wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 03:35 AM JST

PDB ID	:	4UB8 / pdb_00004ub8
Title	:	Native structure of photosystem II (dataset-2) by a femtosecond X-ray laser
Authors	:	Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R.
Deposited on	:	2014-08-12
Resolution	:	1.95 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:

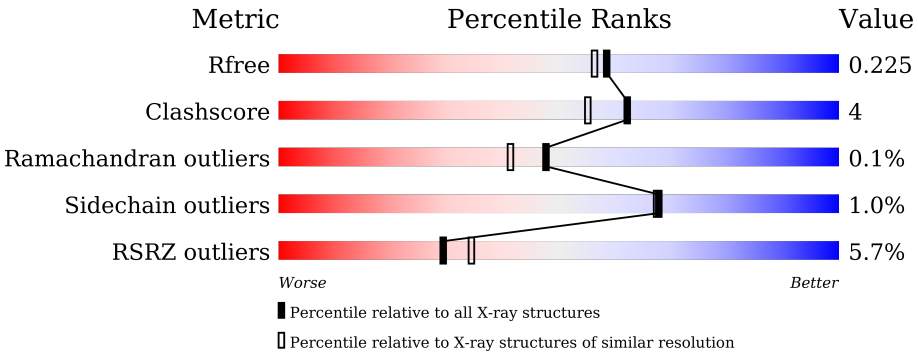
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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.



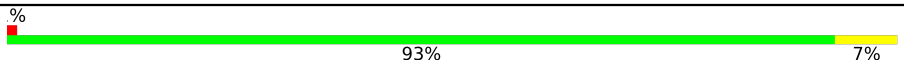
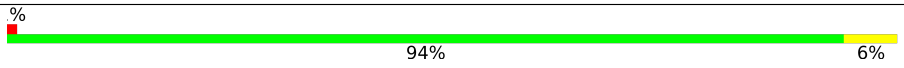
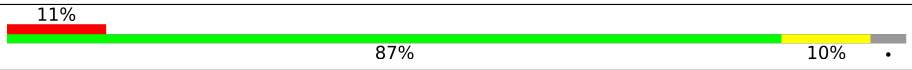
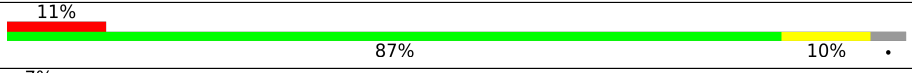
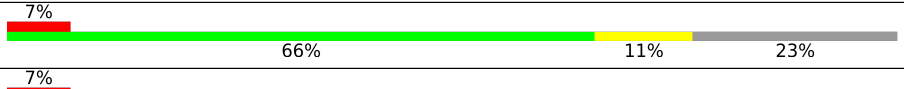
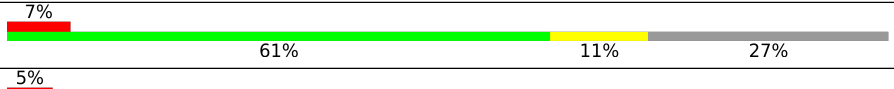
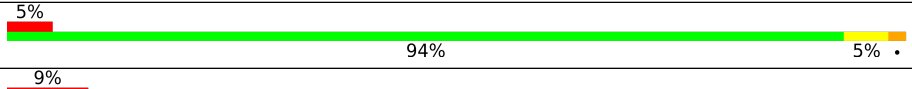
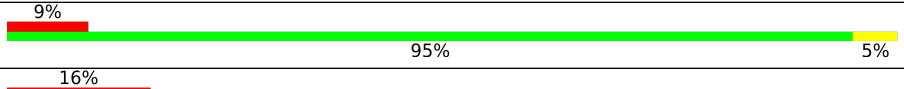
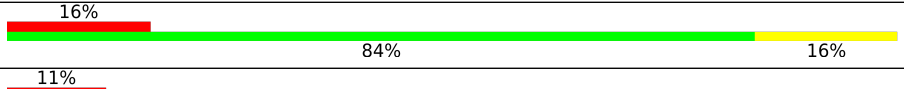
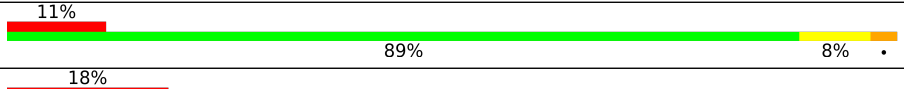
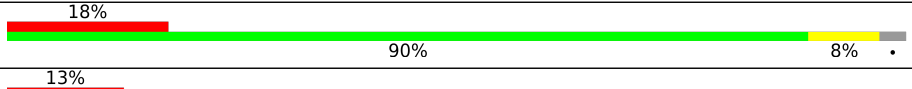
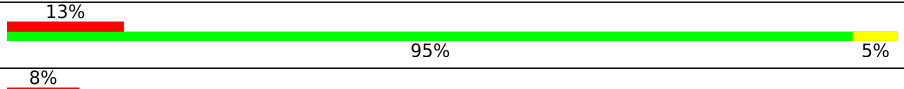
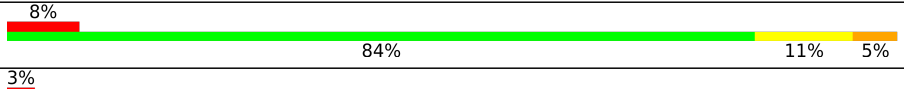
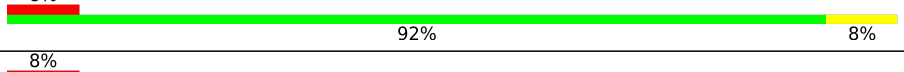
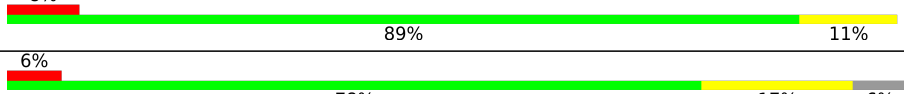
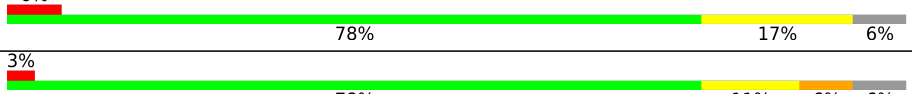
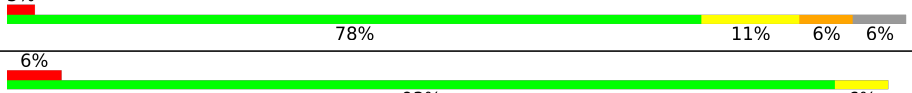
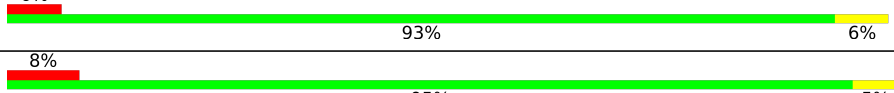
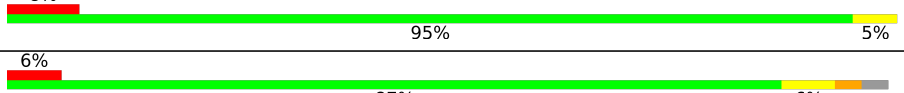
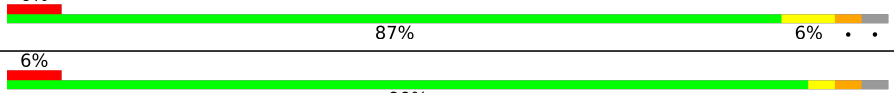
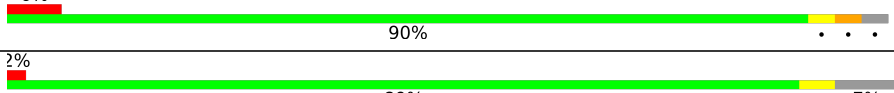
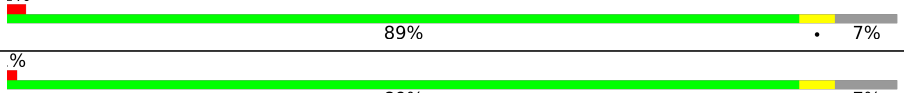
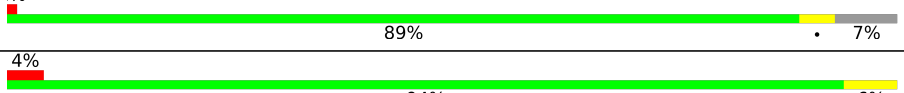
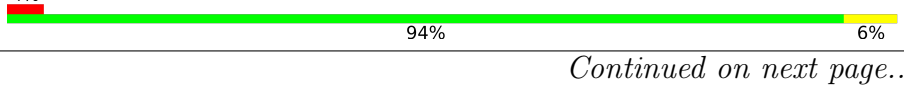
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	92% 5%
1	a	344	2% 90% 7%
2	B	505	3% 93% 7%
2	b	505	5% 94% 6%
3	C	455	2% 93% 6%
3	c	455	2% 93% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	31	
14	t	31	
15	U	104	
15	u	104	
16	V	137	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	v	137	4% 95% 5%
17	Y	30	33% 80% 17%
17	y	30	30% 77% 20%
18	X	40	22% 92% 5%
18	x	40	15% 90% 8%
19	Z	62	32% 94% 6%
19	z	62	34% 90% 10%
20	R	34	88% 79% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CL	u	201	-	-	X	-
40	HEC	V	203	X	-	-	-
40	HEC	v	202	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 53958 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2631	1725	431	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2634	1727	431	461	15			

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4023	2642	667	701	13			
2	b	504	Total	C	N	O	S	0	11	0
			4028	2645	668	702	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total 668	C 436	N 107	O 125	0	2	0
5	e	81	Total 662	C 432	N 107	O 123	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total 275	C 187	N 45	O 42	S 1	0	0	0
6	f	32	Total 257	C 175	N 43	O 38	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 519	C 346	N 85	O 86	S 2	0	1	0
7	h	65	Total 511	C 341	N 82	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	38	Total 314	C 211	N 48	O 54	S 1	0	0	0
8	i	38	Total 314	C 211	N 48	O 54	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	38	Total 272	C 182	N 42	O 47	S 1	0	0	0
9	j	39	Total 282	C 188	N 43	O 49	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 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 309	C 207	N 48	O 53	S 1	0	1	0
11	l	37	Total 309	C 207	N 48	O 53	S 1	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total 274	C 184	N 40	O 49	S 1	0	1	0
12	m	34	Total 269	C 179	N 40	O 49	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 1883	C 1178	N 315	O 385	S 5	0	4	0
13	o	243	Total 1879	C 1175	N 315	O 384	S 5	0	3	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	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	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	1	0
			292	196	46	50			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

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

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

Continued on next page...

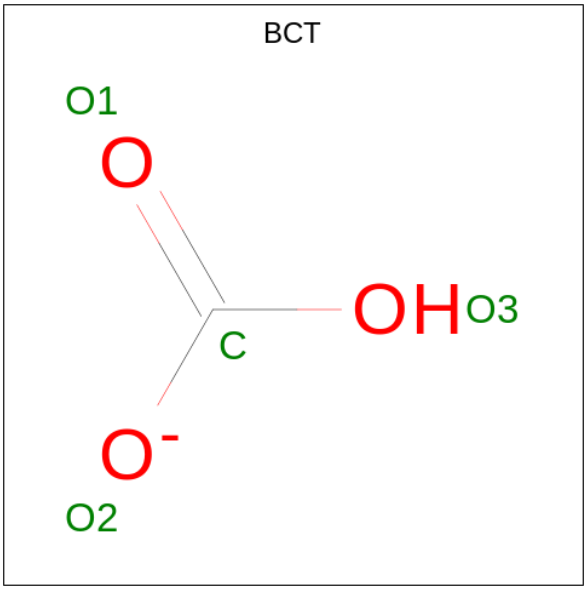
Continued from previous page...

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

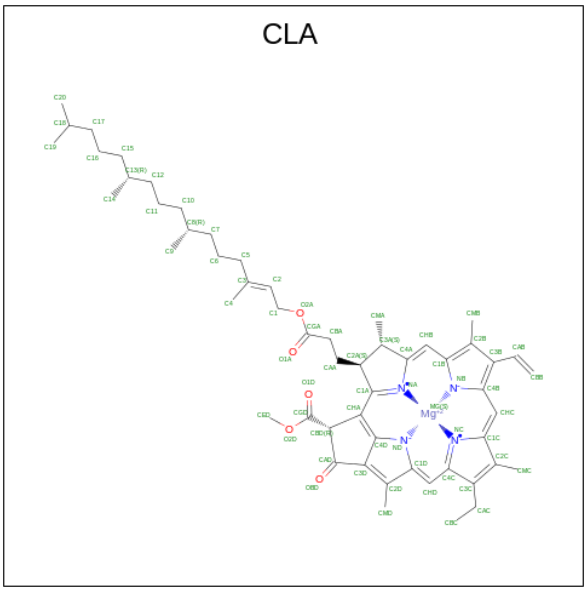
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	2	Total Cl 2 2	0	0
22	V	1	Total Cl 1 1	0	0
22	a	2	Total Cl 2 2	0	0
22	u	1	Total Cl 1 1	0	0

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

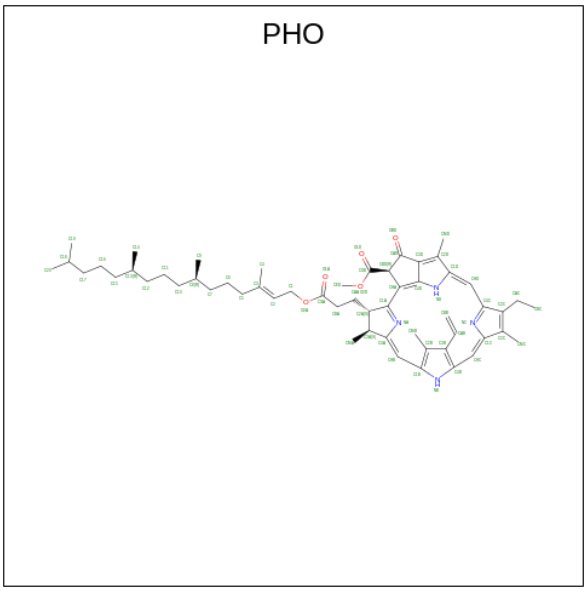
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

Continued on next page...

Continued from previous page...

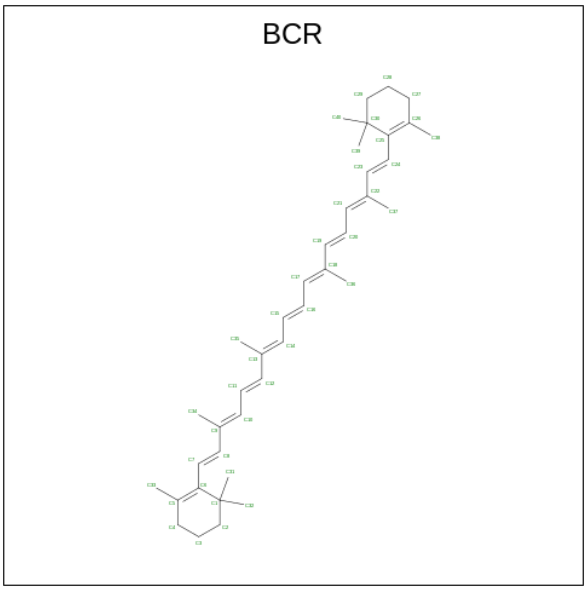
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



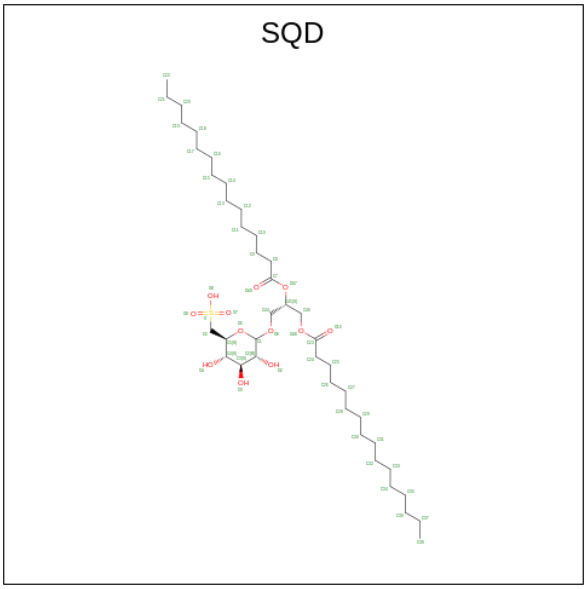
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



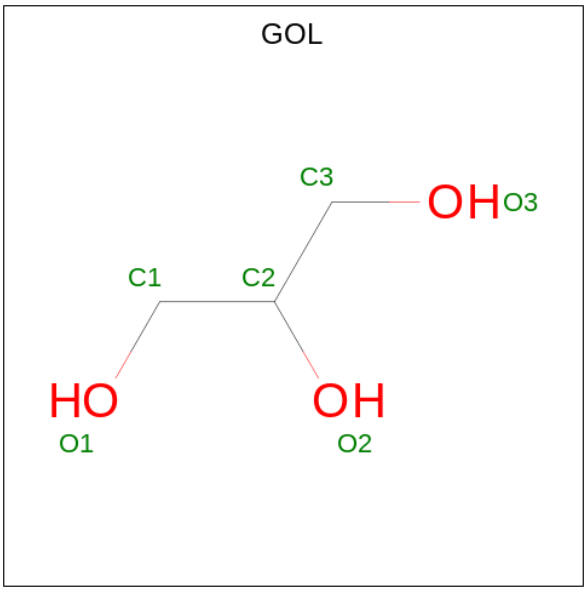
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

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



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

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	F	1	Total C O 6 3 3	0	0
28	O	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	f	1	Total	C	O	0	0
			6	3	3		
28	t	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

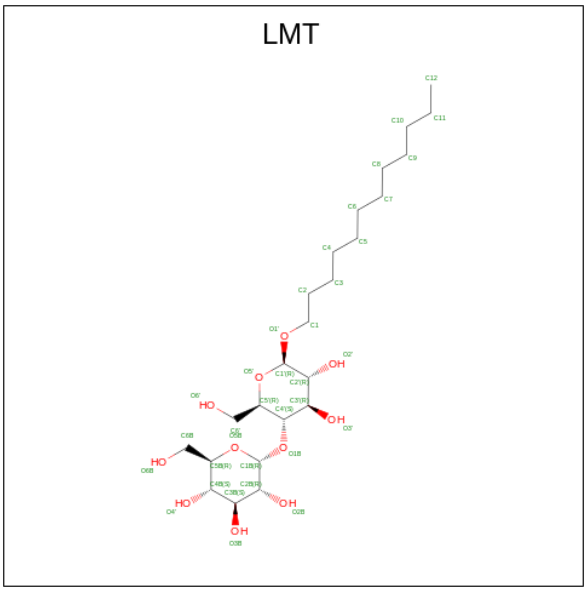
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	v	1	Total C O 6 3 3	0	0
28	v	1	Total C O 6 3 3	0	0

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

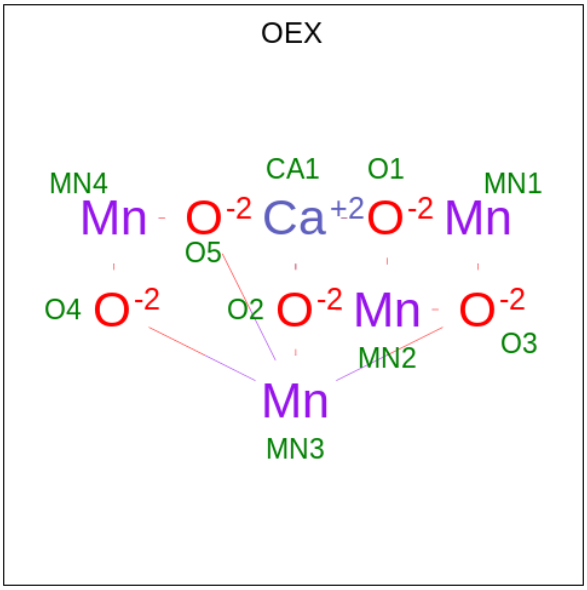
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 28 23 5	0	0
29	B	1	Total C O 33 28 5	0	0
29	C	1	Total C O 34 29 5	0	0
29	D	2	Total C O 57 51 6	0	0
29	I	1	Total C O 40 35 5	0	0
29	J	1	Total C 10 10	0	0
29	M	1	Total C 10 10	0	0
29	X	1	Total C 10 10	0	0
29	a	1	Total C O 30 25 5	0	0
29	b	1	Total C O 33 28 5	0	0
29	d	2	Total C O 53 47 6	0	0
29	i	1	Total C O 40 35 5	0	0
29	j	1	Total C 10 10	0	0
29	k	2	Total C O 42 37 5	0	0
29	m	1	Total C 10 10	0	0
29	x	1	Total C 10 10	0	0

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



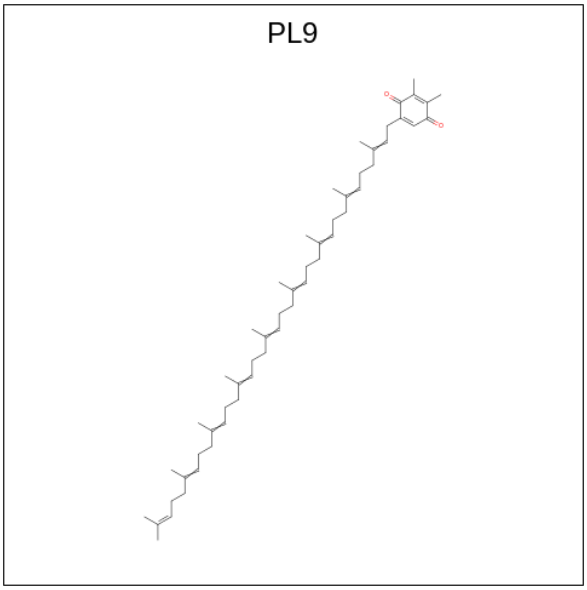
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 33 22 11	0	0
30	B	1	Total C O 25 19 6	0	0
30	D	1	Total C O 35 24 11	0	0
30	E	1	Total C O 35 24 11	0	0
30	I	1	Total C O 35 24 11	0	0
30	M	1	Total C O 35 24 11	0	0
30	M	1	Total C O 35 24 11	0	0
30	a	1	Total C O 35 24 11	0	0
30	a	1	Total C O 35 24 11	0	0
30	b	1	Total C O 25 19 6	0	0
30	b	1	Total C O 25 19 6	0	0
30	f	1	Total C O 35 24 11	0	0
30	m	1	Total C O 35 24 11	0	0
30	m	1	Total C O 35 24 11	0	0

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 32 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: $C_{53}H_{80}O_2$).

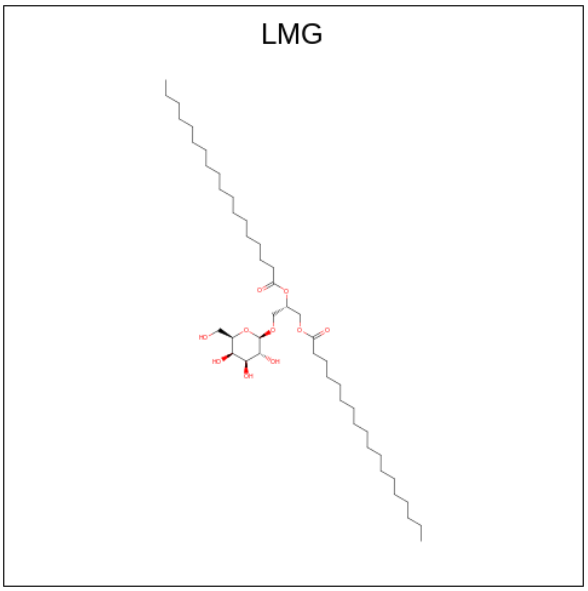


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 55 53 2	0	0
32	D	1	Total C O 55 53 2	0	0
32	a	1	Total C O 55 53 2	0	0
32	d	1	Total C O 55 53 2	0	0

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

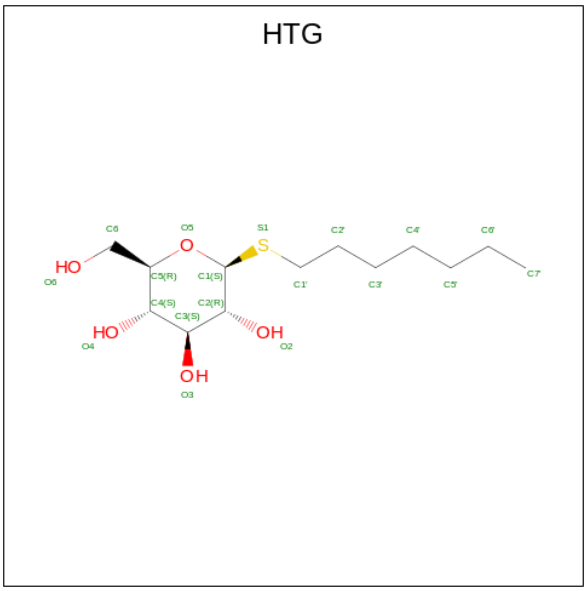
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	f	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	J	1	Total C O 51 41 10	0	0
34	Z	1	Total C O 37 27 10	0	0
34	b	1	Total C O 51 41 10	0	0
34	c	1	Total C O 51 41 10	0	0
34	c	1	Total C O 51 41 10	0	0
34	c	1	Total C O 51 41 10	0	0
34	j	1	Total C O 51 41 10	0	0
34	z	1	Total C O 39 29 10	0	0

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



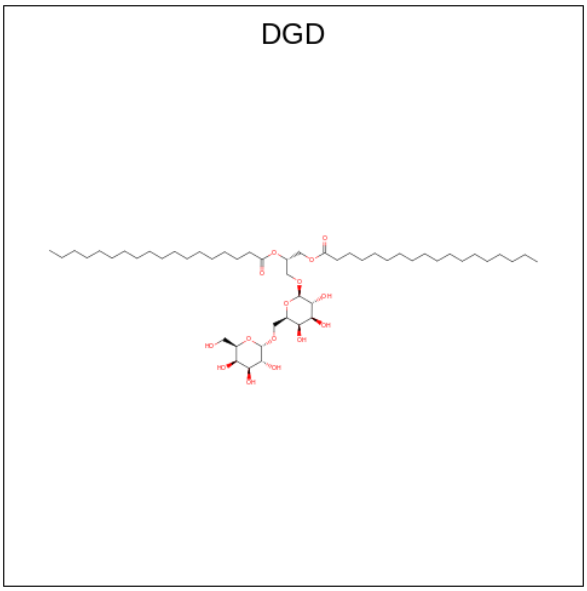
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	c	1	Total C O S 19 13 5 1	0	0
35	c	1	Total C O S 19 13 5 1	0	0
35	d	1	Total C O S 16 10 5 1	0	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



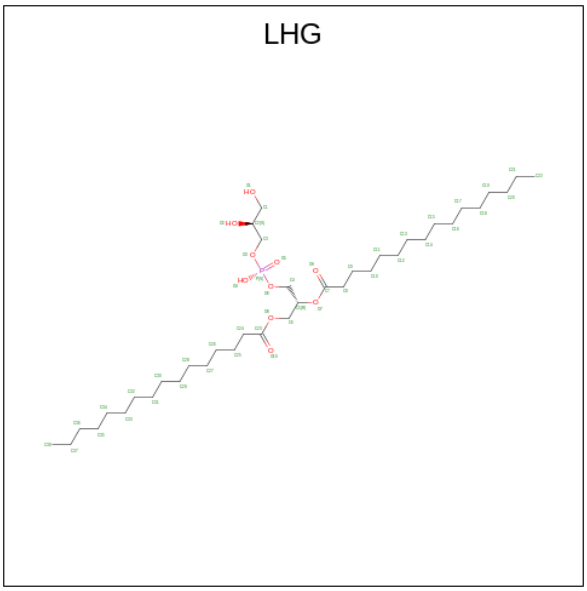
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	D	1	Total C O 62 47 15	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	d	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



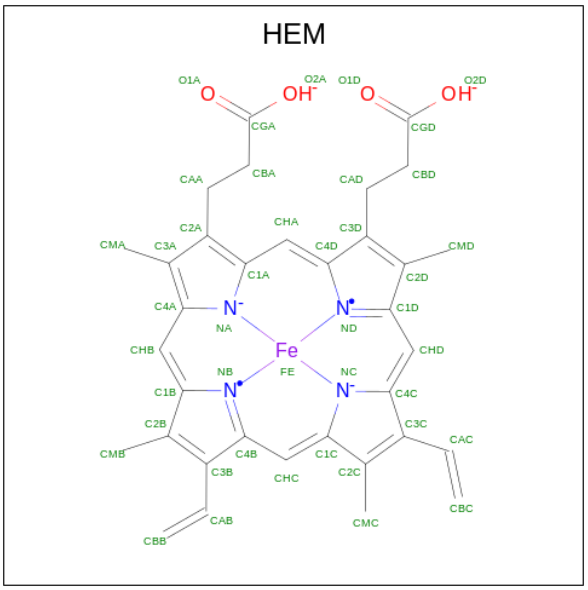
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	E	1	Total C O P 42 31 10 1	0	0
37	L	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49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

Continued on next page...

Continued from previous page...

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

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

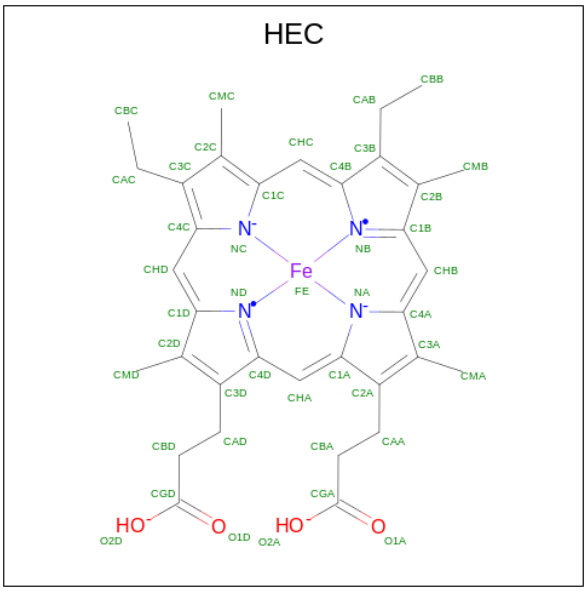


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	146	Total	O	0	3
			149	149		
41	B	277	Total	O	0	3
			280	280		
41	C	206	Total	O	0	3
			209	209		
41	D	157	Total	O	0	4
			161	161		
41	E	28	Total	O	0	0
			28	28		
41	F	7	Total	O	0	0
			7	7		
41	H	39	Total	O	0	1
			40	40		
41	I	8	Total	O	0	0
			8	8		
41	J	12	Total	O	0	0
			12	12		
41	K	6	Total	O	0	0
			6	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	12	Total O 12 12	0	0
41	M	15	Total O 15 15	0	0
41	O	164	Total O 165 165	0	1
41	T	12	Total O 13 13	0	1
41	U	75	Total O 76 76	0	1
41	V	111	Total O 111 111	0	0
41	Y	1	Total O 1 1	0	0
41	X	8	Total O 8 8	0	0
41	a	151	Total O 151 151	0	0
41	b	247	Total O 249 249	0	2
41	c	187	Total O 189 189	0	2
41	d	136	Total O 139 139	0	3
41	e	15	Total O 15 15	0	0
41	f	7	Total O 7 7	0	0
41	h	36	Total O 36 36	0	0
41	i	5	Total O 5 5	0	0
41	j	7	Total O 7 7	0	0
41	k	3	Total O 3 3	0	0
41	l	10	Total O 10 10	0	0
41	m	12	Total O 12 12	0	0
41	o	137	Total O 137 137	0	0

Continued on next page...

Continued from previous page...

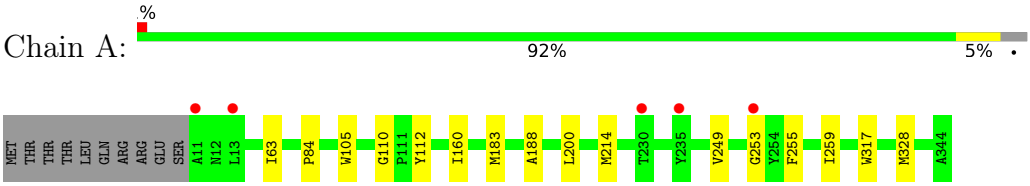
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	t	10	Total O 10 10	0	0
41	u	89	Total O 89 89	0	0
41	v	80	Total O 80 80	0	0
41	y	4	Total O 4 4	0	0
41	x	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

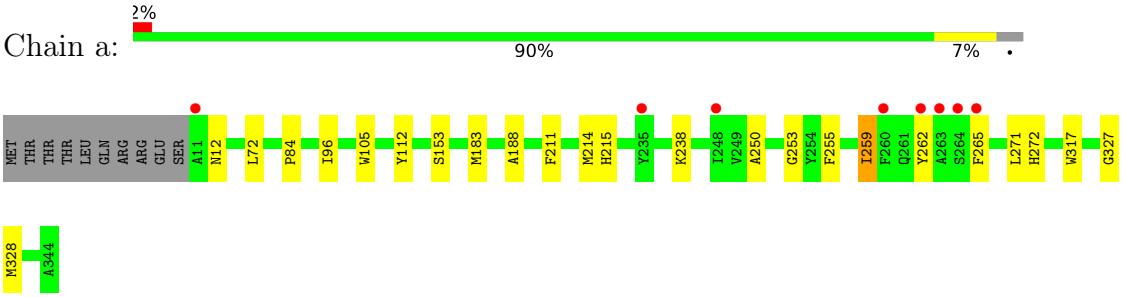
• Molecule 1: Photosystem Q(B) protein

Chain A:



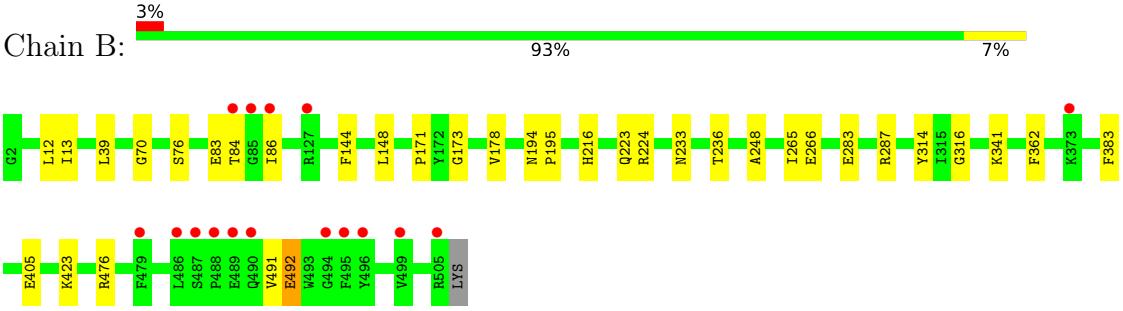
• Molecule 1: Photosystem Q(B) protein

Chain a:



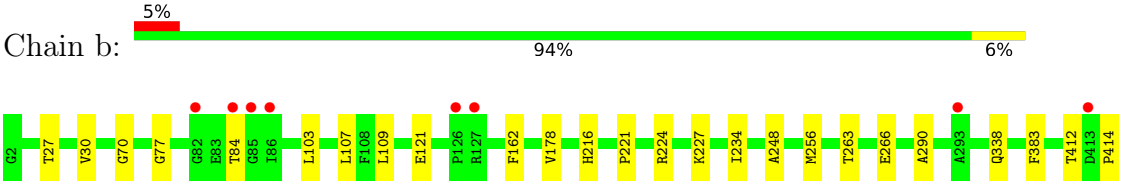
• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

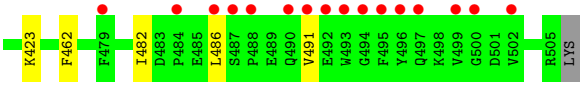
Chain B:



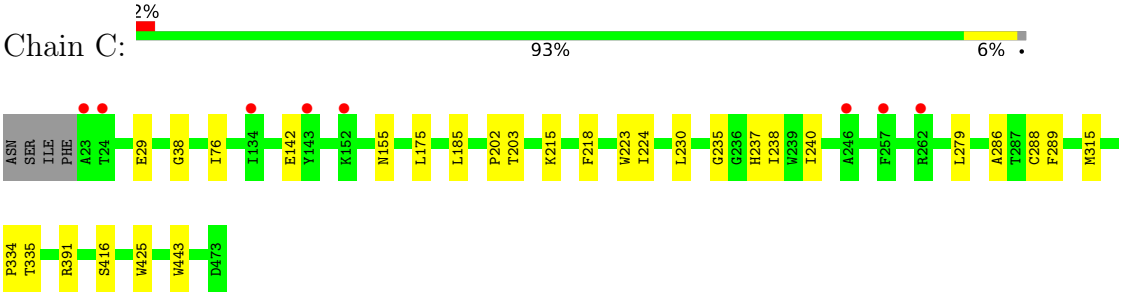
• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

Chain b:

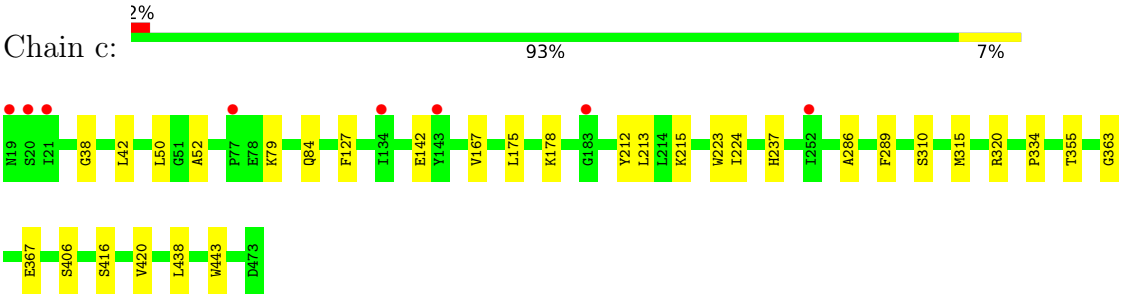




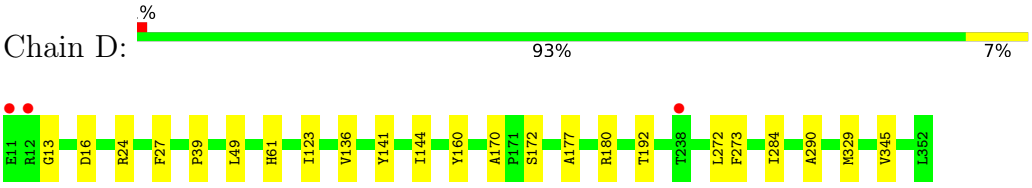
• Molecule 3: Photosystem II 44 kDa reaction center protein



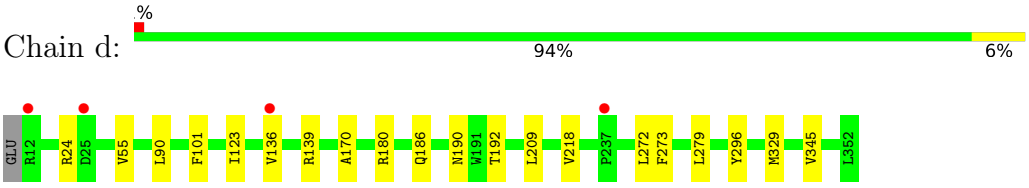
• Molecule 3: Photosystem II 44 kDa reaction center protein



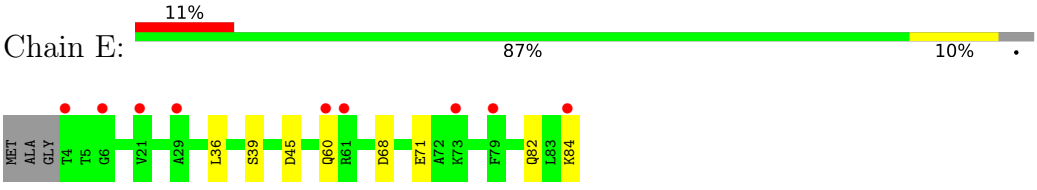
• Molecule 4: Photosystem II D2 protein



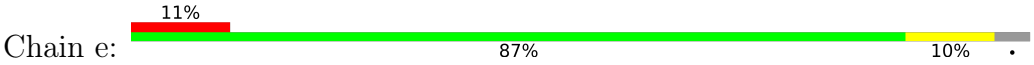
• Molecule 4: Photosystem II D2 protein

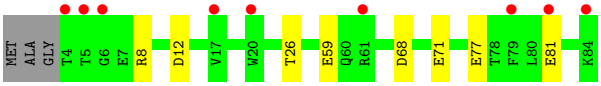


• Molecule 5: Cytochrome b559 subunit alpha



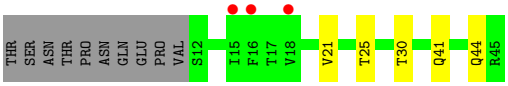
• Molecule 5: Cytochrome b559 subunit alpha





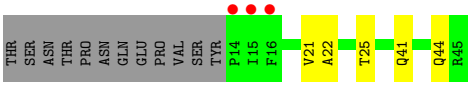
• Molecule 6: Cytochrome b559 subunit beta



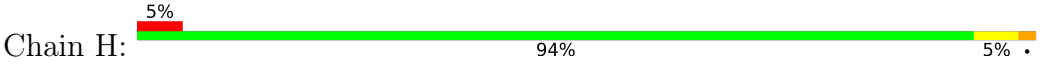


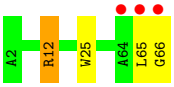
• Molecule 6: Cytochrome b559 subunit beta





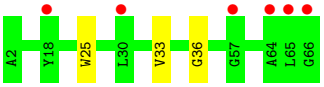
• Molecule 7: Photosystem II reaction center protein H



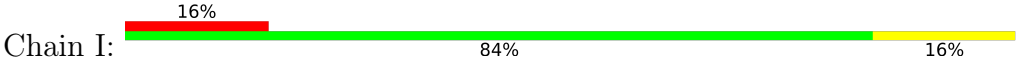


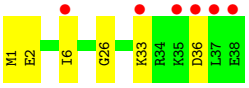
• Molecule 7: Photosystem II reaction center protein H



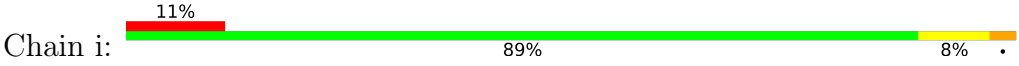


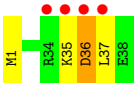
• Molecule 8: Photosystem II reaction center protein I





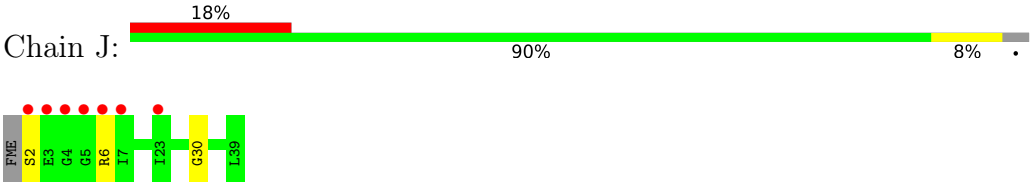
• Molecule 8: Photosystem II reaction center protein I





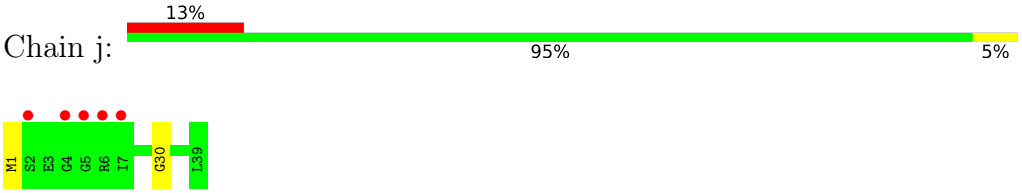
• Molecule 9: Photosystem II reaction center protein J

Chain J:



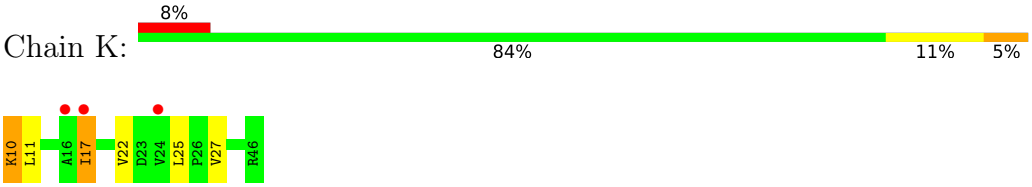
• Molecule 9: Photosystem II reaction center protein J

Chain j:



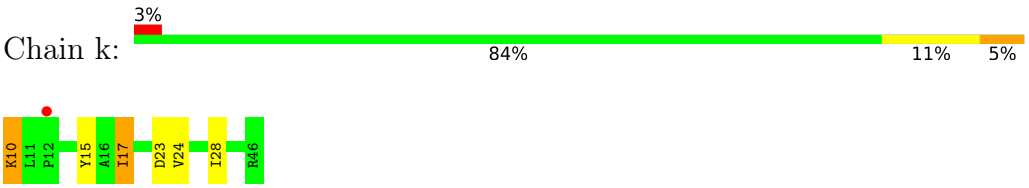
• Molecule 10: Photosystem II reaction center protein K

Chain K:



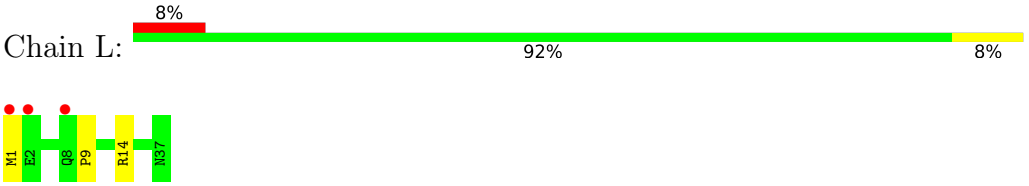
• Molecule 10: Photosystem II reaction center protein K

Chain k:



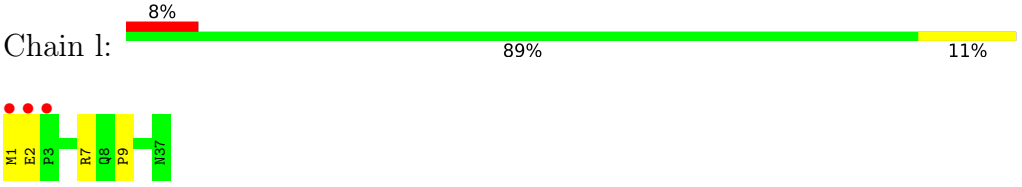
• Molecule 11: Photosystem II reaction center protein L

Chain L:



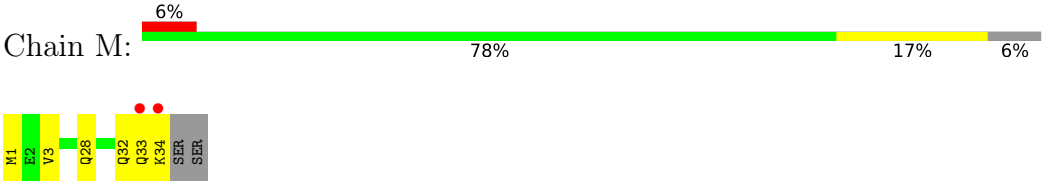
• Molecule 11: Photosystem II reaction center protein L

Chain l:



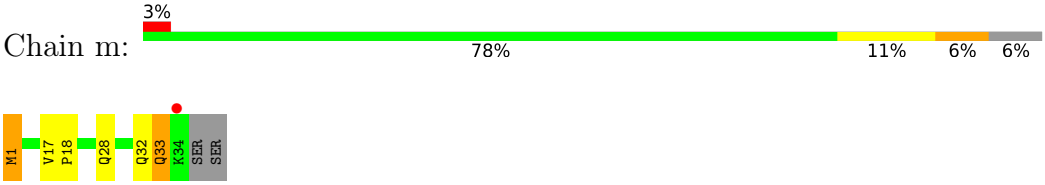
• Molecule 12: Photosystem II reaction center protein M

Chain M:



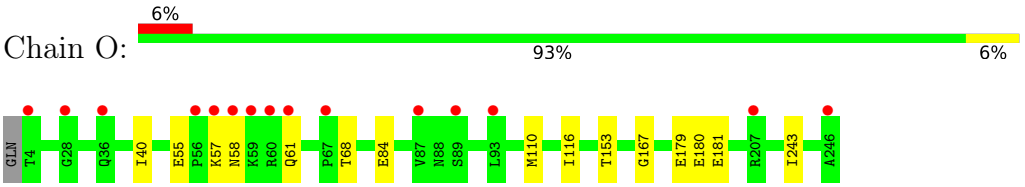
• Molecule 12: Photosystem II reaction center protein M

Chain m:



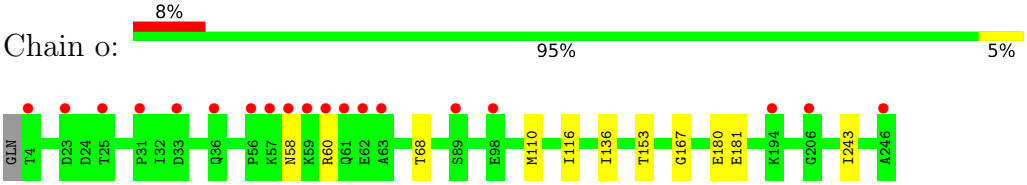
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



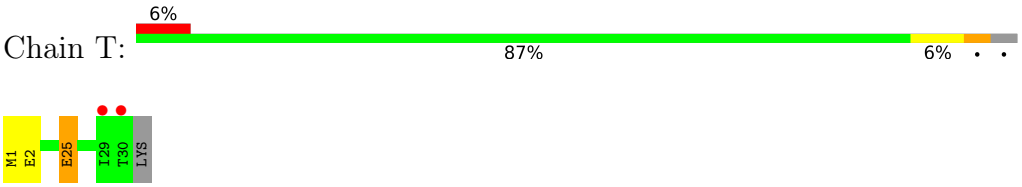
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



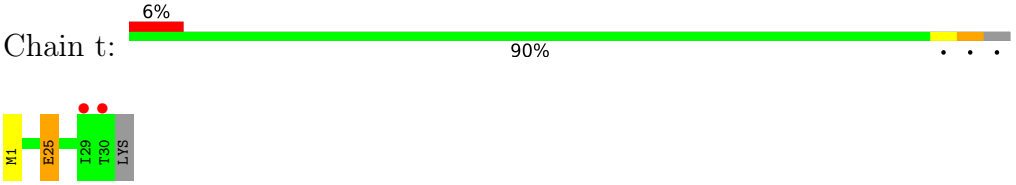
• Molecule 14: Photosystem II reaction center protein T

Chain T:



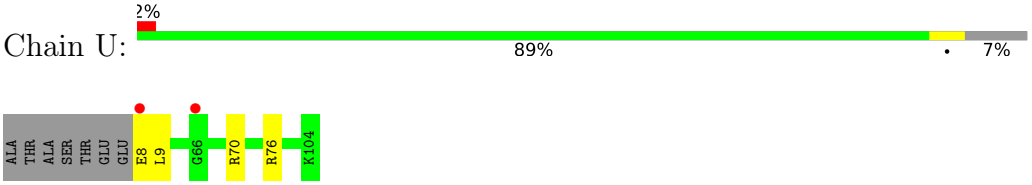
• Molecule 14: Photosystem II reaction center protein T

Chain t:



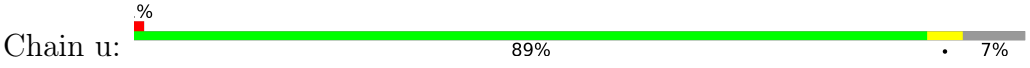
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



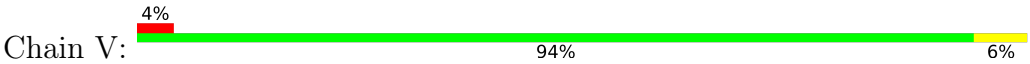
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



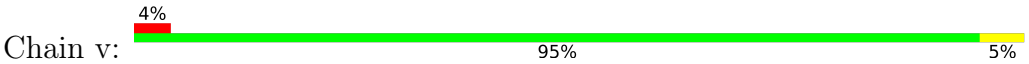


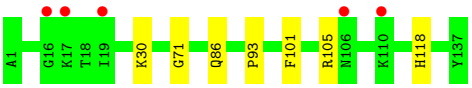
• Molecule 16: Cytochrome c-550



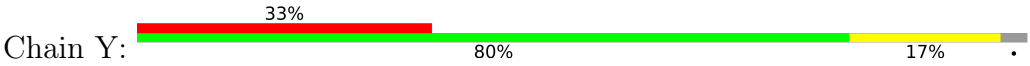


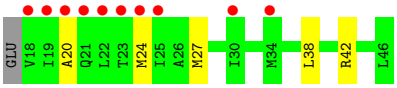
• Molecule 16: Cytochrome c-550



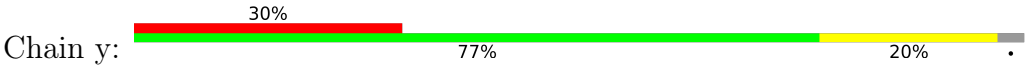


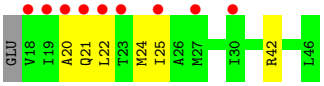
• Molecule 17: Photosystem II reaction center protein Ycf12



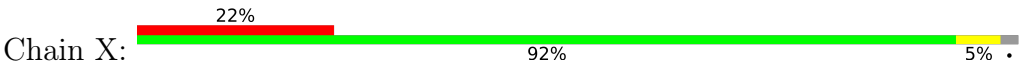


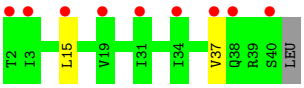
• Molecule 17: Photosystem II reaction center protein Ycf12



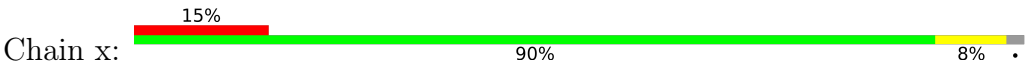


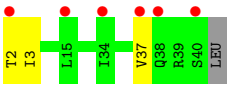
• Molecule 18: Photosystem II reaction center protein X





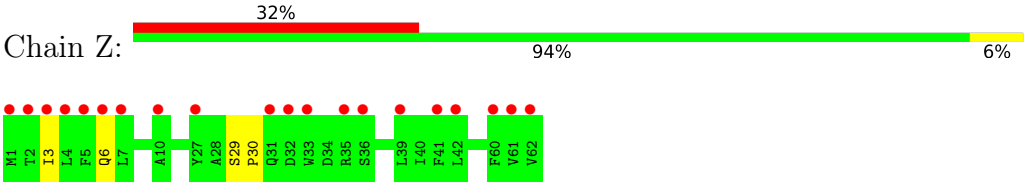
• Molecule 18: Photosystem II reaction center protein X





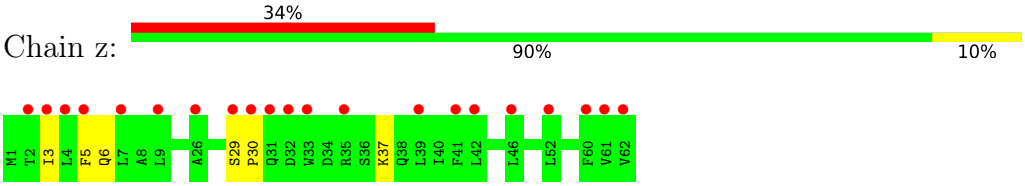
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



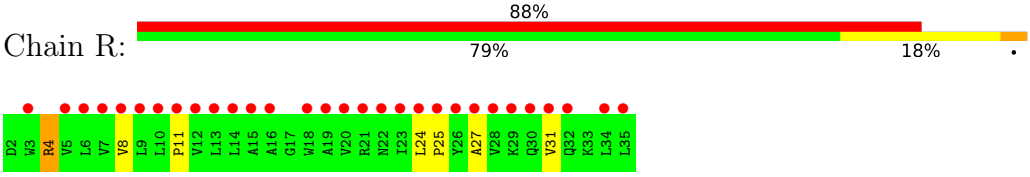
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.81Å 230.00Å 288.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.90 – 1.95 61.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.1 (61.90-1.95) 86.4 (61.90-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.08 (at 1.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.188 , 0.225 0.188 , 0.225	Depositor DCC
R_{free} test set	29342 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	53958	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: UNL, LHG, PHO, BCT, HTG, CL, SQD, HEC, OEX, DGD, CA, MG, HEM, FE2, GOL, LMG, FME, LMT, CLA, BCR, PL9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.67	0/2725	0.86	0/3716
1	a	0.67	1/2731 (0.0%)	0.85	0/3724
2	B	0.60	0/4193	0.83	0/5712
2	b	0.59	0/4201	0.83	3/5723 (0.1%)
3	C	0.56	0/3634	0.82	2/4947 (0.0%)
3	c	0.57	1/3676 (0.0%)	0.82	0/5004
4	D	0.64	0/2821	0.80	2/3844 (0.1%)
4	d	0.64	0/2818	0.82	3/3840 (0.1%)
5	E	0.48	0/693	0.84	0/944
5	e	0.43	0/681	0.82	0/928
6	F	0.57	0/284	0.79	0/387
6	f	0.49	0/265	0.83	0/360
7	H	0.50	0/535	0.78	0/728
7	h	0.43	0/524	0.76	0/713
8	I	0.46	0/311	0.82	0/419
8	i	0.49	0/311	0.74	0/419
9	J	0.47	0/278	0.77	0/376
9	j	0.50	0/278	0.76	0/376
10	K	0.49	0/303	0.75	0/416
10	k	0.59	1/303 (0.3%)	0.83	0/416
11	L	0.55	0/319	0.70	0/433
11	l	0.59	0/319	0.71	0/433
12	M	0.64	0/270	0.88	0/368
12	m	0.72	1/262 (0.4%)	0.92	0/357
13	O	0.52	0/1926	0.82	2/2611 (0.1%)
13	o	0.48	0/1919	0.79	0/2601
14	T	0.65	0/266	0.77	0/362
14	t	0.69	0/266	0.80	0/362
15	U	0.52	0/785	0.78	0/1064
15	u	0.53	0/785	0.73	0/1064
16	V	0.57	0/1096	0.78	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.55	0/1085	0.81	1/1473 (0.1%)
17	Y	0.41	0/216	0.76	0/289
17	y	0.42	0/216	0.78	0/289
18	X	0.41	0/298	0.74	0/403
18	x	0.40	0/290	0.73	0/392
19	Z	0.40	0/490	0.82	0/669
19	z	0.43	0/490	0.81	0/669
20	R	0.36	0/279	0.71	0/383
All	All	0.58	4/43142 (0.0%)	0.81	13/58701 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	17	VAL	CA-CB	7.01	1.58	1.54
10	k	28	ILE	CA-CB	5.54	1.56	1.54
3	c	310	SER	C-O	5.35	1.30	1.24
1	a	327	GLY	C-O	5.09	1.29	1.23

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	v	105	ARG	N-CA-C	6.08	118.70	111.71
4	d	170	ALA	CA-C-N	-5.61	114.15	119.76
4	d	170	ALA	C-N-CA	-5.61	114.15	119.76
2	b	414	PRO	N-CA-C	5.54	117.45	110.70
2	b	221	PRO	O-C-N	5.42	123.80	121.31

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	2631	0	2538	12	0
1	a	2634	0	2543	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4023	0	3904	29	0
2	b	4028	0	3910	25	0
3	C	3506	0	3439	20	0
3	c	3544	0	3480	21	0
4	D	2726	0	2627	20	0
4	d	2720	0	2626	15	0
5	E	668	0	658	7	0
5	e	662	0	648	5	0
6	F	275	0	282	3	0
6	f	257	0	269	3	0
7	H	519	0	545	5	0
7	h	511	0	532	6	0
8	I	314	0	328	4	0
8	i	314	0	328	2	0
9	J	272	0	279	3	0
9	j	282	0	290	1	0
10	K	293	0	305	5	0
10	k	293	0	305	5	0
11	L	309	0	327	2	0
11	l	309	0	327	3	0
12	M	274	0	299	6	0
12	m	269	0	288	5	0
13	O	1883	0	1865	10	0
13	o	1879	0	1858	7	0
14	T	264	0	267	3	0
14	t	264	0	267	1	0
15	U	774	0	773	2	0
15	u	774	0	773	4	0
16	V	1072	0	1086	7	0
16	v	1064	0	1073	3	0
17	Y	215	0	246	3	0
17	y	215	0	246	4	0
18	X	292	0	328	2	0
18	x	287	0	317	2	0
19	Z	479	0	516	1	0
19	z	479	0	516	4	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	V	1	0	0	1	0
22	a	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	u	1	0	0	2	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	195	0	216	6	0
24	B	1040	0	1152	24	0
24	C	845	0	936	20	0
24	D	195	0	216	7	0
24	a	195	0	216	5	0
24	b	1040	0	1152	23	0
24	c	845	0	936	27	0
24	d	195	0	216	5	0
25	A	128	0	148	1	0
25	a	64	0	74	1	0
25	d	64	0	74	1	0
26	A	40	0	56	3	0
26	B	120	0	168	8	0
26	C	80	0	112	3	0
26	D	40	0	56	1	0
26	H	40	0	56	4	0
26	K	40	0	56	1	0
26	T	40	0	56	7	0
26	Y	40	0	56	2	0
26	a	40	0	56	0	0
26	b	120	0	168	8	0
26	c	80	0	112	9	0
26	d	40	0	56	3	0
26	h	40	0	56	4	0
26	k	40	0	56	1	0
26	t	40	0	56	4	0
26	y	40	0	56	1	0
27	A	108	0	156	4	0
27	F	43	0	53	3	0
27	a	108	0	155	4	0
27	b	54	0	78	2	0
27	f	43	0	53	3	0
27	l	54	0	78	2	0
28	A	18	0	24	2	0
28	B	42	0	56	3	0
28	C	12	0	16	1	0
28	F	6	0	8	0	0
28	O	6	0	8	0	0
28	T	12	0	16	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	V	30	0	40	4	0
28	a	12	0	16	2	0
28	b	30	0	40	3	0
28	c	18	0	24	2	0
28	f	6	0	7	0	0
28	t	6	0	8	1	0
28	v	24	0	32	1	0
29	A	28	0	0	0	0
29	B	33	0	0	0	0
29	C	34	0	0	0	0
29	D	57	0	0	0	0
29	I	40	0	0	0	0
29	J	10	0	0	0	0
29	M	10	0	0	0	0
29	X	10	0	0	0	0
29	a	30	0	0	0	0
29	b	33	0	0	0	0
29	d	53	0	0	0	0
29	i	40	0	0	0	0
29	j	10	0	0	0	0
29	k	42	0	0	0	0
29	m	10	0	0	0	0
29	x	10	0	0	0	0
30	A	33	0	39	0	0
30	B	25	0	35	1	0
30	D	35	0	46	1	0
30	E	35	0	46	0	0
30	I	35	0	46	2	0
30	M	70	0	92	3	0
30	a	70	0	92	4	0
30	b	50	0	70	1	0
30	f	35	0	46	0	0
30	m	70	0	92	2	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	A	55	0	80	4	0
32	D	55	0	80	0	0
32	a	55	0	80	10	0
32	d	55	0	80	0	0
33	B	1	0	0	0	0
33	F	1	0	0	0	0
33	O	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	f	1	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	2	0
34	C	153	0	216	7	0
34	J	51	0	72	2	0
34	Z	37	0	44	1	0
34	b	51	0	72	1	0
34	c	153	0	216	3	0
34	j	51	0	72	1	0
34	z	39	0	48	4	0
35	B	95	0	130	4	0
35	C	38	0	52	3	0
35	D	16	0	17	2	0
35	O	19	0	26	0	0
35	V	19	0	26	1	0
35	b	76	0	104	1	0
35	c	38	0	52	0	0
35	d	16	0	17	2	0
36	C	186	0	246	7	0
36	D	62	0	82	1	0
36	H	62	0	82	2	0
36	c	186	0	246	3	0
36	d	62	0	82	5	0
36	h	62	0	82	0	0
37	D	147	0	222	10	0
37	E	42	0	57	2	0
37	L	49	0	74	1	0
37	d	147	0	222	4	0
37	e	42	0	57	4	0
37	l	49	0	74	4	0
38	E	43	0	30	0	0
38	e	43	0	30	2	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	149	0	0	1	0
41	B	280	0	0	4	0
41	C	209	0	0	3	0
41	D	161	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	E	28	0	0	1	0
41	F	7	0	0	0	0
41	H	40	0	0	0	0
41	I	8	0	0	0	0
41	J	12	0	0	1	0
41	K	6	0	0	1	0
41	L	12	0	0	0	0
41	M	15	0	0	0	0
41	O	165	0	0	2	0
41	T	13	0	0	0	0
41	U	76	0	0	2	0
41	V	111	0	0	1	0
41	X	8	0	0	0	0
41	Y	1	0	0	0	0
41	a	151	0	0	1	0
41	b	249	0	0	2	0
41	c	189	0	0	3	0
41	d	139	0	0	1	0
41	e	15	0	0	0	0
41	f	7	0	0	0	0
41	h	36	0	0	0	0
41	i	5	0	0	0	0
41	j	7	0	0	0	0
41	k	3	0	0	0	0
41	l	10	0	0	1	0
41	m	12	0	0	0	0
41	o	137	0	0	0	0
41	t	10	0	0	0	0
41	u	89	0	0	3	0
41	v	80	0	0	1	0
41	x	5	0	0	0	0
41	y	4	0	0	0	0
All	All	53958	0	52755	427	0

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

The worst 5 of 427 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)
1:A:214:MET:HG2	32:A:419:PL9:H102	1.51	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.49	0.92
1:a:214:MET:HG2	32:a:416:PL9:H102	1.54	0.87
24:B:616:CLA:H71	24:B:617:CLA:H192	1.64	0.78
22:u:201:CL:CL	41:u:337:HOH:O	2.40	0.75

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	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	36 28
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	36 28
2	B	512/505 (101%)	507 (99%)	5 (1%)	0	100 100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100 100
3	C	454/455 (100%)	445 (98%)	7 (2%)	2 (0%)	30 21
3	c	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	30 21
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100 100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100 100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100 100
5	e	79/84 (94%)	77 (98%)	2 (2%)	0	100 100
6	F	32/44 (73%)	32 (100%)	0	0	100 100
6	f	30/44 (68%)	30 (100%)	0	0	100 100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100 100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100 100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100 100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	245/244 (100%)	242 (99%)	3 (1%)	0	100	100
13	o	244/244 (100%)	238 (98%)	6 (2%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	29/31 (94%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	130 (96%)	6 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5279/5382 (98%)	5168 (98%)	104 (2%)	7 (0%)	48	41

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
8	i	36	ASP

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	272/279 (98%)	272 (100%)	0	100 100
1	a	273/279 (98%)	272 (100%)	1 (0%)	84 85
2	B	412/403 (102%)	409 (99%)	3 (1%)	76 76
2	b	413/403 (102%)	411 (100%)	2 (0%)	81 82
3	C	357/356 (100%)	353 (99%)	4 (1%)	65 64
3	c	362/356 (102%)	358 (99%)	4 (1%)	65 64
4	D	277/277 (100%)	275 (99%)	2 (1%)	76 76
4	d	277/277 (100%)	274 (99%)	3 (1%)	65 64
5	E	74/73 (101%)	74 (100%)	0	100 100
5	e	72/73 (99%)	71 (99%)	1 (1%)	59 56
6	F	28/38 (74%)	27 (96%)	1 (4%)	31 21
6	f	26/38 (68%)	25 (96%)	1 (4%)	29 19
7	H	55/54 (102%)	52 (94%)	3 (6%)	19 8
7	h	54/54 (100%)	54 (100%)	0	100 100
8	I	34/34 (100%)	34 (100%)	0	100 100
8	i	34/34 (100%)	34 (100%)	0	100 100
9	J	26/26 (100%)	26 (100%)	0	100 100
9	j	26/26 (100%)	26 (100%)	0	100 100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15 5
10	k	30/30 (100%)	28 (93%)	2 (7%)	15 5
11	L	36/35 (103%)	35 (97%)	1 (3%)	38 30
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 30
12	M	31/32 (97%)	31 (100%)	0	100 100
12	m	30/32 (94%)	29 (97%)	1 (3%)	33 24
13	O	210/207 (101%)	209 (100%)	1 (0%)	81 82
13	o	209/207 (101%)	208 (100%)	1 (0%)	81 82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	T	27/27 (100%)	25 (93%)	2 (7%)	13 4
14	t	27/27 (100%)	25 (93%)	2 (7%)	13 4
15	U	84/89 (94%)	83 (99%)	1 (1%)	63 61
15	u	84/89 (94%)	84 (100%)	0	100 100
16	V	118/117 (101%)	117 (99%)	1 (1%)	73 74
16	v	117/117 (100%)	116 (99%)	1 (1%)	70 70
17	Y	22/23 (96%)	22 (100%)	0	100 100
17	y	22/23 (96%)	21 (96%)	1 (4%)	24 14
18	X	33/33 (100%)	33 (100%)	0	100 100
18	x	32/33 (97%)	32 (100%)	0	100 100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29 19
19	z	52/52 (100%)	50 (96%)	2 (4%)	29 19
20	R	29/29 (100%)	28 (97%)	1 (3%)	32 23
All	All	4383/4399 (100%)	4336 (99%)	47 (1%)	68 64

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	289	PHE
6	f	44	GLN
3	c	315	MET
4	d	329	MET
10	k	17	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	490	GLN
3	c	44	ASN
12	m	32	GLN
3	c	28	GLN
3	c	415	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	i	1	8	8,9,10	0.62	0	7,9,11	1.17	1 (14%)
9	FME	j	1	9	8,9,10	0.63	0	7,9,11	1.32	1 (14%)
14	FME	t	1	14	8,9,10	0.85	0	7,9,11	2.28	4 (57%)
12	FME	M	1	12	8,9,10	0.63	0	7,9,11	1.32	0
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.32	2 (28%)
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	1.73	3 (42%)
12	FME	m	1	12	8,9,10	0.69	0	7,9,11	1.05	1 (14%)

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

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

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	C-CA-N	3.68	116.36	109.73
14	t	1	FME	O-C-CA	-3.00	116.92	124.78
14	T	1	FME	O-C-CA	-2.78	117.48	124.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	C-CA-N	2.35	113.97	109.73
14	T	1	FME	CA-N-CN	-2.29	119.31	122.82

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
14	T	1	FME	O1-CN-N-CA
9	j	1	FME	O1-CN-N-CA
9	j	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	2	0
12	m	1	FME	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 252 ligands modelled in this entry, 17 are monoatomic and 19 are unknown - leaving 216 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	$\#\|Z\| > 2$
34	LMG	c	501	-	51,51,55	0.88	2 (3%)	59,59,63	1.25	6 (10%)
37	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.09	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	PHO	A	407	-	58,69,69	2.76	11 (18%)	56,99,99	2.78	14 (25%)
37	LHG	e	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.04	3 (6%)
37	LHG	d	408	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	5 (9%)
24	CLA	B	614	2	69,73,73	2.02	18 (26%)	83,113,113	2.76	33 (39%)
24	CLA	b	611	2	69,73,73	2.01	20 (28%)	83,113,113	2.88	32 (38%)
24	CLA	c	513	3	69,73,73	2.02	19 (27%)	83,113,113	2.75	29 (34%)
24	CLA	b	613	2	69,73,73	2.08	20 (28%)	83,113,113	2.81	32 (38%)
24	CLA	b	606	41	69,73,73	2.09	20 (28%)	83,113,113	2.79	26 (31%)
26	BCR	c	516	-	41,41,41	1.08	1 (2%)	56,56,56	1.41	9 (16%)
31	OEX	A	418	41,3,1	0,14,14	-	-	-		
40	HEC	V	203	16	50,50,50	1.71	9 (18%)	68,82,82	1.82	15 (22%)
24	CLA	b	610	2	69,73,73	2.00	19 (27%)	83,113,113	2.98	31 (37%)
36	DGD	c	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.09	6 (7%)
28	GOL	c	524	-	5,5,5	0.32	0	5,5,5	0.37	0
37	LHG	d	410	-	48,48,48	0.94	2 (4%)	51,54,54	0.97	3 (5%)
24	CLA	C	514	3	69,73,73	2.00	20 (28%)	83,113,113	2.81	31 (37%)
34	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	4 (6%)
28	GOL	c	525	-	5,5,5	0.36	0	5,5,5	0.58	0
38	HEM	e	102	5,6	50,50,50	1.56	7 (14%)	66,82,82	1.76	17 (25%)
36	DGD	c	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	3 (3%)
28	GOL	B	633	-	5,5,5	0.30	0	5,5,5	0.66	0
26	BCR	b	623	-	41,41,41	1.08	1 (2%)	56,56,56	1.13	5 (8%)
24	CLA	B	609	2	69,73,73	2.06	20 (28%)	83,113,113	2.77	29 (34%)
24	CLA	c	504	3	69,73,73	2.01	19 (27%)	83,113,113	2.74	29 (34%)
24	CLA	B	611	41	69,73,73	2.05	20 (28%)	83,113,113	2.79	31 (37%)
26	BCR	A	410	-	41,41,41	1.02	1 (2%)	56,56,56	1.33	7 (12%)
26	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.33	8 (14%)
28	GOL	V	205	-	5,5,5	0.37	0	5,5,5	0.30	0
28	GOL	b	633	-	5,5,5	0.37	0	5,5,5	0.39	0
24	CLA	b	607	2	69,73,73	2.07	20 (28%)	83,113,113	2.89	33 (39%)
36	DGD	H	102	-	63,63,67	0.93	3 (4%)	77,77,81	0.90	3 (3%)
24	CLA	C	503	3	69,73,73	2.05	20 (28%)	83,113,113	2.72	30 (36%)
36	DGD	c	519	-	63,63,67	0.89	2 (3%)	77,77,81	0.97	3 (3%)
30	LMT	a	401	-	36,36,36	0.45	0	47,47,47	0.97	3 (6%)
27	SQD	b	601	-	53,54,54	1.02	3 (5%)	62,65,65	1.63	10 (16%)
28	GOL	A	413	-	5,5,5	0.43	0	5,5,5	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	620	2	69,73,73	2.04	20 (28%)	83,113,113	2.83	28 (33%)
30	LMT	A	417	-	34,34,36	0.38	0	45,45,47	1.06	3 (6%)
30	LMT	m	103	-	36,36,36	0.56	1 (2%)	47,47,47	1.05	4 (8%)
28	GOL	C	524	-	5,5,5	0.34	0	5,5,5	0.89	0
34	LMG	c	521	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	5 (8%)
35	HTG	O	303	-	19,19,19	1.07	1 (5%)	23,24,24	0.93	1 (4%)
36	DGD	D	407	-	63,63,67	0.96	4 (6%)	77,77,81	1.30	9 (11%)
37	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.09	5 (9%)
32	PL9	d	406	-	55,55,55	0.71	1 (1%)	68,69,69	1.55	14 (20%)
30	LMT	m	102	-	36,36,36	0.49	0	47,47,47	0.99	2 (4%)
26	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.39	8 (14%)
28	GOL	T	101	-	5,5,5	0.45	0	5,5,5	0.31	0
30	LMT	B	634	-	25,25,36	0.49	0	30,30,47	0.71	0
24	CLA	c	508	3	69,73,73	2.02	20 (28%)	83,113,113	2.70	31 (37%)
24	CLA	B	607	2	69,73,73	2.03	19 (27%)	83,113,113	2.88	31 (37%)
28	GOL	b	630	-	5,5,5	0.34	0	5,5,5	0.16	0
35	HTG	B	630	-	19,19,19	0.97	2 (10%)	23,24,24	1.31	1 (4%)
37	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.16	5 (9%)
24	CLA	b	612	41	69,73,73	1.96	19 (27%)	83,113,113	2.75	31 (37%)
30	LMT	b	602	-	25,25,36	0.46	0	30,30,47	1.26	3 (10%)
35	HTG	B	623	-	19,19,19	0.88	1 (5%)	23,24,24	1.25	3 (13%)
28	GOL	V	206	-	5,5,5	0.37	0	5,5,5	0.46	0
35	HTG	c	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.50	2 (8%)
34	LMG	c	520	-	51,51,55	0.95	2 (3%)	59,59,63	0.92	2 (3%)
34	LMG	z	101	-	39,39,55	1.11	2 (5%)	47,47,63	1.17	4 (8%)
24	CLA	D	401	41	69,73,73	2.04	20 (28%)	83,113,113	2.82	34 (40%)
26	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	5 (8%)
24	CLA	D	404	4	69,73,73	2.02	19 (27%)	83,113,113	2.88	32 (38%)
36	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.02	5 (6%)
24	CLA	b	619	2	69,73,73	1.99	20 (28%)	83,113,113	2.90	33 (39%)
24	CLA	c	514	3	69,73,73	2.02	20 (28%)	83,113,113	2.91	32 (38%)
28	GOL	V	207	-	5,5,5	0.37	0	5,5,5	0.46	0
24	CLA	C	510	3	69,73,73	2.12	20 (28%)	83,113,113	2.78	31 (37%)
24	CLA	c	510	3	69,73,73	2.07	20 (28%)	83,113,113	2.83	30 (36%)
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	10 (17%)
25	PHO	d	403	-	58,69,69	2.82	11 (18%)	56,99,99	2.88	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	B	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.24	5 (8%)
28	GOL	v	204	-	5,5,5	0.32	0	5,5,5	0.37	0
24	CLA	b	608	2	69,73,73	2.06	20 (28%)	83,113,113	2.89	31 (37%)
37	LHG	D	410	-	48,48,48	0.94	2 (4%)	51,54,54	0.94	3 (5%)
26	BCR	B	620	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	13 (23%)
24	CLA	B	613	2	69,73,73	2.03	21 (30%)	83,113,113	2.72	27 (32%)
28	GOL	B	625	-	5,5,5	0.31	0	5,5,5	0.56	0
35	HTG	b	603	-	19,19,19	1.07	2 (10%)	23,24,24	1.28	1 (4%)
24	CLA	B	616	2	69,73,73	2.05	20 (28%)	83,113,113	2.78	31 (37%)
24	CLA	B	605	2	69,73,73	1.95	22 (31%)	83,113,113	2.91	30 (36%)
24	CLA	b	614	2	69,73,73	2.07	19 (27%)	83,113,113	2.78	31 (37%)
24	CLA	d	404	4	69,73,73	2.05	20 (28%)	83,113,113	2.91	29 (34%)
25	PHO	A	408	-	58,69,69	2.80	13 (22%)	56,99,99	3.01	17 (30%)
24	CLA	c	505	3	69,73,73	2.03	19 (27%)	83,113,113	2.84	29 (34%)
24	CLA	d	401	41	69,73,73	2.01	17 (24%)	83,113,113	2.79	31 (37%)
26	BCR	T	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	11 (19%)
28	GOL	A	412	-	5,5,5	0.26	0	5,5,5	0.68	0
31	OEX	a	415	41,3,1	0,14,14	-	-	-		
27	SQD	l	101	-	53,54,54	1.00	3 (5%)	62,65,65	1.40	9 (14%)
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	7 (9%)
24	CLA	B	610	2	69,73,73	2.00	17 (24%)	83,113,113	2.86	30 (36%)
24	CLA	C	507	3	69,73,73	2.04	20 (28%)	83,113,113	2.71	31 (37%)
35	HTG	b	628	-	19,19,19	1.10	2 (10%)	23,24,24	1.83	3 (13%)
26	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.25	5 (8%)
24	CLA	B	603	2	69,73,73	2.02	21 (30%)	83,113,113	2.91	30 (36%)
24	CLA	B	617	2	69,73,73	1.98	21 (30%)	83,113,113	2.77	29 (34%)
26	BCR	k	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.33	5 (8%)
24	CLA	a	407	41	69,73,73	2.05	20 (28%)	83,113,113	2.86	33 (39%)
28	GOL	B	628	-	5,5,5	0.40	0	5,5,5	0.29	0
37	LHG	D	409	-	48,48,48	0.85	2 (4%)	51,54,54	1.08	5 (9%)
24	CLA	D	403	4	69,73,73	2.04	20 (28%)	83,113,113	2.82	30 (36%)
24	CLA	A	409	1	69,73,73	2.03	20 (28%)	83,113,113	2.85	31 (37%)
24	CLA	B	608	41	69,73,73	2.01	20 (28%)	83,113,113	2.72	33 (39%)
24	CLA	C	512	3	69,73,73	2.01	19 (27%)	83,113,113	2.83	28 (33%)
24	CLA	B	615	2	69,73,73	1.98	20 (28%)	83,113,113	3.03	31 (37%)
28	GOL	T	103	-	5,5,5	0.41	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	HTG	C	523	-	19,19,19	1.02	2 (10%)	23,24,24	1.77	5 (21%)
34	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.14	5 (8%)
27	SQD	a	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.60	11 (17%)
26	BCR	b	622	-	41,41,41	1.14	2 (4%)	56,56,56	1.36	4 (7%)
35	HTG	d	411	-	16,16,19	1.21	2 (12%)	20,21,24	1.55	1 (5%)
34	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.44	7 (15%)
24	CLA	B	606	2	69,73,73	1.99	19 (27%)	83,113,113	2.93	30 (36%)
28	GOL	C	525	-	5,5,5	0.33	0	5,5,5	0.72	0
34	LMG	C	501	-	51,51,55	0.97	2 (3%)	59,59,63	1.10	3 (5%)
24	CLA	A	405	1	69,73,73	2.03	21 (30%)	83,113,113	2.77	31 (37%)
35	HTG	B	624	-	19,19,19	1.06	2 (10%)	23,24,24	1.89	4 (17%)
26	BCR	a	410	-	41,41,41	1.14	1 (2%)	56,56,56	1.35	8 (14%)
26	BCR	D	405	-	41,41,41	1.05	1 (2%)	56,56,56	1.70	12 (21%)
30	LMT	M	101	-	36,36,36	0.57	1 (2%)	47,47,47	0.84	0
24	CLA	C	502	3	69,73,73	1.98	20 (28%)	83,113,113	2.72	29 (34%)
30	LMT	D	402	-	36,36,36	0.48	0	47,47,47	1.01	3 (6%)
30	LMT	E	102	-	36,36,36	0.46	0	47,47,47	0.75	0
30	LMT	f	102	-	36,36,36	0.47	0	47,47,47	0.77	0
35	HTG	b	604	-	19,19,19	1.02	2 (10%)	23,24,24	1.10	2 (8%)
28	GOL	b	629	-	5,5,5	0.38	0	5,5,5	0.29	0
34	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.11	5 (8%)
24	CLA	a	409	1	69,73,73	2.04	19 (27%)	83,113,113	2.83	32 (38%)
28	GOL	v	201	-	5,5,5	0.35	0	5,5,5	0.39	0
23	BCT	a	418	21	2,3,3	0.60	0	2,3,3	0.82	0
32	PL9	a	416	-	55,55,55	0.63	2 (3%)	68,69,69	1.85	18 (26%)
27	SQD	A	416	-	53,54,54	1.05	3 (5%)	62,65,65	1.15	7 (11%)
24	CLA	b	618	2	69,73,73	2.00	20 (28%)	83,113,113	2.83	29 (34%)
35	HTG	V	204	-	19,19,19	1.00	2 (10%)	23,24,24	1.33	3 (13%)
24	CLA	B	604	2	69,73,73	2.05	20 (28%)	83,113,113	2.82	32 (38%)
32	PL9	A	419	-	55,55,55	0.63	1 (1%)	68,69,69	1.85	19 (27%)
24	CLA	a	406	1	69,73,73	2.03	20 (28%)	83,113,113	2.75	29 (34%)
26	BCR	t	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.32	8 (14%)
40	HEC	v	202	16	50,50,50	1.69	8 (16%)	68,82,82	1.77	17 (25%)
24	CLA	C	509	3	69,73,73	2.07	20 (28%)	83,113,113	2.80	28 (33%)
26	BCR	b	624	-	41,41,41	0.99	1 (2%)	56,56,56	1.25	8 (14%)
28	GOL	f	104	33	5,5,5	0.35	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	GOL	t	102	-	5,5,5	0.34	0	5,5,5	0.30	0
27	SQD	f	101	-	42,43,54	1.18	3 (7%)	51,54,65	1.44	7 (13%)
24	CLA	c	506	41	69,73,73	2.02	20 (28%)	83,113,113	2.82	30 (36%)
24	CLA	c	511	3	69,73,73	2.13	20 (28%)	83,113,113	2.79	29 (34%)
28	GOL	B	629	-	5,5,5	0.32	0	5,5,5	0.39	0
24	CLA	B	612	2	69,73,73	2.03	20 (28%)	83,113,113	2.89	29 (34%)
24	CLA	c	515	3	69,73,73	2.06	21 (30%)	83,113,113	2.83	32 (38%)
30	LMT	a	417	-	36,36,36	0.44	0	47,47,47	0.84	2 (4%)
34	LMG	J	101	39	51,51,55	0.84	2 (3%)	59,59,63	1.01	4 (6%)
34	LMG	b	625	-	51,51,55	0.90	2 (3%)	59,59,63	1.03	4 (6%)
28	GOL	V	201	-	5,5,5	0.38	0	5,5,5	0.43	0
35	HTG	c	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	2 (8%)
27	SQD	A	411	-	53,54,54	0.97	3 (5%)	62,65,65	1.58	11 (17%)
24	CLA	b	621	2	69,73,73	2.07	21 (30%)	83,113,113	2.77	30 (36%)
24	CLA	C	505	41	69,73,73	2.05	20 (28%)	83,113,113	2.76	29 (34%)
28	GOL	b	631	-	5,5,5	0.34	0	5,5,5	0.45	0
35	HTG	B	631	-	19,19,19	1.03	2 (10%)	23,24,24	1.44	2 (8%)
24	CLA	B	602	41	69,73,73	2.06	20 (28%)	83,113,113	2.85	30 (36%)
28	GOL	v	203	-	5,5,5	0.27	0	5,5,5	0.49	0
34	LMG	j	101	39	51,51,55	0.93	3 (5%)	59,59,63	0.98	3 (5%)
28	GOL	c	527	-	5,5,5	0.41	0	5,5,5	0.31	0
24	CLA	C	513	3	69,73,73	2.02	20 (28%)	83,113,113	2.81	33 (39%)
30	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.86	0
35	HTG	C	522	-	19,19,19	1.01	2 (10%)	23,24,24	1.28	2 (8%)
28	GOL	a	413	-	5,5,5	0.43	0	5,5,5	0.27	0
23	BCT	A	404	21	2,3,3	0.65	0	2,3,3	0.87	0
36	DGD	d	407	-	63,63,67	0.94	3 (4%)	77,77,81	1.04	6 (7%)
30	LMT	b	626	-	25,25,36	0.50	0	30,30,47	0.64	0
28	GOL	B	627	-	5,5,5	0.34	0	5,5,5	0.71	0
28	GOL	B	635	-	5,5,5	0.40	0	5,5,5	0.25	0
25	PHO	a	408	-	58,69,69	2.78	13 (22%)	56,99,99	2.85	14 (25%)
35	HTG	B	622	-	19,19,19	1.20	1 (5%)	23,24,24	1.43	3 (13%)
24	CLA	C	504	3	69,73,73	2.04	20 (28%)	83,113,113	2.82	28 (33%)
28	GOL	F	103	33	5,5,5	0.36	0	5,5,5	0.37	0
28	GOL	a	412	-	5,5,5	0.34	0	5,5,5	0.57	0
36	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.06	4 (5%)
24	CLA	c	509	41	69,73,73	1.99	19 (27%)	83,113,113	2.79	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	c	503	3	69,73,73	2.02	20 (28%)	83,113,113	2.82	31 (37%)
28	GOL	v	205	-	5,5,5	0.35	0	5,5,5	0.46	0
32	PL9	D	406	-	55,55,55	0.77	2 (3%)	68,69,69	1.50	16 (23%)
24	CLA	b	617	2	69,73,73	2.00	21 (30%)	83,113,113	2.67	30 (36%)
24	CLA	b	616	2	69,73,73	2.04	20 (28%)	83,113,113	2.85	30 (36%)
28	GOL	b	632	-	5,5,5	0.44	0	5,5,5	0.52	0
38	HEM	E	103	5,6	50,50,50	1.52	6 (12%)	66,82,82	1.80	16 (24%)
35	HTG	b	627	-	19,19,19	0.86	1 (5%)	23,24,24	1.35	4 (17%)
24	CLA	C	506	3	69,73,73	2.04	20 (28%)	83,113,113	2.65	27 (32%)
24	CLA	b	615	41	69,73,73	2.05	20 (28%)	83,113,113	2.73	29 (34%)
28	GOL	V	208	-	5,5,5	0.37	0	5,5,5	0.27	0
37	LHG	D	408	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
28	GOL	A	414	-	5,5,5	0.41	0	5,5,5	0.20	0
24	CLA	C	511	3	69,73,73	2.06	20 (28%)	83,113,113	2.76	30 (36%)
26	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	11 (19%)
37	LHG	l	102	-	48,48,48	0.95	2 (4%)	51,54,54	1.02	3 (5%)
24	CLA	d	402	4	69,73,73	2.03	20 (28%)	83,113,113	2.81	28 (33%)
26	BCR	d	405	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	13 (23%)
36	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	0.89	3 (3%)
24	CLA	c	507	3	69,73,73	2.02	19 (27%)	83,113,113	2.66	24 (28%)
26	BCR	Y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	8 (14%)
24	CLA	C	508	41	69,73,73	2.05	20 (28%)	83,113,113	2.80	30 (36%)
24	CLA	b	609	2	69,73,73	2.07	22 (31%)	83,113,113	2.82	29 (34%)
30	LMT	I	102	-	36,36,36	0.45	0	47,47,47	1.18	4 (8%)
28	GOL	B	626	-	5,5,5	0.29	0	5,5,5	0.48	0
26	BCR	c	526	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	10 (17%)
28	GOL	O	302	-	5,5,5	0.36	0	5,5,5	0.35	0
26	BCR	B	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.00	3 (5%)
35	HTG	D	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.03	3 (15%)
24	CLA	c	512	3	69,73,73	2.04	19 (27%)	83,113,113	2.74	31 (37%)
27	SQD	a	402	-	53,54,54	1.03	3 (5%)	62,65,65	1.19	6 (9%)
27	SQD	F	101	-	42,43,54	1.12	3 (7%)	51,54,65	1.55	9 (17%)
24	CLA	A	406	41	69,73,73	2.09	20 (28%)	83,113,113	2.80	32 (38%)

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
34	LMG	c	501	-	-	14/46/66/70	0/1/1/1
37	LHG	E	101	-	-	20/46/46/53	-
25	PHO	A	407	-	-	3/37/103/103	0/5/6/6
37	LHG	e	101	-	-	18/46/46/53	-
37	LHG	d	408	-	-	9/53/53/53	-
24	CLA	B	614	2	-	9/39/115/115	-
24	CLA	b	611	2	-	10/39/115/115	-
24	CLA	c	513	3	-	5/39/115/115	-
24	CLA	b	613	2	-	2/39/115/115	-
24	CLA	b	606	41	-	16/39/115/115	-
26	BCR	c	516	-	-	4/29/63/63	0/2/2/2
40	HEC	V	203	16	1/1/3/7	6/14/54/54	-
24	CLA	b	610	2	-	5/39/115/115	-
36	DGD	c	517	-	-	12/51/91/95	0/2/2/2
28	GOL	c	524	-	-	0/4/4/4	-
37	LHG	d	410	-	-	13/53/53/53	-
24	CLA	C	514	3	-	5/39/115/115	-
34	LMG	B	621	-	-	7/46/66/70	0/1/1/1
28	GOL	c	525	-	-	1/4/4/4	-
38	HEM	e	102	5,6	-	4/14/54/54	-
36	DGD	c	518	-	-	15/51/91/95	0/2/2/2
28	GOL	B	633	-	-	0/4/4/4	-
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
24	CLA	B	609	2	-	1/39/115/115	-
24	CLA	c	504	3	-	5/39/115/115	-
24	CLA	B	611	41	-	3/39/115/115	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
28	GOL	V	205	-	-	4/4/4/4	-
28	GOL	b	633	-	-	2/4/4/4	-
24	CLA	b	607	2	-	3/39/115/115	-
36	DGD	H	102	-	-	11/51/91/95	0/2/2/2
24	CLA	C	503	3	-	10/39/115/115	-
36	DGD	c	519	-	-	12/51/91/95	0/2/2/2
30	LMT	a	401	-	-	9/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	b	601	-	-	20/49/69/69	0/1/1/1
28	GOL	A	413	-	-	2/4/4/4	-
24	CLA	b	620	2	-	5/39/115/115	-
30	LMT	A	417	-	-	3/19/59/61	0/2/2/2
30	LMT	m	103	-	-	6/21/61/61	0/2/2/2
28	GOL	C	524	-	-	2/4/4/4	-
34	LMG	c	521	-	-	6/46/66/70	0/1/1/1
35	HTG	O	303	-	-	2/10/30/30	0/1/1/1
36	DGD	D	407	-	-	17/51/91/95	0/2/2/2
37	LHG	d	409	-	-	11/53/53/53	-
32	PL9	d	406	-	-	3/53/73/73	0/1/1/1
30	LMT	m	102	-	-	3/21/61/61	0/2/2/2
26	BCR	C	516	-	-	3/29/63/63	0/2/2/2
28	GOL	T	101	-	-	2/4/4/4	-
30	LMT	B	634	-	-	5/17/37/61	0/1/1/2
24	CLA	c	508	3	-	8/39/115/115	-
24	CLA	B	607	2	-	4/39/115/115	-
28	GOL	b	630	-	-	0/4/4/4	-
35	HTG	B	630	-	-	1/10/30/30	0/1/1/1
37	LHG	L	101	-	-	12/53/53/53	-
24	CLA	b	612	41	-	5/39/115/115	-
30	LMT	b	602	-	-	7/17/37/61	0/1/1/2
35	HTG	B	623	-	-	5/10/30/30	0/1/1/1
28	GOL	V	206	-	-	2/4/4/4	-
35	HTG	c	522	-	-	1/10/30/30	0/1/1/1
34	LMG	c	520	-	-	5/46/66/70	0/1/1/1
34	LMG	z	101	-	-	13/34/54/70	0/1/1/1
24	CLA	D	401	41	-	5/39/115/115	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	D	404	4	-	7/39/115/115	-
36	DGD	C	518	-	-	19/51/91/95	0/2/2/2
24	CLA	b	619	2	-	14/39/115/115	-
24	CLA	c	514	3	-	14/39/115/115	-
28	GOL	V	207	-	-	0/4/4/4	-
24	CLA	C	510	3	-	4/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	510	3	-	2/39/115/115	-
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
25	PHO	d	403	-	-	3/37/103/103	0/5/6/6
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
28	GOL	v	204	-	-	2/4/4/4	-
24	CLA	b	608	2	-	7/39/115/115	-
37	LHG	D	410	-	-	14/53/53/53	-
26	BCR	B	620	-	-	5/29/63/63	0/2/2/2
24	CLA	B	613	2	-	2/39/115/115	-
28	GOL	B	625	-	-	2/4/4/4	-
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
24	CLA	B	616	2	-	10/39/115/115	-
24	CLA	B	605	2	-	4/39/115/115	-
24	CLA	b	614	2	-	4/39/115/115	-
24	CLA	d	404	4	-	6/39/115/115	-
25	PHO	A	408	-	-	1/37/103/103	0/5/6/6
24	CLA	c	505	3	-	4/39/115/115	-
24	CLA	d	401	41	-	7/39/115/115	-
26	BCR	T	102	-	-	0/29/63/63	0/2/2/2
28	GOL	A	412	-	-	2/4/4/4	-
27	SQD	l	101	-	-	20/49/69/69	0/1/1/1
36	DGD	h	102	-	-	9/51/91/95	0/2/2/2
24	CLA	B	610	2	-	3/39/115/115	-
24	CLA	C	507	3	-	8/39/115/115	-
35	HTG	b	628	-	-	2/10/30/30	0/1/1/1
26	BCR	H	101	-	-	1/29/63/63	0/2/2/2
24	CLA	B	603	2	-	7/39/115/115	-
24	CLA	B	617	2	-	9/39/115/115	-
26	BCR	k	103	-	-	1/29/63/63	0/2/2/2
24	CLA	a	407	41	-	5/39/115/115	-
28	GOL	B	628	-	-	2/4/4/4	-
37	LHG	D	409	-	-	9/53/53/53	-
24	CLA	D	403	4	-	4/39/115/115	-
24	CLA	A	409	1	-	12/39/115/115	-
24	CLA	B	608	41	-	6/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	512	3	-	1/39/115/115	-
24	CLA	B	615	2	-	14/39/115/115	-
28	GOL	T	103	-	-	3/4/4/4	-
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
34	LMG	C	521	-	-	14/46/66/70	0/1/1/1
27	SQD	a	411	-	-	9/49/69/69	0/1/1/1
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
35	HTG	d	411	-	-	2/7/27/30	0/1/1/1
34	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
24	CLA	B	606	2	-	3/39/115/115	-
28	GOL	C	525	-	-	0/4/4/4	-
34	LMG	C	501	-	-	16/46/66/70	0/1/1/1
24	CLA	A	405	1	-	1/39/115/115	-
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
26	BCR	D	405	-	-	6/29/63/63	0/2/2/2
30	LMT	M	101	-	-	8/21/61/61	0/2/2/2
24	CLA	C	502	3	-	11/39/115/115	-
30	LMT	D	402	-	-	9/21/61/61	0/2/2/2
30	LMT	E	102	-	-	9/21/61/61	0/2/2/2
30	LMT	f	102	-	-	7/21/61/61	0/2/2/2
35	HTG	b	604	-	-	1/10/30/30	0/1/1/1
28	GOL	b	629	-	-	2/4/4/4	-
34	LMG	C	520	-	-	13/46/66/70	0/1/1/1
24	CLA	a	409	1	-	11/39/115/115	-
28	GOL	v	201	-	-	0/4/4/4	-
32	PL9	a	416	-	-	17/53/73/73	0/1/1/1
27	SQD	A	416	-	-	17/49/69/69	0/1/1/1
24	CLA	b	618	2	-	6/39/115/115	-
35	HTG	V	204	-	-	3/10/30/30	0/1/1/1
24	CLA	B	604	2	-	3/39/115/115	-
32	PL9	A	419	-	-	8/53/73/73	0/1/1/1
24	CLA	a	406	1	-	3/39/115/115	-
40	HEC	v	202	16	1/1/3/7	6/14/54/54	-
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2
24	CLA	C	509	3	-	3/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
28	GOL	f	104	33	-	3/4/4/4	-
28	GOL	t	102	-	-	0/4/4/4	-
27	SQD	f	101	-	-	16/38/58/69	0/1/1/1
24	CLA	c	506	41	-	8/39/115/115	-
24	CLA	c	511	3	-	9/39/115/115	-
28	GOL	B	629	-	-	0/4/4/4	-
24	CLA	B	612	2	-	3/39/115/115	-
24	CLA	c	515	3	-	6/39/115/115	-
30	LMT	a	417	-	-	2/21/61/61	0/2/2/2
34	LMG	J	101	39	-	9/46/66/70	0/1/1/1
34	LMG	b	625	-	-	18/46/66/70	0/1/1/1
28	GOL	V	201	-	-	0/4/4/4	-
35	HTG	c	523	-	-	1/10/30/30	0/1/1/1
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
24	CLA	b	621	2	-	10/39/115/115	-
24	CLA	C	505	41	-	6/39/115/115	-
28	GOL	b	631	-	-	2/4/4/4	-
35	HTG	B	631	-	-	1/10/30/30	0/1/1/1
24	CLA	B	602	41	-	15/39/115/115	-
28	GOL	v	203	-	-	4/4/4/4	-
34	LMG	j	101	39	-	12/46/66/70	0/1/1/1
28	GOL	c	527	-	-	2/4/4/4	-
24	CLA	C	513	3	-	10/39/115/115	-
30	LMT	M	102	-	-	5/21/61/61	0/2/2/2
35	HTG	C	522	-	-	2/10/30/30	0/1/1/1
28	GOL	a	413	-	-	4/4/4/4	-
36	DGD	d	407	-	-	20/51/91/95	0/2/2/2
30	LMT	b	626	-	-	6/17/37/61	0/1/1/2
28	GOL	B	627	-	-	2/4/4/4	-
28	GOL	B	635	-	-	2/4/4/4	-
25	PHO	a	408	-	-	2/37/103/103	0/5/6/6
35	HTG	B	622	-	-	1/10/30/30	0/1/1/1
24	CLA	C	504	3	-	4/39/115/115	-
28	GOL	F	103	33	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	a	412	-	-	2/4/4/4	-
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
24	CLA	c	509	41	-	3/39/115/115	-
24	CLA	c	503	3	-	5/39/115/115	-
28	GOL	v	205	-	-	2/4/4/4	-
32	PL9	D	406	-	-	1/53/73/73	0/1/1/1
24	CLA	b	617	2	-	3/39/115/115	-
24	CLA	b	616	2	-	4/39/115/115	-
28	GOL	b	632	-	-	2/4/4/4	-
38	HEM	E	103	5,6	-	4/14/54/54	-
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
24	CLA	C	506	3	-	7/39/115/115	-
24	CLA	b	615	41	-	6/39/115/115	-
28	GOL	V	208	-	-	2/4/4/4	-
37	LHG	D	408	-	-	9/53/53/53	-
28	GOL	A	414	-	-	2/4/4/4	-
24	CLA	C	511	3	-	8/39/115/115	-
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
37	LHG	l	102	-	-	18/53/53/53	-
24	CLA	d	402	4	-	3/39/115/115	-
26	BCR	d	405	-	-	6/29/63/63	0/2/2/2
36	DGD	C	519	-	-	5/51/91/95	0/2/2/2
24	CLA	c	507	3	-	5/39/115/115	-
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
24	CLA	C	508	41	-	12/39/115/115	-
24	CLA	b	609	2	-	3/39/115/115	-
30	LMT	I	102	-	-	10/21/61/61	0/2/2/2
28	GOL	B	626	-	-	2/4/4/4	-
26	BCR	c	526	-	-	1/29/63/63	0/2/2/2
28	GOL	O	302	-	-	2/4/4/4	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
35	HTG	D	411	-	-	1/7/27/30	0/1/1/1
24	CLA	c	512	3	-	7/39/115/115	-
27	SQD	a	402	-	-	17/49/69/69	0/1/1/1
27	SQD	F	101	-	-	12/38/58/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	406	41	-	5/39/115/115	-

The worst 5 of 1622 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C1B-C2B	9.08	1.49	1.39
25	d	403	PHO	C1B-C2B	9.05	1.49	1.39
25	d	403	PHO	C1D-C2D	9.03	1.49	1.39
25	a	408	PHO	C1D-C2D	8.84	1.49	1.39
25	A	407	PHO	C1D-C2D	8.67	1.49	1.39

The worst 5 of 2758 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	PHO	C2D-C1D-ND	12.92	118.45	109.53
25	a	408	PHO	C2D-C1D-ND	12.33	118.04	109.53
25	A	407	PHO	C2D-C1D-ND	11.58	117.52	109.53
25	d	403	PHO	C2D-C1D-ND	11.27	117.31	109.53
24	B	615	CLA	C1D-ND-C4D	-10.22	99.08	106.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	203	HEC	NA
40	v	202	HEC	NA

5 of 1243 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

151 monomers are involved in 280 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	c	501	LMG	1	0
37	E	101	LHG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	e	101	LHG	4	0
37	d	408	LHG	1	0
24	B	614	CLA	2	0
24	b	611	CLA	4	0
24	c	513	CLA	3	0
24	b	613	CLA	1	0
24	b	606	CLA	3	0
26	c	516	BCR	4	0
24	b	610	CLA	4	0
37	d	410	LHG	3	0
24	C	514	CLA	4	0
34	B	621	LMG	2	0
28	c	525	GOL	2	0
38	e	102	HEM	2	0
36	c	518	DGD	2	0
26	b	623	BCR	3	0
24	c	504	CLA	2	0
24	B	611	CLA	1	0
26	A	410	BCR	3	0
26	h	101	BCR	4	0
28	V	205	GOL	2	0
28	b	633	GOL	1	0
36	H	102	DGD	2	0
24	C	503	CLA	2	0
36	c	519	DGD	1	0
30	a	401	LMT	4	0
27	b	601	SQD	2	0
28	A	413	GOL	2	0
24	b	620	CLA	4	0
30	m	103	LMT	1	0
28	C	524	GOL	1	0
34	c	521	LMG	1	0
36	D	407	DGD	1	0
30	m	102	LMT	1	0
28	T	101	GOL	1	0
30	B	634	LMT	1	0
24	c	508	CLA	4	0
24	B	607	CLA	2	0
37	L	101	LHG	1	0
35	B	623	HTG	1	0
34	c	520	LMG	1	0
34	z	101	LMG	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	401	CLA	5	0
26	C	515	BCR	3	0
24	D	404	CLA	1	0
36	C	518	DGD	1	0
24	b	619	CLA	1	0
24	c	514	CLA	4	0
28	V	207	GOL	1	0
24	C	510	CLA	2	0
24	c	510	CLA	3	0
26	y	101	BCR	1	0
25	d	403	PHO	1	0
26	B	618	BCR	3	0
24	b	608	CLA	1	0
37	D	410	LHG	8	0
26	B	620	BCR	3	0
24	B	613	CLA	2	0
24	B	616	CLA	1	0
24	b	614	CLA	2	0
24	d	404	CLA	3	0
25	A	408	PHO	1	0
24	c	505	CLA	4	0
26	T	102	BCR	7	0
27	l	101	SQD	2	0
24	B	610	CLA	2	0
24	C	507	CLA	3	0
26	H	101	BCR	4	0
24	B	617	CLA	5	0
26	k	103	BCR	1	0
28	B	628	GOL	1	0
24	D	403	CLA	1	0
24	A	409	CLA	1	0
24	C	512	CLA	1	0
24	B	615	CLA	4	0
28	T	103	GOL	1	0
35	C	523	HTG	2	0
34	C	521	LMG	1	0
27	a	411	SQD	4	0
26	b	622	BCR	2	0
35	d	411	HTG	2	0
34	Z	101	LMG	1	0
24	B	606	CLA	2	0
34	C	501	LMG	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	405	CLA	3	0
26	D	405	BCR	1	0
30	M	101	LMT	1	0
24	C	502	CLA	2	0
30	D	402	LMT	1	0
34	C	520	LMG	2	0
24	a	409	CLA	1	0
32	a	416	PL9	10	0
27	A	416	SQD	2	0
24	b	618	CLA	2	0
35	V	204	HTG	1	0
24	B	604	CLA	3	0
32	A	419	PL9	4	0
24	a	406	CLA	4	0
26	t	101	BCR	4	0
24	C	509	CLA	3	0
26	b	624	BCR	3	0
28	t	102	GOL	1	0
27	f	101	SQD	3	0
24	c	511	CLA	2	0
24	B	612	CLA	1	0
24	c	515	CLA	3	0
34	J	101	LMG	2	0
34	b	625	LMG	1	0
27	A	411	SQD	2	0
24	b	621	CLA	2	0
24	C	505	CLA	1	0
28	b	631	GOL	1	0
24	B	602	CLA	1	0
28	v	203	GOL	1	0
34	j	101	LMG	1	0
24	C	513	CLA	1	0
30	M	102	LMT	2	0
35	C	522	HTG	1	0
36	d	407	DGD	5	0
30	b	626	LMT	1	0
28	B	635	GOL	2	0
25	a	408	PHO	1	0
35	B	622	HTG	3	0
24	C	504	CLA	2	0
28	a	412	GOL	2	0
36	C	517	DGD	4	0

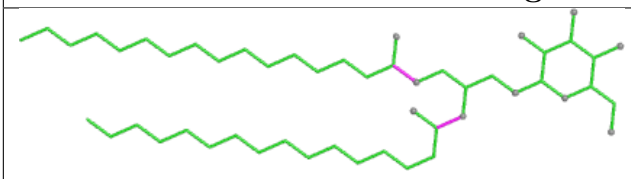
Continued on next page...

