wwPDB X-ray Structure Validation Summary Report (i)

Aug 2, 2026 – 11:33 PM EDT

PDB ID	:	4TNH / pdb_00004tnh
Title	:	RT XFEL structure of Photosystem II in the dark state at 4.9 A resolution
Authors	:	Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on	:	2014-06-04
Resolution	:	4.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

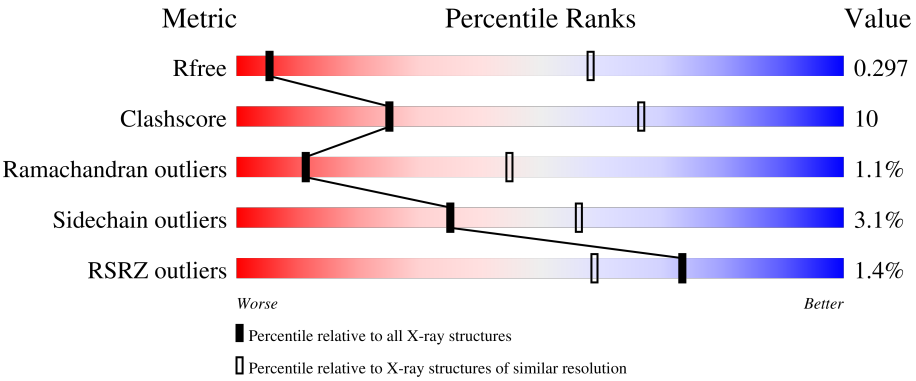
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)

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 4.90 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	1007 (5.82-3.96)
Clashscore	190562	1020 (5.82-3.98)
Ramachandran outliers	187476	1123 (5.90-3.90)
Sidechain outliers	187428	1103 (5.90-3.90)
RSRZ outliers	180081	1002 (5.82-3.96)

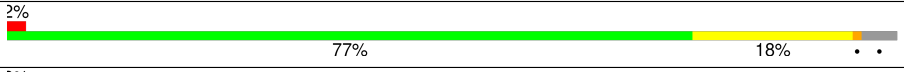
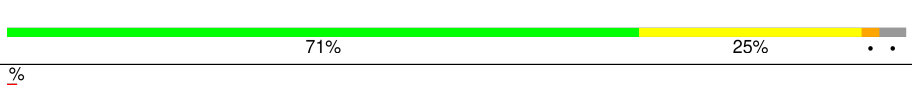
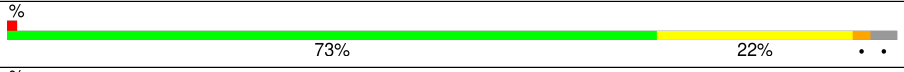
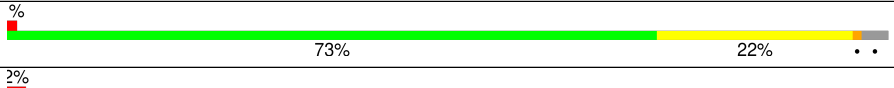
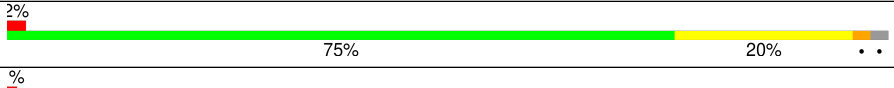
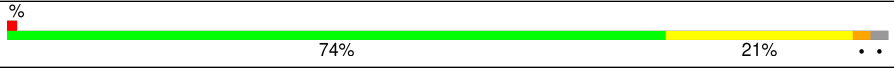
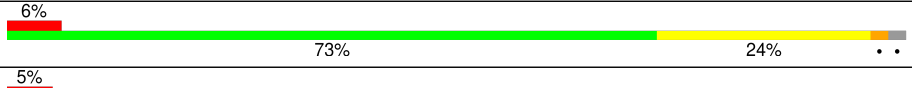
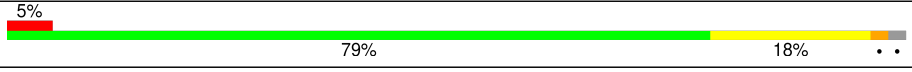
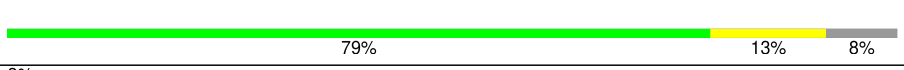
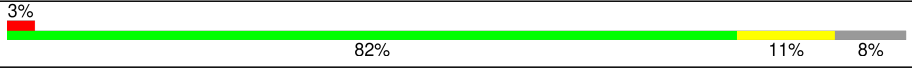
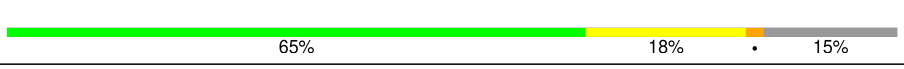
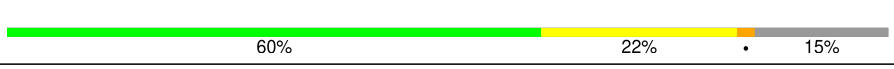
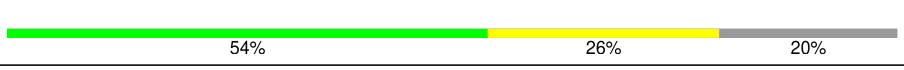
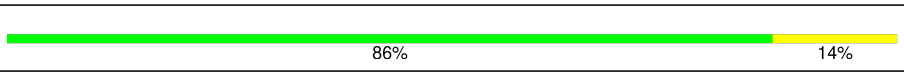
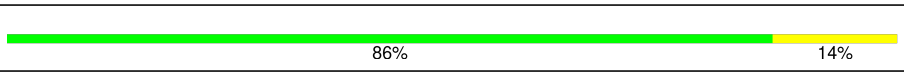
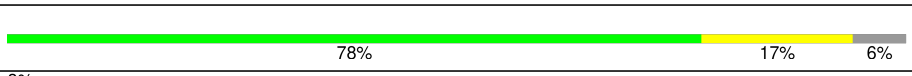
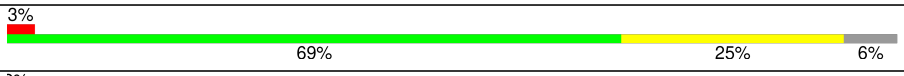
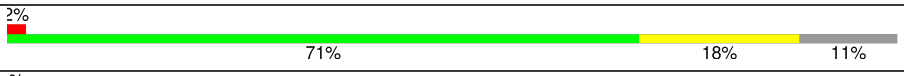
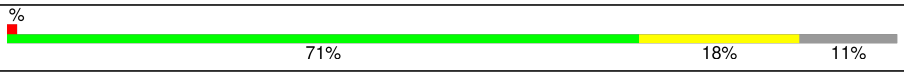
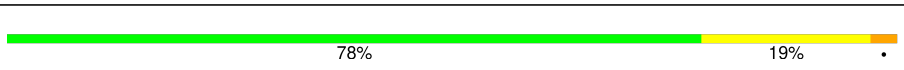
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	% 70% 25%
1	a	344	69% 27%

Continued on next page...

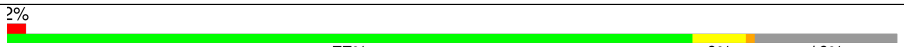
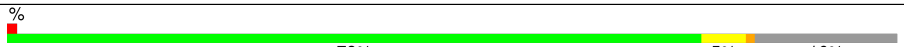
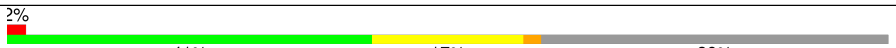
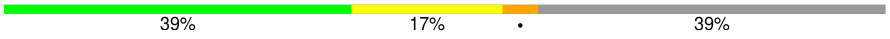
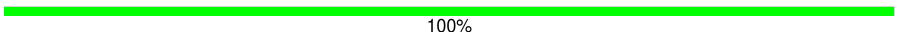
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 50244 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
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	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 Y.

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

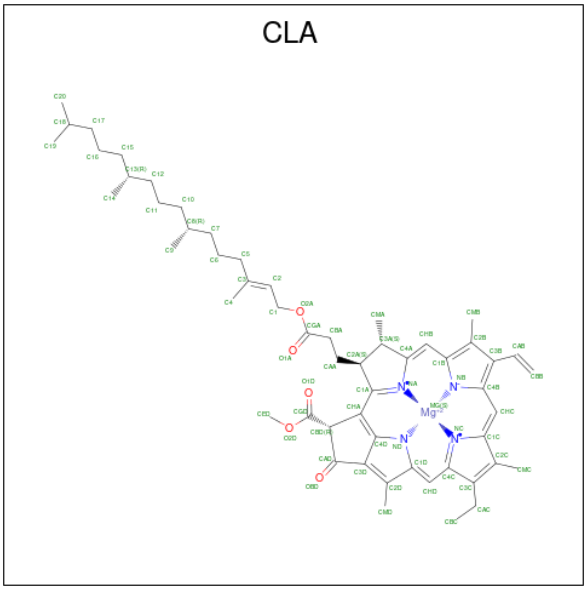
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

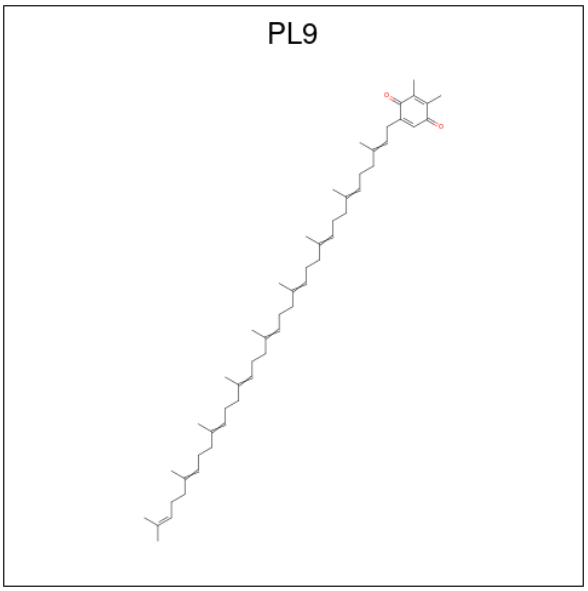
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

Continued on next page...

Continued from previous page...

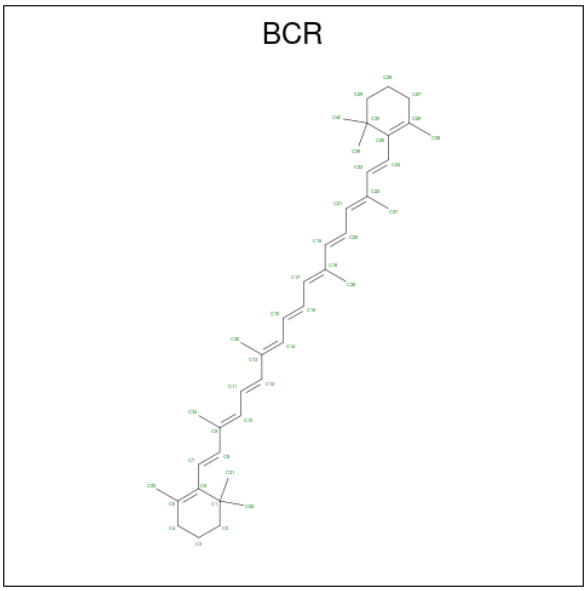
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 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
23	A	1	Total C O 45 43 2	0	0
23	D	1	Total C O 55 53 2	0	0
23	J	1	Total C O 35 33 2	0	0
23	a	1	Total C O 45 43 2	0	0
23	d	1	Total C O 55 53 2	0	0
23	j	1	Total C O 35 33 2	0	0

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



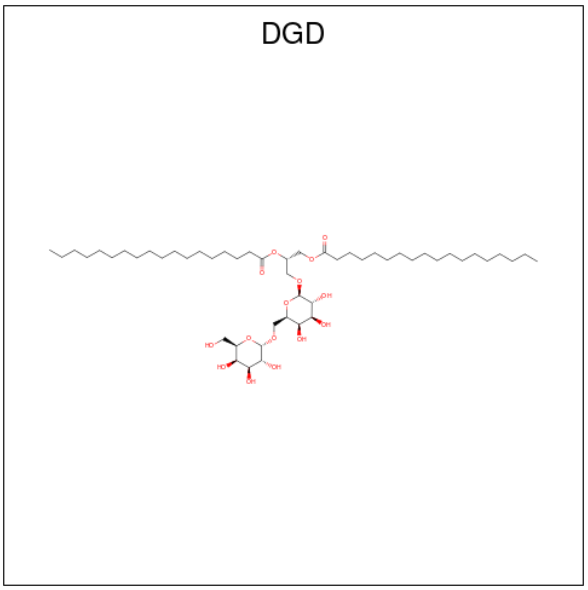
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



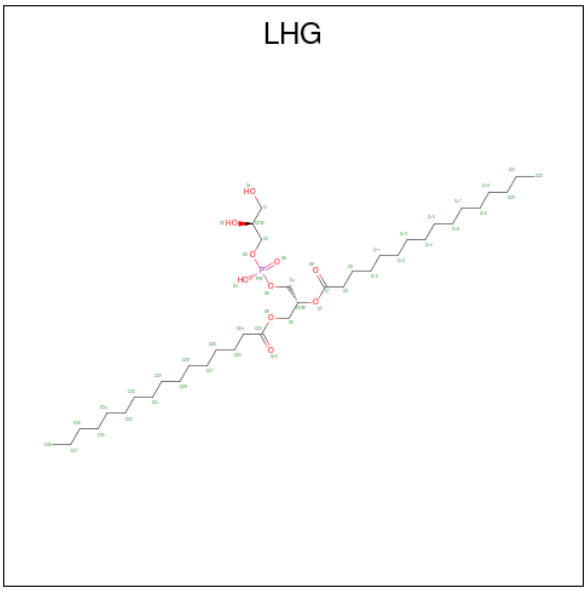
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

Continued on next page...

Continued from previous page...

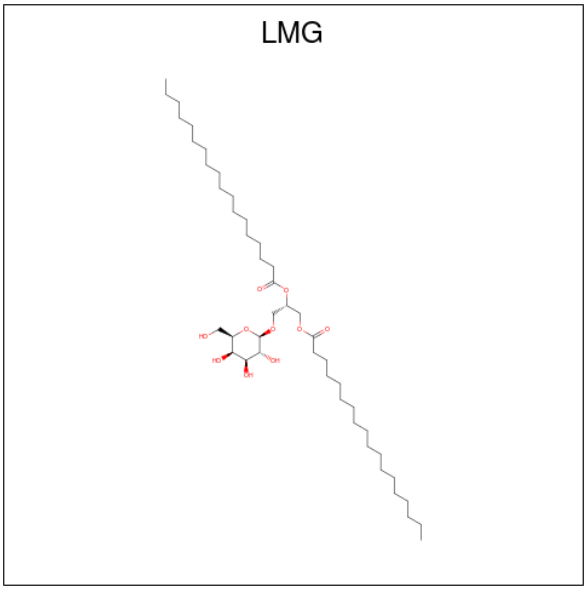
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 58 43 15	0	0
25	B	1	Total C O 52 37 15	0	0
25	C	1	Total C O 53 38 15	0	0
25	C	1	Total C O 62 47 15	0	0
25	C	1	Total C O 66 51 15	0	0
25	D	1	Total C O 63 48 15	0	0
25	a	1	Total C O 56 41 15	0	0
25	b	1	Total C O 52 37 15	0	0
25	b	1	Total C O 58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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

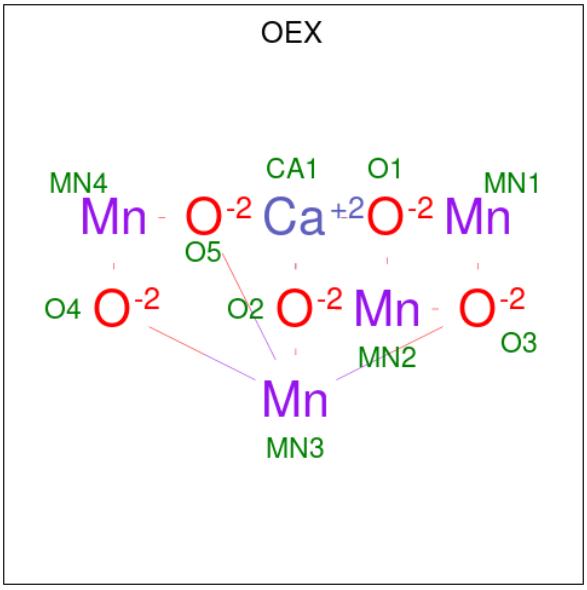


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 51 41 10	0	0
27	A	1	Total C O 42 32 10	0	0
27	B	1	Total C O 49 39 10	0	0
27	C	1	Total C O 45 35 10	0	0
27	C	1	Total C O 48 38 10	0	0
27	D	1	Total C O 49 39 10	0	0
27	D	1	Total C O 48 38 10	0	0
27	D	1	Total C O 46 36 10	0	0
27	E	1	Total C O 44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

- Molecule 28 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

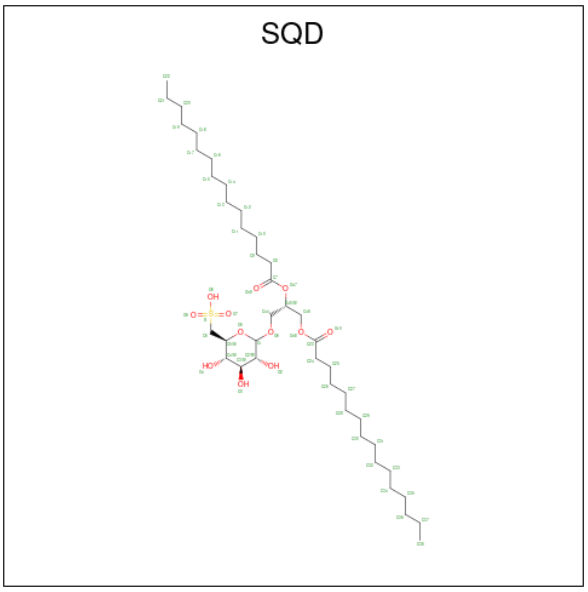
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total Cl 1 1	0	0
28	a	1	Total Cl 1 1	0	0

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



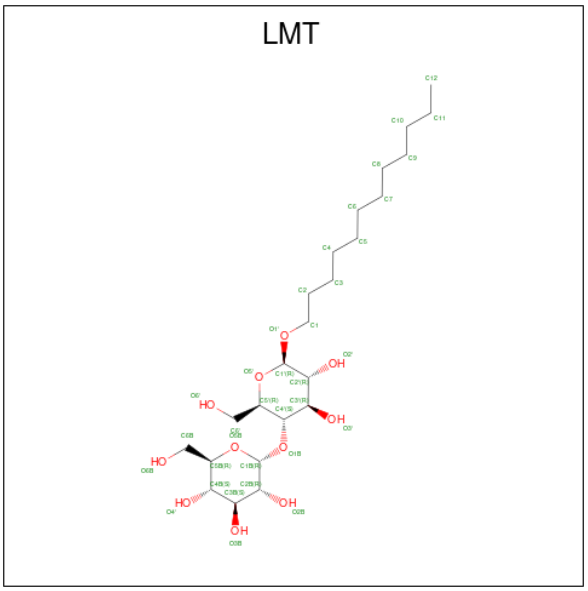
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Ca Mn O 10 1 4 5	0	0
29	a	1	Total Ca Mn O 10 1 4 5	0	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



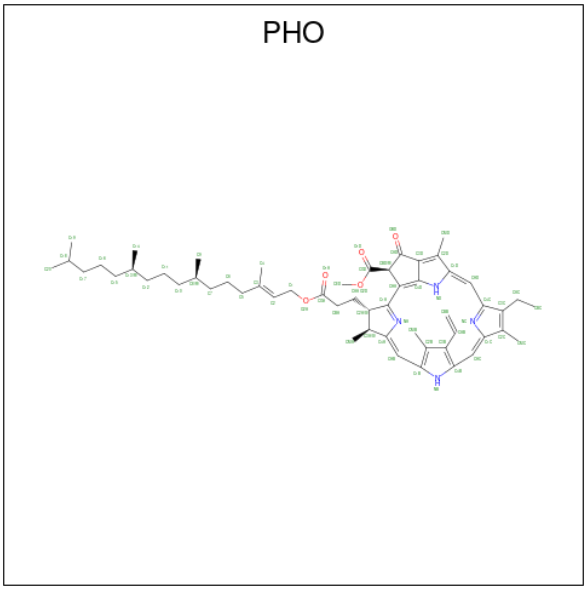
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			43	30	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			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 DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



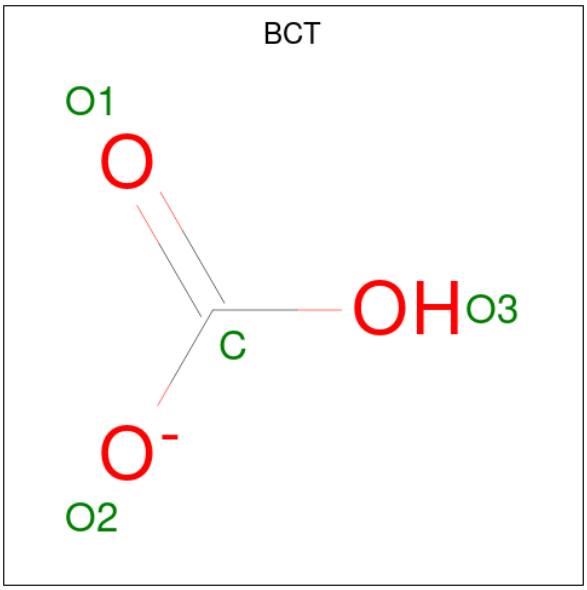
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	D	1	Total C O 31 20 11	0	0
31	I	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35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

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



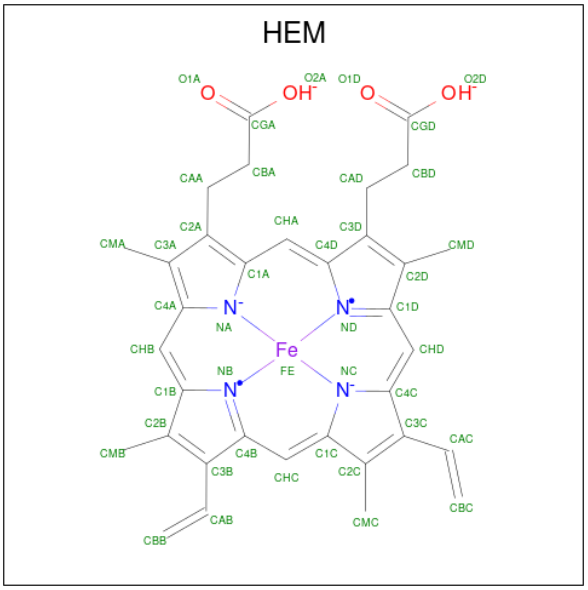
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	D	1	Total C N O 64 55 4 5	0	0
32	D	1	Total C N O 64 55 4 5	0	0
32	a	1	Total C N O 64 55 4 5	0	0
32	d	1	Total C N O 64 55 4 5	0	0

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



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

Continued on next page...

Continued from previous page...

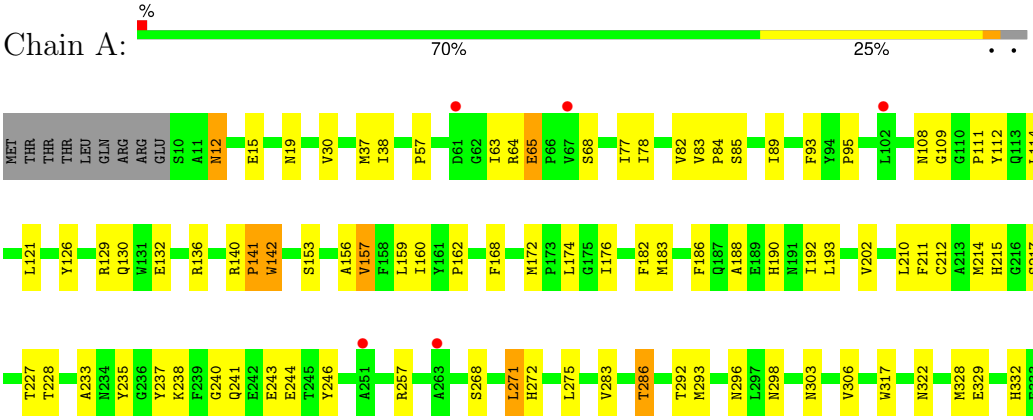
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total	Ca	0	0
			1	1		

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.

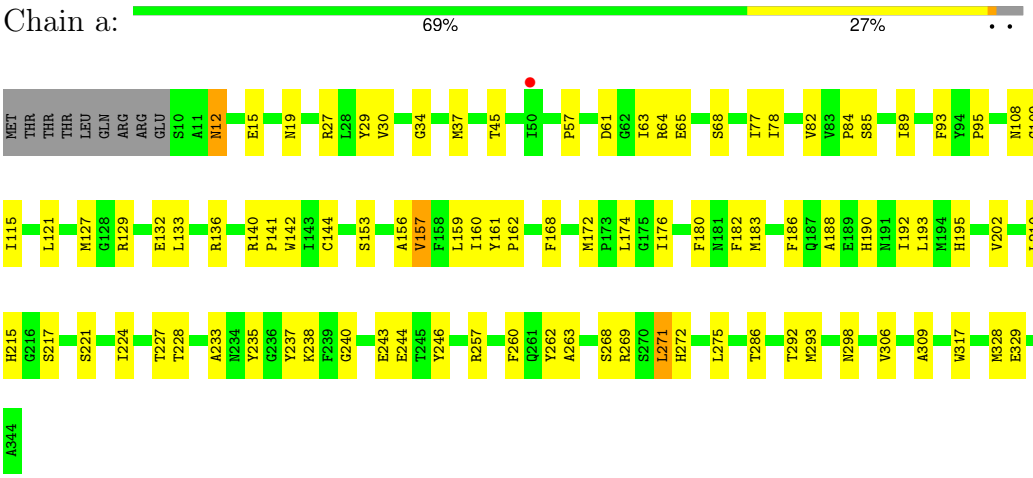
• Molecule 1: Photosystem Q(B) protein 1

Chain A:



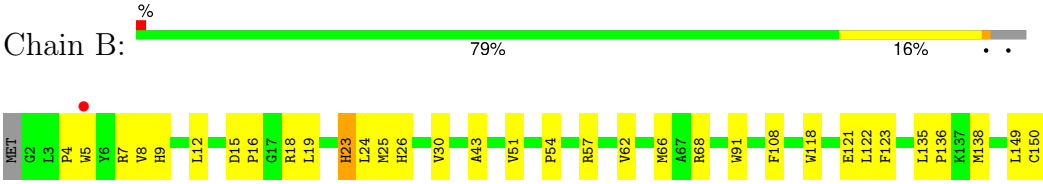
• Molecule 1: Photosystem Q(B) protein 1

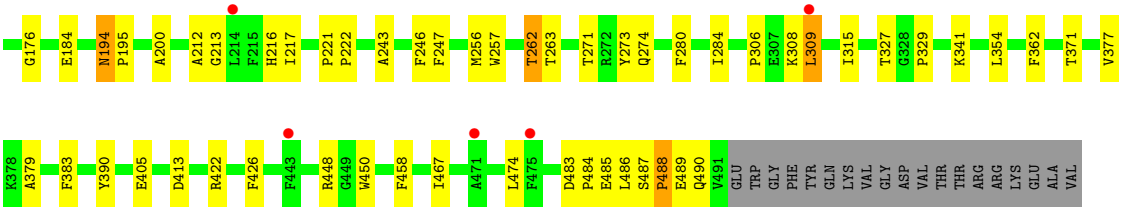
Chain a:



• Molecule 2: Photosystem II core light harvesting protein

Chain B:

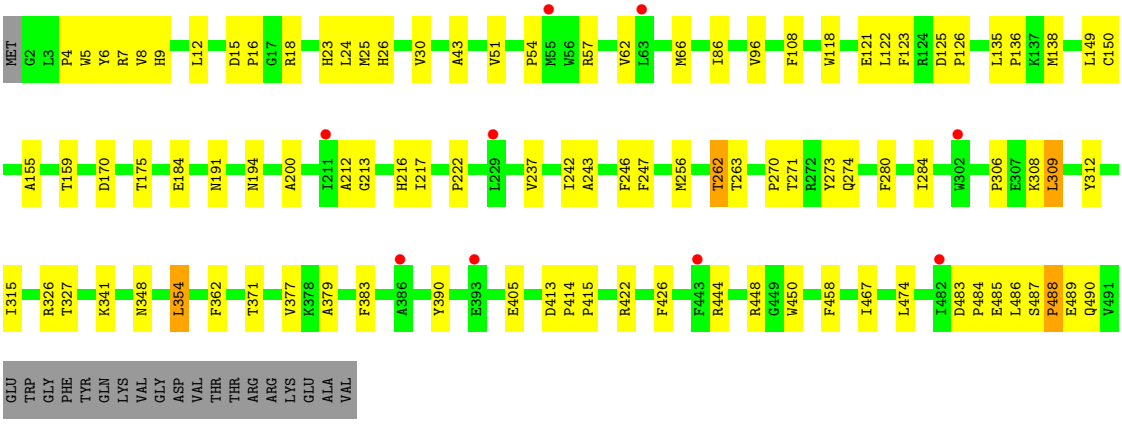




• Molecule 2: Photosystem II core light harvesting protein

Chain b:

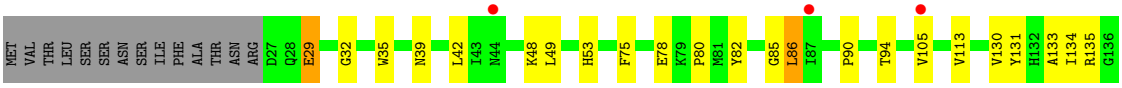


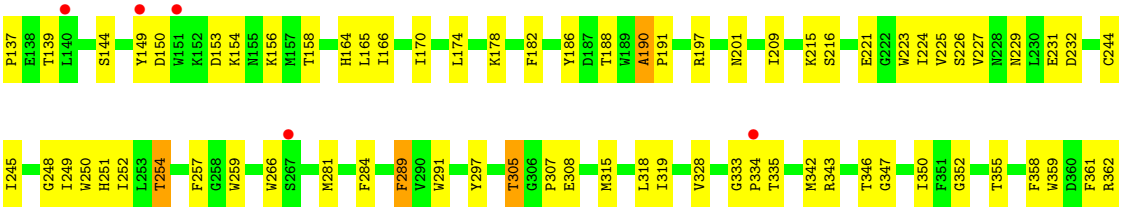


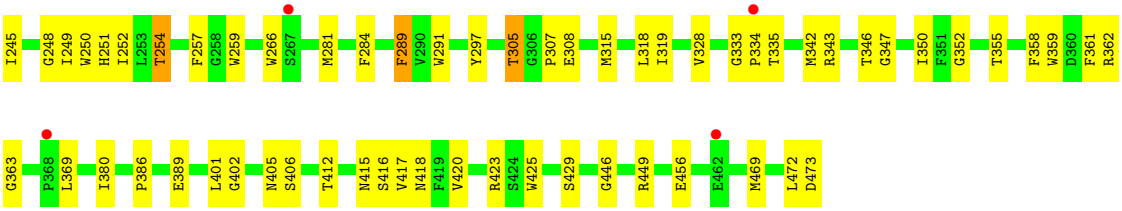
• Molecule 3: Photosystem II CP43 protein

Chain C:







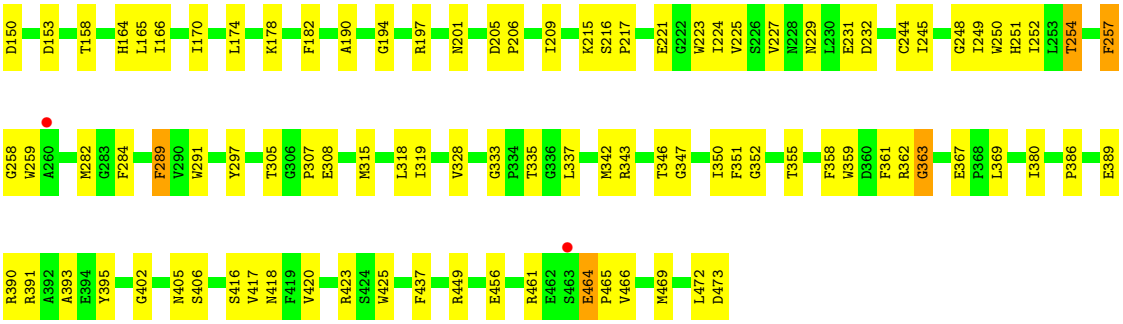


• Molecule 3: Photosystem II CP43 protein

Chain c:



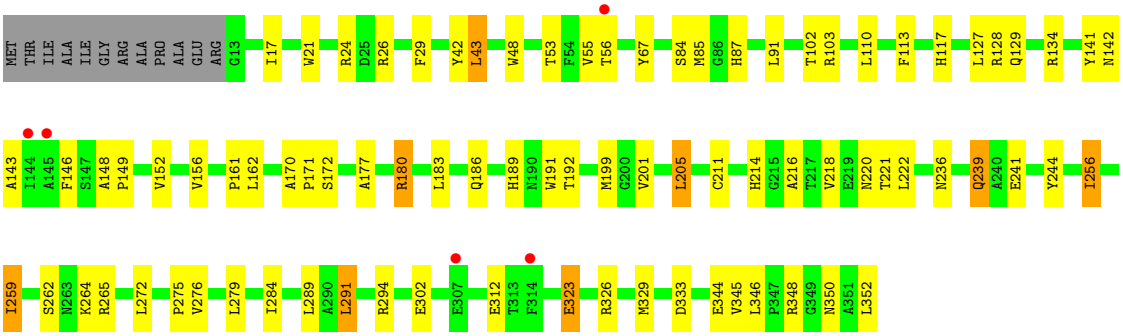




• Molecule 4: Photosystem II D2 protein

Chain D:

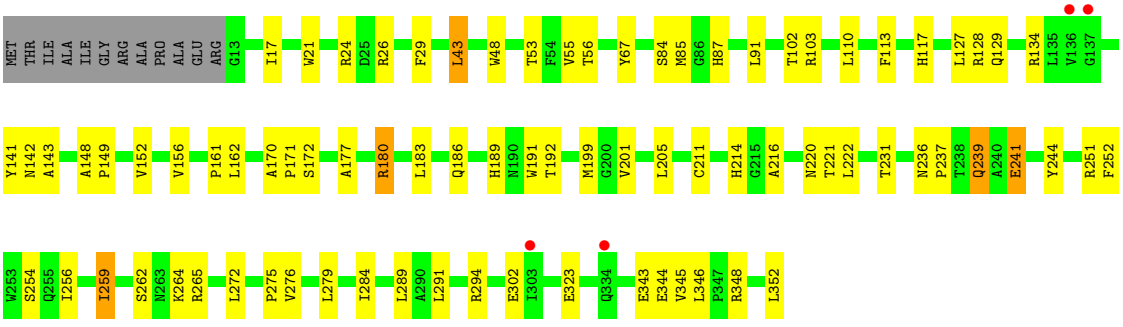




• Molecule 4: Photosystem II D2 protein

Chain d:





• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

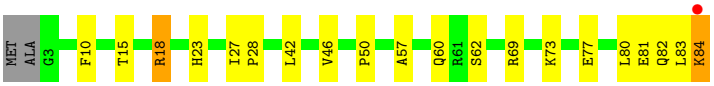




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

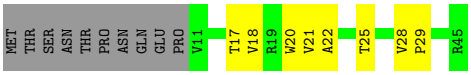




• Molecule 6: Cytochrome b559 subunit beta

Chain F:





• Molecule 6: Cytochrome b559 subunit beta

Chain f:

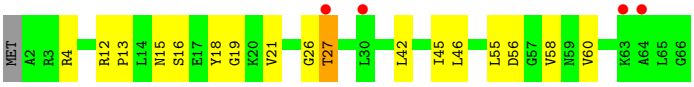




• Molecule 7: Photosystem II reaction center protein H

Chain H:

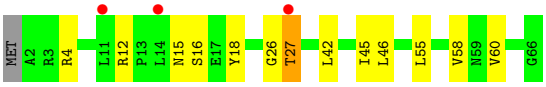




• Molecule 7: Photosystem II reaction center protein H

Chain h:

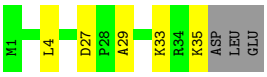




• Molecule 8: Photosystem II reaction center protein I

Chain I:

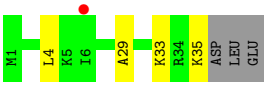




• Molecule 8: Photosystem II reaction center protein I

Chain i:

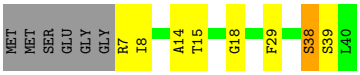




• Molecule 9: Photosystem II reaction center protein J

Chain J:





• Molecule 9: Photosystem II reaction center protein J

Chain j:

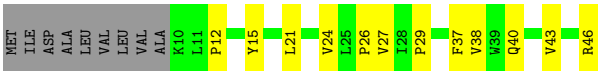




• Molecule 10: Photosystem II reaction center protein K

Chain K:

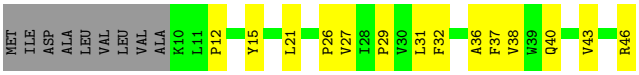




• Molecule 10: Photosystem II reaction center protein K

Chain k:

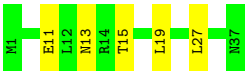




• Molecule 11: Photosystem II reaction center protein L

Chain L:

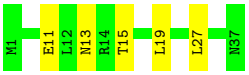




• Molecule 11: Photosystem II reaction center protein L

Chain l:

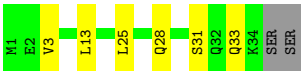




• Molecule 12: Photosystem II reaction center protein M

Chain M:

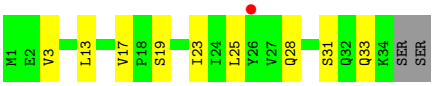




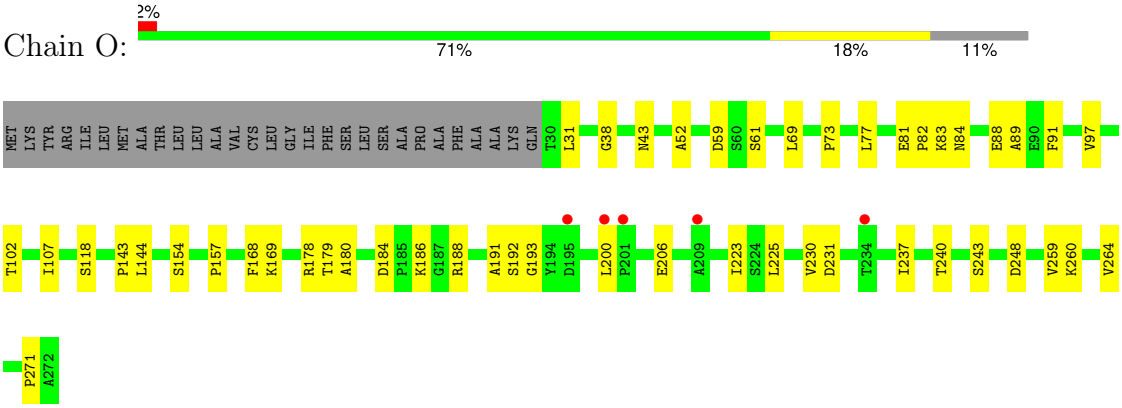
• Molecule 12: Photosystem II reaction center protein M

Chain m:

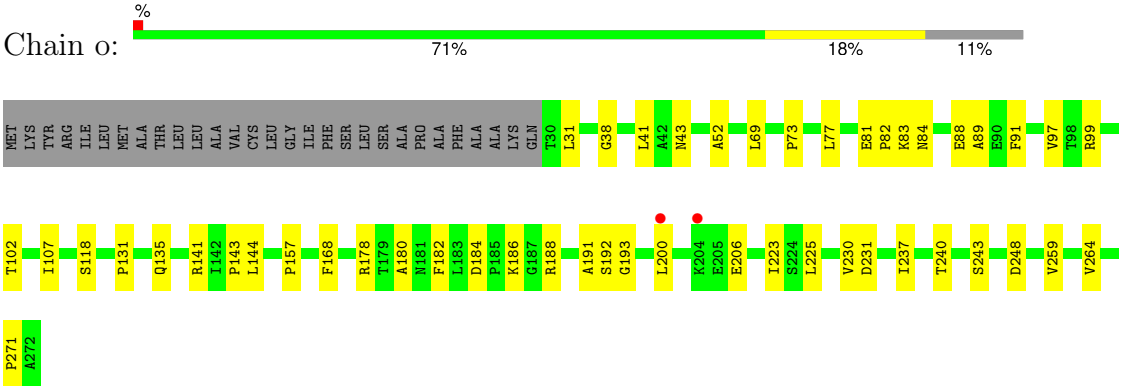




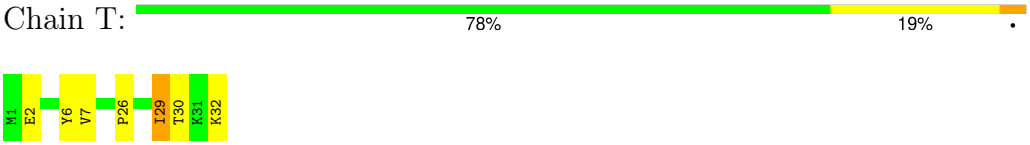
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



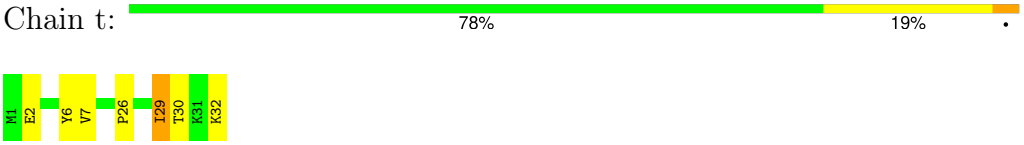
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



• Molecule 14: Photosystem II reaction center protein T

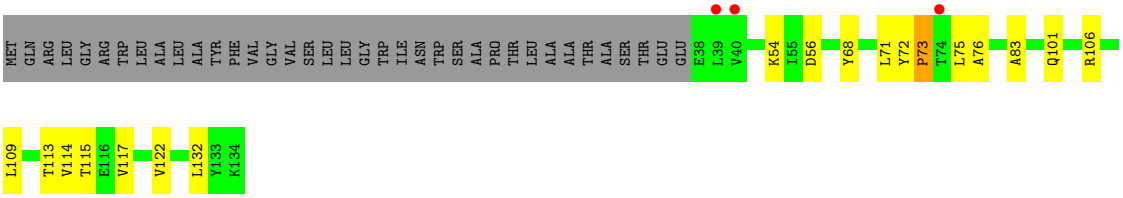


• Molecule 14: Photosystem II reaction center protein T



• Molecule 15: Photosystem II 12 kDa extrinsic protein

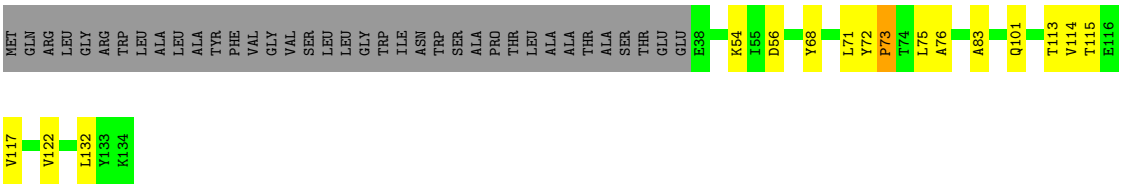




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:

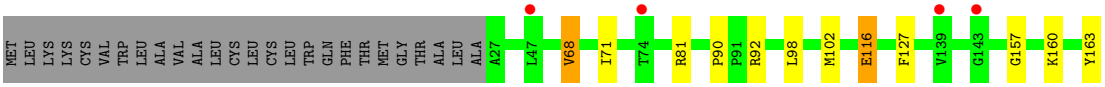




• Molecule 16: Cytochrome c-550

Chain V:

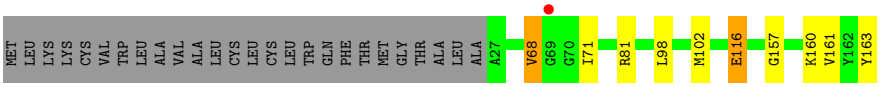




• Molecule 16: Cytochrome c-550

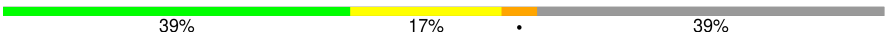
Chain v:

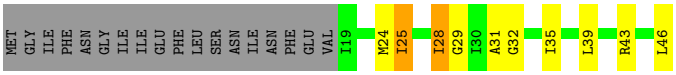




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:

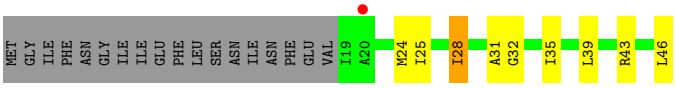




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain 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 Y

Chain Y:



There are no outlier residues recorded for this chain.

• Molecule 19: Photosystem II reaction center protein Y

Chain G:

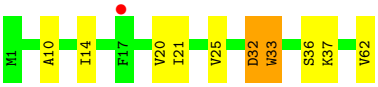


There are no outlier residues recorded for this chain.

• Molecule 20: Photosystem II reaction center protein Z

Chain Z:

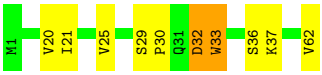




• Molecule 20: Photosystem II reaction center protein Z

Chain z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.88Å 229.03Å 307.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.93 – 4.90 72.93 – 4.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (72.93-4.90) 97.8 (72.93-4.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.281 , 0.292 0.287 , 0.297	Depositor DCC
R_{free} test set	2096 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	173.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 153.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å^2)	206.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: BCR, PL9, CL, LMT, DGD, LMG, SQD, PHO, OEX, LHG, HEM, BCT, FE2, CA, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	0/2713	0.78	2/3700 (0.1%)
1	a	0.31	0/2713	0.78	2/3700 (0.1%)
2	B	0.30	0/3986	0.81	8/5433 (0.1%)
2	b	0.30	0/3986	0.81	8/5433 (0.1%)
3	C	0.30	0/3556	0.79	6/4842 (0.1%)
3	c	0.30	0/3556	0.80	8/4842 (0.2%)
4	D	0.29	0/2801	0.76	0/3818
4	d	0.30	0/2801	0.76	0/3818
5	E	0.31	0/685	0.83	0/933
5	e	0.32	0/685	0.83	0/933
6	F	0.33	0/291	0.75	0/397
6	f	0.33	0/291	0.73	0/397
7	H	0.33	0/520	0.73	0/709
7	h	0.33	0/520	0.74	0/709
8	I	0.30	0/293	0.77	0/395
8	i	0.29	0/293	0.77	0/395
9	J	0.30	0/255	0.84	0/346
9	j	0.31	0/255	0.84	0/346
10	K	0.45	0/303	0.86	0/416
10	k	0.45	0/303	0.86	0/416
11	L	0.28	0/311	0.71	0/422
11	l	0.28	0/311	0.72	0/422
12	M	0.30	0/270	0.78	0/367
12	m	0.33	0/270	0.85	1/367 (0.3%)
13	O	0.28	0/1876	0.71	2/2548 (0.1%)
13	o	0.27	0/1876	0.71	2/2548 (0.1%)
14	T	0.27	0/284	0.75	0/381
14	t	0.27	0/284	0.74	0/381
15	U	0.29	0/785	0.77	0/1064
15	u	0.29	0/785	0.78	0/1064
16	V	0.29	0/1081	0.76	2/1468 (0.1%)
16	v	0.30	0/1081	0.75	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	g	0.32	0/202	0.79	0/272
17	y	0.32	0/202	0.76	0/272
18	X	0.39	0/273	0.80	0/370
18	x	0.37	0/273	0.79	0/370
20	Z	0.31	0/490	0.83	0/669
20	z	0.31	0/490	0.84	0/669
All	All	0.30	0/41950	0.78	41/57100 (0.1%)

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	483	ASP	CA-C-N	10.63	133.13	119.84
2	b	483	ASP	C-N-CA	10.63	133.13	119.84
2	B	483	ASP	CA-C-N	10.59	133.08	119.84
2	B	483	ASP	C-N-CA	10.59	133.08	119.84
3	c	190	ALA	CA-C-N	6.24	125.73	119.24

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	2628	0	2524	75	0
1	a	2628	0	2524	71	0
2	B	3850	0	3718	60	0
2	b	3850	0	3718	64	0
3	C	3444	0	3365	76	0
3	c	3444	0	3365	78	0
4	D	2706	0	2608	66	0
4	d	2706	0	2608	61	0
5	E	666	0	651	13	0
5	e	666	0	651	13	0
6	F	282	0	291	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	282	0	291	6	0
7	H	507	0	521	12	0
7	h	507	0	521	13	0
8	I	286	0	308	3	0
8	i	286	0	308	2	0
9	J	249	0	262	6	0
9	j	249	0	262	7	0
10	K	293	0	305	9	0
10	k	293	0	305	12	0
11	L	304	0	316	4	0
11	l	304	0	316	4	0
12	M	267	0	289	6	0
12	m	267	0	289	8	0
13	O	1845	0	1801	28	0
13	o	1845	0	1801	30	0
14	T	275	0	288	6	0
14	t	275	0	288	6	0
15	U	774	0	773	8	0
15	u	774	0	773	7	0
16	V	1060	0	1068	8	0
16	v	1060	0	1068	8	0
17	g	201	0	226	7	0
17	y	201	0	226	8	0
18	X	270	0	299	10	0
18	x	270	0	299	9	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	8	0
20	z	479	0	516	8	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	27	0
22	B	975	0	1080	56	0
22	C	845	0	936	29	0
22	D	130	0	144	14	0
22	H	65	0	72	9	0
22	a	260	0	288	26	0
22	b	975	0	1080	50	0
22	c	845	0	936	32	0
22	d	130	0	144	11	0
22	h	65	0	72	10	0
23	A	45	0	61	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	D	55	0	80	8	0
23	J	35	0	45	0	0
23	a	45	0	61	4	0
23	d	55	0	80	6	0
23	j	35	0	45	0	0
24	A	40	0	56	2	0
24	B	160	0	224	13	0
24	C	80	0	112	10	0
24	F	40	0	56	3	0
24	H	40	0	56	2	0
24	J	40	0	56	2	0
24	K	40	0	56	3	0
24	a	40	0	56	4	0
24	b	160	0	224	12	0
24	c	120	0	168	13	0
24	f	40	0	56	1	0
24	g	40	0	56	5	0
24	j	40	0	56	1	0
24	x	40	0	56	0	0
24	y	40	0	56	6	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	12	0
25	D	63	0	87	1	0
25	a	56	0	70	3	0
25	b	110	0	136	4	0
25	c	181	0	245	11	0
25	d	63	0	87	1	0
26	A	39	0	51	3	0
26	C	37	0	44	3	0
26	a	39	0	51	1	0
26	c	37	0	44	2	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	2	0
27	D	143	0	196	9	0
27	E	44	0	58	1	0
27	I	43	0	56	0	0
27	M	42	0	54	1	0
27	a	42	0	54	1	0
27	b	49	0	68	4	0
27	c	93	0	126	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	d	143	0	196	10	0
27	e	44	0	58	2	0
27	i	43	0	56	1	0
27	l	51	0	72	2	0
27	m	42	0	54	2	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	8	0
30	B	90	0	111	5	0
30	F	45	0	54	2	0
30	a	105	0	147	8	0
30	b	47	0	61	2	0
30	d	43	0	50	3	0
30	f	45	0	54	3	0
31	B	140	0	184	6	0
31	D	31	0	35	0	0
31	I	35	0	46	0	0
31	M	70	0	92	0	0
31	b	140	0	183	5	0
31	d	31	0	35	0	0
31	i	35	0	46	1	0
32	D	128	0	148	11	0
32	a	64	0	74	4	0
32	d	64	0	74	5	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	4	0
34	f	43	0	30	4	0
34	v	43	0	30	5	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51373	983	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 10.

The worst 5 of 983 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:39:ASN:HB2	22:c:507:CLA:HBA1	1.57	0.86
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.56	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.82
12:M:33:GLN:HB3	12:m:33:GLN:HB3	1.61	0.81
3:c:362:ARG:H	25:c:515:DGD:HE4	1.46	0.80

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	333/344 (97%)	312 (94%)	17 (5%)	4 (1%)	10 42
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	10 42
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	16 52
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	21 58
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	14 49
3	c	445/461 (96%)	405 (91%)	35 (8%)	5 (1%)	11 45
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	36 71
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	36 71
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9 41
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	9 41
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100 100
6	f	33/45 (73%)	29 (88%)	4 (12%)	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%)	6 (18%)	0	100 100
8	i	33/38 (87%)	27 (82%)	6 (18%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3 21
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	3 21
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100 100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100 100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
13	O	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	10 42
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	10 42
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3 20
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3 20
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5 29
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	5 29
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100 100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100 100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2 19
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	2 19
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1 14
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1 14
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7 35
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7 35
All	All	5138/5618 (92%)	4678 (91%)	404 (8%)	56 (1%)	11 45

5 of 56 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

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	271/280 (97%)	261 (96%)	10 (4%)	30	51
1	a	271/280 (97%)	261 (96%)	10 (4%)	30	51
2	B	390/407 (96%)	380 (97%)	10 (3%)	40	61
2	b	390/407 (96%)	380 (97%)	10 (3%)	40	61
3	C	347/362 (96%)	335 (96%)	12 (4%)	32	53
3	c	347/362 (96%)	336 (97%)	11 (3%)	34	55
4	D	275/283 (97%)	263 (96%)	12 (4%)	25	47
4	d	275/283 (97%)	264 (96%)	11 (4%)	28	49
5	E	72/73 (99%)	68 (94%)	4 (6%)	19	41
5	e	72/73 (99%)	68 (94%)	4 (6%)	19	41
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	51
8	I	32/35 (91%)	31 (97%)	1 (3%)	35	56
8	i	32/35 (91%)	31 (97%)	1 (3%)	35	56
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	48
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	48
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	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	76
13	o	202/228 (89%)	200 (99%)	2 (1%)	68	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	82 (98%)	2 (2%)	43	63
16	V	116/138 (84%)	114 (98%)	2 (2%)	53	68
16	v	116/138 (84%)	114 (98%)	2 (2%)	53	68
17	g	20/37 (54%)	17 (85%)	3 (15%)	3	13
17	y	20/37 (54%)	17 (85%)	3 (15%)	3	13
18	X	30/34 (88%)	28 (93%)	2 (7%)	15	37
18	x	30/34 (88%)	28 (93%)	2 (7%)	15	37
20	Z	52/52 (100%)	50 (96%)	2 (4%)	29	51
20	z	52/52 (100%)	50 (96%)	2 (4%)	29	51
All	All	4244/4594 (92%)	4111 (97%)	133 (3%)	35	56

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	h	60	VAL
13	o	31	LEU
18	x	42	GLN
7	H	27	THR
5	E	84	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	322	ASN
12	m	33	GLN
13	o	173	ASN
15	U	93	ASN
13	O	173	ASN

5.3.3 RNA

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	$\#\|Z\| > 2$
22	CLA	B	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
31	LMT	I	102	-	36,36,36	1.09	4 (11%)	47,47,47	1.03	2 (4%)
30	SQD	b	602	-	45,47,54	1.02	3 (6%)	55,58,65	1.72	10 (18%)
22	CLA	C	505	3	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
25	DGD	A	408	-	57,57,67	0.92	0	71,71,81	1.41	9 (12%)
22	CLA	C	520	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
27	LMG	A	410	-	51,51,55	0.75	0	59,59,63	1.36	7 (11%)
22	CLA	c	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
33	BCT	d	403	21	3,3,3	1.11	0	2,3,3	4.23	2 (100%)
24	BCR	A	407	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	7 (12%)
22	CLA	b	617	2	69,73,73	1.18	6 (8%)	82,113,113	1.26	4 (4%)
22	CLA	c	507	3	69,73,73	1.18	7 (10%)	82,113,113	1.30	7 (8%)
24	BCR	c	514	-	41,41,41	1.14	3 (7%)	56,56,56	1.31	8 (14%)
22	CLA	h	101	-	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)
22	CLA	A	405	1	69,73,73	1.19	8 (11%)	82,113,113	1.22	4 (4%)
27	LMG	M	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.22	4 (8%)
22	CLA	c	503	-	69,73,73	1.20	6 (8%)	82,113,113	1.28	5 (6%)
22	CLA	d	404	-	69,73,73	1.19	7 (10%)	82,113,113	1.21	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	b	620	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	5 (8%)
22	CLA	B	609	-	69,73,73	1.19	8 (11%)	82,113,113	1.28	5 (6%)
22	CLA	b	610	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	6 (7%)
26	LHG	a	412	-	38,38,48	0.71	1 (2%)	41,44,54	1.23	3 (7%)
27	LMG	C	518	-	45,45,55	0.76	0	53,53,63	1.29	5 (9%)
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	7 (12%)
22	CLA	b	614	2	69,73,73	1.24	7 (10%)	82,113,113	1.34	7 (8%)
27	LMG	C	521	-	48,48,55	0.76	1 (2%)	56,56,63	1.30	5 (8%)
22	CLA	A	404	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.31	7 (10%)
22	CLA	B	605	2	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
27	LMG	l	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.34	6 (10%)
24	BCR	g	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.31	8 (14%)
22	CLA	B	606	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
34	HEM	V	201	16	50,50,50	1.98	10 (20%)	67,82,82	1.21	3 (4%)
22	CLA	C	502	3	69,73,73	1.19	9 (13%)	82,113,113	1.26	5 (6%)
24	BCR	B	618	-	41,41,41	1.13	2 (4%)	56,56,56	1.40	9 (16%)
32	PHO	D	402	-	58,69,69	2.18	9 (15%)	55,99,99	1.39	5 (9%)
22	CLA	B	608	2	69,73,73	1.20	6 (8%)	82,113,113	1.24	5 (6%)
22	CLA	D	404	-	69,73,73	1.19	8 (11%)	82,113,113	1.20	5 (6%)
27	LMG	i	101	-	43,43,55	0.81	0	51,51,63	1.27	5 (9%)
22	CLA	C	501	3	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	B	614	-	69,73,73	1.19	6 (8%)	82,113,113	1.25	5 (6%)
22	CLA	C	503	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	5 (6%)
22	CLA	b	606	2	69,73,73	1.19	6 (8%)	82,113,113	1.24	7 (8%)
25	DGD	C	515	-	54,54,67	0.96	2 (3%)	68,68,81	1.26	5 (7%)
34	HEM	v	201	16	50,50,50	2.00	10 (20%)	67,82,82	1.25	4 (5%)
24	BCR	B	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
32	PHO	d	401	-	58,69,69	2.14	9 (15%)	55,99,99	1.41	7 (12%)
31	LMT	B	627	-	36,36,36	1.11	4 (11%)	47,47,47	0.97	1 (2%)
25	DGD	c	517	-	67,67,67	0.87	0	81,81,81	1.39	9 (11%)
27	LMG	A	415	-	42,42,55	0.83	1 (2%)	50,50,63	1.26	5 (10%)
22	CLA	C	504	3	69,73,73	1.18	7 (10%)	82,113,113	1.31	7 (8%)
30	SQD	d	402	-	41,43,54	1.05	2 (4%)	51,54,65	1.71	11 (21%)
25	DGD	b	601	-	53,53,67	1.05	2 (3%)	67,67,81	1.33	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	HEM	F	101	6,5	50,50,50	1.96	9 (18%)	67,82,82	1.31	4 (5%)
27	LMG	m	101	-	42,42,55	0.85	1 (2%)	50,50,63	1.25	4 (8%)
22	CLA	b	618	-	69,73,73	1.19	5 (7%)	82,113,113	1.27	5 (6%)
33	BCT	D	403	21	3,3,3	1.10	0	2,3,3	4.25	2 (100%)
30	SQD	f	103	-	43,45,54	1.03	2 (4%)	53,56,65	1.58	10 (18%)
23	PL9	d	406	-	55,55,55	1.03	3 (5%)	68,69,69	1.51	13 (19%)
22	CLA	B	607	2	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
24	BCR	H	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	6 (10%)
25	DGD	a	411	-	57,57,67	0.92	1 (1%)	71,71,81	1.40	8 (11%)
26	LHG	C	519	-	36,36,48	0.71	1 (2%)	39,42,54	1.29	4 (10%)
22	CLA	b	619	2	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.29	4 (7%)
31	LMT	B	624	-	36,36,36	1.09	3 (8%)	47,47,47	1.01	2 (4%)
22	CLA	a	405	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	5 (6%)
22	CLA	a	406	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
24	BCR	b	623	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	9 (16%)
27	LMG	B	621	-	49,49,55	0.76	1 (2%)	57,57,63	1.32	7 (12%)
22	CLA	C	509	3	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
31	LMT	b	626	-	36,36,36	1.10	4 (11%)	47,47,47	0.97	1 (2%)
32	PHO	D	401	-	58,69,69	2.15	9 (15%)	55,99,99	1.40	6 (10%)
23	PL9	a	409	-	45,45,55	1.05	4 (8%)	56,57,69	1.55	11 (19%)
22	CLA	B	601	-	69,73,73	1.20	7 (10%)	82,113,113	1.26	6 (7%)
22	CLA	b	616	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	7 (8%)
22	CLA	A	403	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	5 (6%)
22	CLA	b	608	2	69,73,73	1.18	6 (8%)	82,113,113	1.26	4 (4%)
25	DGD	D	409	-	64,64,67	0.92	0	78,78,81	1.33	9 (11%)
31	LMT	M	102	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	c	510	3	69,73,73	1.20	5 (7%)	82,113,113	1.27	5 (6%)
23	PL9	j	101	-	35,35,55	0.97	2 (5%)	44,45,69	1.59	9 (20%)
24	BCR	b	621	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	8 (14%)
22	CLA	B	602	2	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
31	LMT	b	627	-	36,36,36	1.08	3 (8%)	47,47,47	1.01	2 (4%)
22	CLA	B	615	2	69,73,73	1.18	9 (13%)	82,113,113	1.26	5 (6%)
22	CLA	C	508	3	69,73,73	1.19	7 (10%)	82,113,113	1.24	5 (6%)
22	CLA	c	501	3	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	SQD	a	415	-	49,51,54	0.96	2 (4%)	59,62,65	1.69	9 (15%)
22	CLA	B	603	2	69,73,73	1.19	8 (11%)	82,113,113	1.34	7 (8%)
27	LMG	D	407	-	49,49,55	0.76	1 (2%)	57,57,63	1.31	5 (8%)
22	CLA	B	612	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	7 (8%)
30	SQD	A	413	-	49,51,54	0.96	2 (4%)	59,62,65	1.69	10 (16%)
25	DGD	c	516	-	63,63,67	0.90	1 (1%)	77,77,81	1.42	12 (15%)
23	PL9	D	406	-	55,55,55	1.05	3 (5%)	68,69,69	1.49	13 (19%)
25	DGD	b	624	-	59,59,67	0.90	1 (1%)	73,73,81	1.35	6 (8%)
27	LMG	c	522	-	48,48,55	0.76	0	56,56,63	1.30	5 (8%)
31	LMT	B	628	-	36,36,36	1.13	5 (13%)	47,47,47	1.05	1 (2%)
31	LMT	d	410	-	32,32,36	1.16	4 (12%)	43,43,47	1.01	2 (4%)
31	LMT	b	604	-	36,36,36	1.12	4 (11%)	47,47,47	1.04	1 (2%)
29	OEX	a	414	1,3	0,14,14	-	-	-		
22	CLA	c	504	3	69,73,73	1.18	6 (8%)	82,113,113	1.31	7 (8%)
29	OEX	A	412	1,3	0,14,14	-	-	-		
22	CLA	c	509	3	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)
22	CLA	a	408	1	69,73,73	1.18	6 (8%)	82,113,113	1.25	4 (4%)
27	LMG	I	101	-	43,43,55	0.80	0	51,51,63	1.26	4 (7%)
25	DGD	d	409	-	64,64,67	0.93	1 (1%)	78,78,81	1.34	9 (11%)
30	SQD	A	414	-	52,54,54	0.96	2 (3%)	62,65,65	1.49	9 (14%)
24	BCR	f	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	5 (8%)
22	CLA	b	613	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
24	BCR	C	513	-	41,41,41	1.13	2 (4%)	56,56,56	1.37	9 (16%)
22	CLA	b	607	2	69,73,73	1.19	7 (10%)	82,113,113	1.33	7 (8%)
31	LMT	D	410	-	32,32,36	1.17	4 (12%)	43,43,47	1.01	2 (4%)
24	BCR	j	102	-	41,41,41	1.10	3 (7%)	56,56,56	1.58	13 (23%)
22	CLA	C	512	3	69,73,73	1.19	7 (10%)	82,113,113	1.27	6 (7%)
23	PL9	J	101	-	35,35,55	1.00	2 (5%)	44,45,69	1.59	8 (18%)
22	CLA	c	505	3	69,73,73	1.20	6 (8%)	82,113,113	1.28	4 (4%)
22	CLA	b	605	-	69,73,73	1.21	7 (10%)	82,113,113	1.26	6 (7%)
25	DGD	B	620	-	59,59,67	0.92	1 (1%)	73,73,81	1.34	8 (10%)
22	CLA	C	510	3	69,73,73	1.19	6 (8%)	82,113,113	1.30	6 (7%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.29	6 (11%)
24	BCR	c	521	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	8 (14%)
25	DGD	C	517	-	67,67,67	0.88	1 (1%)	81,81,81	1.39	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	613	2	69,73,73	1.18	6 (8%)	82,113,113	1.26	6 (7%)
22	CLA	b	615	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
27	LMG	D	408	-	48,48,55	0.75	0	56,56,63	1.38	4 (7%)
26	LHG	c	519	-	36,36,48	0.74	2 (5%)	39,42,54	1.28	4 (10%)
24	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	8 (14%)
23	PL9	A	406	-	45,45,55	0.99	3 (6%)	56,57,69	1.55	10 (17%)
31	LMT	B	623	-	36,36,36	1.10	4 (11%)	47,47,47	0.98	1 (2%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.27	5 (7%)
27	LMG	a	402	-	42,42,55	0.82	1 (2%)	50,50,63	1.26	4 (8%)
27	LMG	E	101	-	44,44,55	0.75	0	52,52,63	1.29	3 (5%)
24	BCR	J	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.59	13 (23%)
24	BCR	x	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	5 (8%)
24	BCR	B	616	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	8 (14%)
22	CLA	H	101	-	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	C	507	3	69,73,73	1.18	7 (10%)	82,113,113	1.30	6 (7%)
31	LMT	M	103	-	36,36,36	1.12	4 (11%)	47,47,47	1.00	2 (4%)
24	BCR	y	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.29	7 (12%)
22	CLA	b	609	2	69,73,73	1.17	6 (8%)	82,113,113	1.28	5 (6%)
22	CLA	b	612	2	69,73,73	1.20	6 (8%)	82,113,113	1.23	5 (6%)
22	CLA	c	502	-	69,73,73	1.20	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	C	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
22	CLA	a	404	1	69,73,73	1.19	7 (10%)	82,113,113	1.26	6 (7%)
24	BCR	F	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	6 (10%)
27	LMG	D	411	-	46,46,55	0.76	1 (2%)	54,54,63	1.31	5 (9%)
22	CLA	A	402	1	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
24	BCR	C	514	-	41,41,41	1.14	3 (7%)	56,56,56	1.30	9 (16%)
27	LMG	d	408	-	48,48,55	0.75	0	56,56,63	1.37	4 (7%)
22	CLA	B	610	2	69,73,73	1.24	7 (10%)	82,113,113	1.34	7 (8%)
24	BCR	c	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.38	9 (16%)
26	LHG	A	409	-	38,38,48	0.70	1 (2%)	41,44,54	1.22	3 (7%)
22	CLA	d	405	-	69,73,73	1.19	5 (7%)	82,113,113	1.25	5 (6%)
27	LMG	d	411	-	46,46,55	0.78	1 (2%)	54,54,63	1.30	6 (11%)
27	LMG	d	407	-	49,49,55	0.76	1 (2%)	57,57,63	1.30	5 (8%)
30	SQD	F	103	-	43,45,54	1.03	2 (4%)	53,56,65	1.58	10 (18%)
24	BCR	K	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	SQD	a	401	-	52,54,54	0.96	3 (5%)	62,65,65	1.48	9 (14%)
22	CLA	c	512	3	69,73,73	1.19	5 (7%)	82,113,113	1.27	5 (6%)
30	SQD	B	626	-	45,47,54	1.02	3 (6%)	55,58,65	1.72	10 (18%)
31	LMT	i	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.01	2 (4%)
34	HEM	f	101	6,5	50,50,50	1.96	8 (16%)	67,82,82	1.32	4 (5%)
25	DGD	C	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.43	12 (15%)
22	CLA	c	511	-	69,73,73	1.19	6 (8%)	82,113,113	1.26	5 (6%)
30	SQD	B	622	-	41,43,54	1.05	2 (4%)	51,54,65	1.70	11 (21%)
22	CLA	c	520	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
22	CLA	D	405	-	69,73,73	1.18	6 (8%)	82,113,113	1.25	5 (6%)
22	CLA	b	611	2	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
22	CLA	c	508	3	69,73,73	1.19	7 (10%)	82,113,113	1.24	5 (6%)
24	BCR	b	622	-	41,41,41	1.13	2 (4%)	56,56,56	1.39	10 (17%)
31	LMT	b	603	-	36,36,36	1.11	4 (11%)	47,47,47	0.96	1 (2%)
22	CLA	C	506	-	69,73,73	1.18	6 (8%)	82,113,113	1.28	5 (6%)
24	BCR	a	410	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	7 (12%)
22	CLA	B	604	2	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
32	PHO	a	407	-	58,69,69	2.18	9 (15%)	55,99,99	1.39	5 (9%)

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
22	CLA	B	611	-	-	9/39/115/115	-
31	LMT	I	102	-	-	3/21/61/61	0/2/2/2
30	SQD	b	602	-	-	13/42/62/69	0/1/1/1
22	CLA	C	505	3	-	16/39/115/115	-
25	DGD	A	408	-	-	13/45/85/95	0/2/2/2
22	CLA	C	520	-	-	13/39/115/115	-
27	LMG	A	410	-	-	28/46/66/70	0/1/1/1
22	CLA	c	506	-	-	11/39/115/115	-
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
22	CLA	b	617	2	-	13/39/115/115	-
22	CLA	c	507	3	-	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	c	514	-	-	4/29/63/63	0/2/2/2
22	CLA	h	101	-	-	14/39/115/115	-
22	CLA	A	405	1	-	8/39/115/115	-
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1
22	CLA	c	503	-	-	12/39/115/115	-
22	CLA	d	404	-	-	11/39/115/115	-
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
22	CLA	B	609	-	-	18/39/115/115	-
22	CLA	b	610	-	-	9/39/115/115	-
26	LHG	a	412	-	-	11/43/43/53	-
27	LMG	C	518	-	-	22/40/60/70	0/1/1/1
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
22	CLA	b	614	2	-	11/39/115/115	-
27	LMG	C	521	-	-	19/43/63/70	0/1/1/1
22	CLA	A	404	-	-	8/39/115/115	-
25	DGD	B	625	-	-	19/41/81/95	0/2/2/2
22	CLA	B	605	2	-	14/39/115/115	-
27	LMG	l	101	-	-	25/46/66/70	0/1/1/1
24	BCR	g	101	-	-	4/29/63/63	0/2/2/2
22	CLA	B	606	-	-	9/39/115/115	-
34	HEM	V	201	16	-	5/14/54/54	-
22	CLA	C	502	3	-	10/39/115/115	-
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	PHO	D	402	-	-	11/37/103/103	0/5/6/6
22	CLA	B	608	2	-	9/39/115/115	-
22	CLA	D	404	-	-	14/39/115/115	-
27	LMG	i	101	-	-	19/38/58/70	0/1/1/1
22	CLA	C	501	3	-	15/39/115/115	-
22	CLA	B	614	-	-	10/39/115/115	-
22	CLA	C	503	-	-	12/39/115/115	-
22	CLA	b	606	2	-	14/39/115/115	-
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
34	HEM	v	201	16	-	5/14/54/54	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PHO	d	401	-	-	10/37/103/103	0/5/6/6
31	LMT	B	627	-	-	3/21/61/61	0/2/2/2
25	DGD	c	517	-	-	19/55/95/95	0/2/2/2
27	LMG	A	415	-	-	15/37/57/70	0/1/1/1
22	CLA	C	504	3	-	17/39/115/115	-
30	SQD	d	402	-	-	15/38/58/69	0/1/1/1
25	DGD	b	601	-	-	19/41/81/95	0/2/2/2
34	HEM	F	101	6,5	-	2/14/54/54	-
27	LMG	m	101	-	-	16/37/57/70	0/1/1/1
22	CLA	b	618	-	-	9/39/115/115	-
30	SQD	f	103	-	-	12/40/60/69	0/1/1/1
23	PL9	d	406	-	-	12/53/73/73	0/1/1/1
22	CLA	B	607	2	-	12/39/115/115	-
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
25	DGD	a	411	-	-	14/45/85/95	0/2/2/2
26	LHG	C	519	-	-	16/41/41/53	-
22	CLA	b	619	2	-	19/39/115/115	-
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
31	LMT	B	624	-	-	3/21/61/61	0/2/2/2
22	CLA	a	405	-	-	12/39/115/115	-
22	CLA	a	406	-	-	8/39/115/115	-
24	BCR	b	623	-	-	5/29/63/63	0/2/2/2
27	LMG	B	621	-	-	14/44/64/70	0/1/1/1
22	CLA	C	509	3	-	15/39/115/115	-
31	LMT	b	626	-	-	2/21/61/61	0/2/2/2
32	PHO	D	401	-	-	10/37/103/103	0/5/6/6
23	PL9	a	409	-	-	17/41/61/73	0/1/1/1
22	CLA	B	601	-	-	15/39/115/115	-
22	CLA	b	616	-	-	15/39/115/115	-
22	CLA	A	403	-	-	13/39/115/115	-
22	CLA	b	608	2	-	15/39/115/115	-
25	DGD	D	409	-	-	34/52/92/95	0/2/2/2
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
22	CLA	c	510	3	-	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
24	BCR	b	621	-	-	7/29/63/63	0/2/2/2
22	CLA	B	602	2	-	14/39/115/115	-
31	LMT	b	627	-	-	3/21/61/61	0/2/2/2
22	CLA	B	615	2	-	19/39/115/115	-
22	CLA	C	508	3	-	19/39/115/115	-
22	CLA	c	501	3	-	14/39/115/115	-
30	SQD	a	415	-	-	18/46/66/69	0/1/1/1
22	CLA	B	603	2	-	8/39/115/115	-
27	LMG	D	407	-	-	24/44/64/70	0/1/1/1
22	CLA	B	612	-	-	16/39/115/115	-
30	SQD	A	413	-	-	18/46/66/69	0/1/1/1
25	DGD	c	516	-	-	19/51/91/95	0/2/2/2
23	PL9	D	406	-	-	12/53/73/73	0/1/1/1
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
31	LMT	B	628	-	-	4/21/61/61	0/2/2/2
31	LMT	d	410	-	-	1/17/57/61	0/2/2/2
31	LMT	b	604	-	-	5/21/61/61	0/2/2/2
22	CLA	c	504	3	-	18/39/115/115	-
22	CLA	c	509	3	-	17/39/115/115	-
22	CLA	a	408	1	-	8/39/115/115	-
27	LMG	I	101	-	-	19/38/58/70	0/1/1/1
25	DGD	d	409	-	-	34/52/92/95	0/2/2/2
30	SQD	A	414	-	-	11/49/69/69	0/1/1/1
24	BCR	f	102	-	-	5/29/63/63	0/2/2/2
22	CLA	b	613	-	-	17/39/115/115	-
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2
22	CLA	b	607	2	-	8/39/115/115	-
31	LMT	D	410	-	-	2/17/57/61	0/2/2/2
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
22	CLA	C	512	3	-	14/39/115/115	-
23	PL9	J	101	-	-	9/29/49/73	0/1/1/1
22	CLA	c	505	3	-	16/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	605	-	-	16/39/115/115	-
25	DGD	B	620	-	-	18/47/87/95	0/2/2/2
22	CLA	C	510	3	-	15/39/115/115	-
27	LMG	c	518	-	-	22/40/60/70	0/1/1/1
24	BCR	c	521	-	-	4/29/63/63	0/2/2/2
25	DGD	C	517	-	-	20/55/95/95	0/2/2/2
22	CLA	B	613	2	-	12/39/115/115	-
22	CLA	b	615	-	-	10/39/115/115	-
27	LMG	D	408	-	-	21/43/63/70	0/1/1/1
26	LHG	c	519	-	-	17/41/41/53	-
24	BCR	B	617	-	-	6/29/63/63	0/2/2/2
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
31	LMT	B	623	-	-	3/21/61/61	0/2/2/2
25	DGD	c	515	-	-	19/42/82/95	0/2/2/2
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
27	LMG	E	101	-	-	17/39/59/70	0/1/1/1
24	BCR	J	102	-	-	7/29/63/63	0/2/2/2
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
22	CLA	H	101	-	-	15/39/115/115	-
22	CLA	C	507	3	-	13/39/115/115	-
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	b	609	2	-	18/39/115/115	-
22	CLA	b	612	2	-	10/39/115/115	-
22	CLA	c	502	-	-	10/39/115/115	-
22	CLA	C	511	-	-	17/39/115/115	-
22	CLA	a	404	1	-	8/39/115/115	-
24	BCR	F	102	-	-	5/29/63/63	0/2/2/2
27	LMG	D	411	-	-	15/41/61/70	0/1/1/1
22	CLA	A	402	1	-	8/39/115/115	-
24	BCR	C	514	-	-	4/29/63/63	0/2/2/2
27	LMG	d	408	-	-	21/43/63/70	0/1/1/1
22	CLA	B	610	2	-	11/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	c	513	-	-	5/29/63/63	0/2/2/2
26	LHG	A	409	-	-	11/43/43/53	-
22	CLA	d	405	-	-	8/39/115/115	-
27	LMG	d	411	-	-	16/41/61/70	0/1/1/1
27	LMG	d	407	-	-	24/44/64/70	0/1/1/1
30	SQD	F	103	-	-	12/40/60/69	0/1/1/1
24	BCR	K	102	-	-	4/29/63/63	0/2/2/2
30	SQD	a	401	-	-	13/49/69/69	0/1/1/1
22	CLA	c	512	3	-	16/39/115/115	-
30	SQD	B	626	-	-	13/42/62/69	0/1/1/1
31	LMT	i	102	-	-	3/21/61/61	0/2/2/2
34	HEM	f	101	6,5	-	2/14/54/54	-
25	DGD	C	516	-	-	19/51/91/95	0/2/2/2
22	CLA	c	511	-	-	17/39/115/115	-
30	SQD	B	622	-	-	15/38/58/69	0/1/1/1
22	CLA	c	520	-	-	12/39/115/115	-
22	CLA	D	405	-	-	8/39/115/115	-
22	CLA	b	611	2	-	13/39/115/115	-
22	CLA	c	508	3	-	19/39/115/115	-
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
31	LMT	b	603	-	-	3/21/61/61	0/2/2/2
22	CLA	C	506	-	-	12/39/115/115	-
24	BCR	a	410	-	-	4/29/63/63	0/2/2/2
22	CLA	B	604	2	-	15/39/115/115	-
32	PHO	a	407	-	-	11/37/103/103	0/5/6/6

The worst 5 of 736 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	402	PHO	C1B-C2B	9.63	1.50	1.39
32	D	401	PHO	C1B-C2B	9.55	1.50	1.39
32	d	401	PHO	C1B-C2B	9.52	1.50	1.39
32	a	407	PHO	C1B-C2B	9.52	1.50	1.39
32	a	407	PHO	C3B-C4B	8.72	1.50	1.41

The worst 5 of 1041 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	504	CLA	C4A-NA-C1A	7.26	109.99	106.68
22	B	611	CLA	C4A-NA-C1A	7.22	109.97	106.68
22	c	504	CLA	C4A-NA-C1A	7.21	109.97	106.68
22	b	615	CLA	C4A-NA-C1A	7.12	109.93	106.68
22	B	603	CLA	C4A-NA-C1A	7.07	109.91	106.68

There are no chirality outliers.

5 of 2084 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C1A-C2A-CAA-CBA
22	A	403	CLA	C3A-C2A-CAA-CBA
22	A	404	CLA	C2B-C3B-CAB-CBB
22	A	404	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

155 monomers are involved in 449 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	611	CLA	3	0
30	b	602	SQD	2	0
22	C	505	CLA	2	0
25	A	408	DGD	1	0
22	C	520	CLA	3	0
27	A	410	LMG	2	0
22	c	506	CLA	4	0
24	A	407	BCR	2	0
22	b	617	CLA	2	0
22	c	507	CLA	5	0
24	c	514	BCR	3	0
22	h	101	CLA	10	0
22	A	405	CLA	1	0
27	M	101	LMG	1	0
22	c	503	CLA	2	0
22	d	404	CLA	9	0
24	b	620	BCR	5	0
22	b	610	CLA	5	0
26	a	412	LHG	1	0
27	C	518	LMG	2	0
27	b	625	LMG	4	0
22	b	614	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	404	CLA	5	0
25	B	625	DGD	2	0
22	B	605	CLA	7	0
27	l	101	LMG	2	0
24	g	101	BCR	5	0
22	B	606	CLA	7	0
34	V	201	HEM	4	0
24	B	618	BCR	4	0
32	D	402	PHO	5	0
22	B	608	CLA	5	0
22	D	404	CLA	10	0
27	i	101	LMG	1	0
22	C	501	CLA	2	0
22	B	614	CLA	2	0
22	C	503	CLA	3	0
22	b	606	CLA	8	0
25	C	515	DGD	3	0
34	v	201	HEM	5	0
24	B	619	BCR	1	0
32	d	401	PHO	5	0
31	B	627	LMT	2	0
25	c	517	DGD	5	0
27	A	415	LMG	1	0
22	C	504	CLA	3	0
30	d	402	SQD	3	0
25	b	601	DGD	2	0
34	F	101	HEM	4	0
27	m	101	LMG	2	0
22	b	618	CLA	1	0
30	f	103	SQD	3	0
23	d	406	PL9	6	0
22	B	607	CLA	8	0
24	H	102	BCR	2	0
25	a	411	DGD	3	0
26	C	519	LHG	3	0
22	b	619	CLA	4	0
27	e	101	LMG	2	0
22	a	405	CLA	10	0
22	a	406	CLA	6	0
24	b	623	BCR	4	0
27	B	621	LMG	3	0
22	C	509	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b	626	LMT	1	0
32	D	401	PHO	6	0
23	a	409	PL9	4	0
22	B	601	CLA	1	0
22	b	616	CLA	3	0
22	A	403	CLA	12	0
22	b	608	CLA	8	0
25	D	409	DGD	1	0
22	c	510	CLA	4	0
24	b	621	BCR	1	0
22	B	602	CLA	10	0
22	B	615	CLA	4	0
22	C	508	CLA	1	0
22	c	501	CLA	4	0
30	a	415	SQD	3	0
22	B	603	CLA	3	0
27	D	407	LMG	2	0
22	B	612	CLA	2	0
30	A	413	SQD	3	0
25	c	516	DGD	3	0
23	D	406	PL9	8	0
25	b	624	DGD	2	0
27	c	522	LMG	1	0
31	B	628	LMT	2	0
31	b	604	LMT	2	0
22	c	504	CLA	3	0
22	c	509	CLA	3	0
22	a	408	CLA	2	0
25	d	409	DGD	1	0
30	A	414	SQD	5	0
24	f	102	BCR	1	0
22	b	613	CLA	1	0
24	C	513	BCR	5	0
22	b	607	CLA	3	0
24	j	102	BCR	1	0
22	C	512	CLA	3	0
22	c	505	CLA	1	0
25	B	620	DGD	2	0
22	C	510	CLA	4	0
27	c	518	LMG	2	0
24	c	521	BCR	3	0
25	C	517	DGD	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	613	CLA	4	0
22	b	615	CLA	4	0
27	D	408	LMG	6	0
26	c	519	LHG	2	0
24	B	617	BCR	2	0
23	A	406	PL9	5	0
31	B	623	LMT	2	0
25	c	515	DGD	3	0
27	a	402	LMG	1	0
27	E	101	LMG	1	0
24	J	102	BCR	2	0
24	B	616	BCR	7	0
22	H	101	CLA	9	0
22	C	507	CLA	4	0
24	y	101	BCR	6	0
22	b	609	CLA	5	0
22	b	612	CLA	5	0
22	C	511	CLA	1	0
22	a	404	CLA	9	0
24	F	102	BCR	3	0
27	D	411	LMG	1	0
22	A	402	CLA	11	0
24	C	514	BCR	5	0
27	d	408	LMG	6	0
22	B	610	CLA	2	0
24	c	513	BCR	7	0
26	A	409	LHG	3	0
22	d	405	CLA	2	0
27	d	411	LMG	1	0
27	d	407	LMG	3	0
30	F	103	SQD	2	0
24	K	102	BCR	3	0
30	a	401	SQD	5	0
22	c	512	CLA	2	0
30	B	626	SQD	2	0
31	i	102	LMT	1	0
34	f	101	HEM	4	0
25	C	516	DGD	4	0
30	B	622	SQD	3	0
22	c	520	CLA	5	0
22	D	405	CLA	4	0
22	b	611	CLA	8	0

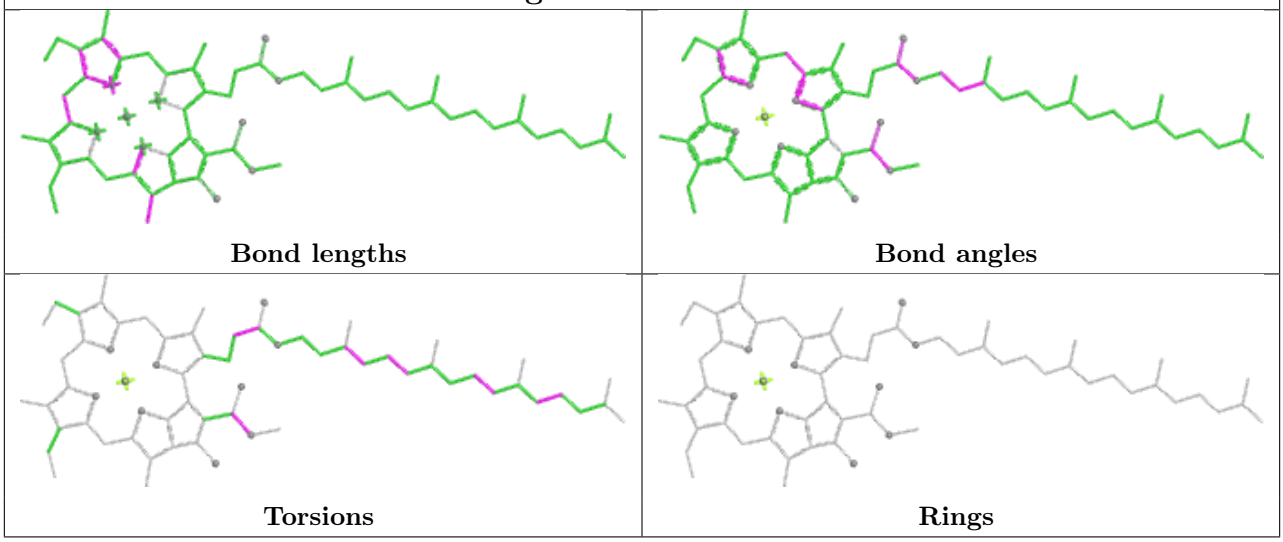
Continued on next page...

