL9	J	101	35/55	0.67	0.43	119,157,178,182	0
33	LMT	I	102	35/35	0.68	0.18	99,135,144,145	0
33	LMT	b	626	35/35	0.70	0.18	76,139,174,176	0
33	LMT	b	627	35/35	0.70	0.16	100,140,152,154	0
28	DGD	B	627	52/66	0.70	0.25	75,105,178,180	0
22	BCT	d	401	4/4	0.70	0.26	87,91,92,94	0
23	CLA	B	601	65/65	0.72	0.19	92,108,131,137	0
23	CLA	C	507	65/65	0.73	0.23	79,93,100,104	0
23	CLA	c	513	65/65	0.74	0.17	93,109,142,148	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	BCR	z	101	40/40	0.74	0.26	86,96,112,115	0
30	SQD	b	601	47/54	0.75	0.21	81,103,147,151	0
33	LMT	B	628	35/35	0.75	0.24	72,126,141,144	0
28	DGD	D	409	63/66	0.75	0.27	104,127,181,188	0
28	DGD	d	409	63/66	0.76	0.27	106,128,181,190	0
27	BCR	B	618	40/40	0.76	0.26	75,82,94,95	0
23	CLA	C	513	65/65	0.76	0.18	95,109,142,149	0
25	PL9	j	101	35/55	0.76	0.37	120,160,178,182	0
32	CL	a	418	1/1	0.77	0.16	49,49,49,49	0
30	SQD	d	408	43/54	0.77	0.20	67,109,152,157	0
30	SQD	B	626	47/54	0.77	0.20	75,100,144,148	0
33	LMT	b	603	35/35	0.77	0.26	73,119,136,138	0
31	LMG	k	103	48/55	0.78	0.27	79,100,112,115	0
28	DGD	C	519	66/66	0.78	0.23	55,72,100,114	0
29	LHG	A	415	37/49	0.78	0.18	104,133,190,202	0
31	LMG	M	101	42/55	0.78	0.21	83,111,135,144	0
31	LMG	E	101	44/55	0.79	0.23	87,123,132,139	0
25	PL9	A	408	45/55	0.79	0.26	89,101,119,127	0
31	LMG	c	519	45/55	0.79	0.19	86,119,142,171	0
31	LMG	b	625	49/55	0.80	0.30	51,75,86,89	0
25	PL9	a	410	45/55	0.81	0.29	82,103,121,125	0
27	BCR	H	101	40/40	0.81	0.23	83,96,130,131	0
33	LMT	B	625	35/35	0.81	0.20	95,139,149,152	0
27	BCR	k	102	40/40	0.81	0.20	72,80,109,111	0
27	BCR	T	102	40/40	0.82	0.24	71,79,86,86	0
31	LMG	A	418	42/55	0.82	0.25	81,105,123,147	0
27	BCR	a	412	40/40	0.82	0.24	54,71,84,87	0
29	LHG	a	417	37/49	0.82	0.17	110,135,197,206	0
27	BCR	B	620	40/40	0.82	0.20	75,86,98,103	0
31	LMG	a	402	42/55	0.82	0.27	72,100,119,143	0
27	BCR	C	516	40/40	0.82	0.24	74,86,95,100	0
27	BCR	b	621	40/40	0.83	0.28	63,73,84,87	0
28	DGD	b	602	52/66	0.83	0.18	79,107,180,186	0
23	CLA	b	620	65/65	0.84	0.21	75,98,145,147	0
30	SQD	F	102	45/54	0.84	0.23	87,127,149,152	0
30	SQD	a	415	51/54	0.84	0.19	88,101,128,129	0
23	CLA	C	506	65/65	0.84	0.22	79,91,125,133	0
31	LMG	i	101	43/55	0.84	0.19	84,120,162,177	0
33	LMT	b	604	35/35	0.84	0.16	69,133,158,160	0
27	BCR	c	514	40/40	0.84	0.21	76,82,88,89	0
28	DGD	C	518	62/66	0.84	0.19	58,81,134,144	0
23	CLA	b	613	65/65	0.84	0.19	65,93,104,114	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	413	51/54	0.84	0.20	81,99,128,131	0
23	CLA	c	511	65/65	0.85	0.16	75,91,102,108	0
23	CLA	c	512	65/65	0.85	0.17	83,104,146,152	0
28	DGD	C	517	53/66	0.85	0.20	61,79,96,101	0
31	LMG	a	416	51/55	0.85	0.24	62,80,93,100	0
23	CLA	B	616	65/65	0.85	0.23	79,93,147,152	0
23	CLA	c	506	65/65	0.85	0.20	78,92,122,128	0
27	BCR	B	619	40/40	0.85	0.26	62,75,83,86	0
33	LMT	m	101	35/35	0.85	0.22	68,93,112,114	0
35	CA	K	101	1/1	0.85	0.16	86,86,86,86	0
32	CL	A	416	1/1	0.86	0.25	49,49,49,49	0
23	CLA	a	406	65/65	0.86	0.25	55,71,140,147	0
28	DGD	A	411	56/66	0.86	0.19	77,102,146,153	0
27	BCR	h	101	40/40	0.86	0.22	85,94,124,127	0
25	PL9	d	404	55/55	0.86	0.23	45,65,78,85	0
30	SQD	a	401	54/54	0.86	0.23	76,114,149,152	0
27	BCR	b	622	40/40	0.86	0.20	72,83,94,96	0
31	LMG	m	102	42/55	0.86	0.26	73,111,128,138	0
28	DGD	c	517	62/66	0.87	0.19	64,84,132,141	0
31	LMG	B	622	49/55	0.87	0.21	61,79,105,117	0
28	DGD	c	518	66/66	0.87	0.17	54,73,105,118	0
23	CLA	C	504	65/65	0.87	0.19	62,83,138,145	0
31	LMG	I	101	43/55	0.87	0.18	73,118,166,178	0
27	BCR	y	101	40/40	0.87	0.20	79,86,106,109	0
23	CLA	c	502	65/65	0.87	0.17	63,75,100,106	0
27	BCR	C	515	40/40	0.87	0.19	85,92,115,116	0
27	BCR	A	410	40/40	0.87	0.19	52,68,85,90	0
27	BCR	B	617	40/40	0.87	0.19	67,74,81,84	0
31	LMG	e	101	44/55	0.87	0.17	91,122,132,136	0
27	BCR	c	515	40/40	0.87	0.19	75,86,95,101	0
23	CLA	C	511	65/65	0.87	0.18	74,88,102,109	0
28	DGD	a	413	56/66	0.87	0.16	76,100,145,148	0
27	BCR	T	101	40/40	0.87	0.23	68,75,82,83	0
35	CA	k	101	1/1	0.87	0.13	103,103,103,103	0
31	LMG	b	624	49/55	0.88	0.24	59,82,102,113	0
30	SQD	f	102	45/54	0.88	0.18	88,133,148,152	0
23	CLA	b	619	65/65	0.88	0.16	85,97,108,116	0
23	CLA	C	510	65/65	0.88	0.16	67,74,83,93	0
31	LMG	C	520	48/55	0.88	0.21	89,100,109,112	0
23	CLA	a	409	65/65	0.88	0.18	55,67,129,133	0
31	LMG	D	406	46/55	0.88	0.20	58,73,116,129	0
27	BCR	C	514	40/40	0.88	0.18	73,80,87,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	610	65/65	0.88	0.17	69,81,88,92	0
23	CLA	b	606	65/65	0.88	0.23	70,87,96,97	0
23	CLA	C	509	65/65	0.88	0.17	62,81,95,98	0
23	CLA	b	614	65/65	0.88	0.17	66,82,88,91	0
28	DGD	b	623	58/66	0.89	0.19	57,74,99,107	0
30	SQD	A	417	54/54	0.89	0.20	77,113,147,154	0
28	DGD	c	516	53/66	0.89	0.21	63,77,96,103	0
31	LMG	B	623	49/55	0.89	0.19	58,76,84,87	0
24	PHO	A	406	64/64	0.89	0.15	50,69,77,81	0
23	CLA	B	608	65/65	0.89	0.18	64,75,93,97	0
27	BCR	D	405	40/40	0.89	0.20	68,81,105,110	0
23	CLA	C	505	65/65	0.89	0.19	69,77,86,91	0
23	CLA	c	507	65/65	0.89	0.17	83,93,105,111	0
23	CLA	c	505	65/65	0.90	0.19	70,77,83,85	0
23	CLA	C	501	65/65	0.90	0.14	69,82,90,95	0
23	CLA	b	607	65/65	0.90	0.15	68,82,92,103	0
23	CLA	c	508	65/65	0.90	0.18	70,85,118,134	0
23	CLA	B	603	65/65	0.90	0.19	65,81,94,109	0
23	CLA	B	605	65/65	0.90	0.15	58,78,86,92	0
23	CLA	B	614	65/65	0.90	0.17	63,83,125,129	0
23	CLA	d	402	65/65	0.90	0.17	49,57,81,95	0
23	CLA	B	615	65/65	0.90	0.15	83,96,106,116	0
23	CLA	c	501	65/65	0.90	0.15	67,82,92,94	0
25	PL9	D	404	55/55	0.90	0.21	42,61,71,77	0
23	CLA	B	606	65/65	0.90	0.19	67,81,110,121	0
29	LHG	A	412	39/49	0.90	0.18	59,79,89,93	0
23	CLA	c	503	65/65	0.90	0.14	77,89,97,103	0
29	LHG	a	414	39/49	0.90	0.17	60,78,94,102	0
23	CLA	a	405	65/65	0.91	0.17	44,53,69,73	0
23	CLA	A	407	65/65	0.91	0.17	56,66,127,129	0
22	BCT	A	402	4/4	0.91	0.09	85,90,90,94	0
23	CLA	c	509	65/65	0.91	0.13	67,85,91,97	0
23	CLA	A	405	65/65	0.91	0.18	44,69,140,145	0
23	CLA	C	512	65/65	0.91	0.16	89,101,144,149	0
23	CLA	B	604	65/65	0.91	0.15	59,67,104,124	0
23	CLA	b	610	65/65	0.91	0.15	70,83,112,126	0
23	CLA	b	611	65/65	0.91	0.18	54,64,89,92	0
35	CA	O	301	1/1	0.91	0.12	112,112,112,112	0
24	PHO	a	408	64/64	0.91	0.16	58,68,79,86	0
35	CA	o	301	1/1	0.91	0.09	98,98,98,98	0
23	CLA	D	401	65/65	0.92	0.15	49,59,87,97	0
23	CLA	d	403	65/65	0.92	0.16	72,88,121,128	0

Continued on next page...

Continued from previous page...

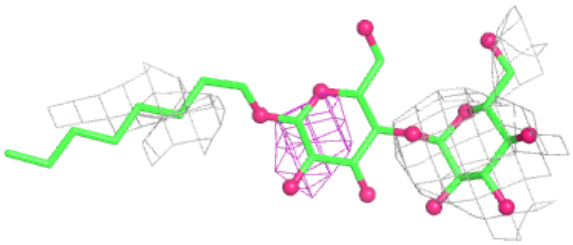
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LMT	M	102	35/35	0.92	0.17	69,96,112,115	0
31	LMG	d	406	46/55	0.92	0.17	63,73,116,130	0
23	CLA	a	404	65/65	0.92	0.15	53,60,67,74	0
23	CLA	C	508	65/65	0.92	0.18	71,86,117,132	0
23	CLA	b	608	65/65	0.92	0.15	61,68,107,117	0
31	LMG	D	407	48/55	0.92	0.19	54,72,81,120	0
23	CLA	B	609	65/65	0.92	0.16	74,89,104,106	0
23	CLA	c	510	65/65	0.92	0.13	67,75,84,89	0
34	HEM	f	101	43/43	0.92	0.12	89,105,124,126	0
23	CLA	B	602	65/65	0.92	0.15	68,87,95,96	0
23	CLA	b	612	65/65	0.92	0.17	63,75,95,98	0
31	LMG	A	414	51/55	0.92	0.16	63,77,92,95	0
23	CLA	c	504	65/65	0.92	0.15	75,83,133,138	0
23	CLA	A	404	65/65	0.93	0.15	44,54,67,74	0
28	DGD	B	621	58/66	0.93	0.17	46,71,101,105	0
31	LMG	d	407	48/55	0.93	0.19	58,70,85,120	0
23	CLA	B	612	65/65	0.93	0.16	61,72,82,86	0
23	CLA	C	503	65/65	0.93	0.13	71,88,99,105	0
24	PHO	D	402	64/64	0.93	0.13	51,62,72,74	0
24	PHO	a	407	64/64	0.93	0.14	53,63,70,73	0
23	CLA	C	502	65/65	0.94	0.15	59,75,108,111	0
23	CLA	B	607	65/65	0.94	0.13	52,66,82,85	0
23	CLA	b	616	65/65	0.94	0.12	61,73,83,86	0
34	HEM	V	201	43/43	0.94	0.16	58,69,74,76	0
23	CLA	b	617	65/65	0.94	0.15	57,67,91,93	0
23	CLA	b	618	65/65	0.94	0.14	60,82,123,130	0
23	CLA	B	613	65/65	0.94	0.13	46,64,88,93	0
30	SQD	D	408	43/54	0.94	0.17	71,103,148,152	0
23	CLA	B	611	65/65	0.94	0.13	63,72,80,87	0
23	CLA	A	403	65/65	0.95	0.13	52,58,66,70	0
23	CLA	D	403	65/65	0.95	0.15	74,87,123,124	0
34	HEM	v	201	43/43	0.95	0.12	57,68,75,76	0
23	CLA	b	615	65/65	0.95	0.13	54,72,80,87	0
23	CLA	b	609	65/65	0.95	0.12	61,76,84,88	0
27	BCR	d	405	40/40	0.95	0.12	69,82,102,106	0
34	HEM	F	101	43/43	0.95	0.13	89,105,127,130	0
21	FE2	a	403	1/1	0.98	0.12	72,72,72,72	0
26	OEC	a	411	5/9	0.98	0.14	35,44,62,68	0
26	OEC	A	409	5/9	0.99	0.18	35,44,57,62	0
21	FE2	A	401	1/1	0.99	0.06	64,64,64,64	0

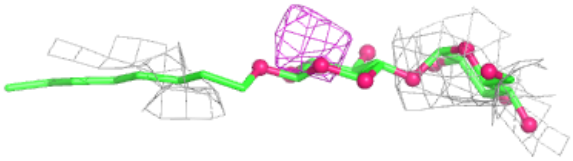
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

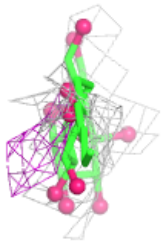
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMT 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)

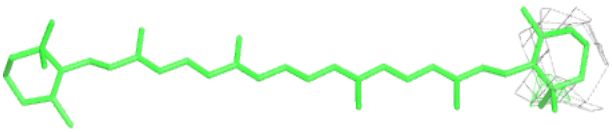


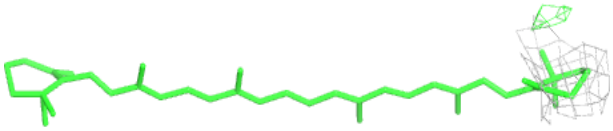




Electron density around BCR j 102:

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

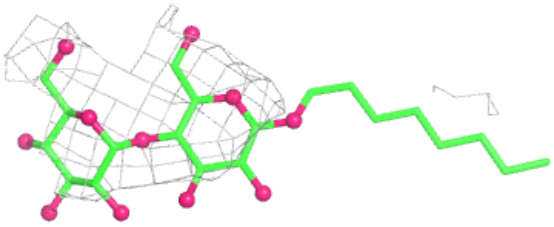


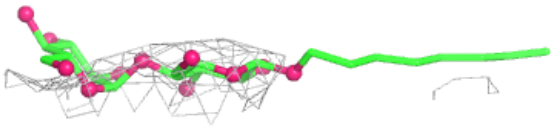


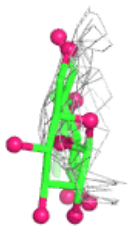


Electron density around LMT D 410:

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

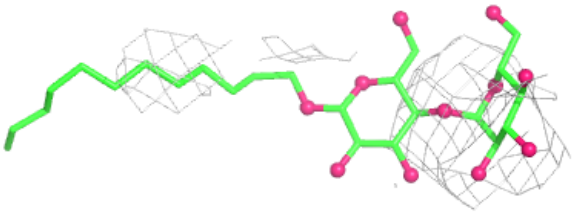


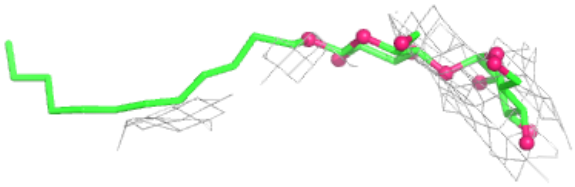


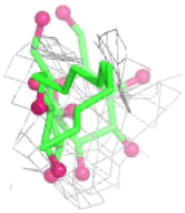


Electron density around LMT B 624:

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

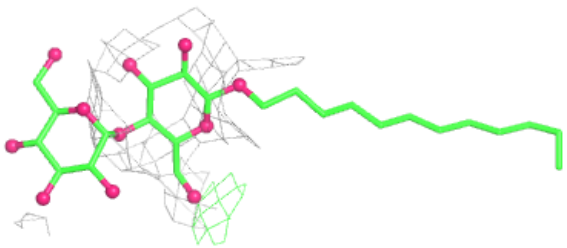


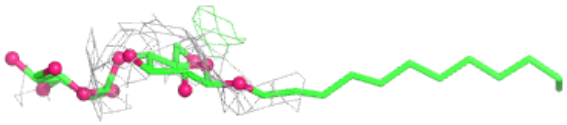




Electron density around LMT B 629:

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

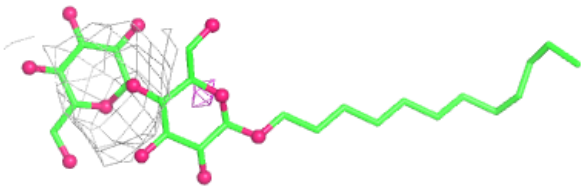


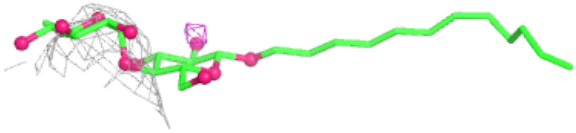


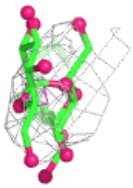


Electron density around LMT i 102:

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

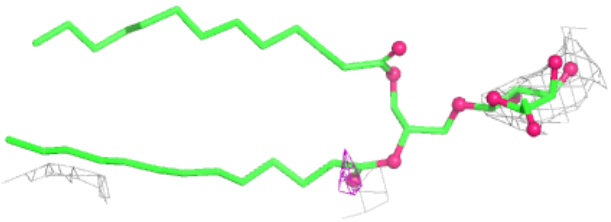


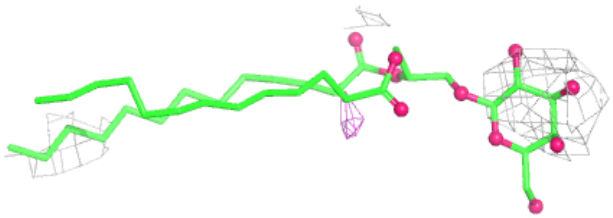


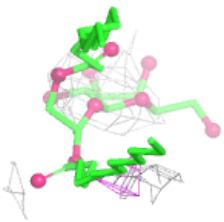


Electron density around LMG C 521:

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

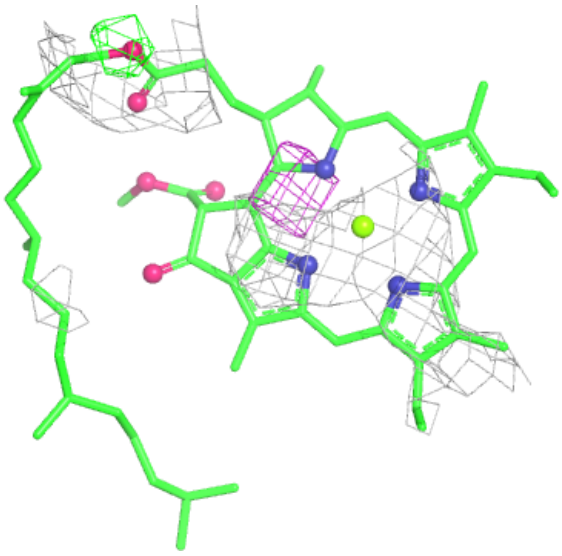


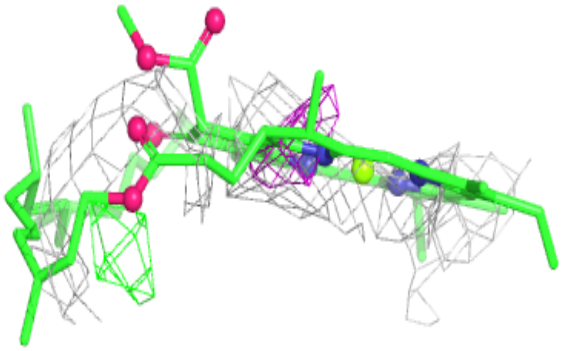


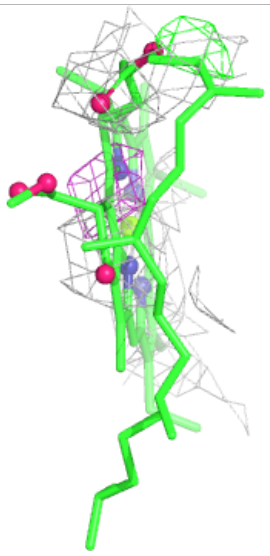


Electron density around CLA b 605:

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

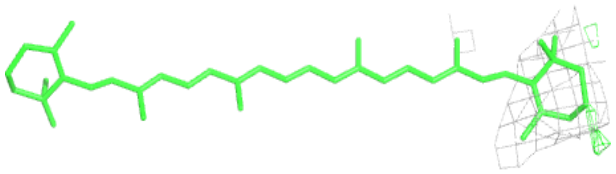


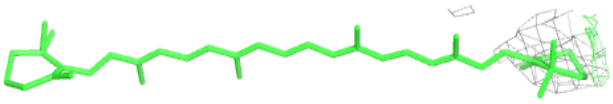




Electron density around BCR J 102:

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

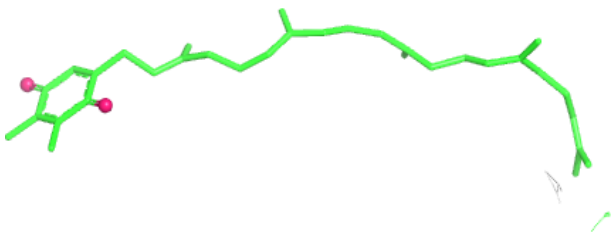


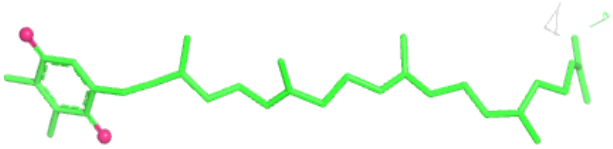


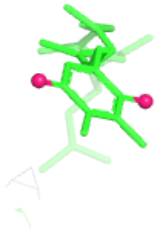


Electron density around PL9 J 101:

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

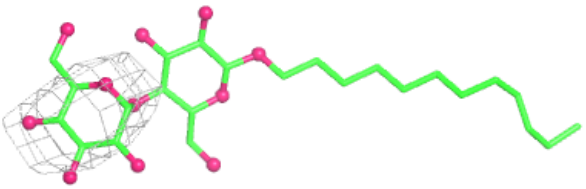


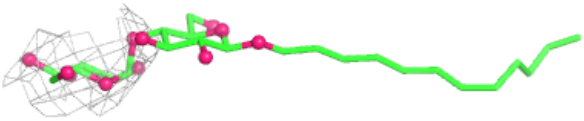


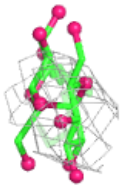


Electron density around LMT I 102:

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

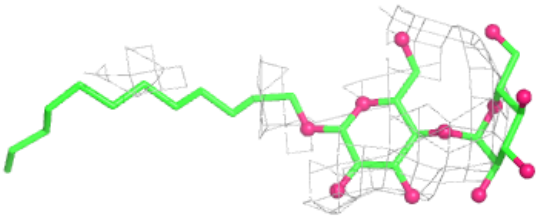


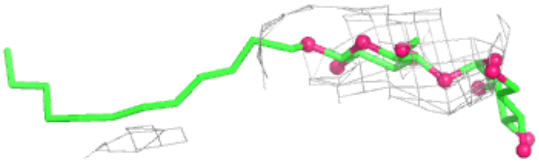




Electron density around LMT b 626:

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

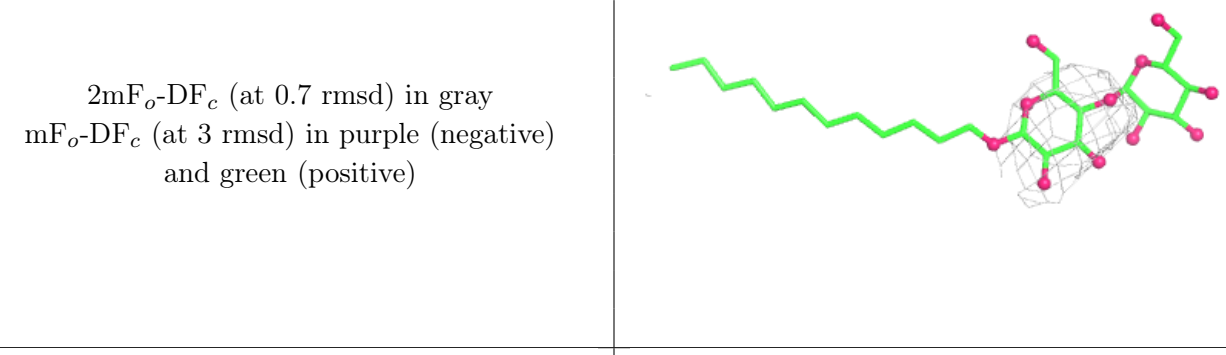


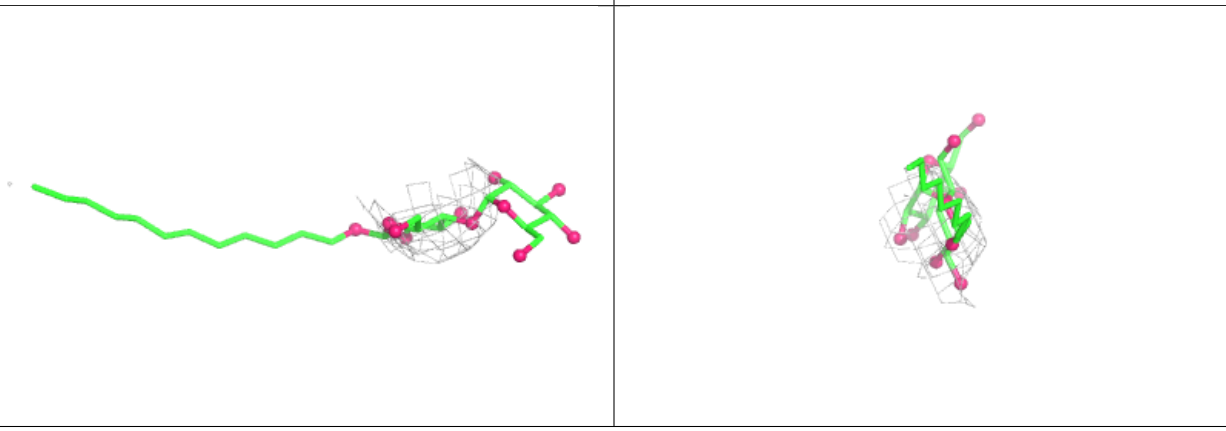




Electron density around LMT b 627:

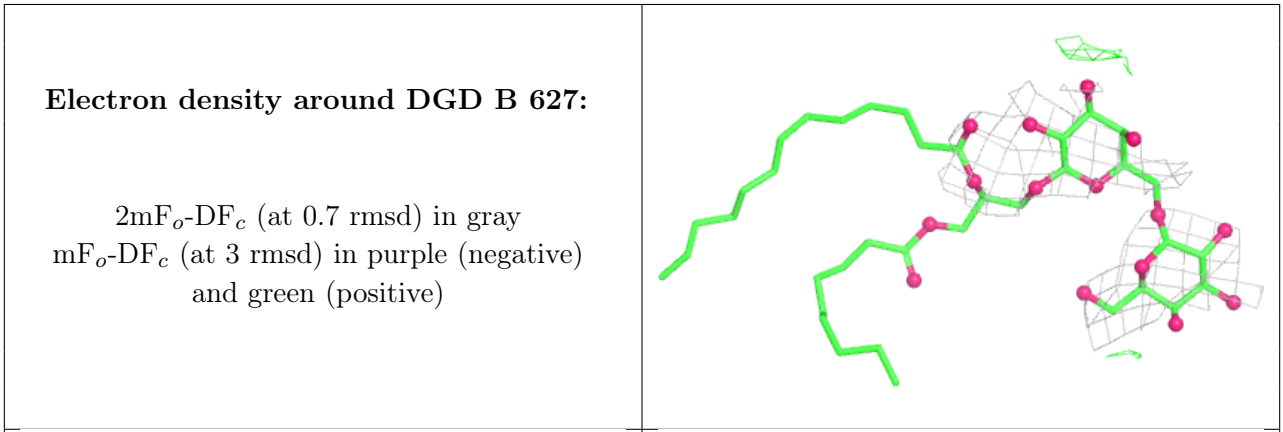
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

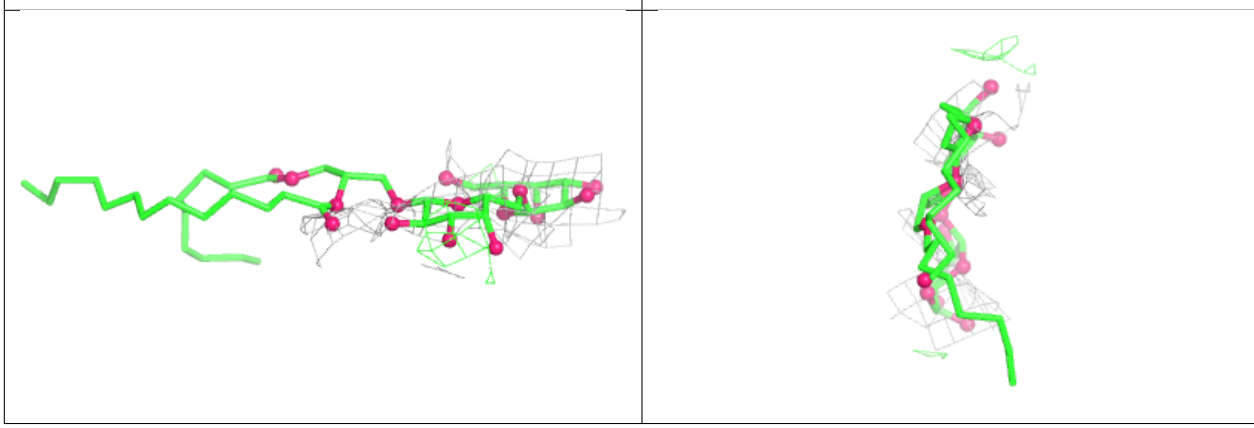




Electron density around DGD B 627:

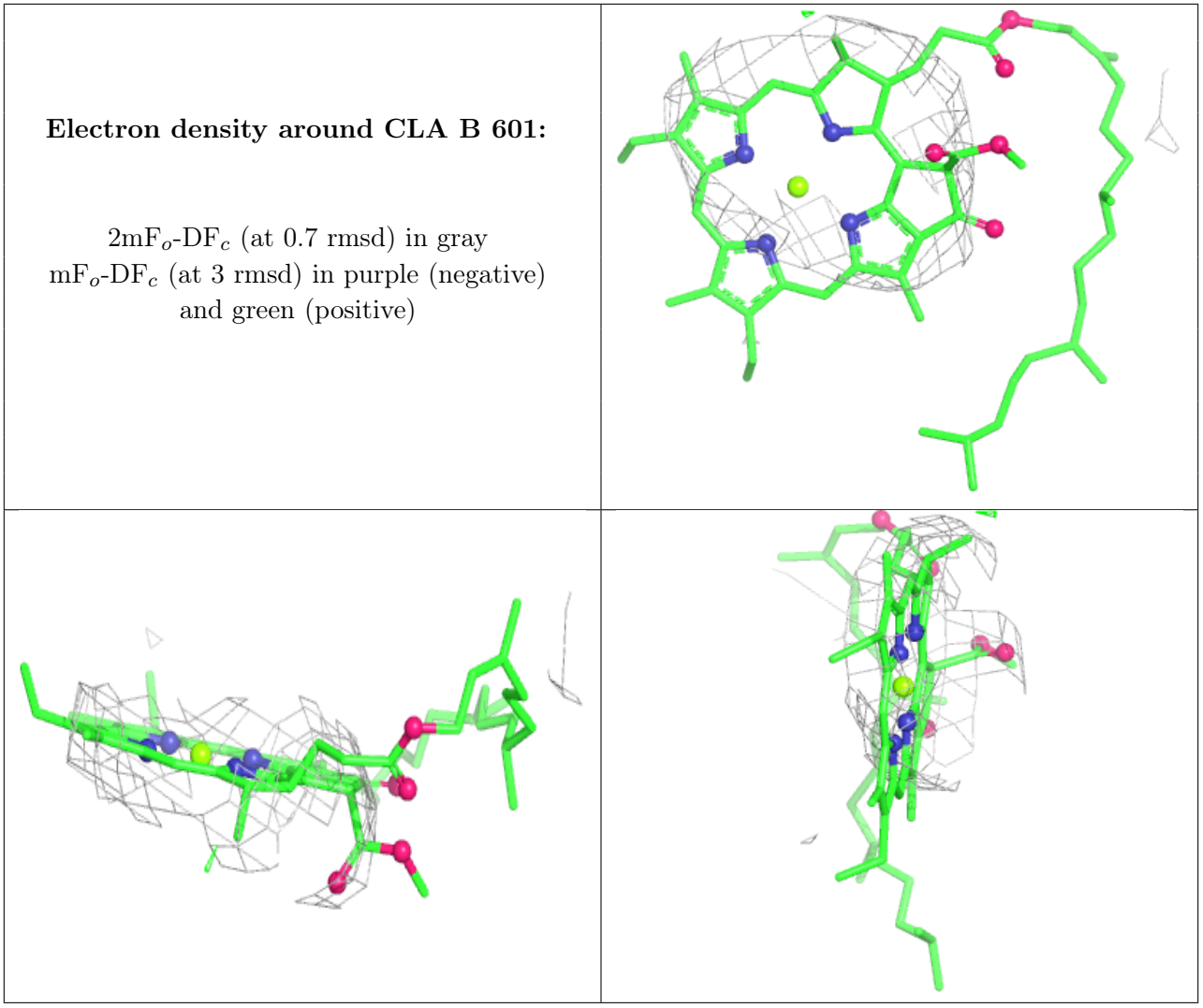
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





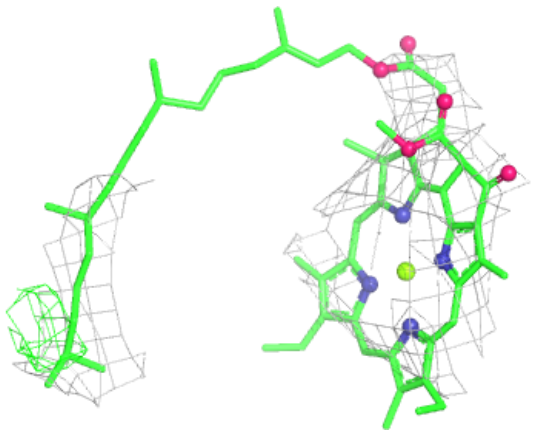
Electron density around CLA B 601:

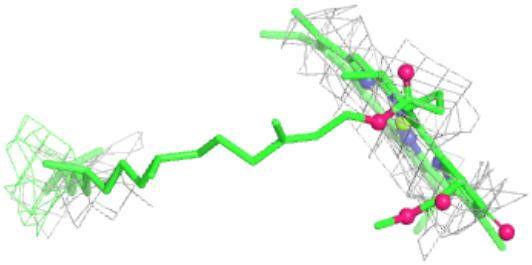
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

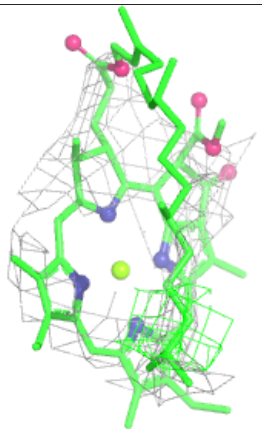


Electron density around CLA C 507:

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

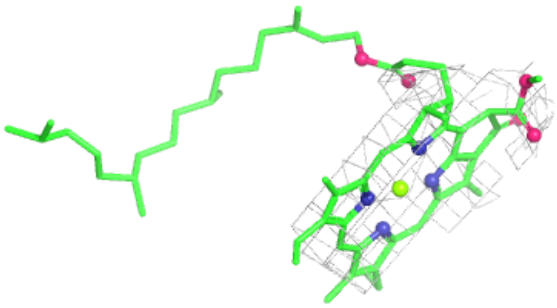


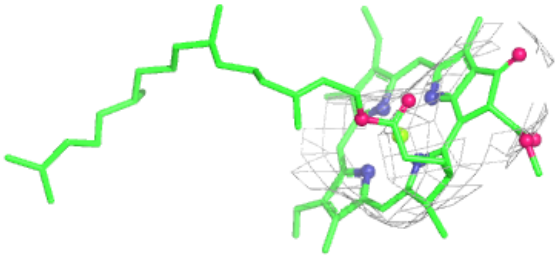


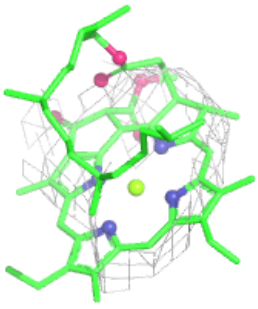


Electron density around CLA c 513:

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

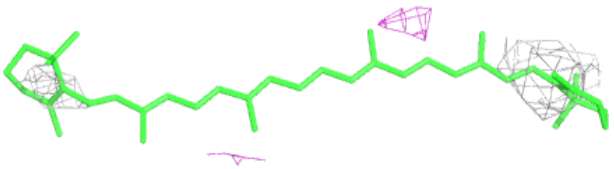


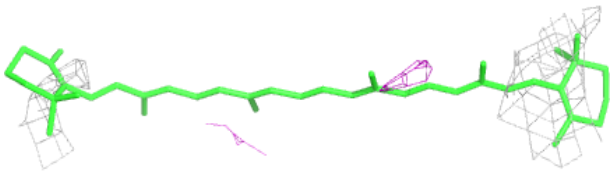


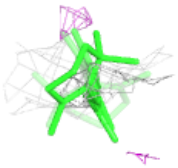


Electron density around BCR z 101:

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

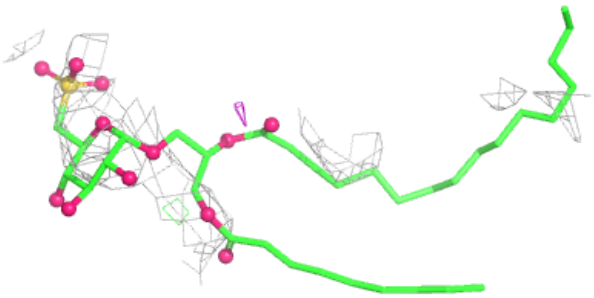


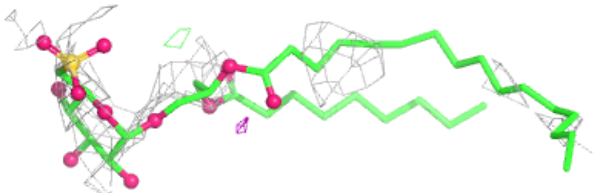




Electron density around SQD b 601:

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

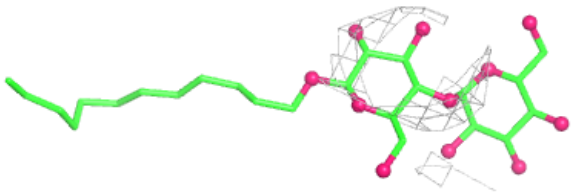


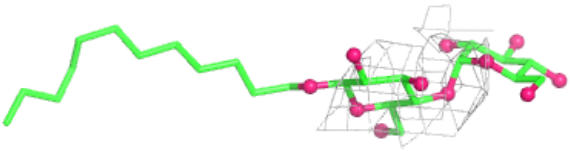


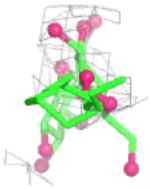


Electron density around LMT B 628:

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

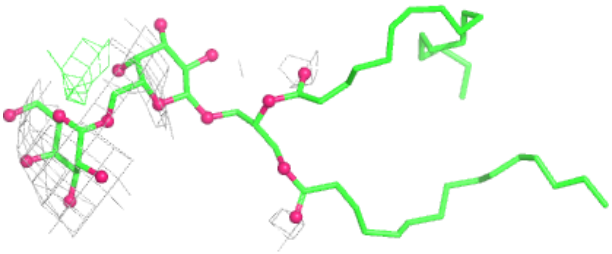


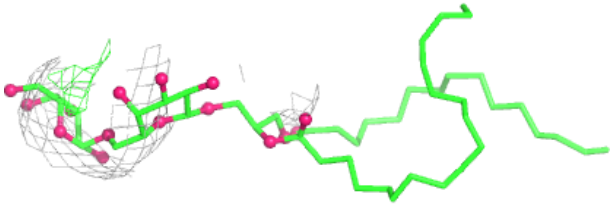




Electron density around DGD D 409:

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

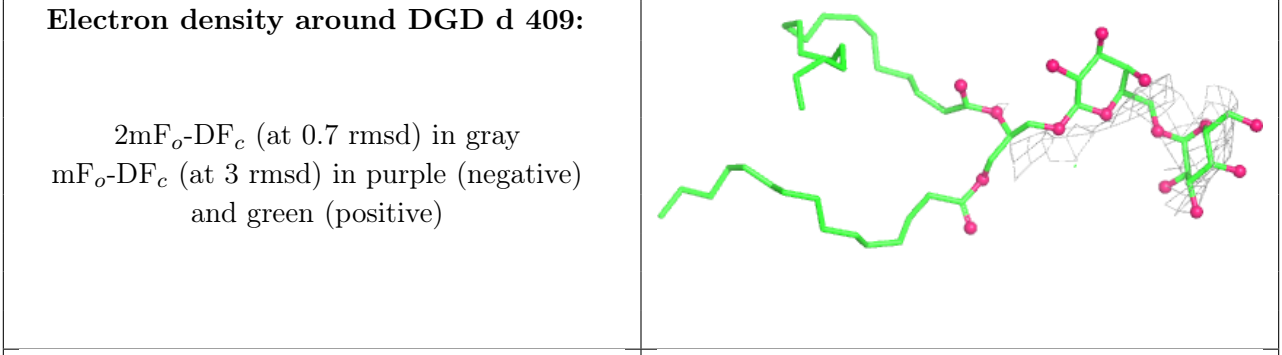


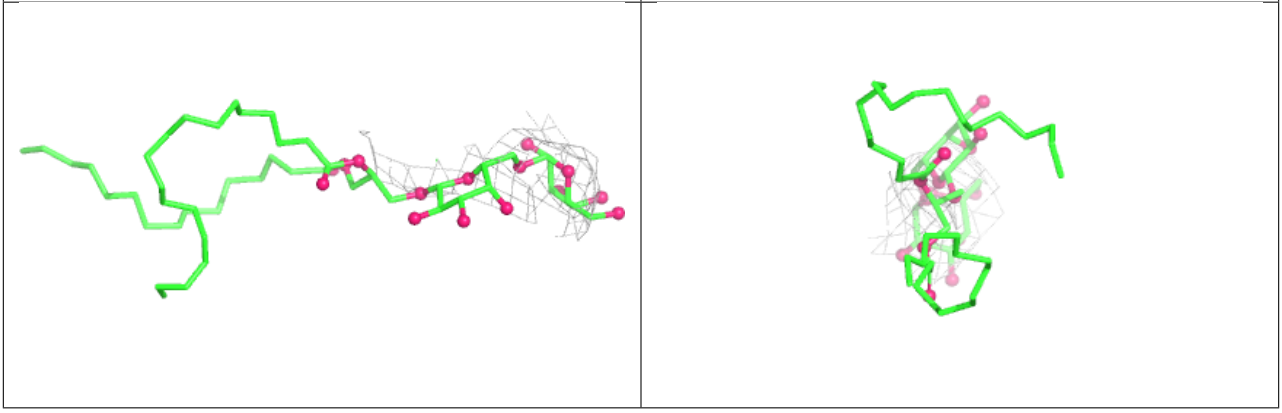




Electron density around DGD d 409:

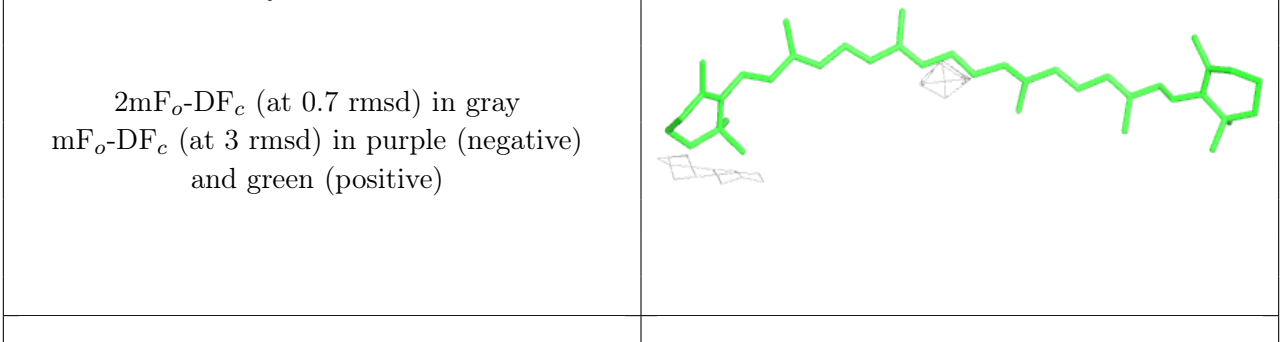
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

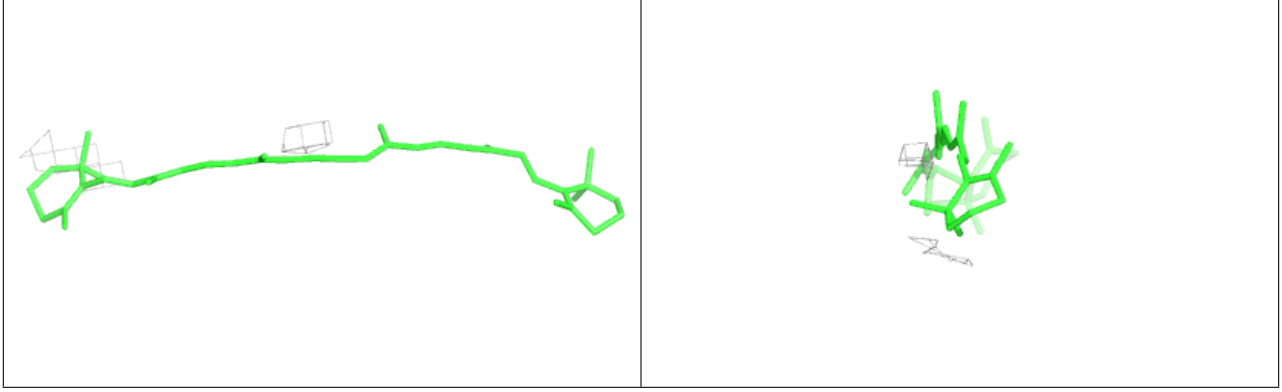




Electron density around BCR B 618:

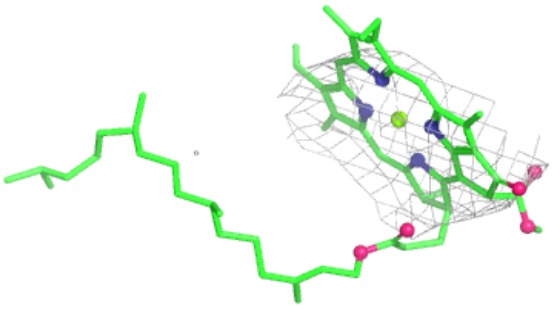
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

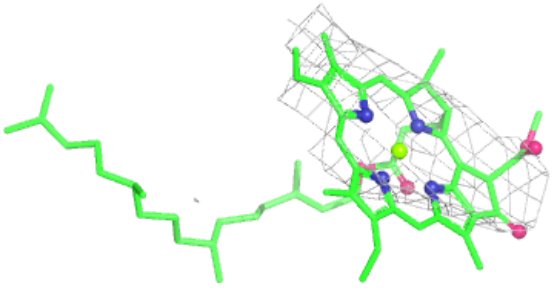


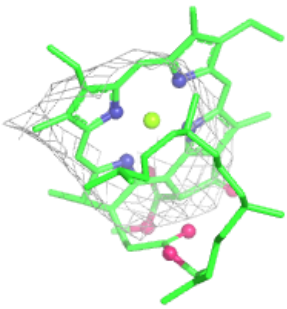


Electron density around CLA C 513:

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

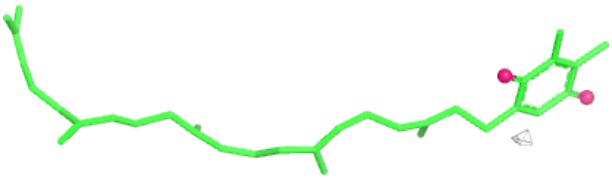


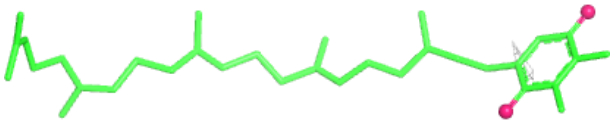


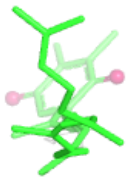


Electron density around PL9 j 101:

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



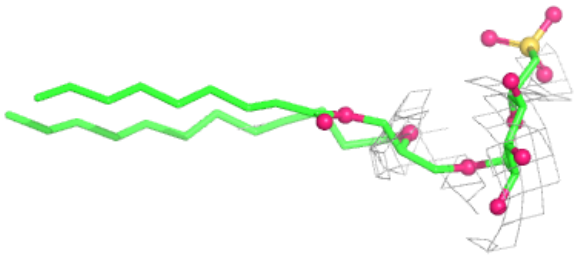


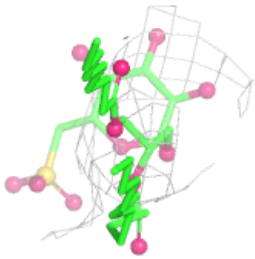


Electron density around SQD d 408:

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

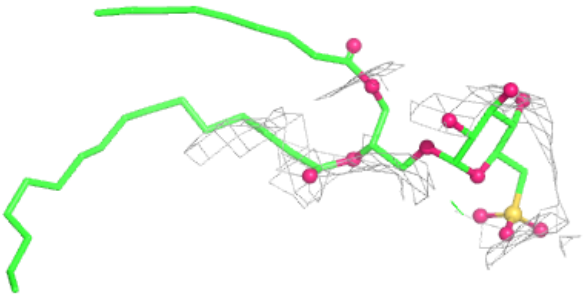


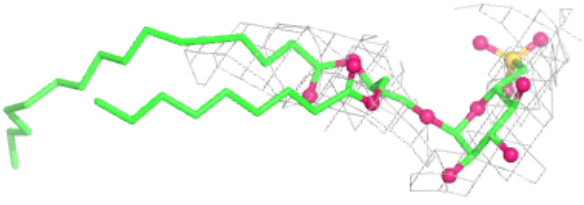


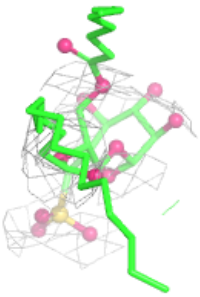


Electron density around SQD B 626:

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

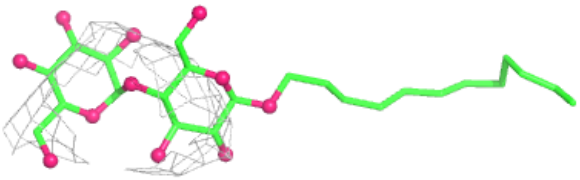


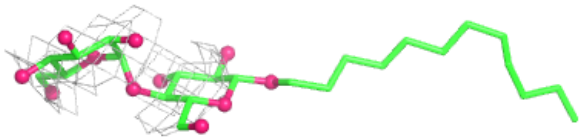


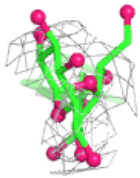


Electron density around LMT b 603:

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

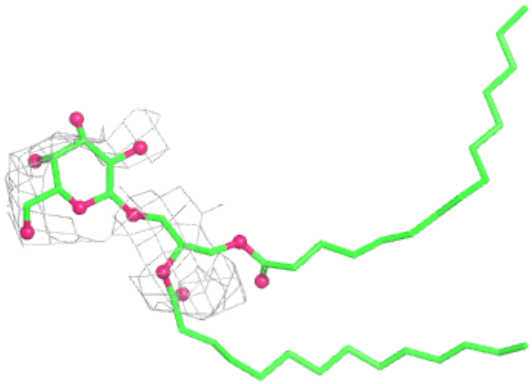


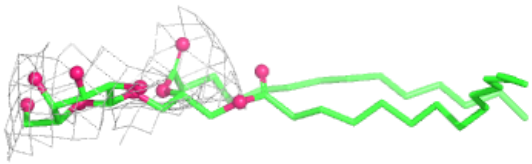


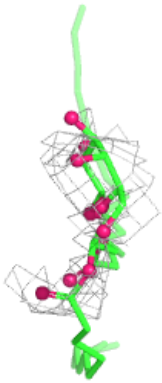


Electron density around LMG k 103:

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

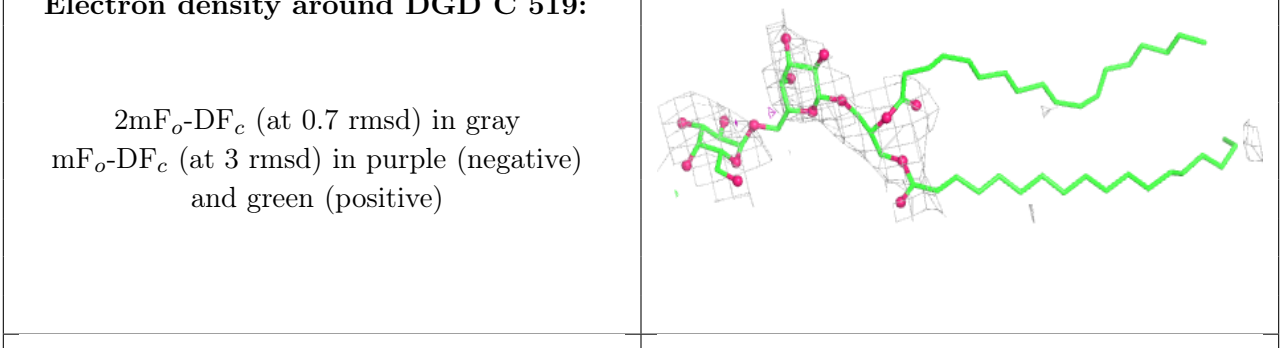






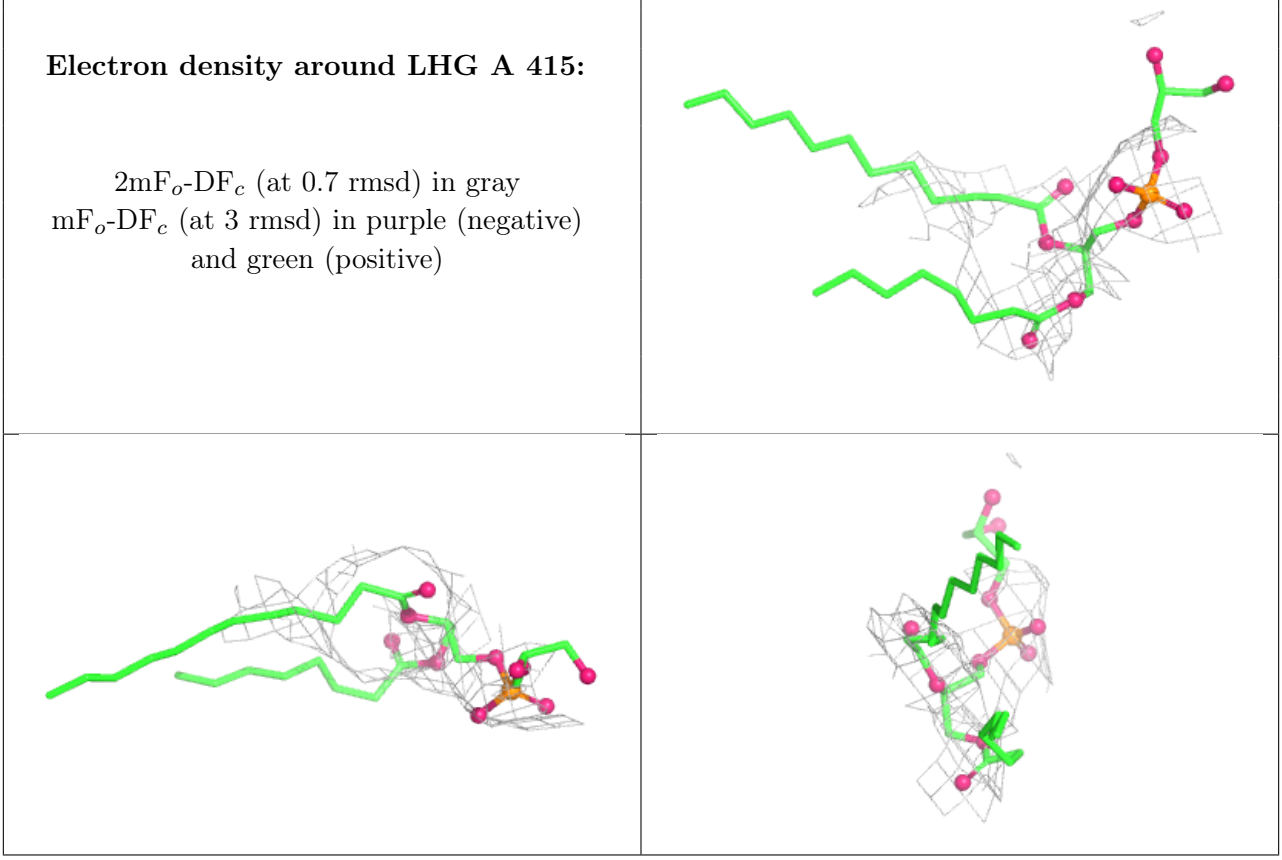
Electron density around DGD C 519:

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



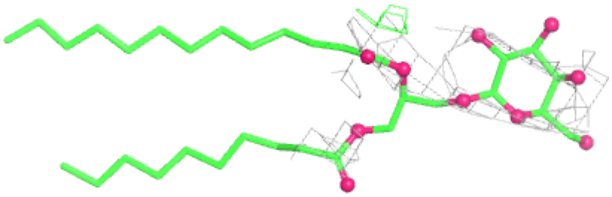
Electron density around LHG A 415:

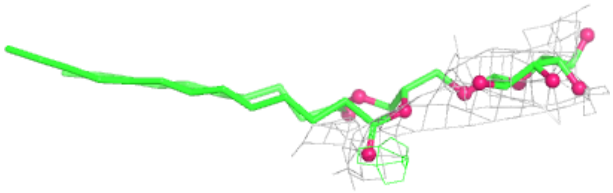
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

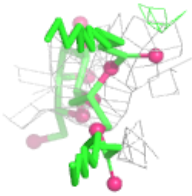


Electron density around LMG M 101:

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

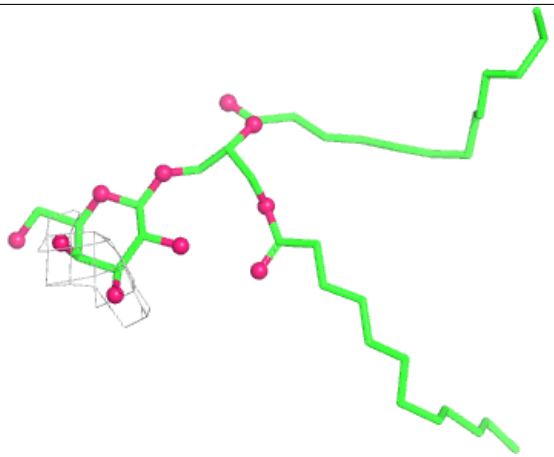


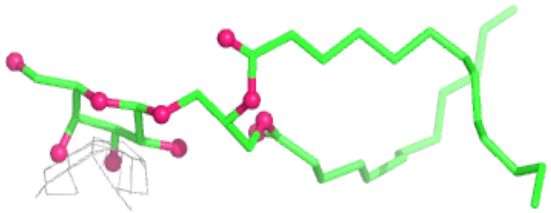


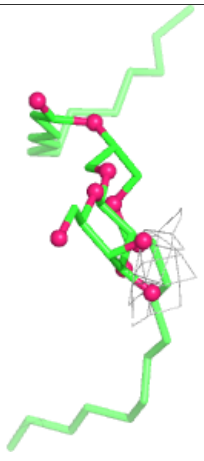


Electron density around LMG E 101:

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

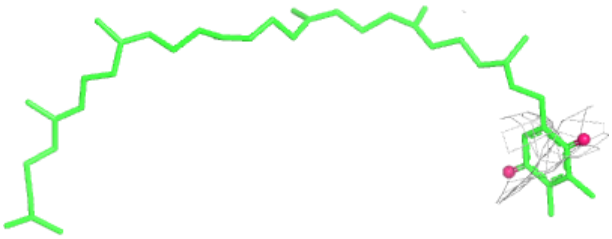


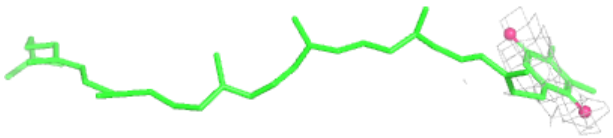




Electron density around PL9 A 408:

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

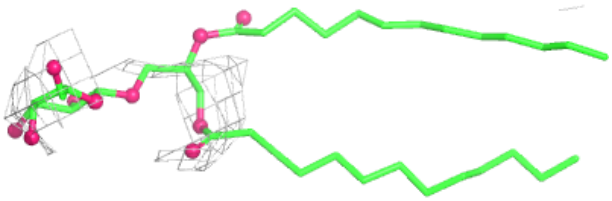


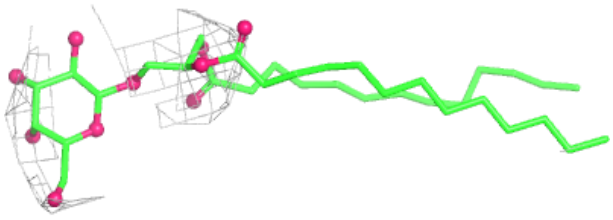


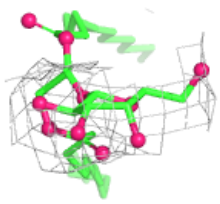


Electron density around LMG c 519:

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

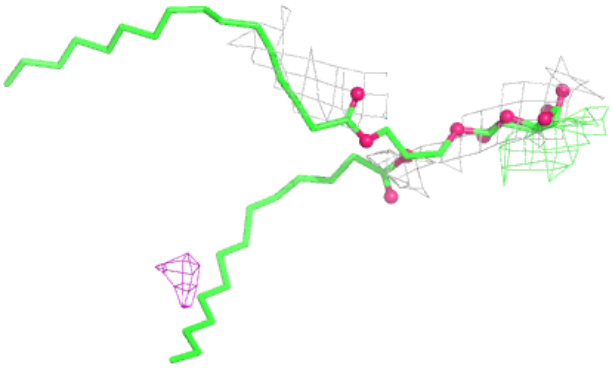


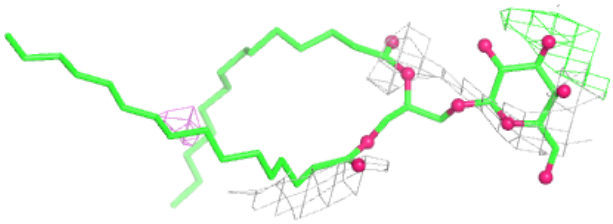


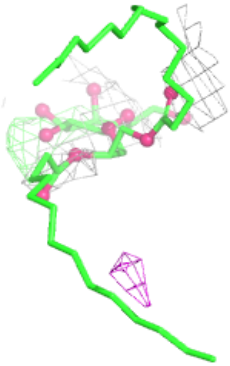


Electron density around LMG b 625:

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

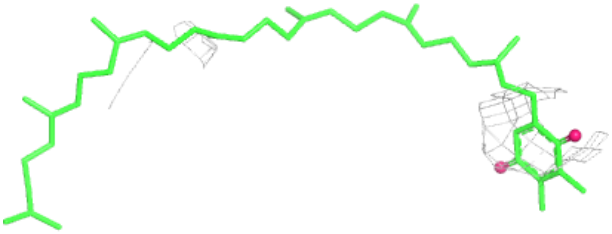


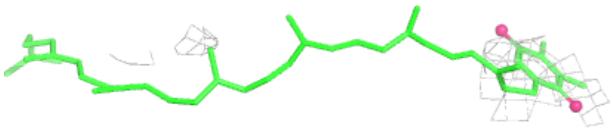




Electron density around PL9 a 410:

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

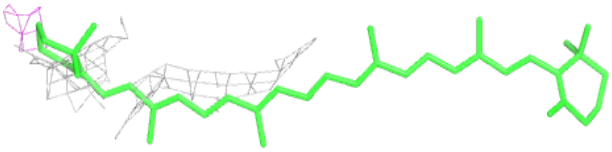


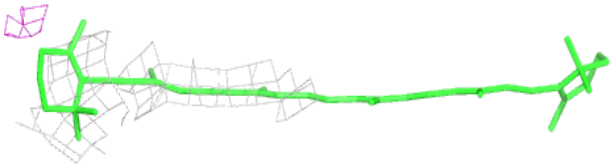


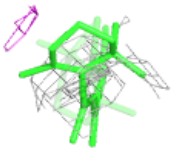


Electron density around BCR H 101:

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

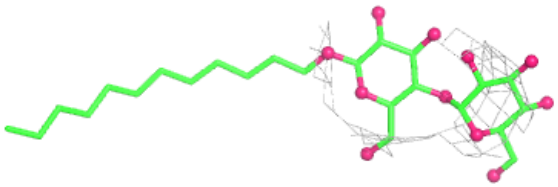


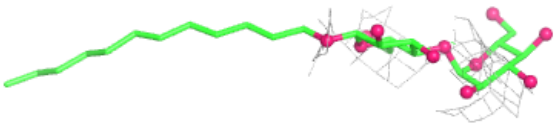


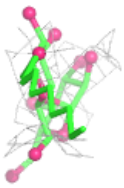


Electron density around LMT B 625:

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

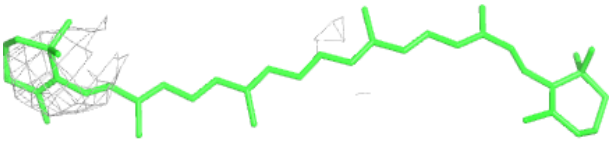




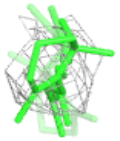


Electron density around BCR k 102:

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

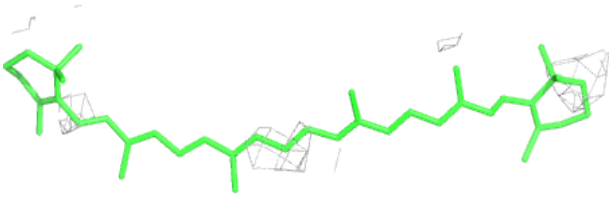


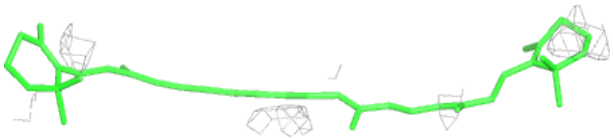


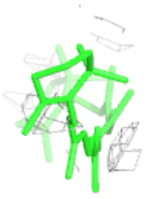


Electron density around BCR T 102:

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

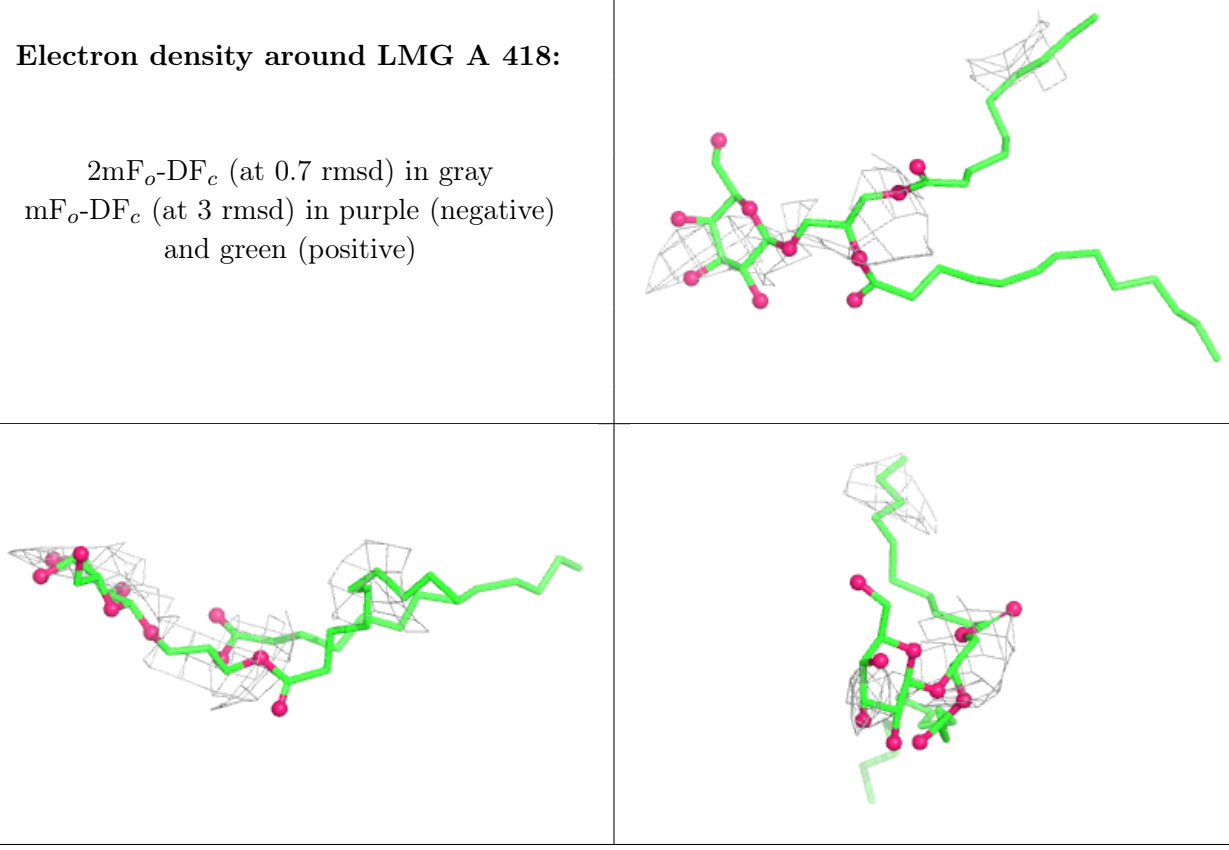






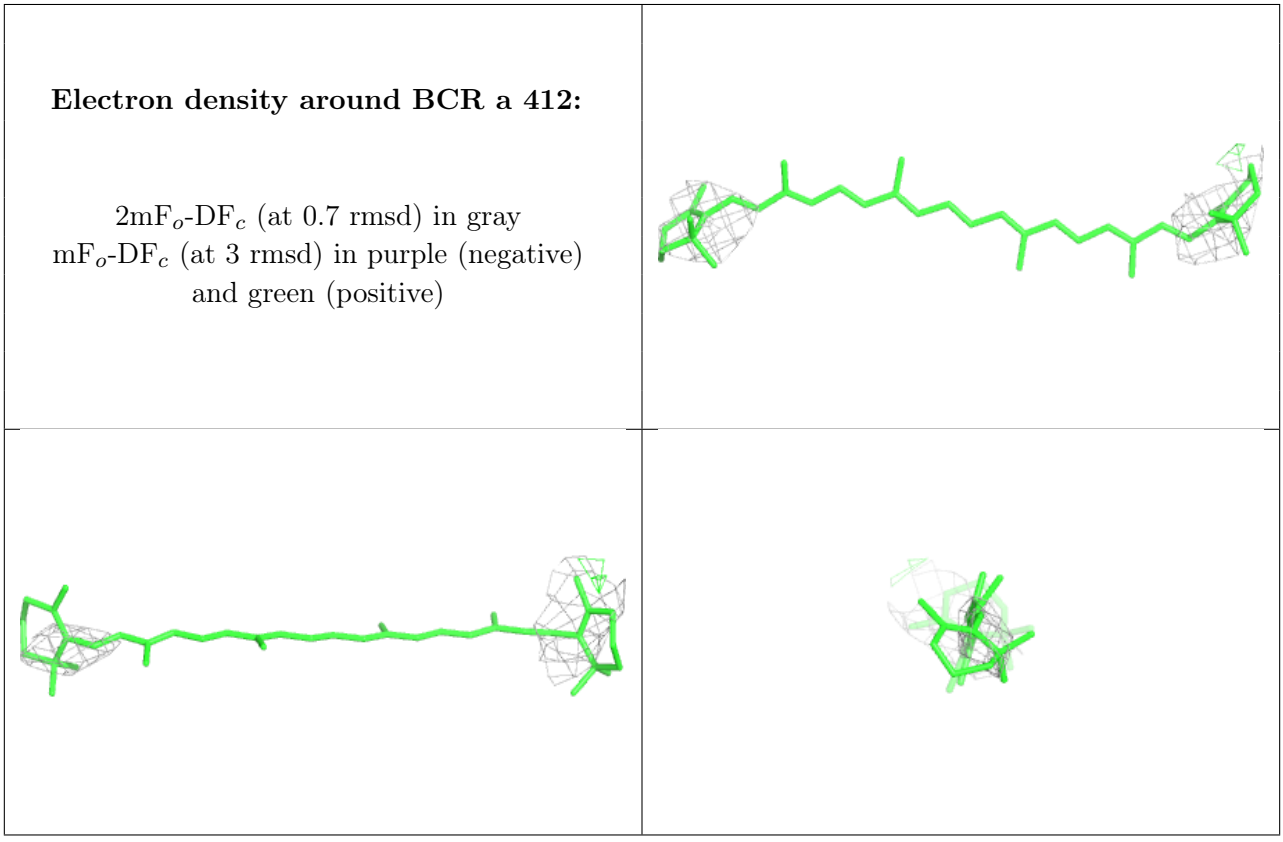
Electron density around LMG A 418:

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



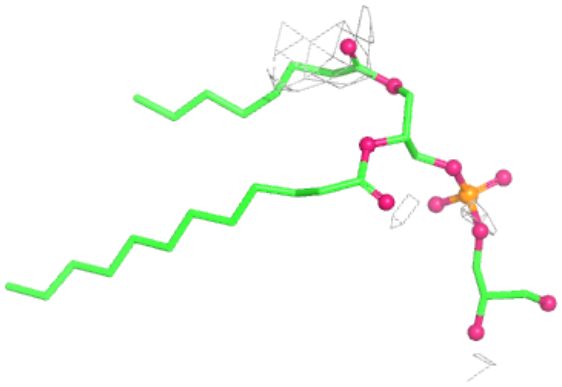
Electron density around BCR a 412:

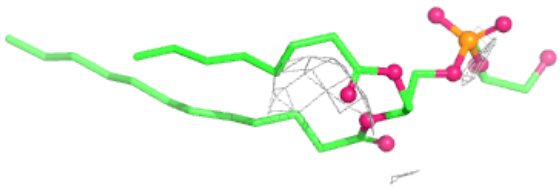
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

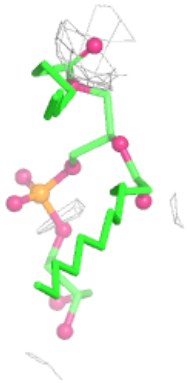


Electron density around LHG a 417:

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

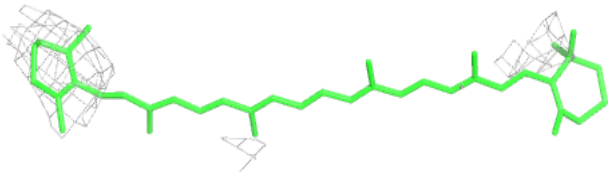


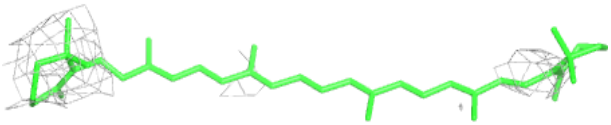


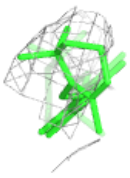


Electron density around BCR B 620:

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

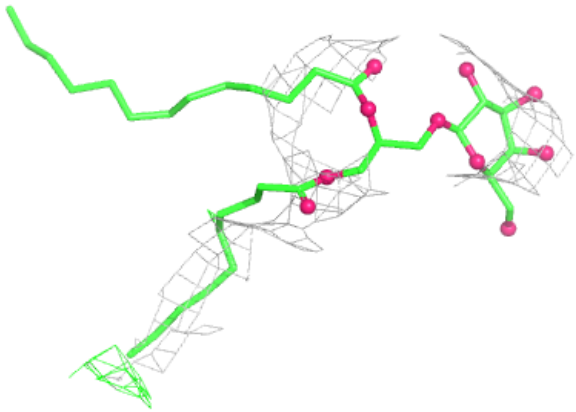


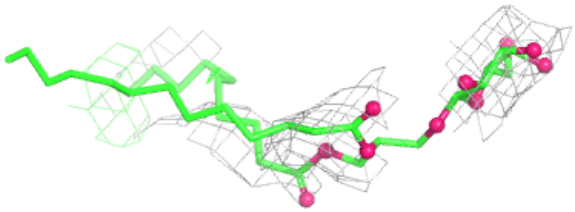


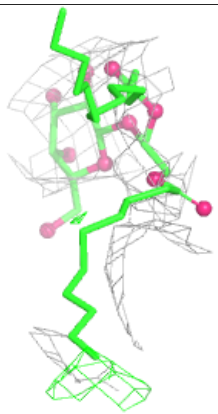


Electron density around LMG a 402:

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

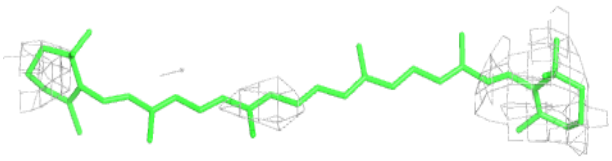


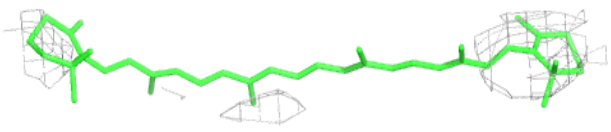


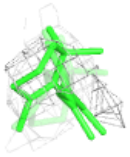


Electron density around BCR C 516:

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

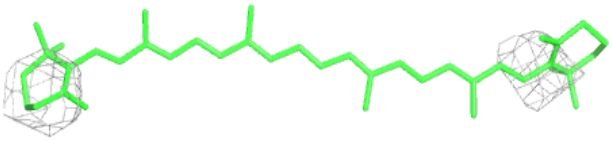




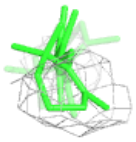


Electron density around BCR b 621:

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

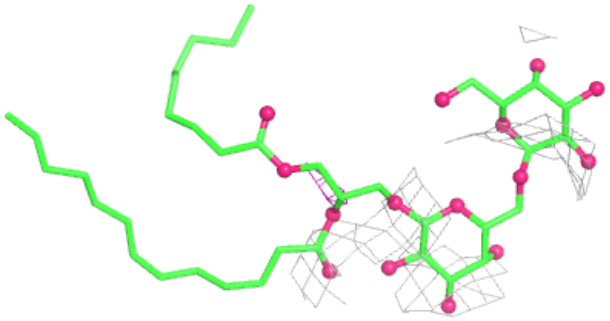


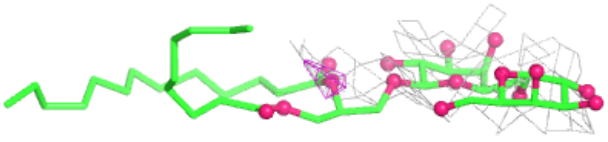




Electron density around DGD b 602:

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

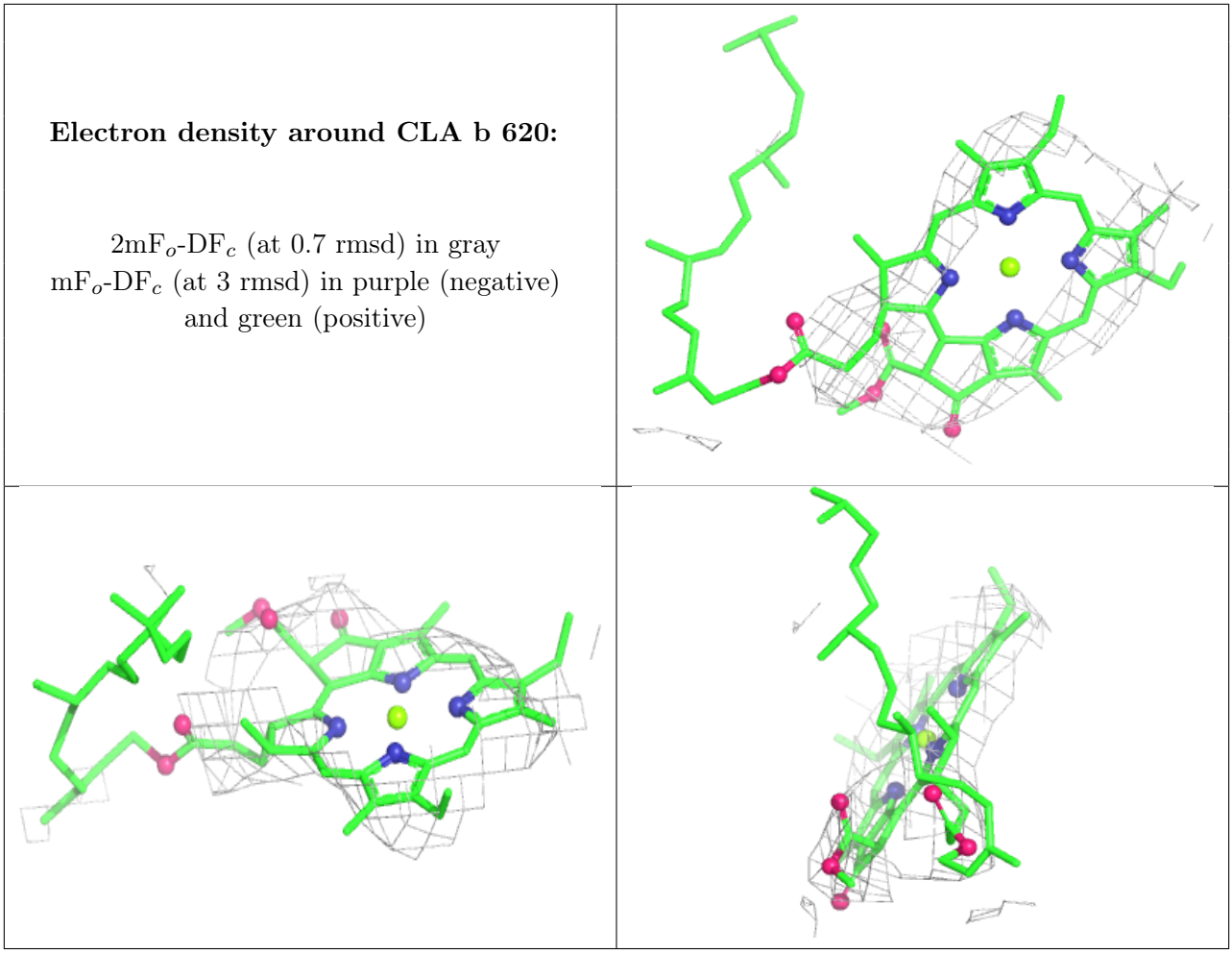






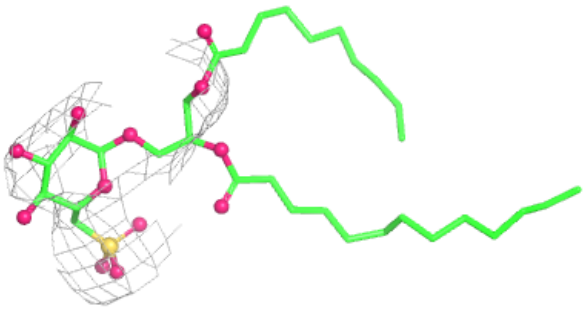
Electron density around CLA b 620:

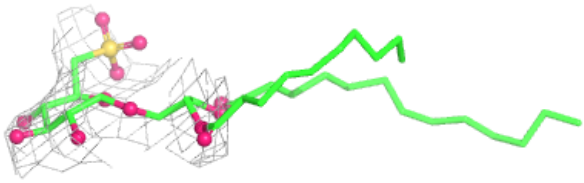
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

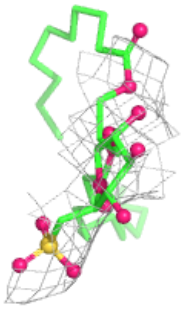


Electron density around SQD F 102:

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

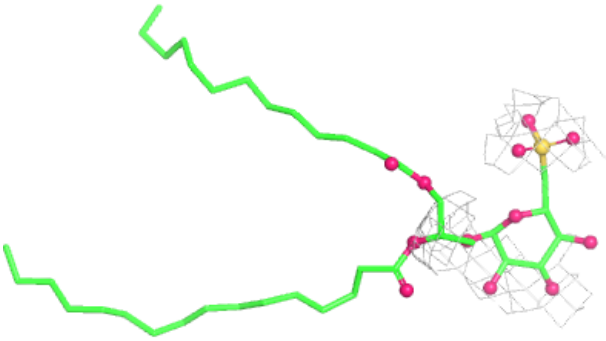


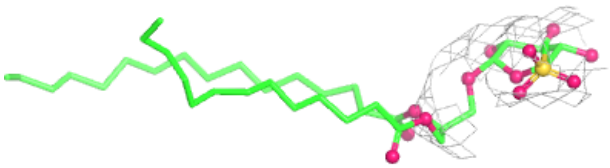


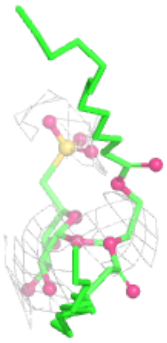


Electron density around SQD a 415:

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

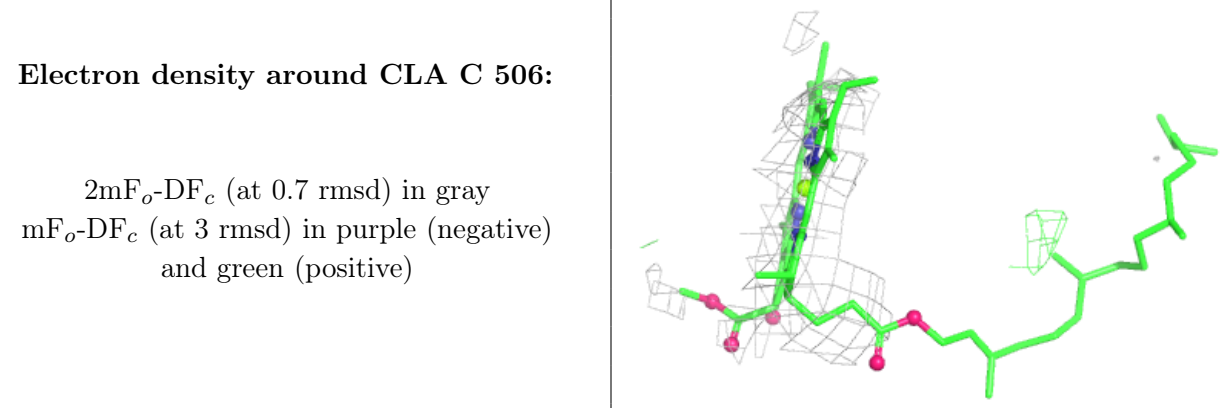






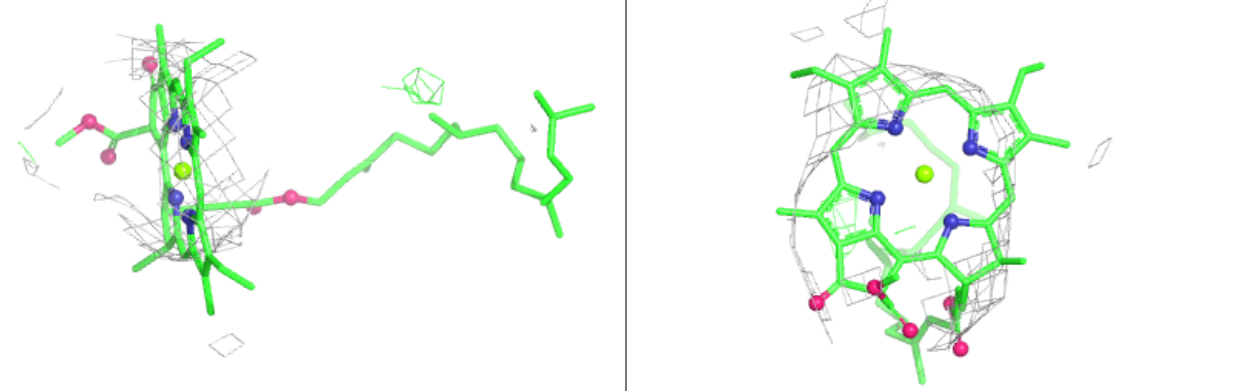
Electron density around CLA C 506:

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



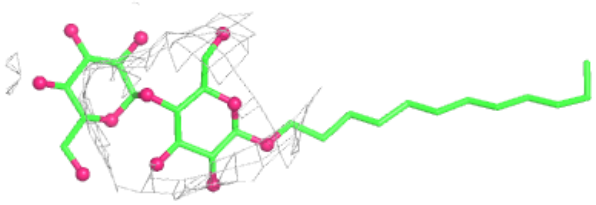
Electron density around LMG i 101:

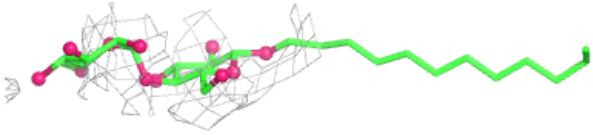
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT b 604:

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

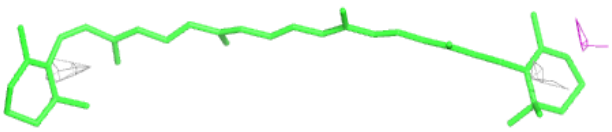


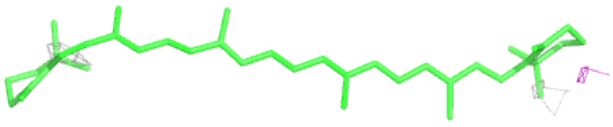


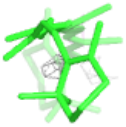


Electron density around BCR c 514:

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

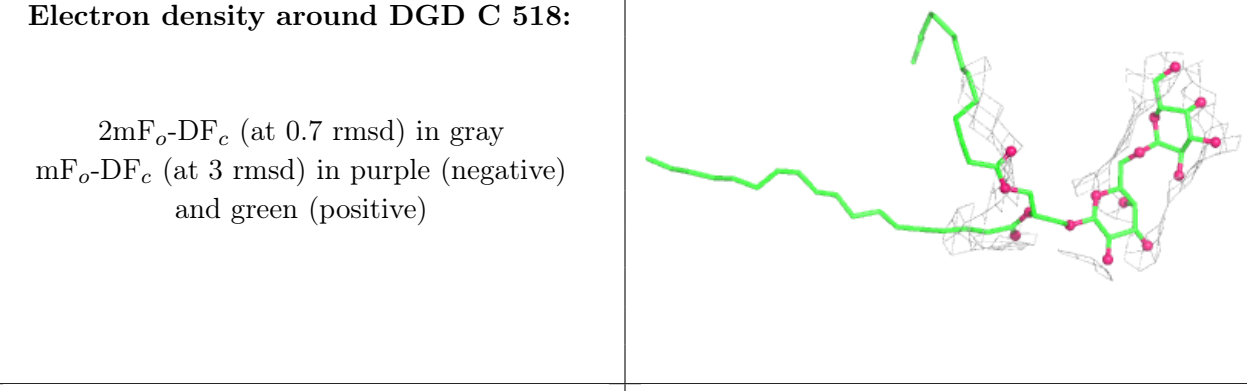






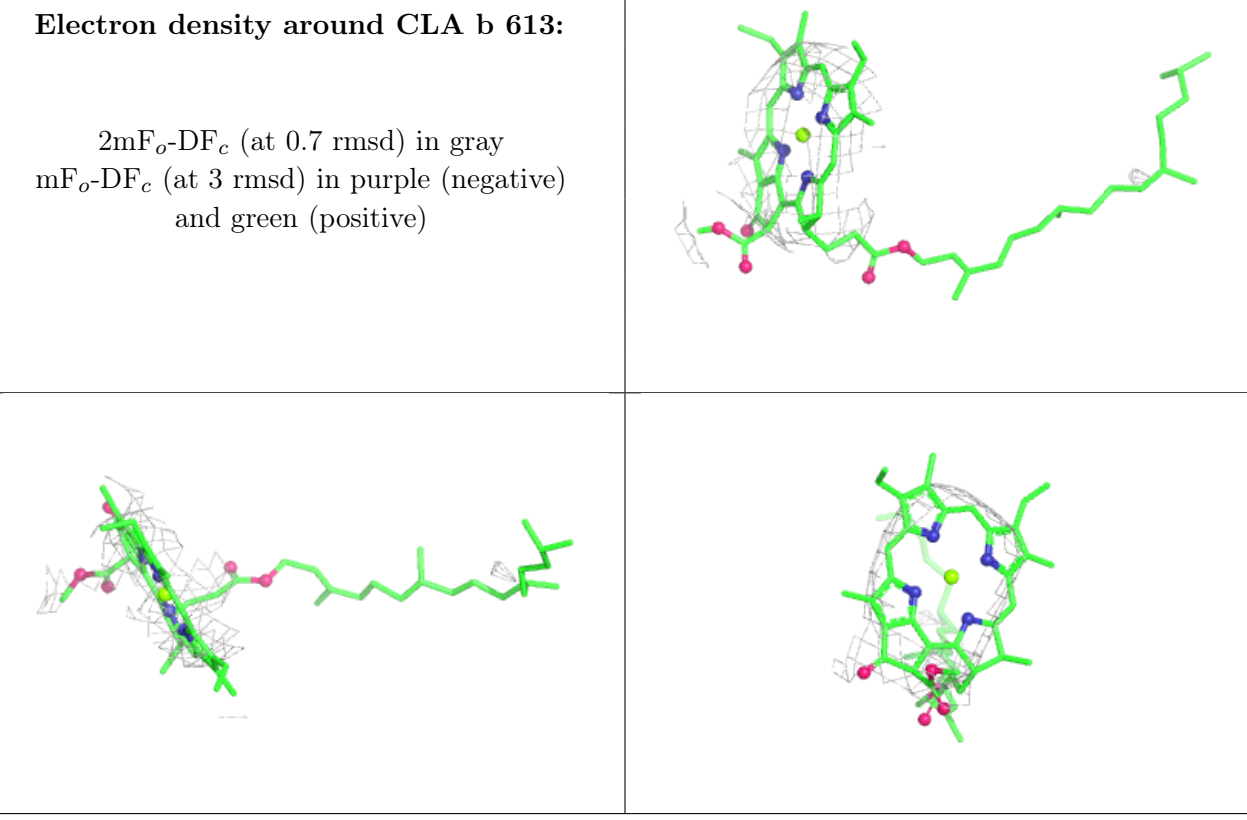
Electron density around DGD C 518:

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



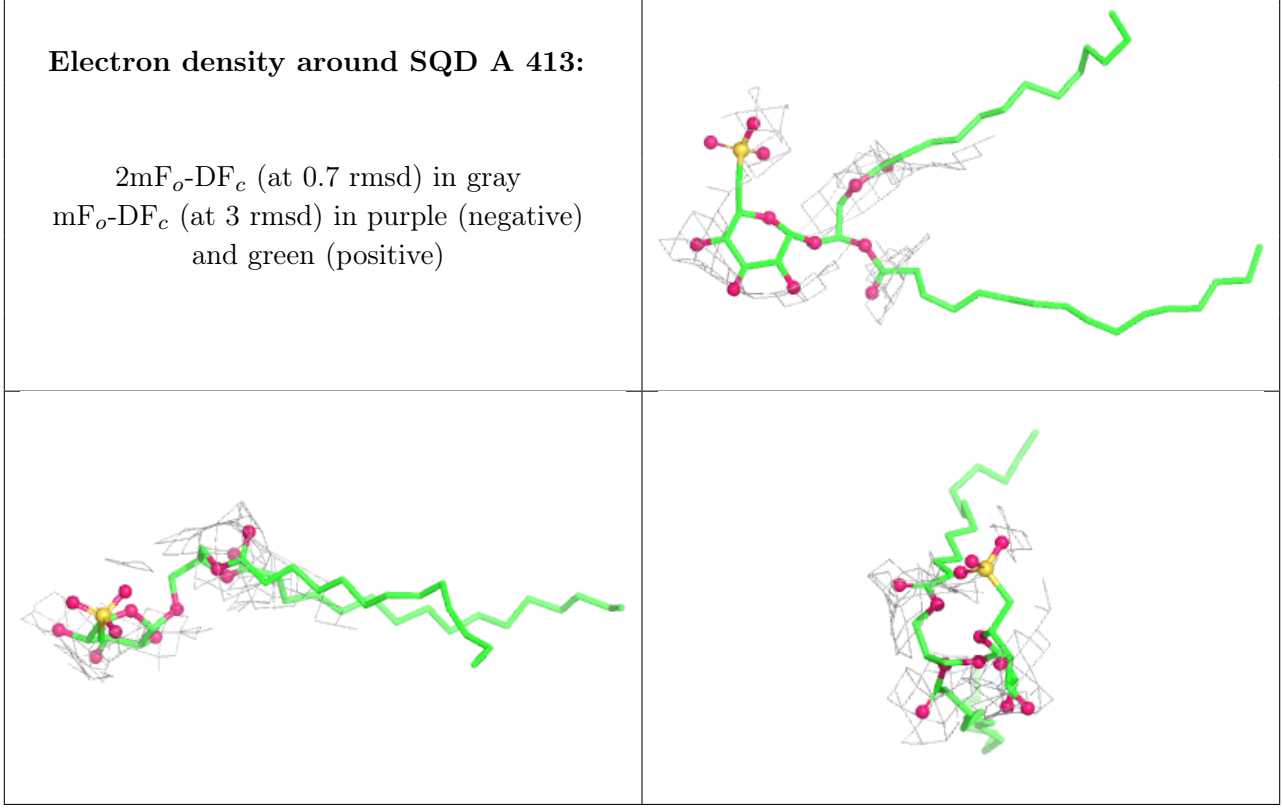
Electron density around CLA b 613:

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



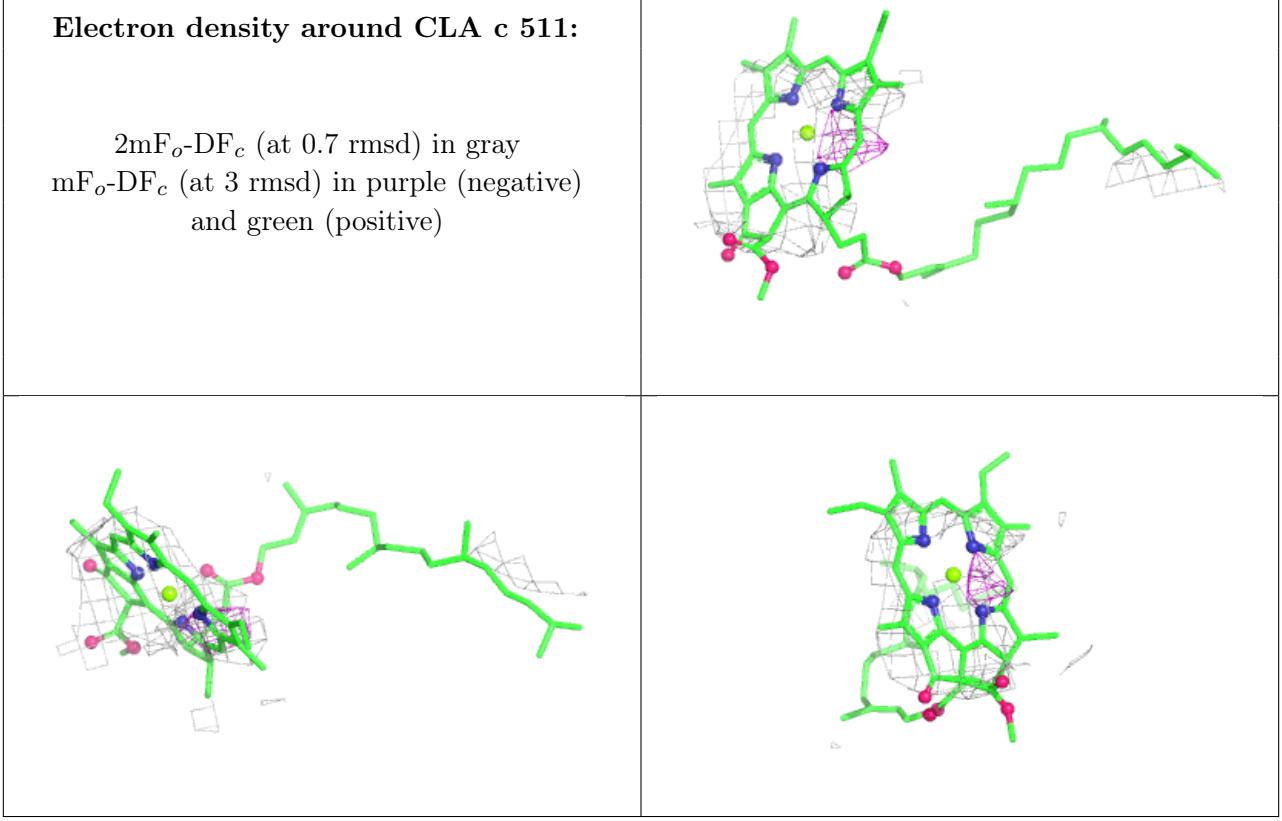
Electron density around SQD A 413:

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



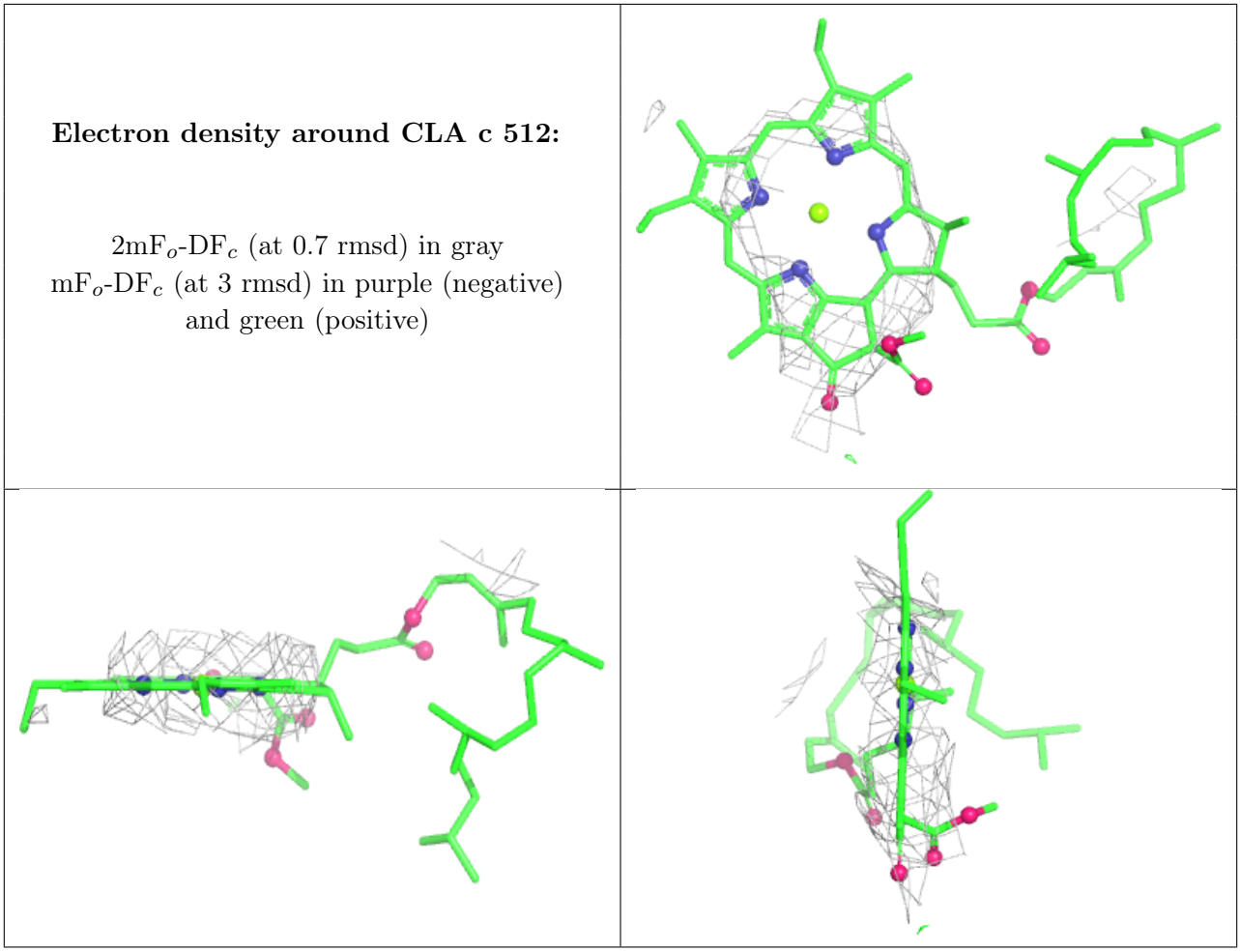
Electron density around CLA c 511:

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



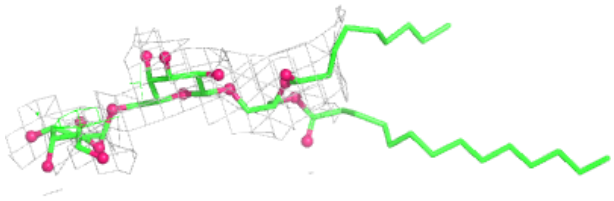
Electron density around CLA c 512:

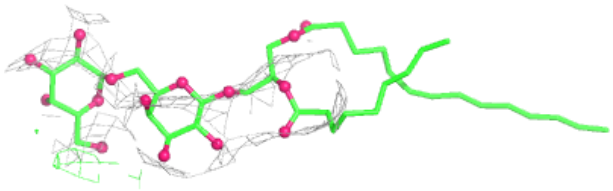
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

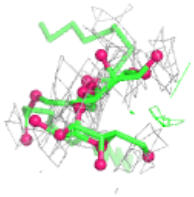


Electron density around DGD C 517:

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



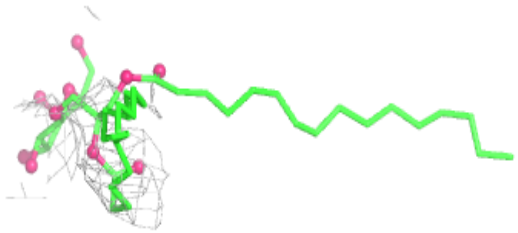




Electron density around LMG a 416:

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

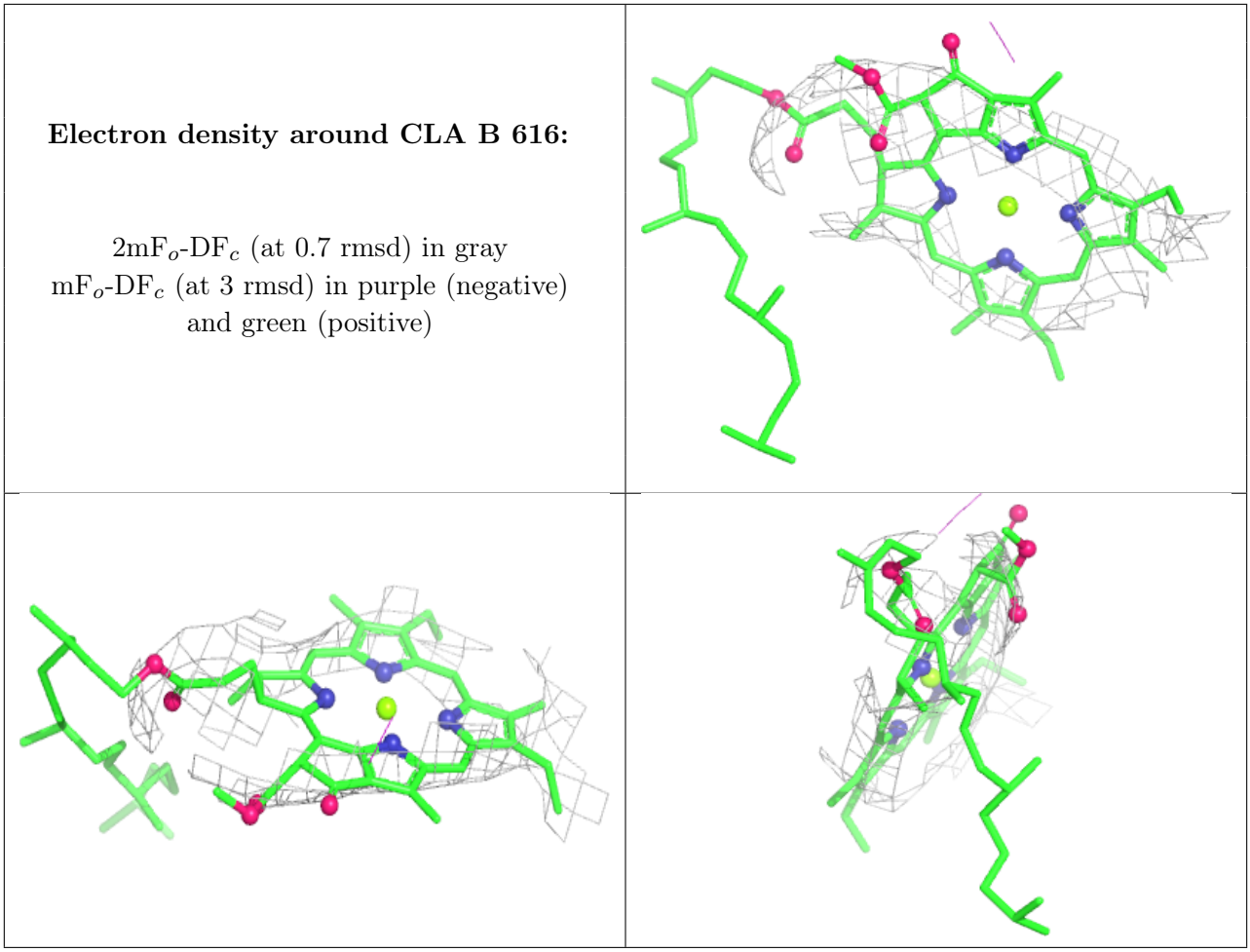






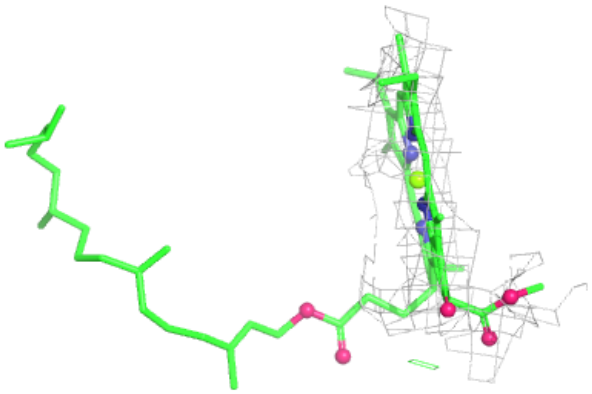
Electron density around CLA B 616:

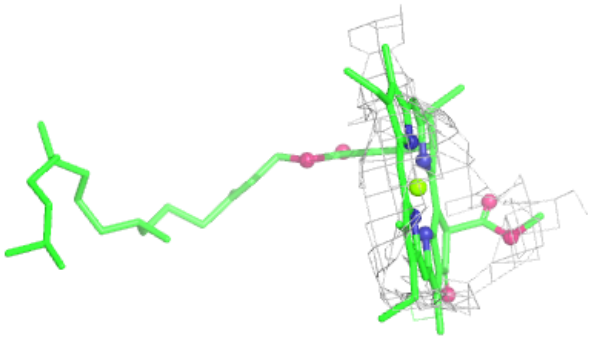
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

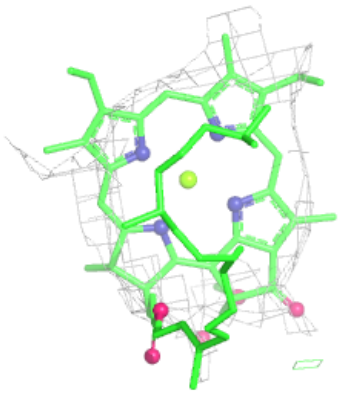


Electron density around CLA c 506:

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

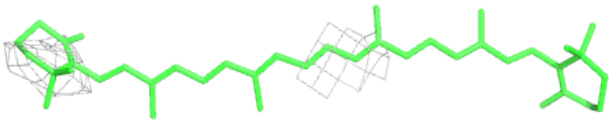


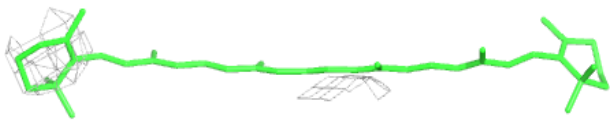


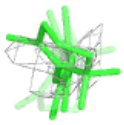


Electron density around BCR B 619:

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

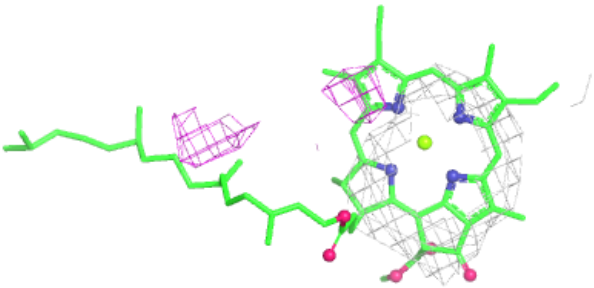


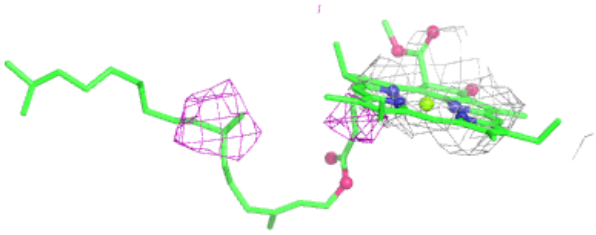


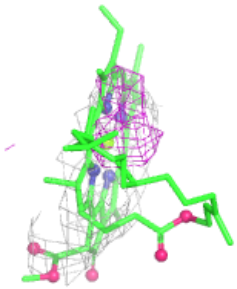


Electron density around CLA a 406:

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

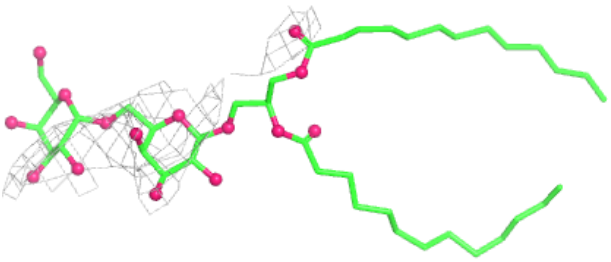


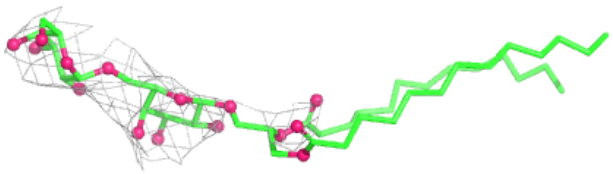


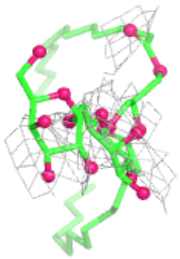


Electron density around DGD A 411:

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

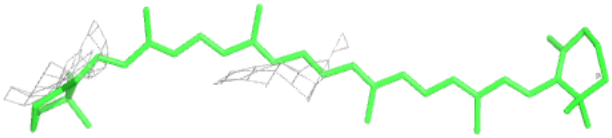


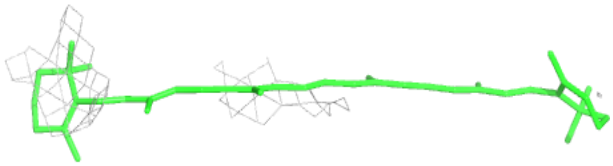


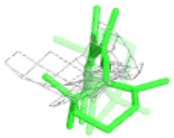


Electron density around BCR h 101:

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

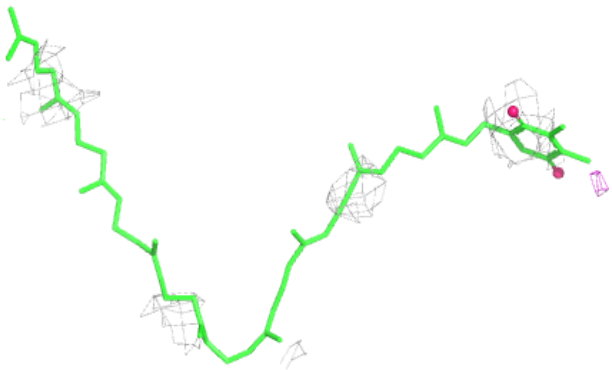


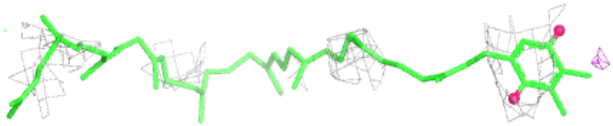




Electron density around PL9 d 404:

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

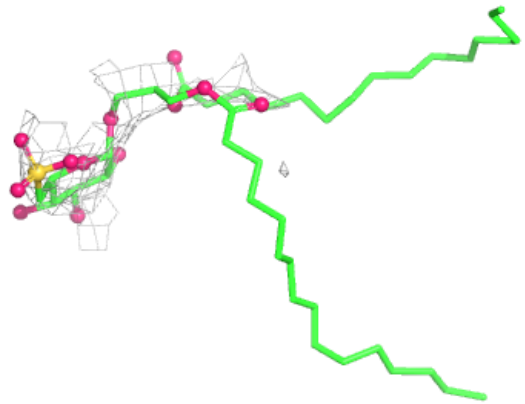




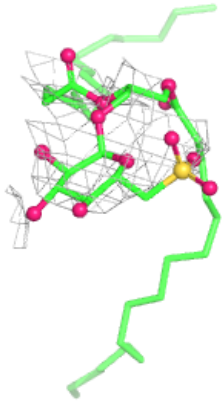


Electron density around SQD a 401:

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

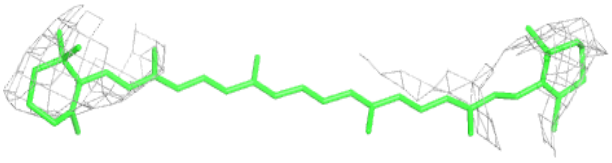


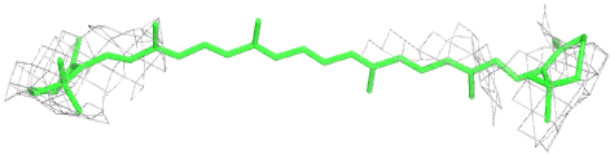


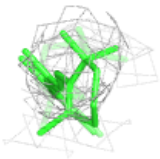


Electron density around BCR b 622:

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

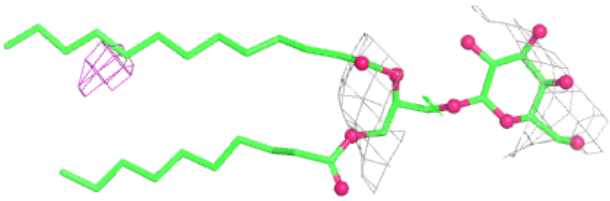


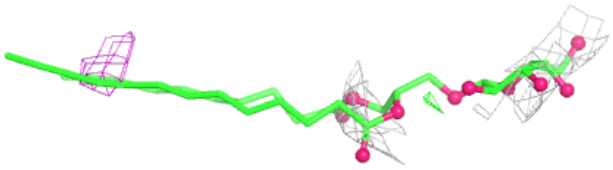


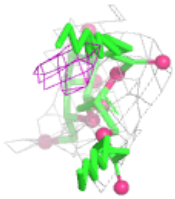


Electron density around LMG m 102:

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



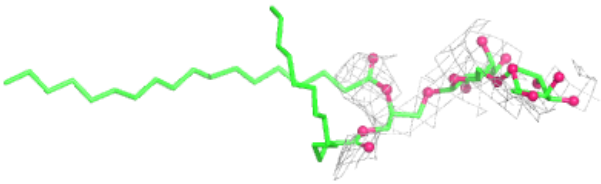




Electron density around DGD c 517:

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

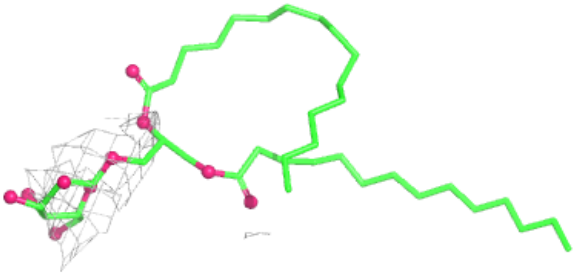




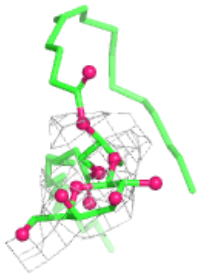


Electron density around LMG B 622:

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

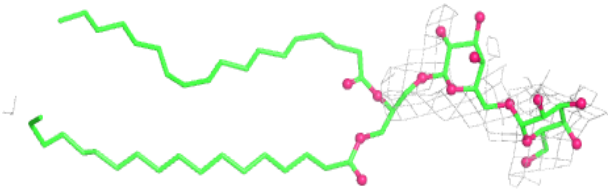


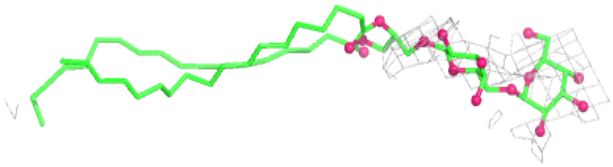




Electron density around DGD c 518:

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

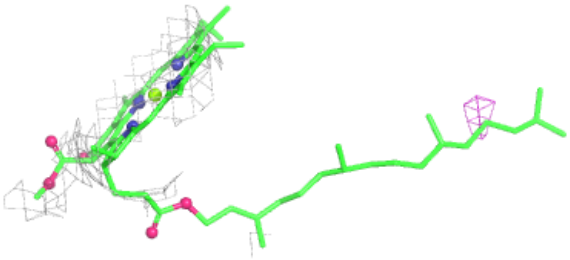


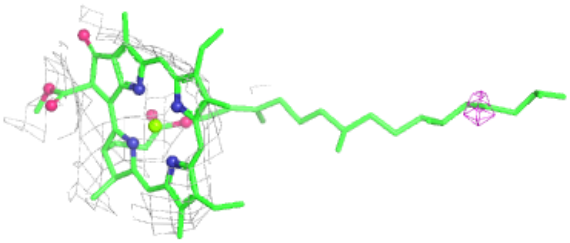


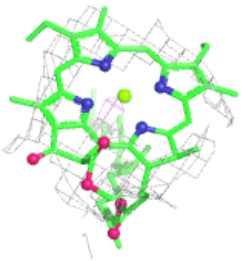


Electron density around CLA C 504:

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

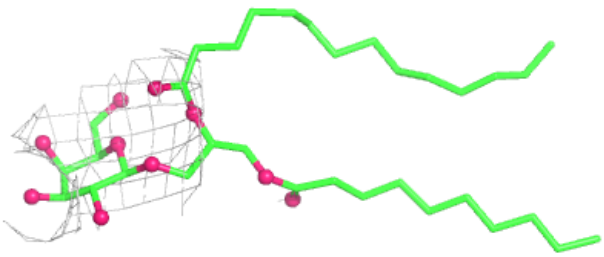


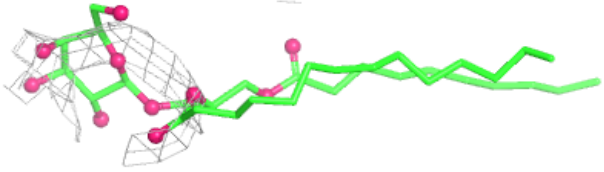




Electron density around LMG I 101:

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

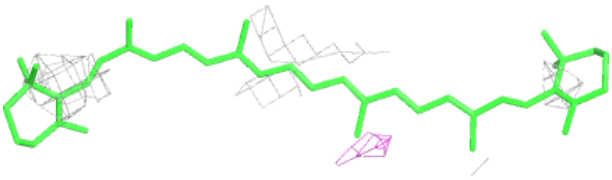


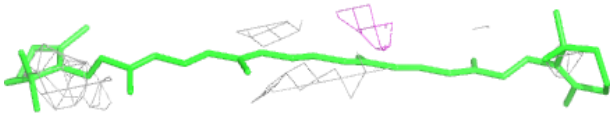


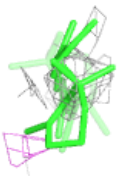


Electron density around BCR y 101:

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

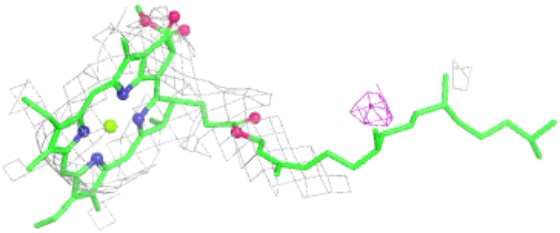


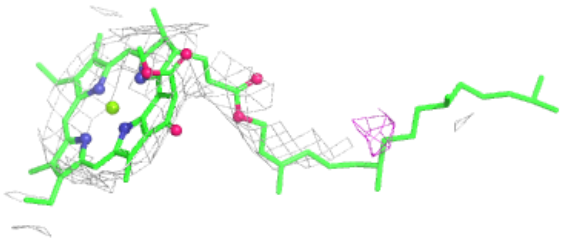


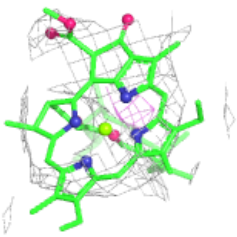


Electron density around CLA c 502:

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

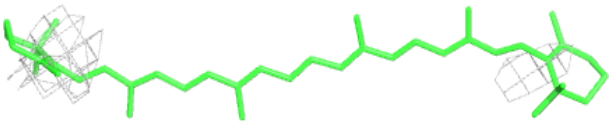


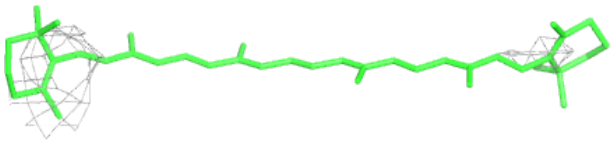


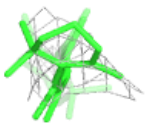


Electron density around BCR C 515:

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





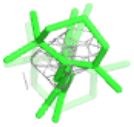


Electron density around BCR A 410:

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

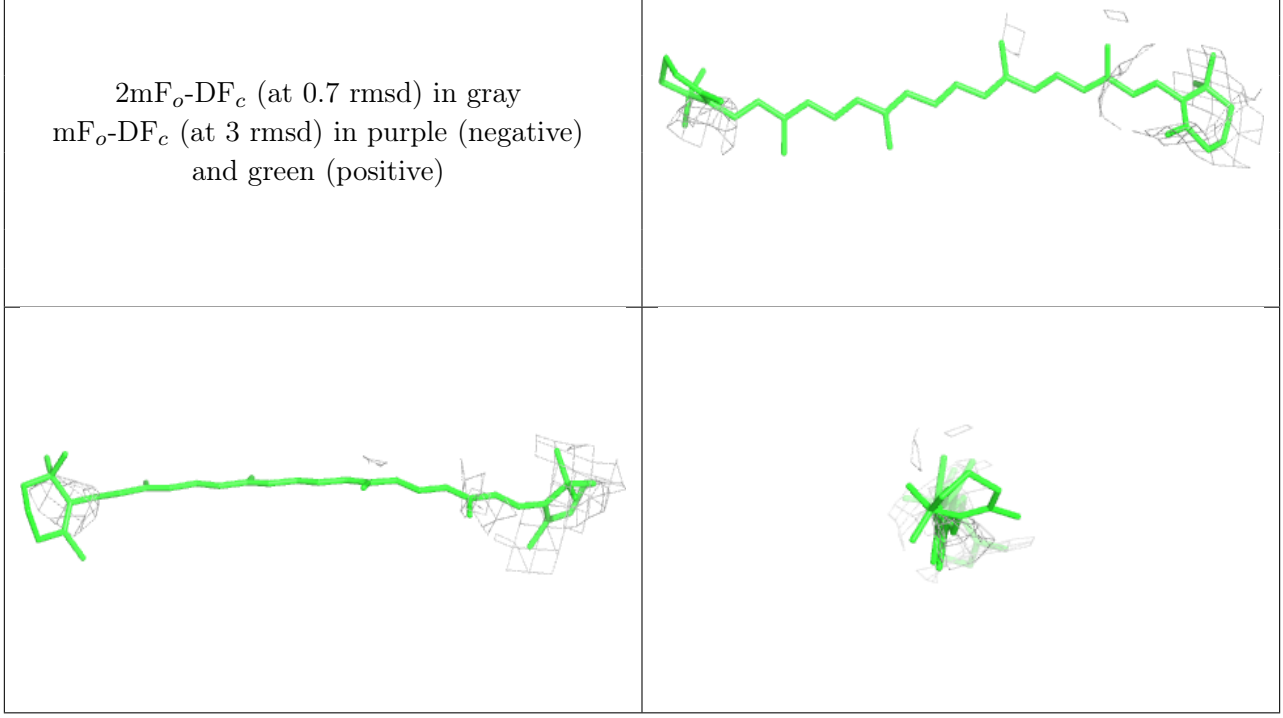






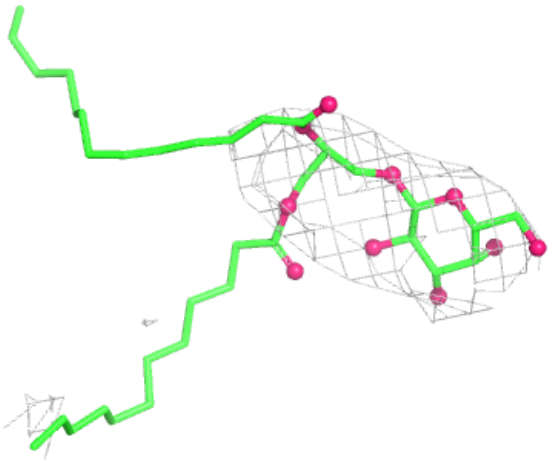
Electron density around BCR B 617:

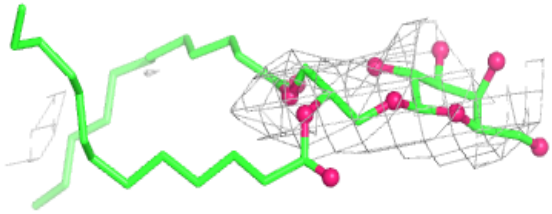
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 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)

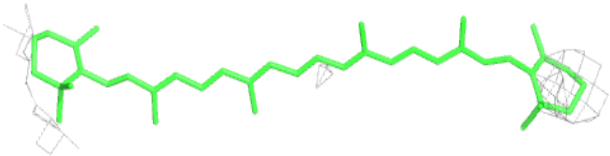


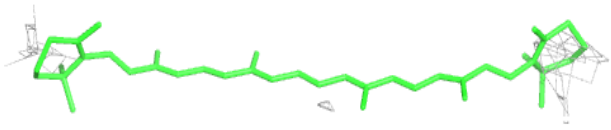




Electron density around BCR c 515:

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

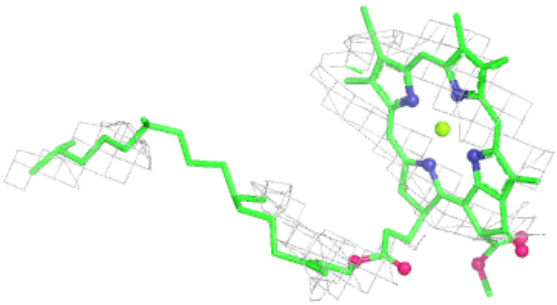


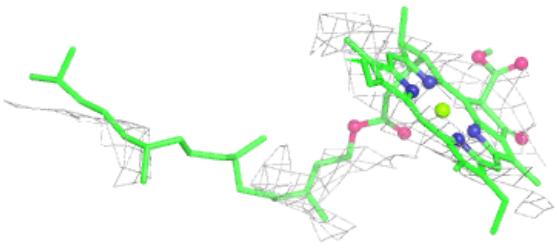


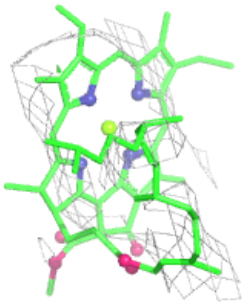


Electron density around CLA C 511:

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

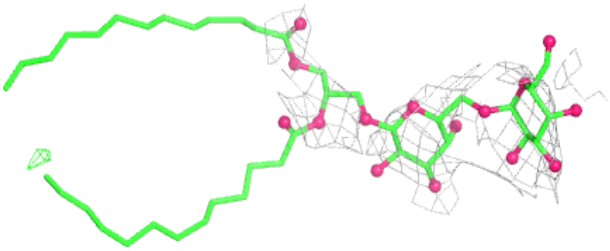


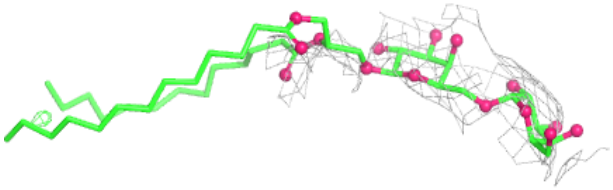




Electron density around DGD a 413:

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

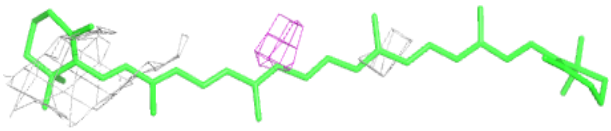


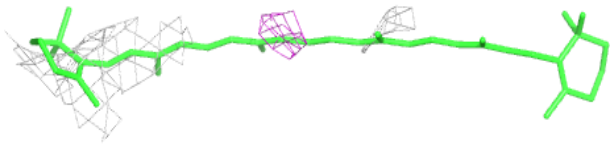


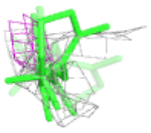


Electron density around BCR T 101:

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

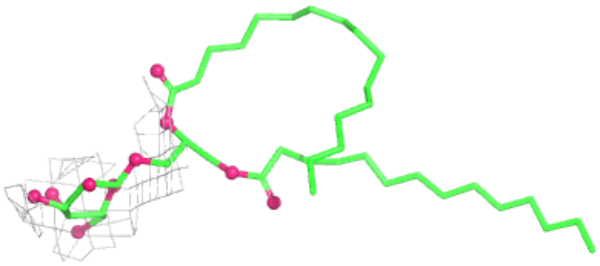






Electron density around LMG b 624:

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

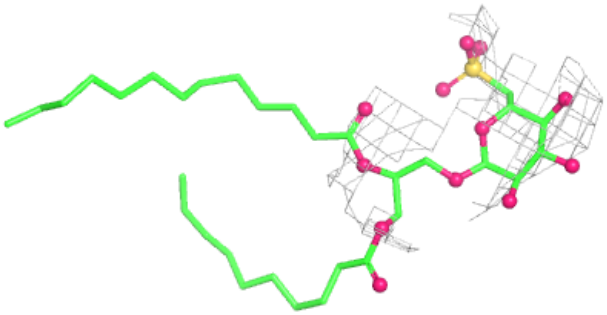


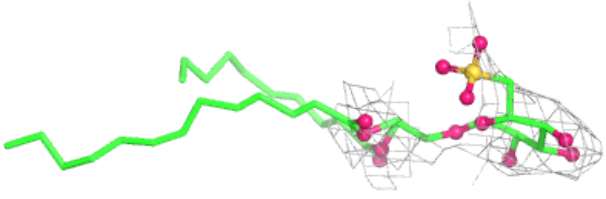




Electron density around SQD f 102:

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

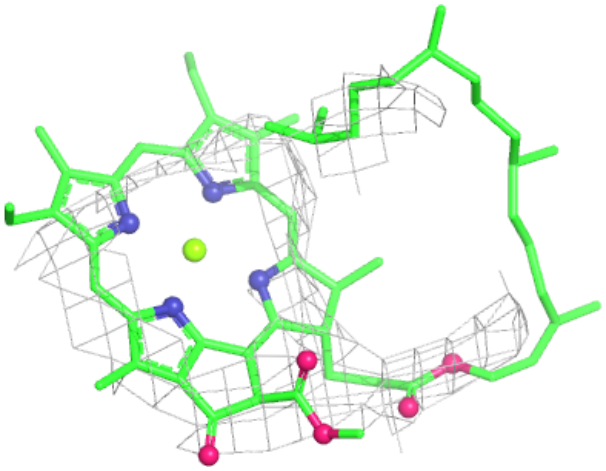


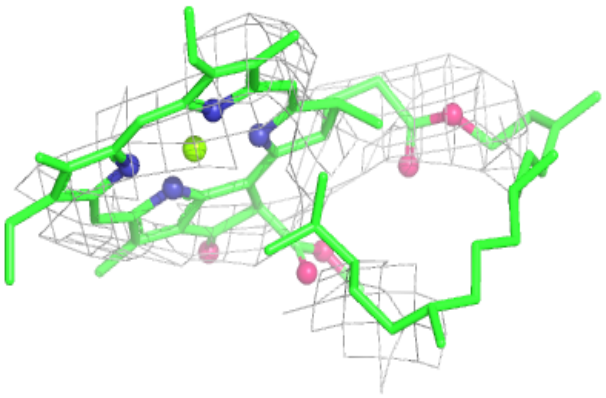


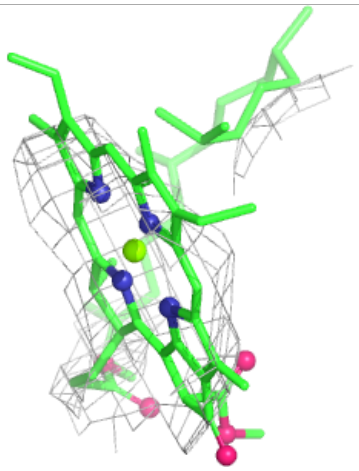


Electron density around CLA b 619:

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

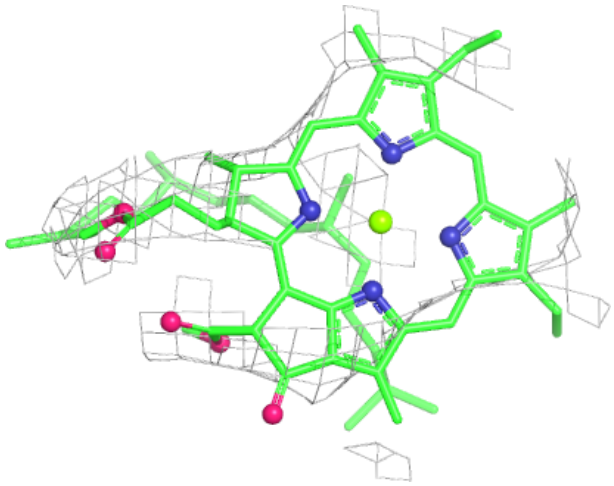


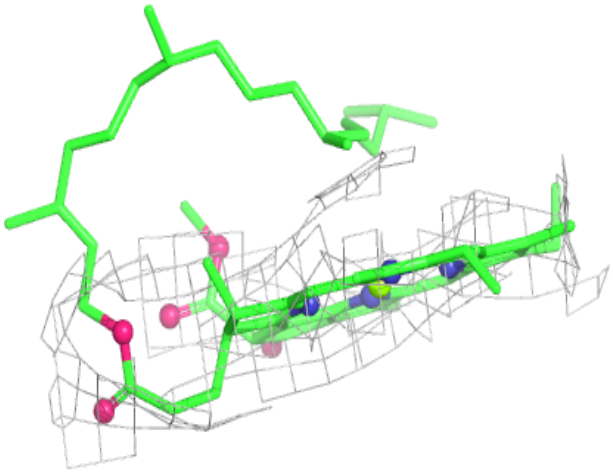


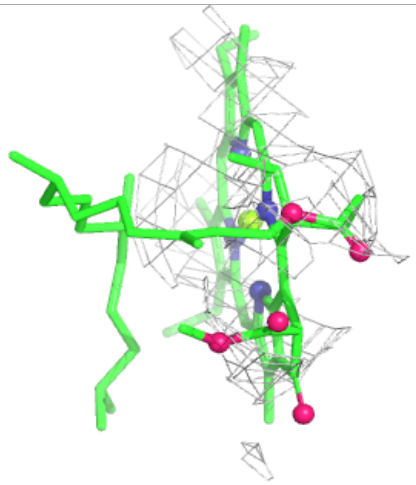


Electron density around CLA C 510:

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

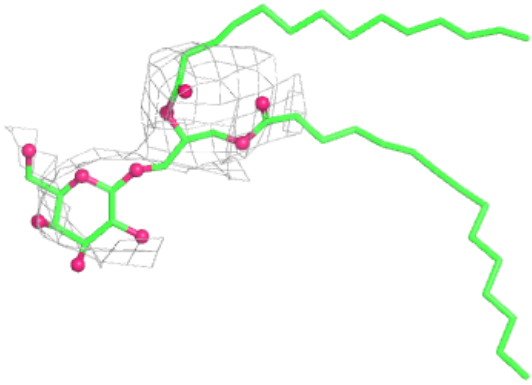


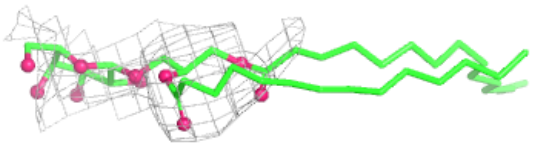


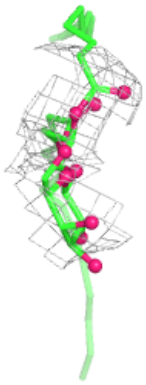


Electron density around LMG C 520:

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

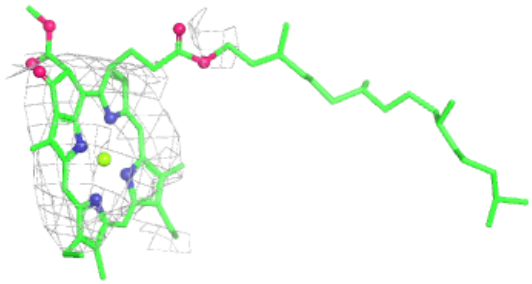


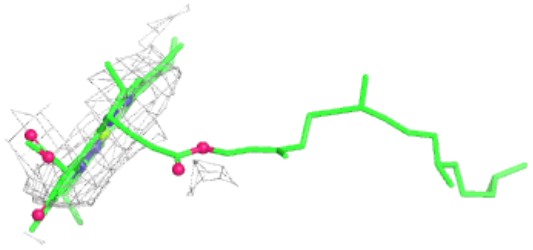


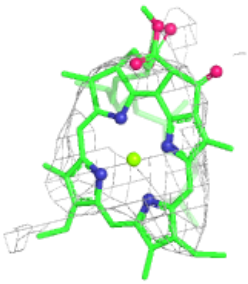


Electron density around CLA a 409:

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

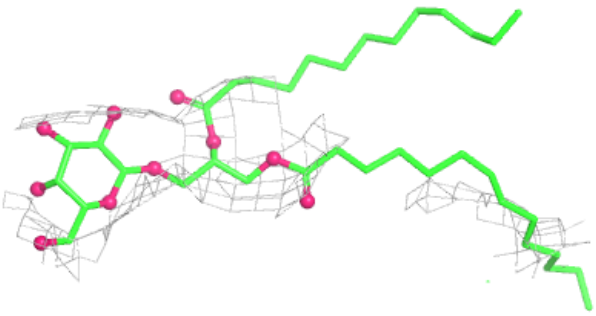


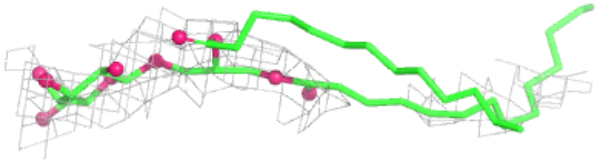


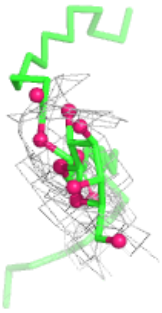


Electron density around LMG D 406:

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

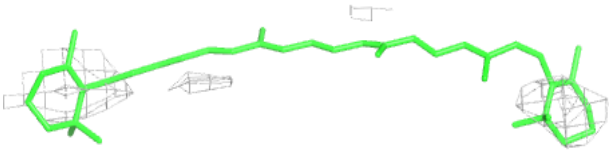


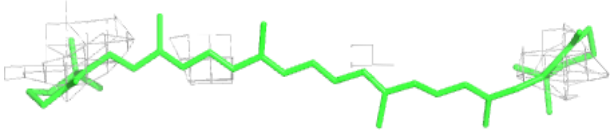


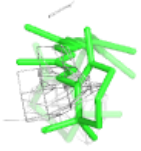


Electron density around BCR C 514:

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

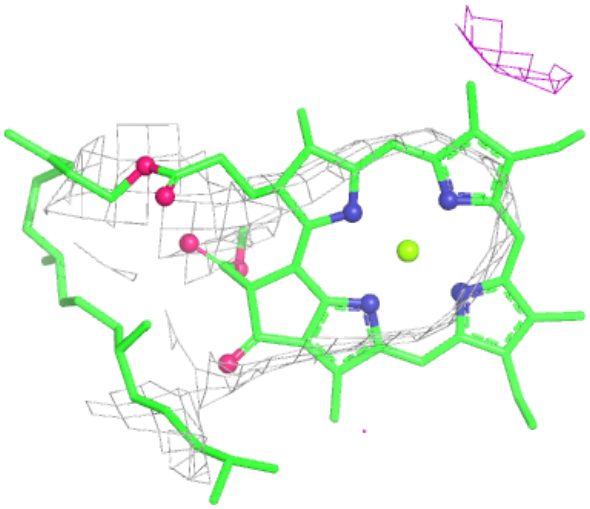






Electron density around CLA B 610:

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

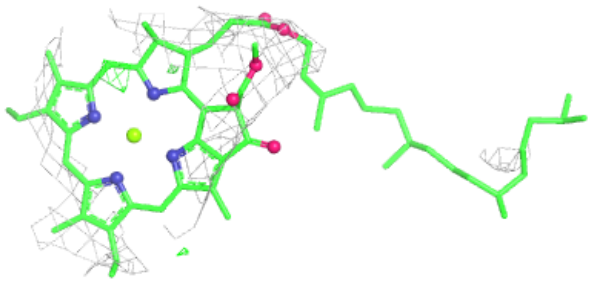


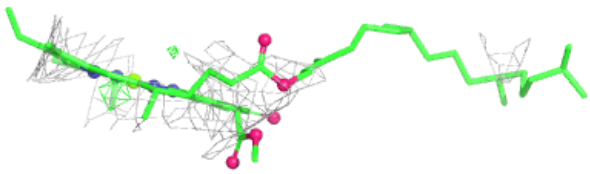


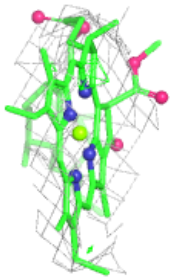


Electron density around CLA b 606:

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

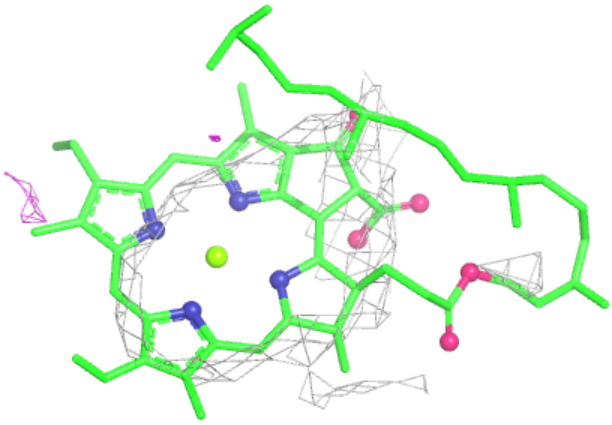


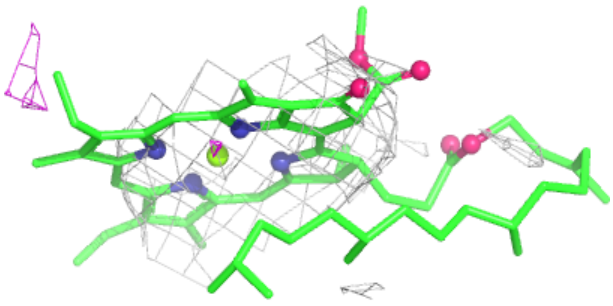


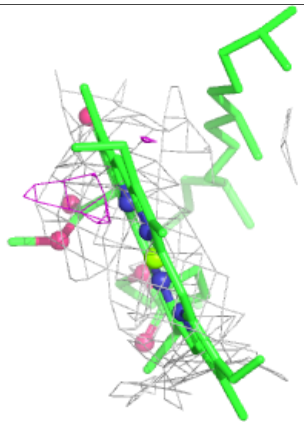


Electron density around CLA C 509:

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

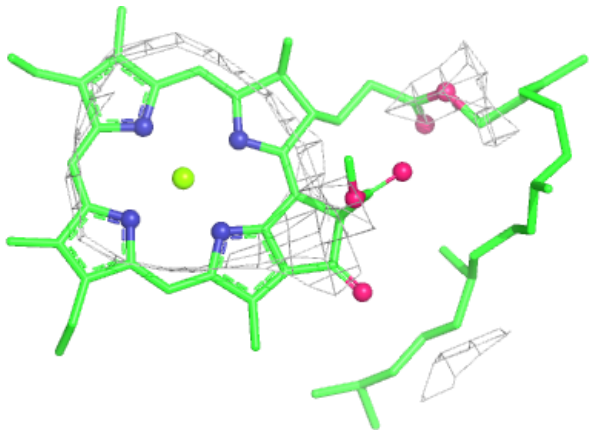


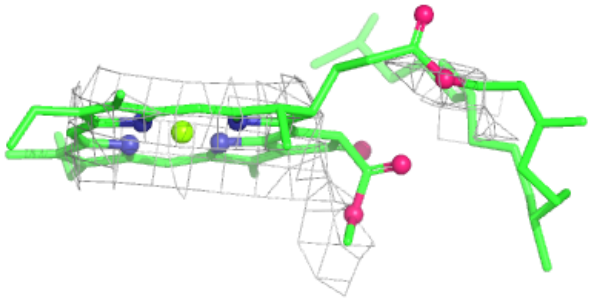




Electron density around CLA b 614:

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





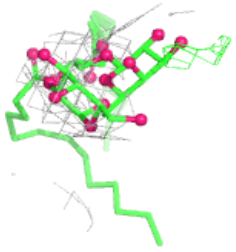


Electron density around DGD b 623:

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

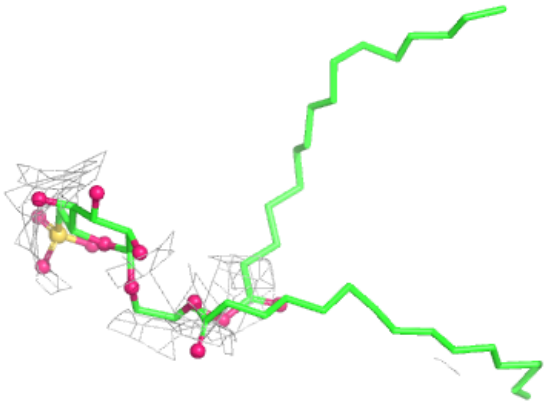


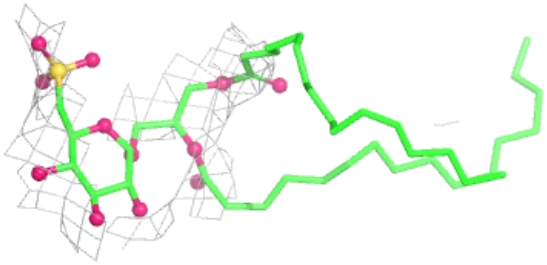


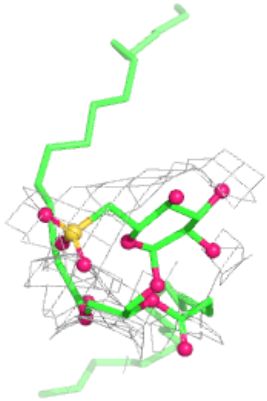


Electron density around SQD A 417:

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

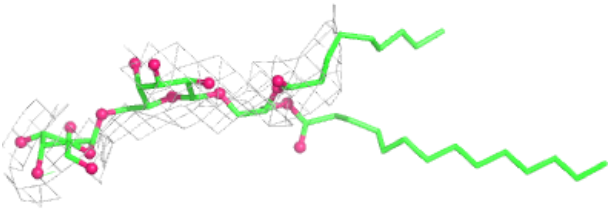


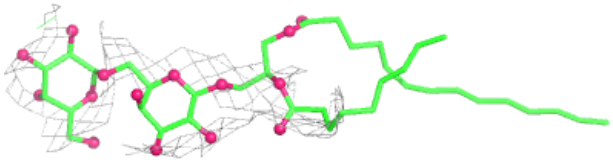


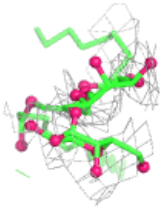


Electron density around DGD c 516:

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

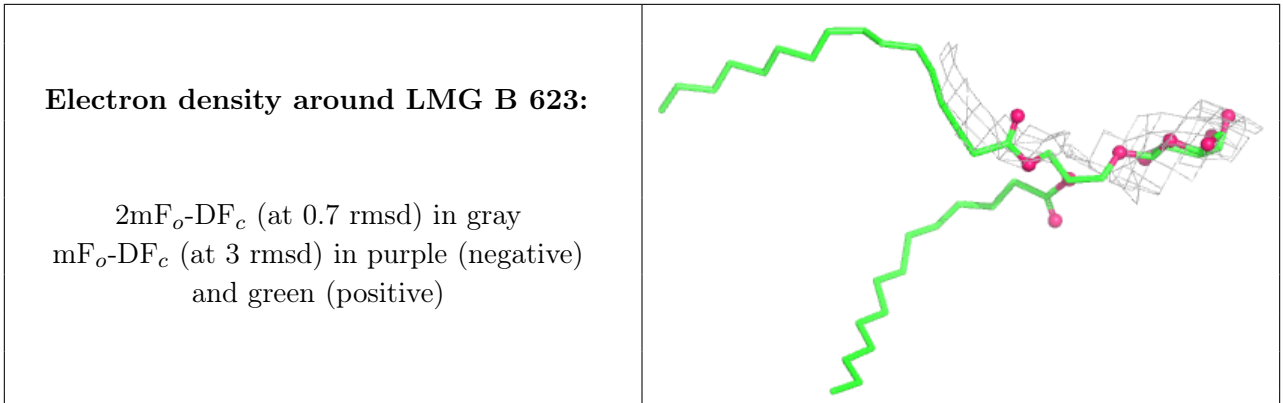


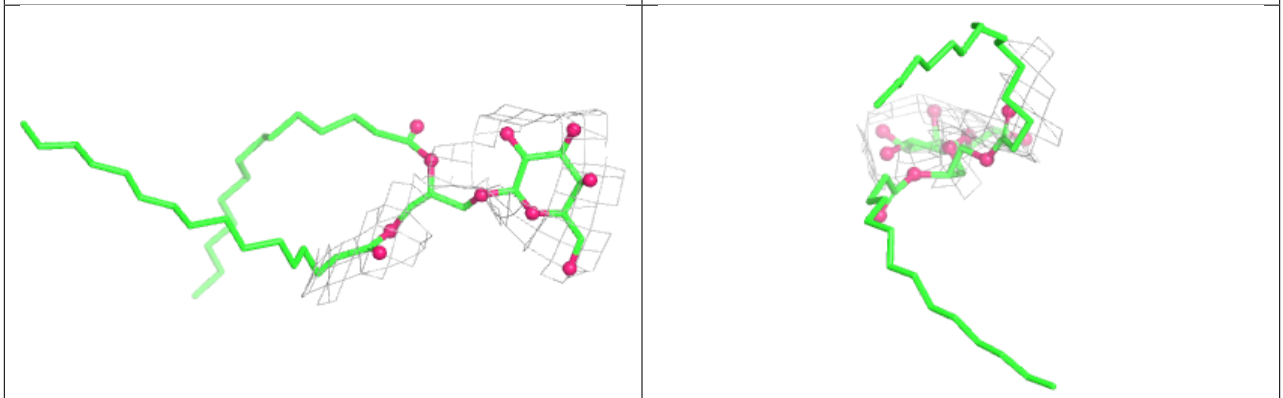




Electron density around LMG B 623:

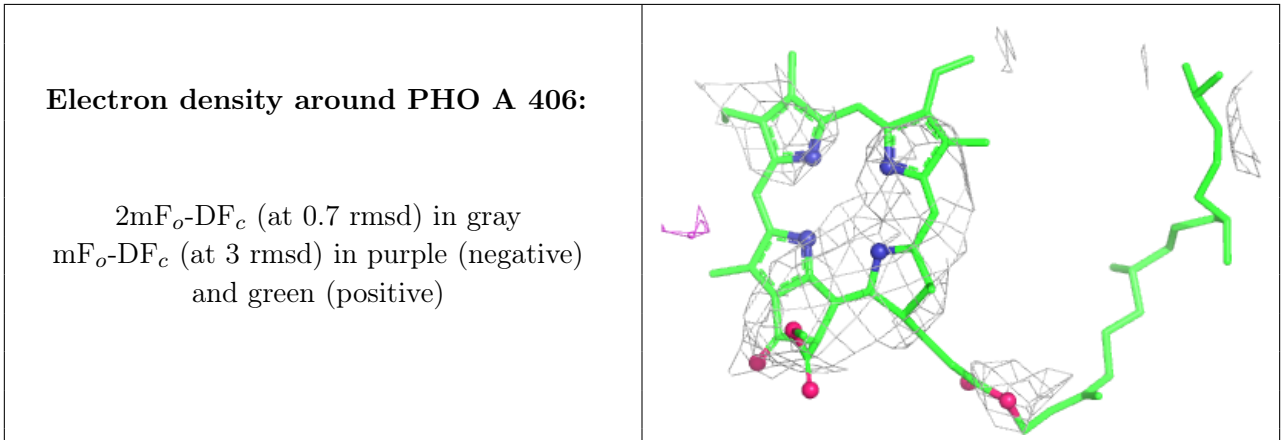
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

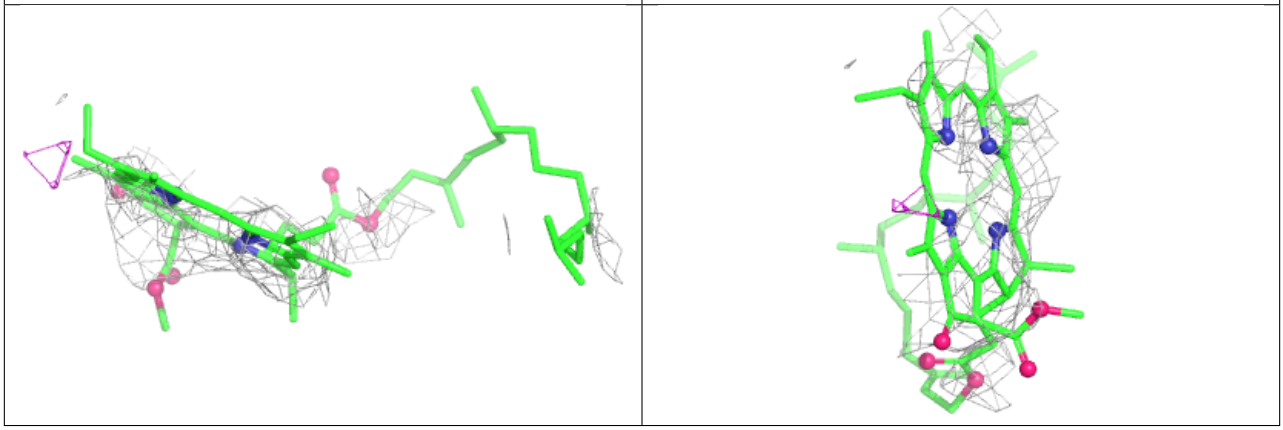




Electron density around PHO A 406:

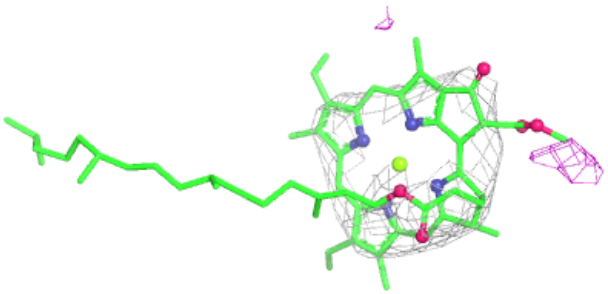
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

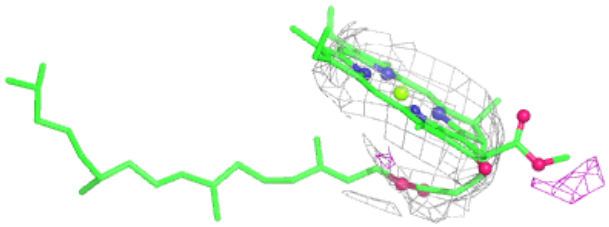


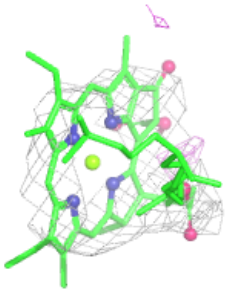


Electron density around CLA B 608:

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

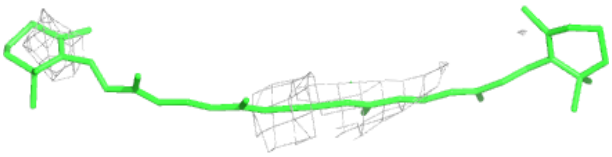


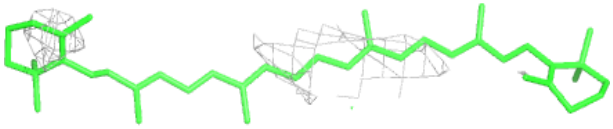


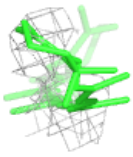


Electron density around BCR D 405:

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

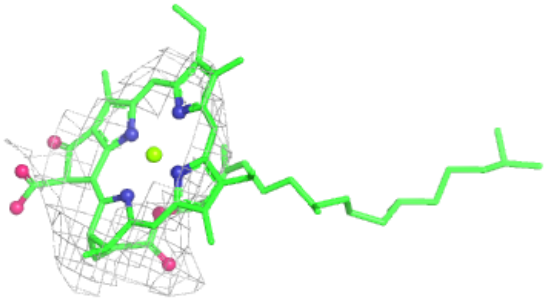


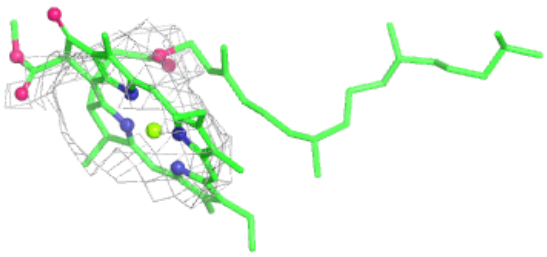


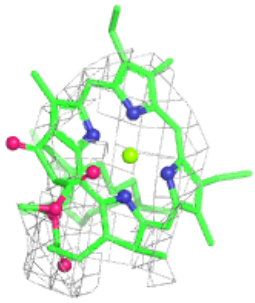


Electron density around CLA C 505:

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

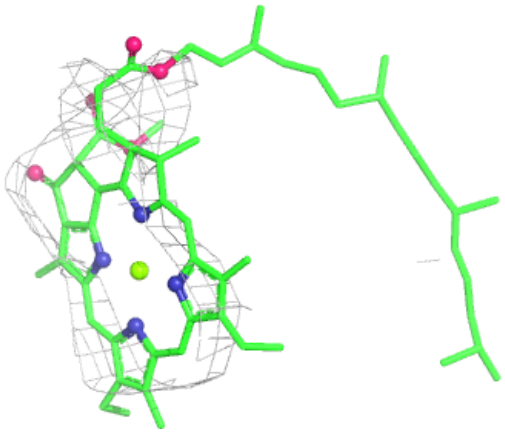


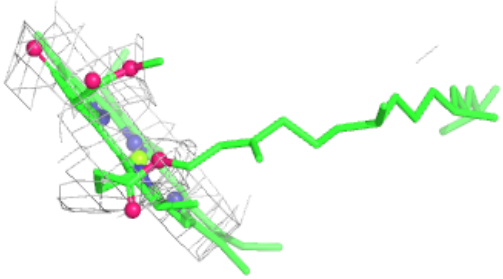


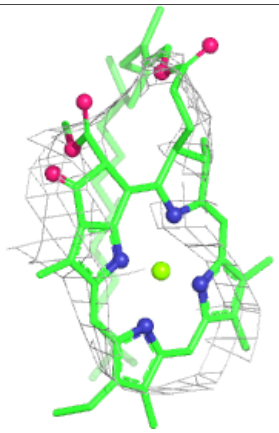


Electron density around CLA c 507:

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

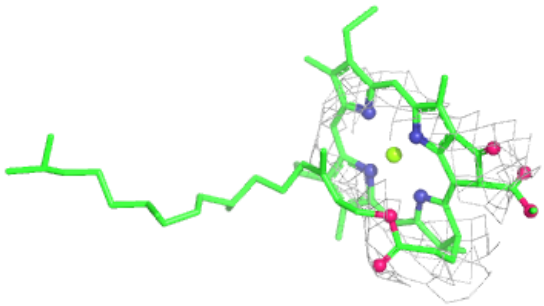






Electron density around CLA c 505:

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

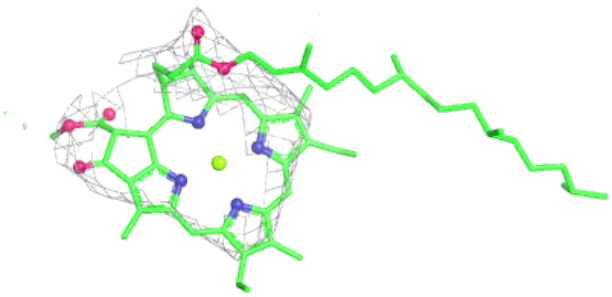


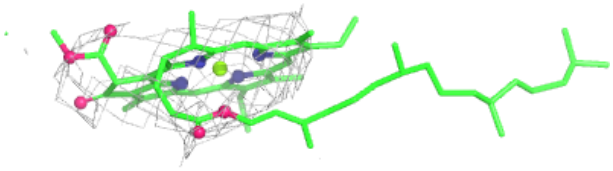


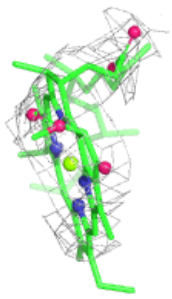


Electron density around CLA C 501:

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

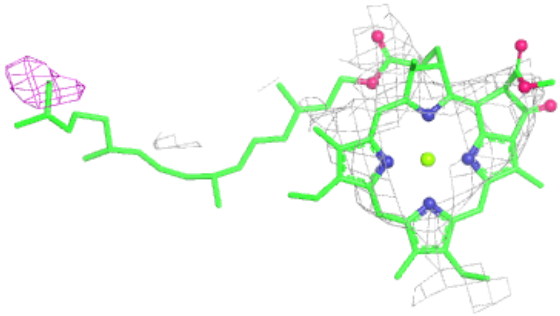


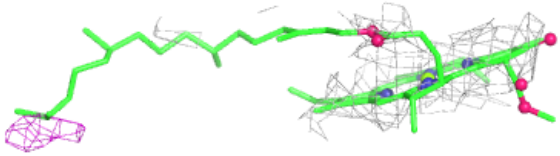




Electron density around CLA b 607:

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

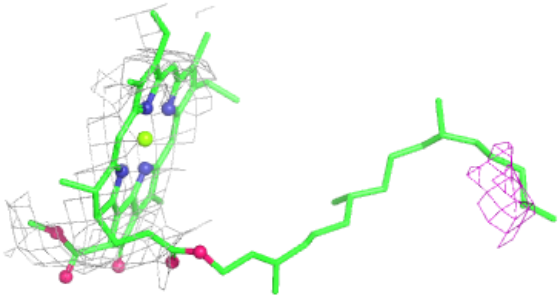


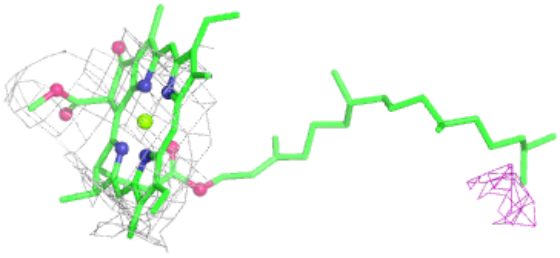


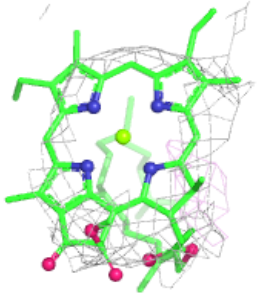


Electron density around CLA c 508:

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

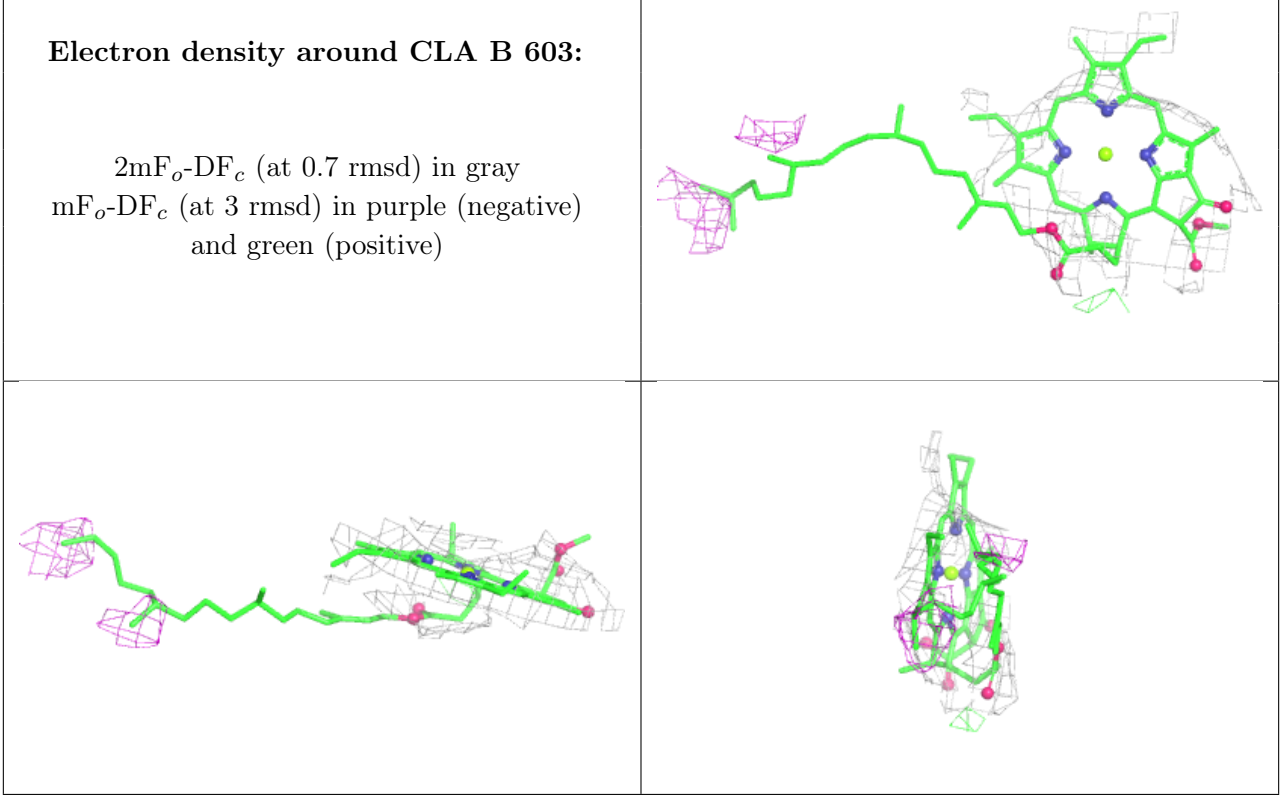






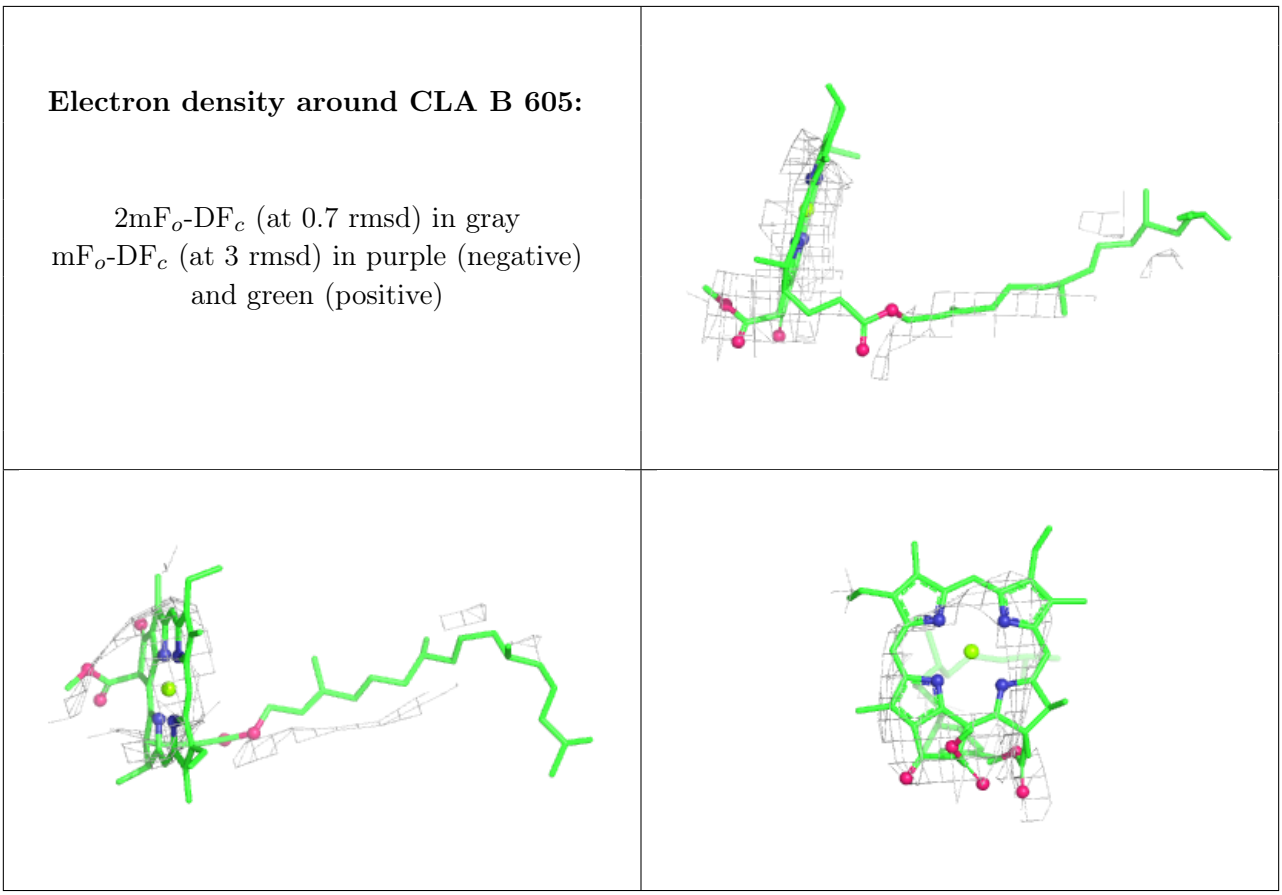
Electron density around CLA B 603:

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



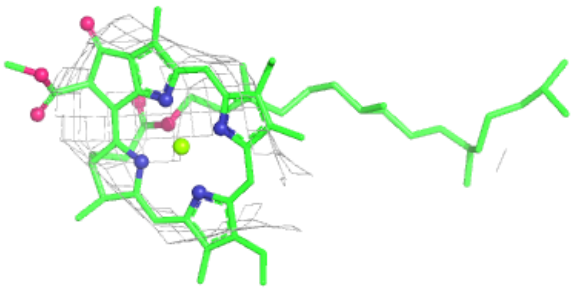
Electron density around CLA B 605:

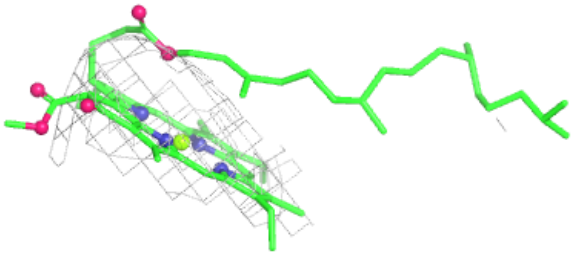
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

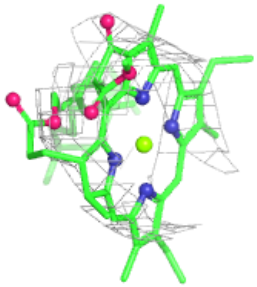


Electron density around CLA B 614:

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

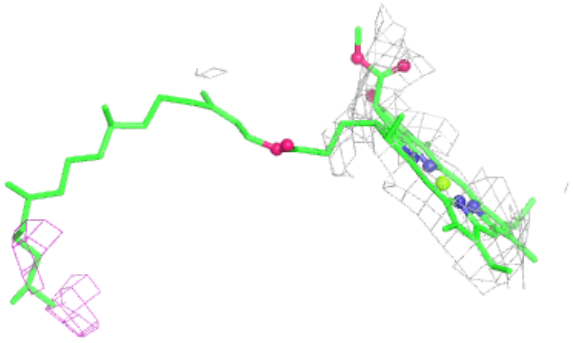


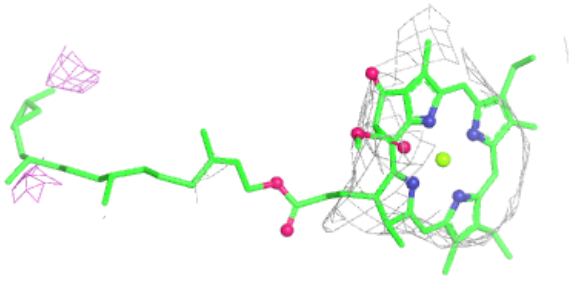




Electron density around CLA d 402:

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

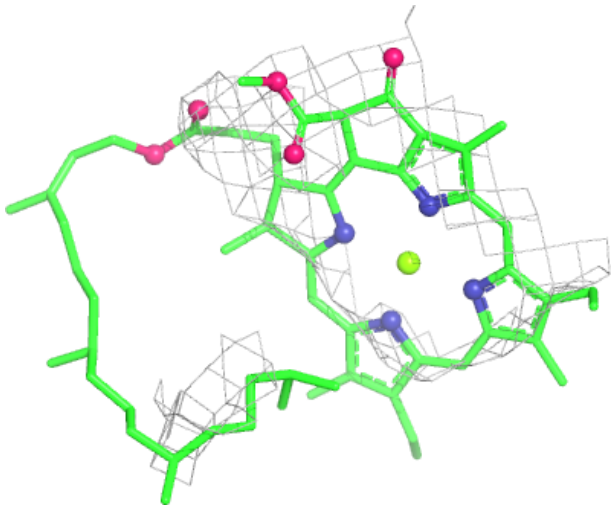


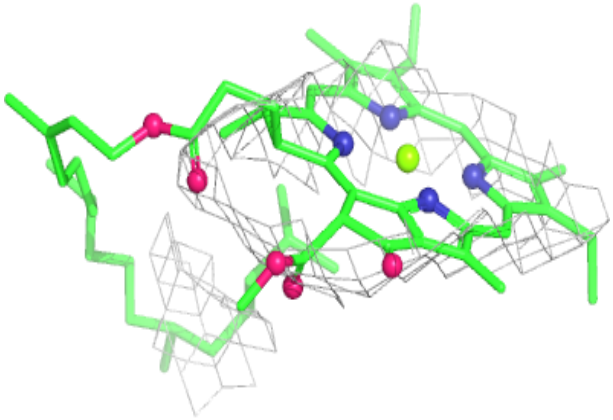


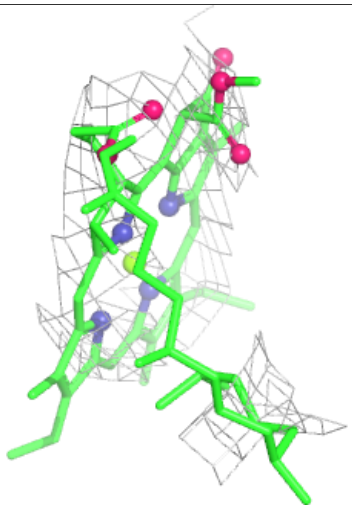


Electron density around CLA B 615:

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

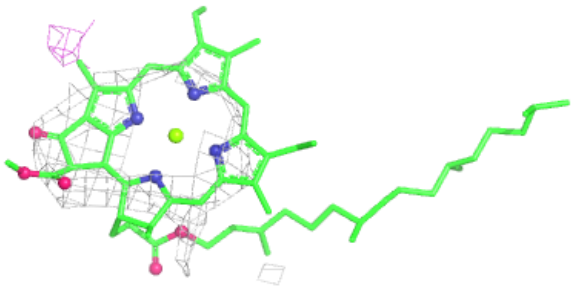


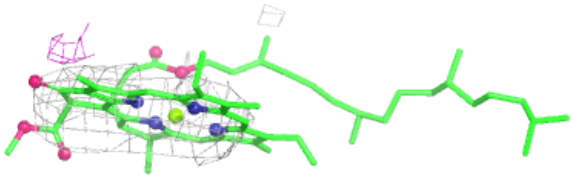


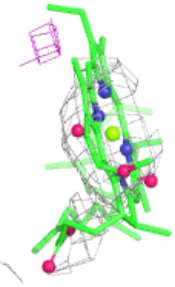


Electron density around CLA c 501:

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

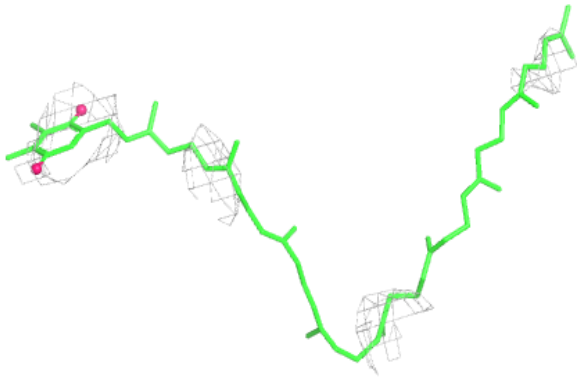




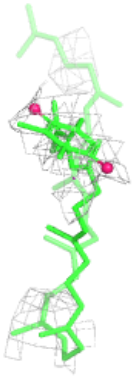


Electron density around PL9 D 404:

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

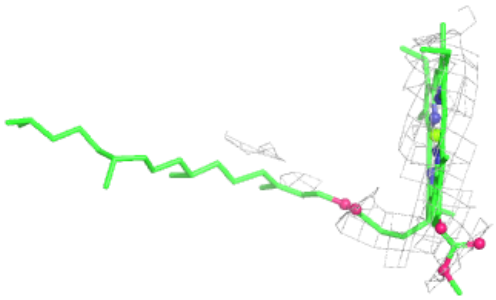


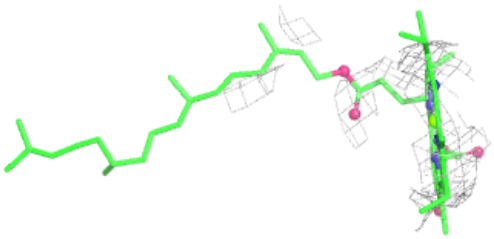


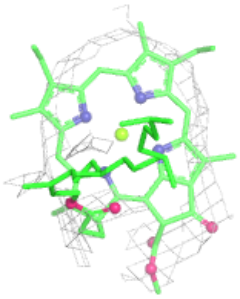


Electron density around CLA B 606:

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

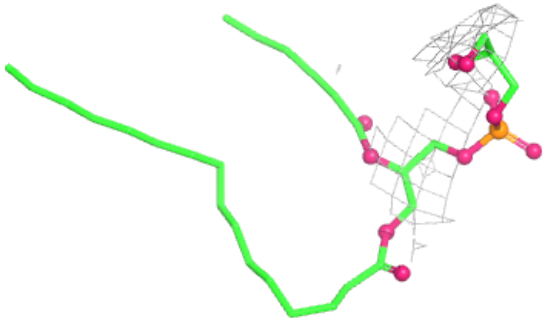


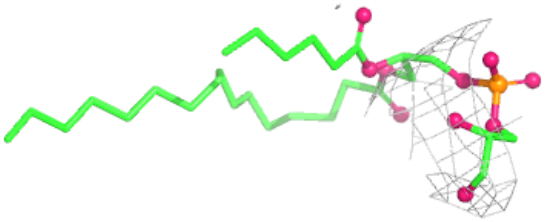




Electron density around LHG A 412:

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

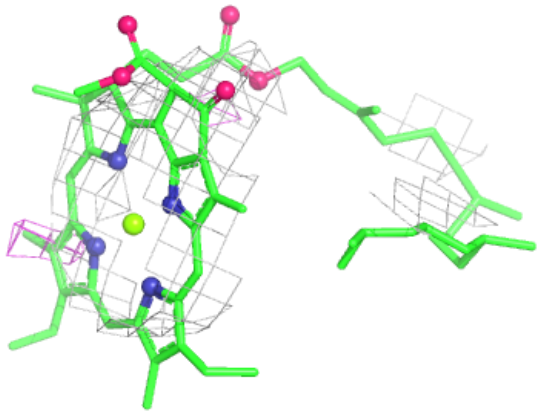


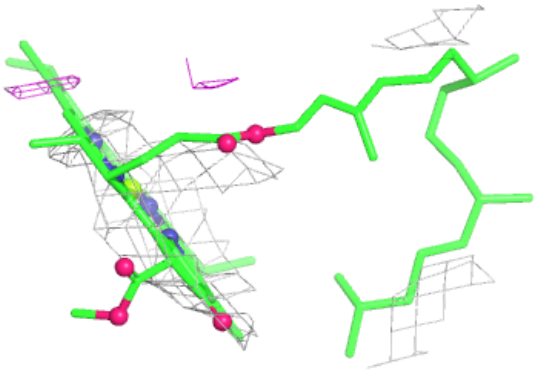


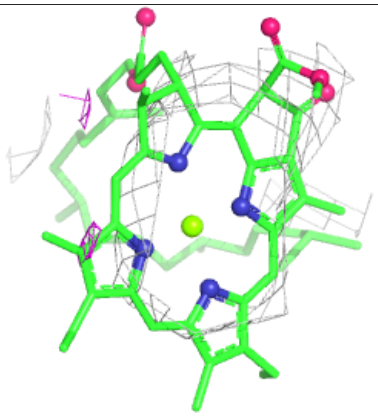


Electron density around CLA c 503:

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

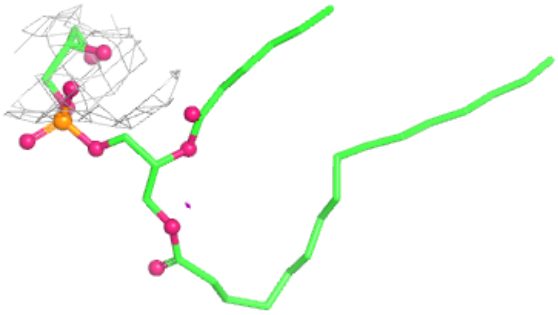


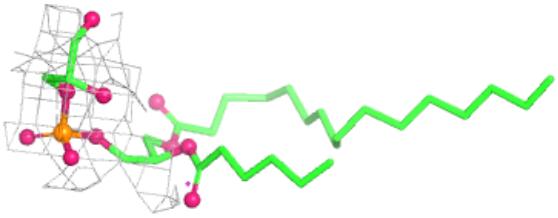


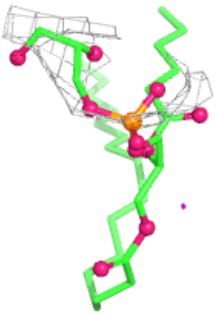


Electron density around LHG a 414:

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

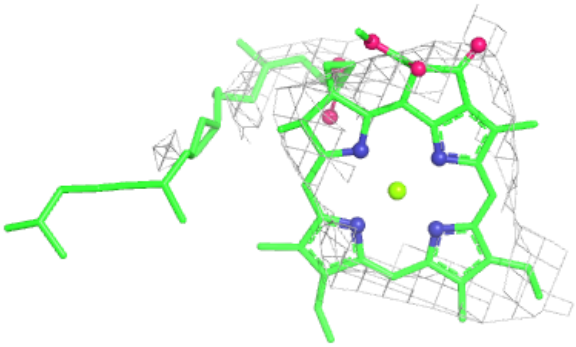


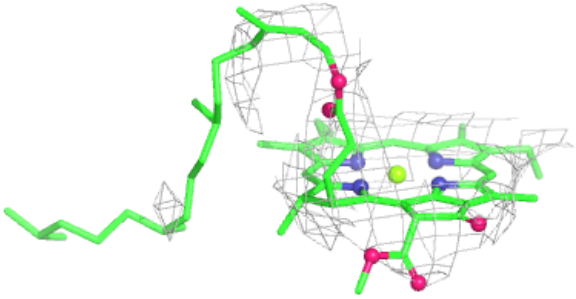


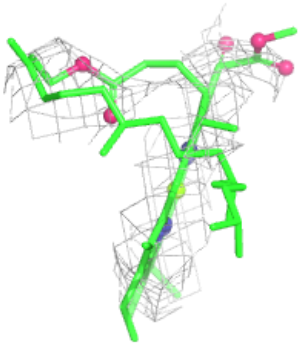


Electron density around CLA a 405:

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

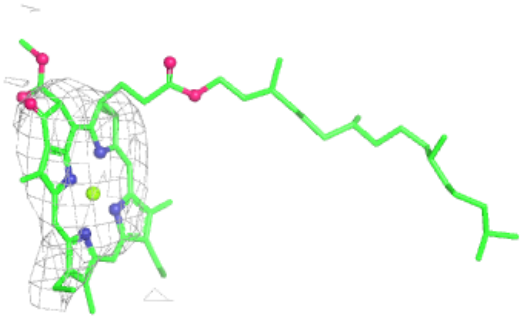


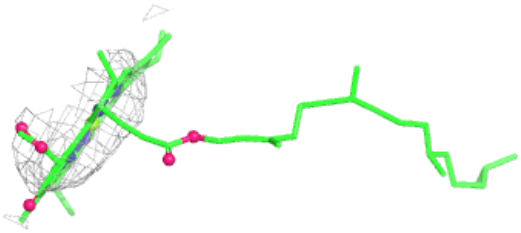


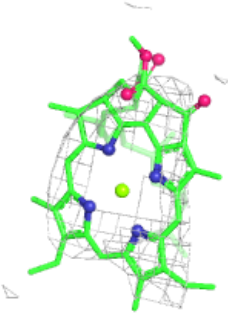


Electron density around CLA A 407:

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

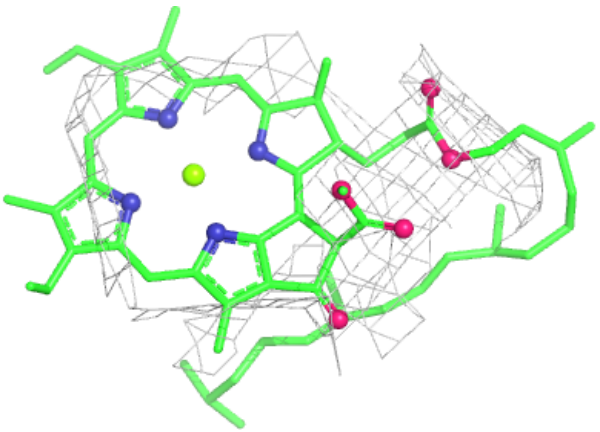


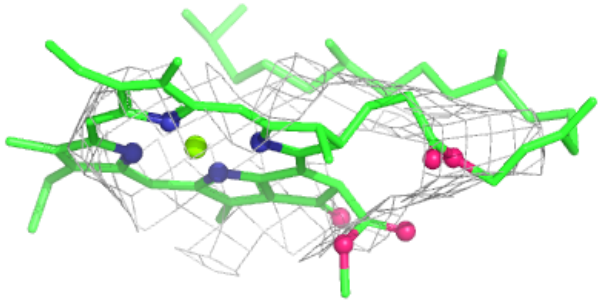


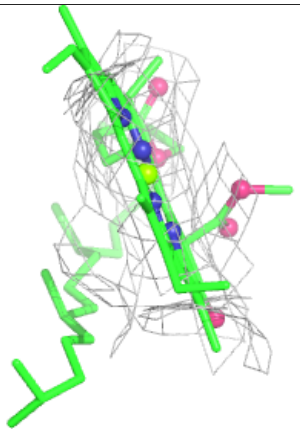


Electron density around CLA c 509:

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

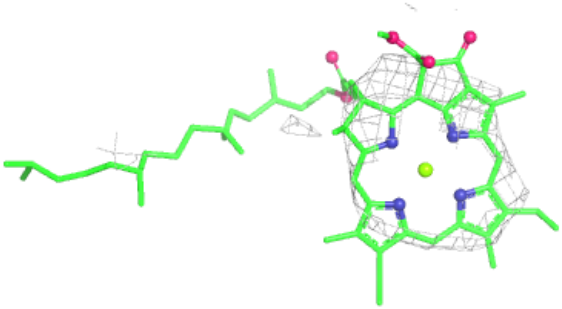


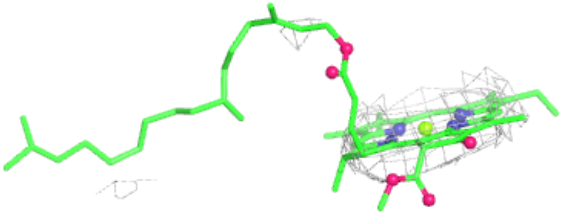


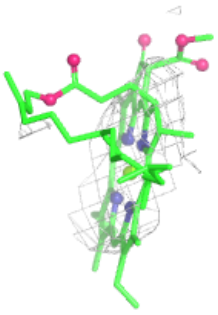


Electron density around CLA A 405:

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

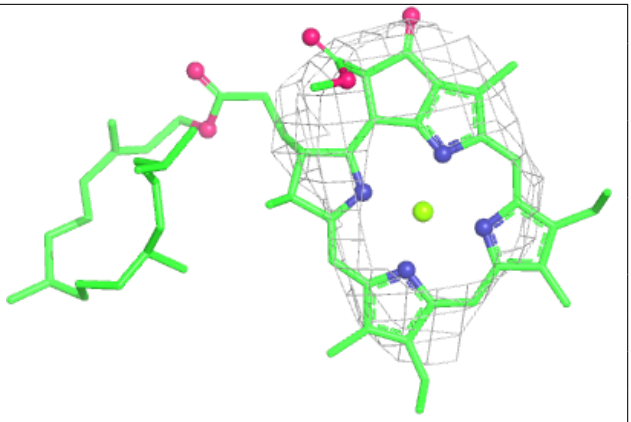


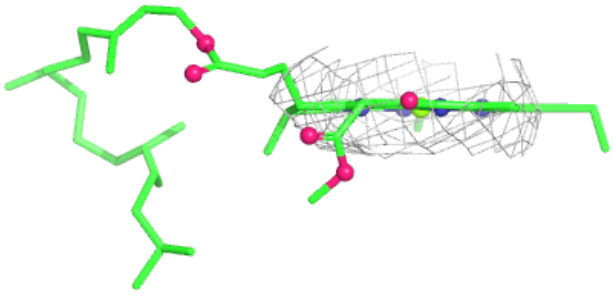


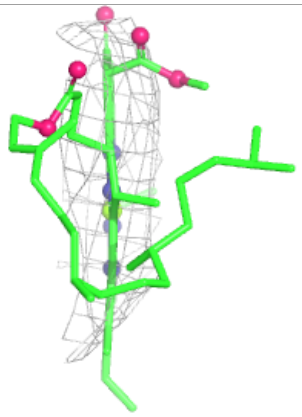


Electron density around CLA C 512:

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

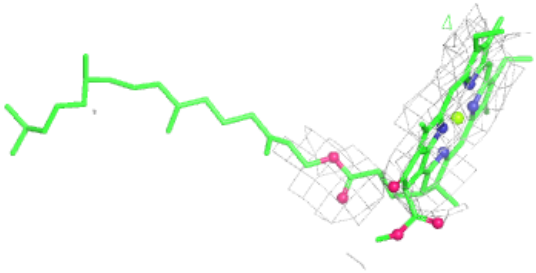


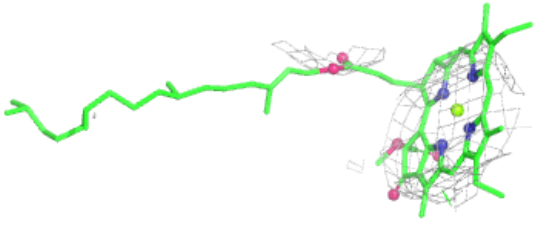


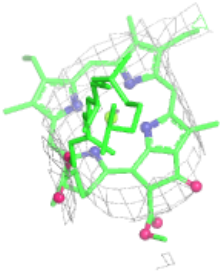


Electron density around CLA B 604:

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

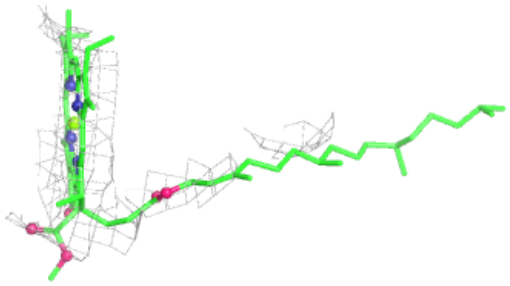




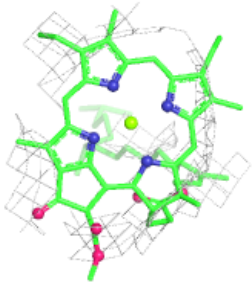


Electron density around CLA b 610:

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

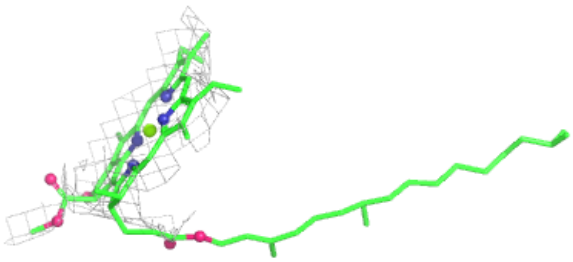


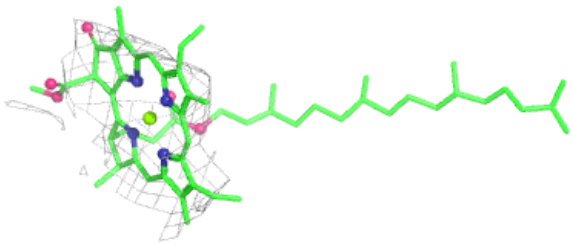


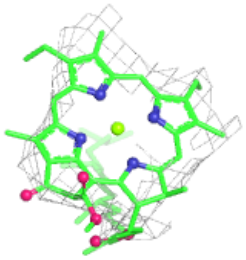


Electron density around CLA b 611:

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

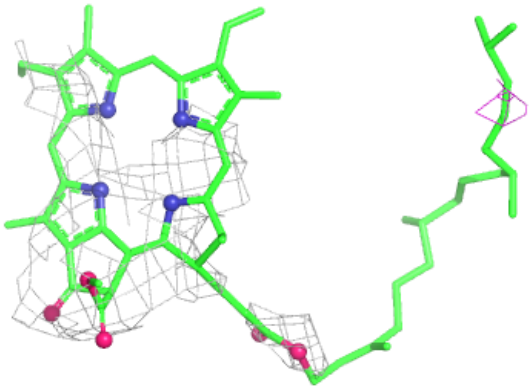


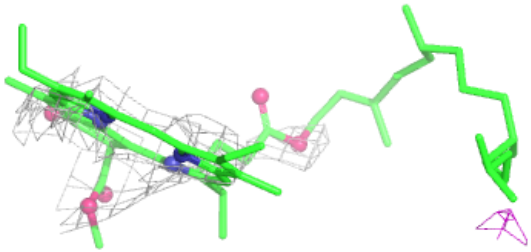




Electron density around PHO a 408:

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

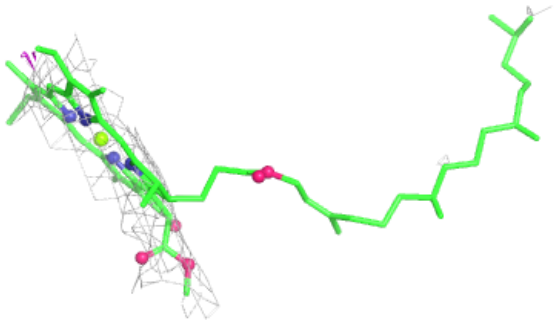


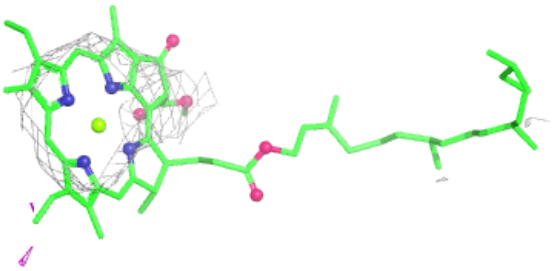


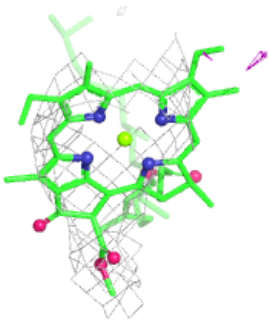


Electron density around CLA D 401:

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

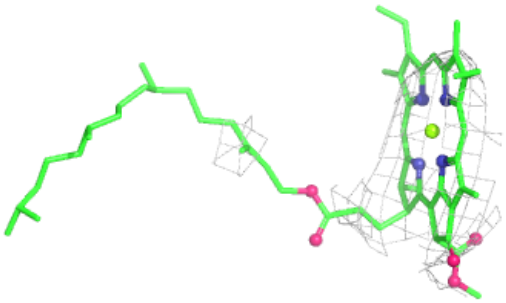


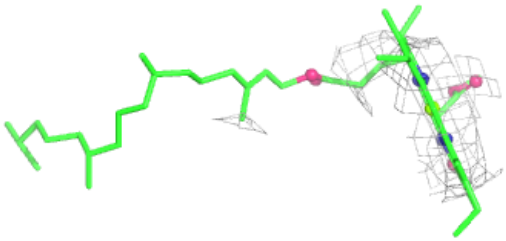


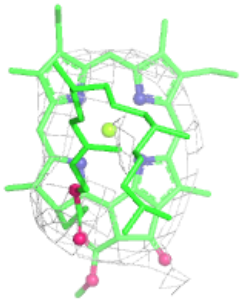


Electron density around CLA d 403:

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

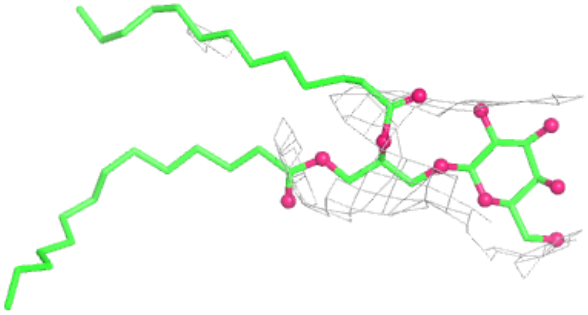


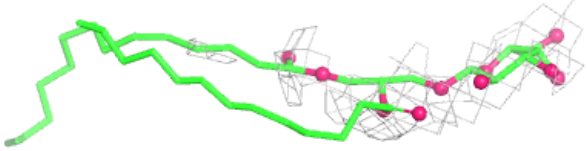


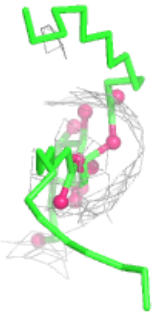


Electron density around LMG d 406:

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

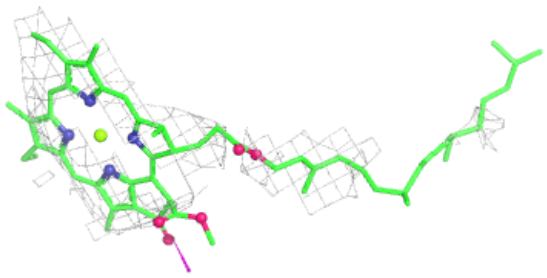


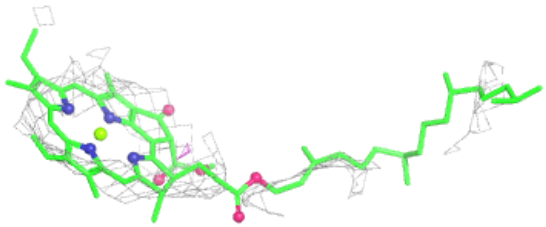


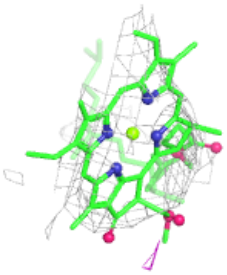


Electron density around CLA a 404:

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

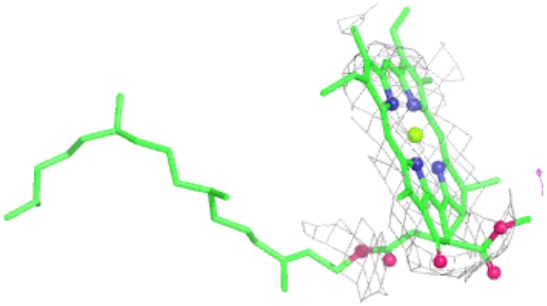


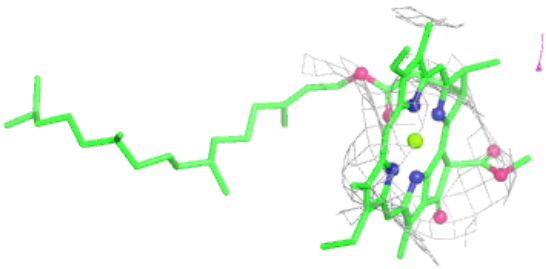


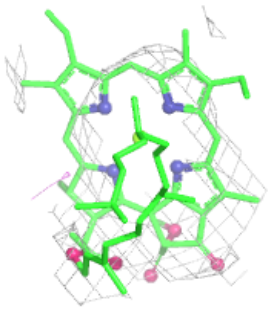


Electron density around CLA C 508:

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

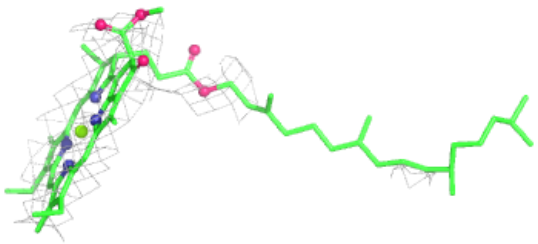


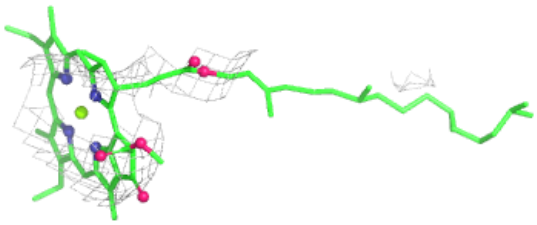


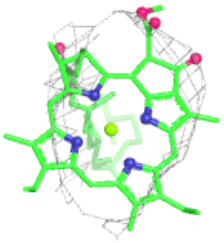


Electron density around CLA b 608:

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



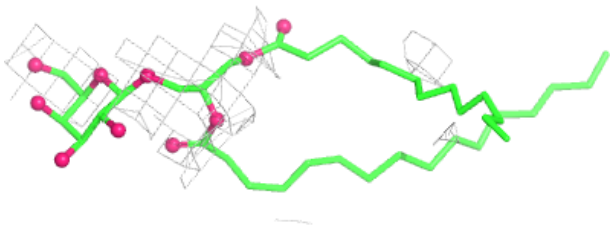


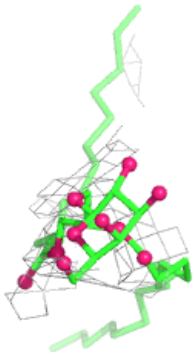


Electron density around LMG D 407:

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

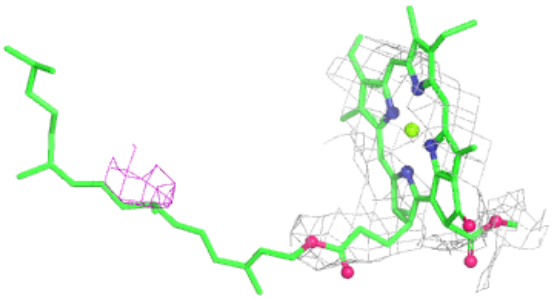


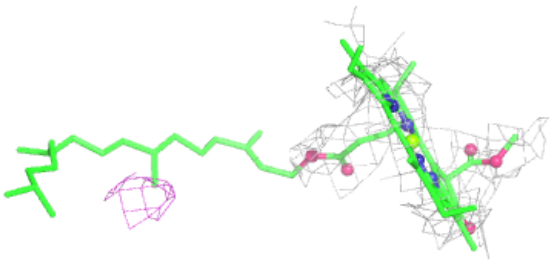


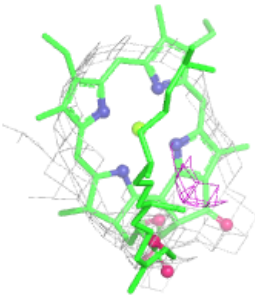


Electron density around CLA B 609:

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

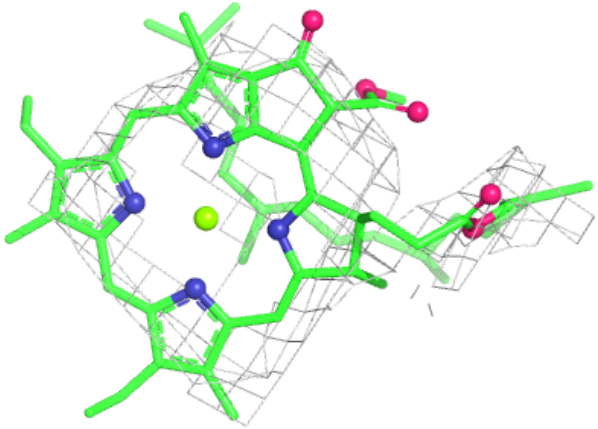


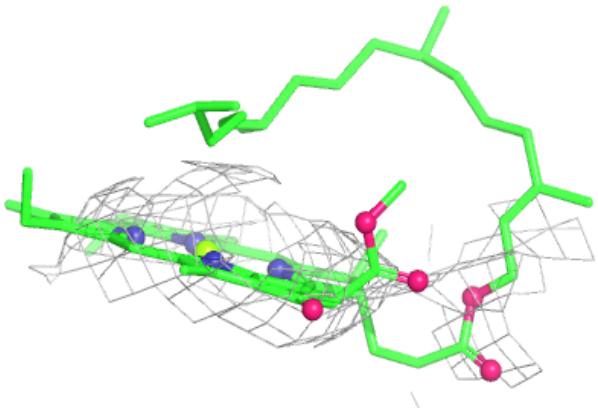


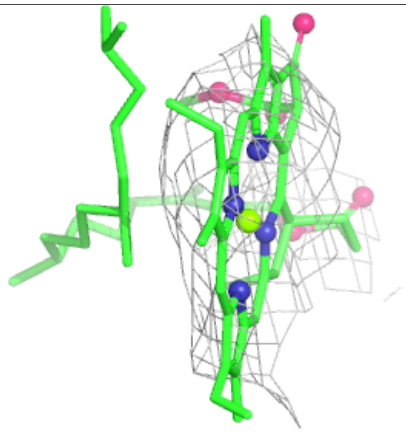


Electron density around CLA c 510:

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

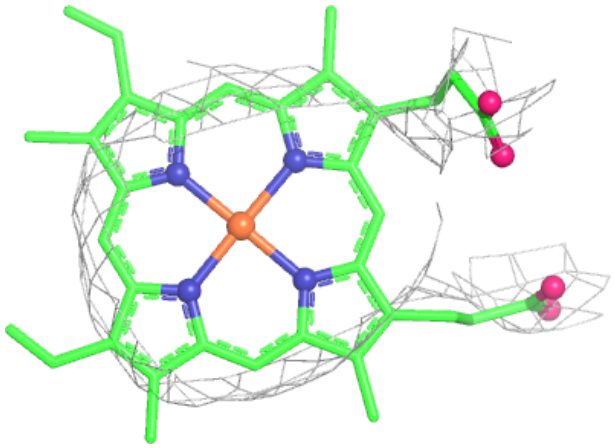


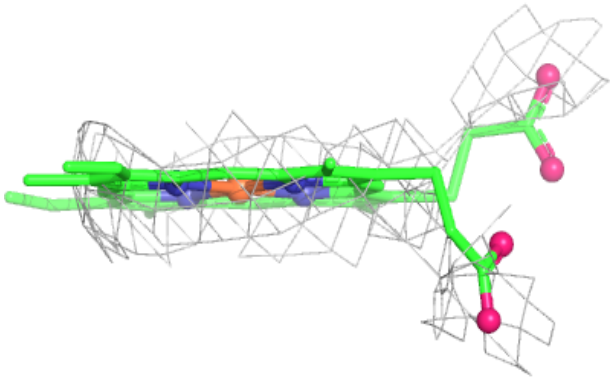


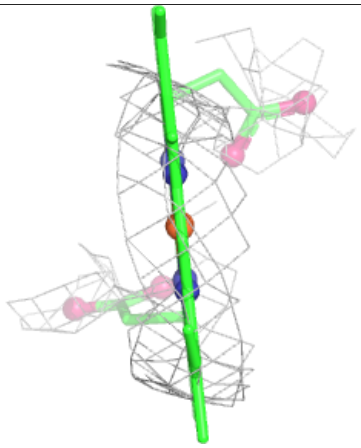


Electron density around HEM f 101:

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

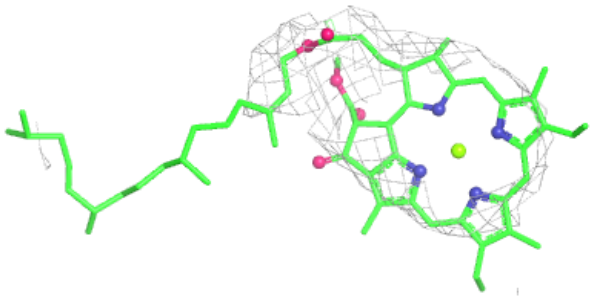


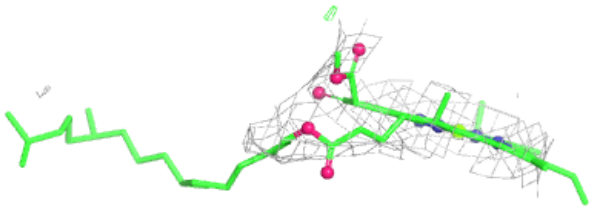


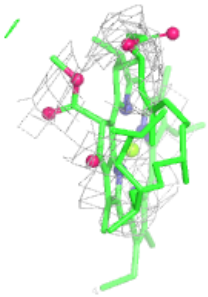


Electron density around CLA B 602:

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

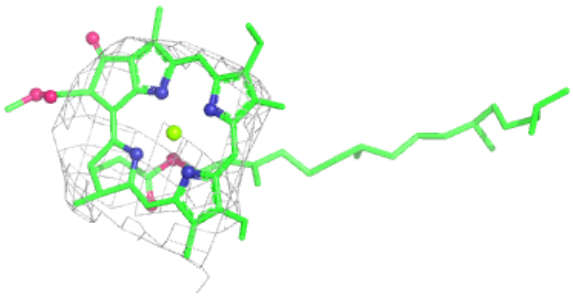


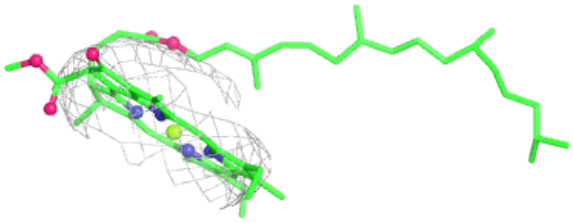


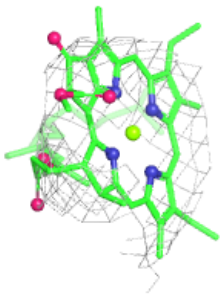


Electron density around CLA b 612:

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

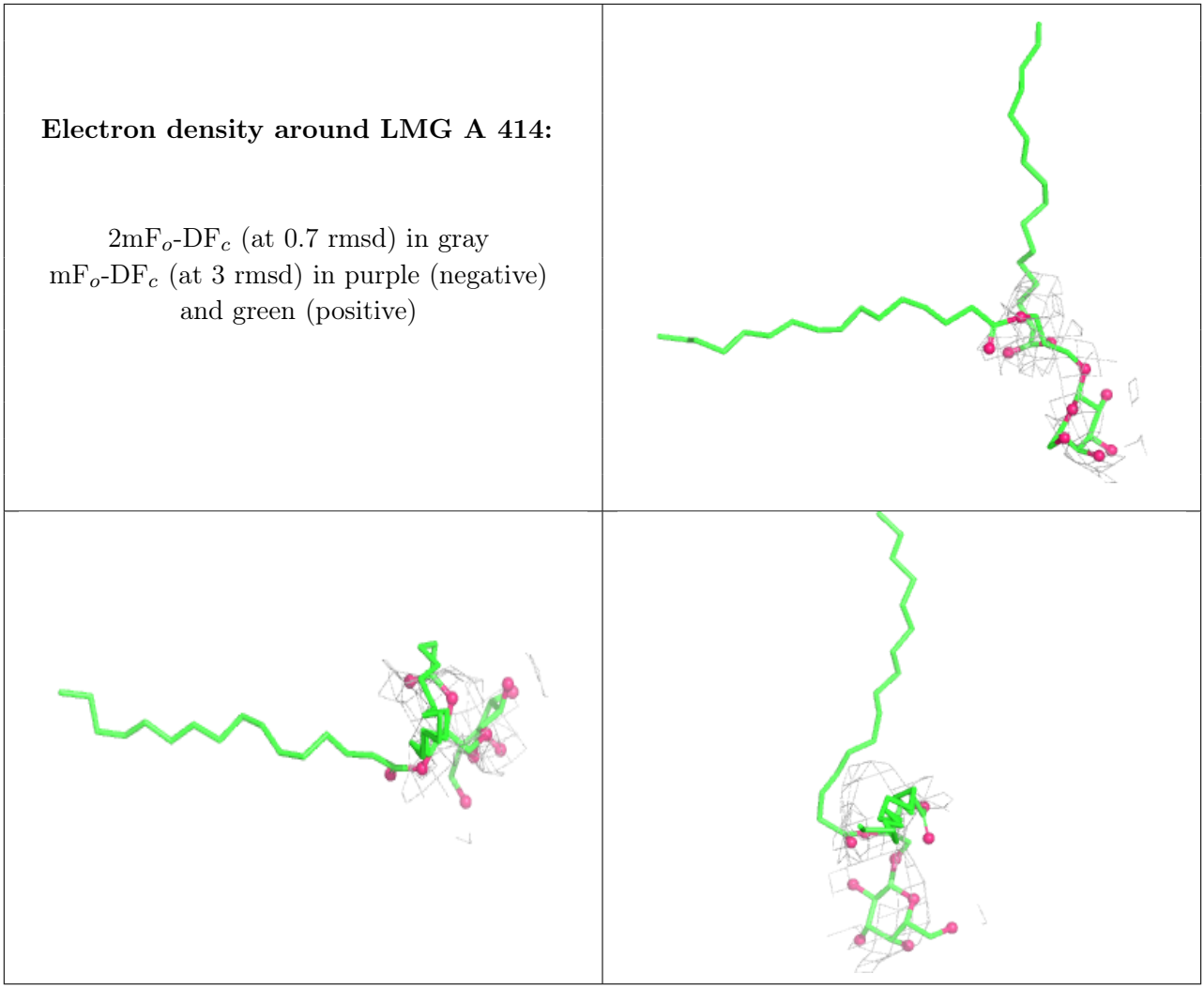






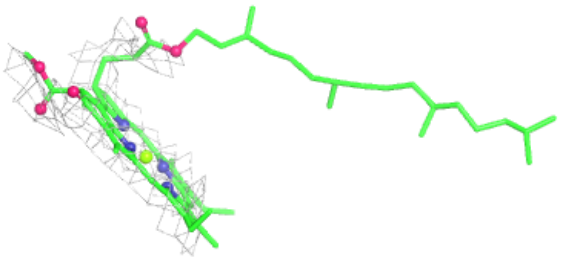
Electron density around LMG A 414:

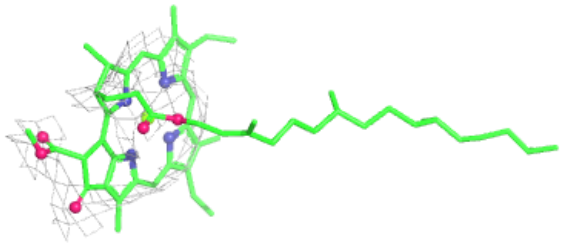
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

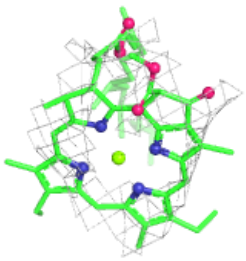


Electron density around CLA c 504:

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

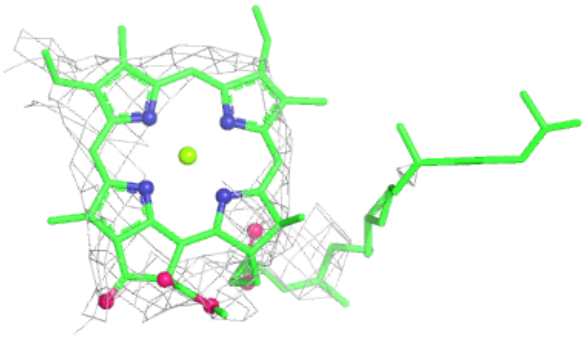


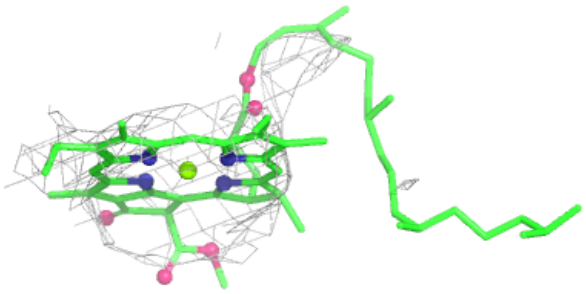


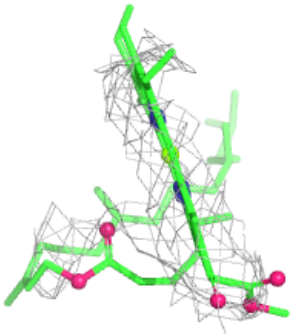


Electron density around CLA A 404:

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

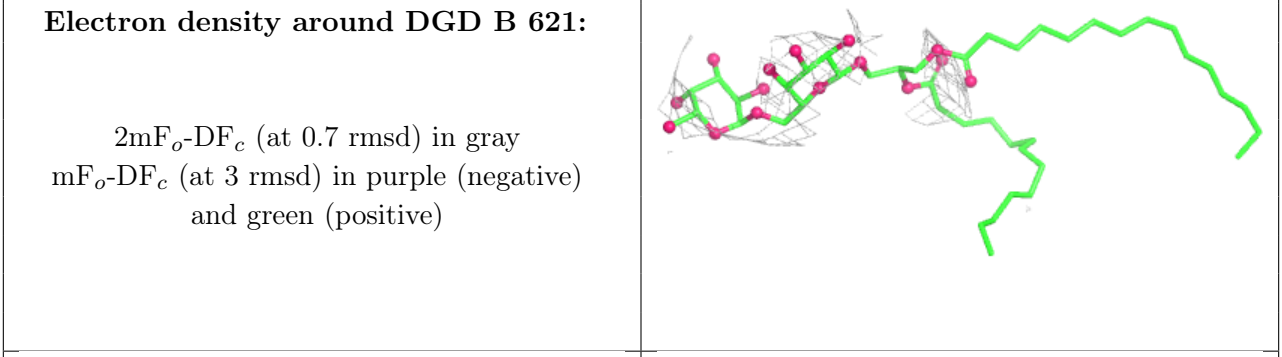






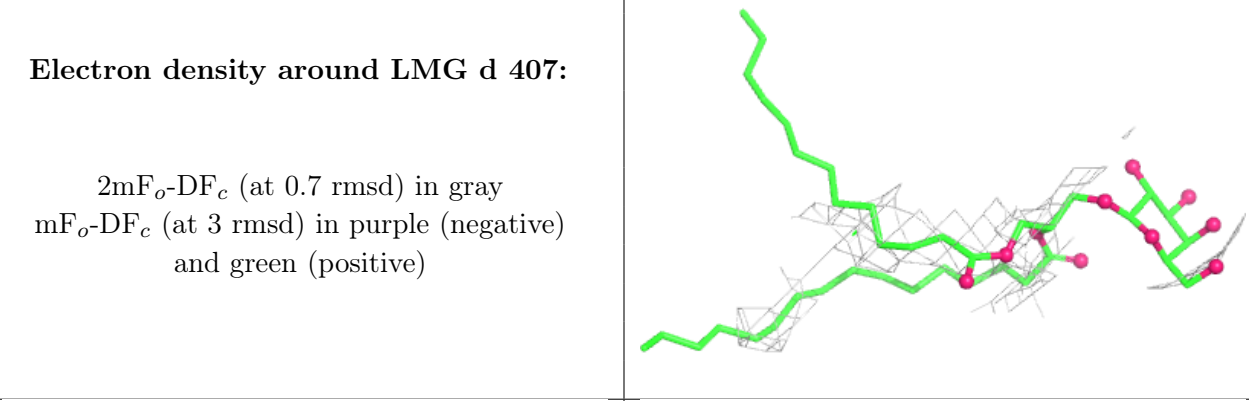
Electron density around DGD B 621:

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



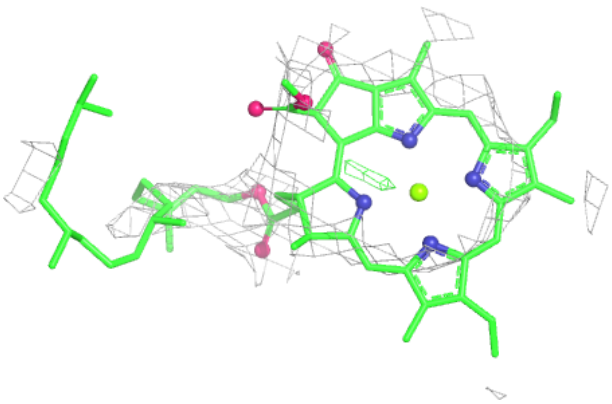
Electron density around LMG d 407:

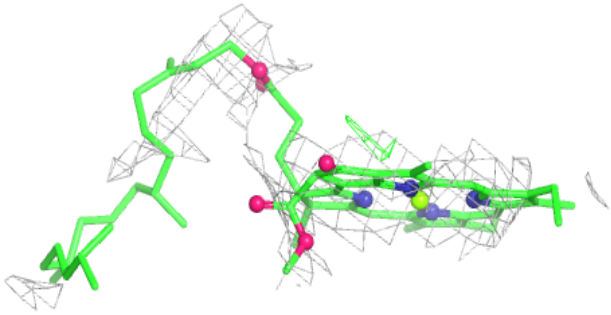
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

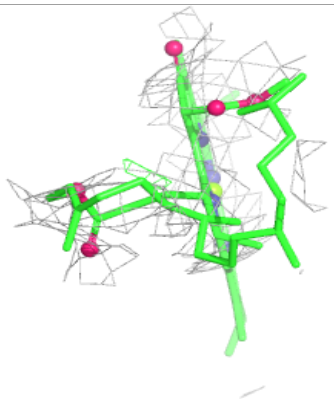


Electron density around CLA B 612:

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

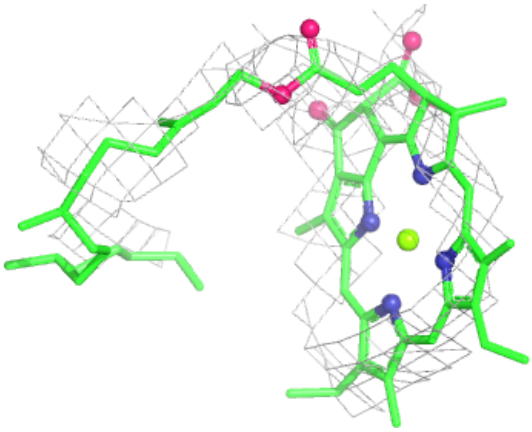


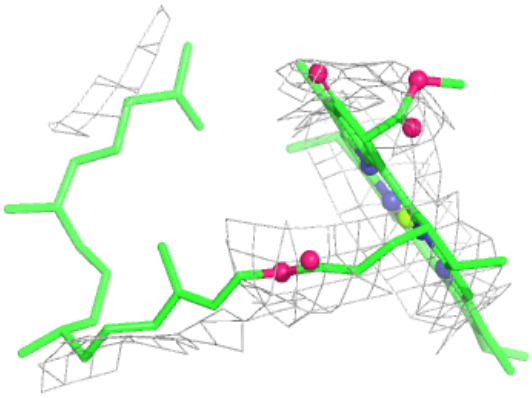


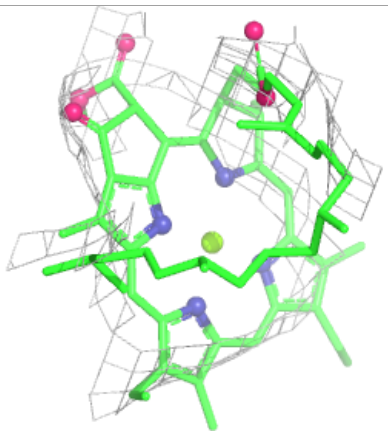


Electron density around CLA C 503:

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

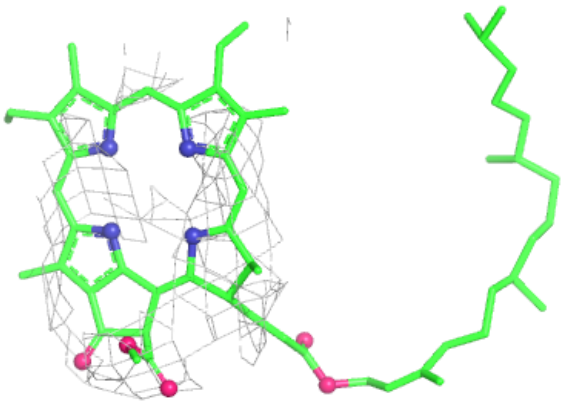


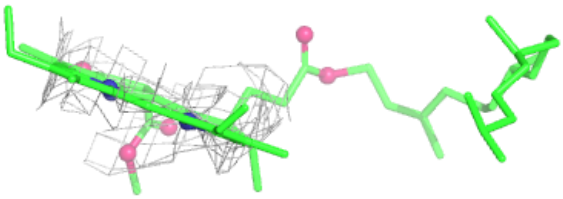


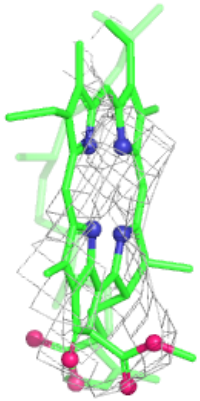


Electron density around PHO D 402:

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

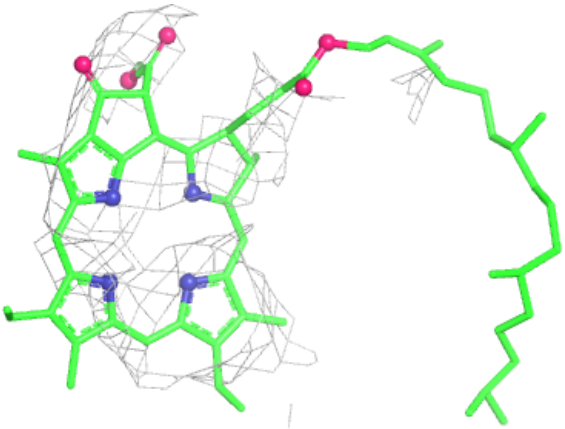


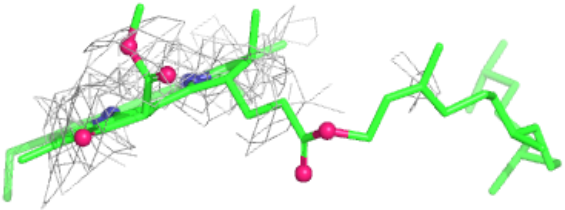




Electron density around PHO a 407:

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

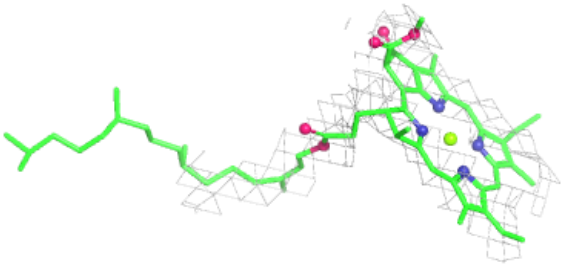


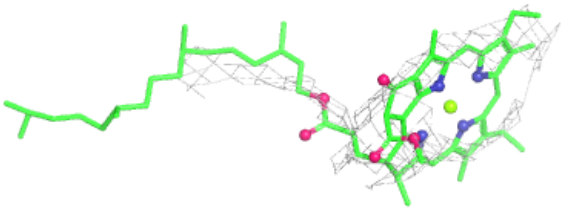


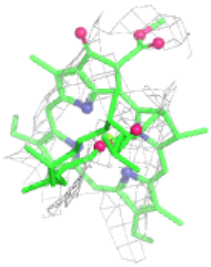


Electron density around CLA C 502:

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

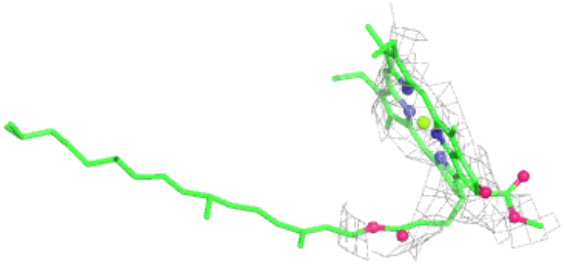


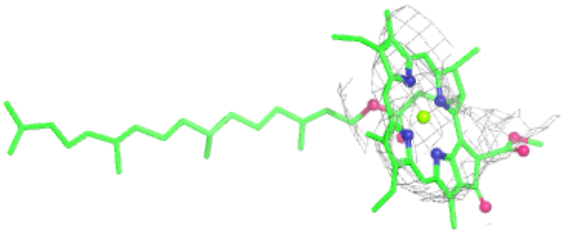


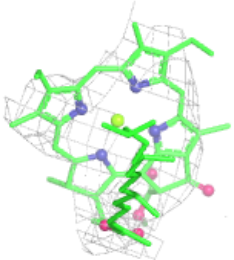


Electron density around CLA B 607:

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

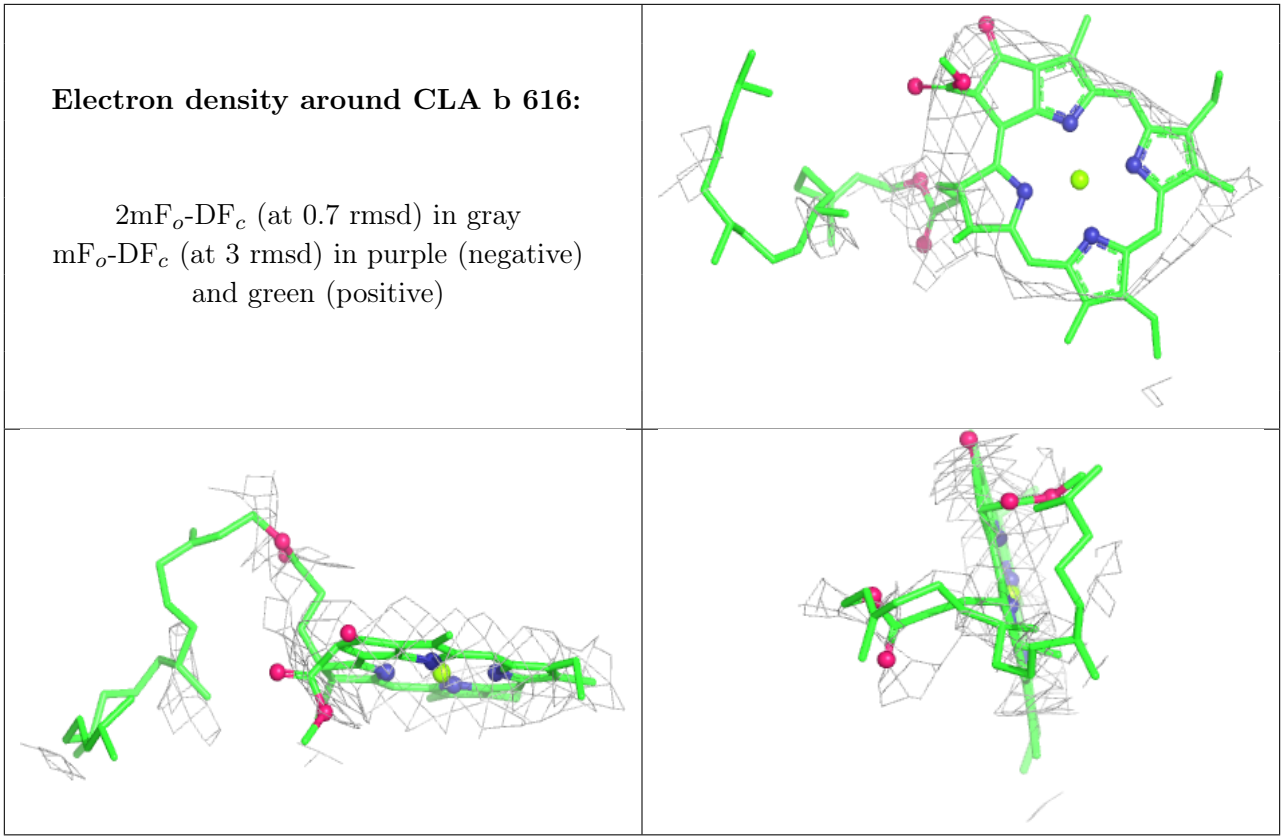






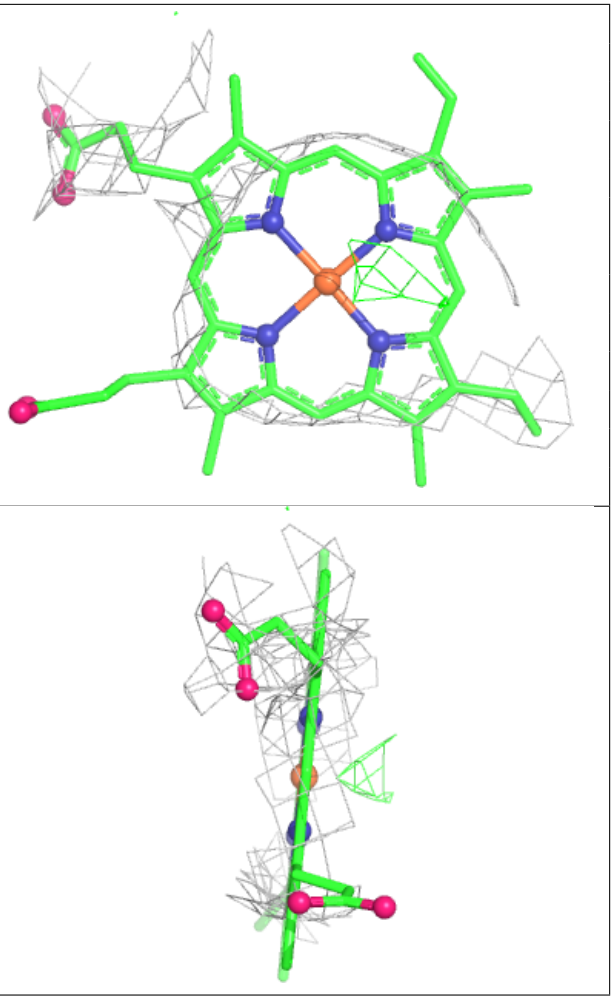
Electron density around CLA b 616:

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



Electron density around HEM V 201:

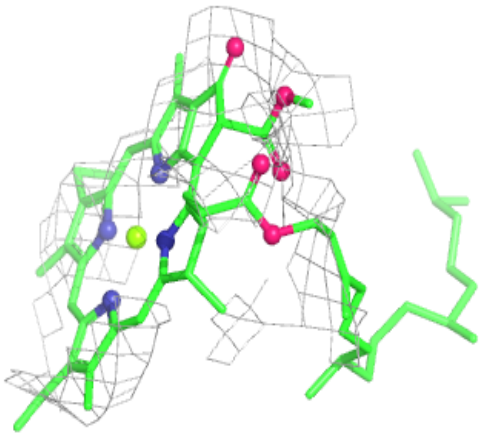
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

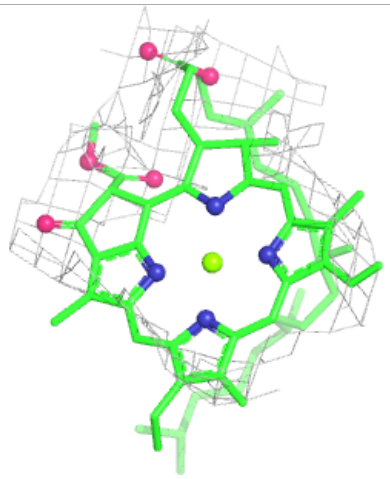


Electron density around CLA b 617:

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

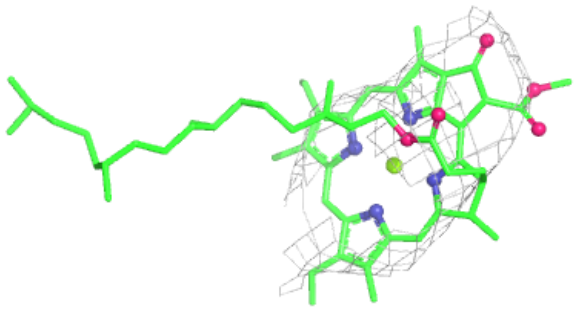


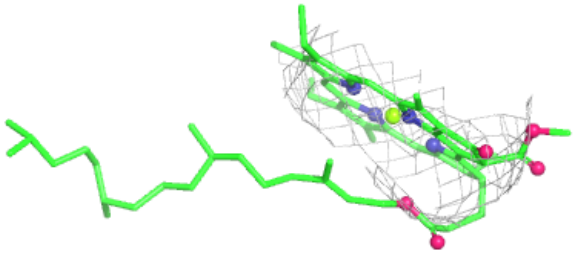




Electron density around CLA b 618:

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



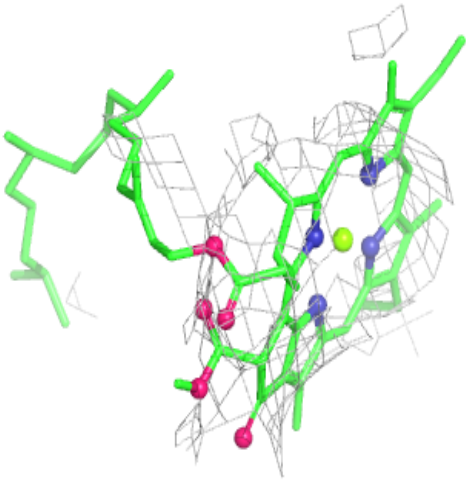


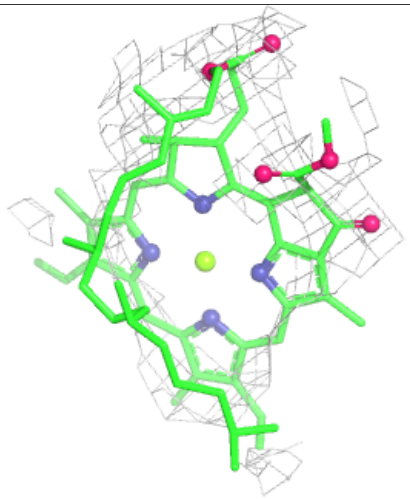


Electron density around CLA B 613:

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

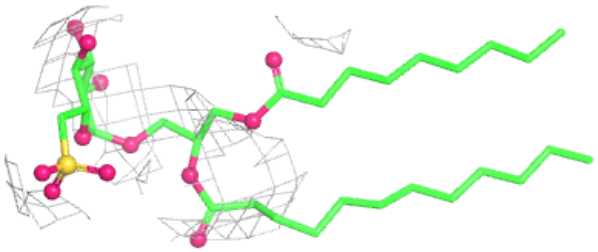


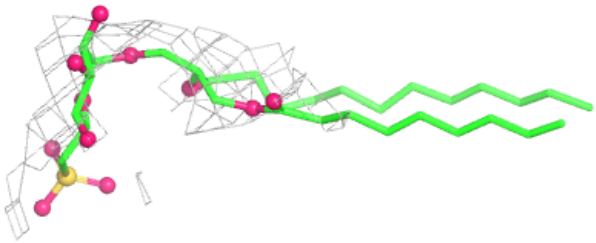


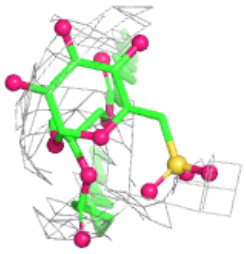


Electron density around SQD D 408:

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

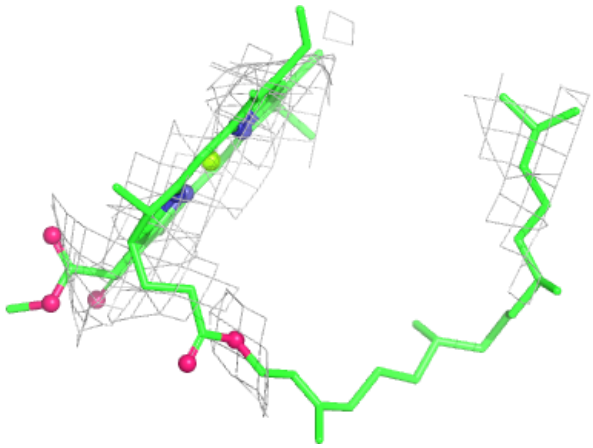


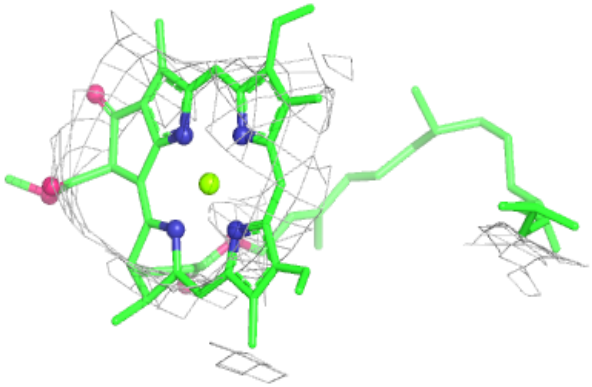


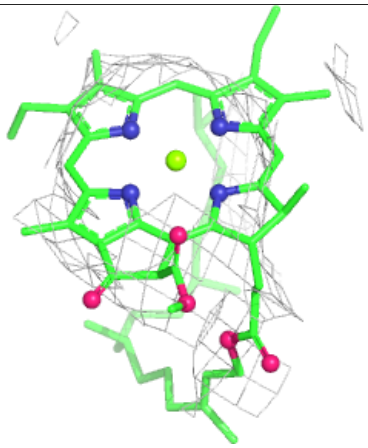


Electron density around CLA B 611:

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

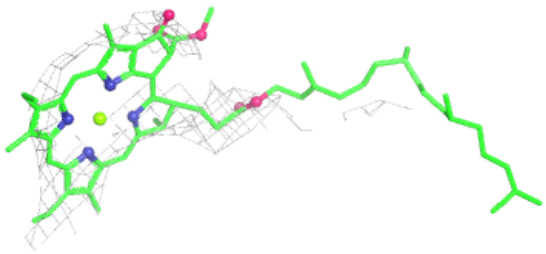


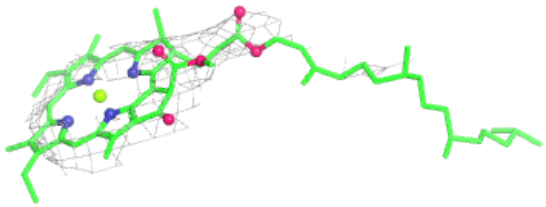


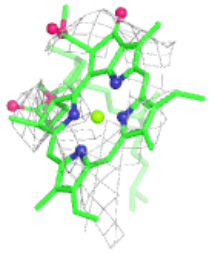


Electron density around CLA A 403:

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



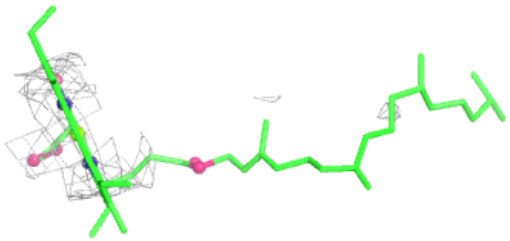


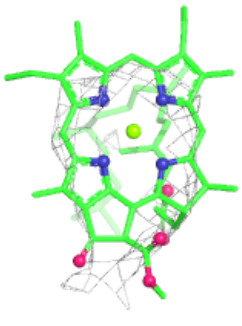


Electron density around CLA D 403:

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

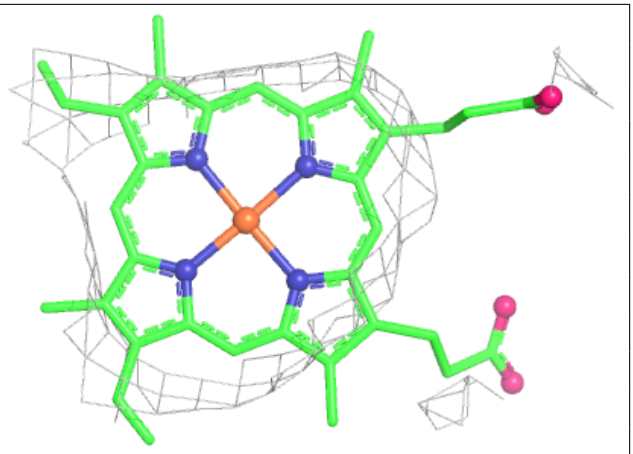


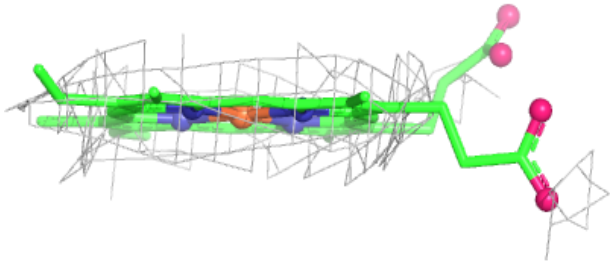


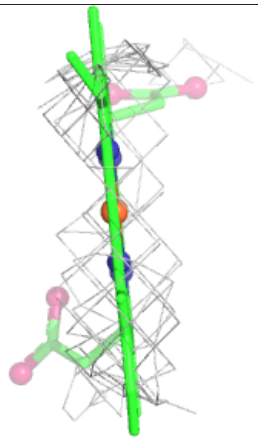


Electron density around HEM v 201:

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

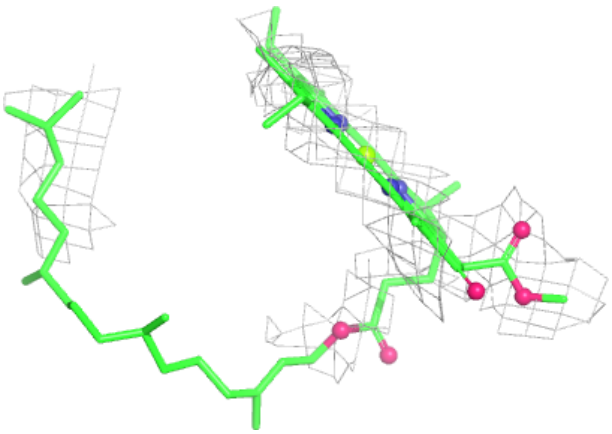


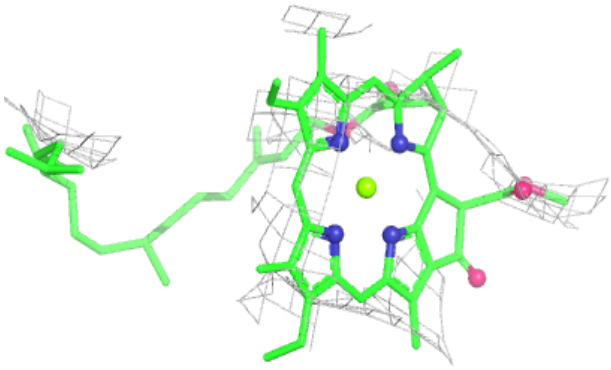


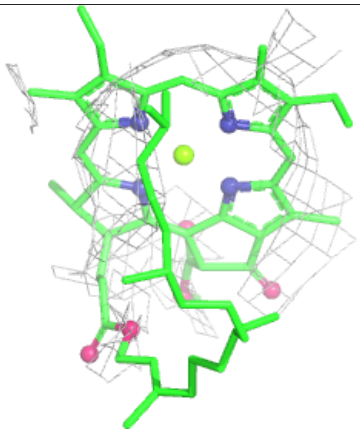


Electron density around CLA b 615:

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

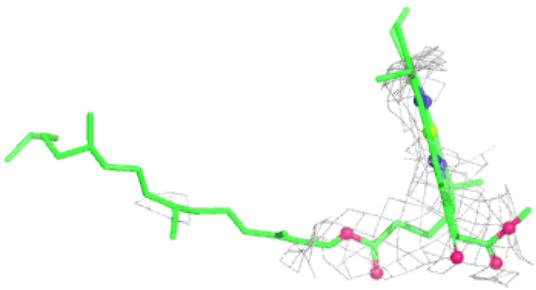


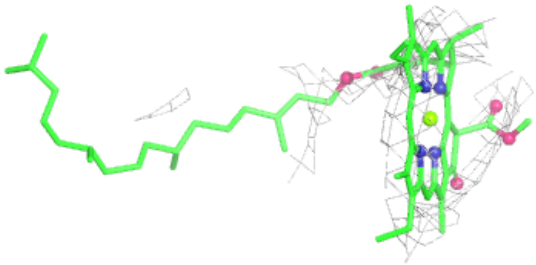


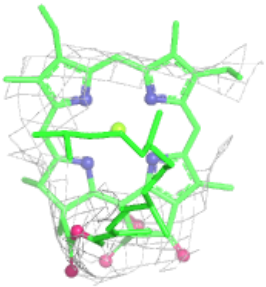


Electron density around CLA b 609:

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

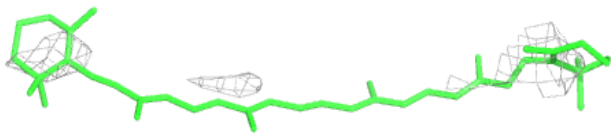


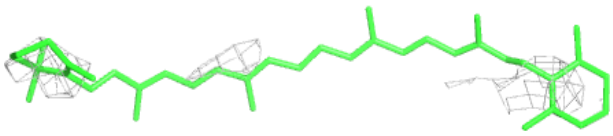


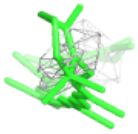


Electron density around BCR d 405:

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

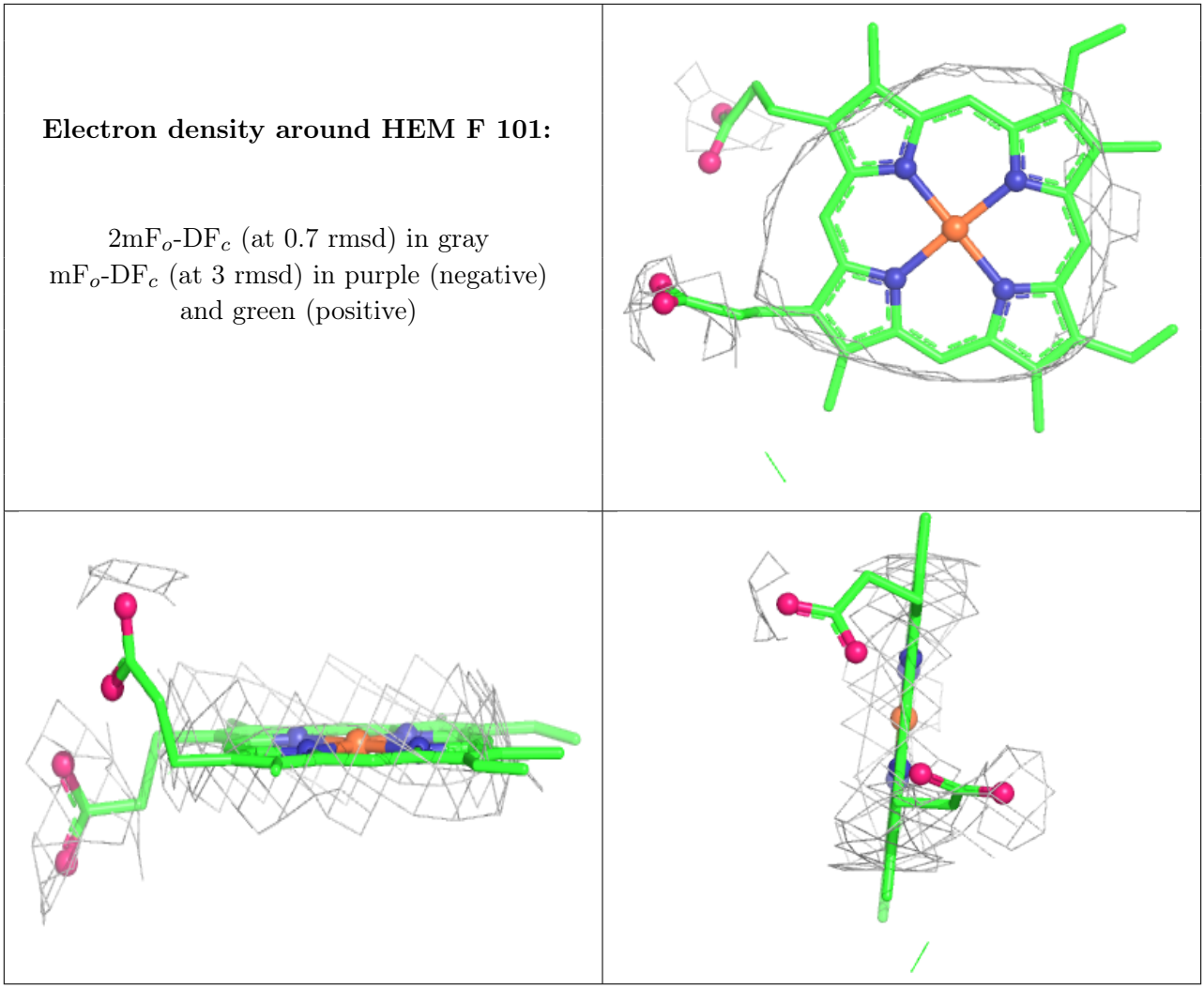






Electron density around HEM F 101:

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



6.5 Other polymers (i)

There are no such residues in this entry.