Continued from previous page...

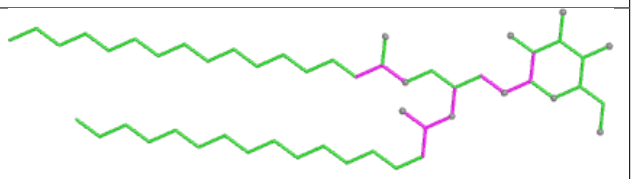
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	509	CLA	3	0
24	c	503	CLA	3	0
24	b	616	CLA	1	0
28	b	632	GOL	1	0
35	b	627	HTG	1	0
28	V	208	GOL	1	0
37	D	408	LHG	2	0
24	C	511	CLA	2	0
26	K	101	BCR	1	0
37	l	102	LHG	4	0
24	d	402	CLA	2	0
26	d	405	BCR	3	0
36	C	519	DGD	2	0
24	c	507	CLA	3	0
26	Y	101	BCR	2	0
24	C	508	CLA	2	0
24	b	609	CLA	1	0
30	I	102	LMT	2	0
26	c	526	BCR	5	0
26	B	619	BCR	2	0
35	D	411	HTG	2	0
27	F	101	SQD	3	0
24	A	406	CLA	2	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.

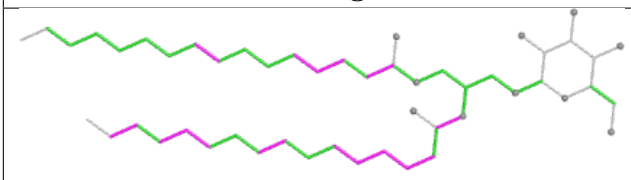
Ligand LMG c 501



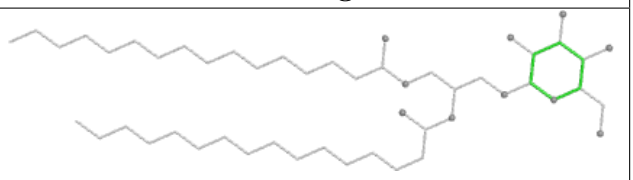
Bond lengths



Bond angles

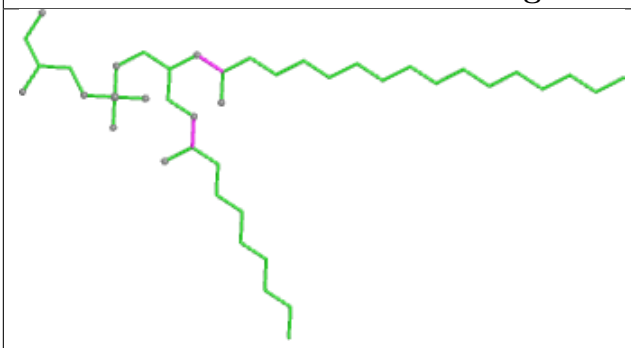


Torsions

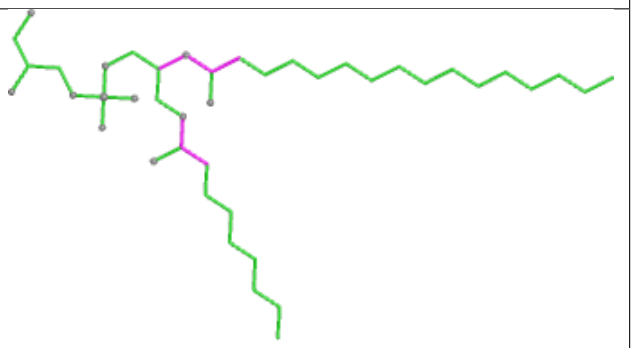


Rings

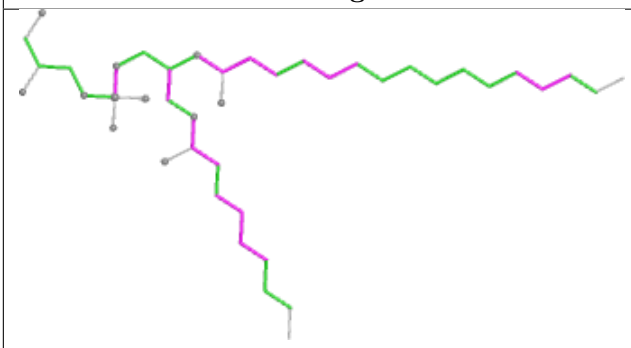
Ligand LHG E 101



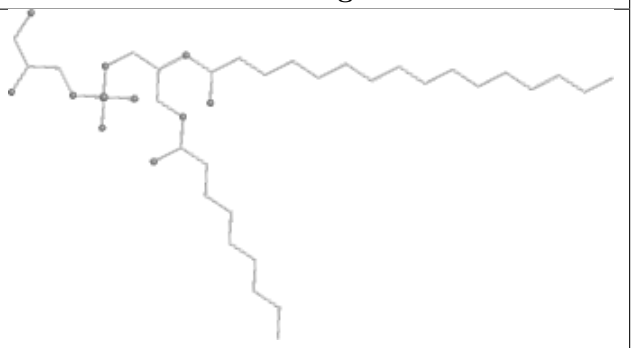
Bond lengths



Bond angles

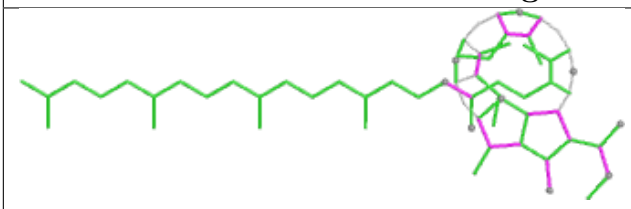


Torsions

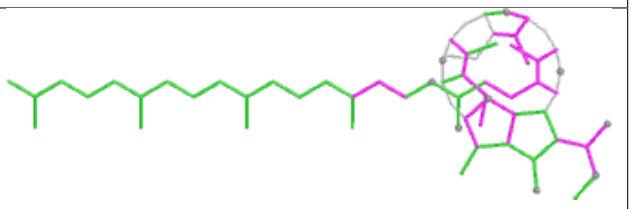


Rings

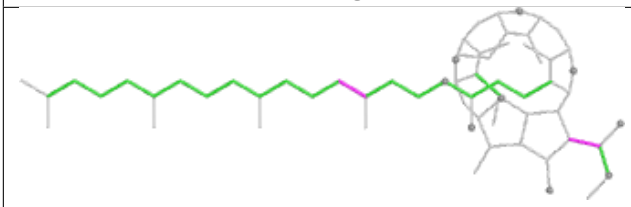
Ligand PHO A 407



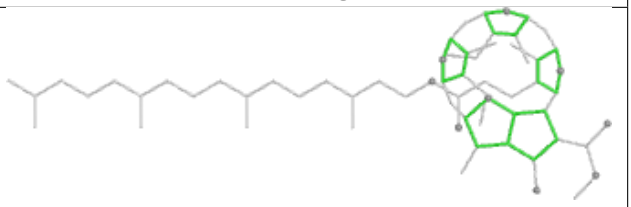
Bond lengths



Bond angles

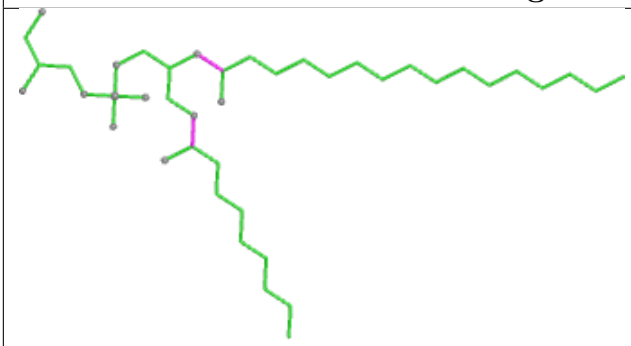


Torsions

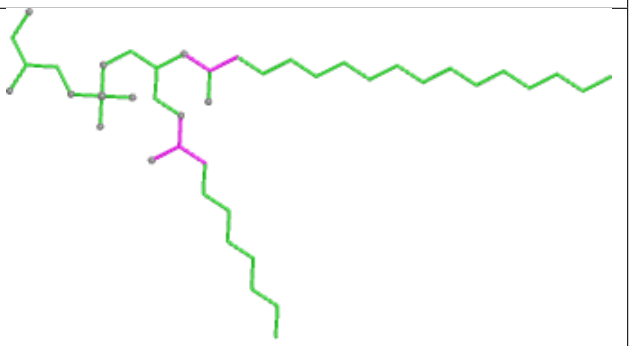


Rings

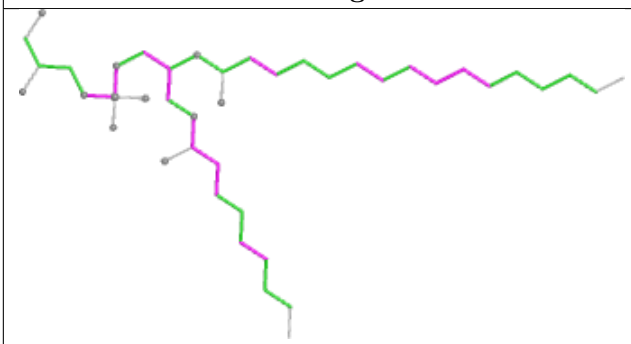
Ligand LHG e 101



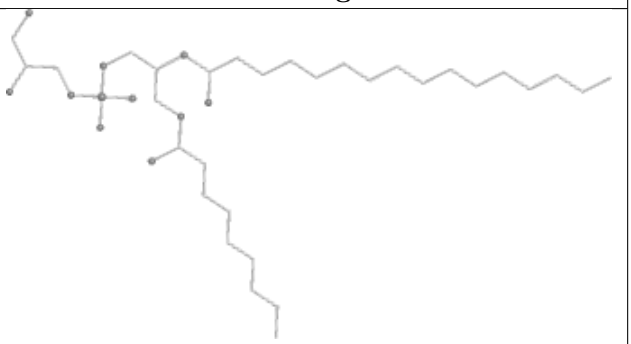
Bond lengths



Bond angles

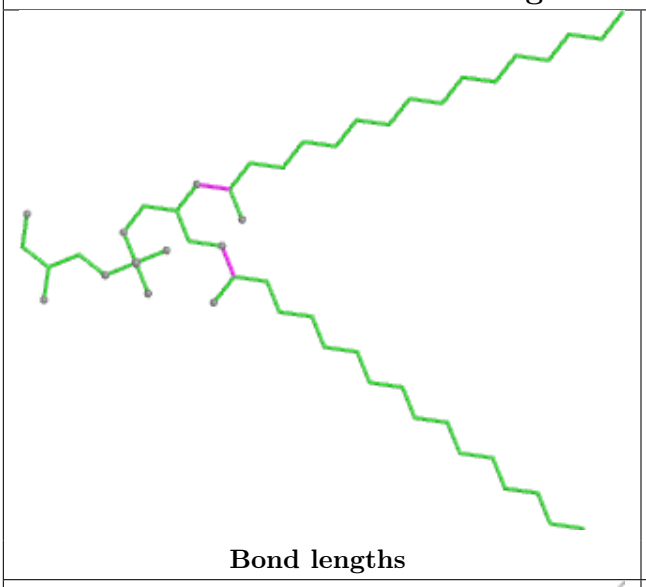


Torsions

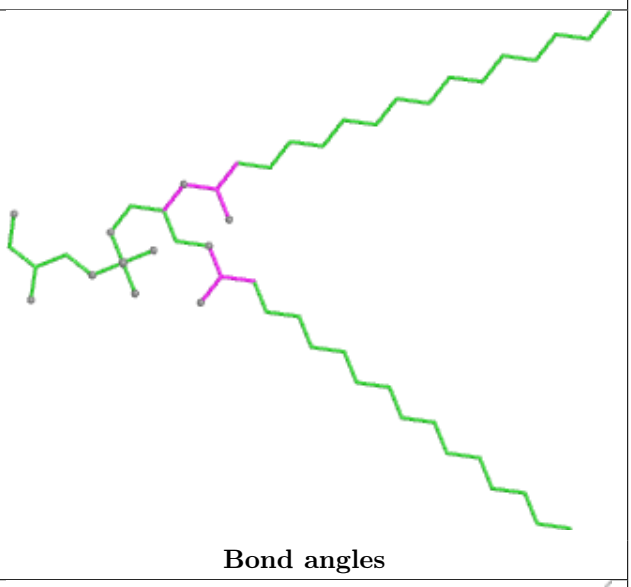


Rings

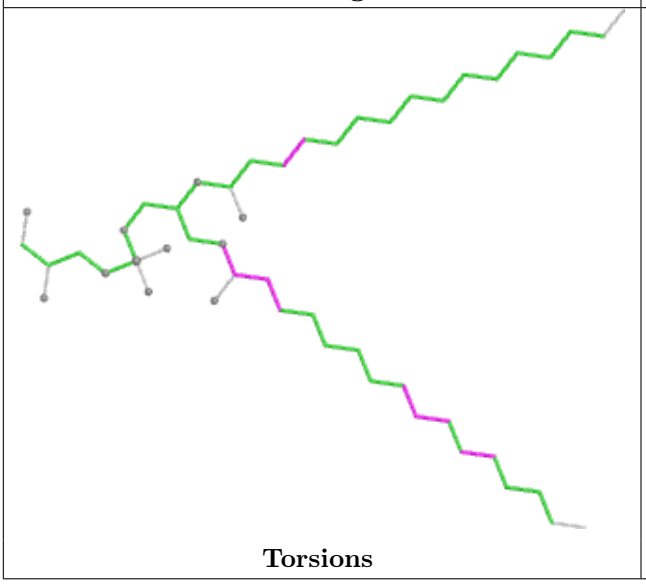
Ligand LHG d 408



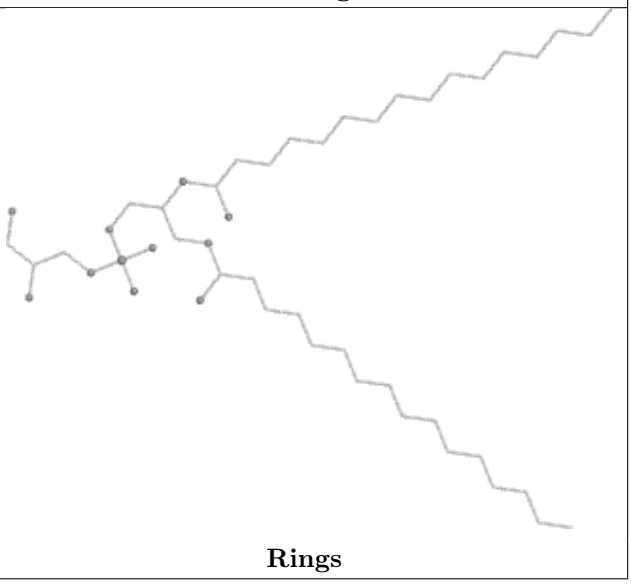
Bond lengths



Bond angles

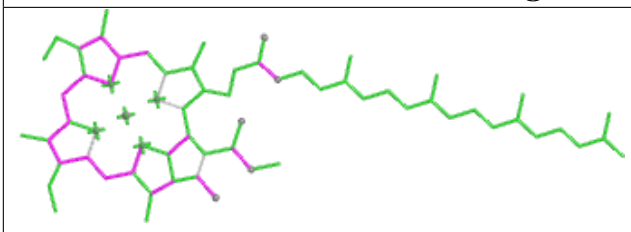


Torsions

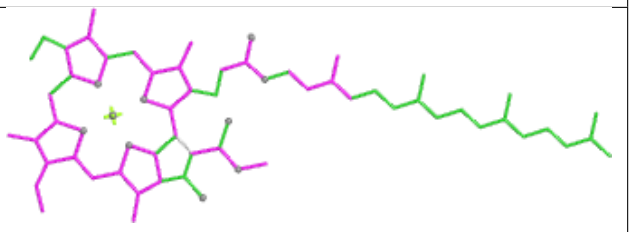


Rings

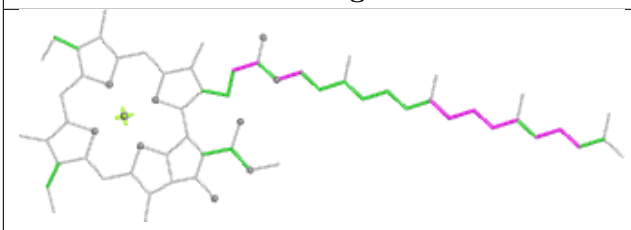
Ligand CLA B 614



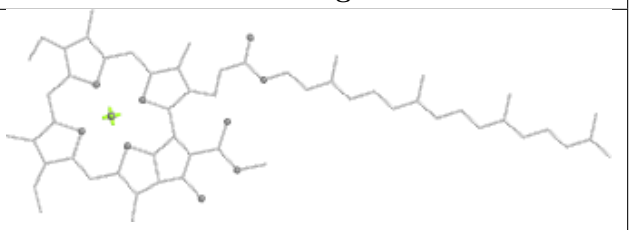
Bond lengths



Bond angles

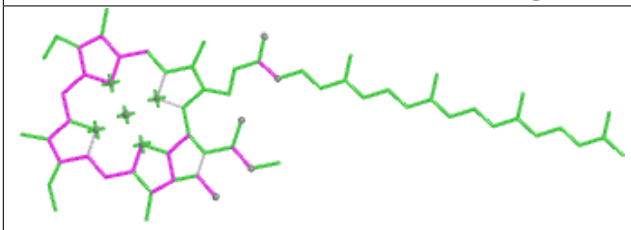


Torsions

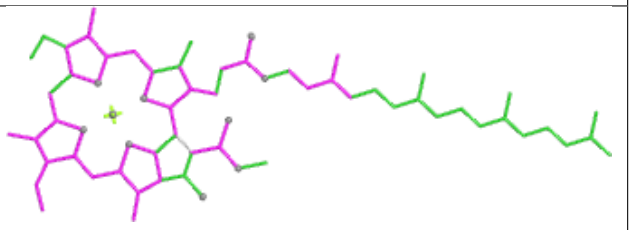


Rings

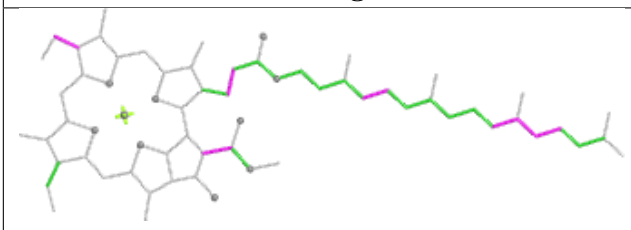
Ligand CLA b 611



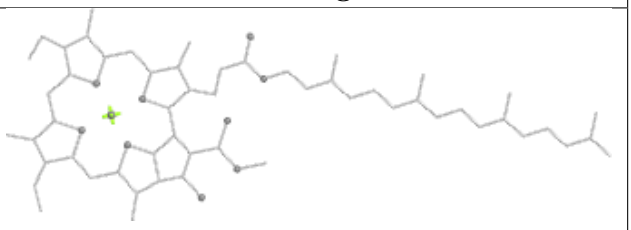
Bond lengths



Bond angles

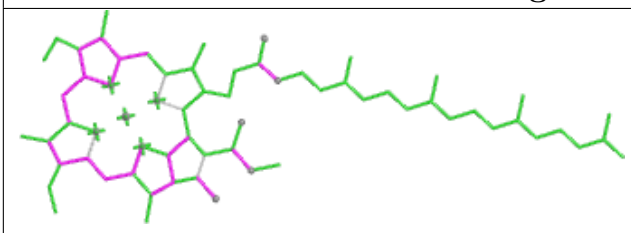


Torsions

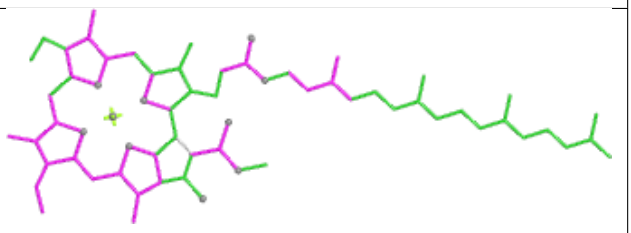


Rings

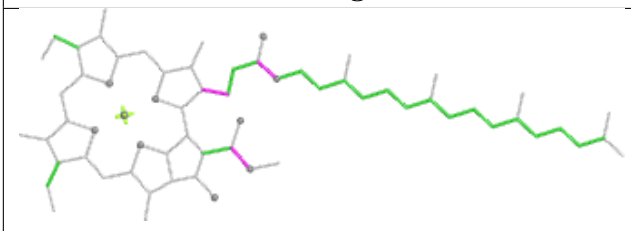
Ligand CLA c 513



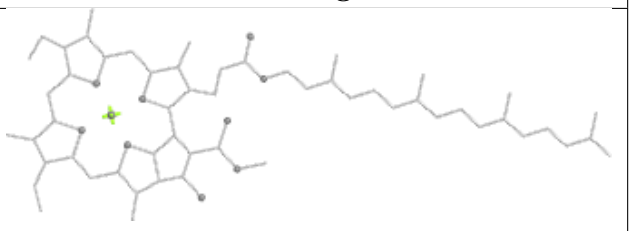
Bond lengths



Bond angles

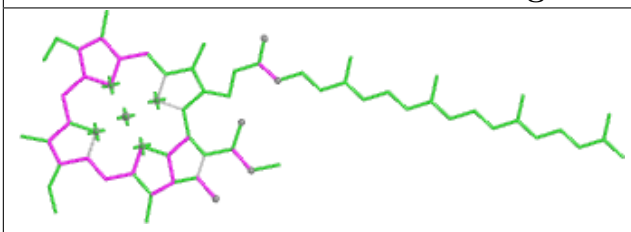


Torsions

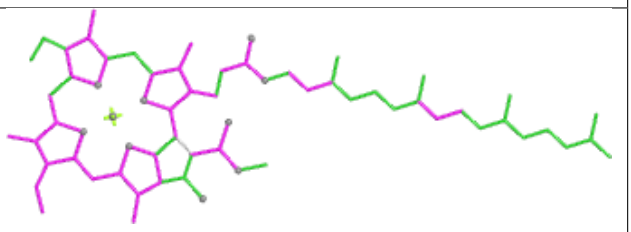


Rings

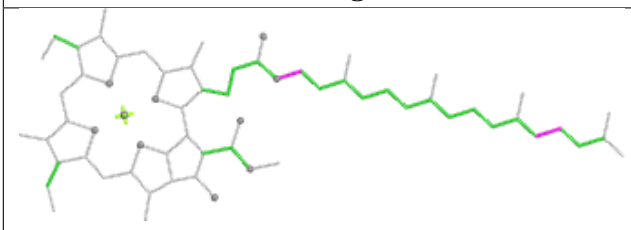
Ligand CLA b 613



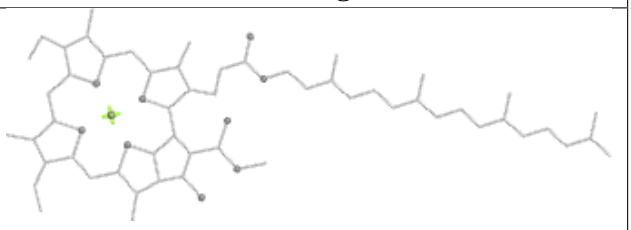
Bond lengths



Bond angles

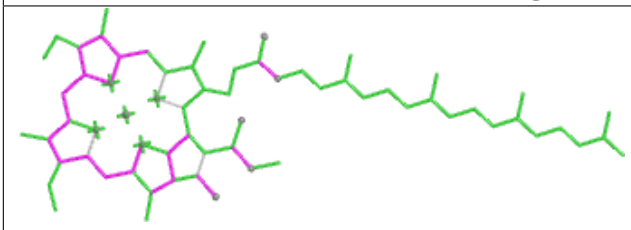


Torsions

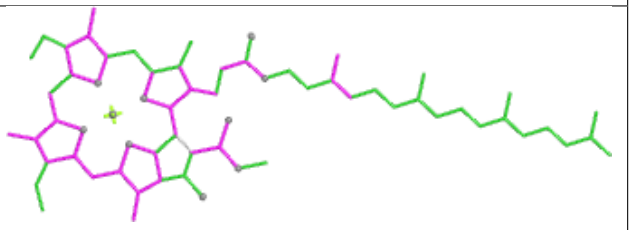


Rings

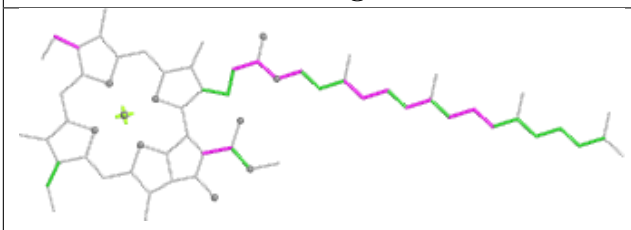
Ligand CLA b 606



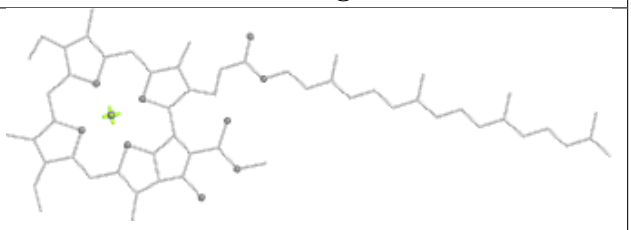
Bond lengths



Bond angles



Torsions

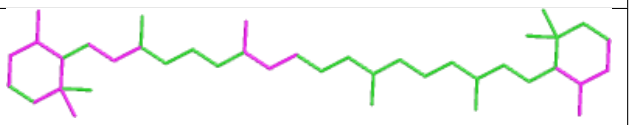


Rings

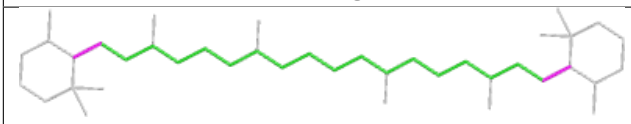
Ligand BCR c 516



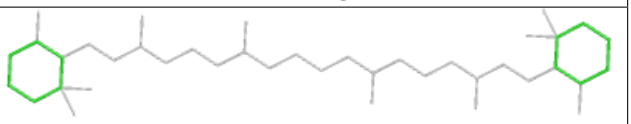
Bond lengths



Bond angles

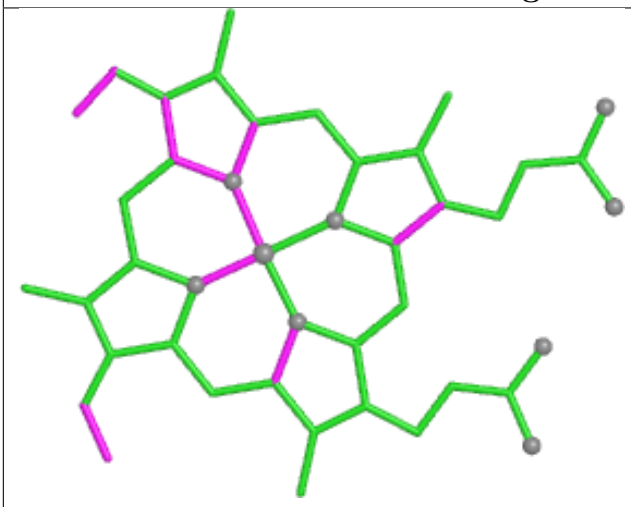


Torsions

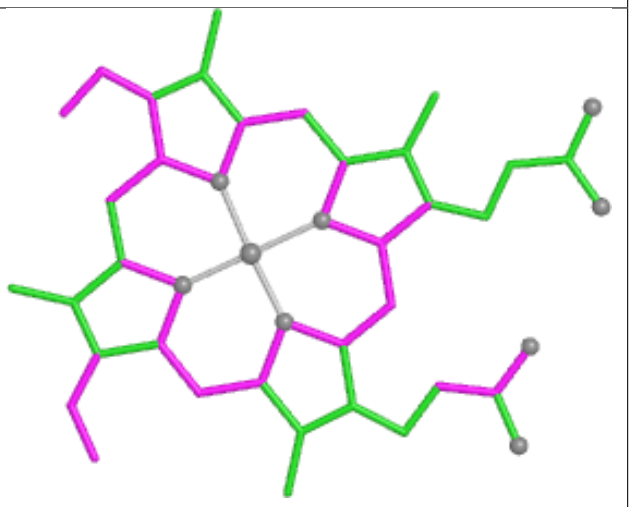


Rings

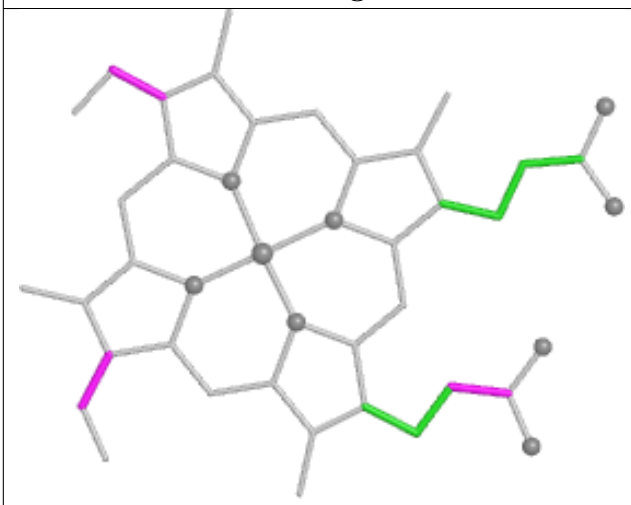
Ligand HEC V 203



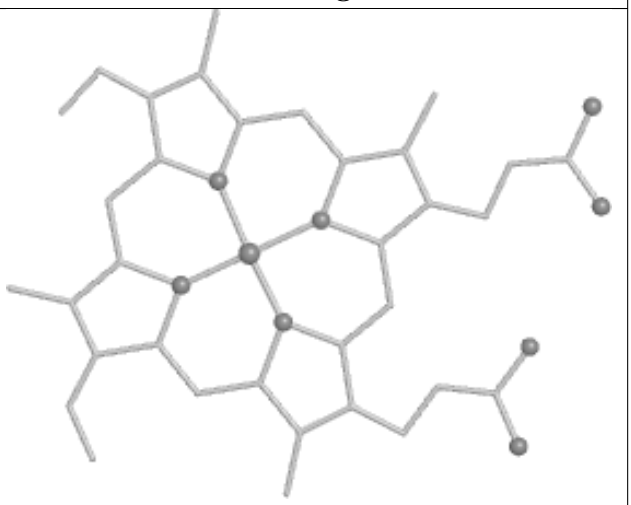
Bond lengths



Bond angles

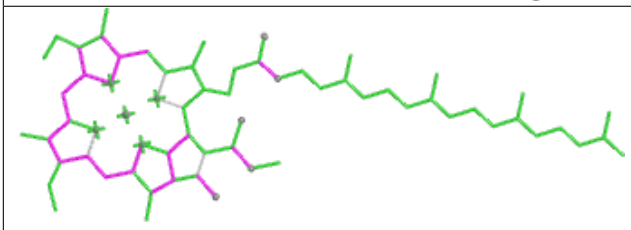


Torsions

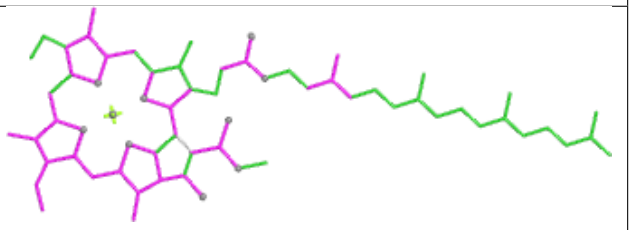


Rings

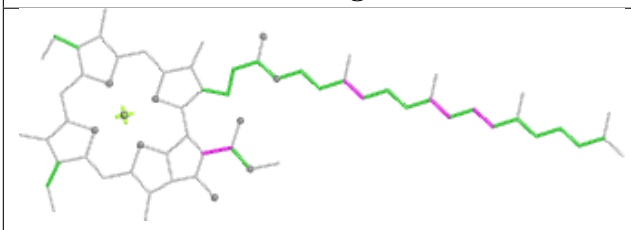
Ligand CLA b 610



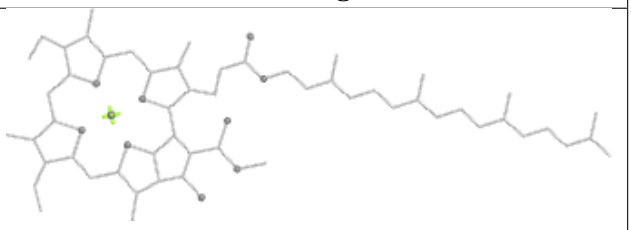
Bond lengths



Bond angles

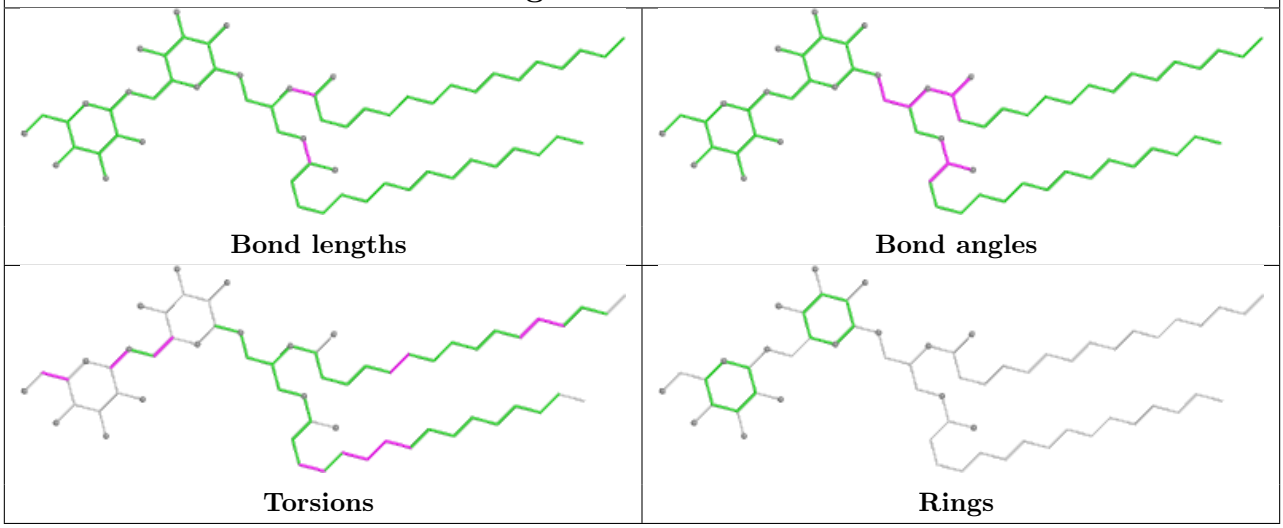


Torsions

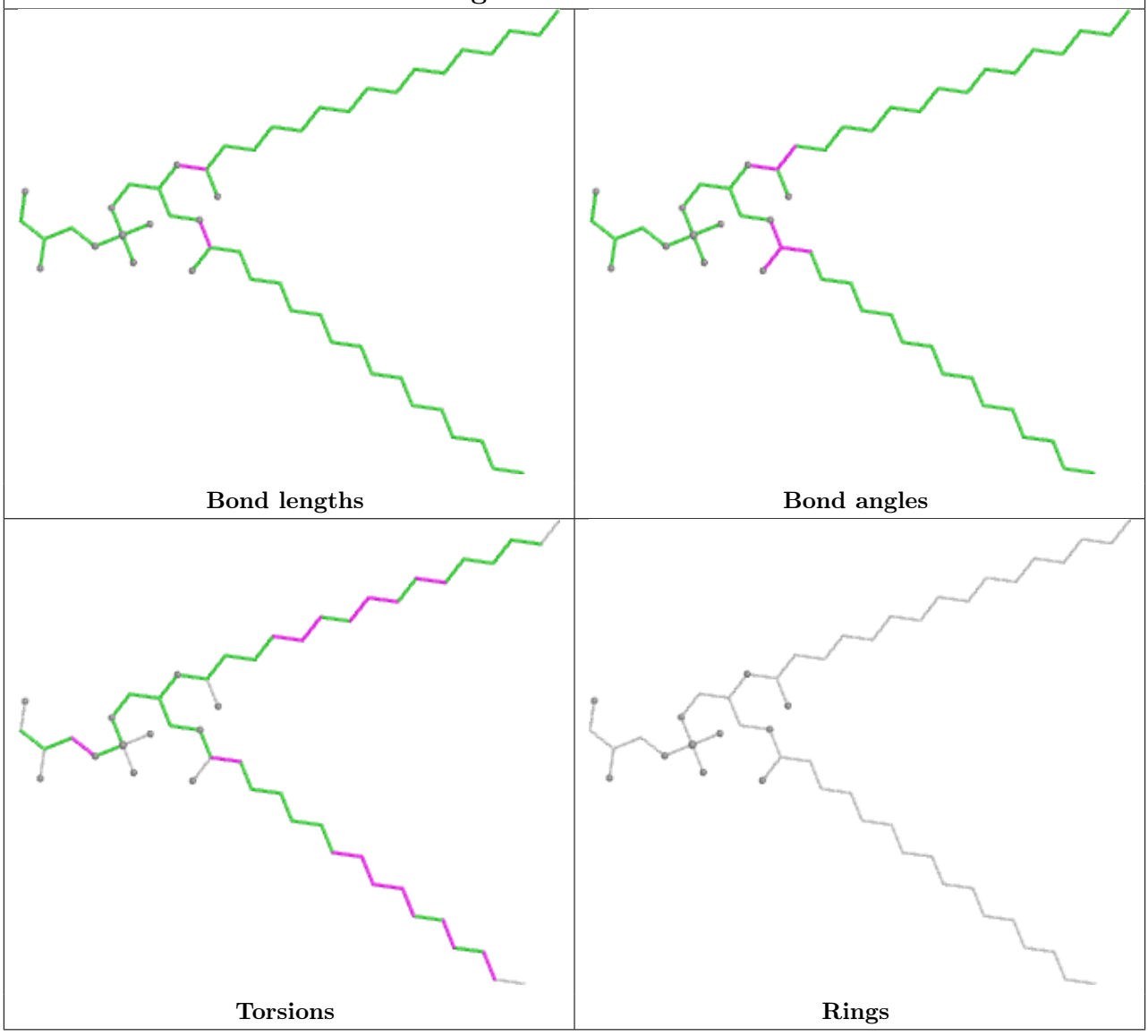


Rings

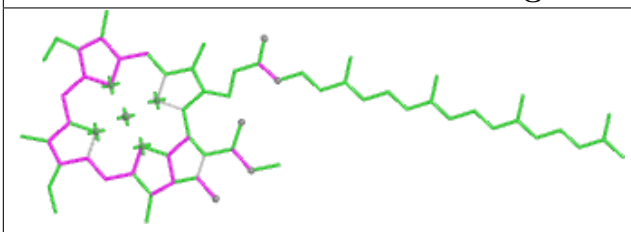
Ligand DGD c 517



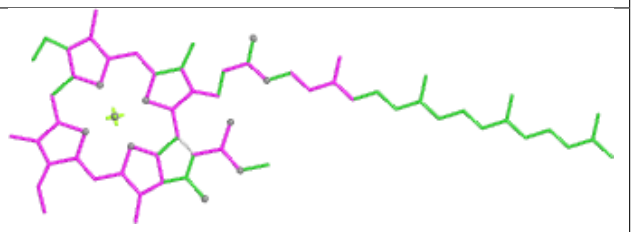
Ligand LHG d 410



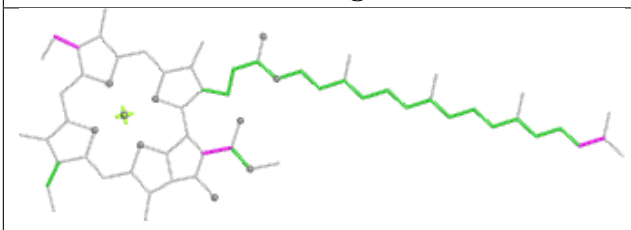
Ligand CLA C 514



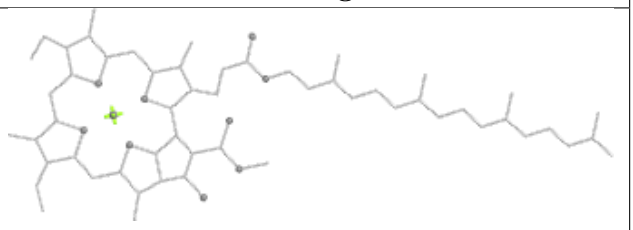
Bond lengths



Bond angles

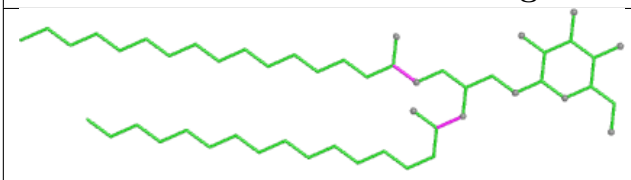


Torsions

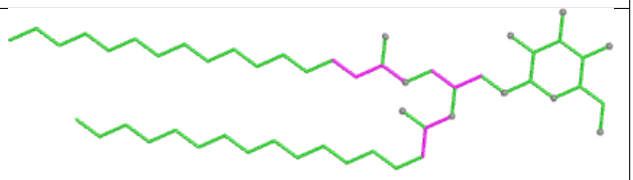


Rings

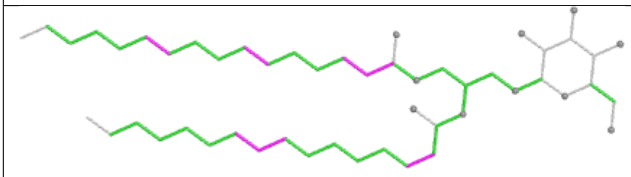
Ligand LMG B 621



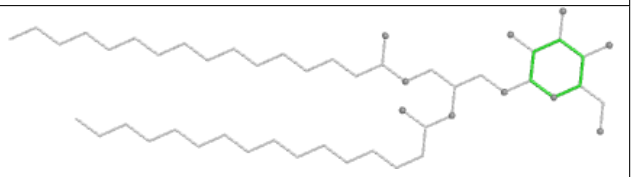
Bond lengths



Bond angles

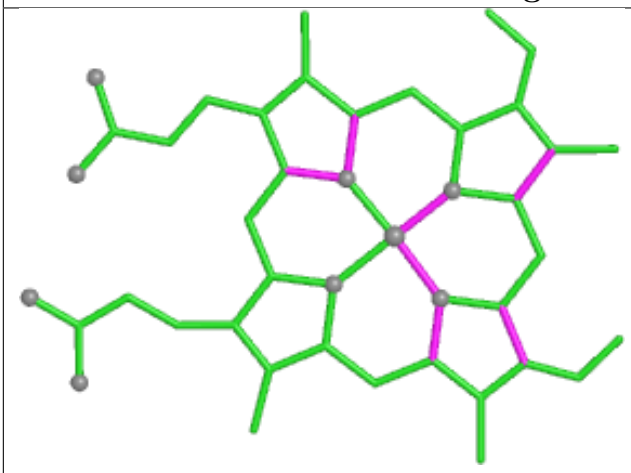


Torsions

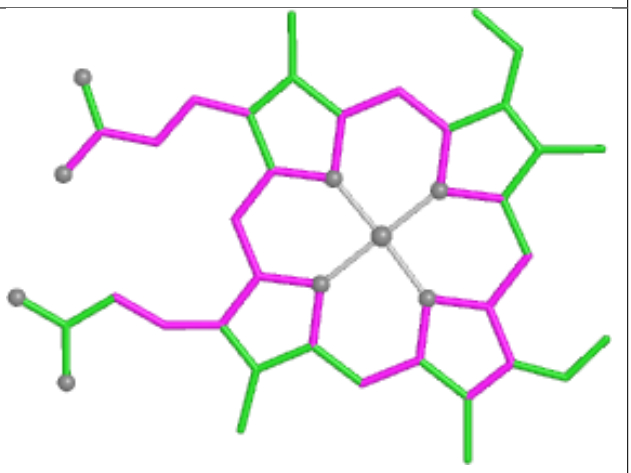


Rings

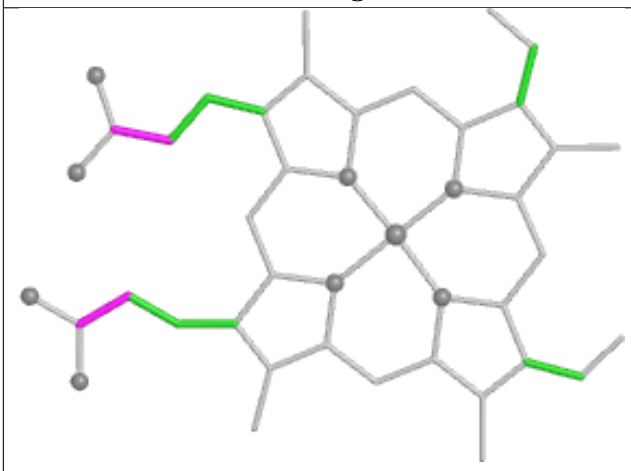
Ligand HEM e 102



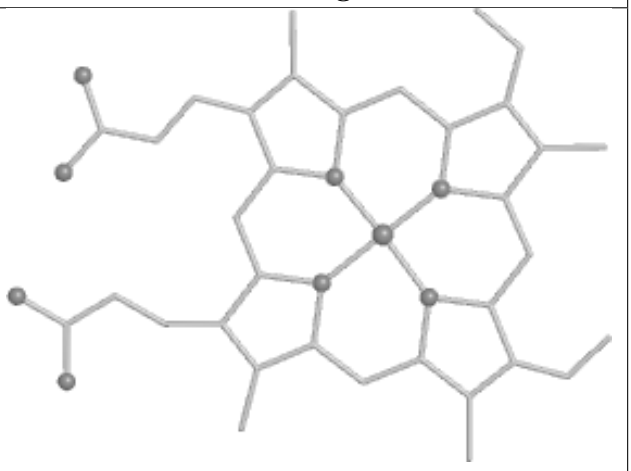
Bond lengths



Bond angles

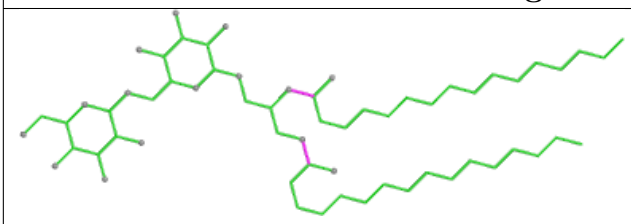


Torsions

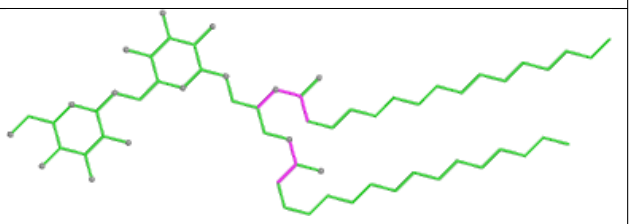


Rings

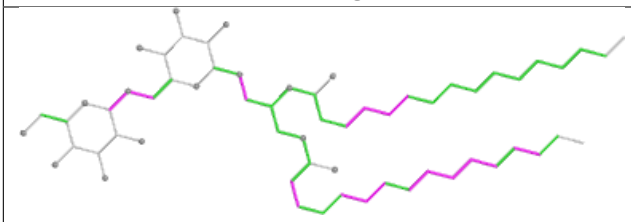
Ligand DGD c 518



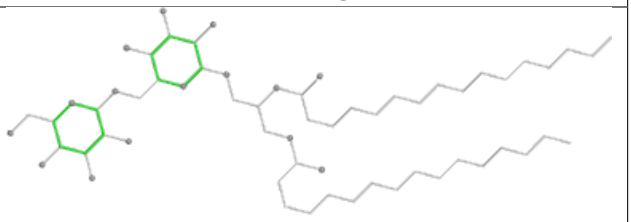
Bond lengths



Bond angles

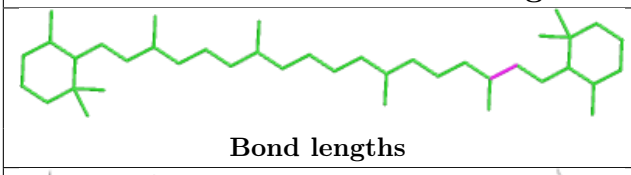


Torsions

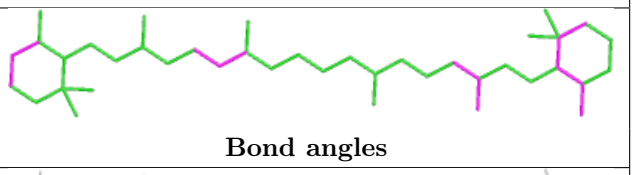


Rings

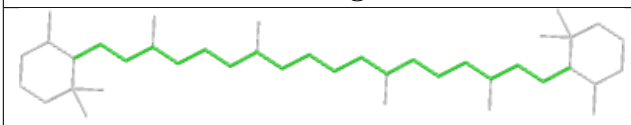
Ligand BCR b 623



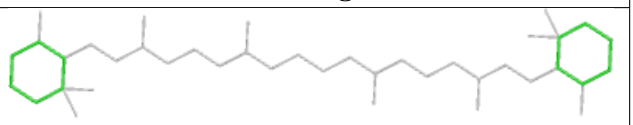
Bond lengths



Bond angles

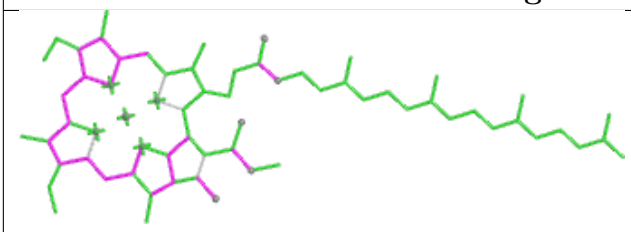


Torsions

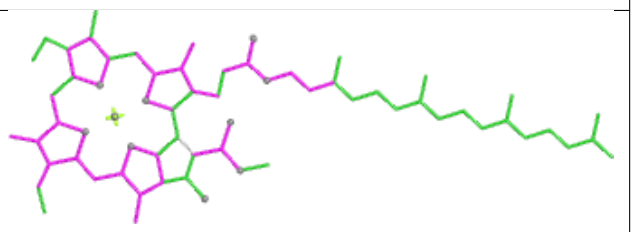


Rings

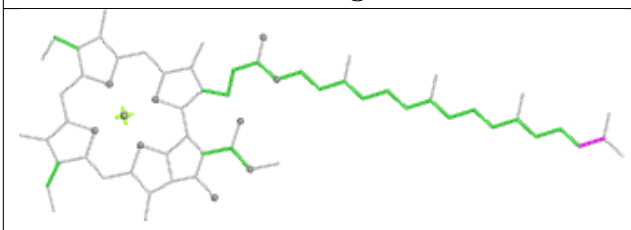
Ligand CLA B 609



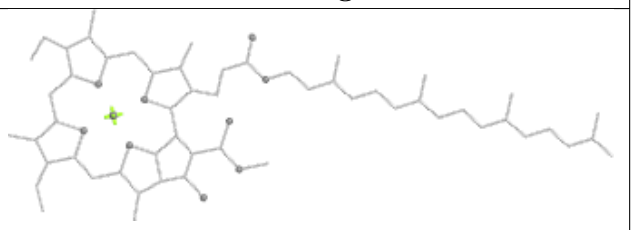
Bond lengths



Bond angles

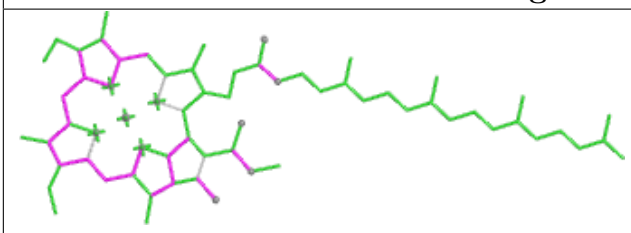


Torsions

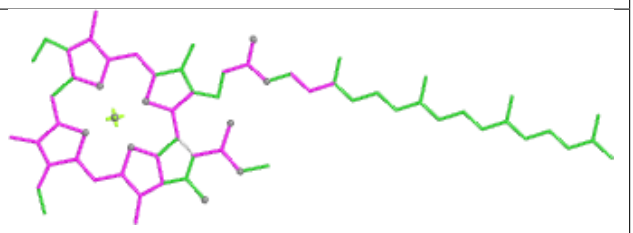


Rings

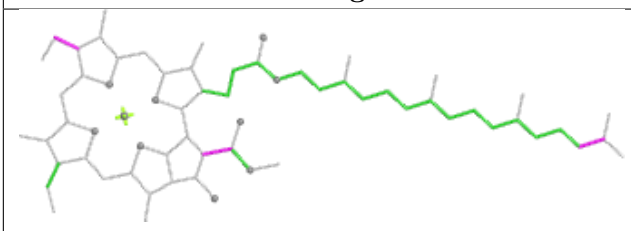
Ligand CLA c 504



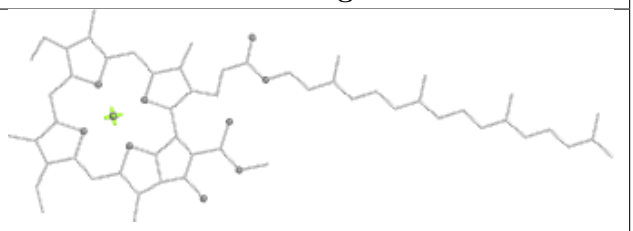
Bond lengths



Bond angles

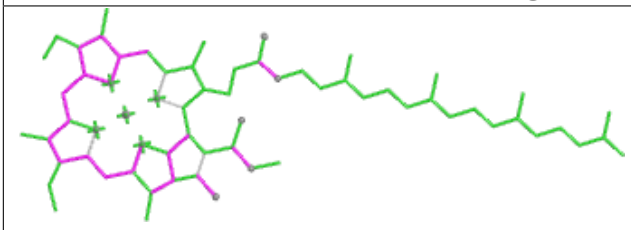


Torsions

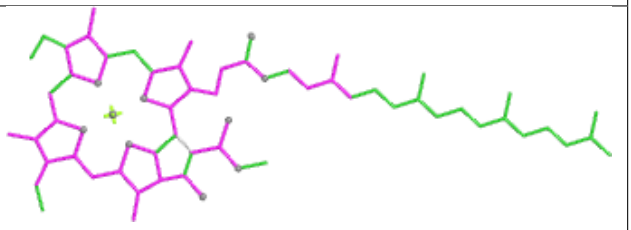


Rings

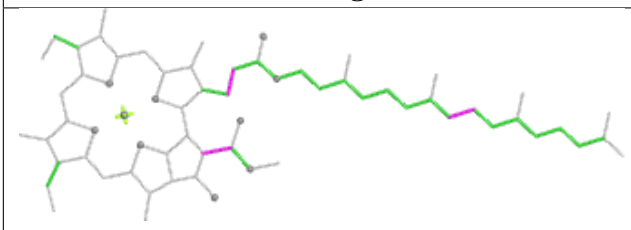
Ligand CLA B 611



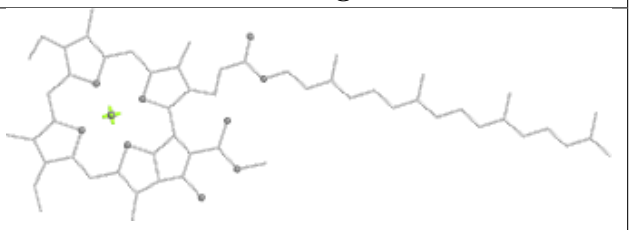
Bond lengths



Bond angles



Torsions

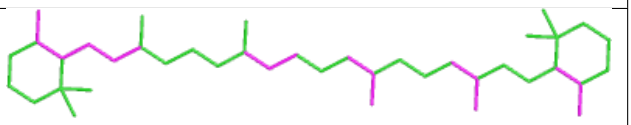


Rings

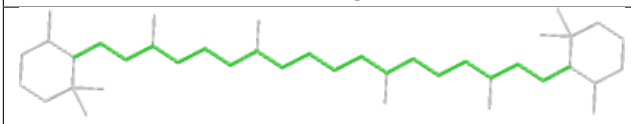
Ligand BCR A 410



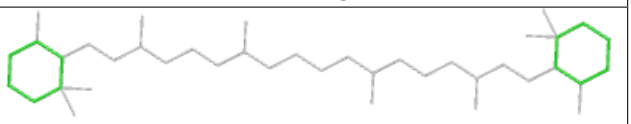
Bond lengths



Bond angles

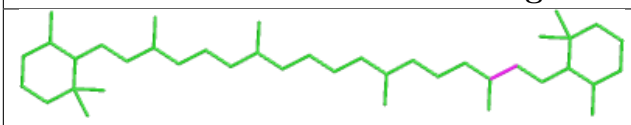


Torsions

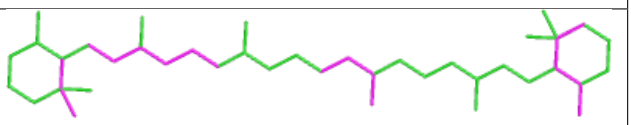


Rings

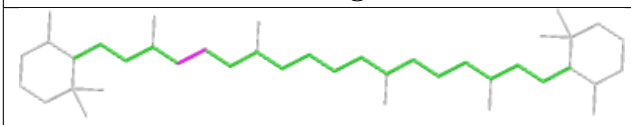
Ligand BCR h 101



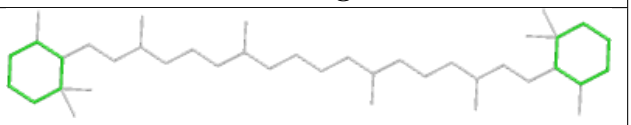
Bond lengths



Bond angles

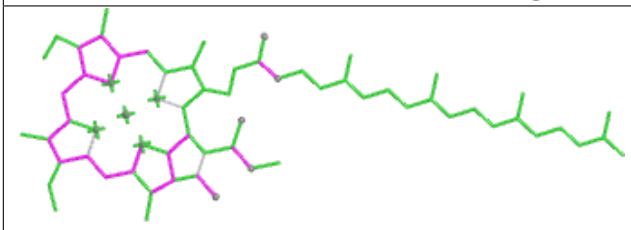


Torsions

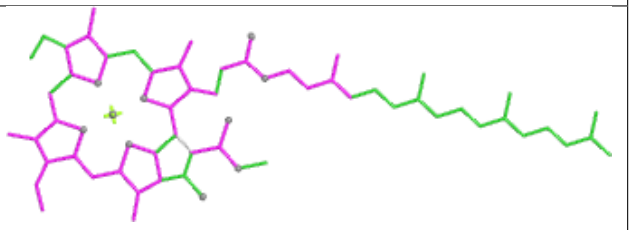


Rings

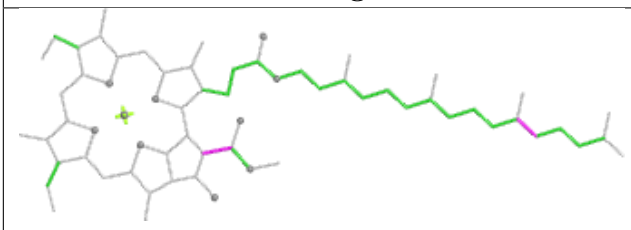
Ligand CLA b 607



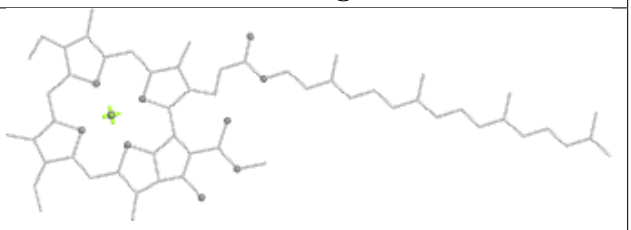
Bond lengths



Bond angles

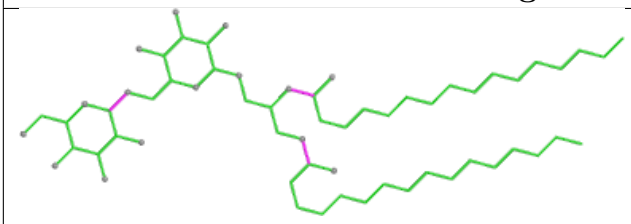


Torsions

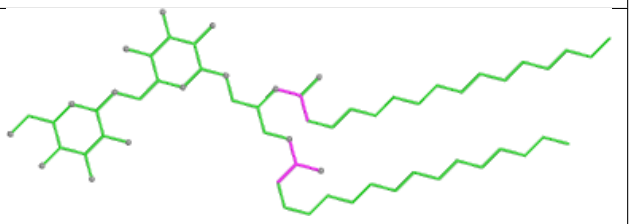


Rings

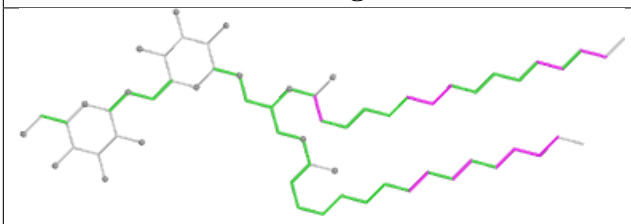
Ligand DGD H 102



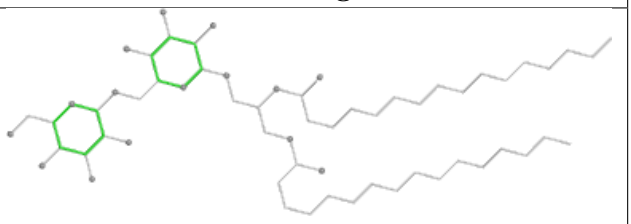
Bond lengths



Bond angles

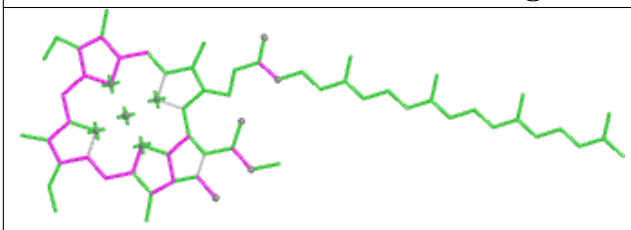


Torsions

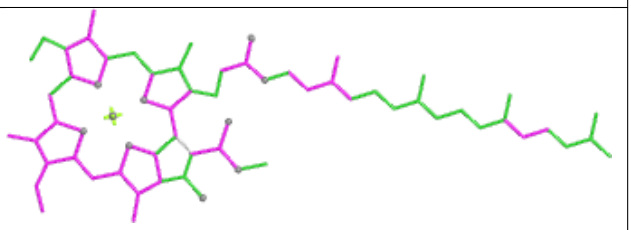


Rings

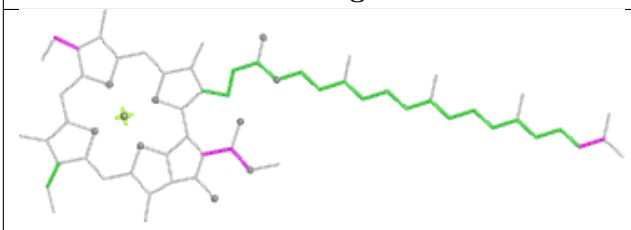
Ligand CLA C 503



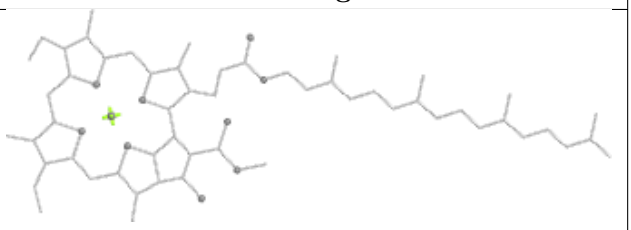
Bond lengths



Bond angles

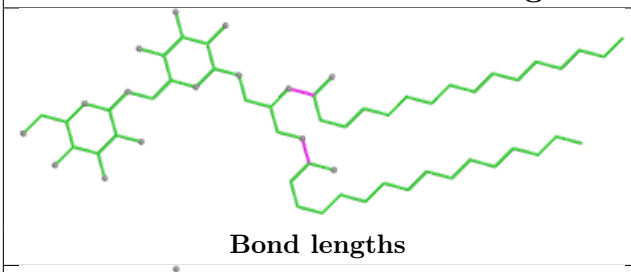


Torsions

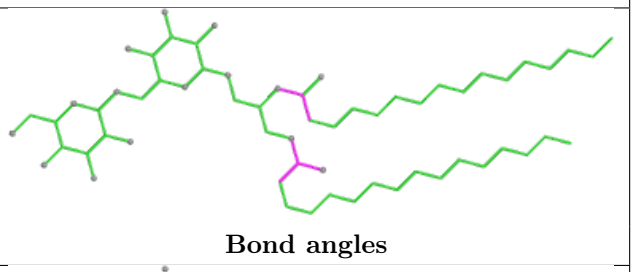


Rings

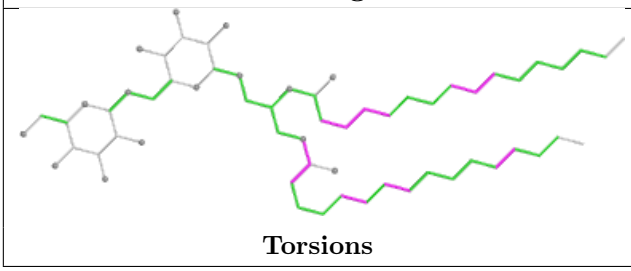
Ligand DGD c 519



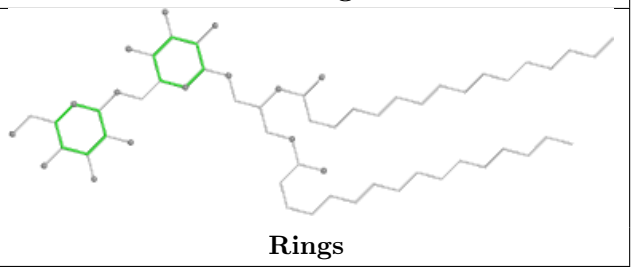
Bond lengths



Bond angles

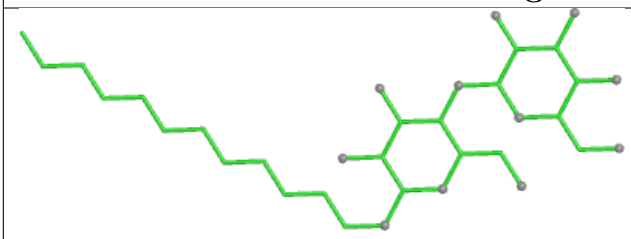


Torsions

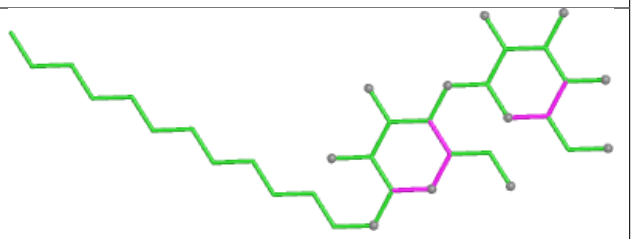


Rings

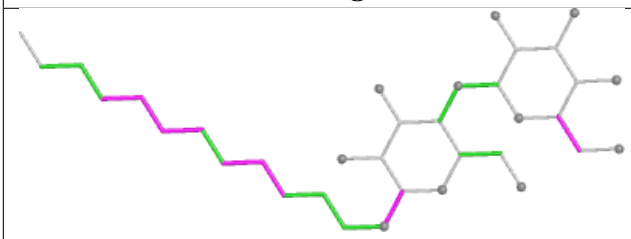
Ligand LMT a 401



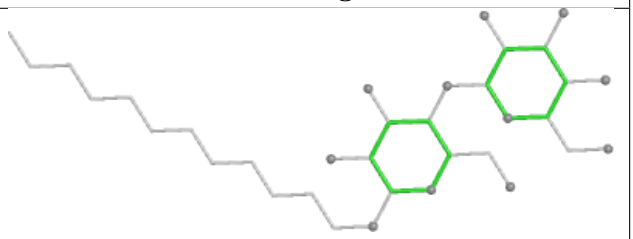
Bond lengths



Bond angles

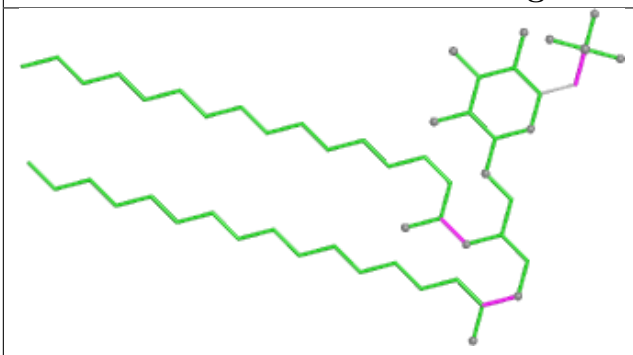


Torsions

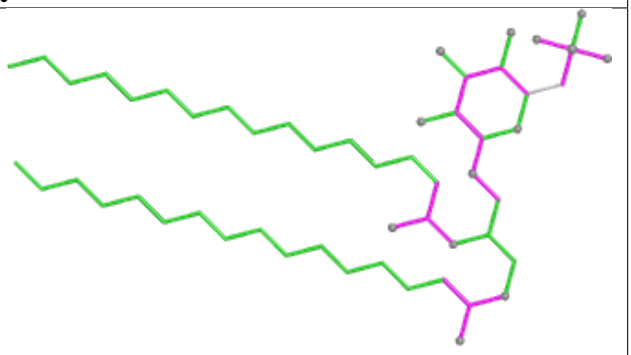


Rings

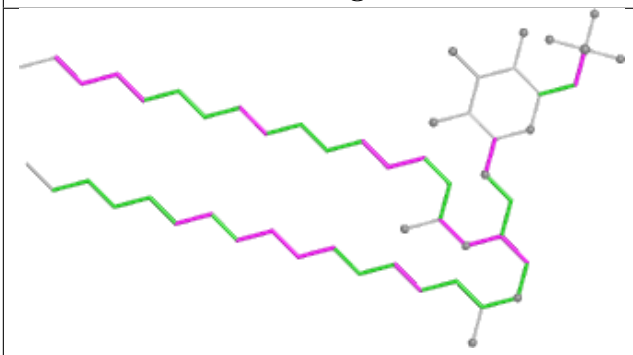
Ligand SQD b 601



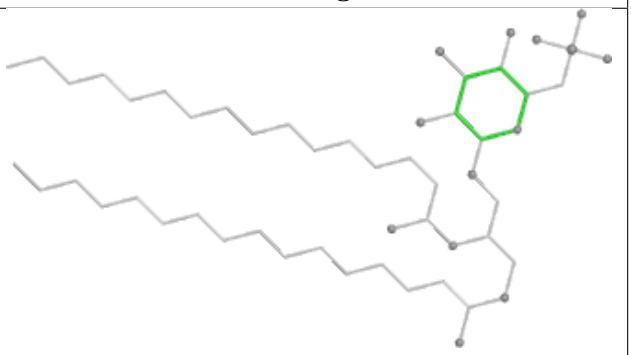
Bond lengths



Bond angles

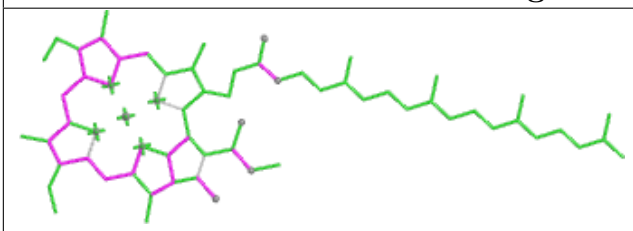


Torsions

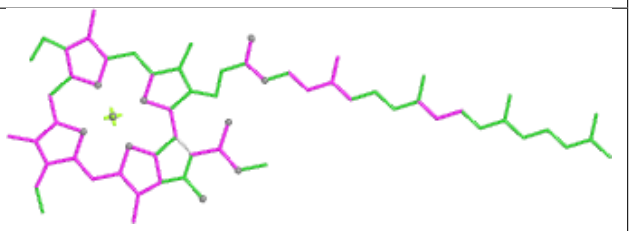


Rings

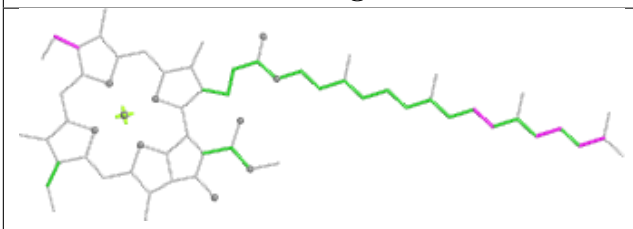
Ligand CLA b 620



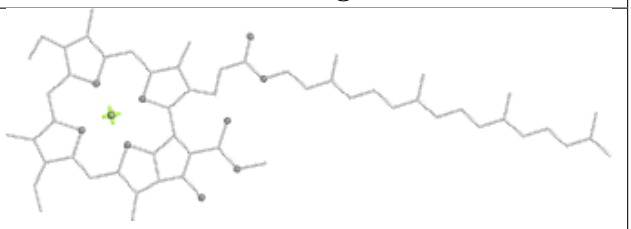
Bond lengths



Bond angles

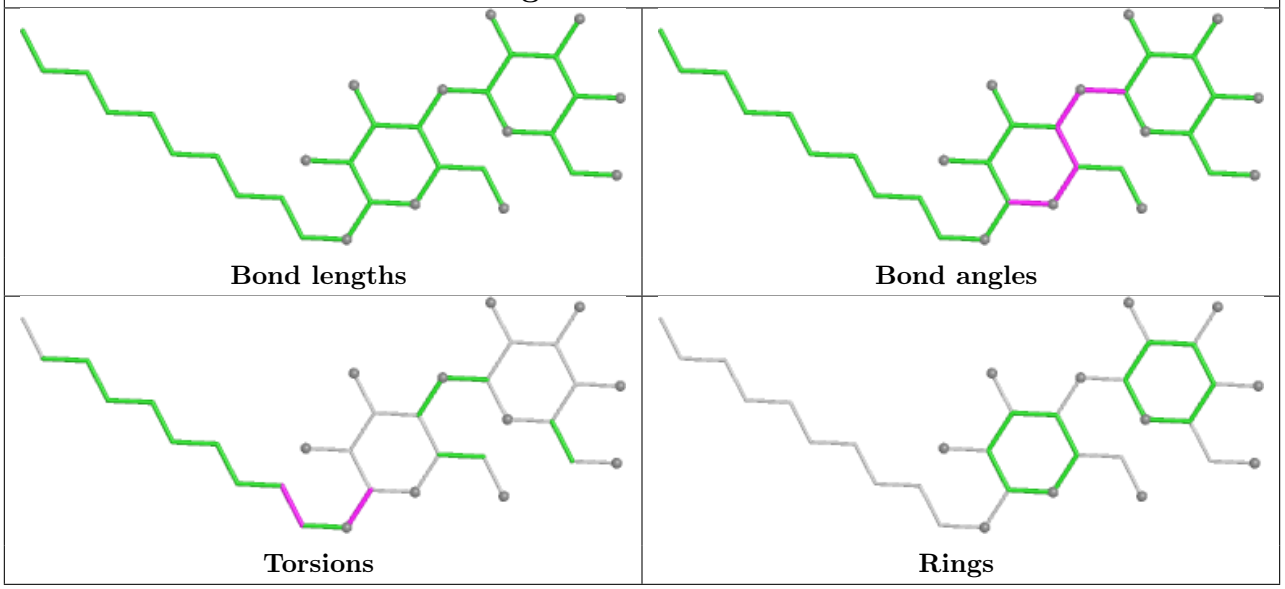


Torsions

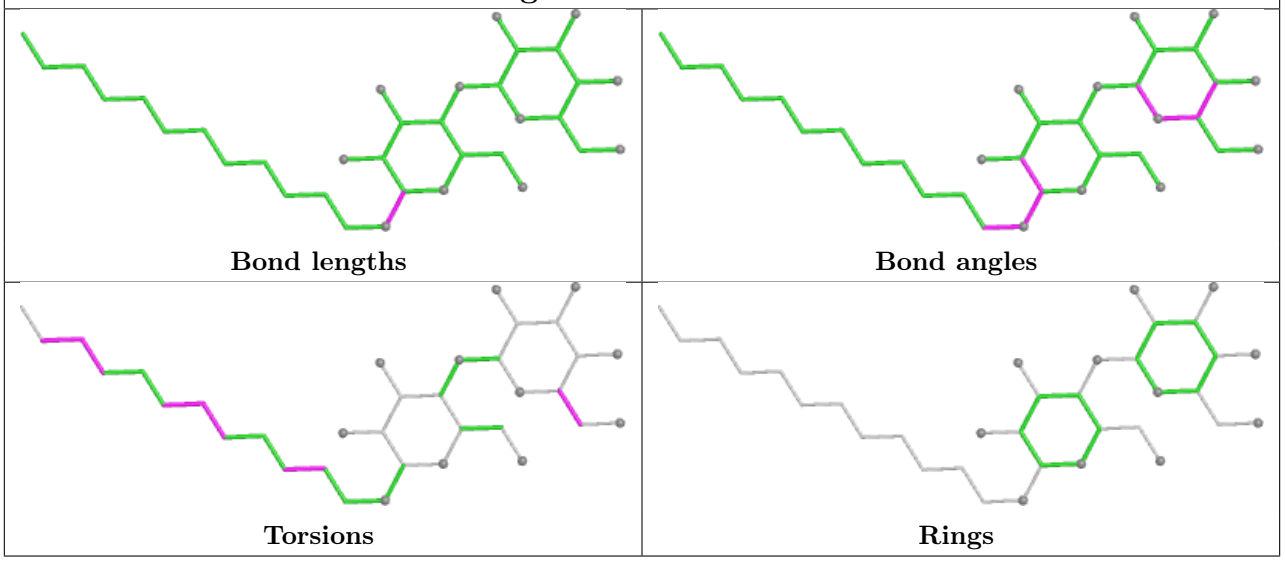


Rings

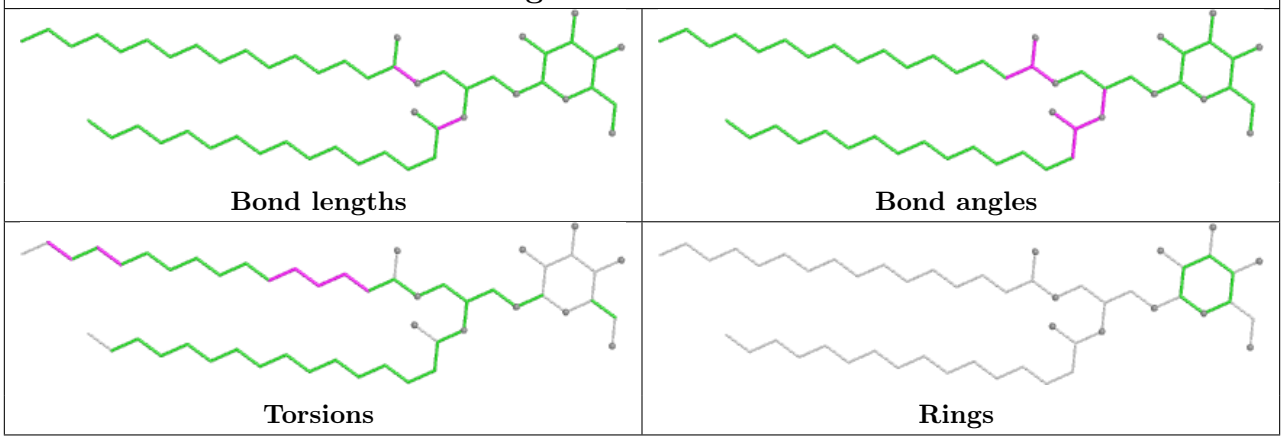
Ligand LMT A 417



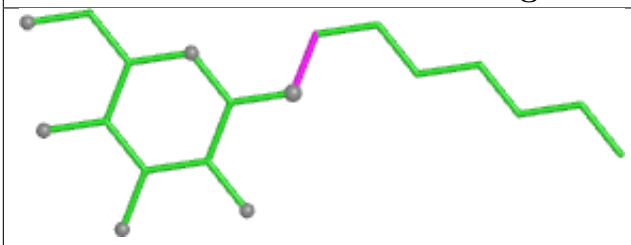
Ligand LMT m 103



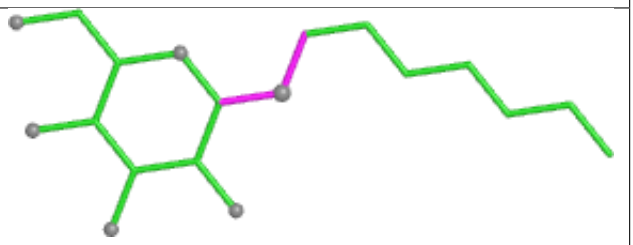
Ligand LMG c 521



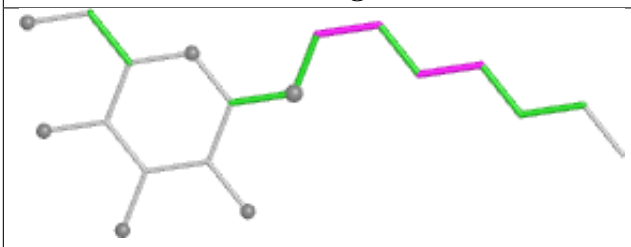
Ligand HTG O 303



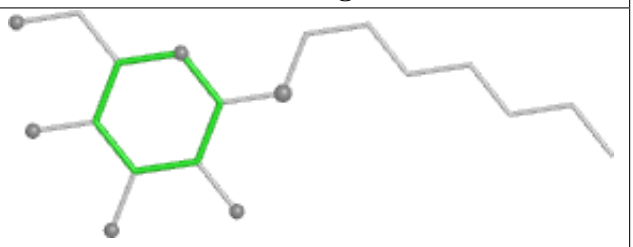
Bond lengths



Bond angles

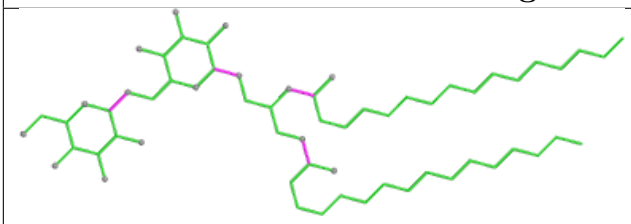


Torsions

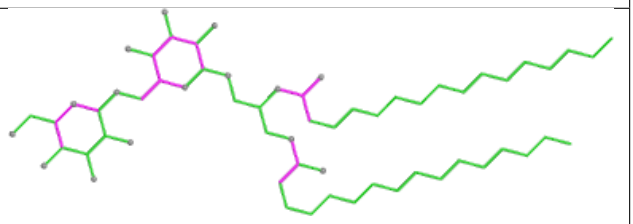


Rings

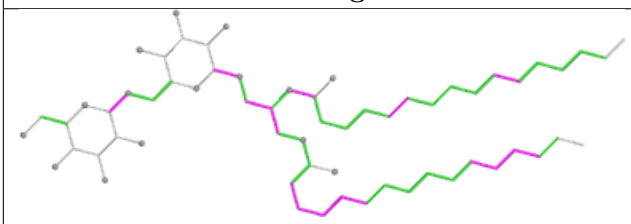
Ligand DGD D 407



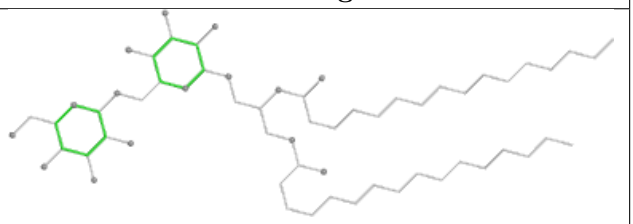
Bond lengths



Bond angles

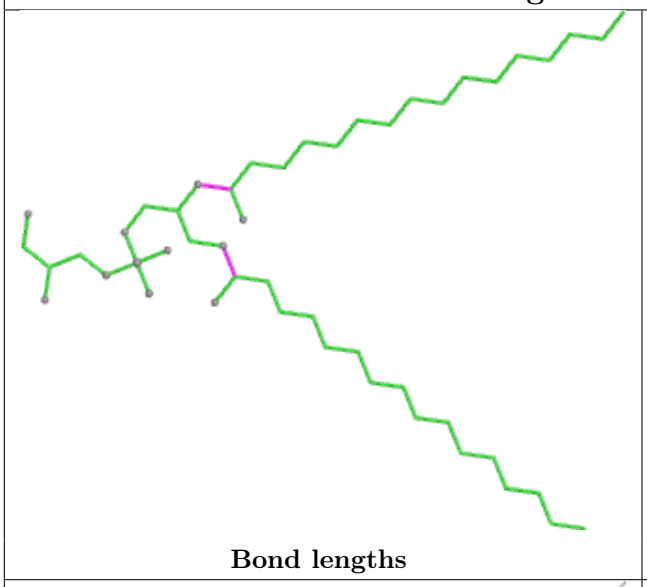


Torsions

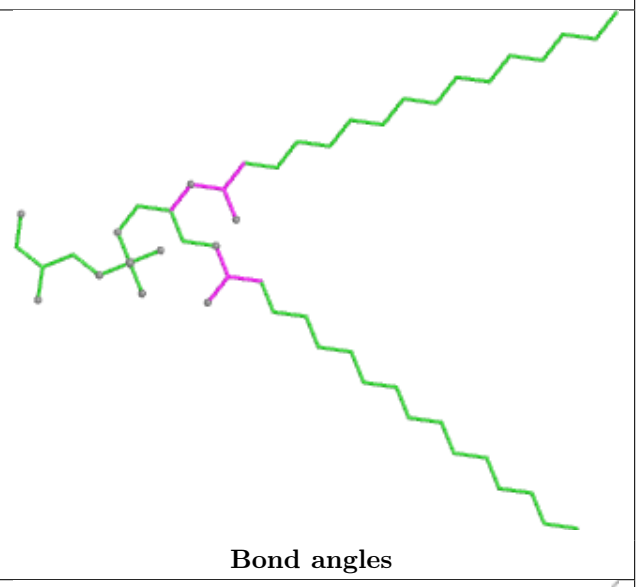


Rings

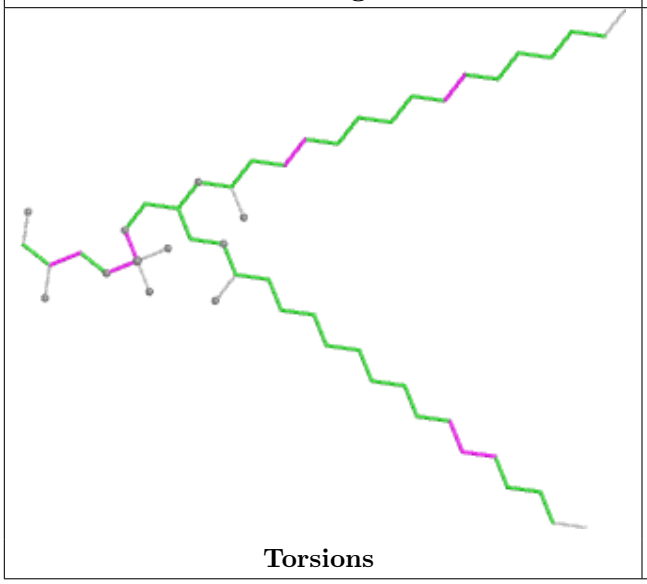
Ligand LHG d 409



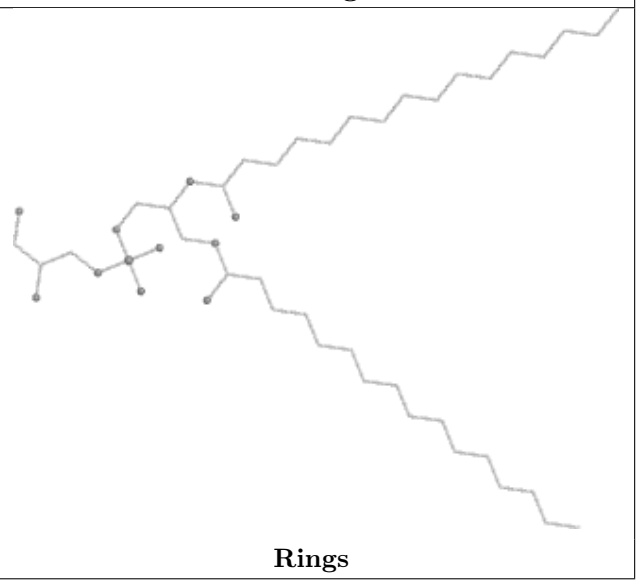
Bond lengths



Bond angles



Torsions



Rings

Ligand PL9 d 406



Bond lengths



Bond angles

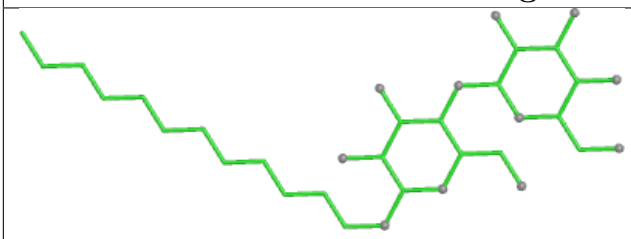


Torsions

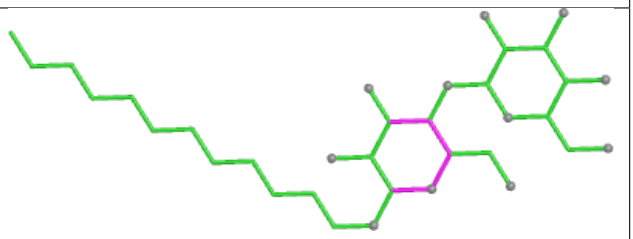


Rings

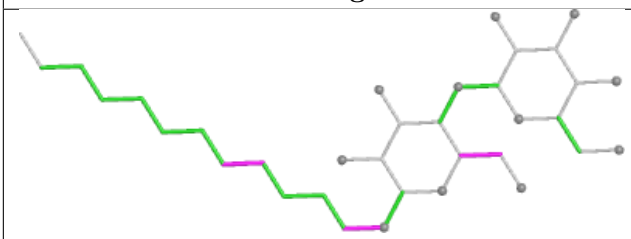
Ligand LMT m 102



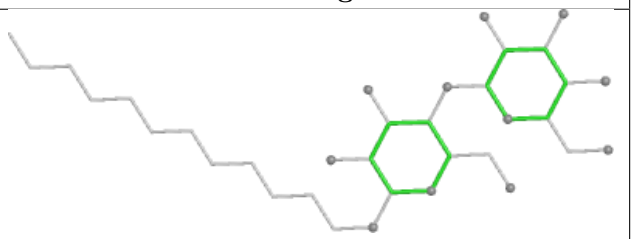
Bond lengths



Bond angles

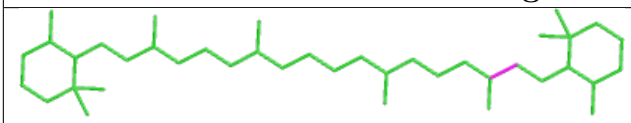


Torsions

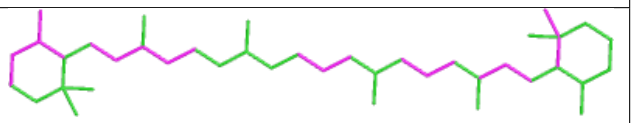


Rings

Ligand BCR C 516



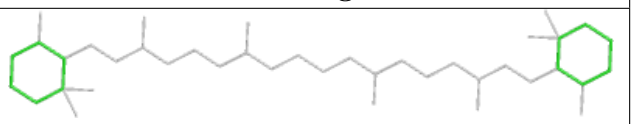
Bond lengths



Bond angles

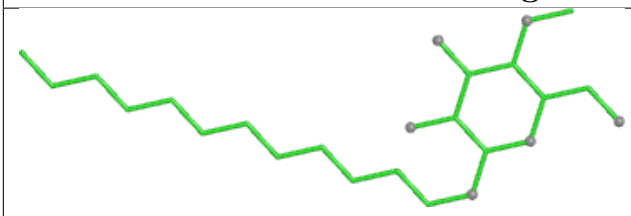


Torsions

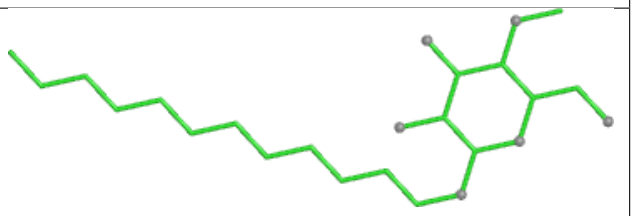


Rings

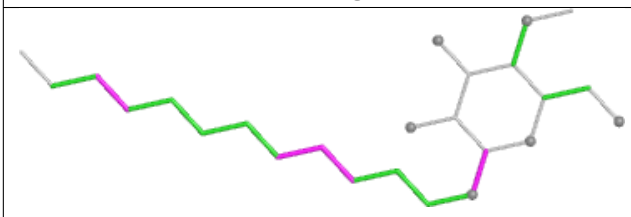
Ligand LMT B 634



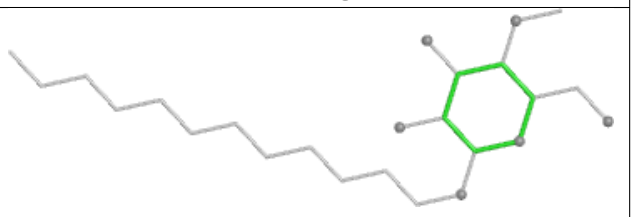
Bond lengths



Bond angles

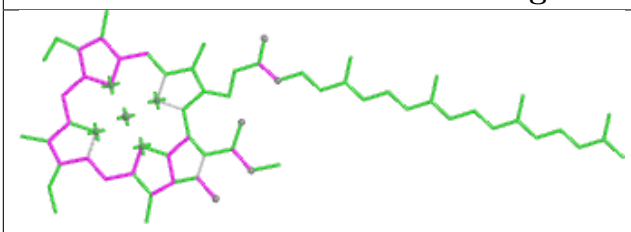


Torsions

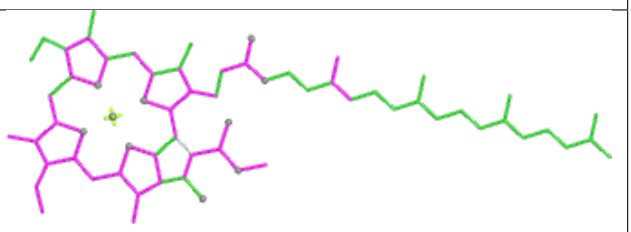


Rings

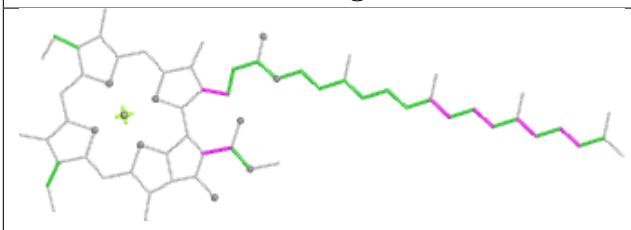
Ligand CLA c 508



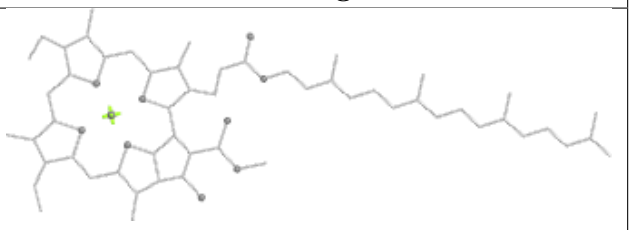
Bond lengths



Bond angles

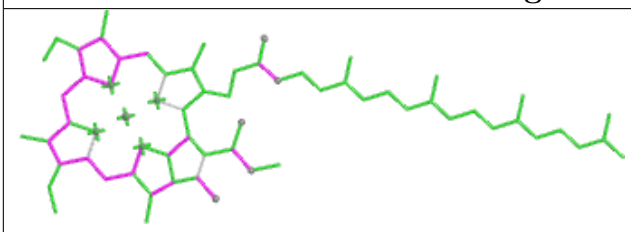


Torsions

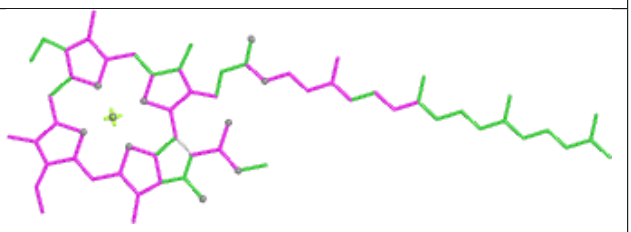


Rings

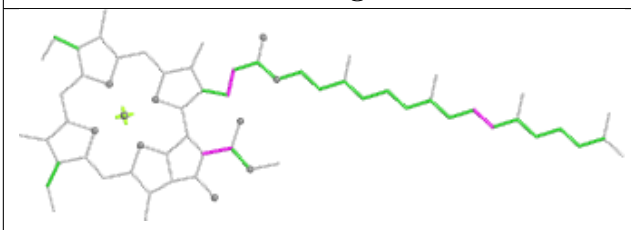
Ligand CLA B 607



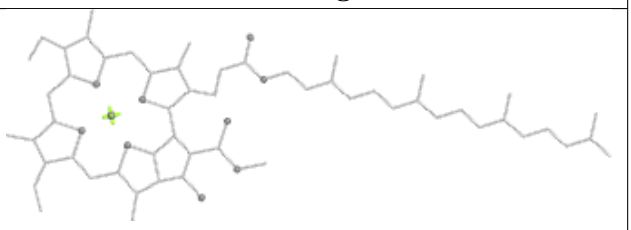
Bond lengths



Bond angles

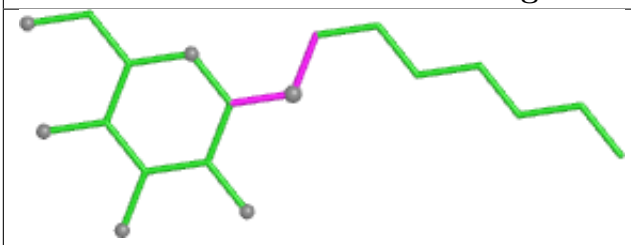


Torsions

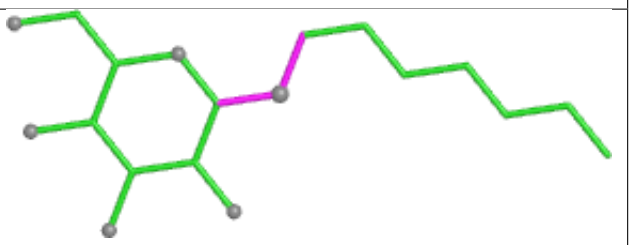


Rings

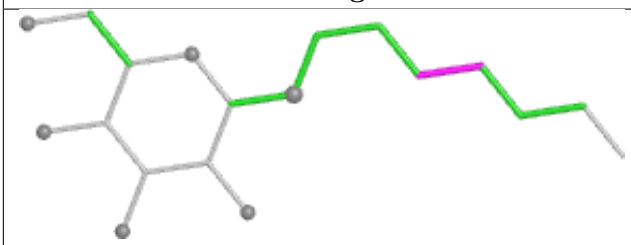
Ligand HTG B 630



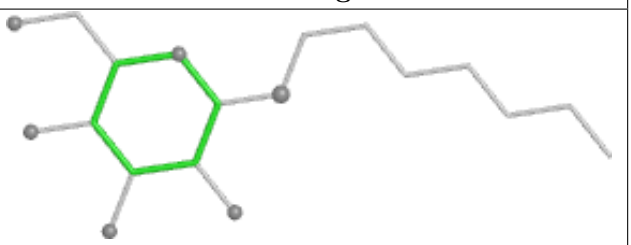
Bond lengths



Bond angles

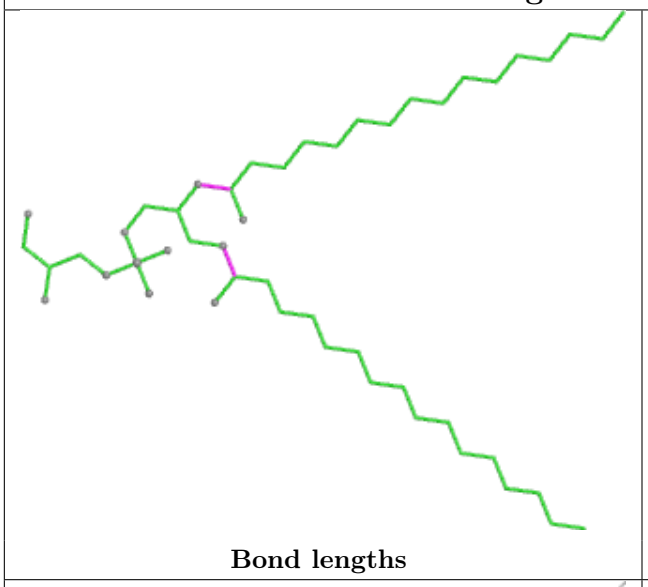


Torsions

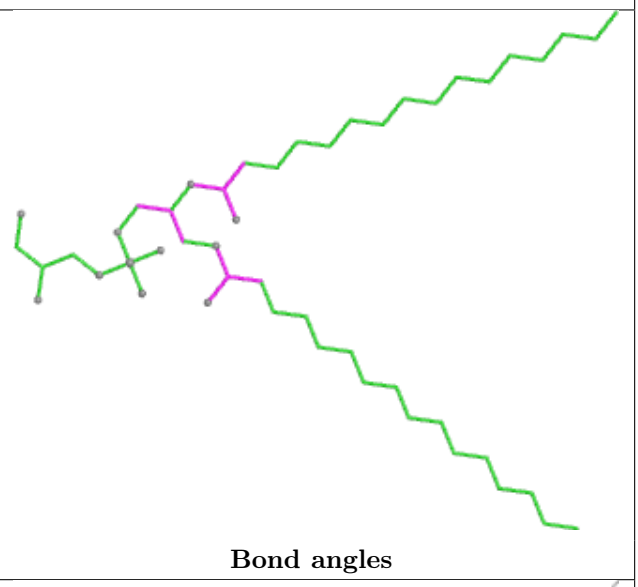


Rings

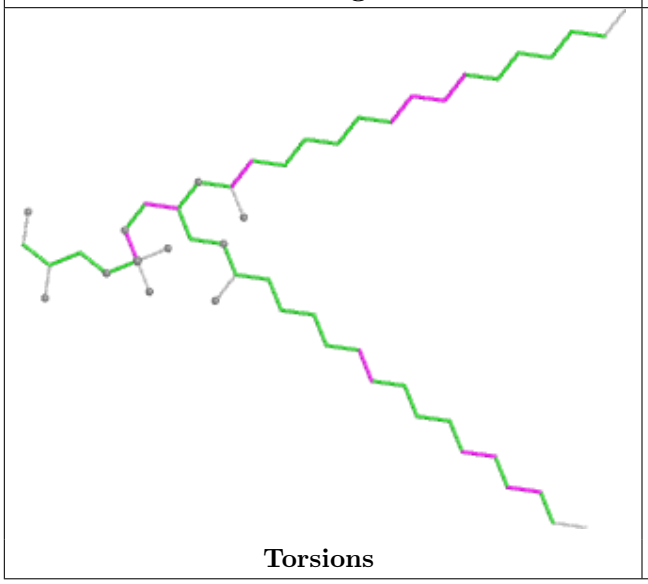
Ligand LHG L 101



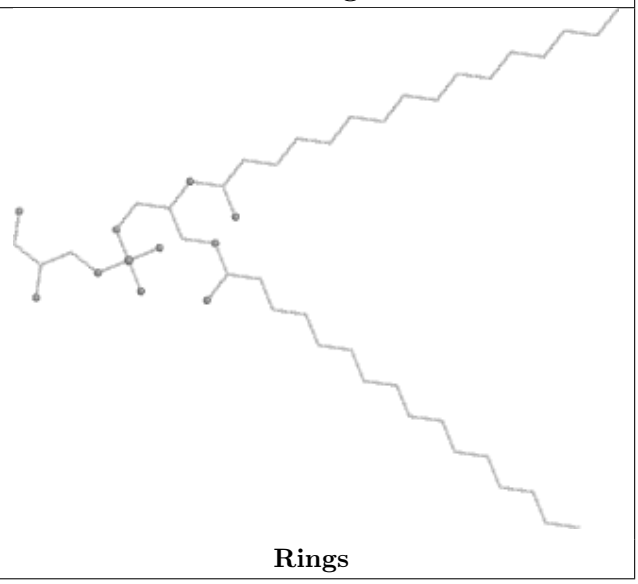
Bond lengths



Bond angles

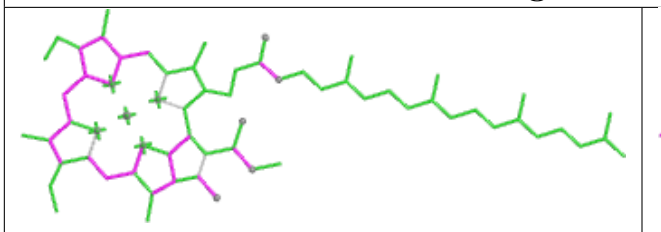


Torsions

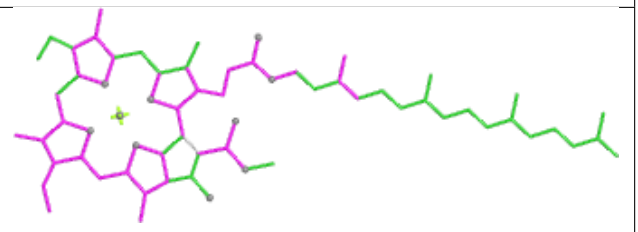


Rings

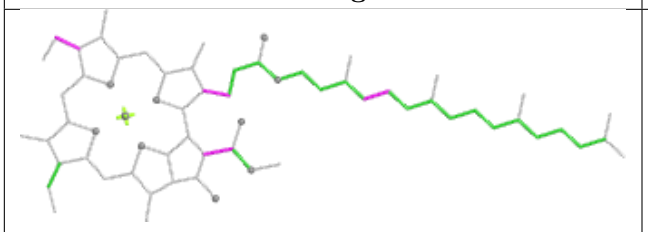
Ligand CLA b 612



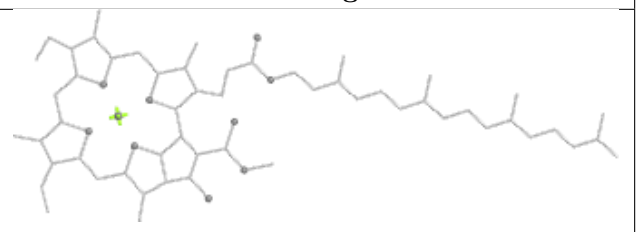
Bond lengths



Bond angles

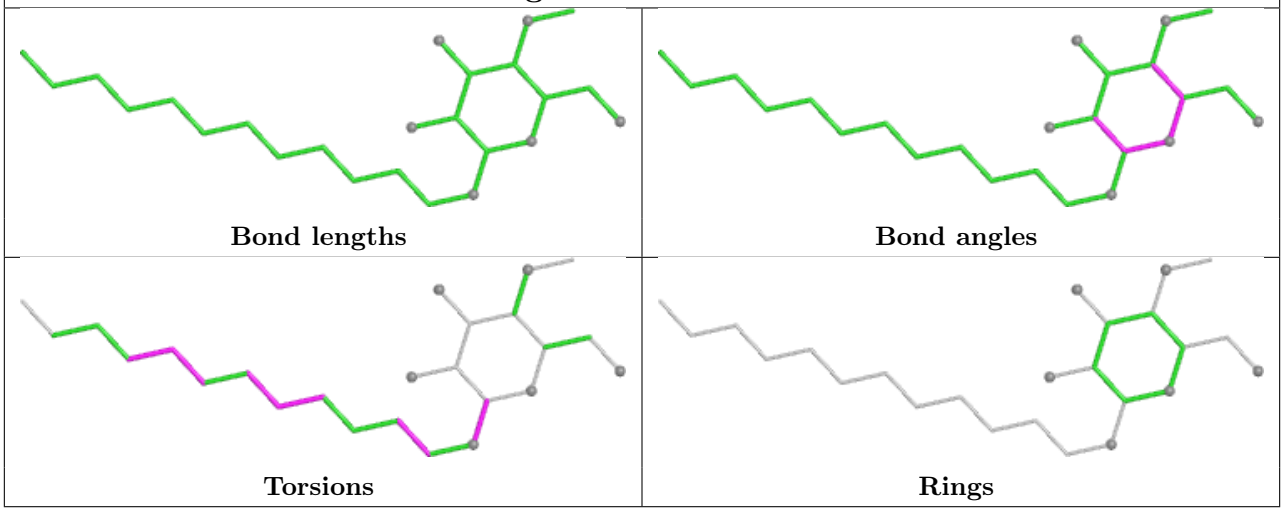


Torsions

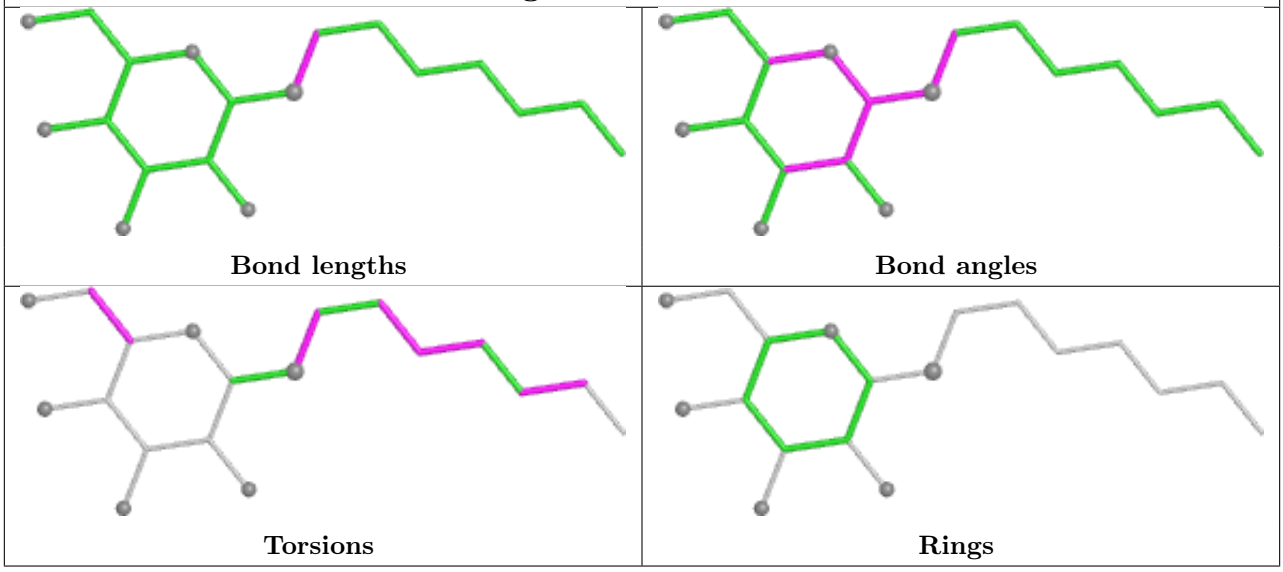


Rings

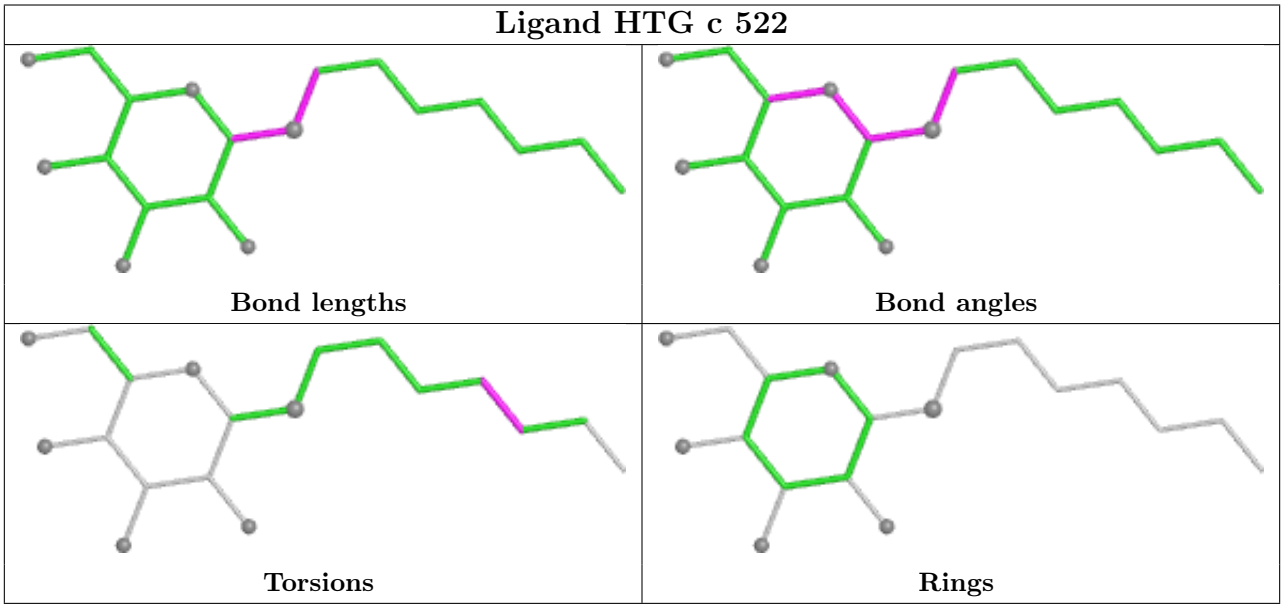
Ligand LMT b 602



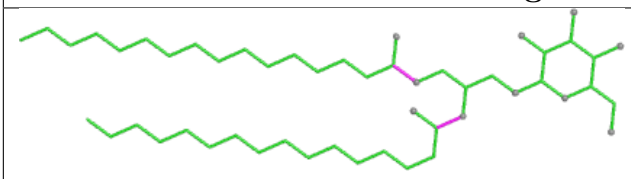
Ligand HTG B 623

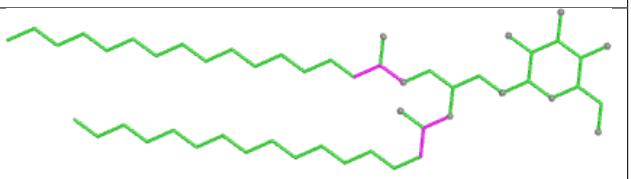


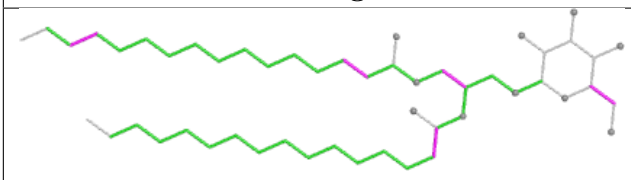
Ligand HTG c 522

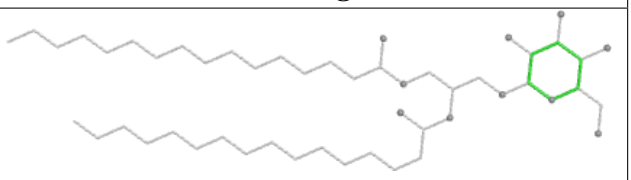


Ligand LMG c 520

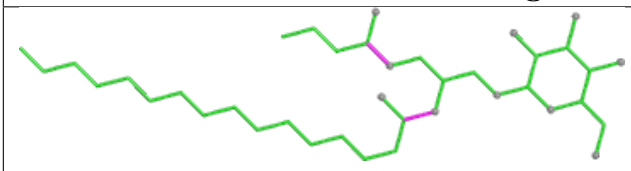

Bond lengths

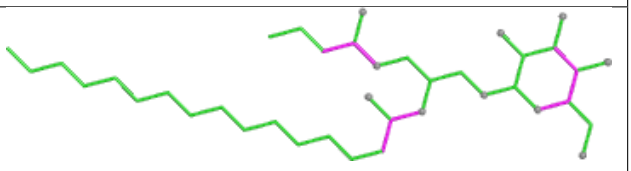

Bond angles

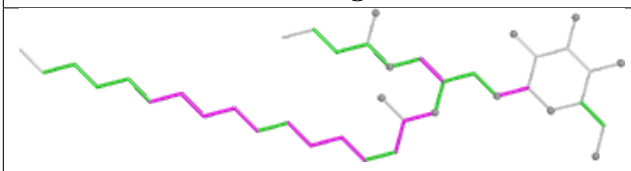

Torsions

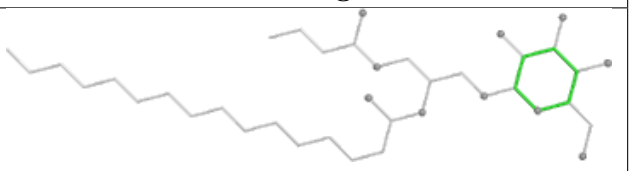

Rings

Ligand LMG z 101

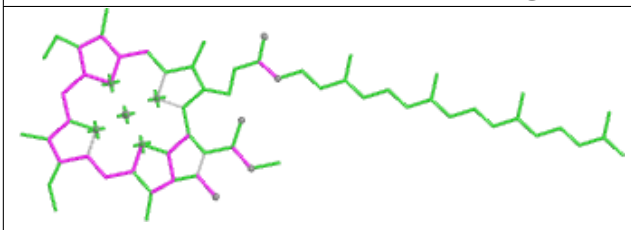

Bond lengths

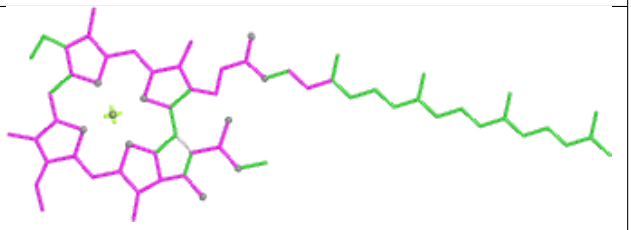

Bond angles

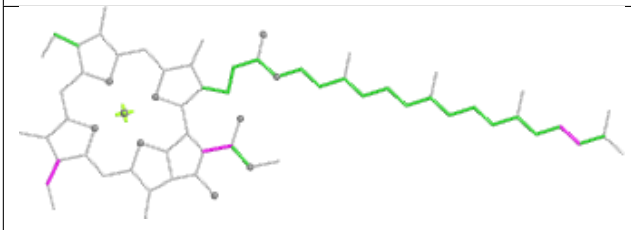

Torsions

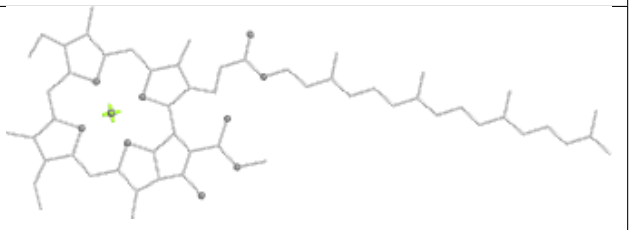

Rings

Ligand CLA D 401

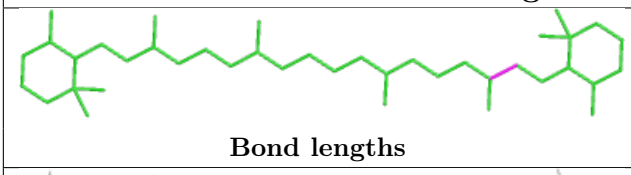

Bond lengths


Bond angles

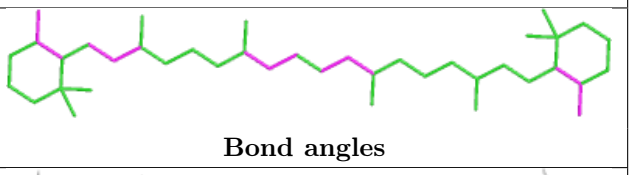

Torsions


Rings

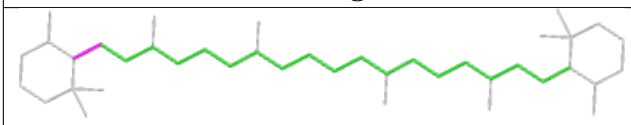
Ligand BCR C 515



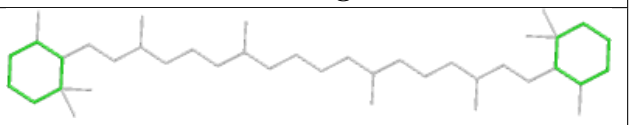
Bond lengths



Bond angles

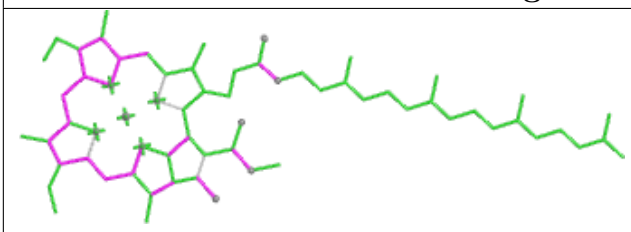


Torsions

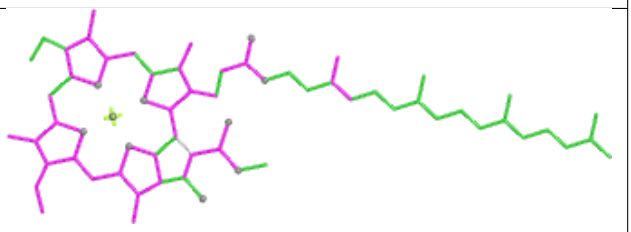


Rings

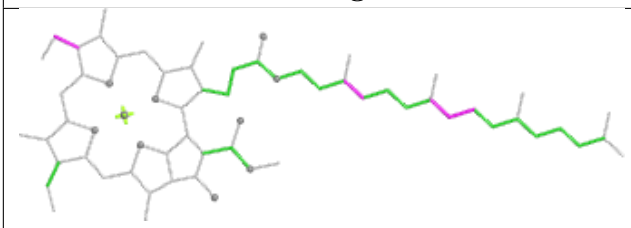
Ligand CLA D 404



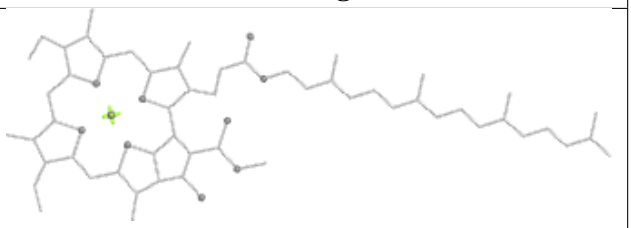
Bond lengths



Bond angles

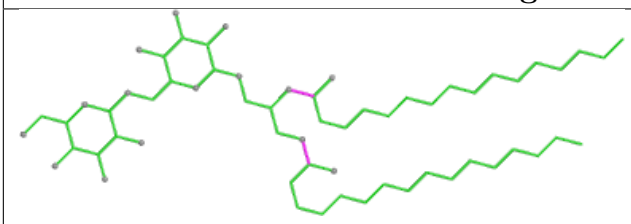


Torsions

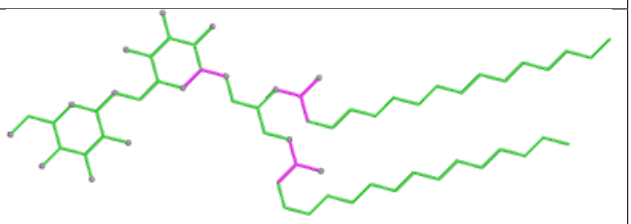


Rings

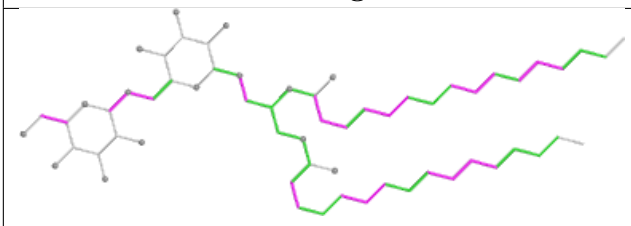
Ligand DGD C 518



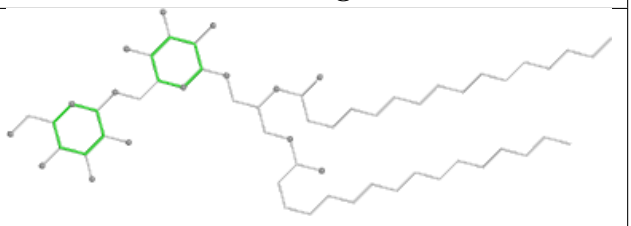
Bond lengths



Bond angles

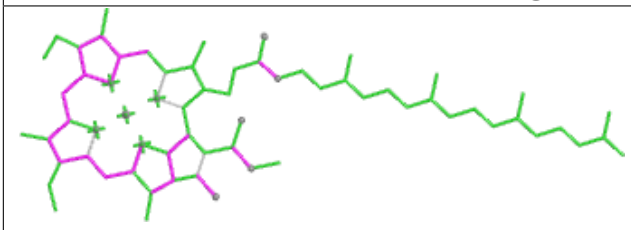


Torsions

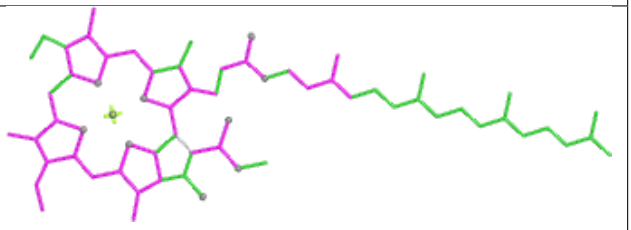


Rings

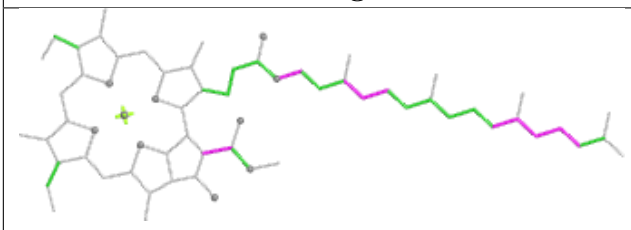
Ligand CLA b 619



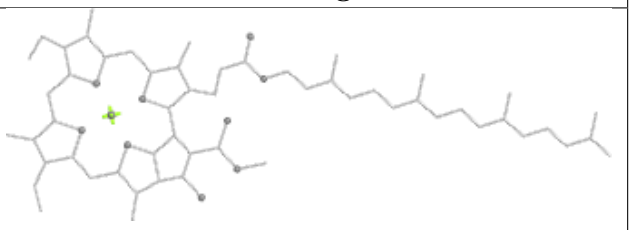
Bond lengths



Bond angles

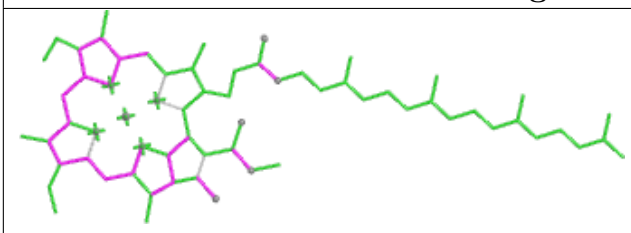


Torsions

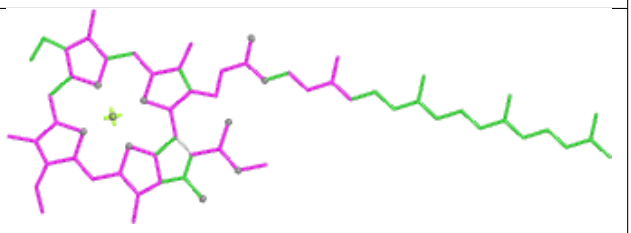


Rings