Continued from previous page...

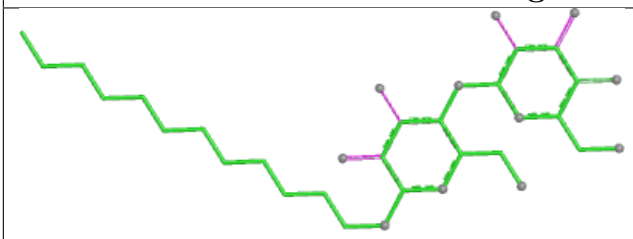
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	508	CLA	3	0
24	b	622	BCR	3	0
31	b	603	LMT	2	0
22	C	506	CLA	3	0
24	a	410	BCR	4	0
22	B	604	CLA	8	0
32	a	407	PHO	4	0

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

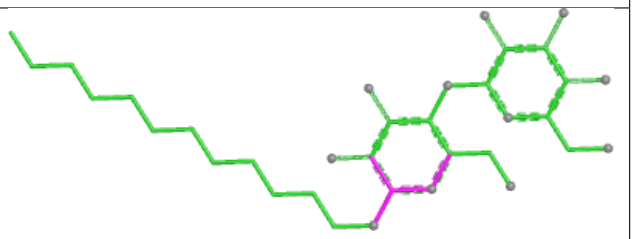
Ligand CLA B 611



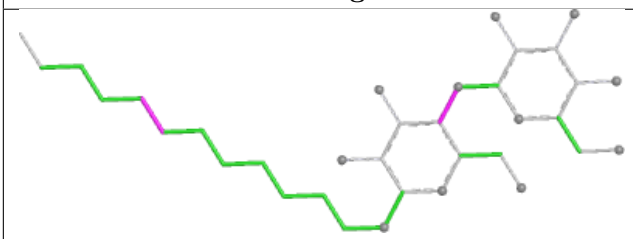
Ligand LMT I 102



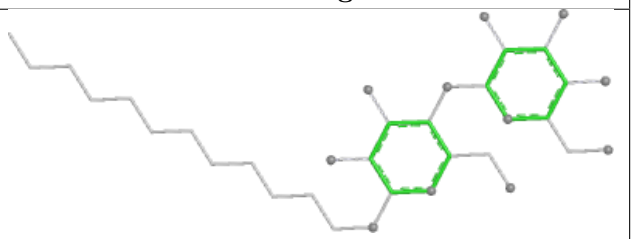
Bond lengths



Bond angles

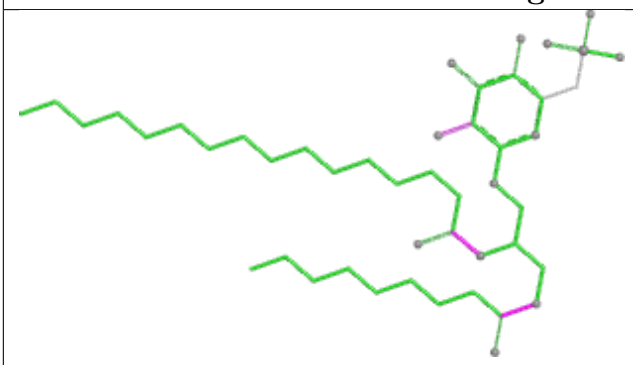


Torsions

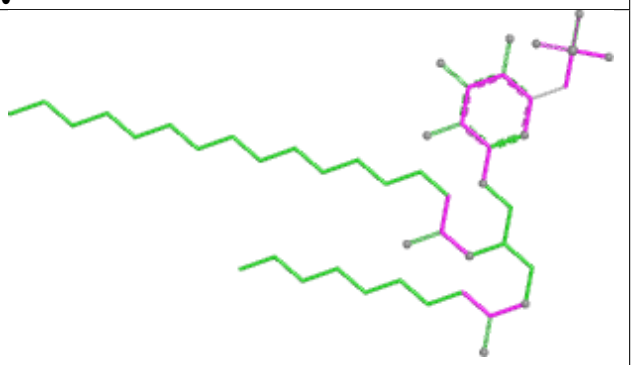


Rings

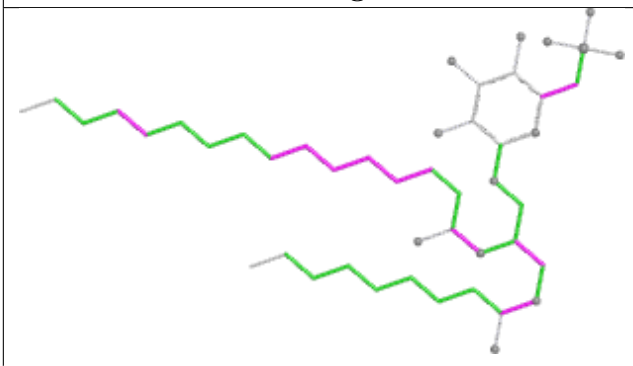
Ligand SQD b 602



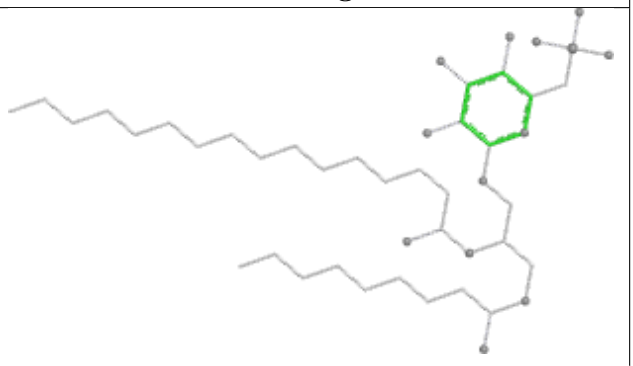
Bond lengths



Bond angles

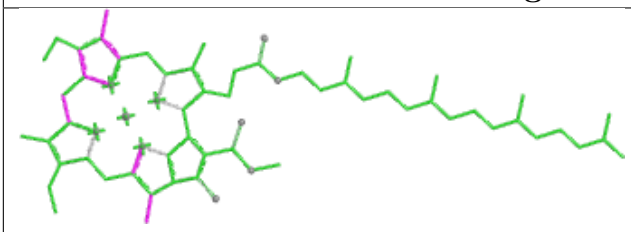


Torsions

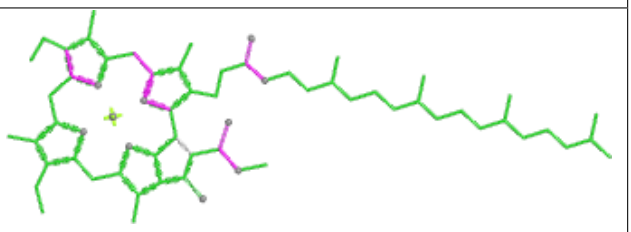


Rings

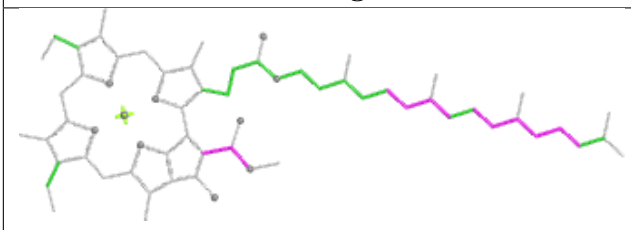
Ligand CLA C 505



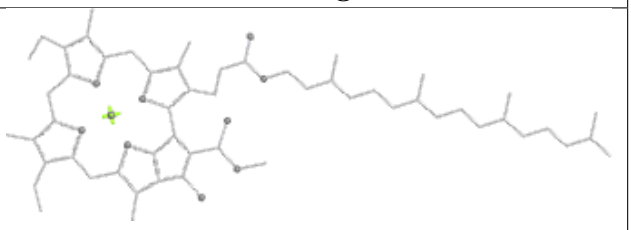
Bond lengths



Bond angles

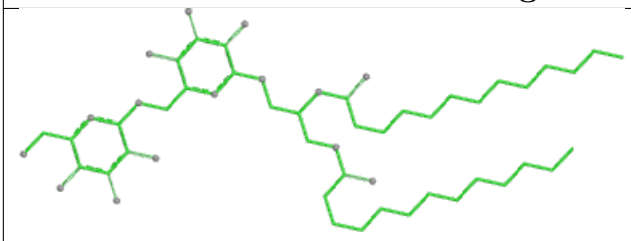


Torsions

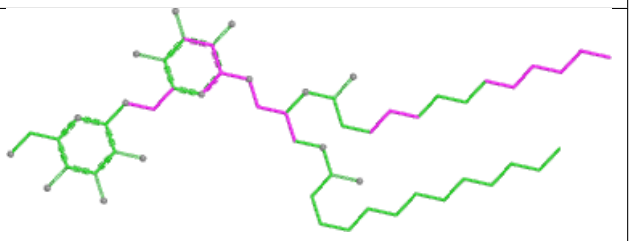


Rings

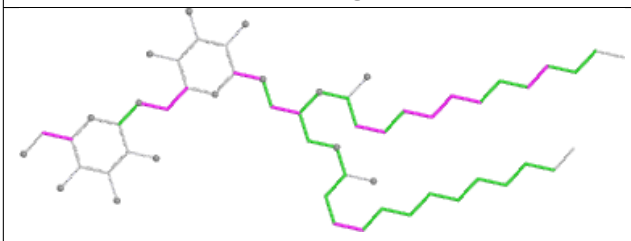
Ligand DGD A 408



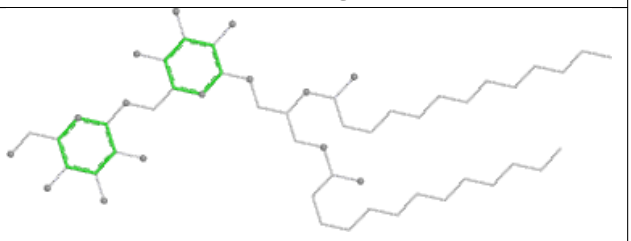
Bond lengths



Bond angles

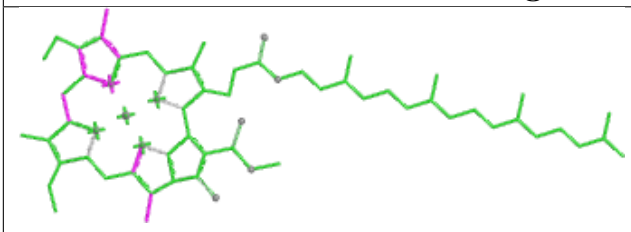


Torsions

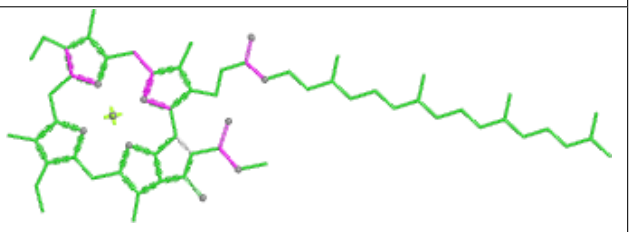


Rings

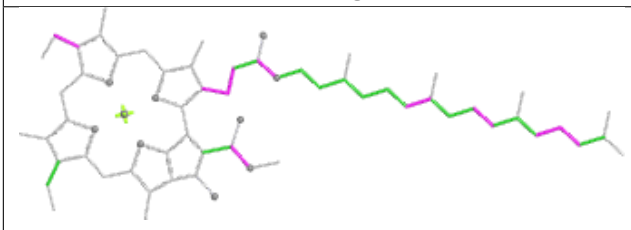
Ligand CLA C 520



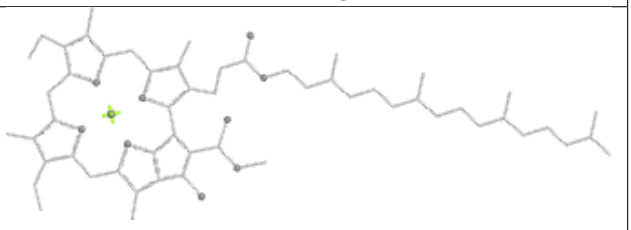
Bond lengths



Bond angles

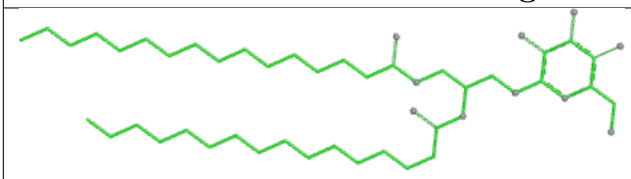


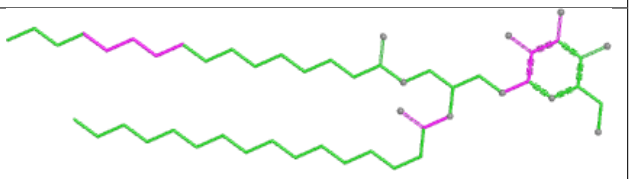
Torsions

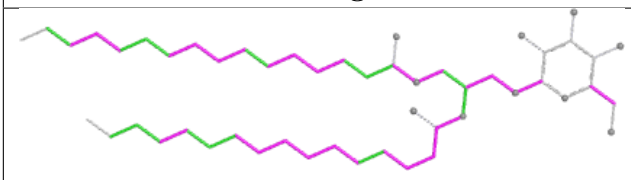


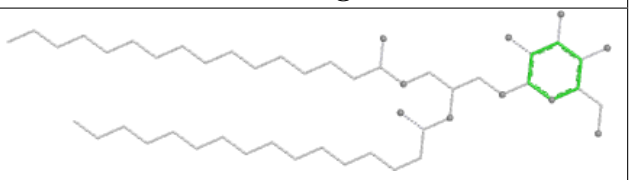
Rings

Ligand LMG A 410

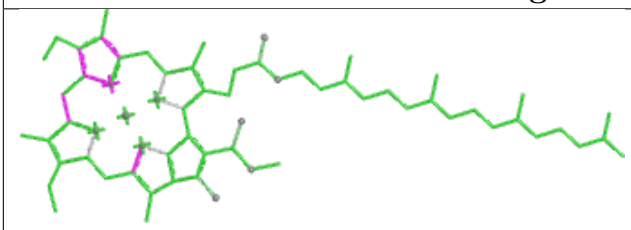

Bond lengths

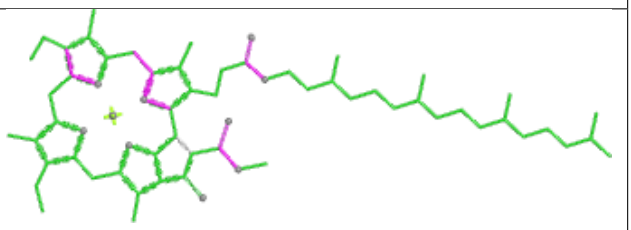

Bond angles

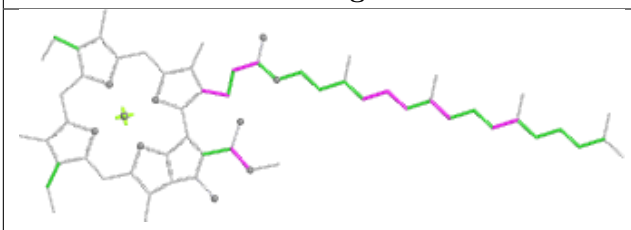

Torsions

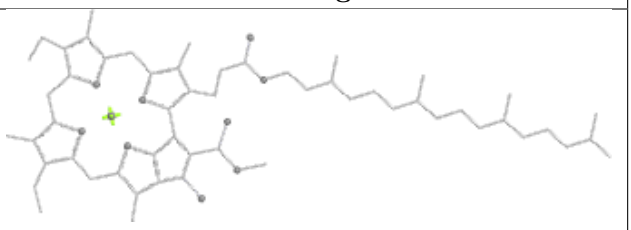

Rings

Ligand CLA c 506

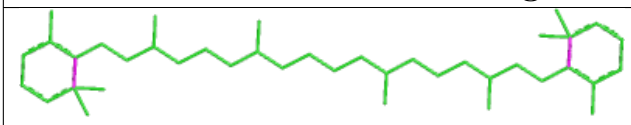

Bond lengths

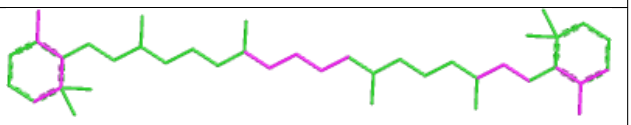

Bond angles

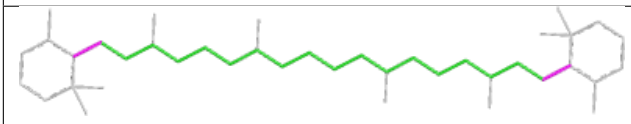

Torsions

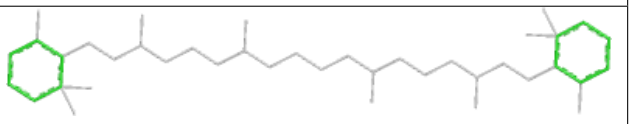

Rings

Ligand BCR A 407

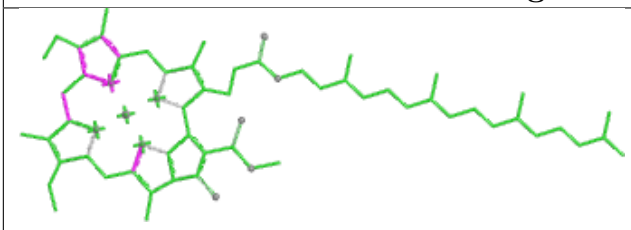

Bond lengths


Bond angles

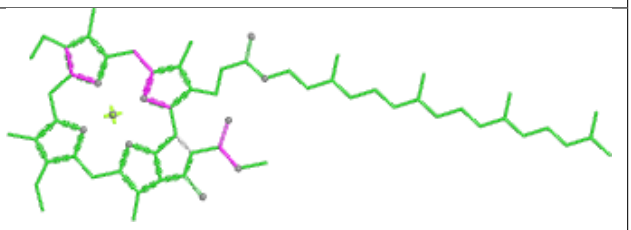

Torsions


Rings

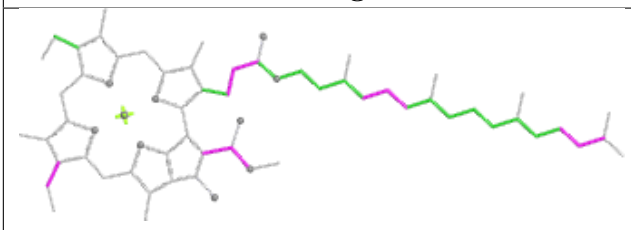
Ligand CLA b 617



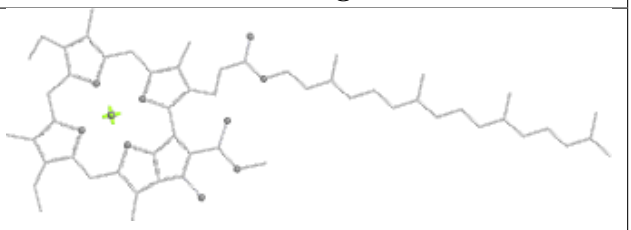
Bond lengths



Bond angles

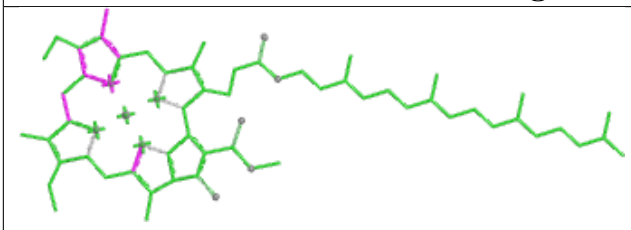


Torsions

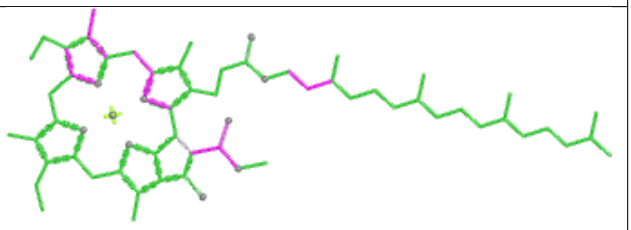


Rings

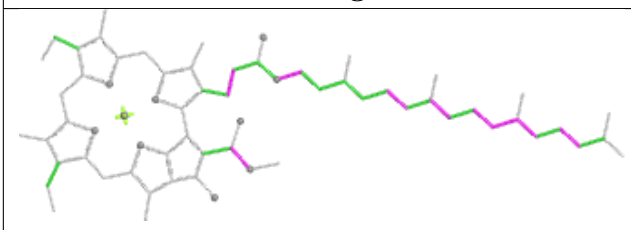
Ligand CLA c 507



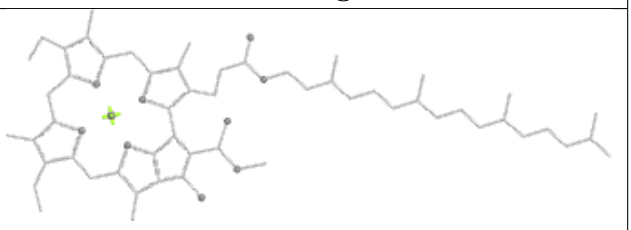
Bond lengths



Bond angles

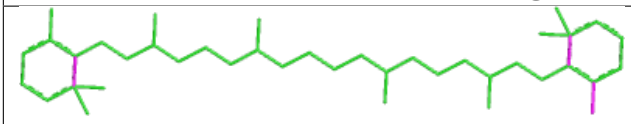


Torsions

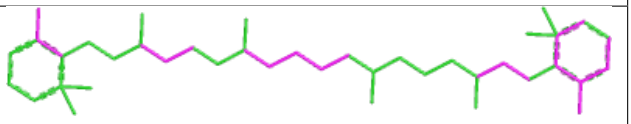


Rings

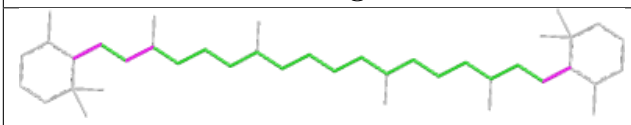
Ligand BCR c 514



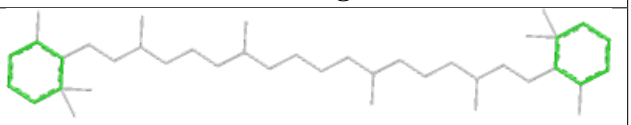
Bond lengths



Bond angles

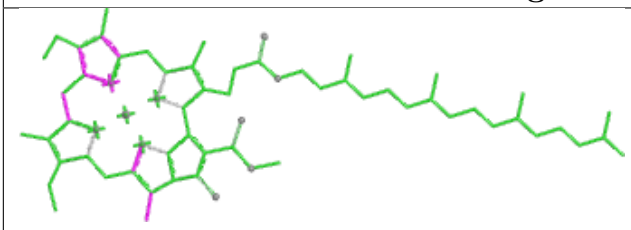


Torsions

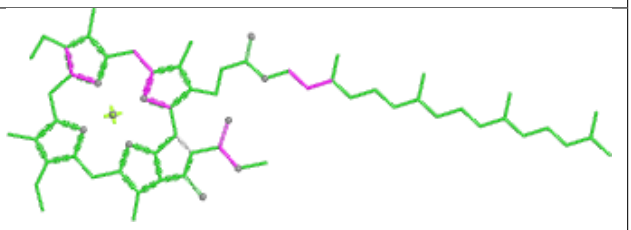


Rings

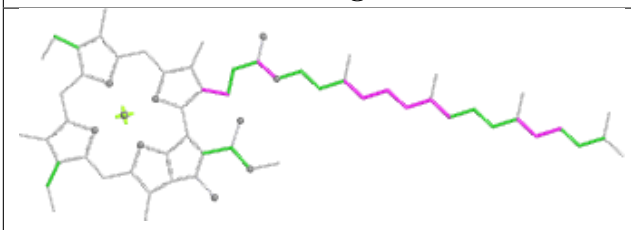
Ligand CLA h 101



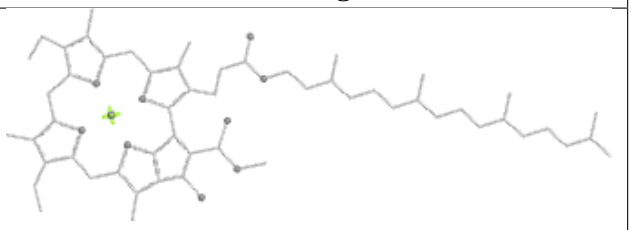
Bond lengths



Bond angles

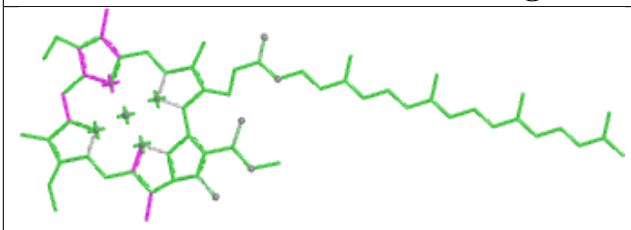


Torsions

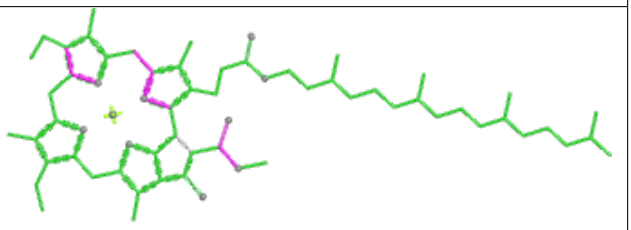


Rings

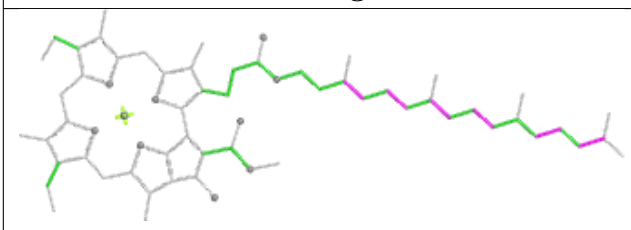
Ligand CLA A 405



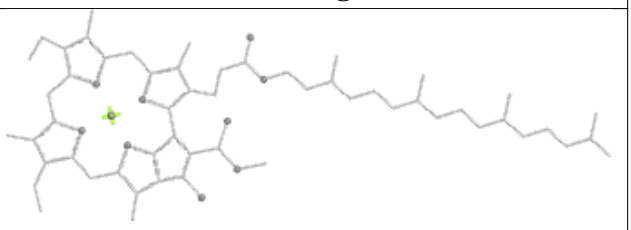
Bond lengths



Bond angles

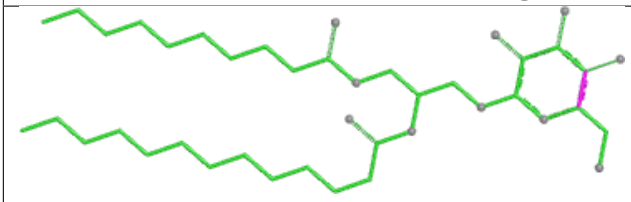


Torsions

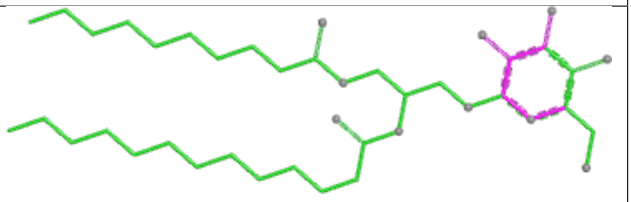


Rings

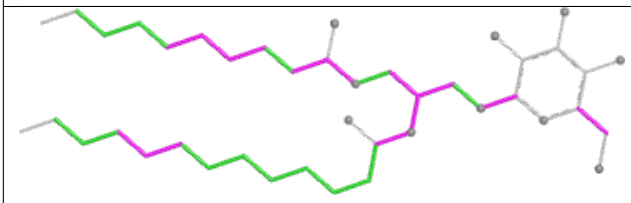
Ligand LMG M 101



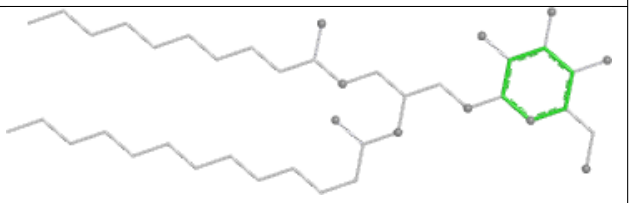
Bond lengths



Bond angles

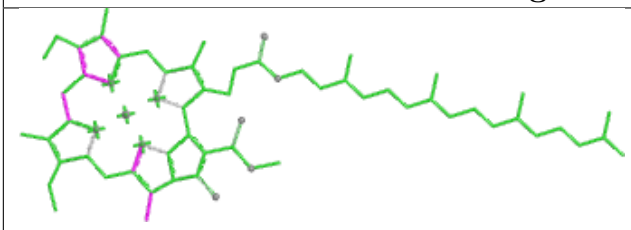


Torsions

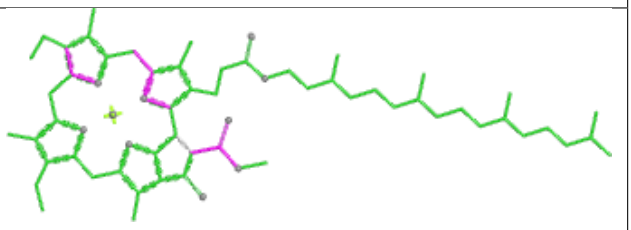


Rings

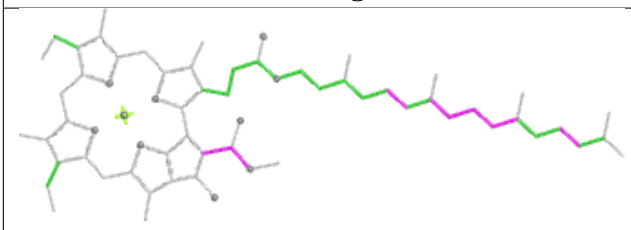
Ligand CLA c 503



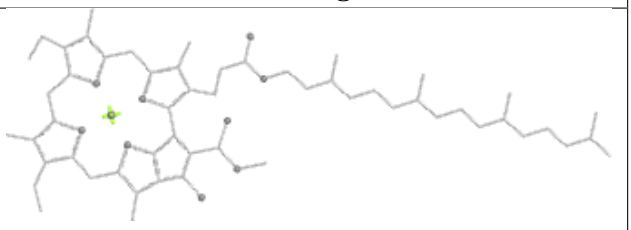
Bond lengths



Bond angles

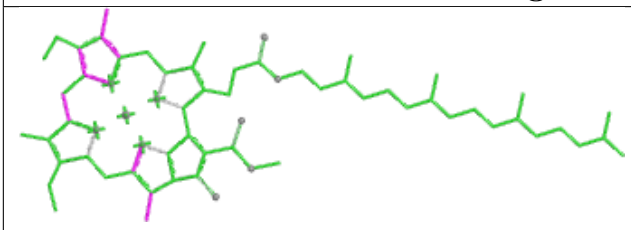


Torsions

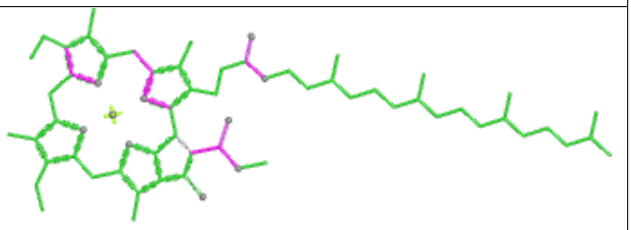


Rings

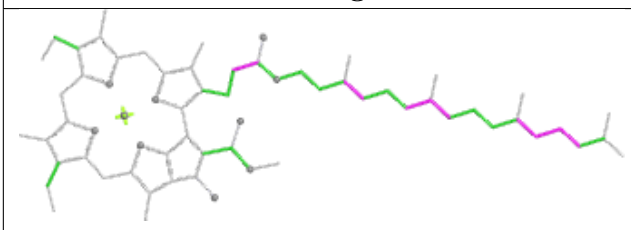
Ligand CLA d 404



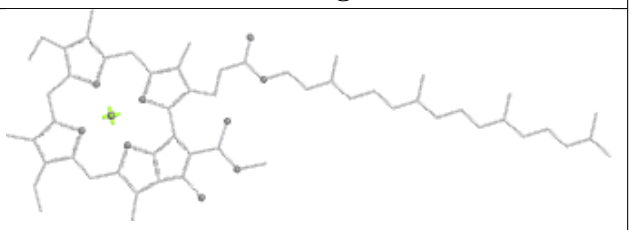
Bond lengths



Bond angles

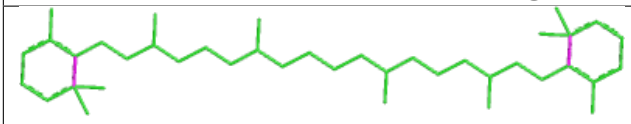


Torsions

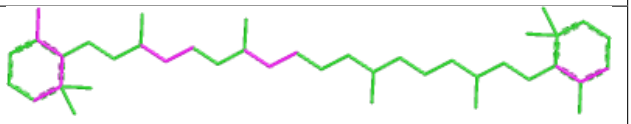


Rings

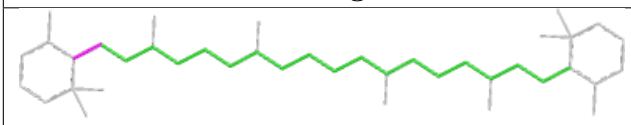
Ligand BCR b 620



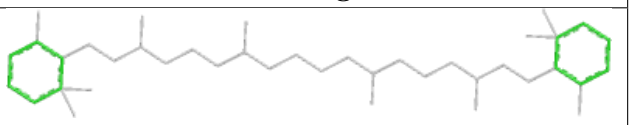
Bond lengths



Bond angles

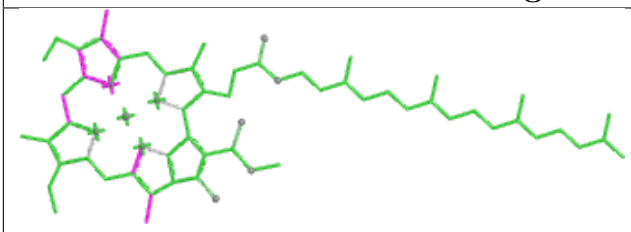


Torsions

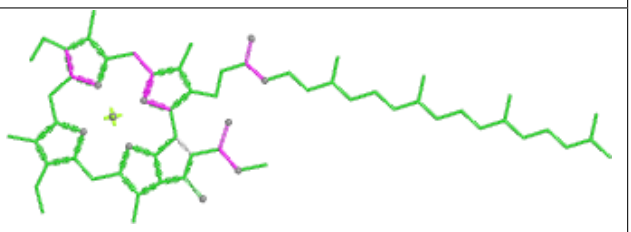


Rings

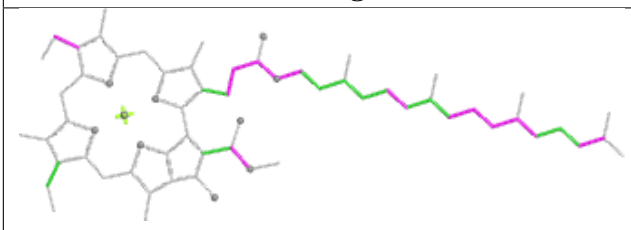
Ligand CLA B 609



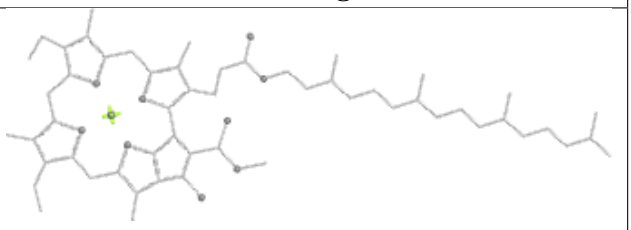
Bond lengths



Bond angles

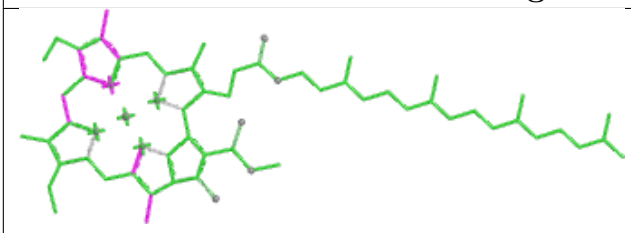


Torsions

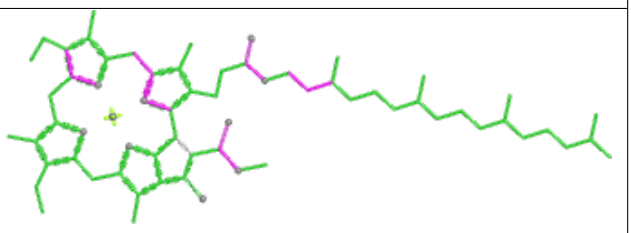


Rings

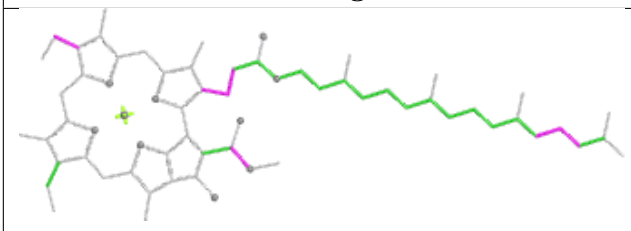
Ligand CLA b 610



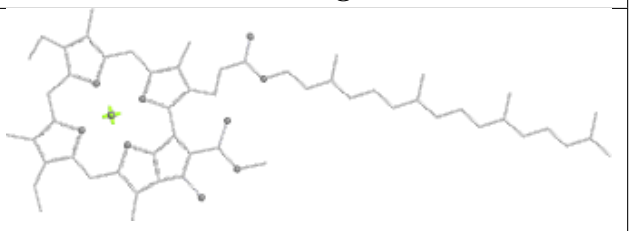
Bond lengths



Bond angles

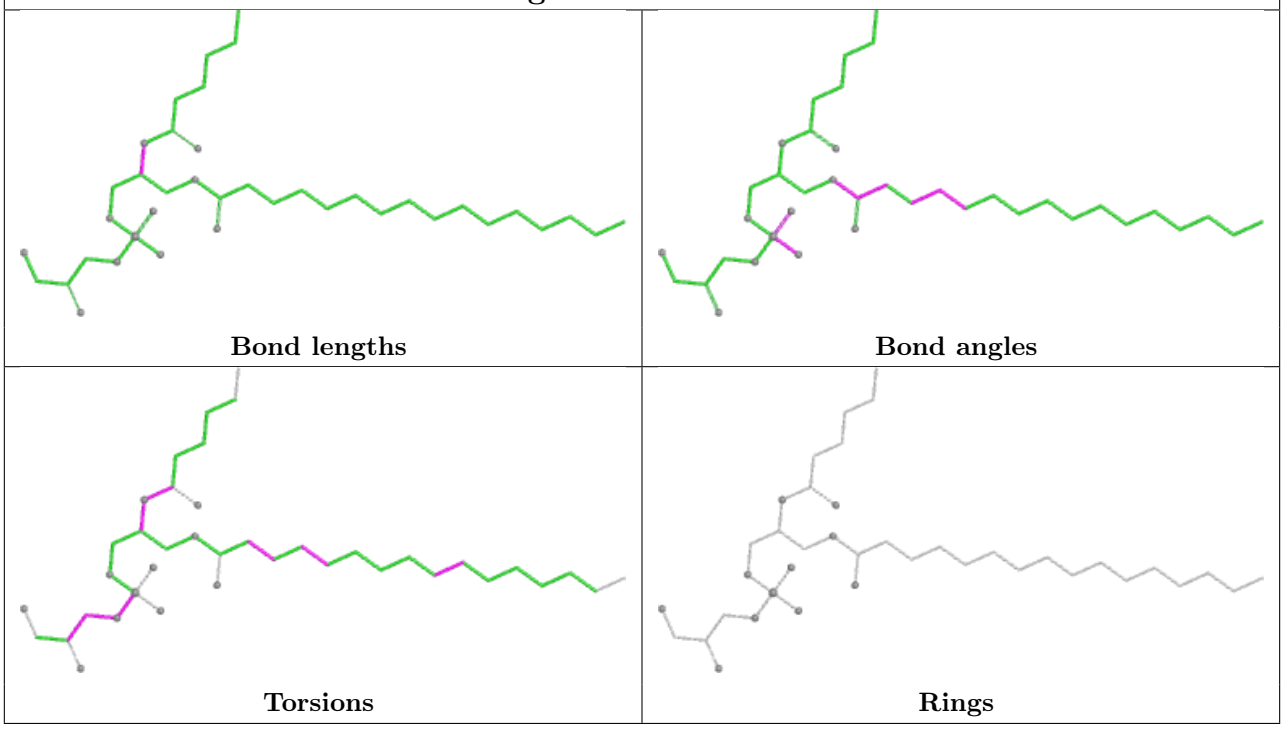


Torsions

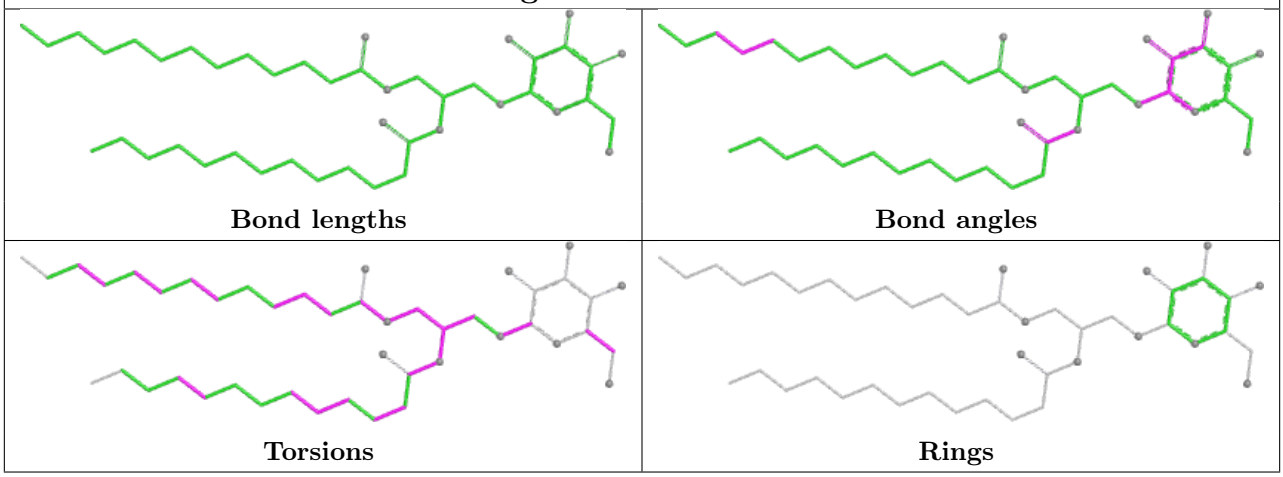


Rings

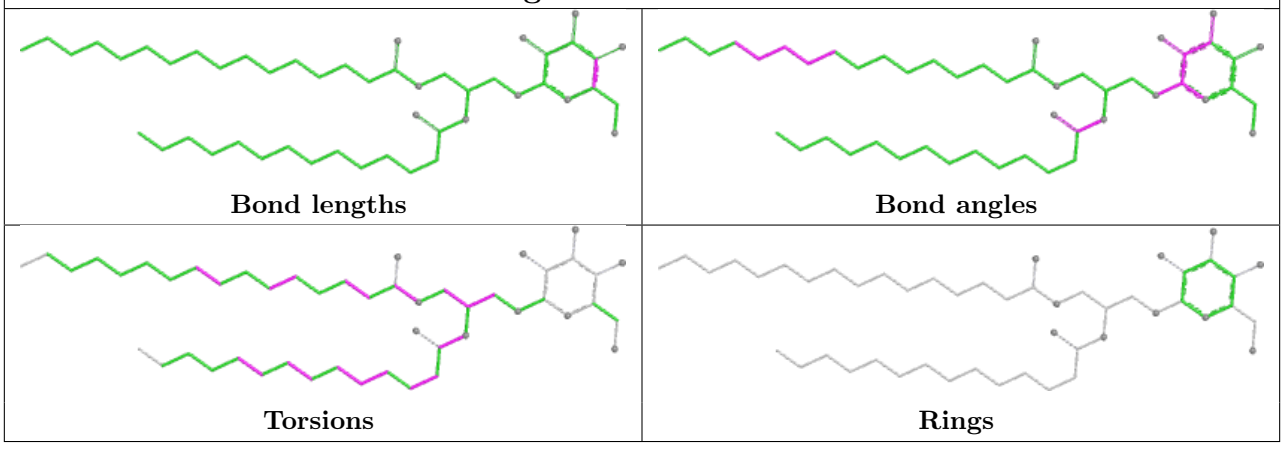
Ligand LHG a 412



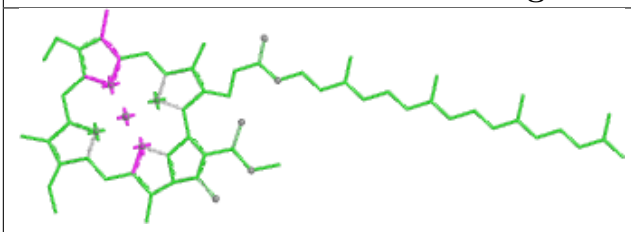
Ligand LMG C 518

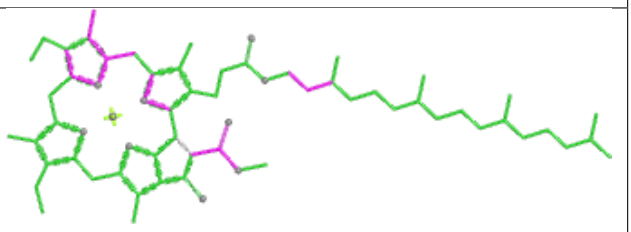


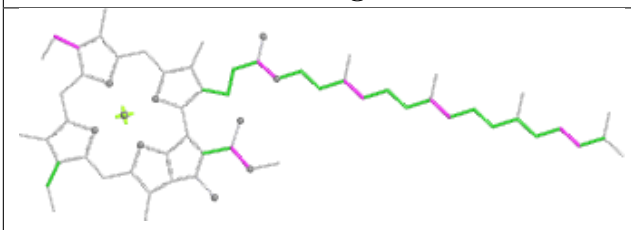
Ligand LMG b 625

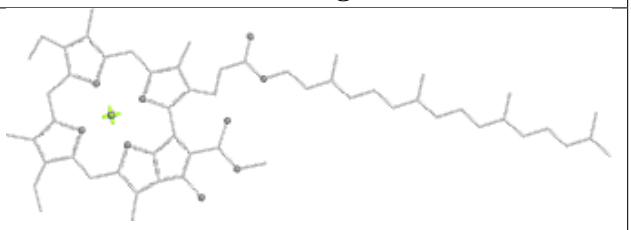


Ligand CLA b 614

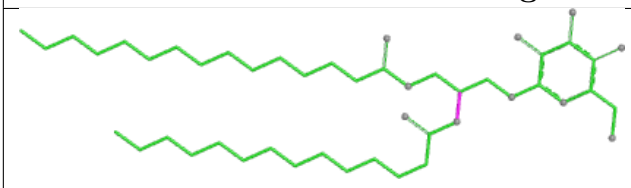

Bond lengths

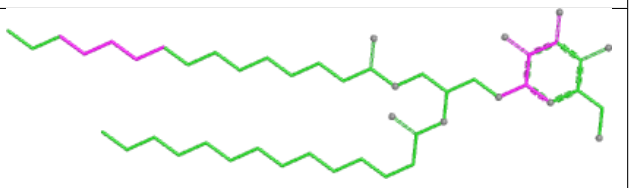

Bond angles

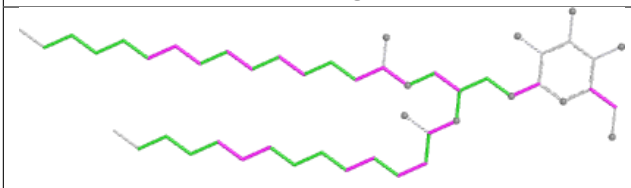

Torsions

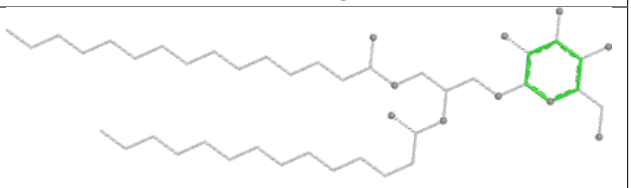

Rings

Ligand LMG C 521

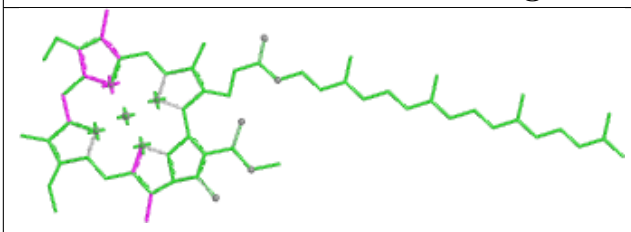

Bond lengths

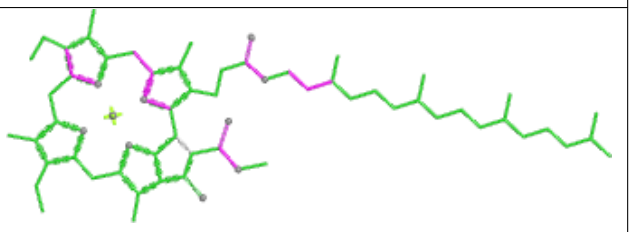

Bond angles

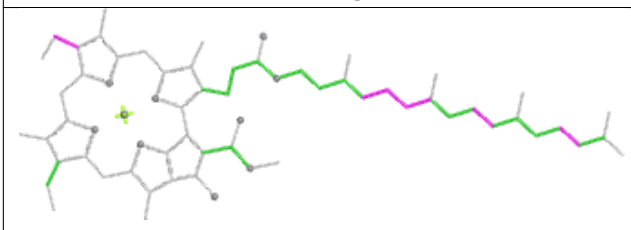

Torsions

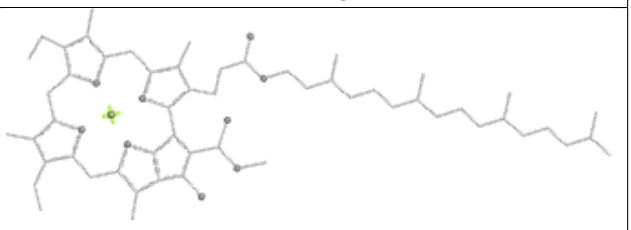

Rings

Ligand CLA A 404

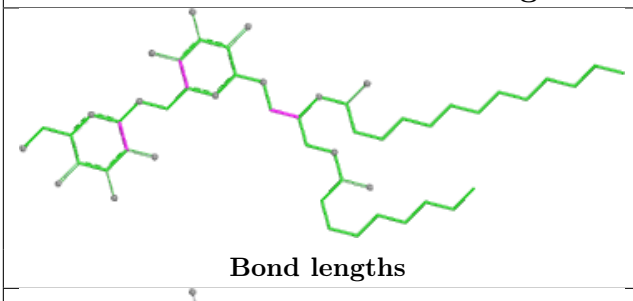

Bond lengths


Bond angles

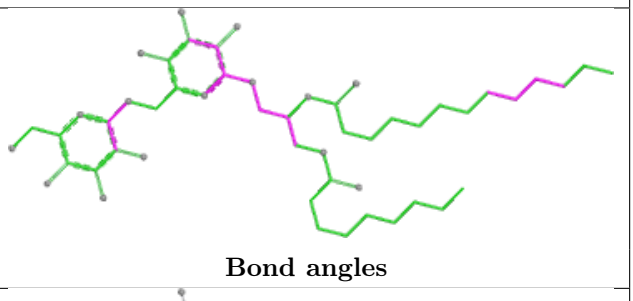

Torsions


Rings

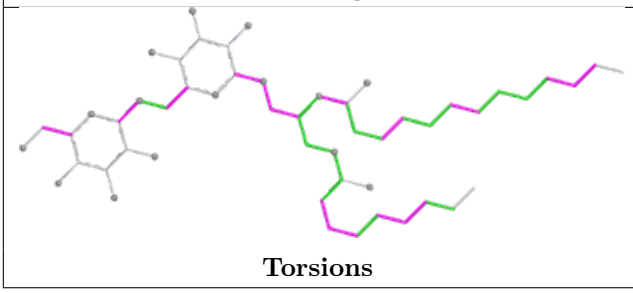
Ligand DGD B 625



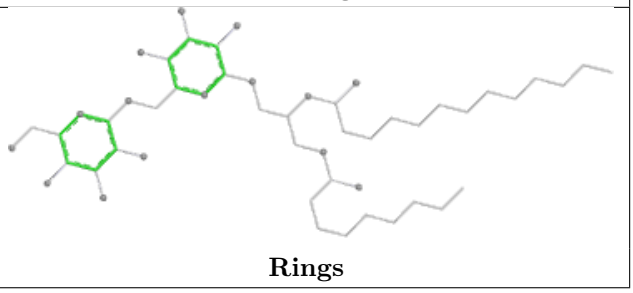
Bond lengths



Bond angles

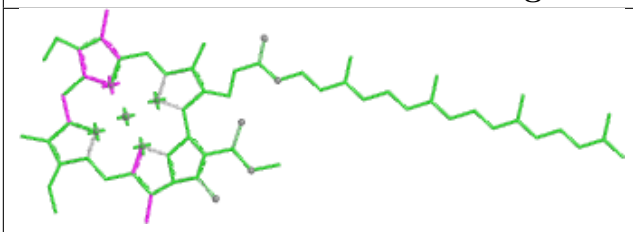


Torsions

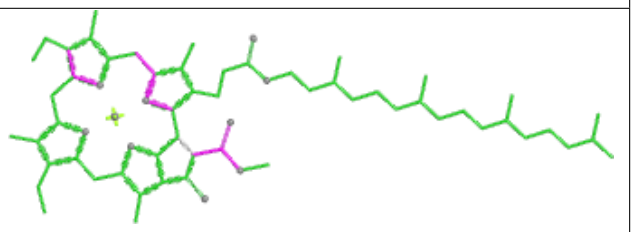


Rings

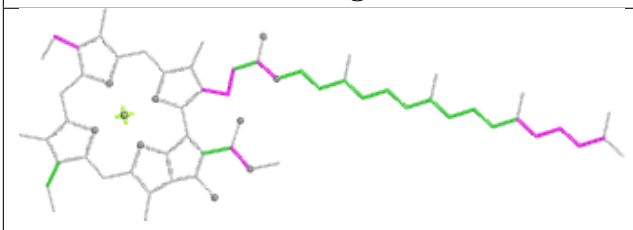
Ligand CLA B 605



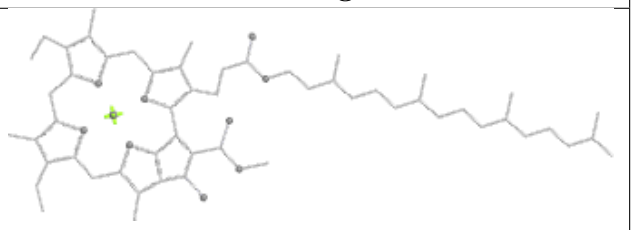
Bond lengths



Bond angles

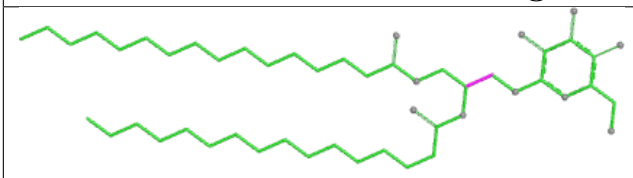


Torsions

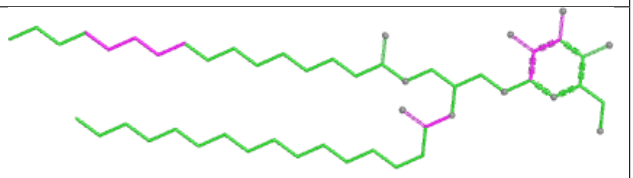


Rings

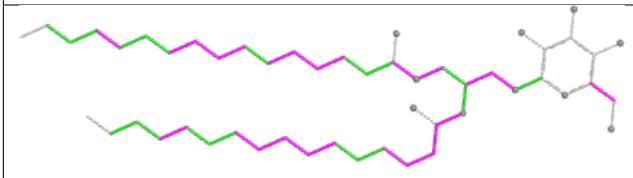
Ligand LMG l 101



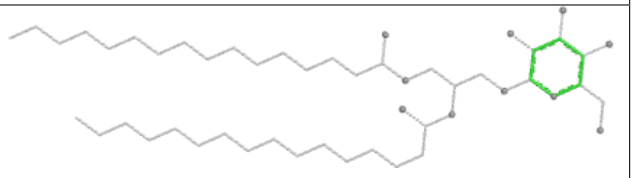
Bond lengths



Bond angles

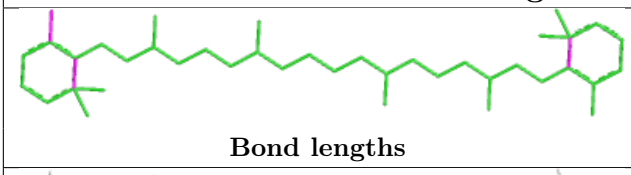


Torsions

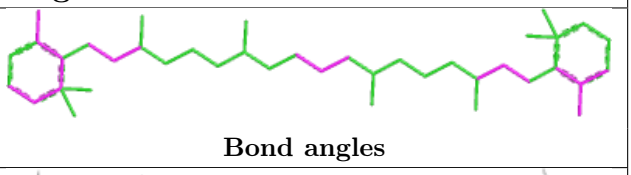


Rings

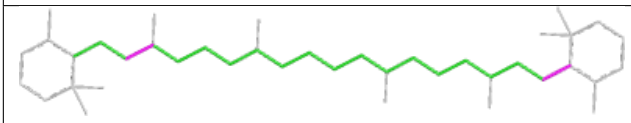
Ligand BCR g 101



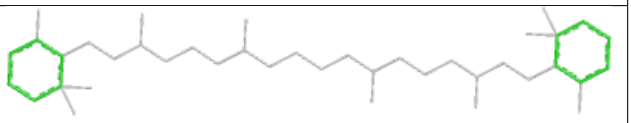
Bond lengths



Bond angles

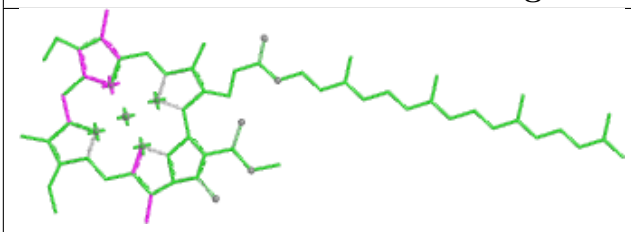


Torsions

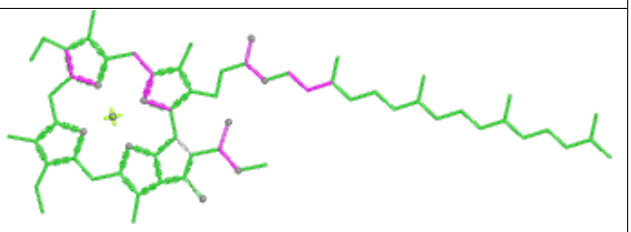


Rings

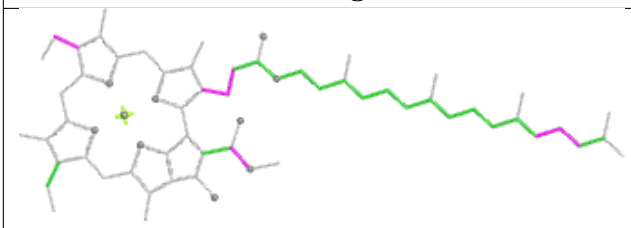
Ligand CLA B 606



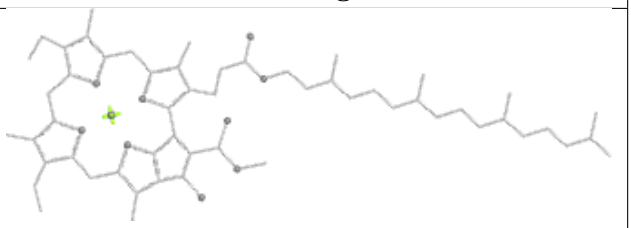
Bond lengths



Bond angles

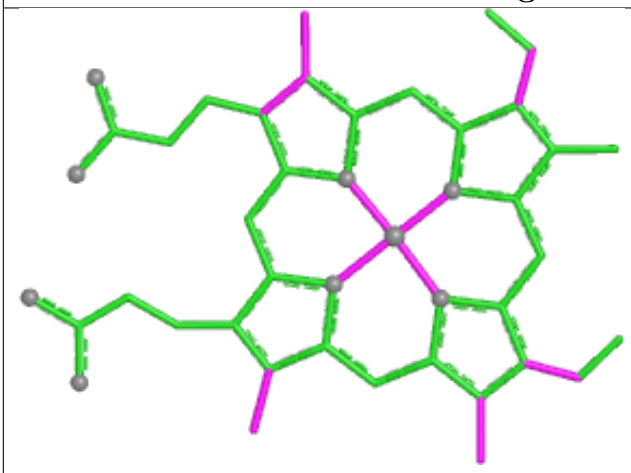


Torsions

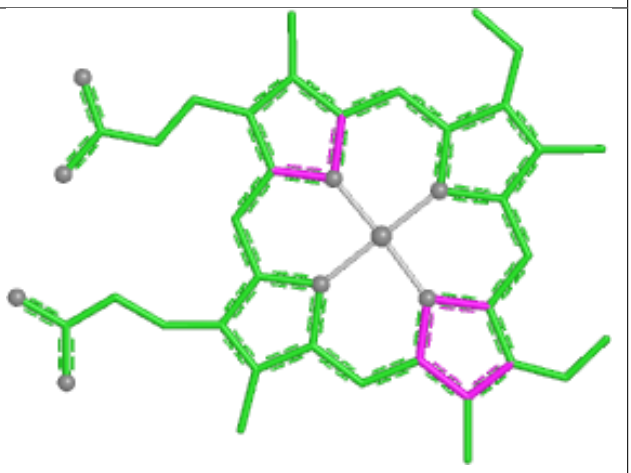


Rings

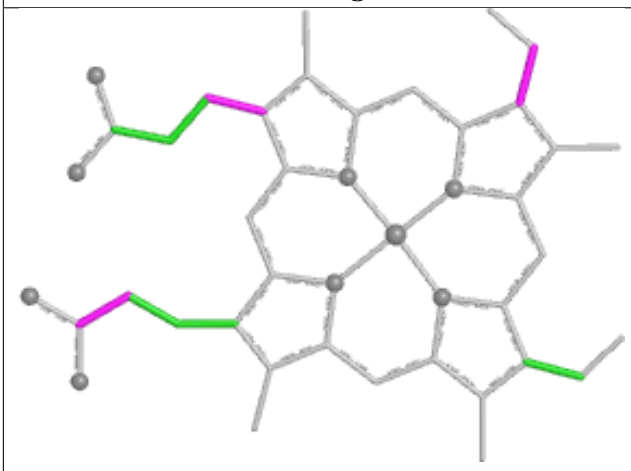
Ligand HEM V 201



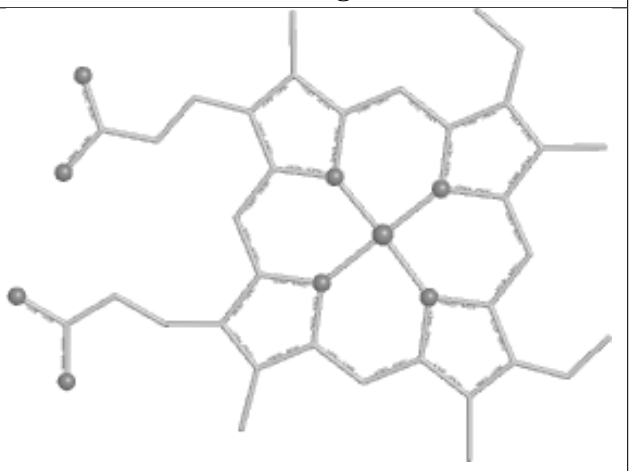
Bond lengths



Bond angles

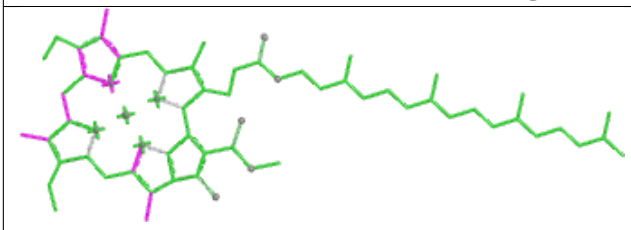


Torsions

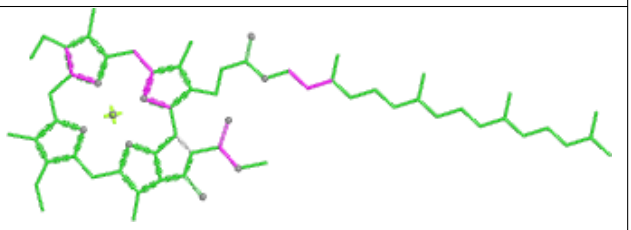


Rings

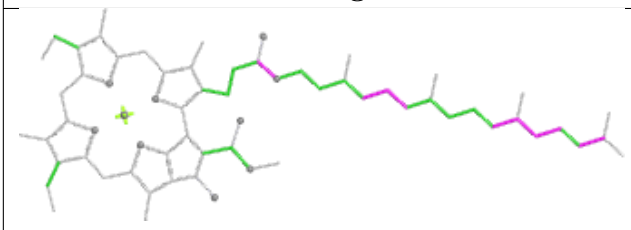
Ligand CLA C 502



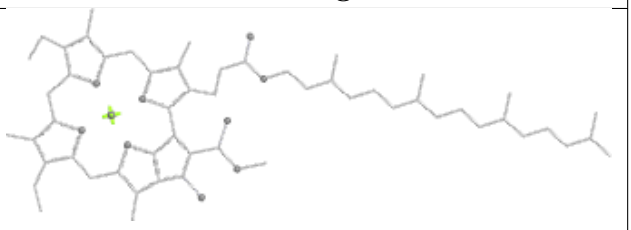
Bond lengths



Bond angles

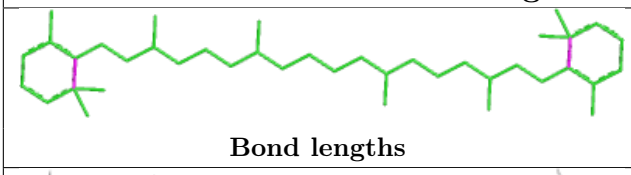


Torsions

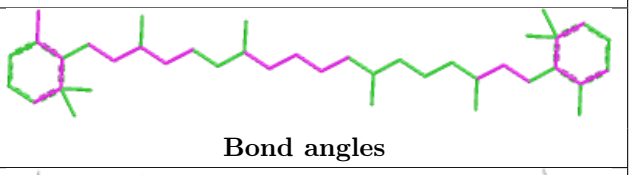


Rings

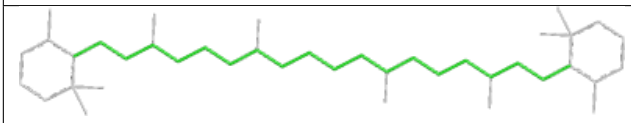
Ligand BCR B 618



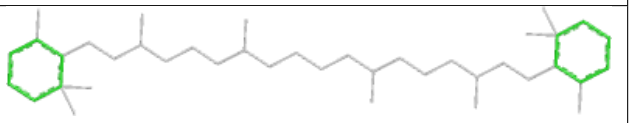
Bond lengths



Bond angles



Torsions



Rings

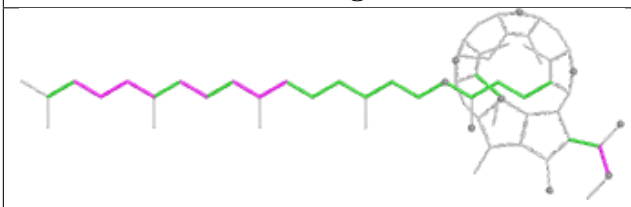
Ligand PHO D 402



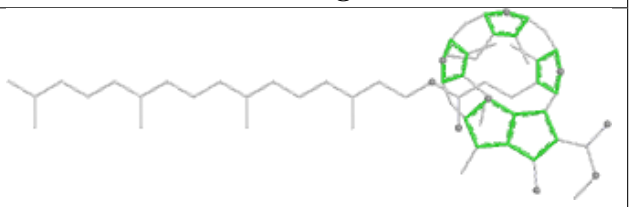
Bond lengths



Bond angles

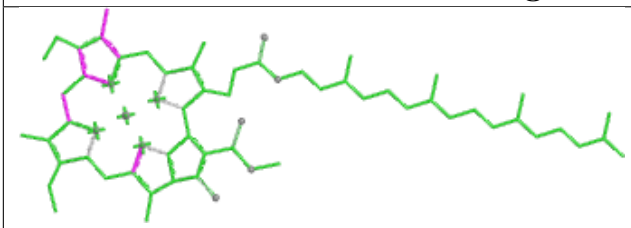


Torsions

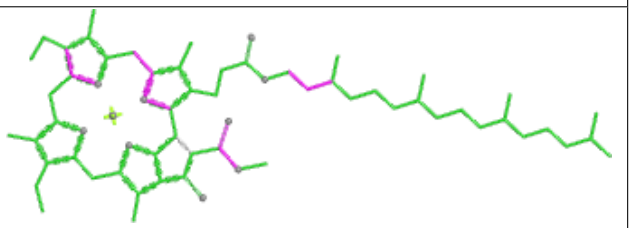


Rings

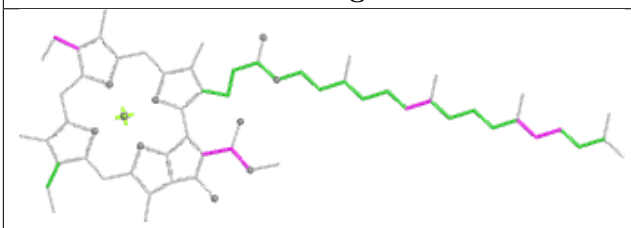
Ligand CLA B 608



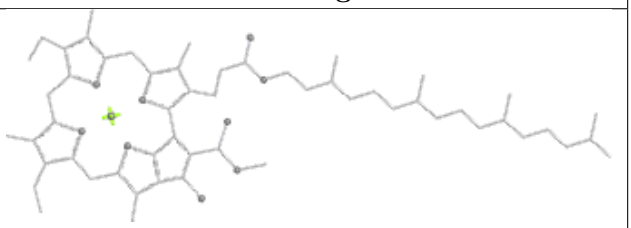
Bond lengths



Bond angles

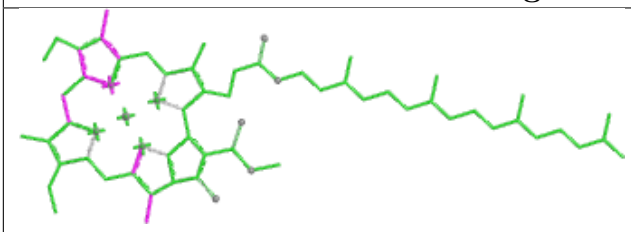


Torsions

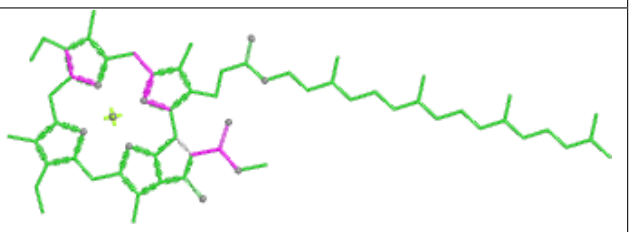


Rings

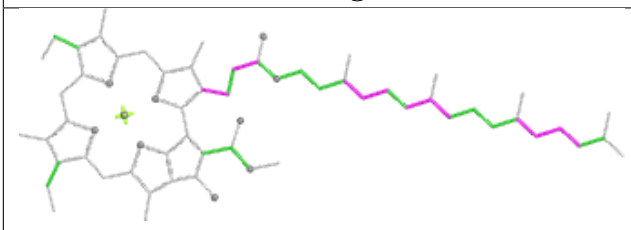
Ligand CLA D 404



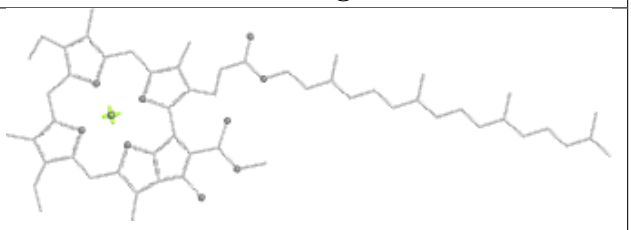
Bond lengths



Bond angles

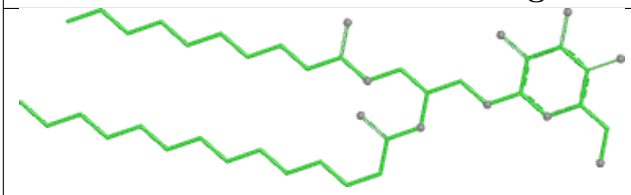


Torsions

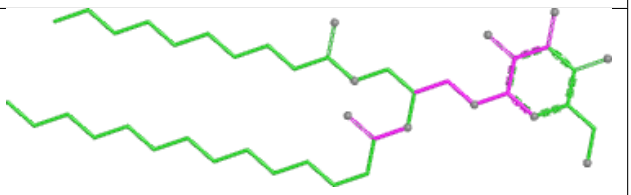


Rings

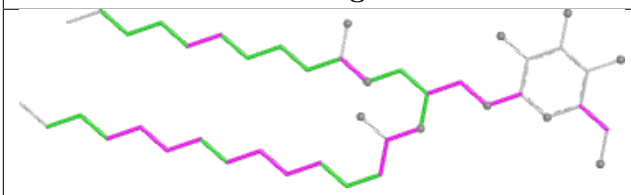
Ligand LMG i 101



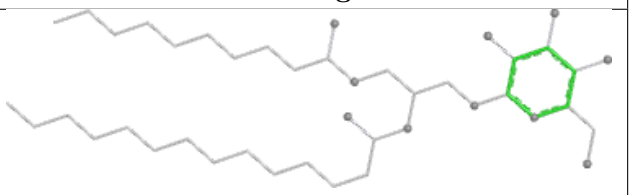
Bond lengths



Bond angles

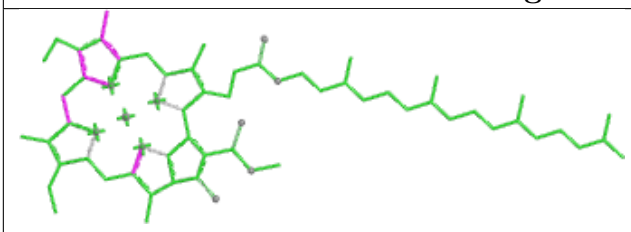


Torsions

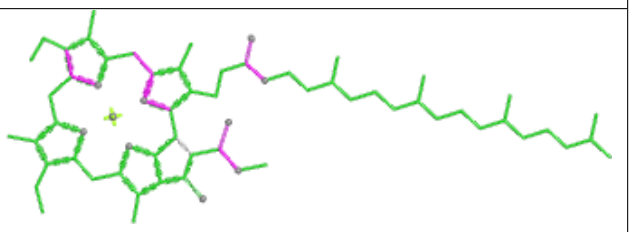


Rings

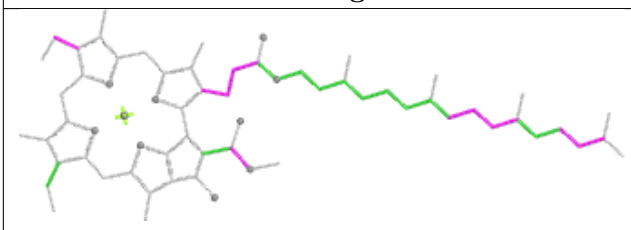
Ligand CLA C 501



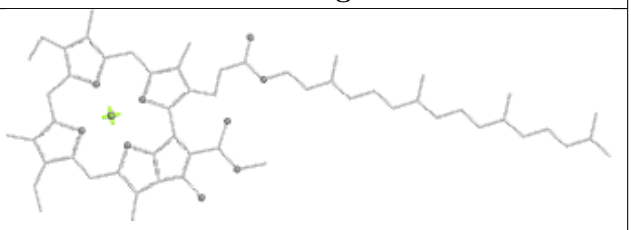
Bond lengths



Bond angles

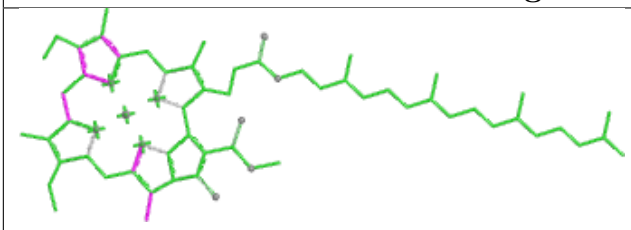


Torsions

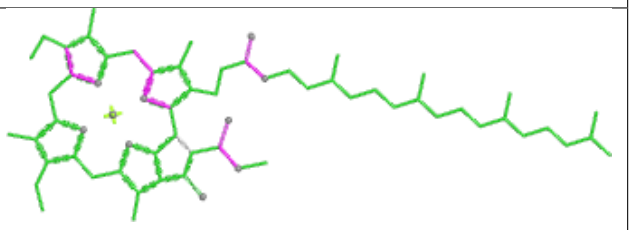


Rings

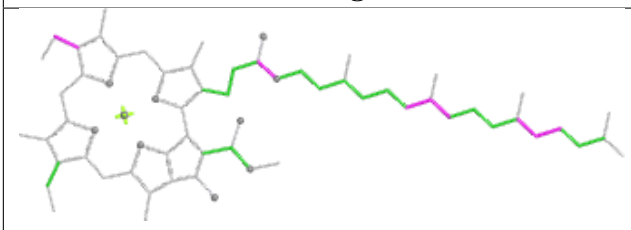
Ligand CLA B 614



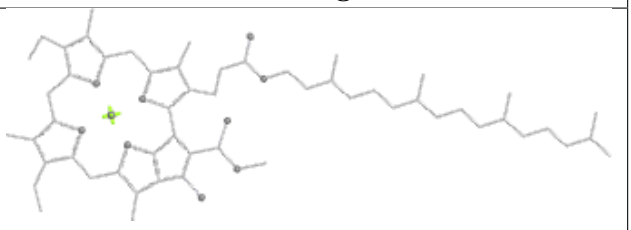
Bond lengths



Bond angles

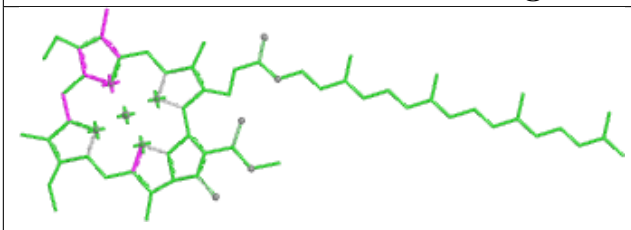


Torsions

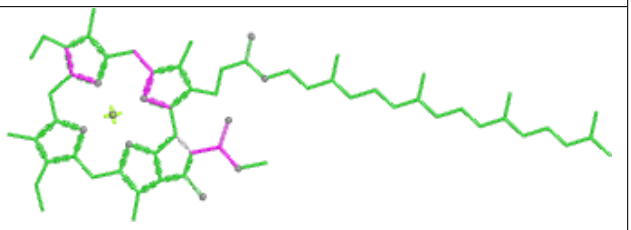


Rings

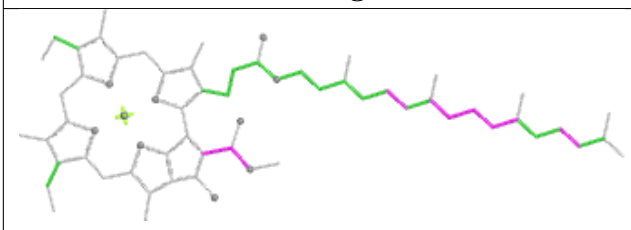
Ligand CLA C 503



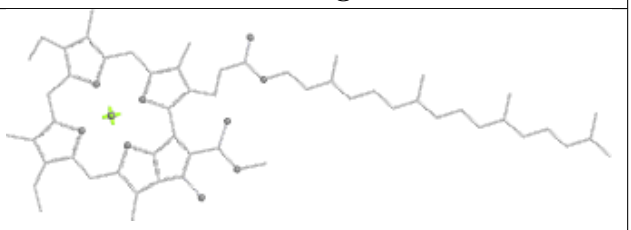
Bond lengths



Bond angles

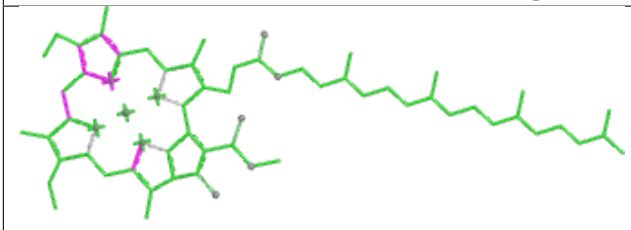


Torsions

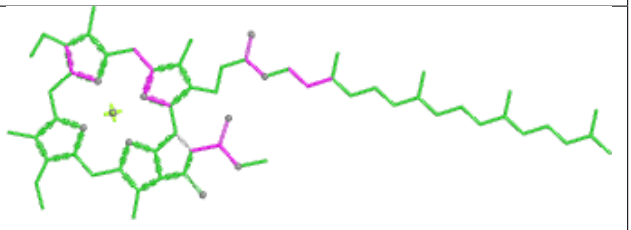


Rings

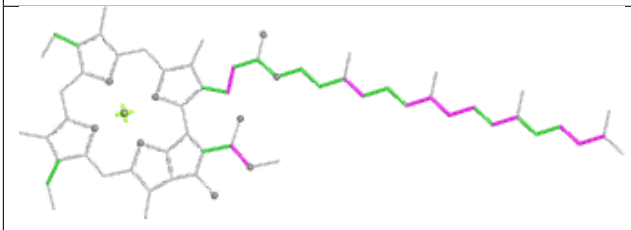
Ligand CLA b 606



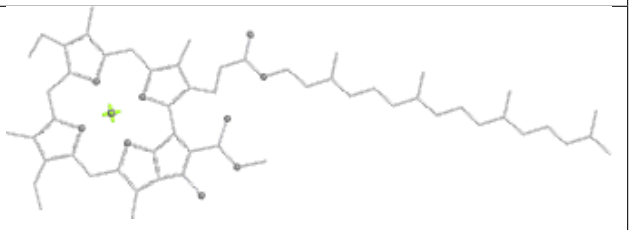
Bond lengths



Bond angles

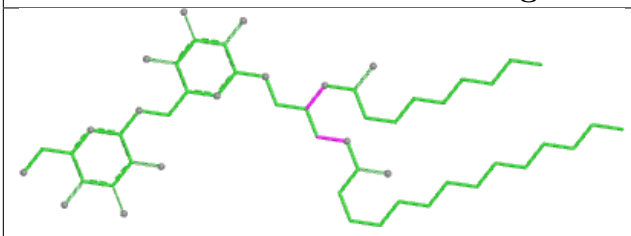


Torsions

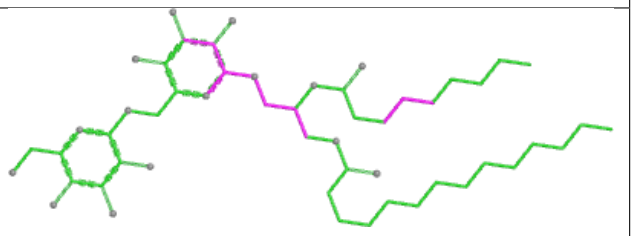


Rings

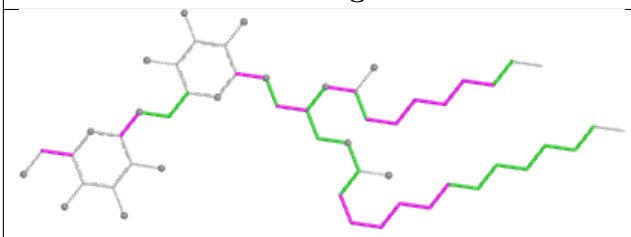
Ligand DGD C 515



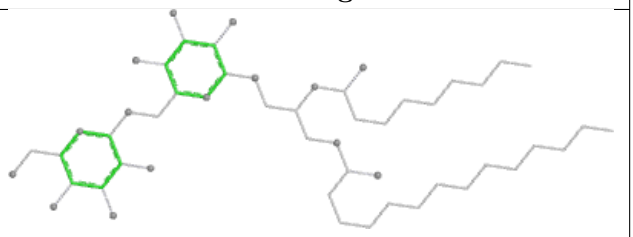
Bond lengths



Bond angles

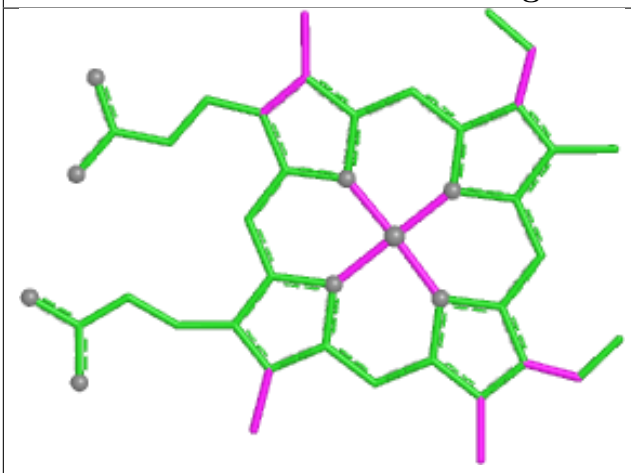


Torsions

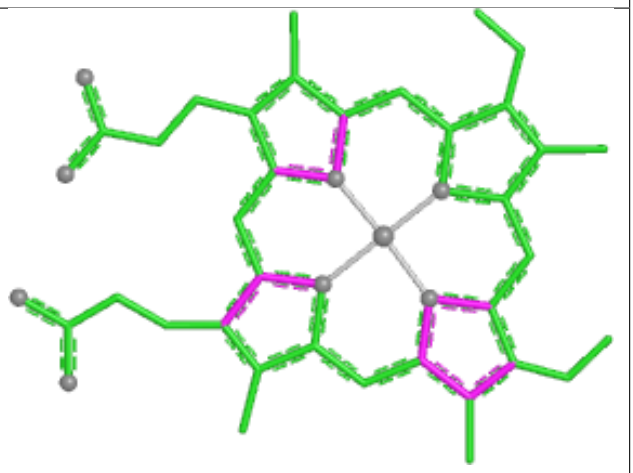


Rings

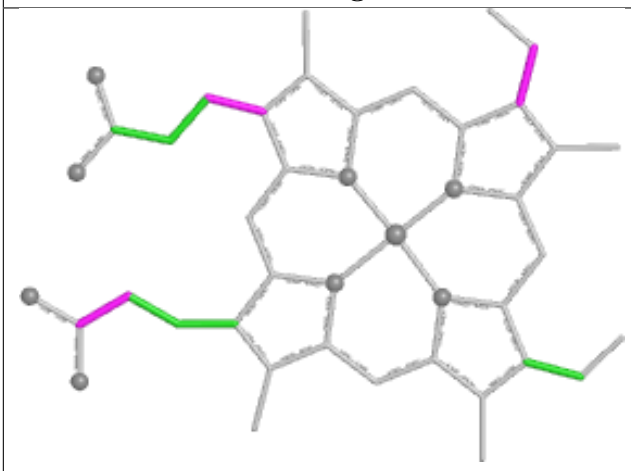
Ligand HEM v 201



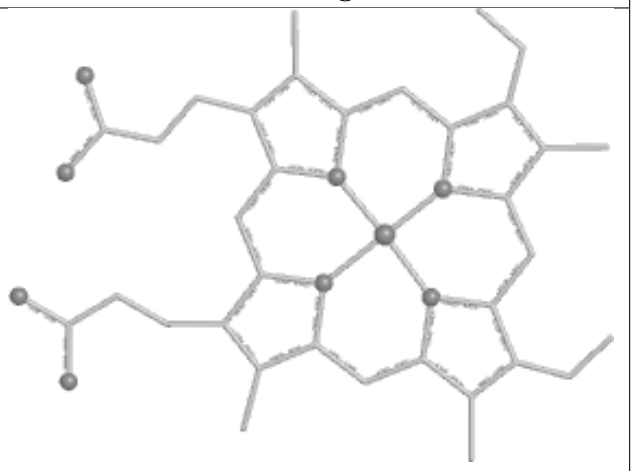
Bond lengths



Bond angles

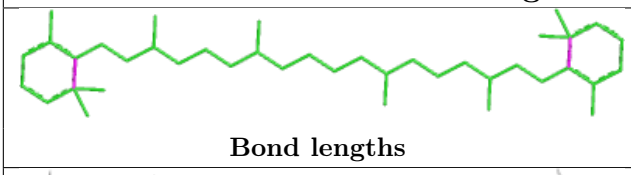


Torsions

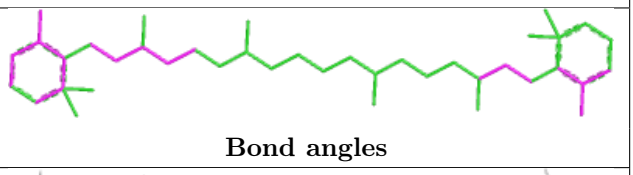


Rings

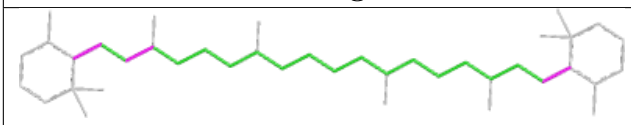
Ligand BCR B 619



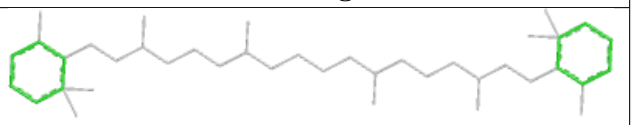
Bond lengths



Bond angles

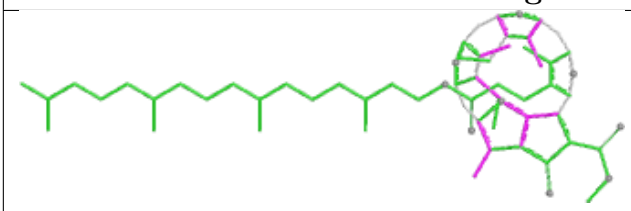


Torsions

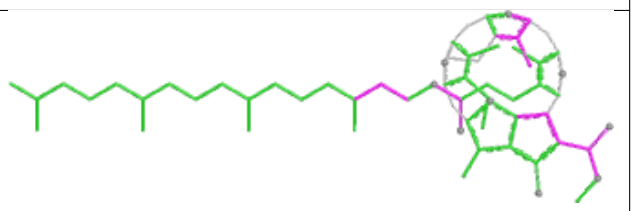


Rings

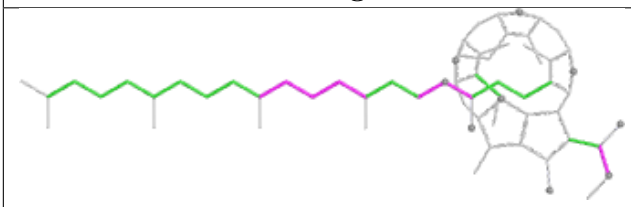
Ligand PHO d 401



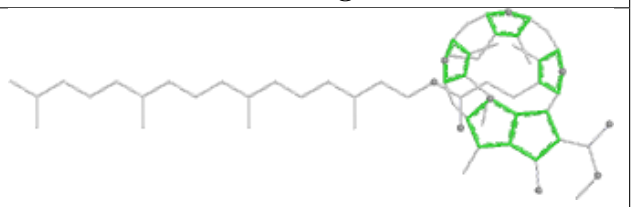
Bond lengths



Bond angles

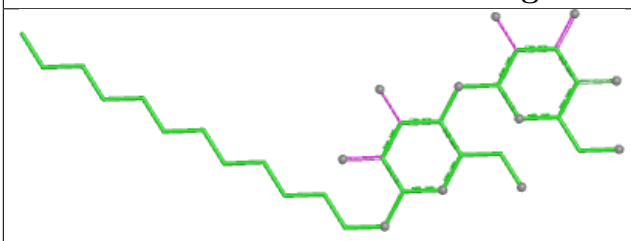


Torsions

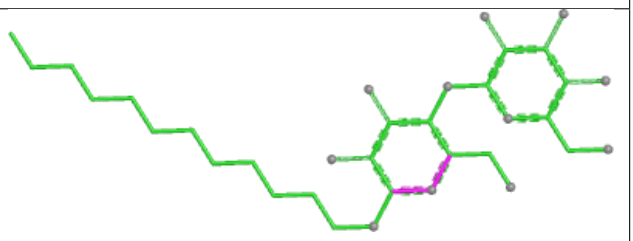


Rings

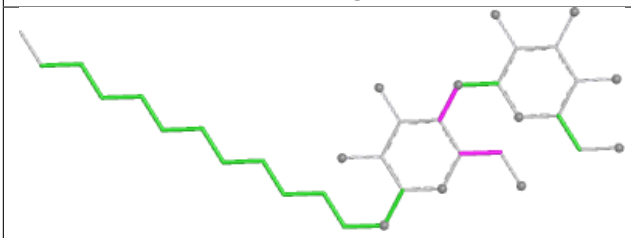
Ligand LMT B 627



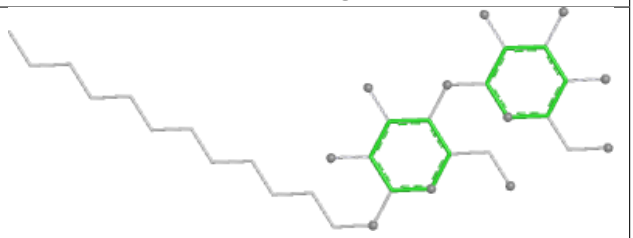
Bond lengths



Bond angles

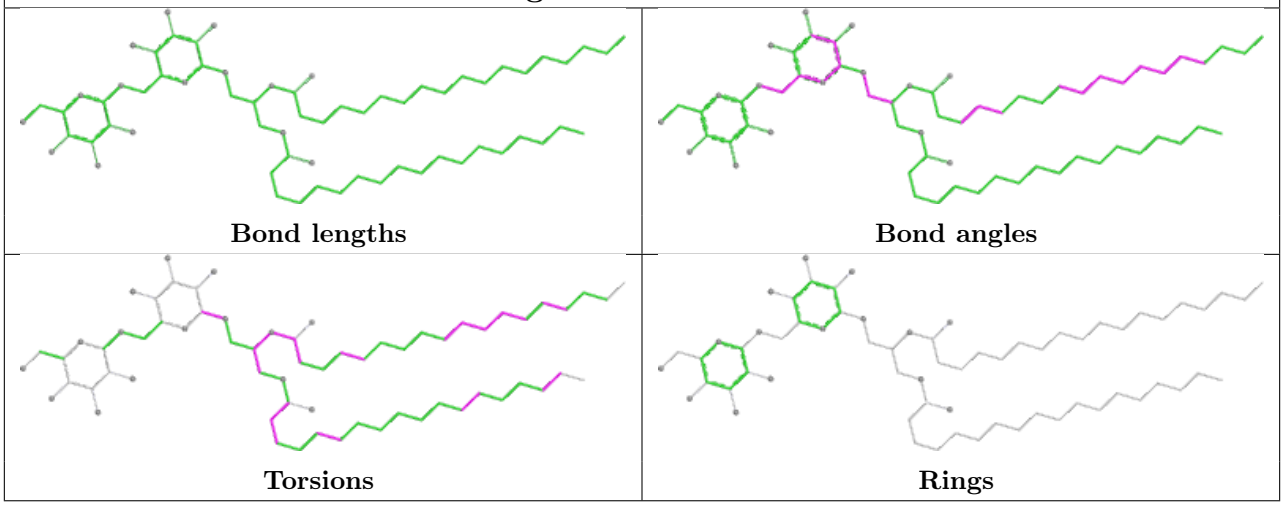


Torsions

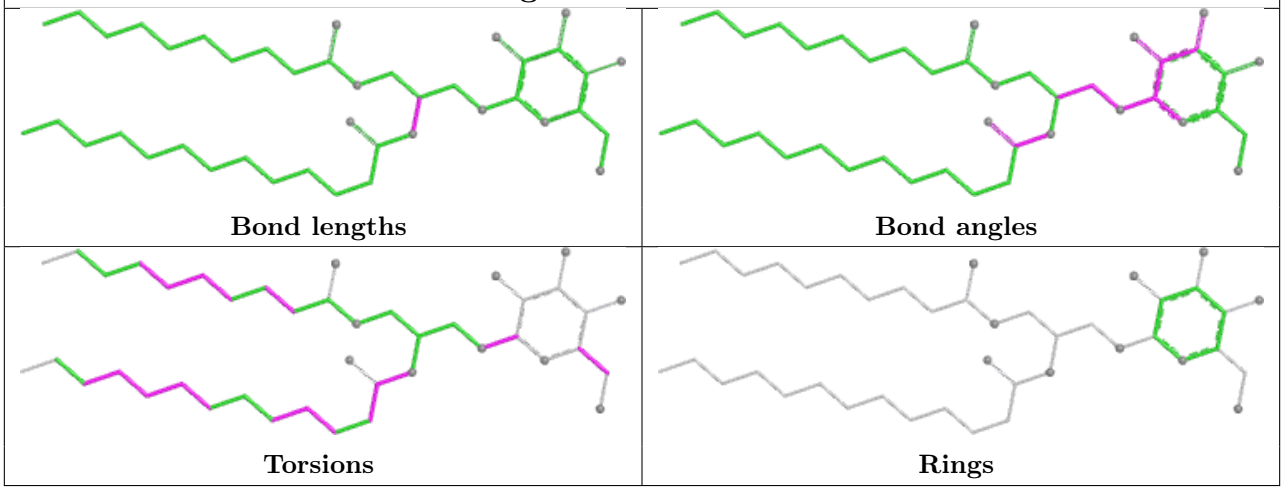


Rings

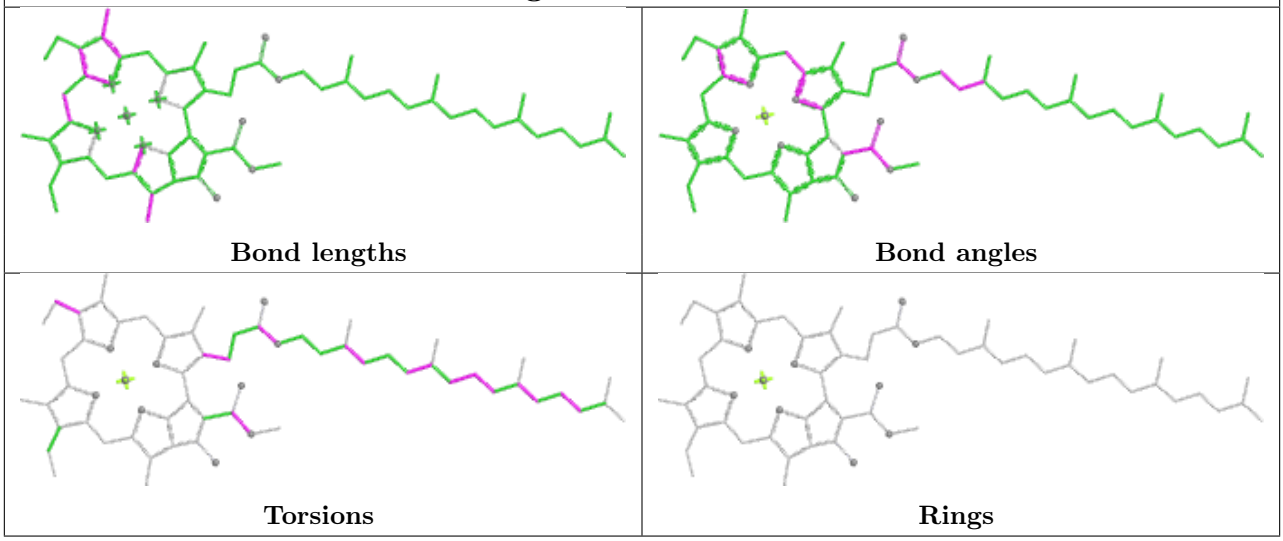
Ligand DGD c 517



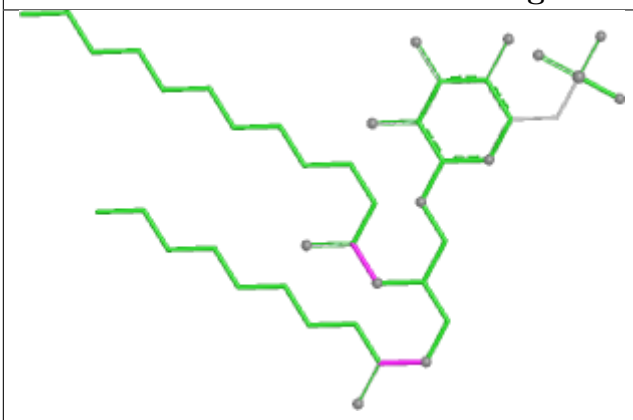
Ligand LMG A 415



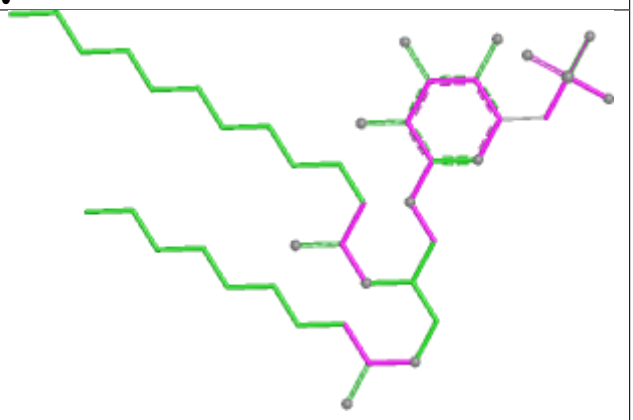
Ligand CLA C 504



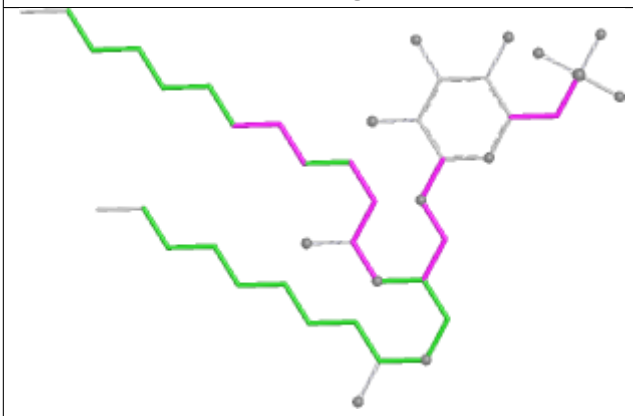
Ligand SQD d 402



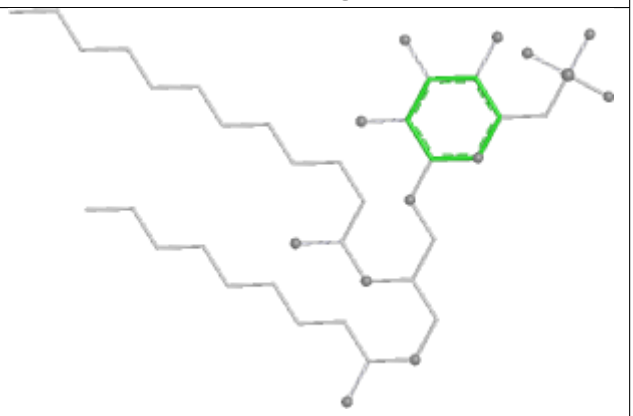
Bond lengths



Bond angles

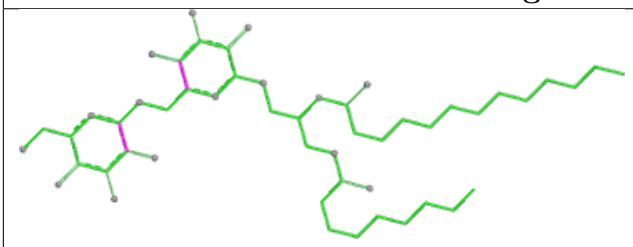


Torsions

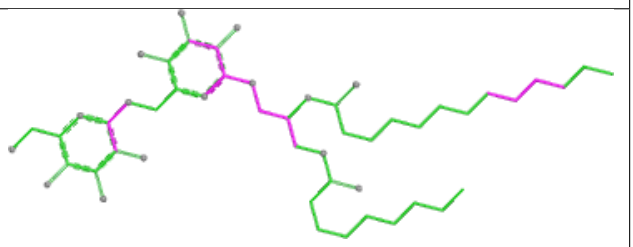


Rings

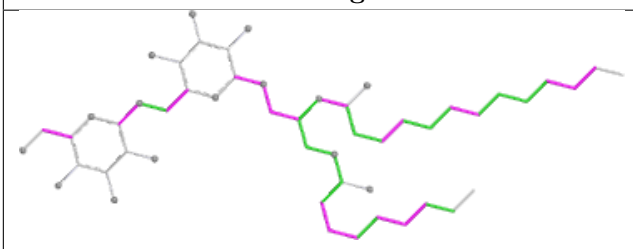
Ligand DGD b 601



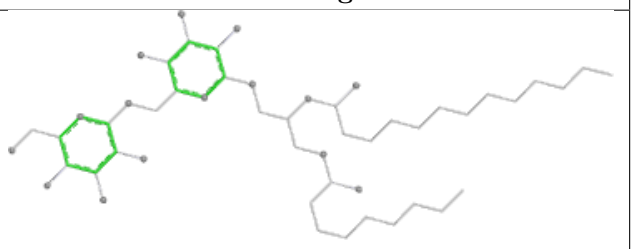
Bond lengths



Bond angles

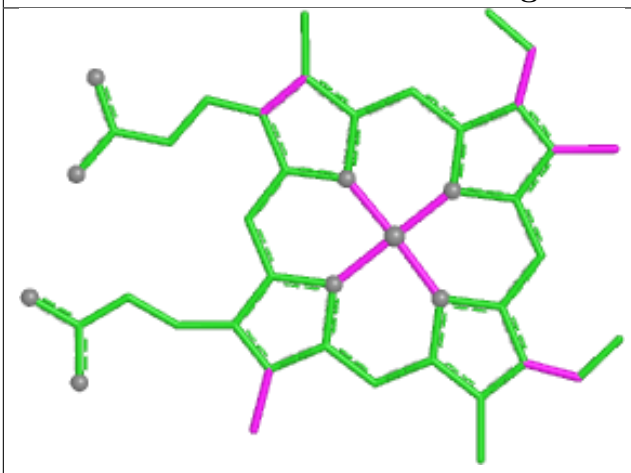


Torsions

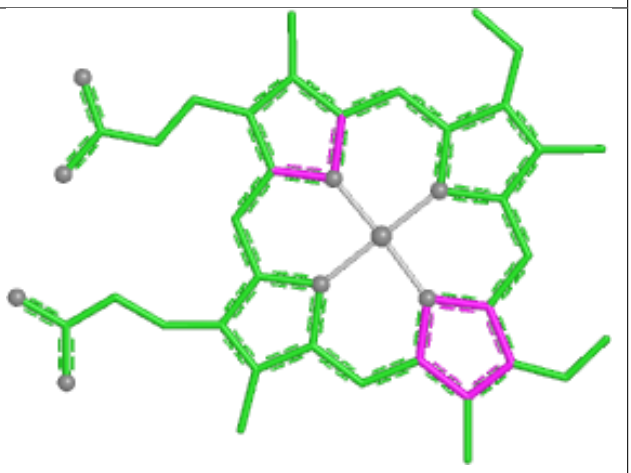


Rings

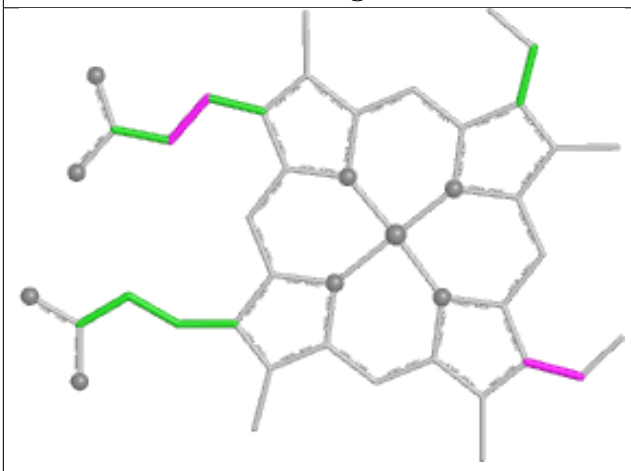
Ligand HEM F 101



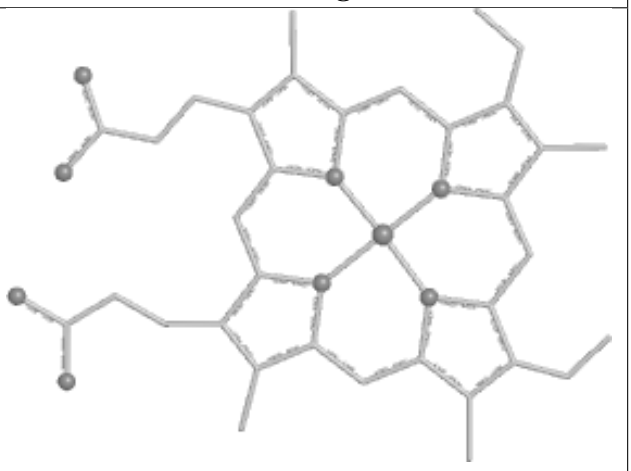
Bond lengths



Bond angles

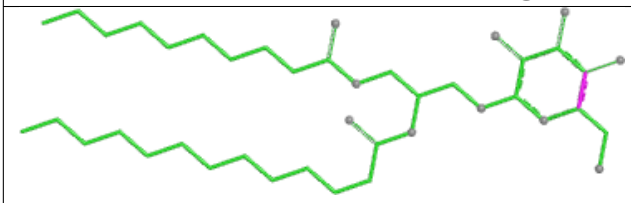


Torsions

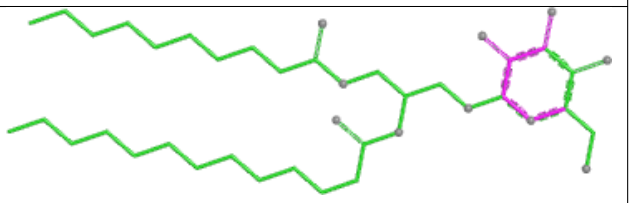


Rings

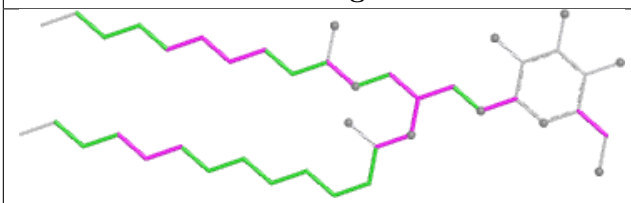