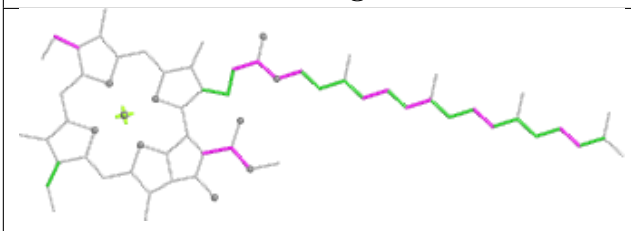
Ligand CLA c 514



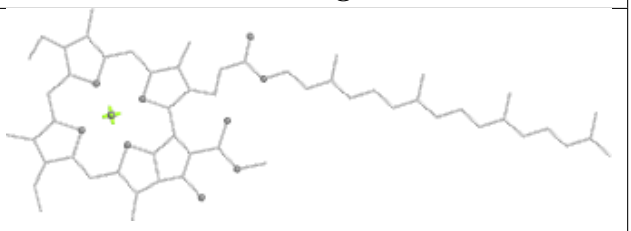
Bond lengths



Bond angles

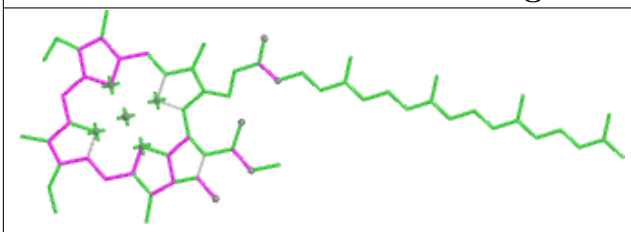


Torsions

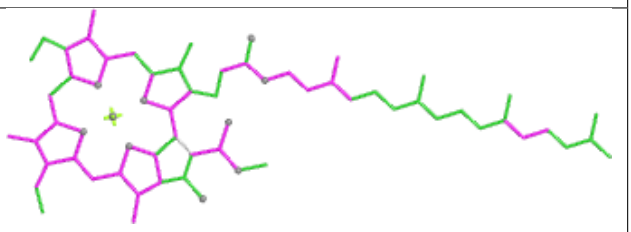


Rings

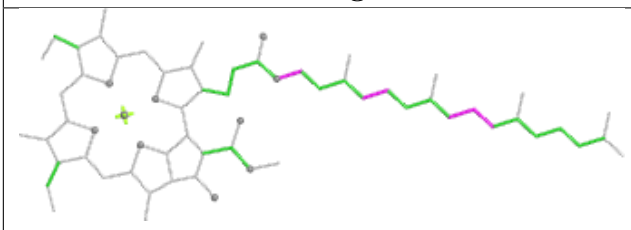
Ligand CLA C 510



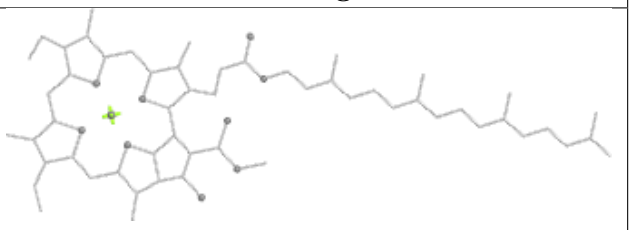
Bond lengths



Bond angles

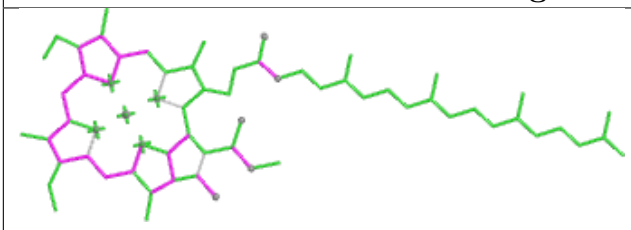


Torsions

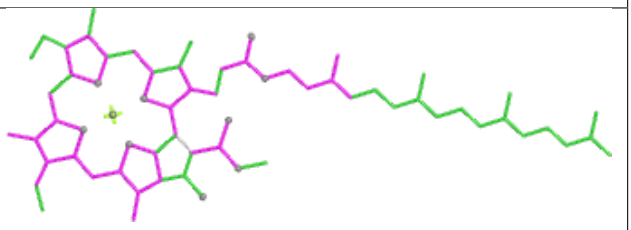


Rings

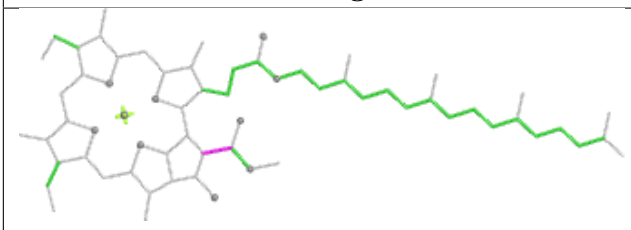
Ligand CLA c 510



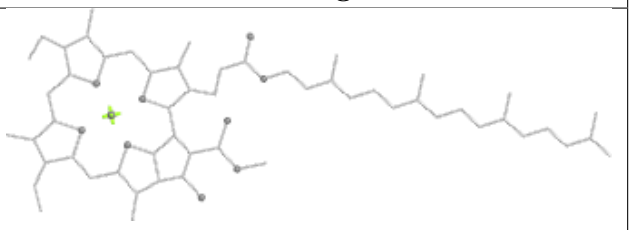
Bond lengths



Bond angles

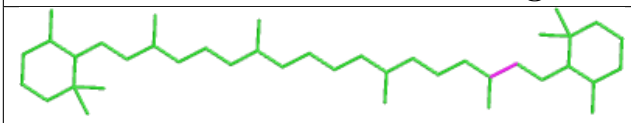


Torsions

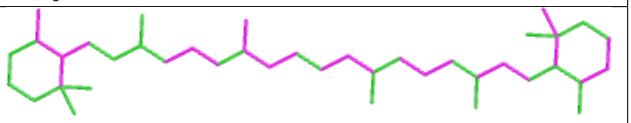


Rings

Ligand BCR y 101



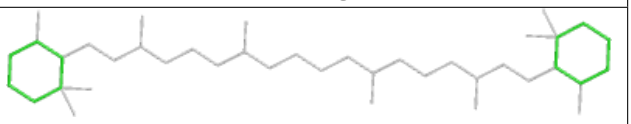
Bond lengths



Bond angles

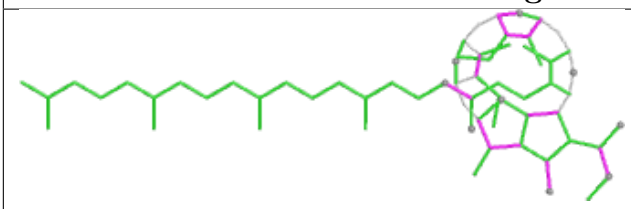


Torsions

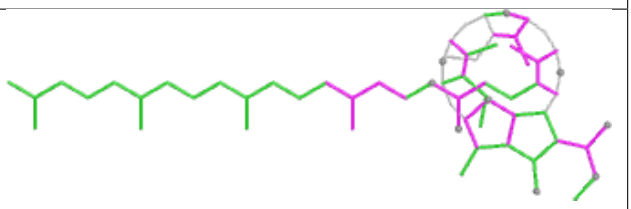


Rings

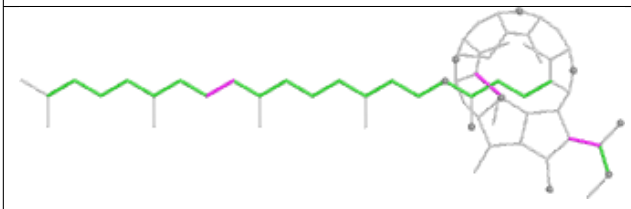
Ligand PHO d 403



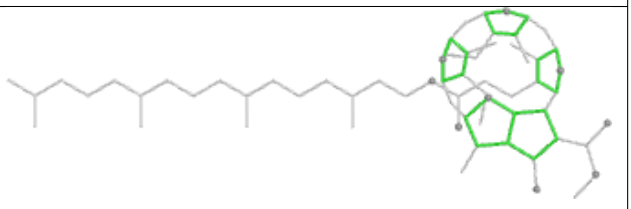
Bond lengths



Bond angles

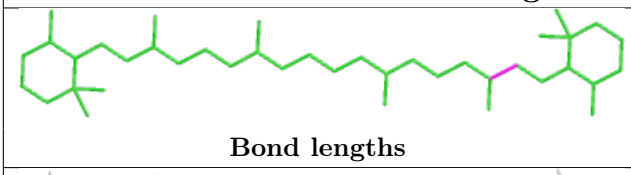


Torsions

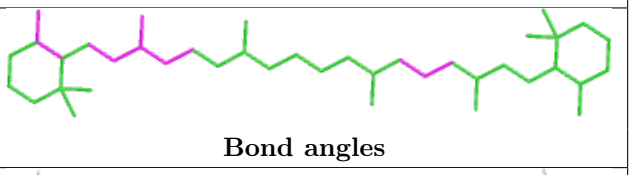


Rings

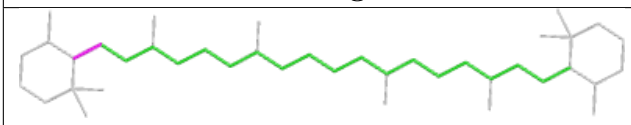
Ligand BCR B 618



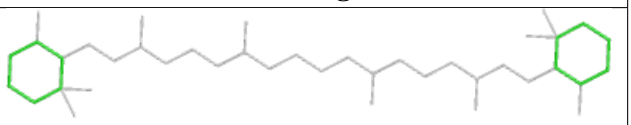
Bond lengths



Bond angles

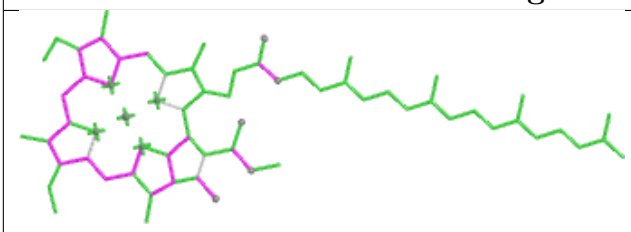


Torsions

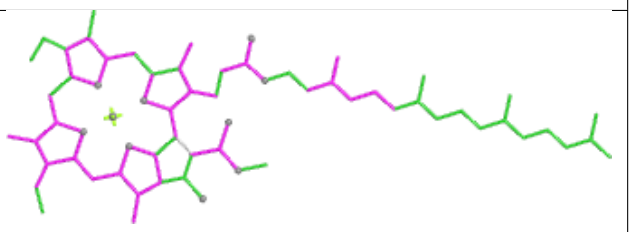


Rings

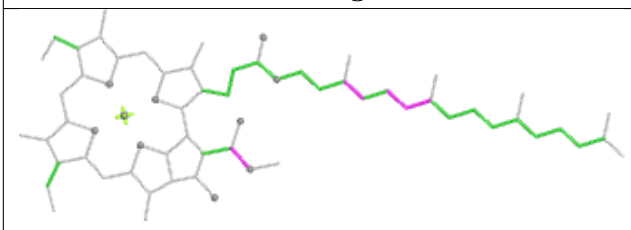
Ligand CLA b 608



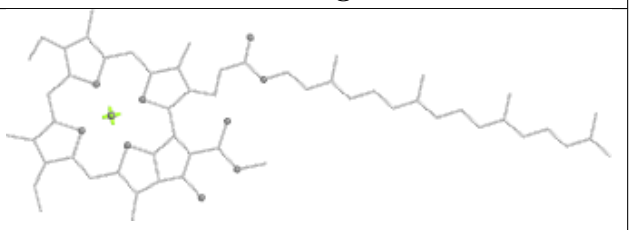
Bond lengths



Bond angles

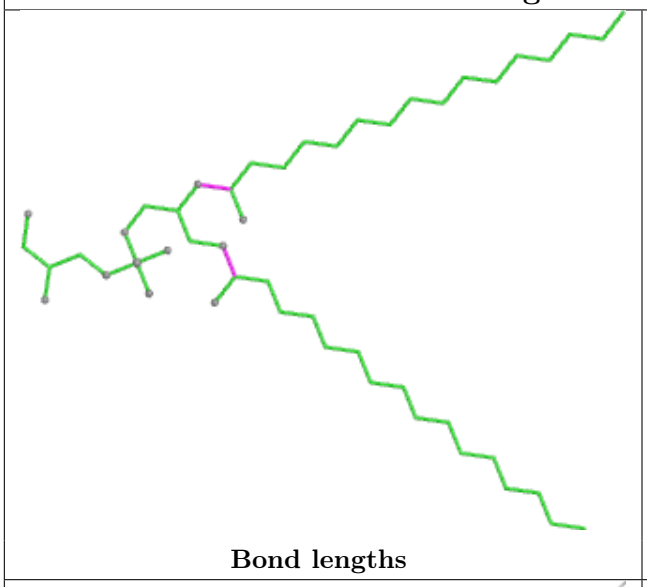


Torsions

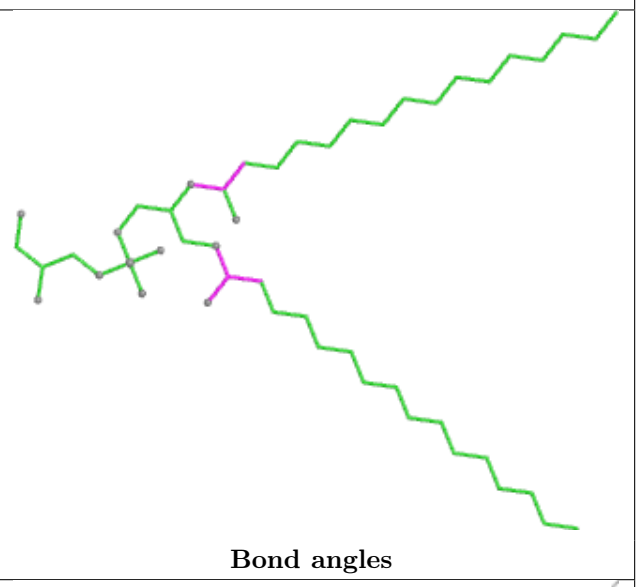


Rings

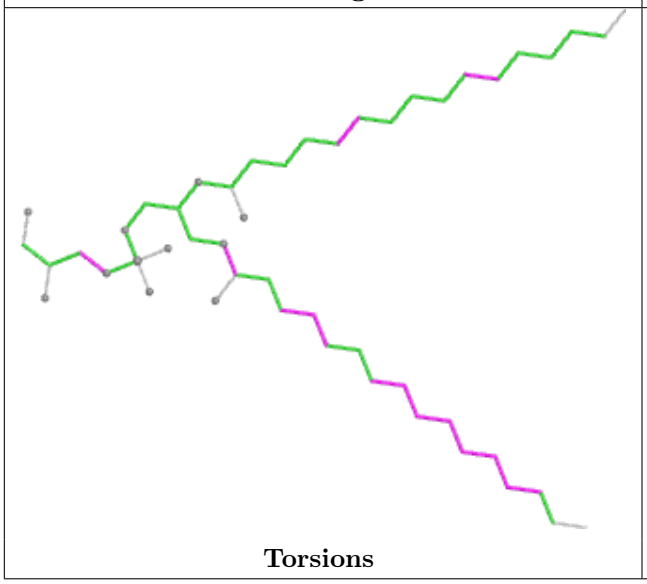
Ligand LHG D 410



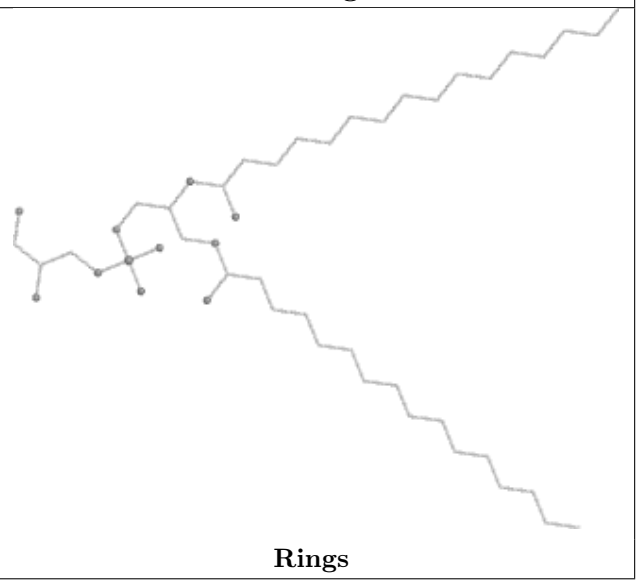
Bond lengths



Bond angles



Torsions

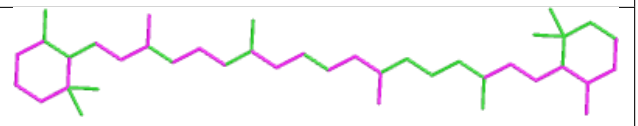


Rings

Ligand BCR B 620



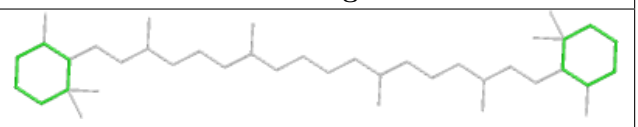
Bond lengths



Bond angles

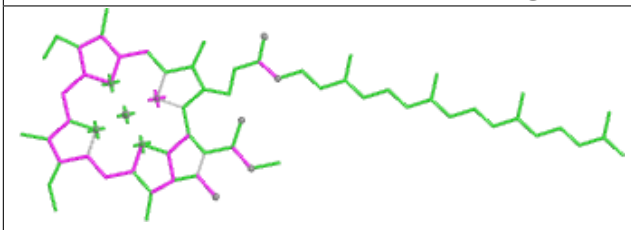


Torsions

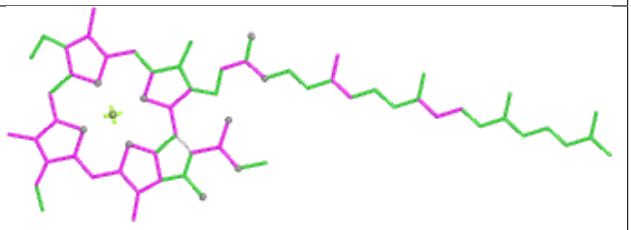


Rings

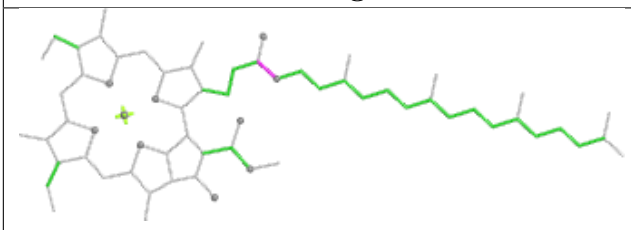
Ligand CLA B 613



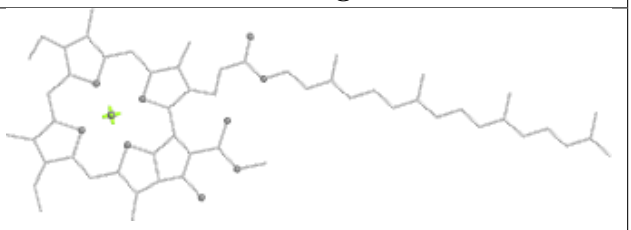
Bond lengths



Bond angles

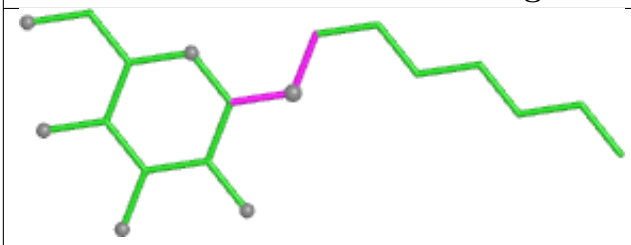


Torsions

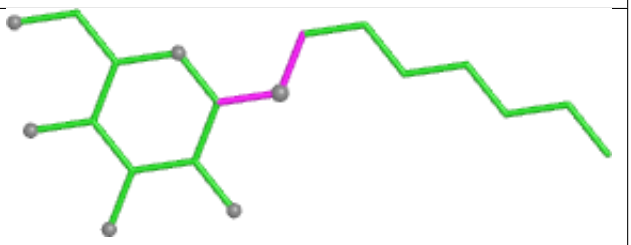


Rings

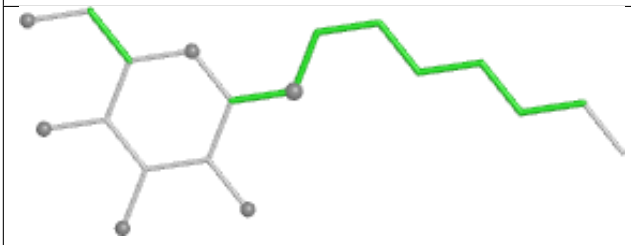
Ligand HTG b 603



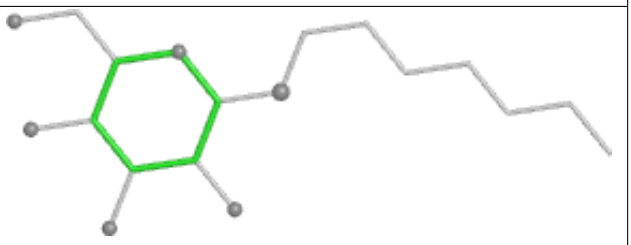
Bond lengths



Bond angles

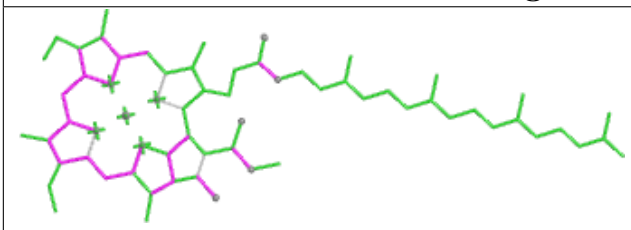


Torsions

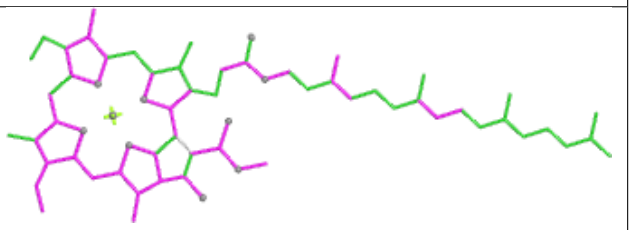


Rings

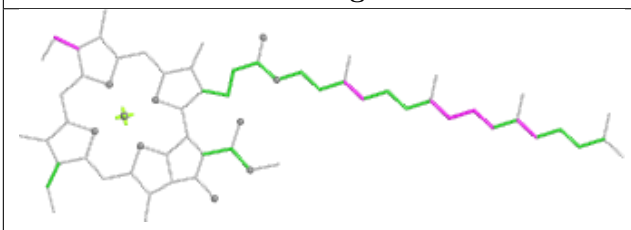
Ligand CLA B 616



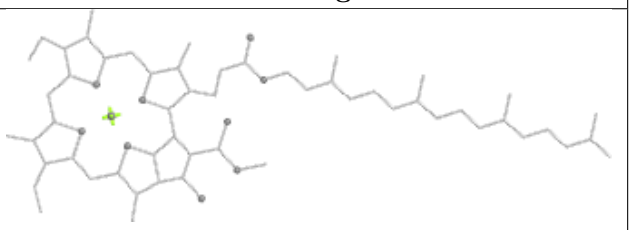
Bond lengths



Bond angles

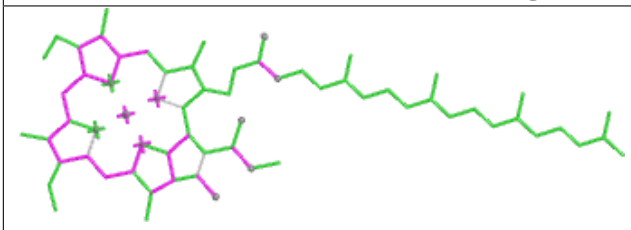


Torsions

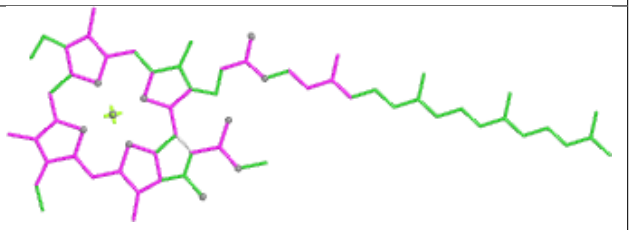


Rings

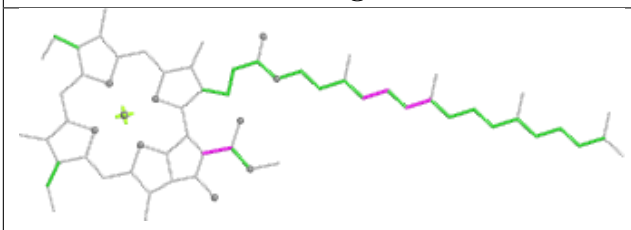
Ligand CLA B 605



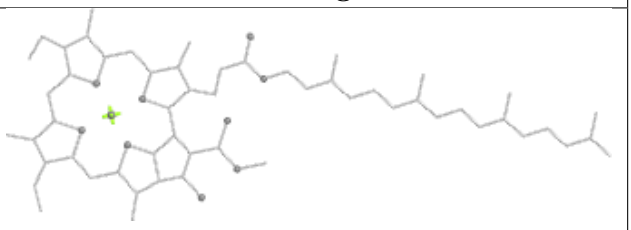
Bond lengths



Bond angles

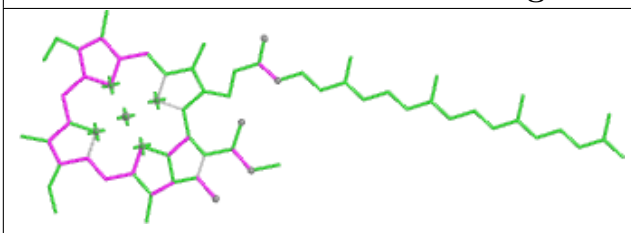


Torsions

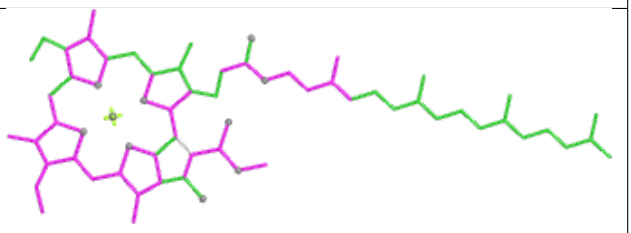


Rings

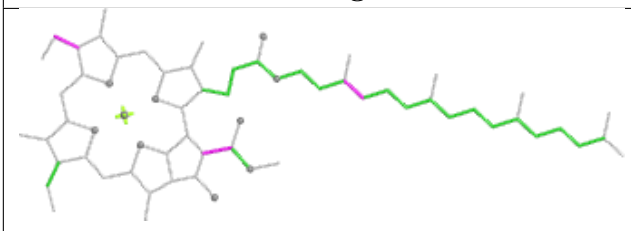
Ligand CLA b 614



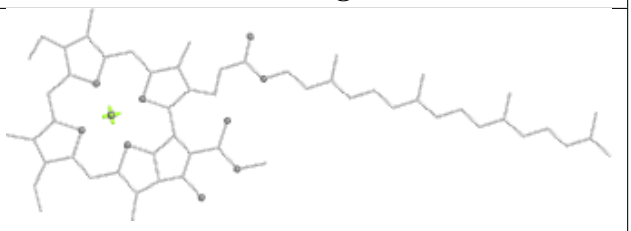
Bond lengths



Bond angles

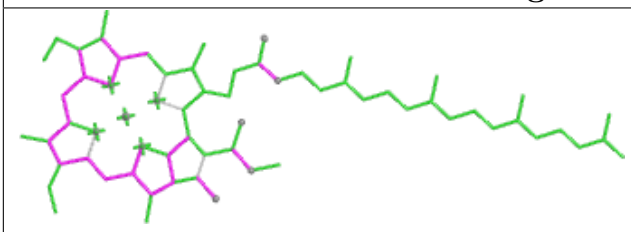


Torsions

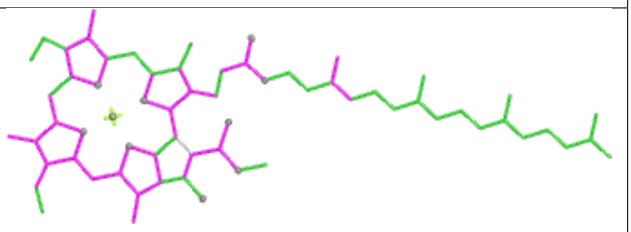


Rings

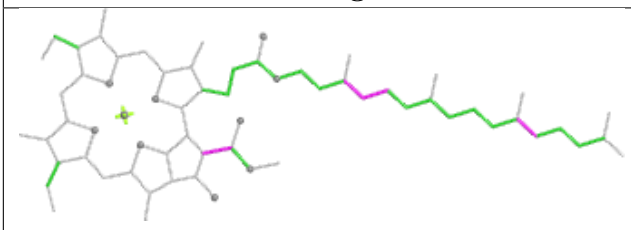
Ligand CLA d 404



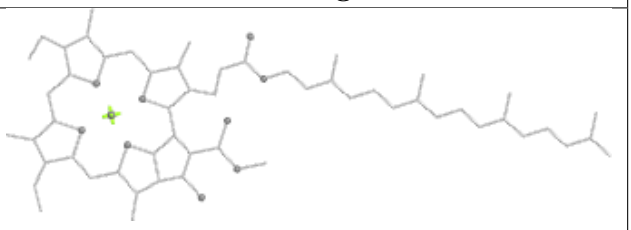
Bond lengths



Bond angles

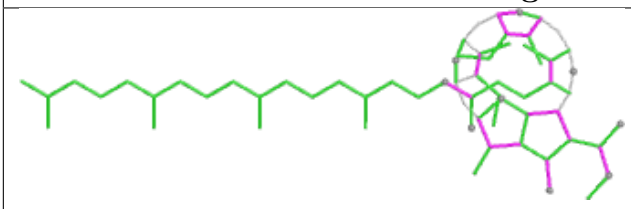


Torsions

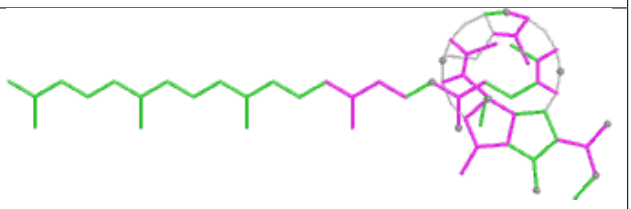


Rings

Ligand PHO A 408



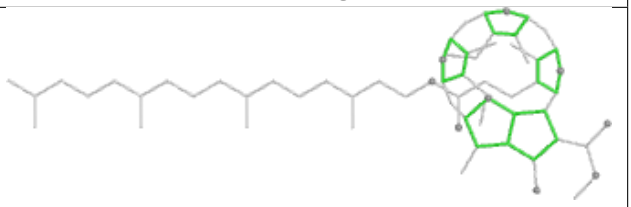
Bond lengths



Bond angles

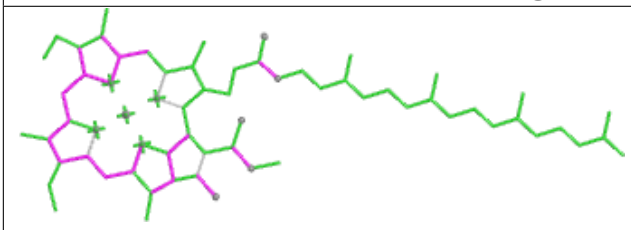


Torsions

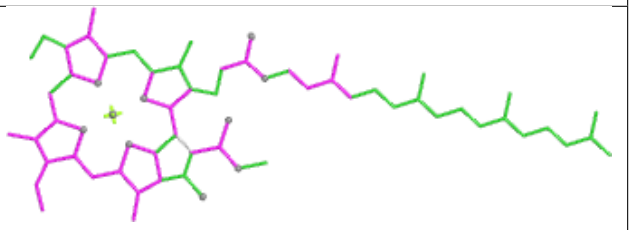


Rings

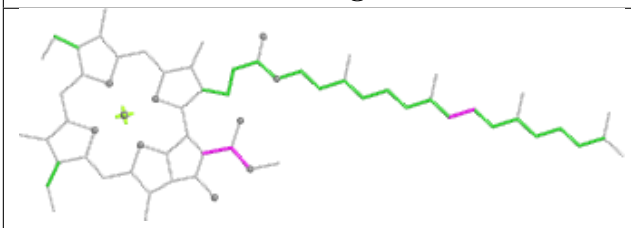
Ligand CLA c 505



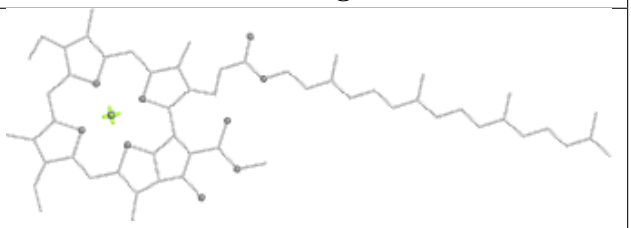
Bond lengths



Bond angles

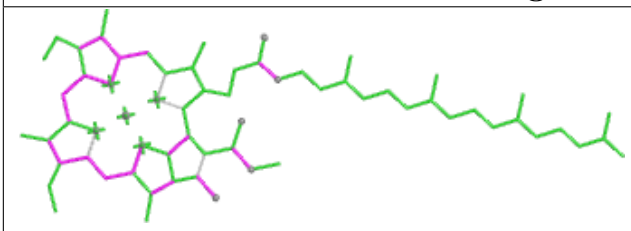


Torsions

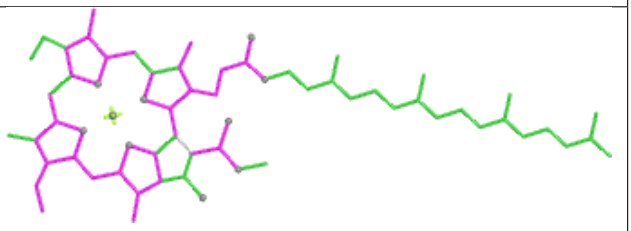


Rings

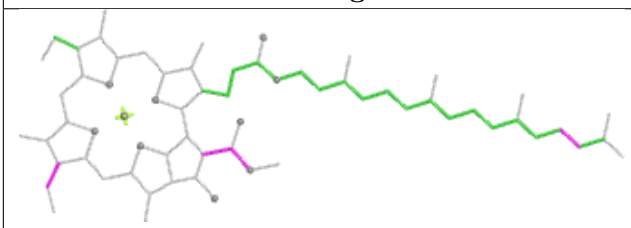
Ligand CLA d 401



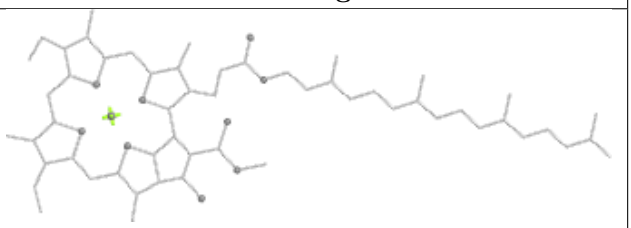
Bond lengths



Bond angles

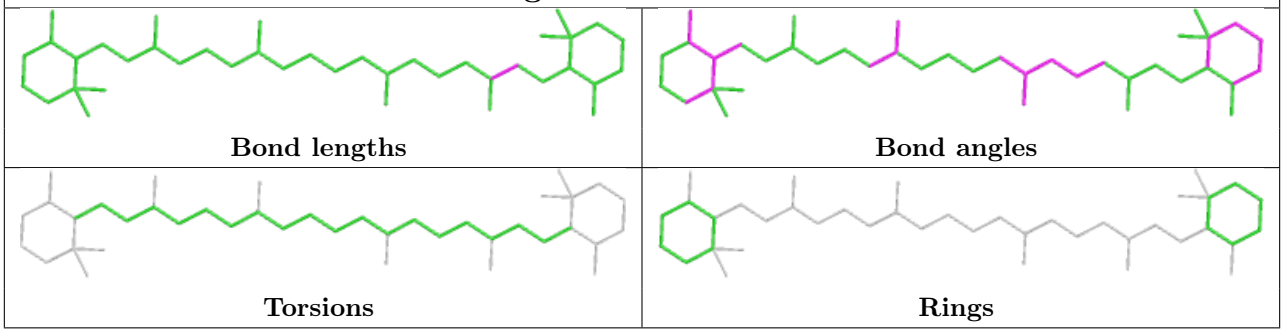


Torsions

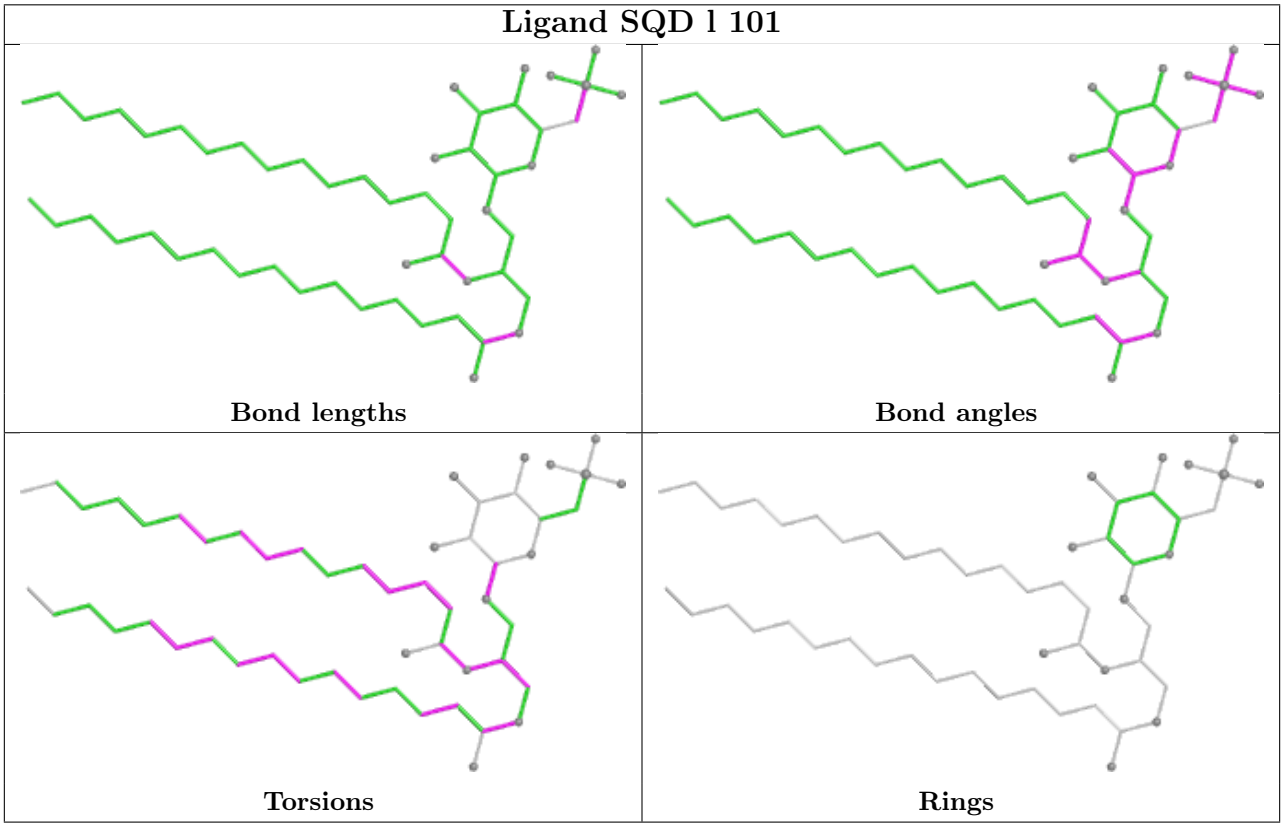


Rings

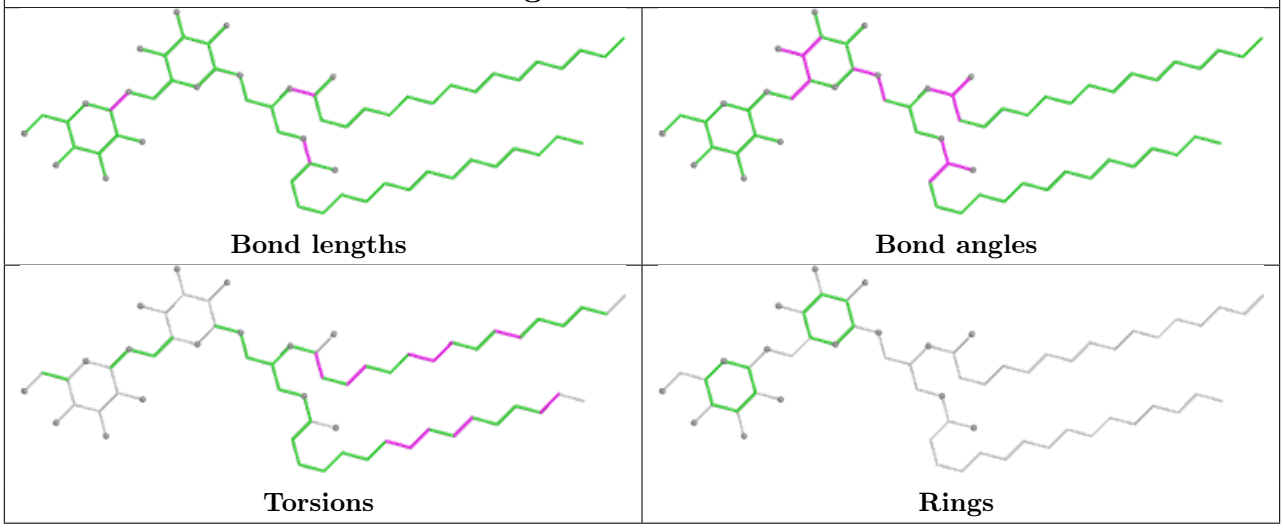
Ligand BCR T 102



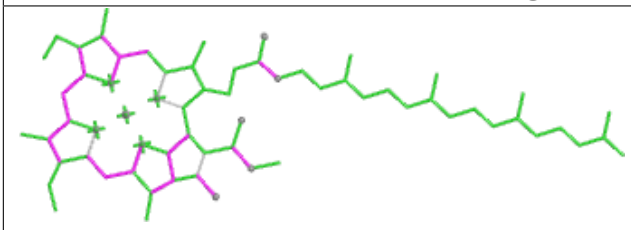
Ligand SQD l 101



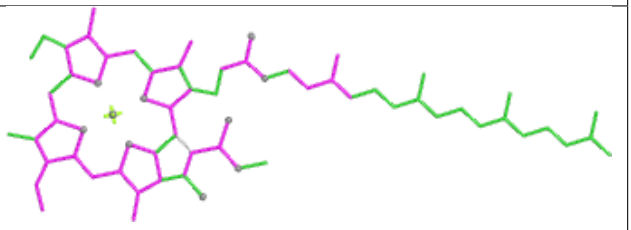
Ligand DGD h 102



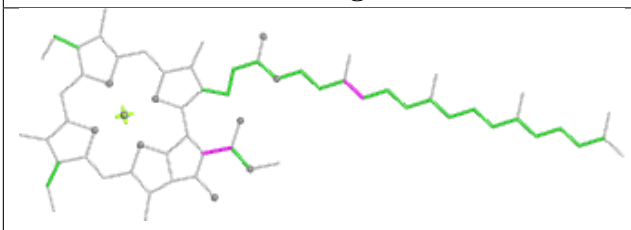
Ligand CLA B 610



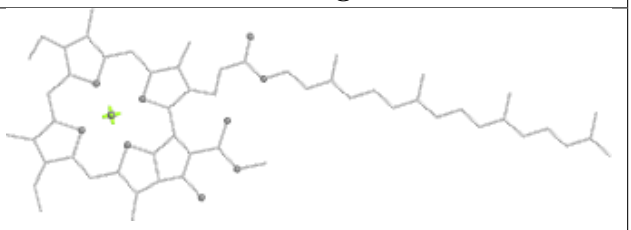
Bond lengths



Bond angles

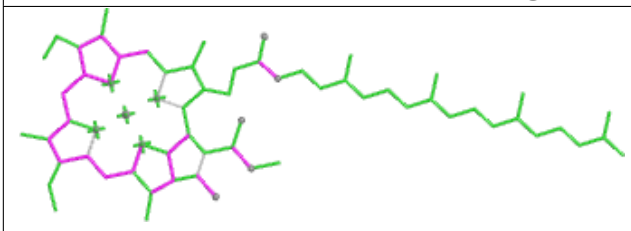


Torsions

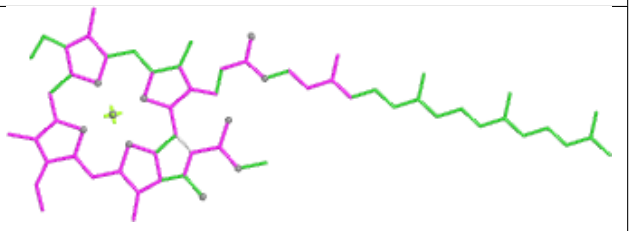


Rings

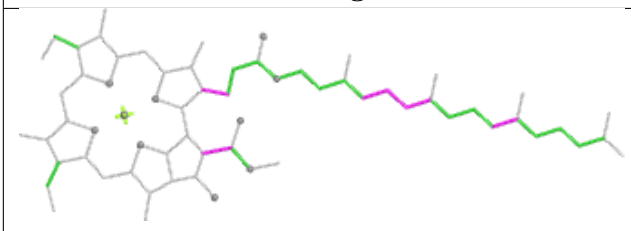
Ligand CLA C 507



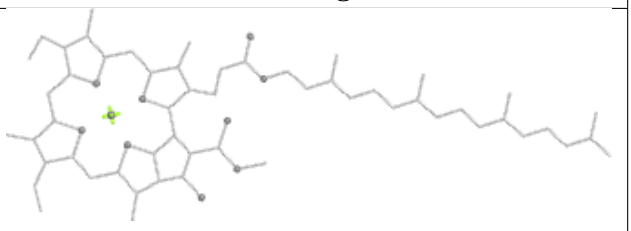
Bond lengths



Bond angles

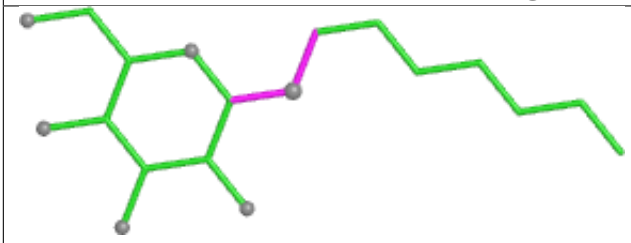


Torsions

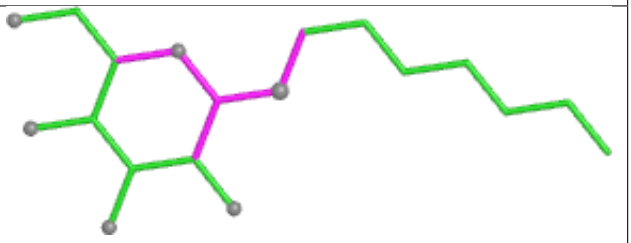


Rings

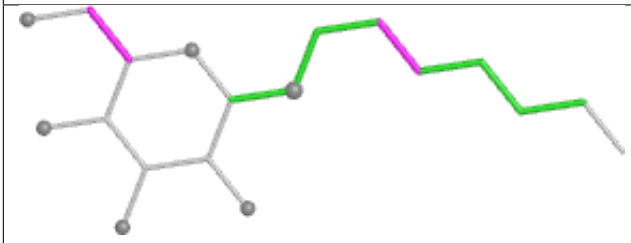
Ligand HTG b 628



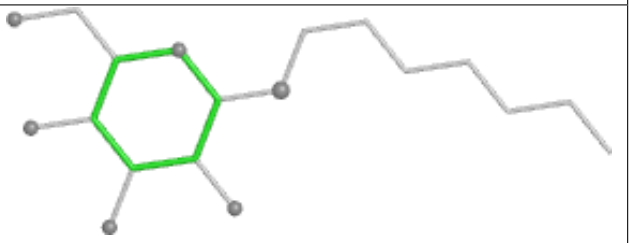
Bond lengths



Bond angles

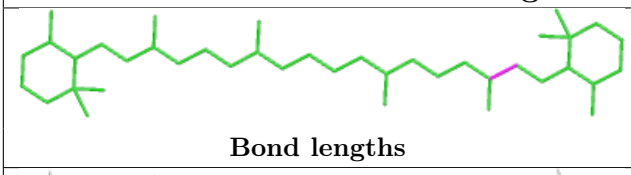


Torsions

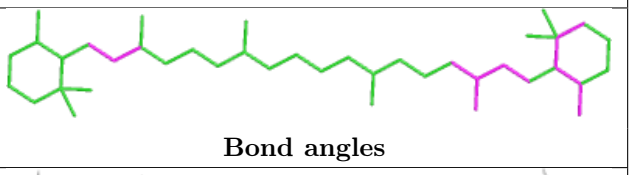


Rings

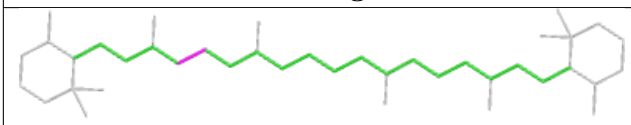
Ligand BCR H 101



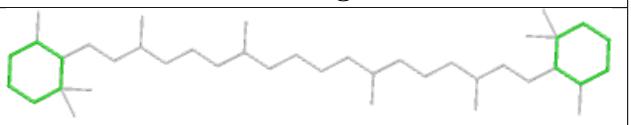
Bond lengths



Bond angles

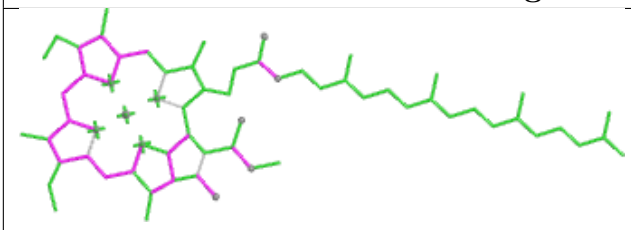


Torsions

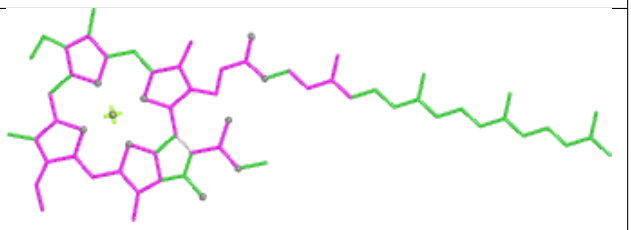


Rings

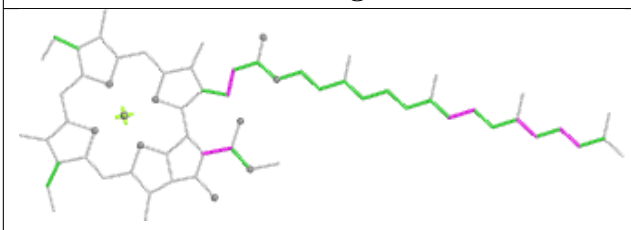
Ligand CLA B 603



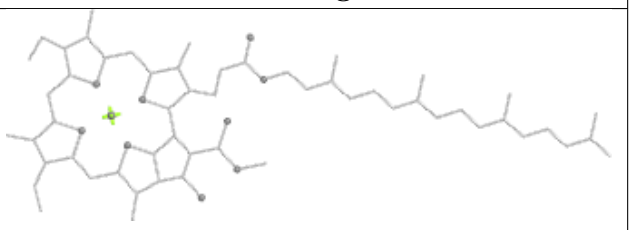
Bond lengths



Bond angles

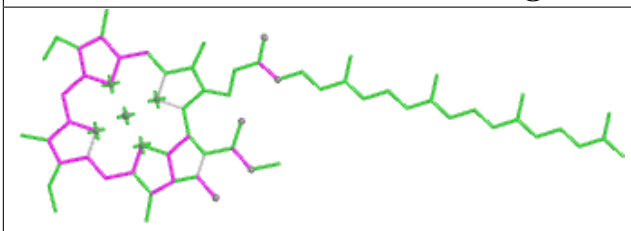


Torsions

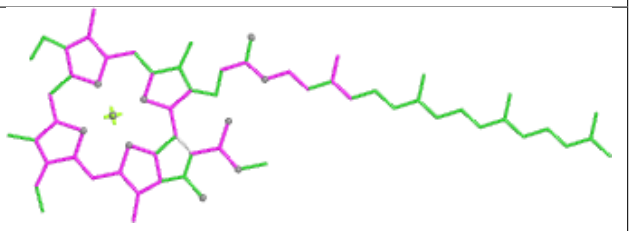


Rings

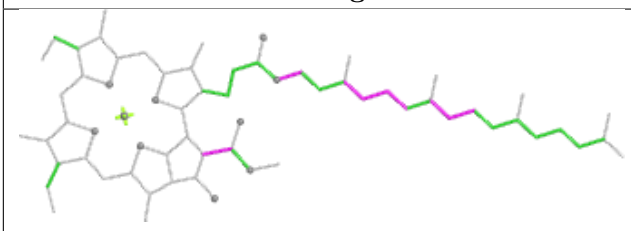
Ligand CLA B 617



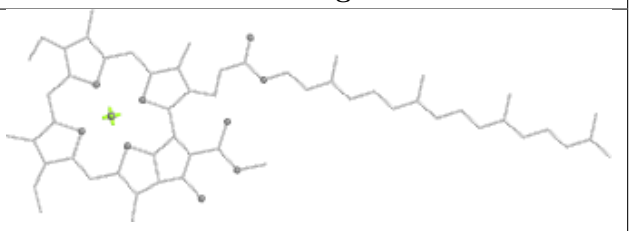
Bond lengths



Bond angles

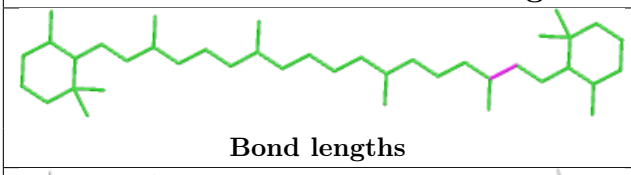


Torsions

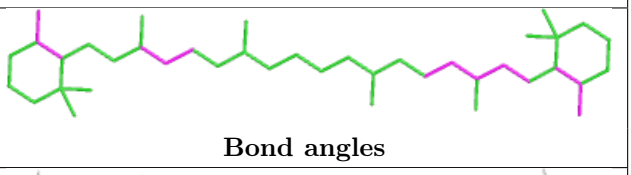


Rings

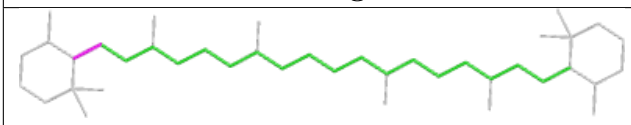
Ligand BCR k 103



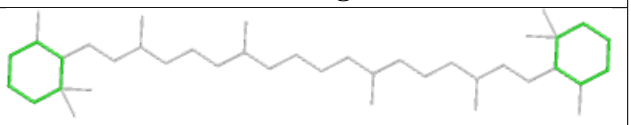
Bond lengths



Bond angles

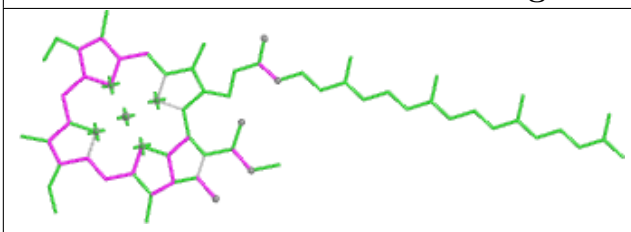


Torsions

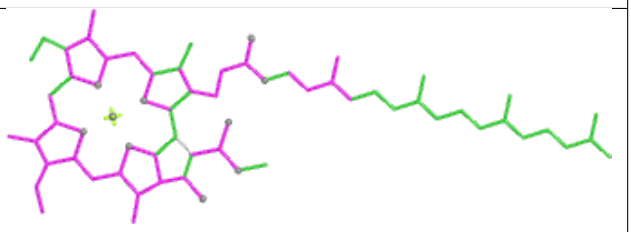


Rings

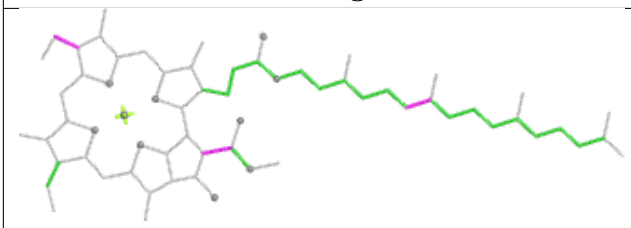
Ligand CLA a 407



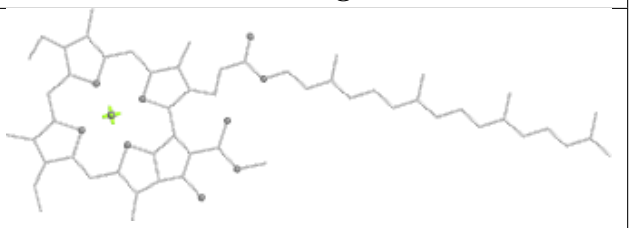
Bond lengths



Bond angles

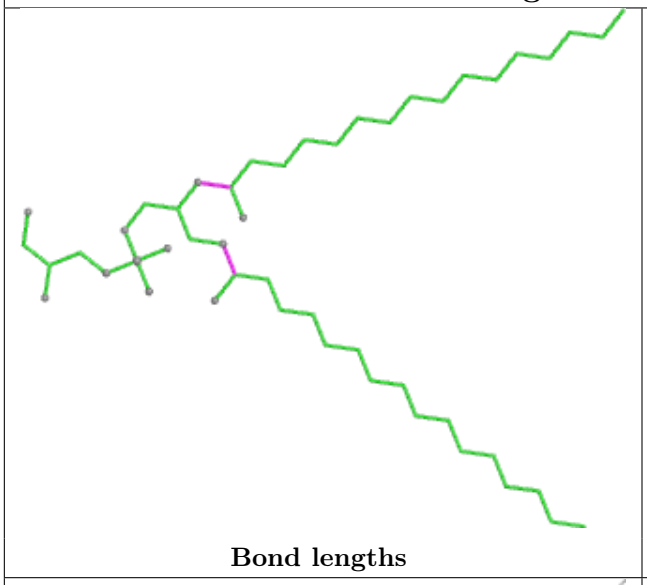


Torsions

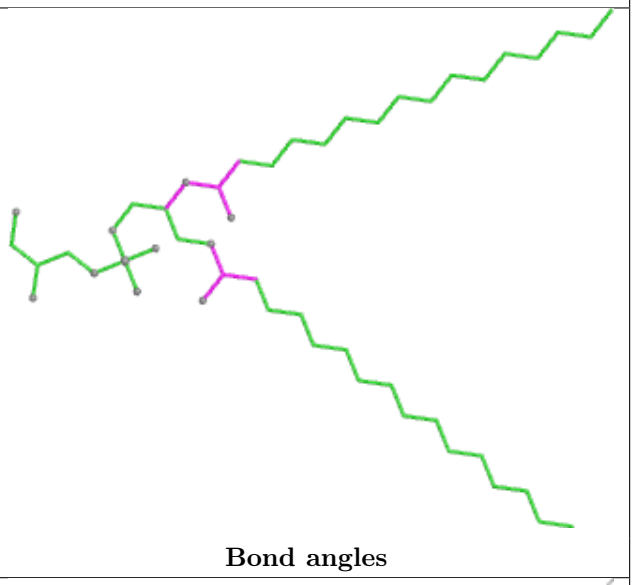


Rings

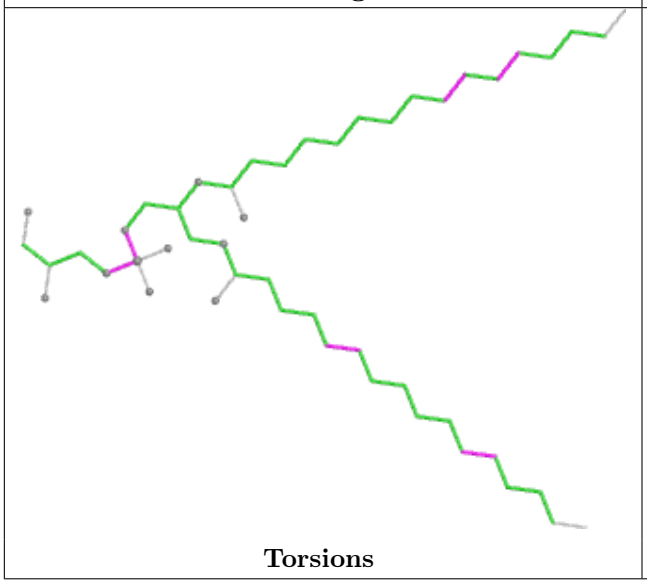
Ligand LHG D 409



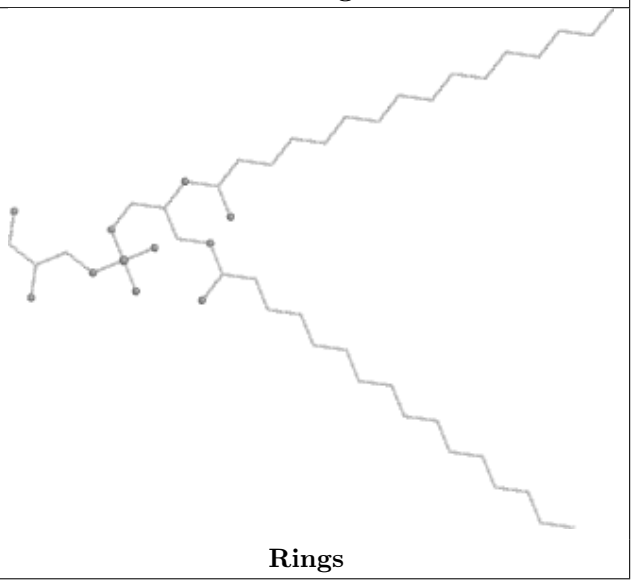
Bond lengths



Bond angles

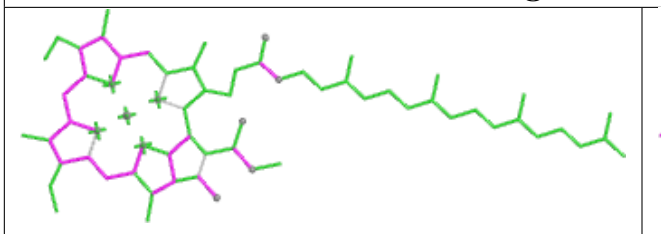


Torsions

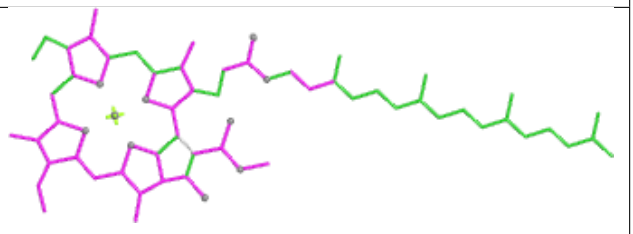


Rings

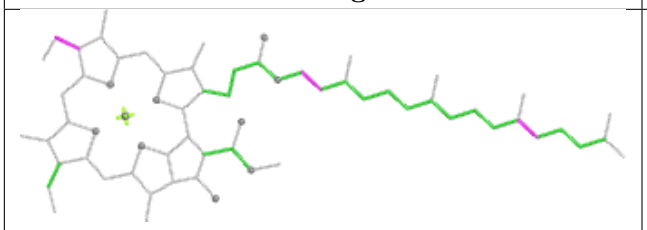
Ligand CLA D 403



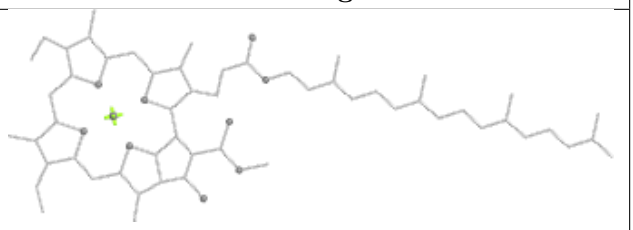
Bond lengths



Bond angles

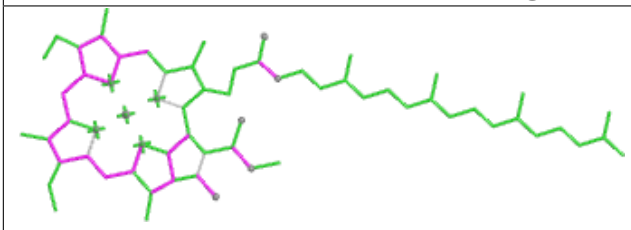


Torsions

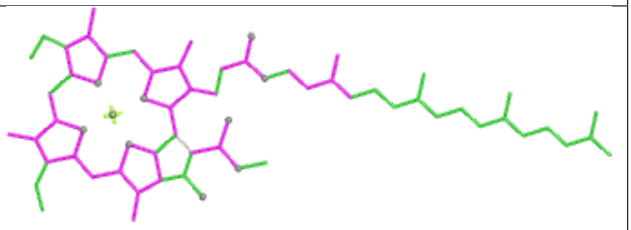


Rings

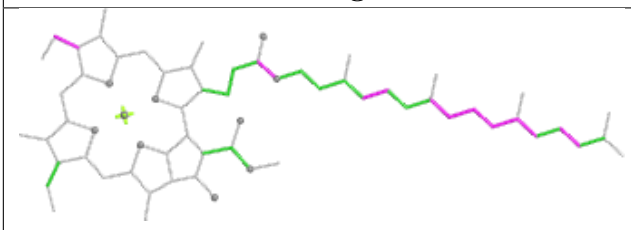
Ligand CLA A 409



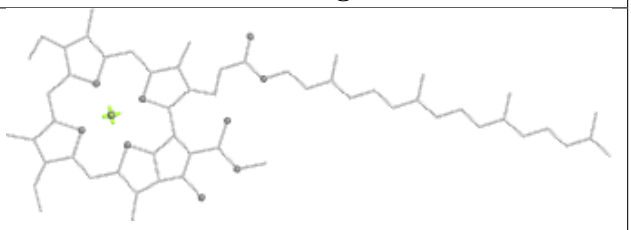
Bond lengths



Bond angles

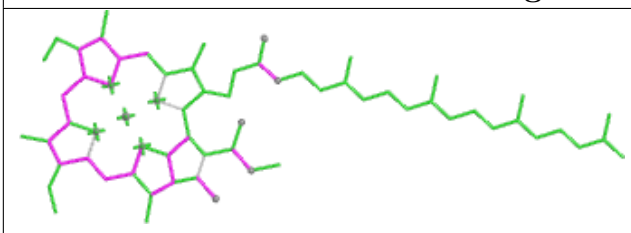


Torsions

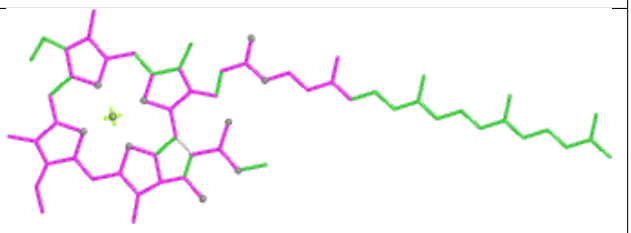


Rings

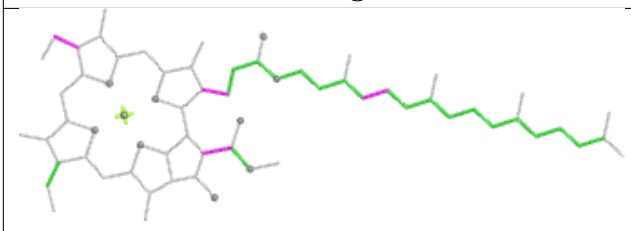
Ligand CLA B 608



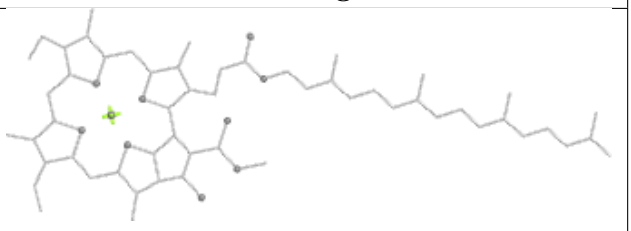
Bond lengths



Bond angles

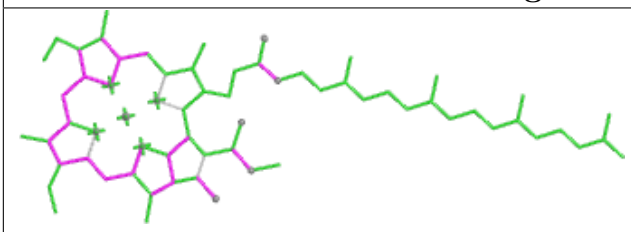


Torsions

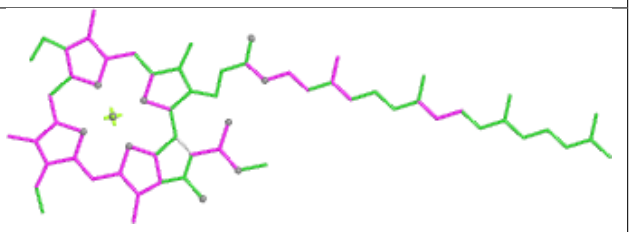


Rings

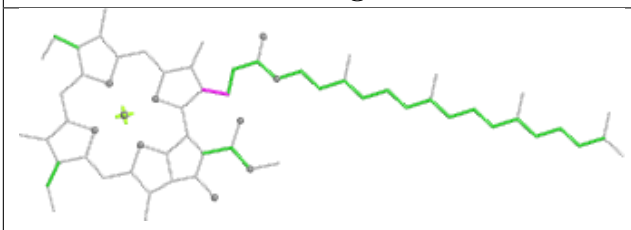
Ligand CLA C 512



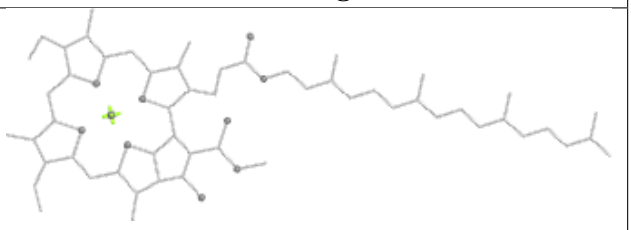
Bond lengths



Bond angles

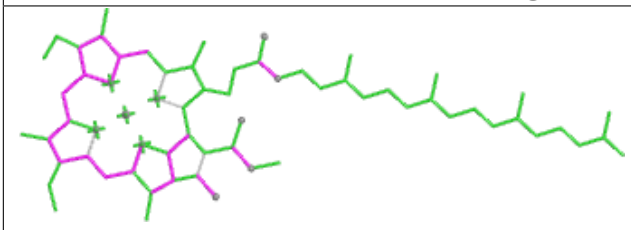


Torsions

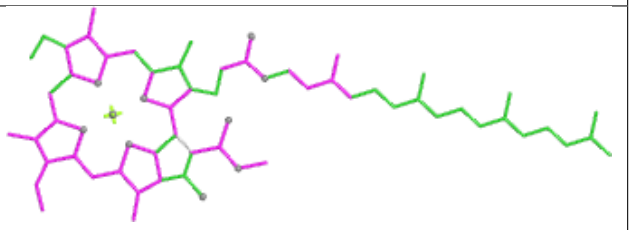


Rings

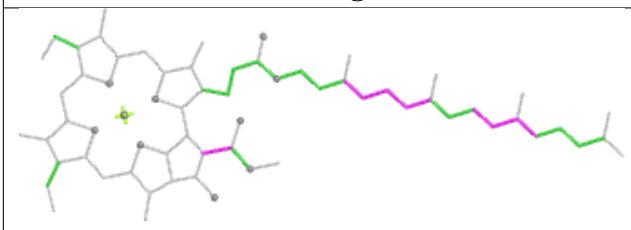
Ligand CLA B 615



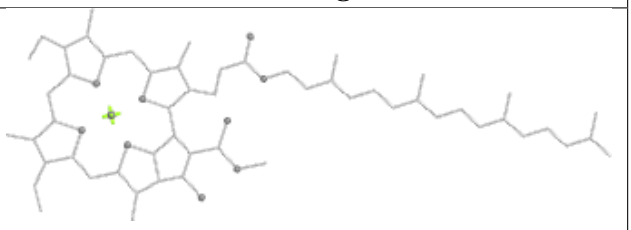
Bond lengths



Bond angles

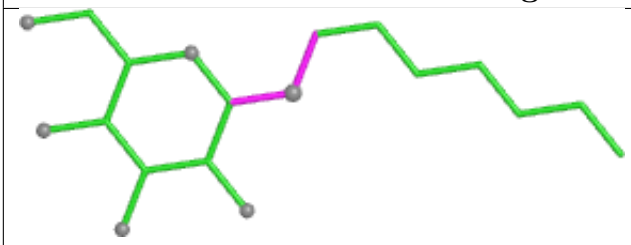


Torsions

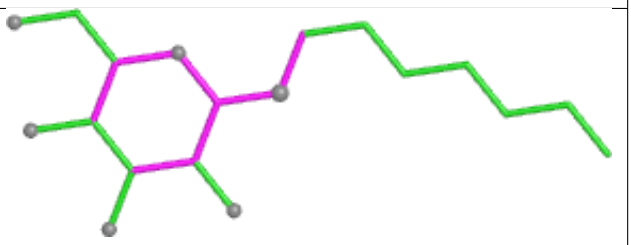


Rings

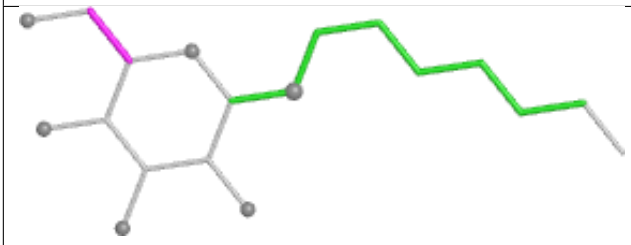
Ligand HTG C 523



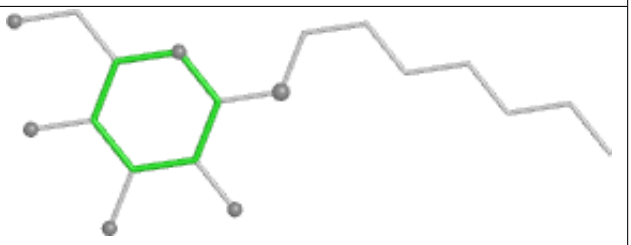
Bond lengths



Bond angles

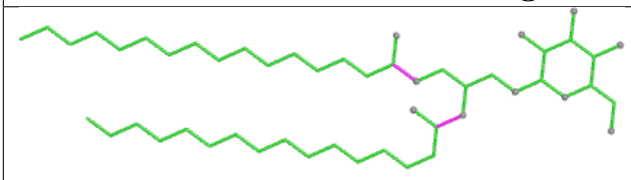


Torsions

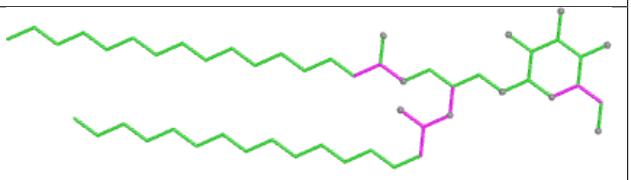


Rings

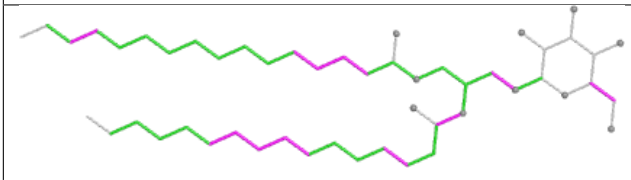
Ligand LMG C 521



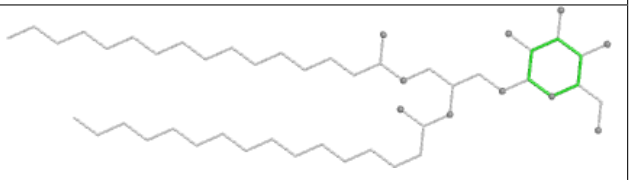
Bond lengths



Bond angles

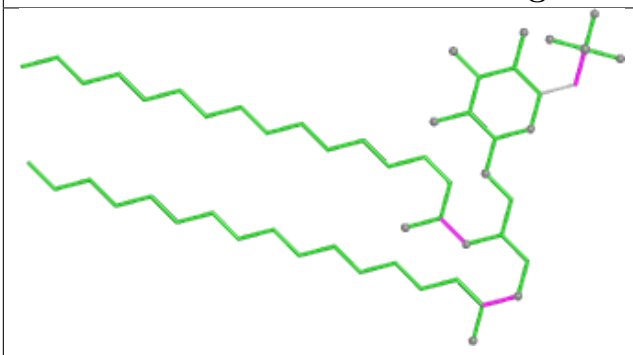


Torsions

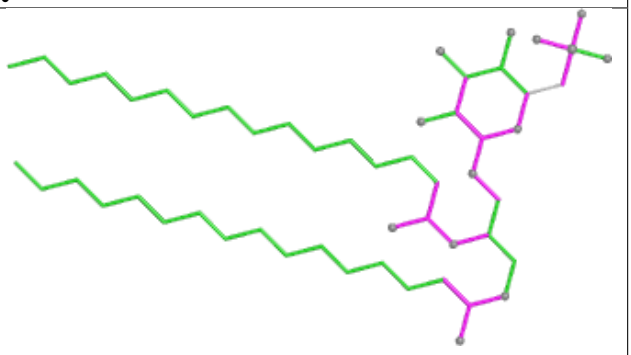


Rings

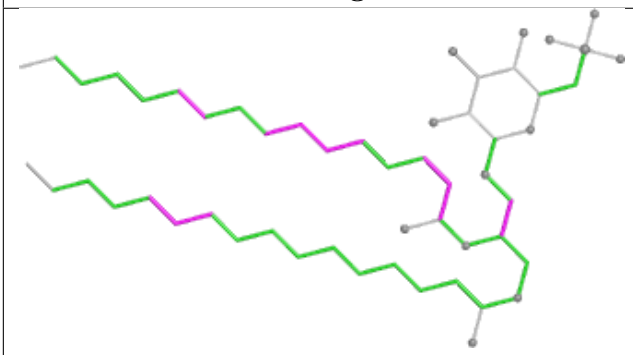
Ligand SQD a 411



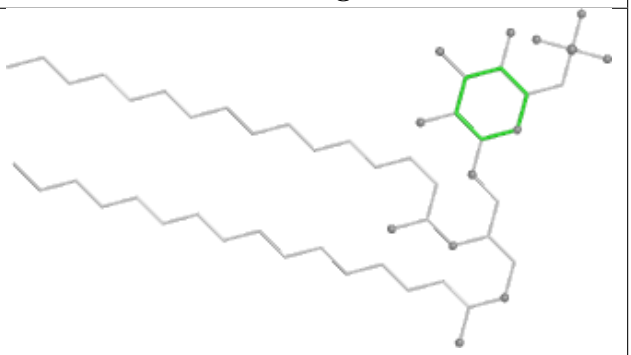
Bond lengths



Bond angles



Torsions

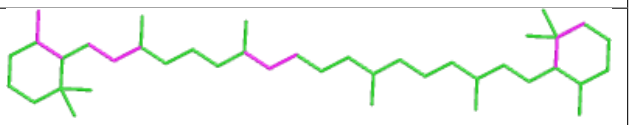


Rings

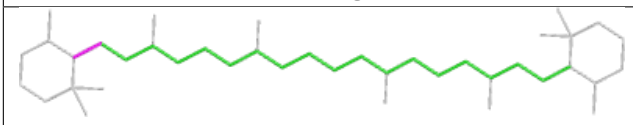
Ligand BCR b 622



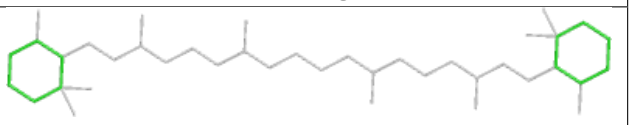
Bond lengths



Bond angles

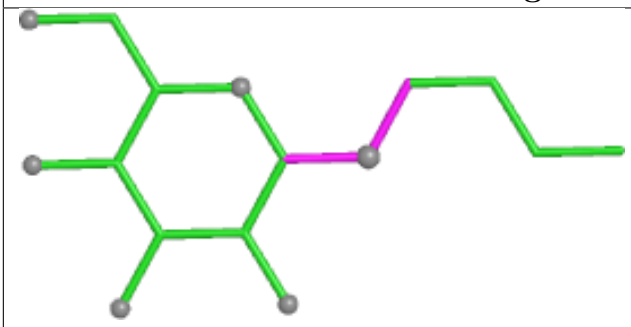


Torsions

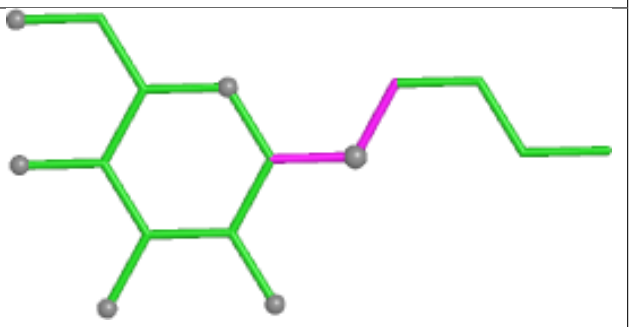


Rings

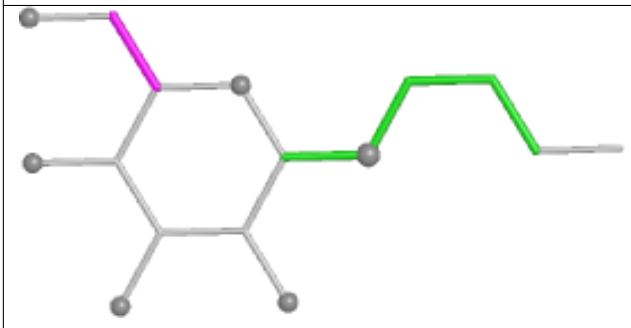
Ligand HTG d 411



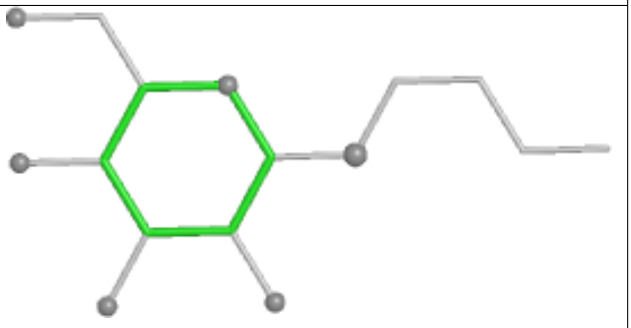
Bond lengths



Bond angles

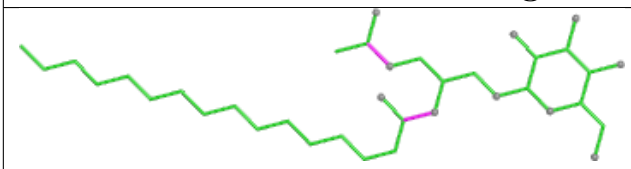


Torsions



Rings

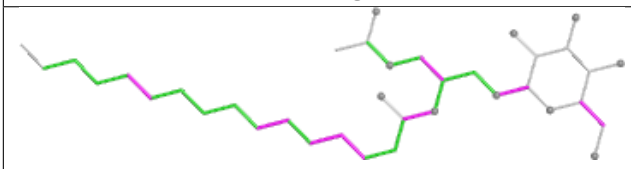
Ligand LMG Z 101



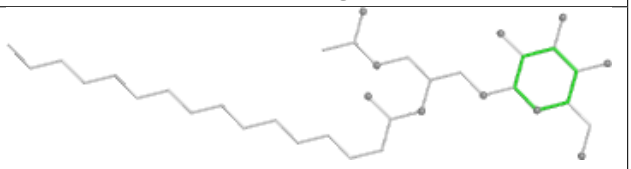
Bond lengths



Bond angles

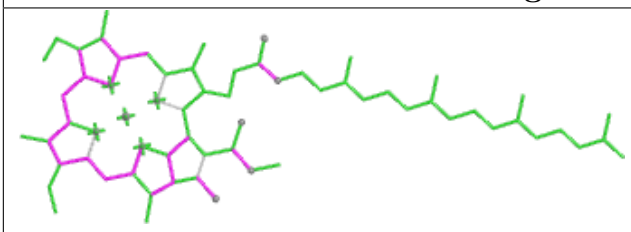


Torsions

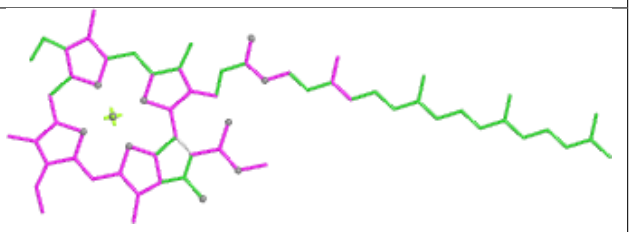


Rings

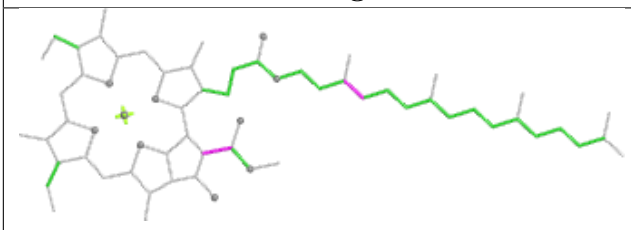
Ligand CLA B 606



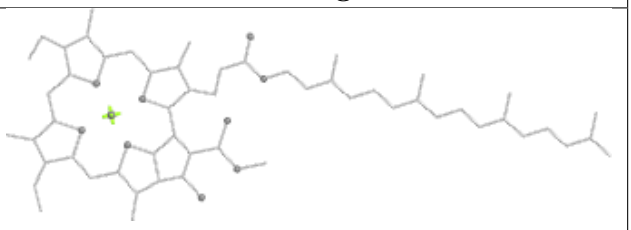
Bond lengths



Bond angles

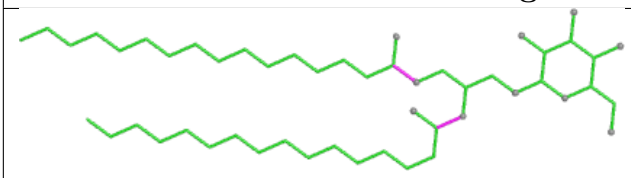


Torsions

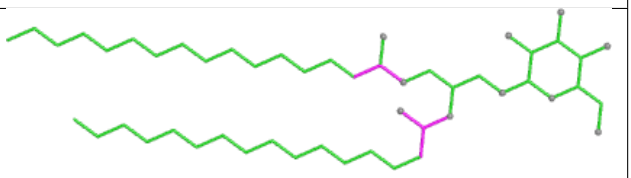


Rings

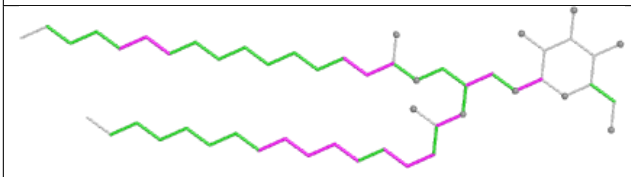
Ligand LMG C 501



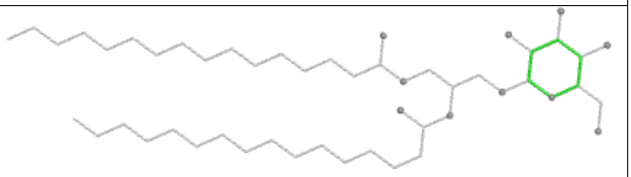
Bond lengths



Bond angles

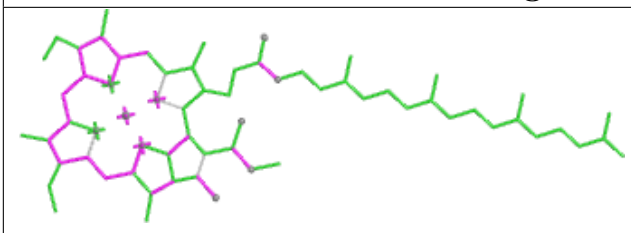


Torsions

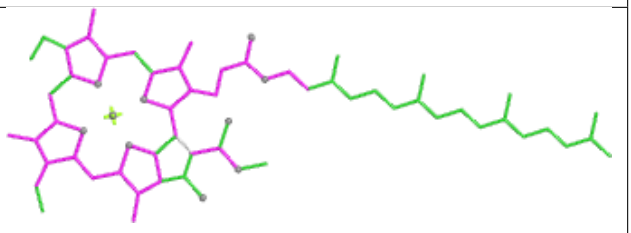


Rings

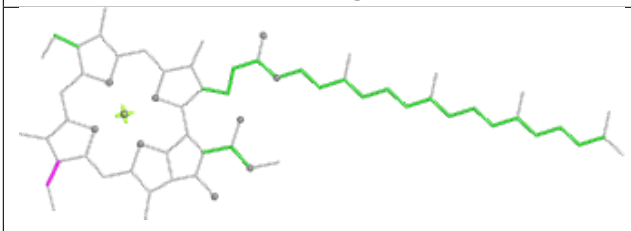
Ligand CLA A 405



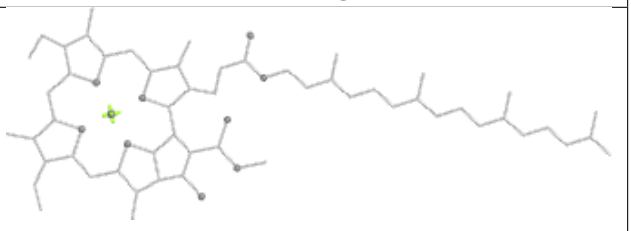
Bond lengths



Bond angles

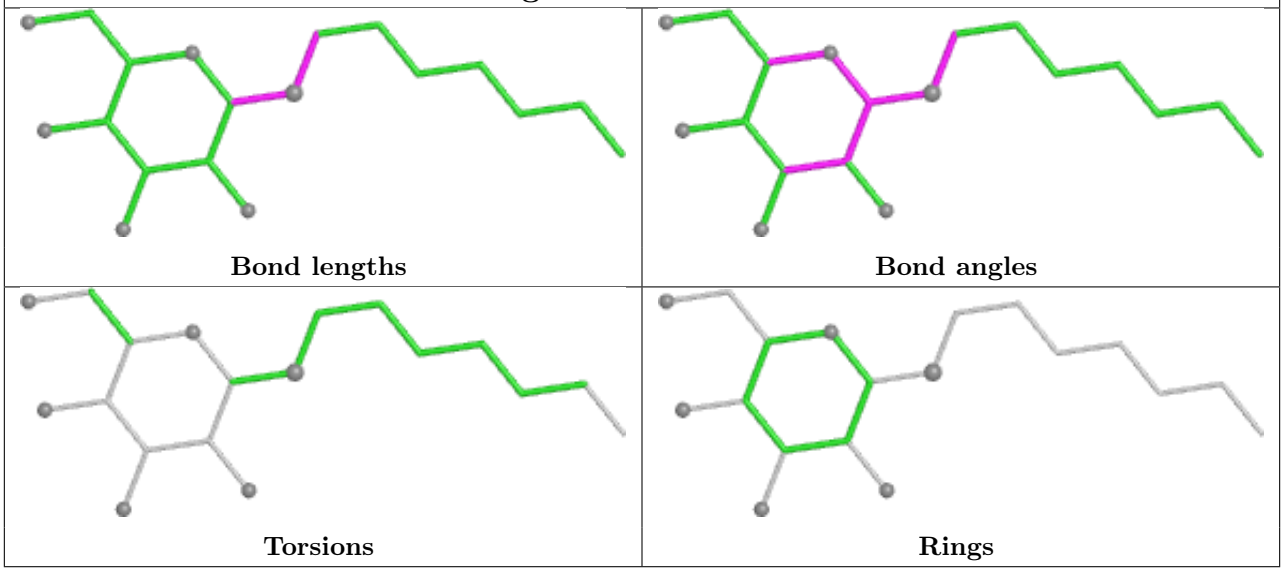


Torsions

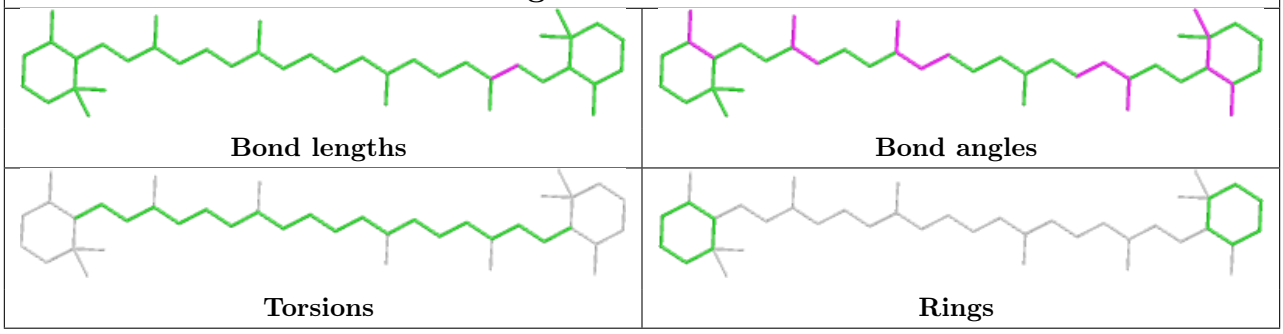


Rings

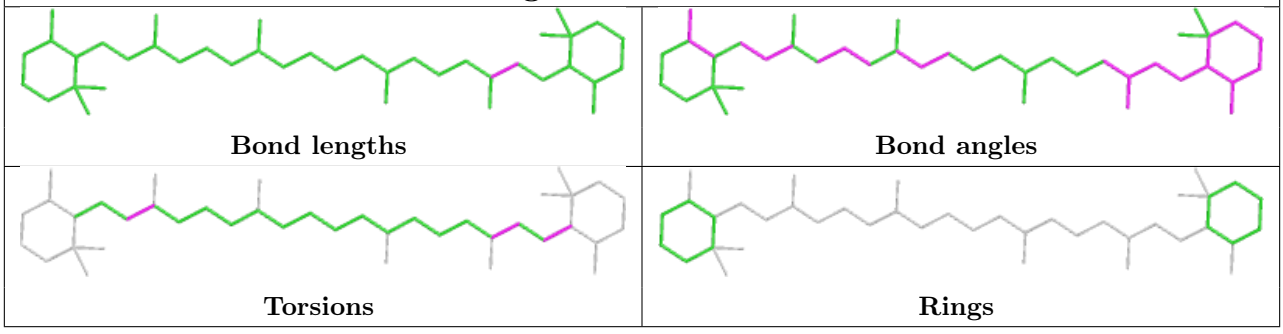
Ligand HTG B 624



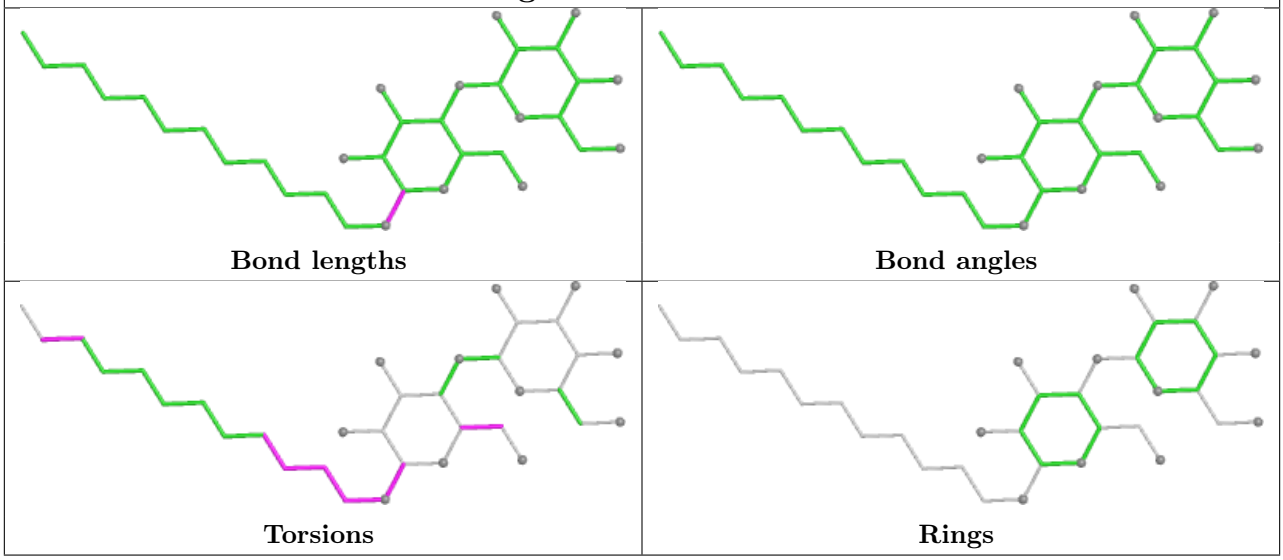
Ligand BCR a 410



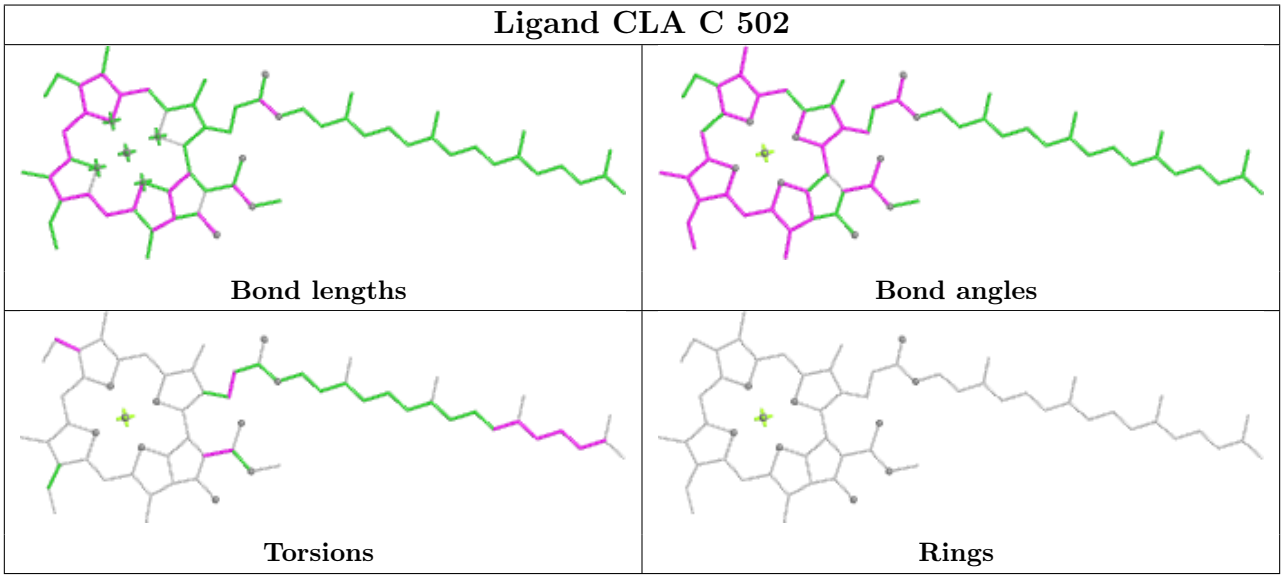
Ligand BCR D 405



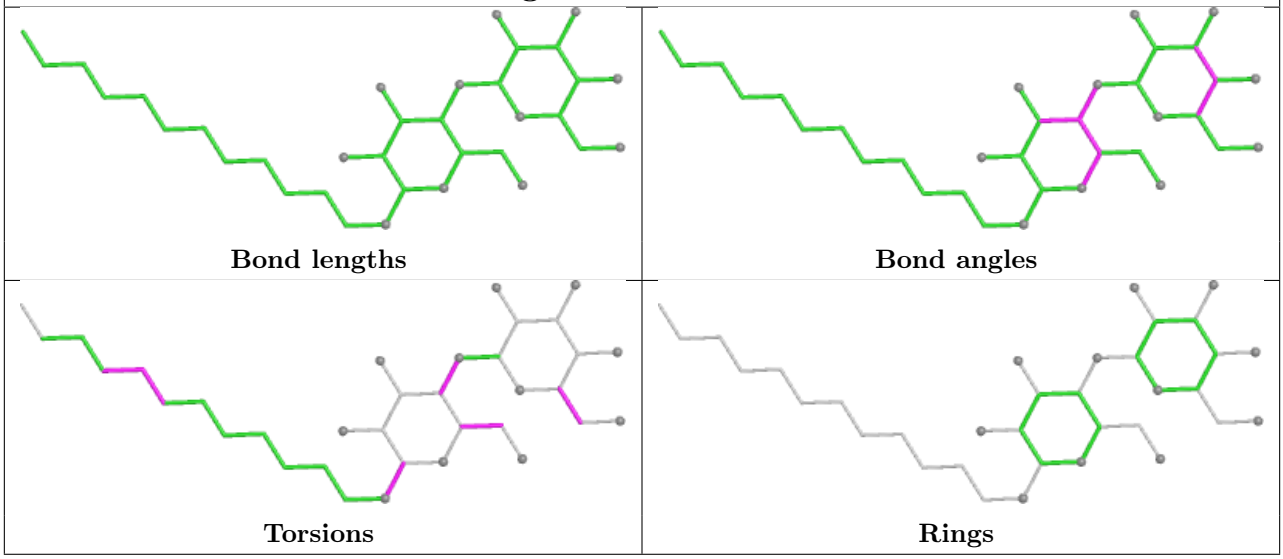
Ligand LMT M 101



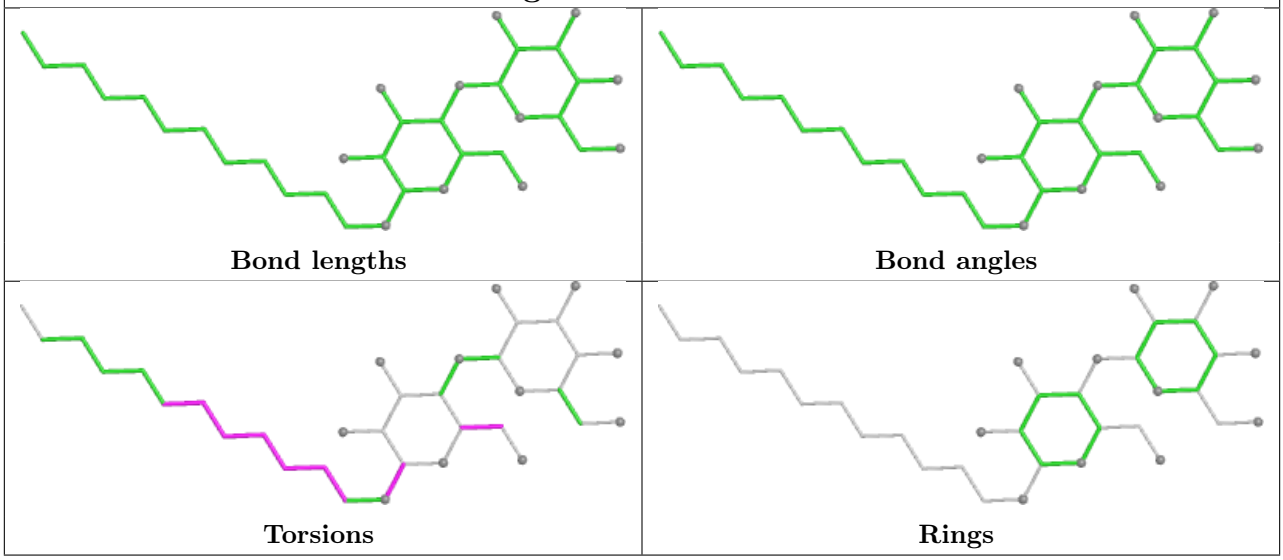
Ligand CLA C 502



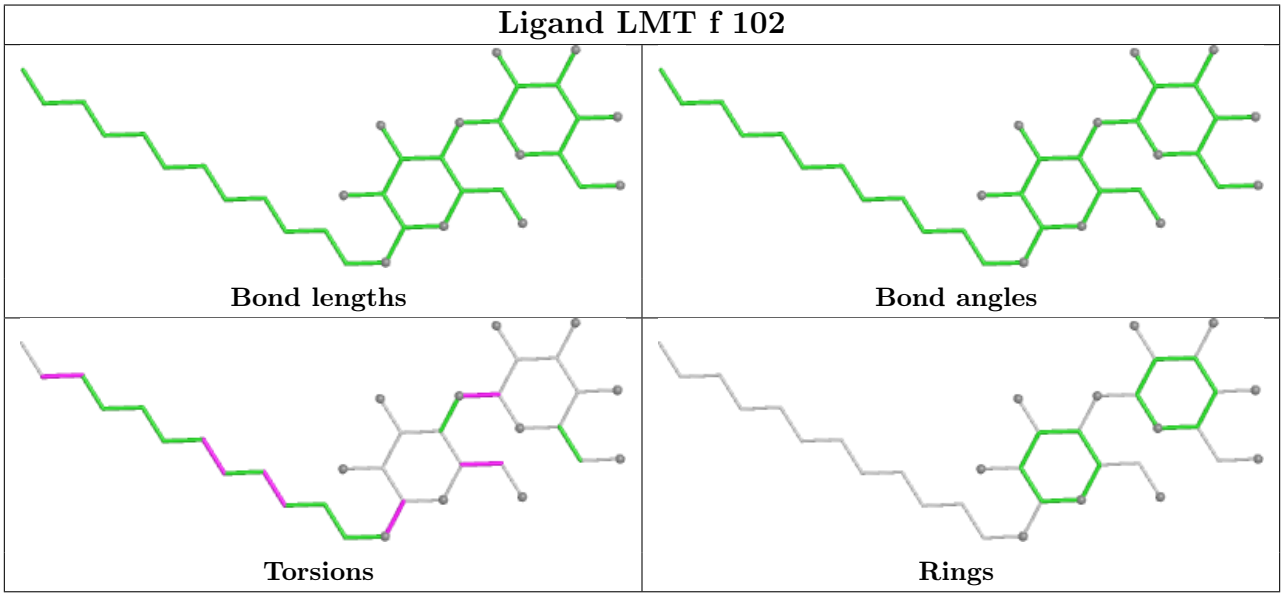
Ligand LMT D 402



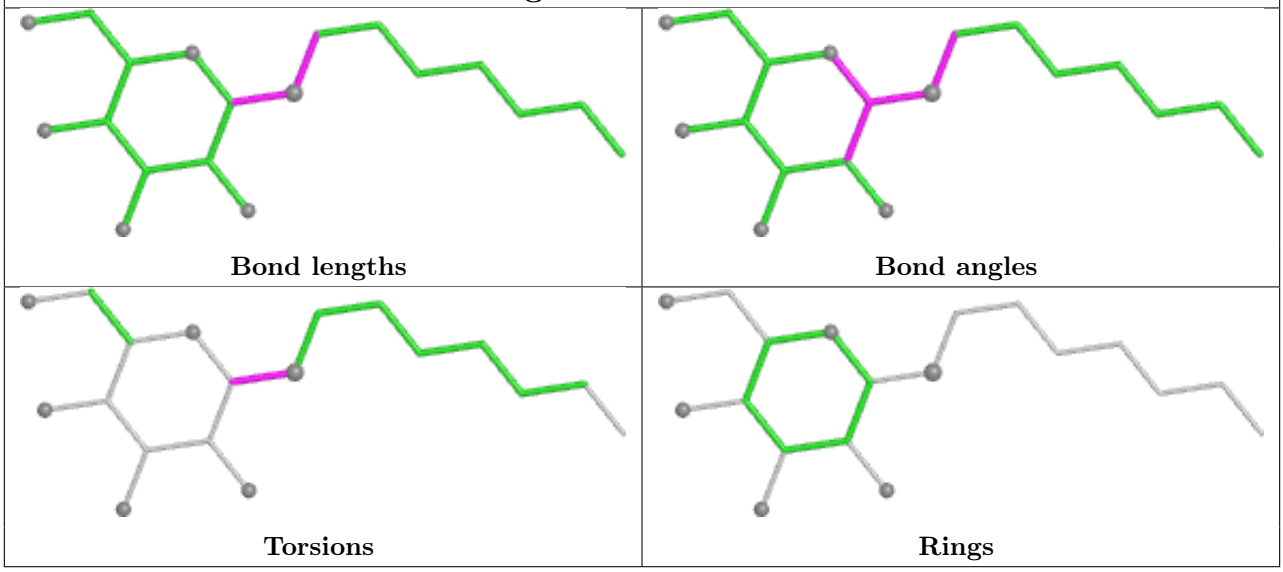
Ligand LMT E 102



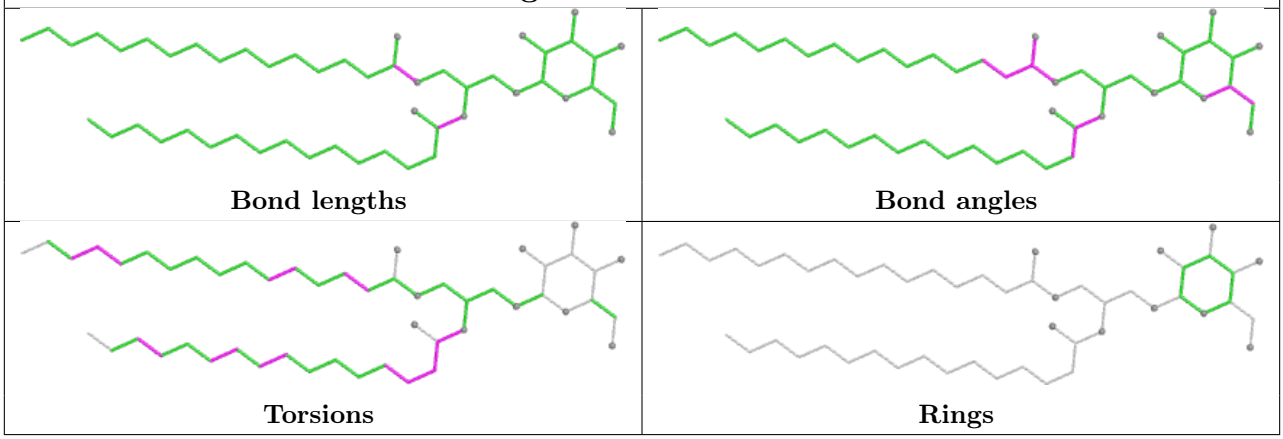
Ligand LMT f 102



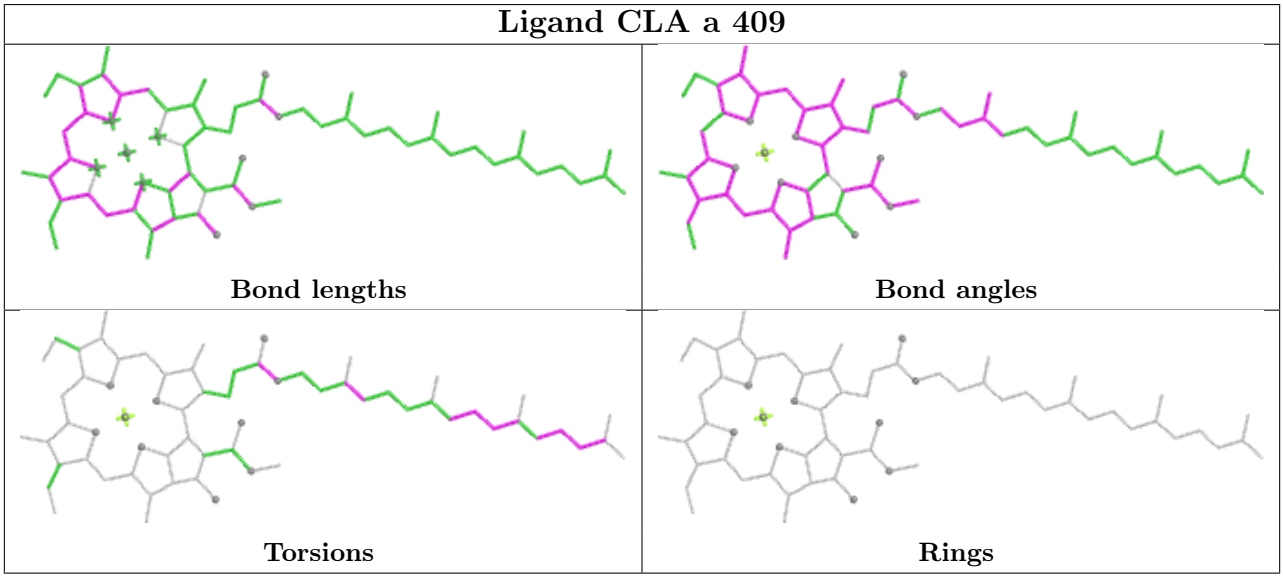
Ligand HTG b 604



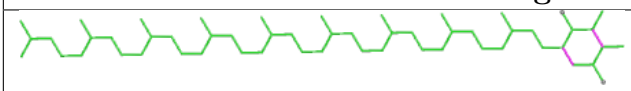
Ligand LMG C 520



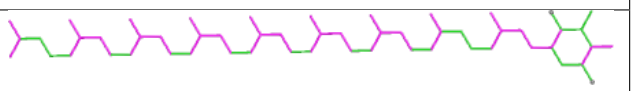
Ligand CLA a 409



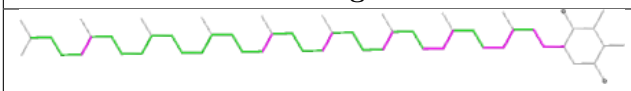
Ligand PL9 a 416



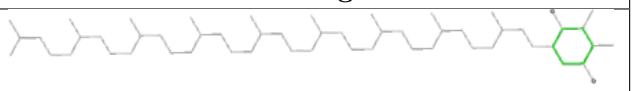
Bond lengths



Bond angles

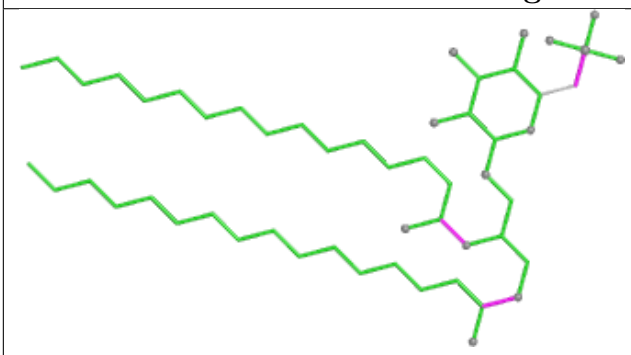


Torsions

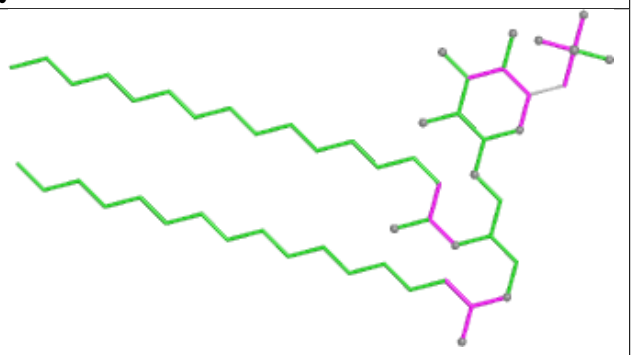


Rings

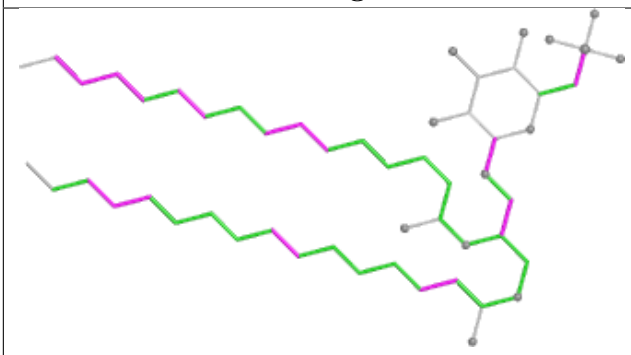
Ligand SQD A 416



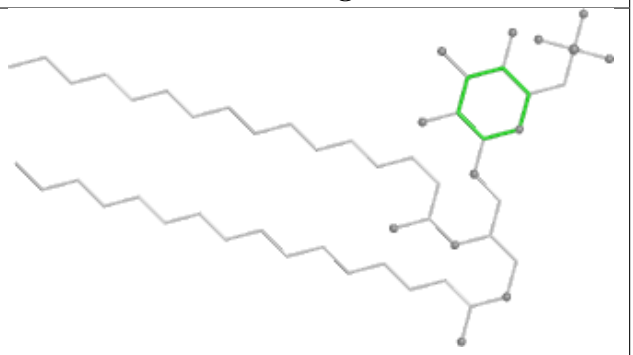
Bond lengths



Bond angles

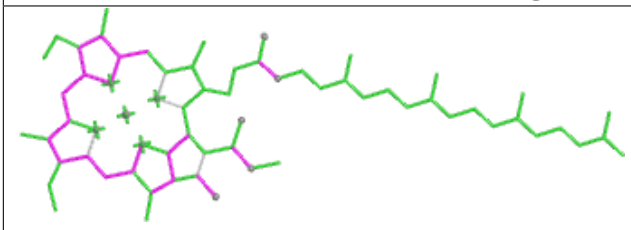


Torsions

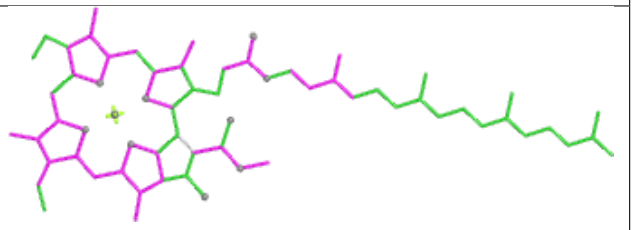


Rings

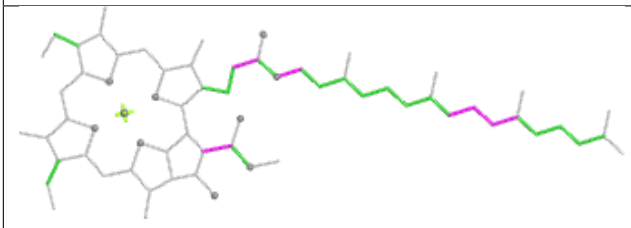
Ligand CLA b 618



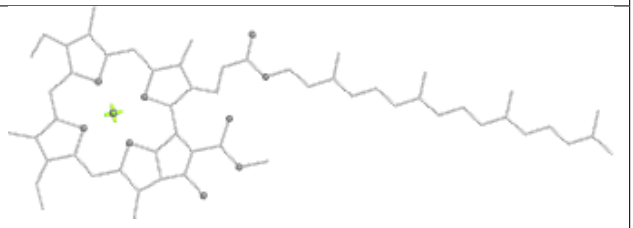
Bond lengths



Bond angles

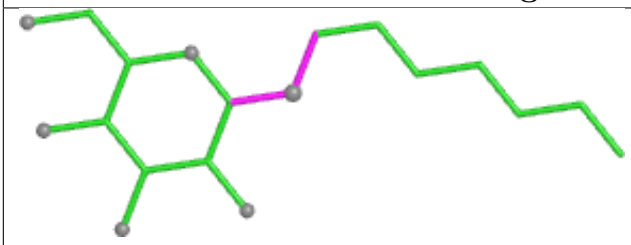


Torsions

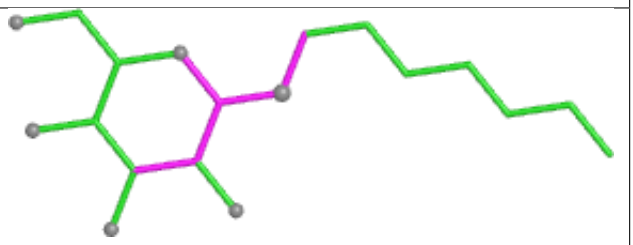


Rings

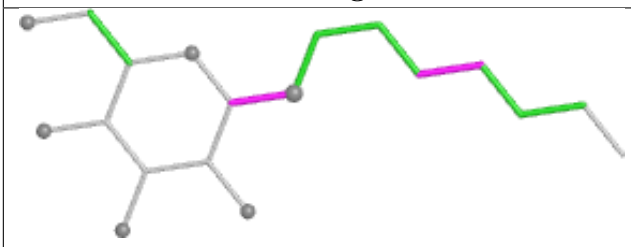
Ligand HTG V 204



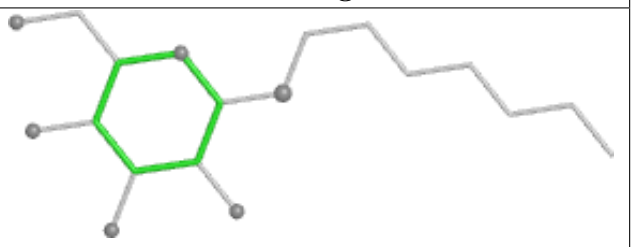
Bond lengths



Bond angles

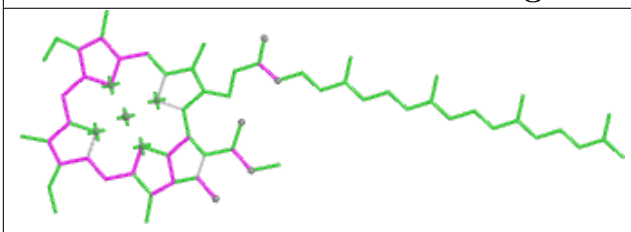


Torsions

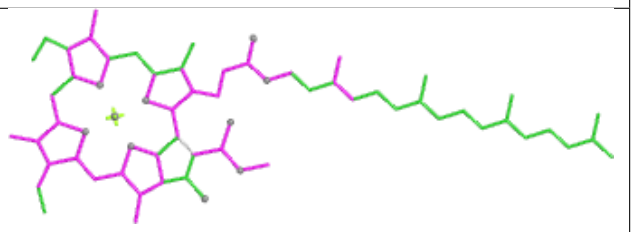


Rings

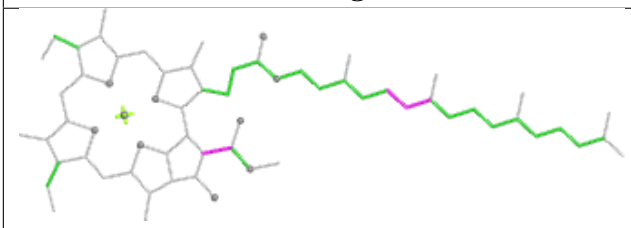
Ligand CLA B 604



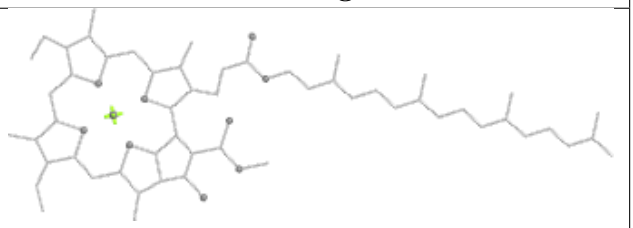
Bond lengths



Bond angles

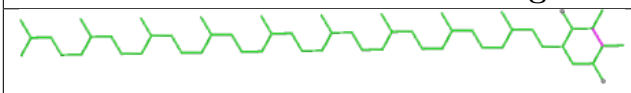


Torsions

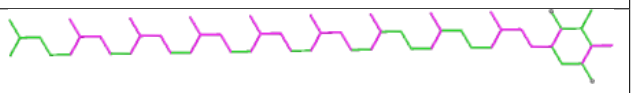


Rings

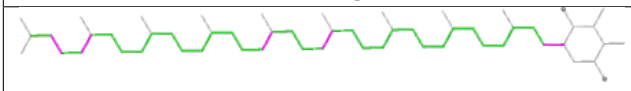
Ligand PL9 A 419



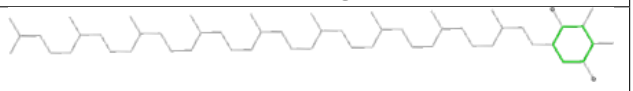
Bond lengths



Bond angles

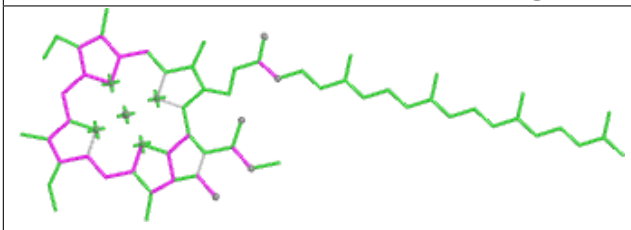


Torsions

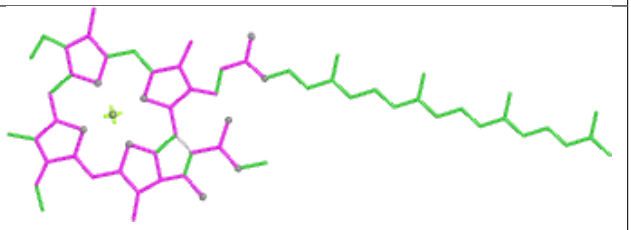


Rings

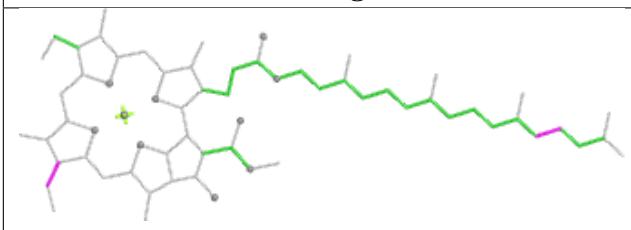
Ligand CLA a 406



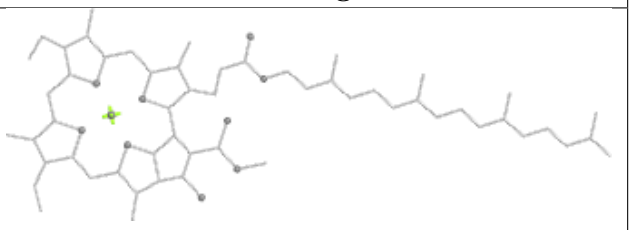
Bond lengths



Bond angles



Torsions

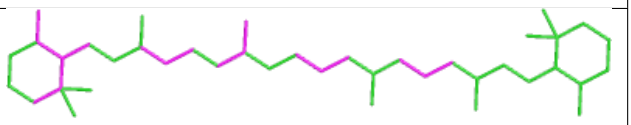


Rings

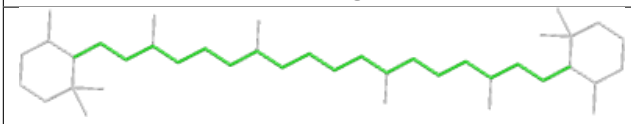
Ligand BCR t 101



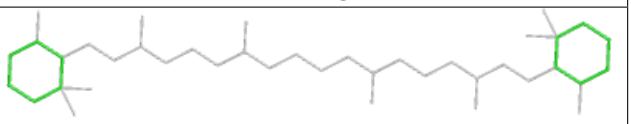
Bond lengths



Bond angles

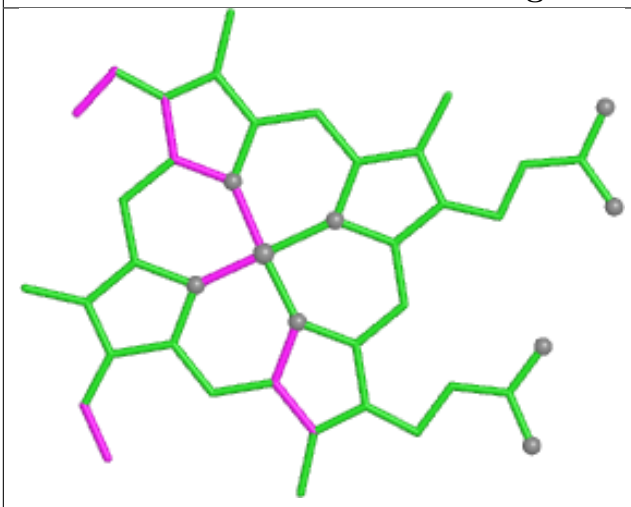


Torsions

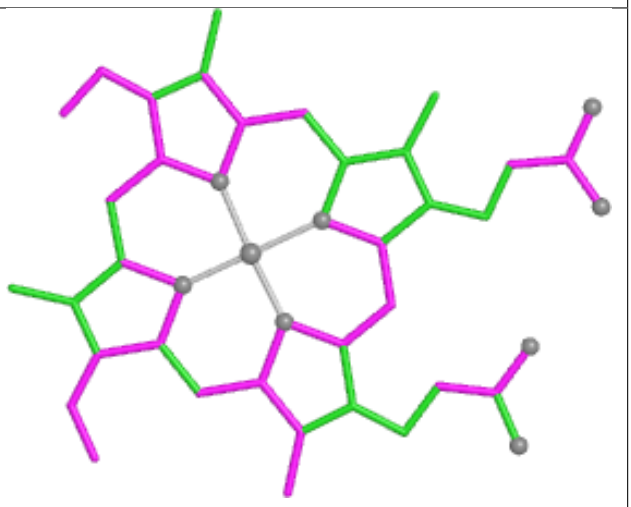


Rings

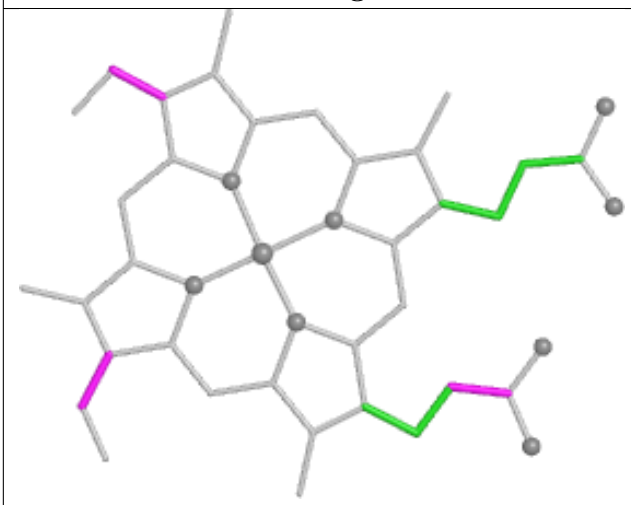
Ligand HEC v 202



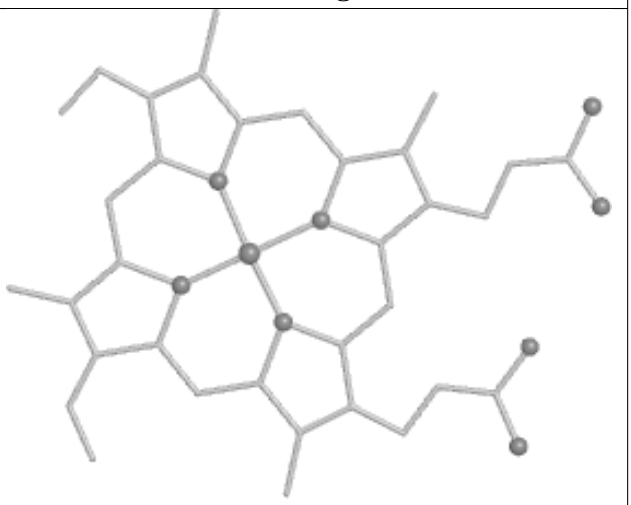
Bond lengths



Bond angles

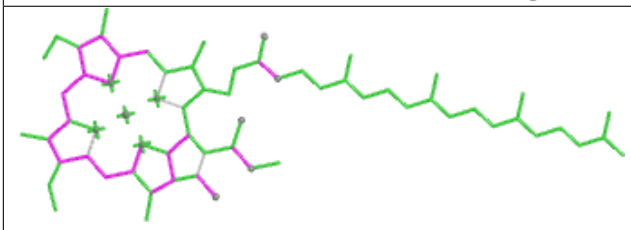


Torsions

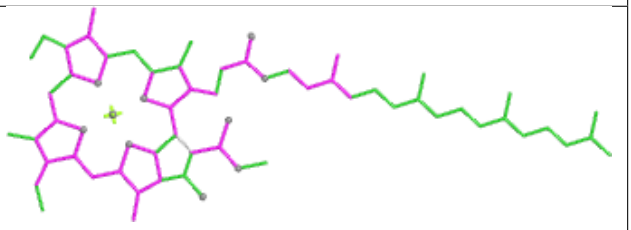


Rings

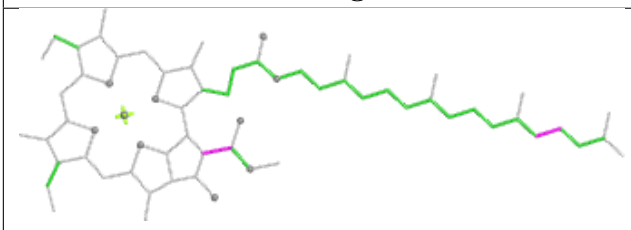
Ligand CLA C 509



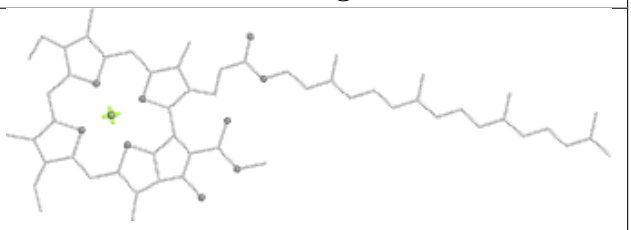
Bond lengths



Bond angles

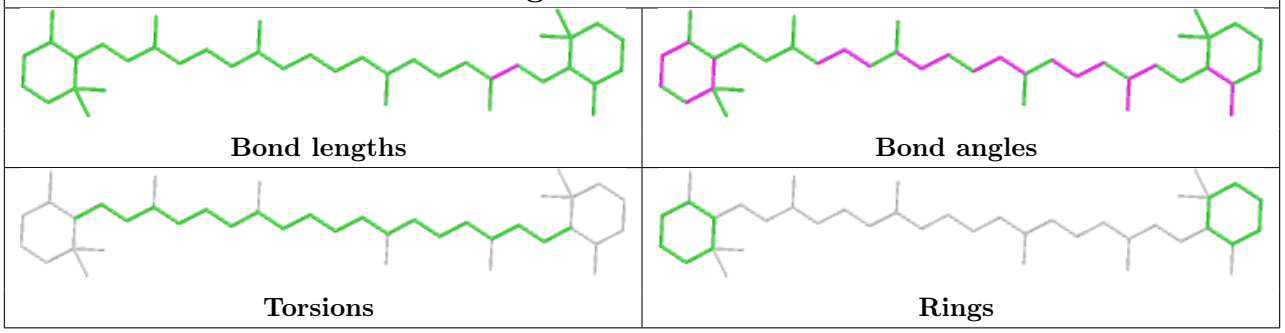


Torsions

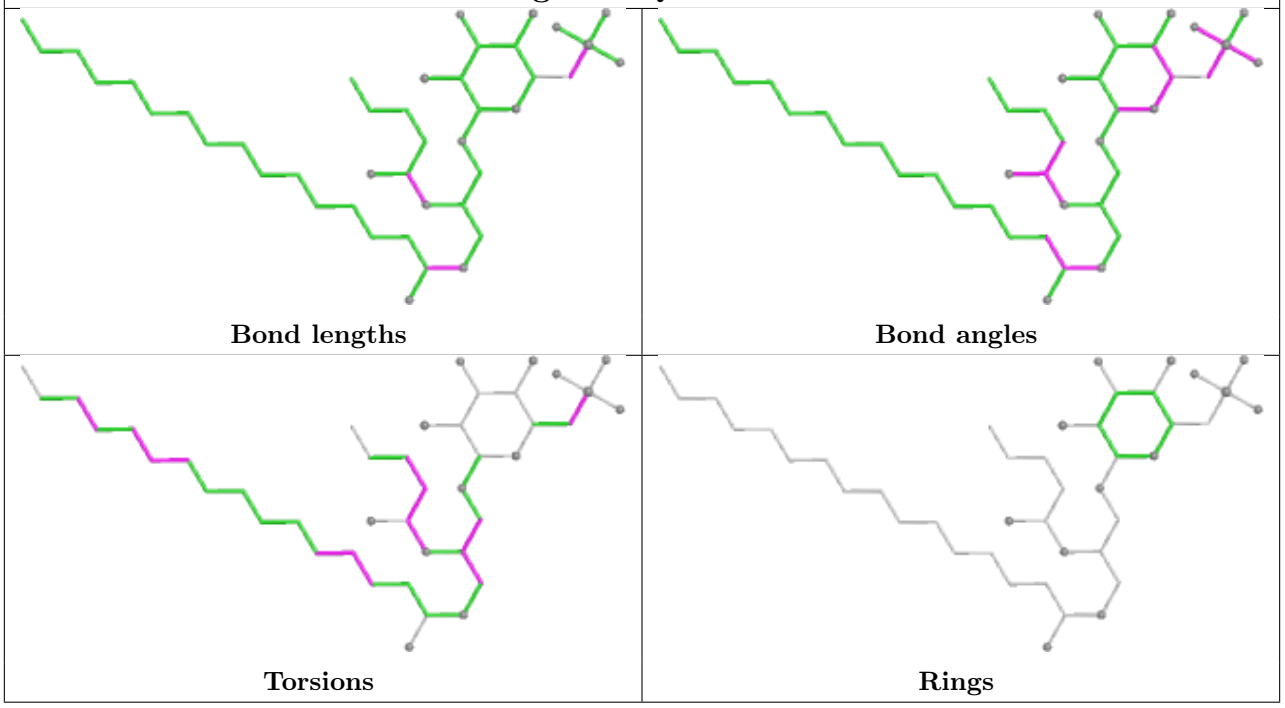


Rings

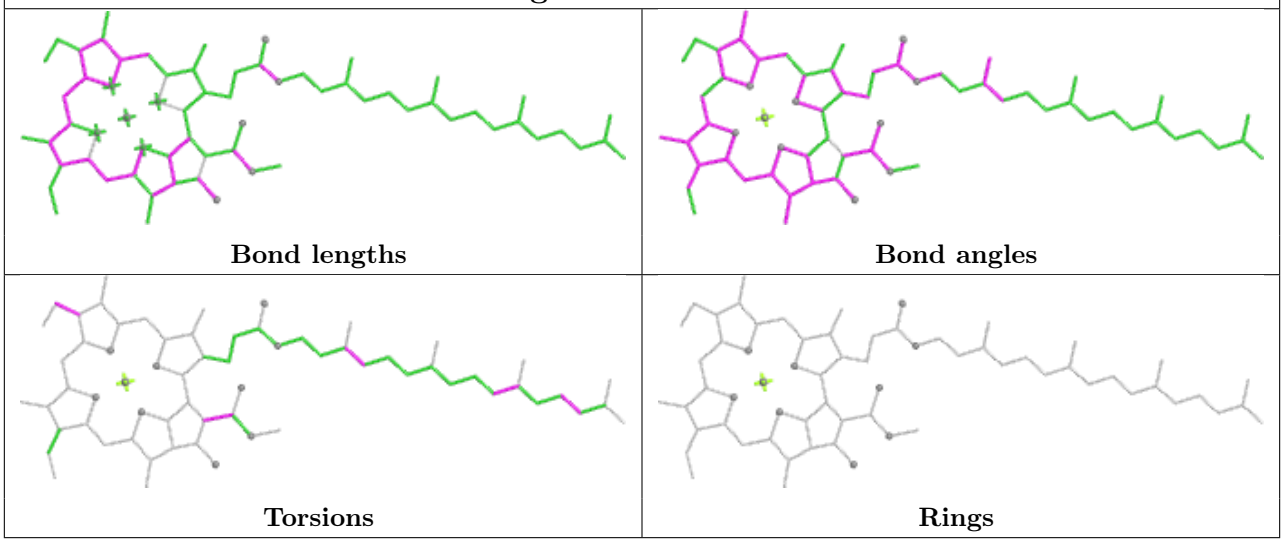
Ligand BCR b 624



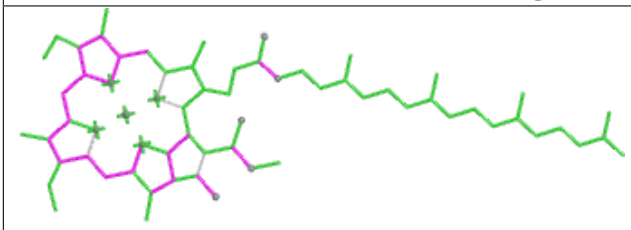
Ligand SQD f 101



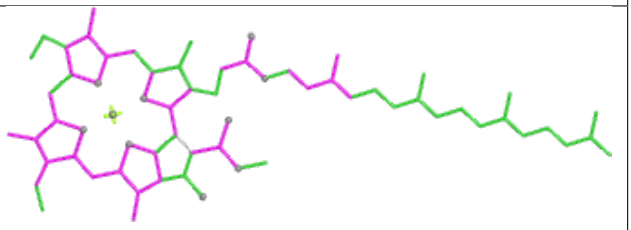
Ligand CLA c 506



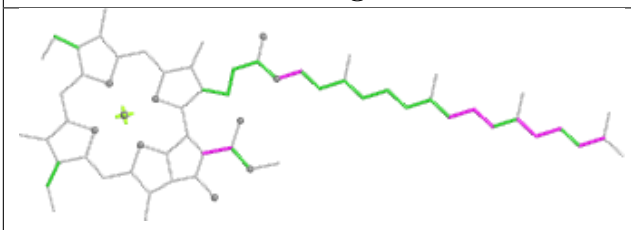
Ligand CLA c 511



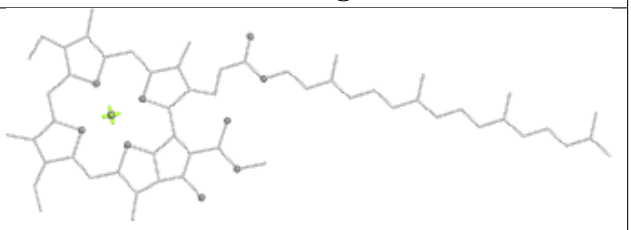
Bond lengths



Bond angles

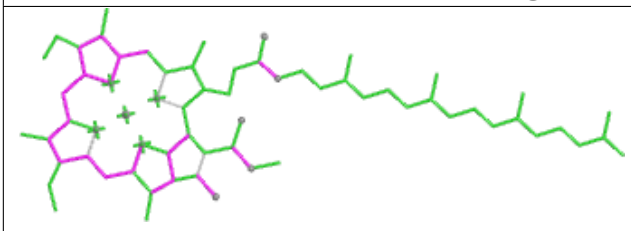


Torsions

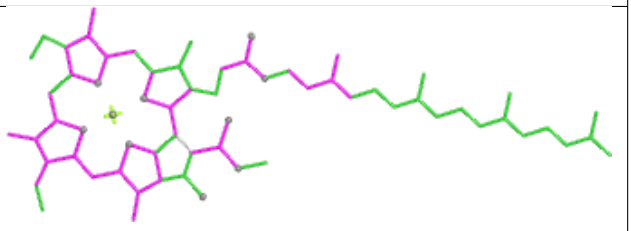


Rings

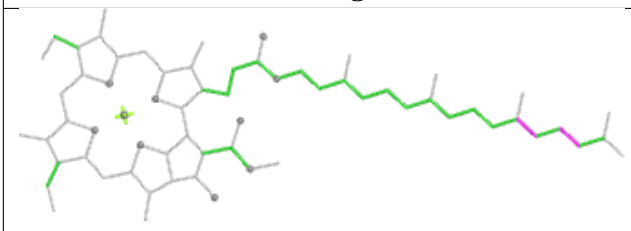
Ligand CLA B 612



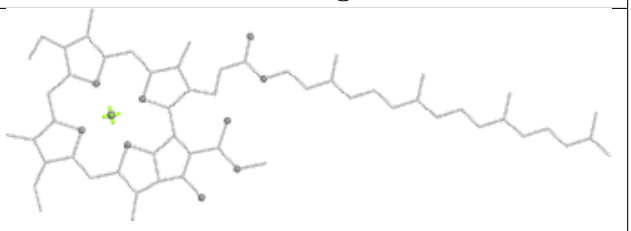
Bond lengths



Bond angles

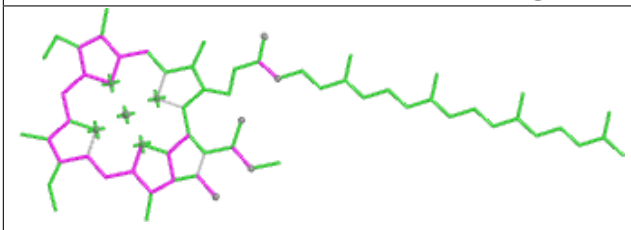


Torsions

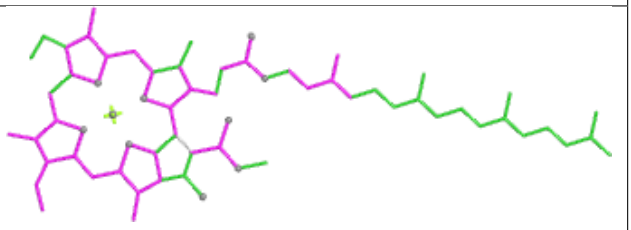


Rings

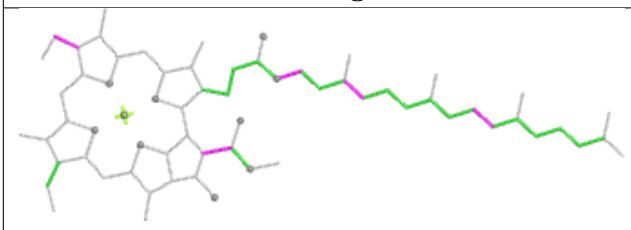
Ligand CLA c 515



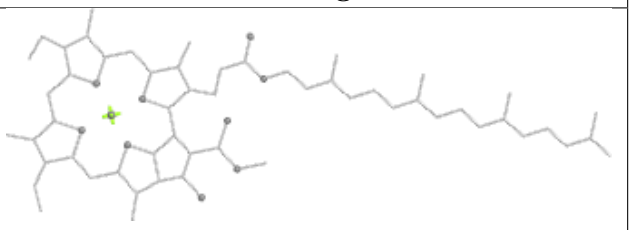
Bond lengths



Bond angles

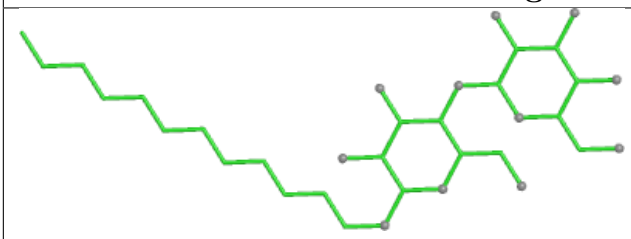


Torsions

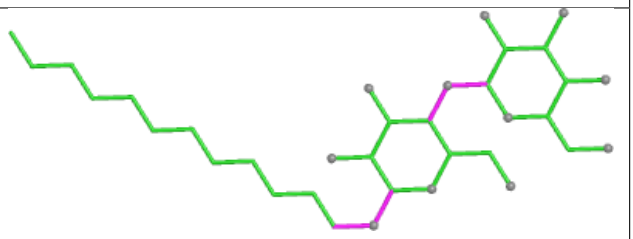


Rings

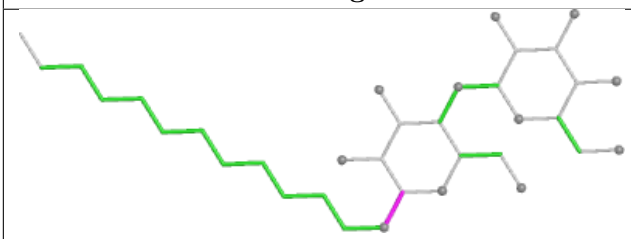
Ligand LMT a 417



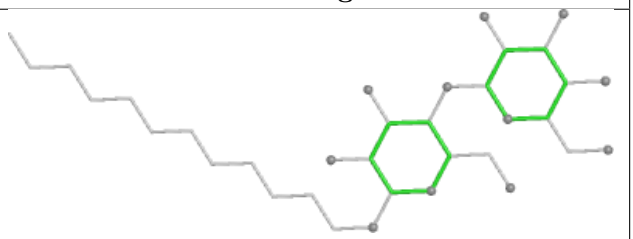
Bond lengths



Bond angles

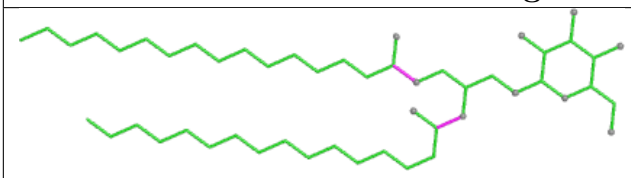


Torsions

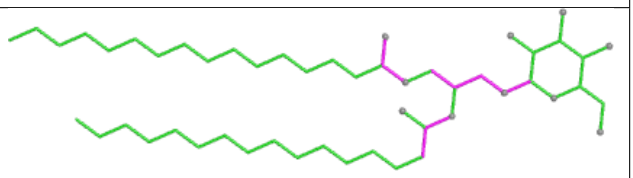


Rings

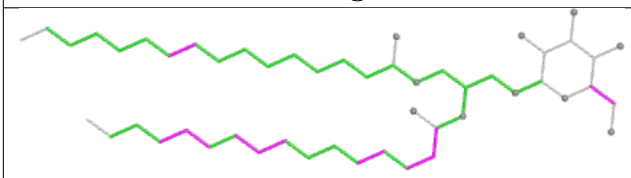
Ligand LMG J 101



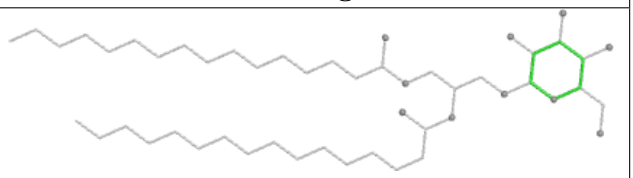
Bond lengths



Bond angles

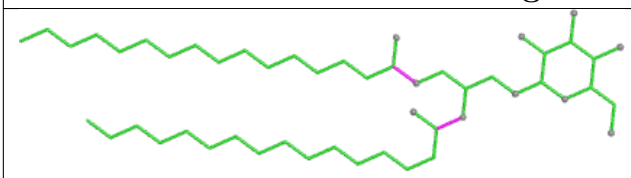


Torsions

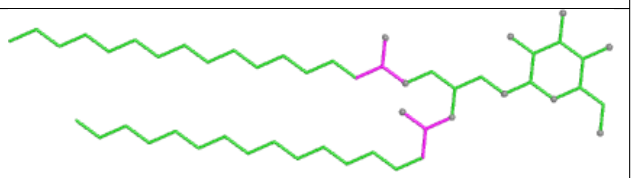


Rings

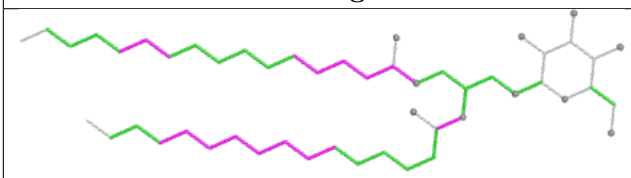
Ligand LMG b 625



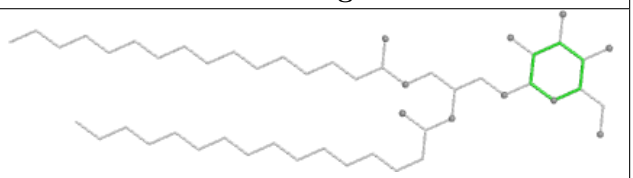
Bond lengths



Bond angles

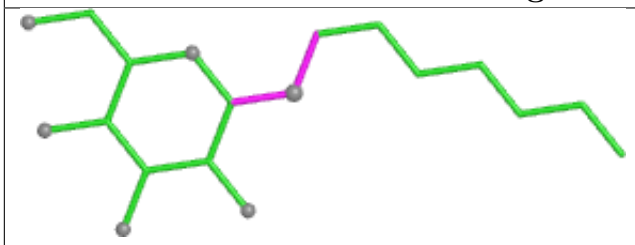


Torsions

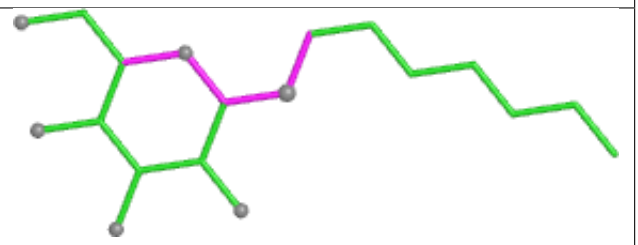


Rings

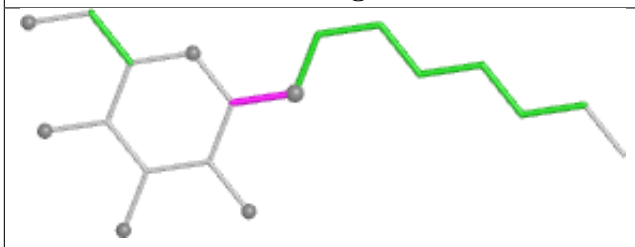
Ligand HTG c 523



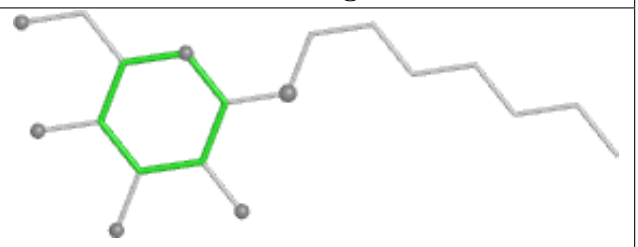
Bond lengths



Bond angles

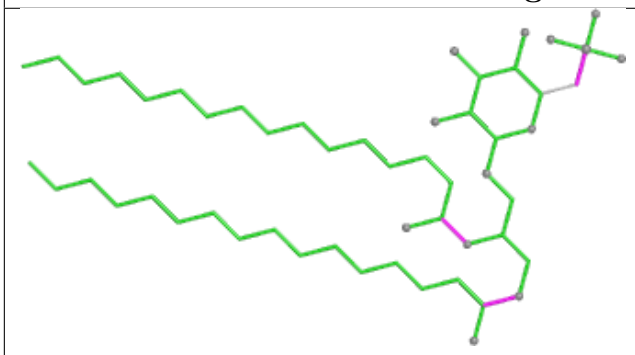


Torsions

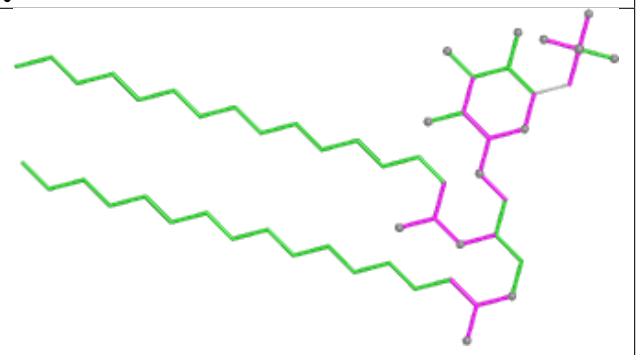


Rings

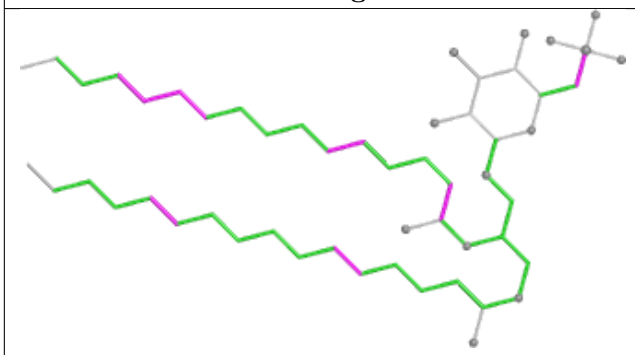
Ligand SQD A 411



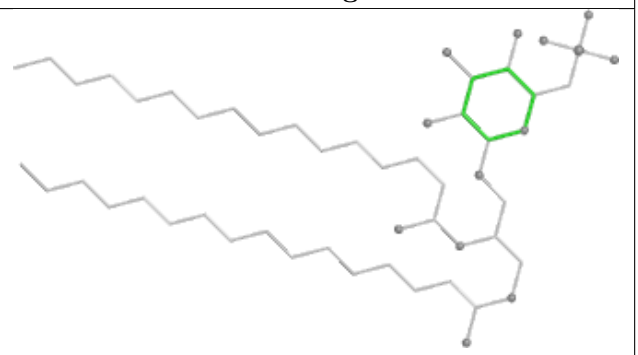
Bond lengths



Bond angles

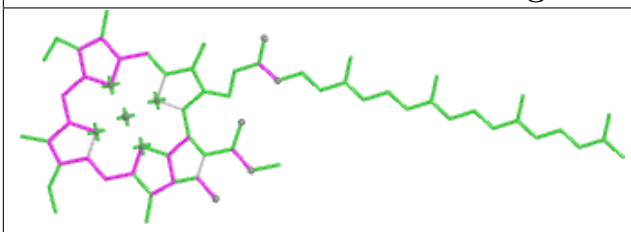


Torsions

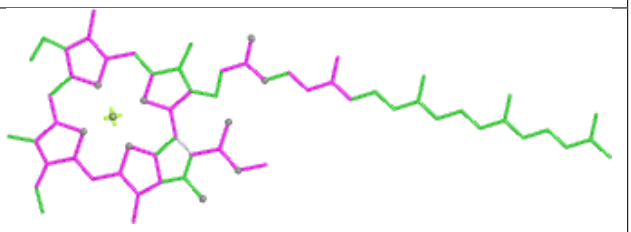


Rings

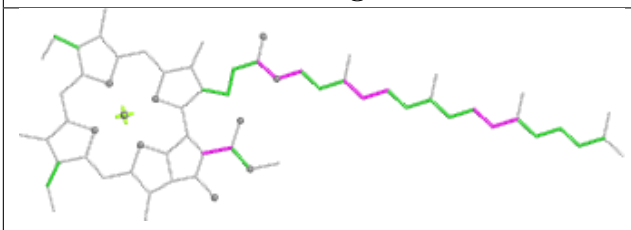
Ligand CLA b 621



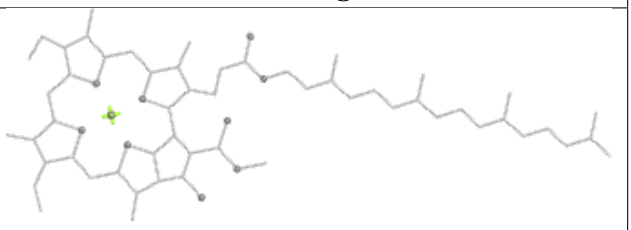
Bond lengths



Bond angles

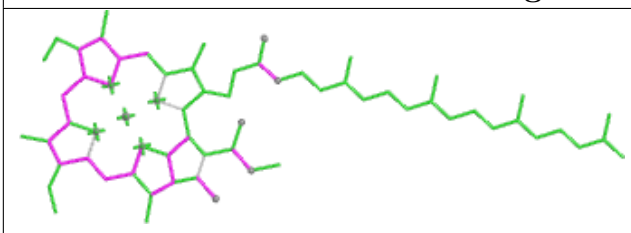


Torsions

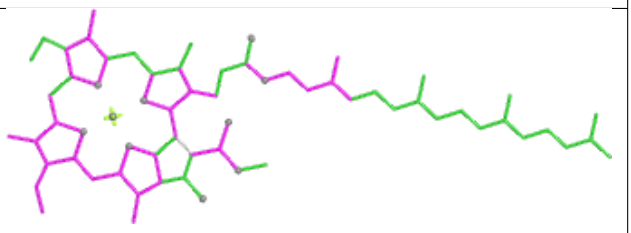


Rings

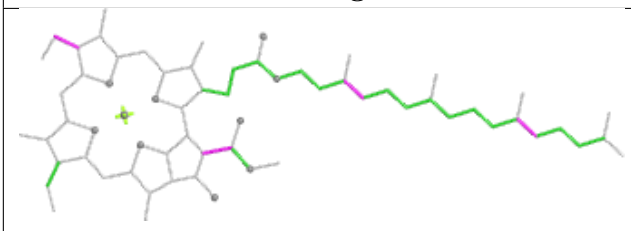
Ligand CLA C 505



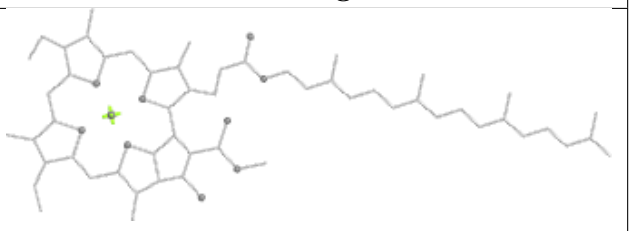
Bond lengths



Bond angles

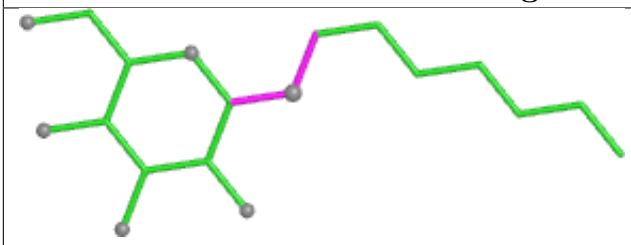


Torsions

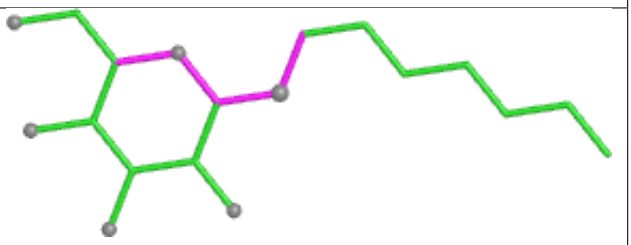


Rings

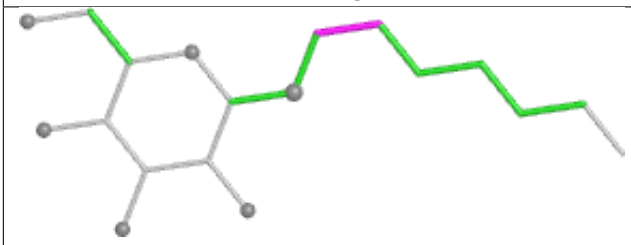
Ligand HTG B 631



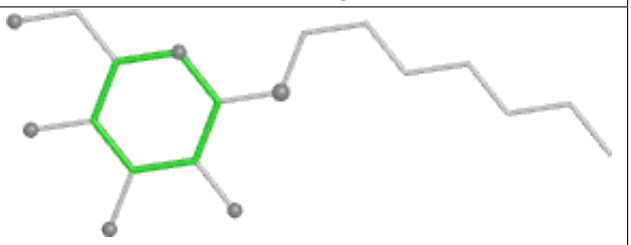
Bond lengths



Bond angles

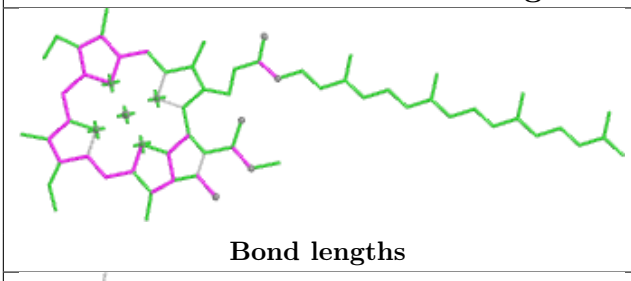


Torsions

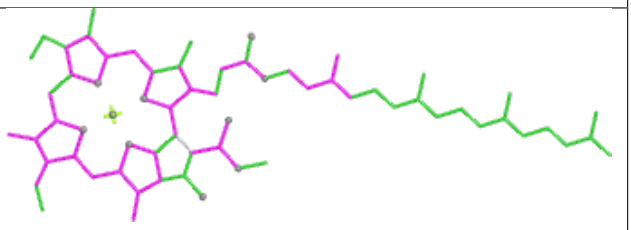


Rings

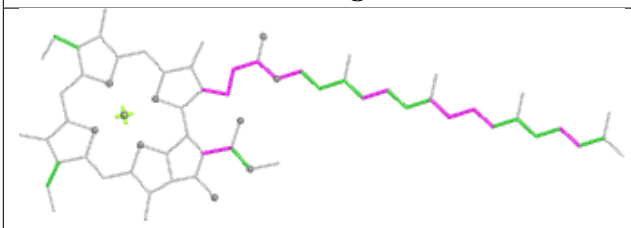
Ligand CLA B 602



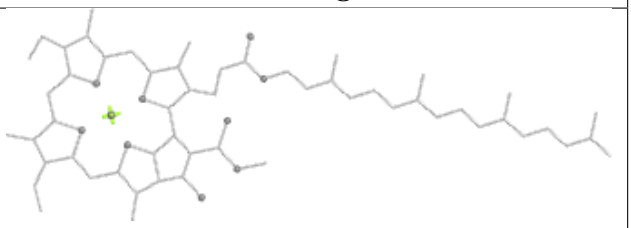
Bond lengths



Bond angles

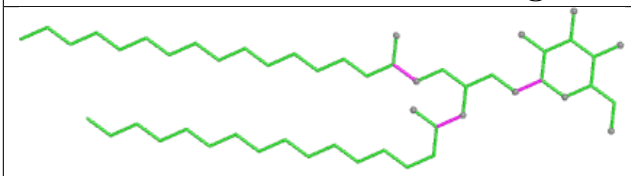


Torsions

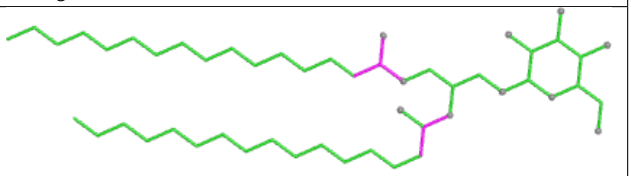


Rings

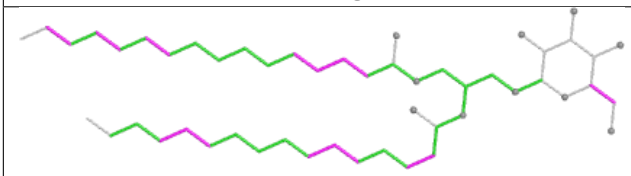
Ligand LMG j 101



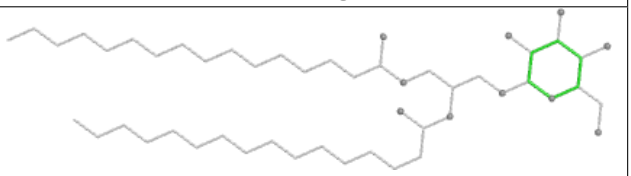
Bond lengths



Bond angles

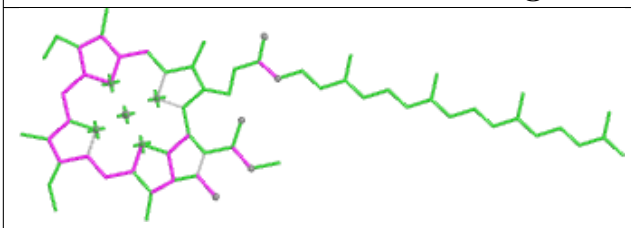


Torsions

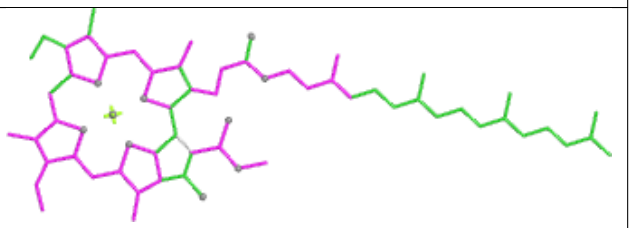


Rings

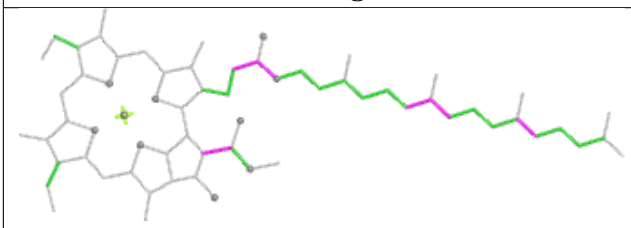
Ligand CLA C 513



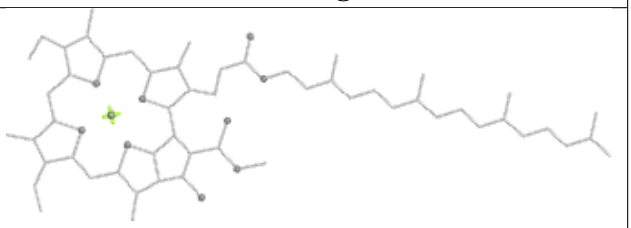
Bond lengths



Bond angles

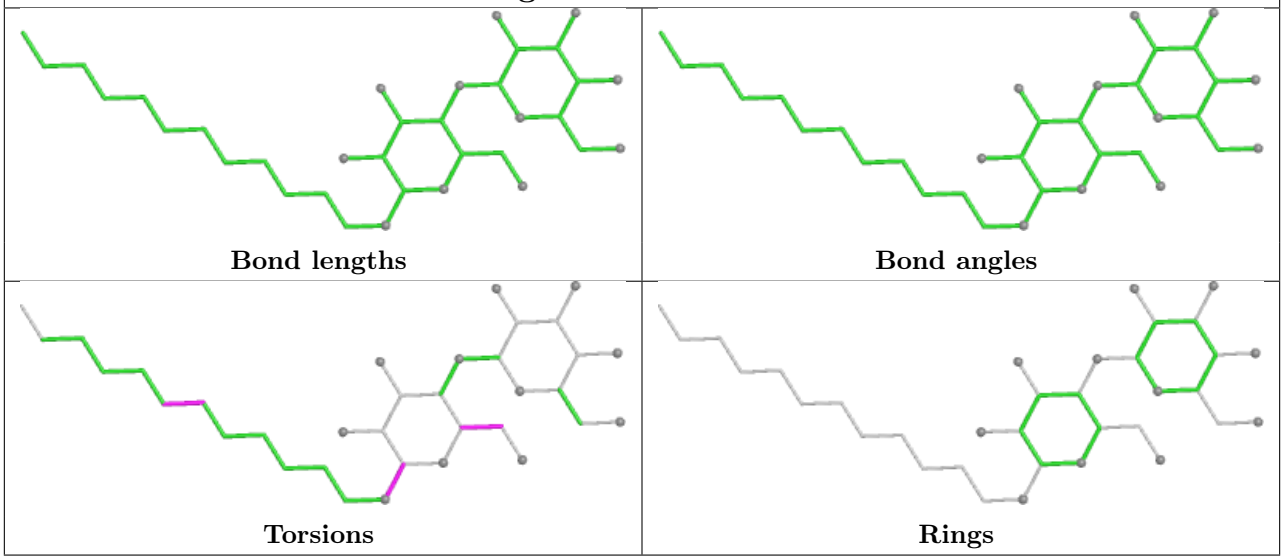


Torsions

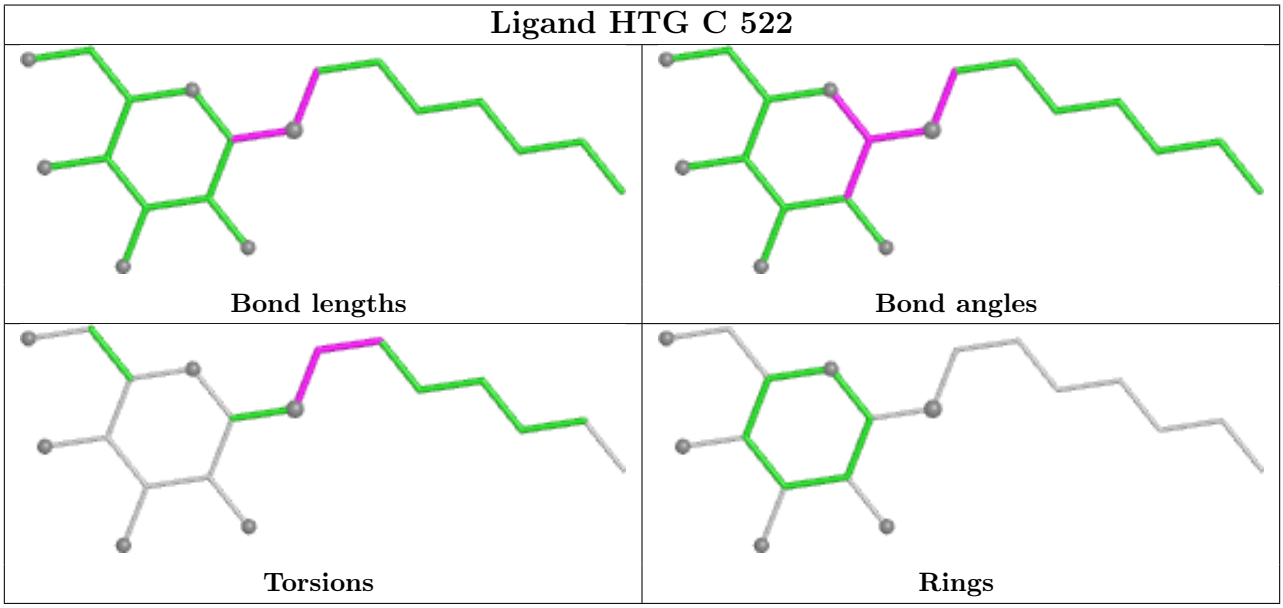


Rings

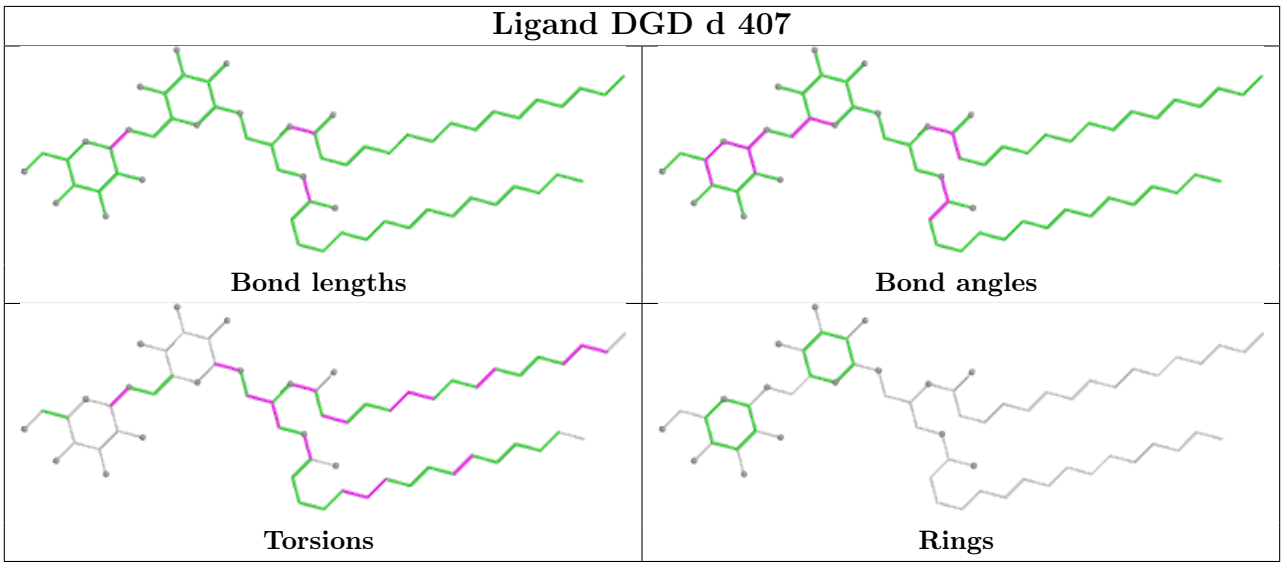
Ligand LMT M 102



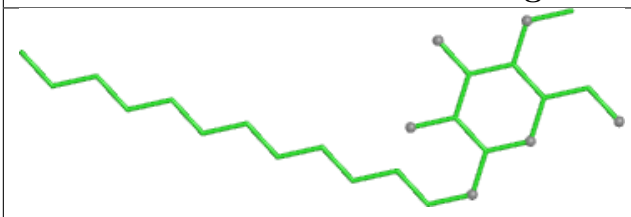
Ligand HTG C 522



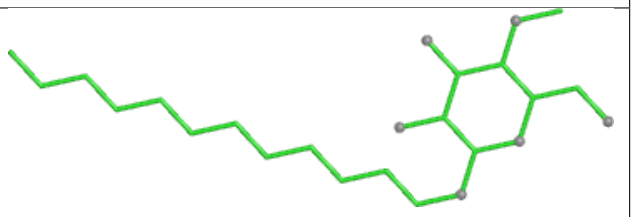
Ligand DGD d 407



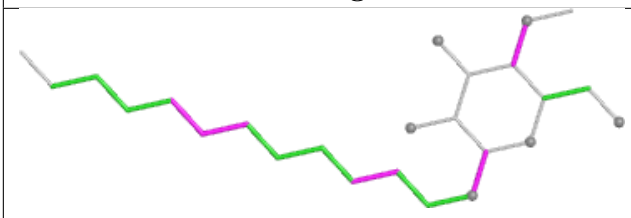
Ligand LMT b 626



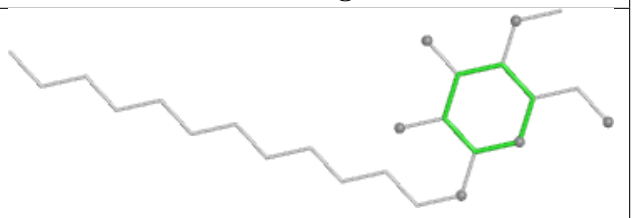
Bond lengths



Bond angles

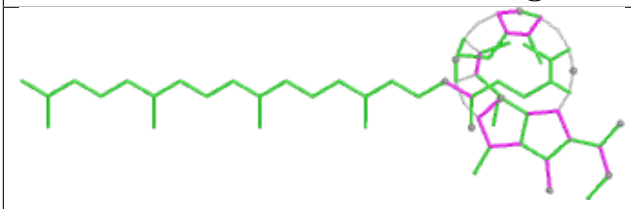


Torsions

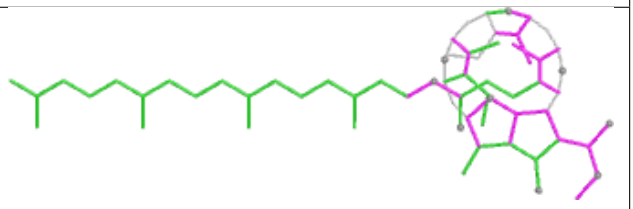


Rings

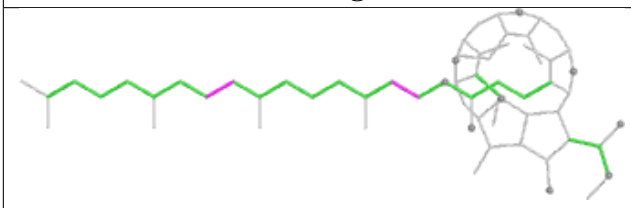
Ligand PHO a 408



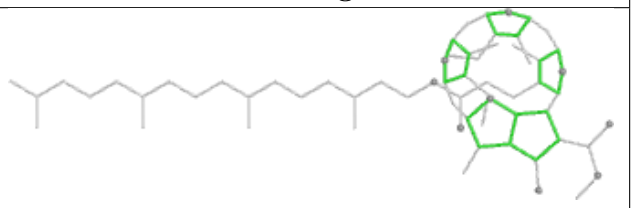
Bond lengths



Bond angles

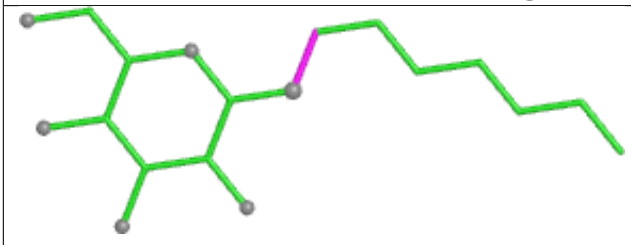


Torsions

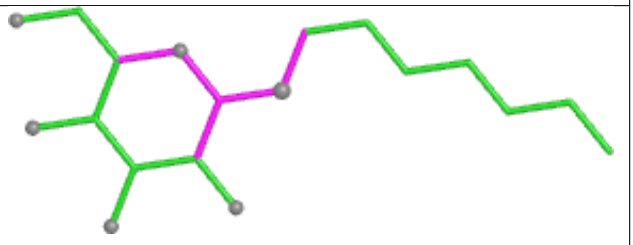


Rings

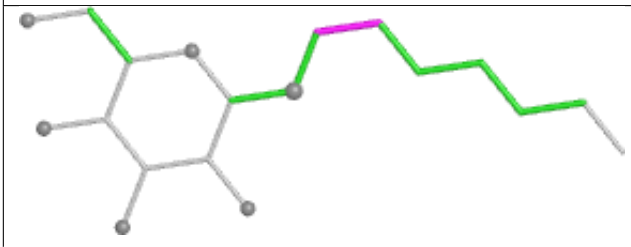
Ligand HTG B 622



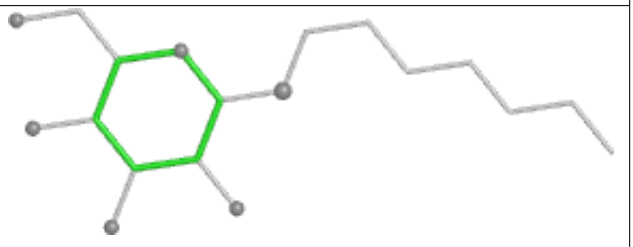
Bond lengths



Bond angles

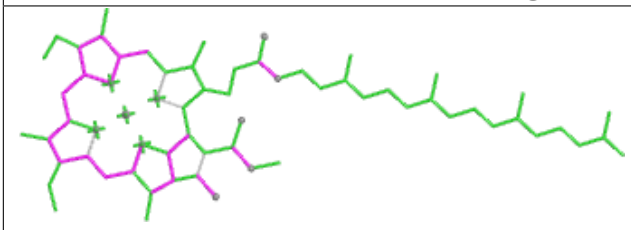


Torsions

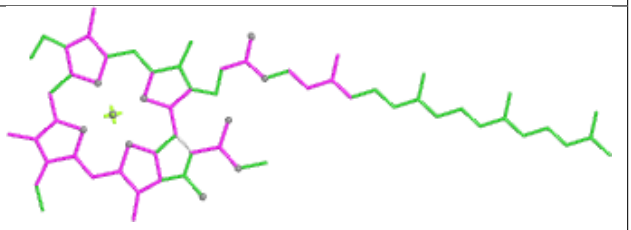


Rings

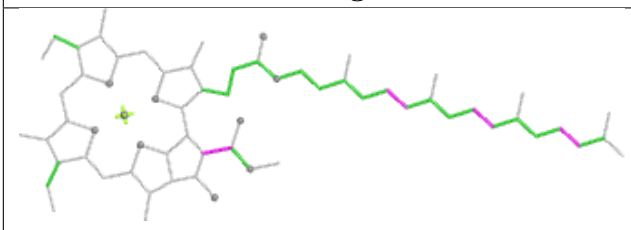
Ligand CLA C 504



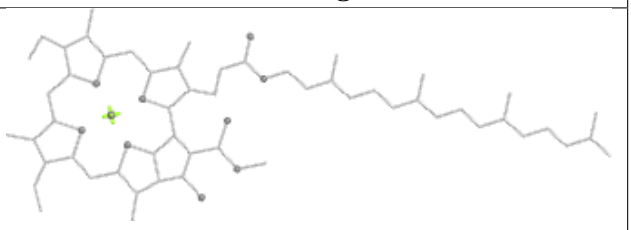
Bond lengths



Bond angles

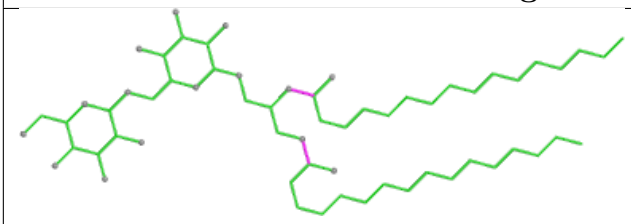


Torsions

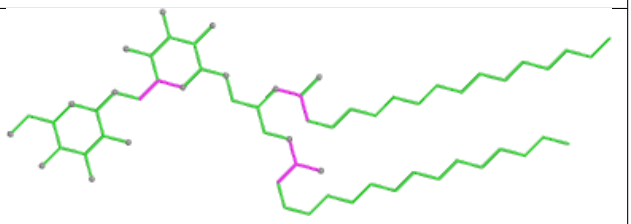


Rings

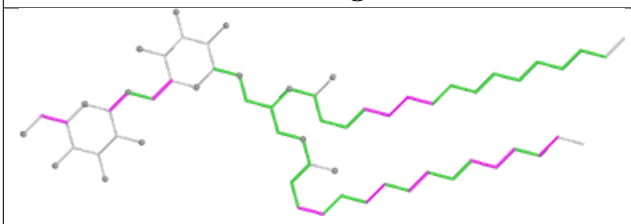
Ligand DGD C 517



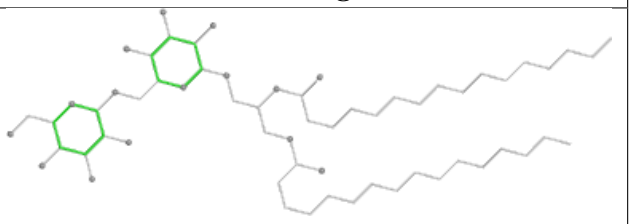
Bond lengths



Bond angles

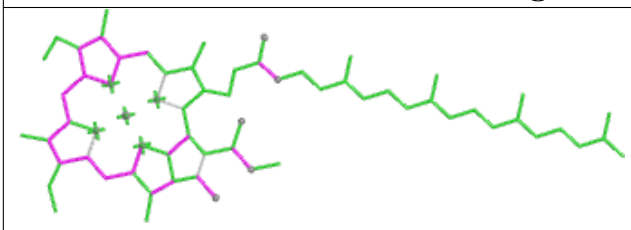


Torsions

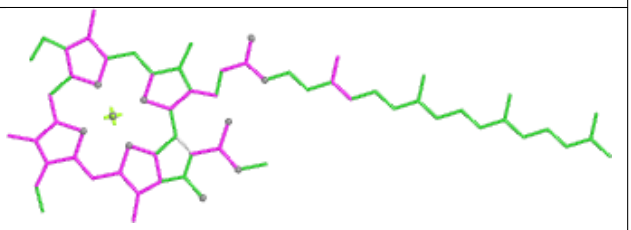


Rings

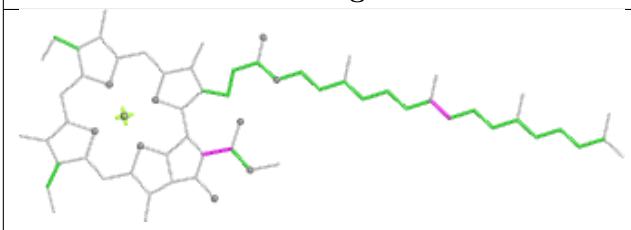
Ligand CLA c 509



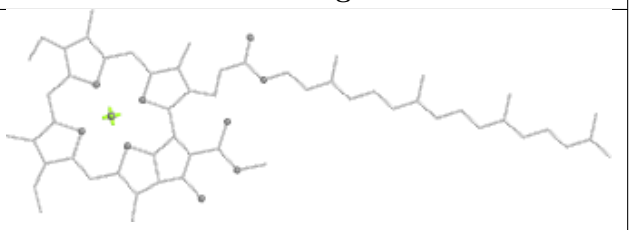
Bond lengths



Bond angles

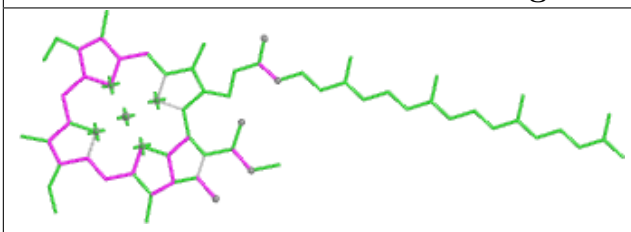


Torsions

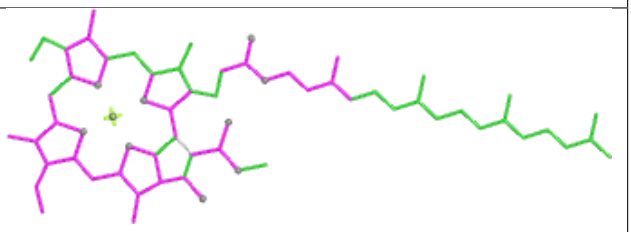


Rings

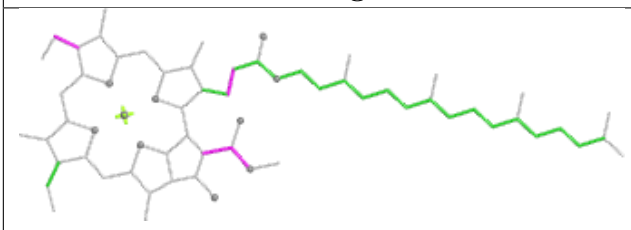
Ligand CLA c 503



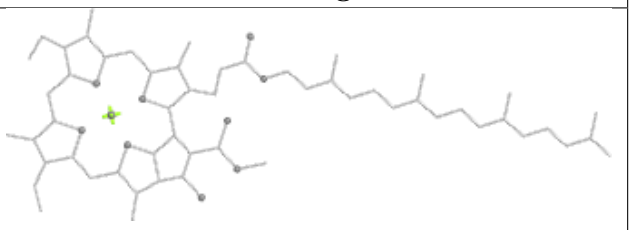
Bond lengths



Bond angles



Torsions

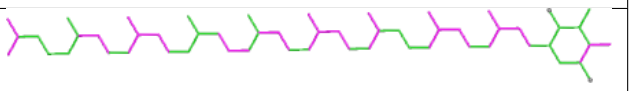


Rings

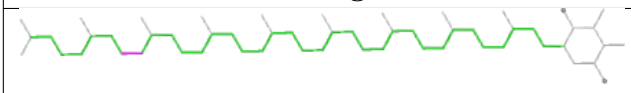
Ligand PL9 D 406



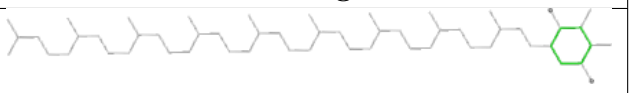
Bond lengths



Bond angles

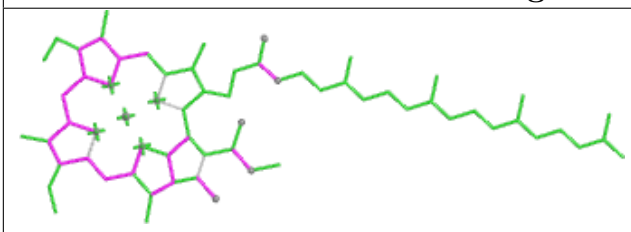


Torsions

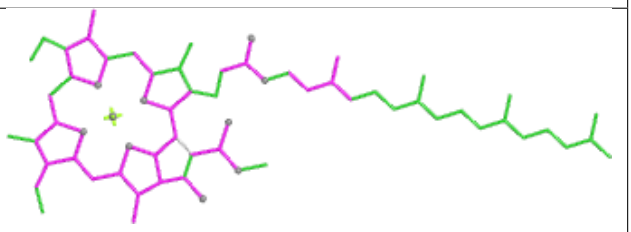


Rings

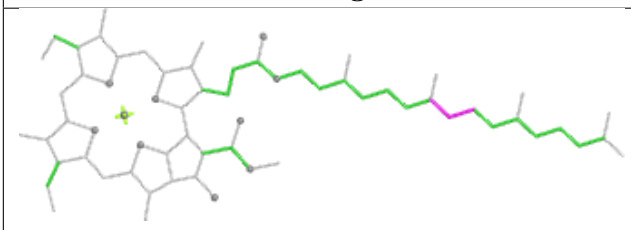
Ligand CLA b 617



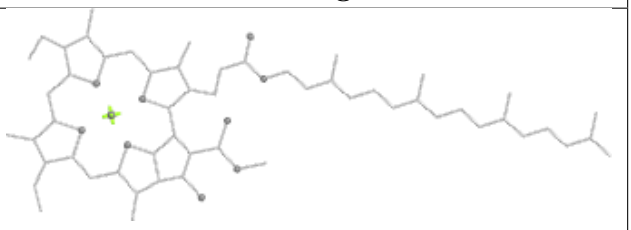
Bond lengths



Bond angles

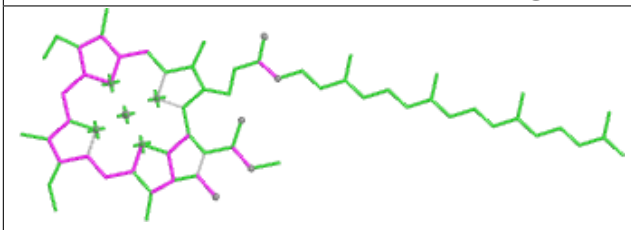


Torsions

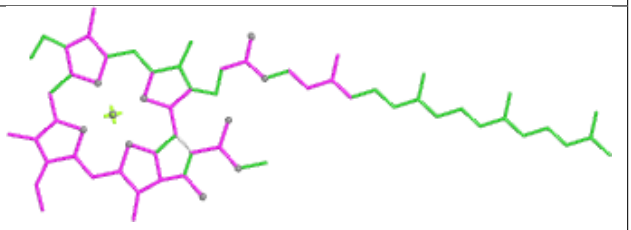


Rings

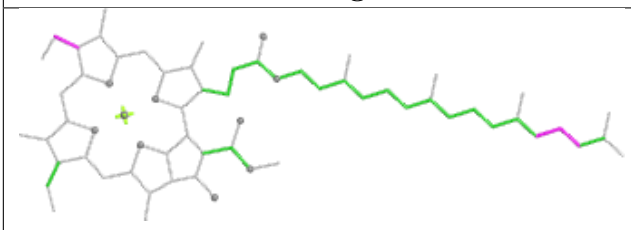
Ligand CLA b 616



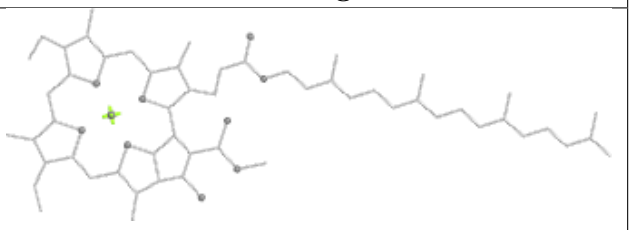
Bond lengths



Bond angles

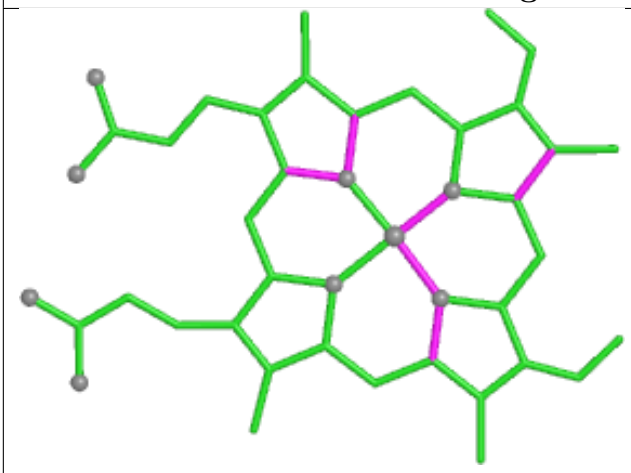


Torsions

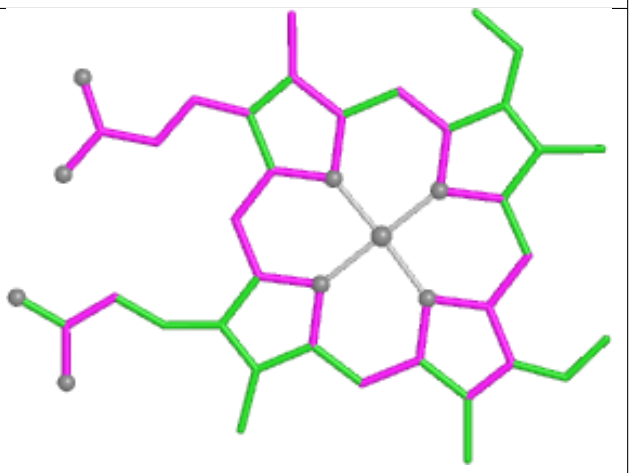


Rings

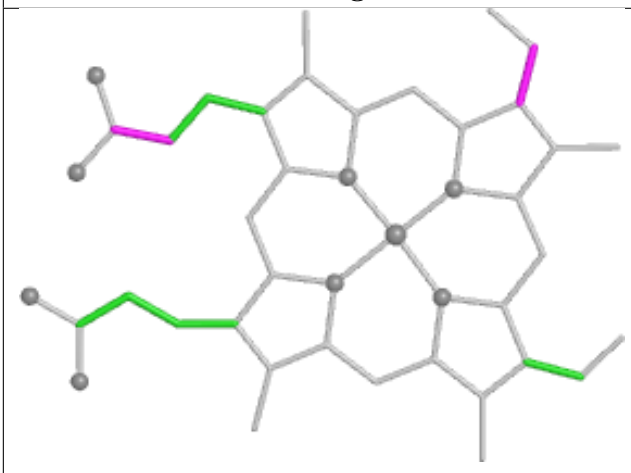
Ligand HEM E 103



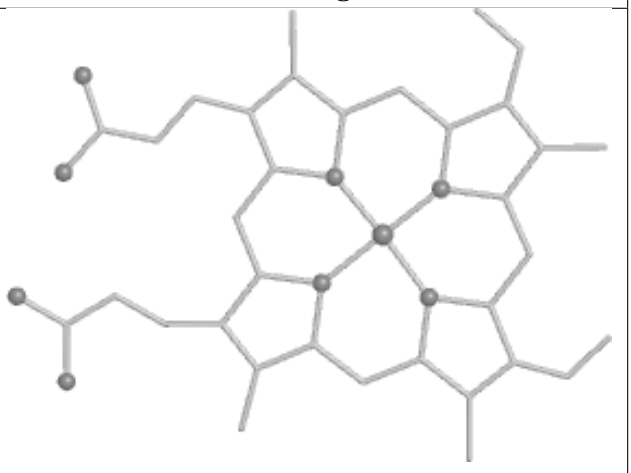
Bond lengths



Bond angles

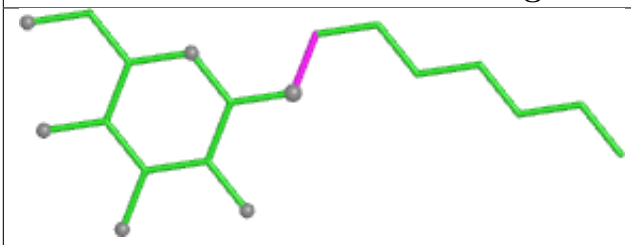


Torsions

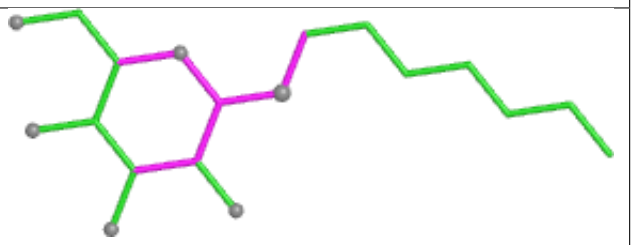


Rings

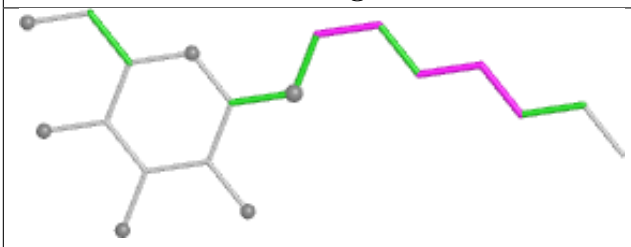
Ligand HTG b 627



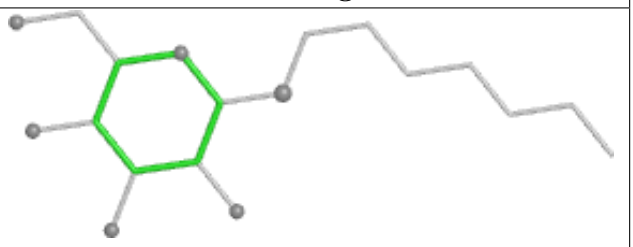
Bond lengths



Bond angles

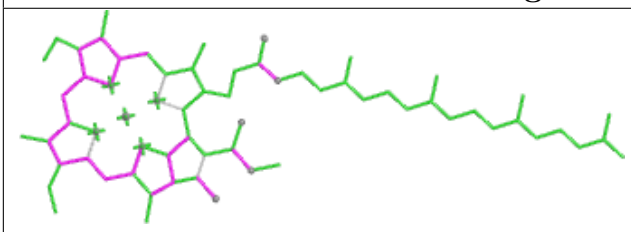


Torsions

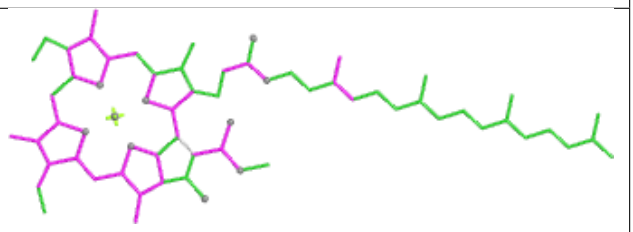


Rings

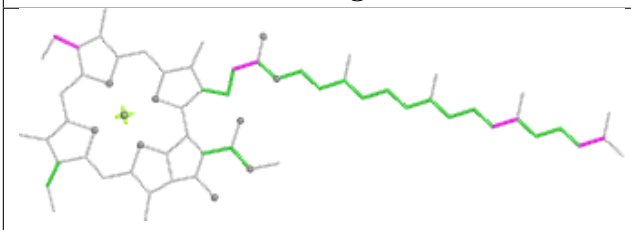
Ligand CLA C 506



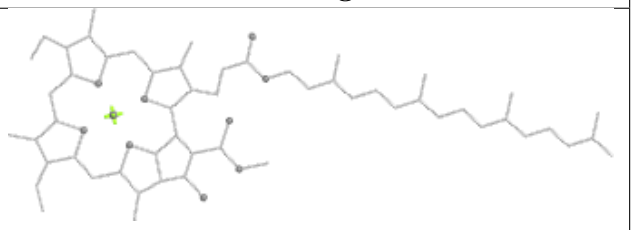
Bond lengths



Bond angles

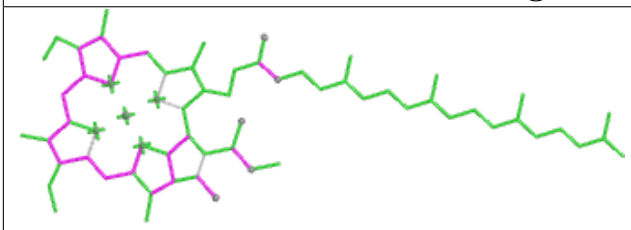


Torsions

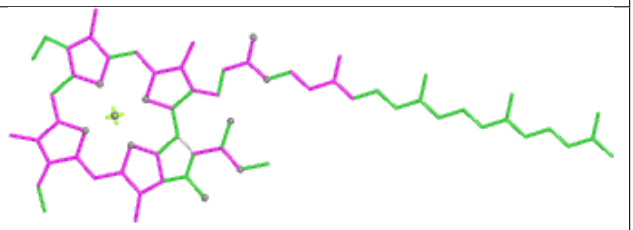


Rings

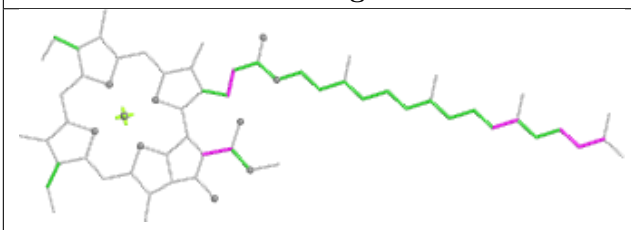
Ligand CLA b 615



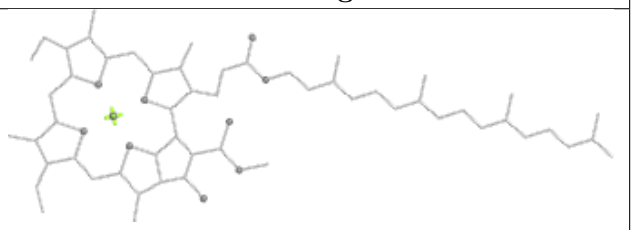
Bond lengths



Bond angles

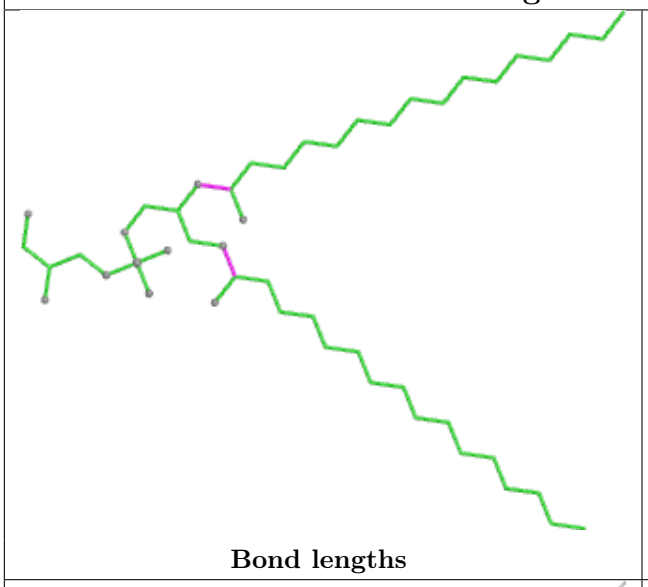


Torsions

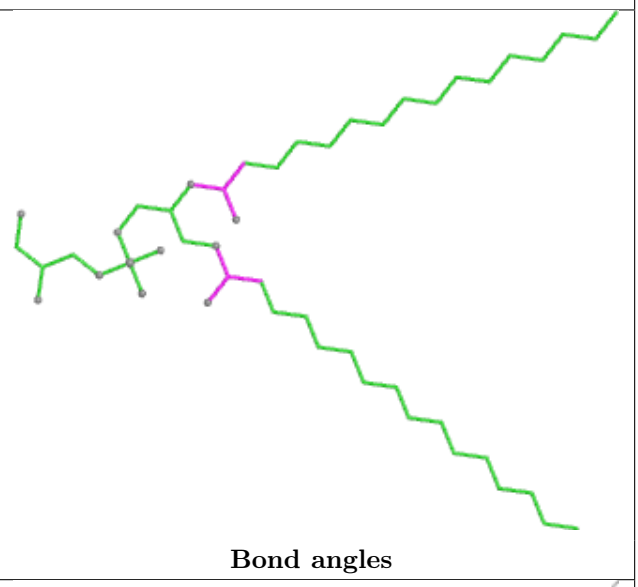


Rings

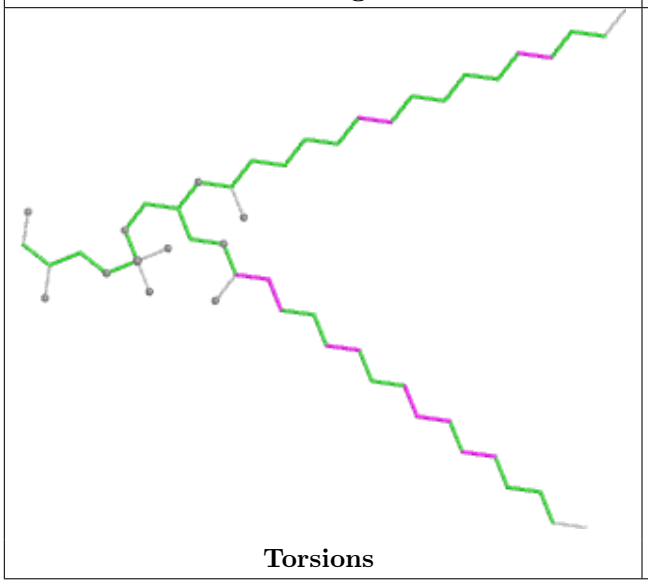
Ligand LHG D 408



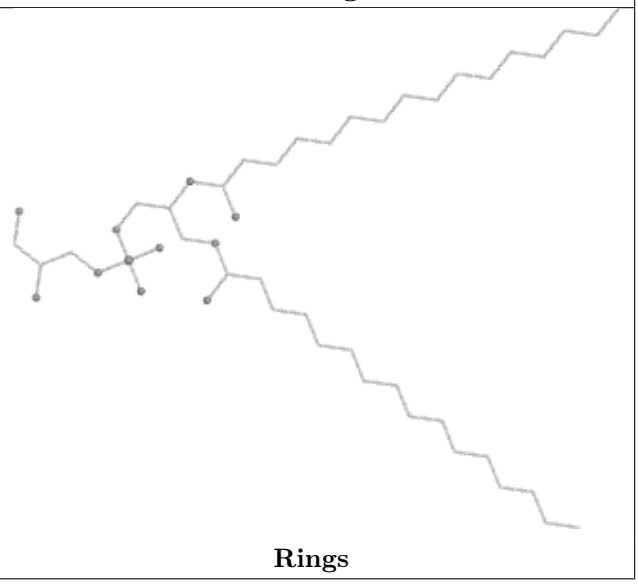
Bond lengths



Bond angles

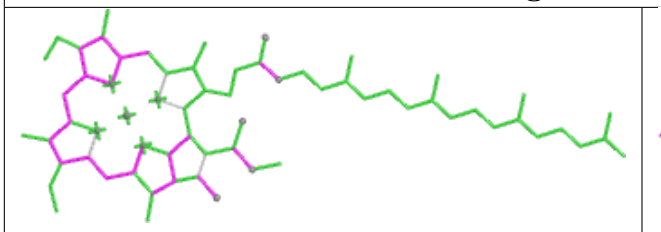


Torsions

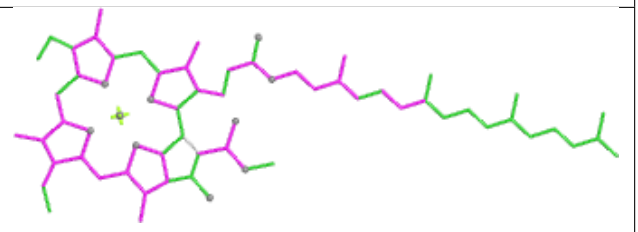


Rings

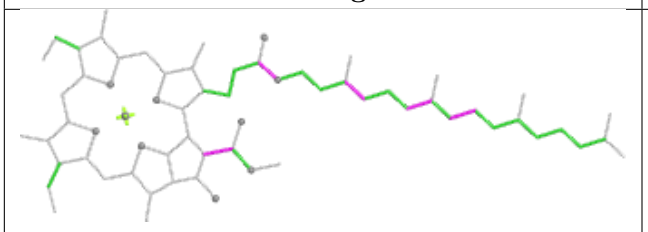
Ligand CLA C 511



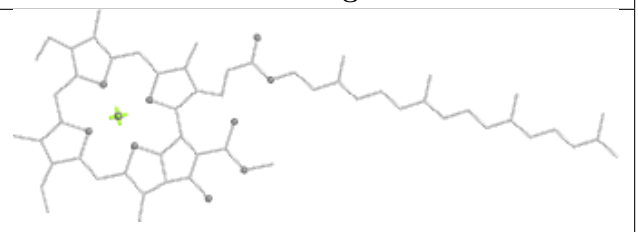
Bond lengths



Bond angles

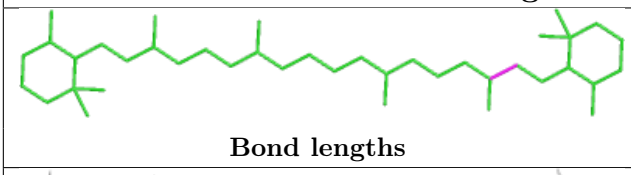


Torsions

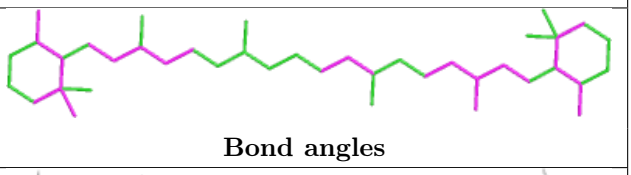


Rings

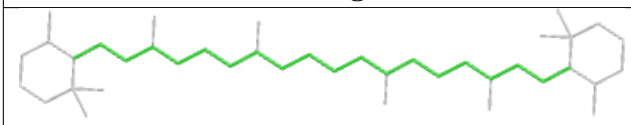
Ligand BCR K 101



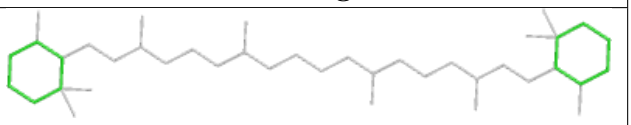
Bond lengths



Bond angles

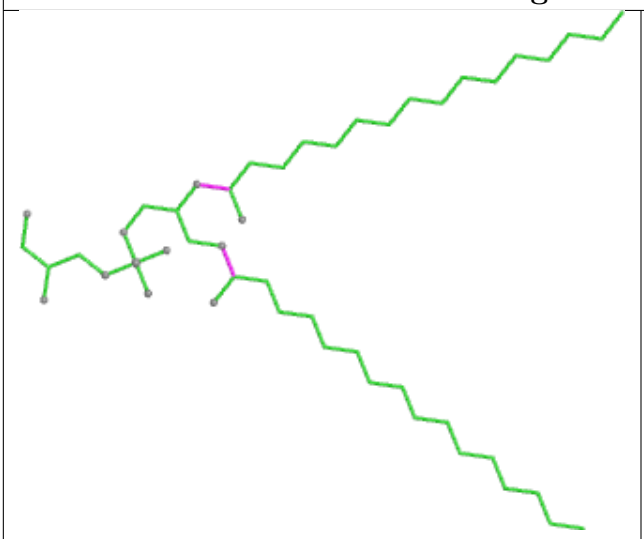


Torsions

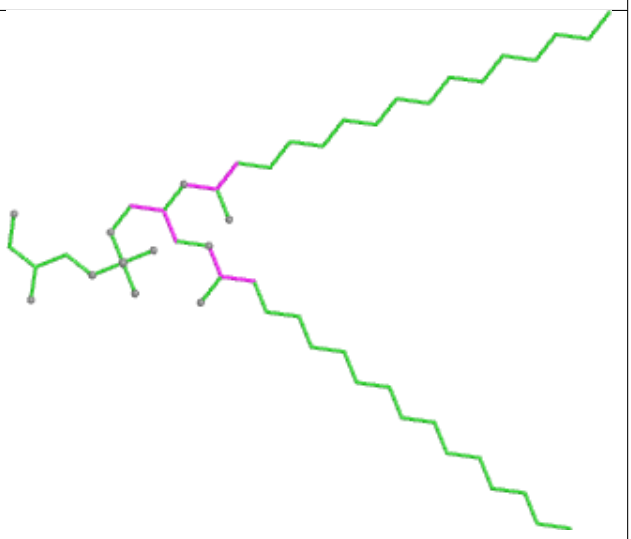


Rings

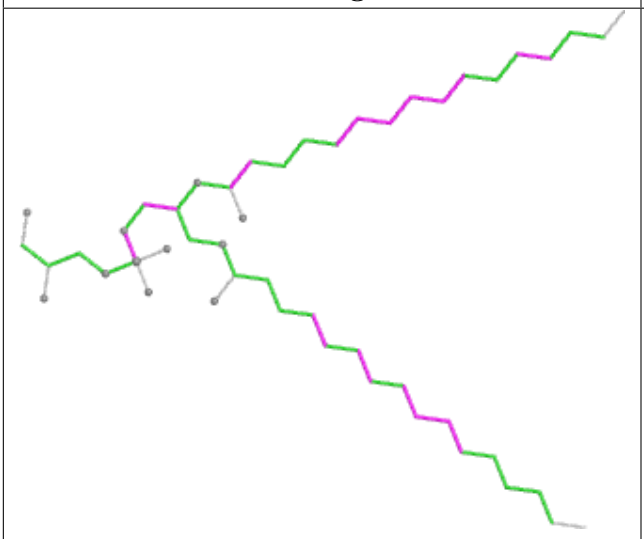
Ligand LHG l 102



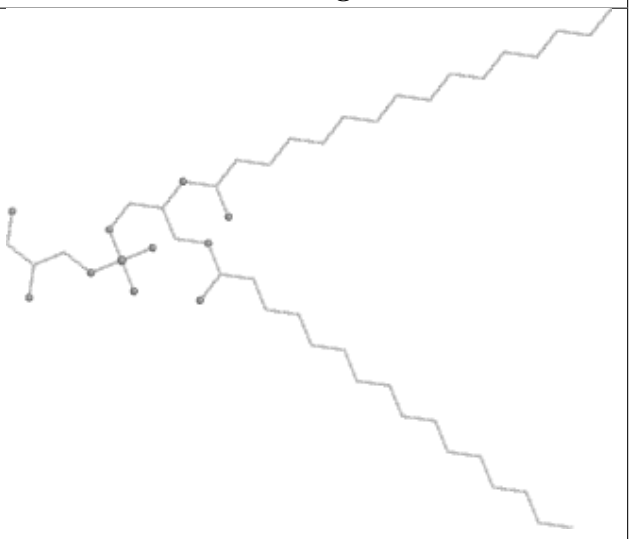
Bond lengths



Bond angles

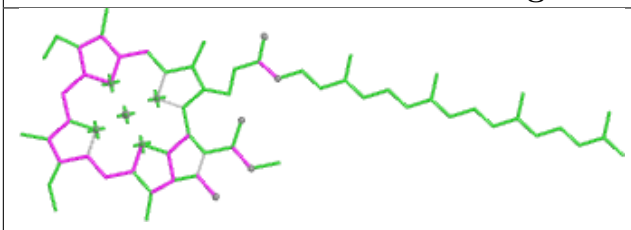


Torsions

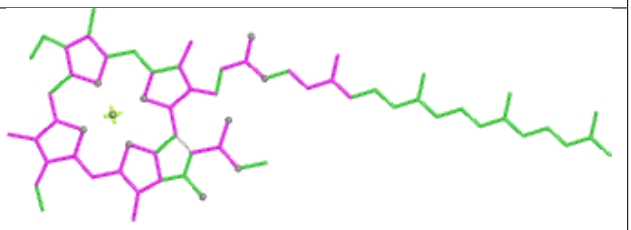


Rings

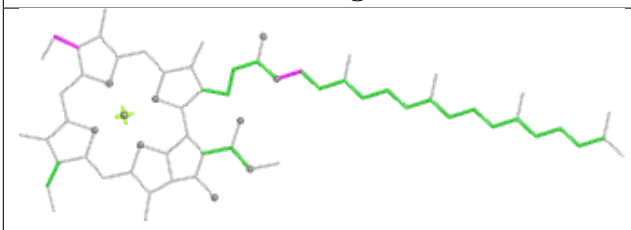
Ligand CLA d 402



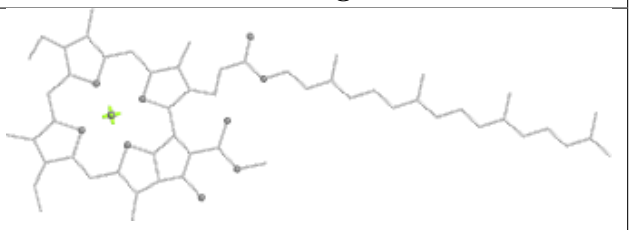
Bond lengths



Bond angles

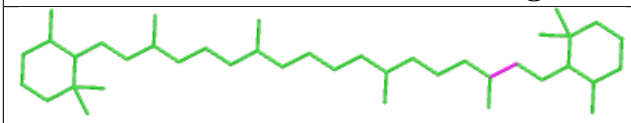


Torsions

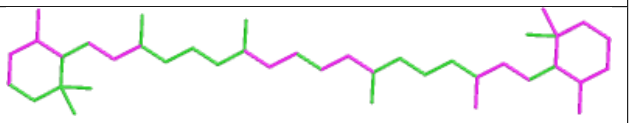


Rings

Ligand BCR d 405



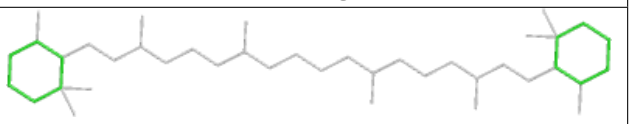
Bond lengths



Bond angles

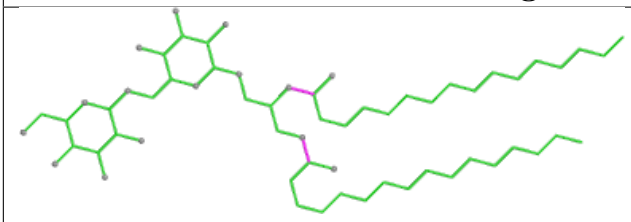


Torsions

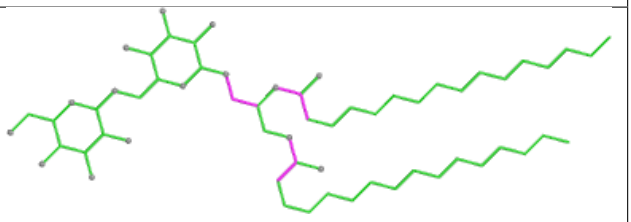


Rings

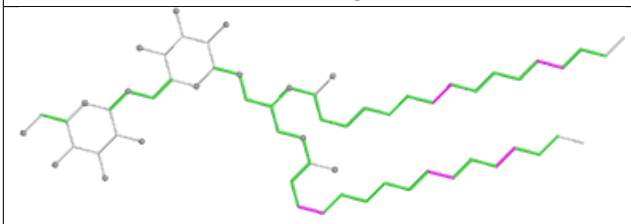
Ligand DGD C 519



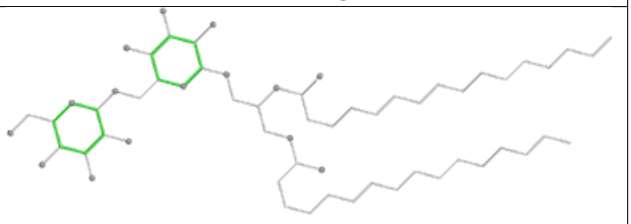
Bond lengths



Bond angles

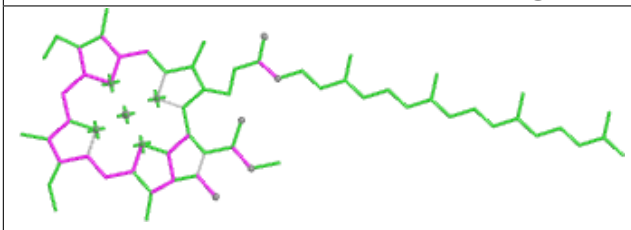


Torsions

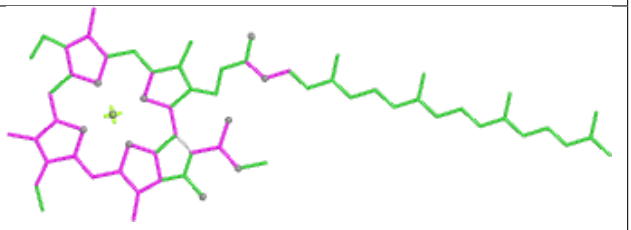


Rings

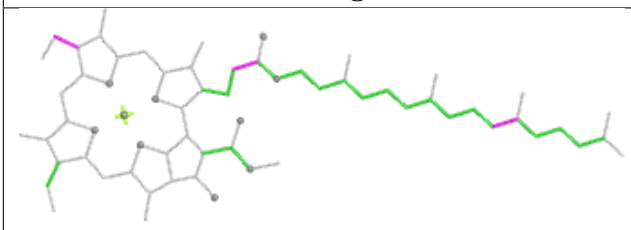
Ligand CLA c 507



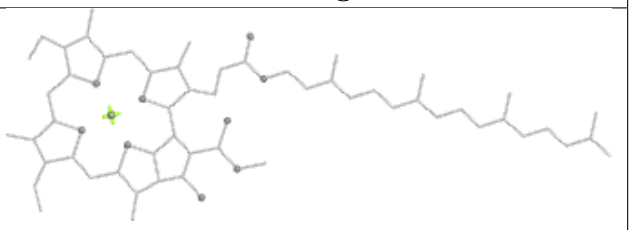
Bond lengths



Bond angles



Torsions

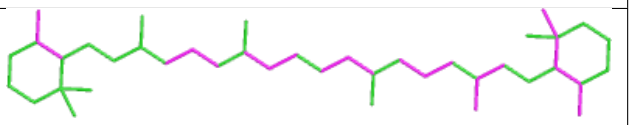


Rings

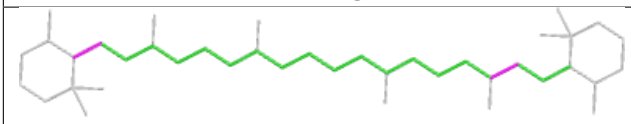
Ligand BCR Y 101



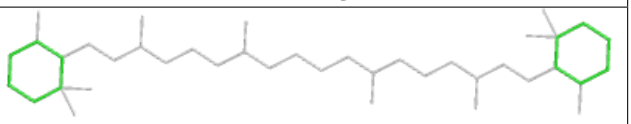
Bond lengths



Bond angles

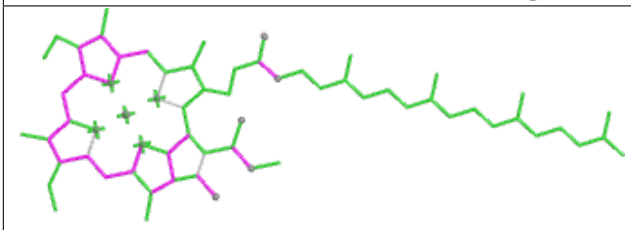


Torsions

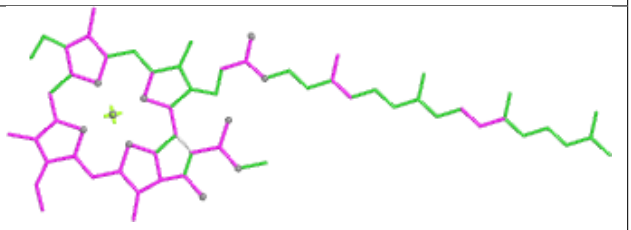


Rings

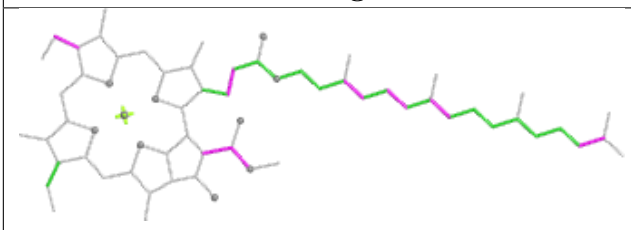
Ligand CLA C 508



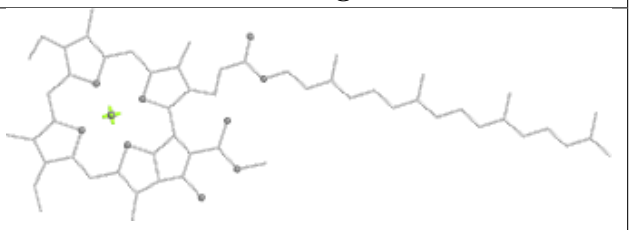
Bond lengths



Bond angles

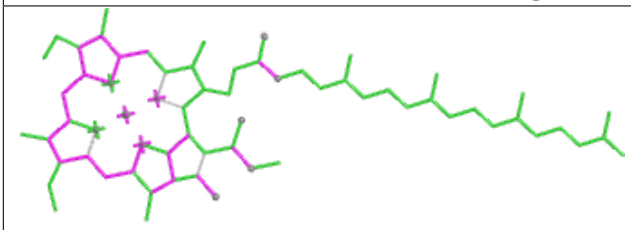


Torsions

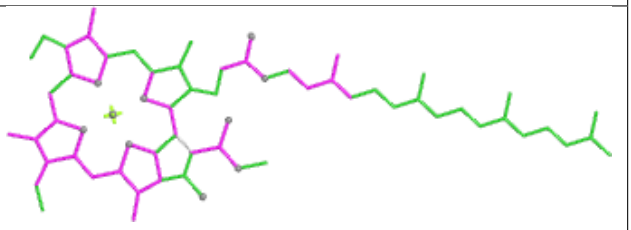


Rings

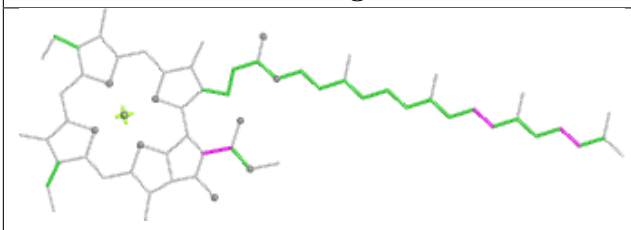
Ligand CLA b 609



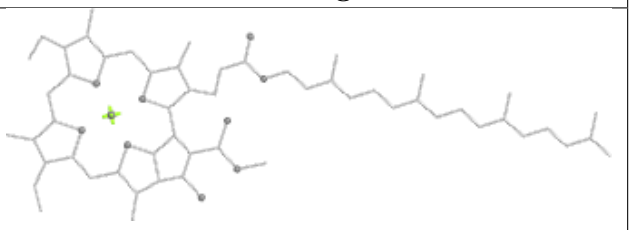
Bond lengths



Bond angles

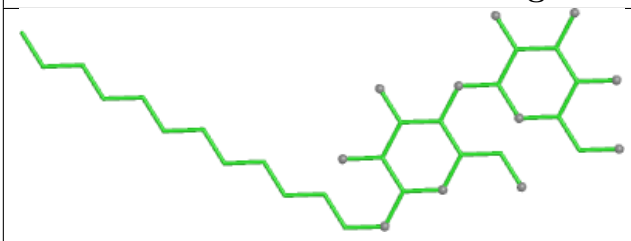


Torsions

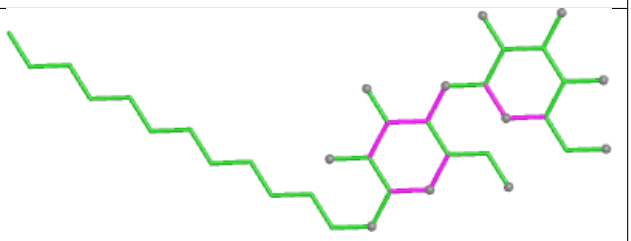


Rings

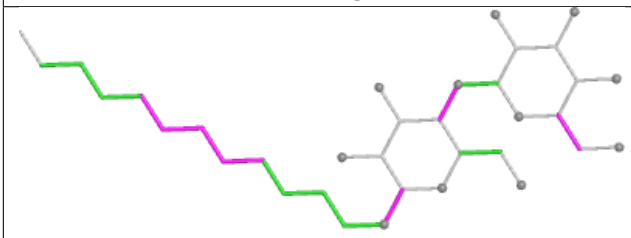
Ligand LMT I 102



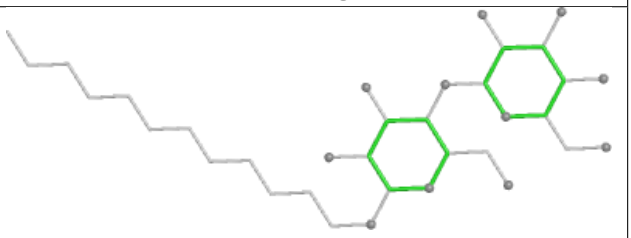
Bond lengths



Bond angles



Torsions

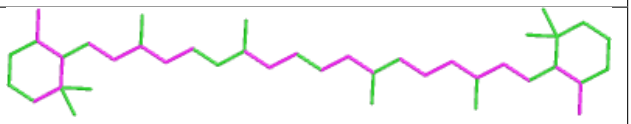


Rings

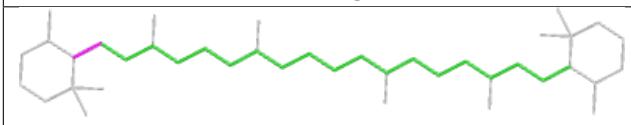
Ligand BCR c 526



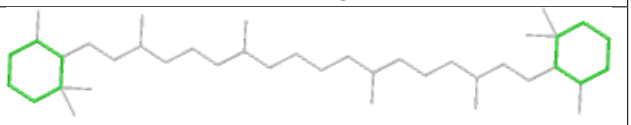
Bond lengths



Bond angles

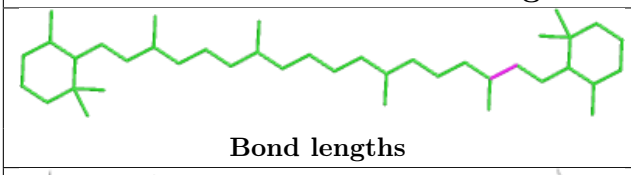


Torsions

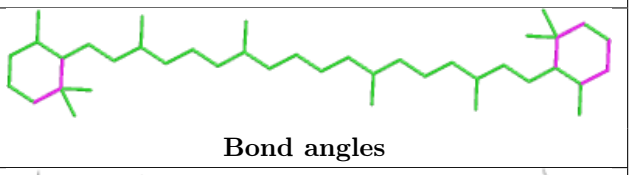


Rings

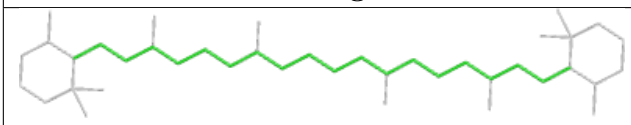
Ligand BCR B 619



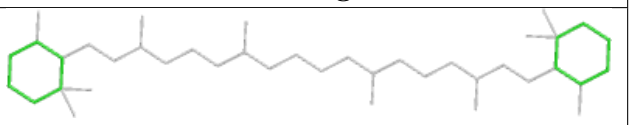
Bond lengths



Bond angles

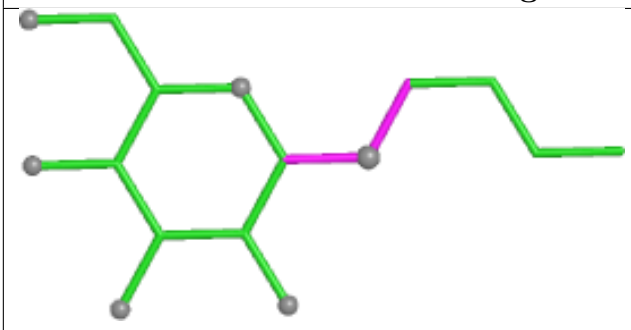


Torsions

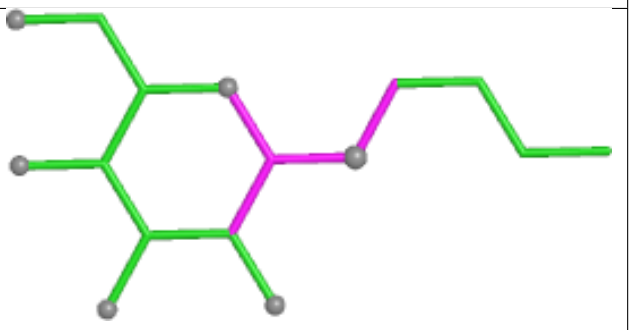


Rings

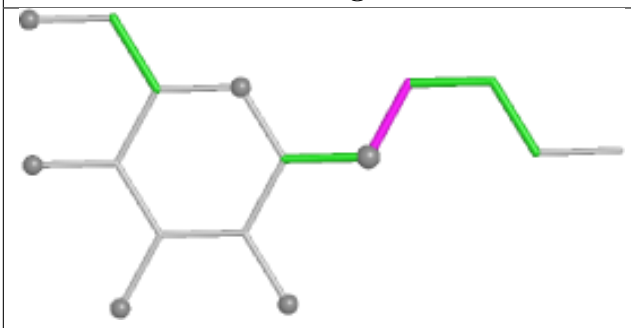
Ligand HTG D 411



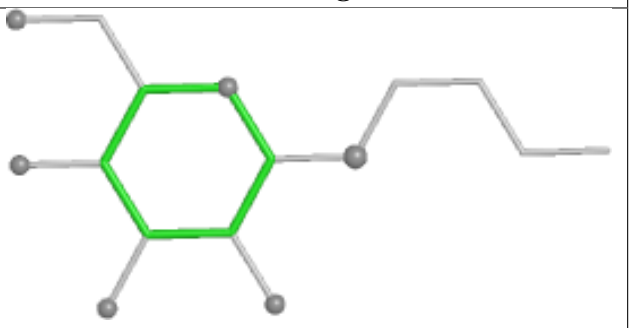
Bond lengths



Bond angles

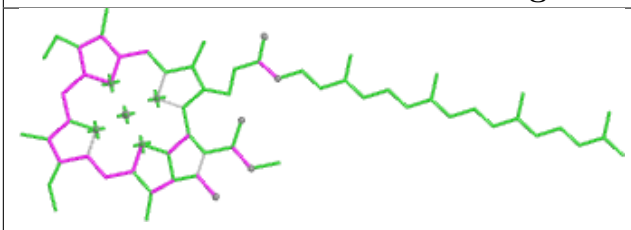


Torsions

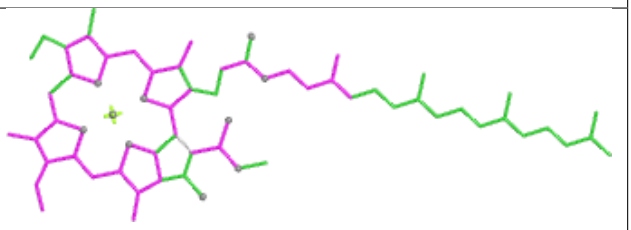


Rings

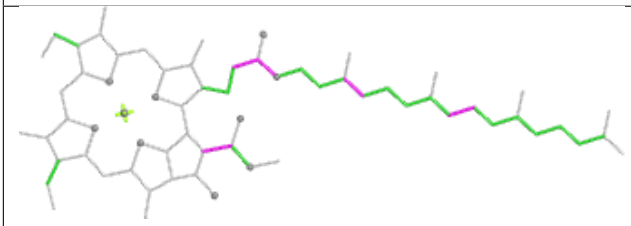
Ligand CLA c 512



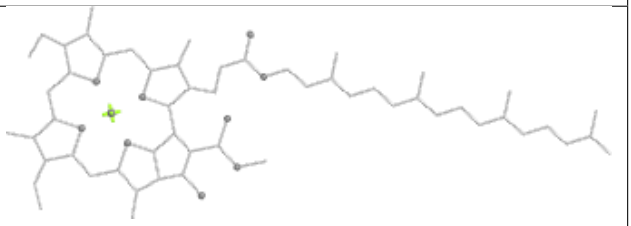
Bond lengths



Bond angles

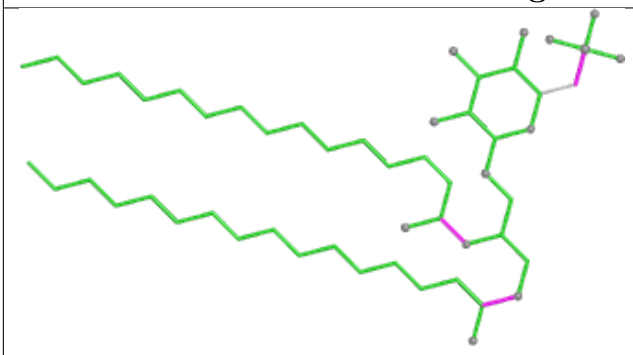


Torsions

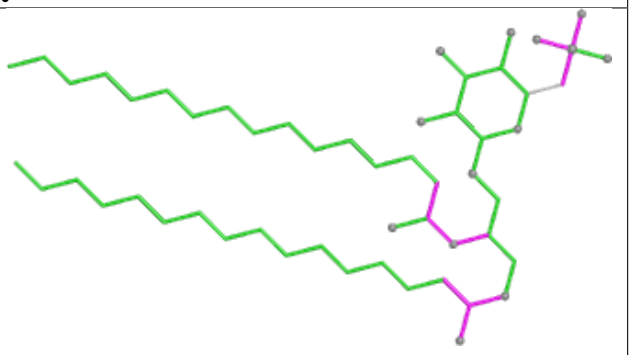


Rings

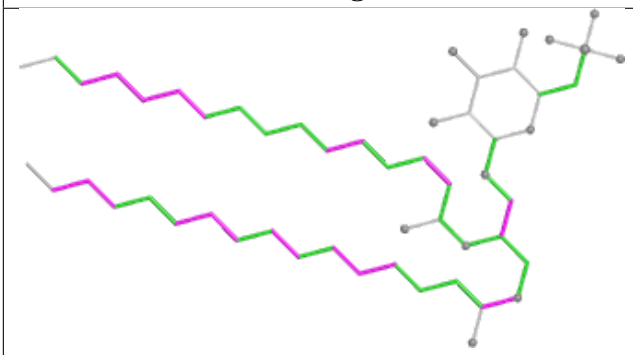
Ligand SQD a 402



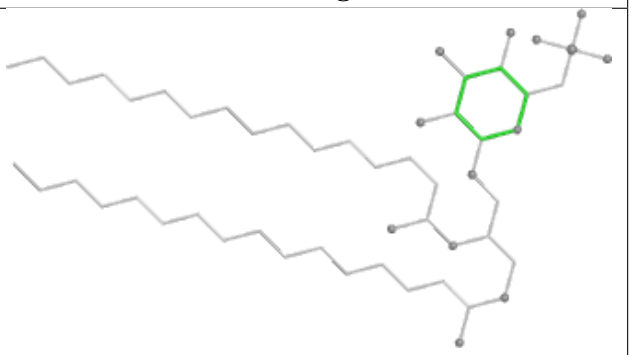
Bond lengths



Bond angles

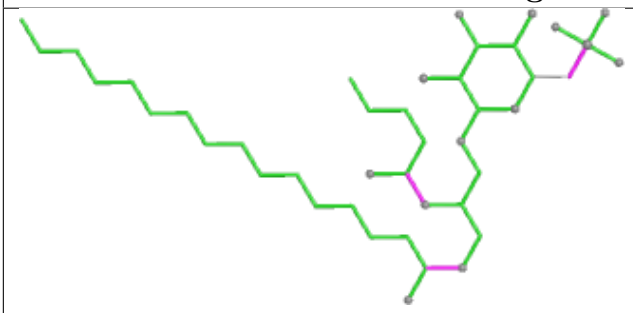


Torsions

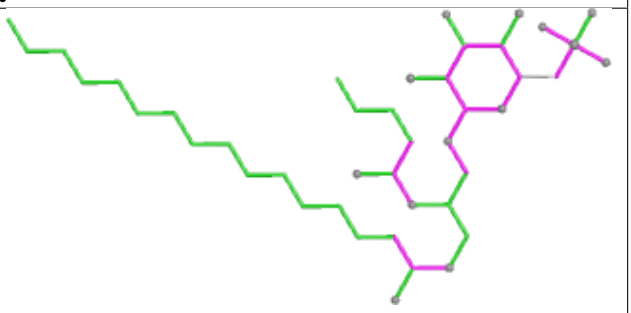


Rings

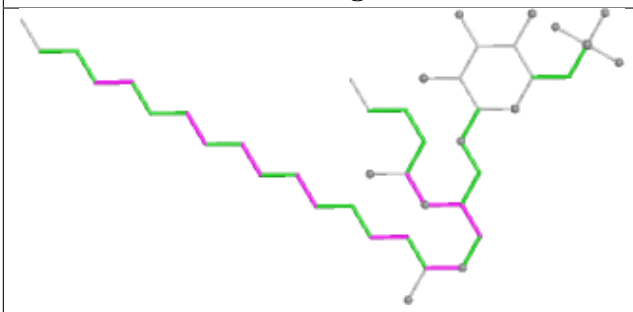
Ligand SQD F 101



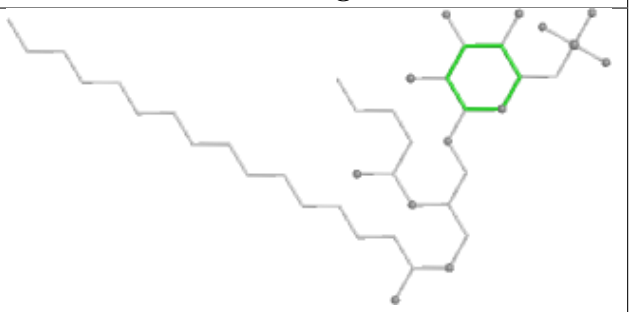
Bond lengths



Bond angles

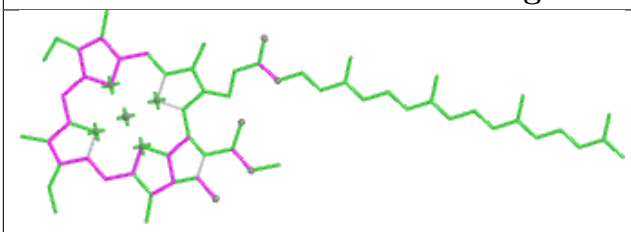


Torsions

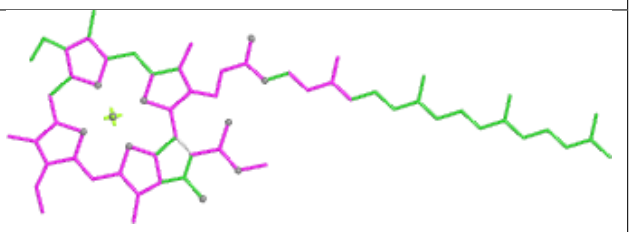


Rings

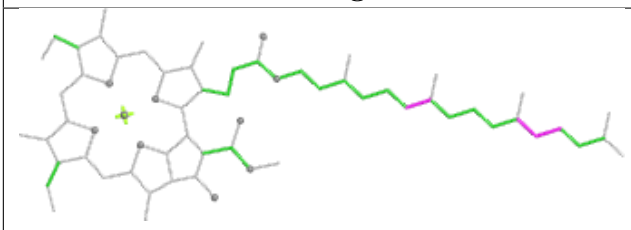
Ligand CLA A 406



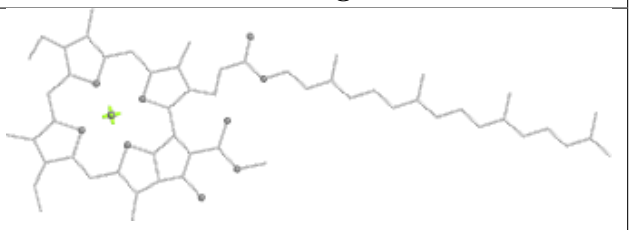
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.11	5 (1%)	72	78	15, 23, 42, 79	3 (0%)
1	a	334/344 (97%)	-0.06	8 (2%)	59	66	17, 24, 48, 82	4 (1%)
2	B	504/505 (99%)	0.07	16 (3%)	50	56	13, 27, 51, 90	10 (1%)
2	b	504/505 (99%)	0.17	24 (4%)	35	41	17, 29, 60, 108	11 (2%)
3	C	451/455 (99%)	0.20	8 (1%)	67	75	19, 32, 49, 89	5 (1%)
3	c	455/455 (100%)	0.30	8 (1%)	67	75	18, 35, 50, 87	6 (1%)
4	D	342/342 (100%)	-0.15	3 (0%)	81	85	15, 24, 40, 114	0
4	d	341/342 (99%)	-0.12	4 (1%)	76	82	14, 26, 42, 90	1 (0%)
5	E	81/84 (96%)	0.92	9 (11%)	10	12	23, 40, 68, 97	2 (2%)
5	e	81/84 (96%)	0.97	9 (11%)	10	12	32, 45, 77, 97	0
6	F	34/44 (77%)	0.51	3 (8%)	15	18	26, 35, 56, 64	0
6	f	32/44 (72%)	0.69	3 (9%)	14	16	31, 37, 84, 99	0
7	H	65/65 (100%)	0.47	3 (4%)	37	43	20, 34, 52, 97	1 (1%)
7	h	65/65 (100%)	0.65	6 (9%)	14	16	28, 37, 58, 113	0
8	I	37/38 (97%)	0.85	6 (16%)	4	5	30, 34, 91, 101	0
8	i	37/38 (97%)	0.82	4 (10%)	11	12	29, 34, 79, 102	0