Ligand LMG m 101



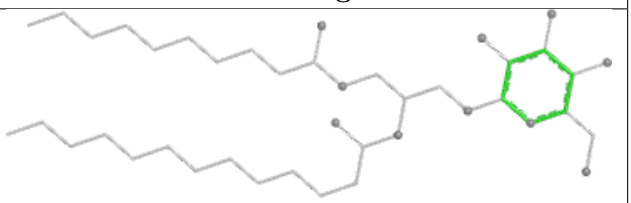
Bond lengths



Bond angles

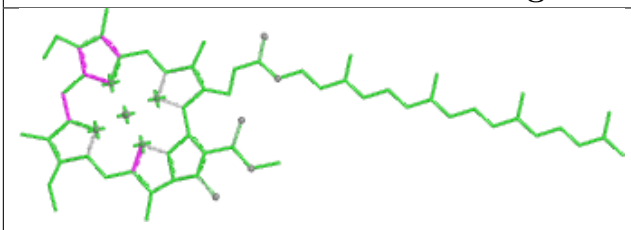


Torsions

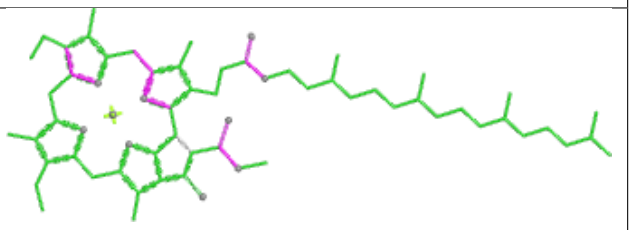


Rings

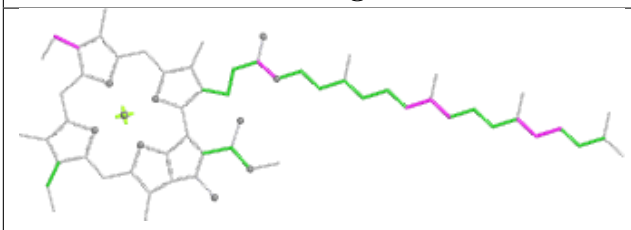
Ligand CLA b 618



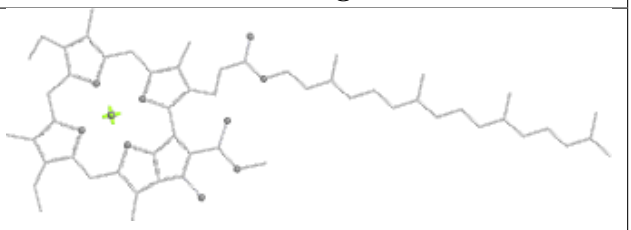
Bond lengths



Bond angles

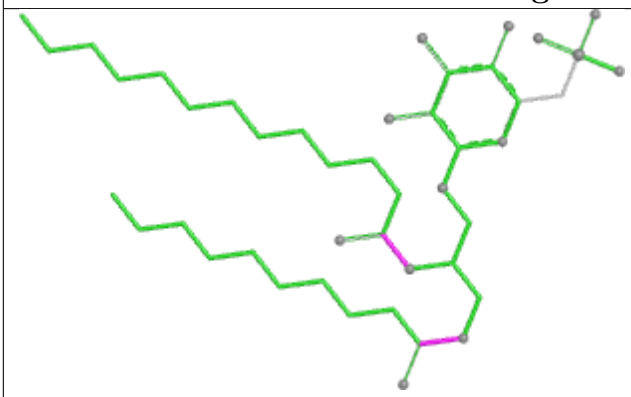


Torsions

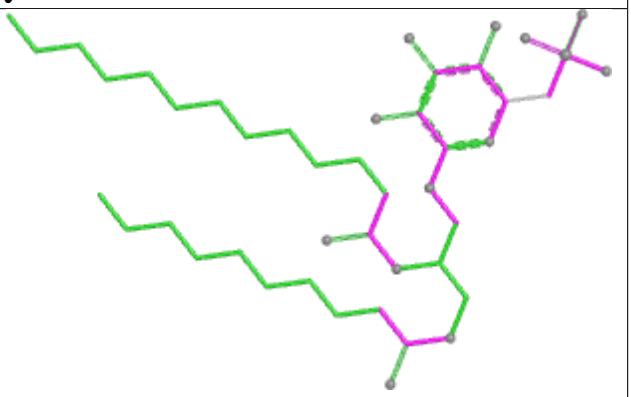


Rings

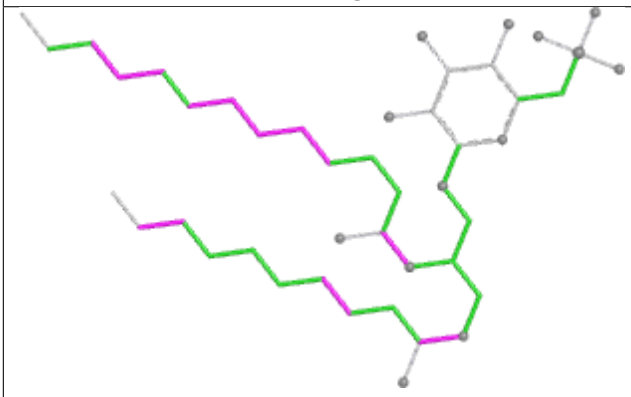
Ligand SQD f 103



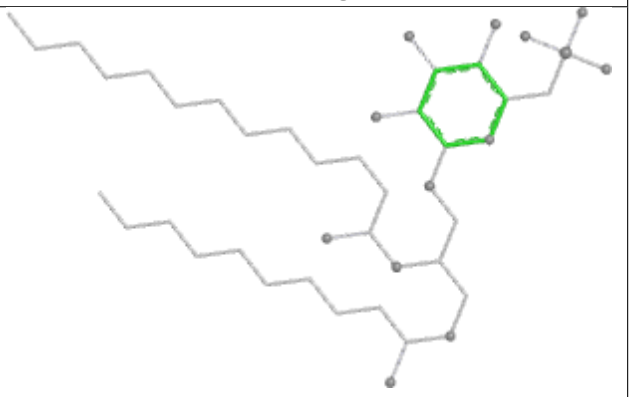
Bond lengths



Bond angles



Torsions



Rings

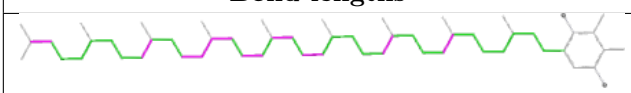
Ligand PL9 d 406



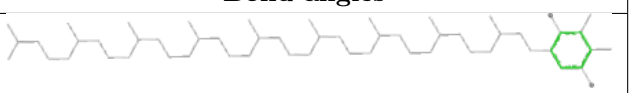
Bond lengths



Bond angles

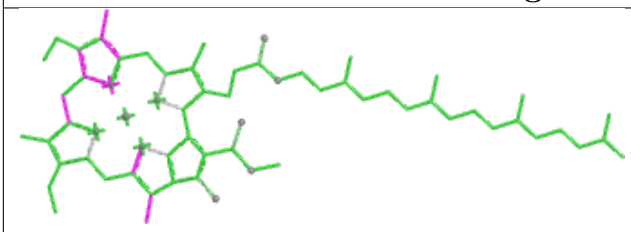


Torsions

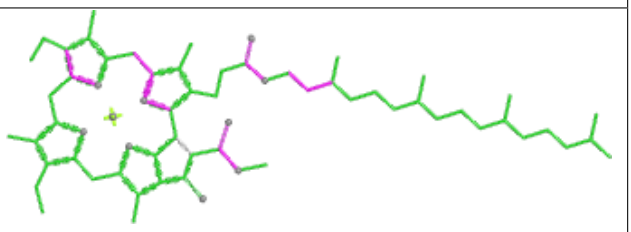


Rings

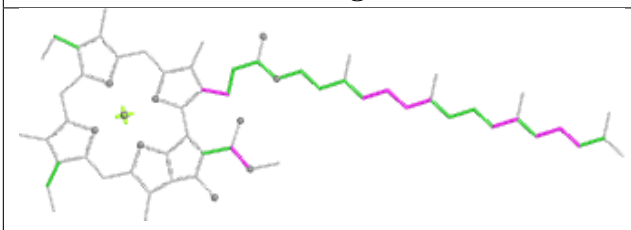
Ligand CLA B 607



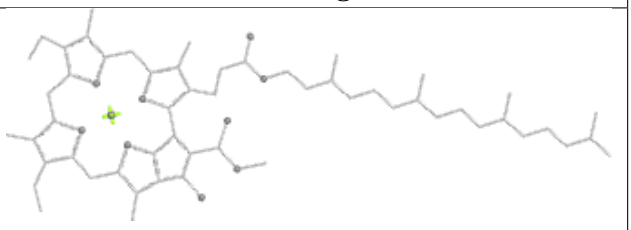
Bond lengths



Bond angles



Torsions

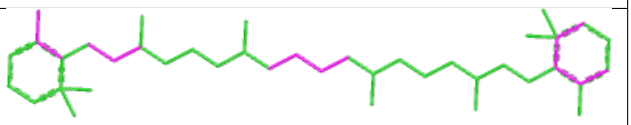


Rings

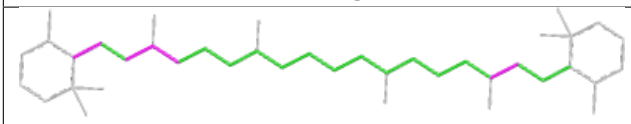
Ligand BCR H 102



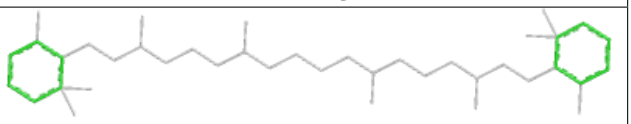
Bond lengths



Bond angles

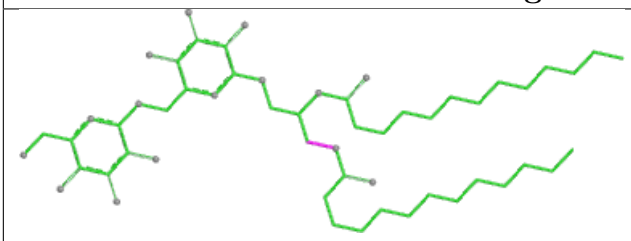


Torsions

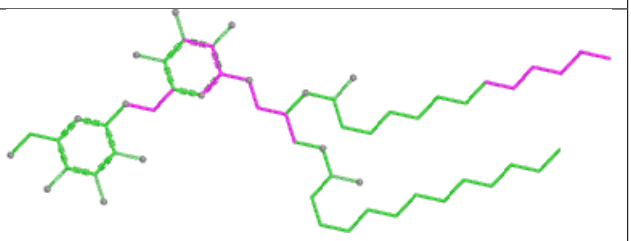


Rings

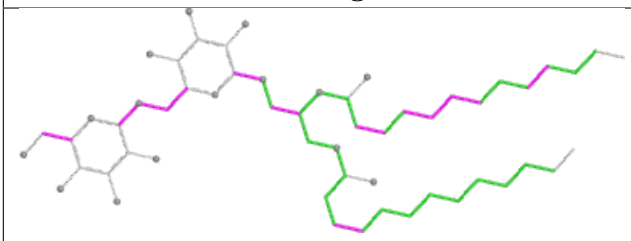
Ligand DGD a 411



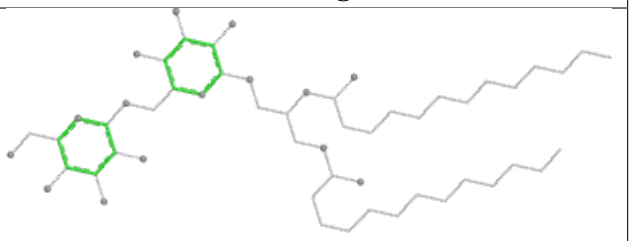
Bond lengths



Bond angles

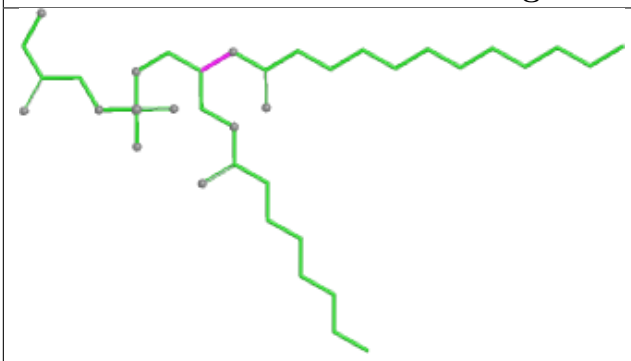


Torsions

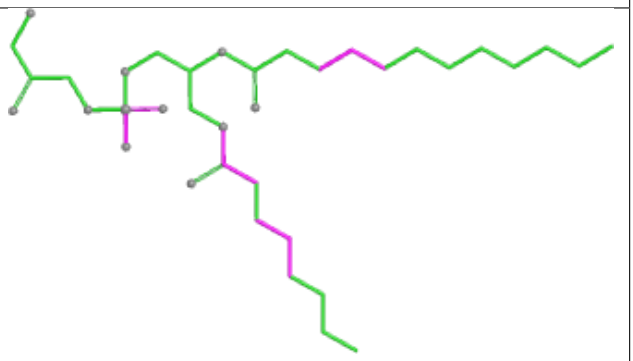


Rings

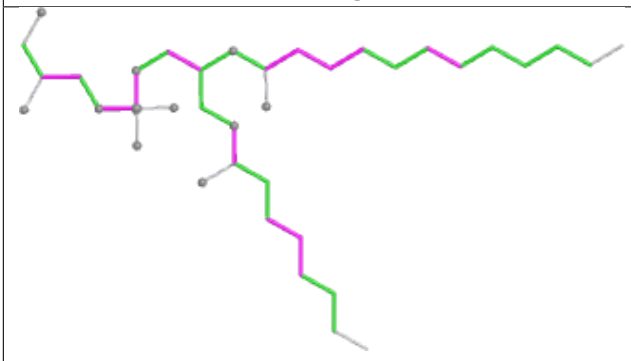
Ligand LHG C 519



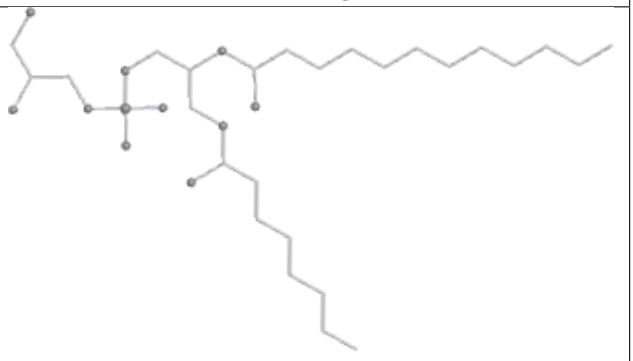
Bond lengths



Bond angles

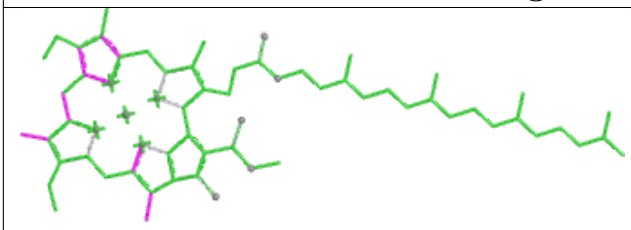


Torsions

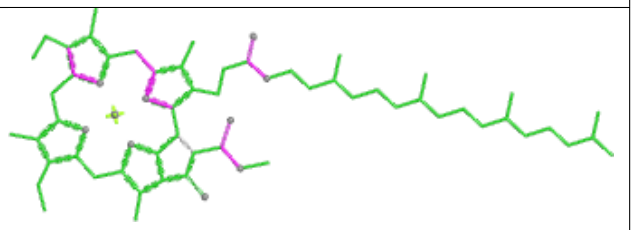


Rings

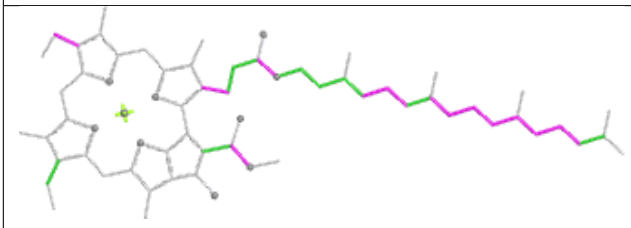
Ligand CLA b 619



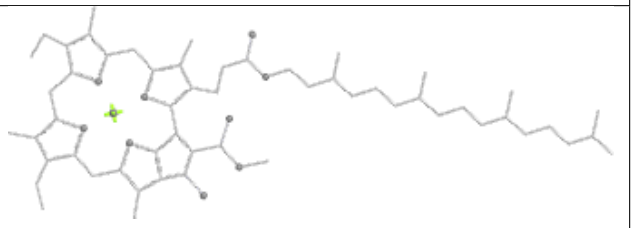
Bond lengths



Bond angles

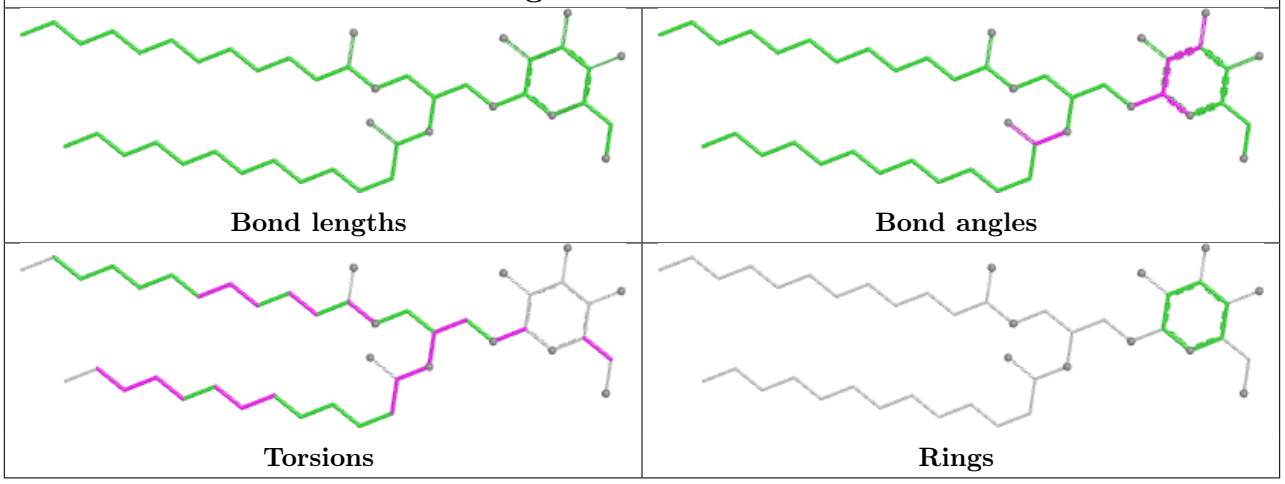


Torsions

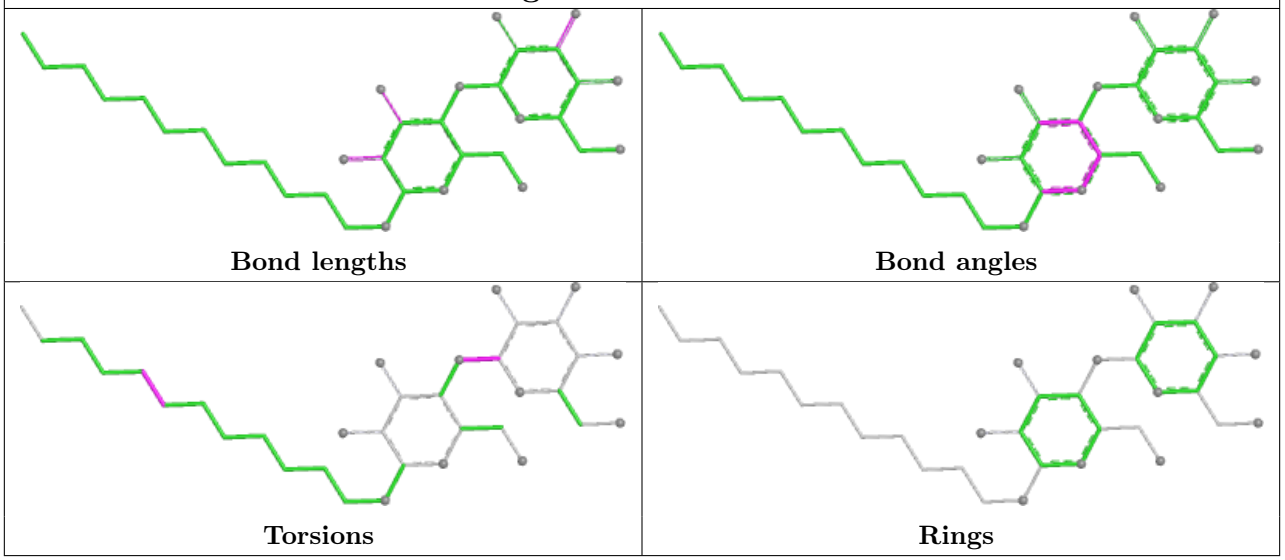


Rings

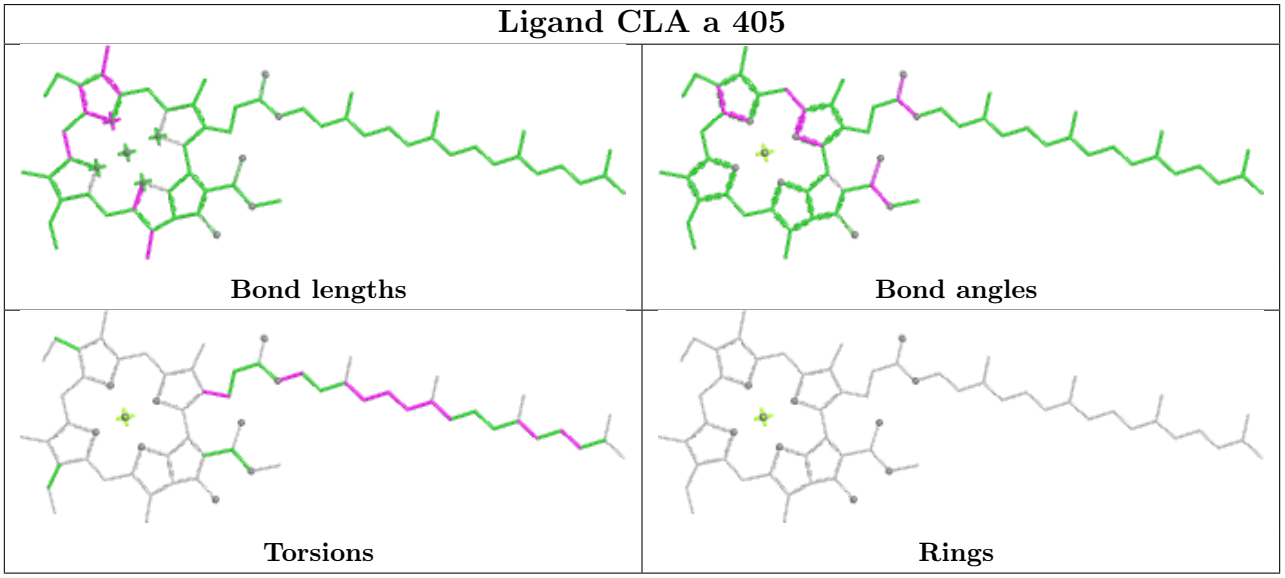
Ligand LMG e 101



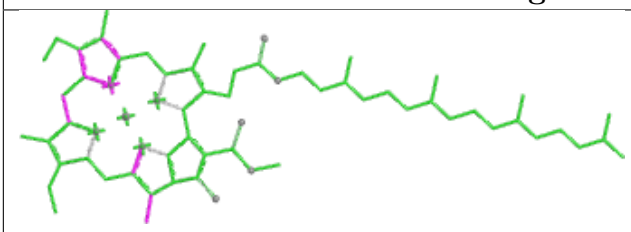
Ligand LMT B 624



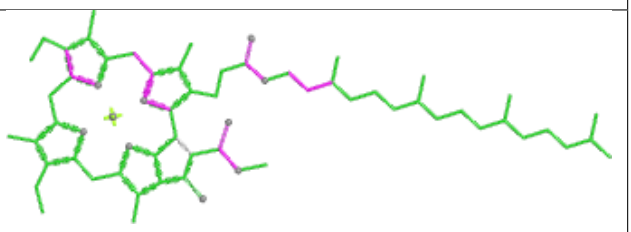
Ligand CLA a 405



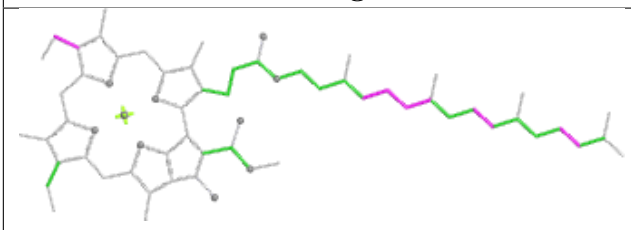
Ligand CLA a 406



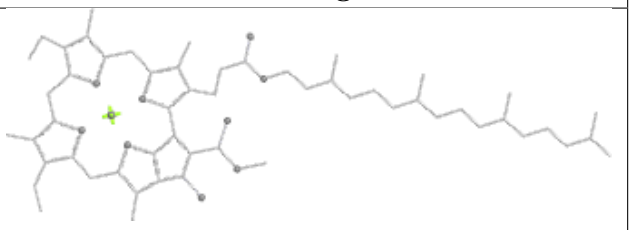
Bond lengths



Bond angles

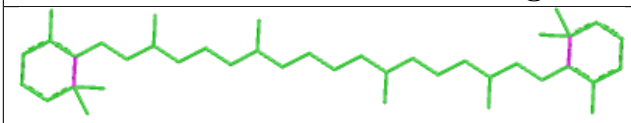


Torsions

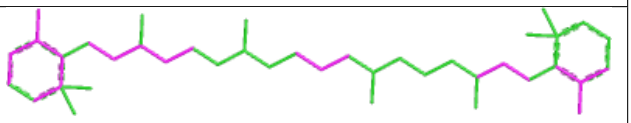


Rings

Ligand BCR b 623



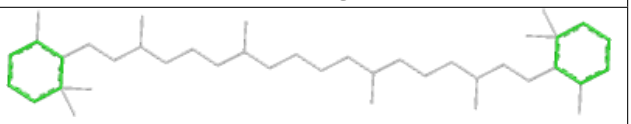
Bond lengths



Bond angles

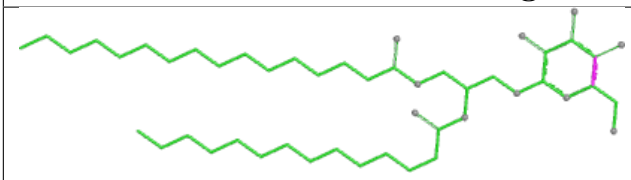


Torsions

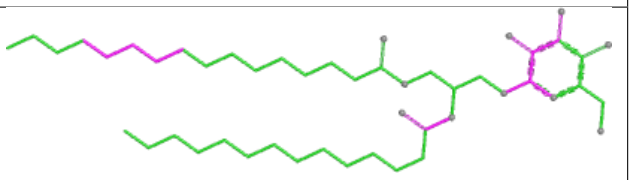


Rings

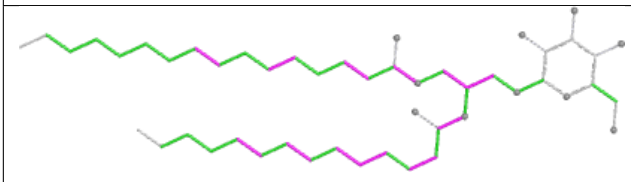
Ligand LMG B 621



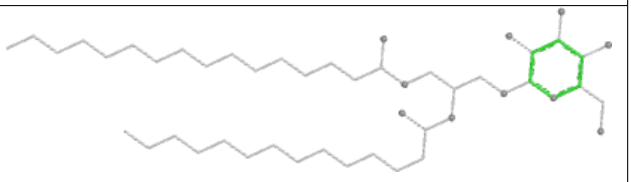
Bond lengths



Bond angles

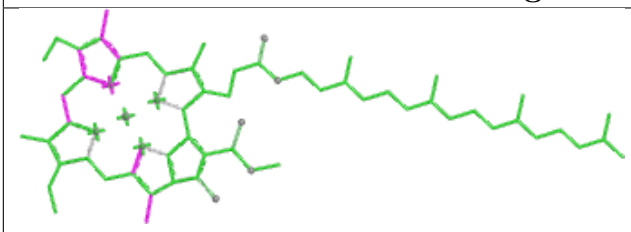


Torsions

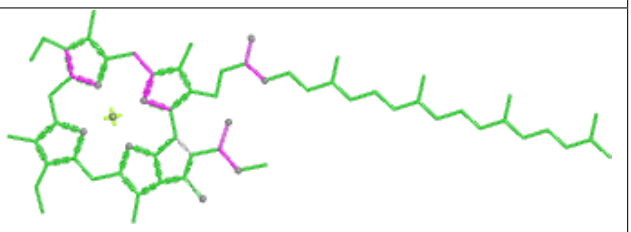


Rings

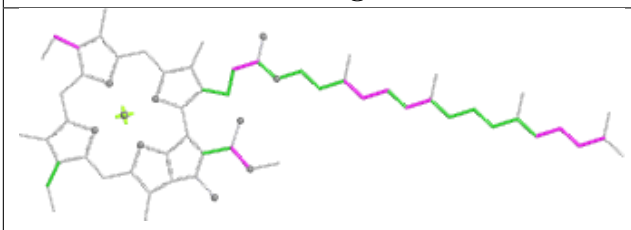
Ligand CLA C 509



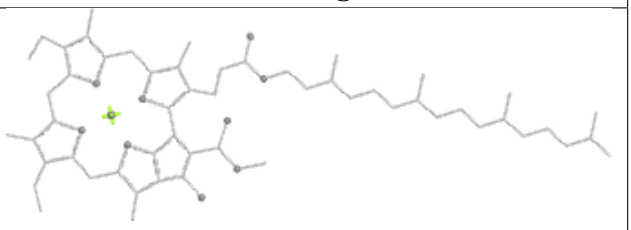
Bond lengths



Bond angles

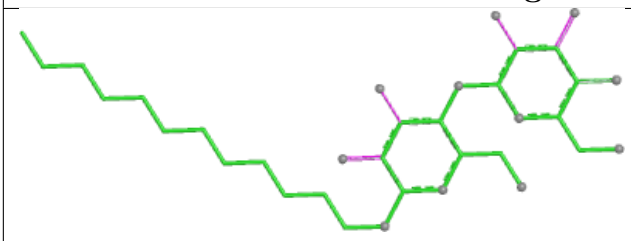


Torsions

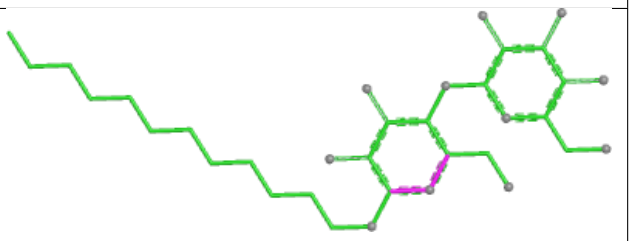


Rings

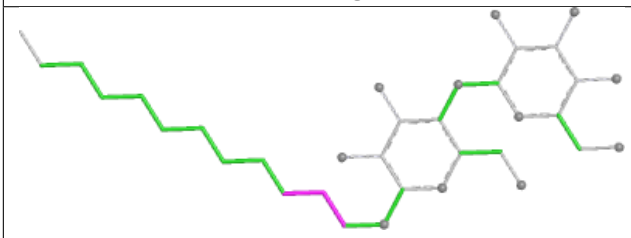
Ligand LMT b 626



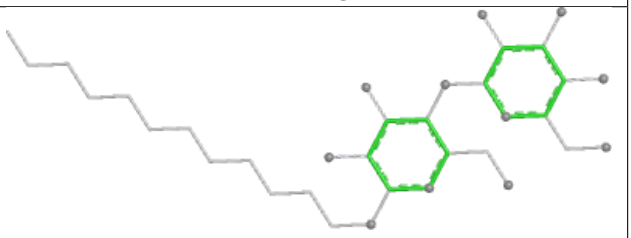
Bond lengths



Bond angles

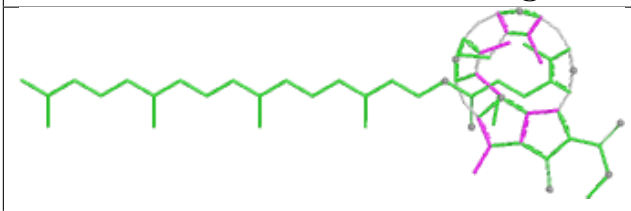


Torsions

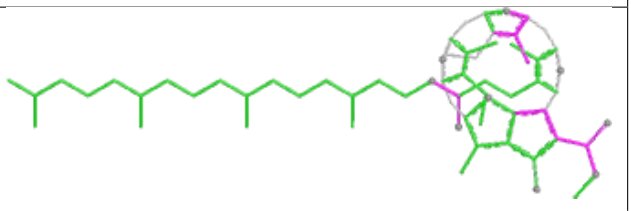


Rings

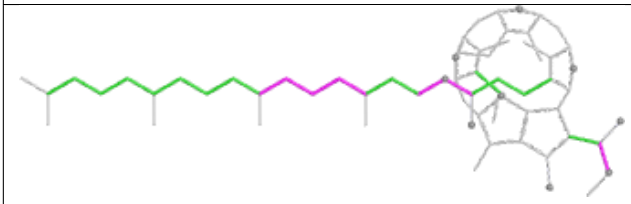
Ligand PHO D 401



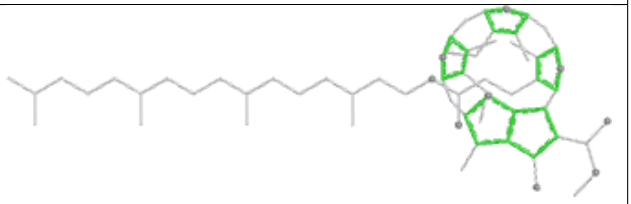
Bond lengths



Bond angles

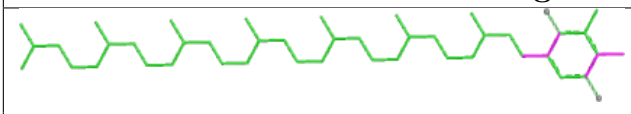


Torsions

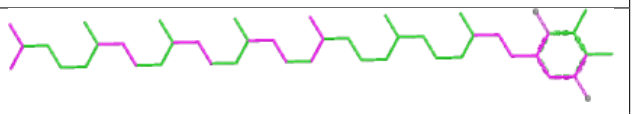


Rings

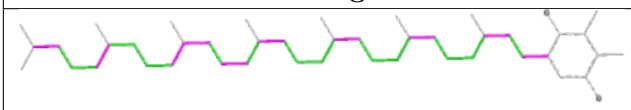
Ligand PL9 a 409



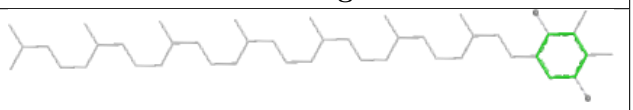
Bond lengths



Bond angles

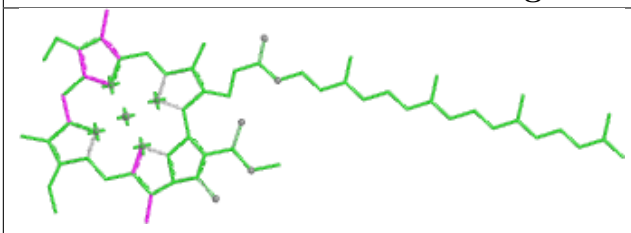


Torsions

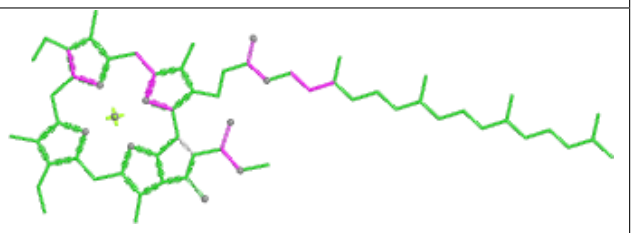


Rings

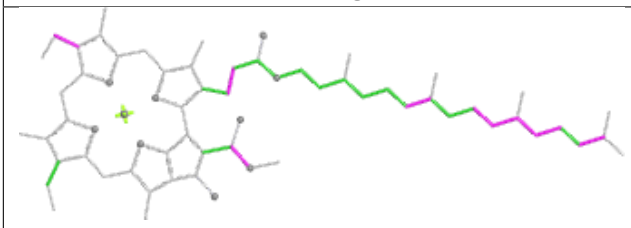
Ligand CLA B 601



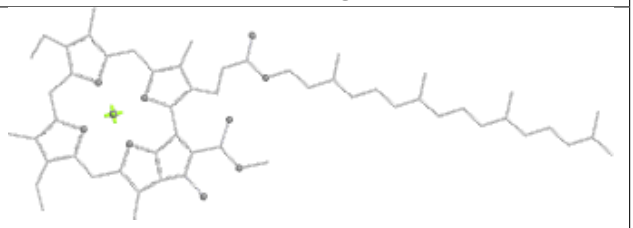
Bond lengths



Bond angles

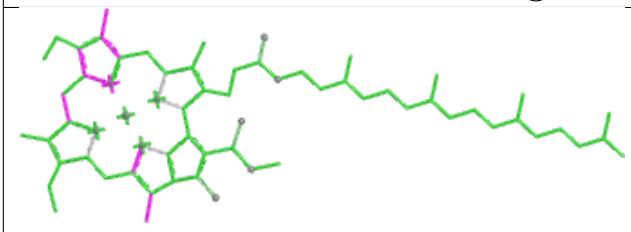


Torsions

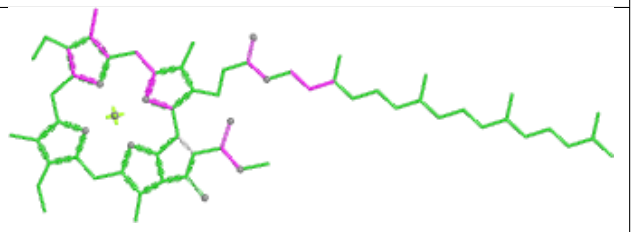


Rings

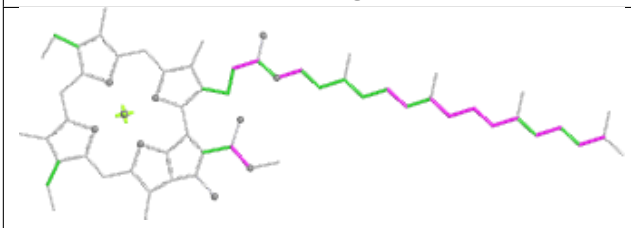
Ligand CLA b 616



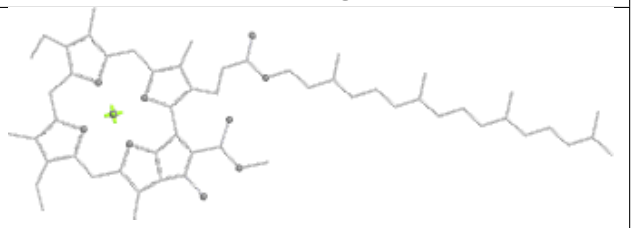
Bond lengths



Bond angles

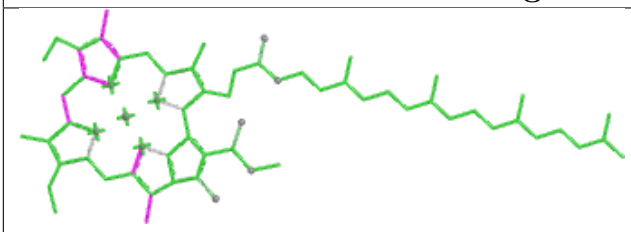


Torsions

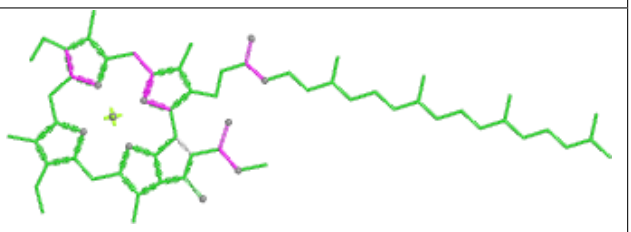


Rings

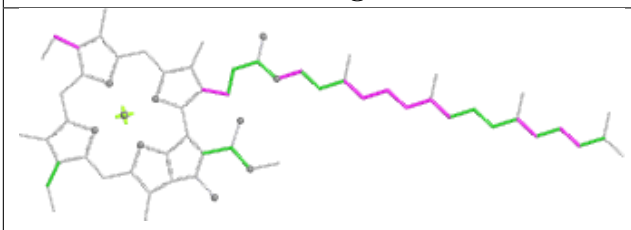
Ligand CLA A 403



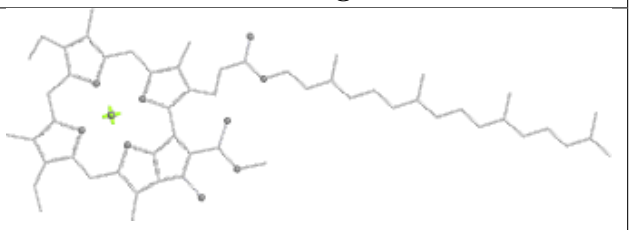
Bond lengths



Bond angles

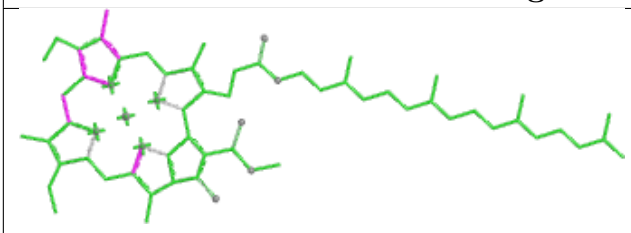


Torsions

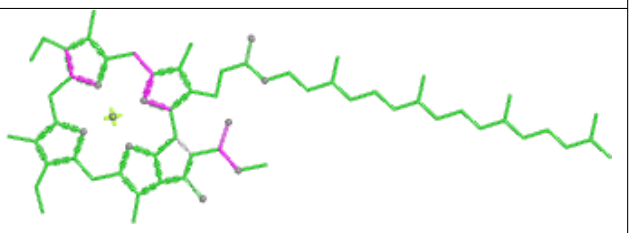


Rings

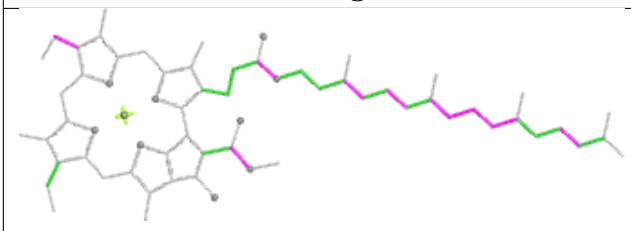
Ligand CLA b 608



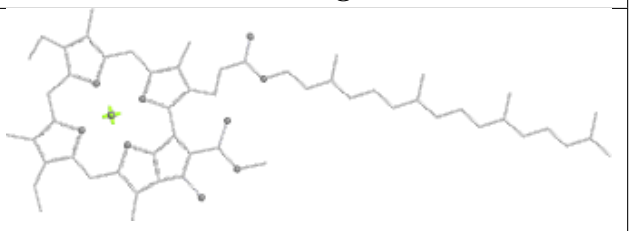
Bond lengths



Bond angles

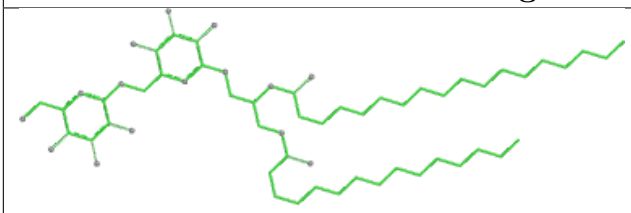


Torsions

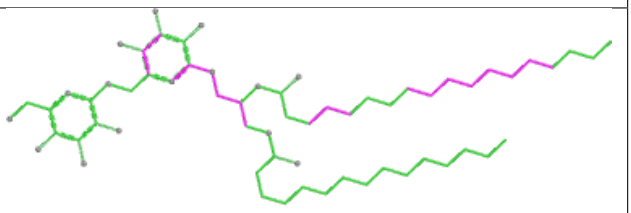


Rings

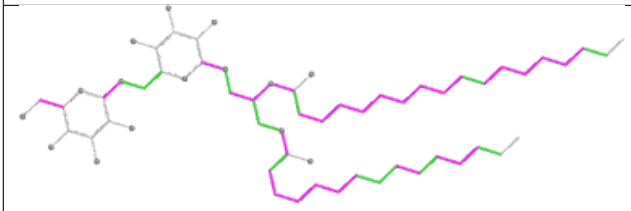
Ligand DGD D 409



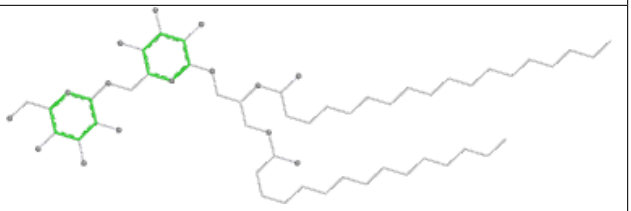
Bond lengths



Bond angles

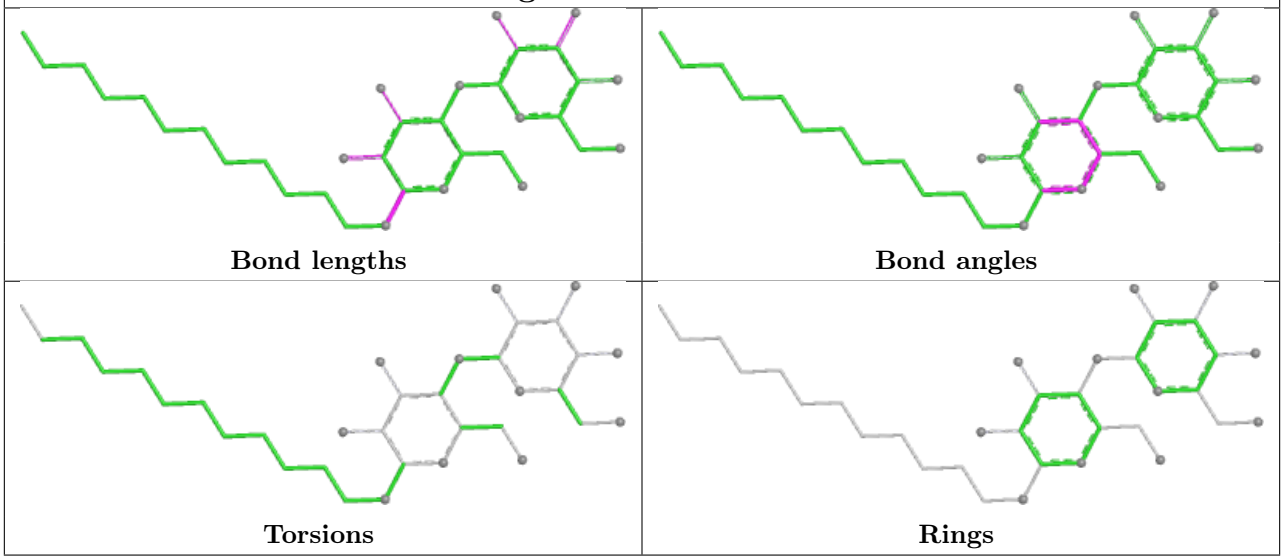


Torsions

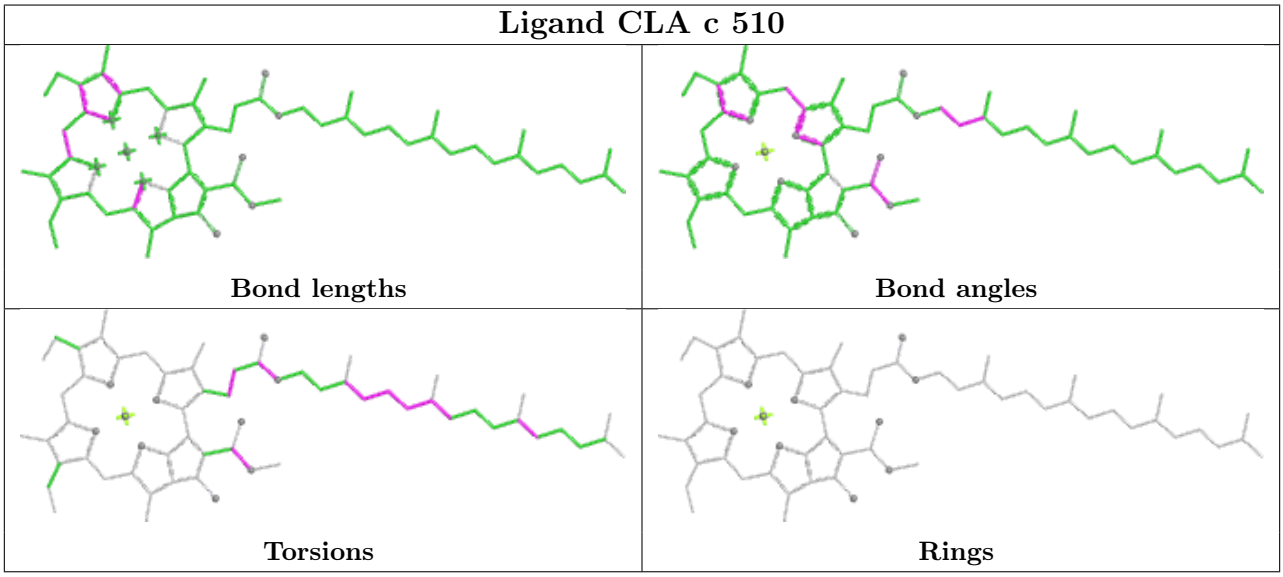


Rings

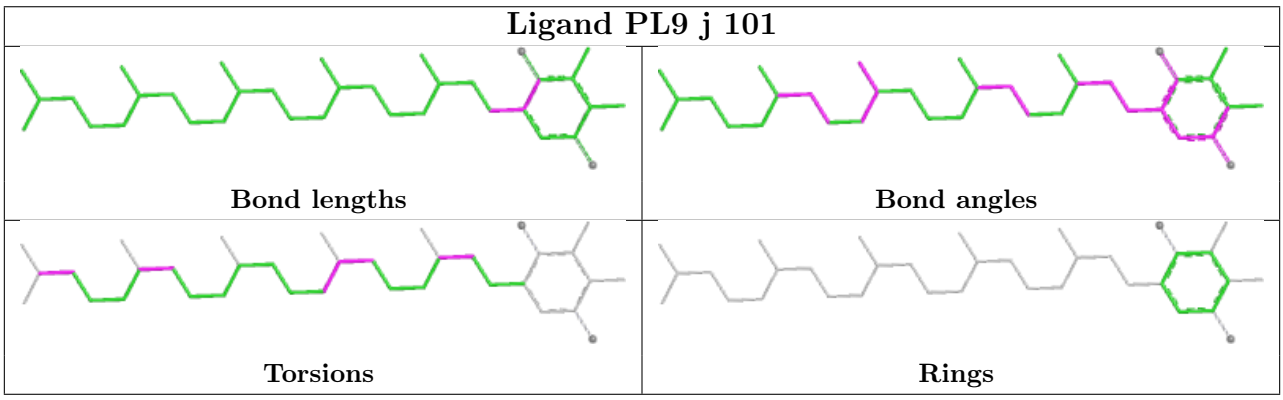
Ligand LMT M 102



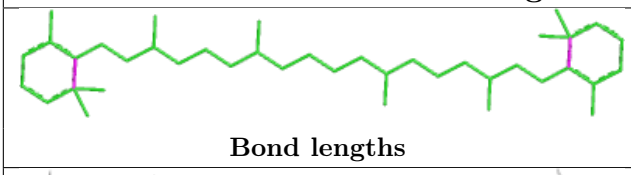
Ligand CLA c 510

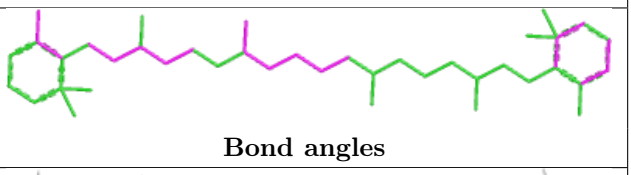


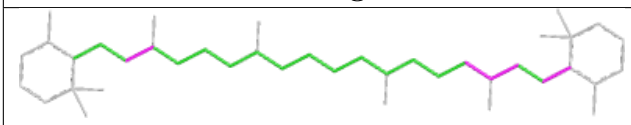
Ligand PL9 j 101

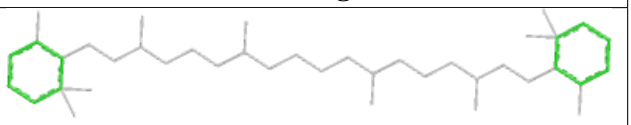


Ligand BCR b 621

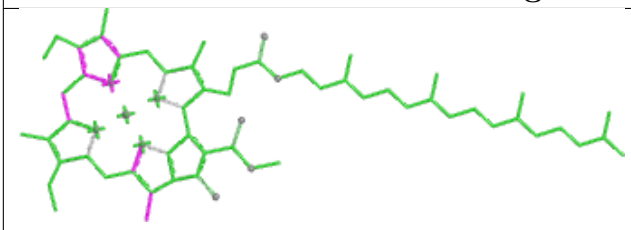

Bond lengths

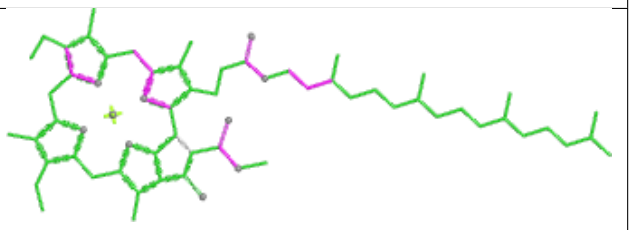

Bond angles

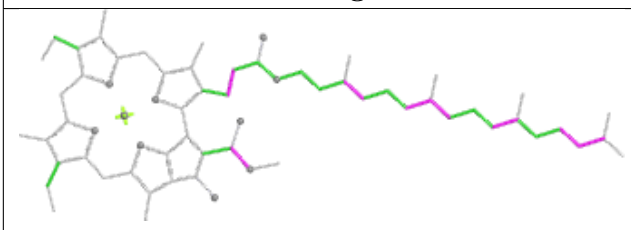

Torsions

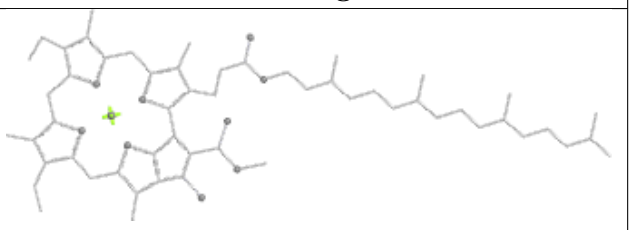

Rings

Ligand CLA B 602

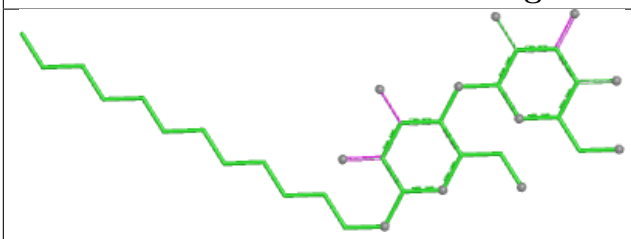

Bond lengths

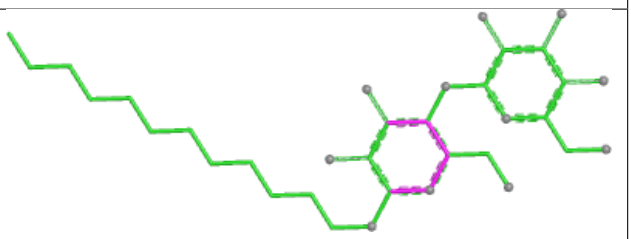

Bond angles

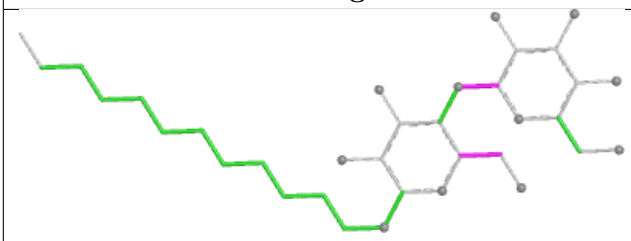

Torsions

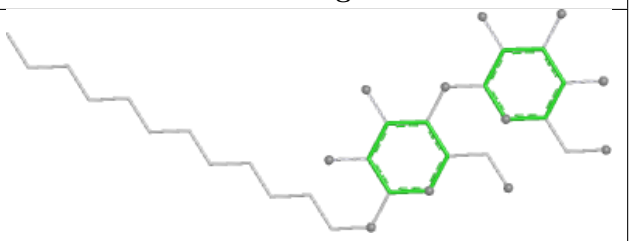

Rings

Ligand LMT b 627

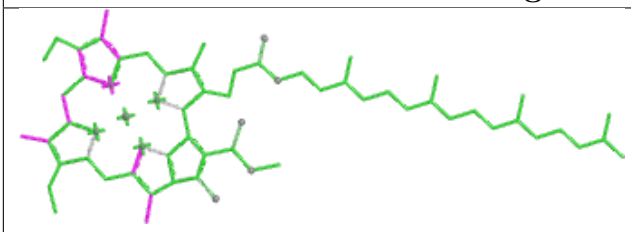

Bond lengths


Bond angles

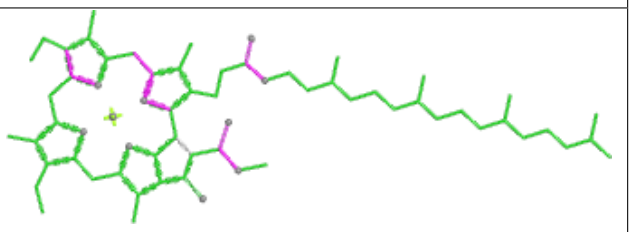

Torsions


Rings

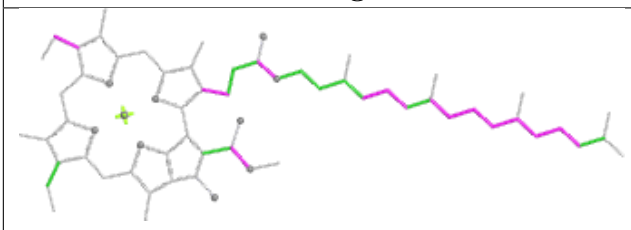
Ligand CLA B 615



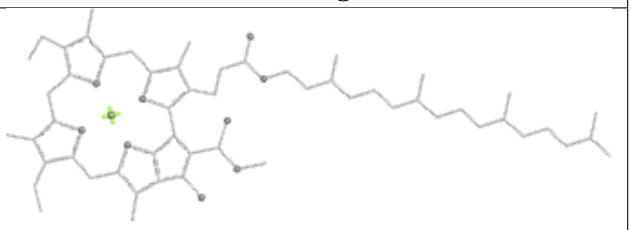
Bond lengths



Bond angles

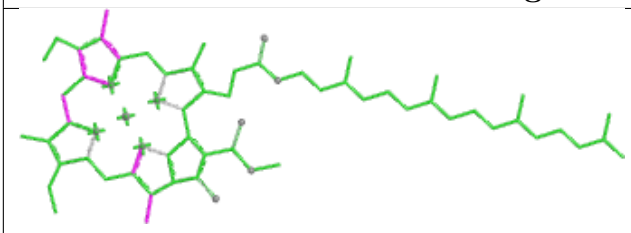


Torsions

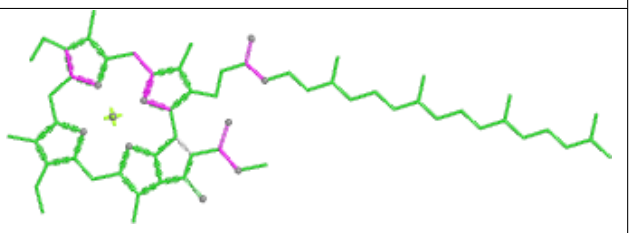


Rings

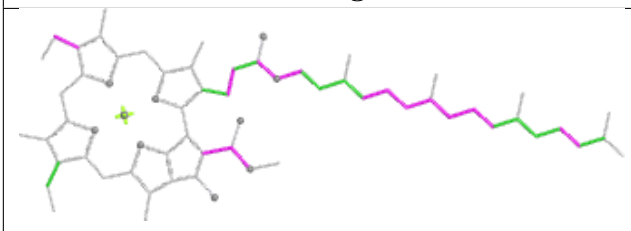
Ligand CLA C 508



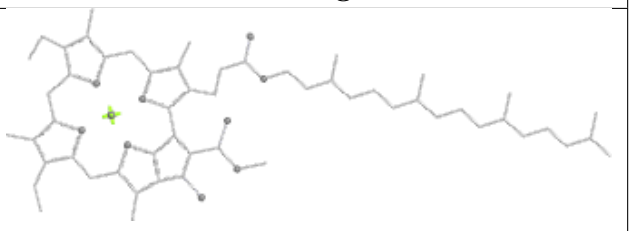
Bond lengths



Bond angles

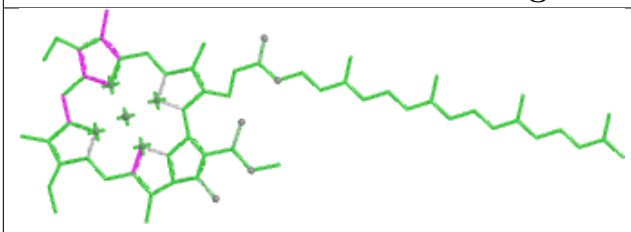


Torsions

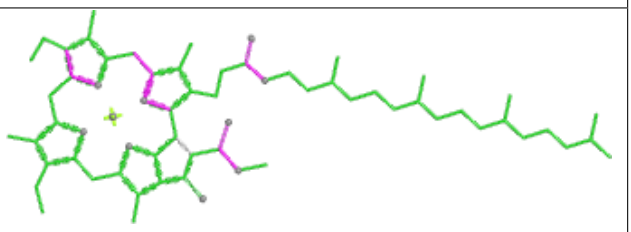


Rings

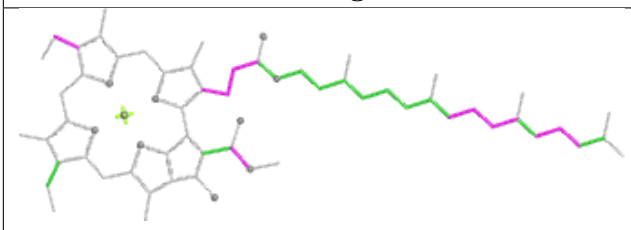
Ligand CLA c 501



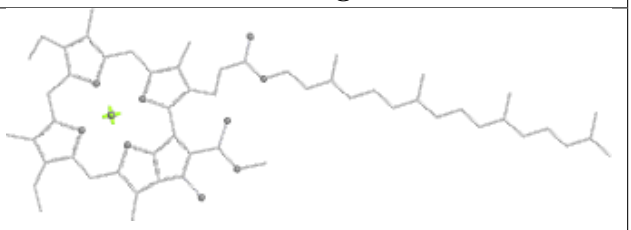
Bond lengths



Bond angles

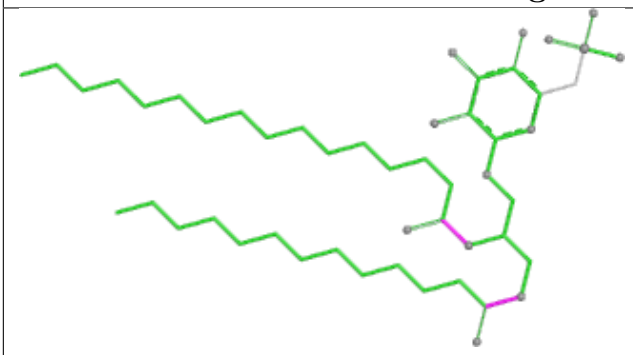


Torsions

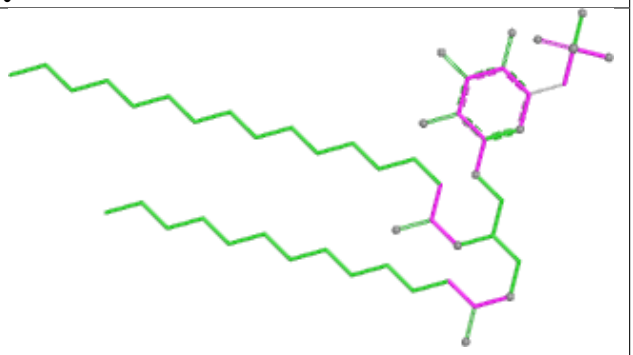


Rings

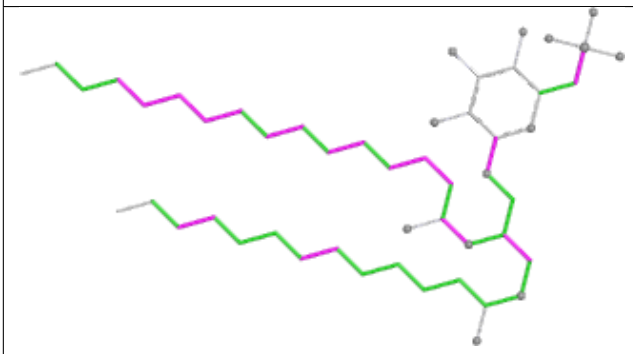
Ligand SQD a 415



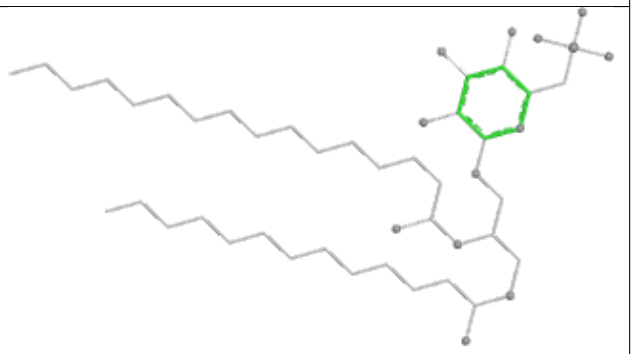
Bond lengths



Bond angles

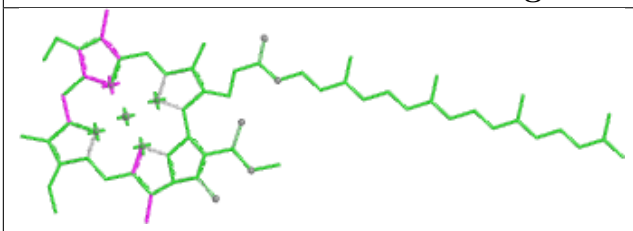


Torsions

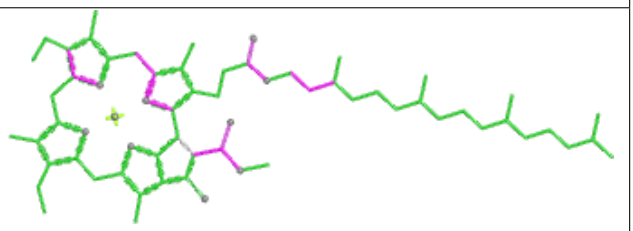


Rings

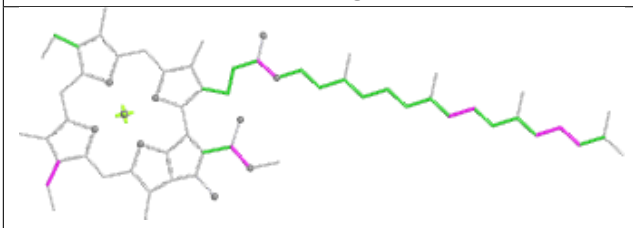
Ligand CLA B 603



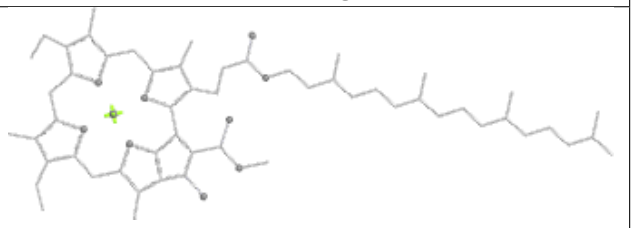
Bond lengths



Bond angles

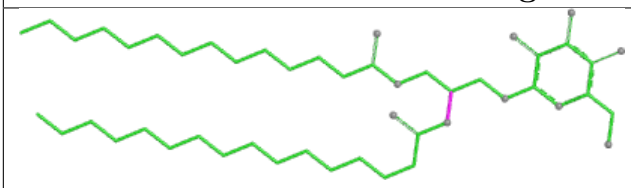


Torsions

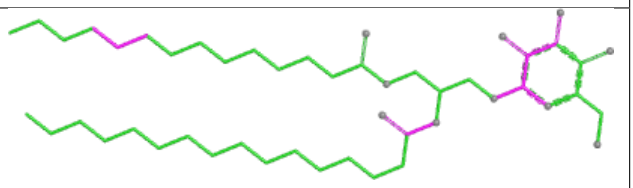


Rings

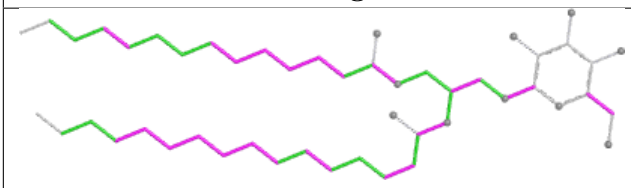
Ligand LMG D 407



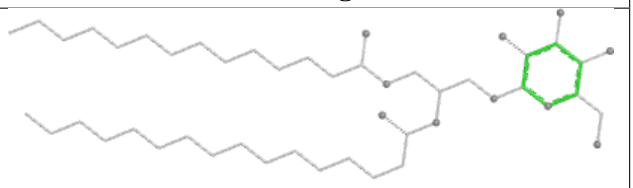
Bond lengths



Bond angles

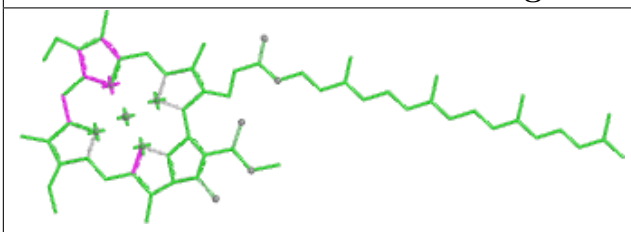


Torsions

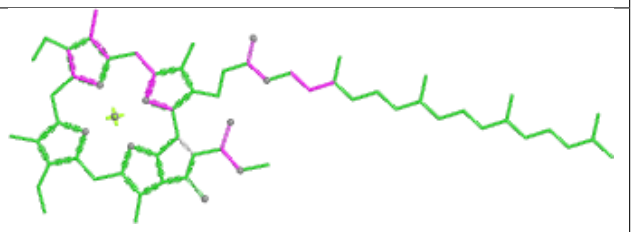


Rings

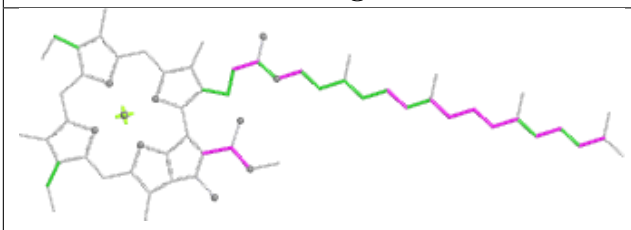
Ligand CLA B 612



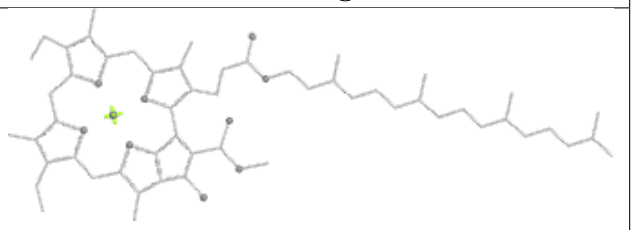
Bond lengths



Bond angles

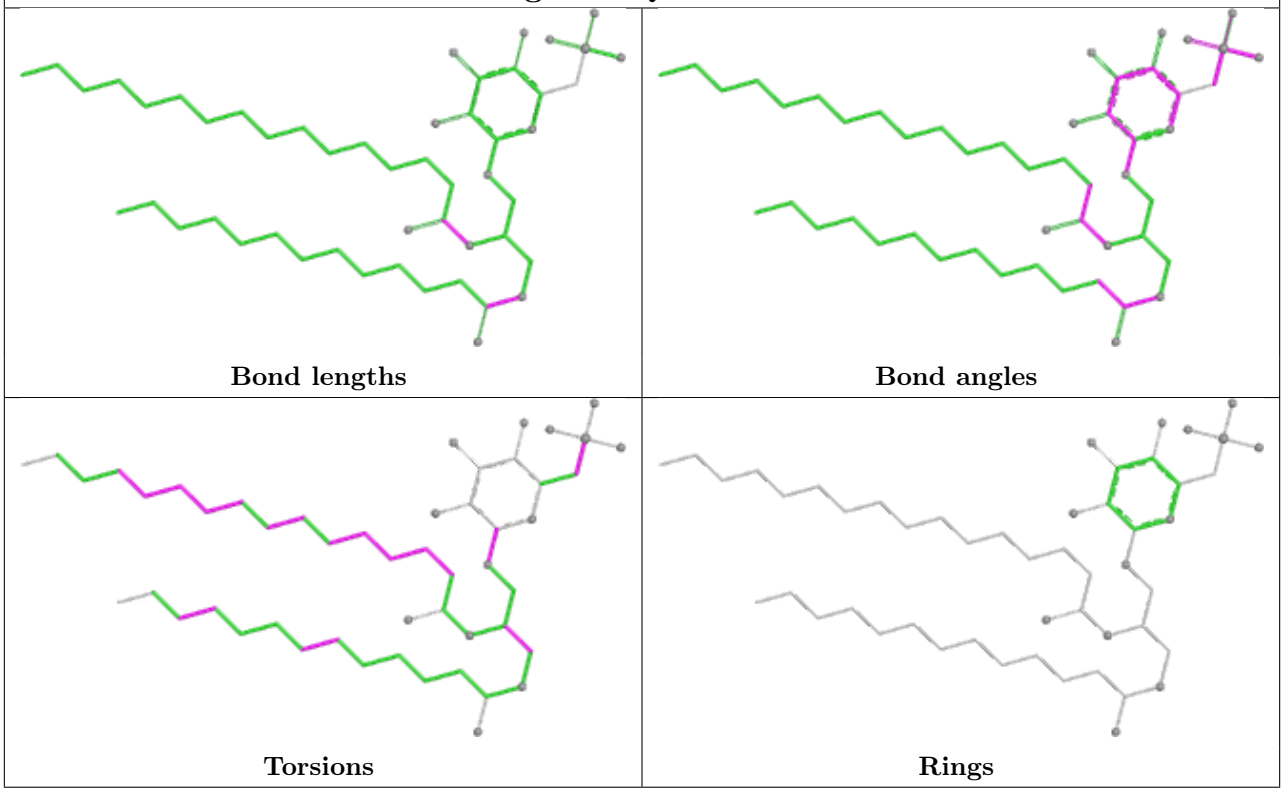


Torsions

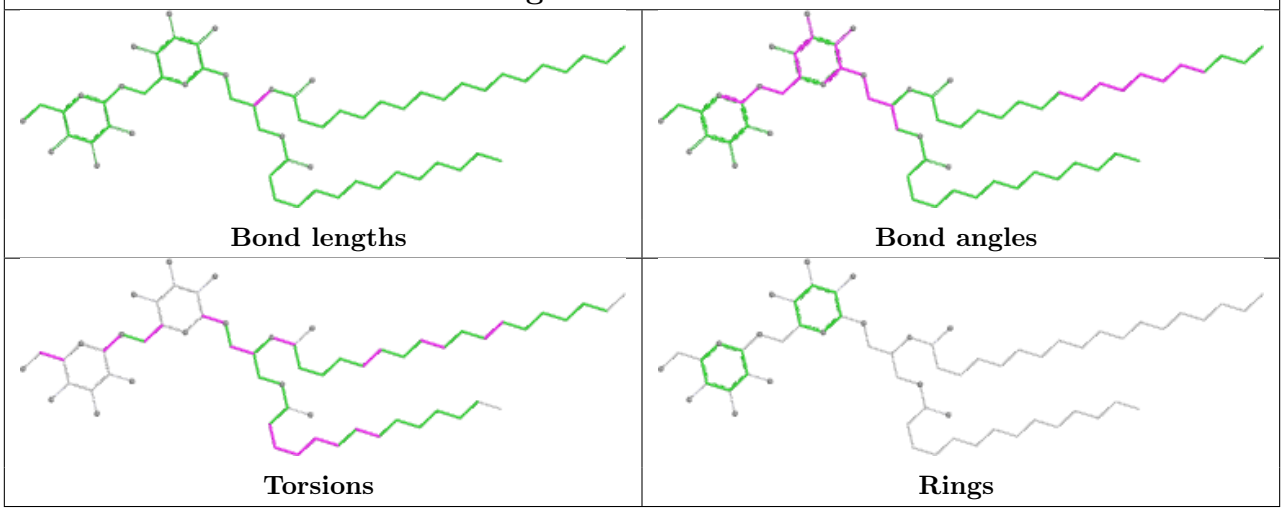


Rings

Ligand SQD A 413



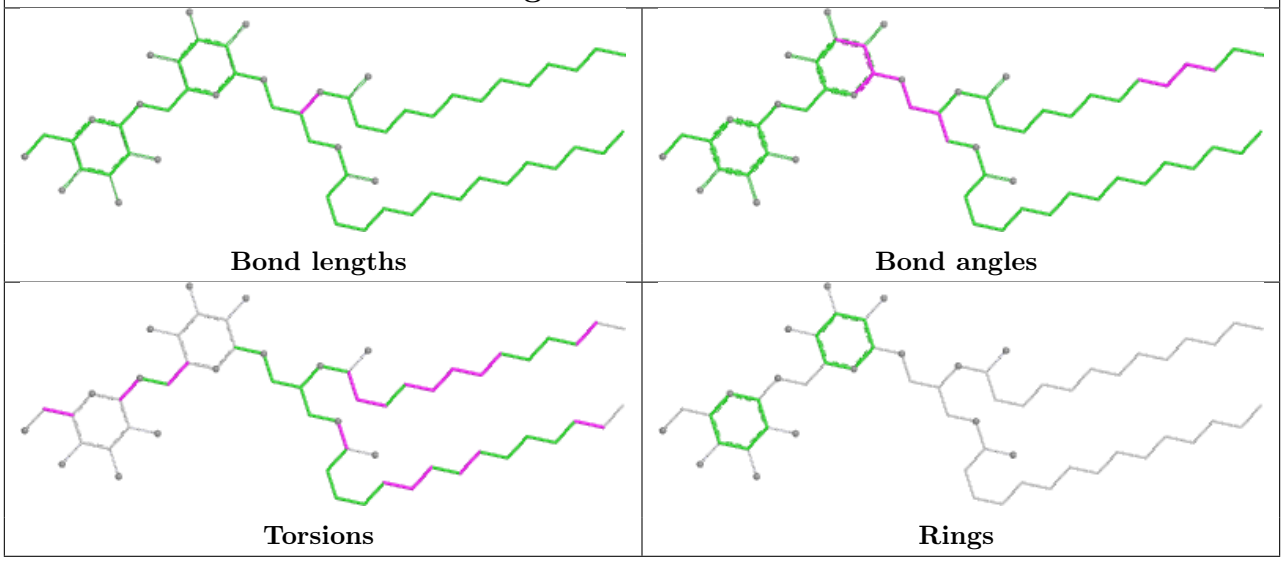
Ligand DGD c 516



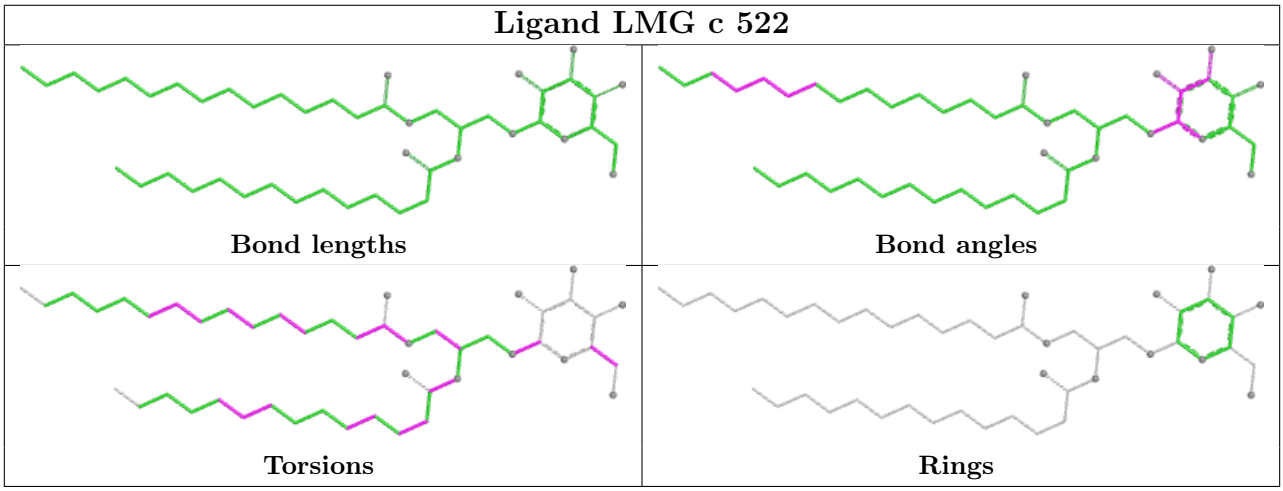
Ligand PL9 D 406



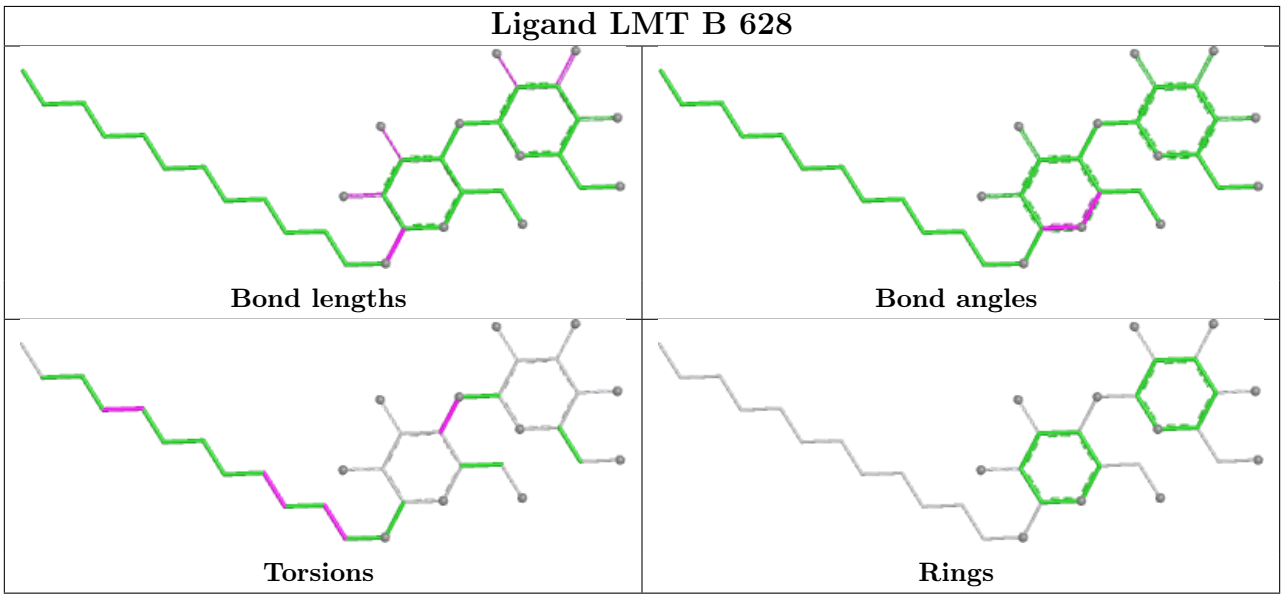
Ligand DGD b 624



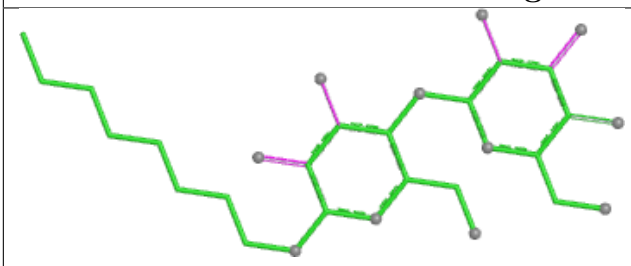
Ligand LMG c 522



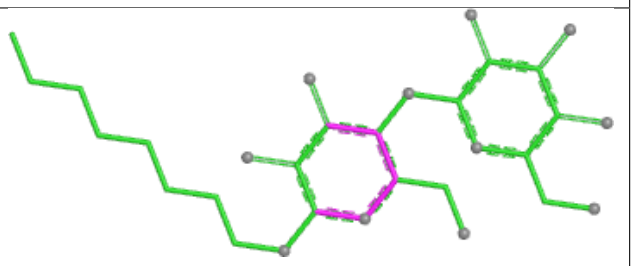
Ligand LMT B 628



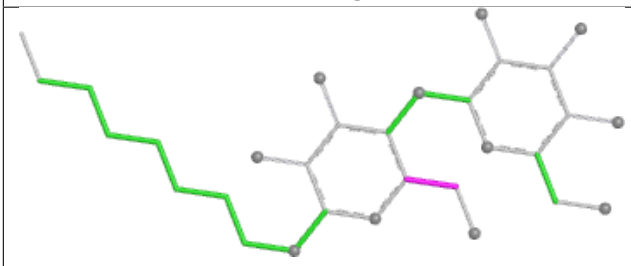
Ligand LMT d 410



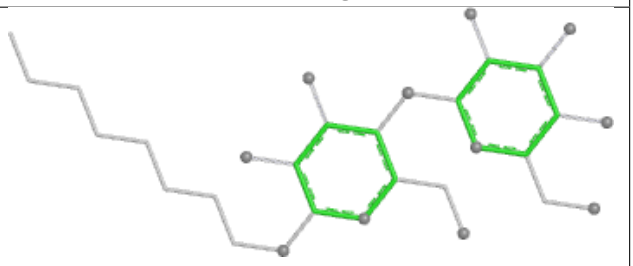
Bond lengths



Bond angles

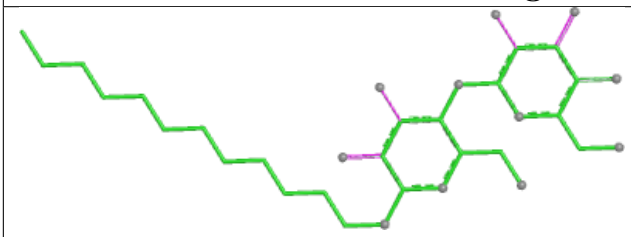


Torsions

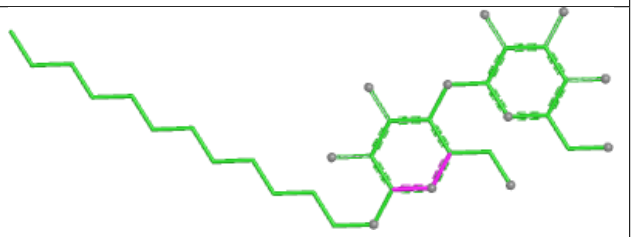


Rings

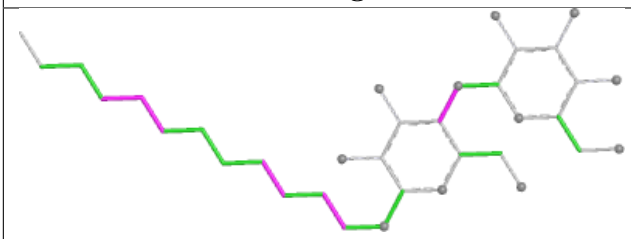
Ligand LMT b 604



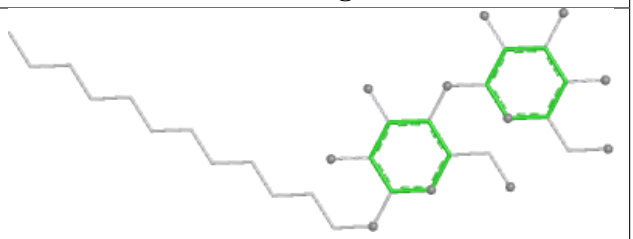
Bond lengths



Bond angles

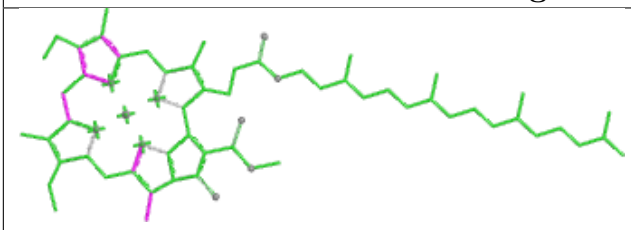


Torsions

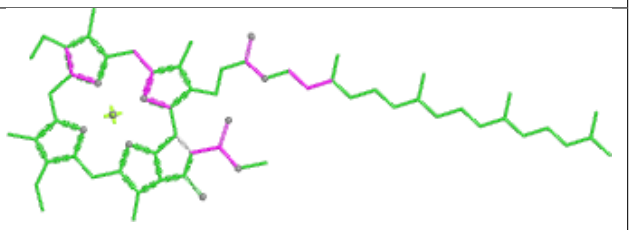


Rings

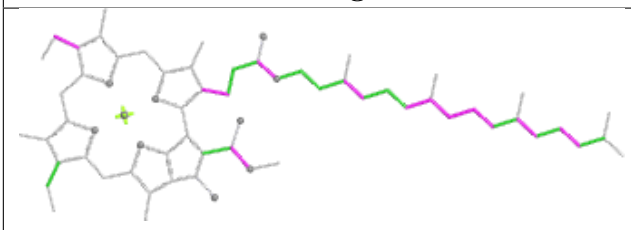
Ligand CLA c 504



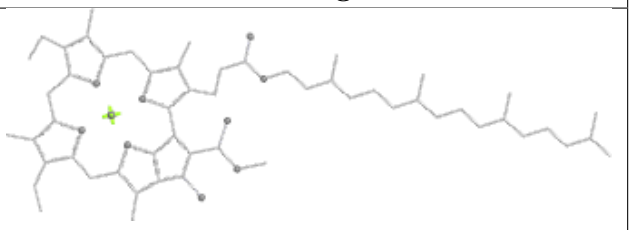
Bond lengths



Bond angles

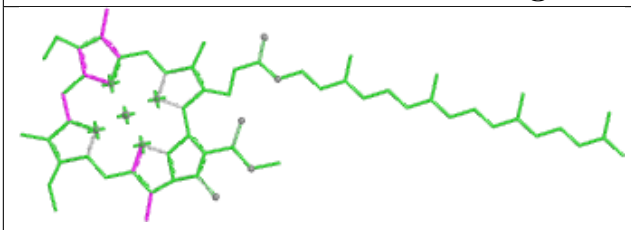


Torsions

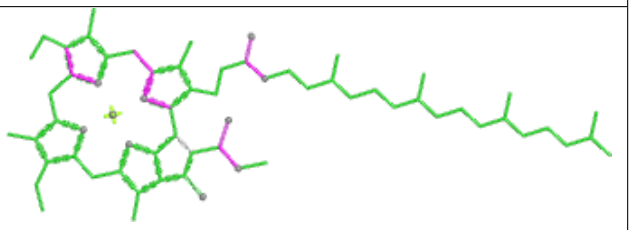


Rings

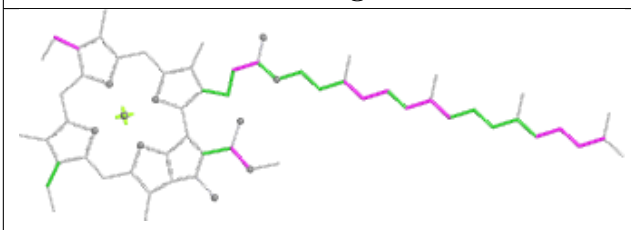
Ligand CLA c 509



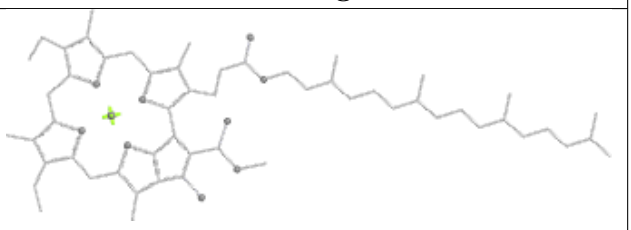
Bond lengths



Bond angles

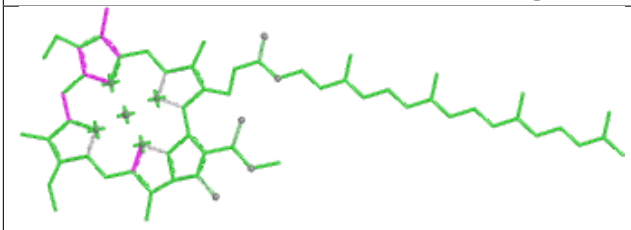


Torsions

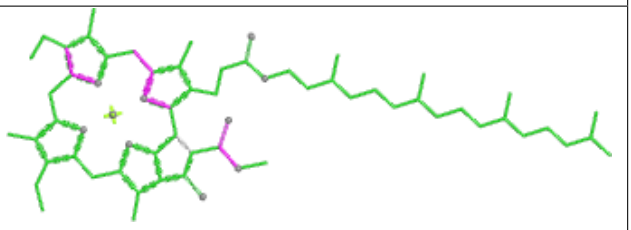


Rings

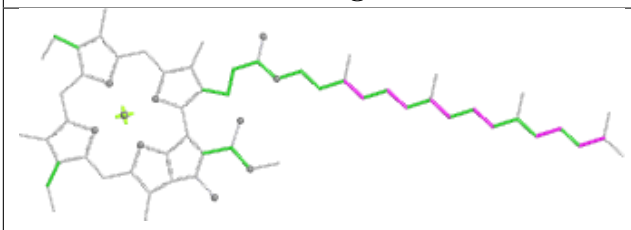
Ligand CLA a 408



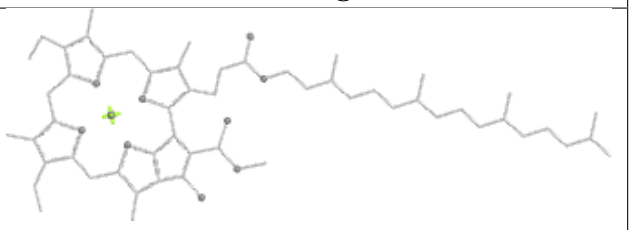
Bond lengths



Bond angles

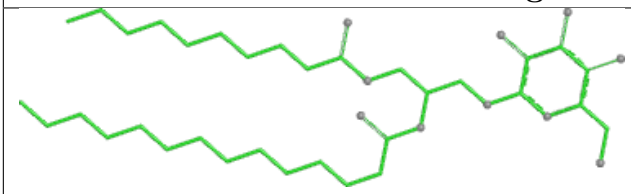


Torsions

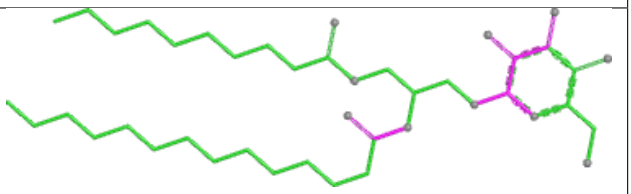


Rings

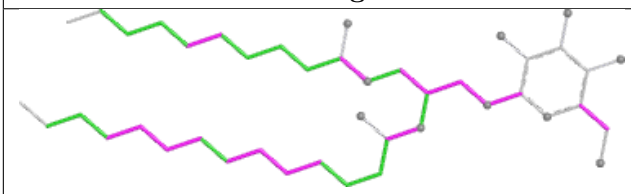
Ligand LMG I 101



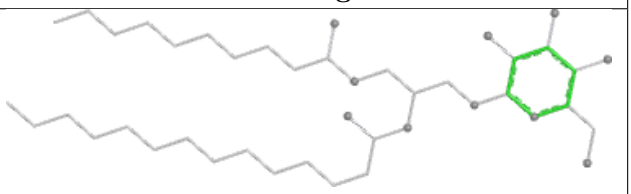
Bond lengths



Bond angles

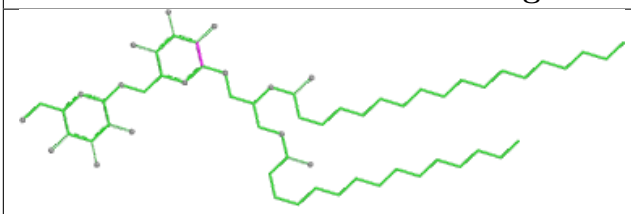


Torsions

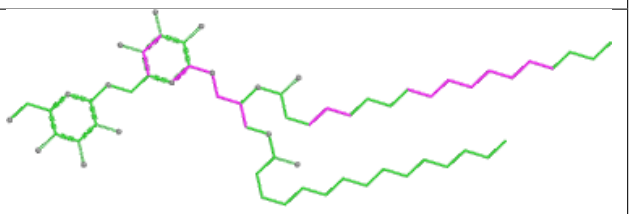


Rings

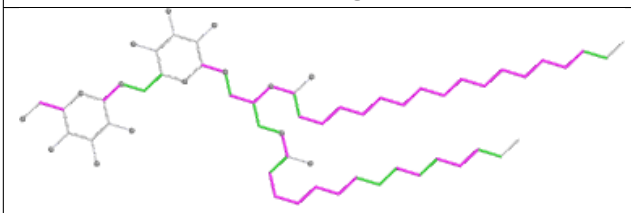
Ligand DGD d 409



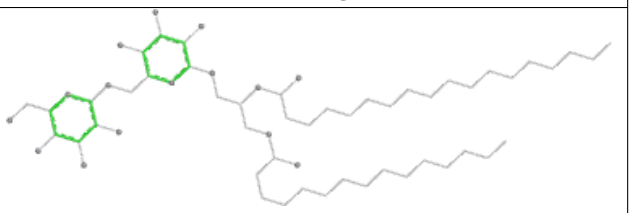
Bond lengths



Bond angles

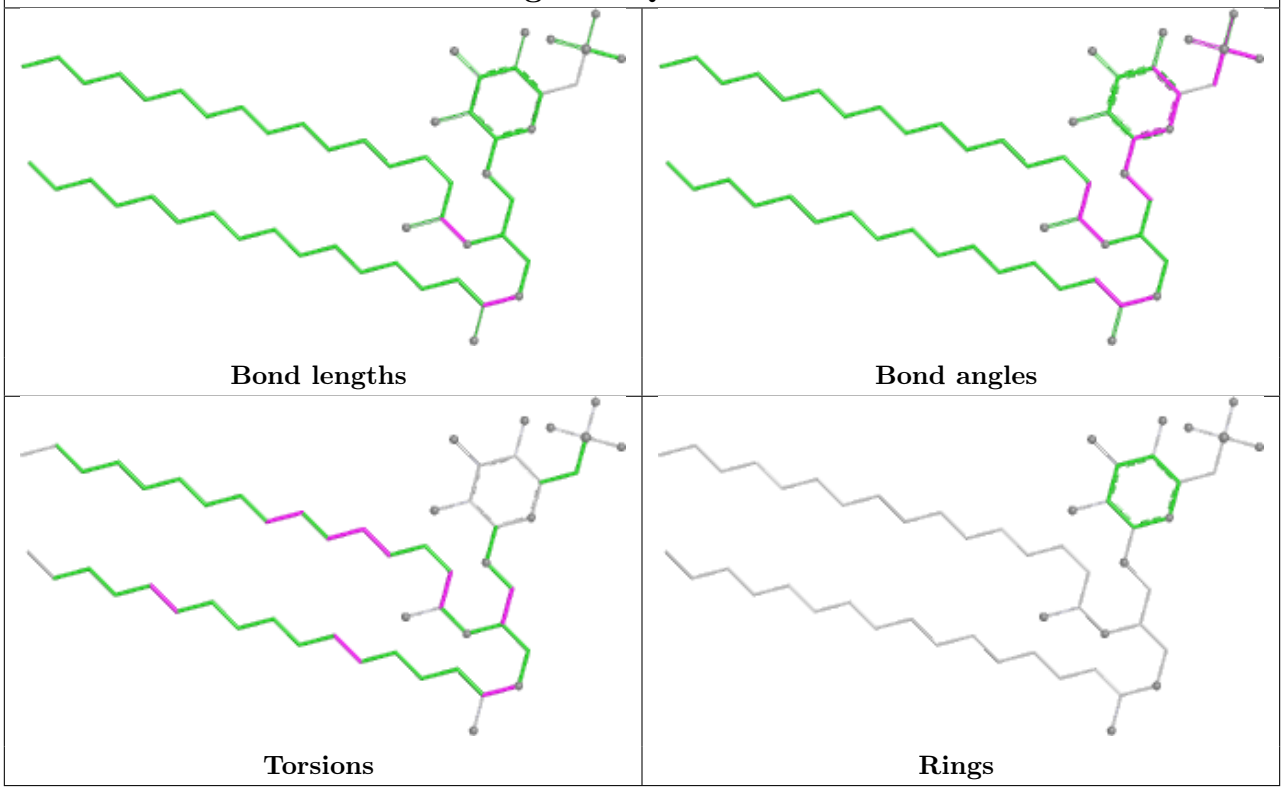


Torsions

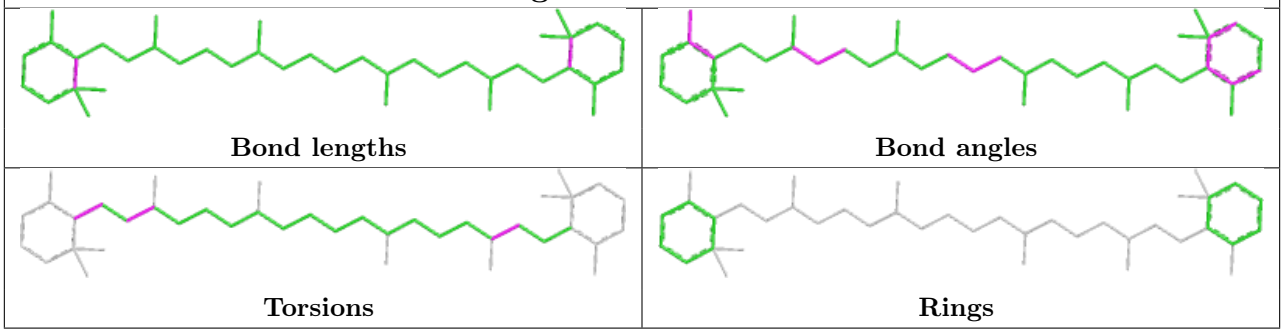


Rings

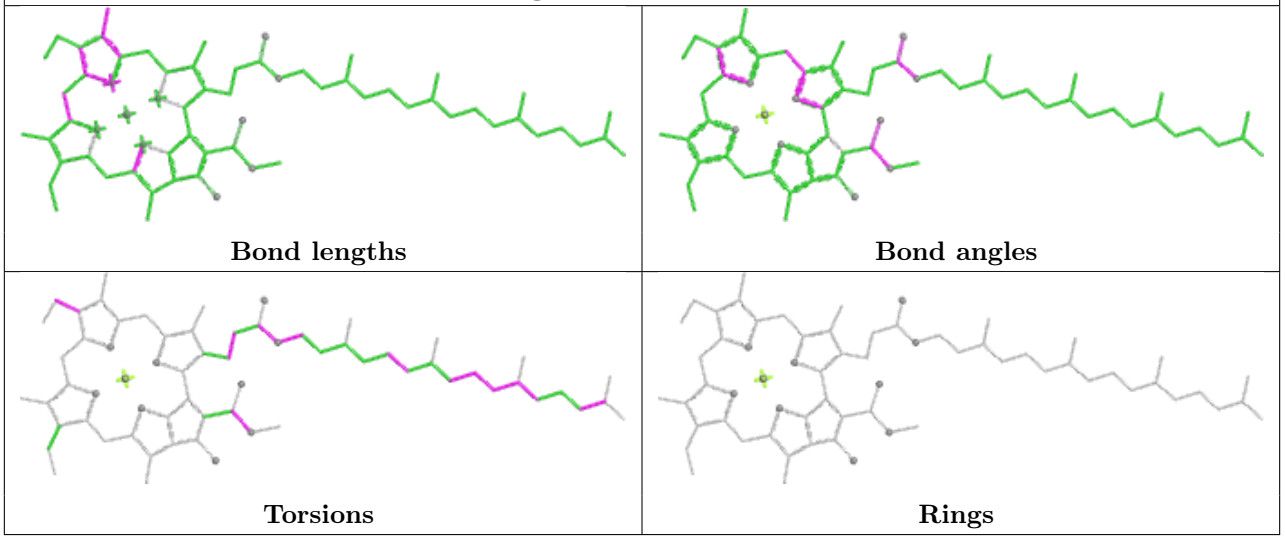
Ligand SQD A 414



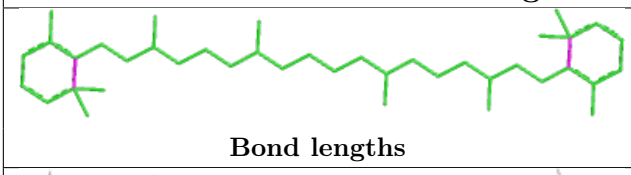
Ligand BCR f 102



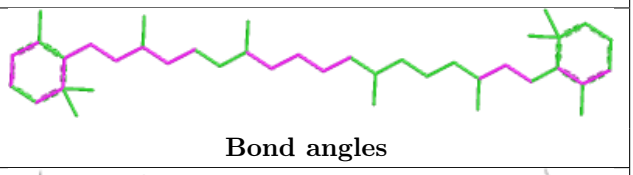
Ligand CLA b 613



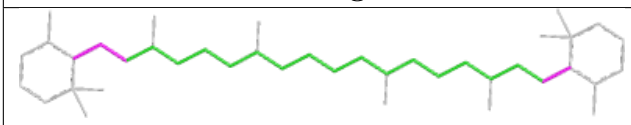
Ligand BCR C 513



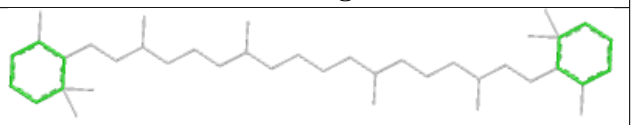
Bond lengths



Bond angles

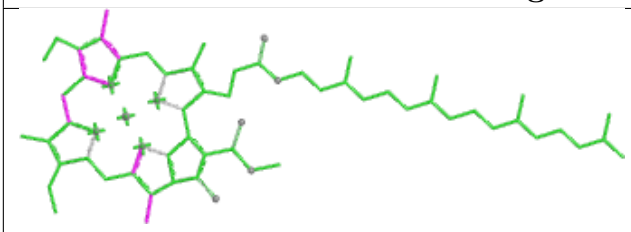


Torsions

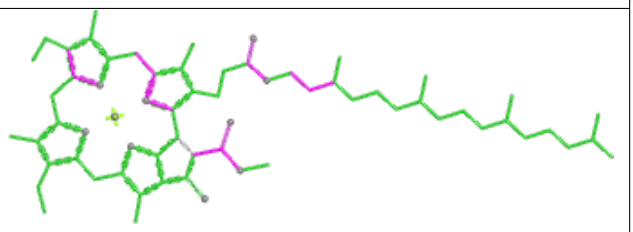


Rings

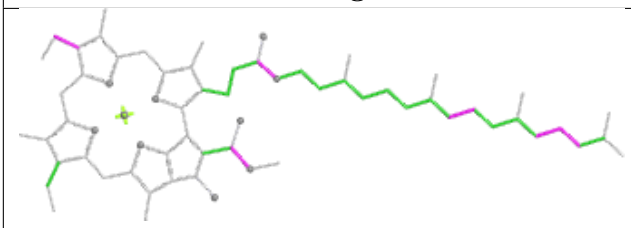
Ligand CLA b 607



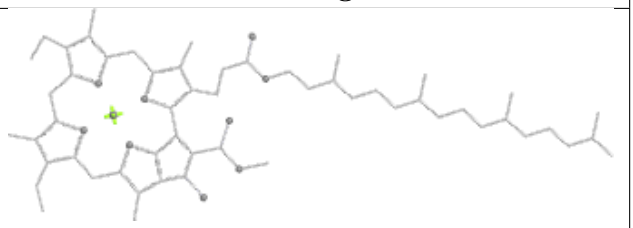
Bond lengths



Bond angles

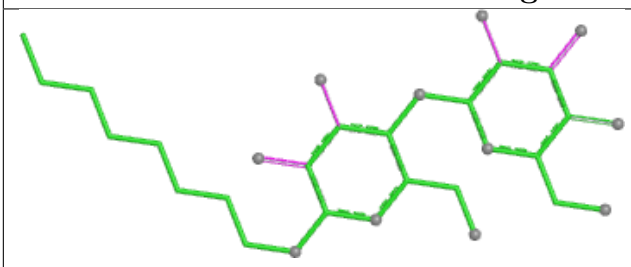


Torsions

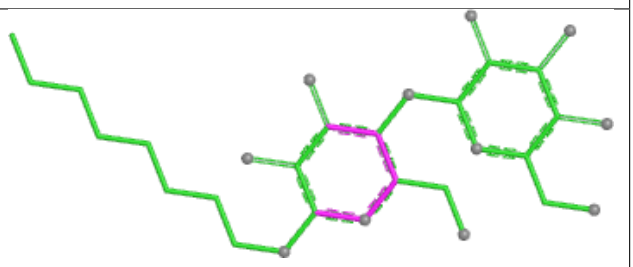


Rings

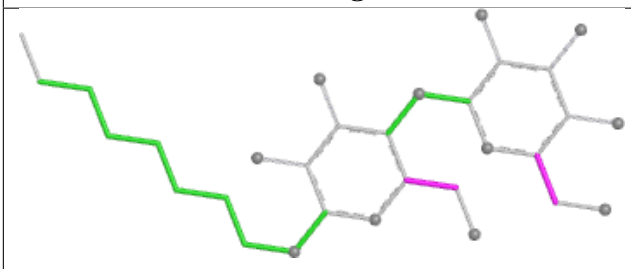
Ligand LMT D 410



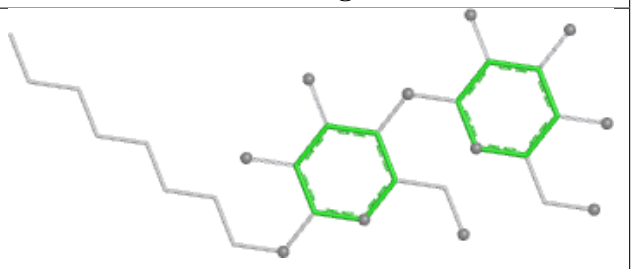
Bond lengths



Bond angles

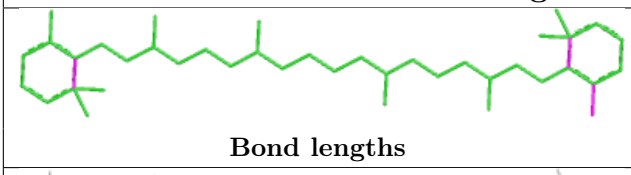


Torsions

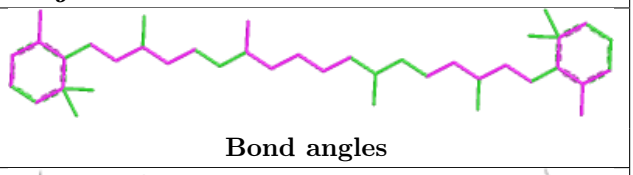


Rings

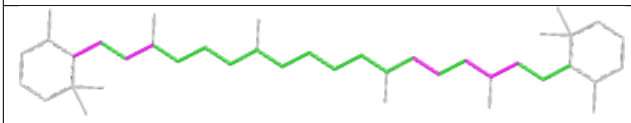
Ligand BCR j 102



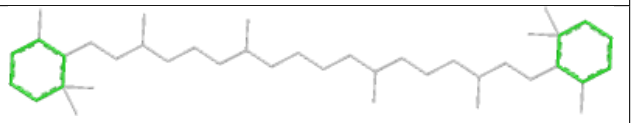
Bond lengths



Bond angles

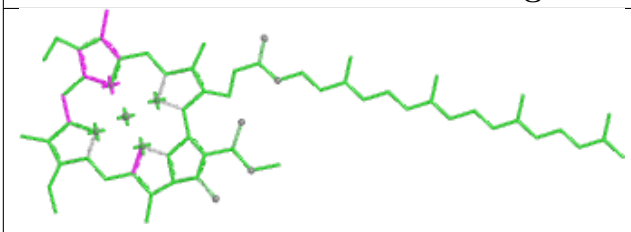


Torsions

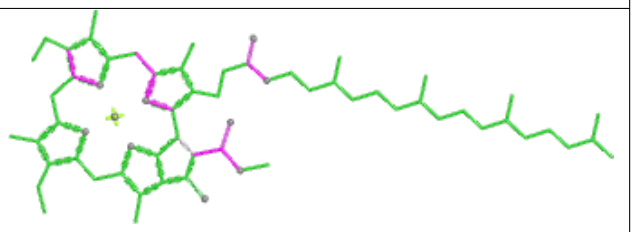


Rings

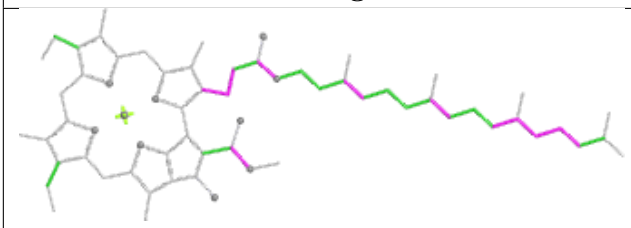
Ligand CLA C 512



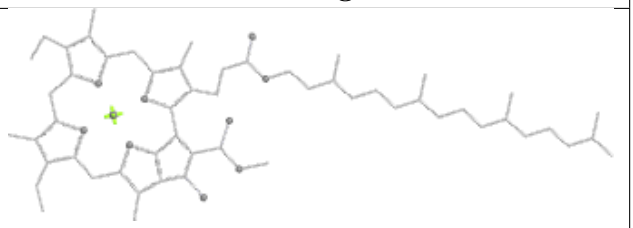
Bond lengths



Bond angles

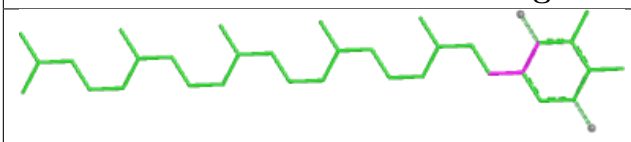


Torsions

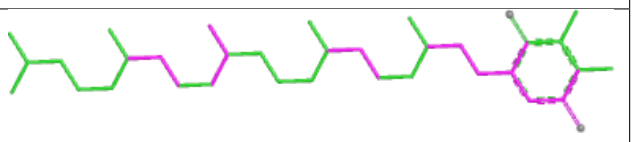


Rings

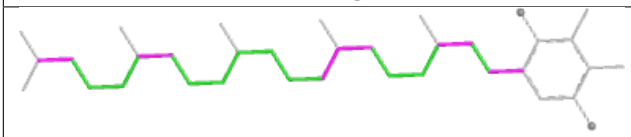
Ligand PL9 J 101



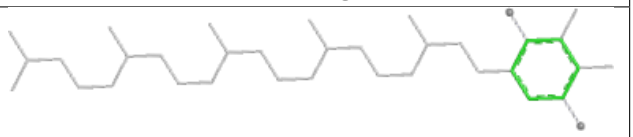
Bond lengths



Bond angles

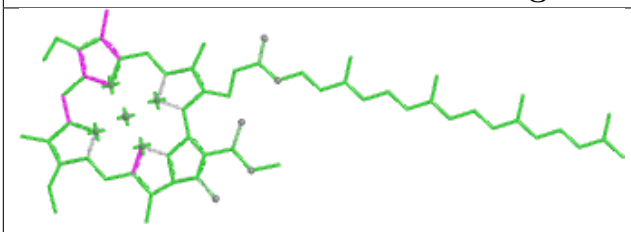


Torsions

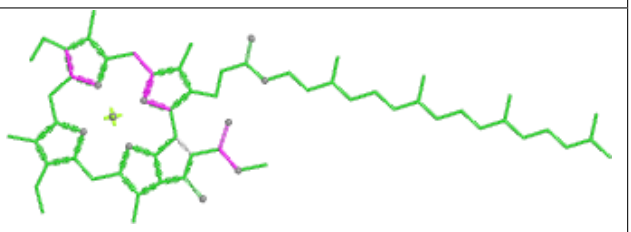


Rings

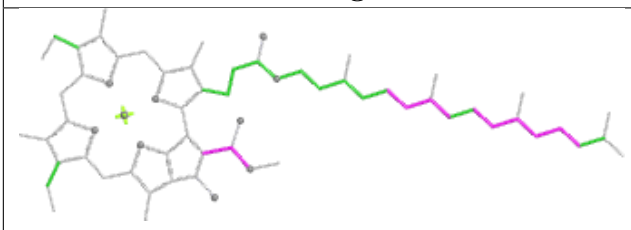
Ligand CLA c 505



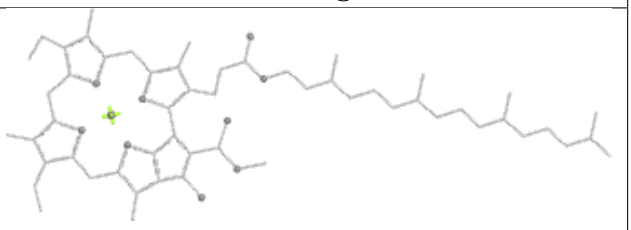
Bond lengths



Bond angles

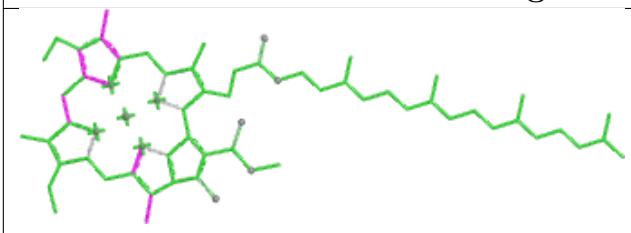


Torsions

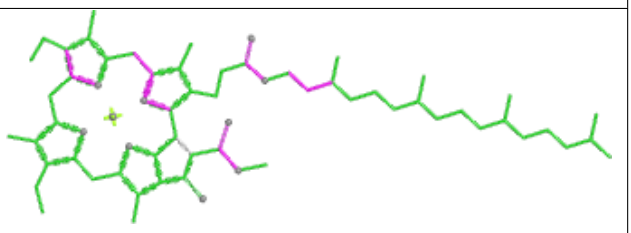


Rings

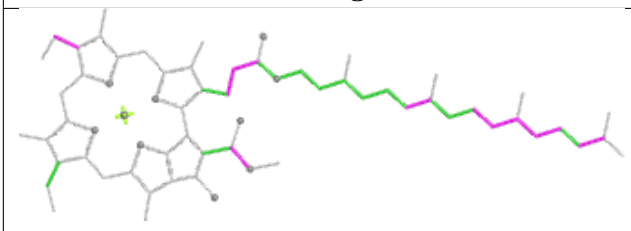
Ligand CLA b 605



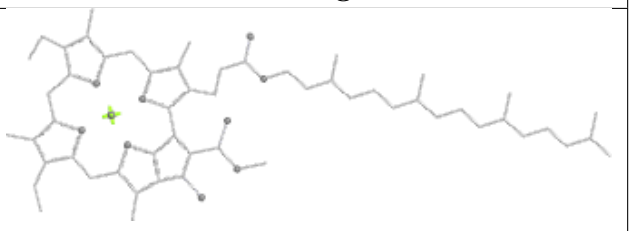
Bond lengths



Bond angles

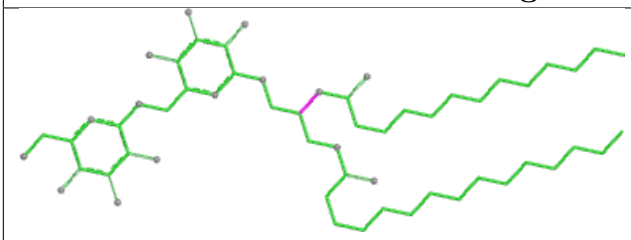


Torsions

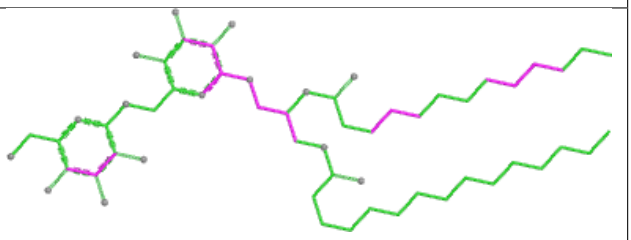


Rings

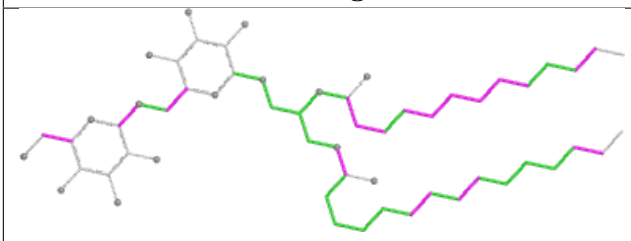
Ligand DGD B 620



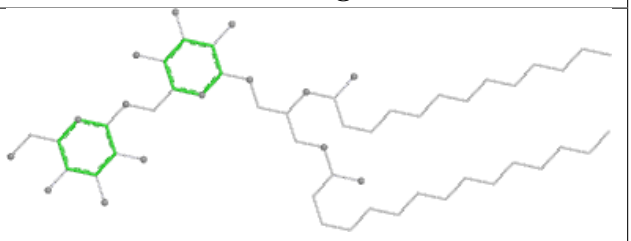
Bond lengths



Bond angles

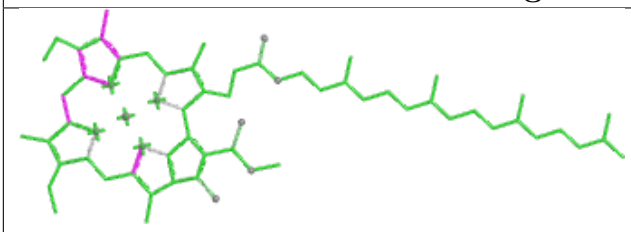


Torsions

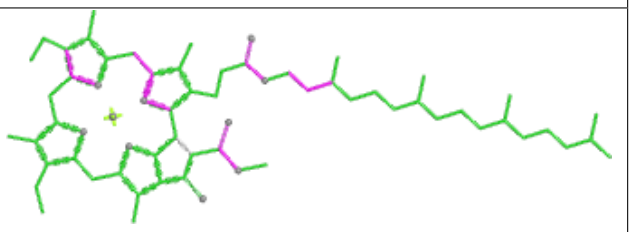


Rings

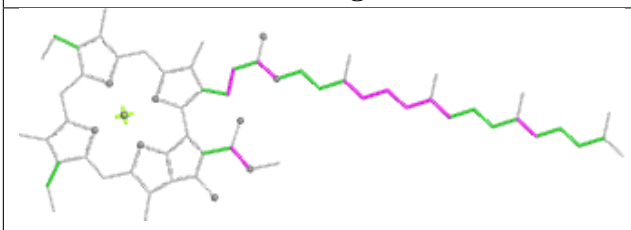
Ligand CLA C 510



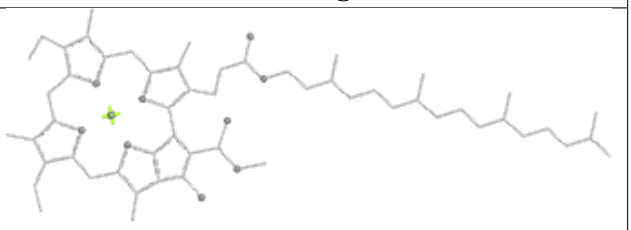
Bond lengths



Bond angles

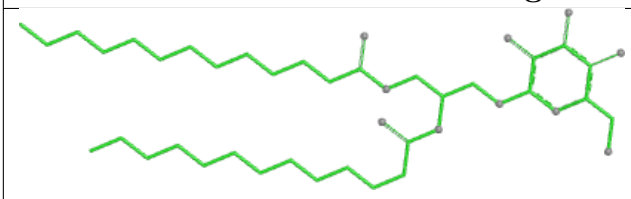


Torsions

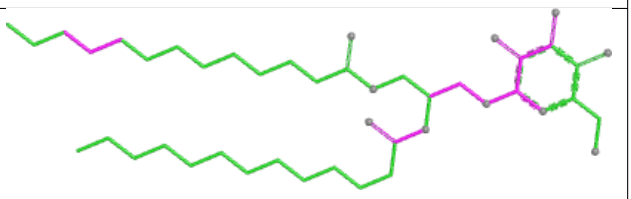


Rings

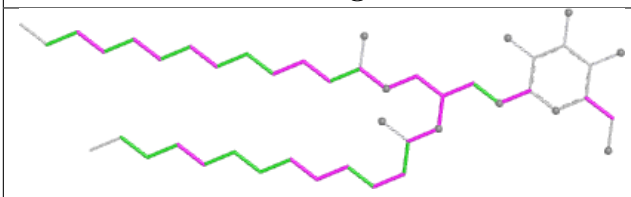
Ligand LMG c 518



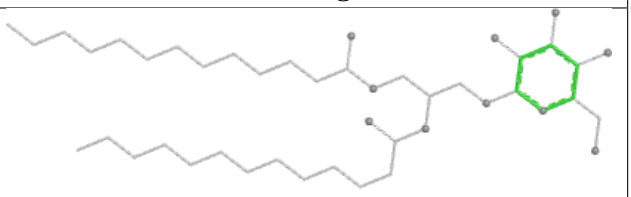
Bond lengths



Bond angles

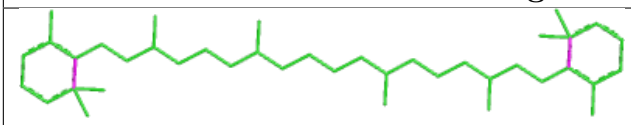


Torsions

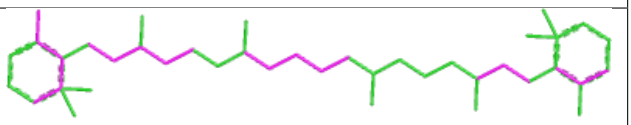


Rings

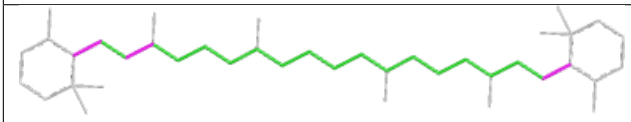
Ligand BCR c 521



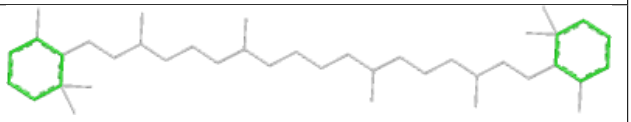
Bond lengths



Bond angles

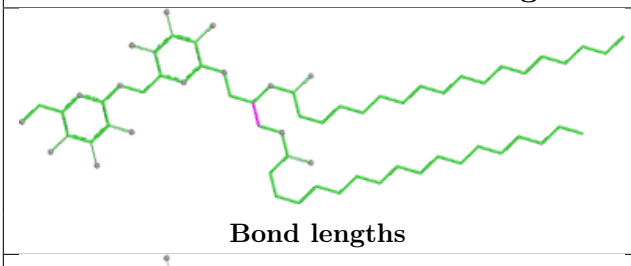


Torsions

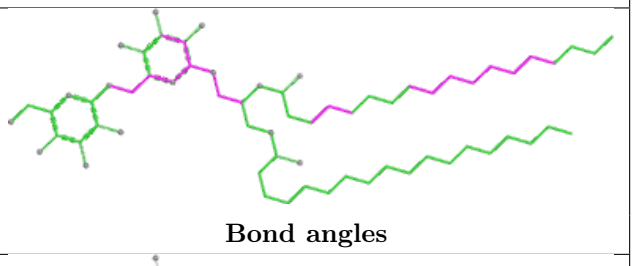


Rings

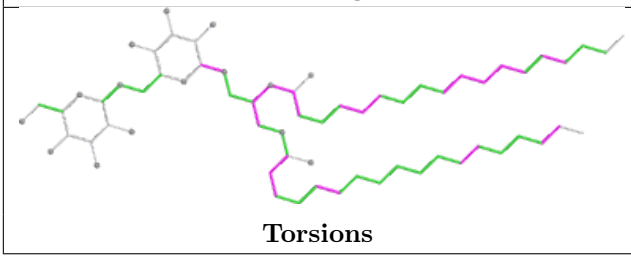
Ligand DGD C 517



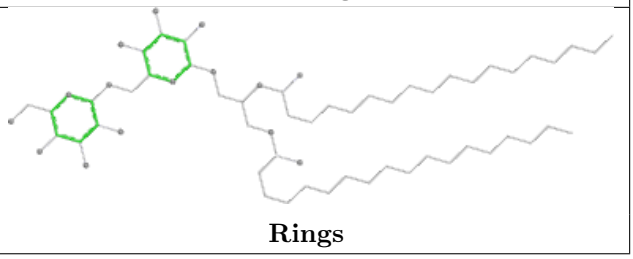
Bond lengths



Bond angles

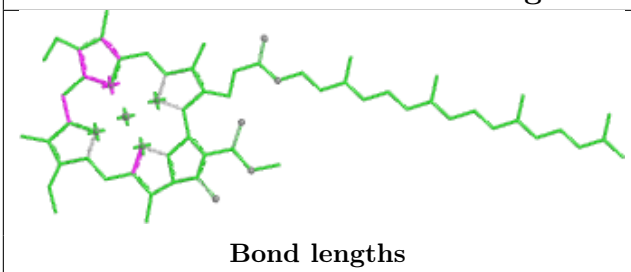


Torsions

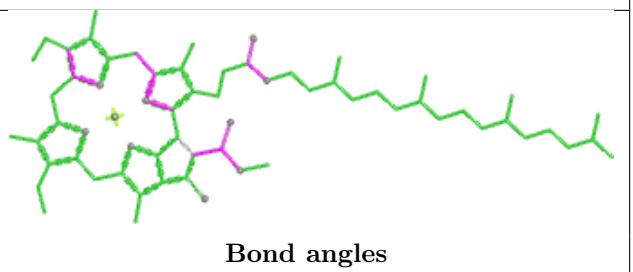


Rings

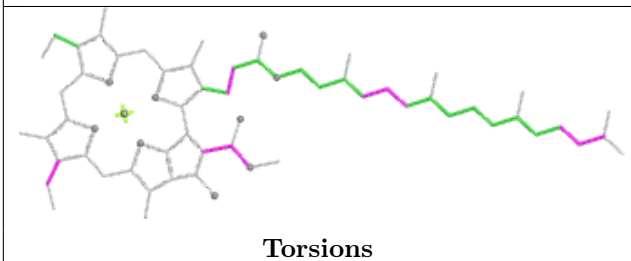
Ligand CLA B 613



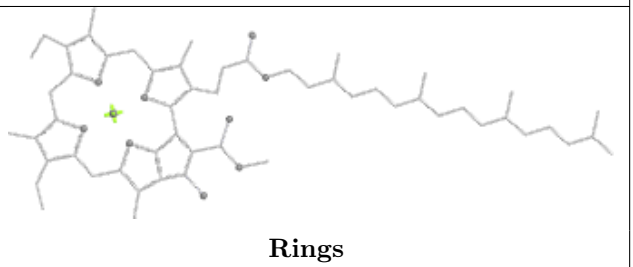
Bond lengths



Bond angles

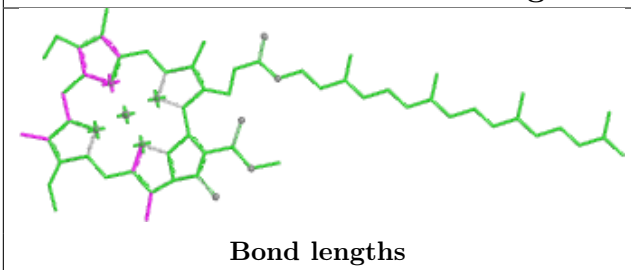


Torsions

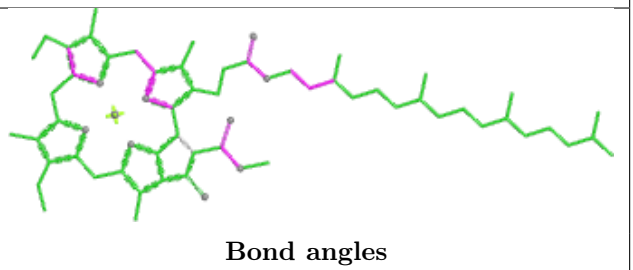


Rings

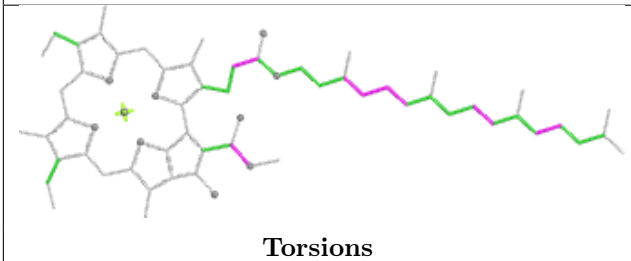
Ligand CLA b 615



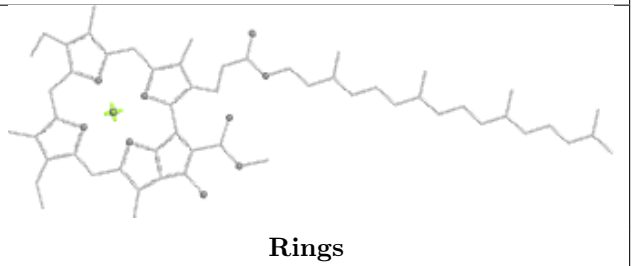
Bond lengths



Bond angles

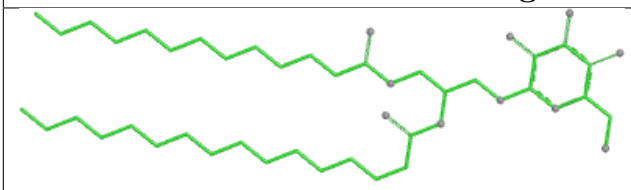


Torsions

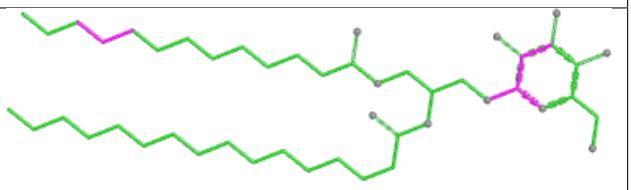


Rings

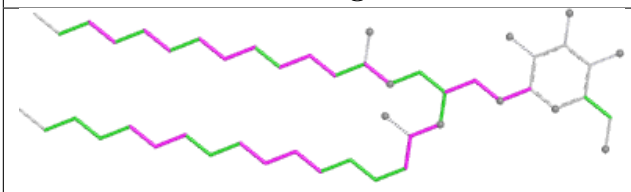
Ligand LMG D 408



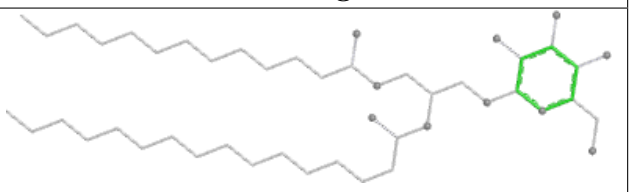
Bond lengths



Bond angles

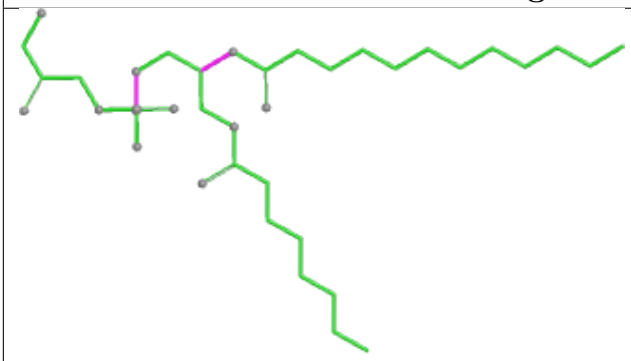


Torsions

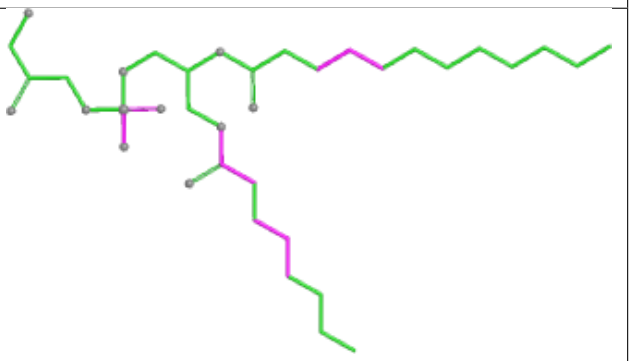


Rings

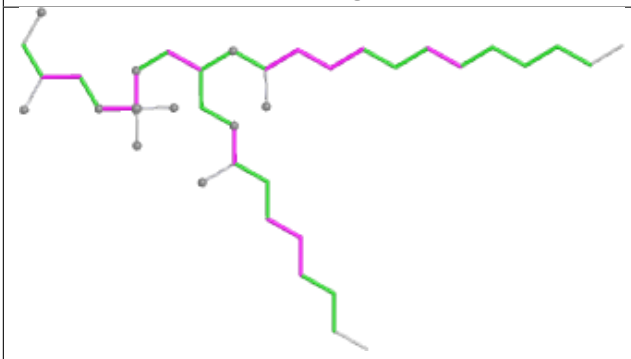
Ligand LHG c 519



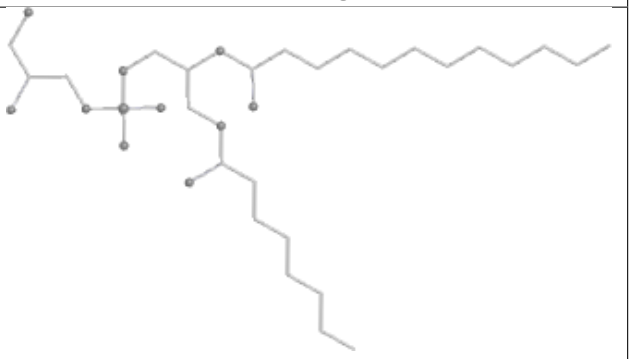
Bond lengths



Bond angles

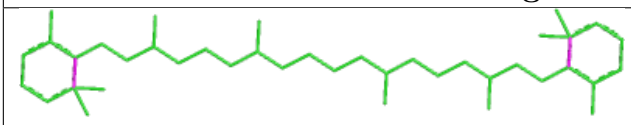


Torsions

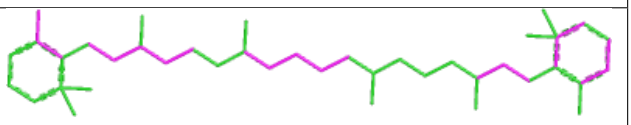


Rings

Ligand BCR B 617



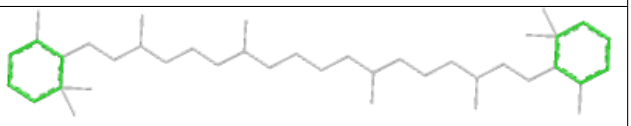
Bond lengths



Bond angles

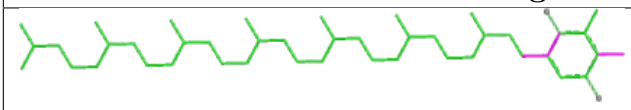


Torsions

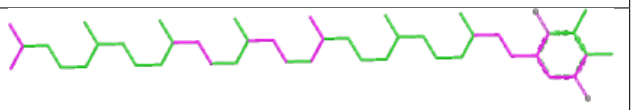


Rings

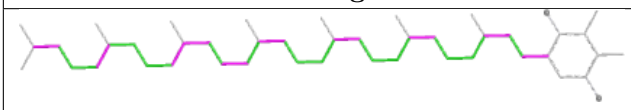
Ligand PL9 A 406



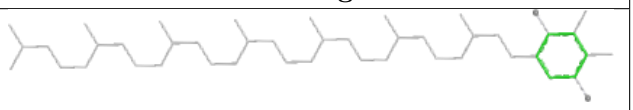
Bond lengths



Bond angles

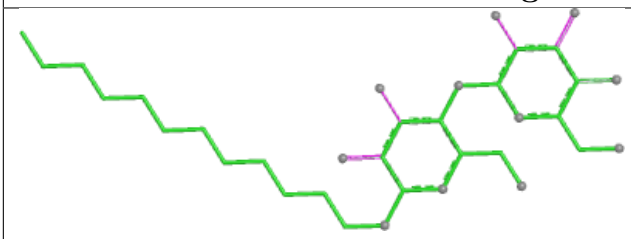


Torsions

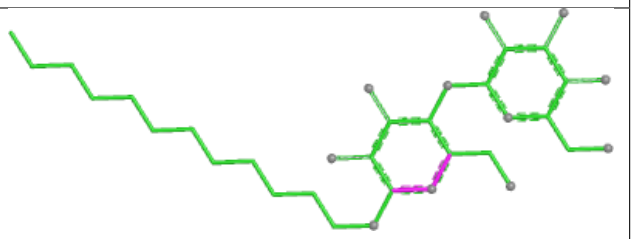


Rings

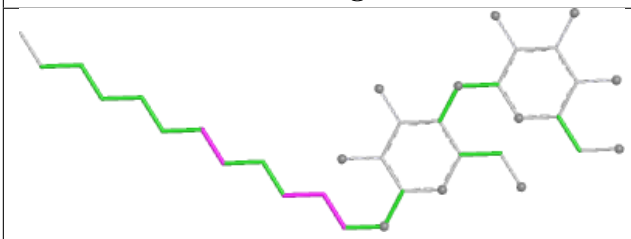
Ligand LMT B 623



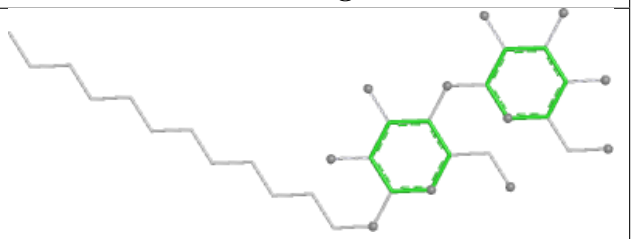
Bond lengths



Bond angles

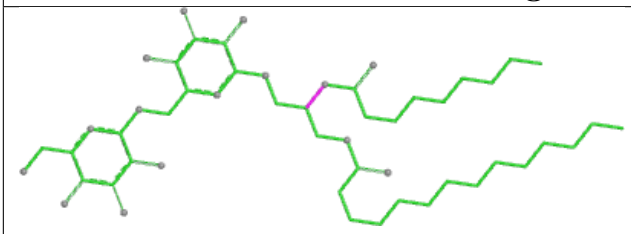


Torsions

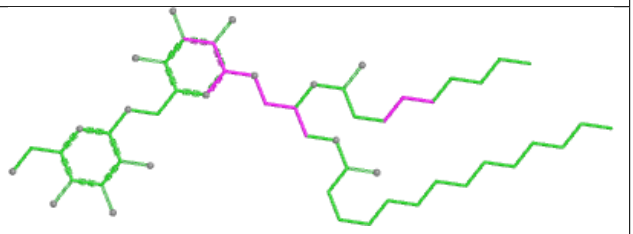


Rings

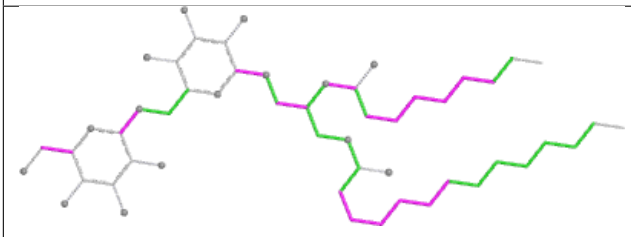
Ligand DGD c 515



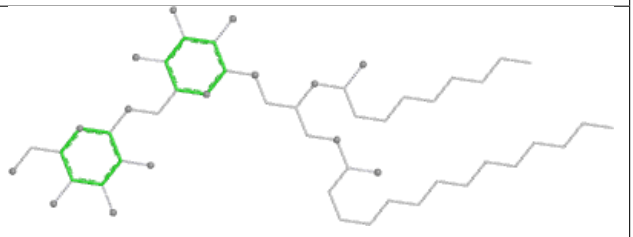
Bond lengths



Bond angles

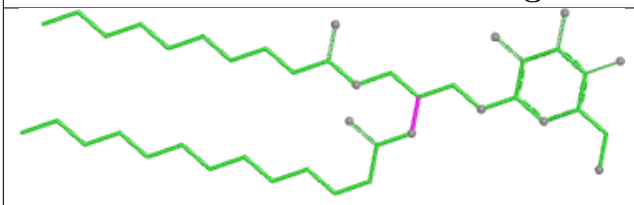


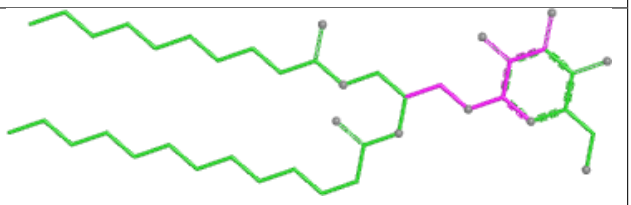
Torsions

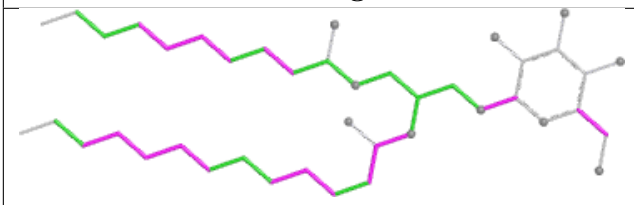


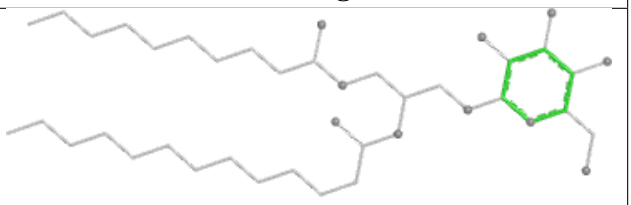
Rings

Ligand LMG a 402

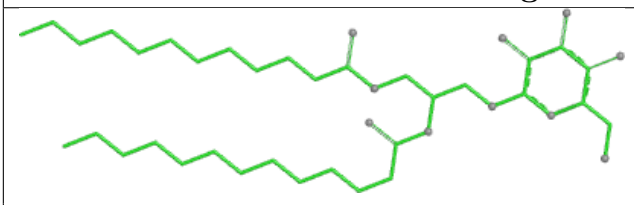

Bond lengths

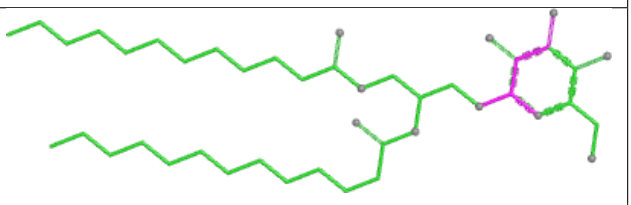

Bond angles

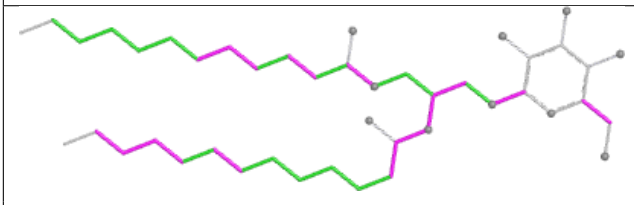

Torsions

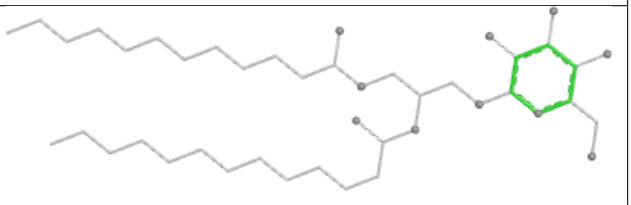

Rings

Ligand LMG E 101


Bond lengths

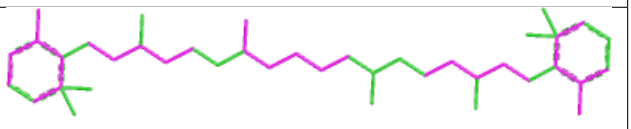

Bond angles

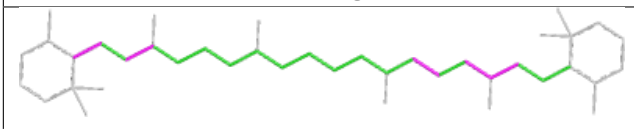

Torsions

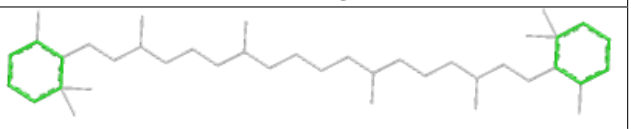

Rings

Ligand BCR J 102

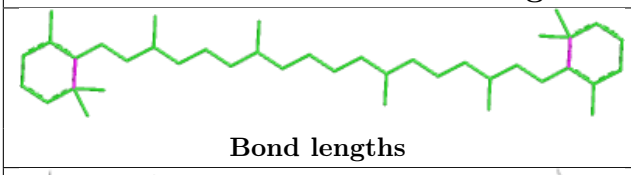

Bond lengths


Bond angles

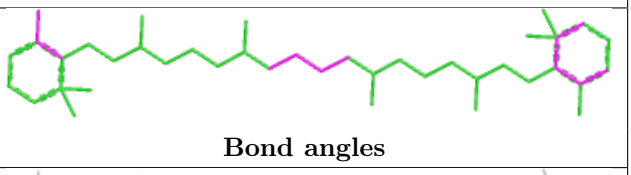

Torsions


Rings

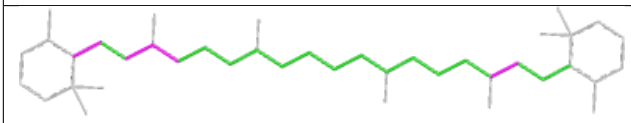
Ligand BCR x 101



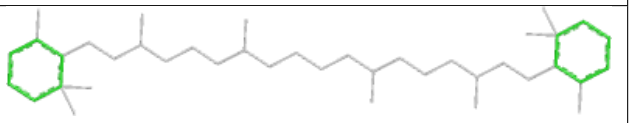
Bond lengths



Bond angles



Torsions

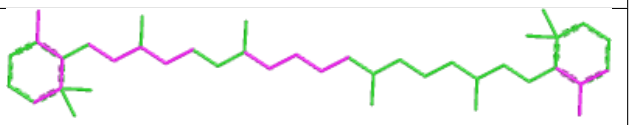


Rings

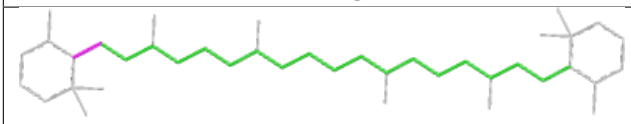
Ligand BCR B 616



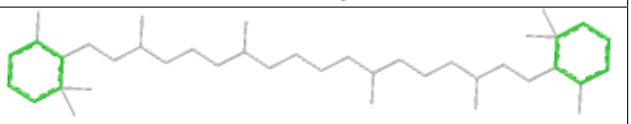
Bond lengths



Bond angles

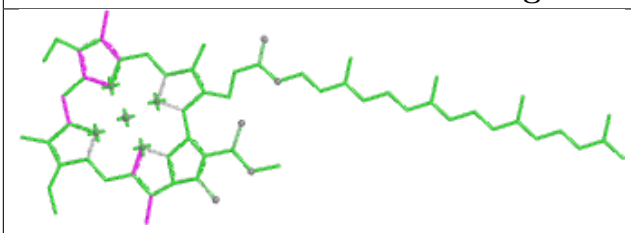


Torsions

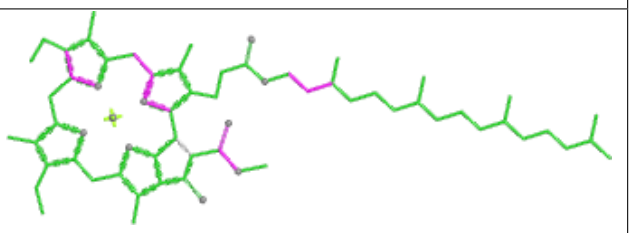


Rings

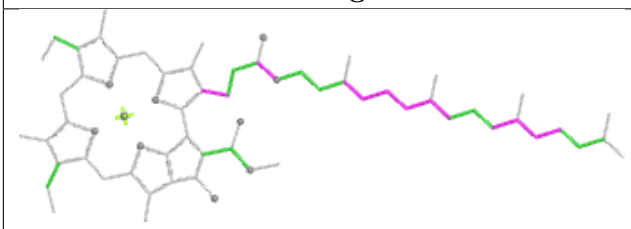
Ligand CLA H 101



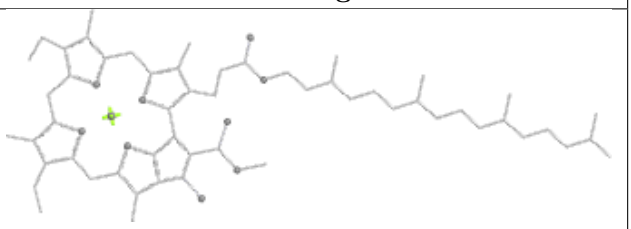
Bond lengths



Bond angles

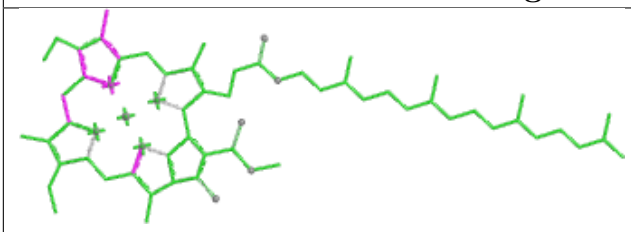


Torsions

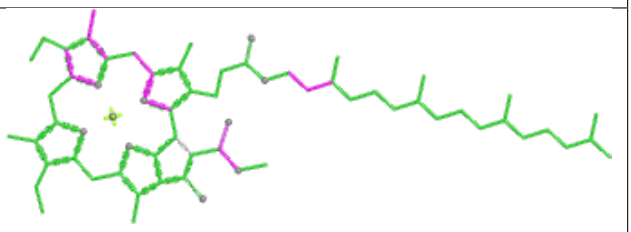


Rings

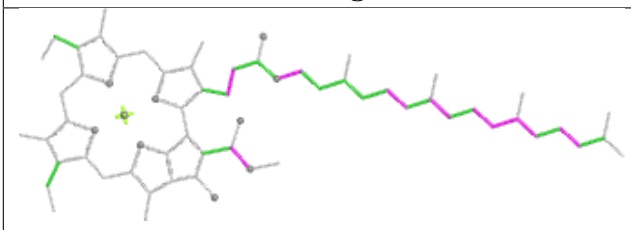
Ligand CLA C 507



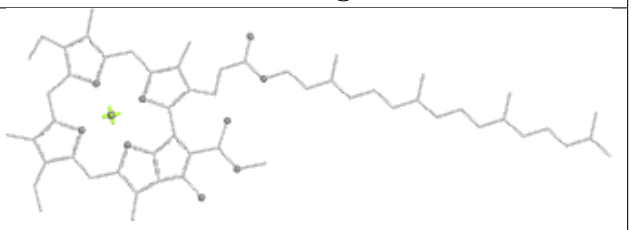
Bond lengths



Bond angles

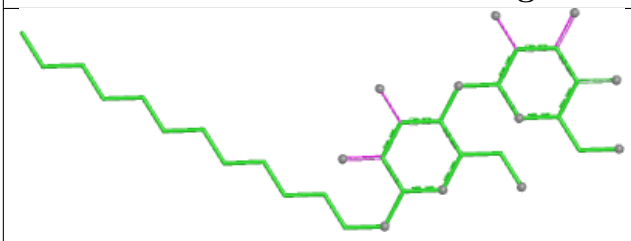


Torsions

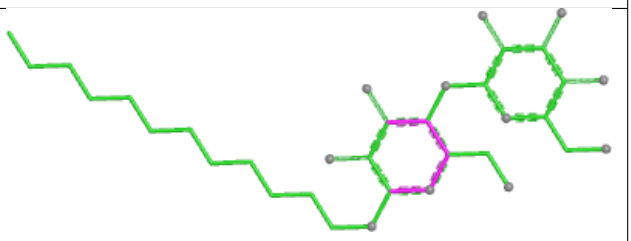


Rings

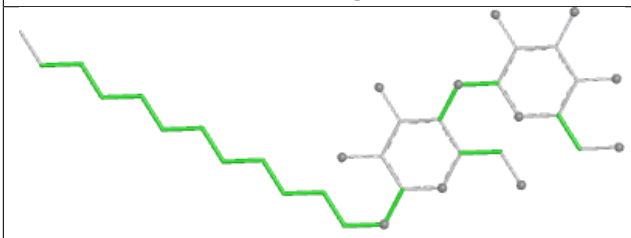
Ligand LMT M 103



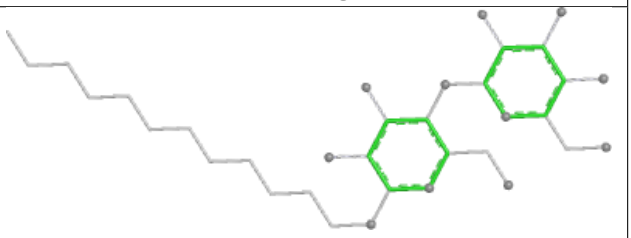
Bond lengths



Bond angles



Torsions

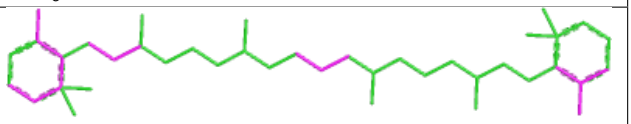


Rings

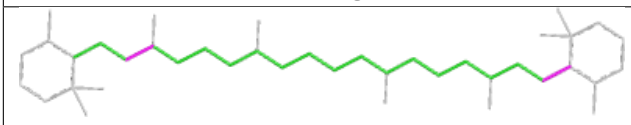
Ligand BCR y 101



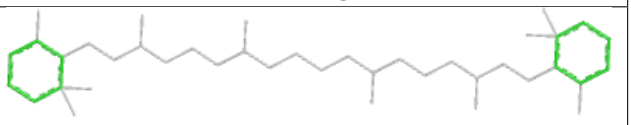
Bond lengths



Bond angles

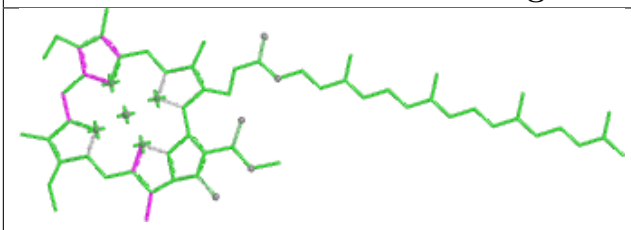


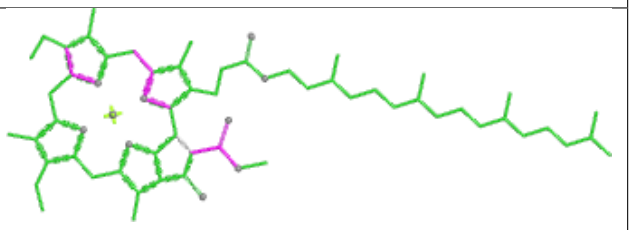
Torsions

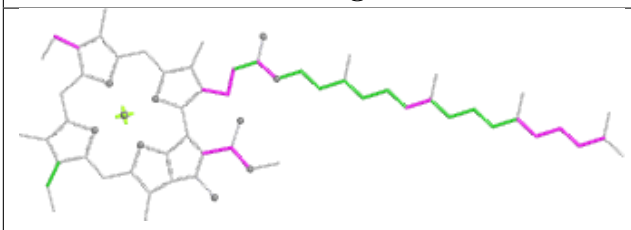


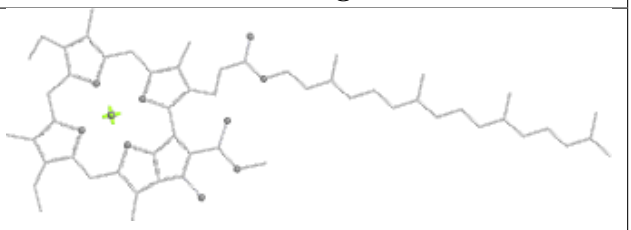
Rings

Ligand CLA b 609

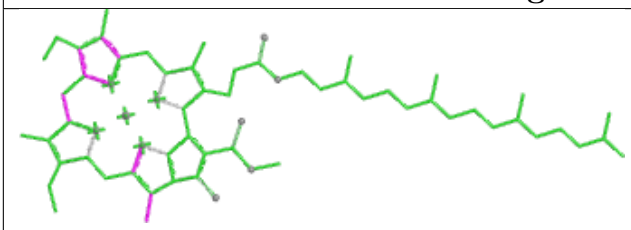

Bond lengths

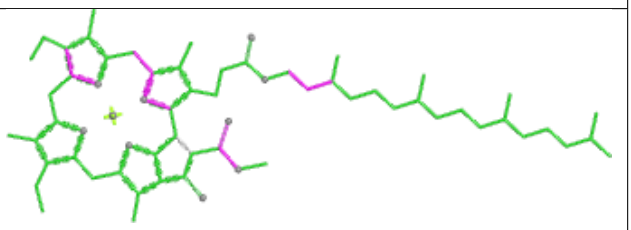

Bond angles

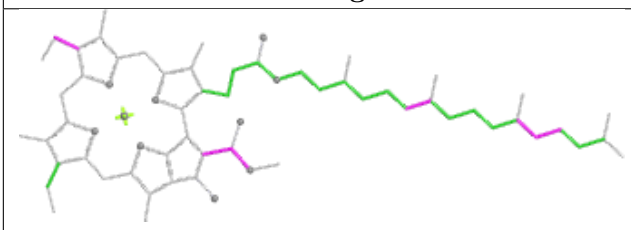

Torsions

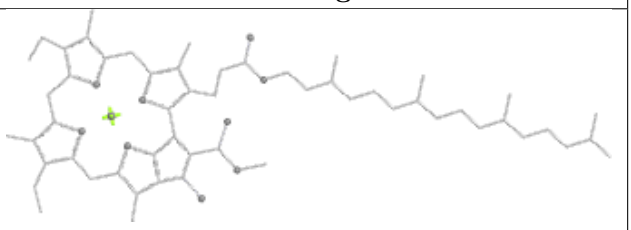

Rings

Ligand CLA b 612

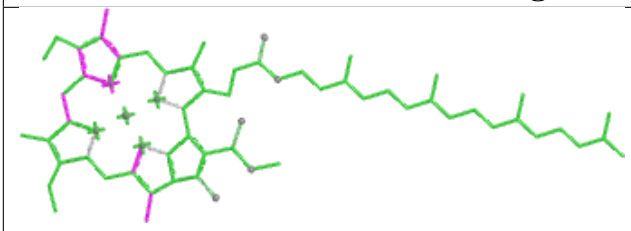

Bond lengths

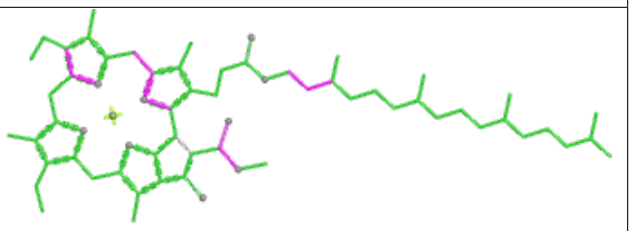

Bond angles

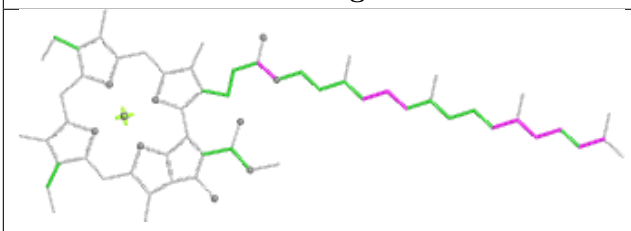

Torsions

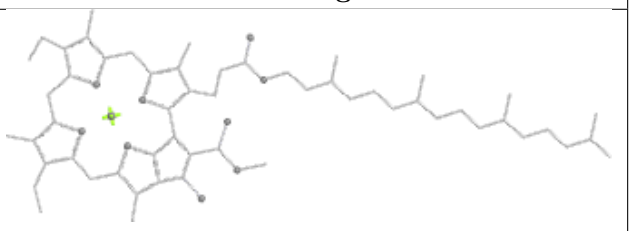

Rings

Ligand CLA c 502

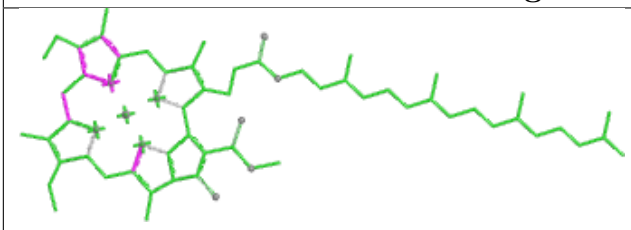

Bond lengths


Bond angles

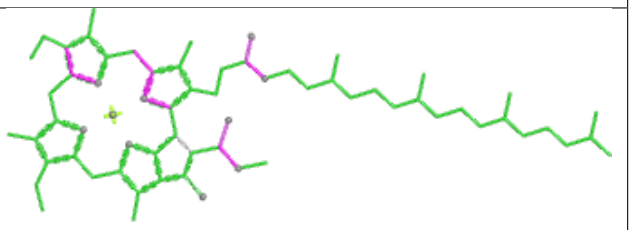

Torsions


Rings

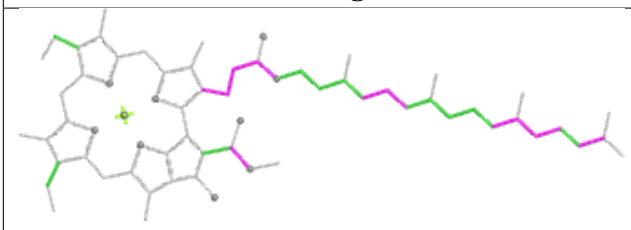
Ligand CLA C 511



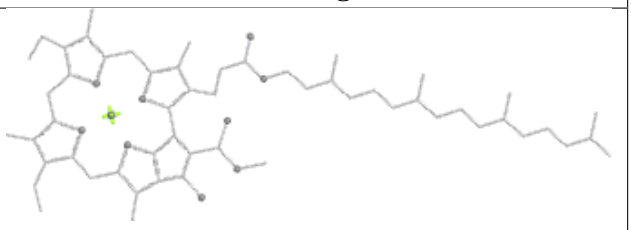
Bond lengths



Bond angles

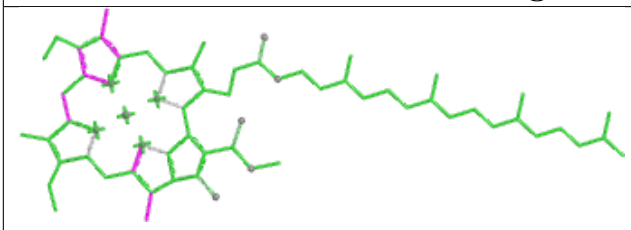


Torsions

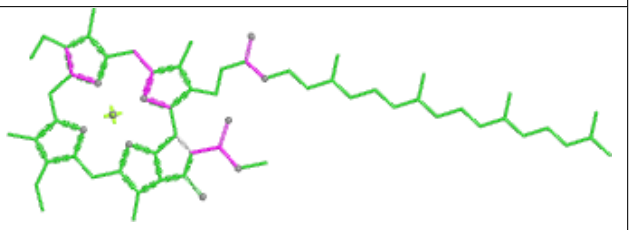


Rings

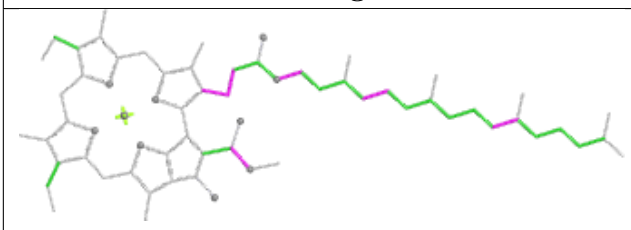
Ligand CLA a 404



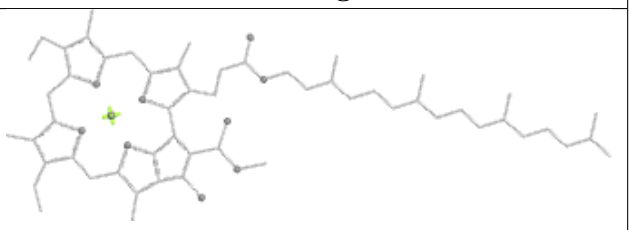
Bond lengths



Bond angles

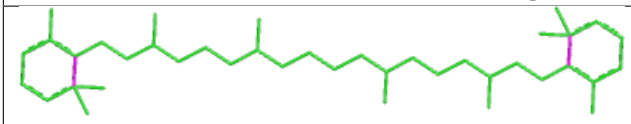


Torsions

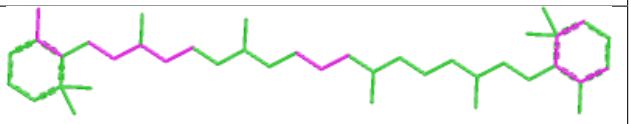


Rings

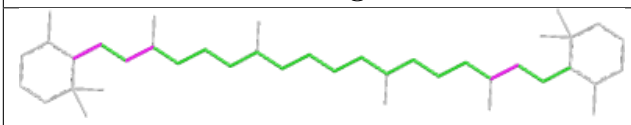
Ligand BCR F 102



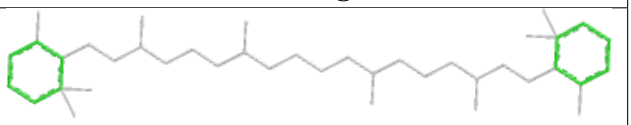
Bond lengths



Bond angles

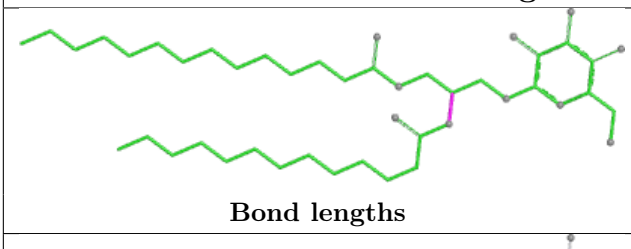


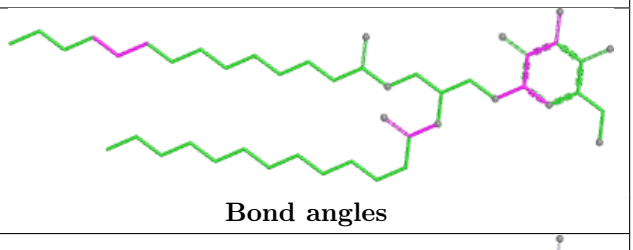
Torsions

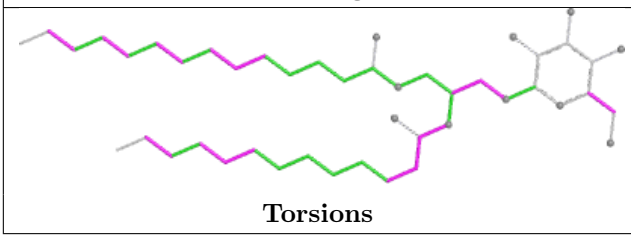


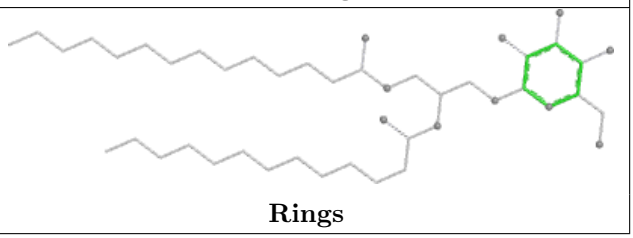
Rings

Ligand LMG D 411

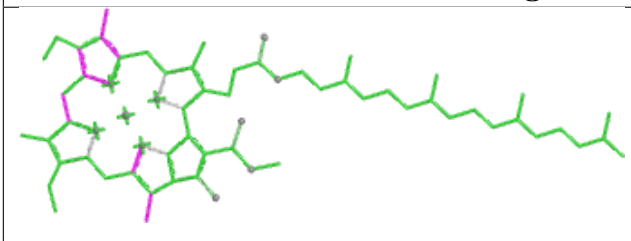

Bond lengths

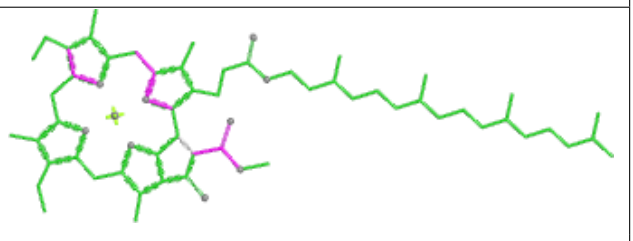

Bond angles

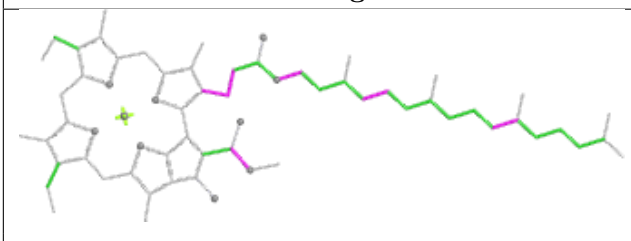

Torsions

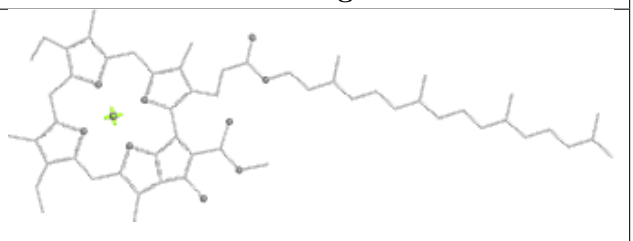

Rings

Ligand CLA A 402

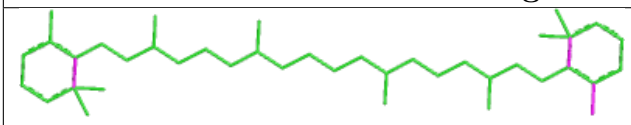

Bond lengths

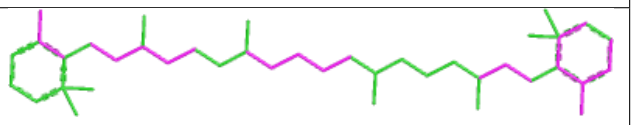

Bond angles


Torsions

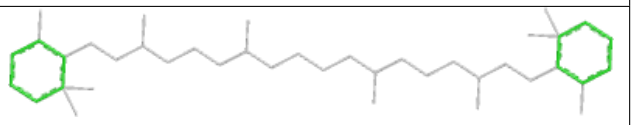

Rings

Ligand BCR C 514

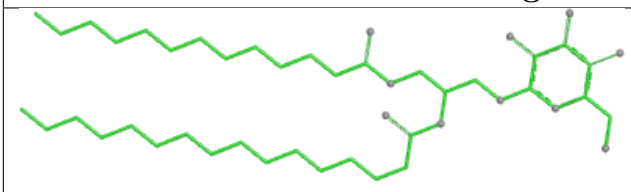

Bond lengths


Bond angles

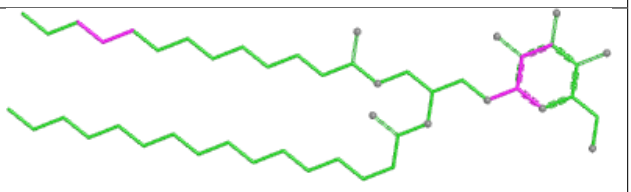

Torsions


Rings

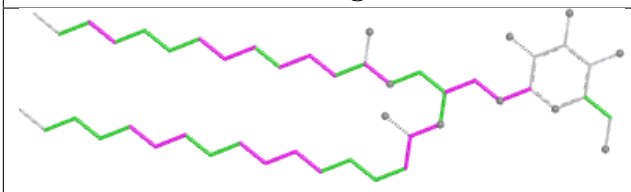
Ligand LMG d 408



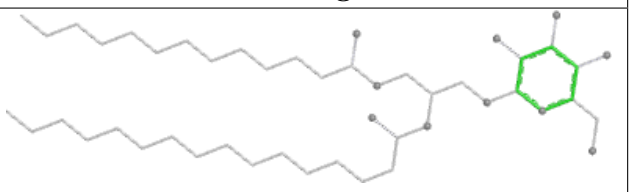
Bond lengths



Bond angles

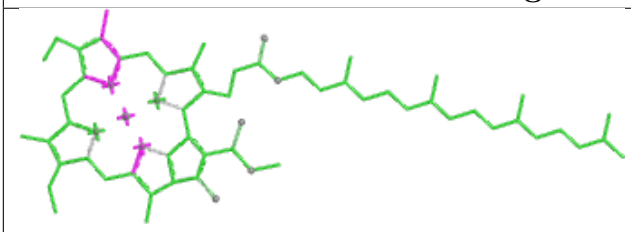


Torsions

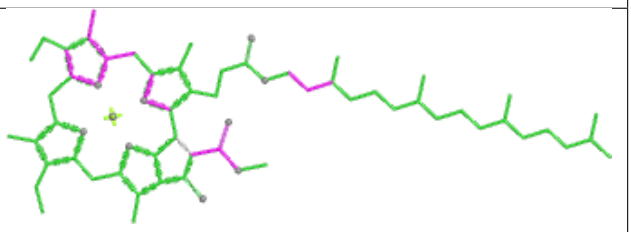


Rings

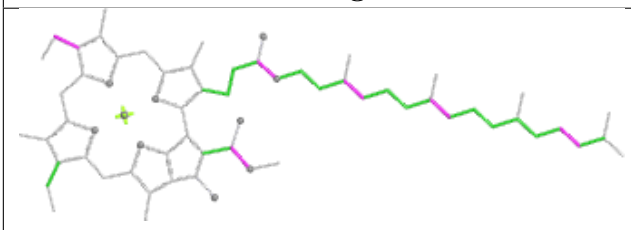
Ligand CLA B 610



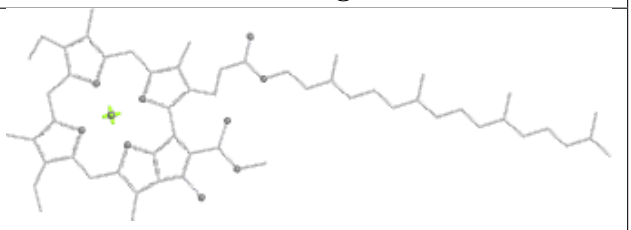
Bond lengths



Bond angles

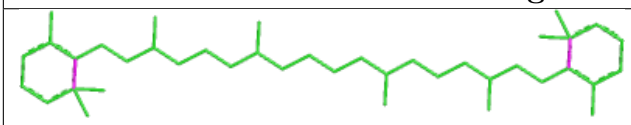


Torsions

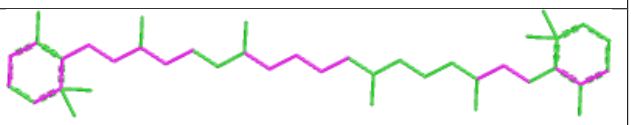


Rings

Ligand BCR c 513



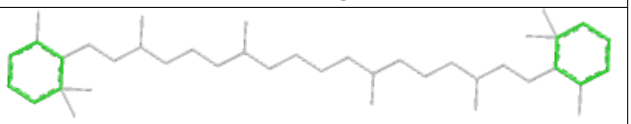
Bond lengths



Bond angles

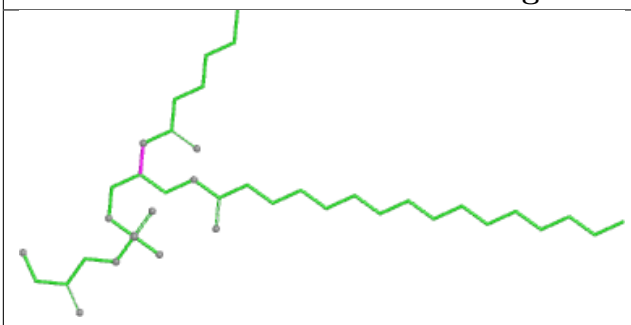


Torsions

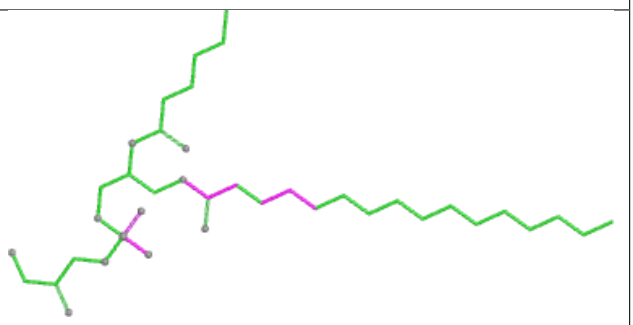


Rings

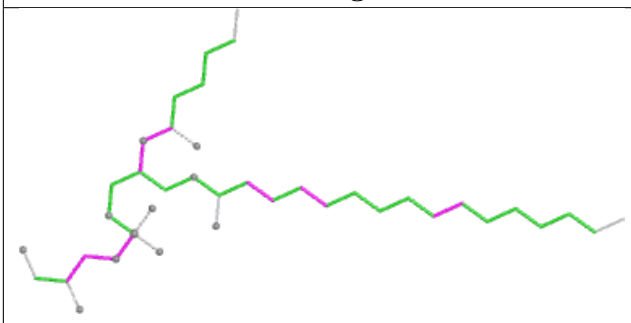
Ligand LHG A 409



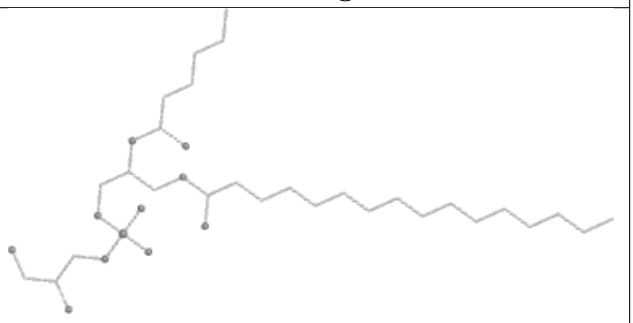
Bond lengths



Bond angles

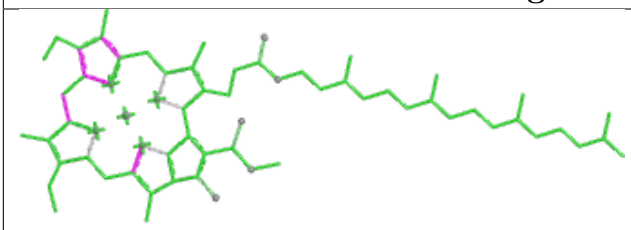


Torsions

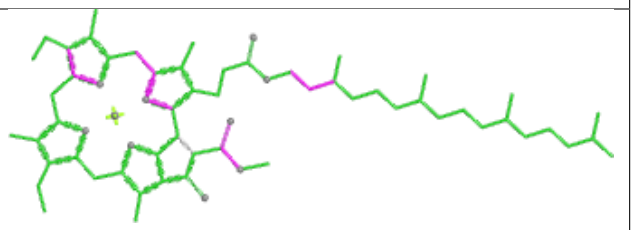


Rings

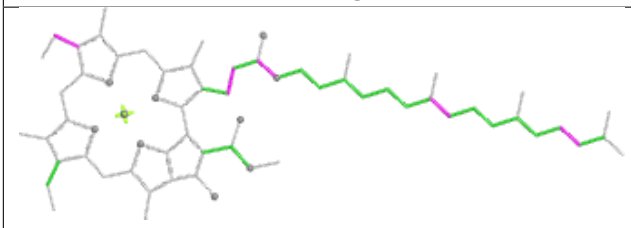
Ligand CLA d 405



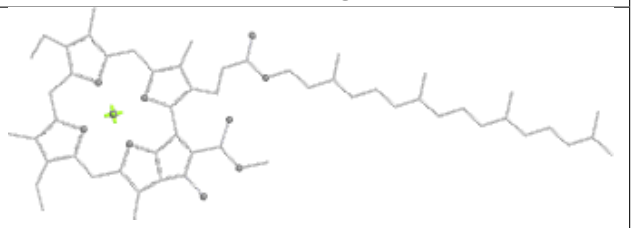
Bond lengths



Bond angles

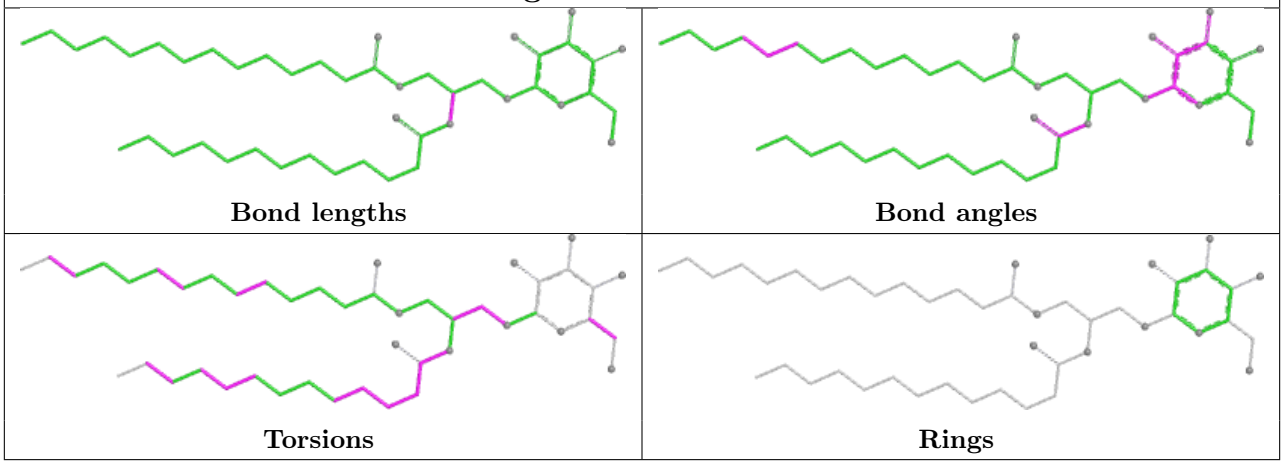


Torsions

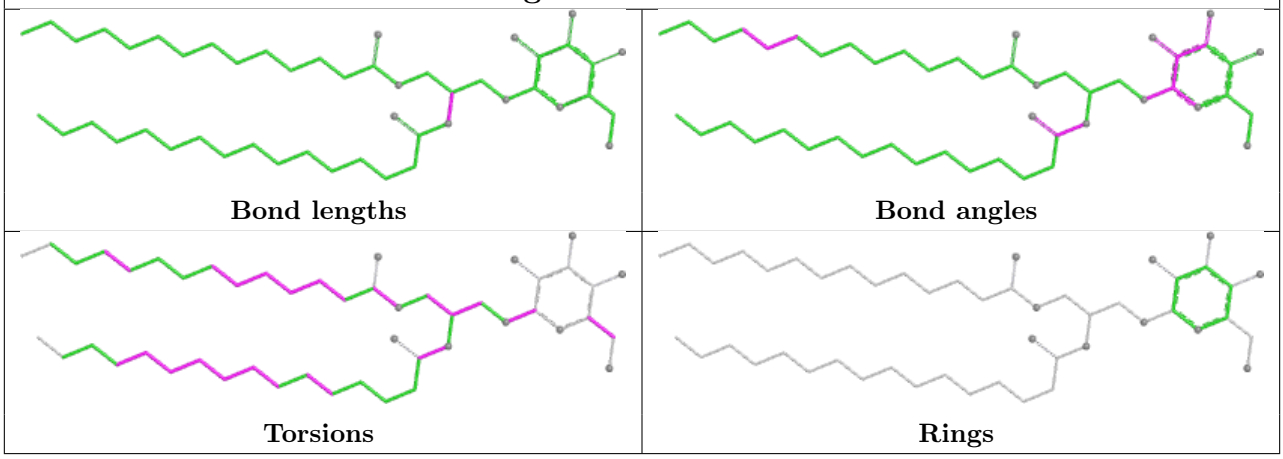


Rings

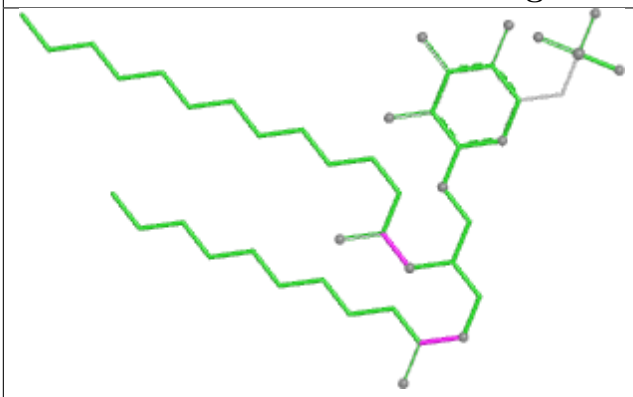
Ligand LMG d 411



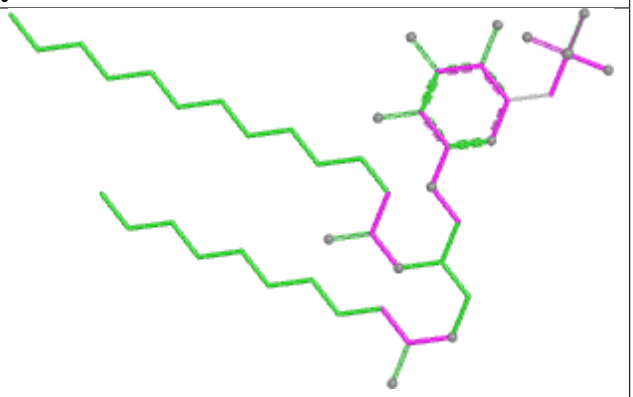
Ligand LMG d 407



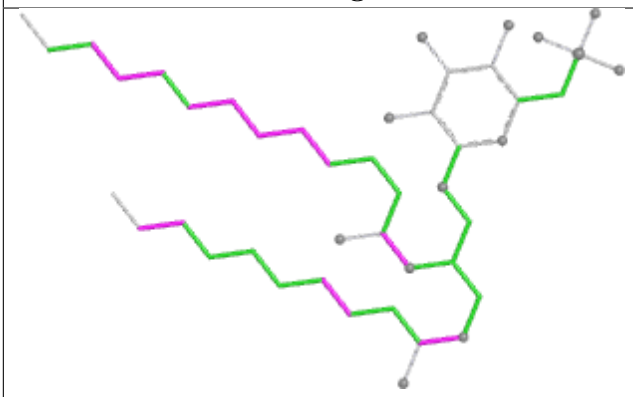
Ligand SQD F 103



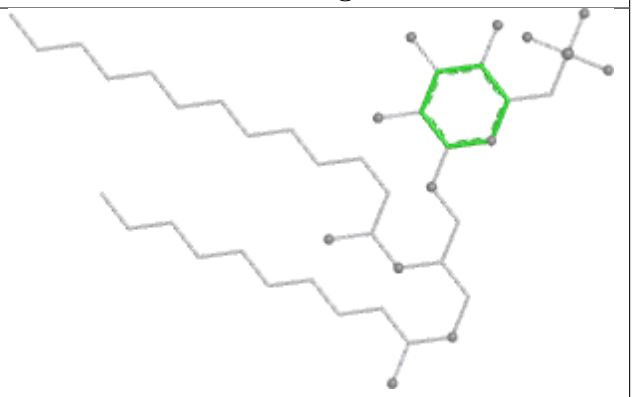
Bond lengths



Bond angles

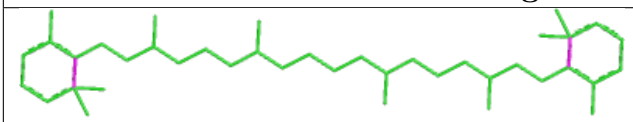


Torsions

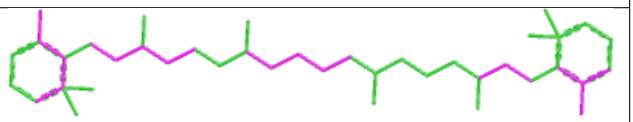


Rings

Ligand BCR K 102



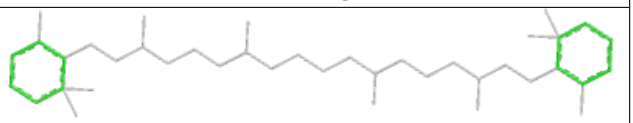
Bond lengths



Bond angles

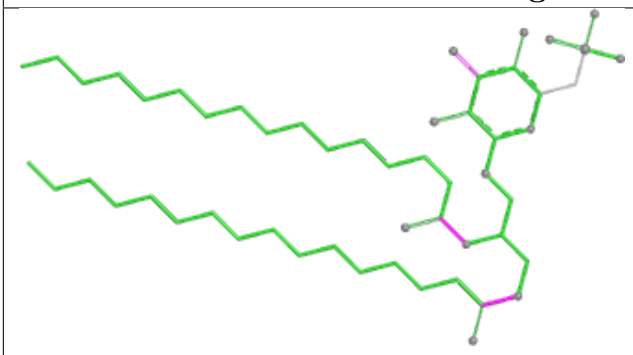


Torsions

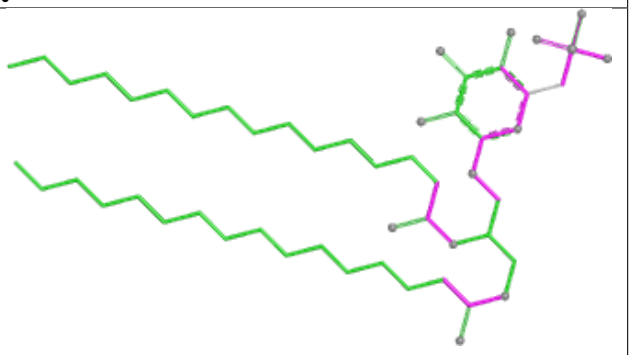


Rings

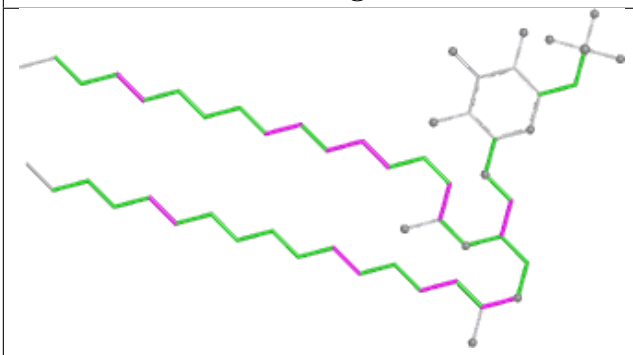
Ligand SQD a 401



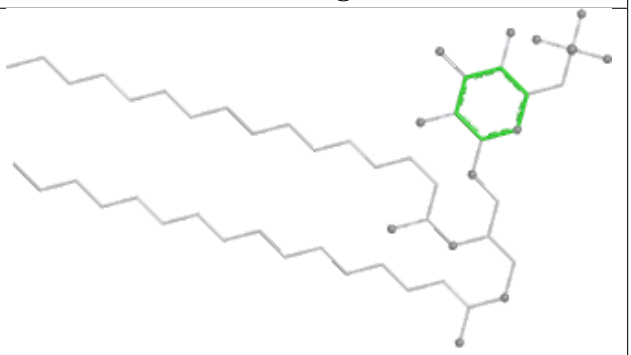
Bond lengths



Bond angles

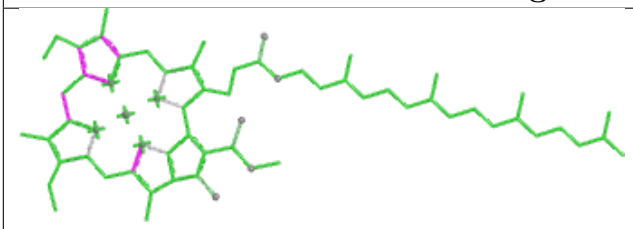


Torsions

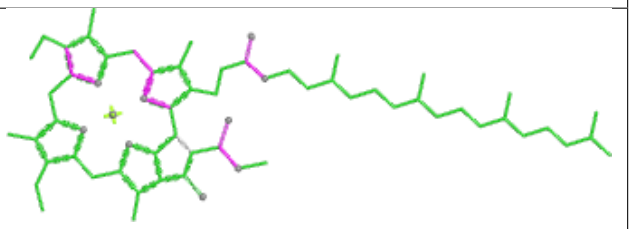


Rings

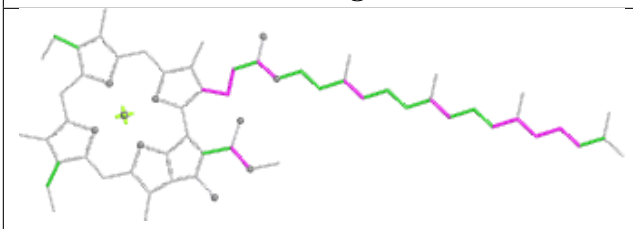
Ligand CLA c 512



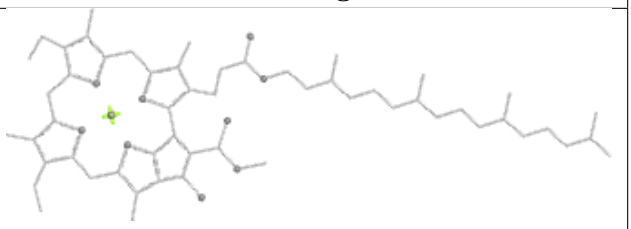
Bond lengths



Bond angles

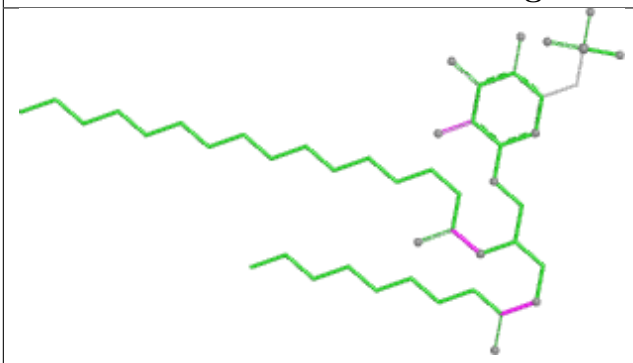


Torsions

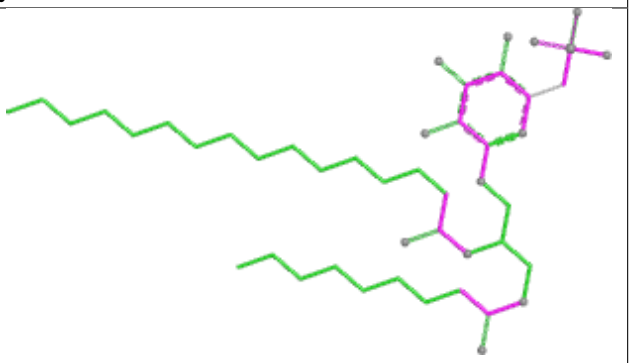


Rings

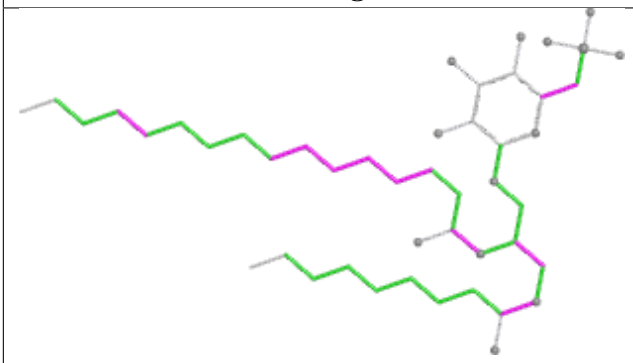
Ligand SQD B 626



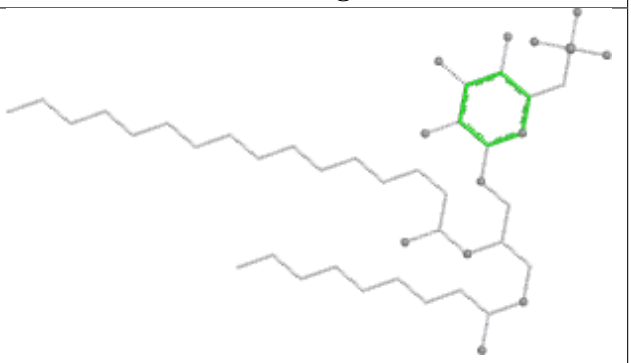
Bond lengths



Bond angles

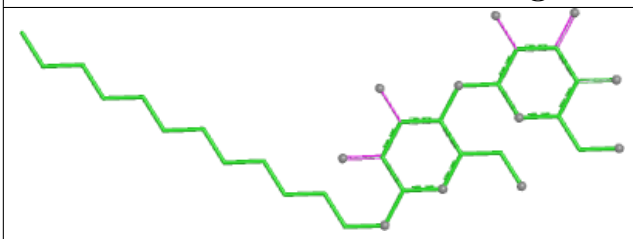


Torsions

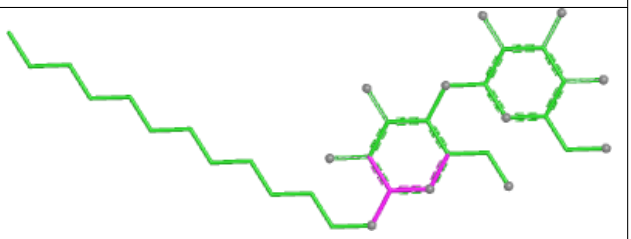


Rings

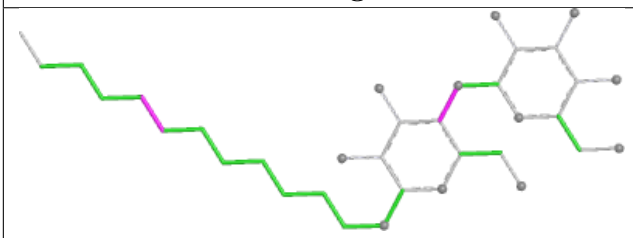
Ligand LMT i 102



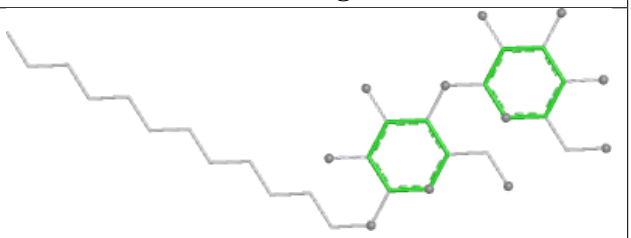
Bond lengths



Bond angles

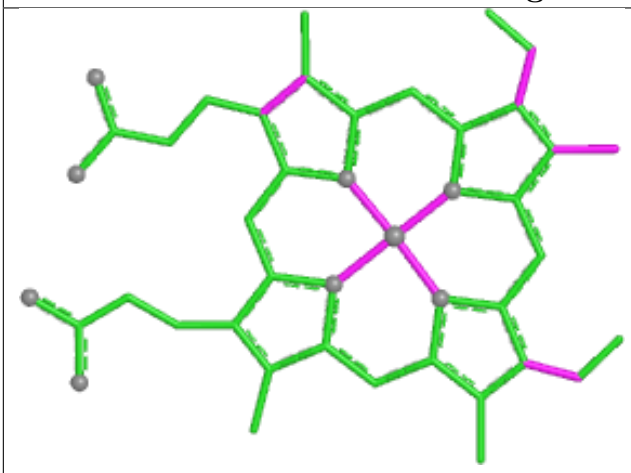


Torsions

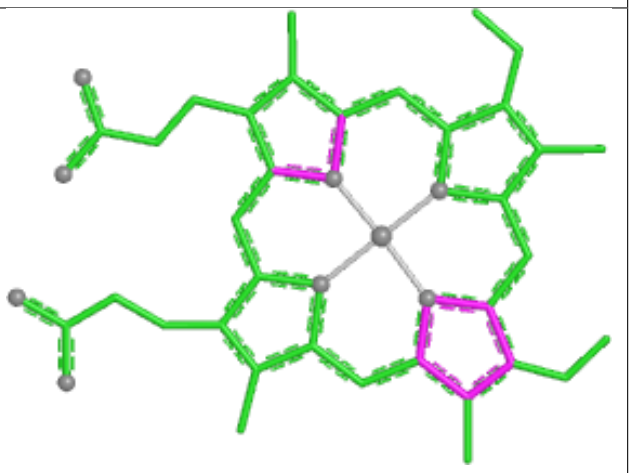


Rings

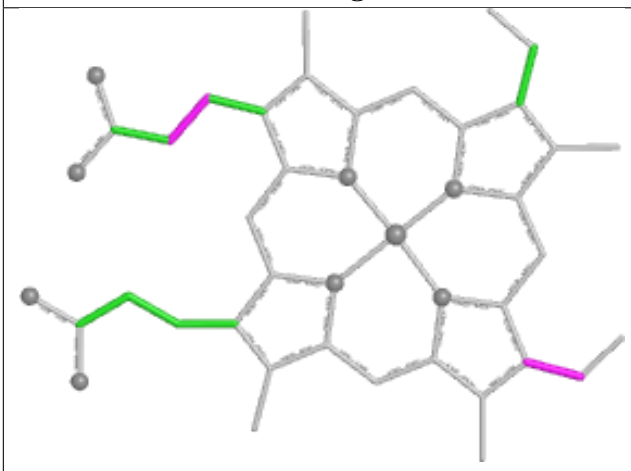
Ligand HEM f 101



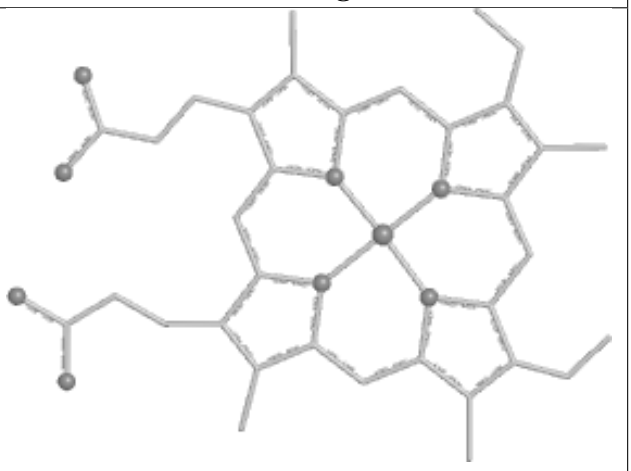
Bond lengths



Bond angles

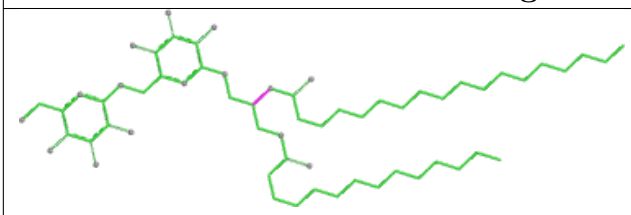


Torsions

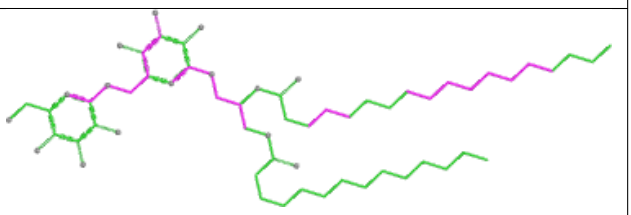


Rings

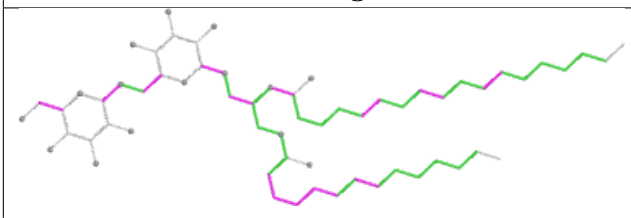
Ligand DGD C 516



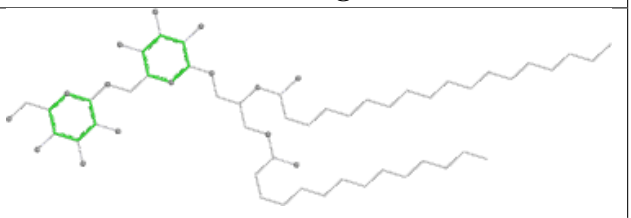
Bond lengths



Bond angles

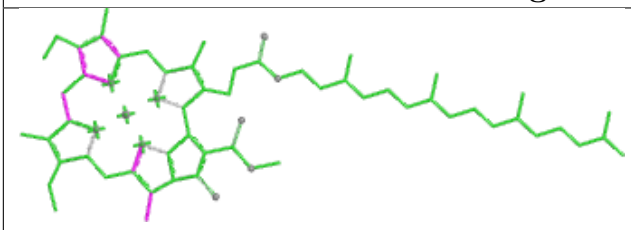


Torsions

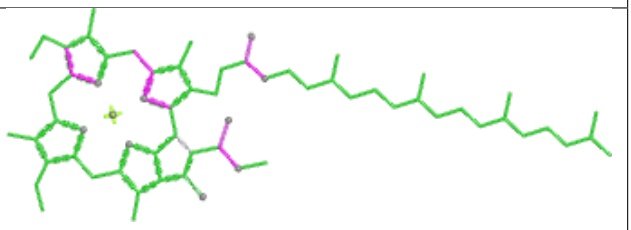


Rings

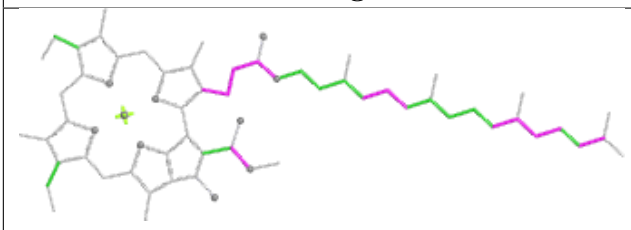
Ligand CLA c 511



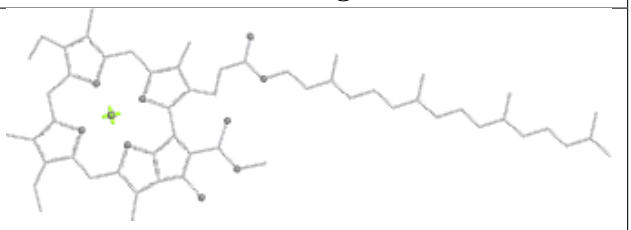
Bond lengths



Bond angles

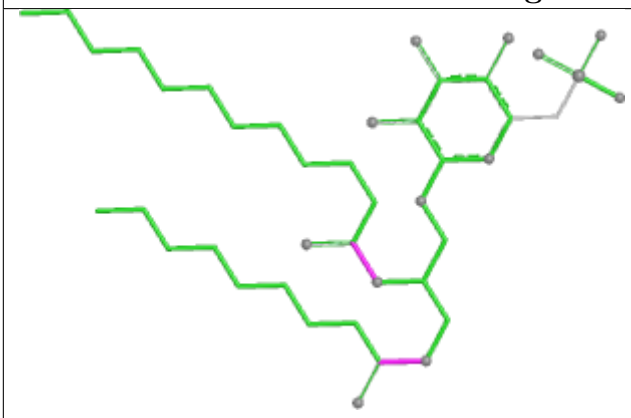


Torsions

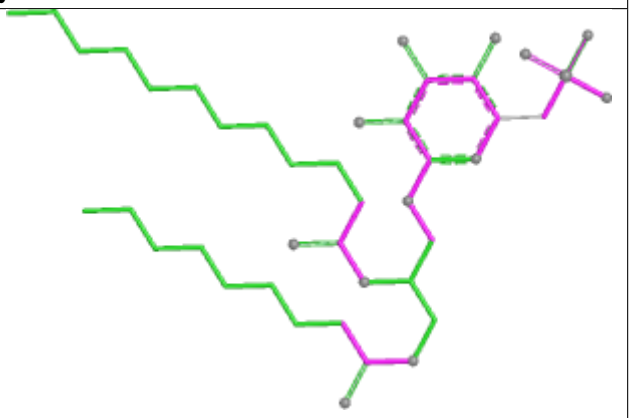


Rings

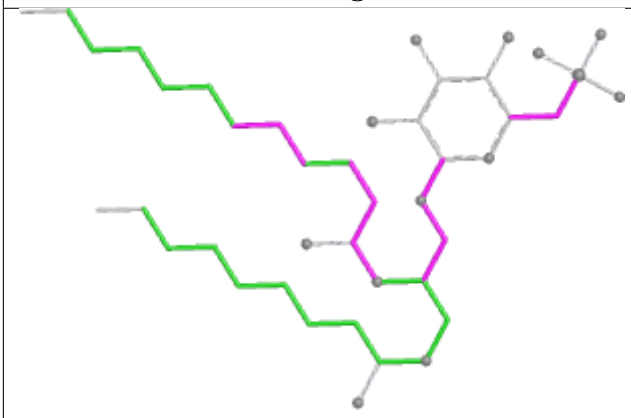
Ligand SQD B 622



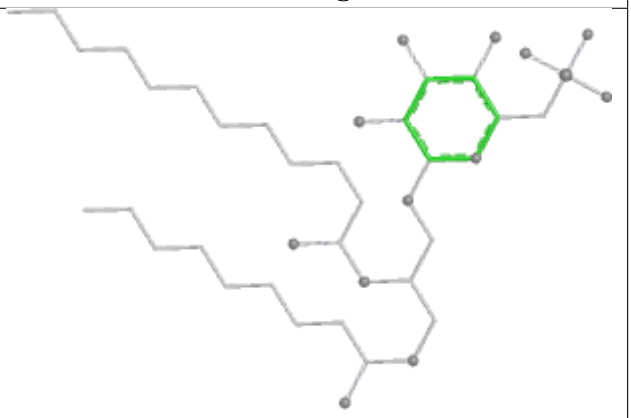
Bond lengths



Bond angles

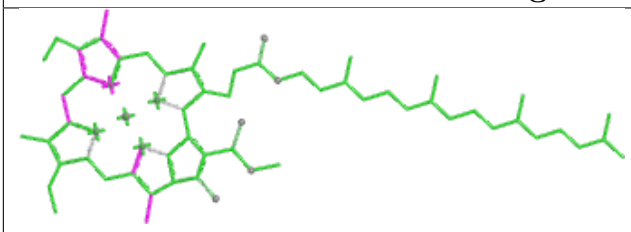


Torsions

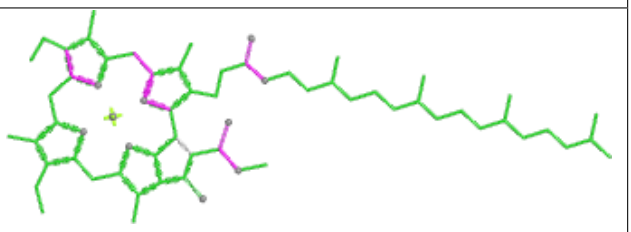


Rings

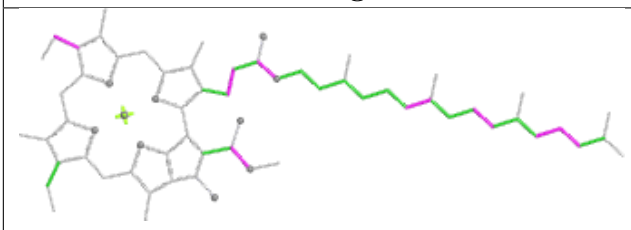
Ligand CLA c 520



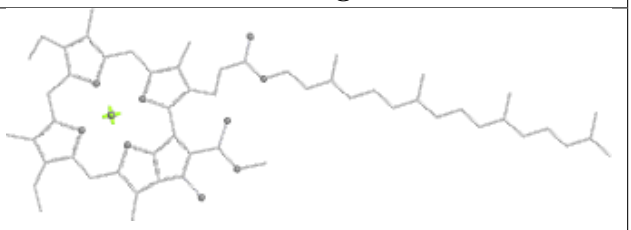
Bond lengths



Bond angles

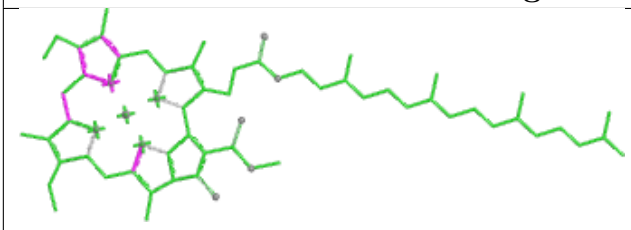


Torsions

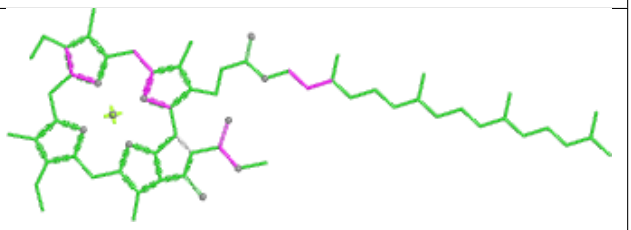


Rings

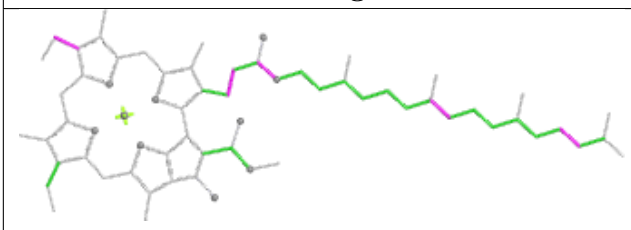
Ligand CLA D 405



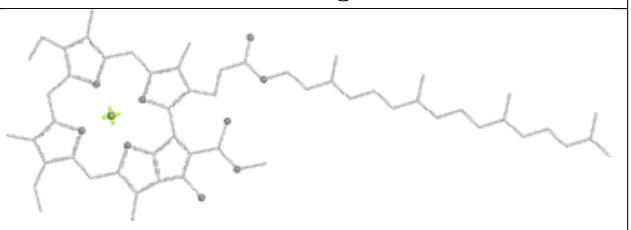
Bond lengths



Bond angles

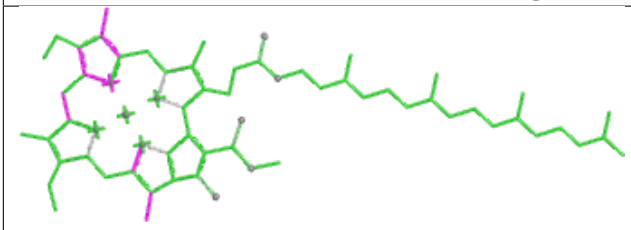


Torsions

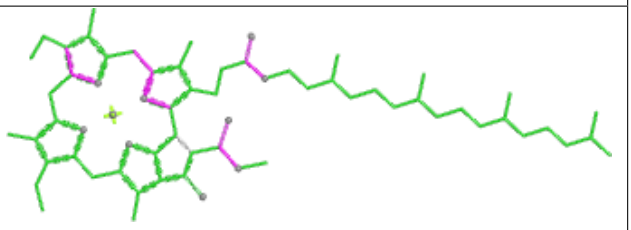


Rings

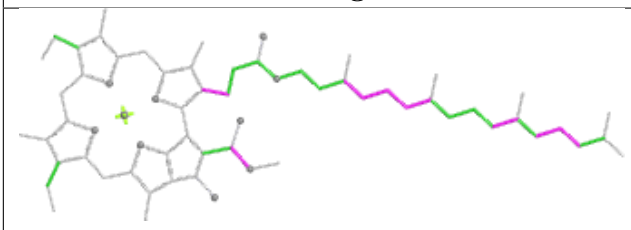
Ligand CLA b 611



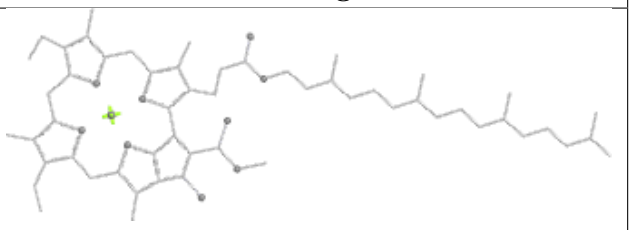
Bond lengths



Bond angles

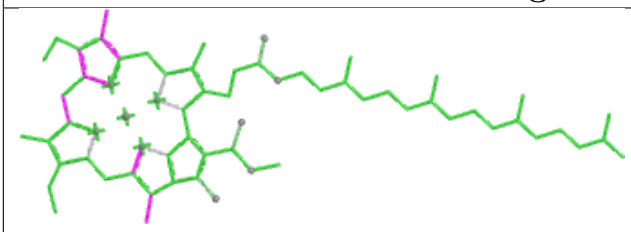


Torsions

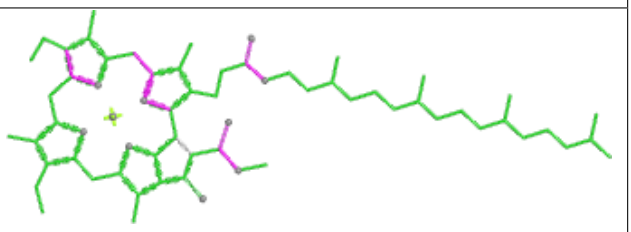


Rings

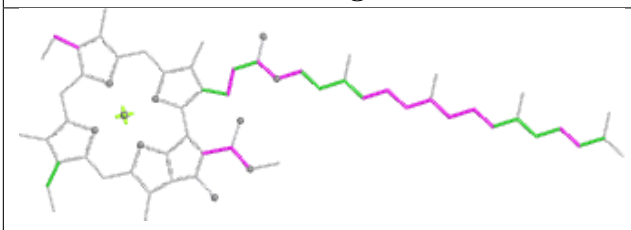
Ligand CLA c 508



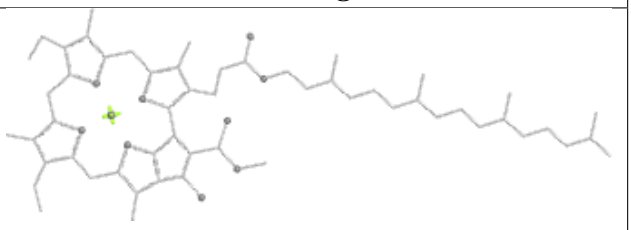
Bond lengths



Bond angles



Torsions

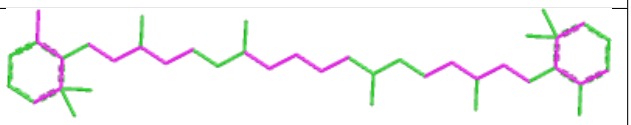