9	J	38/39 (97%)	0.78	7 (18%)	3	3	26, 38, 85, 109	0
9	j	38/39 (97%)	0.77	5 (13%)	7	8	30, 41, 84, 85	0
10	K	37/37 (100%)	0.52	3 (8%)	18	21	31, 38, 55, 64	0
10	k	37/37 (100%)	0.81	1 (2%)	56	62	33, 42, 56, 66	0
11	L	37/37 (100%)	0.02	3 (8%)	18	21	12, 20, 66, 91	1 (2%)
11	l	37/37 (100%)	0.06	3 (8%)	18	21	12, 21, 61, 91	1 (2%)
12	M	33/36 (91%)	0.00	2 (6%)	27	31	14, 23, 44, 100	1 (3%)
12	m	33/36 (91%)	0.01	1 (3%)	52	59	19, 23, 44, 100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.34	15 (6%) 26 31	16, 34, 65, 113	4 (1%)
13	o	243/244 (99%)	0.48	19 (7%) 19 22	17, 35, 75, 122	3 (1%)
14	T	29/31 (93%)	0.02	2 (6%) 23 26	17, 22, 48, 85	1 (3%)
14	t	29/31 (93%)	0.09	2 (6%) 23 26	17, 23, 49, 85	1 (3%)
15	U	97/104 (93%)	0.23	2 (2%) 63 70	22, 33, 53, 85	0
15	u	97/104 (93%)	0.13	1 (1%) 79 84	25, 34, 51, 85	0
16	V	137/137 (100%)	0.19	6 (4%) 39 45	17, 33, 54, 70	1 (0%)
16	v	137/137 (100%)	0.32	5 (3%) 46 53	26, 38, 57, 72	0
17	Y	29/30 (96%)	1.92	10 (34%) 1 0	38, 50, 91, 107	0
17	y	29/30 (96%)	1.80	9 (31%) 1 1	40, 54, 91, 107	0
18	X	39/40 (97%)	1.25	9 (23%) 2 2	31, 42, 80, 92	1 (2%)
18	x	39/40 (97%)	1.18	6 (15%) 5 5	35, 45, 93, 96	0
19	Z	62/62 (100%)	1.59	20 (32%) 1 0	40, 52, 87, 98	0
19	z	62/62 (100%)	1.72	21 (33%) 1 0	44, 53, 87, 98	0
20	R	34/34 (100%)	3.68	30 (88%) 0 0	69, 93, 111, 118	0
All	All	5293/5382 (98%)	0.28	301 (5%) 29 34	12, 31, 63, 122	57 (1%)

The worst 5 of 301 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	i	37	LEU	7.1
17	Y	18	VAL	7.0
20	R	18	TRP	6.5
2	b	486	LEU	6.2
7	h	65	LEU	6.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
9	FME	j	1	10/11	0.76	0.23	53,71,94,136	0
14	FME	t	1	10/11	0.92	0.10	13,22,33,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	m	1	10/11	0.93	0.12	25,31,61,62	0
12	FME	M	1	10/11	0.94	0.11	23,34,56,61	0
14	FME	T	1	10/11	0.95	0.08	21,27,45,56	0
8	FME	i	1	10/11	0.96	0.09	23,34,37,42	0
8	FME	I	1	10/11	0.97	0.07	22,34,37,40	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	DGD	D	407	62/66	0.65	0.23	44,89,114,119	0
28	GOL	B	635	6/6	0.66	0.28	82,91,97,98	0
36	DGD	d	407	62/66	0.68	0.21	41,88,117,122	0
29	UNL	k	101	32/-	0.69	0.22	42,75,105,108	0
30	LMT	E	102	35/35	0.71	0.18	43,81,105,107	0
30	LMT	f	102	35/35	0.71	0.18	56,83,109,113	0
30	LMT	b	626	25/35	0.74	0.19	33,67,110,115	0
29	UNL	j	103	10/-	0.74	0.23	44,61,67,73	0
28	GOL	O	302	6/6	0.74	0.16	52,61,64,70	0
29	UNL	i	101	40/-	0.74	0.23	36,64,96,108	0
28	GOL	v	203	6/6	0.75	0.20	50,69,71,78	0
29	UNL	I	101	40/-	0.75	0.23	27,63,114,119	0
35	HTG	d	411	16/19	0.75	0.18	54,73,84,87	0
29	UNL	k	102	10/-	0.75	0.37	54,83,94,102	0
28	GOL	T	103	6/6	0.75	0.22	63,76,80,81	0
37	LHG	e	101	42/49	0.75	0.18	49,87,117,128	0
35	HTG	B	624	19/19	0.76	0.15	38,95,102,121	0
35	HTG	B	631	19/19	0.76	0.16	25,84,104,120	0
35	HTG	V	204	19/19	0.76	0.19	40,65,99,175	0
35	HTG	b	628	19/19	0.76	0.17	48,90,106,124	0
35	HTG	c	523	19/19	0.76	0.16	60,84,93,98	0
28	GOL	t	102	6/6	0.76	0.22	29,60,65,69	0
30	LMT	M	101	35/35	0.76	0.16	35,60,79,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	UNL	a	414	30/-	0.76	0.18	45,65,86,89	0
28	GOL	v	204	6/6	0.76	0.19	47,64,70,92	0
30	LMT	a	417	35/35	0.77	0.17	52,76,90,94	0
27	SQD	a	402	54/54	0.77	0.16	34,61,79,100	0
35	HTG	D	411	16/19	0.77	0.17	38,100,111,113	0
29	UNL	b	634	33/-	0.77	0.22	42,71,112,116	0
34	LMG	Z	101	37/55	0.77	0.21	32,81,104,105	0
29	UNL	A	415	28/-	0.78	0.20	55,65,84,90	0
29	UNL	B	632	33/-	0.78	0.20	32,70,105,113	0
30	LMT	I	102	35/35	0.78	0.18	59,81,95,100	0
29	UNL	C	526	34/-	0.78	0.19	46,71,82,84	0
37	LHG	E	101	42/49	0.78	0.19	38,73,93,103	0
34	LMG	z	101	39/55	0.78	0.18	47,74,94,101	0
30	LMT	m	103	35/35	0.79	0.16	30,60,86,90	0
32	PL9	a	416	55/55	0.79	0.23	50,76,94,95	0
28	GOL	a	413	6/6	0.79	0.18	38,67,69,71	0
28	GOL	c	525	6/6	0.79	0.18	43,46,61,62	0
27	SQD	l	101	54/54	0.79	0.18	31,67,98,101	0
28	GOL	b	632	6/6	0.80	0.20	40,46,68,69	0
30	LMT	B	634	25/35	0.80	0.20	32,63,105,111	0
30	LMT	D	402	35/35	0.80	0.15	32,75,96,97	0
29	UNL	M	103	10/-	0.81	0.17	34,42,59,64	0
34	LMG	c	521	51/55	0.81	0.17	35,79,91,98	0
29	UNL	d	413	36/-	0.81	0.17	35,58,94,99	0
29	UNL	J	103	10/-	0.81	0.21	38,53,73,75	0
29	UNL	m	101	10/-	0.81	0.18	37,51,60,62	0
29	UNL	x	101	10/-	0.81	0.19	35,44,57,58	0
34	LMG	C	521	51/55	0.81	0.17	31,74,90,96	0
30	LMT	b	602	25/35	0.82	0.18	22,63,102,106	0
35	HTG	c	522	19/19	0.82	0.15	63,69,80,85	0
32	PL9	A	419	55/55	0.82	0.21	38,66,87,92	0
27	SQD	f	101	43/54	0.82	0.19	55,82,109,117	0
33	CA	b	605	1/1	0.82	0.14	95,95,95,95	0
35	HTG	C	523	19/19	0.82	0.16	46,75,97,109	0
29	UNL	D	413	40/-	0.82	0.20	33,55,105,108	0
30	LMT	m	102	35/35	0.82	0.14	16,51,73,79	0
28	GOL	C	524	6/6	0.83	0.16	39,45,57,60	0
27	SQD	F	101	43/54	0.83	0.18	39,70,96,105	0
27	SQD	A	416	54/54	0.83	0.15	28,52,75,76	0
35	HTG	b	604	19/19	0.83	0.16	50,80,106,112	0
28	GOL	A	414	6/6	0.83	0.19	40,60,69,70	0
27	SQD	b	601	54/54	0.83	0.16	36,58,91,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	LMT	a	401	35/35	0.84	0.15	28,61,79,86	0
28	GOL	V	205	6/6	0.84	0.15	37,54,59,72	0
28	GOL	A	413	6/6	0.84	0.14	35,38,41,42	0
30	LMT	A	417	33/35	0.84	0.16	27,65,78,85	0
28	GOL	B	627	6/6	0.84	0.16	31,35,43,44	0
34	LMG	C	520	51/55	0.84	0.18	26,61,82,87	0
35	HTG	b	627	19/19	0.86	0.17	27,44,80,80	0
33	CA	B	601	1/1	0.86	0.09	79,79,79,79	0
35	HTG	B	623	19/19	0.86	0.17	29,42,64,71	0
29	UNL	d	412	17/-	0.87	0.17	31,48,79,85	0
29	UNL	X	101	10/-	0.87	0.12	29,37,41,42	0
34	LMG	c	501	51/55	0.87	0.15	39,60,77,85	0
30	LMT	M	102	35/35	0.87	0.12	22,50,66,76	0
28	GOL	B	628	6/6	0.87	0.17	35,46,67,70	0
34	LMG	C	501	51/55	0.87	0.14	37,54,74,82	0
28	GOL	F	103	6/6	0.87	0.15	52,59,65,68	0
28	GOL	b	631	6/6	0.88	0.12	39,46,48,60	0
34	LMG	c	520	51/55	0.88	0.16	33,63,86,88	0
35	HTG	C	522	19/19	0.89	0.15	53,65,89,95	0
28	GOL	V	206	6/6	0.89	0.15	21,38,44,48	0
27	SQD	a	411	54/54	0.89	0.15	32,56,75,78	0
28	GOL	T	101	6/6	0.89	0.16	35,60,64,65	0
24	CLA	c	515	65/65	0.89	0.13	37,51,79,88	0
35	HTG	B	630	19/19	0.89	0.13	30,54,78,81	0
28	GOL	B	633	6/6	0.89	0.11	27,36,40,41	0
28	GOL	B	626	6/6	0.90	0.10	32,37,40,59	0
26	BCR	c	526	40/40	0.90	0.12	39,48,59,63	0
24	CLA	b	606	65/65	0.90	0.12	30,46,82,98	0
34	LMG	B	621	51/55	0.90	0.12	20,35,52,64	0
28	GOL	V	208	6/6	0.90	0.10	41,56,62,63	0
28	GOL	c	527	6/6	0.91	0.12	36,57,61,63	0
34	LMG	b	625	51/55	0.91	0.12	24,39,59,71	0
26	BCR	C	515	40/40	0.91	0.10	31,42,49,53	0
26	BCR	H	101	40/40	0.91	0.10	21,32,48,52	0
26	BCR	Y	101	40/40	0.91	0.10	28,35,49,50	0
24	CLA	C	507	65/65	0.91	0.12	28,42,81,88	0
26	BCR	h	101	40/40	0.91	0.10	27,35,46,49	0
28	GOL	b	630	6/6	0.91	0.12	37,48,50,52	0
27	SQD	A	411	54/54	0.91	0.14	26,51,71,78	0
24	CLA	c	514	65/65	0.91	0.11	34,43,67,76	0
28	GOL	b	633	6/6	0.91	0.13	32,54,63,71	0
24	CLA	C	514	65/65	0.91	0.11	32,42,69,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	D	405	40/40	0.92	0.10	22,31,61,77	0
28	GOL	B	629	6/6	0.92	0.14	24,40,61,78	0
26	BCR	k	103	40/40	0.92	0.10	32,40,48,52	0
24	CLA	B	602	65/65	0.92	0.11	24,39,82,104	0
28	GOL	b	629	6/6	0.92	0.10	32,40,48,57	0
35	HTG	b	603	19/19	0.92	0.11	34,44,64,67	0
26	BCR	T	102	40/40	0.92	0.08	14,28,36,42	0
29	UNL	D	412	17/-	0.92	0.12	24,45,74,78	0
24	CLA	b	621	65/65	0.92	0.12	21,35,82,84	0
28	GOL	B	625	6/6	0.92	0.12	28,43,48,55	0
24	CLA	c	508	65/65	0.92	0.12	30,41,65,70	0
34	LMG	j	101	51/55	0.92	0.12	26,39,70,82	0
26	BCR	d	405	40/40	0.92	0.11	29,35,63,64	0
36	DGD	H	102	62/66	0.92	0.10	20,29,42,58	0
28	GOL	V	201	6/6	0.92	0.10	27,29,40,41	0
36	DGD	h	102	62/66	0.92	0.10	23,35,52,69	0
37	LHG	D	408	49/49	0.92	0.10	16,31,43,54	0
32	PL9	d	406	55/55	0.92	0.09	16,23,35,47	0
37	LHG	d	408	49/49	0.92	0.11	26,34,46,50	0
28	GOL	f	104	6/6	0.92	0.10	45,51,59,61	0
24	CLA	b	620	65/65	0.93	0.09	22,31,51,74	0
28	GOL	V	207	6/6	0.93	0.14	35,38,41,44	0
24	CLA	C	508	65/65	0.93	0.09	25,35,48,57	0
28	GOL	a	412	6/6	0.93	0.11	22,37,41,45	0
28	GOL	A	412	6/6	0.93	0.08	29,31,34,37	0
24	CLA	c	505	65/65	0.93	0.09	29,35,46,60	0
26	BCR	a	410	40/40	0.93	0.07	16,24,31,33	0
32	PL9	D	406	55/55	0.93	0.08	14,23,36,43	0
26	BCR	b	624	40/40	0.93	0.09	20,32,46,52	0
26	BCR	c	516	40/40	0.93	0.09	29,36,47,57	0
24	CLA	c	506	65/65	0.93	0.09	26,33,51,61	0
24	CLA	c	507	65/65	0.93	0.09	22,31,52,62	0
24	CLA	C	509	65/65	0.93	0.10	21,29,78,80	0
24	CLA	C	512	65/65	0.93	0.09	26,32,41,48	0
26	BCR	t	101	40/40	0.93	0.09	15,24,45,49	0
36	DGD	C	518	62/66	0.93	0.11	22,32,76,92	0
28	GOL	v	201	6/6	0.93	0.10	31,40,49,50	0
26	BCR	y	101	40/40	0.93	0.09	31,40,53,60	0
36	DGD	c	518	62/66	0.93	0.11	24,35,79,94	0
24	CLA	C	513	65/65	0.93	0.10	29,42,67,74	0
25	PHO	d	403	64/64	0.93	0.07	20,25,34,38	0
26	BCR	B	620	40/40	0.93	0.08	22,29,42,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	C	502	65/65	0.93	0.09	25,32,47,58	0
26	BCR	C	516	40/40	0.93	0.09	25,34,43,46	0
37	LHG	d	410	49/49	0.93	0.14	23,35,85,104	0
22	CL	u	201	1/1	0.93	0.07	63,63,63,63	0
37	LHG	l	102	49/49	0.93	0.10	19,30,48,57	0
26	BCR	B	619	40/40	0.94	0.08	17,25,44,46	0
24	CLA	b	612	65/65	0.94	0.07	14,23,30,36	0
24	CLA	b	613	65/65	0.94	0.07	22,29,38,42	0
24	CLA	b	614	65/65	0.94	0.08	24,31,41,50	0
24	CLA	b	619	65/65	0.94	0.10	15,25,72,77	0
24	CLA	B	604	65/65	0.94	0.08	18,25,32,40	0
26	BCR	K	101	40/40	0.94	0.09	27,33,42,47	0
24	CLA	B	607	65/65	0.94	0.09	18,26,51,75	0
24	CLA	c	503	65/65	0.94	0.09	29,34,45,54	0
24	CLA	B	612	65/65	0.94	0.08	15,21,37,41	0
26	BCR	b	622	40/40	0.94	0.07	16,26,33,36	0
33	CA	f	103	1/1	0.94	0.07	72,72,72,72	0
24	CLA	B	615	65/65	0.94	0.10	15,24,67,78	0
23	BCT	a	418	4/4	0.94	0.10	30,33,42,44	0
36	DGD	C	517	62/66	0.94	0.10	22,33,75,83	0
24	CLA	C	504	65/65	0.94	0.08	24,33,42,48	0
24	CLA	c	509	65/65	0.94	0.09	27,34,49,58	0
34	LMG	J	101	51/55	0.94	0.12	20,37,78,86	0
36	DGD	c	517	62/66	0.94	0.10	23,32,68,76	0
24	CLA	c	512	65/65	0.94	0.08	26,32,44,59	0
36	DGD	c	519	62/66	0.94	0.09	26,34,65,72	0
24	CLA	c	513	65/65	0.94	0.09	30,39,50,54	0
28	GOL	v	205	6/6	0.94	0.11	25,39,52,58	0
24	CLA	C	505	65/65	0.94	0.09	22,29,59,77	0
37	LHG	D	410	49/49	0.94	0.14	20,33,91,95	0
24	CLA	b	607	65/65	0.94	0.08	23,30,38,41	0
24	CLA	b	611	65/65	0.94	0.09	19,31,58,74	0
26	BCR	A	410	40/40	0.94	0.08	16,26,33,35	0
35	HTG	B	622	19/19	0.94	0.10	26,30,44,56	0
26	BCR	B	618	40/40	0.94	0.07	15,23,33,41	0
24	CLA	b	616	65/65	0.95	0.07	18,26,38,52	0
24	CLA	b	617	65/65	0.95	0.07	18,26,36,50	0
24	CLA	A	405	65/65	0.95	0.07	15,18,26,50	0
24	CLA	B	608	65/65	0.95	0.07	13,20,31,35	0
24	CLA	B	609	65/65	0.95	0.06	17,22,32,36	0
24	CLA	B	610	65/65	0.95	0.07	19,26,36,40	0
35	HTG	O	303	19/19	0.95	0.09	24,32,47,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	c	504	65/65	0.95	0.09	26,32,45,55	0
24	CLA	C	510	65/65	0.95	0.09	25,32,51,57	0
28	GOL	C	525	6/6	0.95	0.08	20,24,26,27	0
26	BCR	b	623	40/40	0.95	0.07	15,27,40,46	0
24	CLA	C	511	65/65	0.95	0.08	23,29,41,62	0
24	CLA	B	611	65/65	0.95	0.07	19,26,36,39	0
23	BCT	A	404	4/4	0.95	0.07	27,30,39,40	0
33	CA	F	102	1/1	0.95	0.07	72,72,72,72	0
24	CLA	B	613	65/65	0.95	0.07	15,23,32,35	0
24	CLA	c	510	65/65	0.95	0.09	24,31,70,87	0
36	DGD	C	519	62/66	0.95	0.09	20,30,58,63	0
24	CLA	c	511	65/65	0.95	0.08	29,36,49,55	0
24	CLA	a	409	65/65	0.95	0.12	20,27,83,88	0
24	CLA	B	603	65/65	0.95	0.07	18,25,32,38	0
24	CLA	B	616	65/65	0.95	0.09	19,28,48,60	0
24	CLA	b	608	65/65	0.95	0.07	22,29,38,42	0
24	CLA	d	402	65/65	0.95	0.07	18,22,38,46	0
24	CLA	d	404	65/65	0.95	0.10	27,34,74,81	0
25	PHO	A	407	64/64	0.95	0.06	15,18,23,28	0
24	CLA	b	610	65/65	0.95	0.07	18,24,37,42	0
24	CLA	B	617	65/65	0.95	0.11	19,28,88,91	0
22	CL	V	202	1/1	0.95	0.07	63,63,63,63	0
37	LHG	d	409	49/49	0.95	0.08	17,26,39,55	0
24	CLA	C	503	65/65	0.95	0.07	22,28,40,51	0
24	CLA	B	606	65/65	0.95	0.07	16,22,34,38	0
24	CLA	b	615	65/65	0.95	0.08	21,28,39,46	0
38	HEM	e	102	43/43	0.95	0.11	38,48,65,84	0
24	CLA	C	506	65/65	0.96	0.08	21,29,45,53	0
25	PHO	A	408	64/64	0.96	0.06	16,22,30,32	0
25	PHO	a	408	64/64	0.96	0.06	16,21,29,37	0
24	CLA	b	618	65/65	0.96	0.07	15,23,48,56	0
24	CLA	b	609	65/65	0.96	0.08	16,25,56,66	0
24	CLA	D	401	65/65	0.96	0.07	13,18,30,32	0
37	LHG	D	409	49/49	0.96	0.08	17,27,48,60	0
24	CLA	D	403	65/65	0.96	0.06	14,19,36,42	0
33	CA	o	301	1/1	0.96	0.05	62,62,62,62	0
37	LHG	L	101	49/49	0.96	0.08	15,29,47,58	0
24	CLA	D	404	65/65	0.96	0.09	21,28,73,84	0
24	CLA	a	407	65/65	0.96	0.09	19,25,72,79	0
24	CLA	B	605	65/65	0.96	0.08	15,22,51,63	0
24	CLA	d	401	65/65	0.96	0.06	16,19,26,42	0
24	CLA	B	614	65/65	0.96	0.07	14,22,45,52	0

Continued on next page...

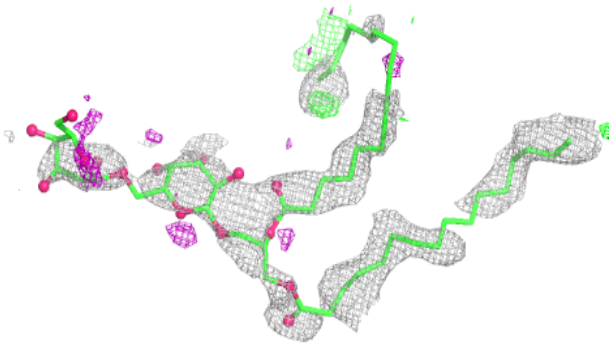
Continued from previous page...