Rings

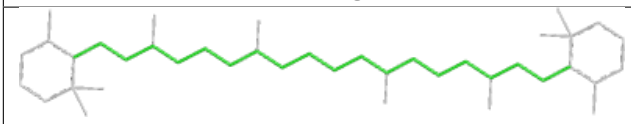
Ligand BCR b 622



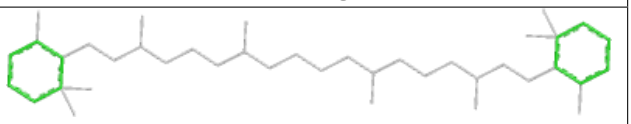
Bond lengths



Bond angles

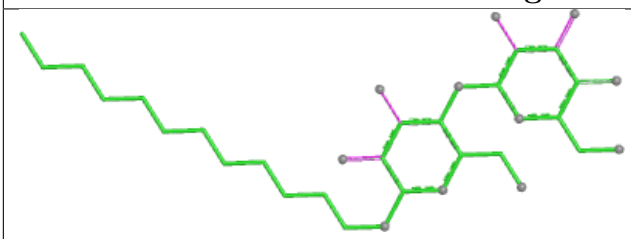


Torsions

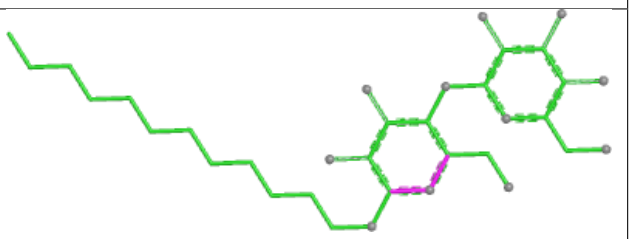


Rings

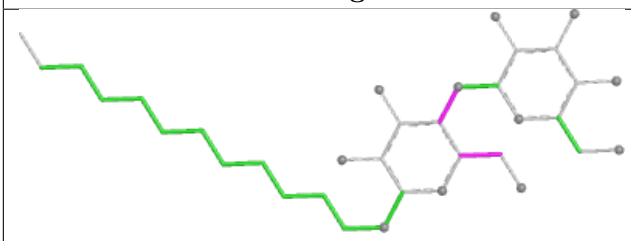
Ligand LMT b 603



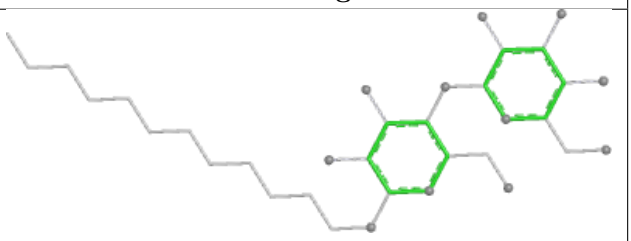
Bond lengths



Bond angles

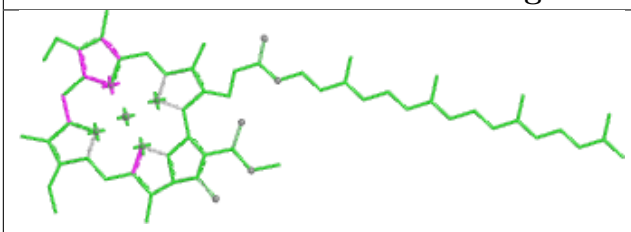


Torsions

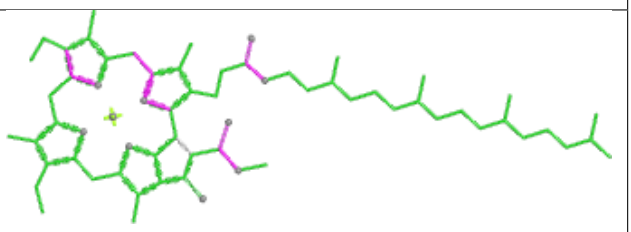


Rings

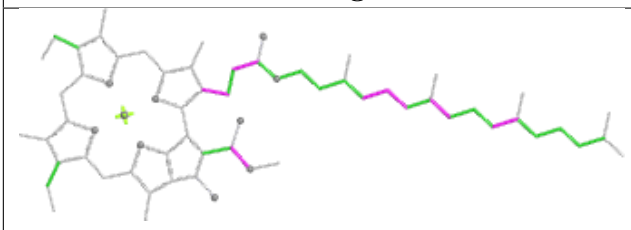
Ligand CLA C 506



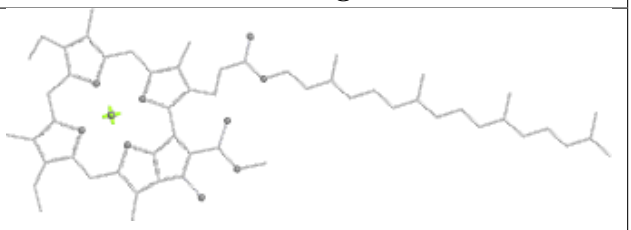
Bond lengths



Bond angles

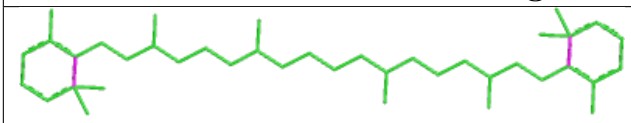


Torsions

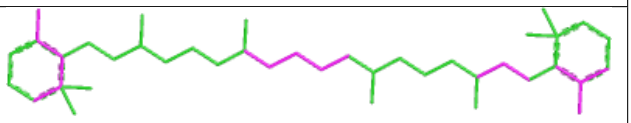


Rings

Ligand BCR a 410



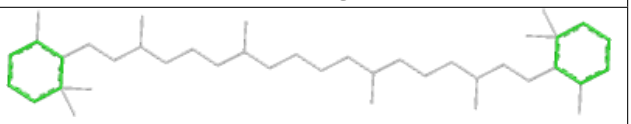
Bond lengths



Bond angles

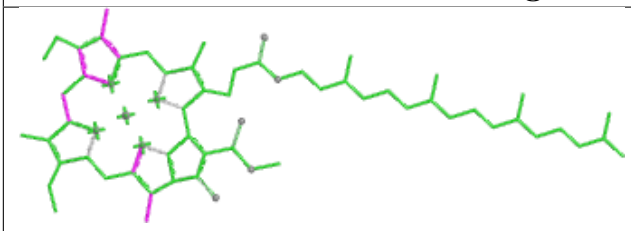


Torsions

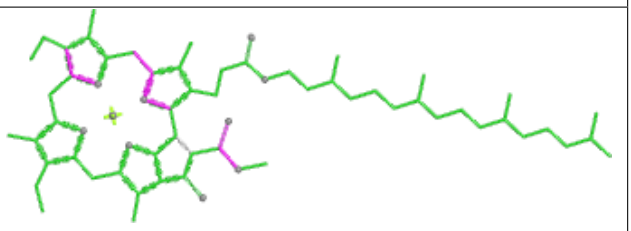


Rings

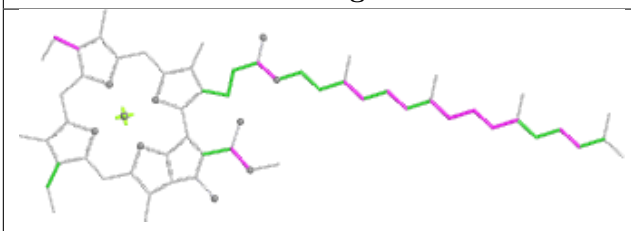
Ligand CLA B 604



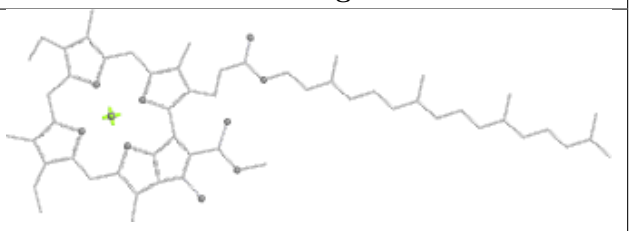
Bond lengths



Bond angles

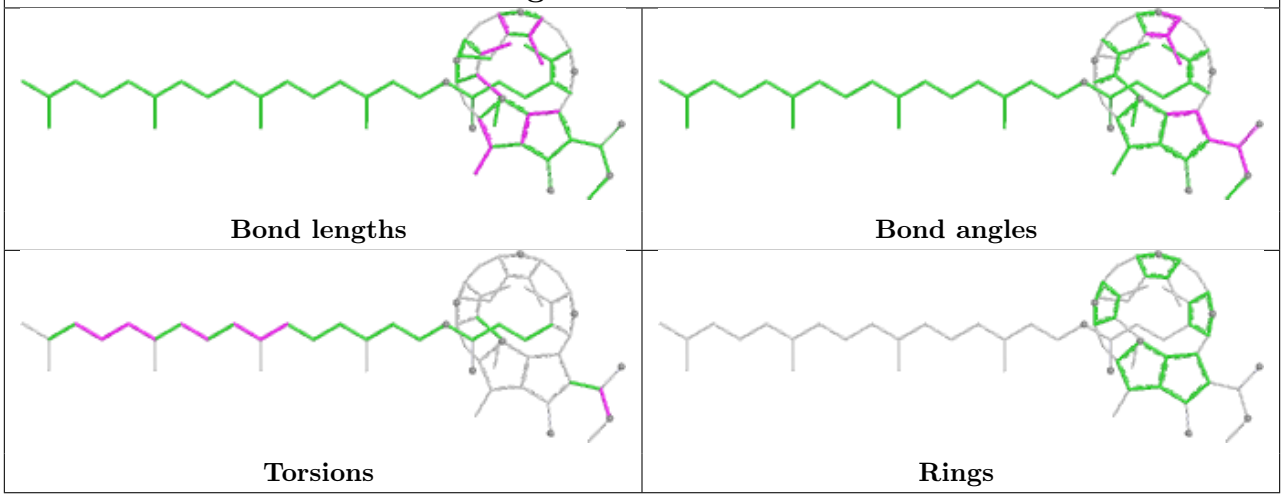


Torsions



Rings

Ligand PHO a 407



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	335/344 (97%)	0.04	5 (1%) 72 57	205, 207, 208, 208	0
1	a	335/344 (97%)	-0.15	1 (0%) 90 80	204, 207, 208, 209	0
2	B	490/510 (96%)	-0.14	6 (1%) 76 62	205, 207, 208, 208	0
2	b	490/510 (96%)	-0.09	9 (1%) 67 54	205, 207, 208, 209	0
3	C	447/461 (96%)	-0.05	10 (2%) 62 50	205, 207, 208, 209	0
3	c	447/461 (96%)	-0.13	2 (0%) 88 77	206, 207, 208, 209	0
4	D	340/352 (96%)	-0.01	5 (1%) 72 57	204, 207, 208, 209	0
4	d	340/352 (96%)	-0.15	4 (1%) 76 62	204, 207, 208, 208	0
5	E	82/84 (97%)	-0.13	2 (2%) 59 49	205, 207, 208, 208	0
5	e	82/84 (97%)	-0.06	1 (1%) 76 62	206, 207, 208, 208	0
6	F	35/45 (77%)	-0.08	0 100 100	206, 207, 208, 208	0
6	f	35/45 (77%)	-0.20	0 100 100	206, 207, 208, 208	0
7	H	65/66 (98%)	0.31	4 (6%) 26 28	206, 207, 208, 209	0
7	h	65/66 (98%)	0.15	3 (4%) 37 34	206, 207, 208, 208	0
8	I	35/38 (92%)	-0.15	0 100 100	206, 207, 208, 208	0
8	i	35/38 (92%)	-0.15	1 (2%) 53 43	206, 207, 208, 208	0
9	J	34/40 (85%)	-0.25	0 100 100	205, 207, 207, 208	0
9	j	34/40 (85%)	-0.16	0 100 100	206, 207, 208, 209	0
10	K	37/46 (80%)	-0.22	0 100 100	206, 207, 208, 208	0
10	k	37/46 (80%)	-0.13	0 100 100	206, 207, 208, 209	0
11	L	37/37 (100%)	-0.19	0 100 100	205, 207, 208, 208	0
11	l	37/37 (100%)	-0.13	0 100 100	206, 207, 208, 209	0
12	M	34/36 (94%)	-0.00	0 100 100	205, 206, 207, 208	0
12	m	34/36 (94%)	0.06	1 (2%) 53 43	205, 207, 207, 208	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%)	-0.03	5 (2%) 63 51	205, 207, 208, 209	0
13	o	243/272 (89%)	-0.12	2 (0%) 82 69	205, 207, 208, 209	0
14	T	32/32 (100%)	-0.11	0 100 100	206, 207, 208, 209	0
14	t	32/32 (100%)	0.03	0 100 100	205, 206, 208, 208	0
15	U	97/134 (72%)	0.00	3 (3%) 51 42	205, 207, 208, 208	0
15	u	97/134 (72%)	0.14	0 100 100	205, 207, 208, 208	0
16	V	137/163 (84%)	0.04	4 (2%) 53 43	205, 207, 208, 208	0
16	v	137/163 (84%)	-0.09	1 (0%) 84 71	206, 207, 208, 208	0
17	g	28/46 (60%)	-0.04	1 (3%) 46 39	206, 207, 208, 209	0
17	y	28/46 (60%)	-0.20	0 100 100	206, 207, 208, 208	0
18	X	37/41 (90%)	0.06	0 100 100	205, 207, 208, 209	0
18	x	37/41 (90%)	0.06	0 100 100	206, 207, 208, 208	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	-0.15	1 (1%) 70 56	205, 207, 208, 209	0
20	z	62/62 (100%)	-0.21	0 100 100	206, 207, 208, 209	0
All	All	5214/5674 (91%)	-0.07	71 (1%) 73 59	204, 207, 208, 209	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	63	LEU	4.4
2	B	309	LEU	4.3
7	H	27	THR	4.3
16	V	47	LEU	3.9
4	D	145	ALA	3.8

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	LMT	d	410	31/35	0.48	0.17	206,208,209,210	0
31	LMT	i	102	35/35	0.50	0.17	206,208,209,210	0
31	LMT	I	102	35/35	0.54	0.18	205,207,209,210	0
22	CLA	b	605	65/65	0.61	0.22	205,208,209,209	0
31	LMT	B	623	35/35	0.65	0.14	205,208,209,210	0
35	CA	K	101	1/1	0.65	0.17	210,210,210,210	0
31	LMT	b	626	35/35	0.67	0.14	205,208,210,210	0
31	LMT	b	627	35/35	0.68	0.13	205,208,210,210	0
22	CLA	B	601	65/65	0.69	0.17	206,207,208,209	0
31	LMT	D	410	31/35	0.70	0.13	206,208,208,209	0
24	BCR	J	102	40/40	0.71	0.26	205,207,208,209	0
27	LMG	E	101	44/55	0.71	0.24	204,207,209,210	0
26	LHG	c	519	37/49	0.72	0.19	205,207,211,214	0
33	BCT	d	403	4/4	0.74	0.24	207,207,207,208	0
35	CA	O	301	1/1	0.75	0.08	207,207,207,207	0
25	DGD	B	625	52/66	0.76	0.18	205,208,210,210	0
27	LMG	c	518	45/55	0.76	0.17	206,207,208,208	0
23	PL9	A	406	45/55	0.76	0.29	205,206,207,208	0
22	CLA	b	619	65/65	0.77	0.15	205,207,208,209	0
35	CA	o	301	1/1	0.77	0.12	209,209,209,209	0
31	LMT	b	603	35/35	0.78	0.12	205,207,208,209	0
27	LMG	C	518	45/55	0.78	0.16	205,206,208,208	0
22	CLA	c	512	65/65	0.78	0.15	205,207,208,208	0
25	DGD	D	409	63/66	0.78	0.18	205,208,209,211	0
25	DGD	d	409	63/66	0.78	0.19	205,208,210,211	0
31	LMT	B	628	35/35	0.78	0.17	204,207,209,209	0
24	BCR	j	102	40/40	0.78	0.24	206,207,209,209	0
27	LMG	A	415	42/55	0.78	0.22	204,207,208,209	0
31	LMT	M	102	35/35	0.78	0.20	205,207,208,209	0
30	SQD	B	626	47/54	0.79	0.15	204,207,209,211	0
30	SQD	d	402	43/54	0.80	0.17	205,207,209,211	0
27	LMG	a	402	42/55	0.80	0.19	204,207,209,209	0
31	LMT	B	627	35/35	0.80	0.11	205,207,209,209	0
30	SQD	F	103	45/54	0.80	0.21	205,207,209,210	0
31	LMT	B	624	35/35	0.81	0.13	205,207,210,210	0
25	DGD	C	517	66/66	0.81	0.18	205,206,207,208	0
23	PL9	J	101	35/55	0.81	0.27	204,207,208,209	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	C	506	65/65	0.81	0.18	204,207,207,208	0
30	SQD	A	413	51/54	0.81	0.18	205,207,208,208	0
26	LHG	C	519	37/49	0.82	0.14	204,207,210,212	0
25	DGD	C	516	62/66	0.82	0.13	204,206,208,208	0
25	DGD	A	408	56/66	0.82	0.18	206,207,209,210	0
25	DGD	c	517	66/66	0.83	0.17	204,206,207,208	0
24	BCR	c	521	40/40	0.83	0.16	205,207,208,209	0
27	LMG	b	625	49/55	0.83	0.20	205,206,207,208	0
25	DGD	b	601	52/66	0.83	0.15	204,207,208,209	0
30	SQD	b	602	47/54	0.84	0.16	205,207,209,212	0
24	BCR	H	102	40/40	0.84	0.20	206,207,208,208	0
27	LMG	I	101	43/55	0.84	0.16	204,207,209,210	0
22	CLA	a	406	65/65	0.84	0.21	205,207,208,209	0
24	BCR	a	410	40/40	0.84	0.22	205,206,207,207	0
24	BCR	b	621	40/40	0.84	0.19	204,206,207,207	0
24	BCR	c	513	40/40	0.84	0.18	204,206,207,208	0
22	CLA	C	512	65/65	0.84	0.15	205,207,208,209	0
25	DGD	a	411	56/66	0.84	0.16	205,207,209,209	0
27	LMG	l	101	51/55	0.85	0.19	205,206,208,208	0
25	DGD	c	516	62/66	0.85	0.16	205,207,208,209	0
23	PL9	d	406	55/55	0.85	0.16	204,206,207,208	0
32	PHO	D	402	64/64	0.85	0.16	205,206,207,208	0
30	SQD	a	401	54/54	0.86	0.16	205,207,209,211	0
22	CLA	c	506	65/65	0.86	0.15	206,207,208,208	0
24	BCR	x	101	40/40	0.86	0.21	205,207,208,208	0
27	LMG	m	101	42/55	0.86	0.18	203,207,208,209	0
22	CLA	c	505	65/65	0.87	0.14	204,206,208,208	0
22	CLA	b	613	65/65	0.87	0.13	205,207,208,209	0
24	BCR	g	101	40/40	0.87	0.17	204,206,207,207	0
27	LMG	e	101	44/55	0.87	0.17	204,207,208,209	0
22	CLA	c	510	65/65	0.87	0.13	206,207,208,209	0
22	CLA	A	405	65/65	0.87	0.15	204,206,208,208	0
31	LMT	b	604	35/35	0.87	0.16	205,207,209,209	0
27	LMG	M	101	42/55	0.87	0.17	205,207,209,210	0
25	DGD	C	515	53/66	0.88	0.15	204,206,207,208	0
22	CLA	B	605	65/65	0.88	0.12	205,206,207,208	0
24	BCR	K	102	40/40	0.88	0.20	204,207,208,209	0
23	PL9	j	101	35/55	0.88	0.23	205,208,209,209	0
24	BCR	C	514	40/40	0.88	0.17	205,206,207,207	0
27	LMG	B	621	49/55	0.88	0.16	204,206,207,208	0
24	BCR	b	623	40/40	0.88	0.13	204,206,207,207	0
22	CLA	c	502	65/65	0.88	0.15	205,207,208,208	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	LMG	i	101	43/55	0.89	0.12	205,207,209,209	0
22	CLA	C	520	65/65	0.89	0.15	205,207,208,209	0
24	BCR	b	622	40/40	0.89	0.22	204,206,207,207	0
22	CLA	c	503	65/65	0.89	0.13	205,207,208,208	0
30	SQD	B	622	43/54	0.89	0.15	205,207,209,212	0
32	PHO	D	401	64/64	0.89	0.14	203,206,207,208	0
22	CLA	b	606	65/65	0.89	0.14	205,206,207,207	0
27	LMG	C	521	48/55	0.89	0.18	204,206,207,208	0
27	LMG	c	522	48/55	0.89	0.19	205,206,207,208	0
31	LMT	M	103	35/35	0.89	0.14	205,206,208,210	0
24	BCR	b	620	40/40	0.89	0.21	205,206,207,208	0
30	SQD	A	414	54/54	0.90	0.14	204,207,208,210	0
22	CLA	C	508	65/65	0.90	0.13	205,206,207,208	0
25	DGD	b	624	58/66	0.90	0.19	205,206,207,208	0
22	CLA	C	510	65/65	0.90	0.12	205,206,207,208	0
24	BCR	y	101	40/40	0.90	0.18	205,206,207,207	0
30	SQD	a	415	51/54	0.90	0.15	205,206,208,208	0
22	CLA	C	511	65/65	0.90	0.13	205,207,208,208	0
23	PL9	D	406	55/55	0.90	0.17	204,206,207,207	0
22	CLA	c	501	65/65	0.90	0.13	205,207,208,209	0
22	CLA	B	613	65/65	0.90	0.13	205,206,207,208	0
22	CLA	B	615	65/65	0.90	0.13	205,206,208,208	0
22	CLA	C	505	65/65	0.90	0.14	205,206,207,208	0
21	FE2	a	403	1/1	0.90	0.17	211,211,211,211	0
35	CA	k	101	1/1	0.90	0.07	204,204,204,204	0
27	LMG	D	408	48/55	0.90	0.13	202,206,208,208	0
27	LMG	d	408	48/55	0.91	0.16	204,206,207,208	0
26	LHG	A	409	39/49	0.91	0.19	205,206,208,209	0
22	CLA	B	607	65/65	0.91	0.15	205,206,207,209	0
25	DGD	B	620	58/66	0.91	0.16	203,206,208,209	0
23	PL9	a	409	45/55	0.91	0.18	204,206,207,208	0
22	CLA	c	508	65/65	0.91	0.10	205,207,208,208	0
22	CLA	b	607	65/65	0.91	0.11	205,206,207,209	0
24	BCR	A	407	40/40	0.91	0.15	205,206,207,208	0
24	BCR	B	616	40/40	0.91	0.11	205,206,207,207	0
27	LMG	D	411	46/55	0.91	0.15	205,206,207,208	0
24	BCR	B	619	40/40	0.91	0.12	205,206,207,207	0
24	BCR	c	514	40/40	0.91	0.17	205,206,207,208	0
22	CLA	b	609	65/65	0.91	0.11	205,207,208,209	0
25	DGD	c	515	53/66	0.91	0.16	205,207,208,209	0
30	SQD	f	103	45/54	0.91	0.14	205,207,208,210	0
22	CLA	h	101	65/65	0.91	0.15	204,207,208,209	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	b	610	65/65	0.91	0.13	205,206,207,208	0
22	CLA	A	404	65/65	0.91	0.16	204,206,207,208	0
22	CLA	a	405	65/65	0.92	0.14	202,206,207,208	0
22	CLA	c	511	65/65	0.92	0.12	205,207,208,209	0
24	BCR	F	102	40/40	0.92	0.17	205,206,207,208	0
22	CLA	b	617	65/65	0.92	0.13	205,206,208,209	0
22	CLA	B	604	65/65	0.92	0.12	205,207,208,208	0
22	CLA	B	602	65/65	0.92	0.13	204,206,208,209	0
22	CLA	C	504	65/65	0.92	0.13	205,206,207,207	0
22	CLA	B	603	65/65	0.92	0.12	204,206,207,208	0
22	CLA	c	504	65/65	0.92	0.15	205,207,208,208	0
32	PHO	d	401	64/64	0.92	0.13	204,206,207,207	0
22	CLA	b	608	65/65	0.92	0.12	205,206,207,208	0
22	CLA	B	609	65/65	0.92	0.11	205,206,208,208	0
22	CLA	D	404	65/65	0.92	0.12	203,206,207,208	0
22	CLA	c	509	65/65	0.92	0.12	204,206,208,209	0
24	BCR	B	617	40/40	0.92	0.15	204,206,207,208	0
27	LMG	d	407	49/55	0.93	0.17	205,206,207,207	0
22	CLA	c	520	65/65	0.93	0.13	205,207,207,208	0
27	LMG	D	407	49/55	0.93	0.15	205,206,207,208	0
22	CLA	d	404	65/65	0.93	0.15	204,206,207,207	0
22	CLA	C	509	65/65	0.93	0.12	205,206,207,208	0
22	CLA	B	611	65/65	0.93	0.10	204,206,207,208	0
28	CL	A	411	1/1	0.93	0.15	207,207,207,207	0
32	PHO	a	407	64/64	0.93	0.11	205,207,207,208	0
22	CLA	b	618	65/65	0.93	0.12	205,207,208,208	0
26	LHG	a	412	39/49	0.93	0.14	205,207,208,210	0
24	BCR	B	618	40/40	0.93	0.18	204,205,207,207	0
22	CLA	C	503	65/65	0.93	0.12	205,207,207,208	0
24	BCR	C	513	40/40	0.93	0.12	205,206,207,208	0
22	CLA	H	101	65/65	0.93	0.14	205,206,207,208	0
22	CLA	b	615	65/65	0.94	0.09	205,206,207,208	0
22	CLA	C	502	65/65	0.94	0.13	205,206,207,208	0
24	BCR	f	102	40/40	0.94	0.15	206,206,207,208	0
27	LMG	d	411	46/55	0.94	0.14	204,206,207,208	0
22	CLA	A	402	65/65	0.94	0.14	205,206,207,208	0
22	CLA	D	405	65/65	0.94	0.14	205,206,207,207	0
22	CLA	B	614	65/65	0.94	0.11	205,206,207,208	0
22	CLA	B	608	65/65	0.94	0.12	205,207,208,209	0
22	CLA	C	501	65/65	0.94	0.10	205,206,207,208	0
22	CLA	d	405	65/65	0.94	0.14	204,206,207,208	0
22	CLA	b	611	65/65	0.94	0.12	205,206,207,208	0

Continued on next page...

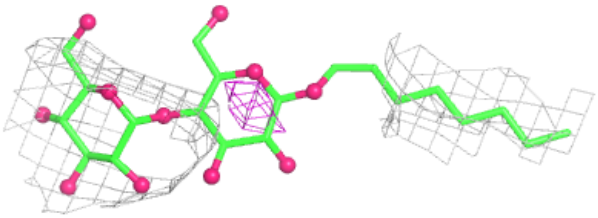
Continued from previous page...

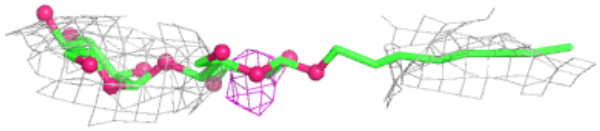
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	b	612	65/65	0.94	0.12	205,206,207,209	0
22	CLA	a	408	65/65	0.94	0.12	205,206,207,209	0
27	LMG	A	410	51/55	0.94	0.14	204,206,207,208	0
22	CLA	A	403	65/65	0.95	0.12	204,206,207,207	0
28	CL	a	413	1/1	0.95	0.14	204,204,204,204	0
22	CLA	a	404	65/65	0.95	0.10	205,206,207,208	0
34	HEM	f	101	43/43	0.95	0.12	206,207,207,208	0
34	HEM	v	201	43/43	0.95	0.12	205,207,207,208	0
22	CLA	B	610	65/65	0.95	0.09	205,206,207,207	0
22	CLA	B	606	65/65	0.95	0.12	205,206,207,208	0
22	CLA	c	507	65/65	0.95	0.10	205,207,208,208	0
22	CLA	C	507	65/65	0.95	0.14	205,206,208,210	0
33	BCT	D	403	4/4	0.96	0.06	206,206,206,206	0
21	FE2	A	401	1/1	0.96	0.07	206,206,206,206	0
34	HEM	F	101	43/43	0.96	0.10	205,207,208,209	0
34	HEM	V	201	43/43	0.96	0.16	203,206,207,208	0
22	CLA	B	612	65/65	0.96	0.10	204,206,207,207	0
22	CLA	b	616	65/65	0.97	0.17	204,206,208,209	0
22	CLA	b	614	65/65	0.97	0.12	205,206,207,208	0
29	OEX	A	412	10/10	0.98	0.07	198,204,206,206	0
29	OEX	a	414	10/10	0.98	0.08	198,203,205,207	0

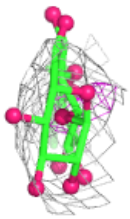
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

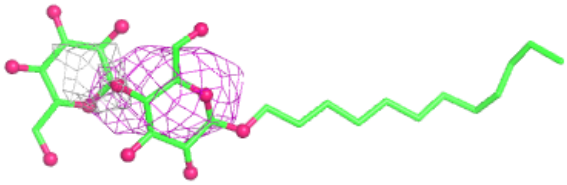


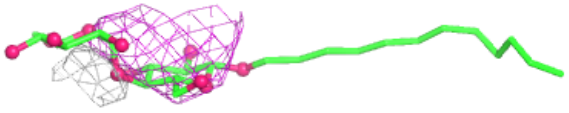


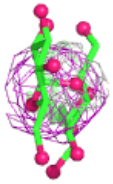


Electron density around LMT i 102:

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

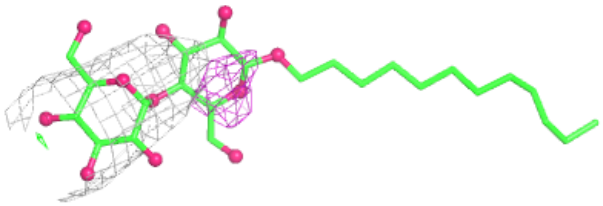


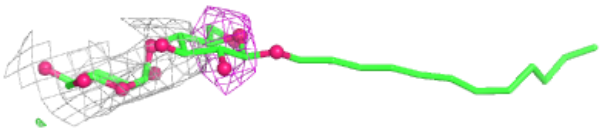


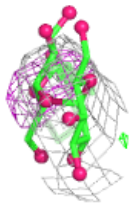


Electron density around LMT I 102:

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

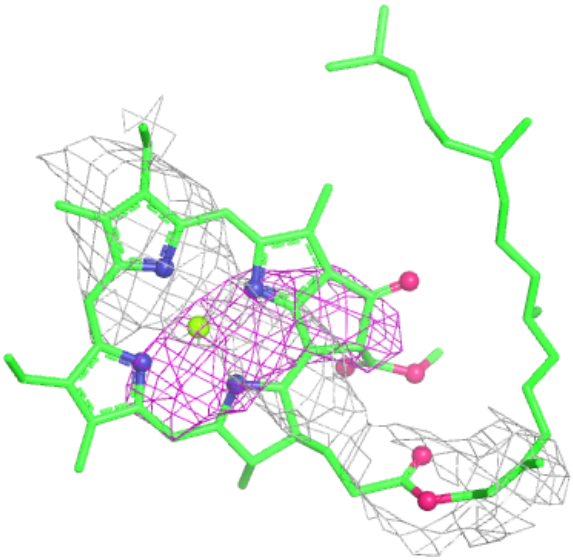


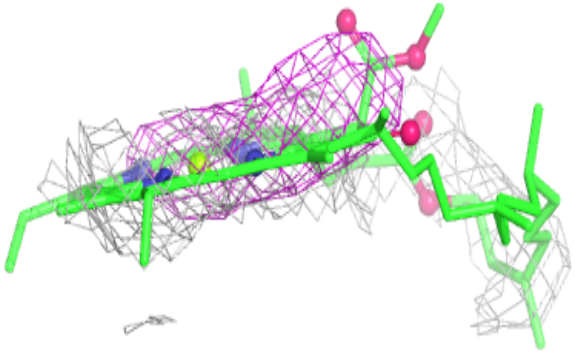


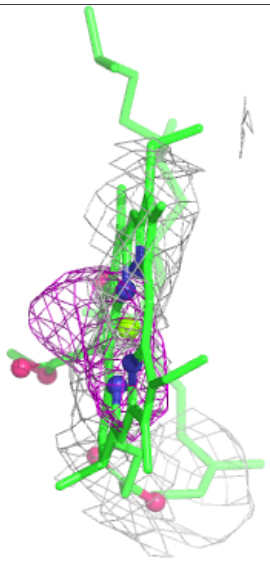


Electron density around CLA b 605:

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

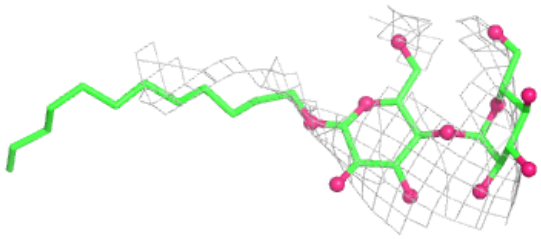


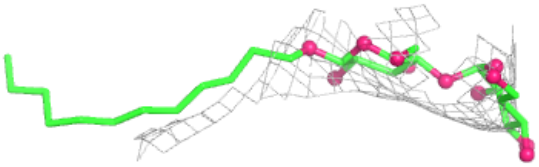


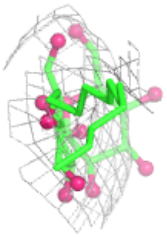


Electron density around LMT B 623:

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

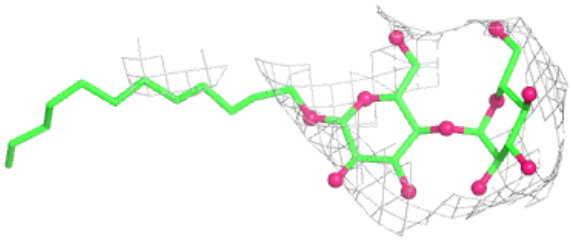


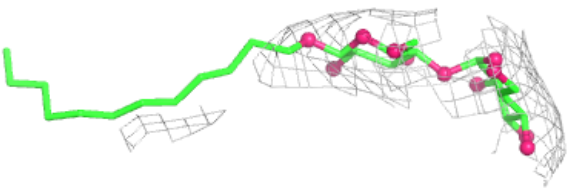


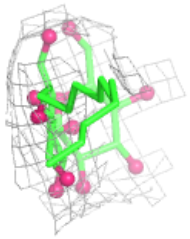


Electron density around LMT b 626:

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

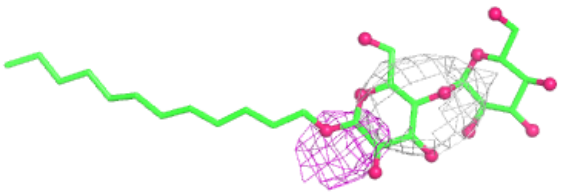


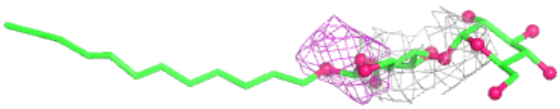




Electron density around LMT b 627:

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

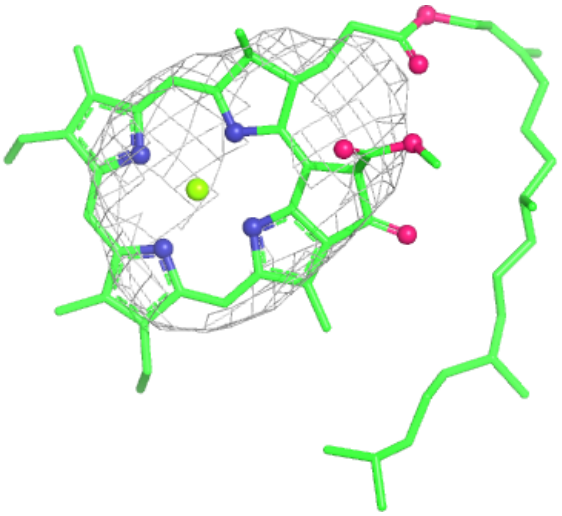


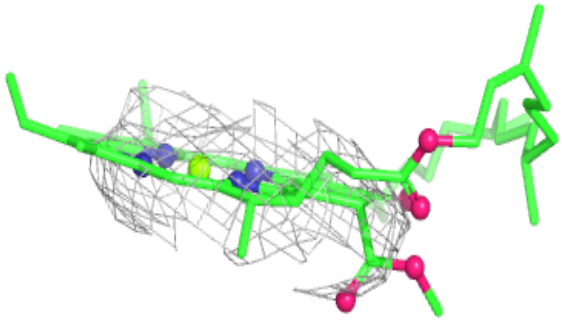


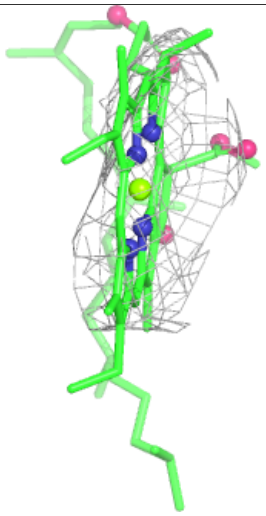


Electron density around CLA B 601:

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

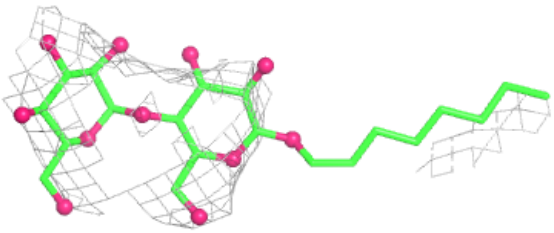


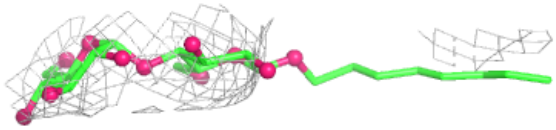


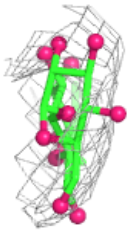


Electron density around LMT D 410:

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

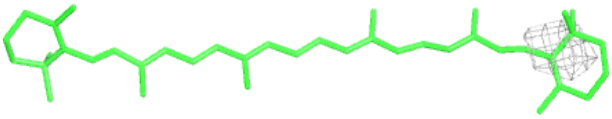


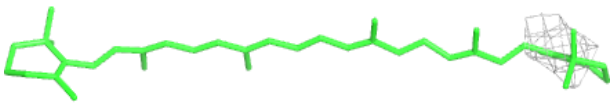


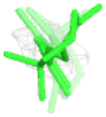


Electron density around BCR J 102:

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

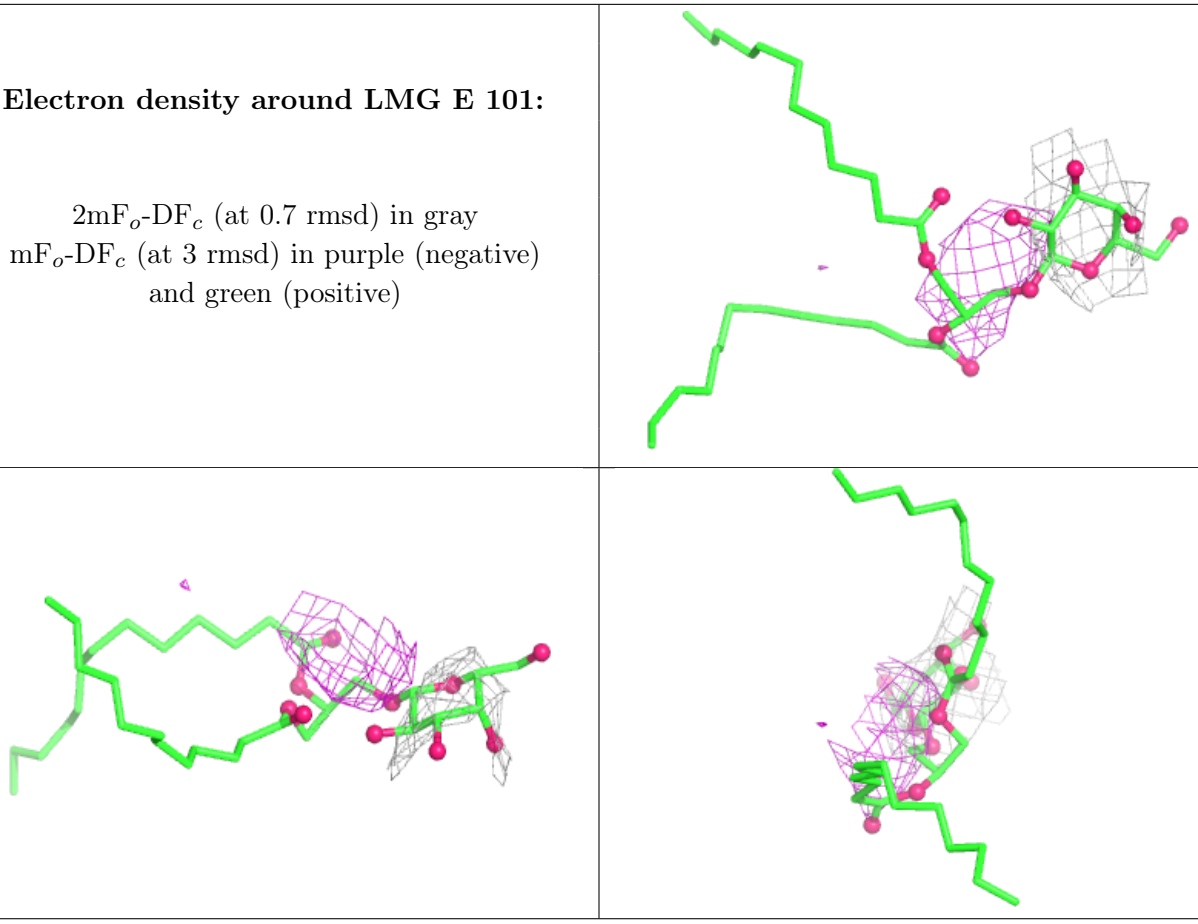






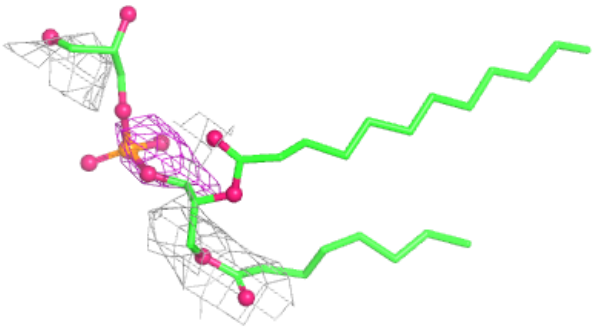
Electron density around LMG E 101:

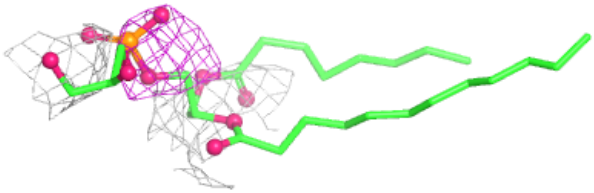
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

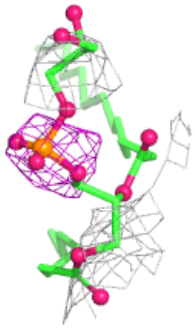


Electron density around LHG c 519:

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

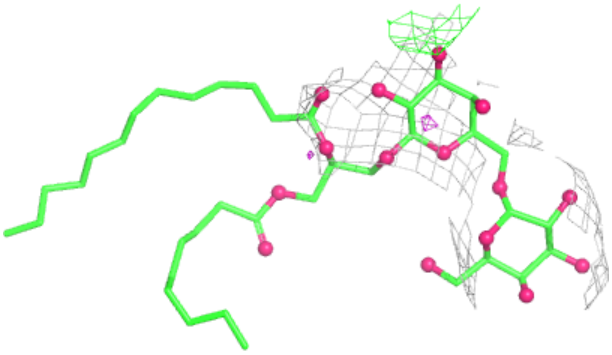


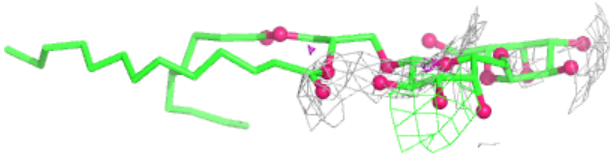


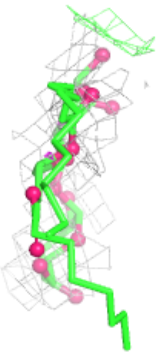


Electron density around DGD B 625:

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

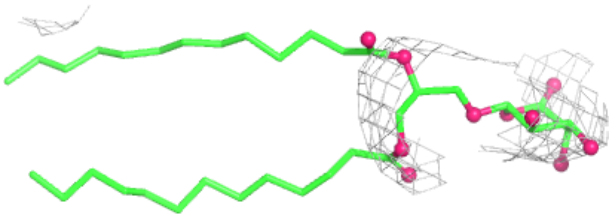


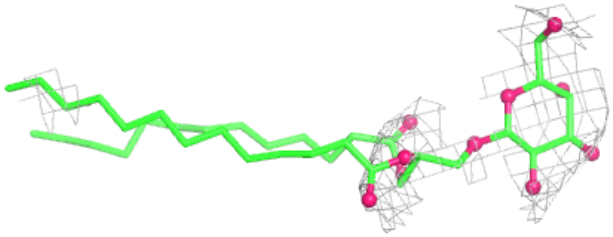


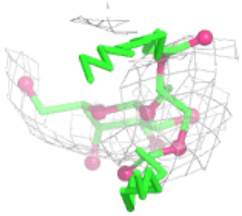


Electron density around LMG c 518:

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

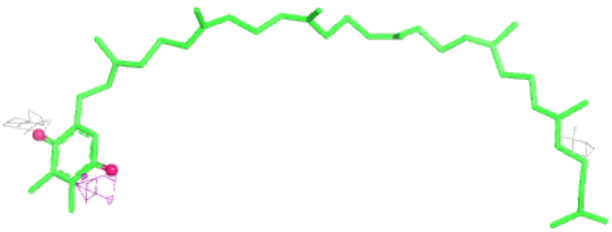


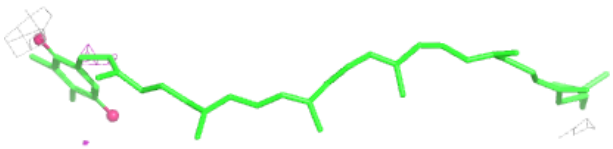


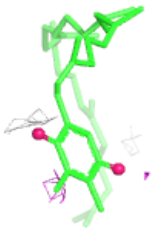


Electron density around PL9 A 406:

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

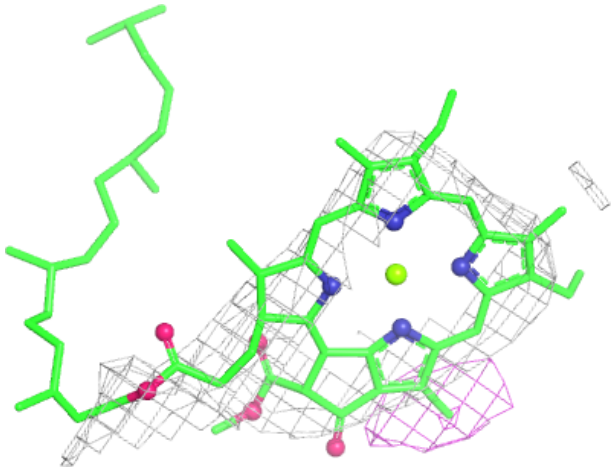


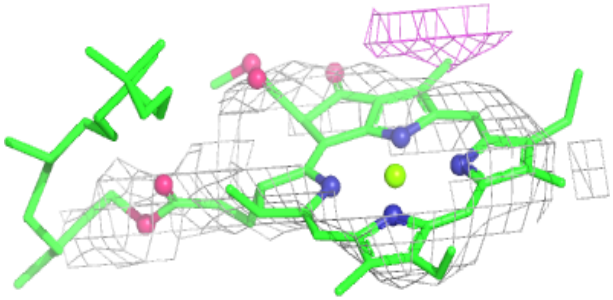


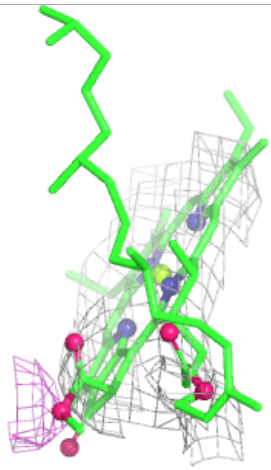


Electron density around CLA b 619:

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

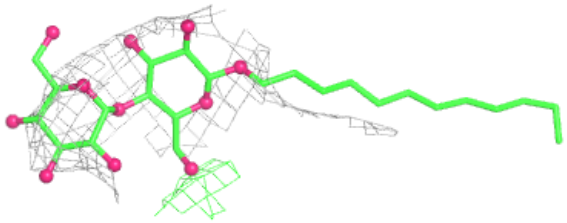


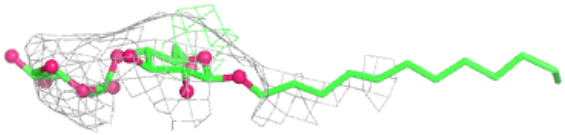


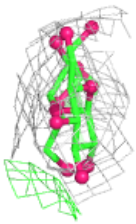


Electron density around LMT b 603:

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

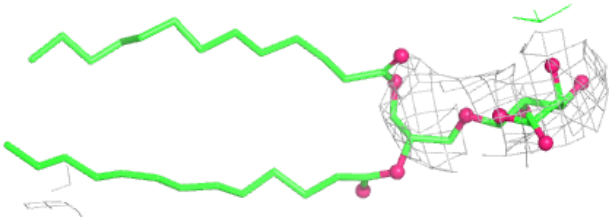


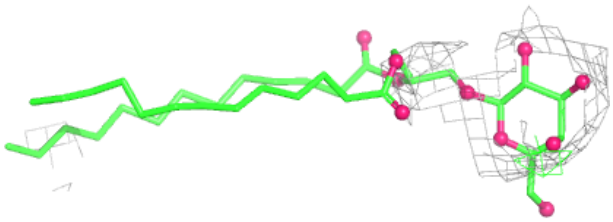


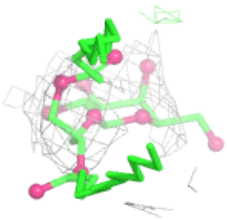


Electron density around LMG C 518:

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

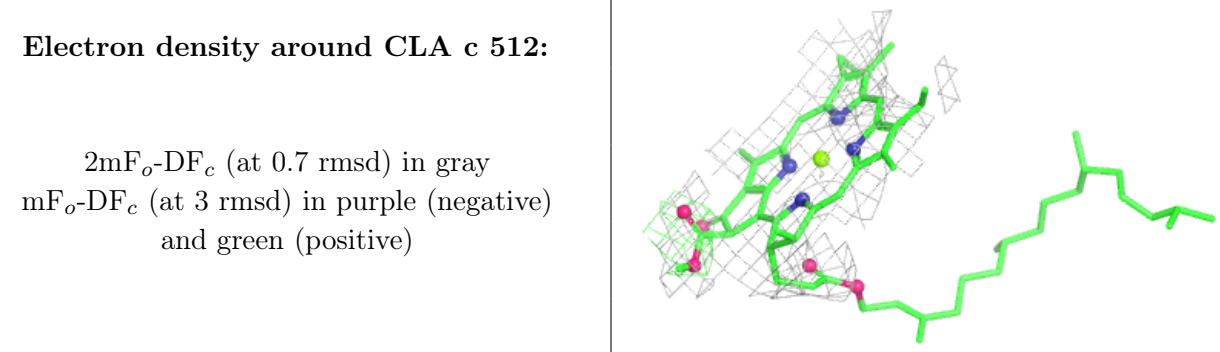


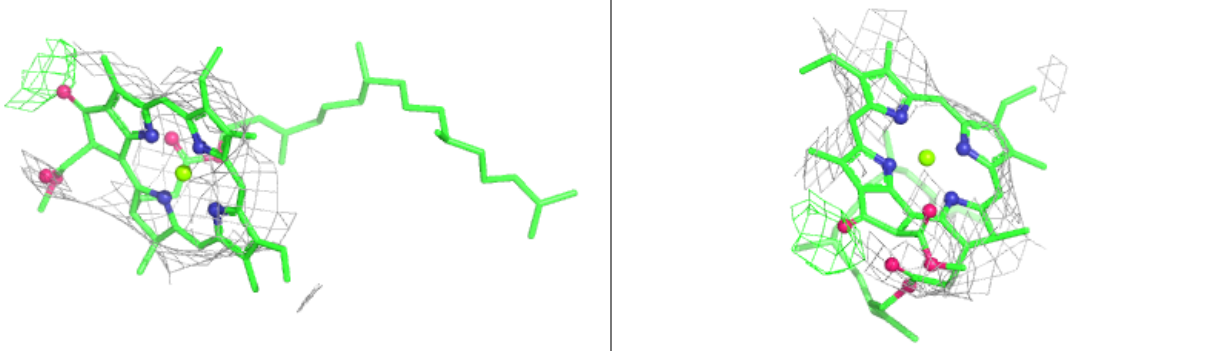




Electron density around CLA c 512:

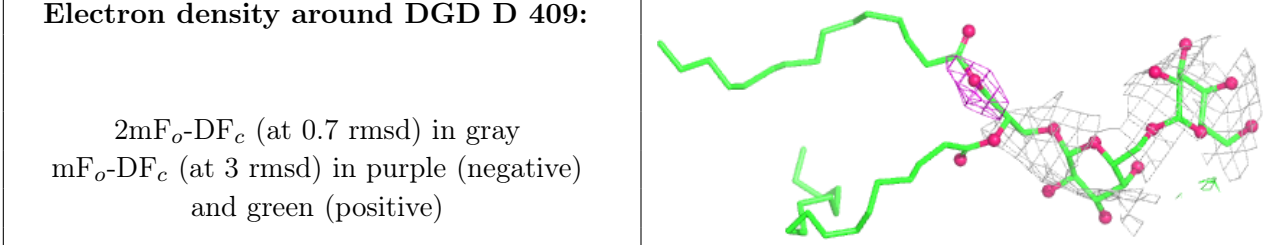
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

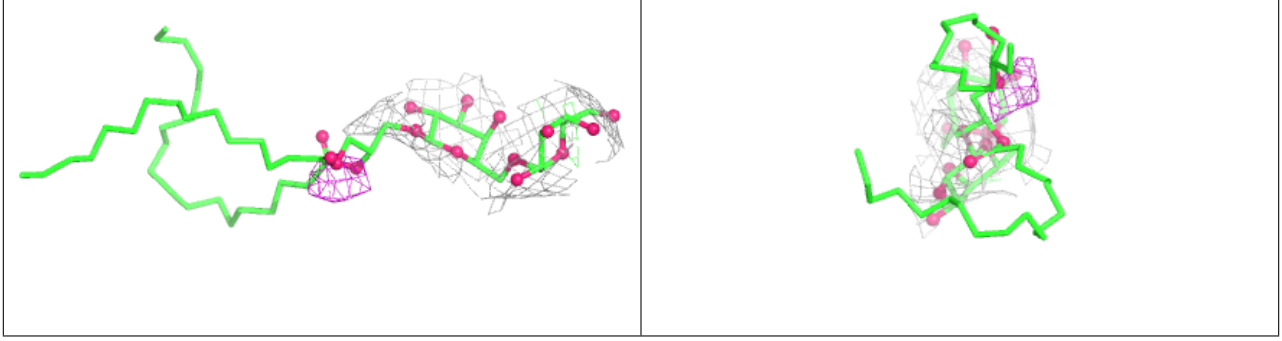




Electron density around DGD D 409:

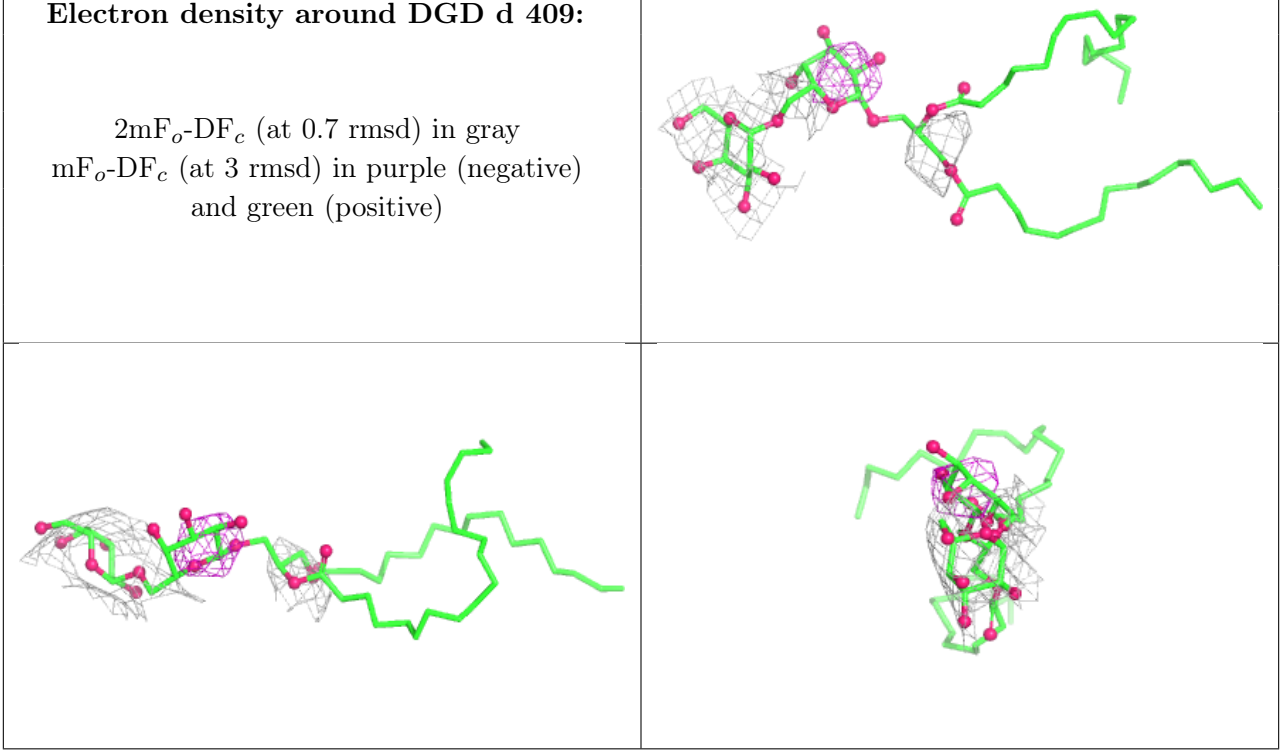
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





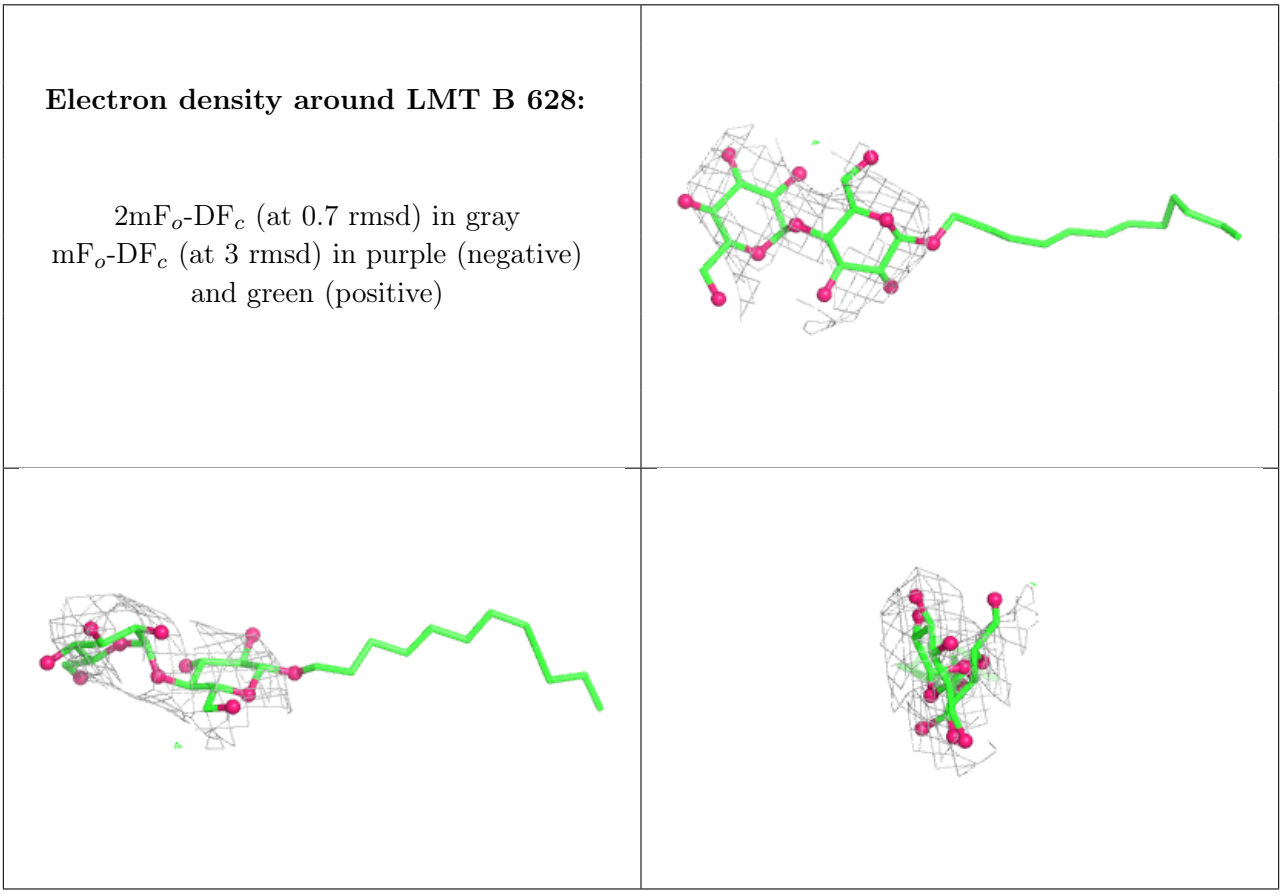
Electron density around DGD d 409:

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



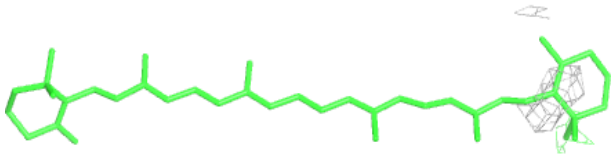
Electron density around LMT B 628:

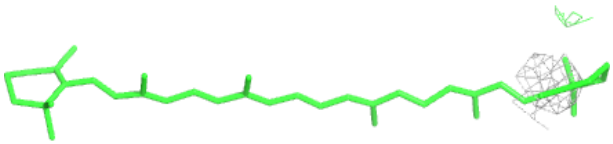
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

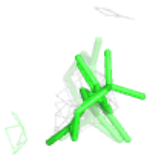


Electron density around BCR j 102:

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

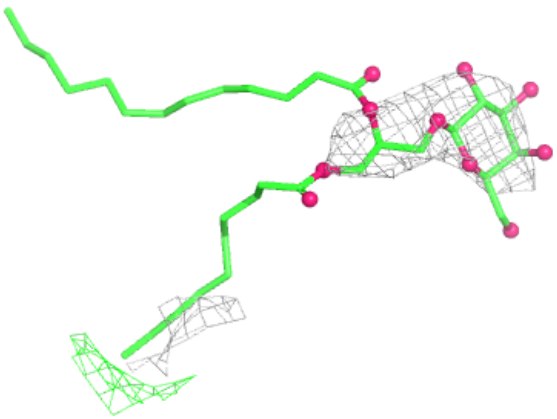


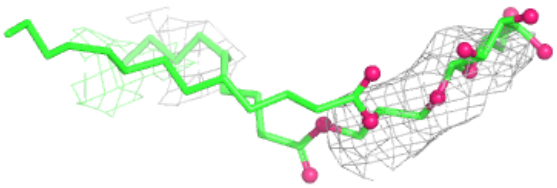


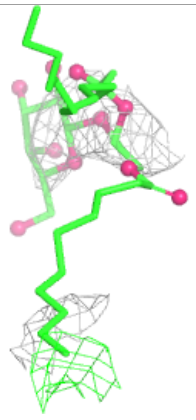


Electron density around LMG A 415:

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

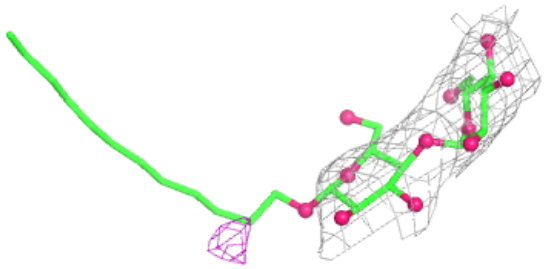


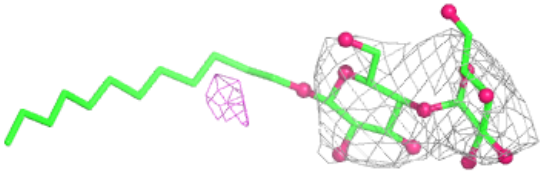




Electron density around LMT M 102:

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

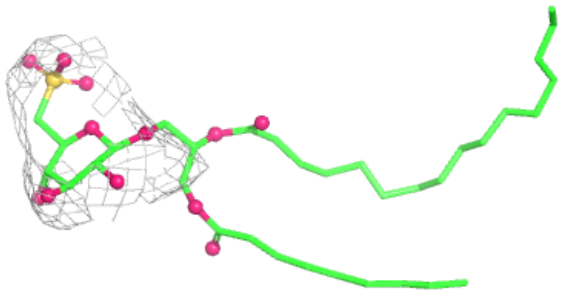


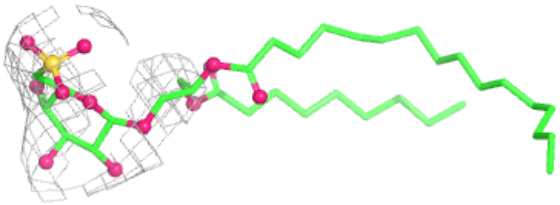


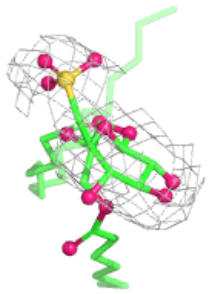


Electron density around SQD B 626:

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

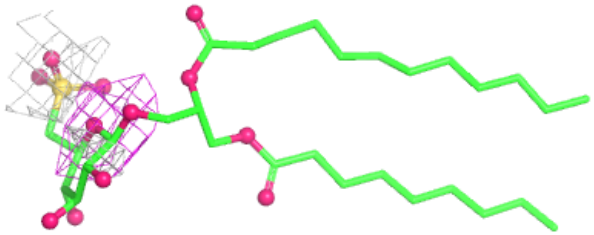


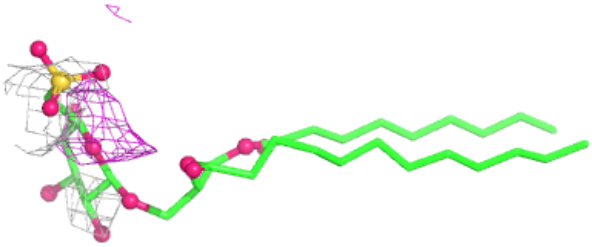


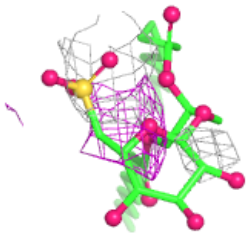


Electron density around SQD d 402:

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

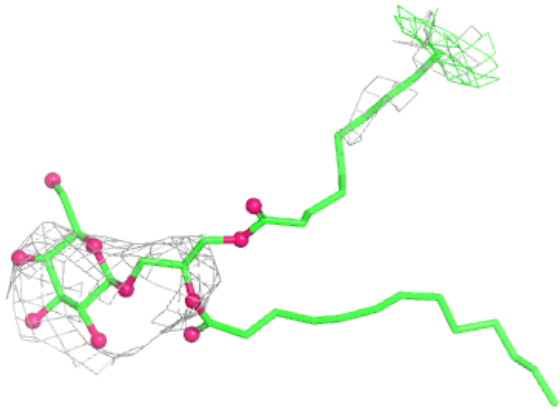


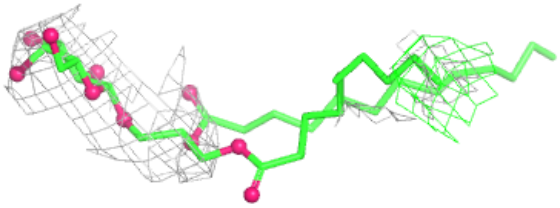


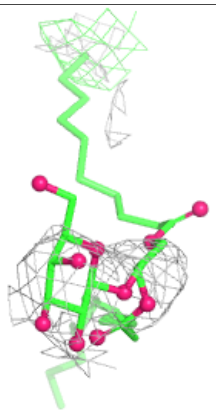


Electron density around LMG a 402:

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

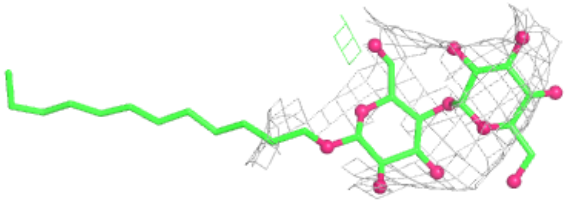


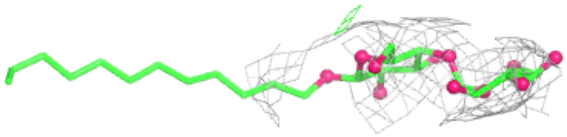




Electron density around LMT B 627:

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



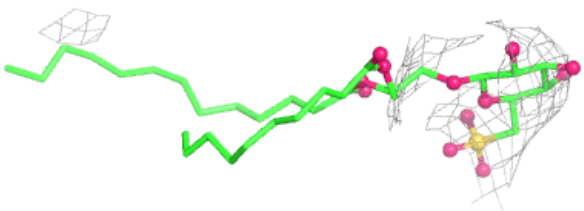


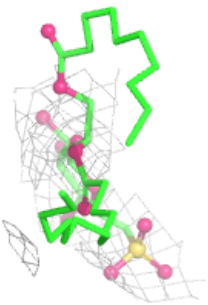


Electron density around SQD F 103:

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

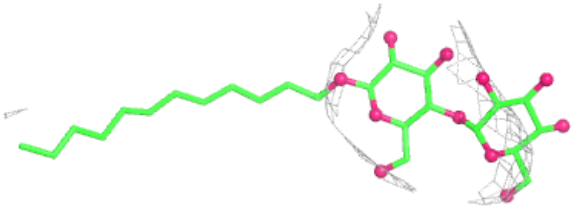


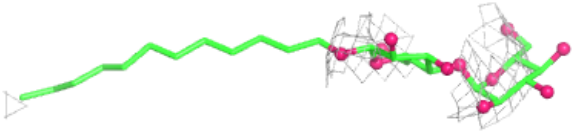


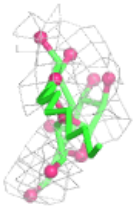


Electron density around LMT B 624:

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

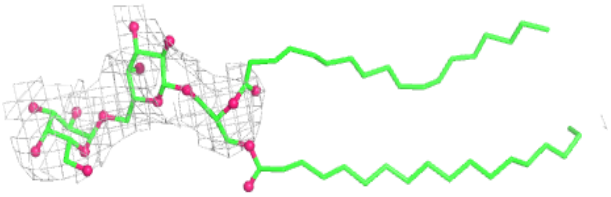


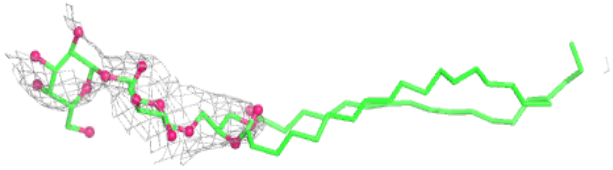


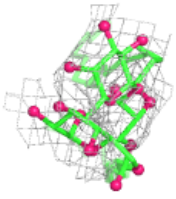


Electron density around DGD C 517:

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

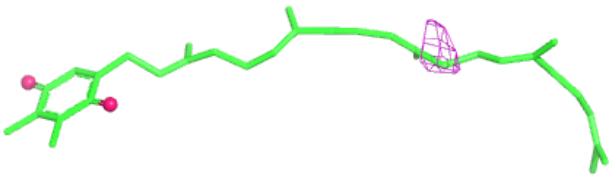


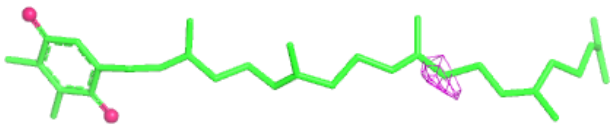


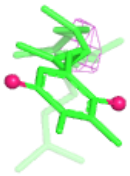


Electron density around PL9 J 101:

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

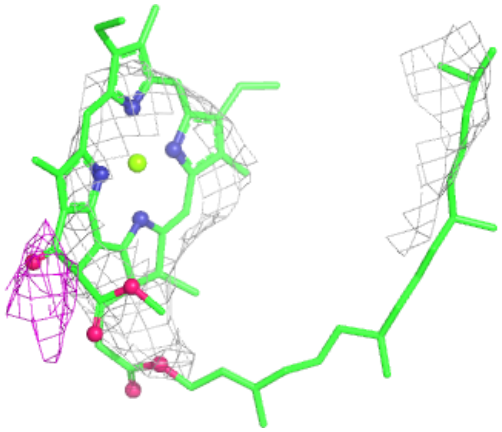


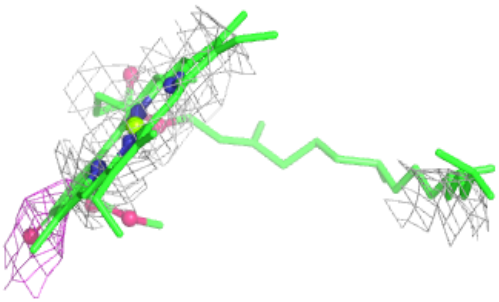


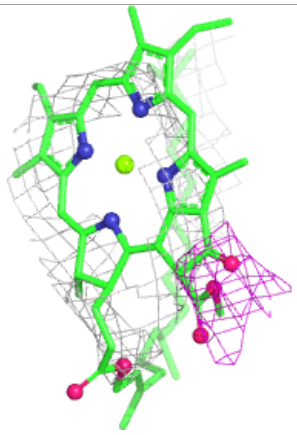


Electron density around CLA C 506:

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

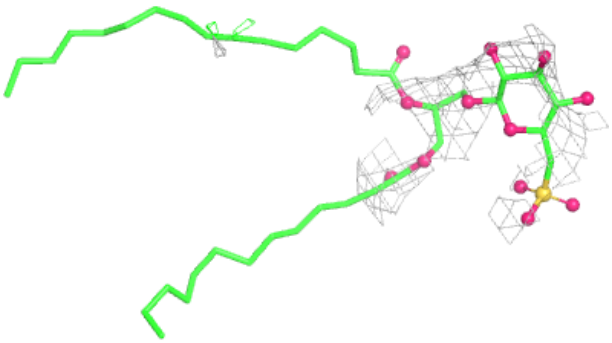


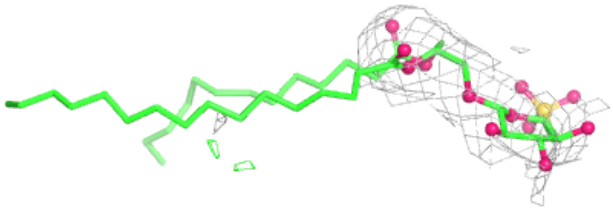


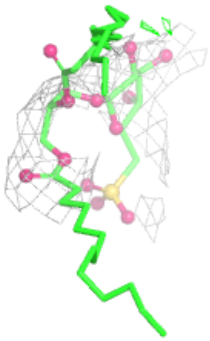


Electron density around SQD A 413:

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

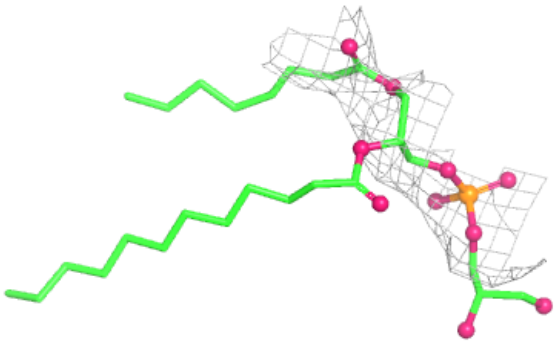


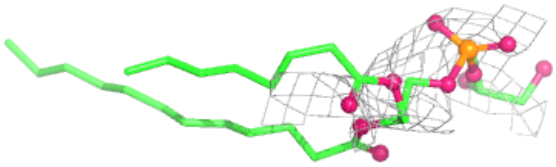


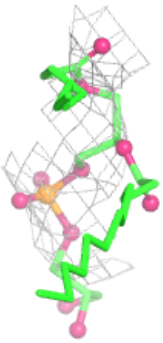


Electron density around LHG C 519:

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



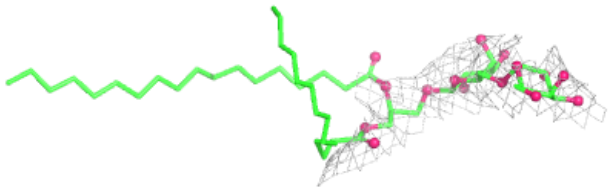




Electron density around DGD C 516:

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

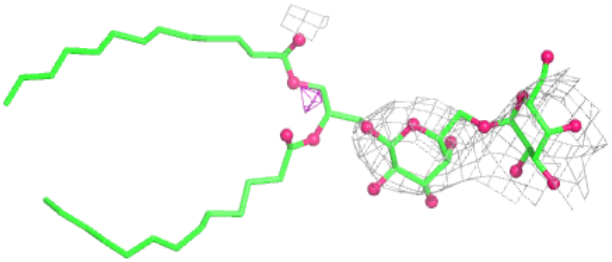


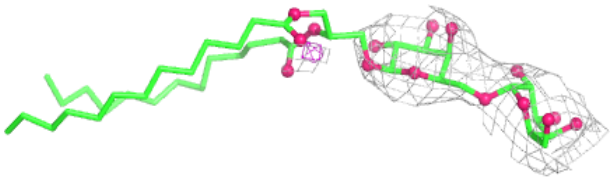


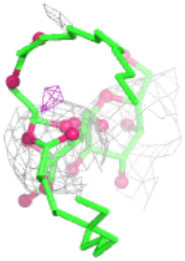


Electron density around DGD A 408:

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

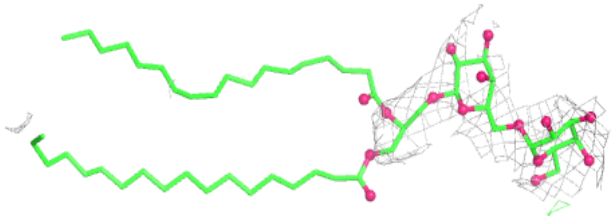


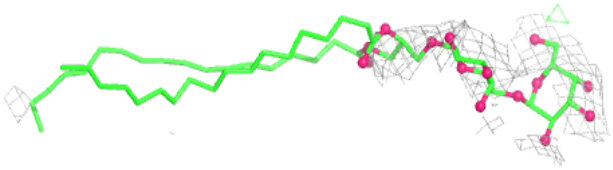


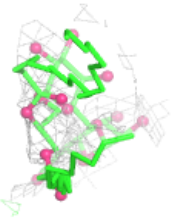


Electron density around DGD c 517:

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

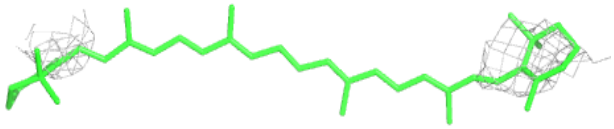


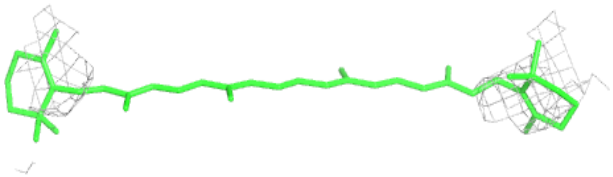


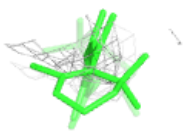


Electron density around BCR c 521:

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

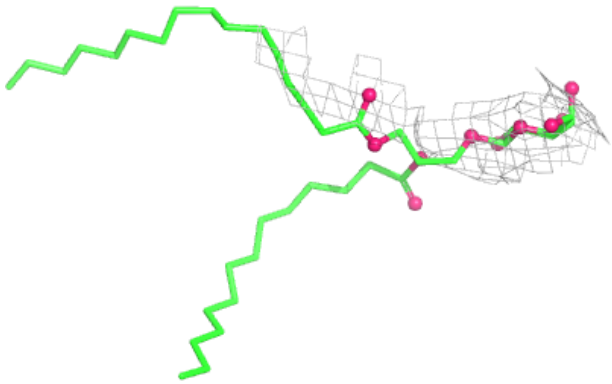


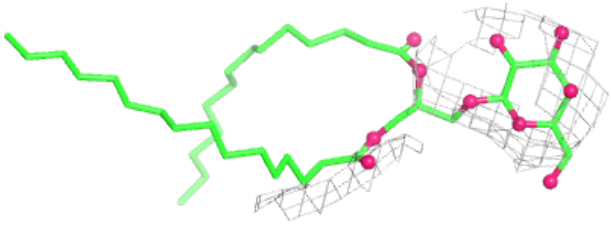


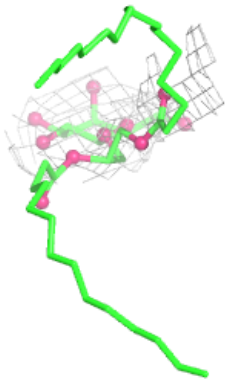


Electron density around LMG b 625:

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

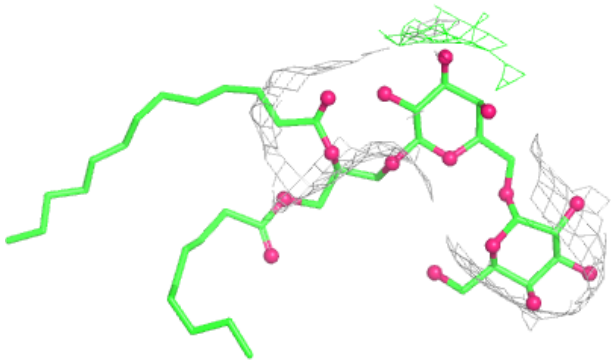


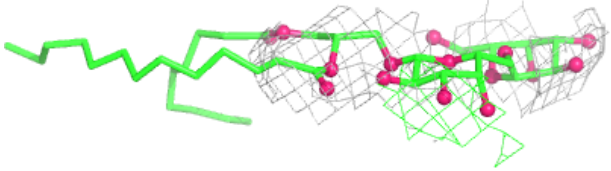


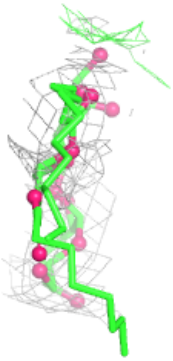


Electron density around DGD b 601:

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

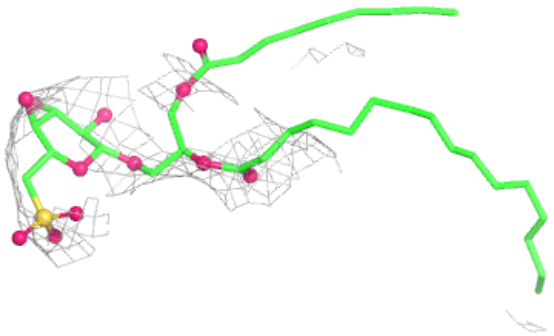


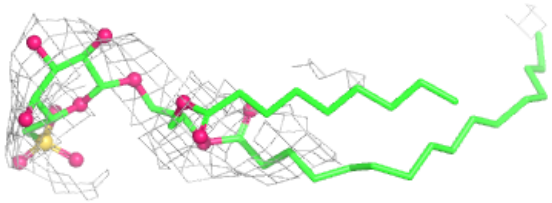


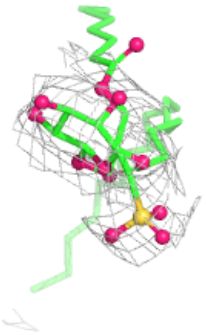


Electron density around SQD b 602:

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

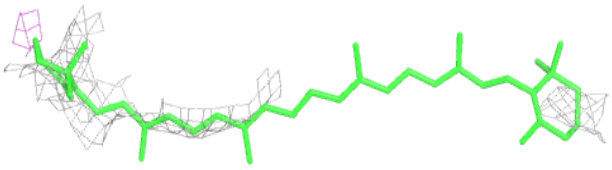


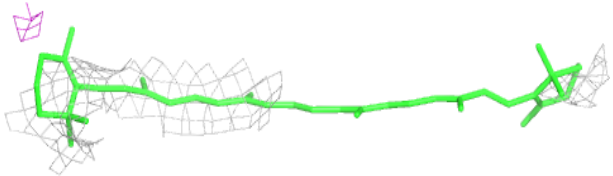


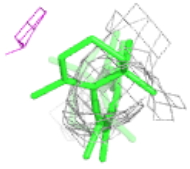


Electron density around BCR H 102:

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

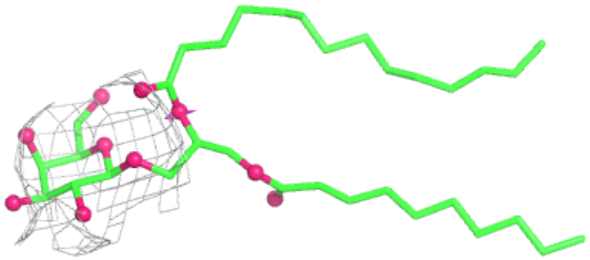


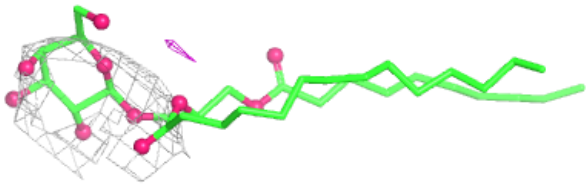


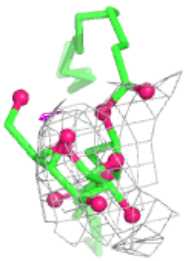


Electron density around LMG I 101:

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

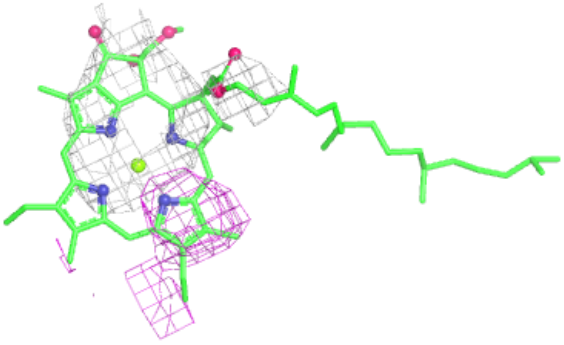


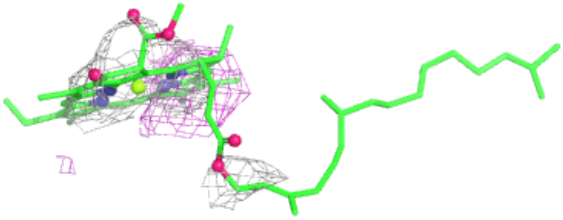


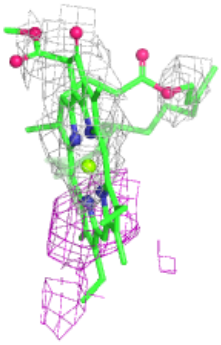


Electron density around CLA a 406:

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

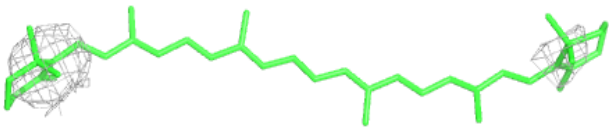


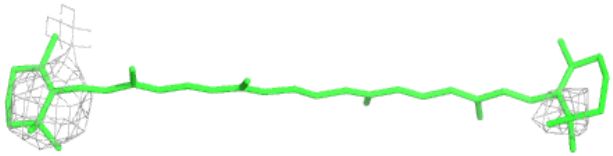


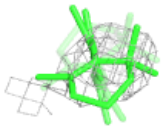


Electron density around BCR a 410:

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

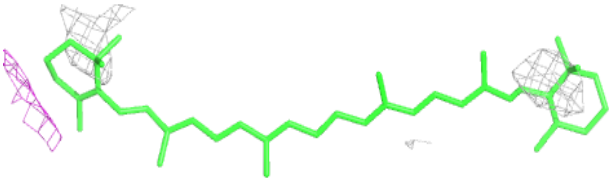


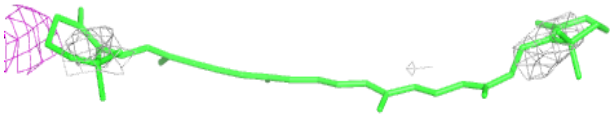


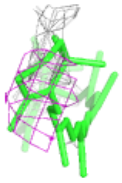


Electron density around BCR b 621:

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

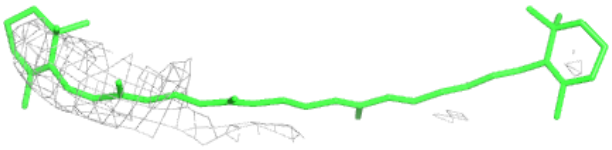


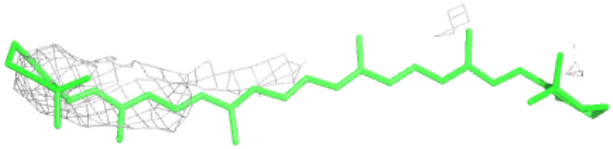


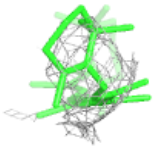


Electron density around BCR c 513:

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

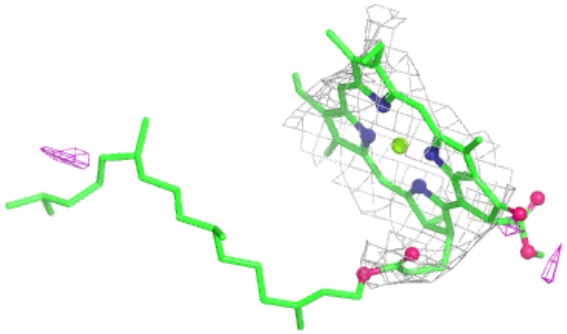


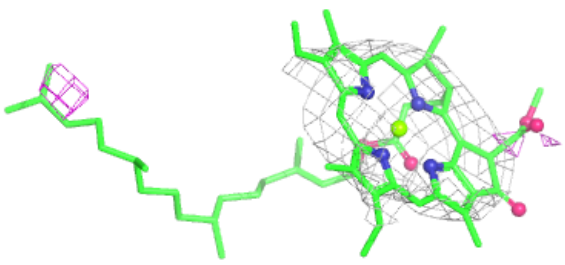


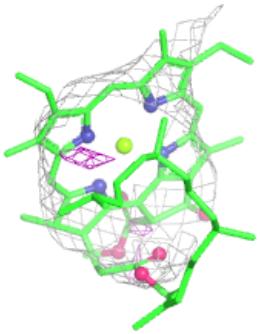


Electron density around CLA C 512:

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



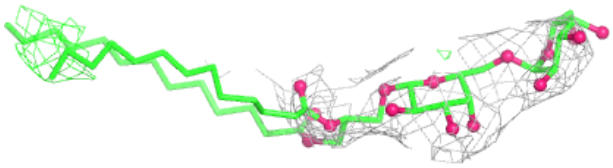




Electron density around DGD a 411:

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

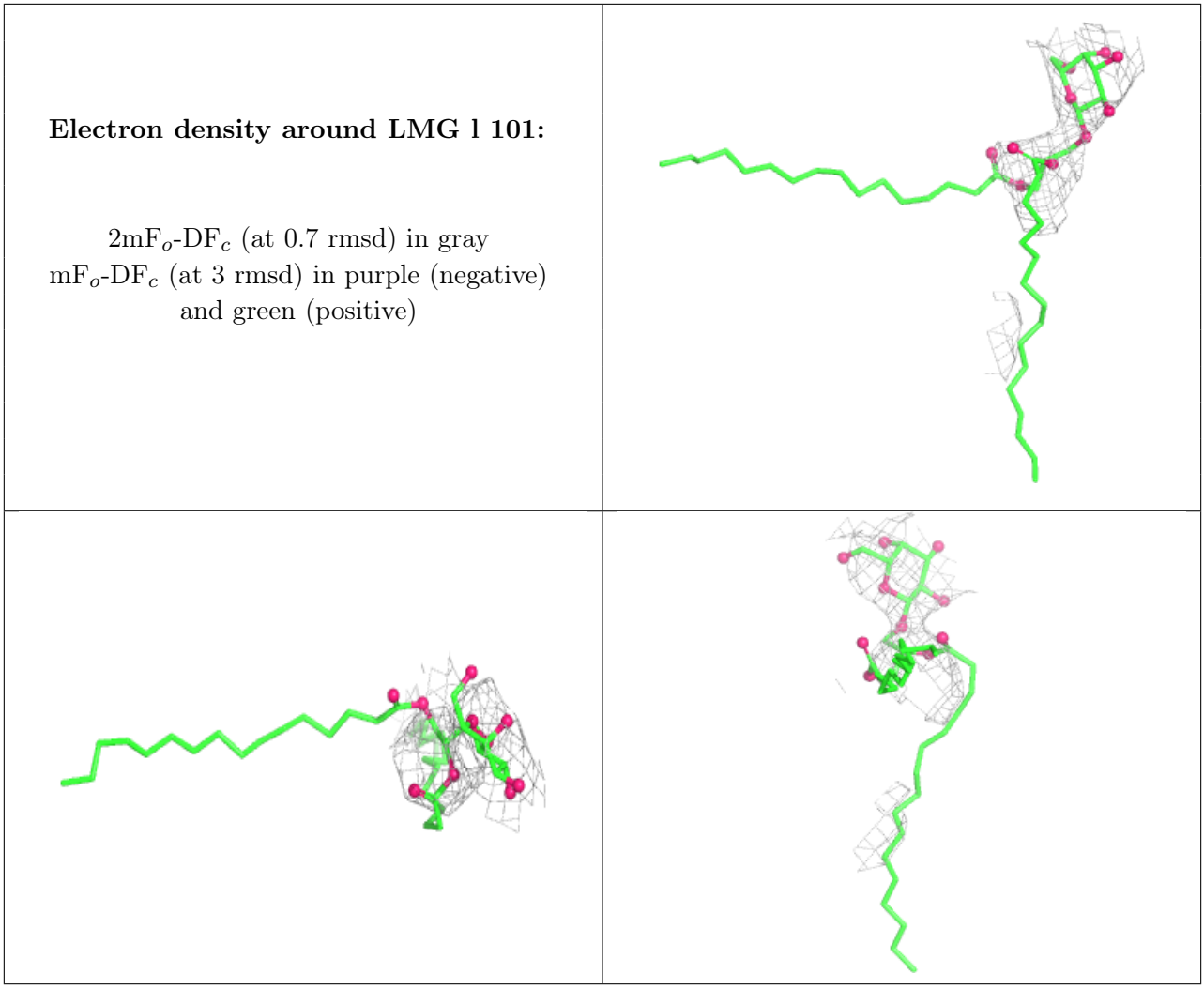






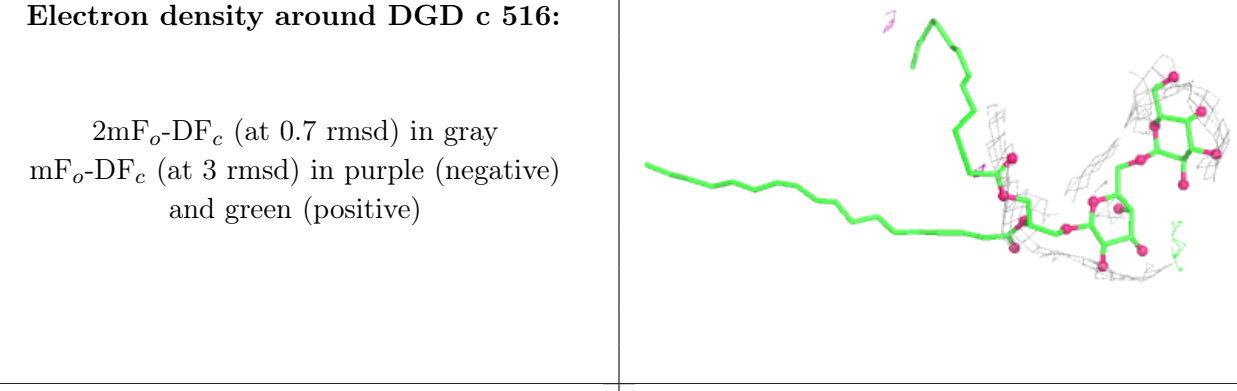
Electron density around LMG l 101:

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



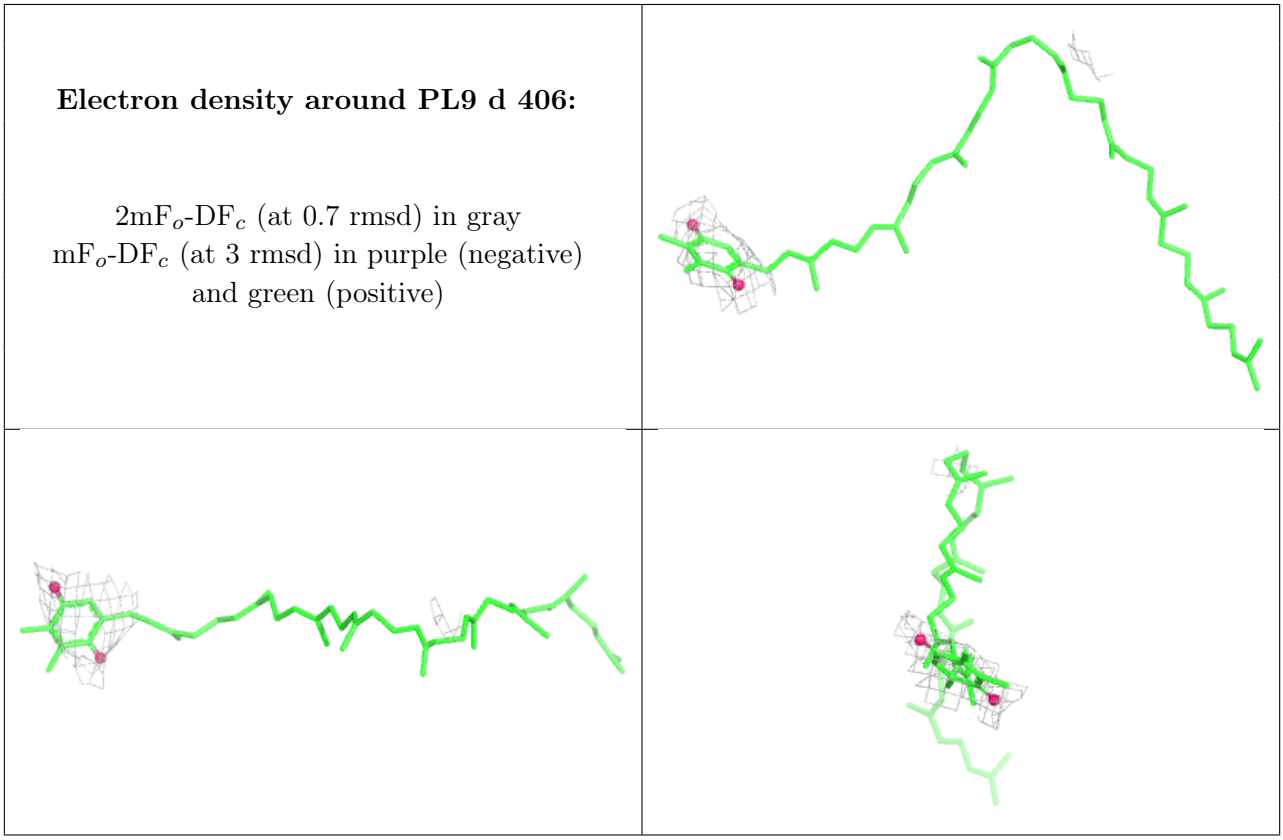
Electron density around DGD c 516:

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



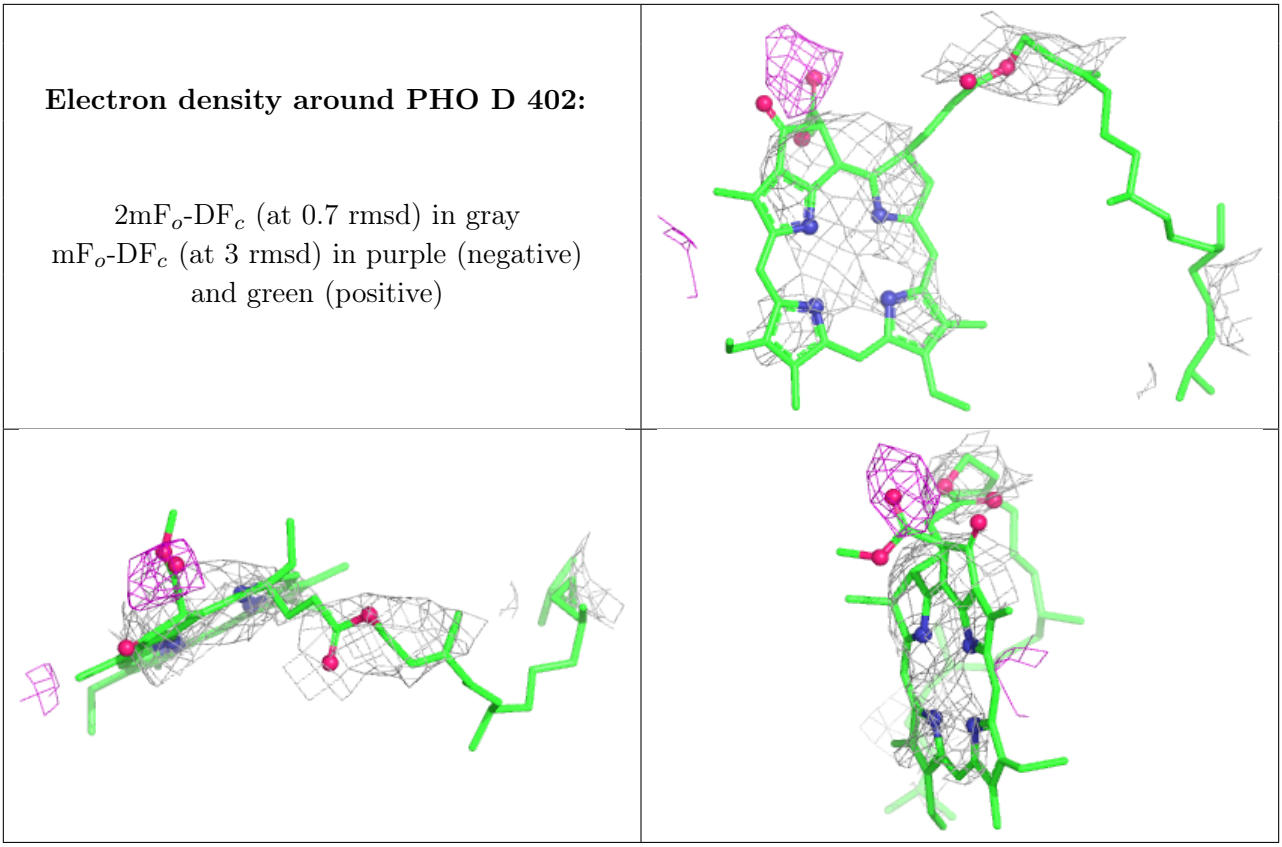
Electron density around PL9 d 406:

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



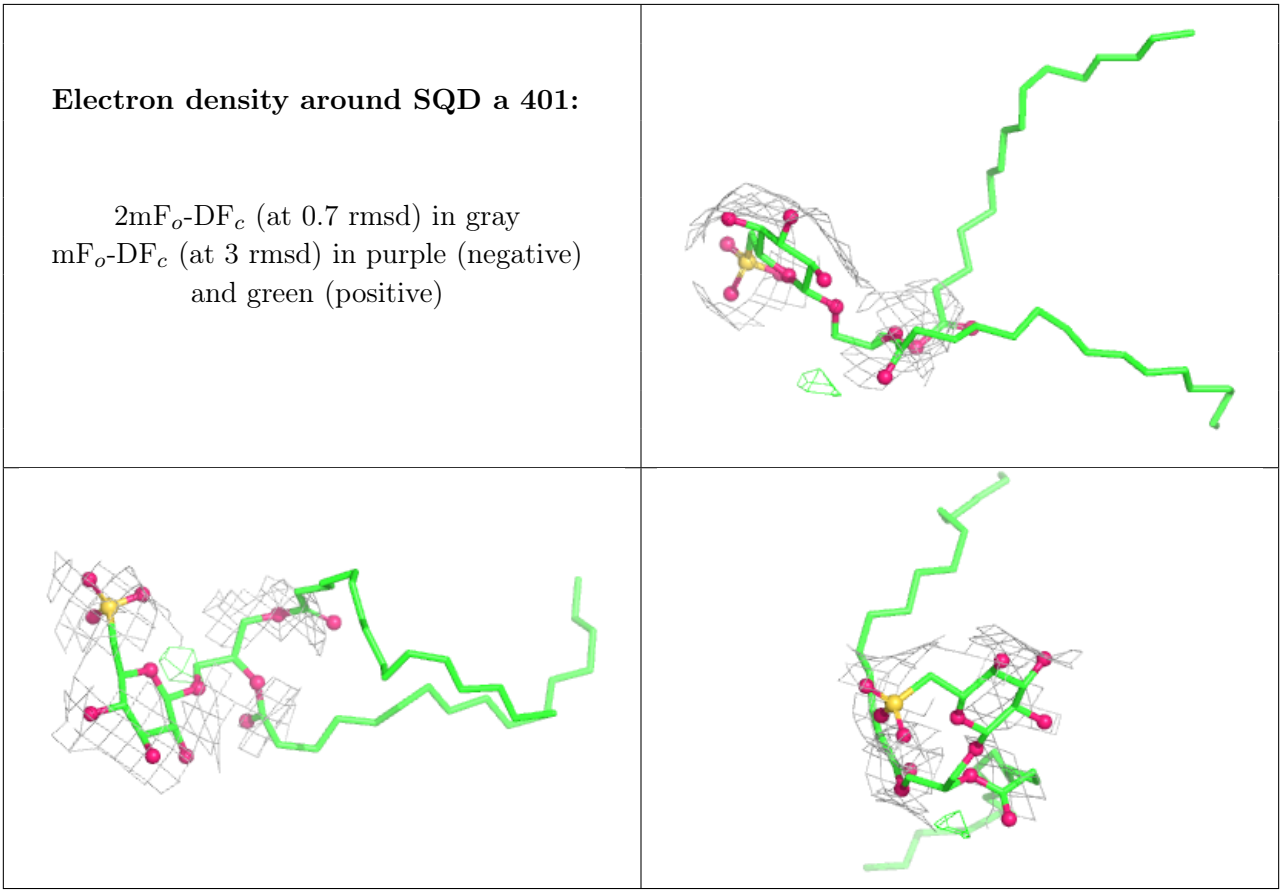
Electron density around PHO D 402:

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



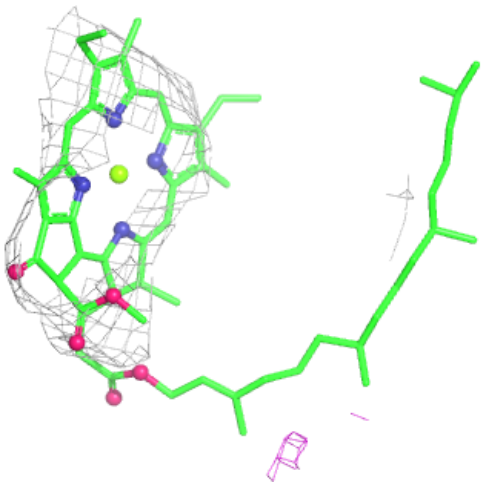
Electron density around SQD a 401:

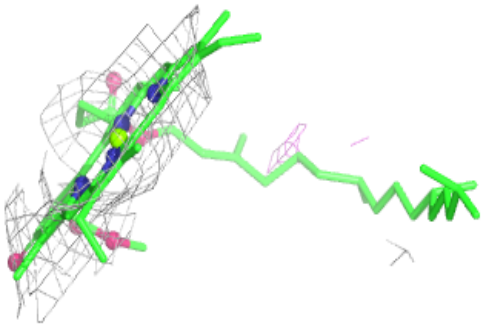
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

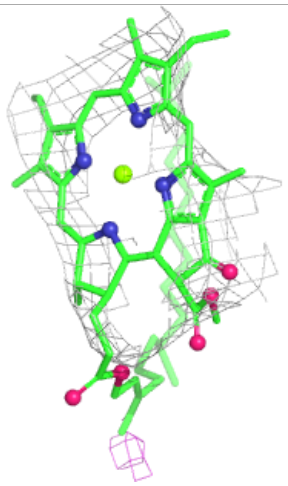


Electron density around CLA c 506:

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

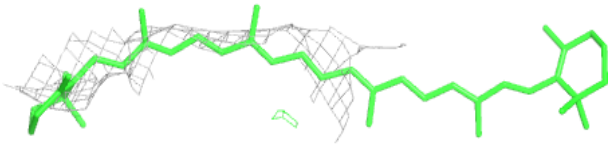


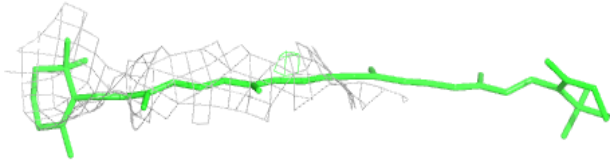


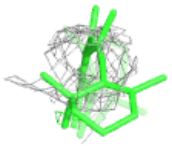


Electron density around BCR x 101:

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

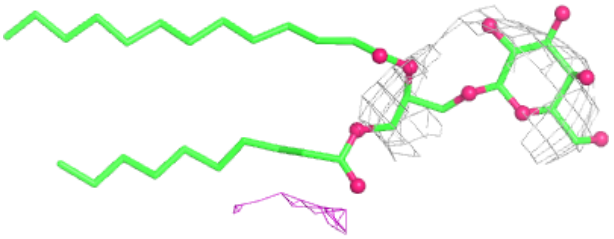


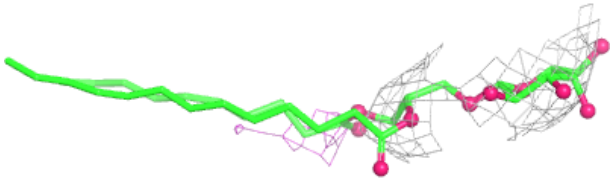


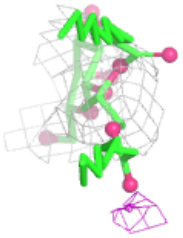


Electron density around LMG m 101:

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

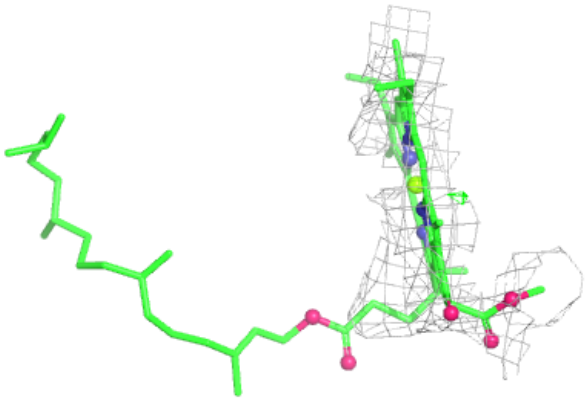


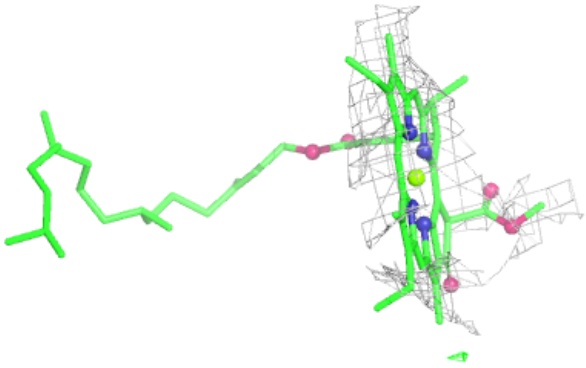


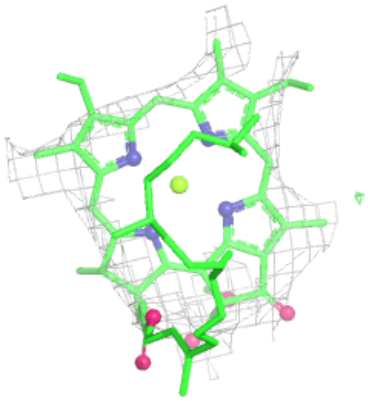


Electron density around CLA c 505:

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

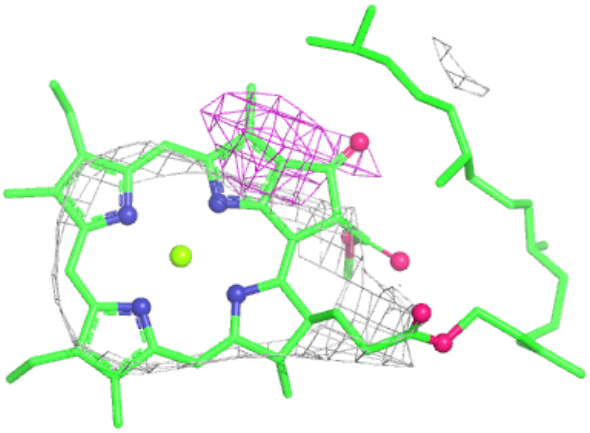


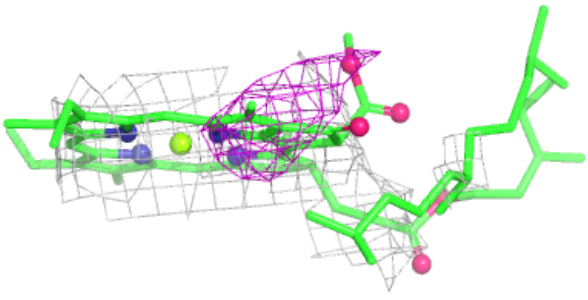


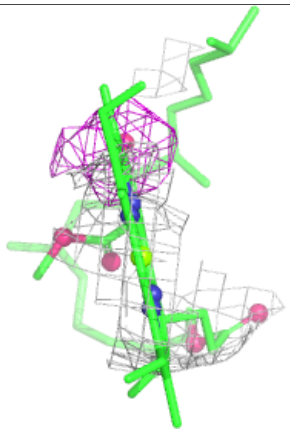


Electron density around CLA b 613:

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

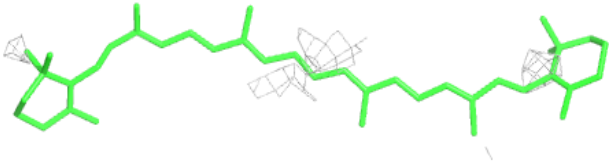




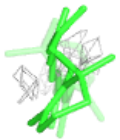


Electron density around BCR g 101:

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

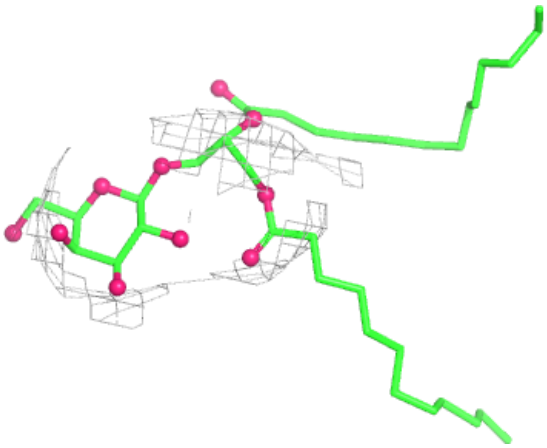


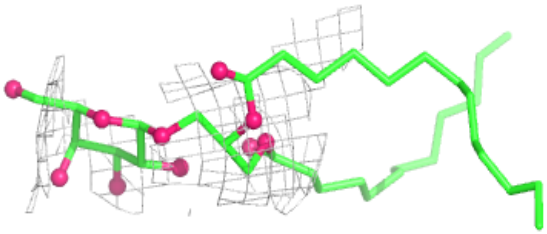


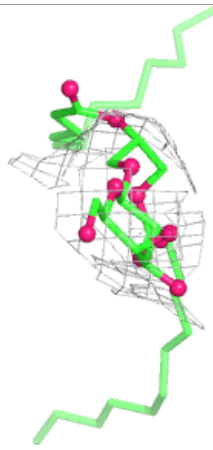


Electron density around LMG e 101:

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

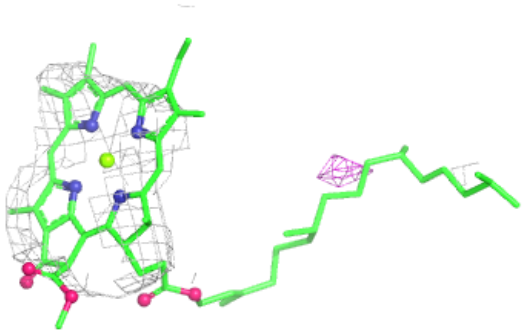


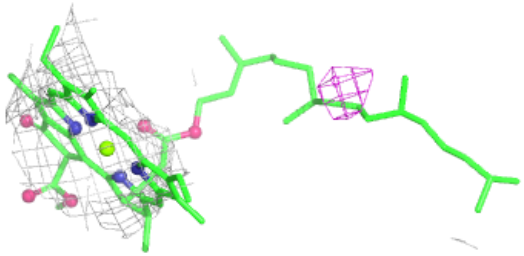


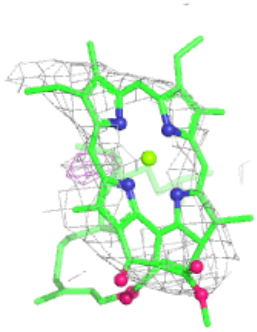


Electron density around CLA c 510:

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

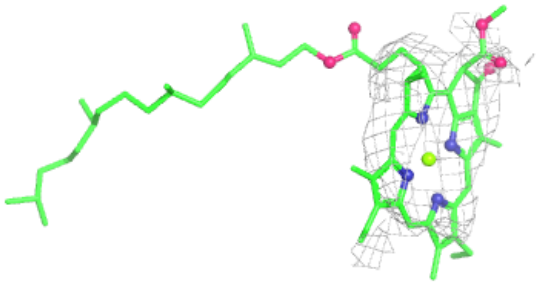


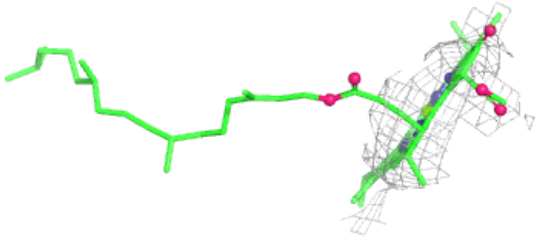




Electron density around CLA A 405:

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

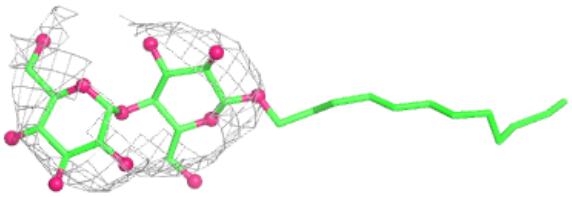


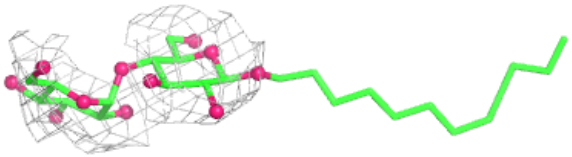


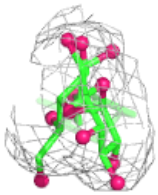


Electron density around LMT b 604:

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

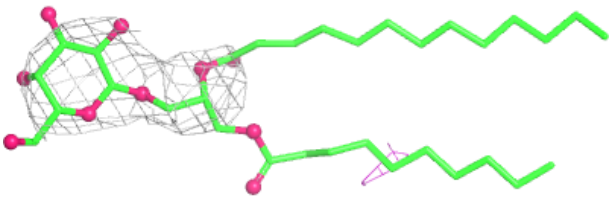


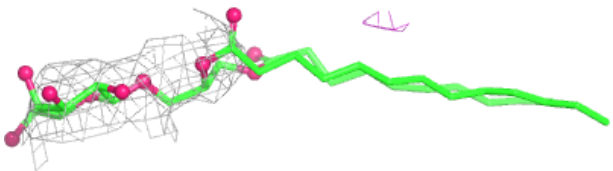


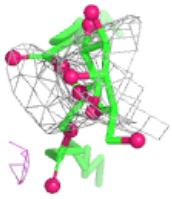


Electron density around LMG M 101:

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

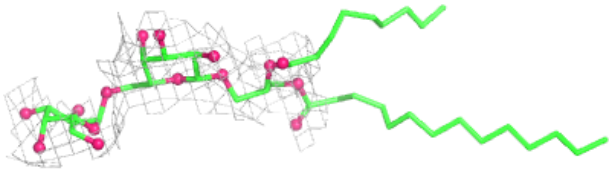


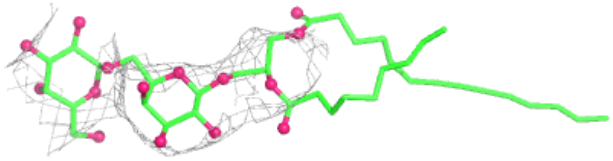


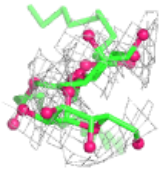


Electron density around DGD C 515:

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

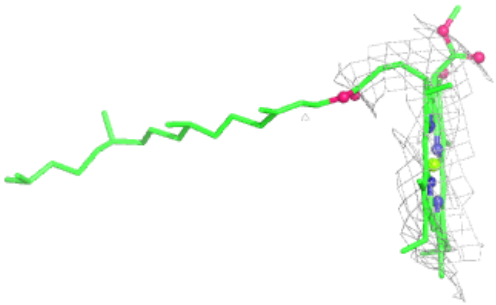


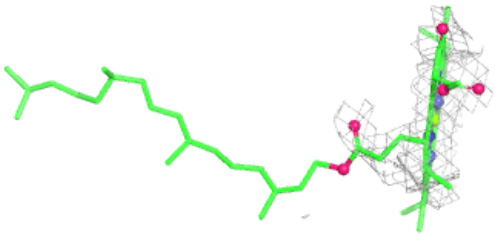


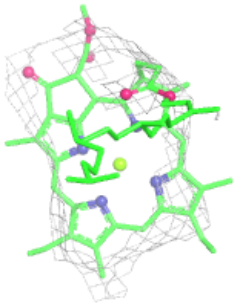


Electron density around CLA B 605:

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

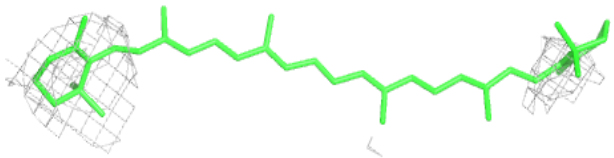


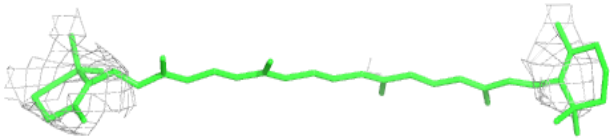


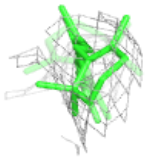


Electron density around BCR K 102:

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

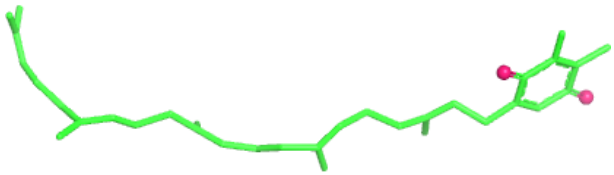


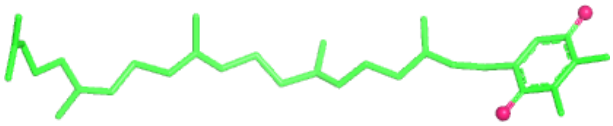


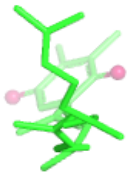


Electron density around PL9 j 101:

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

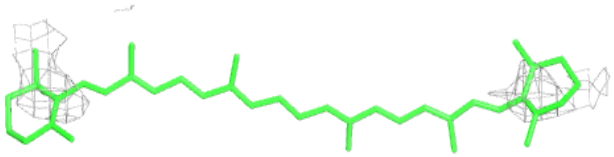


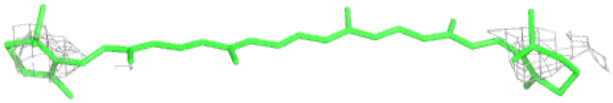


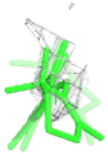


Electron density around BCR C 514:

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

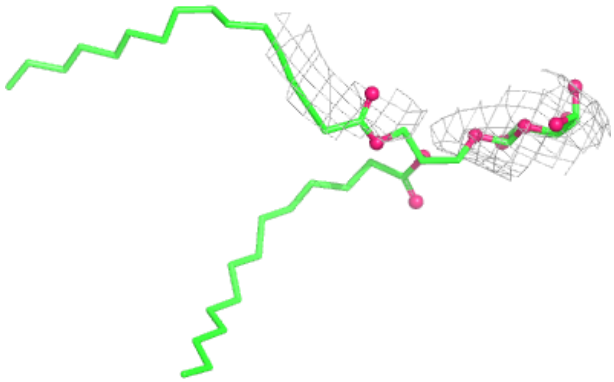


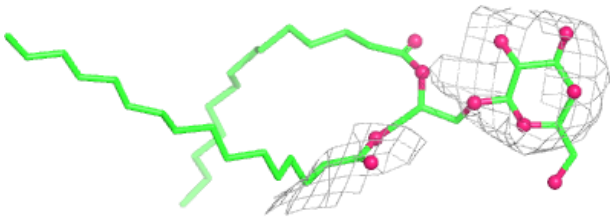


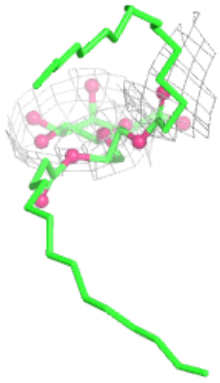


Electron density around LMG B 621:

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

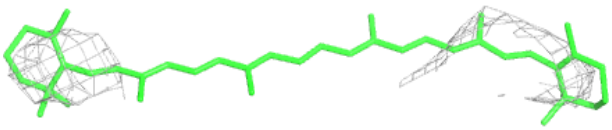


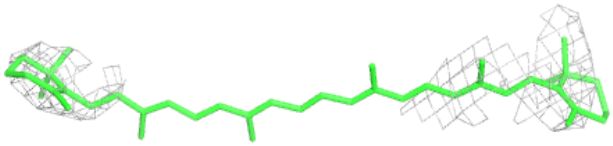


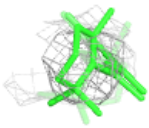


Electron density around BCR b 623:

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



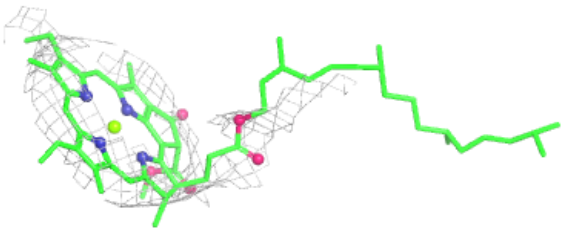


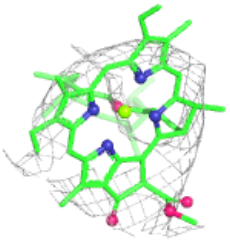


Electron density around CLA c 502:

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

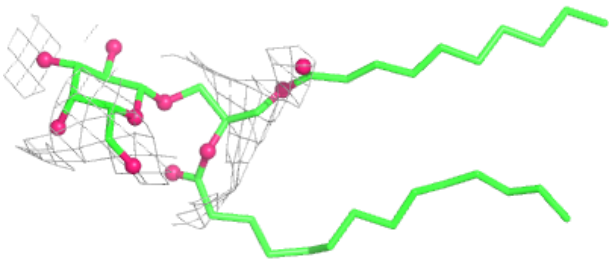


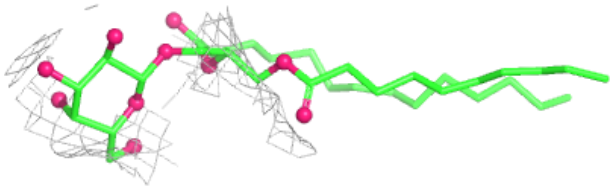


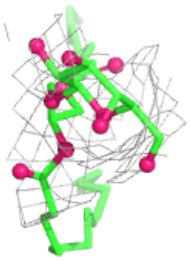


Electron density around LMG i 101:

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

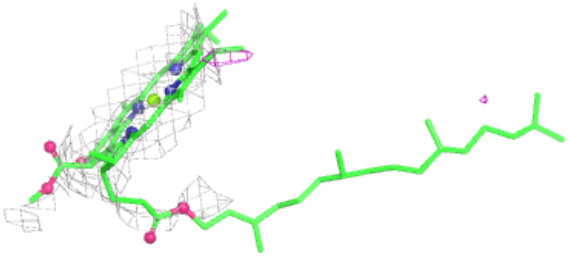


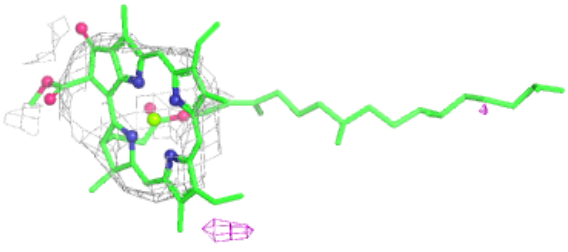


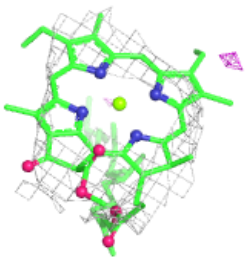


Electron density around CLA C 520:

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

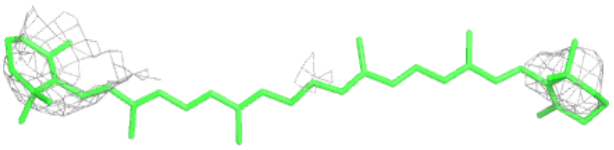




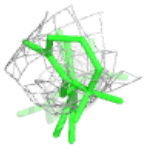


Electron density around BCR b 622:

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

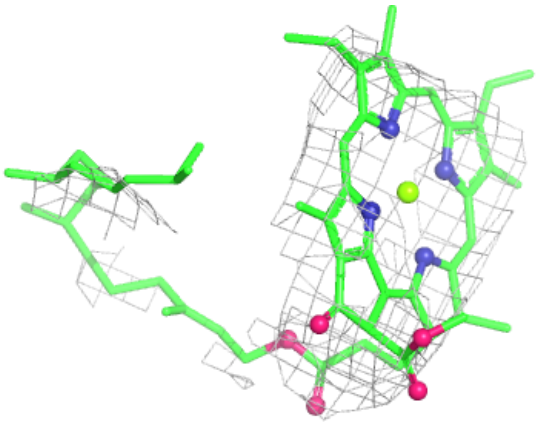


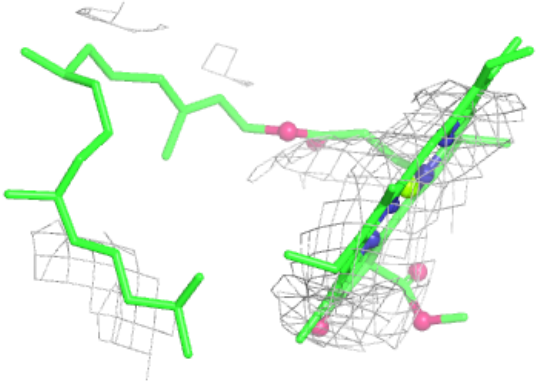


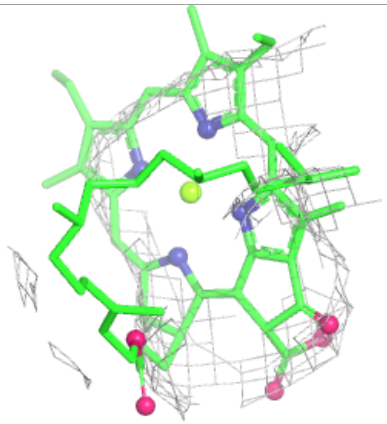


Electron density around CLA c 503:

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

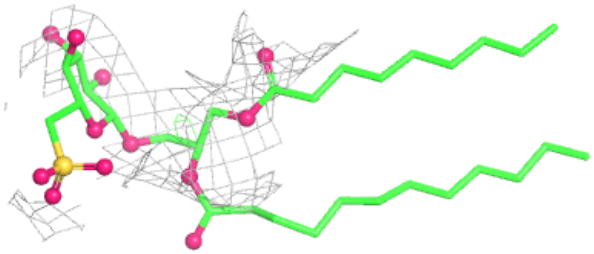


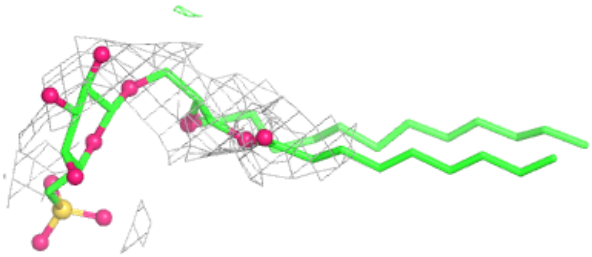


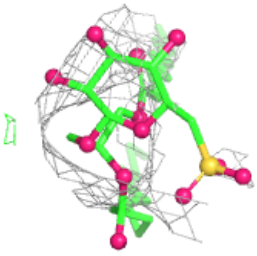


Electron density around SQD B 622:

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

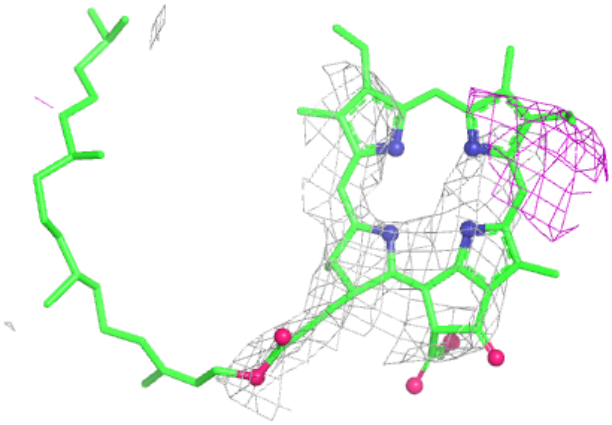


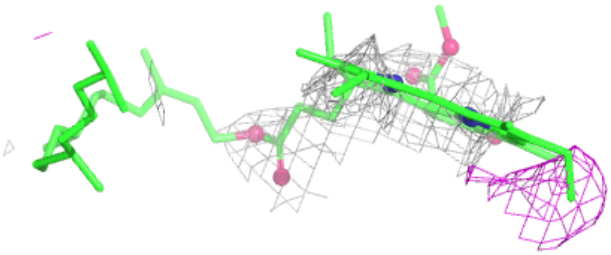




Electron density around PHO D 401:

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

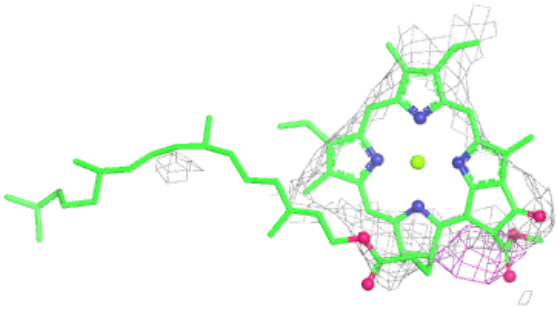


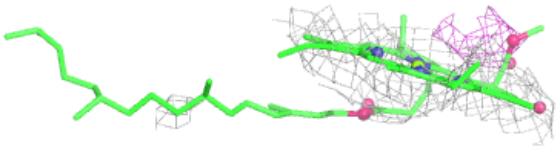


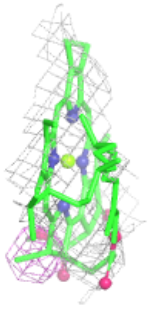


Electron density around CLA b 606:

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

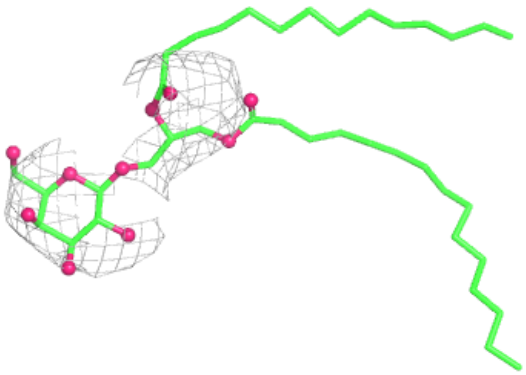


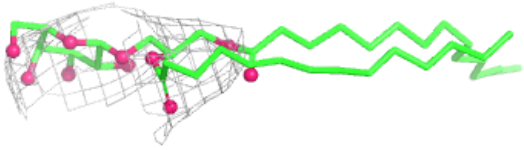


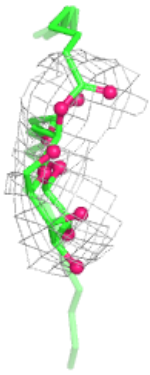


Electron density around LMG C 521:

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

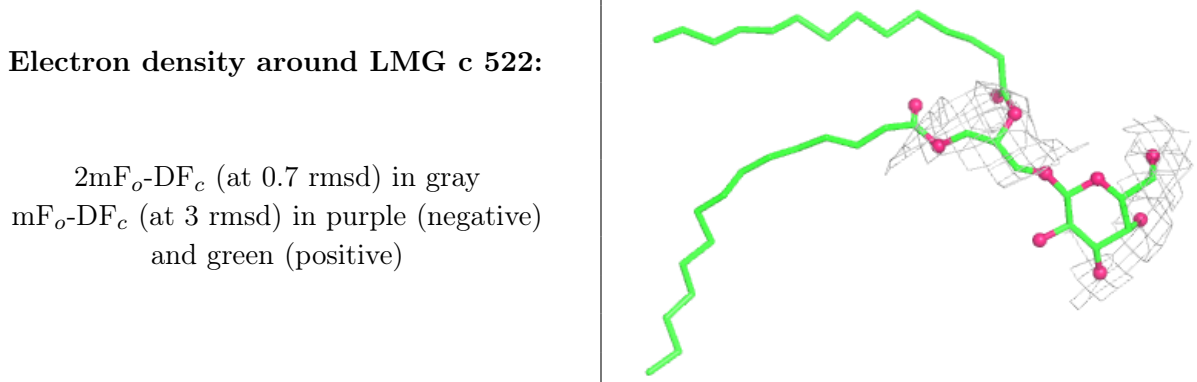


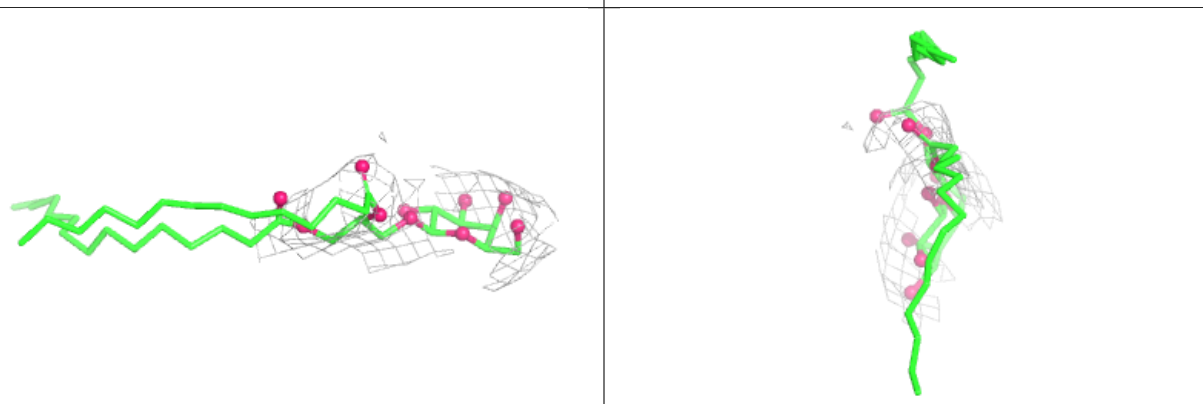




Electron density around LMG c 522:

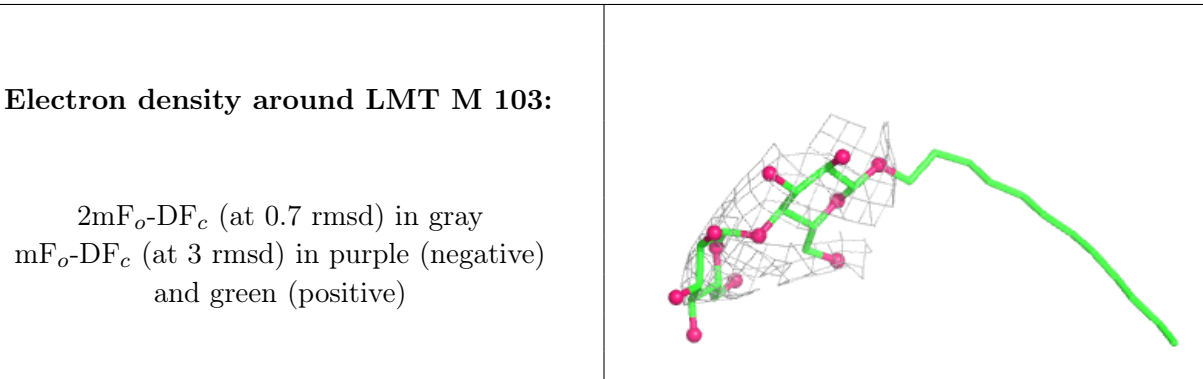
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

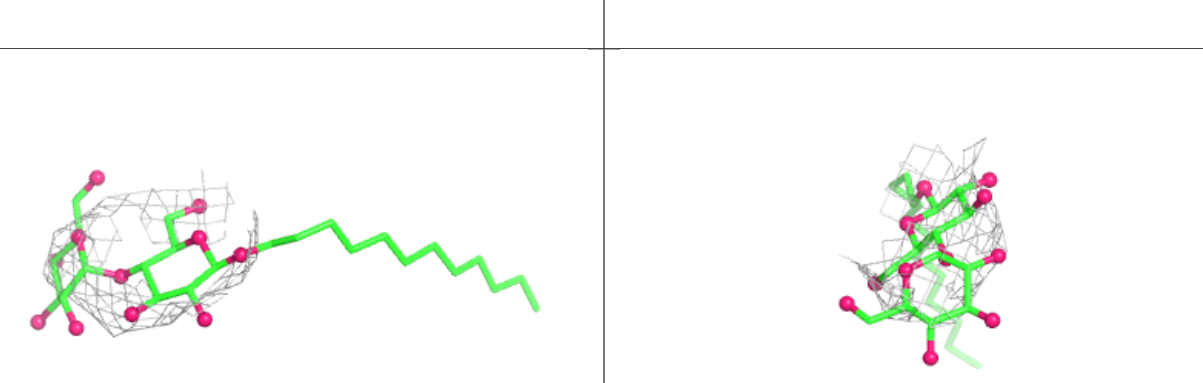




Electron density around LMT M 103:

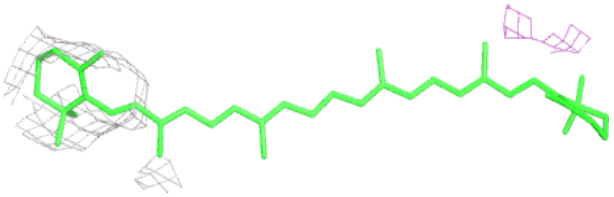
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



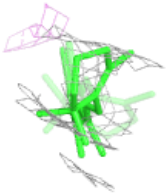


Electron density around BCR b 620:

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

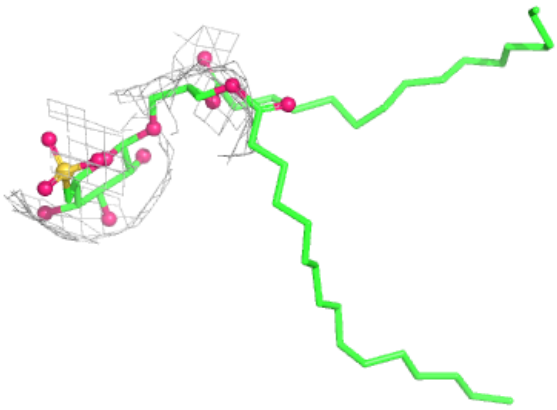


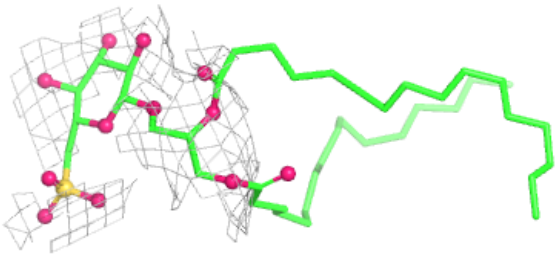




Electron density around SQD A 414:

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

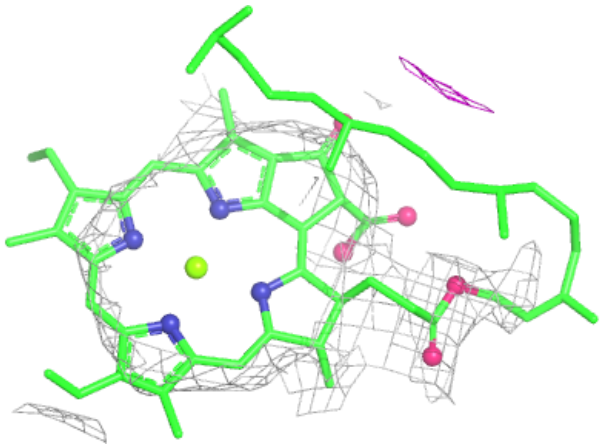


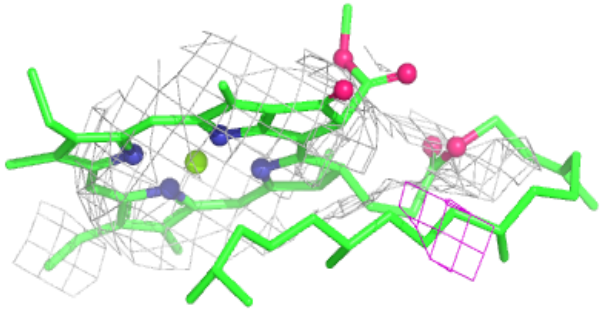


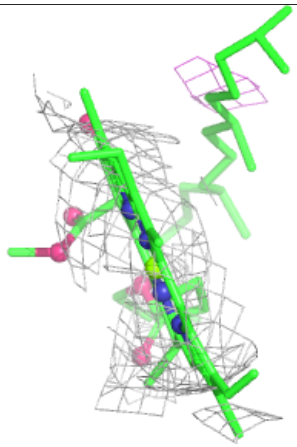


Electron density around CLA C 508:

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

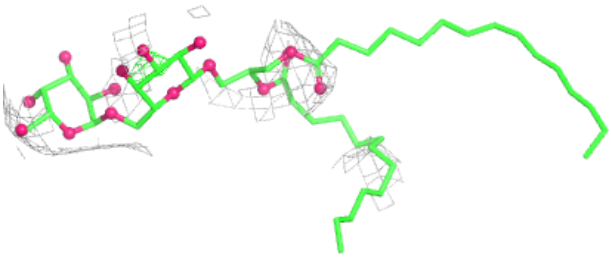


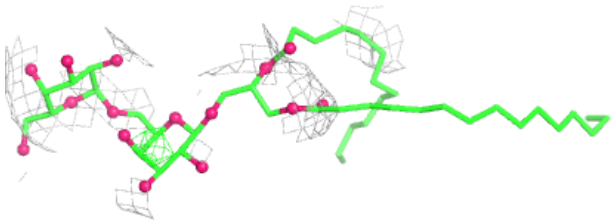




Electron density around DGD b 624:

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

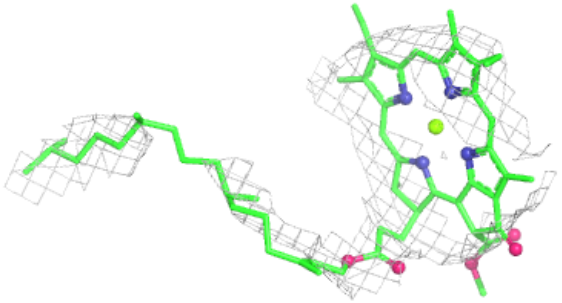


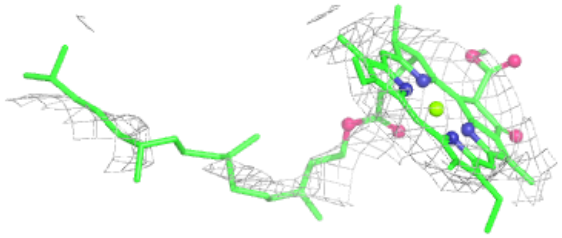


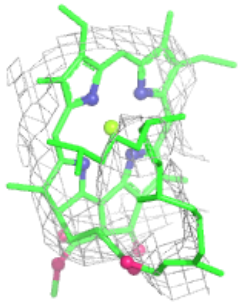


Electron density around CLA C 510:

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

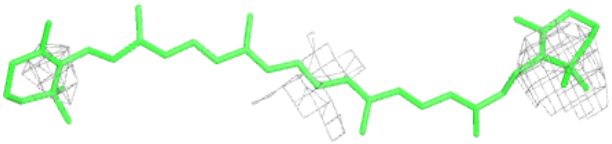


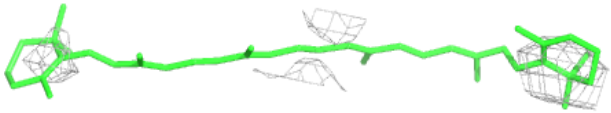


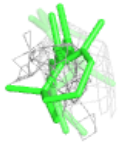


Electron density around BCR y 101:

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

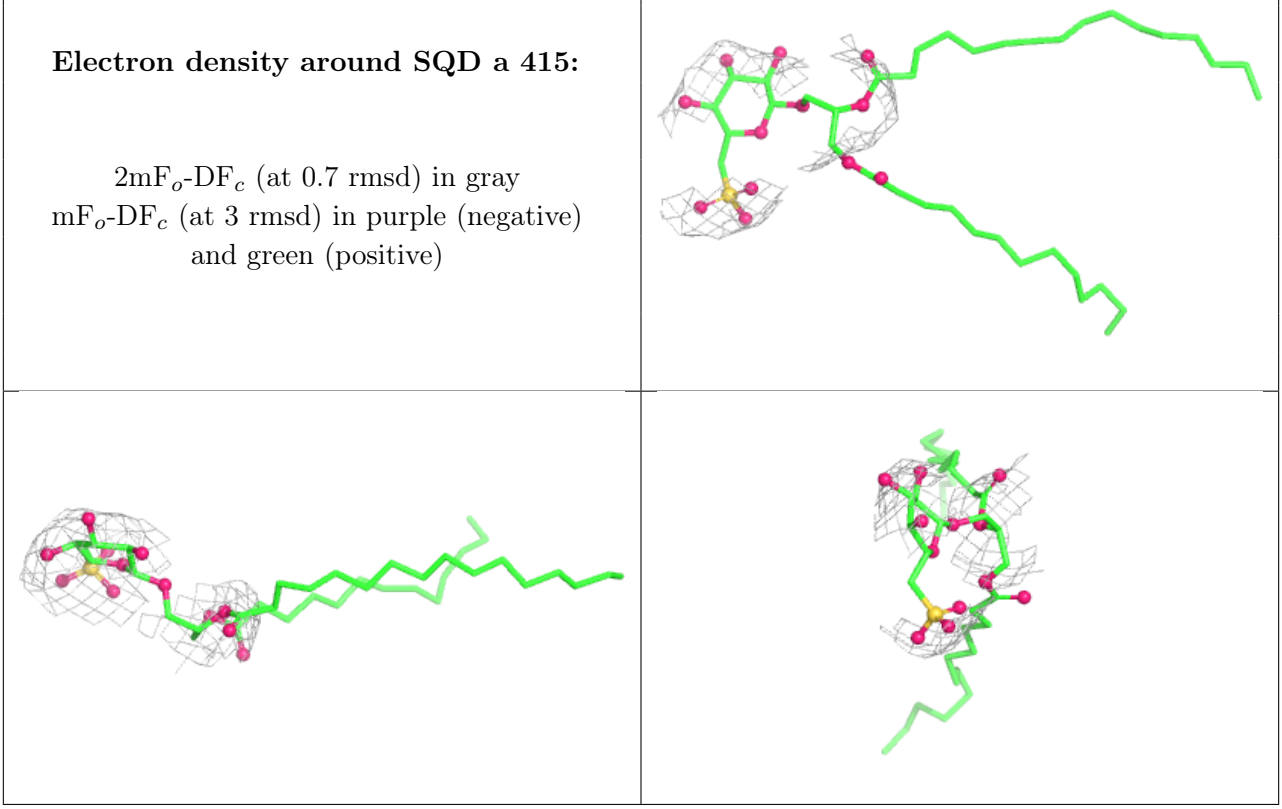






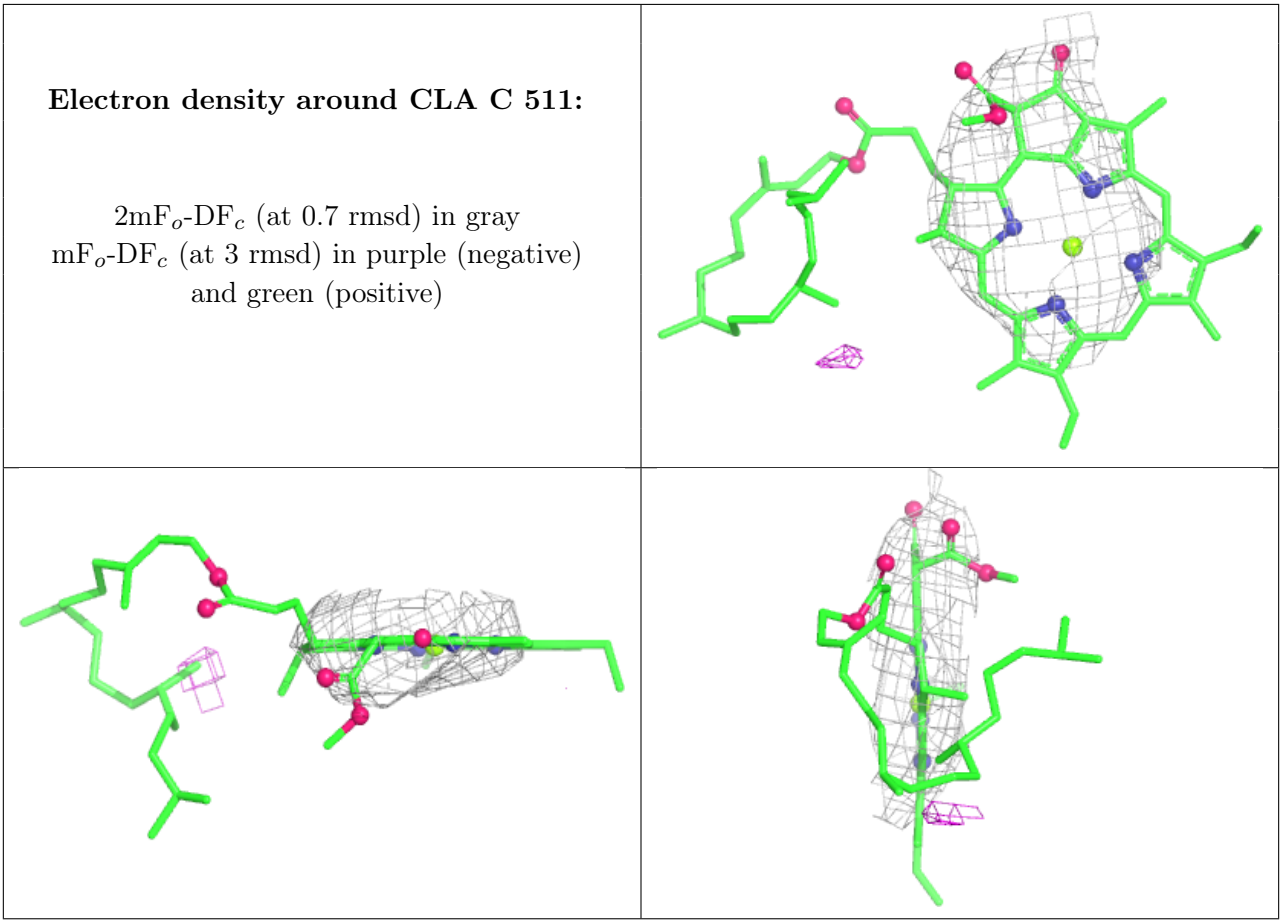
Electron density around SQD a 415:

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



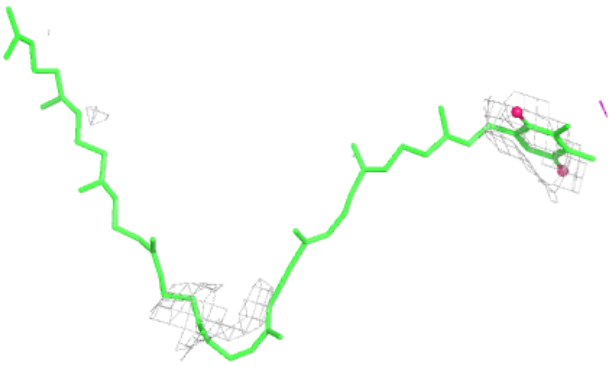
Electron density around CLA C 511:

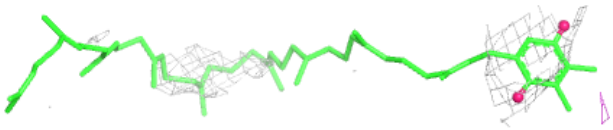
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PL9 D 406:

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

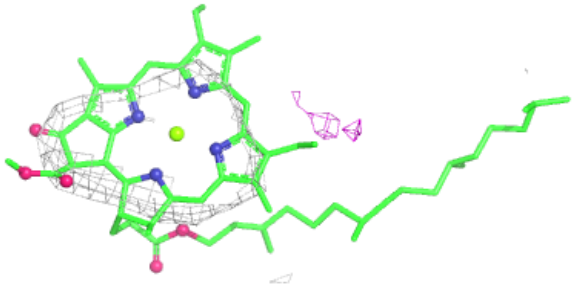




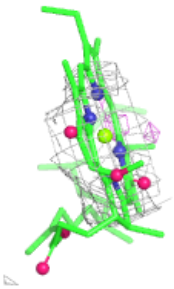


Electron density around CLA c 501:

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

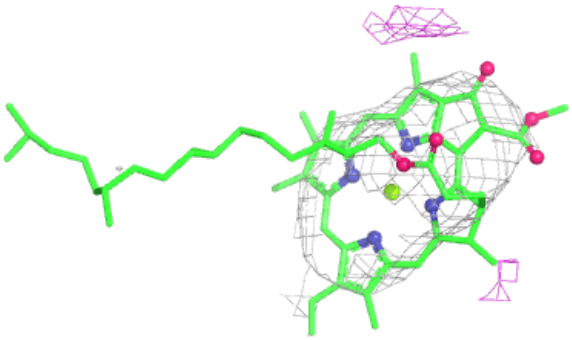


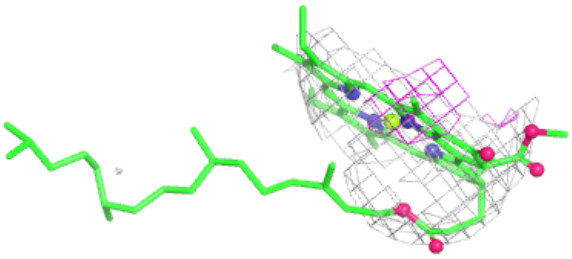


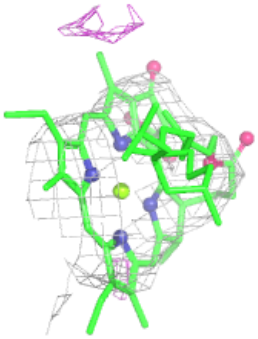


Electron density around CLA B 613:

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

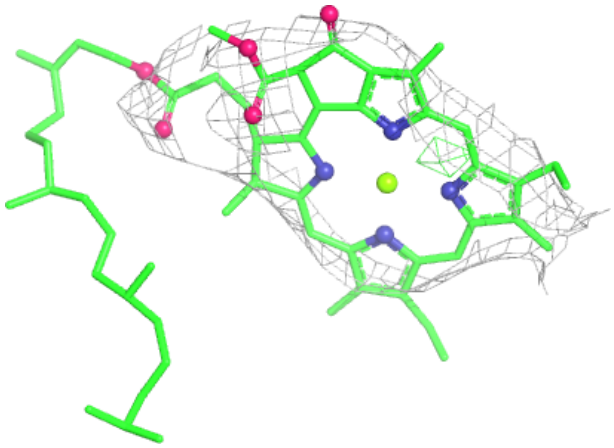


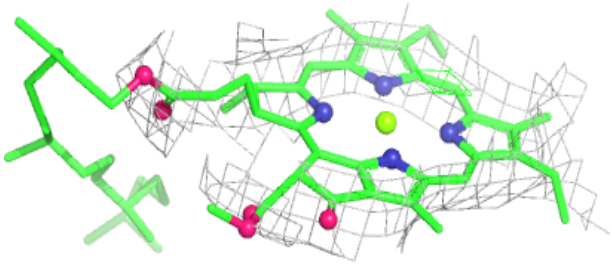


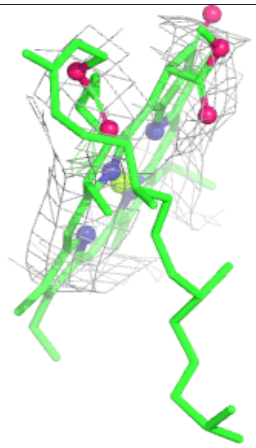


Electron density around CLA B 615:

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

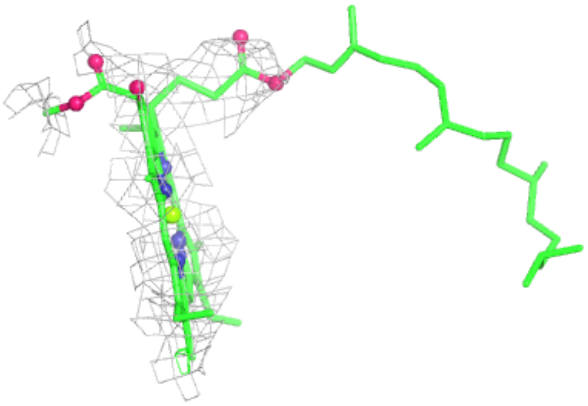


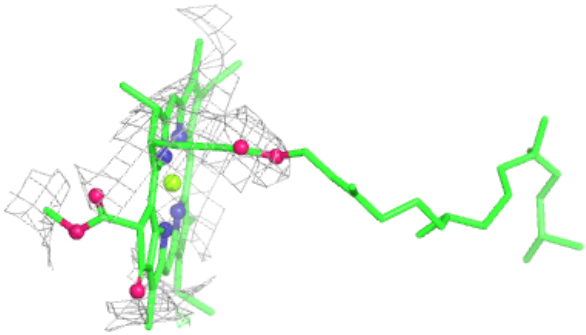


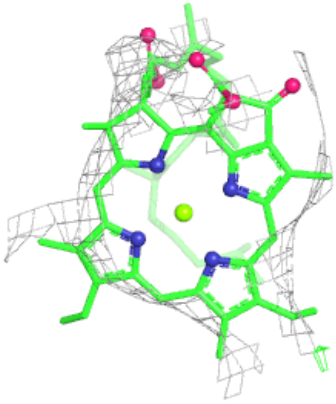


Electron density around CLA C 505:

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

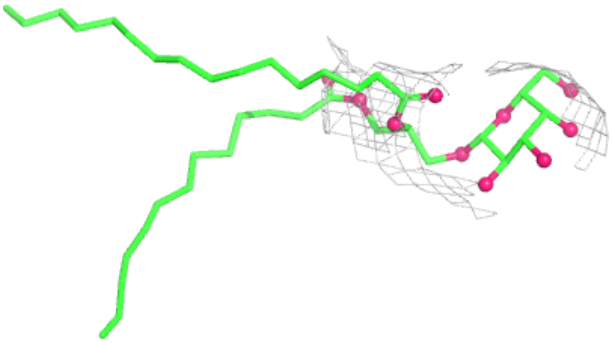


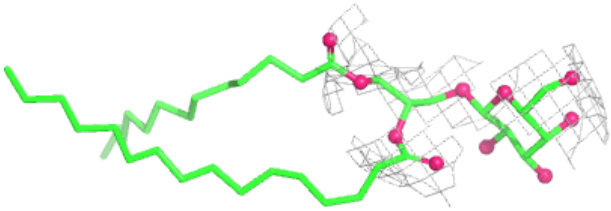


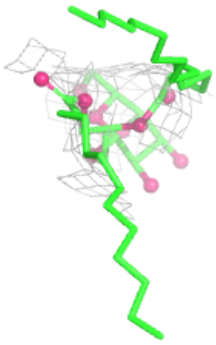


Electron density around LMG D 408:

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

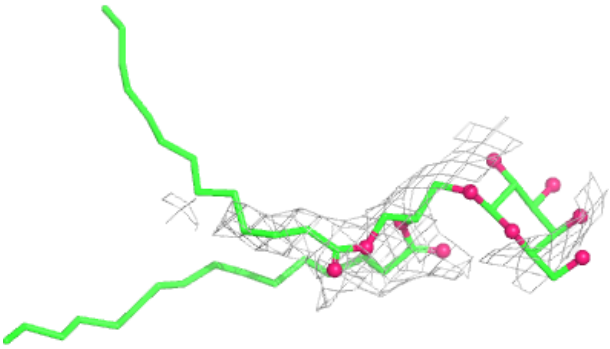


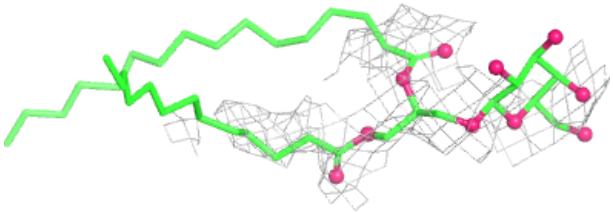


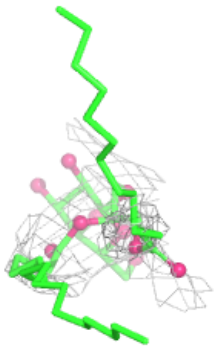


Electron density around LMG d 408:

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

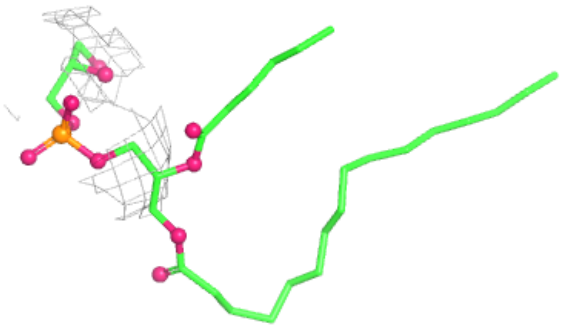


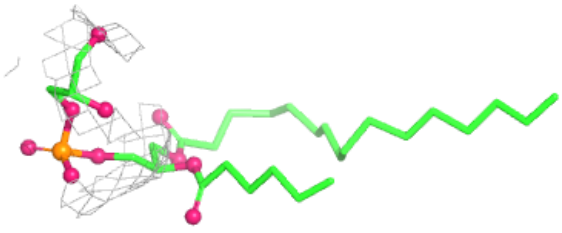


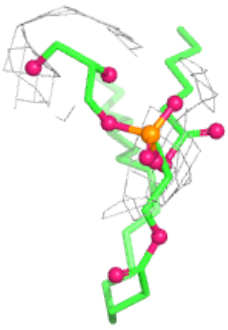


Electron density around LHG A 409:

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

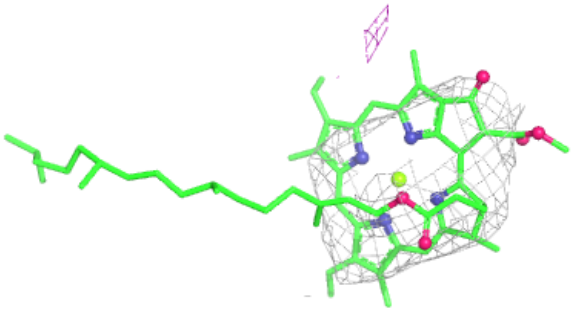


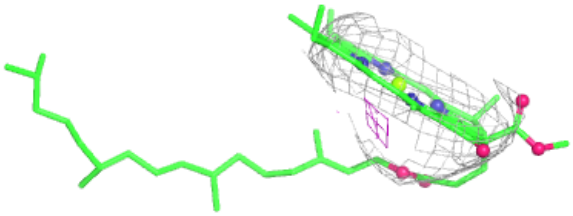


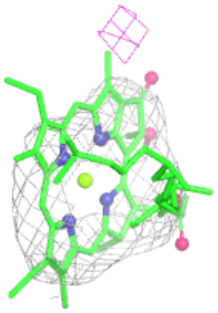


Electron density around CLA B 607:

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

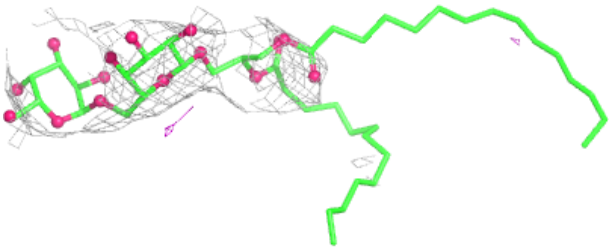




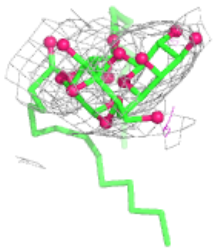


Electron density around DGD B 620:

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

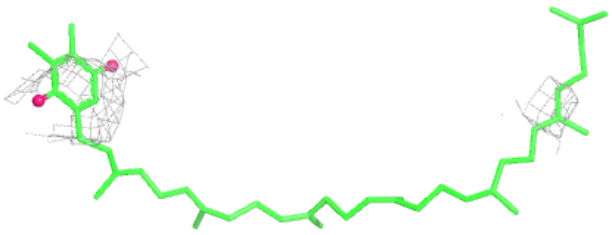


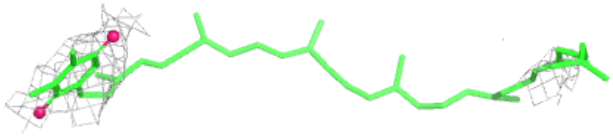


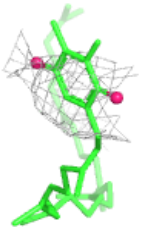


Electron density around PL9 a 409:

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

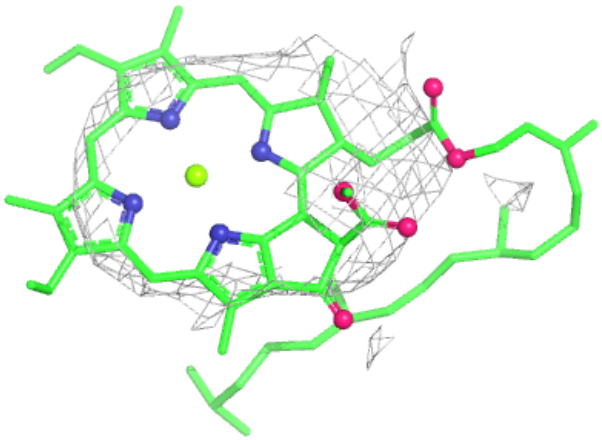


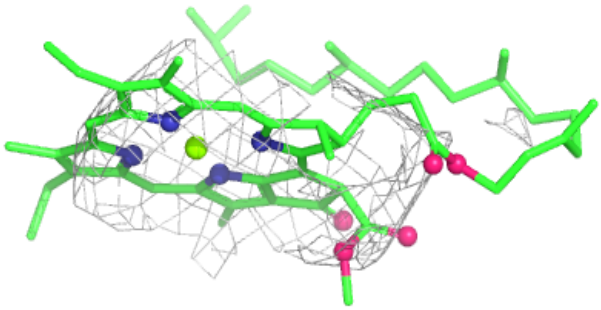


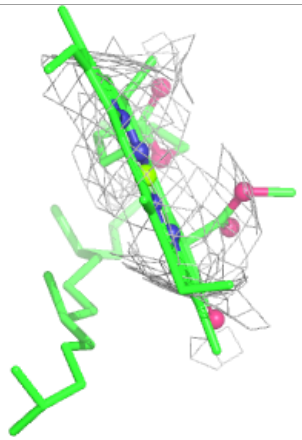


Electron density around CLA c 508:

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

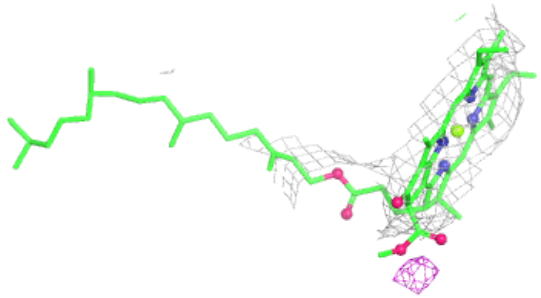


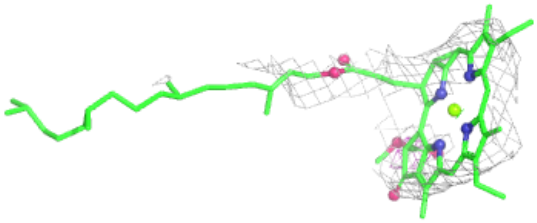


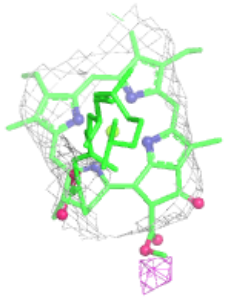


Electron density around CLA b 607:

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

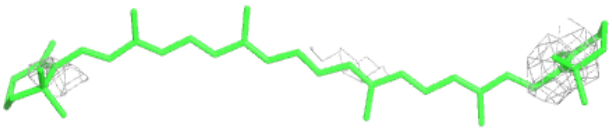


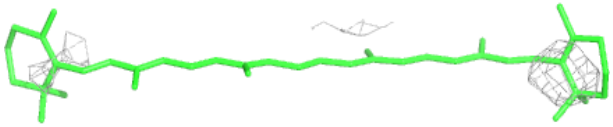


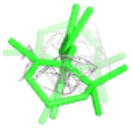


Electron density around BCR A 407:

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

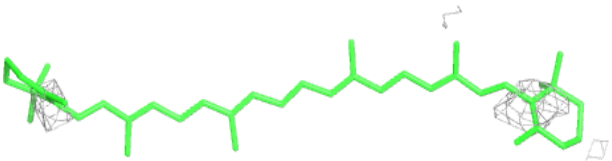




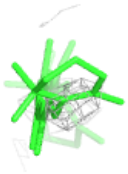


Electron density around BCR B 616:

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

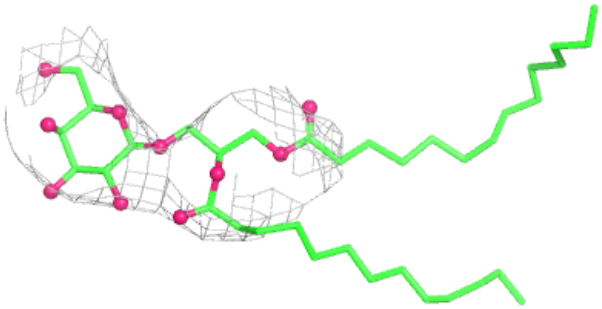




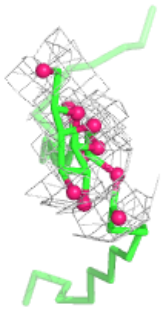


Electron density around LMG D 411:

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

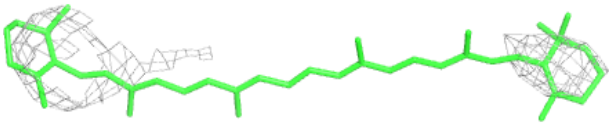


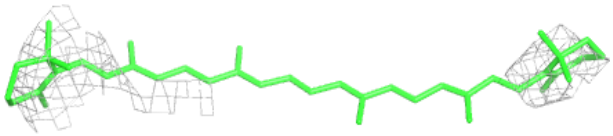


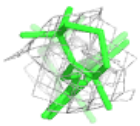


Electron density around BCR B 619:

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

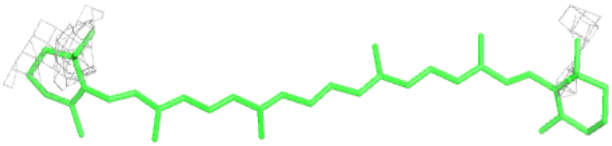


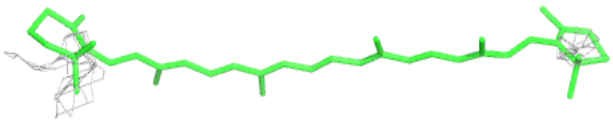


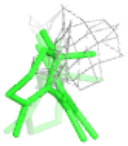


Electron density around BCR c 514:

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

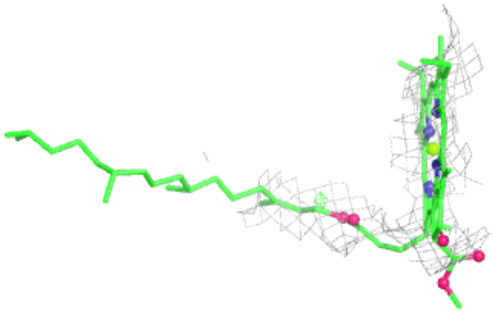


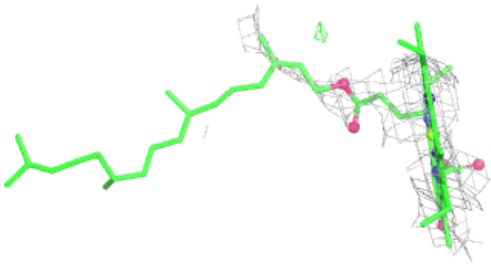


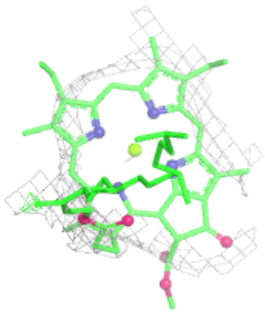


Electron density around CLA b 609:

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

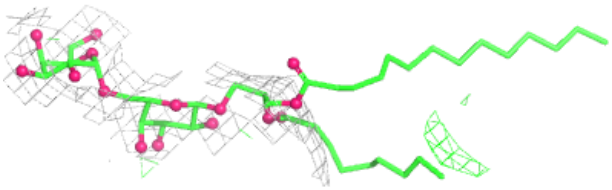


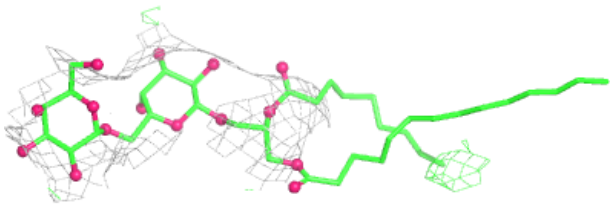


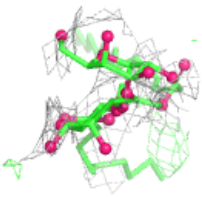


Electron density around DGD c 515:

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

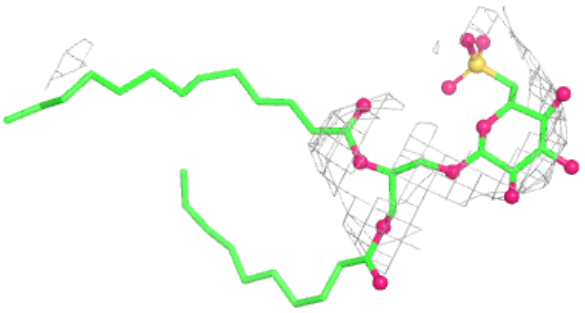


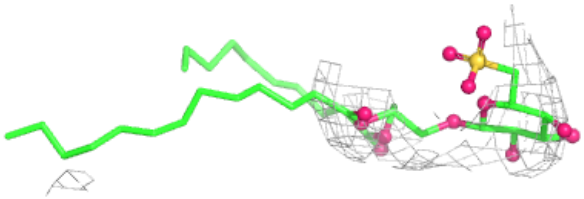




Electron density around SQD f 103:

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

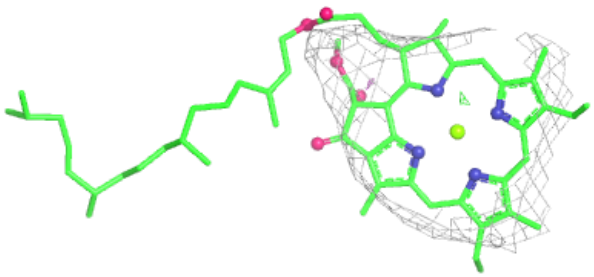


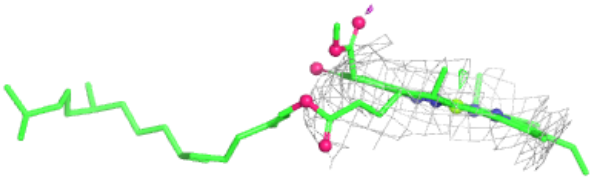


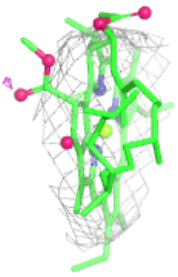


Electron density around CLA h 101:

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

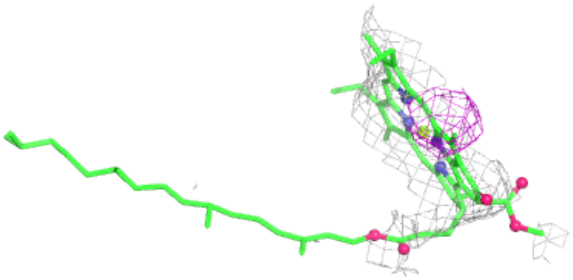


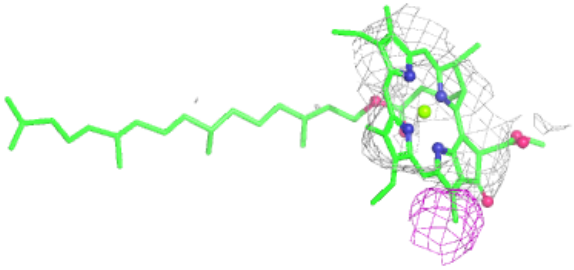


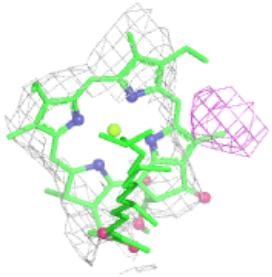


Electron density around CLA b 610:

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

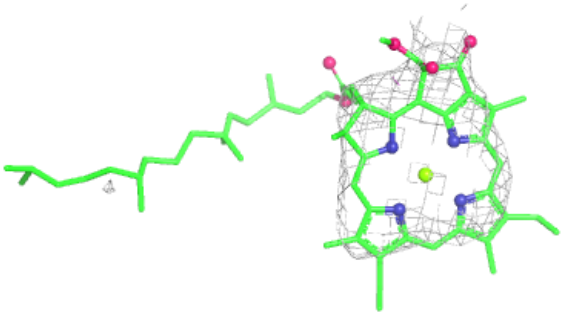


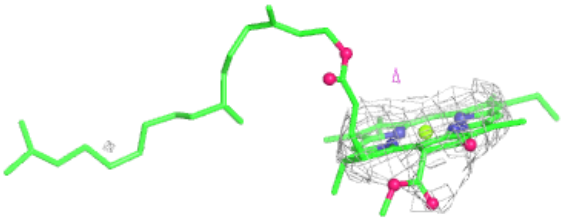


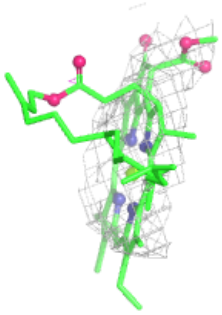


Electron density around CLA A 404:

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

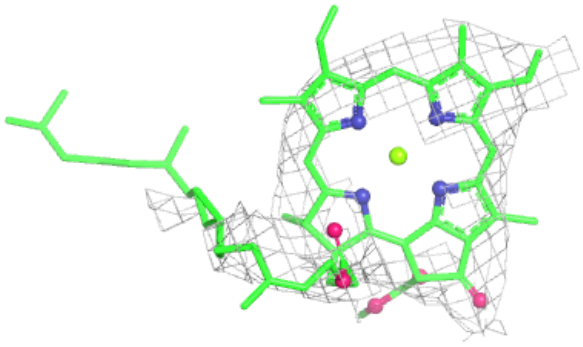


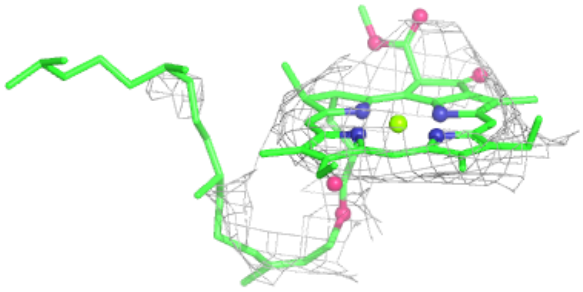




Electron density around CLA a 405:

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

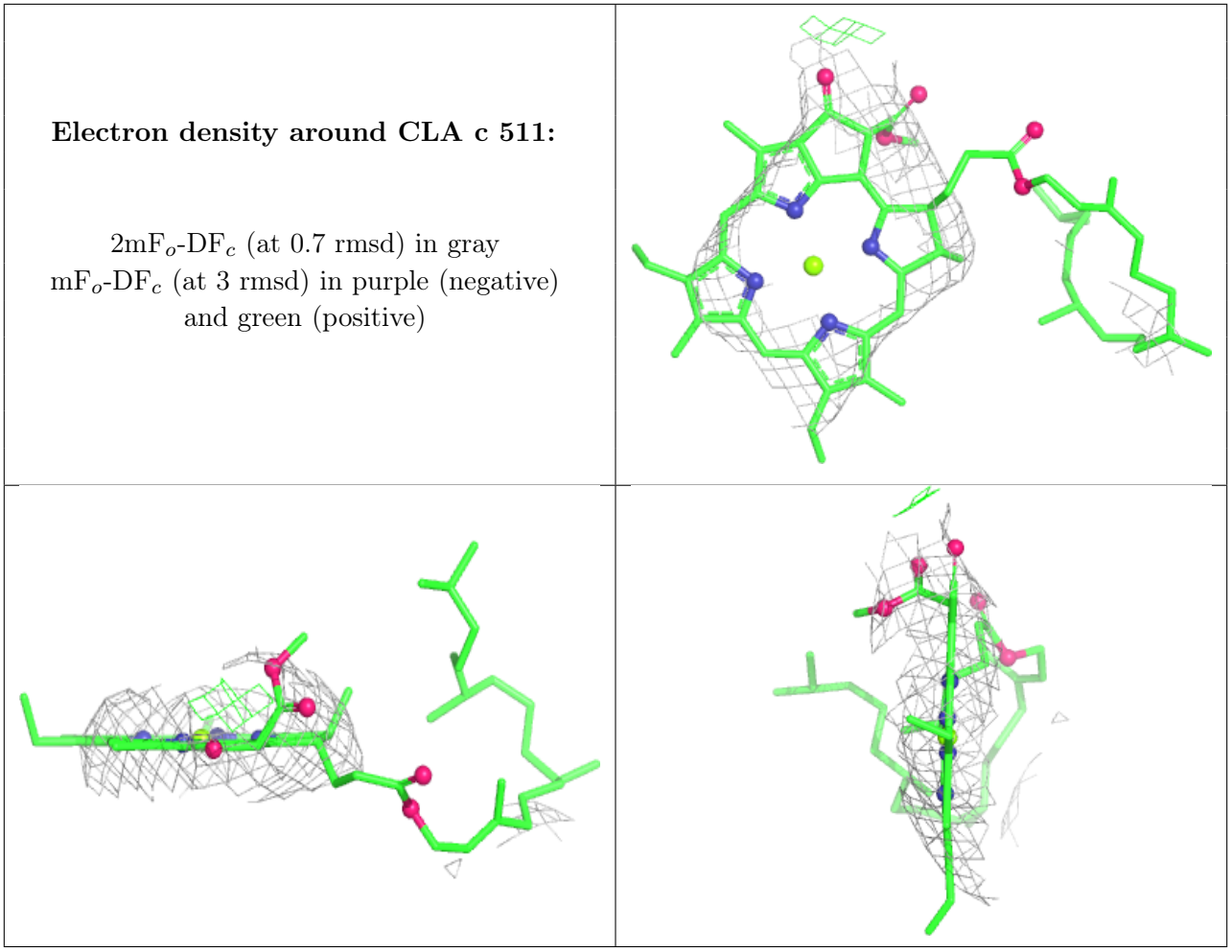






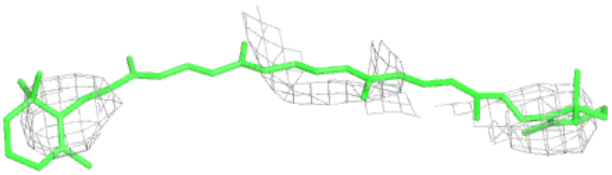
Electron density around CLA c 511:

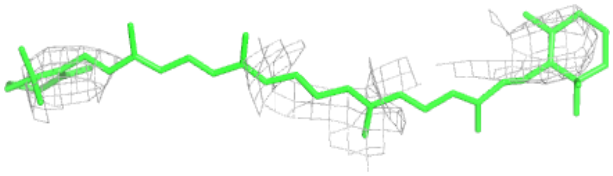
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

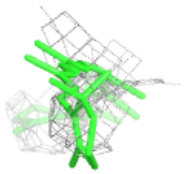


Electron density around BCR F 102:

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

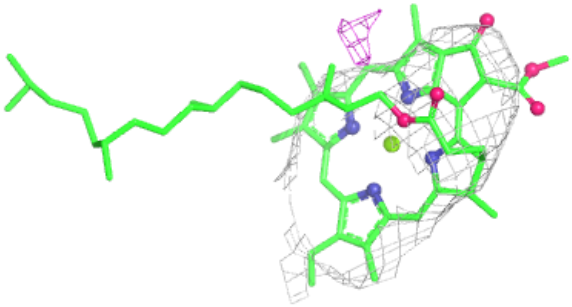


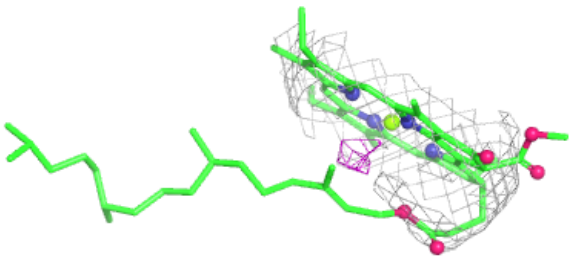




Electron density around CLA b 617:

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

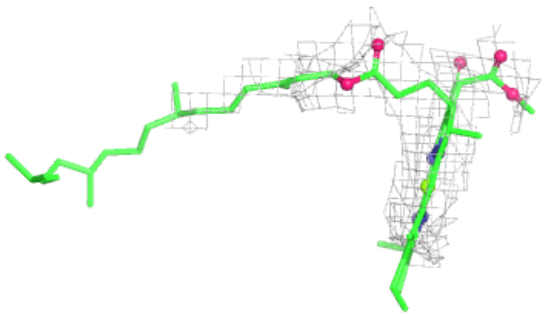


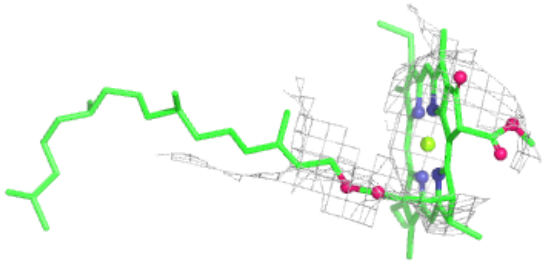


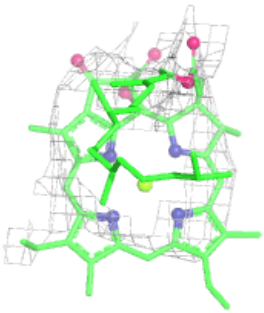


Electron density around CLA B 604:

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

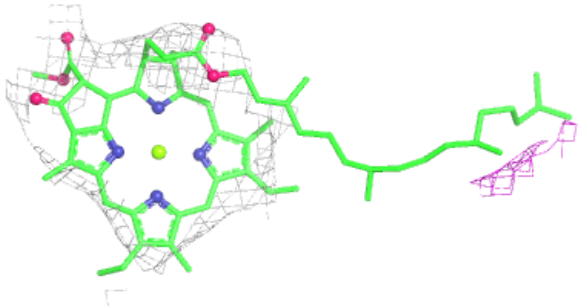


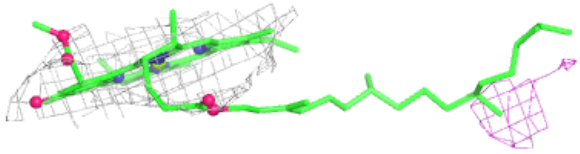


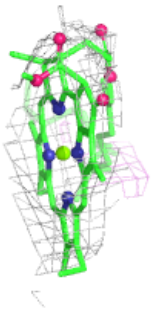


Electron density around CLA B 602:

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

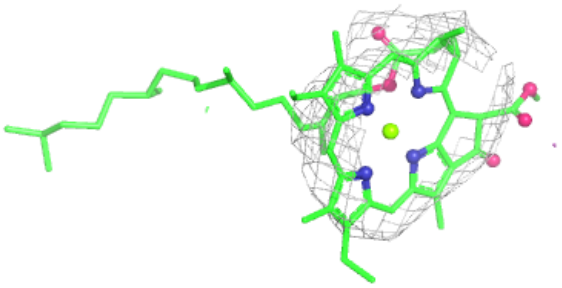


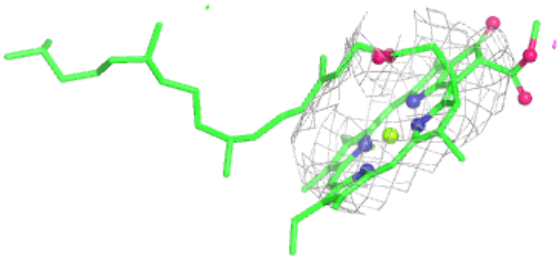


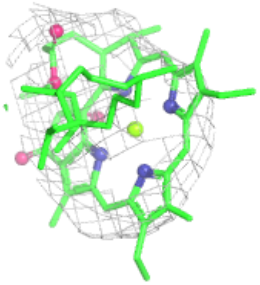


Electron density around CLA C 504:

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

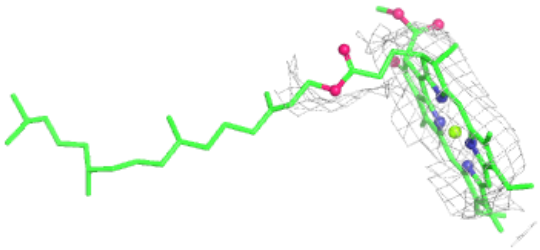


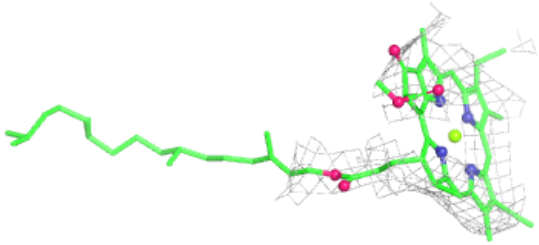


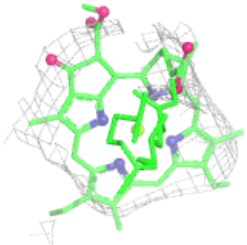


Electron density around CLA B 603:

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

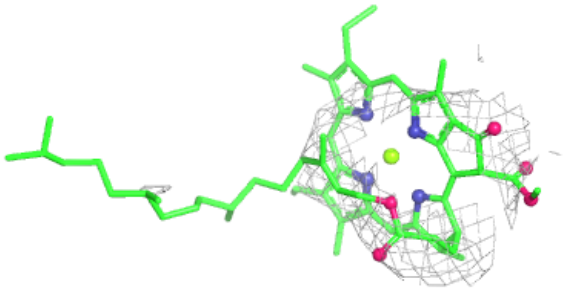


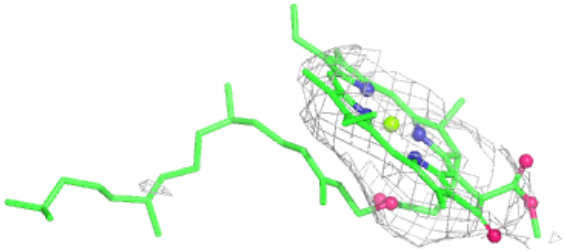


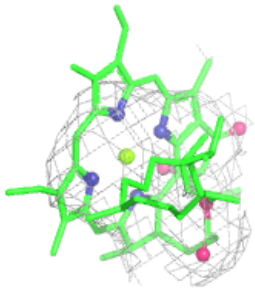


Electron density around CLA c 504:

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

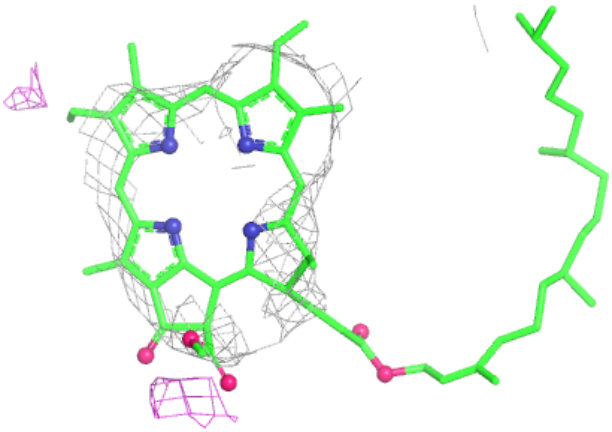


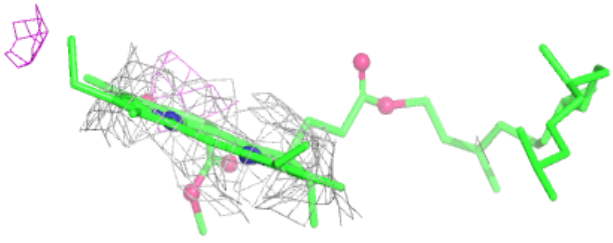


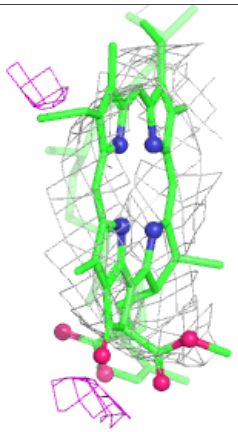


Electron density around PHO d 401:

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



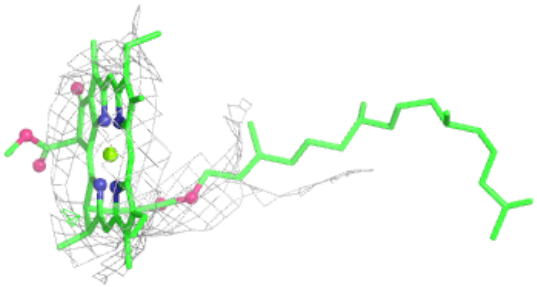


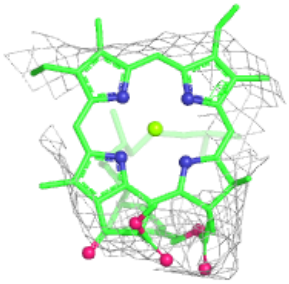


Electron density around CLA b 608:

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

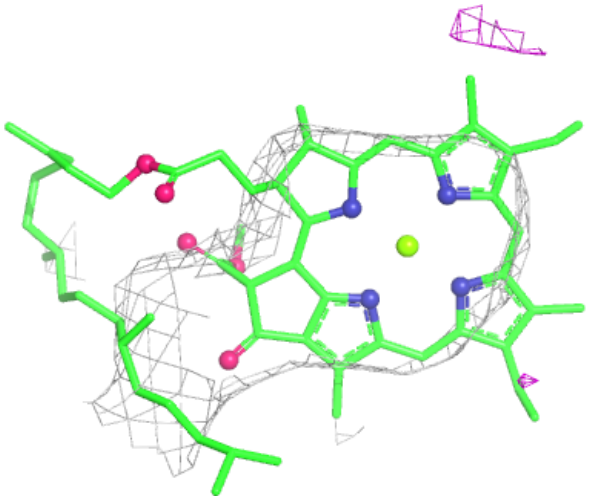


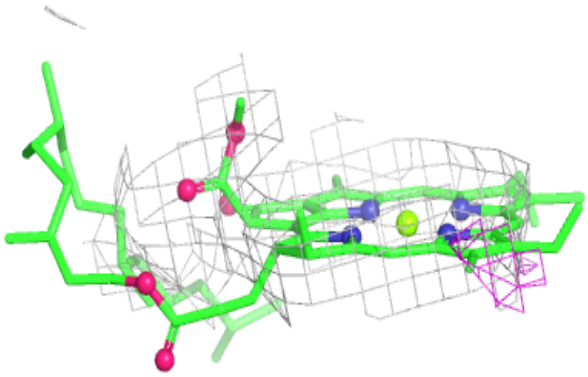




Electron density around CLA B 609:

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

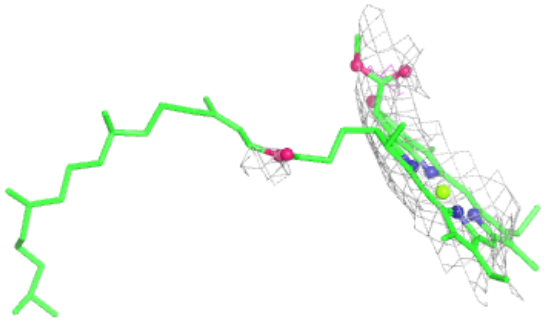


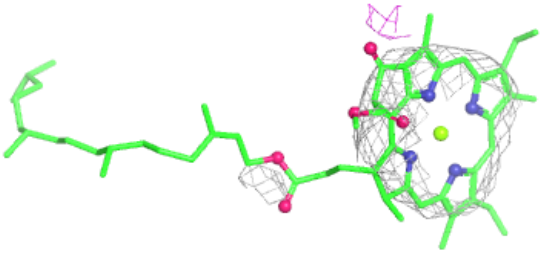


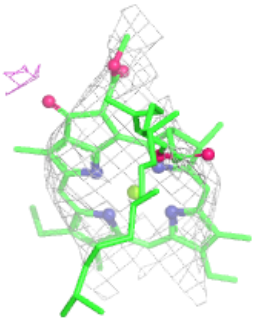


Electron density around CLA D 404:

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

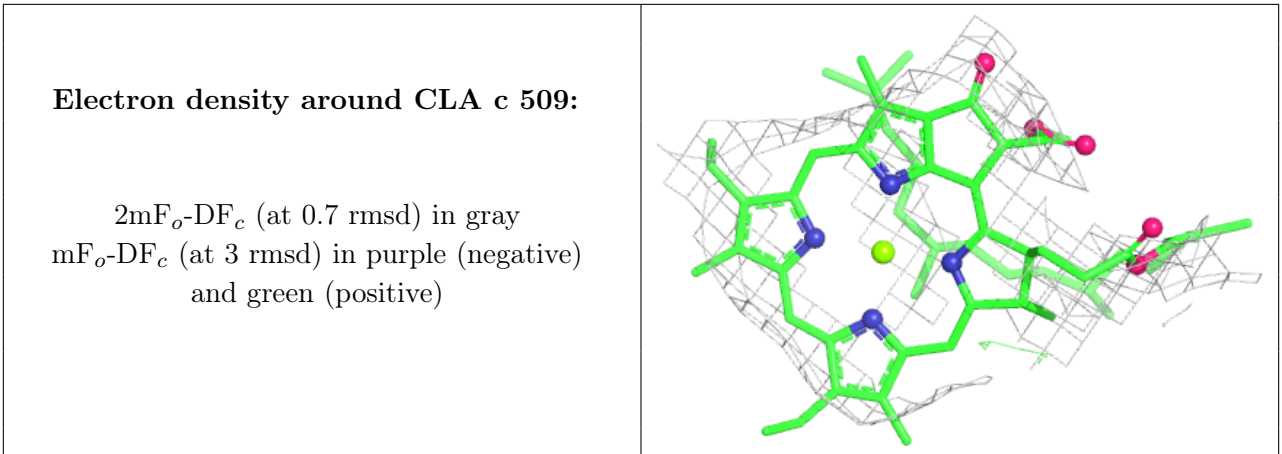


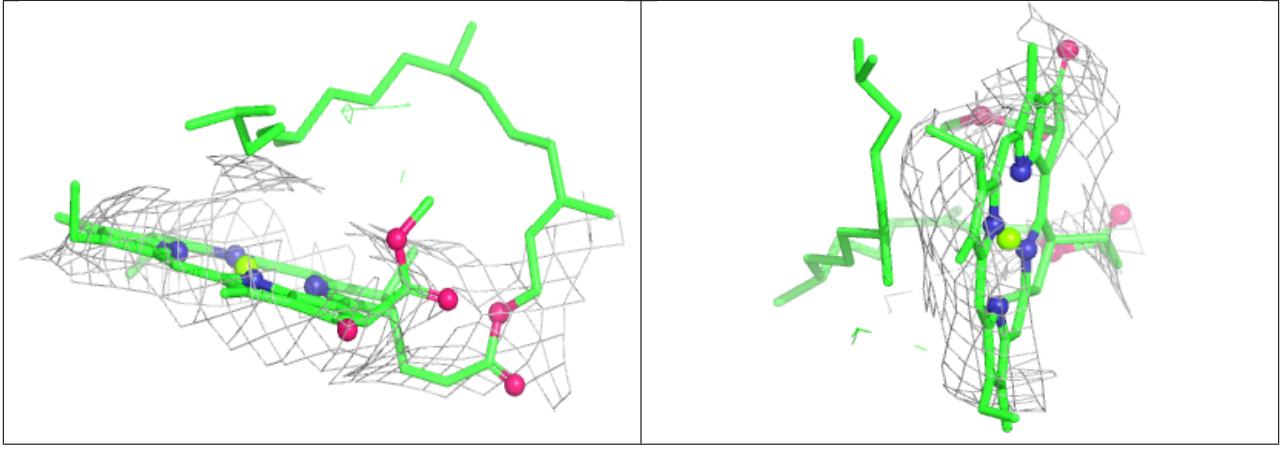




Electron density around CLA c 509:

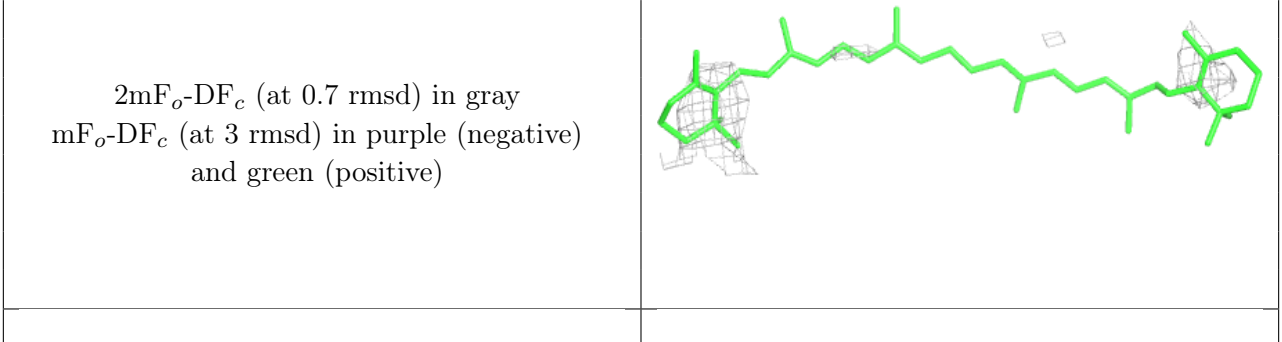
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

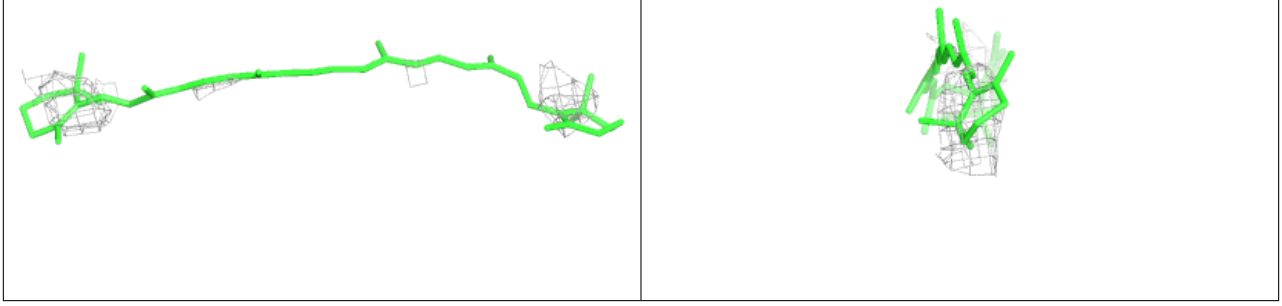




Electron density around BCR B 617:

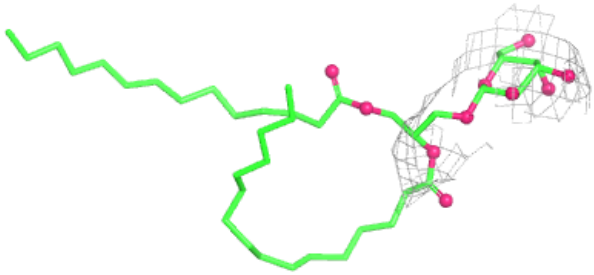
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

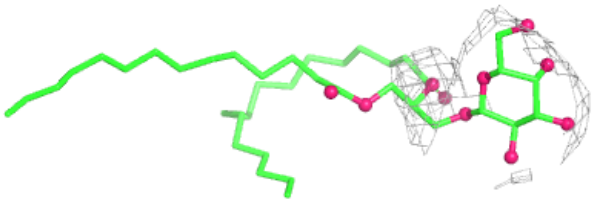




Electron density around LMG d 407:

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

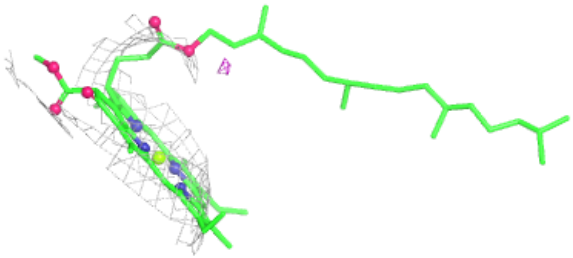


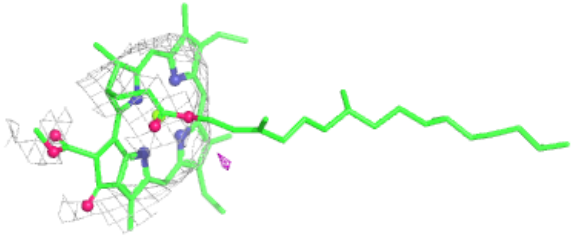


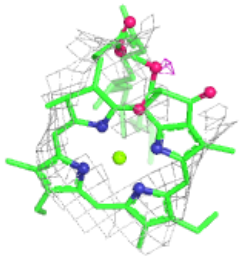


Electron density around CLA c 520:

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

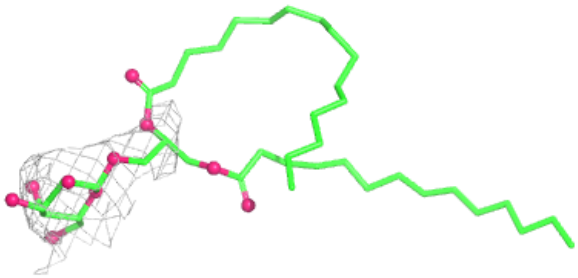




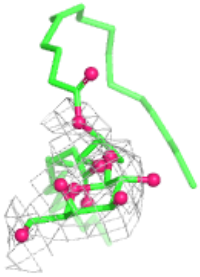


Electron density around LMG D 407:

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

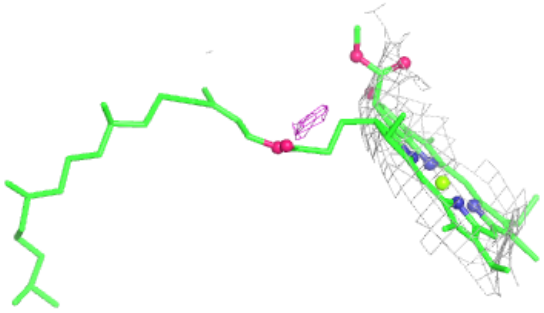


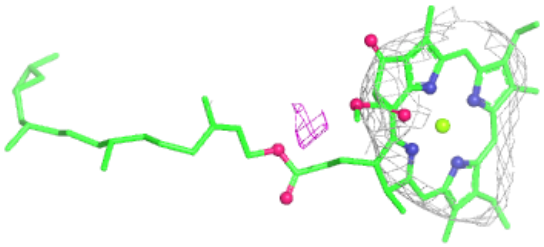


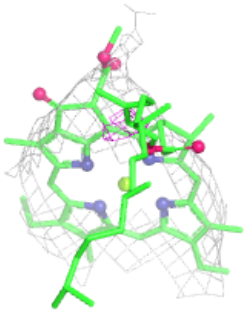


Electron density around CLA d 404:

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

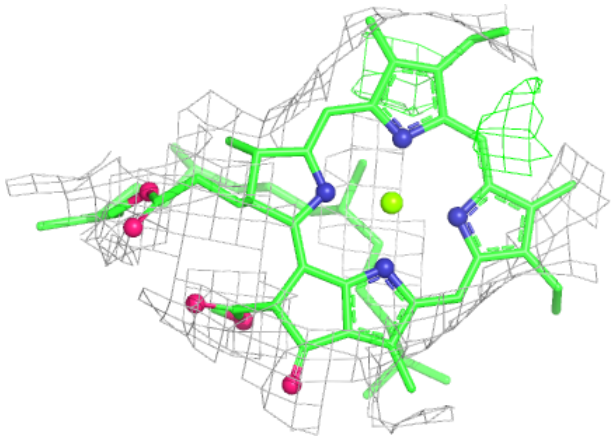


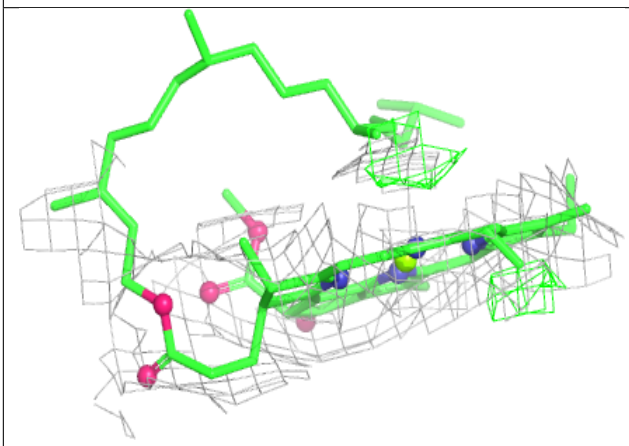




Electron density around CLA C 509:

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

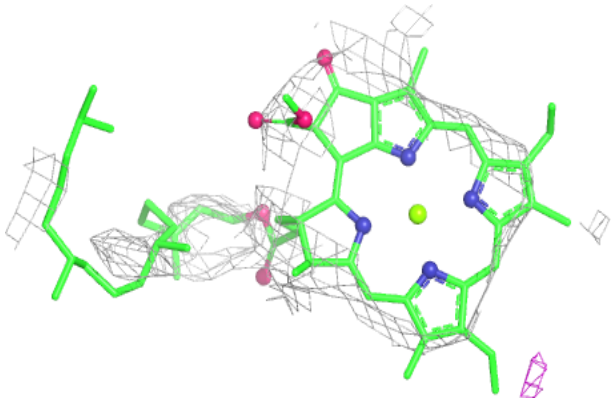


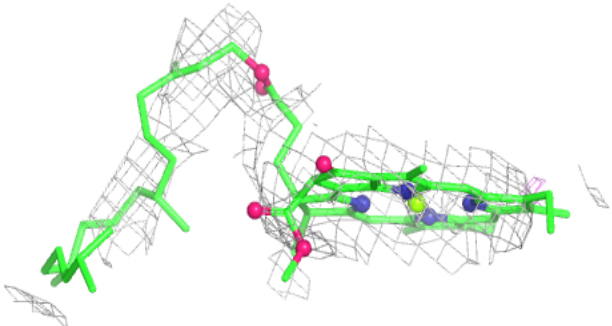




Electron density around CLA B 611:

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

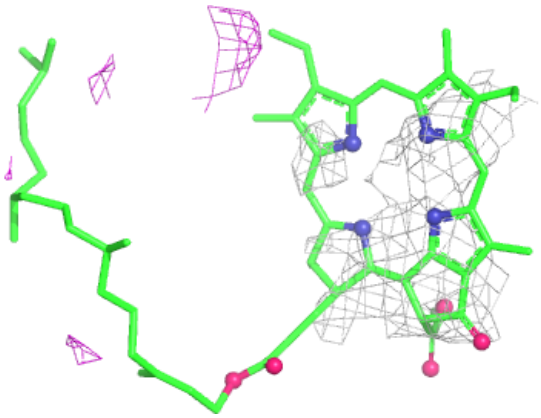


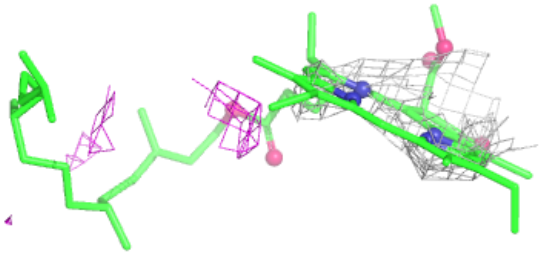




Electron density around PHO a 407:

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

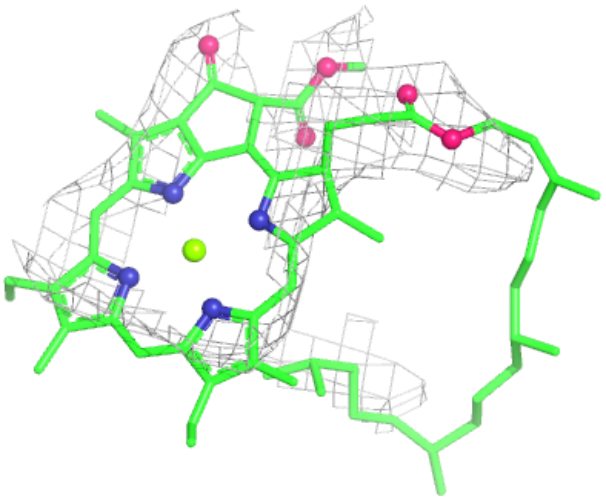


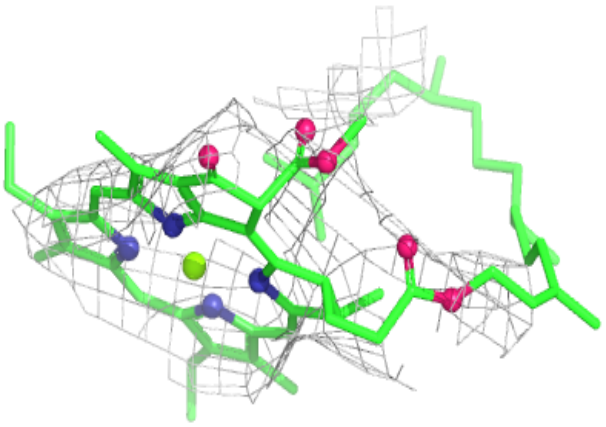




Electron density around CLA b 618:

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

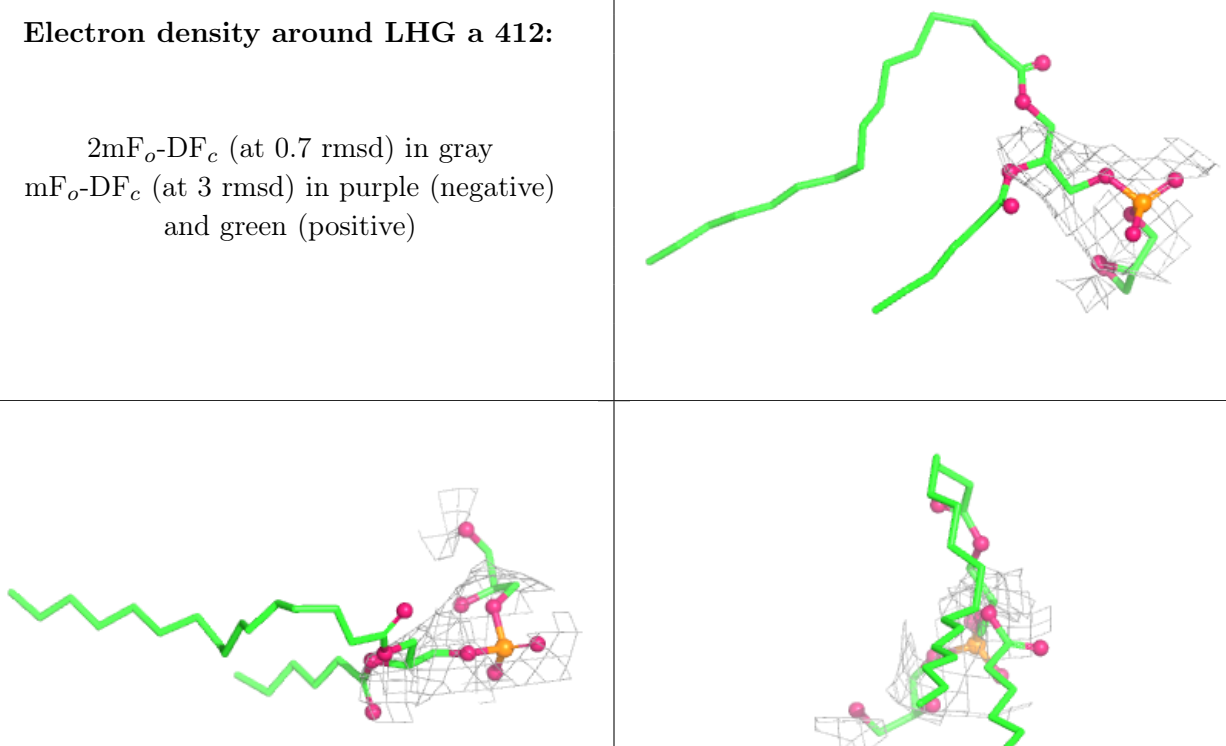






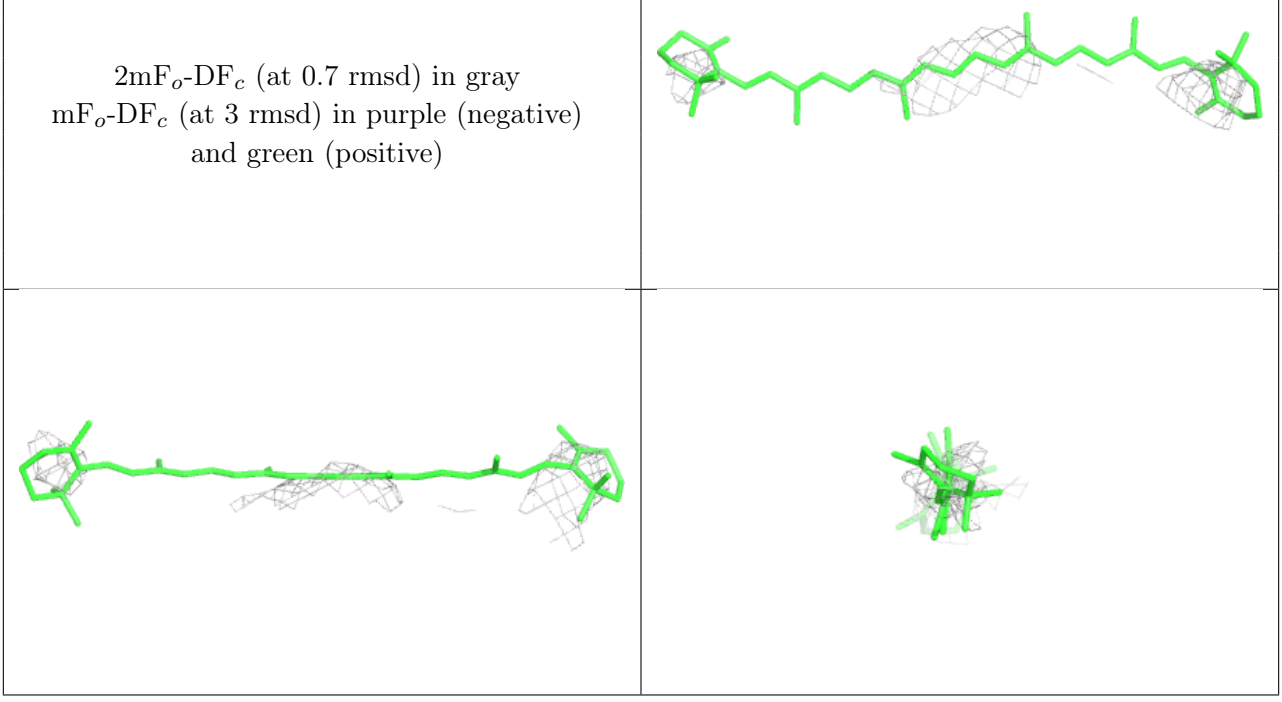
Electron density around LHG a 412:

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



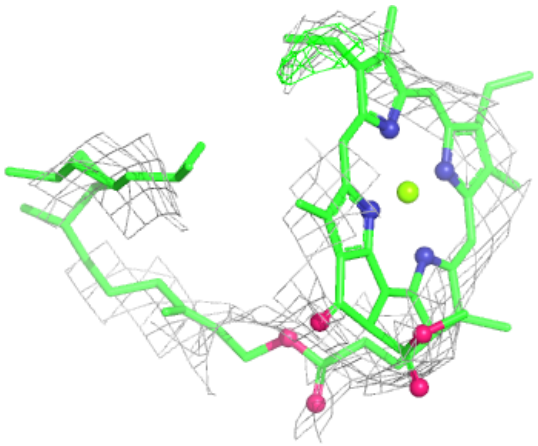
Electron density around BCR B 618:

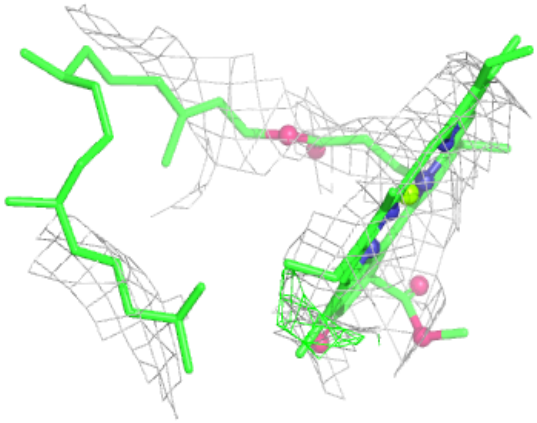
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

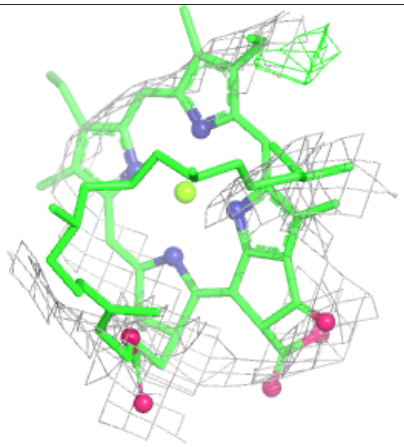


Electron density around CLA C 503:

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

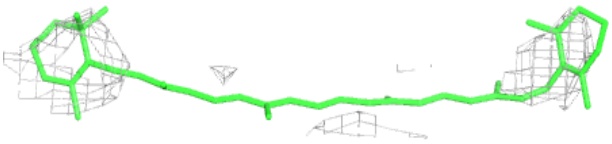


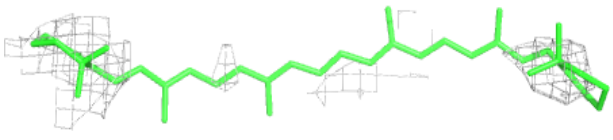


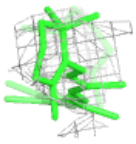


Electron density around BCR C 513:

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

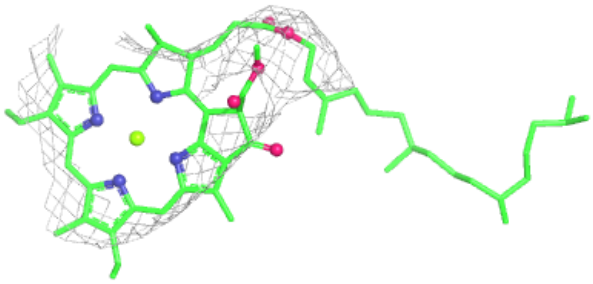


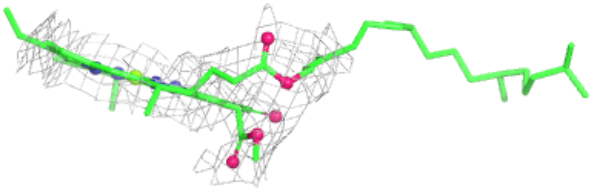


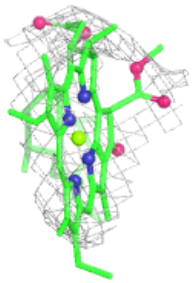


Electron density around CLA H 101:

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

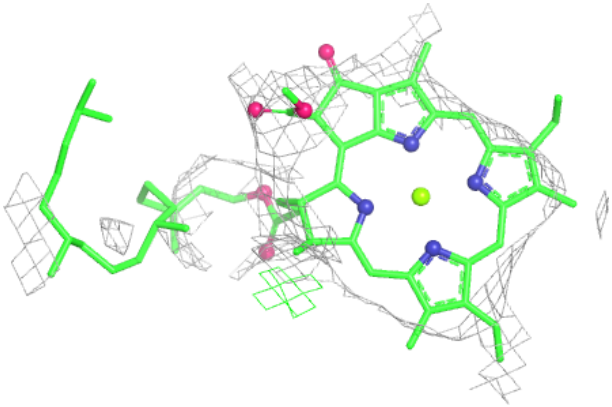


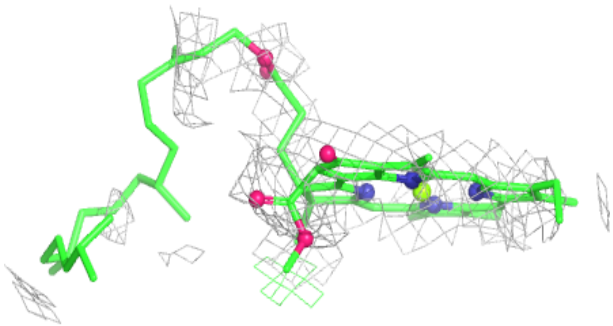


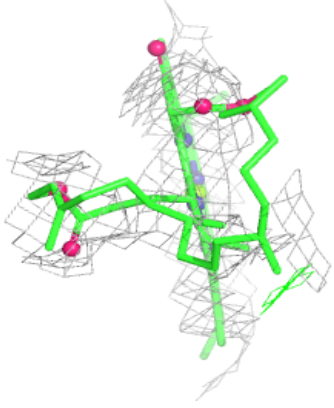


Electron density around CLA b 615:

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



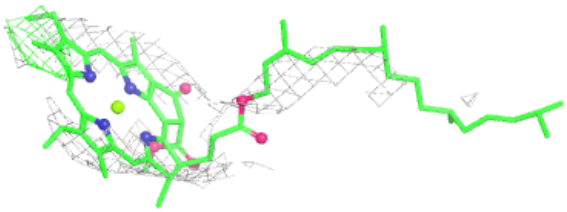


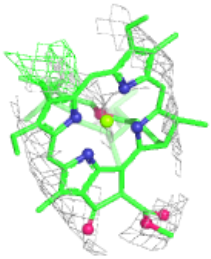


Electron density around CLA C 502:

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



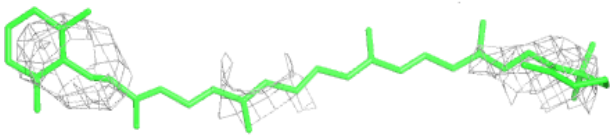


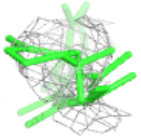


Electron density around BCR f 102:

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

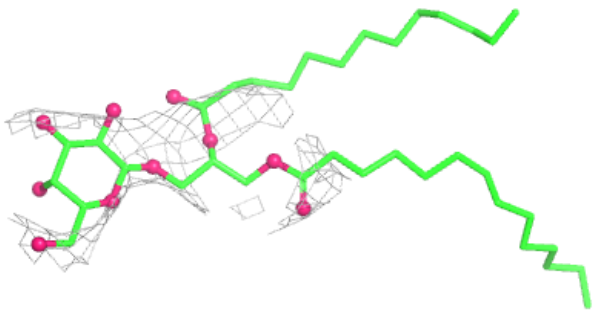


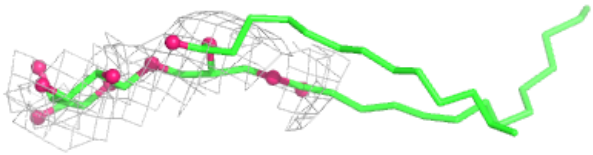




Electron density around LMG d 411:

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



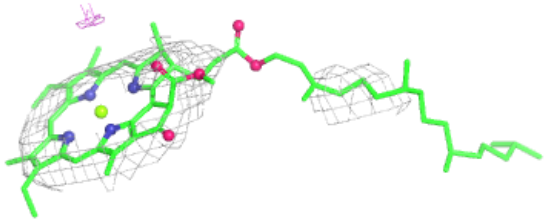


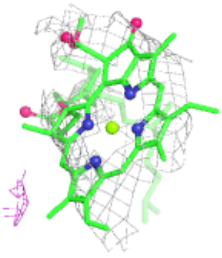


Electron density around CLA A 402:

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

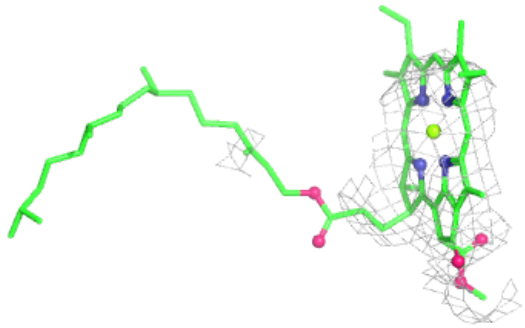


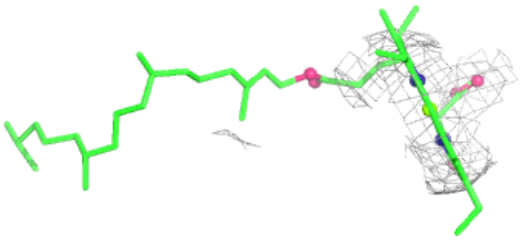


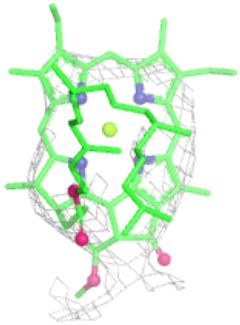


Electron density around CLA D 405:

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

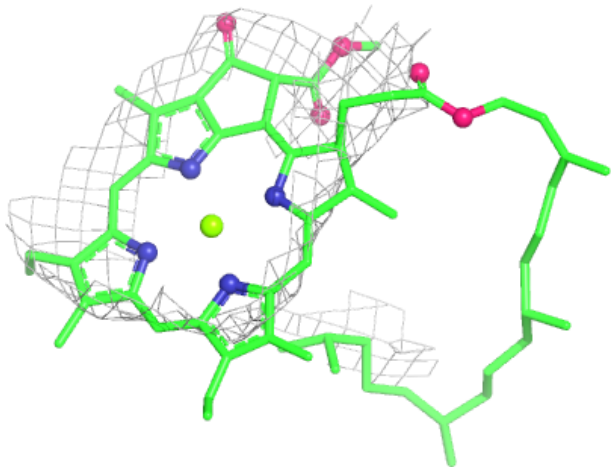


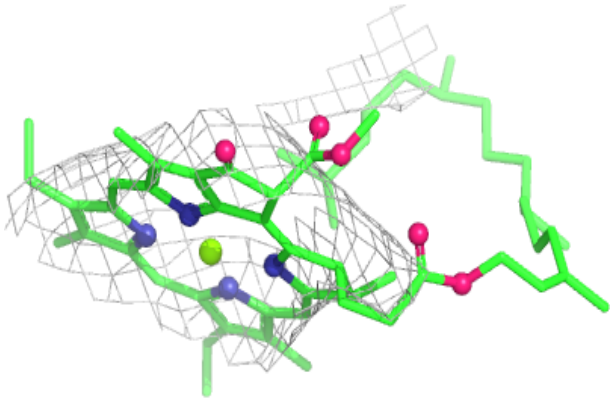


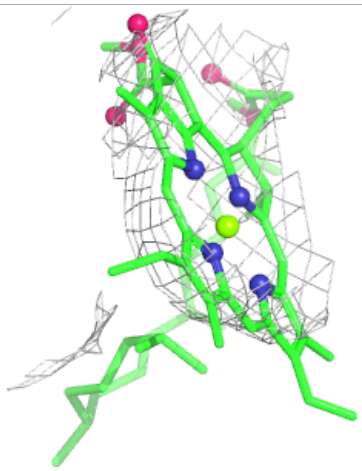


Electron density around CLA B 614:

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

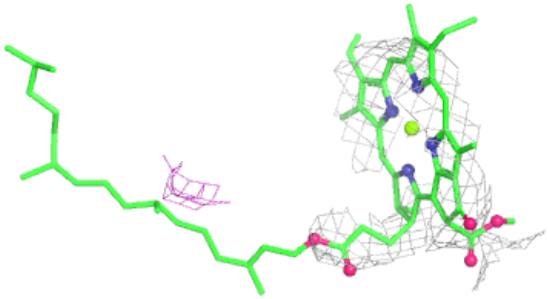


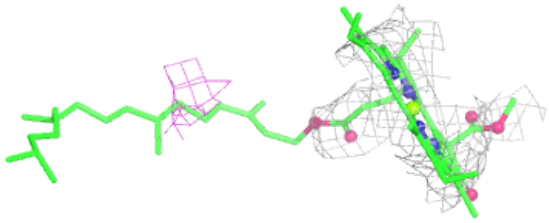


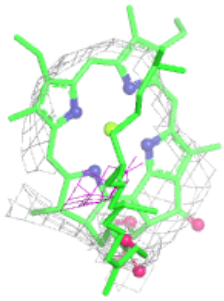


Electron density around CLA B 608:

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

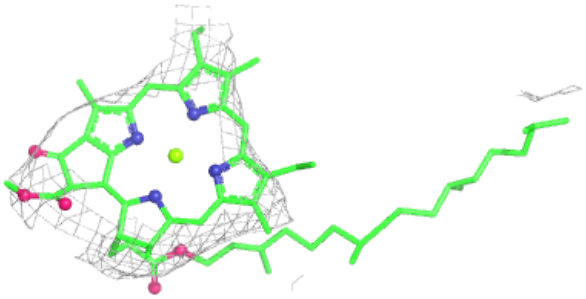


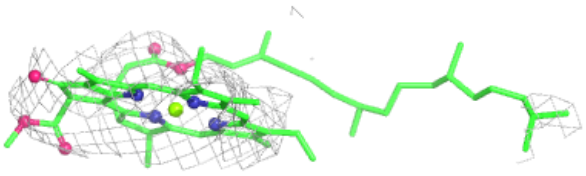


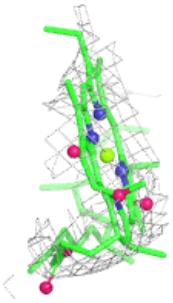


Electron density around CLA C 501:

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



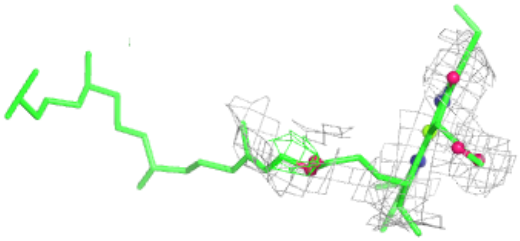


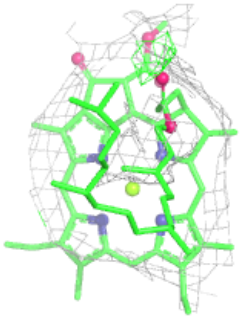


Electron density around CLA d 405:

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

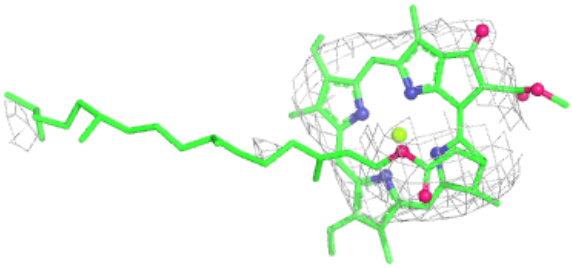


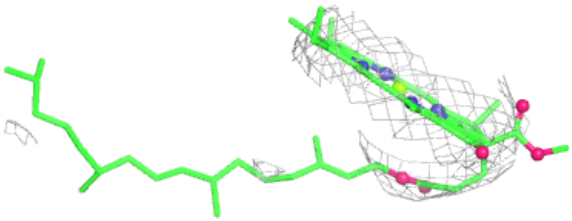


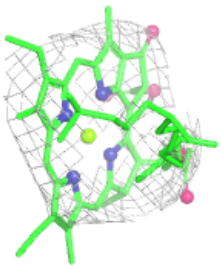


Electron density around CLA b 611:

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

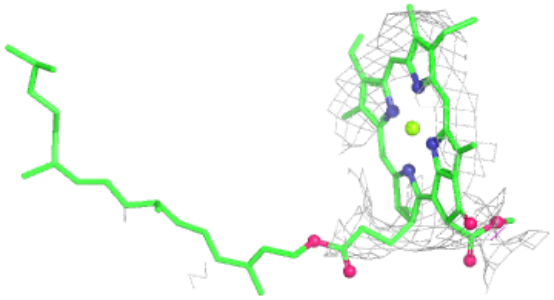


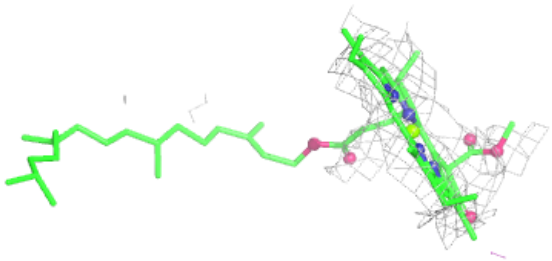


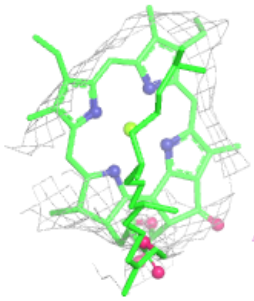


Electron density around CLA b 612:

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

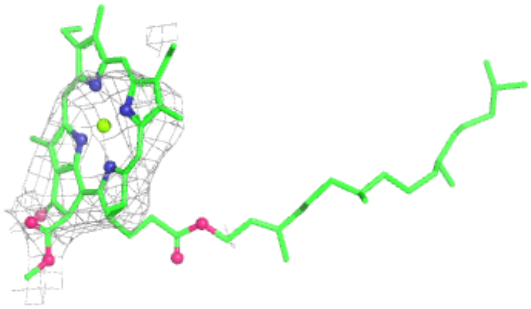


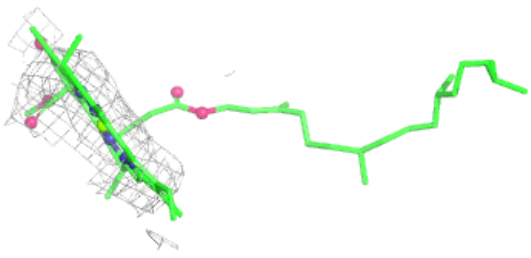


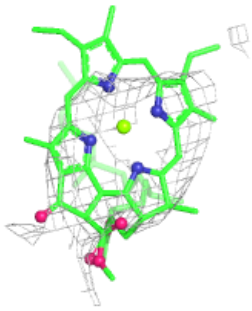


Electron density around CLA a 408:

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

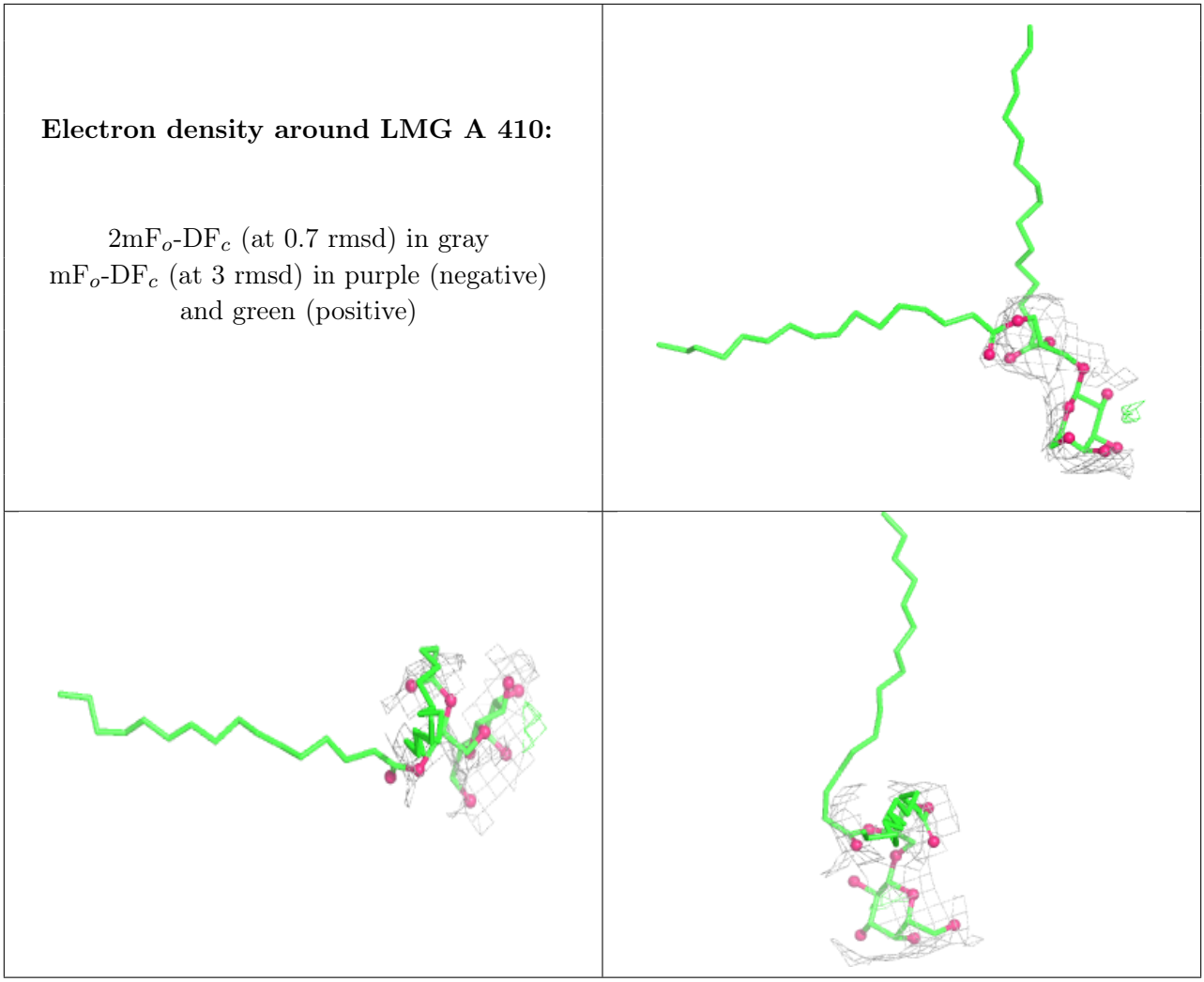






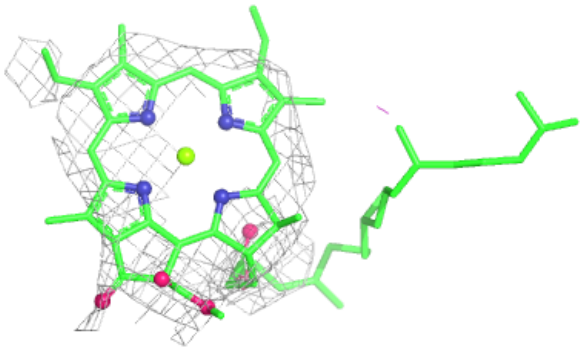
Electron density around LMG A 410:

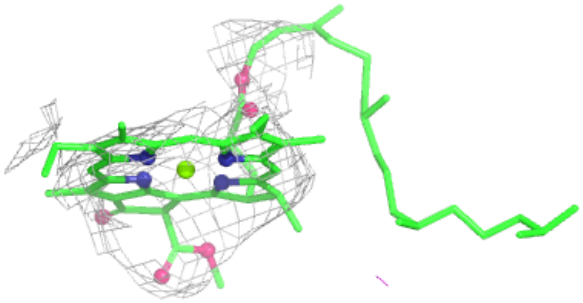
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

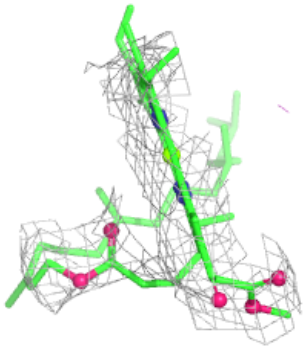


Electron density around CLA A 403:

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

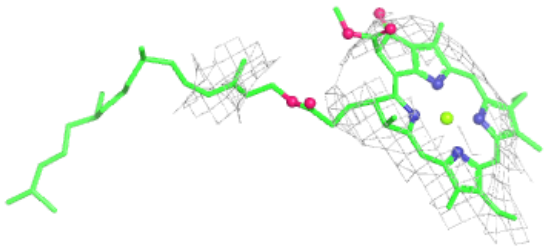


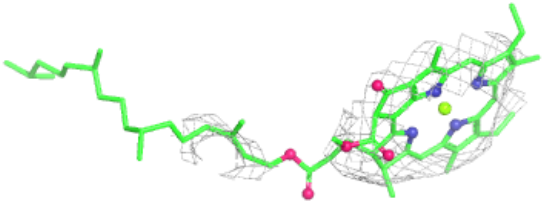


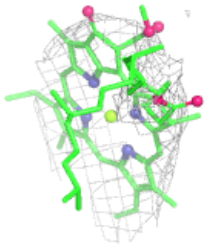


Electron density around CLA a 404:

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

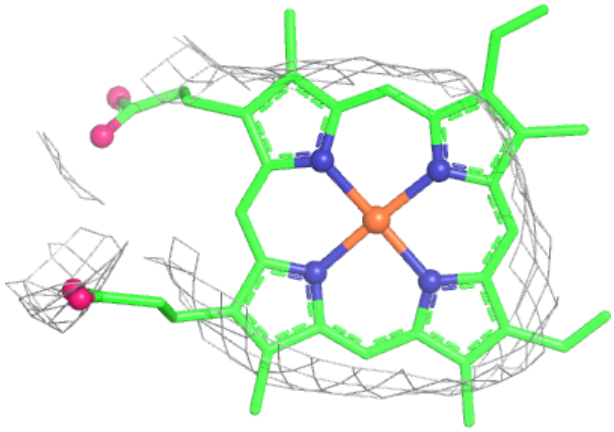


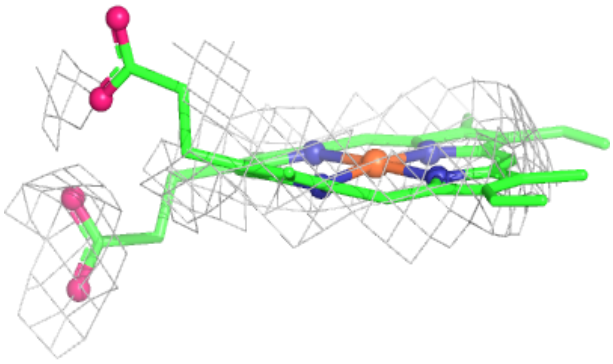


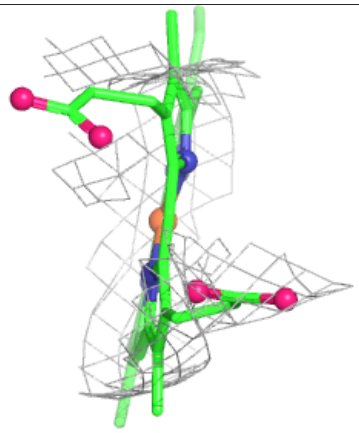


Electron density around HEM f 101:

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

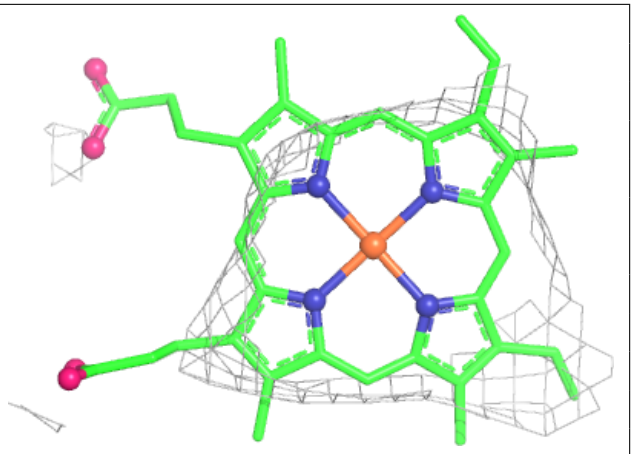


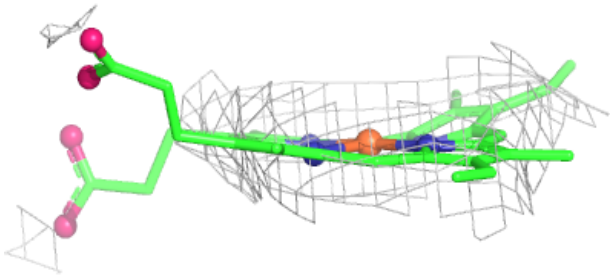


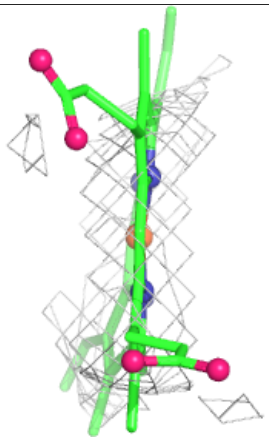


Electron density around HEM v 201:

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

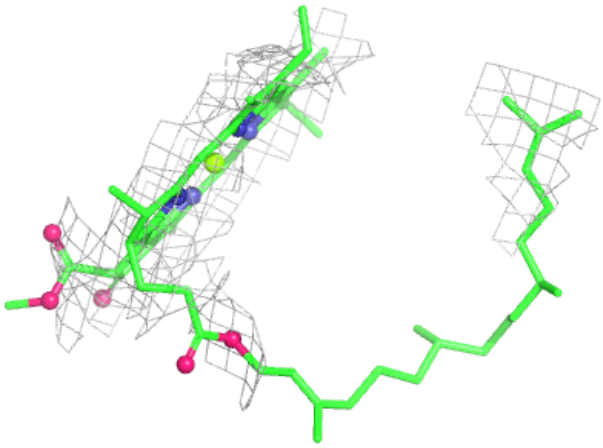


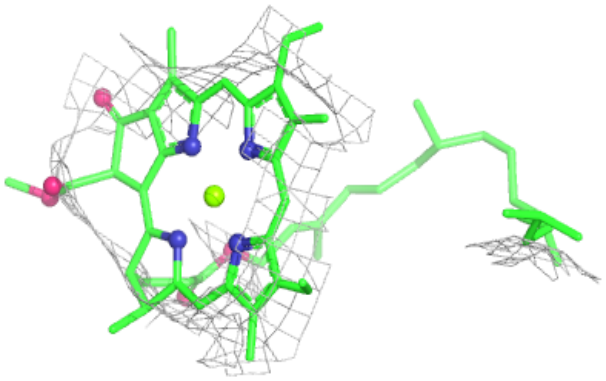


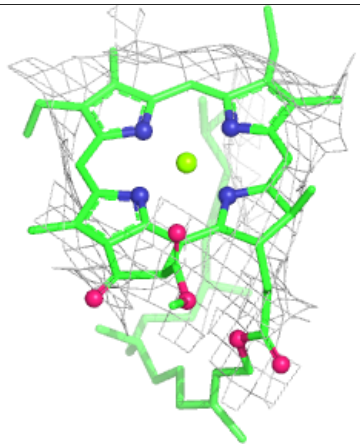


Electron density around CLA B 610:

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

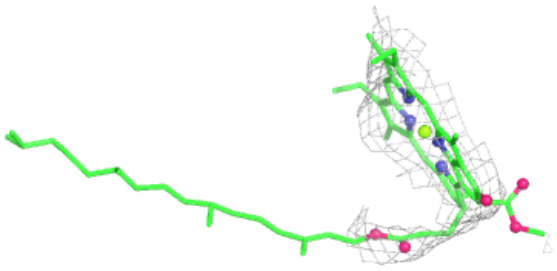


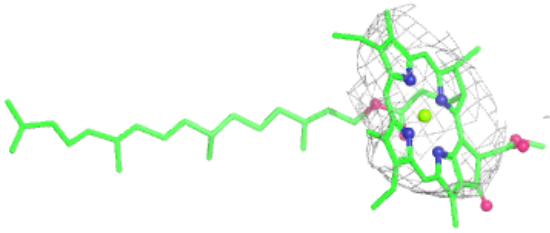


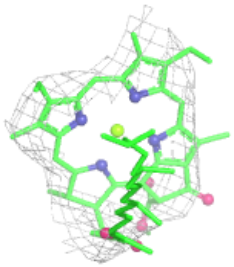


Electron density around CLA B 606:

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

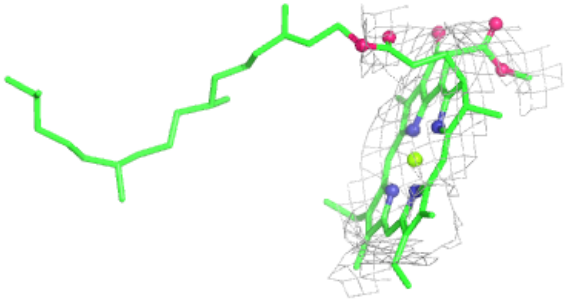


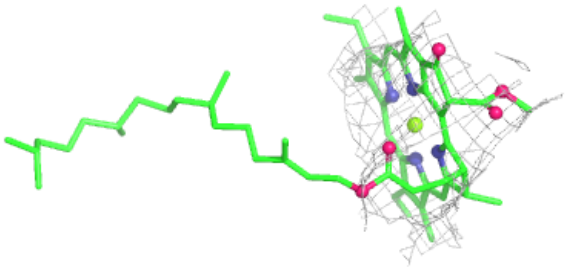


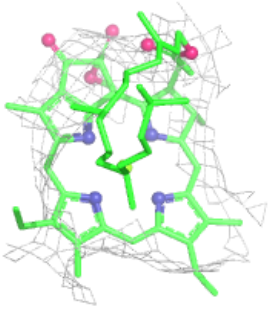


Electron density around CLA c 507:

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

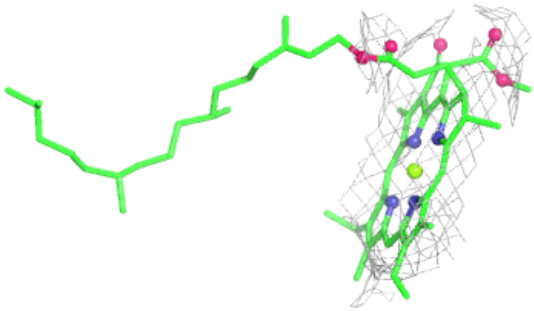


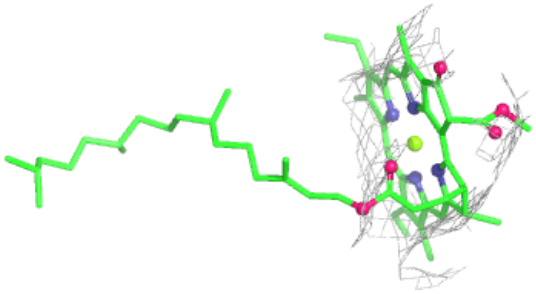


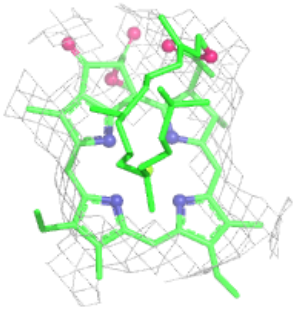


Electron density around CLA C 507:

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

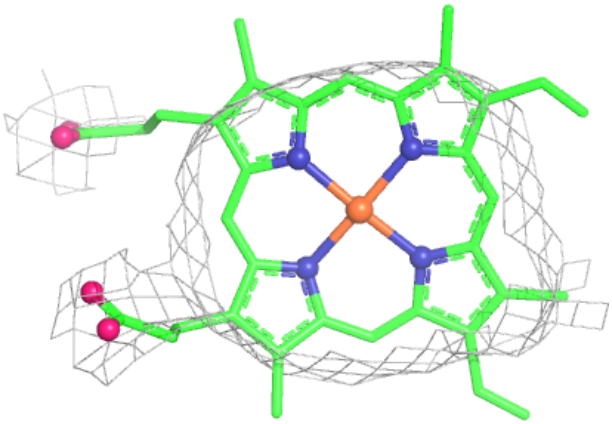


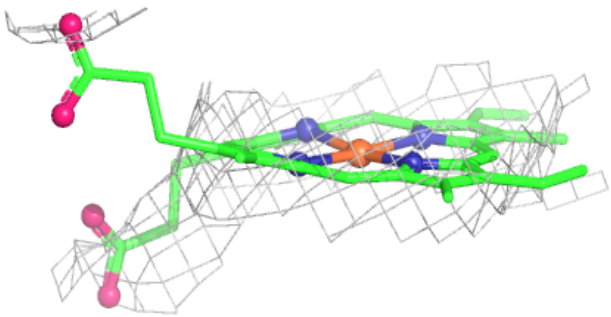


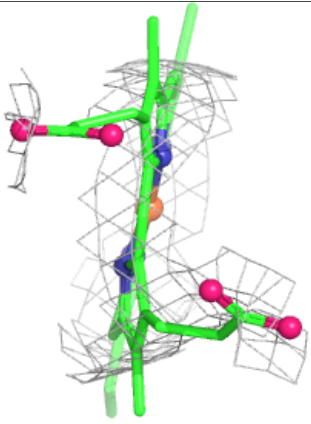


Electron density around HEM F 101:

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

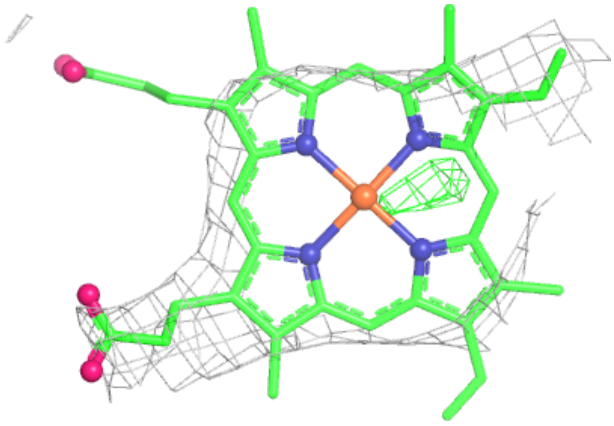


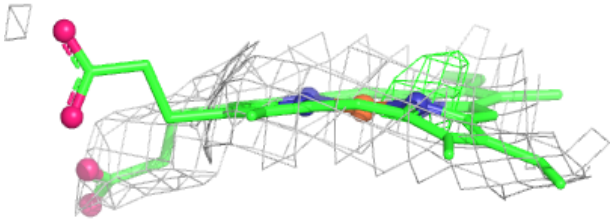


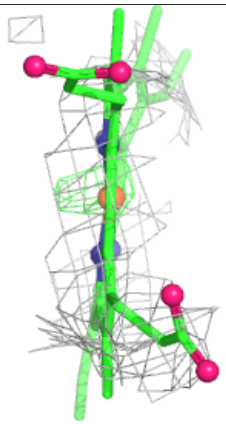


Electron density around HEM V 201:

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

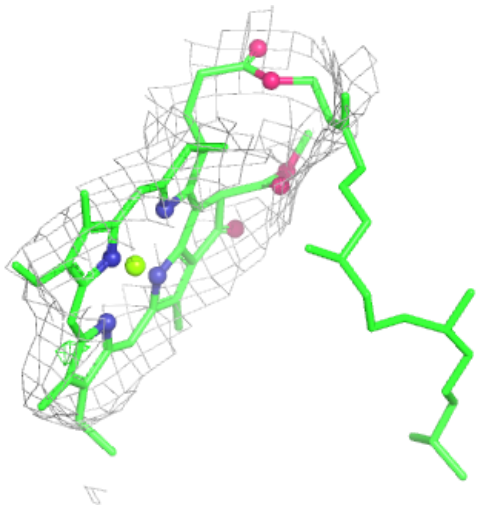


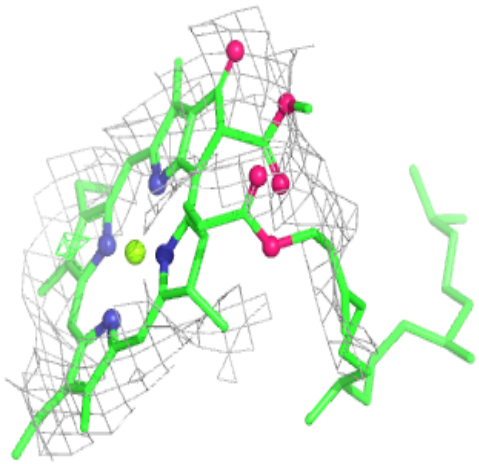


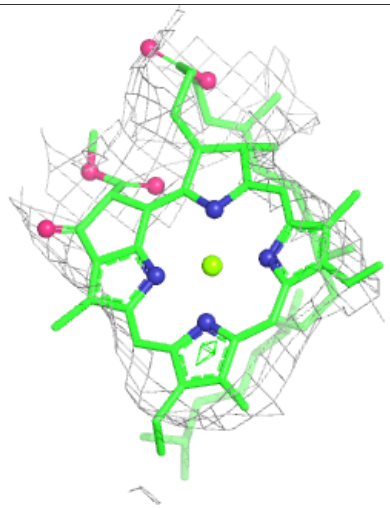


Electron density around CLA B 612:

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

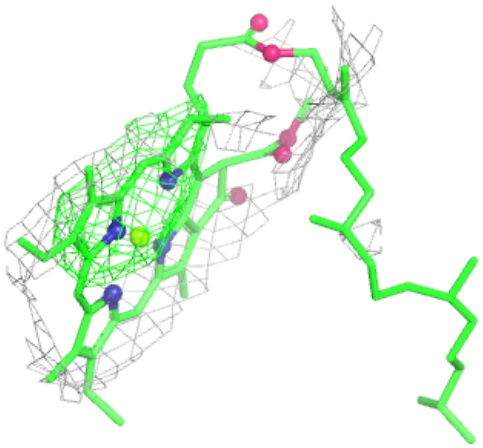


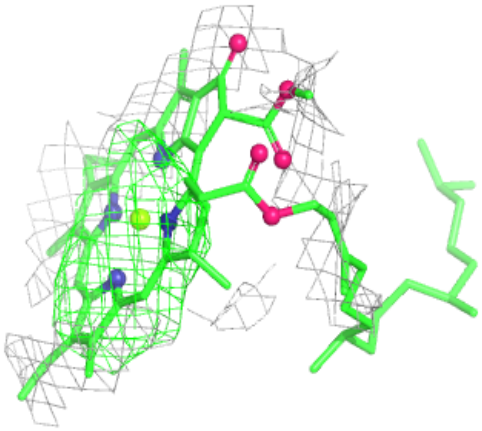


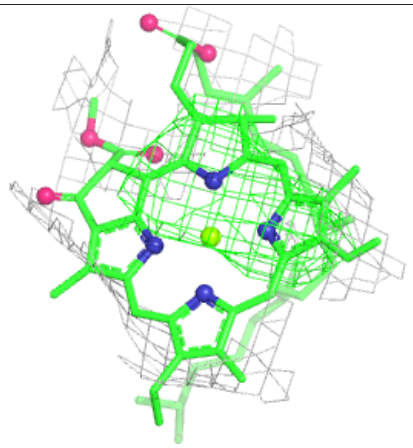


Electron density around CLA b 616:

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

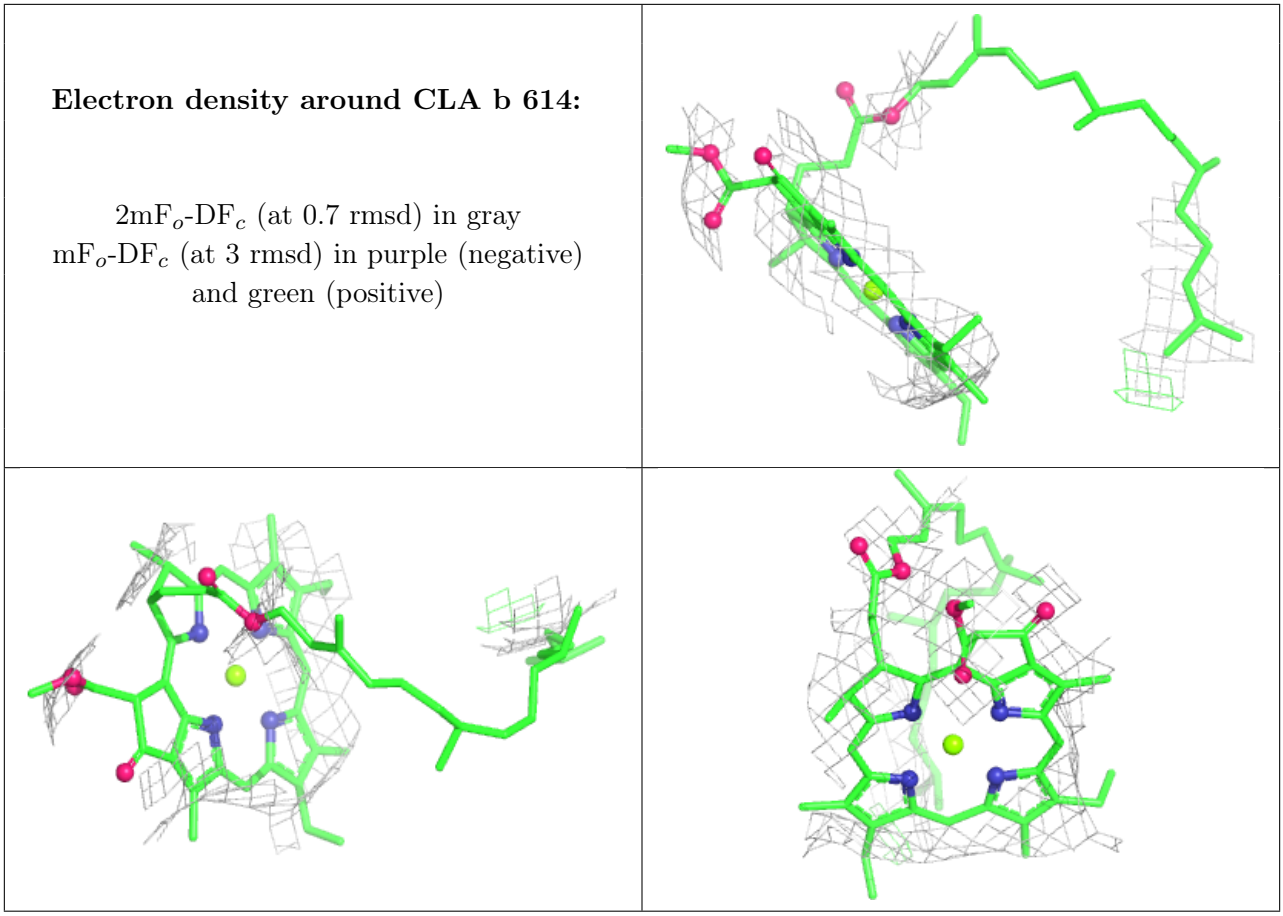






Electron density around CLA b 614:

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



6.5 Other polymers

There are no such residues in this entry.