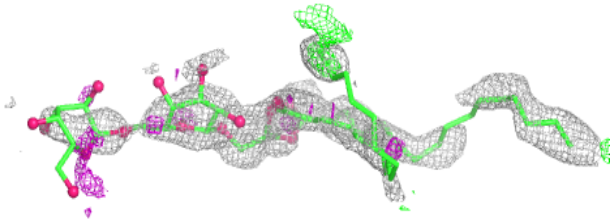
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	A	409	65/65	0.96	0.10	18,27,83,92	0
24	CLA	a	406	65/65	0.97	0.06	17,20,35,51	0
28	GOL	c	524	6/6	0.97	0.06	25,28,30,34	0
38	HEM	E	103	43/43	0.97	0.08	27,38,50,56	0
24	CLA	A	406	65/65	0.97	0.08	15,19,84,88	0
39	MG	j	102	1/1	0.97	0.12	34,34,34,34	0
39	MG	J	102	1/1	0.98	0.07	28,28,28,28	0
33	CA	O	301	1/1	0.98	0.04	56,56,56,56	0
40	HEC	V	203	43/43	0.98	0.06	23,26,31,36	0
40	HEC	v	202	43/43	0.98	0.07	29,33,40,48	0
21	FE2	a	403	1/1	0.99	0.06	30,30,30,30	0
22	CL	A	402	1/1	0.99	0.03	19,19,19,19	0
22	CL	A	403	1/1	0.99	0.05	23,23,23,23	0
31	OEX	A	418	10/10	0.99	0.04	16,23,28,32	0
31	OEX	a	415	10/10	0.99	0.04	20,24,35,37	0
33	CA	c	502	1/1	0.99	0.03	44,44,44,44	0
21	FE2	A	401	1/1	0.99	0.03	27,27,27,27	0
22	CL	a	404	1/1	0.99	0.05	20,20,20,20	0
22	CL	a	405	1/1	0.99	0.04	26,26,26,26	0

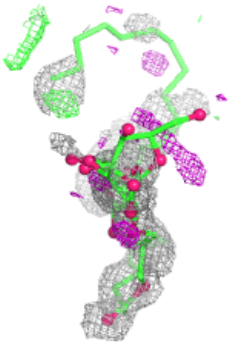
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGD D 407:

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

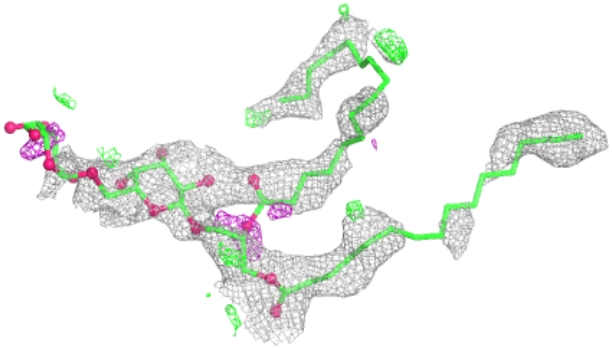


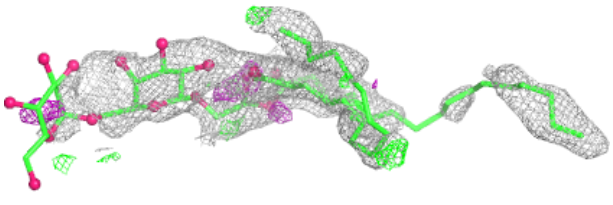


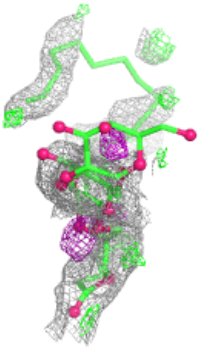


Electron density around DGD d 407:

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

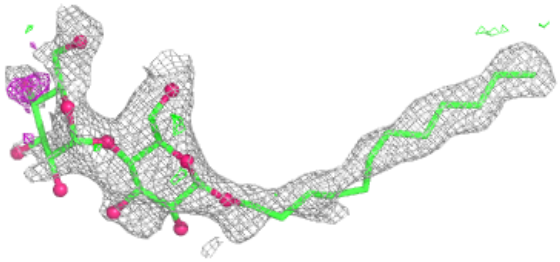


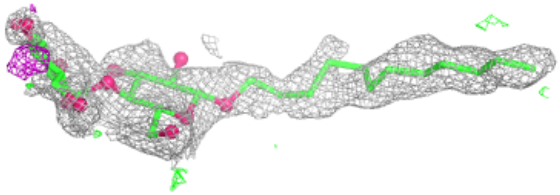


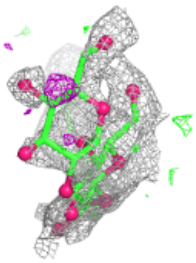


Electron density around LMT E 102:

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

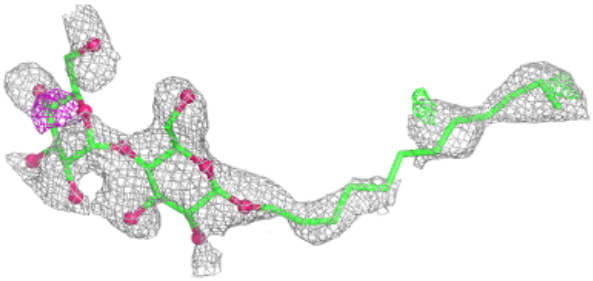


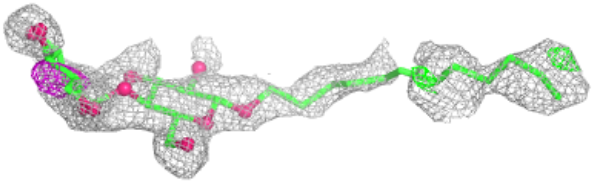


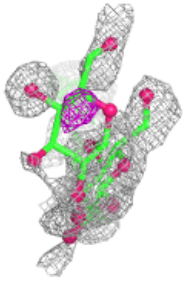


Electron density around LMT f 102:

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

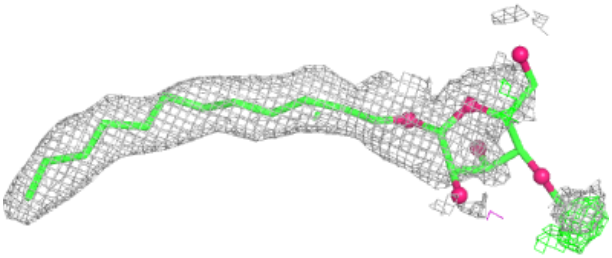


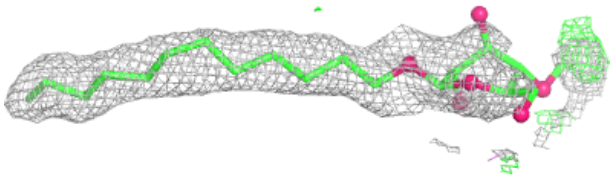


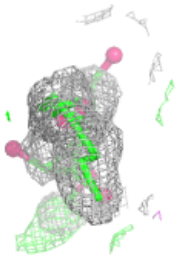


Electron density around LMT b 626:

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



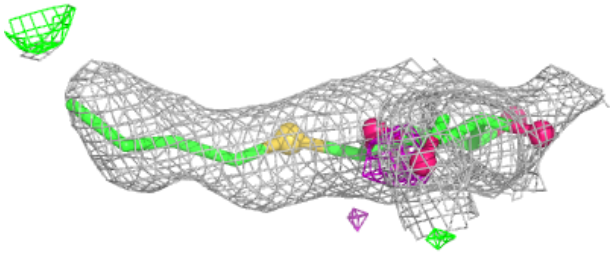


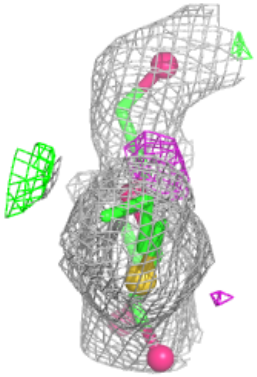


Electron density around HTG d 411:

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

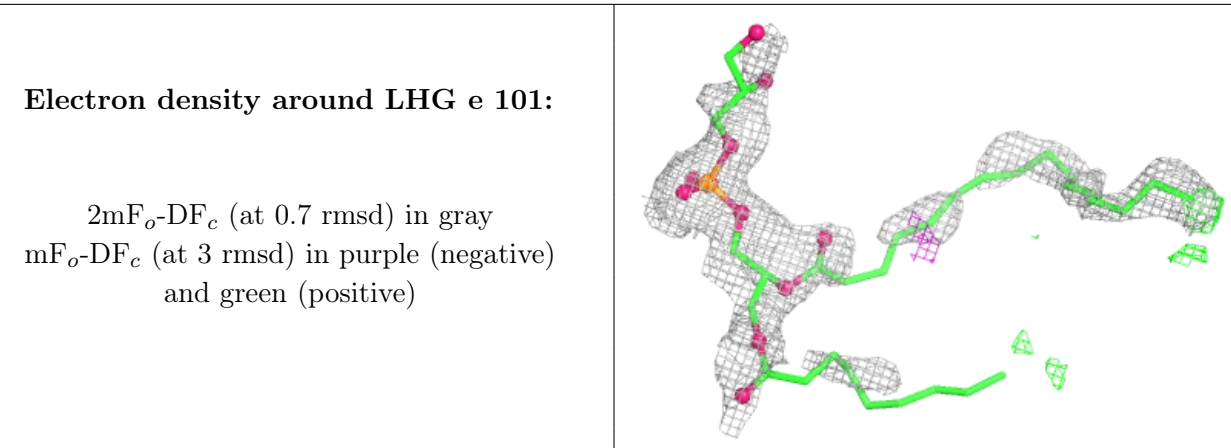






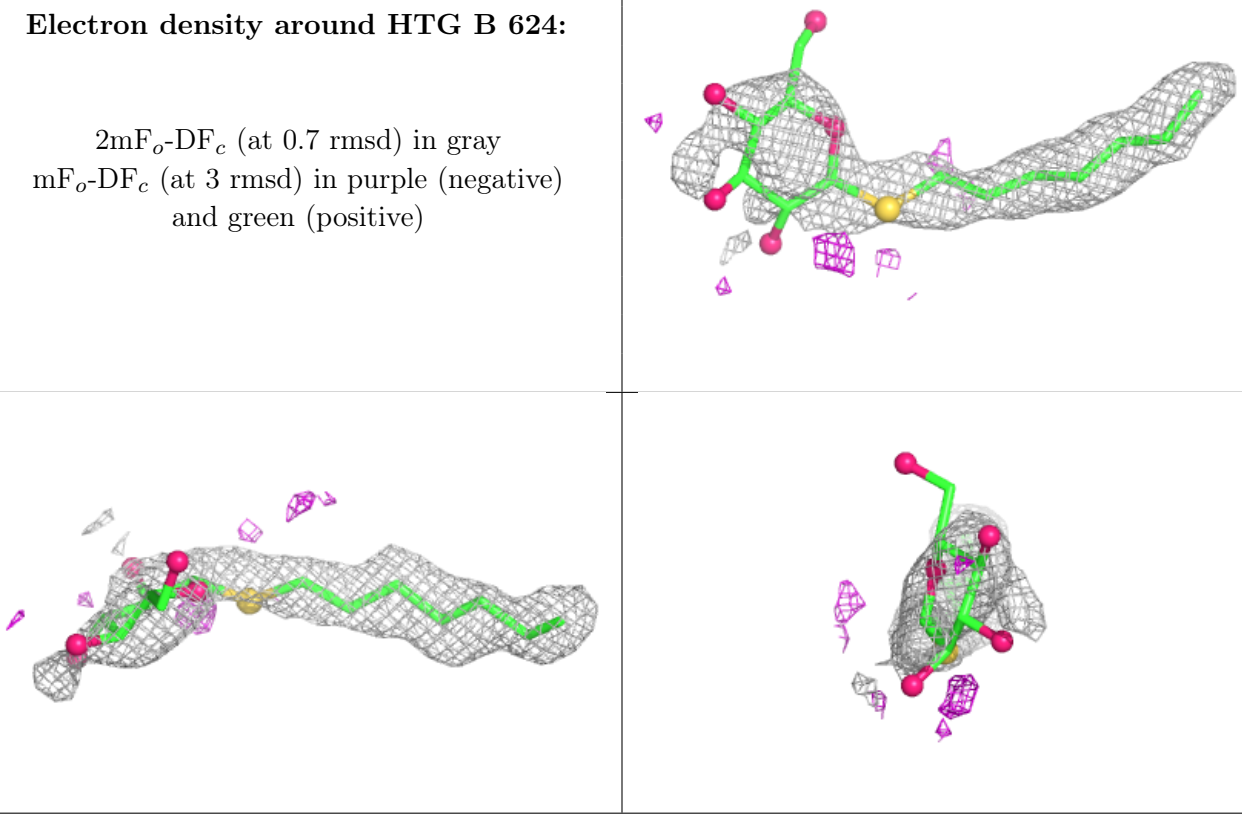
Electron density around LHG e 101:

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



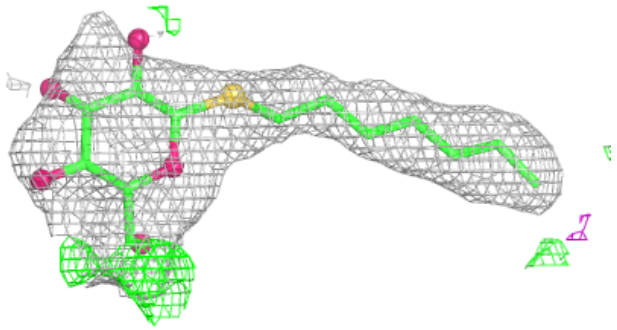
Electron density around HTG B 624:

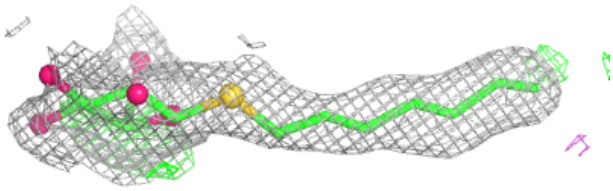
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

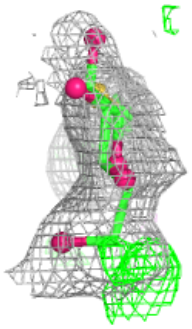


Electron density around HTG B 631:

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

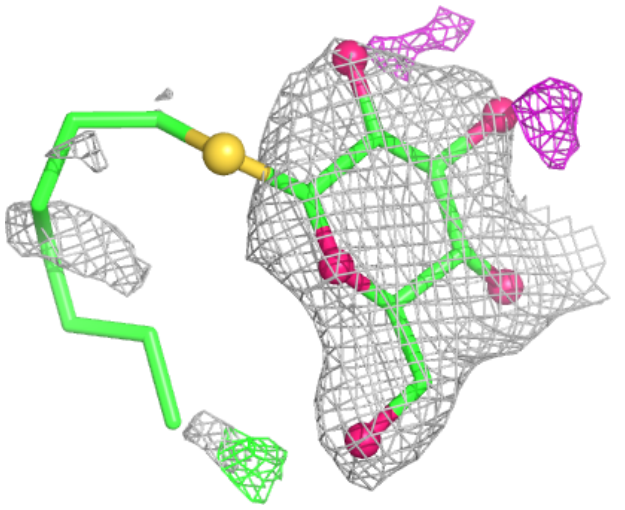


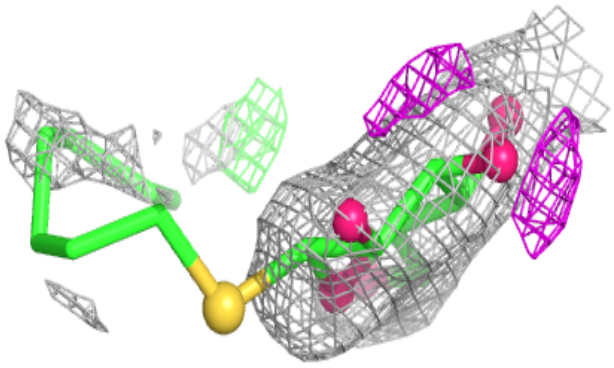


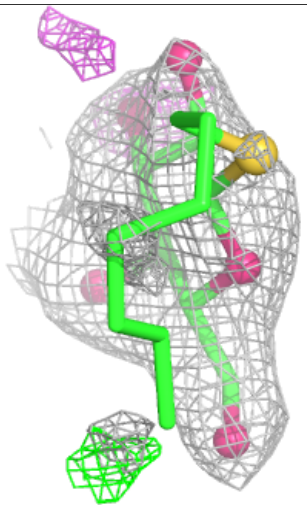


Electron density around HTG V 204:

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



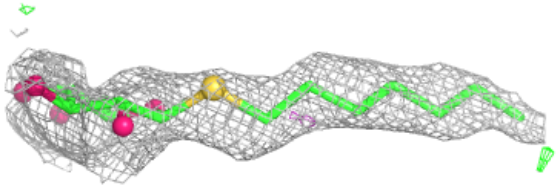


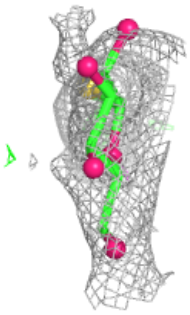


Electron density around HTG b 628:

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

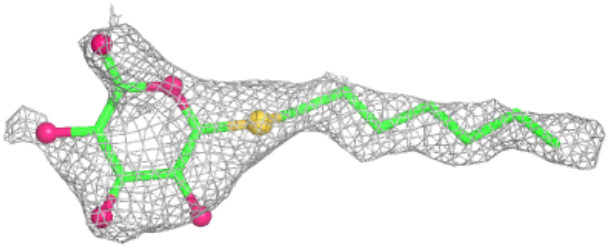


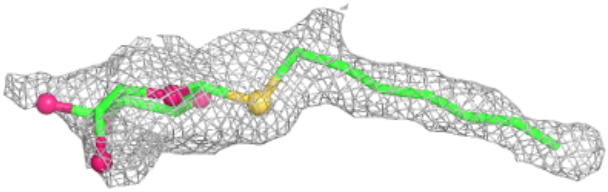


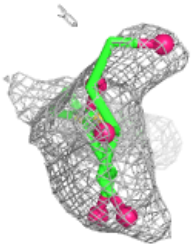


Electron density around HTG c 523:

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

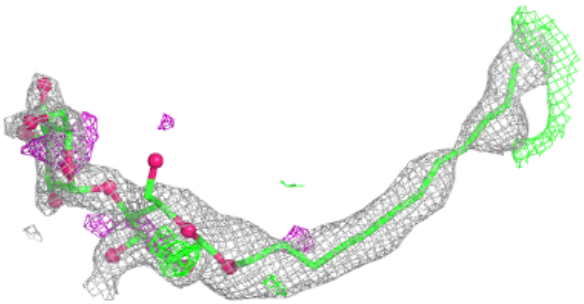


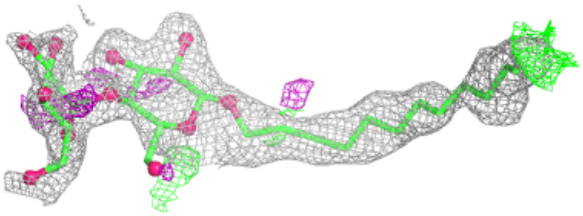


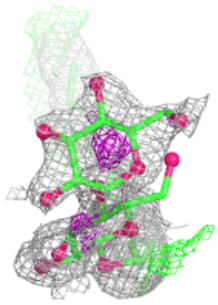


Electron density around LMT M 101:

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

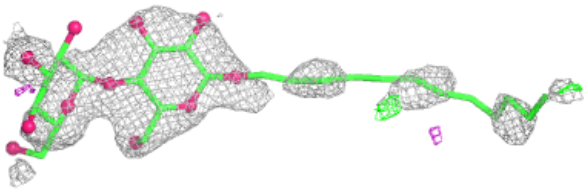


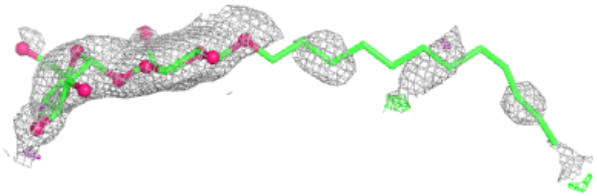


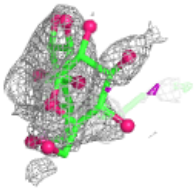


Electron density around LMT a 417:

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

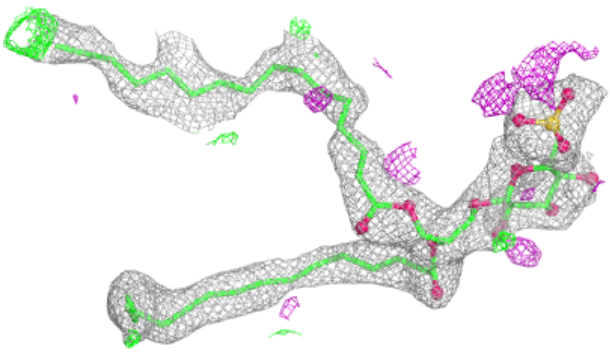


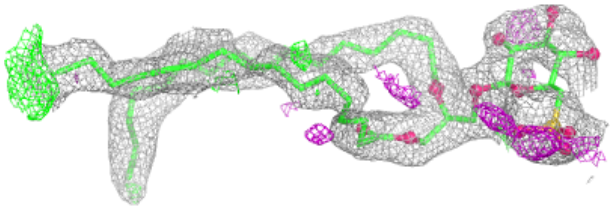




Electron density around SQD a 402:

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

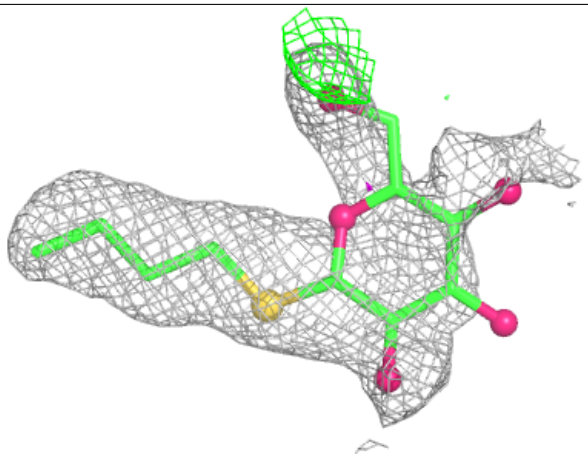


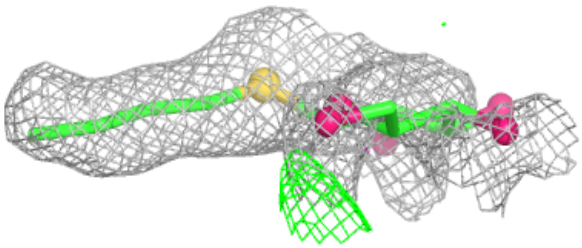


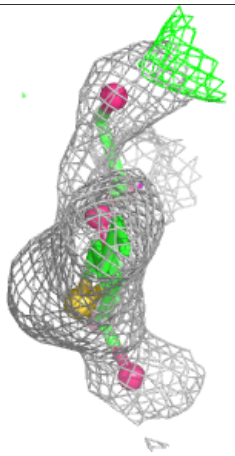


Electron density around HTG D 411:

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

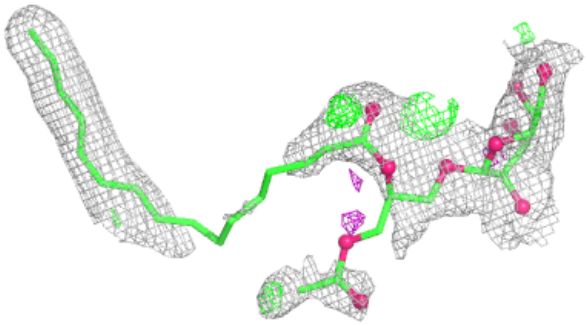


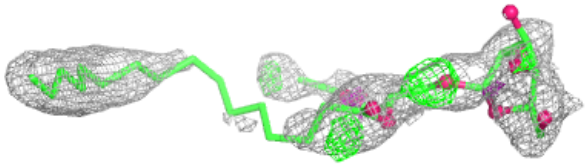


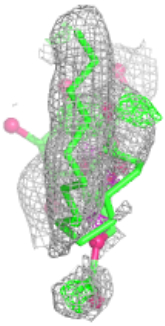


Electron density around LMG Z 101:

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

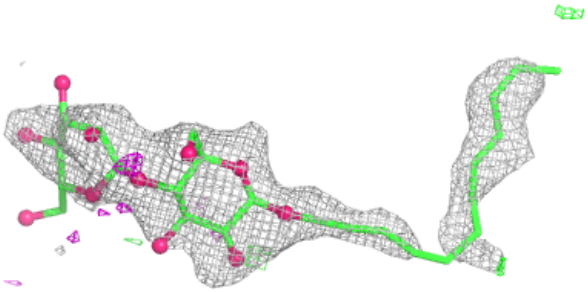


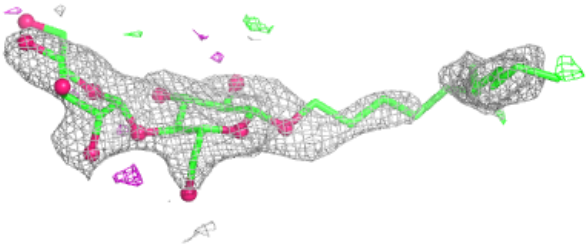


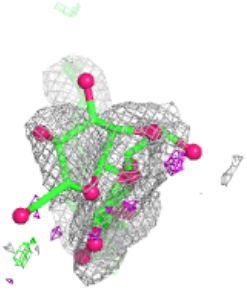


Electron density around LMT I 102:

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

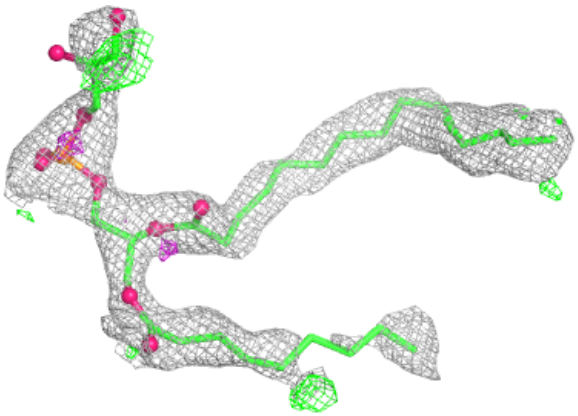


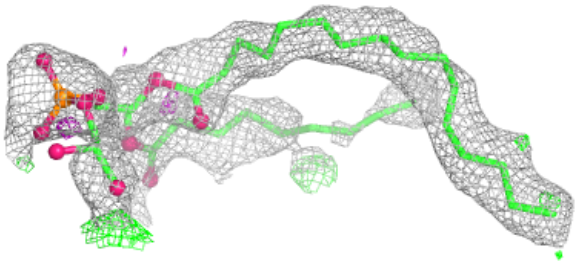




Electron density around LHG E 101:

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

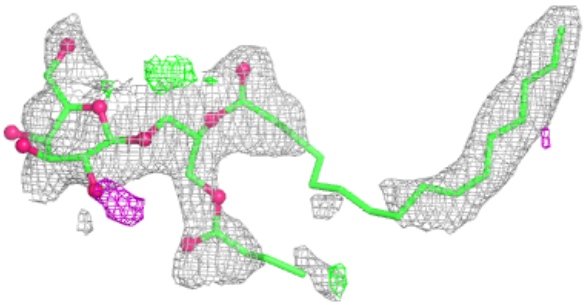


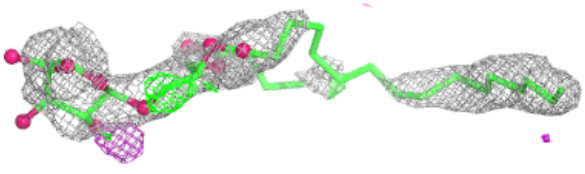


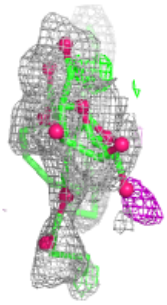


Electron density around LMG z 101:

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

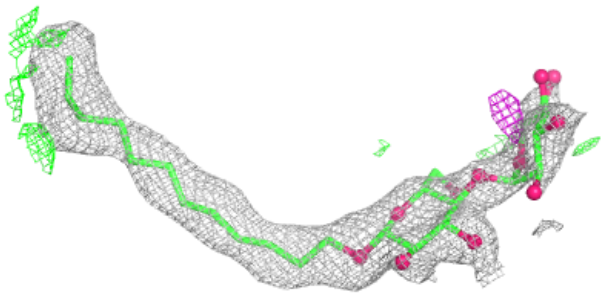


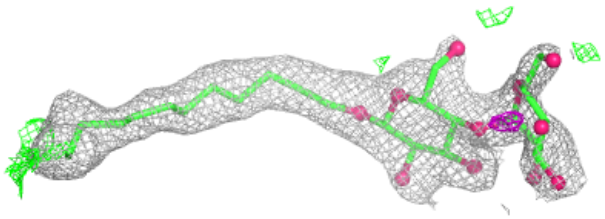


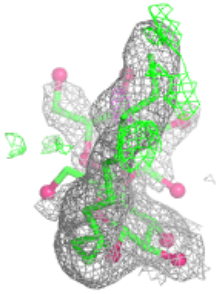


Electron density around LMT m 103:

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

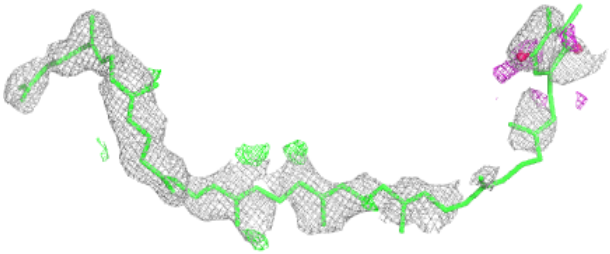


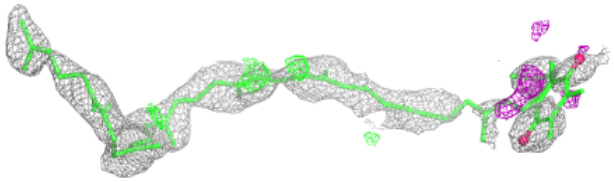


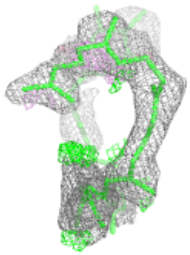


Electron density around PL9 a 416:

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

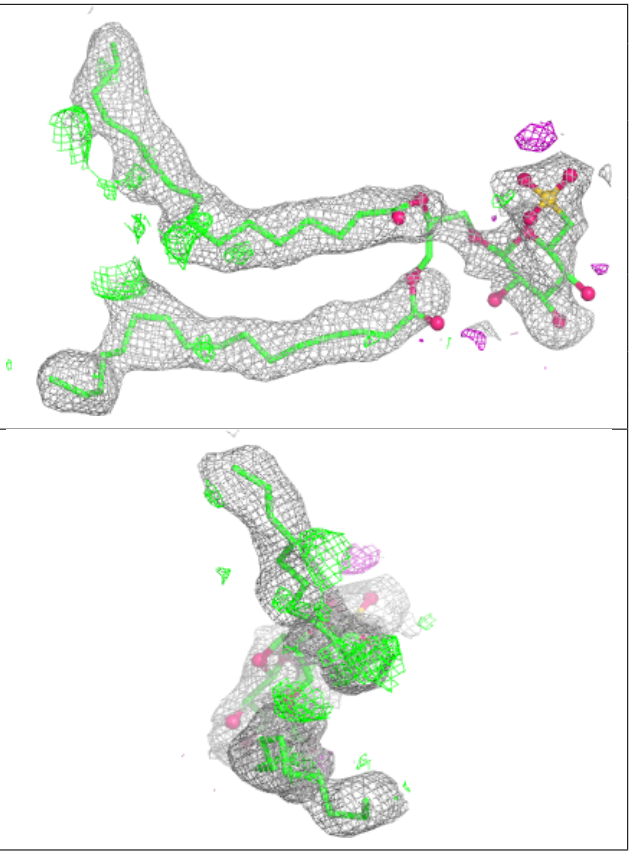






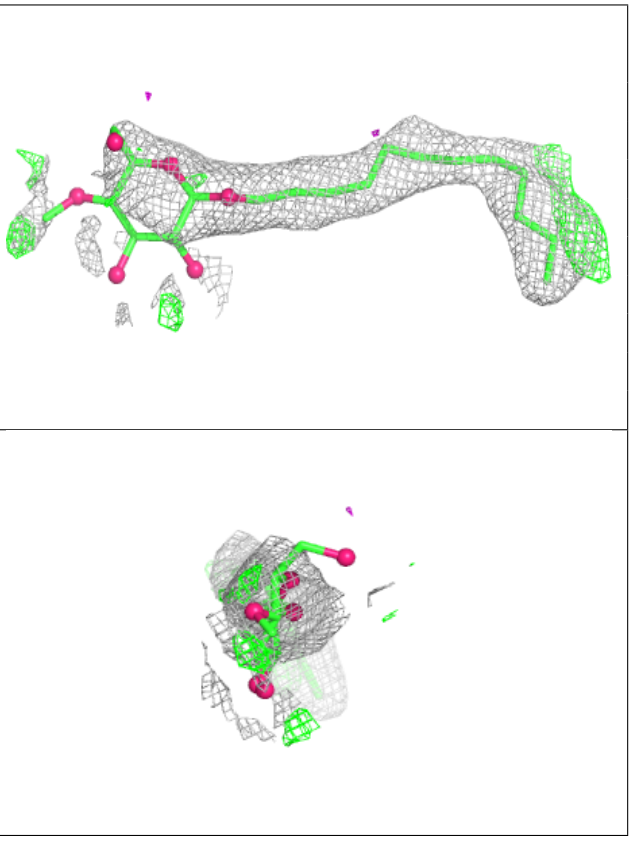
Electron density around SQD l 101:

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



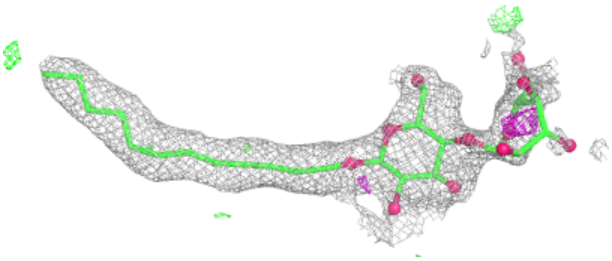
Electron density around LMT B 634:

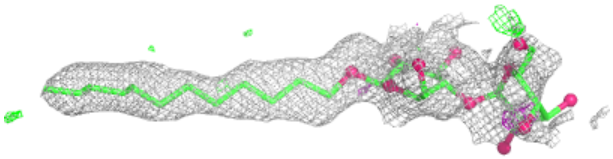
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

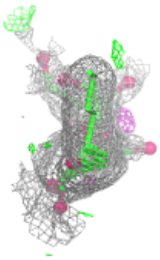


Electron density around LMT D 402:

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

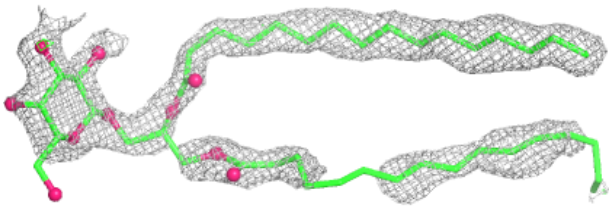


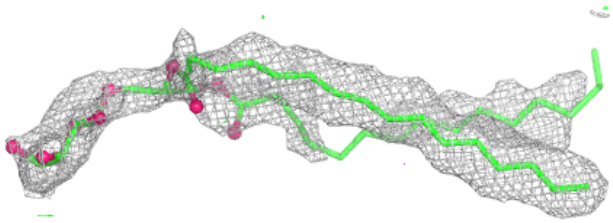


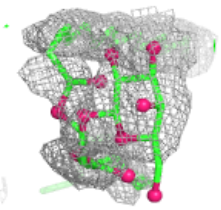


Electron density around LMG c 521:

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

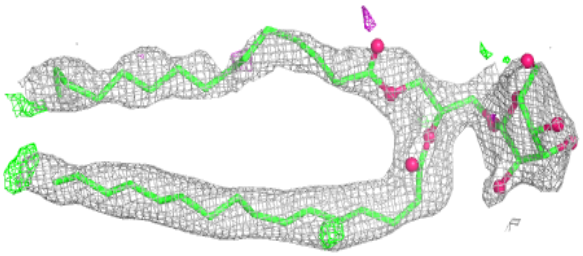


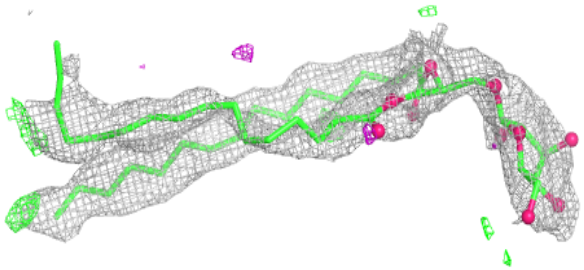


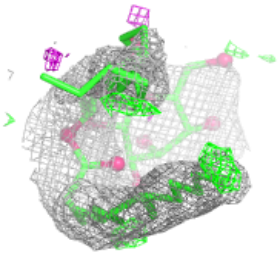


Electron density around LMG C 521:

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

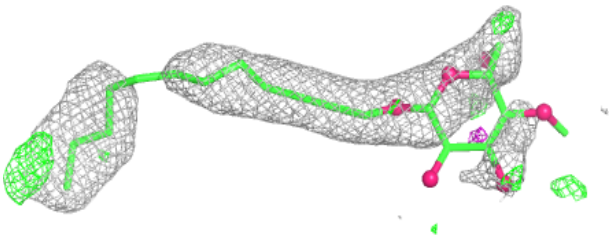


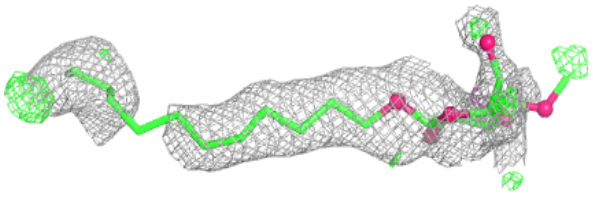


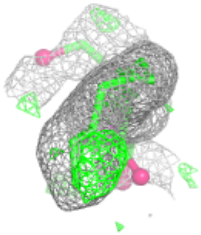


Electron density around LMT b 602:

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

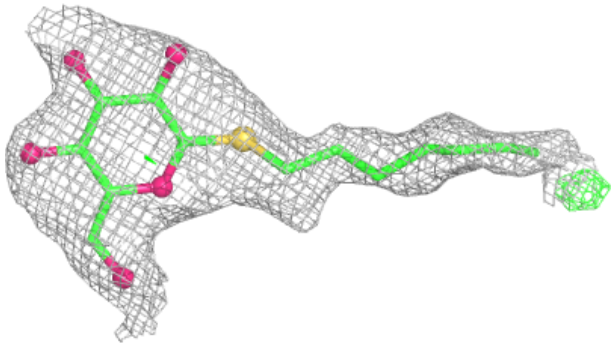


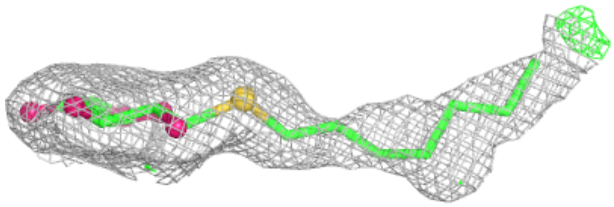


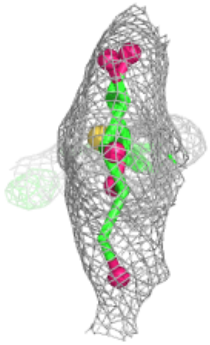


Electron density around HTG c 522:

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

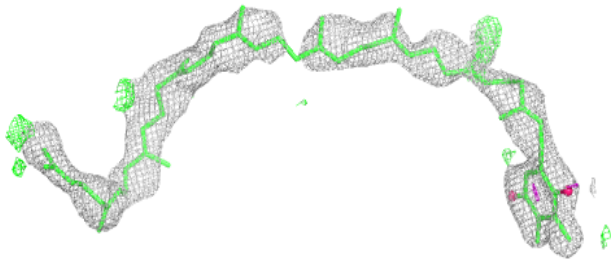


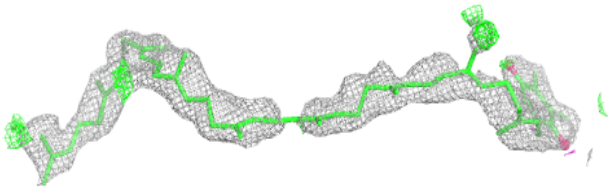


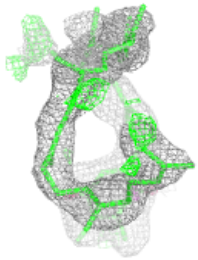


Electron density around PL9 A 419:

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

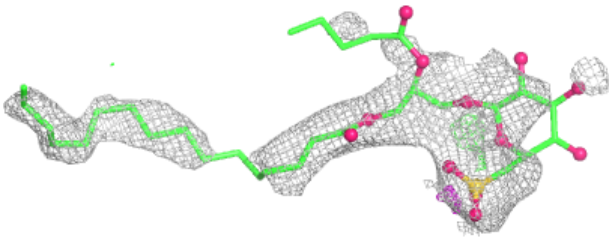


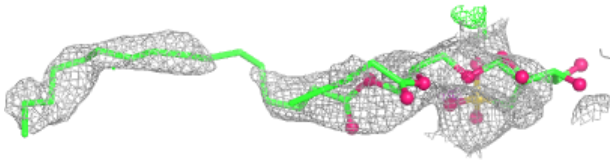


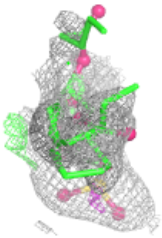


Electron density around SQD f 101:

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

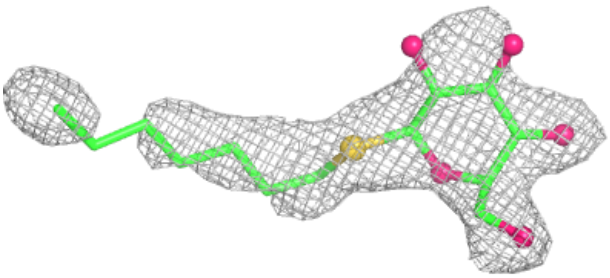


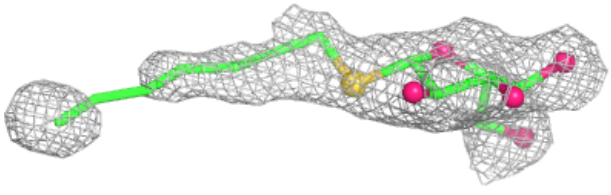


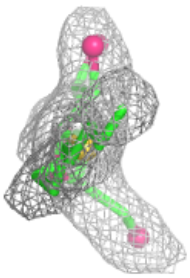


Electron density around HTG C 523:

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

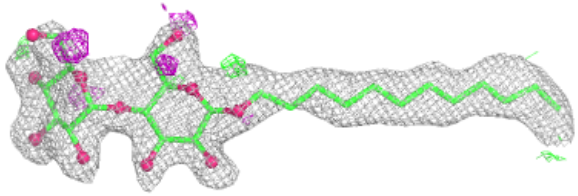


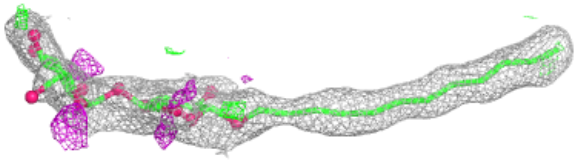


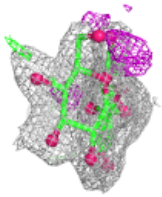


Electron density around LMT m 102:

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

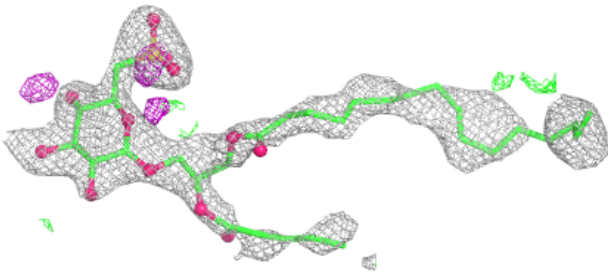


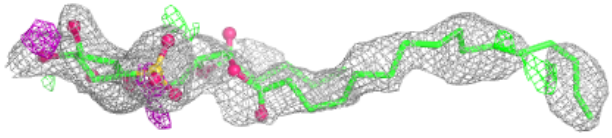


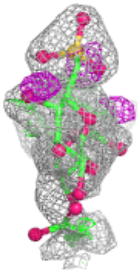


Electron density around SQD F 101:

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

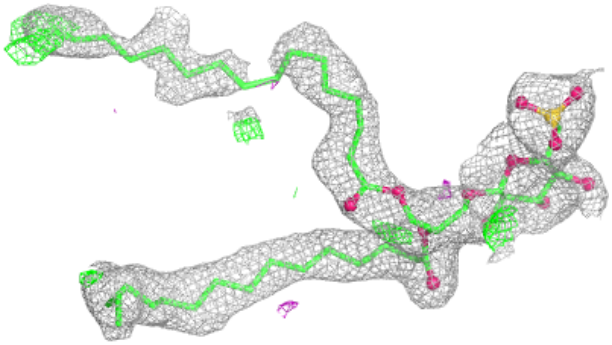


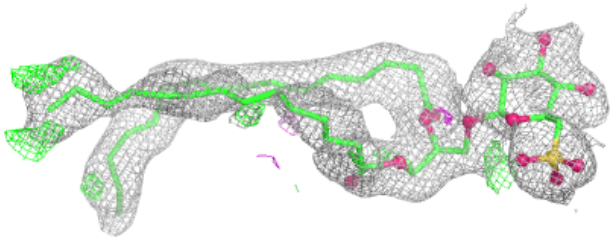


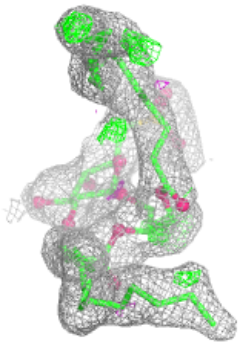


Electron density around SQD A 416:

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

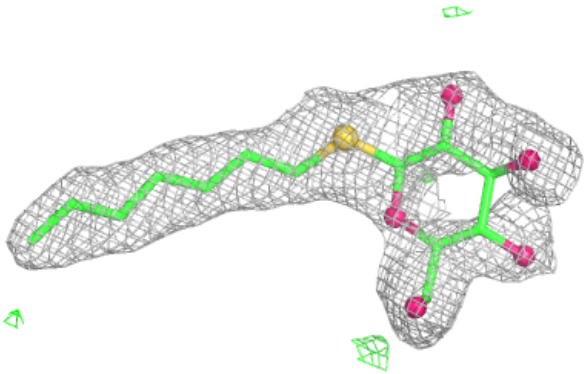


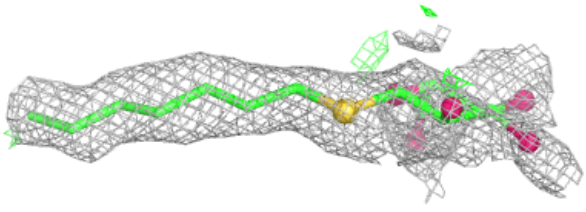


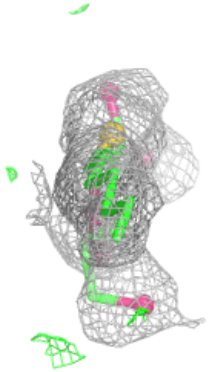


Electron density around HTG b 604:

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

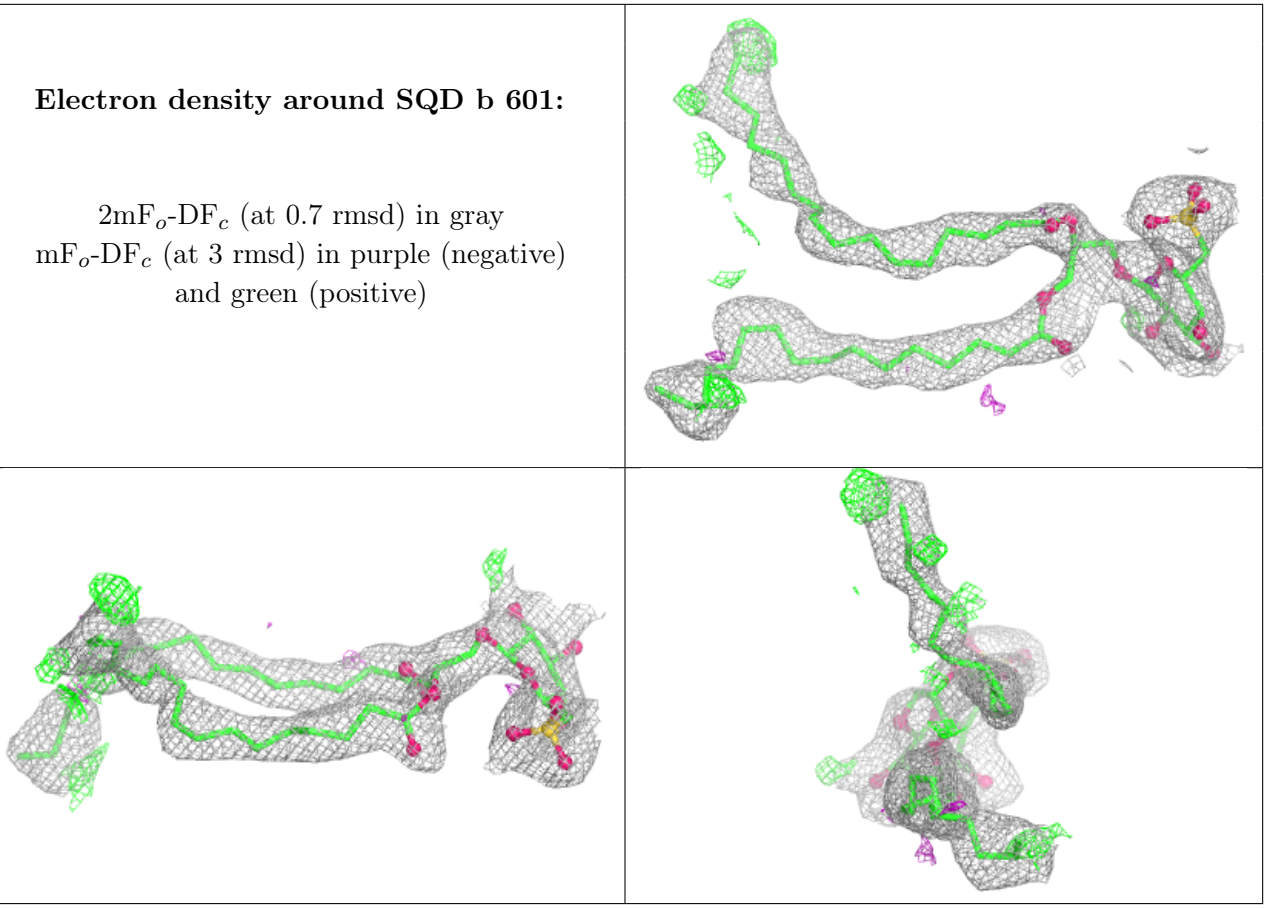






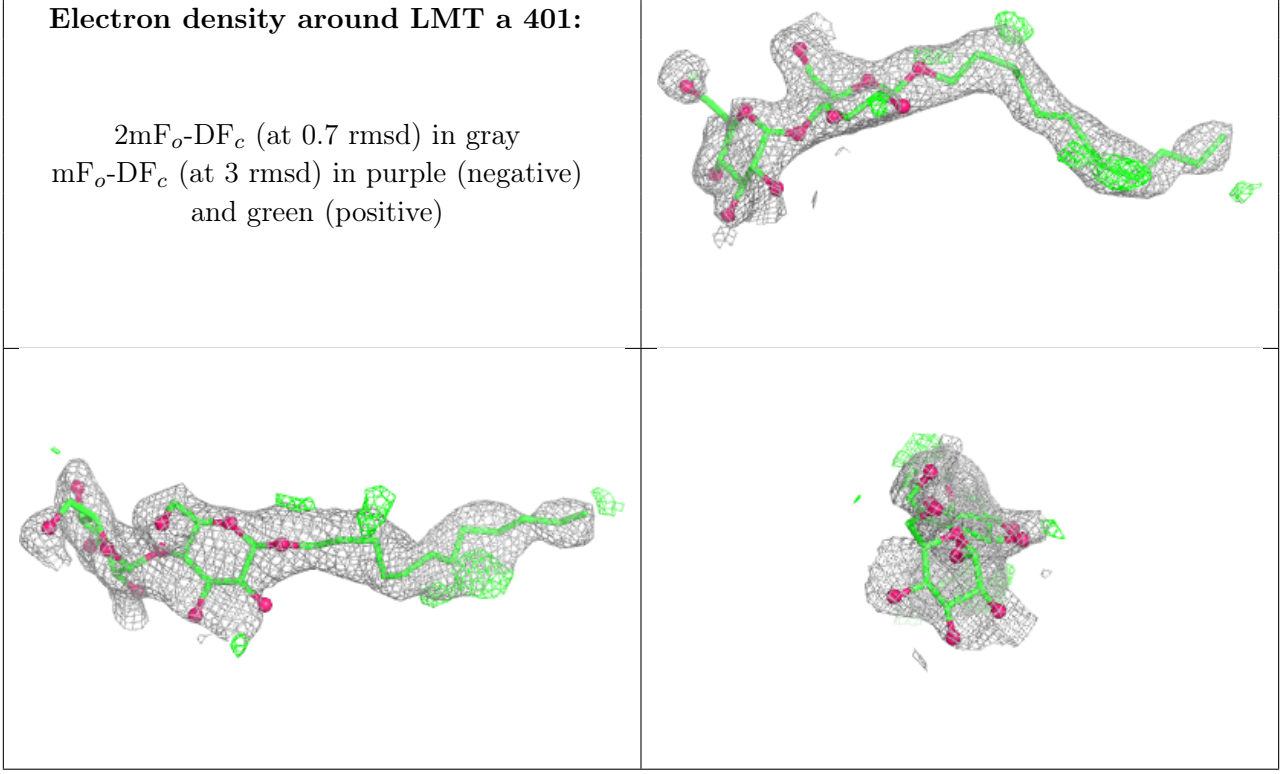
Electron density around SQD b 601:

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



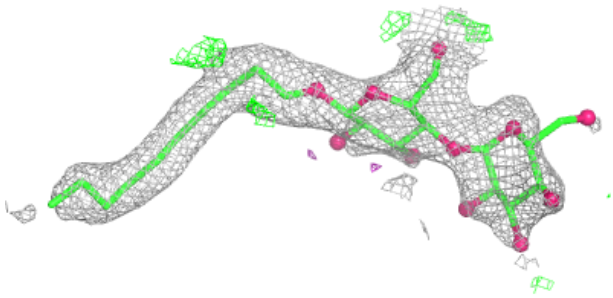
Electron density around LMT a 401:

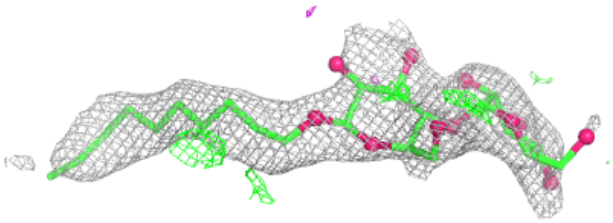
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

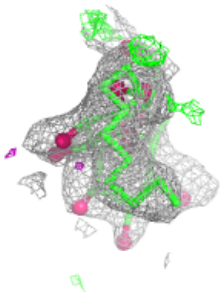


Electron density around LMT A 417:

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

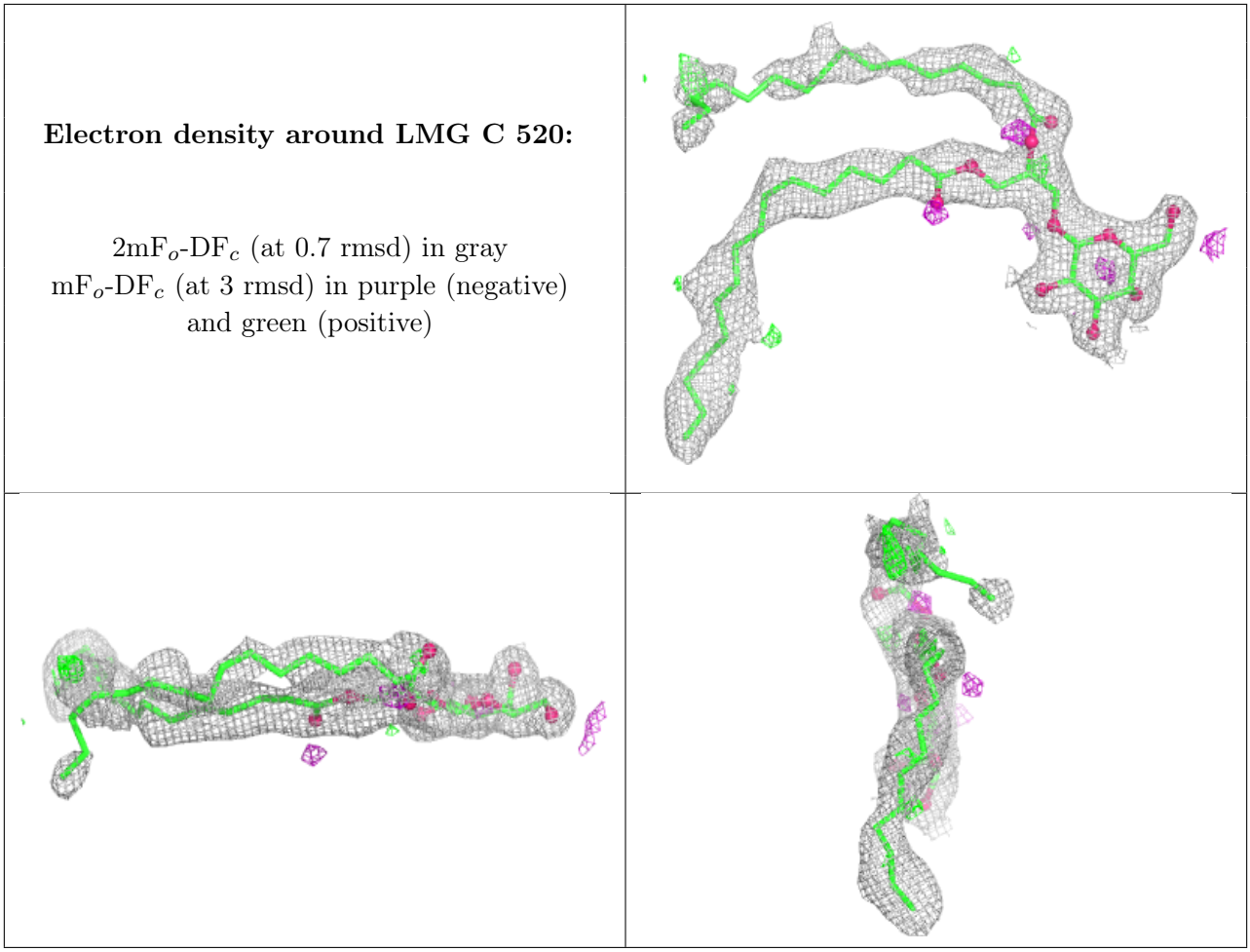






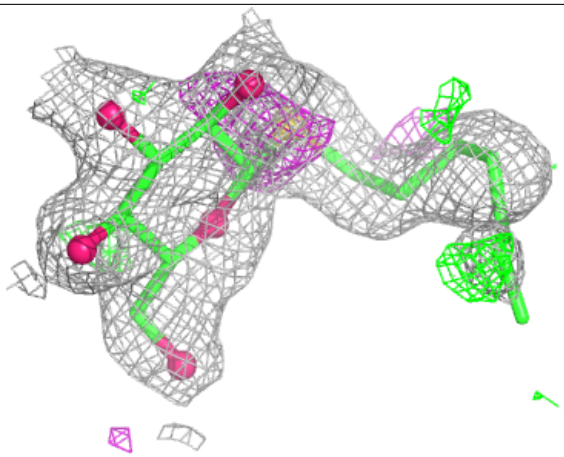
Electron density around LMG C 520:

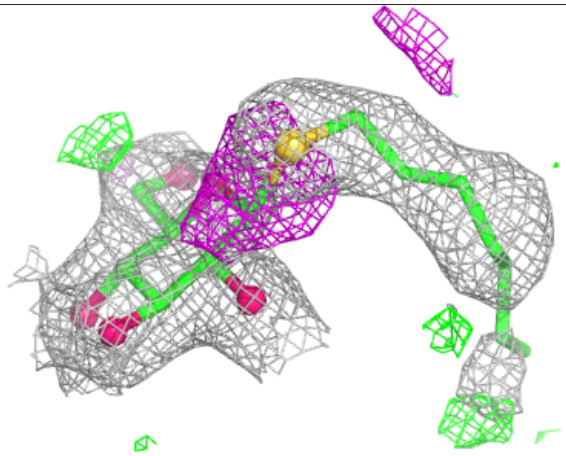
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

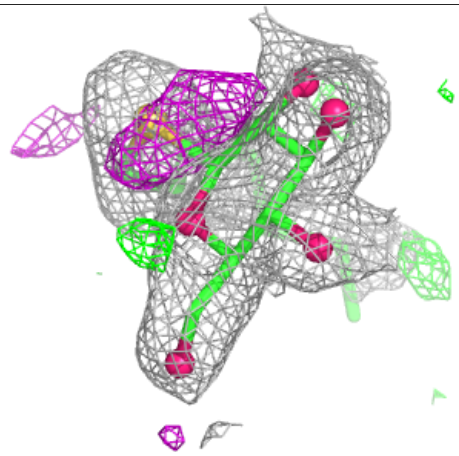


Electron density around HTG b 627:

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

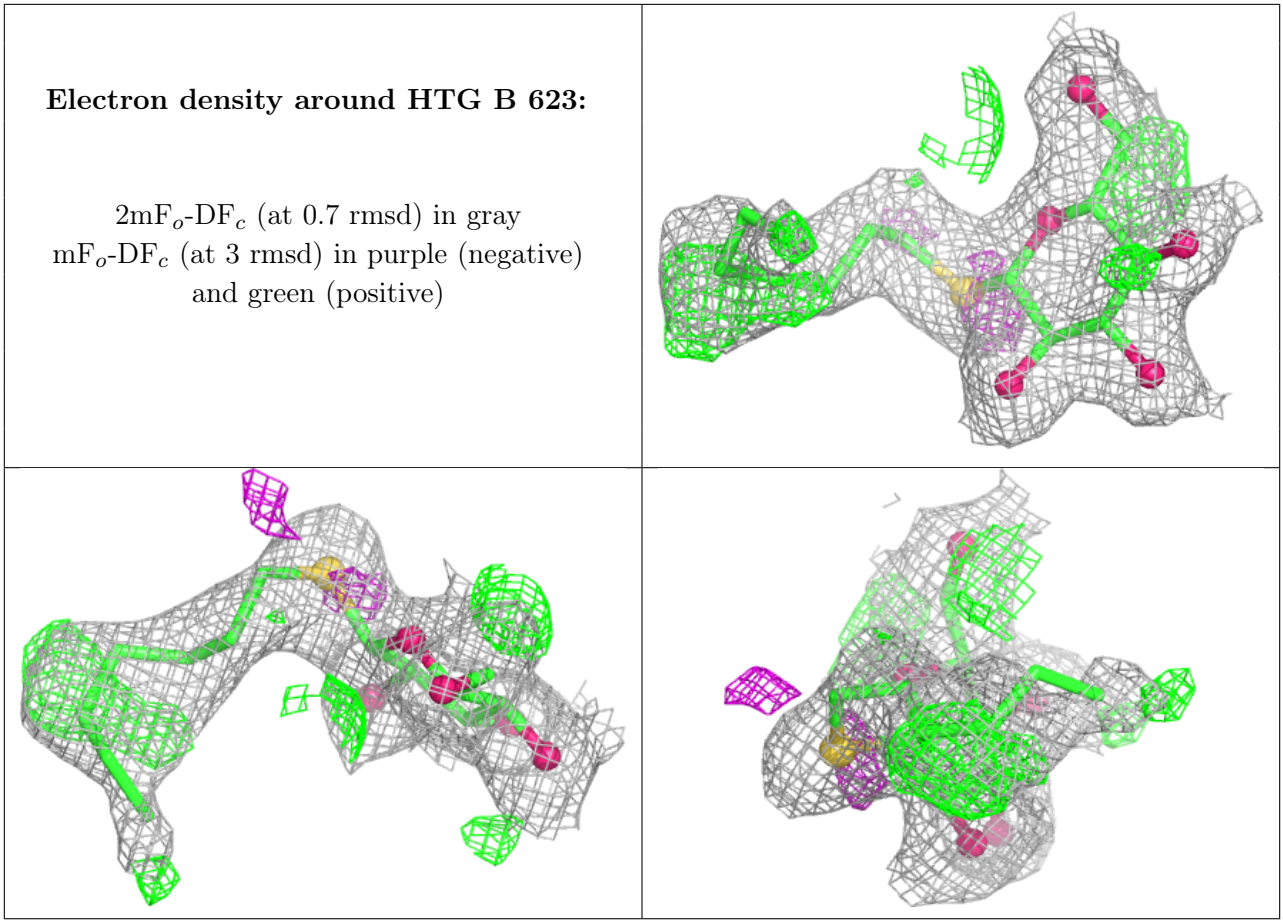






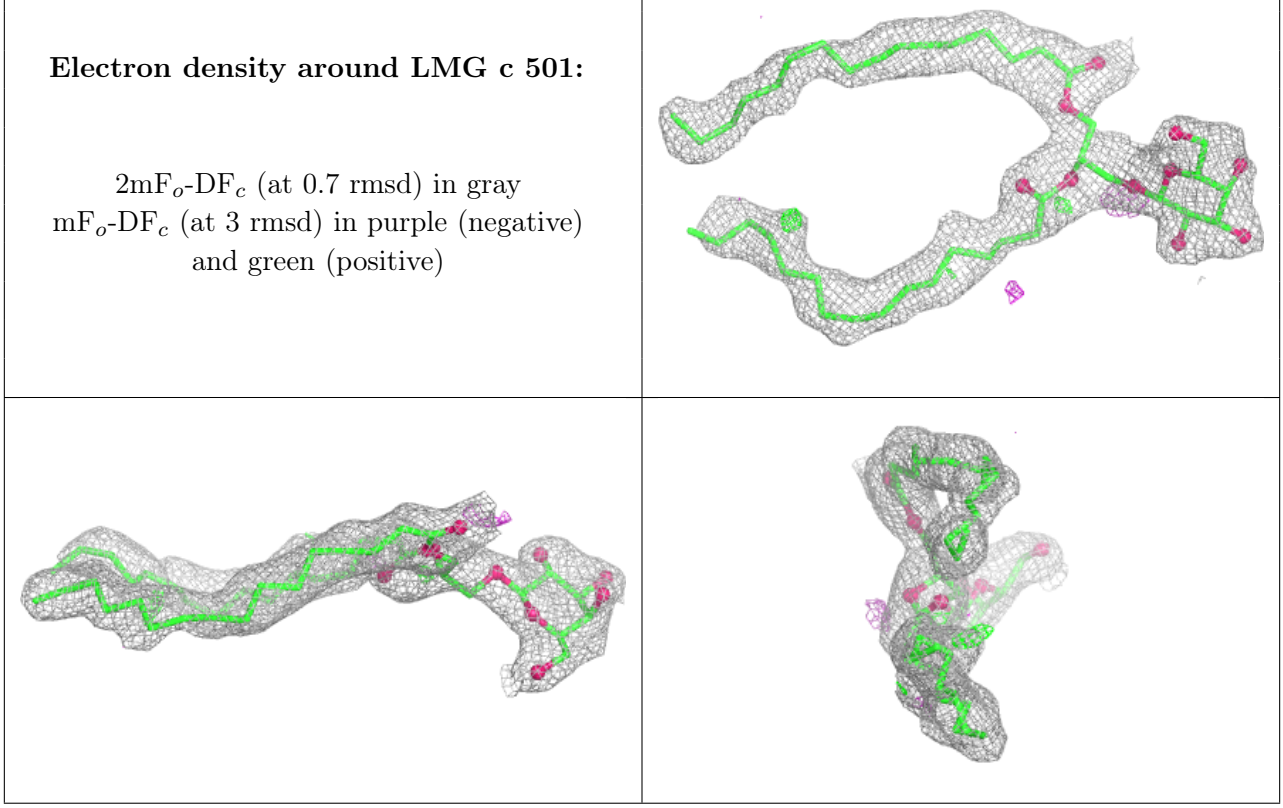
Electron density around HTG B 623:

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



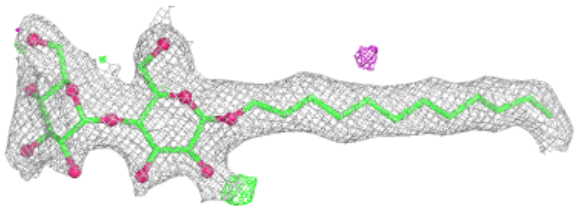
Electron density around LMG c 501:

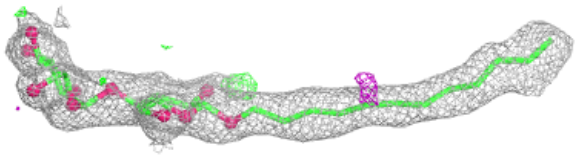
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

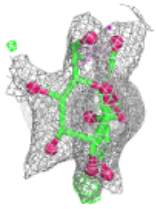


Electron density around LMT M 102:

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

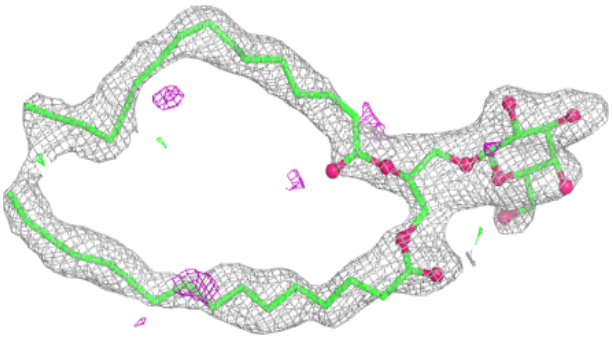


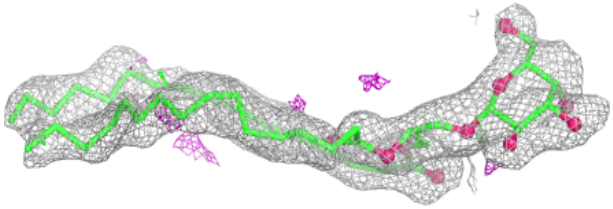


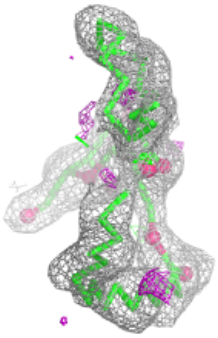


Electron density around LMG C 501:

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

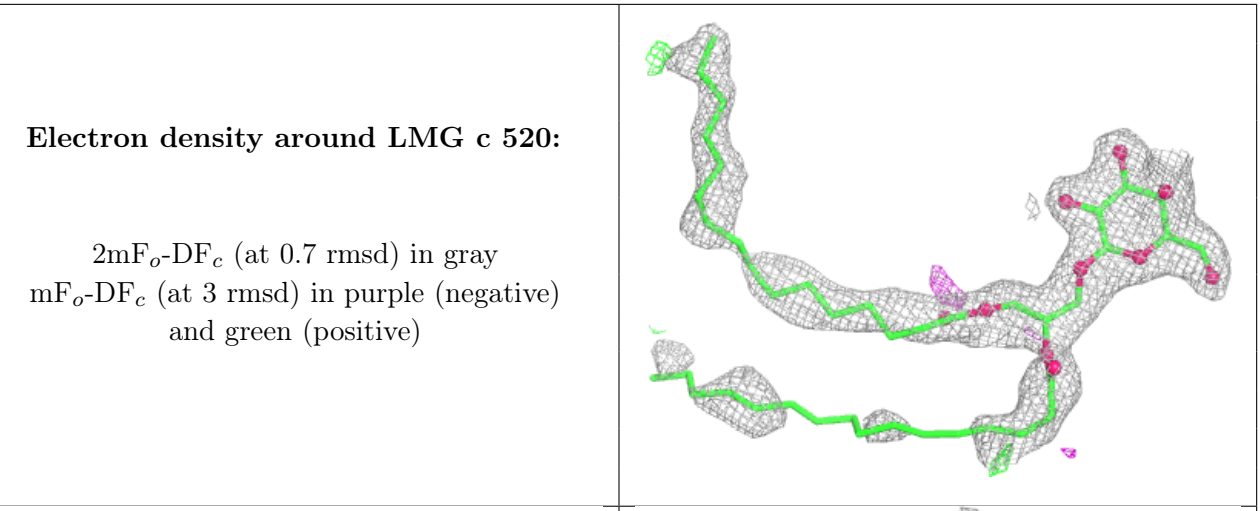


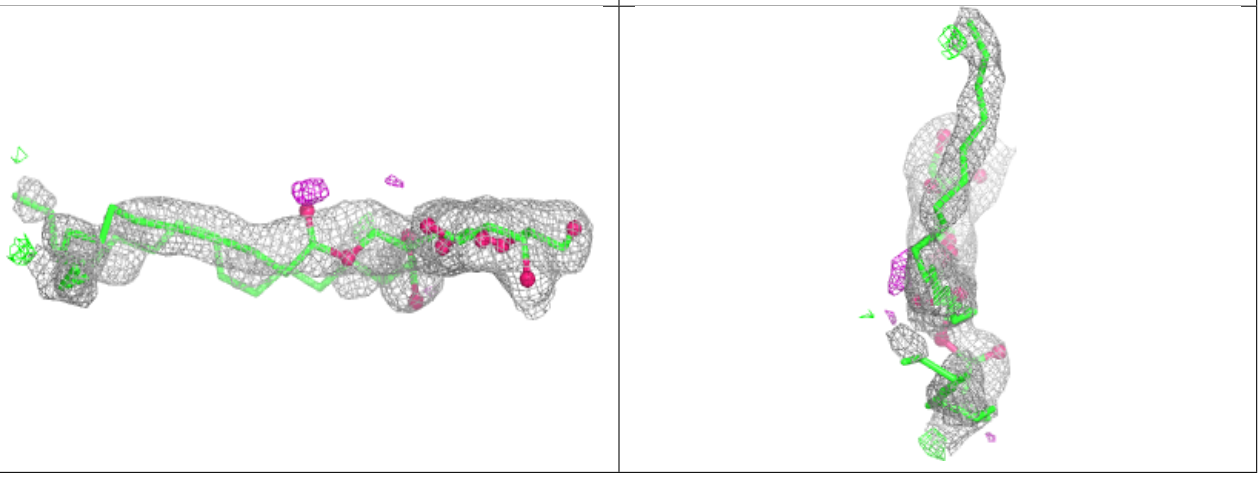




Electron density around LMG c 520:

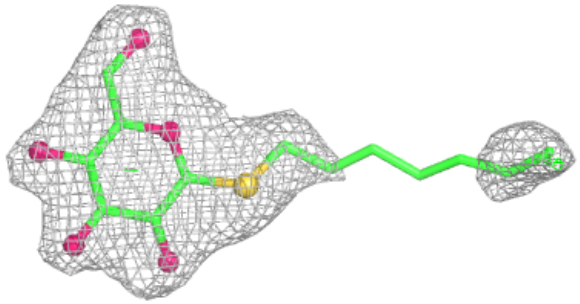
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

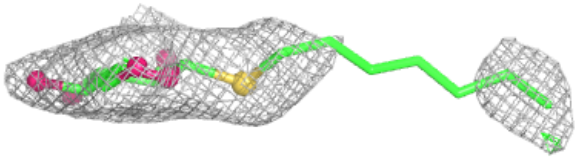


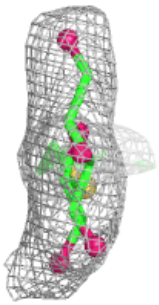


Electron density around HTG C 522:

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

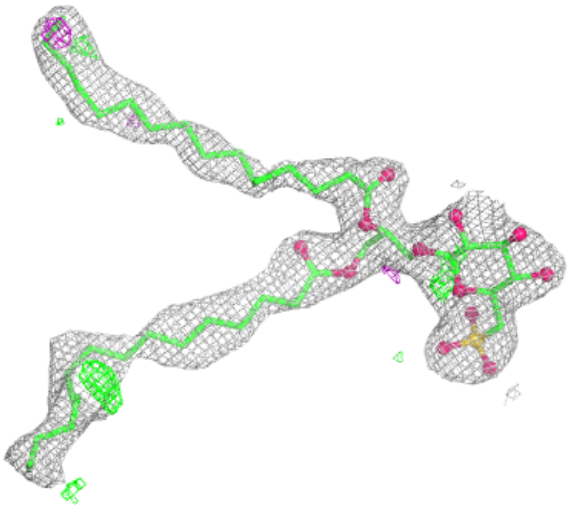


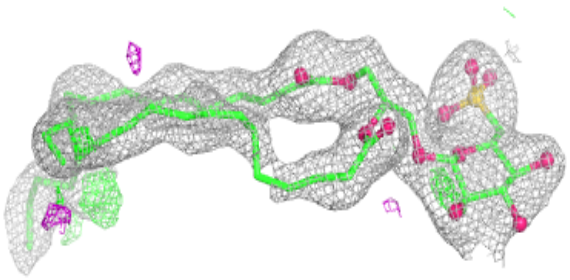


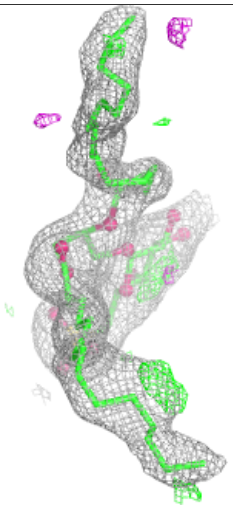


Electron density around SQD a 411:

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

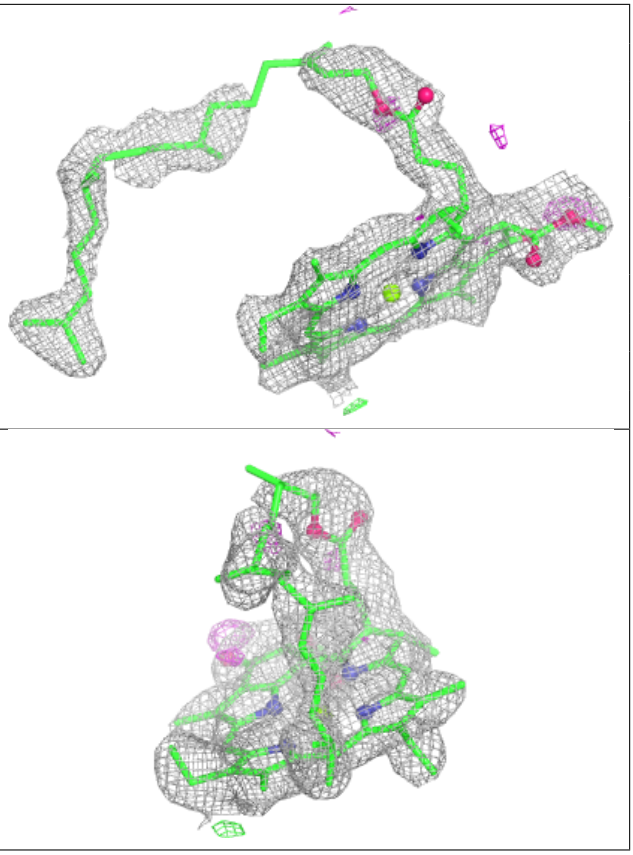






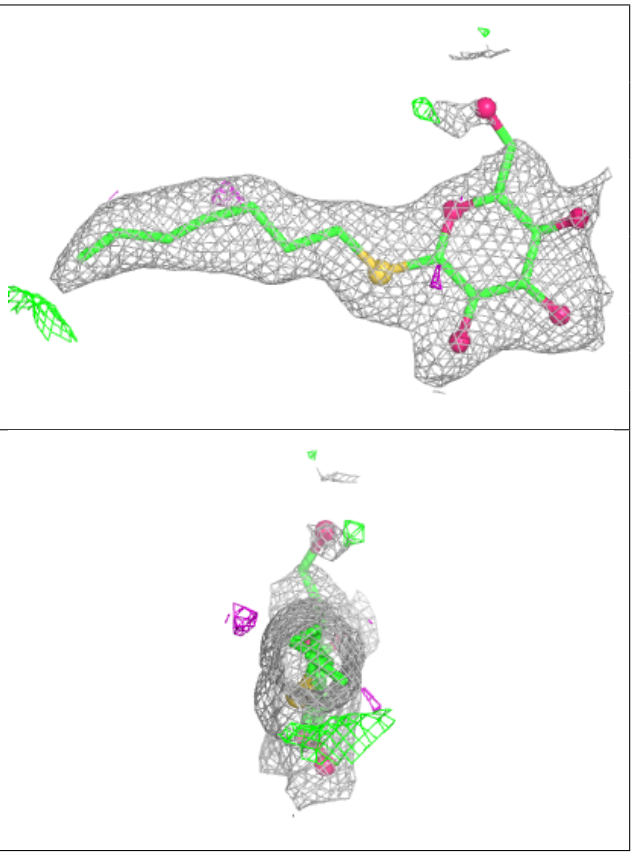
Electron density around CLA c 515:

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



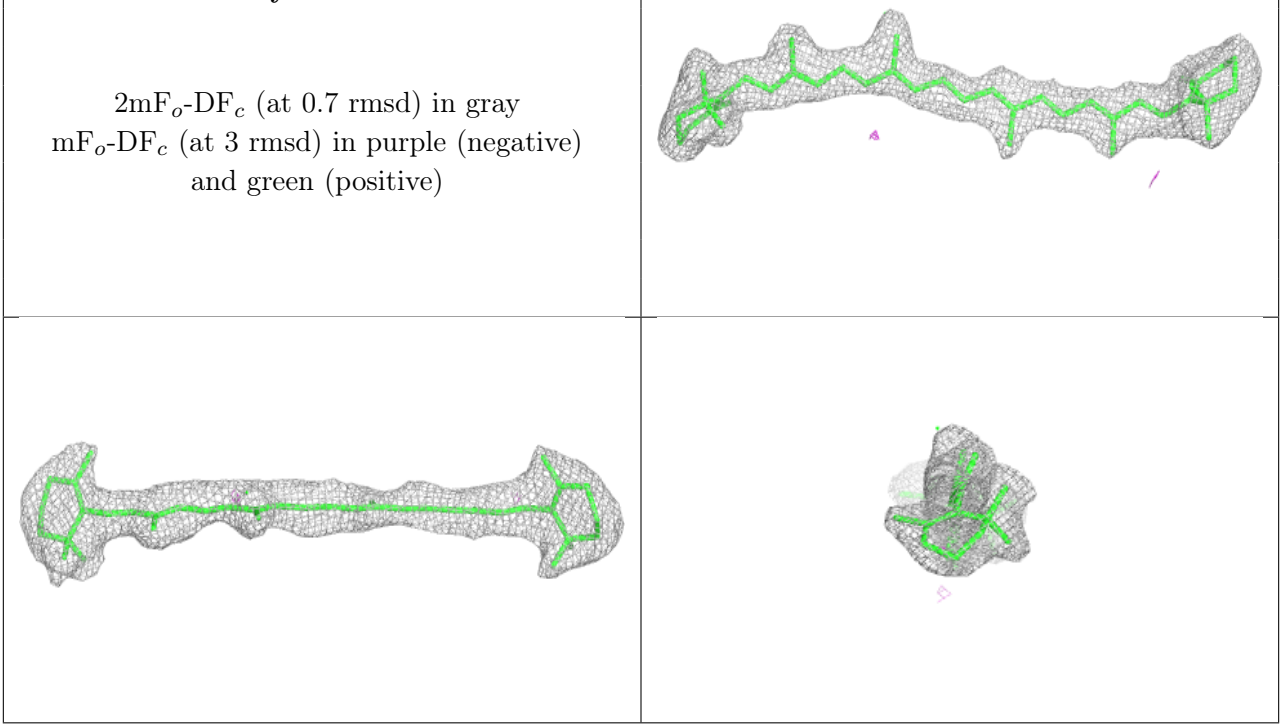
Electron density around HTG B 630:

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



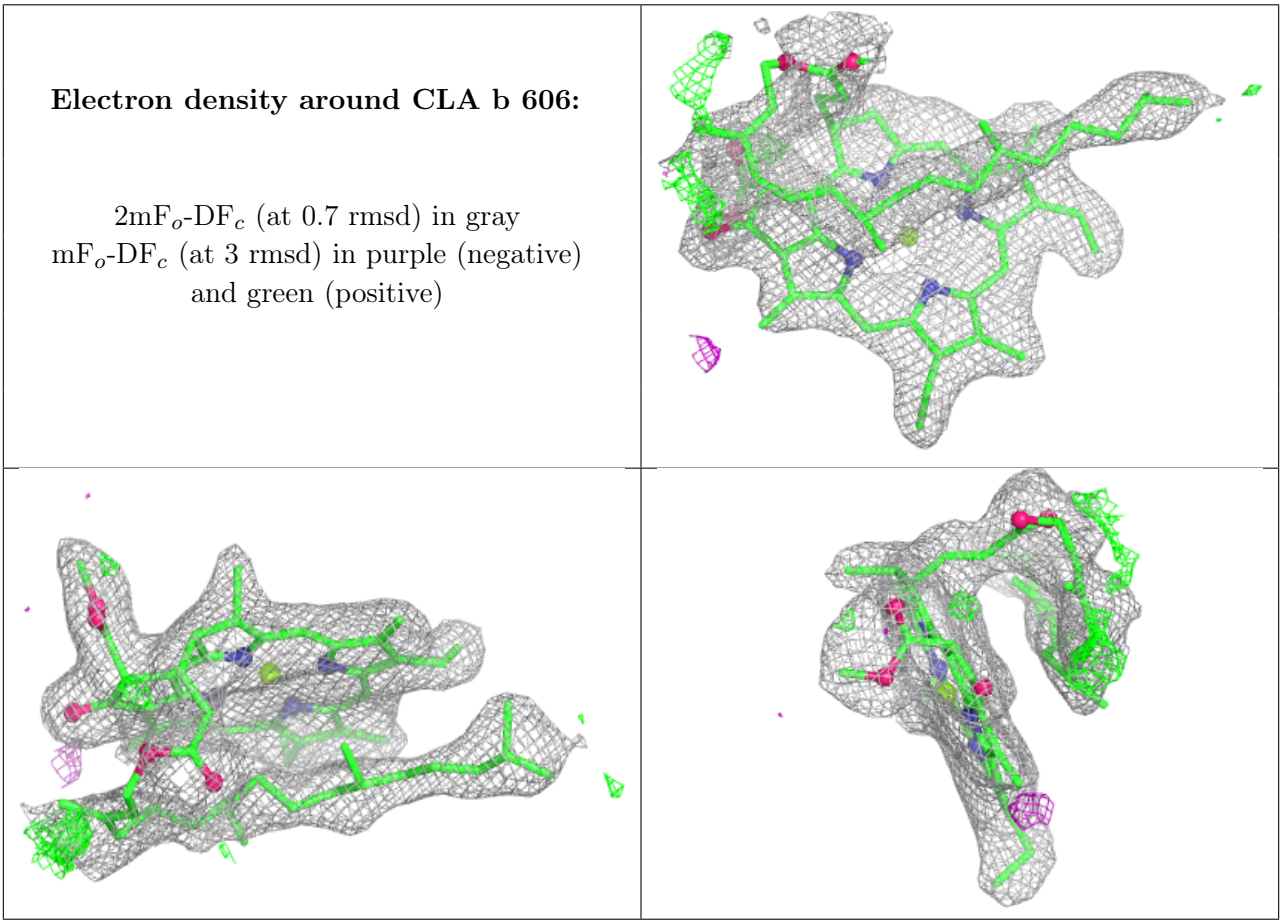
Electron density around BCR c 526:

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



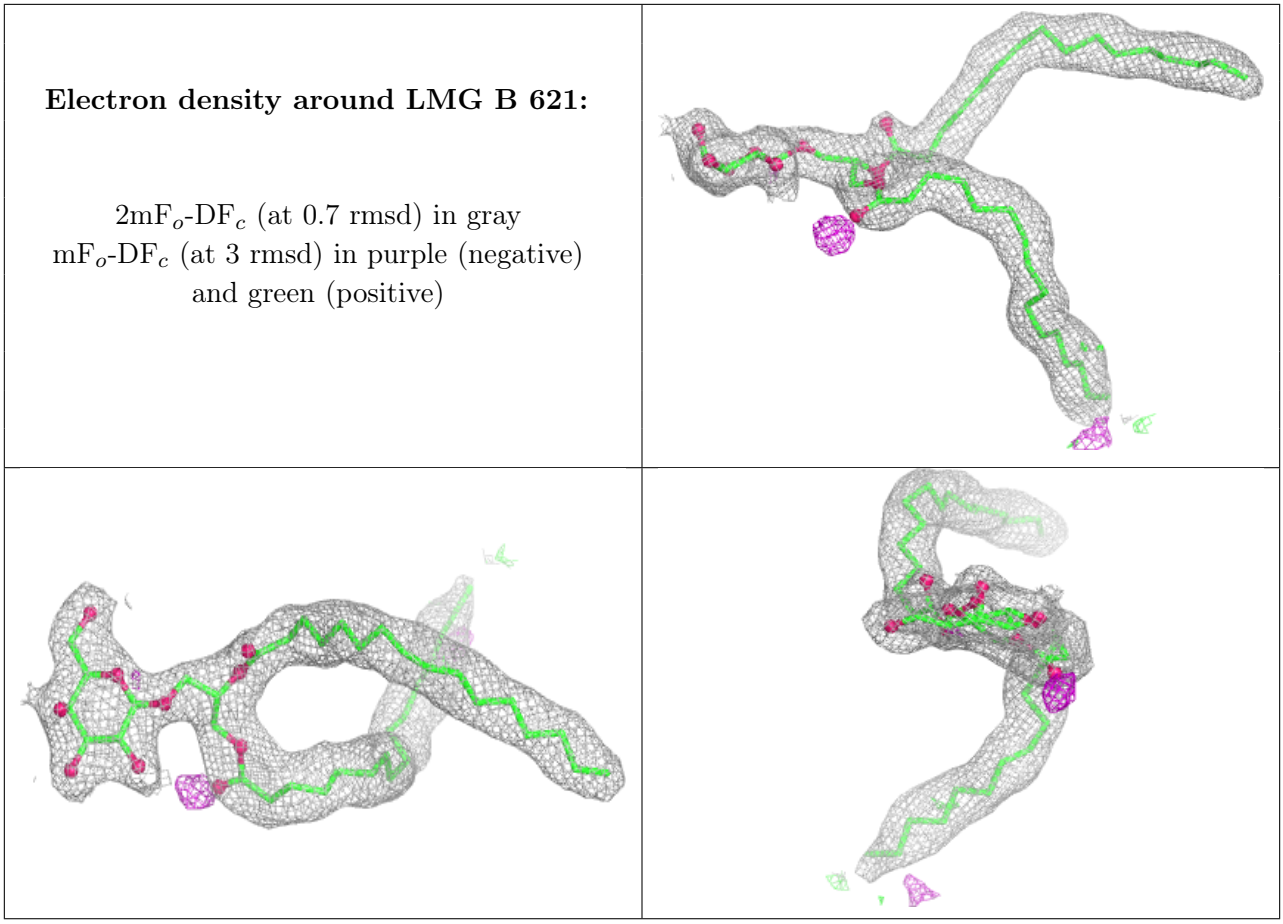
Electron density around CLA b 606:

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



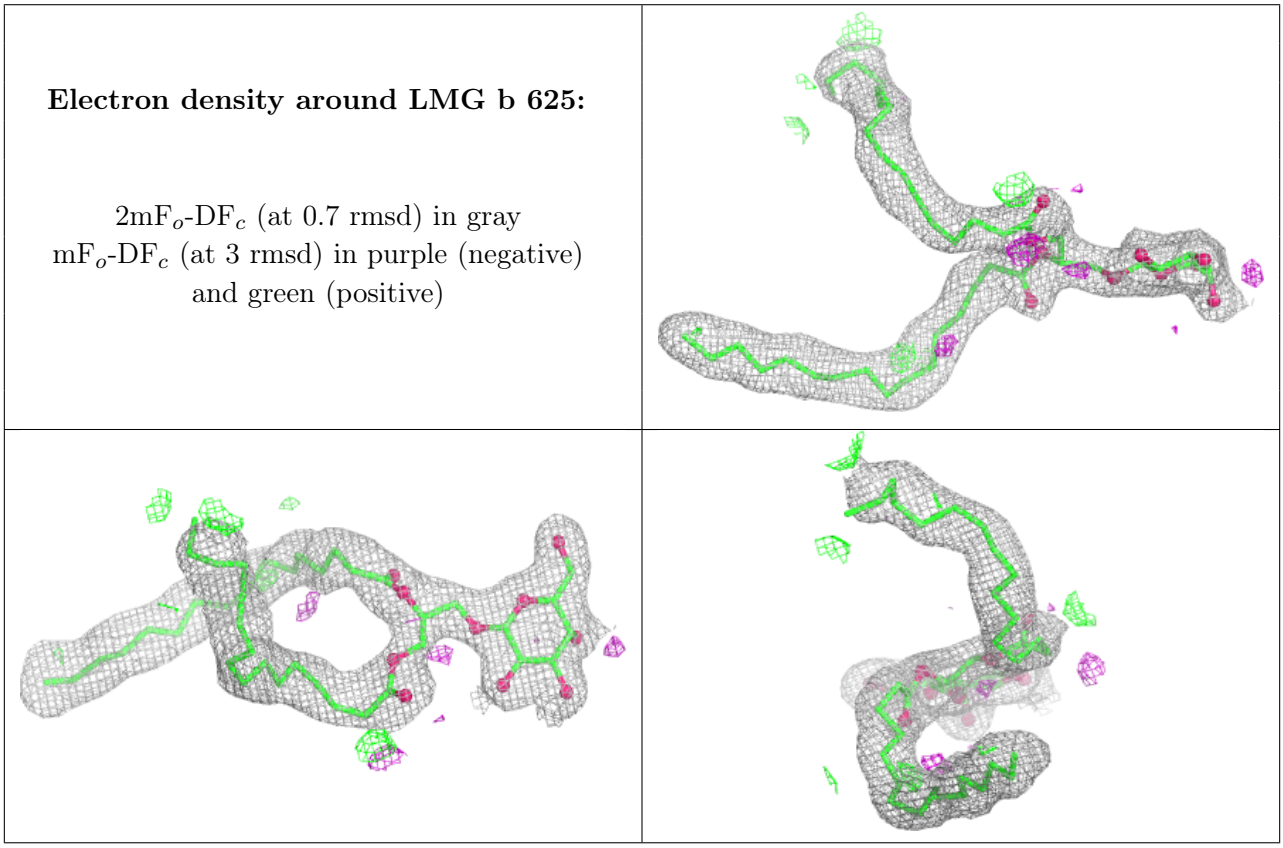
Electron density around LMG B 621:

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



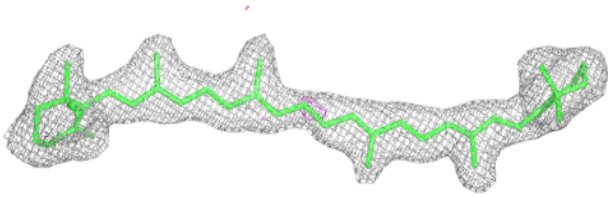
Electron density around LMG b 625:

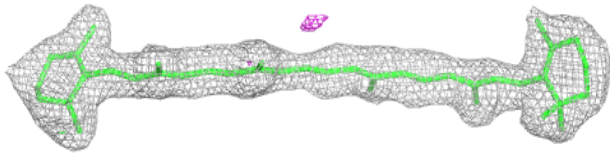
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

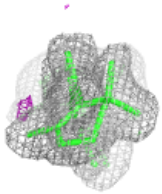


Electron density around BCR C 515:

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

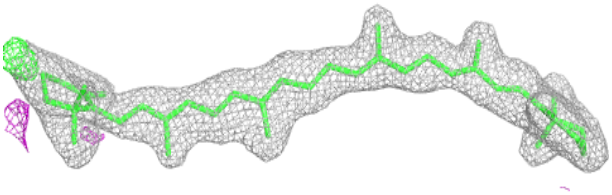


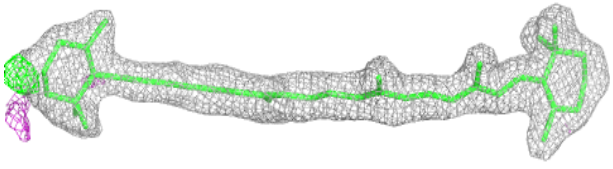


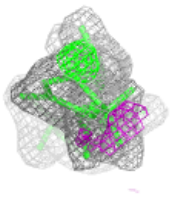


Electron density around BCR H 101:

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

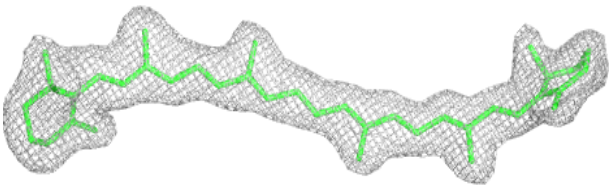


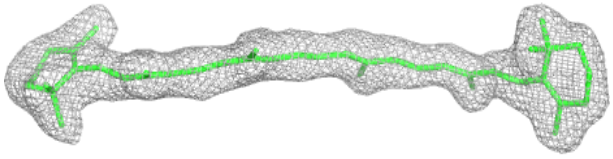


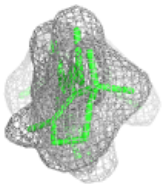


Electron density around BCR Y 101:

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

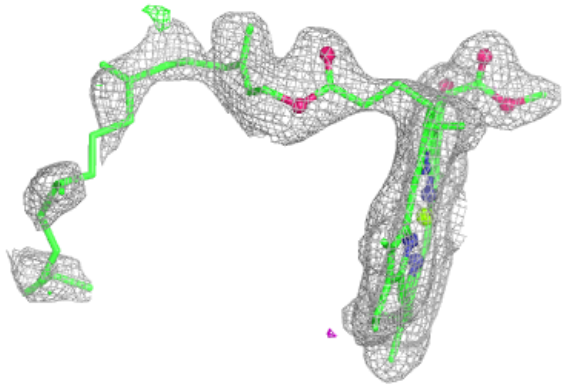


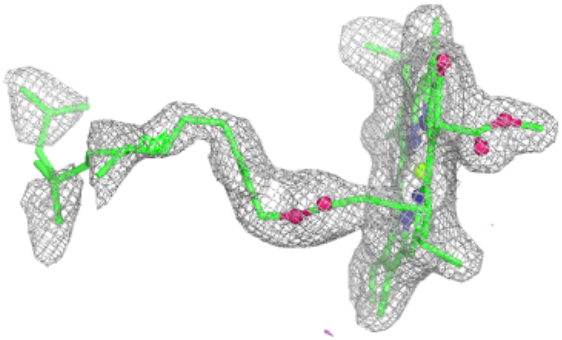


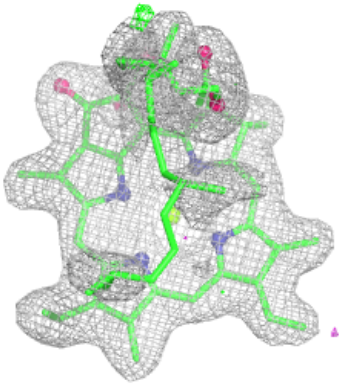


Electron density around CLA C 507:

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

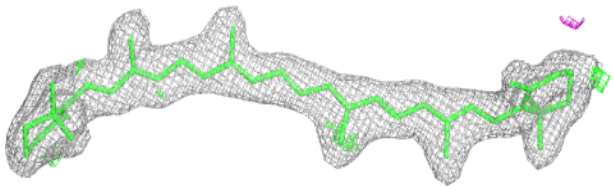


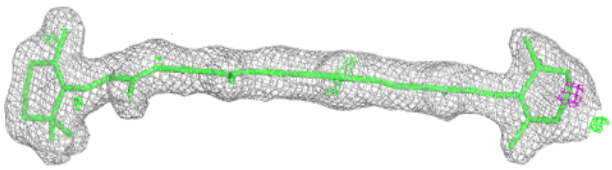


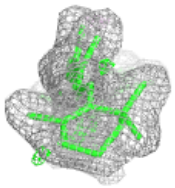


Electron density around BCR h 101:

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

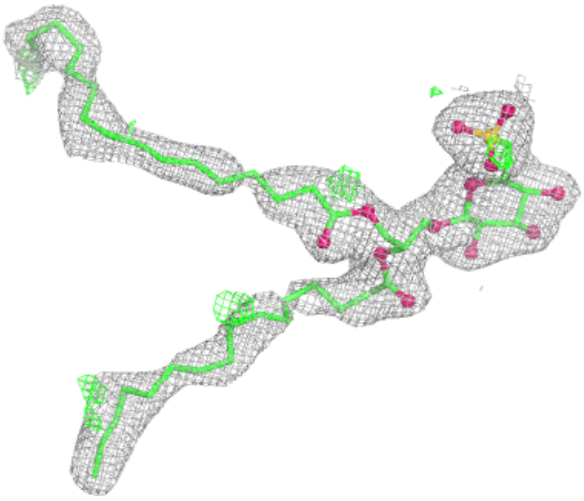


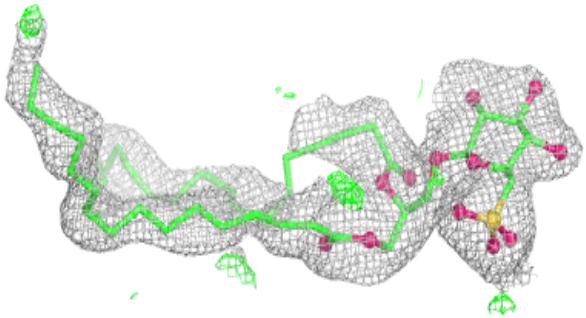


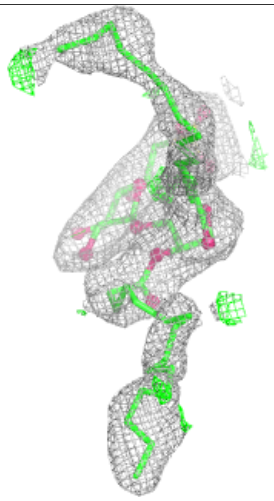


Electron density around SQD A 411:

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

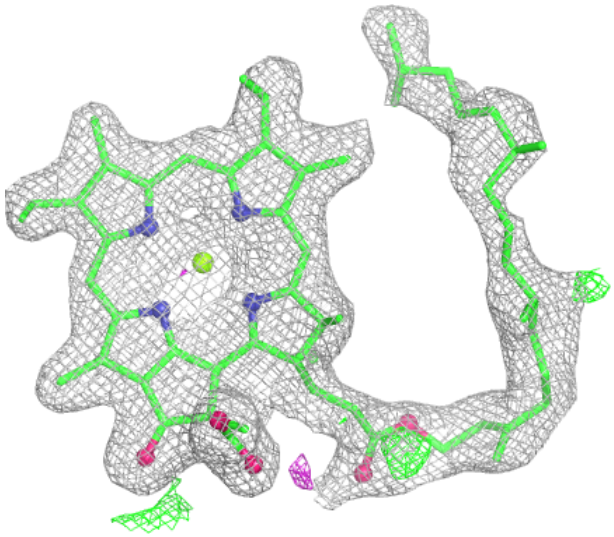


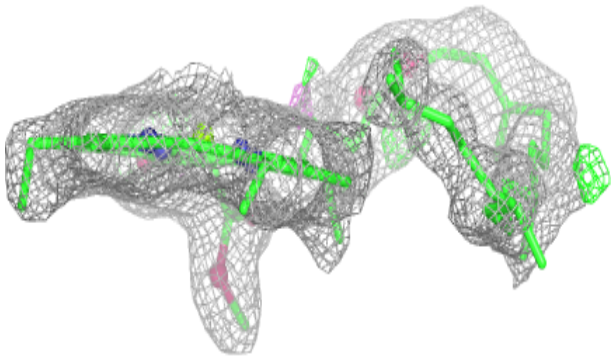


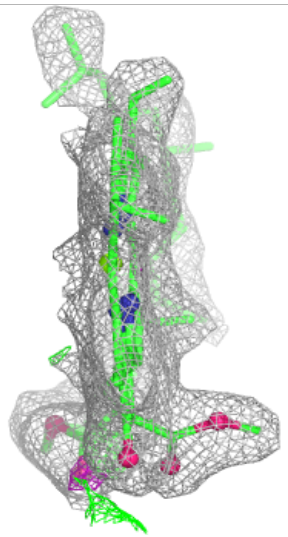


Electron density around CLA c 514:

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

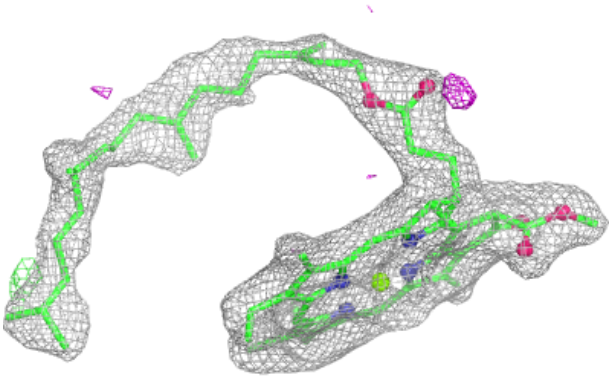


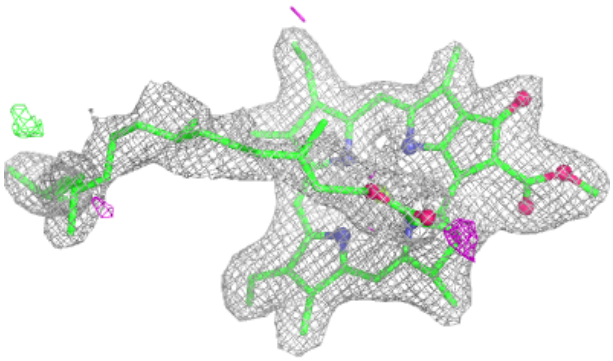


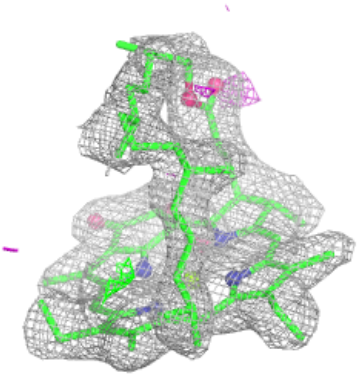


Electron density around CLA C 514:

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

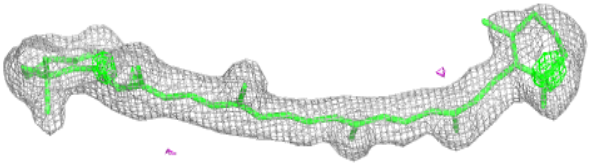


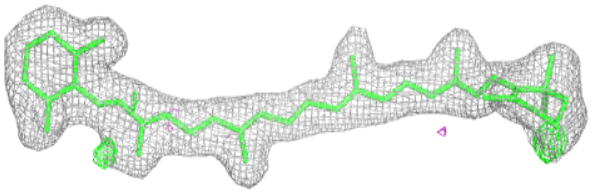


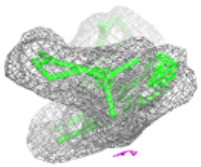


Electron density around BCR D 405:

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

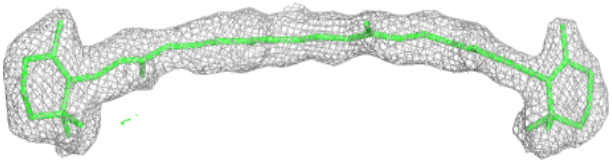


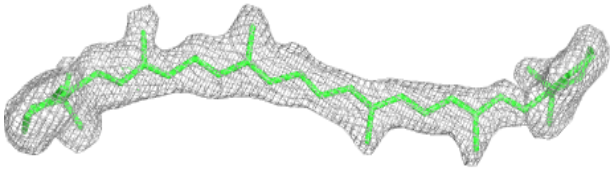


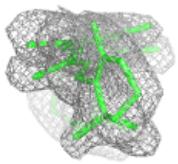


Electron density around BCR k 103:

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

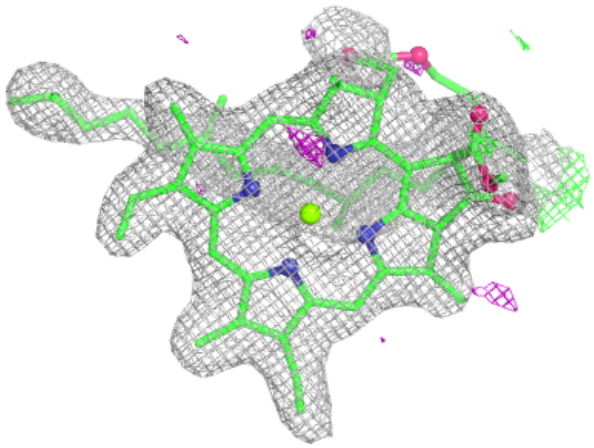


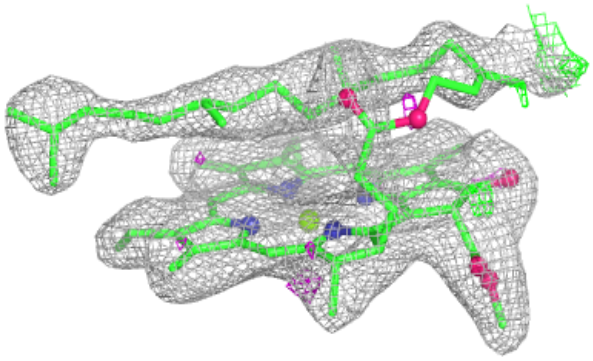


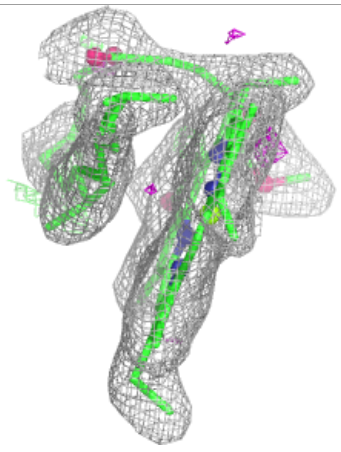


Electron density around CLA B 602:

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

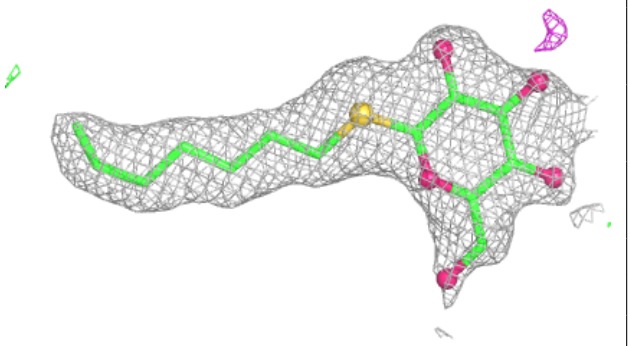


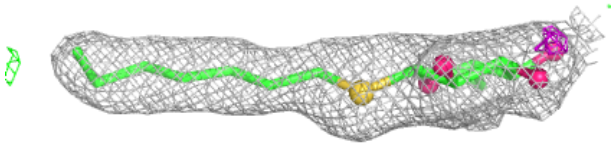


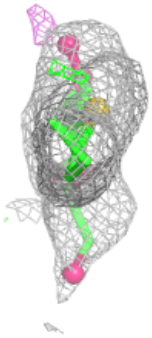


Electron density around HTG b 603:

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

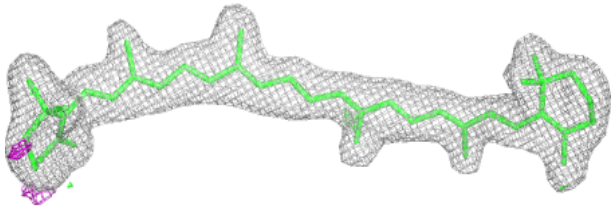


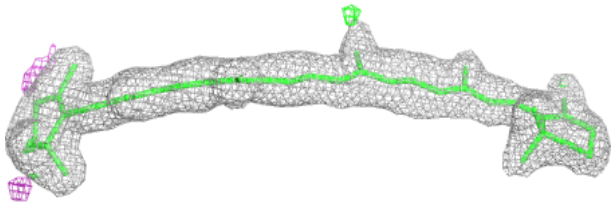


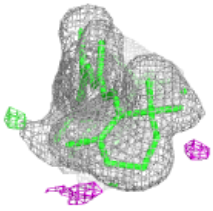


Electron density around BCR T 102:

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

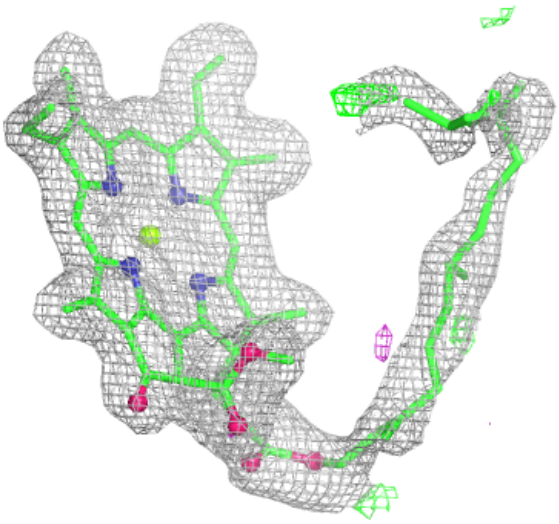


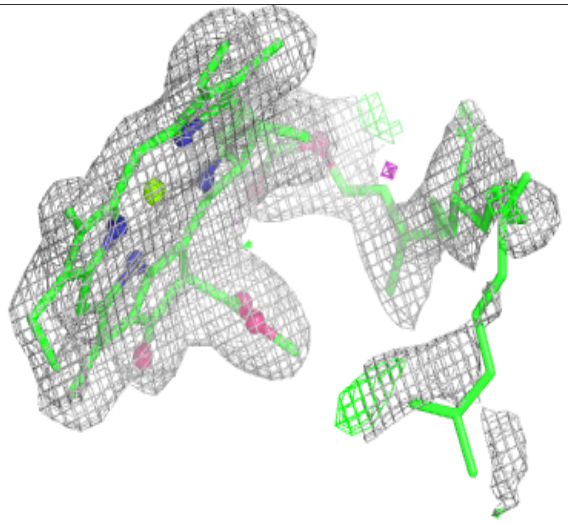


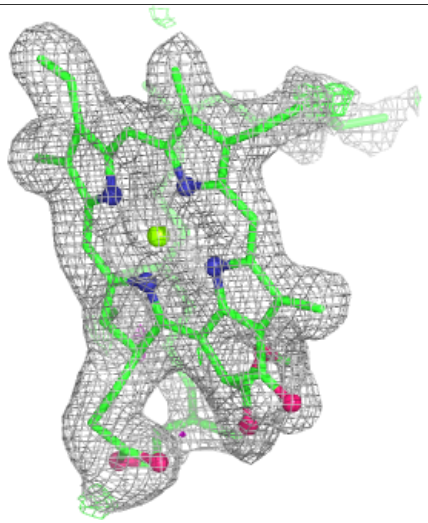


Electron density around CLA b 621:

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

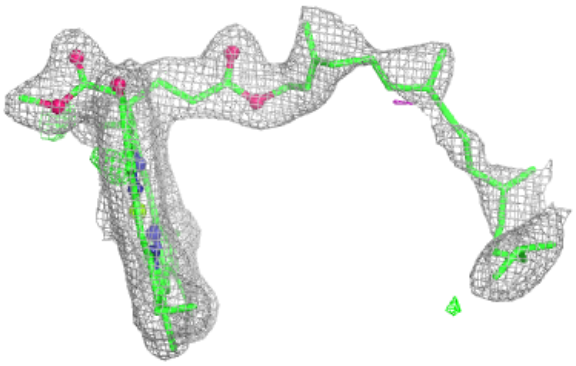


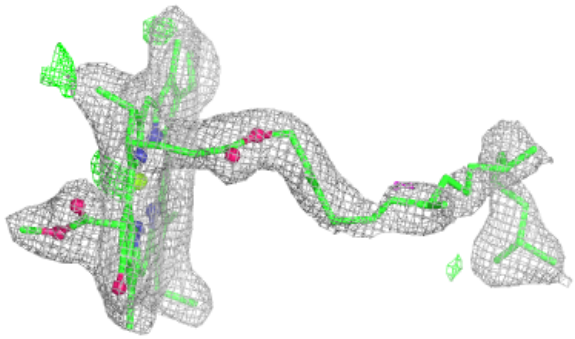


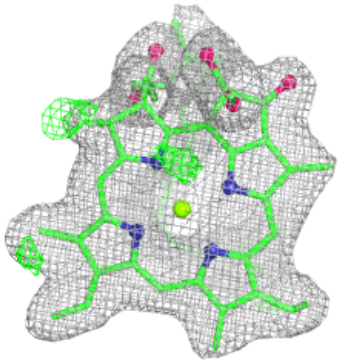


Electron density around CLA c 508:

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

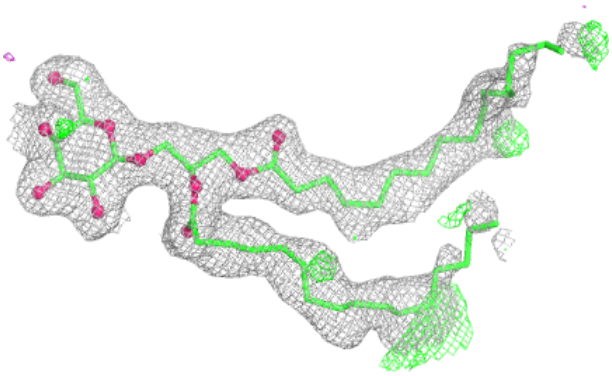


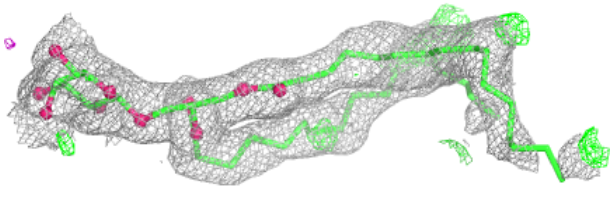


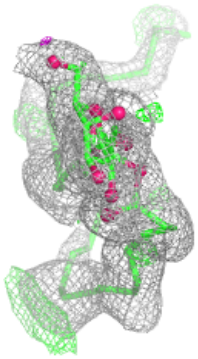


Electron density around LMG j 101:

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

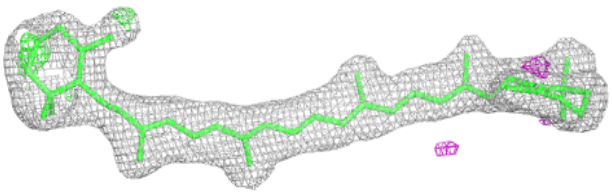


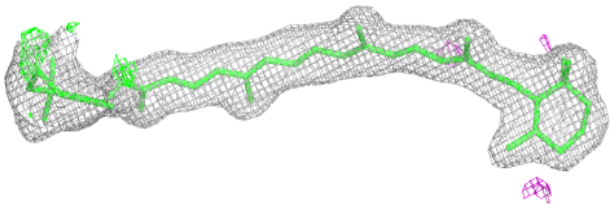


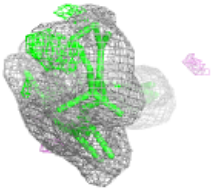


Electron density around BCR d 405:

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

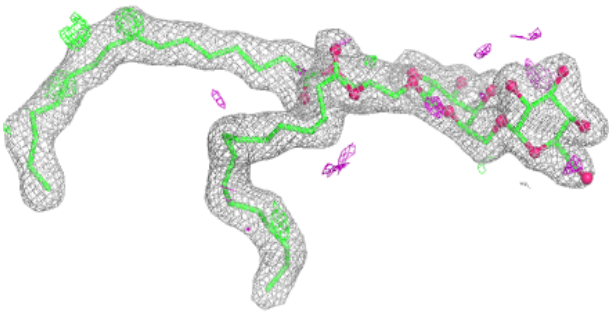


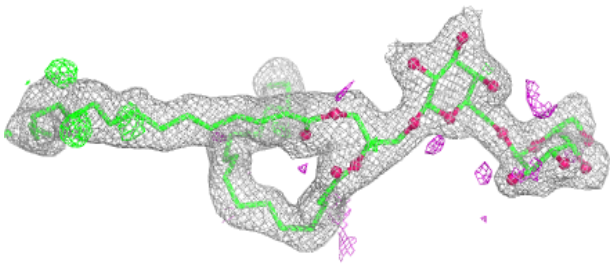


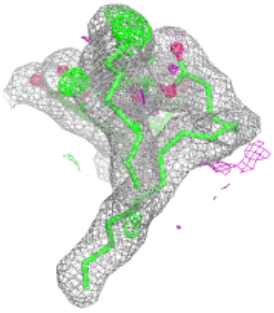


Electron density around DGD H 102:

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

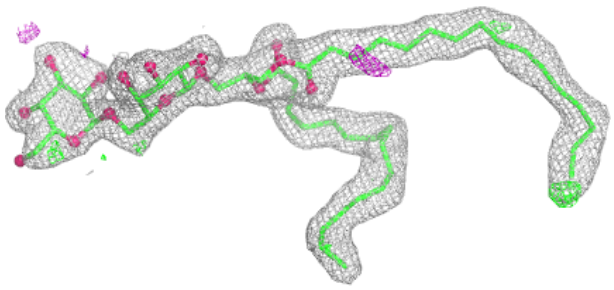


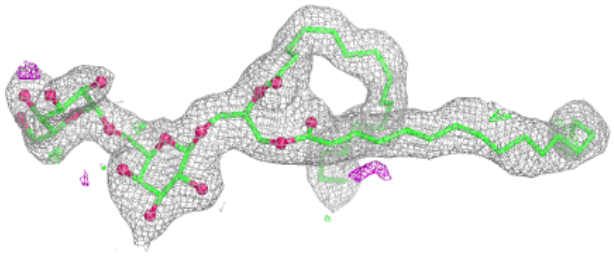


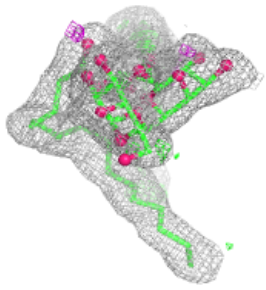


Electron density around DGD h 102:

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

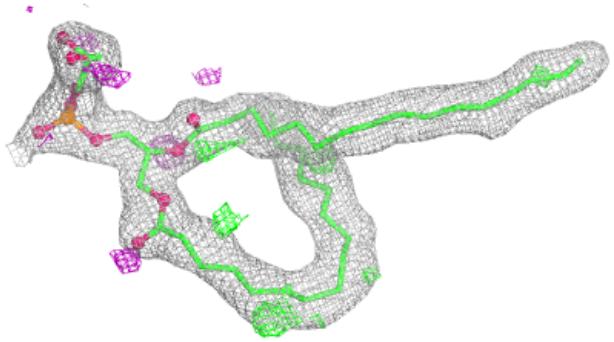


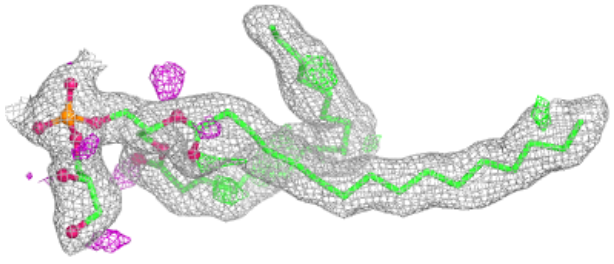




Electron density around LHG D 408:

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

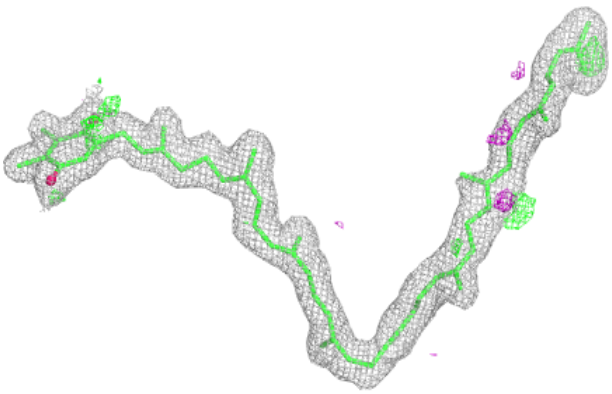


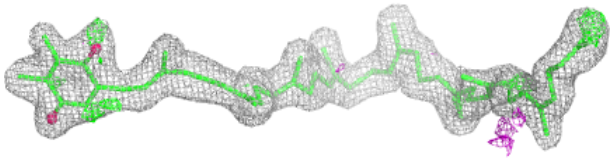




Electron density around PL9 d 406:

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

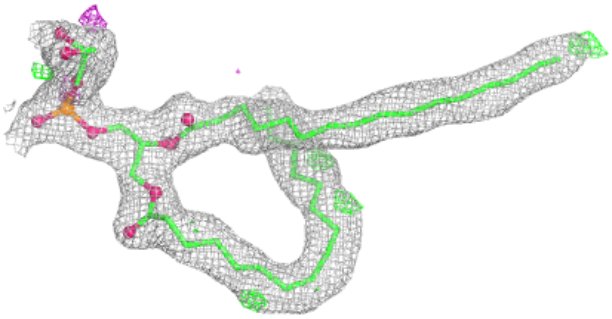


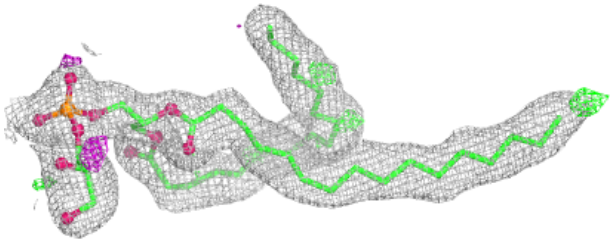


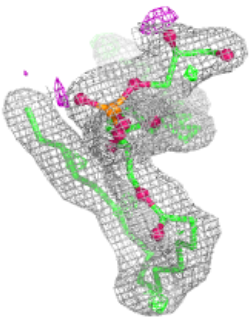


Electron density around LHG d 408:

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

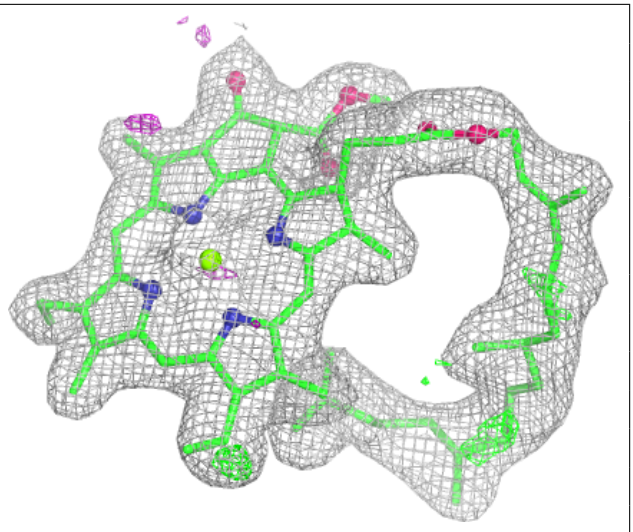


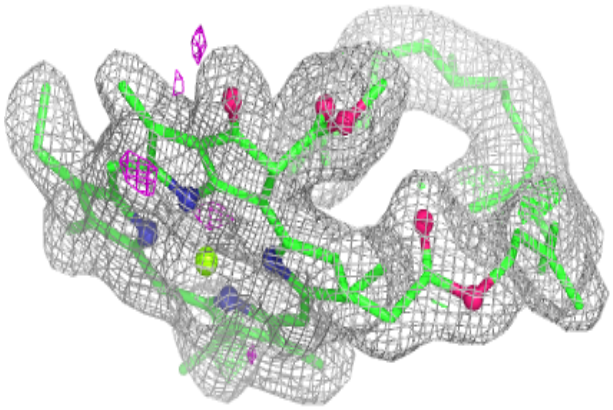


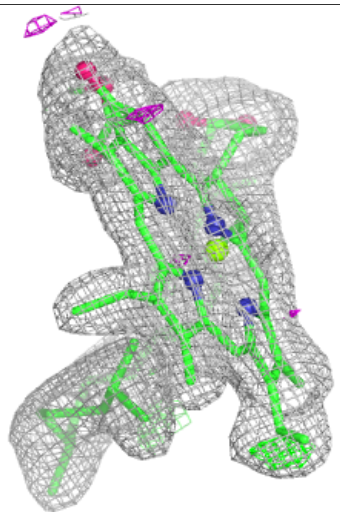


Electron density around CLA b 620:

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

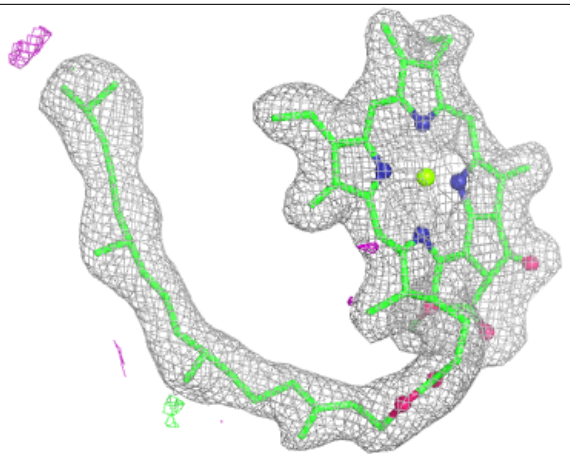


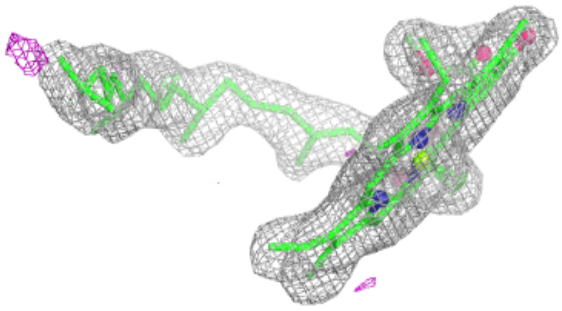


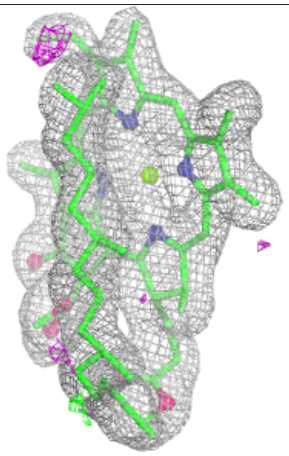


Electron density around CLA C 508:

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

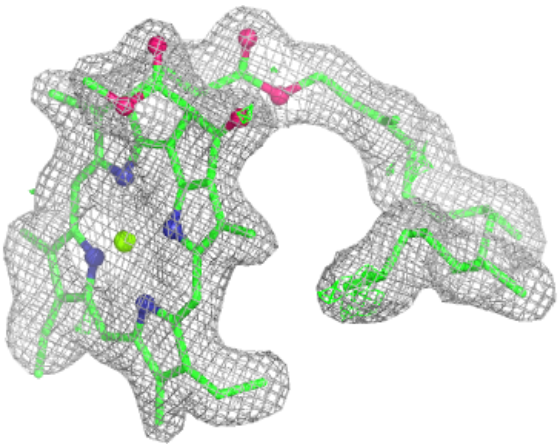


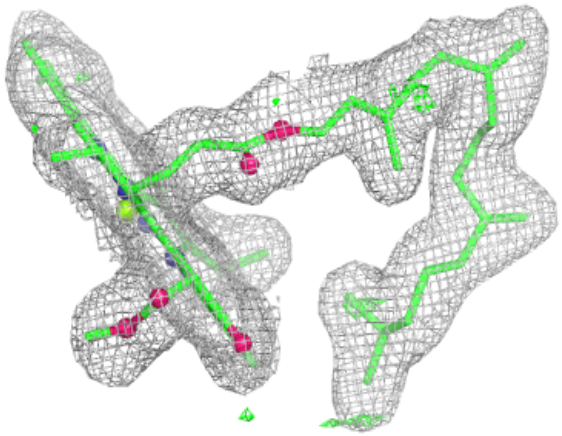


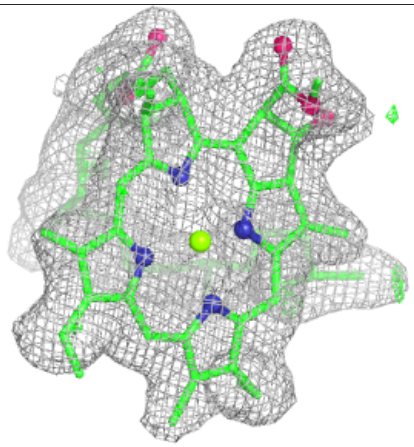


Electron density around CLA c 505:

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

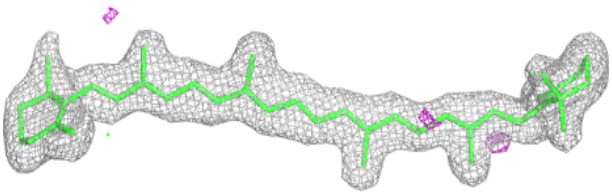


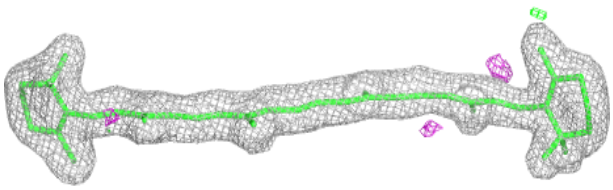


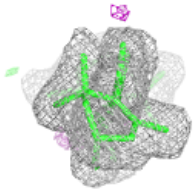


Electron density around BCR a 410:

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

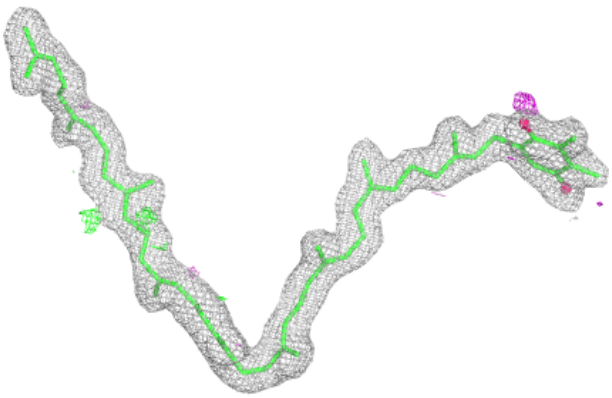


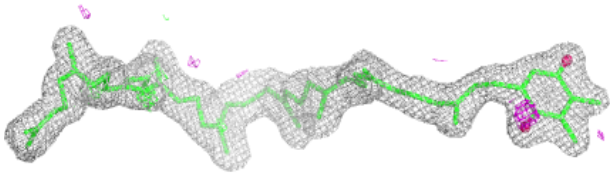


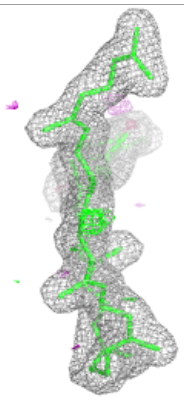


Electron density around PL9 D 406:

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

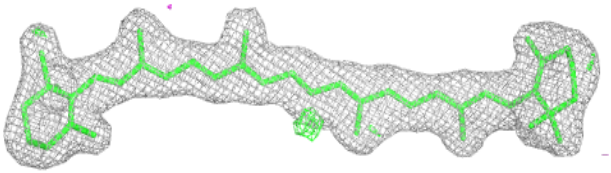


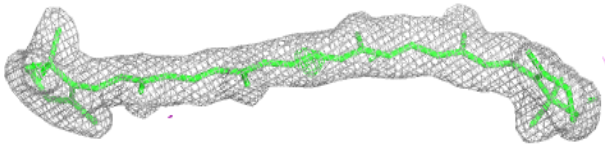


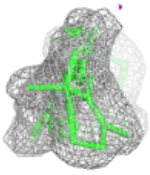


Electron density around BCR b 624:

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

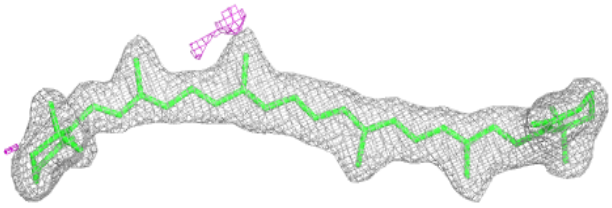


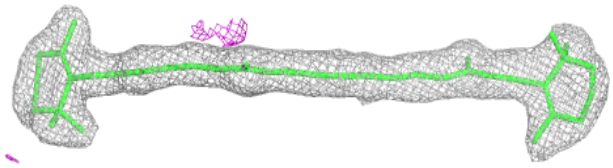


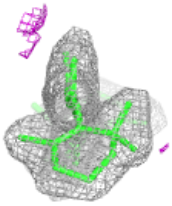


Electron density around BCR c 516:

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

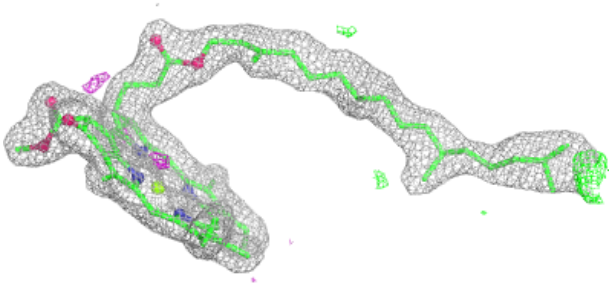


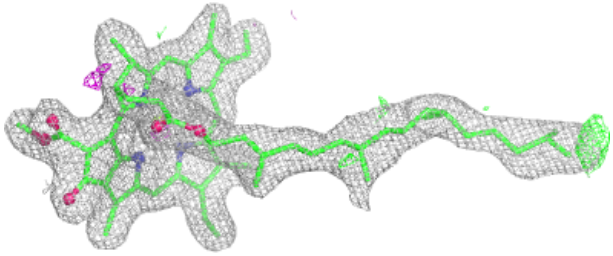


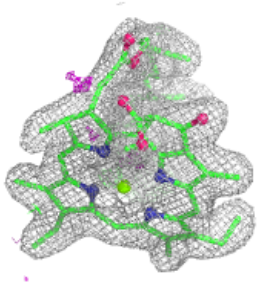


Electron density around CLA c 506:

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

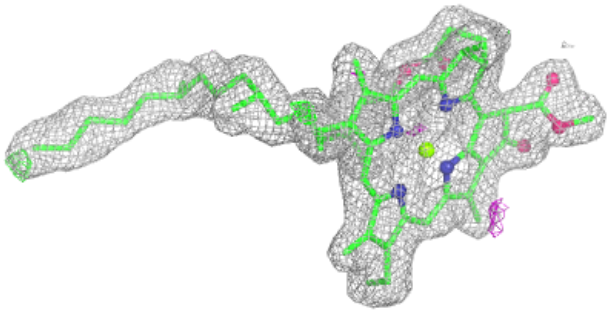


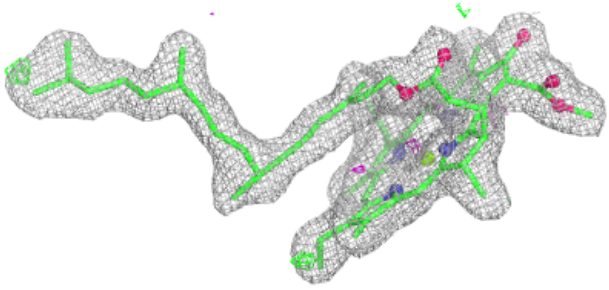


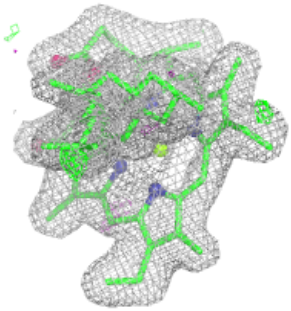


Electron density around CLA c 507:

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

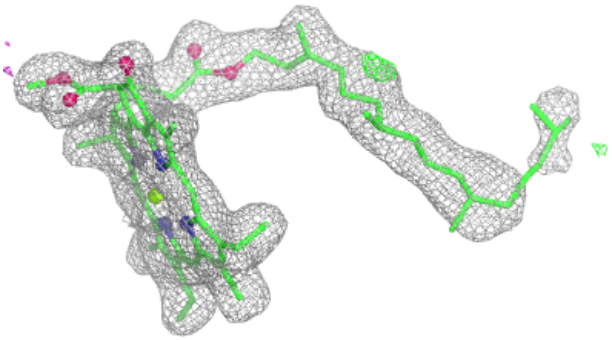


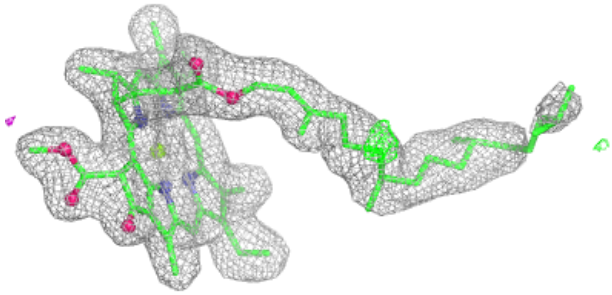


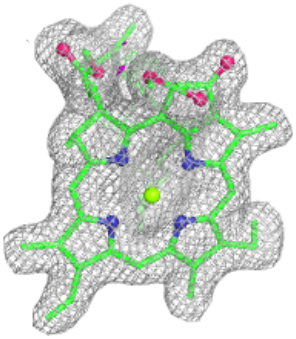


Electron density around CLA C 509:

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

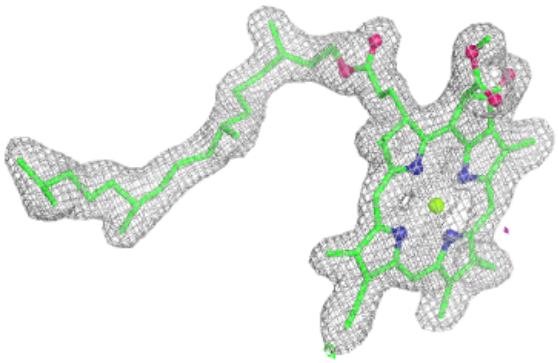


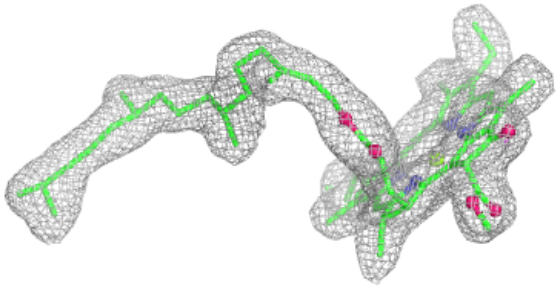


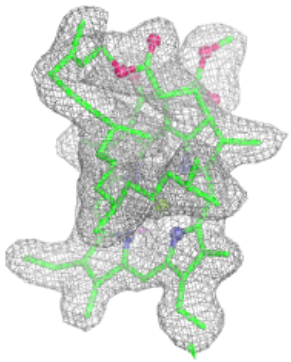


Electron density around CLA C 512:

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

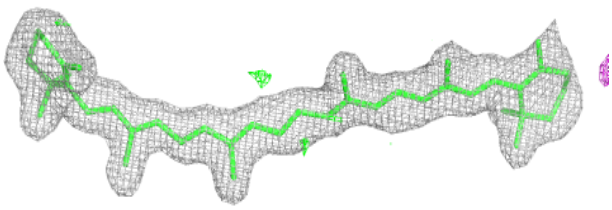


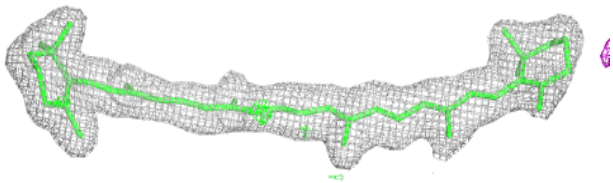


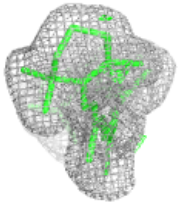


Electron density around BCR t 101:

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

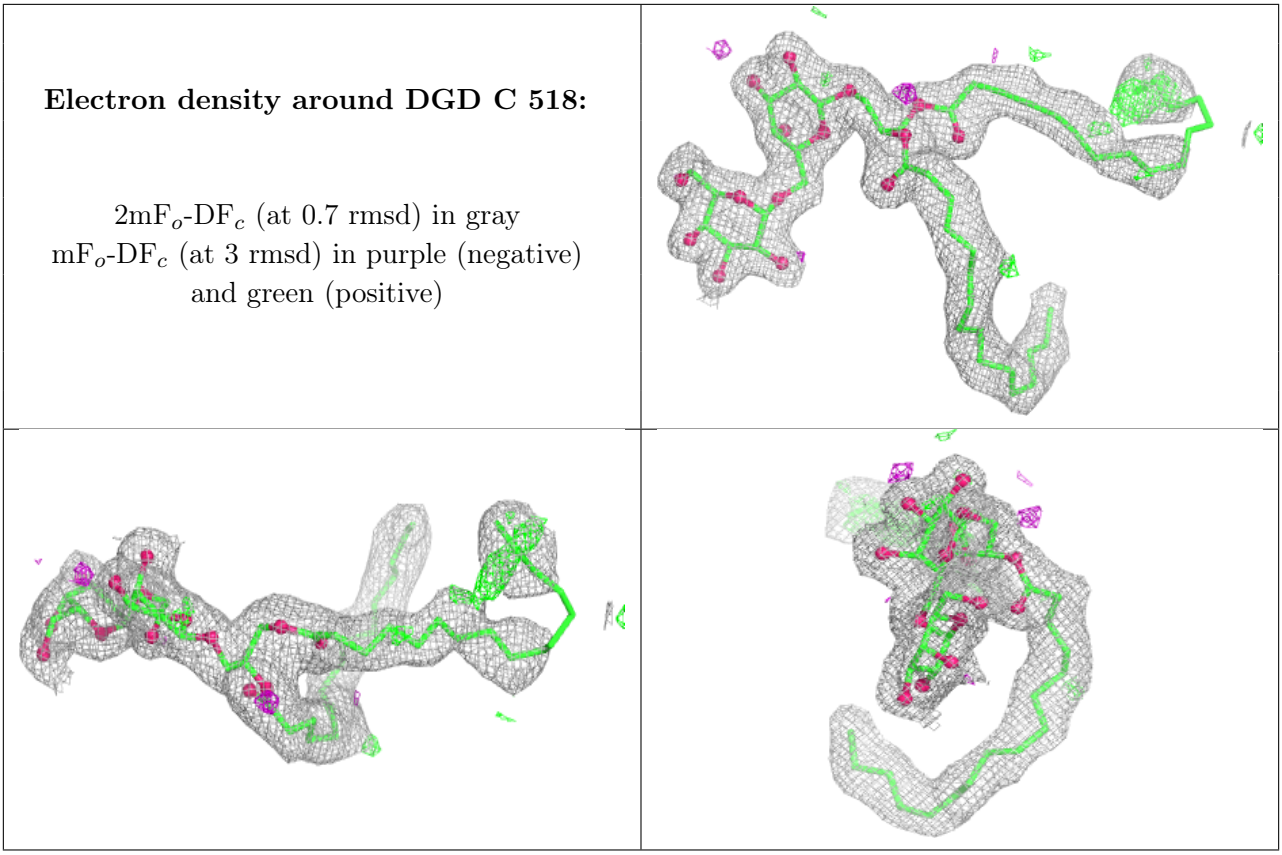






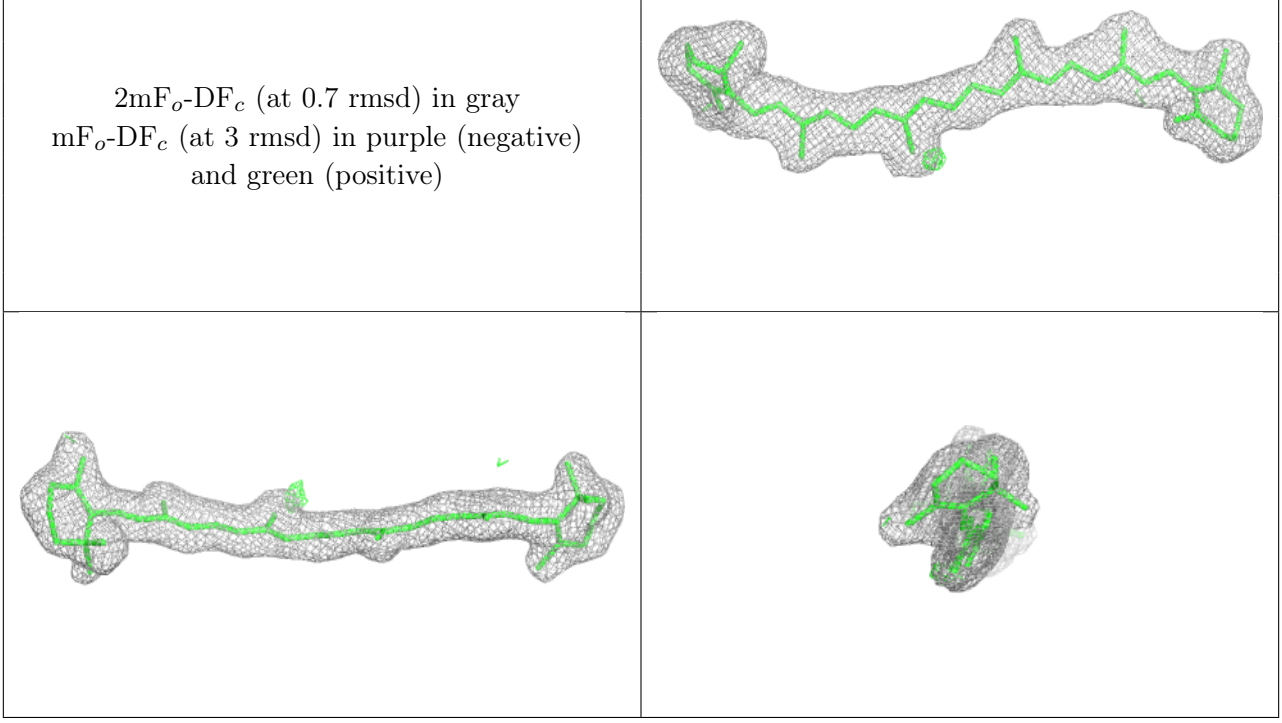
Electron density around DGD C 518:

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



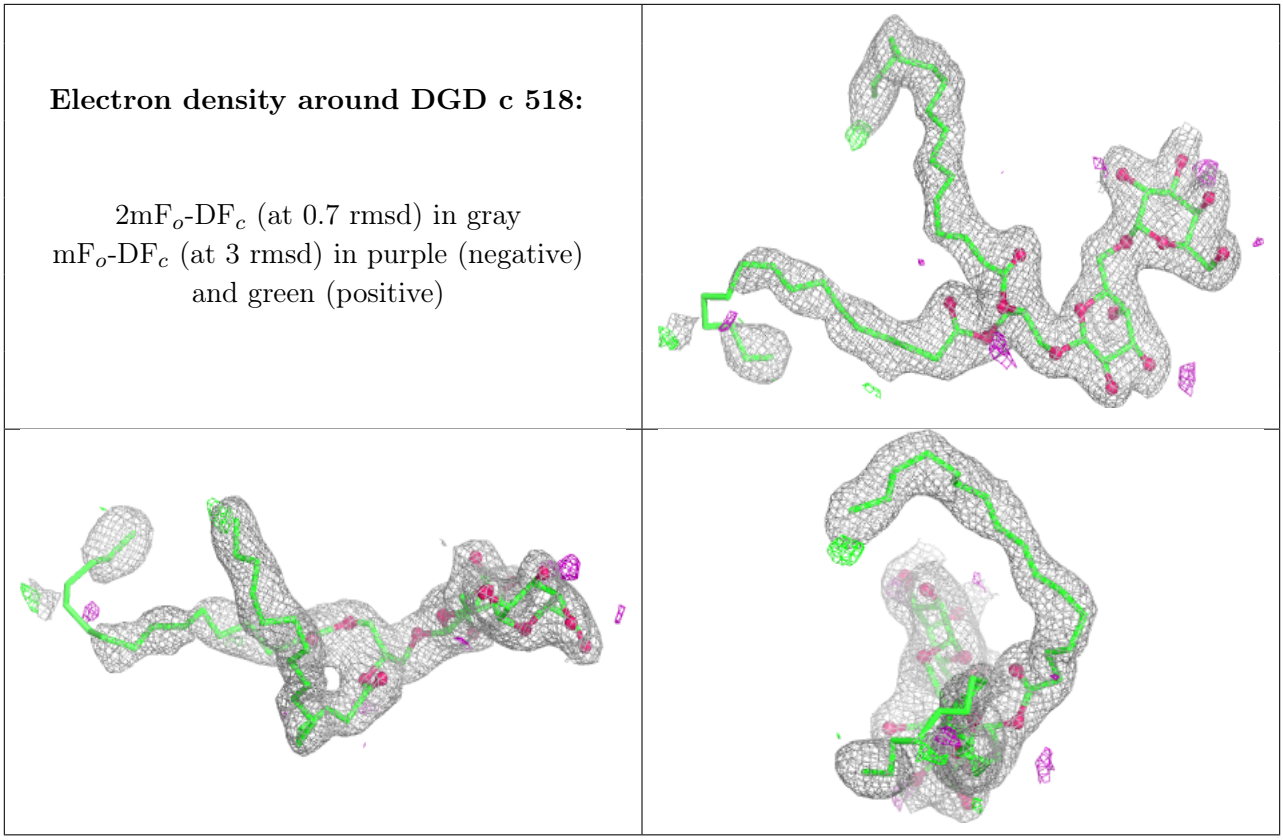
Electron density around BCR y 101:

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



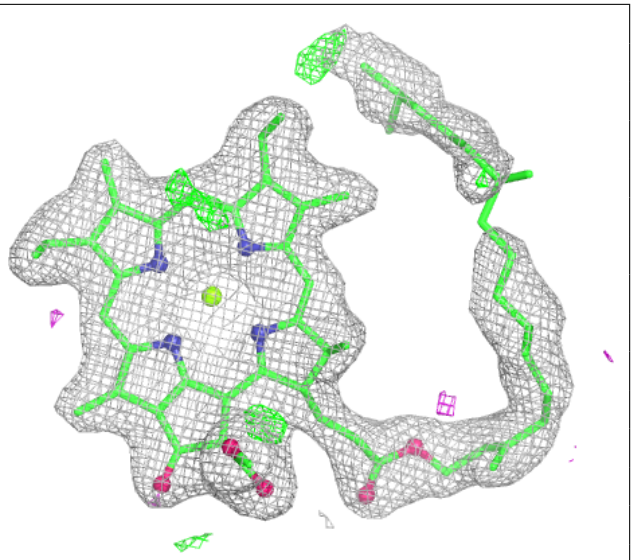
Electron density around DGD c 518:

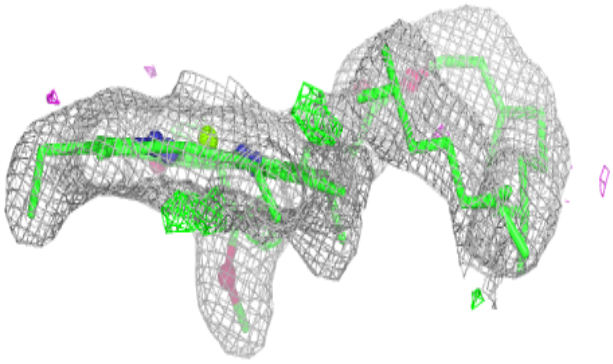
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

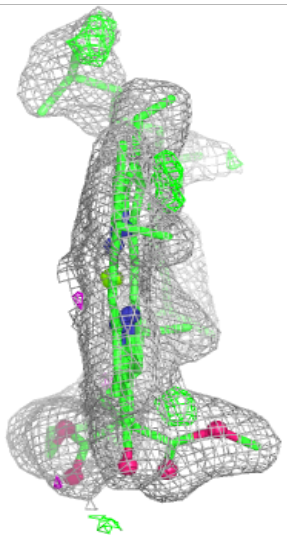


Electron density around CLA C 513:

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

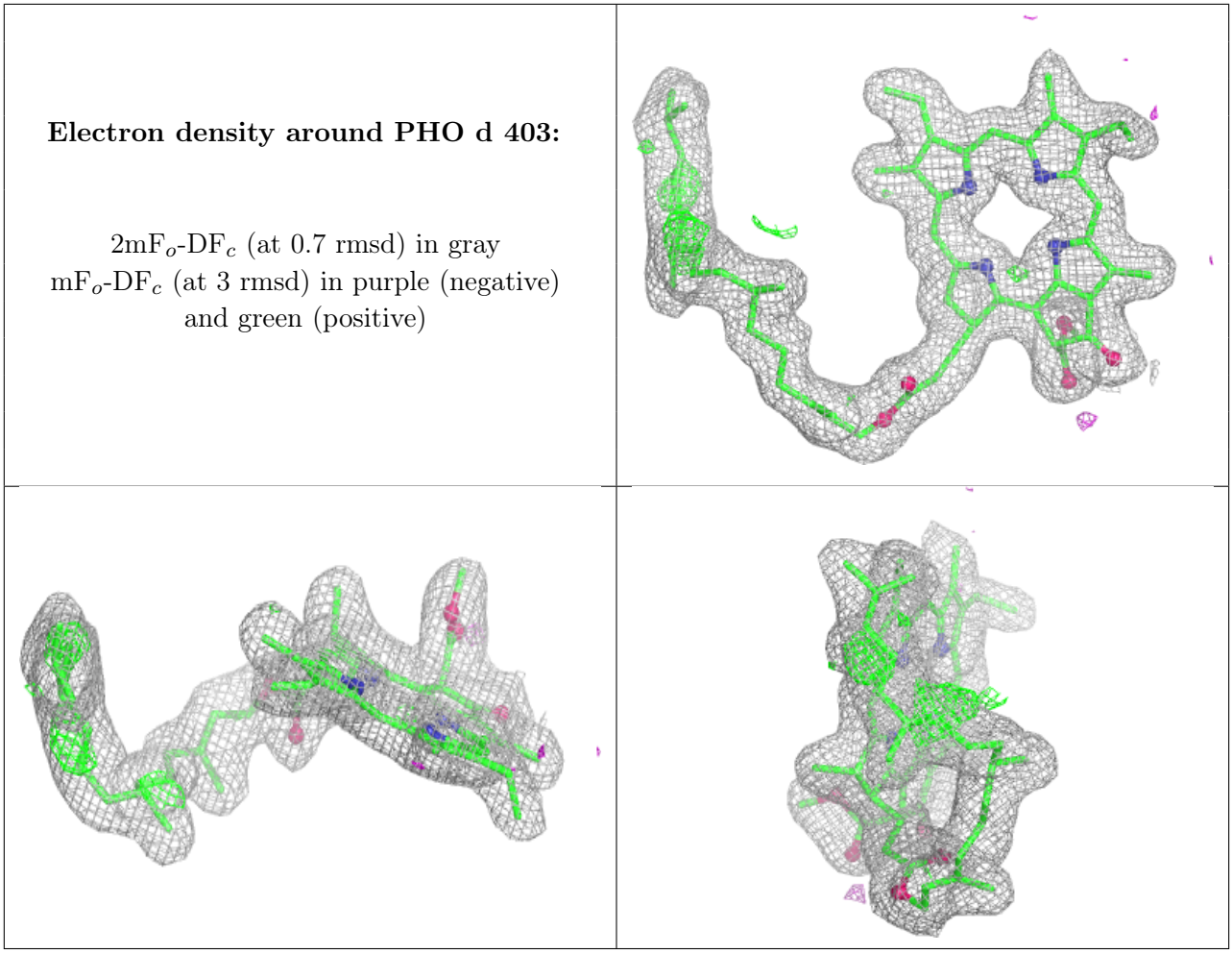






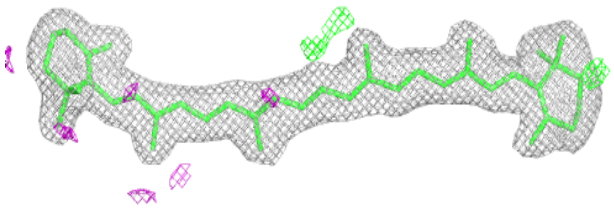
Electron density around PHO d 403:

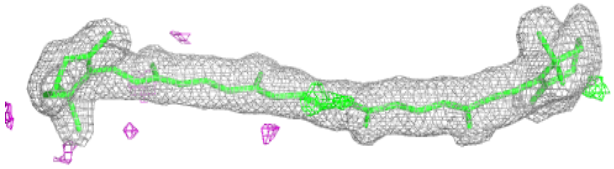
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

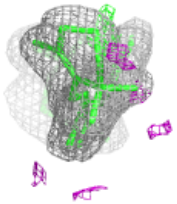


Electron density around BCR B 620:

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

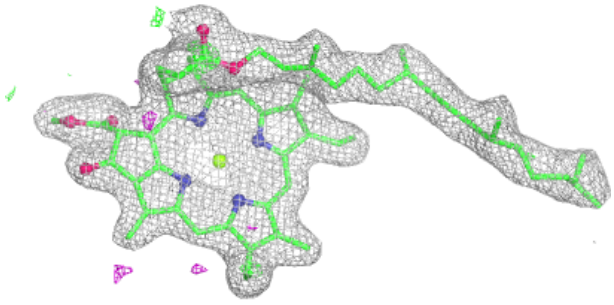


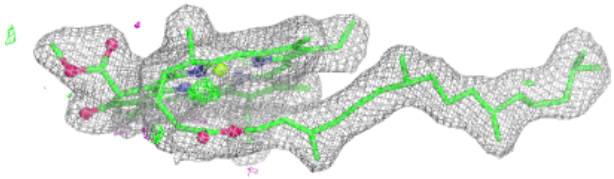


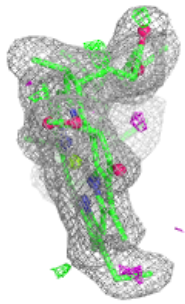


Electron density around CLA C 502:

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

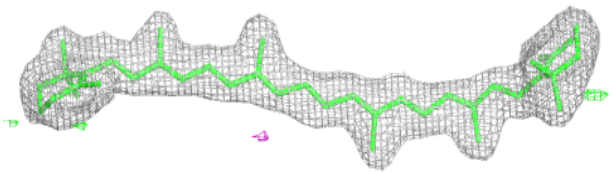


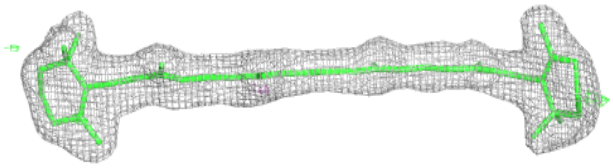


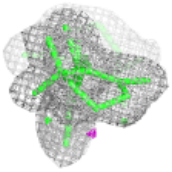


Electron density around BCR C 516:

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

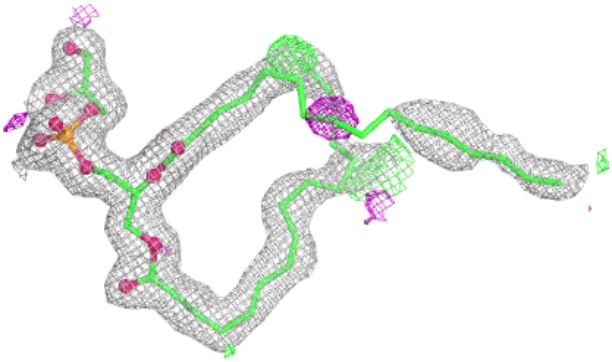


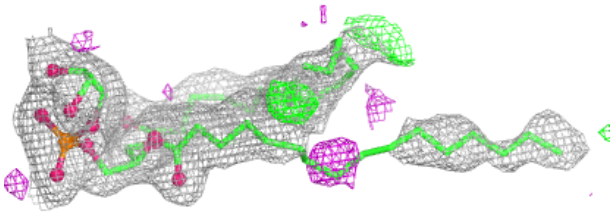


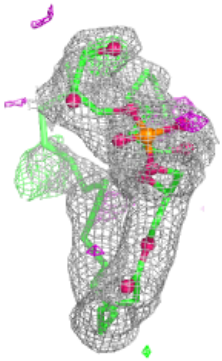


Electron density around LHG d 410:

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

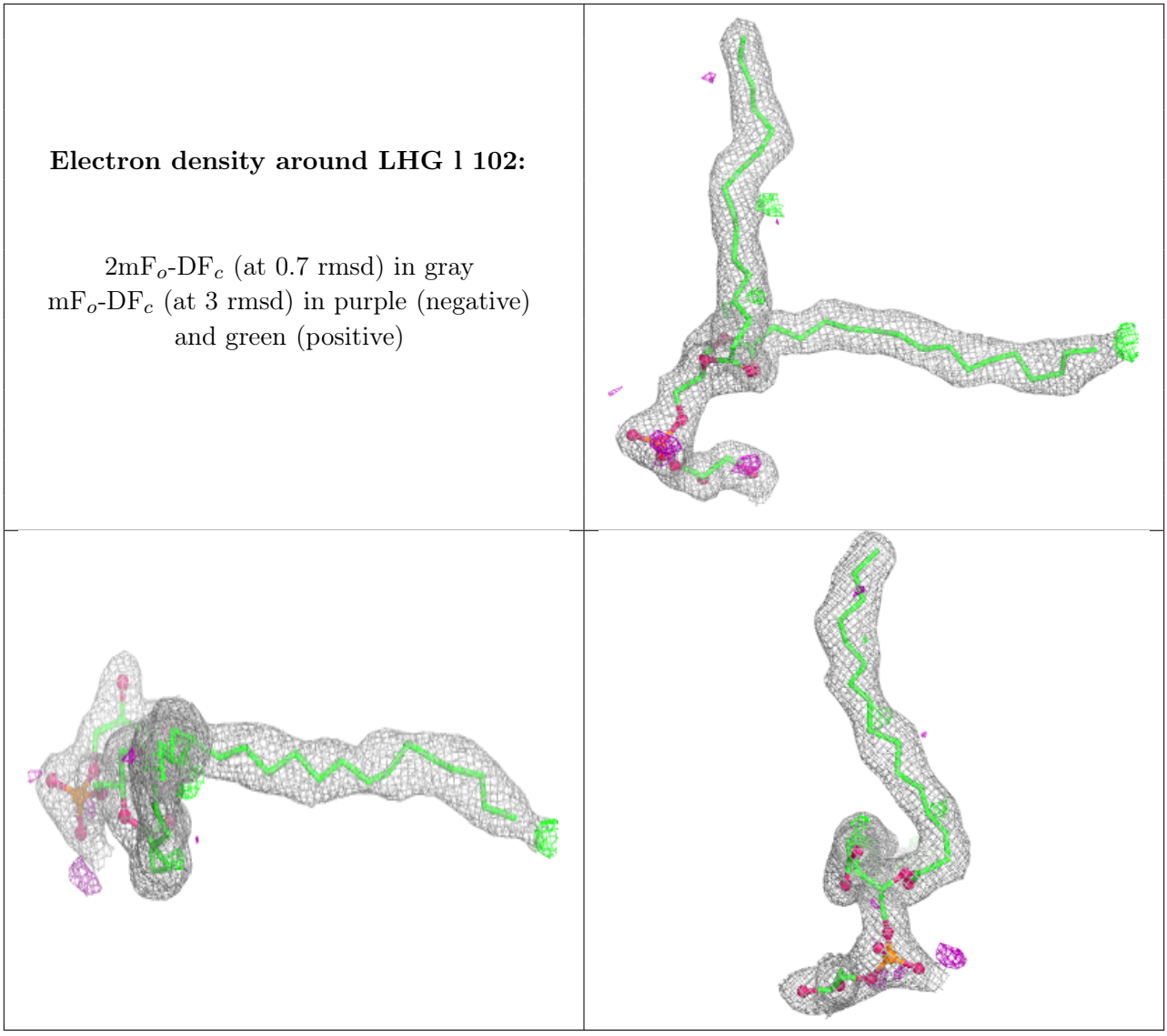






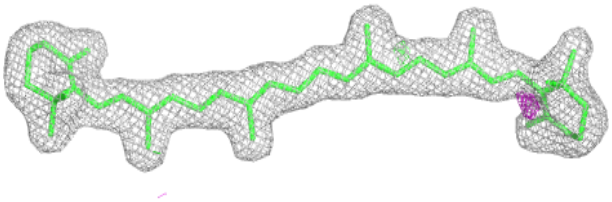
Electron density around LHG l 102:

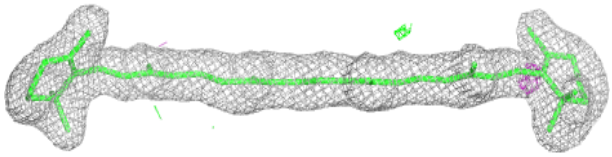
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

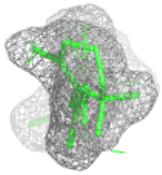


Electron density around BCR B 619:

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

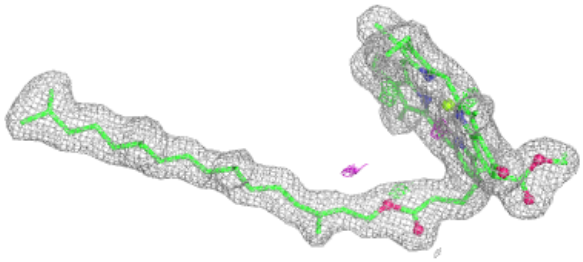


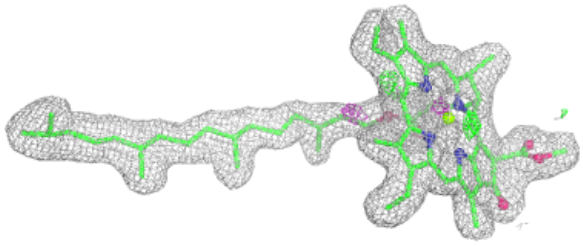


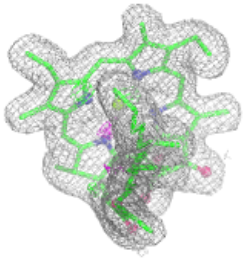


Electron density around CLA b 612:

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

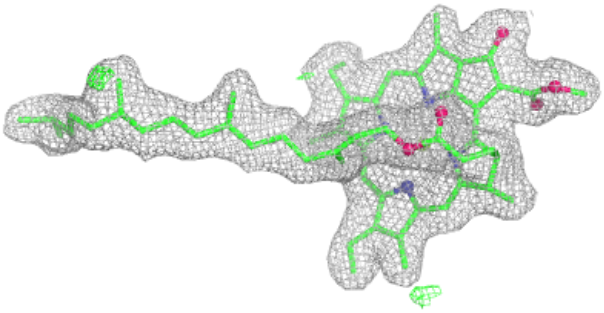


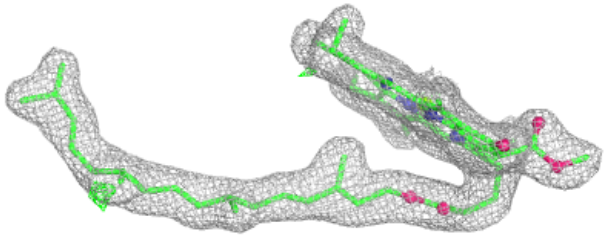


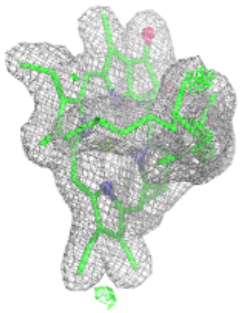


Electron density around CLA b 613:

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

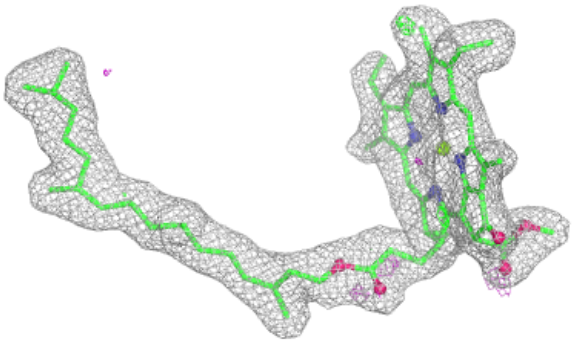


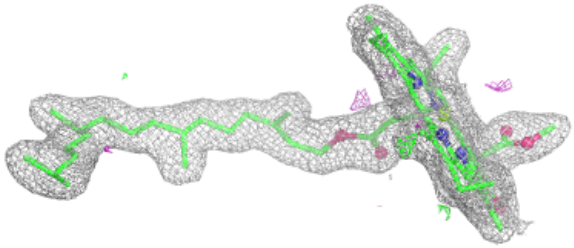


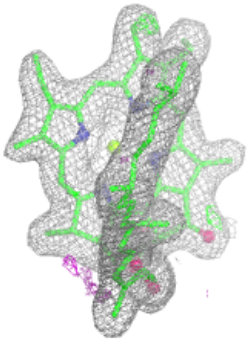


Electron density around CLA b 614:

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

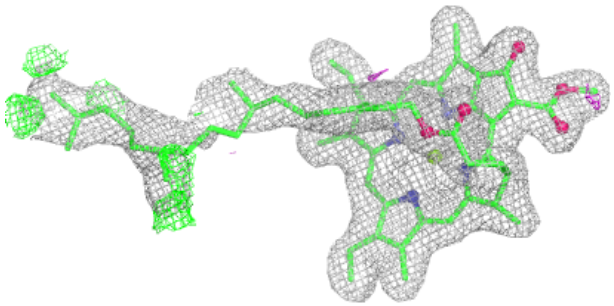


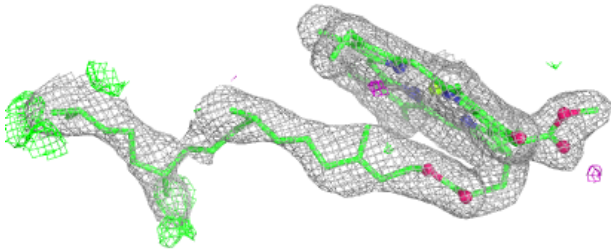


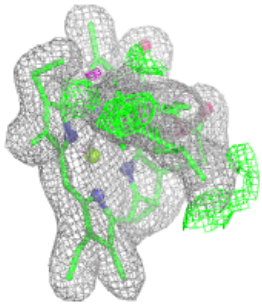


Electron density around CLA b 619:

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

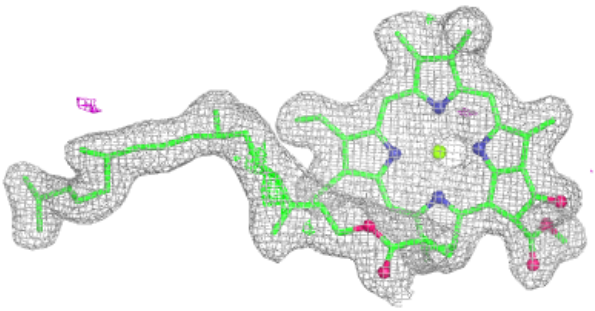


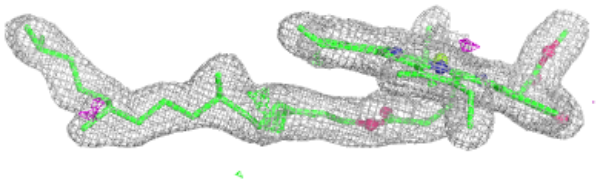


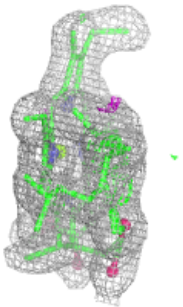


Electron density around CLA B 604:

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

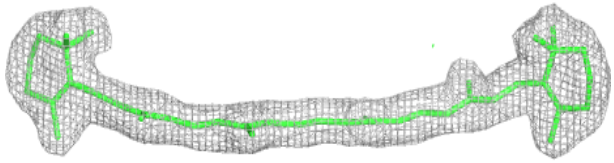


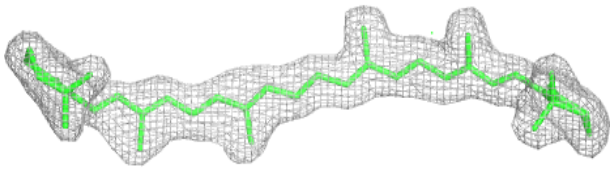


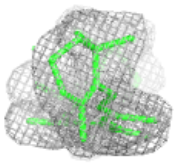


Electron density around BCR K 101:

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

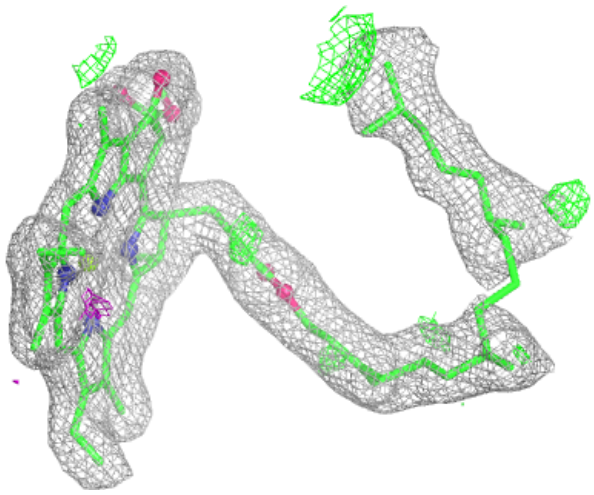


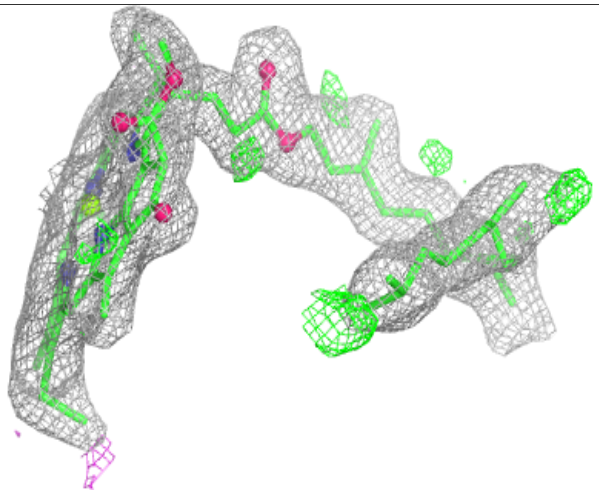


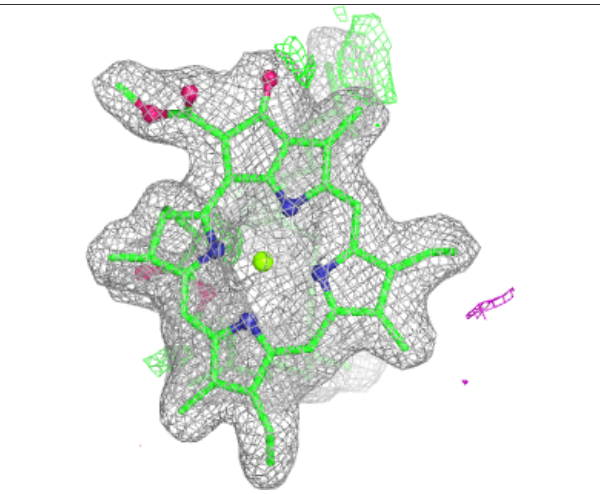


Electron density around CLA B 607:

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

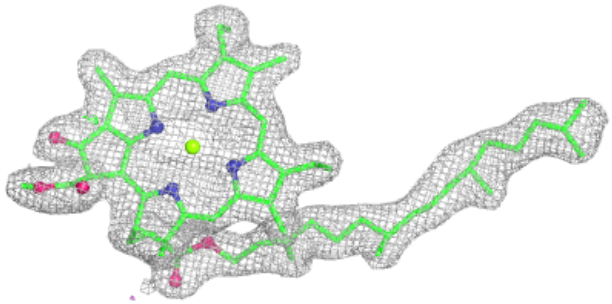


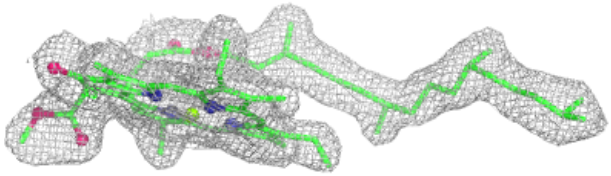


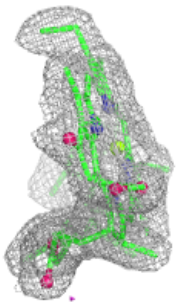


Electron density around CLA c 503:

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

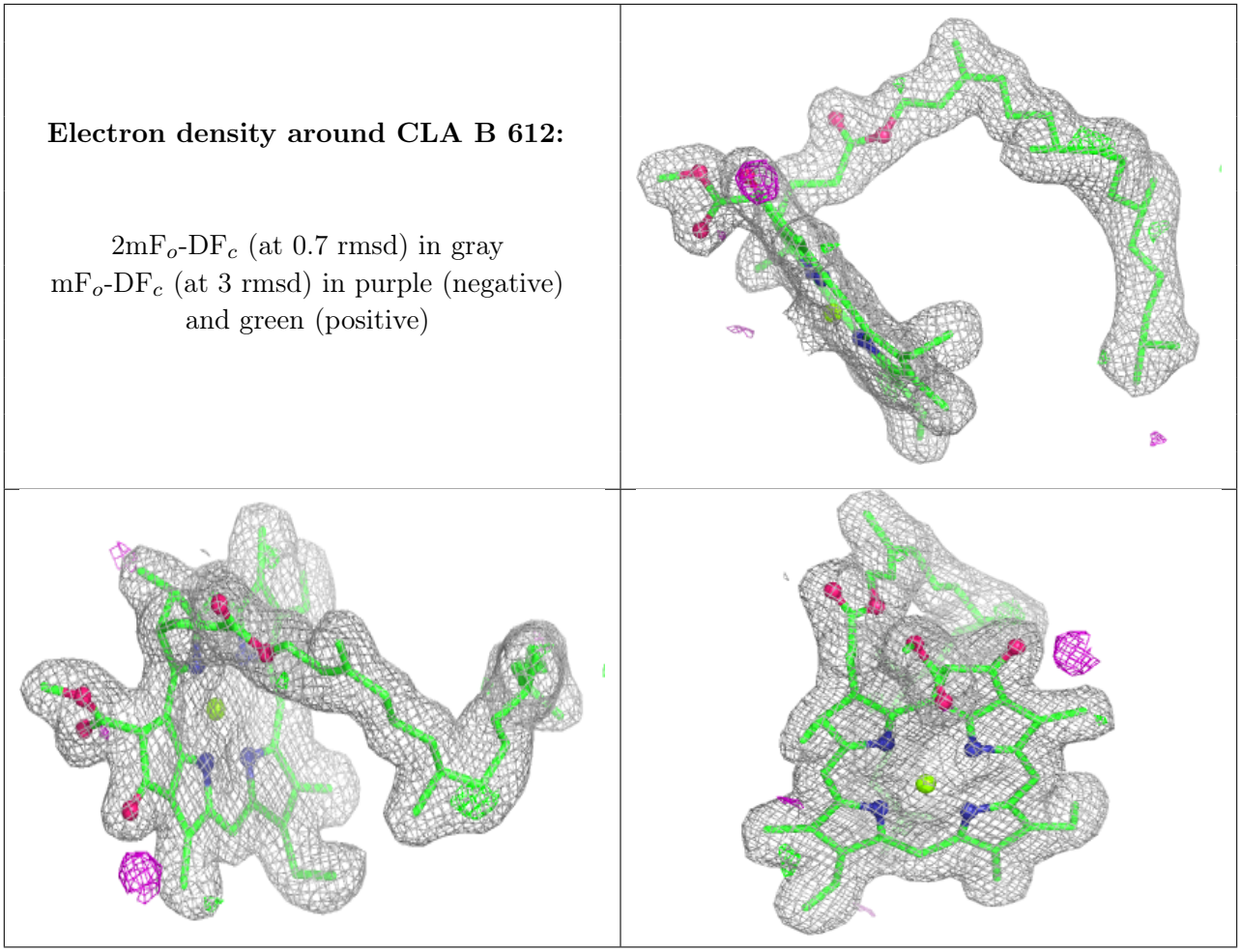






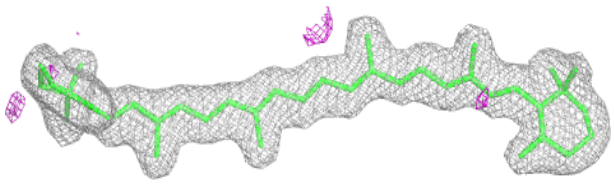
Electron density around CLA B 612:

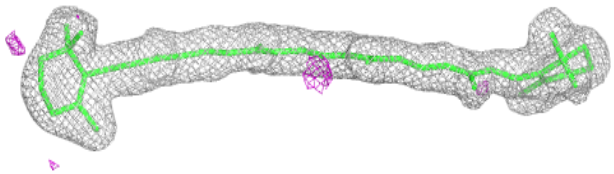
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

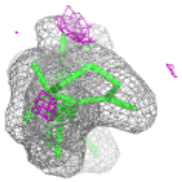


Electron density around BCR b 622:

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

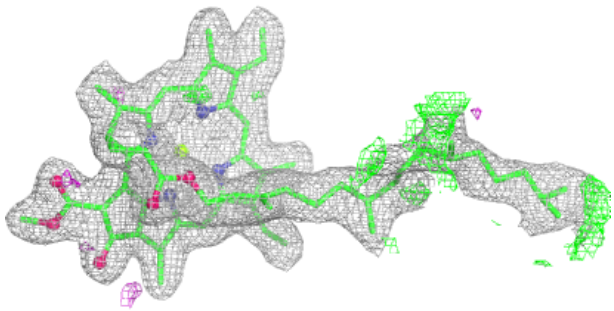


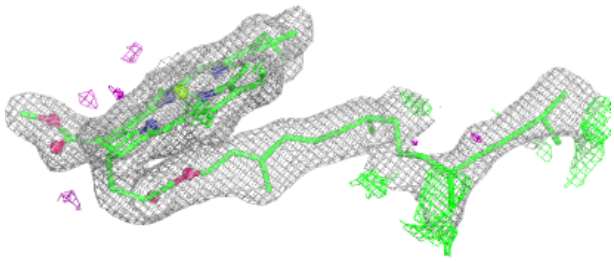


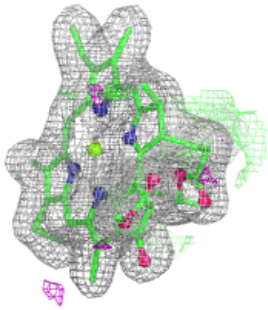


Electron density around CLA B 615:

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

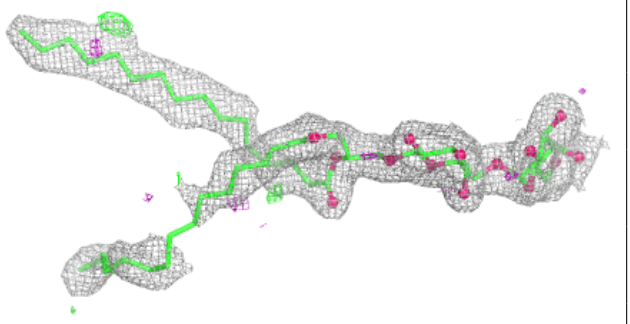


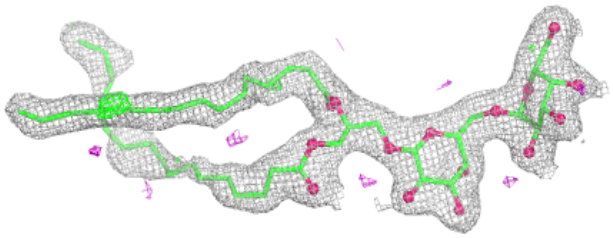


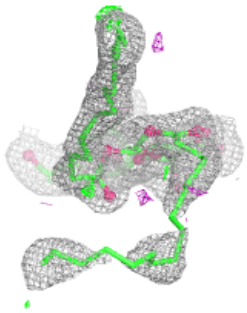


Electron density around DGD C 517:

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

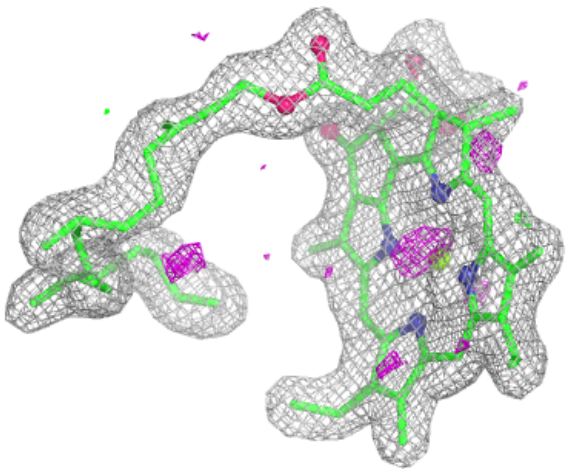


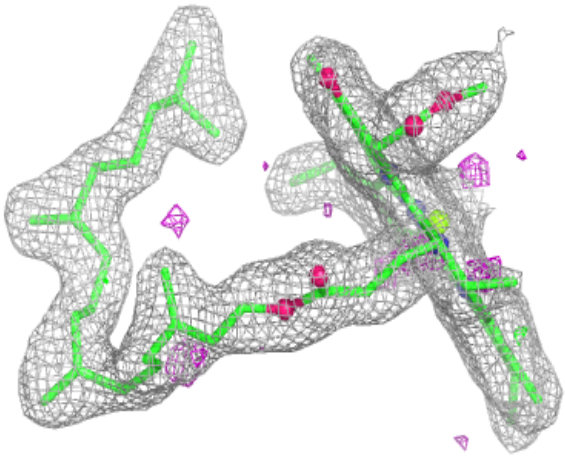


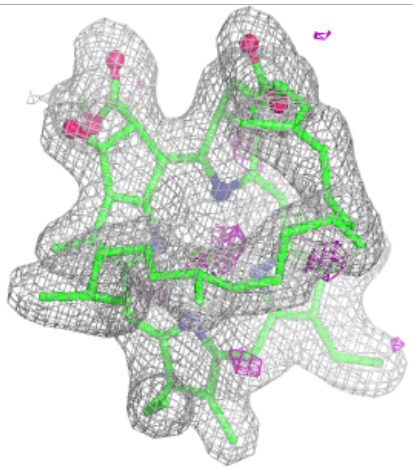


Electron density around CLA C 504:

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

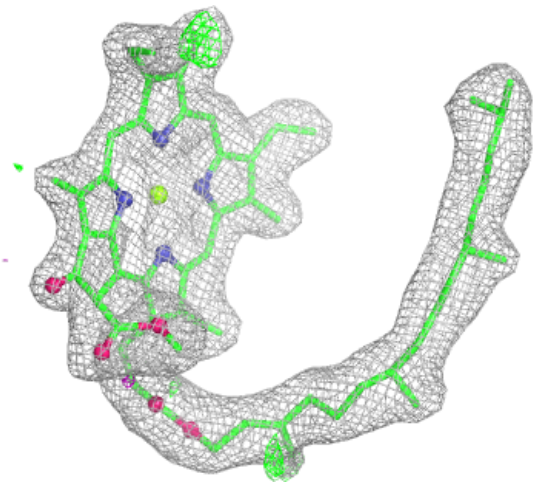


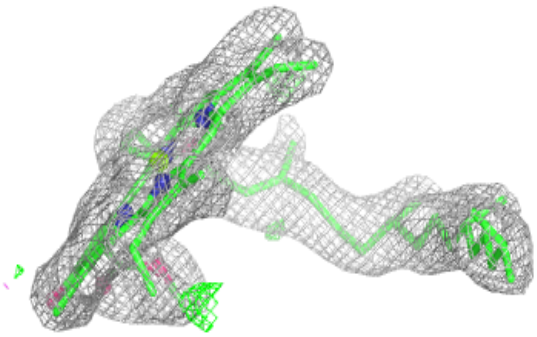


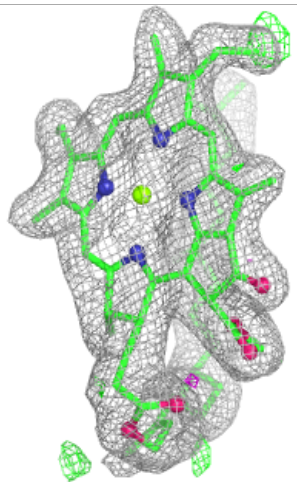


Electron density around CLA c 509:

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

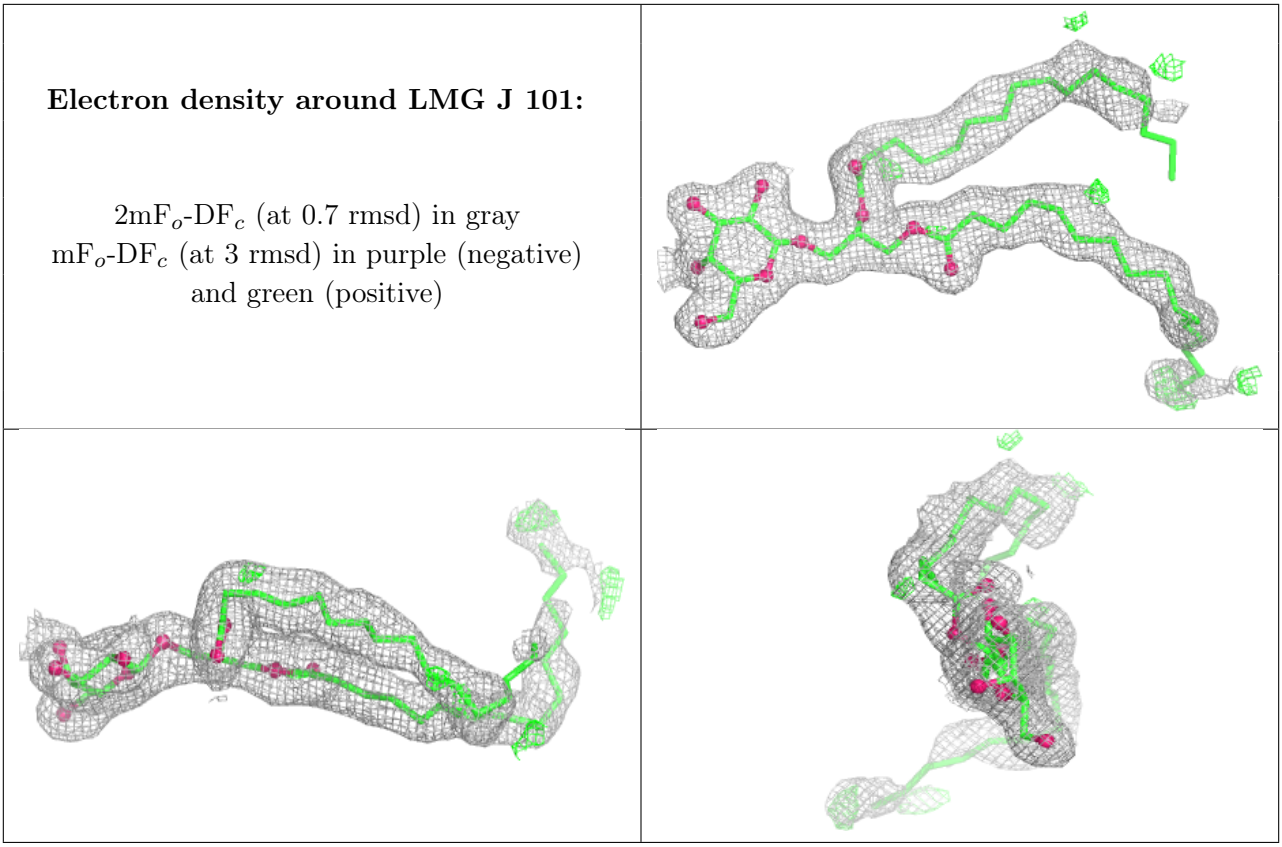






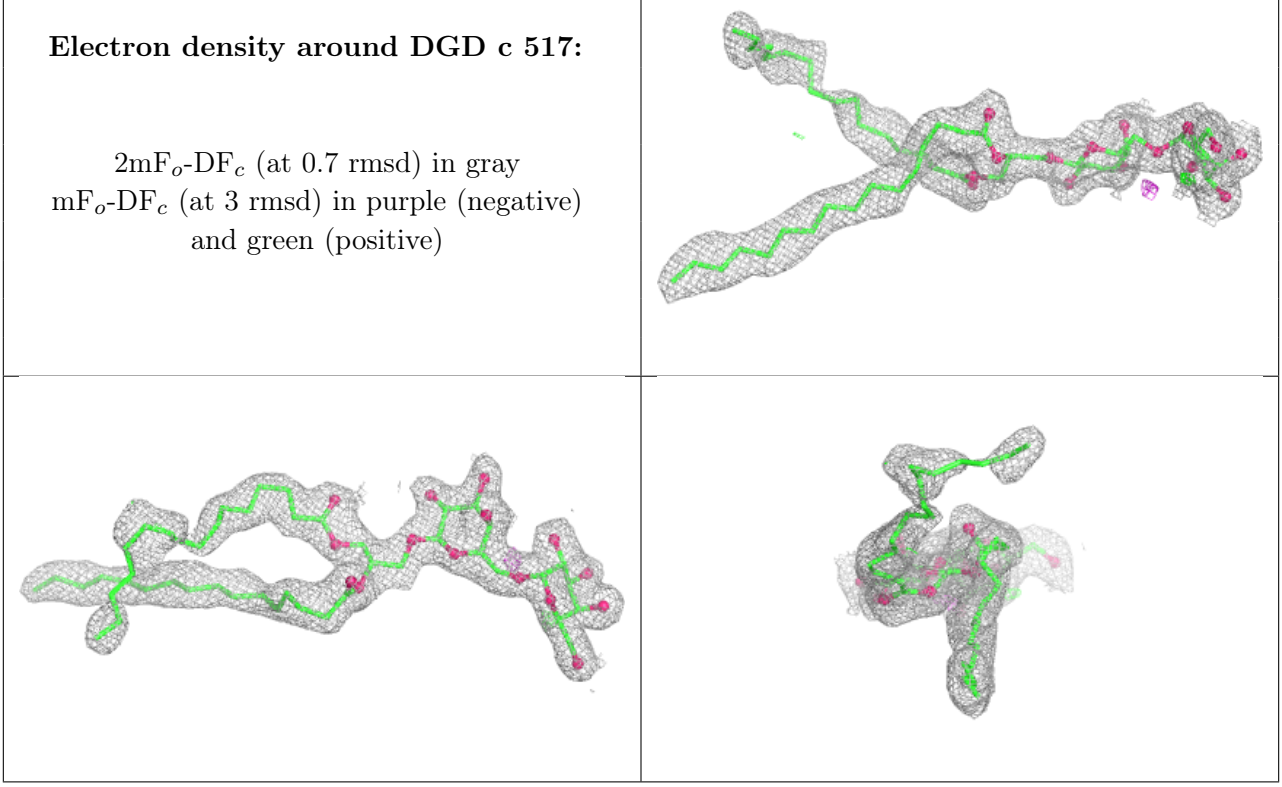
Electron density around LMG J 101:

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



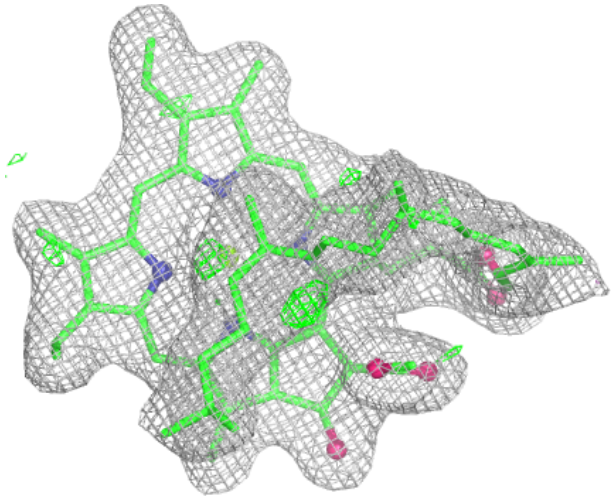
Electron density around DGD c 517:

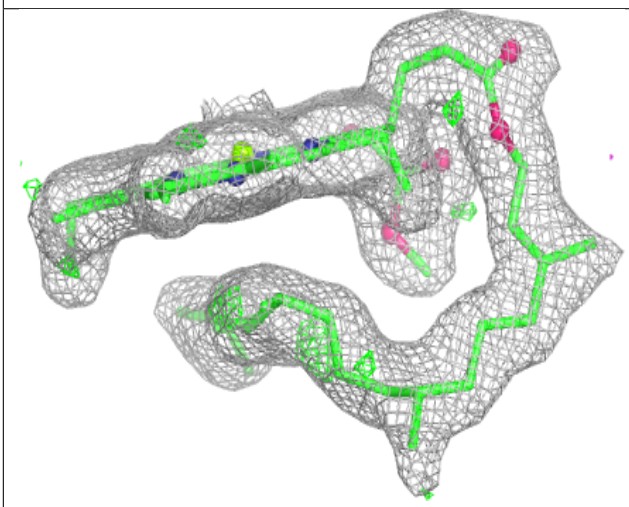
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA c 512:

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

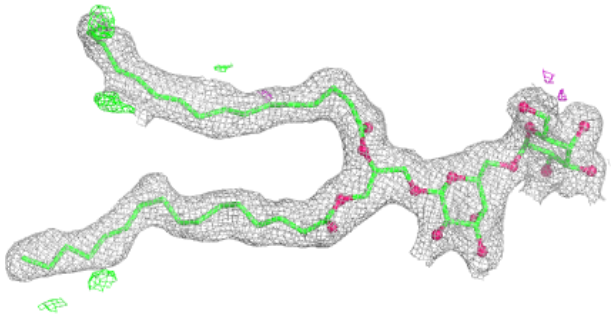


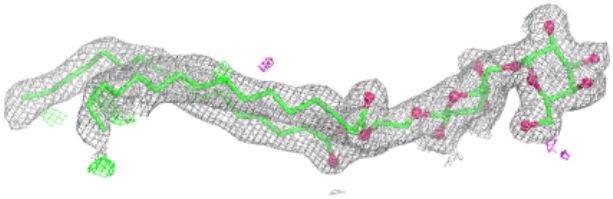


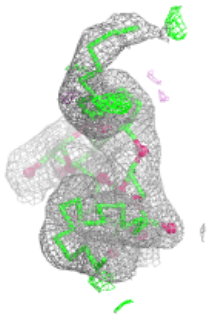


Electron density around DGD c 519:

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

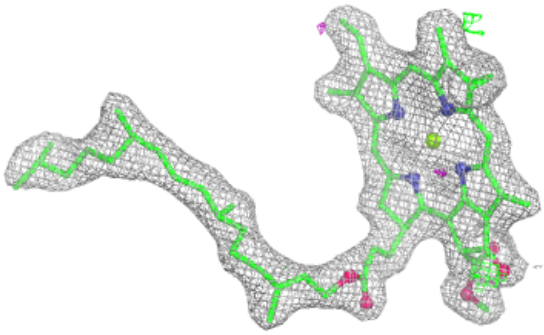


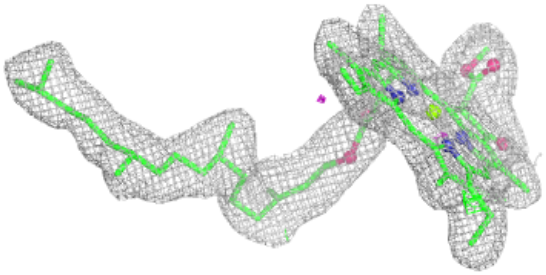


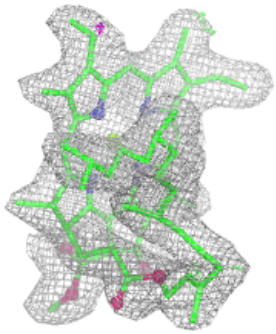


Electron density around CLA c 513:

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

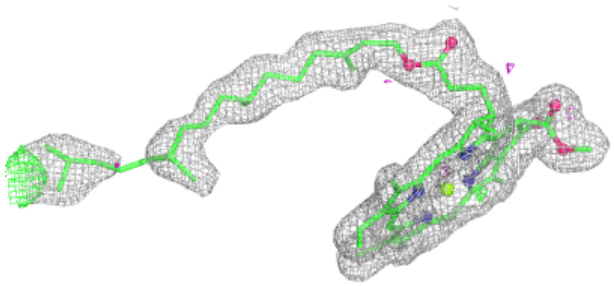


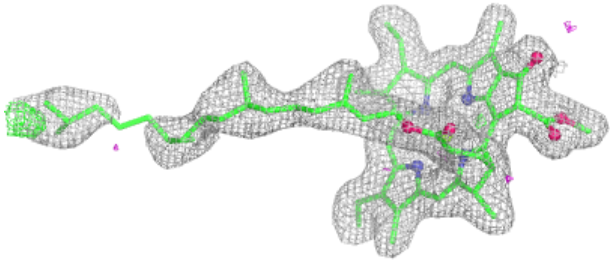


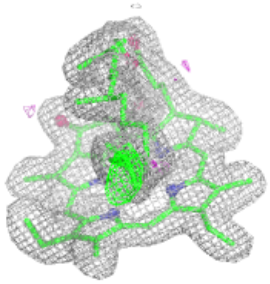


Electron density around CLA C 505:

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

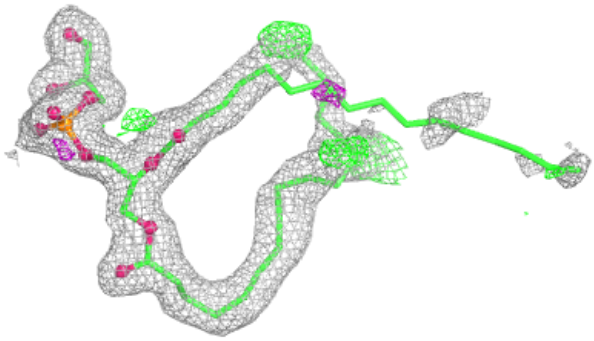


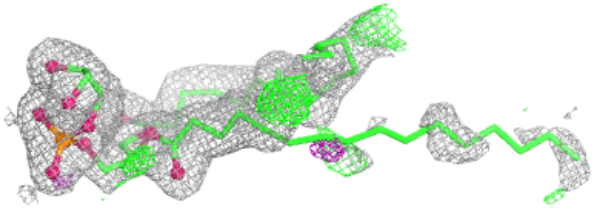


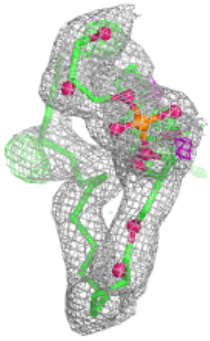


Electron density around LHG D 410:

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

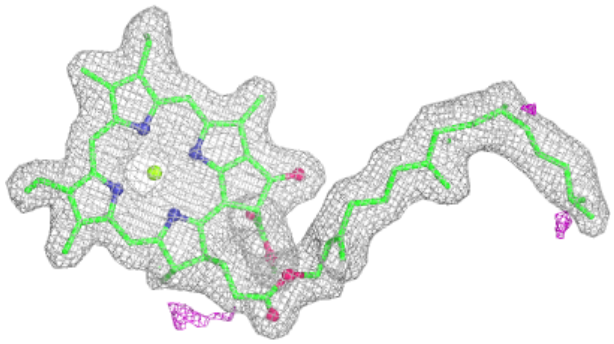


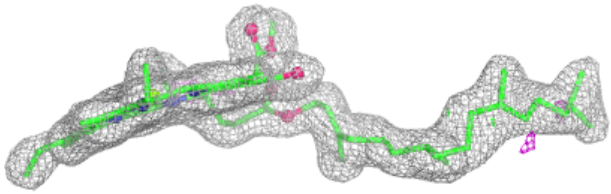


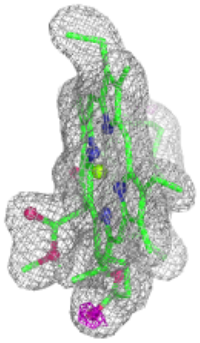


Electron density around CLA b 607:

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

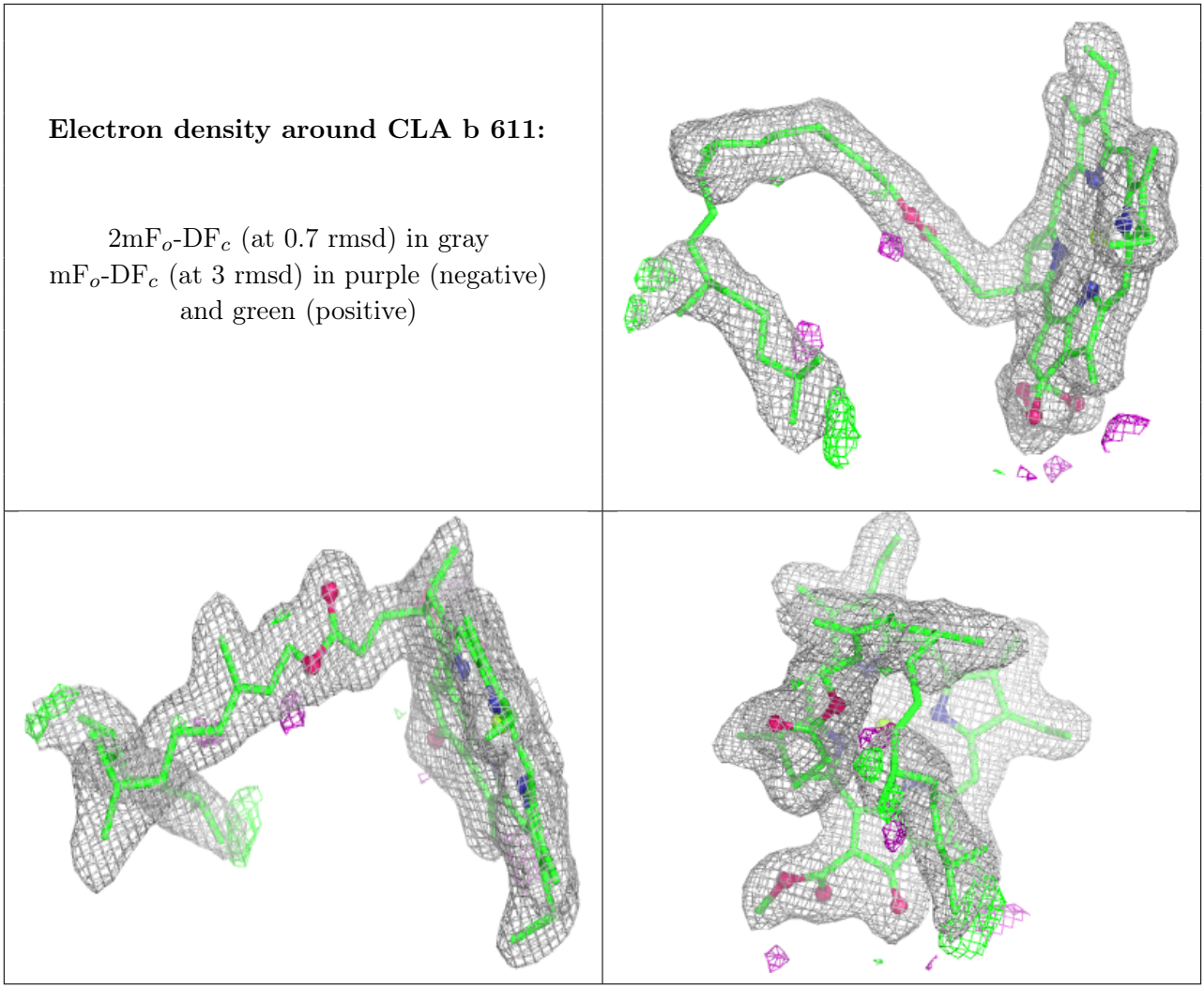






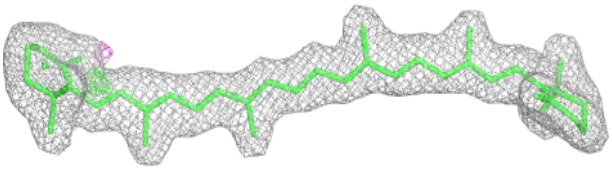
Electron density around CLA b 611:

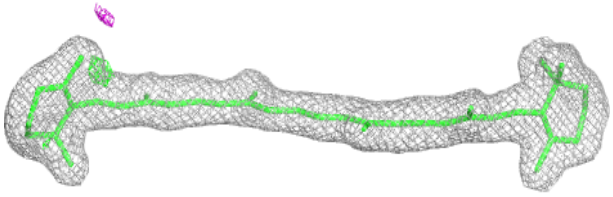
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

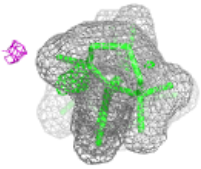


Electron density around BCR A 410:

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

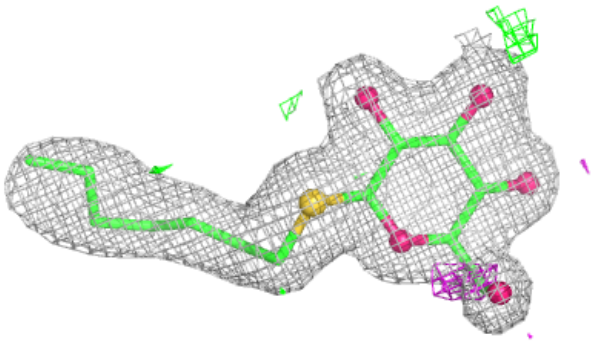


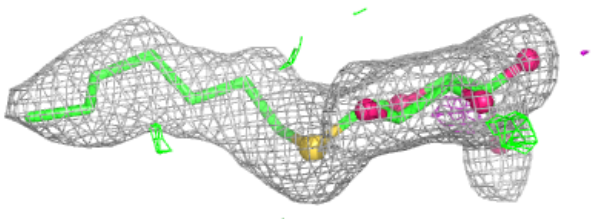


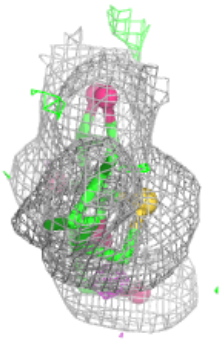


Electron density around HTG B 622:

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

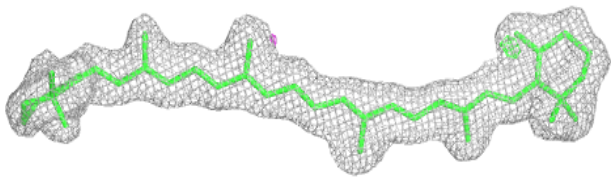


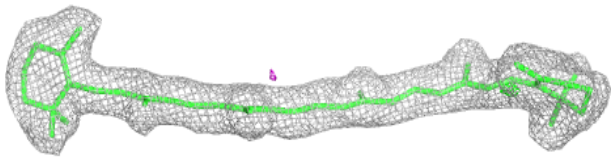


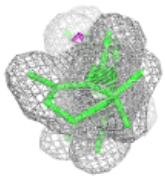


Electron density around BCR B 618:

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

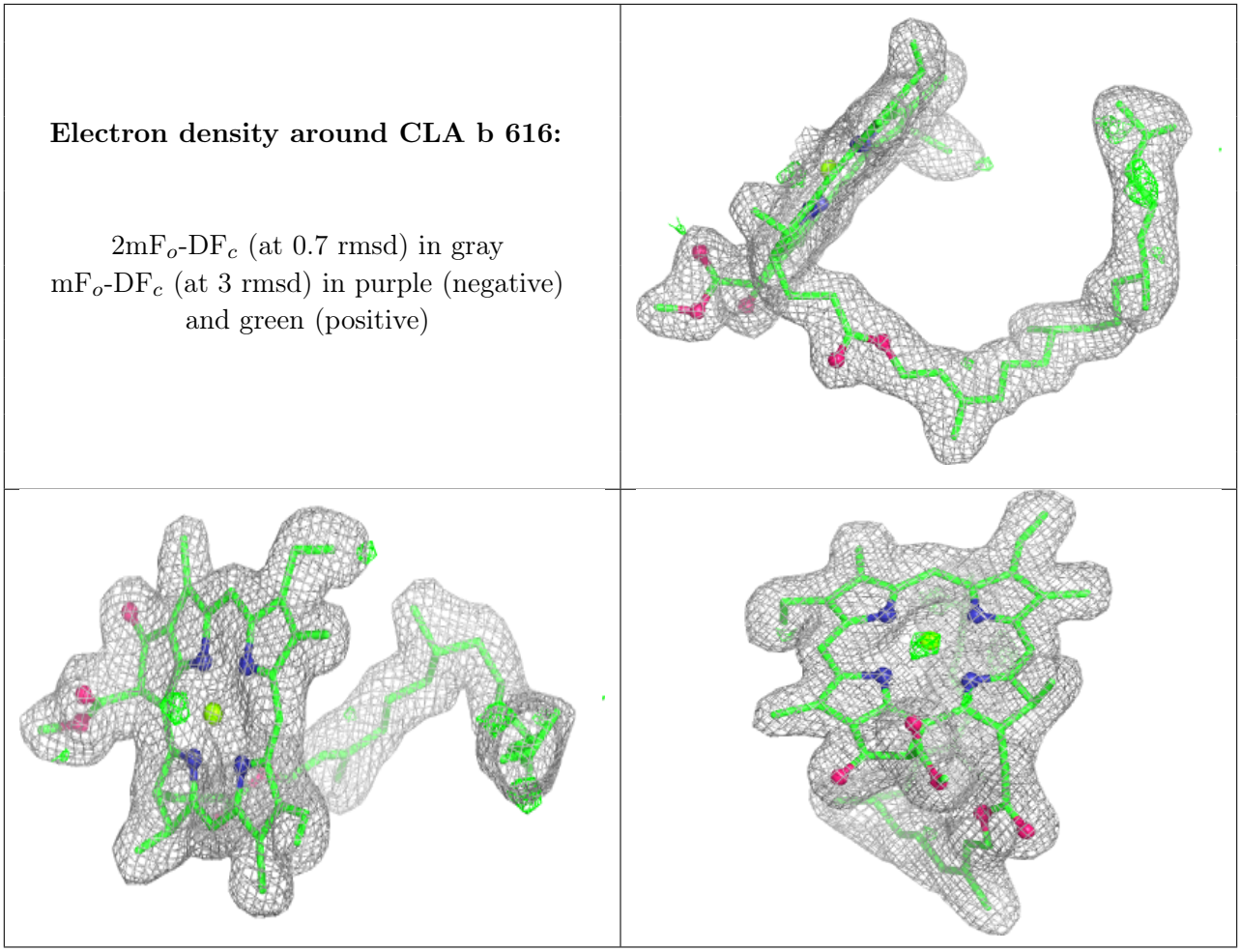






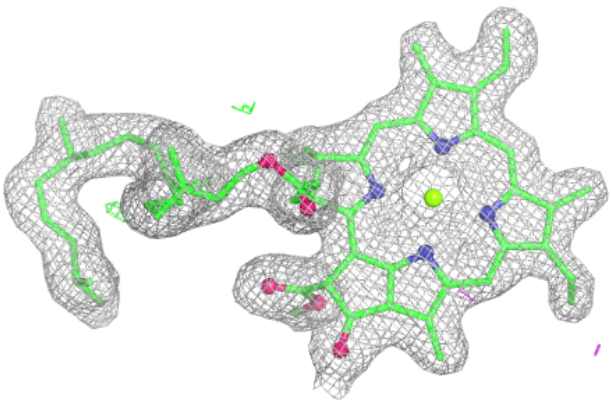
Electron density around CLA b 616:

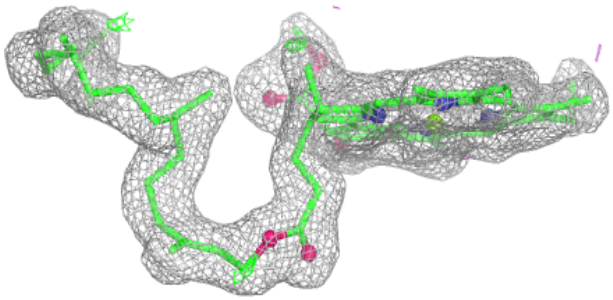
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 617:

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

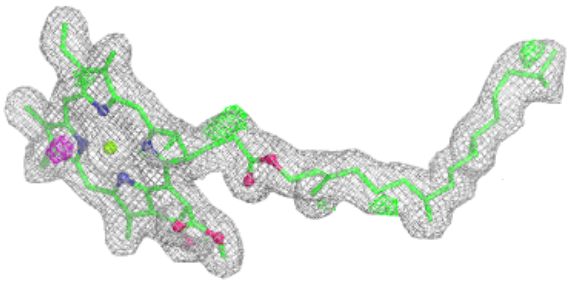


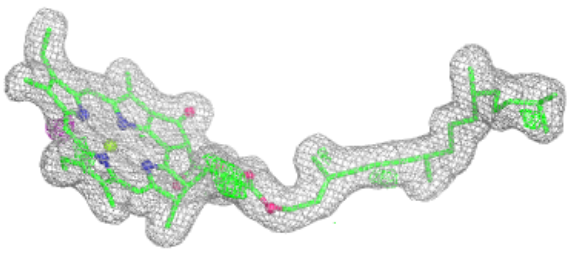


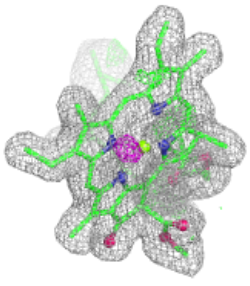


Electron density around CLA A 405:

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

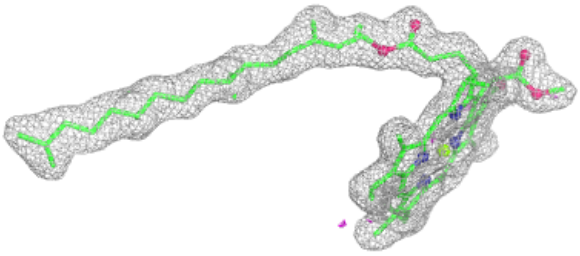


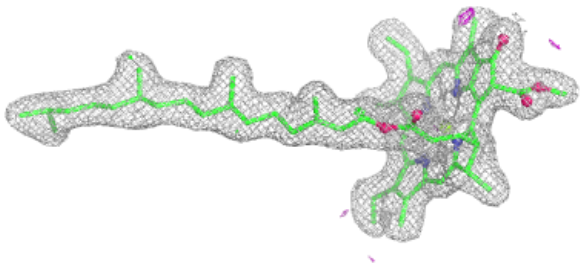


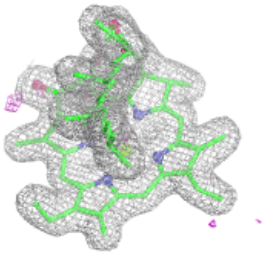


Electron density around CLA B 608:

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

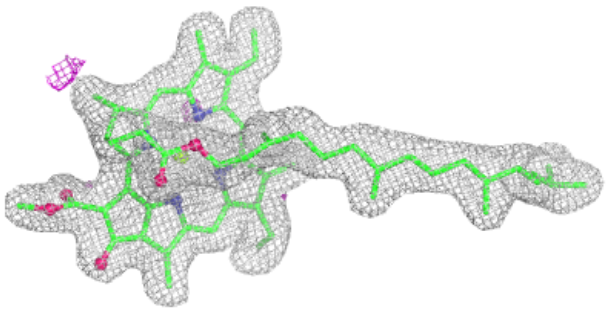


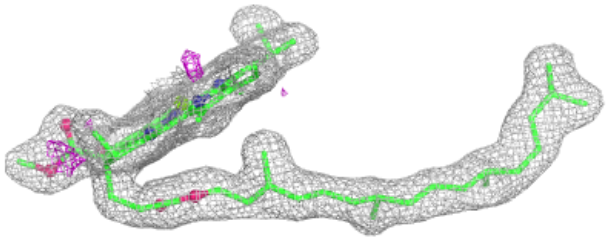


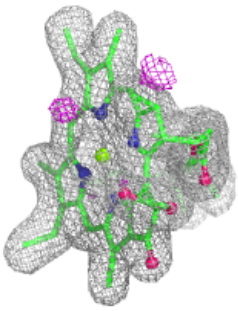


Electron density around CLA B 609:

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

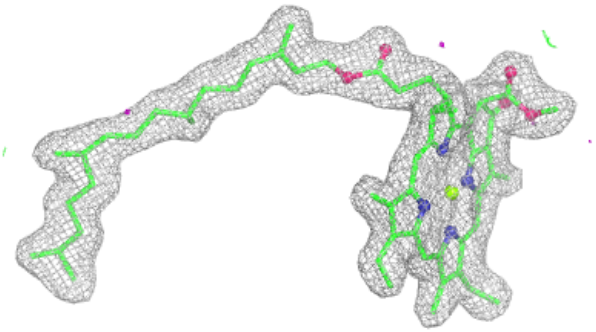


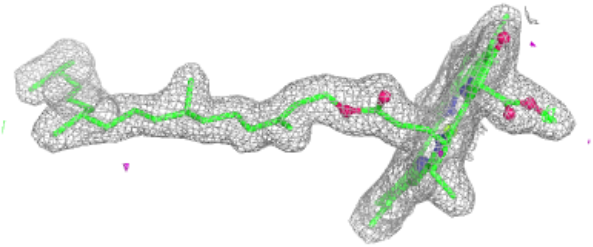


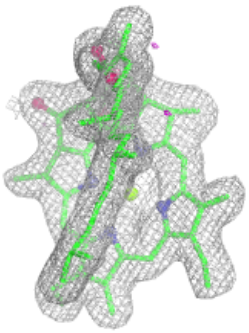


Electron density around CLA B 610:

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

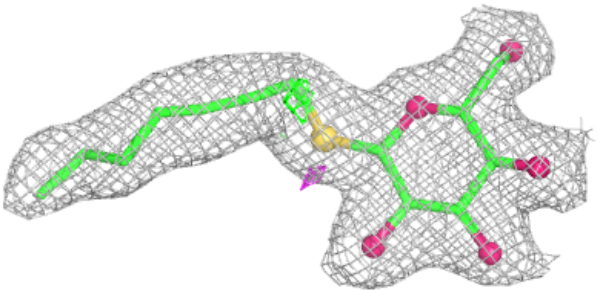


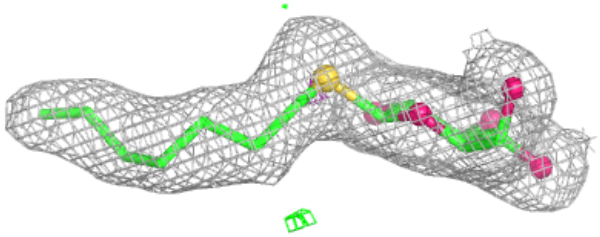


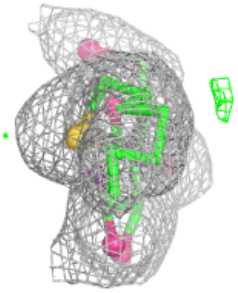


Electron density around HTG O 303:

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

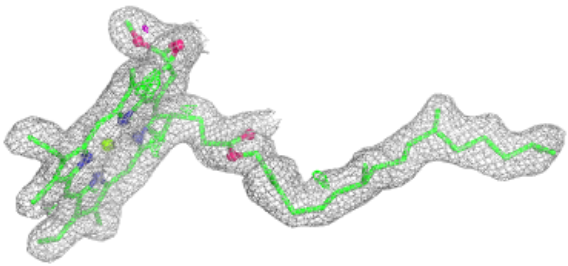


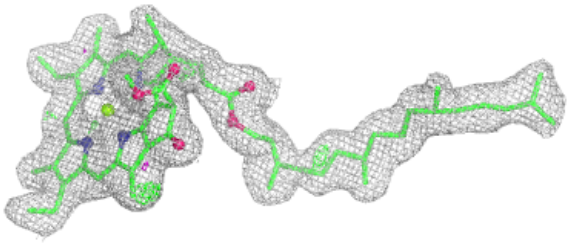


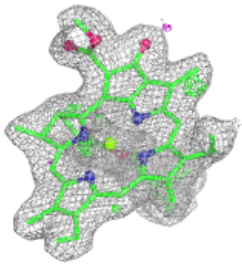


Electron density around CLA c 504:

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

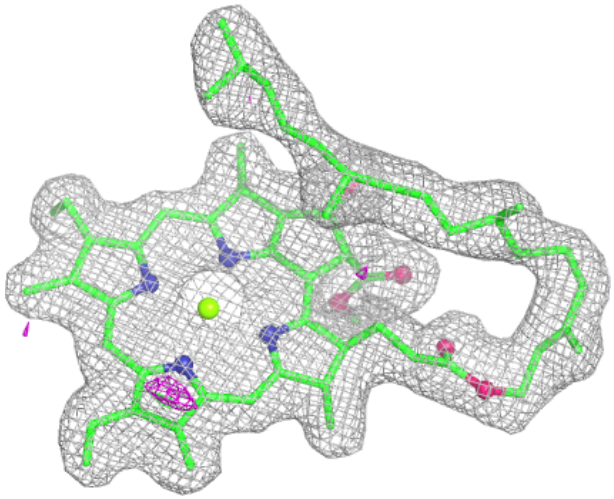


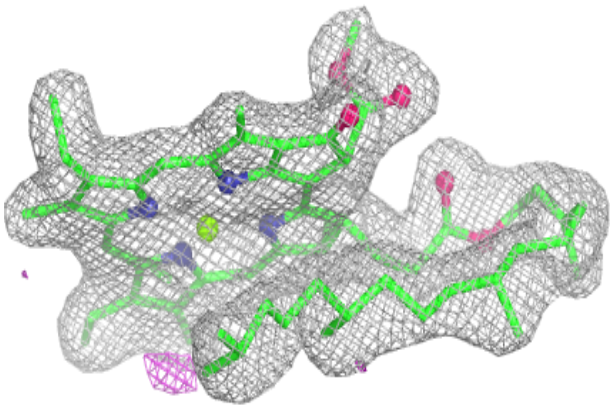


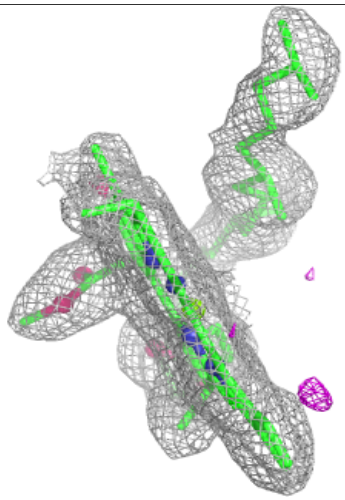


Electron density around CLA C 510:

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

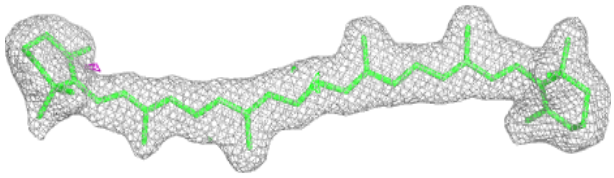


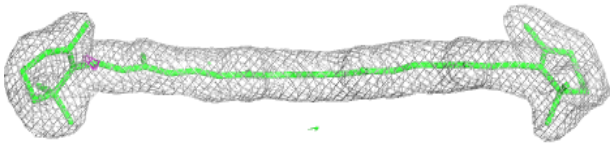


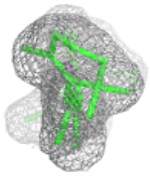


Electron density around BCR b 623:

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

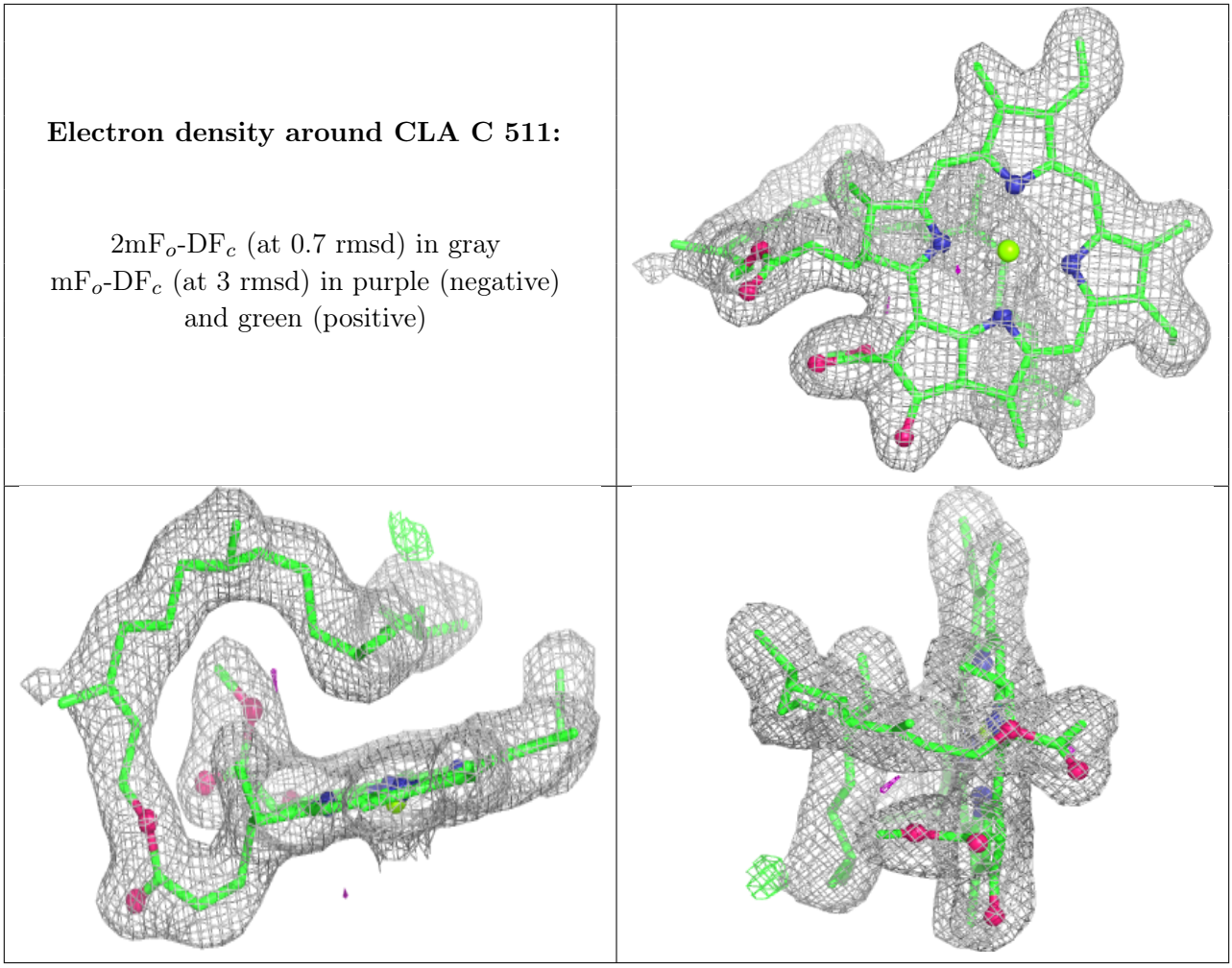






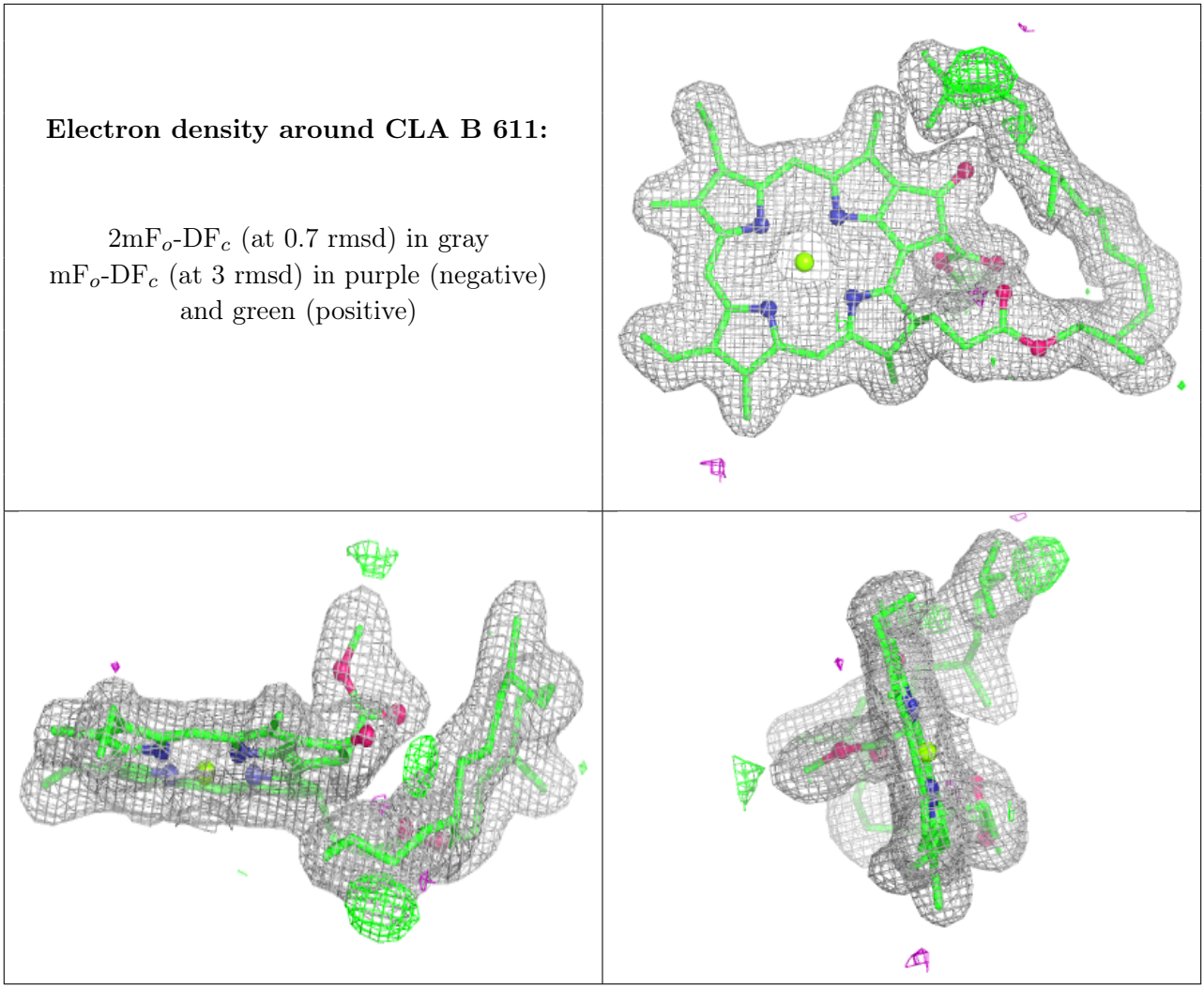
Electron density around CLA C 511:

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



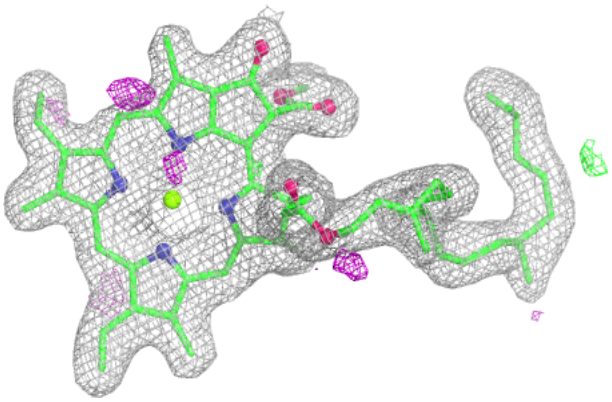
Electron density around CLA B 611:

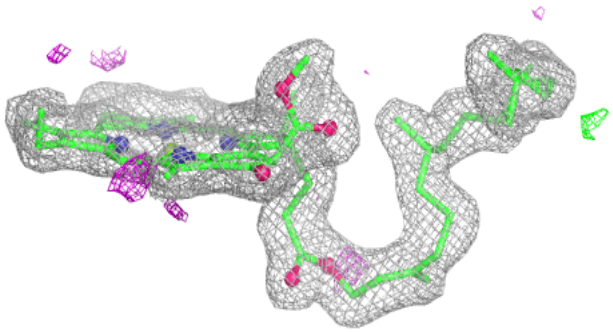
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 613:

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

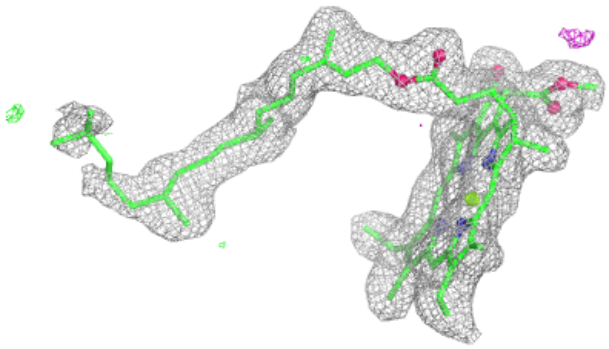


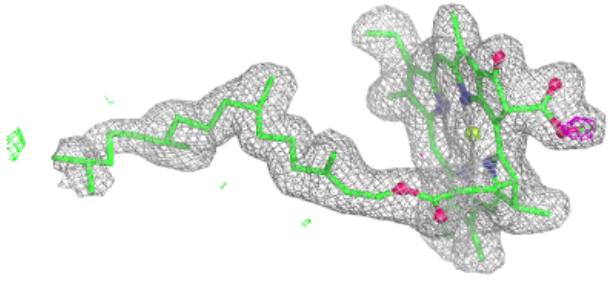


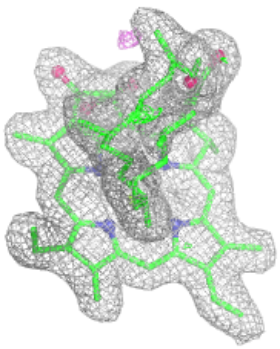


Electron density around CLA c 510:

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

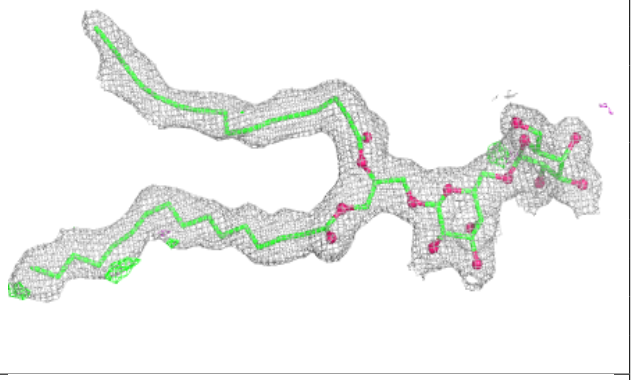


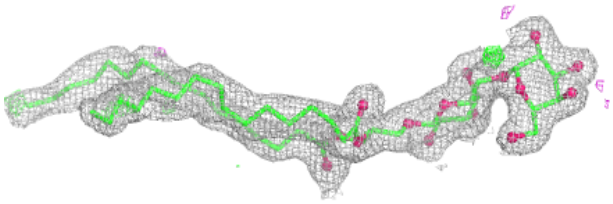




Electron density around DGD C 519:

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

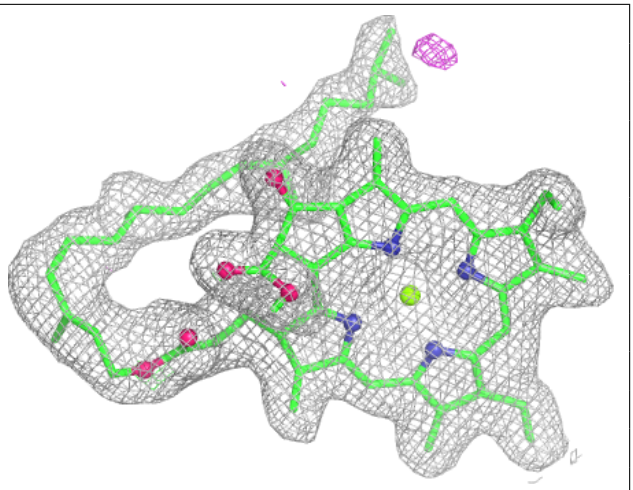


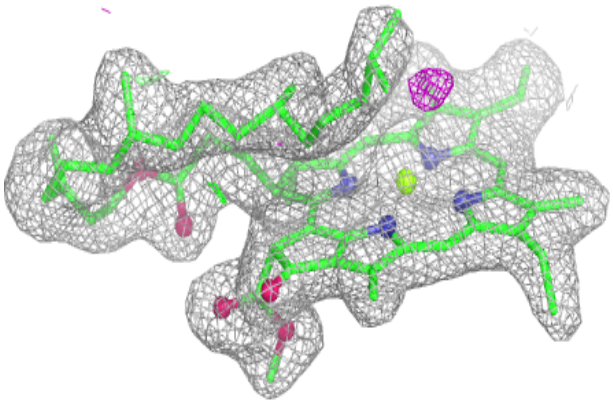




Electron density around CLA c 511:

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

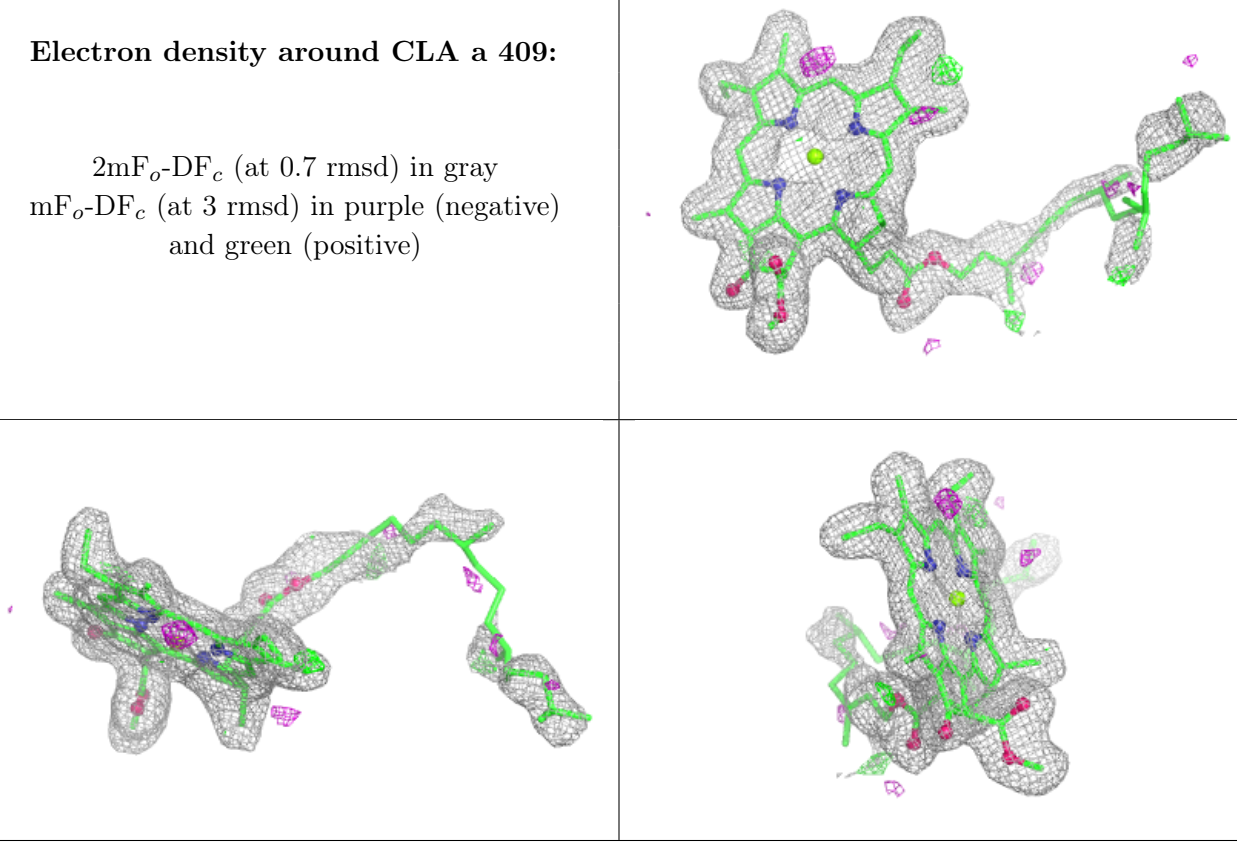






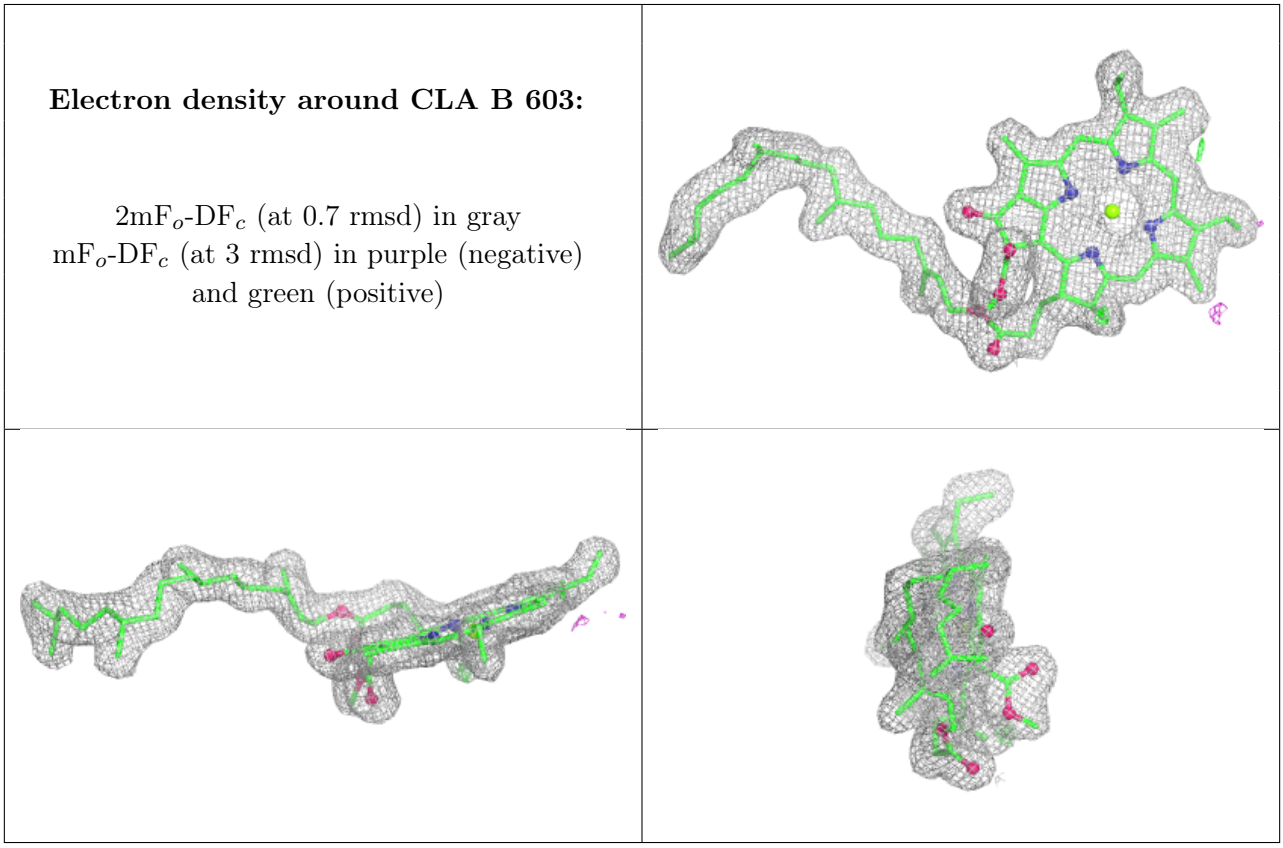
Electron density around CLA a 409:

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



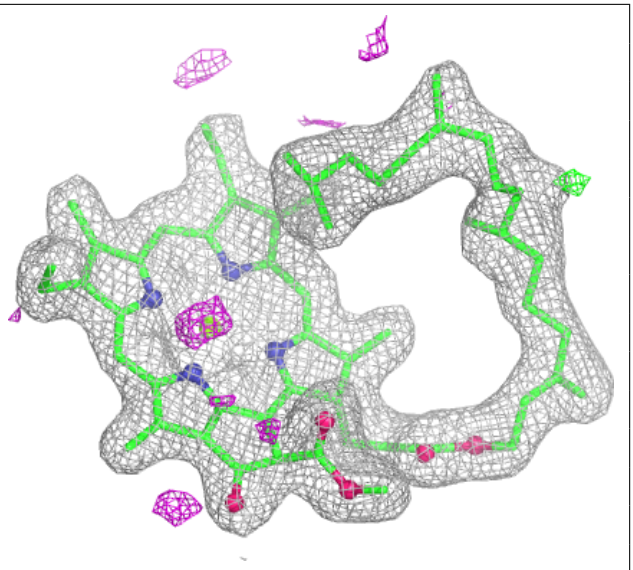
Electron density around CLA B 603:

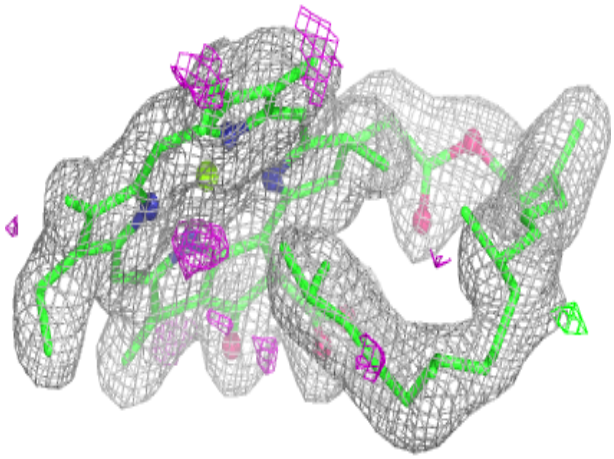
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

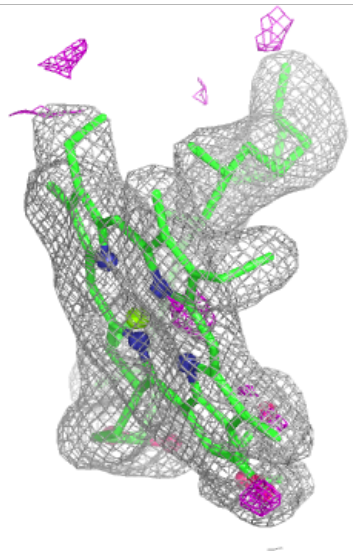


Electron density around CLA B 616:

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

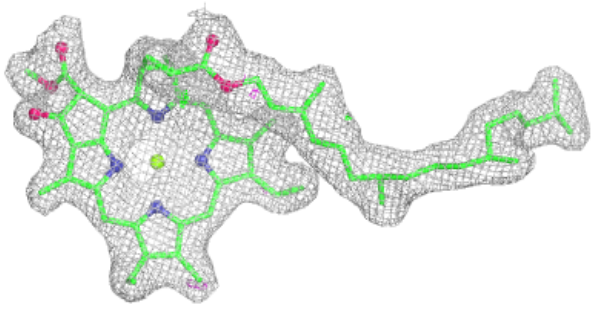


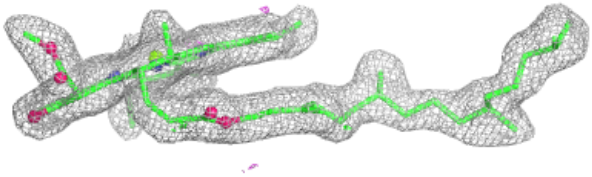


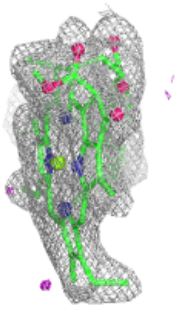


Electron density around CLA b 608:

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

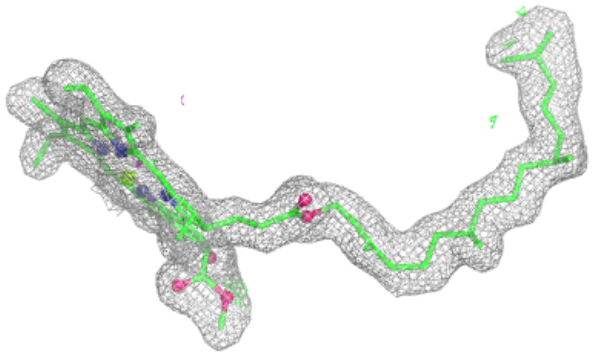


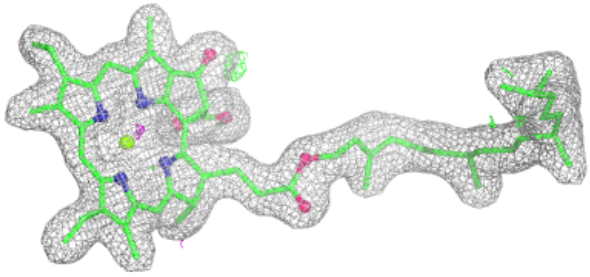


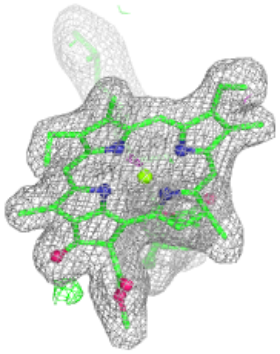


Electron density around CLA d 402:

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

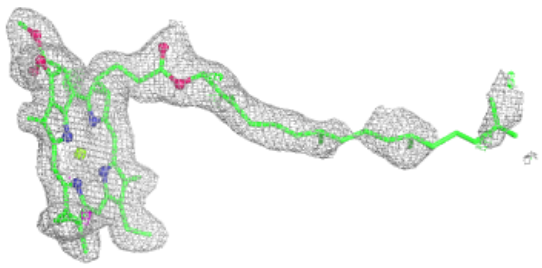


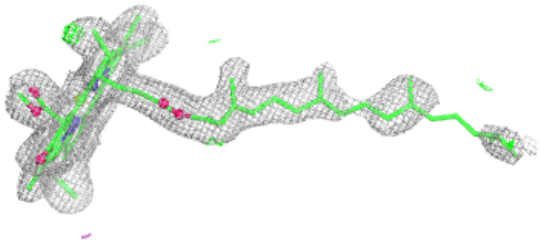


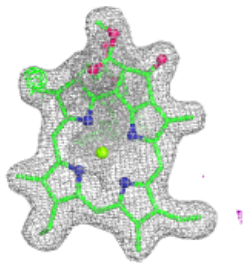


Electron density around CLA d 404:

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

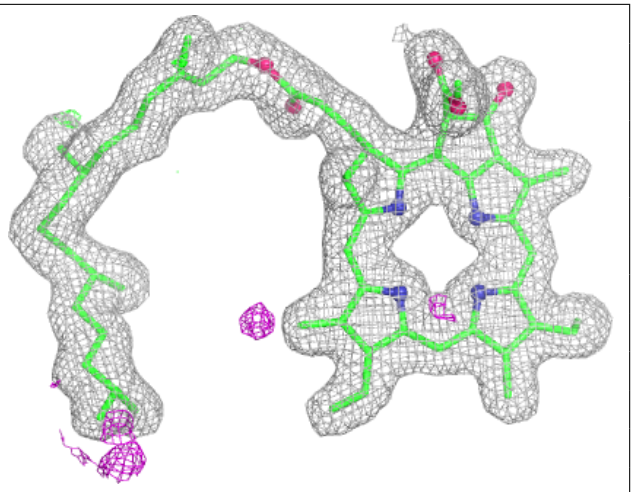


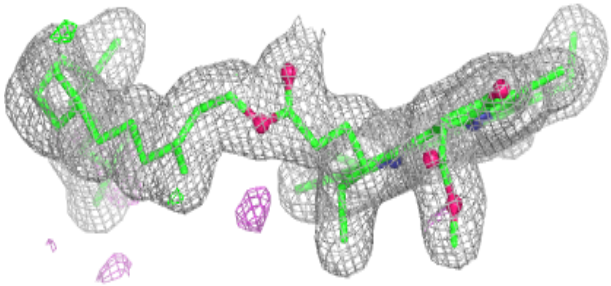


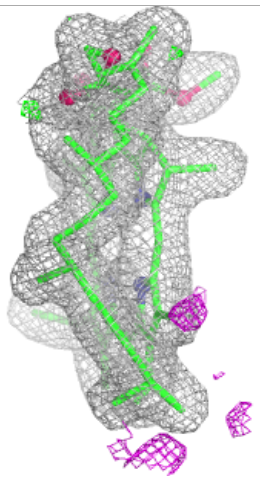


Electron density around PHO A 407:

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

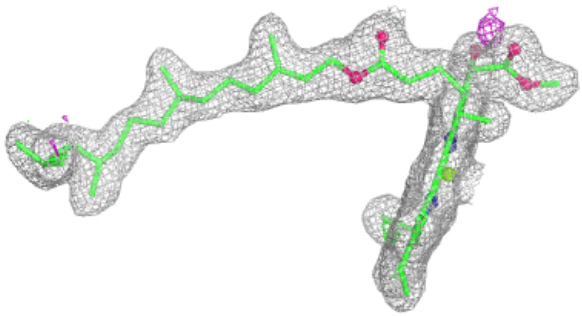


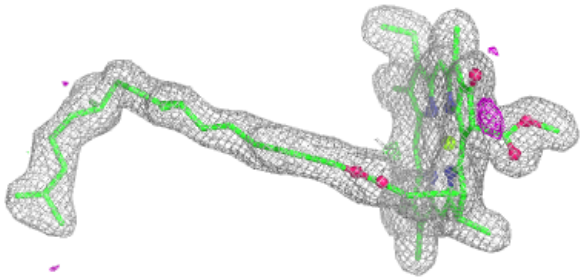


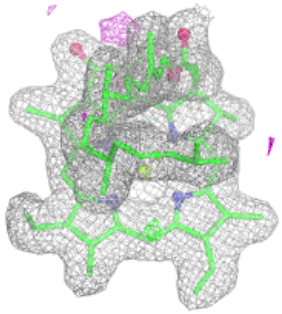


Electron density around CLA b 610:

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

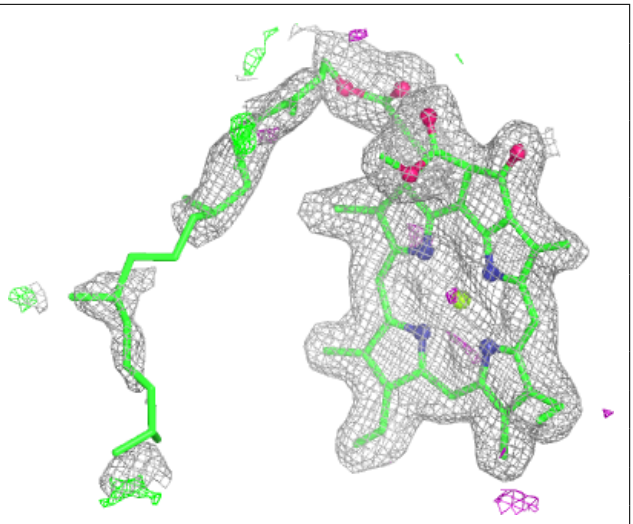


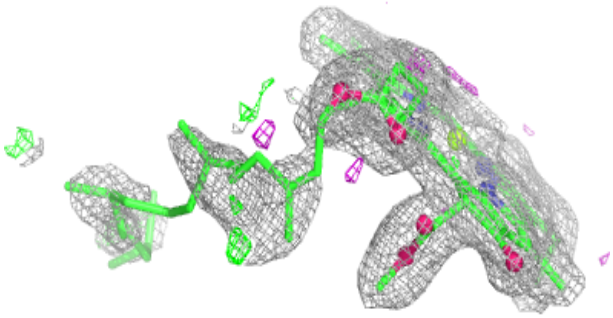


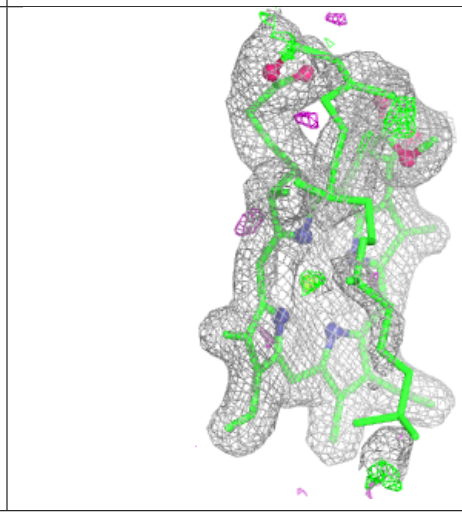


Electron density around CLA B 617:

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

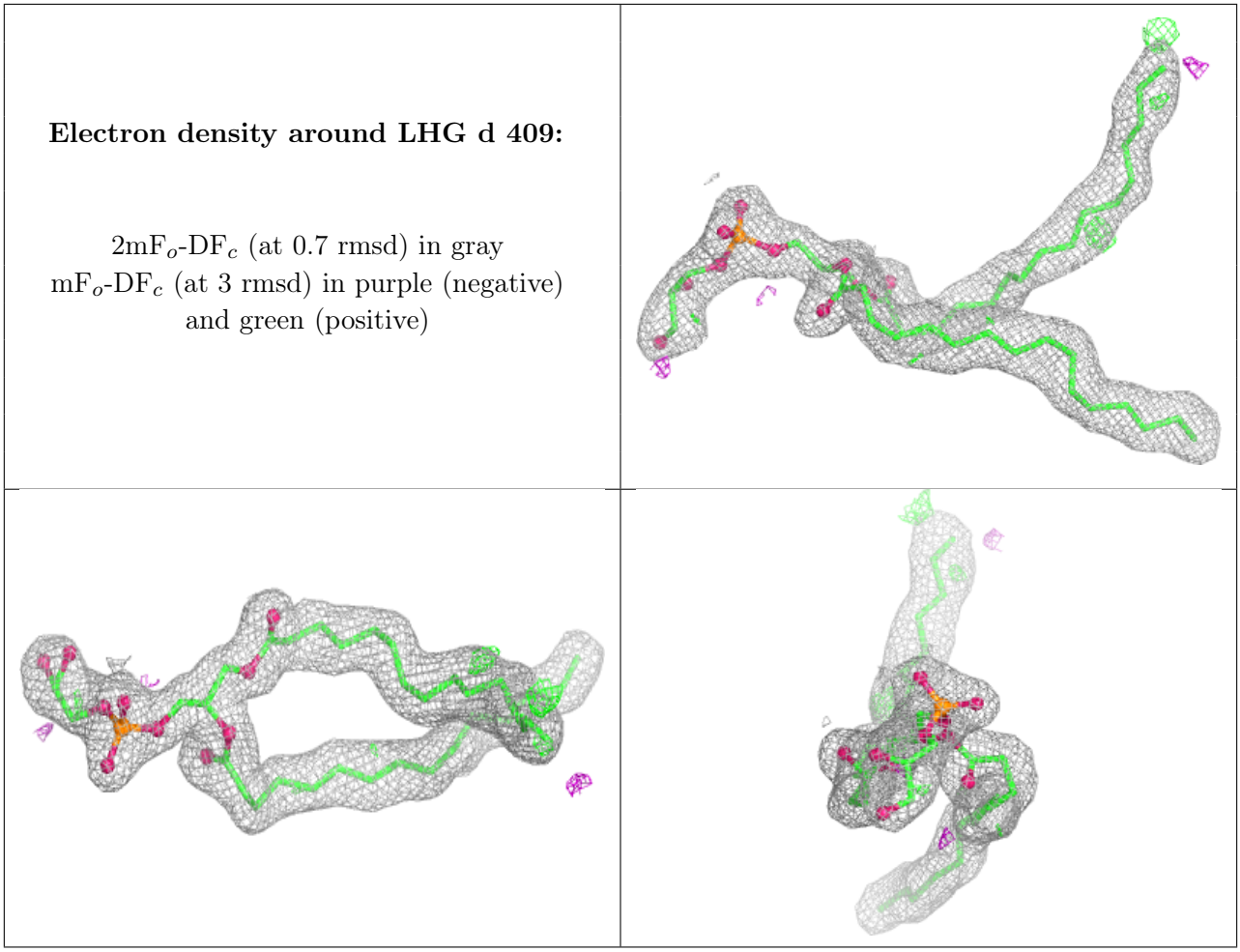






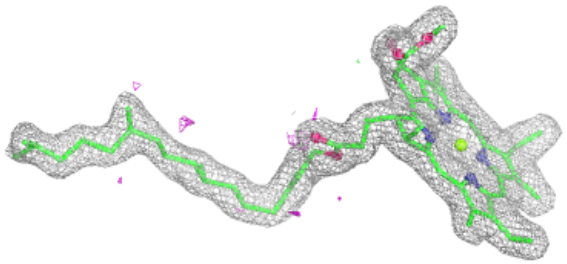
Electron density around LHG d 409:

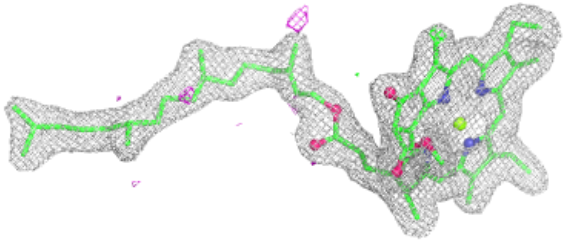
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

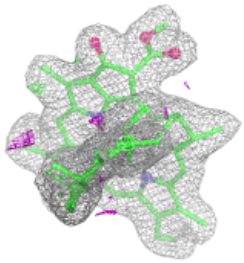


Electron density around CLA C 503:

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

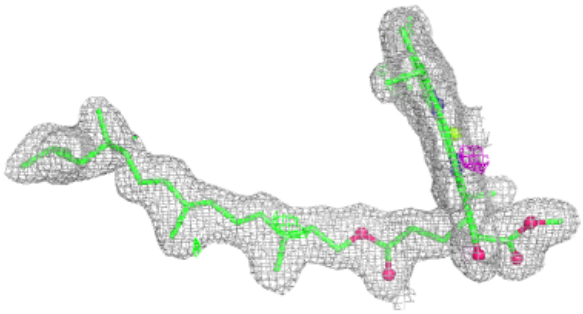


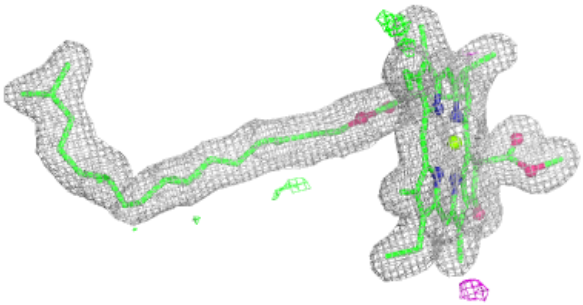


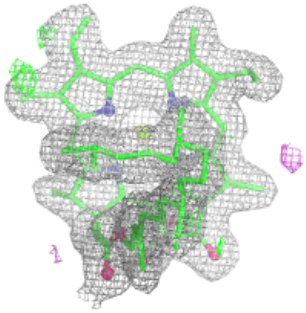


Electron density around CLA B 606:

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

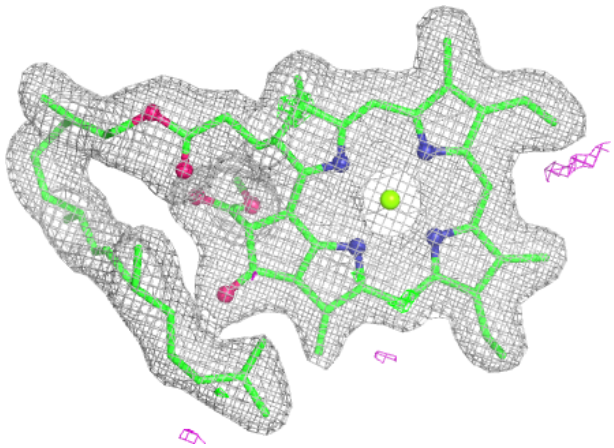


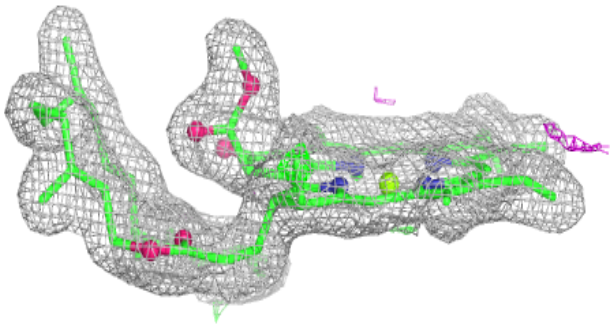


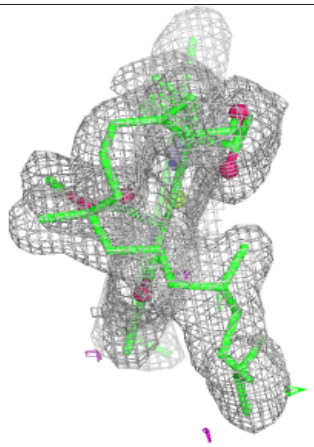


Electron density around CLA b 615:

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

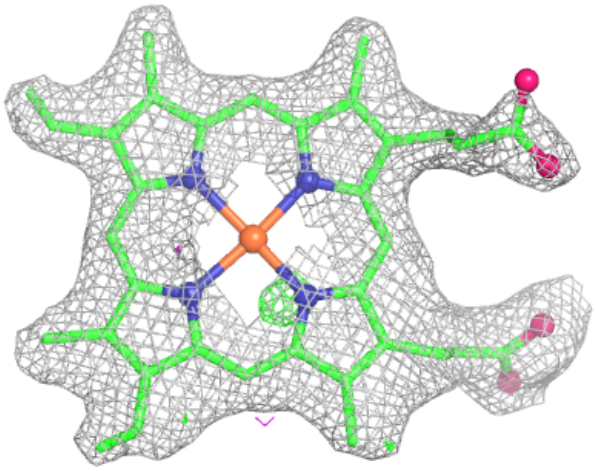


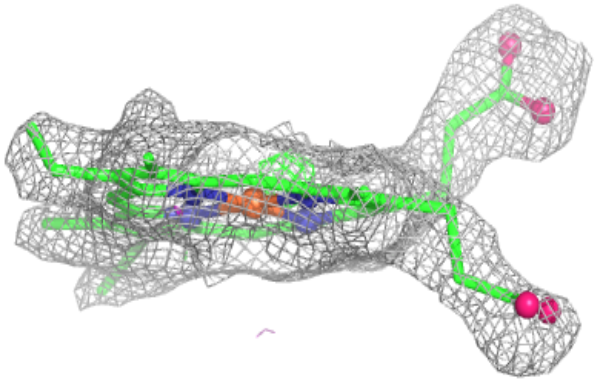


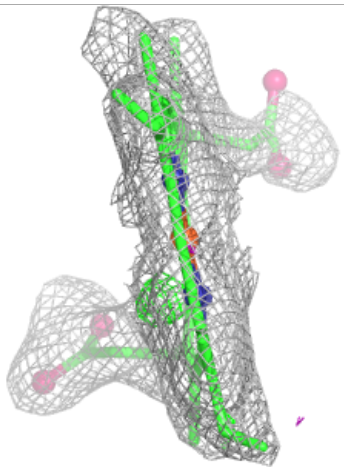


Electron density around HEM e 102:

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

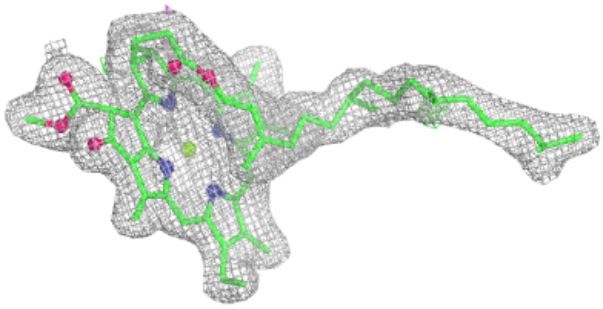


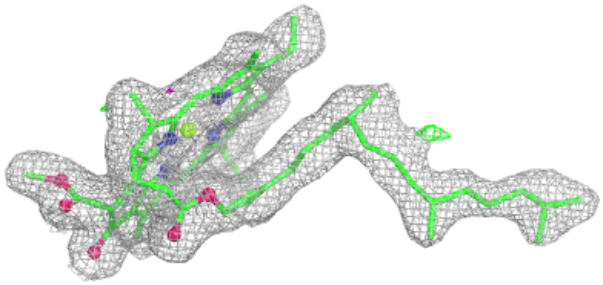


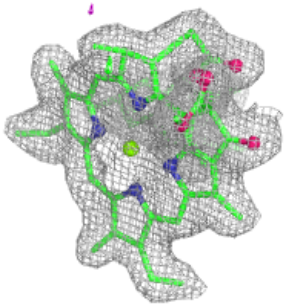


Electron density around CLA C 506:

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

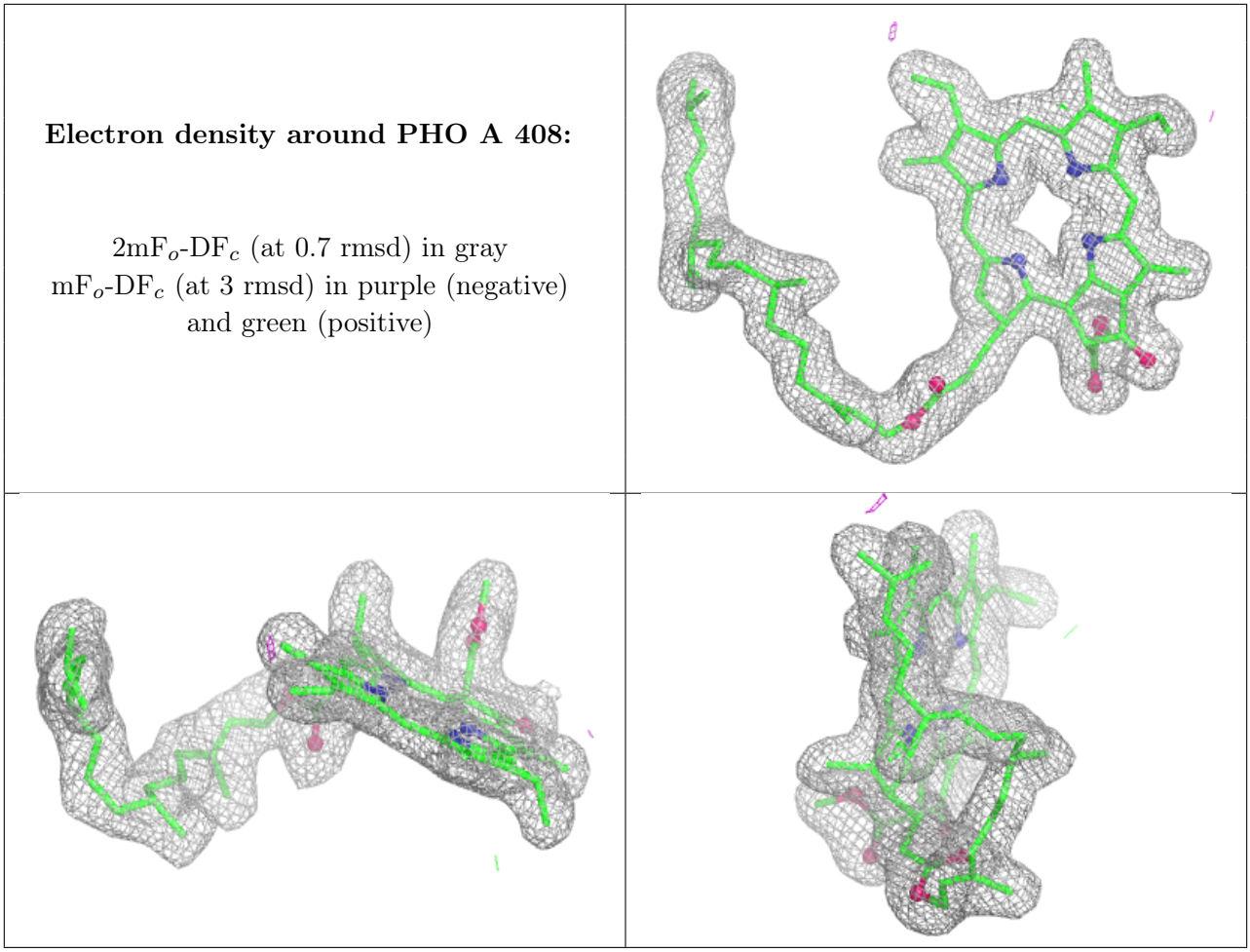






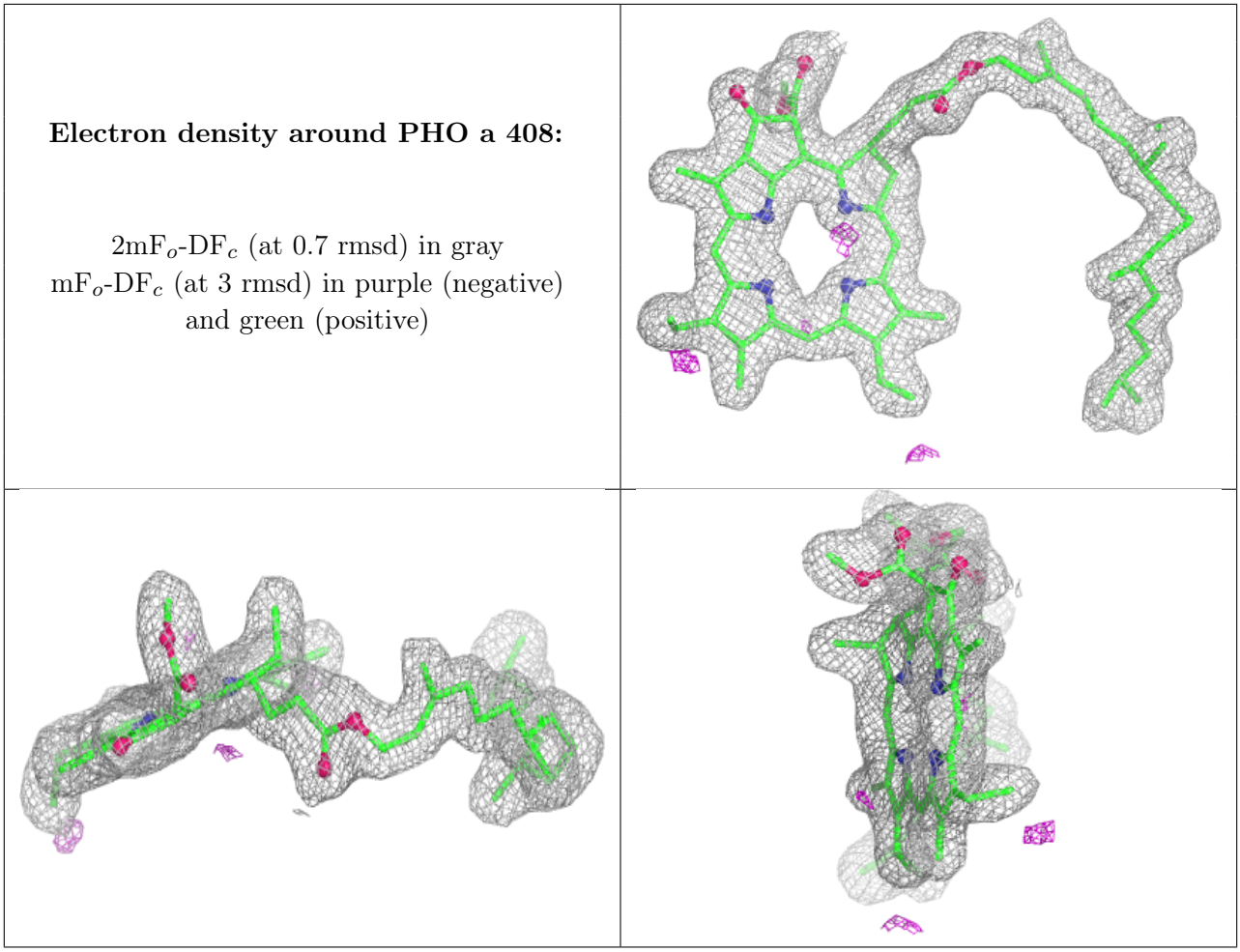
Electron density around PHO A 408:

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



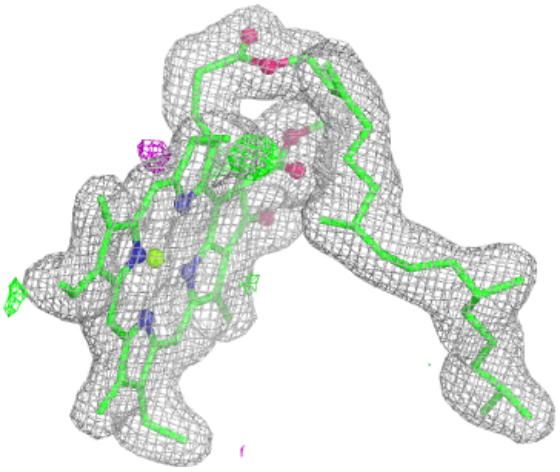
Electron density around PHO a 408:

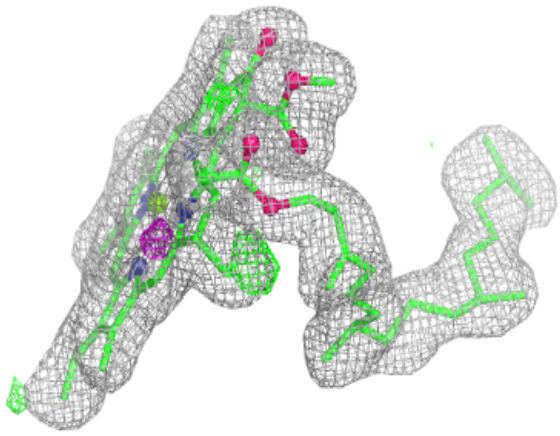
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

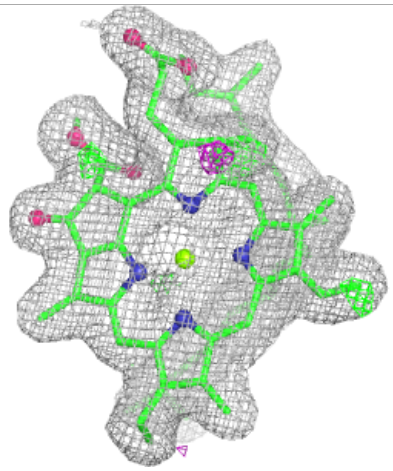


Electron density around CLA b 618:

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

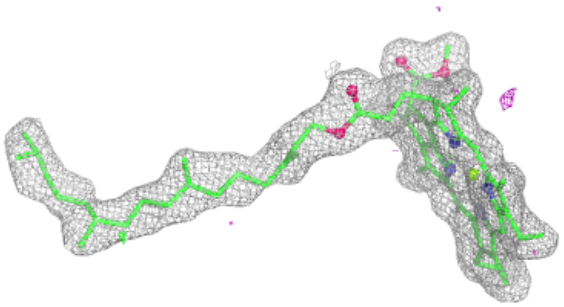


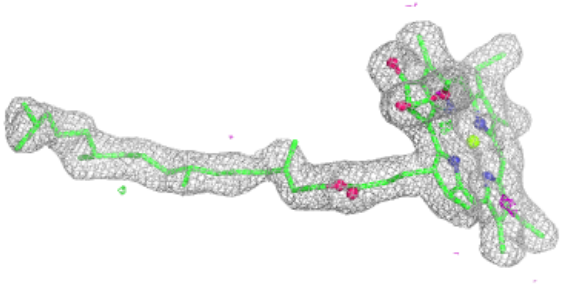


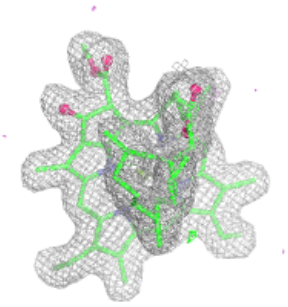


Electron density around CLA b 609:

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

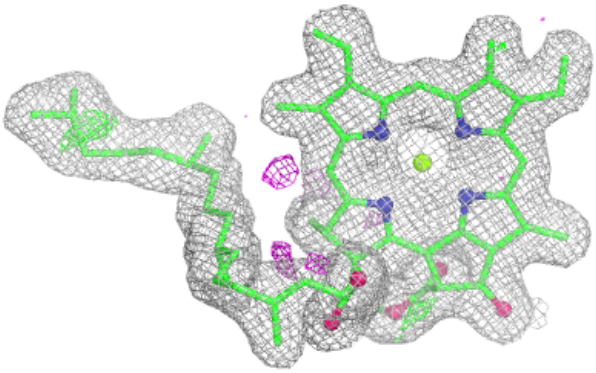


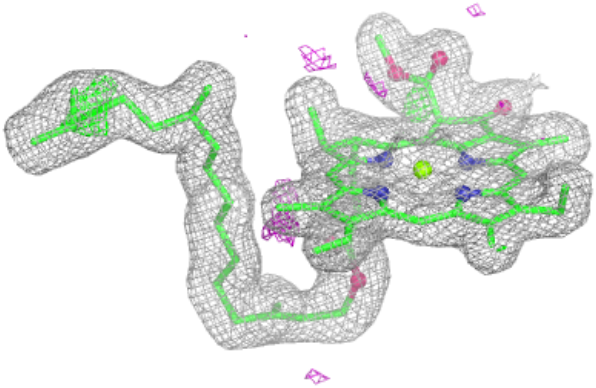


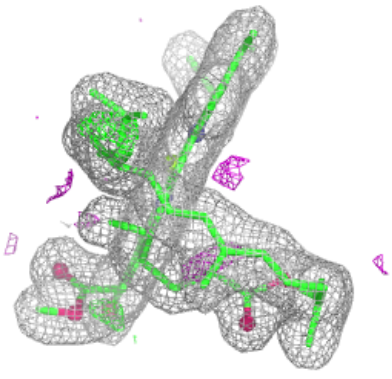


Electron density around CLA D 401:

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

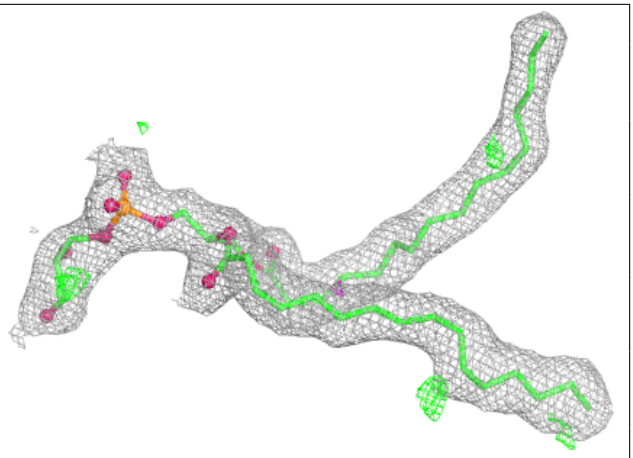


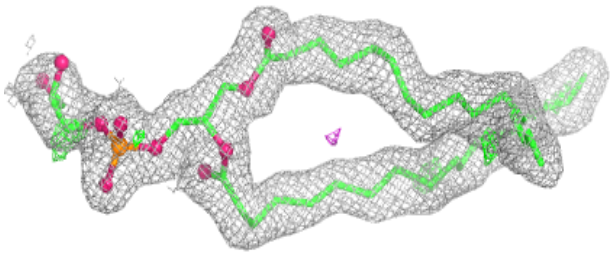


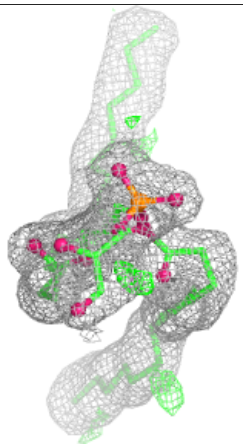


Electron density around LHG D 409:

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

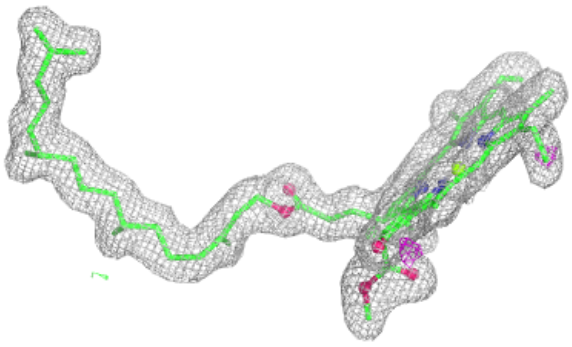


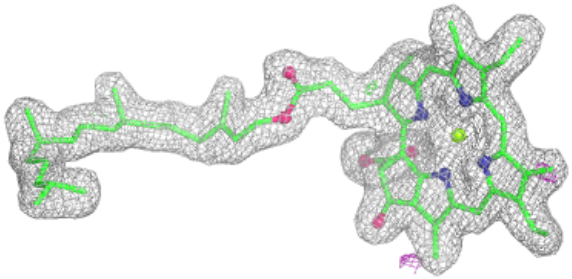


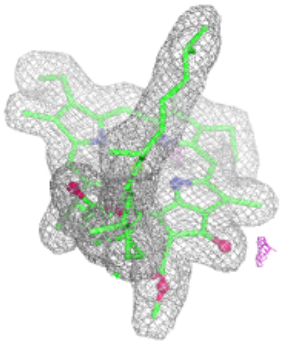


Electron density around CLA D 403:

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

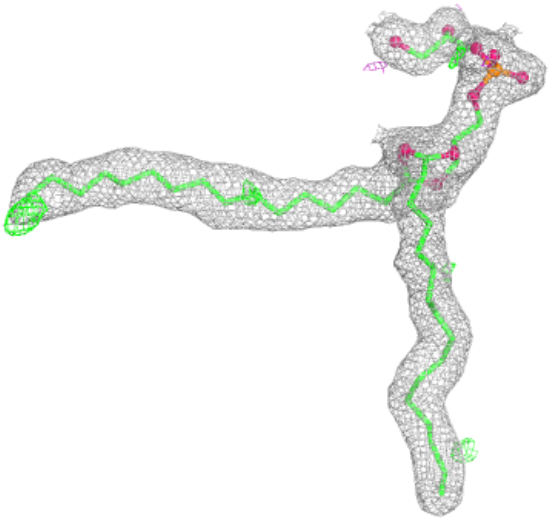


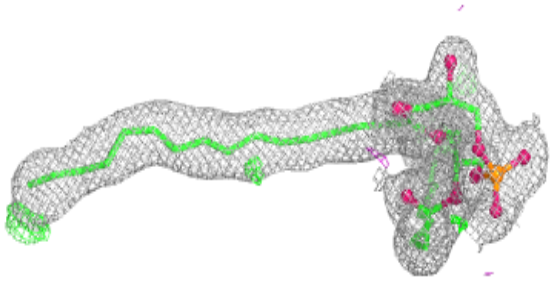


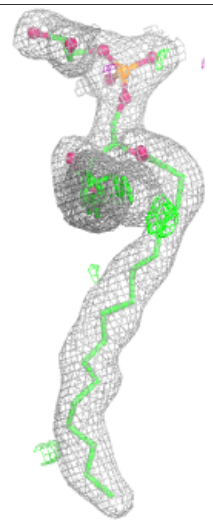


Electron density around LHG L 101:

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

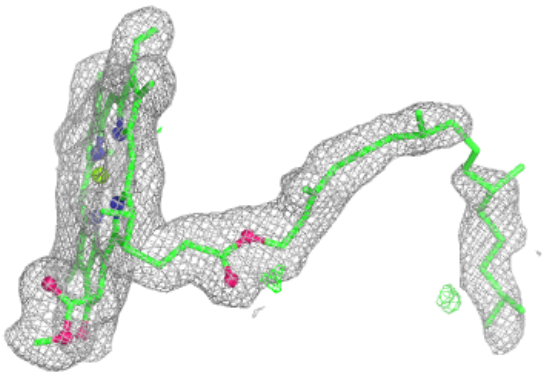


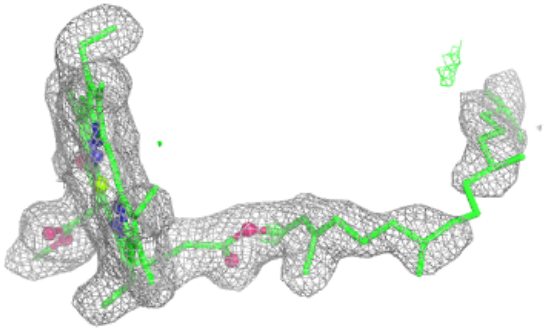


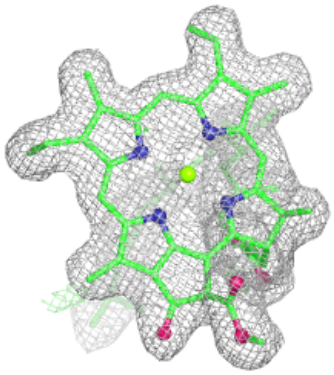


Electron density around CLA D 404:

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

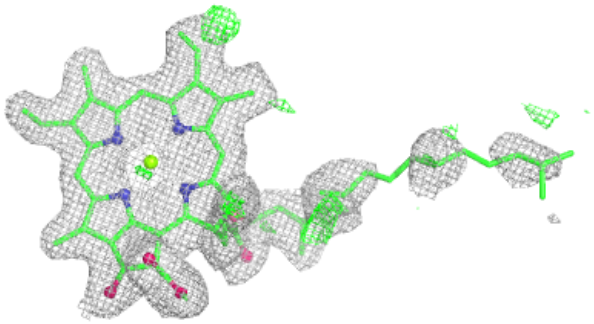


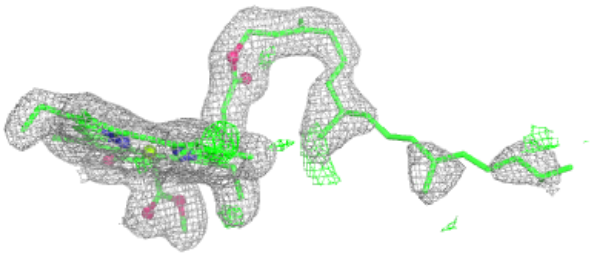


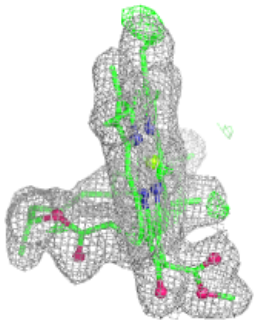


Electron density around CLA a 407:

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

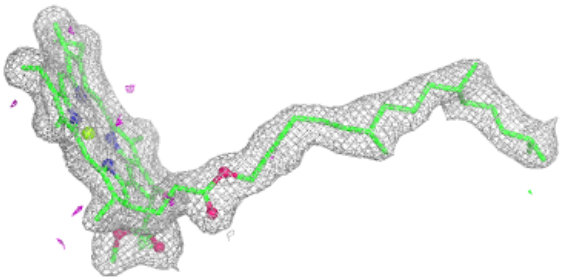


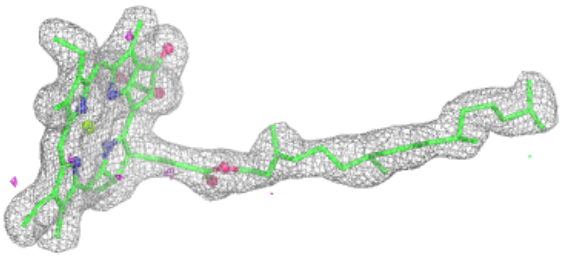


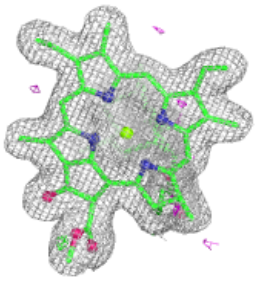


Electron density around CLA B 605:

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

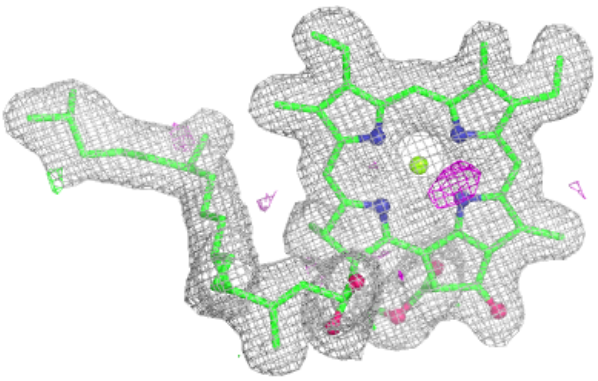


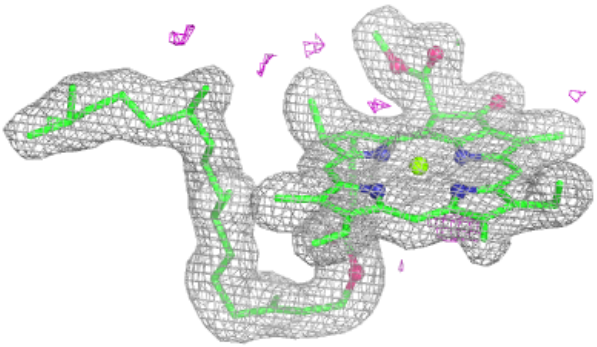


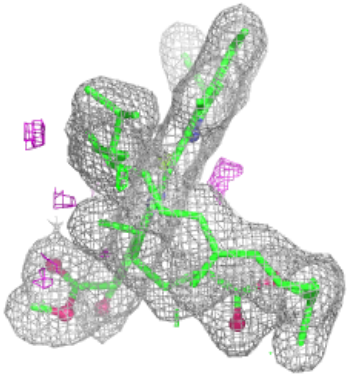


Electron density around CLA d 401:

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

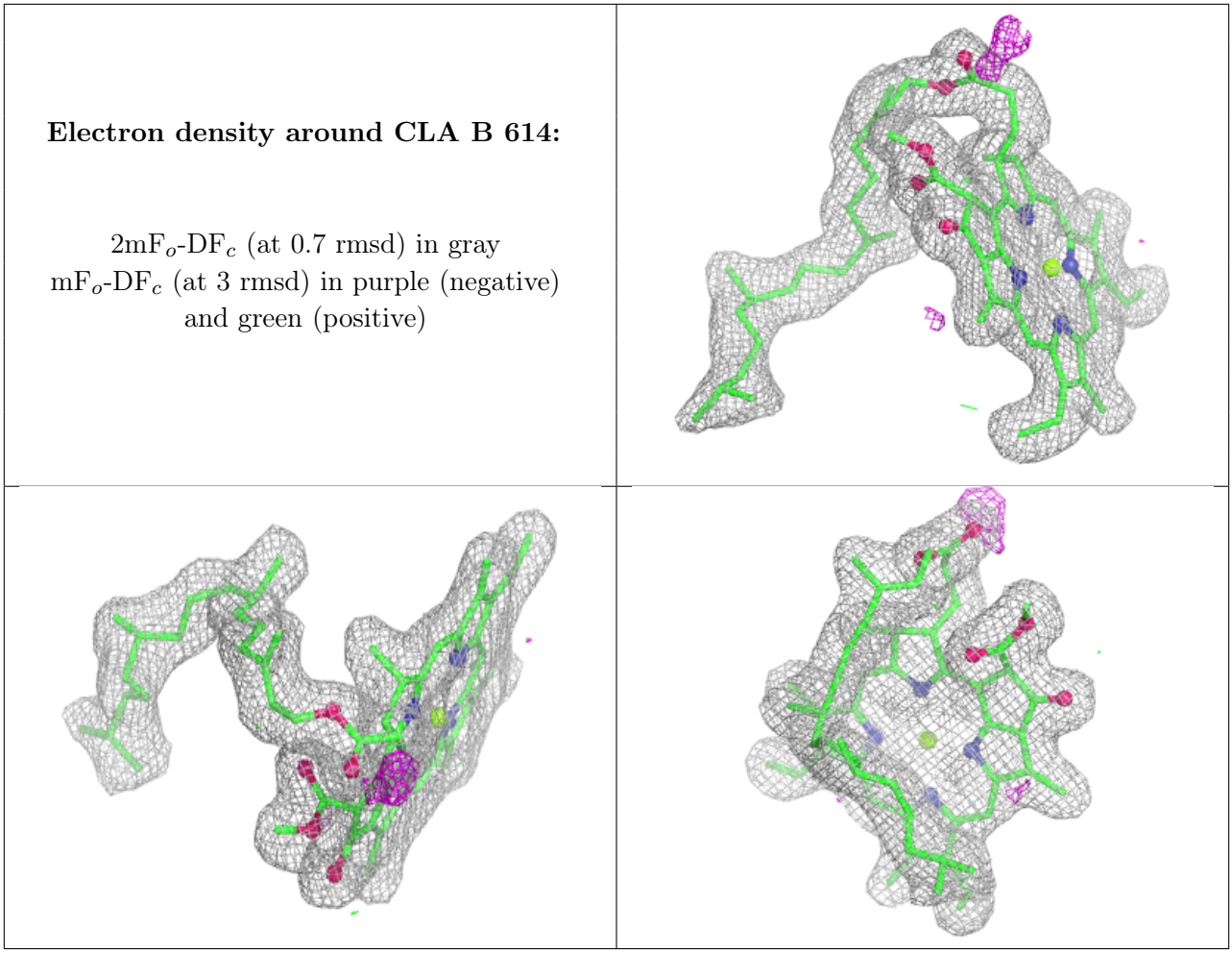






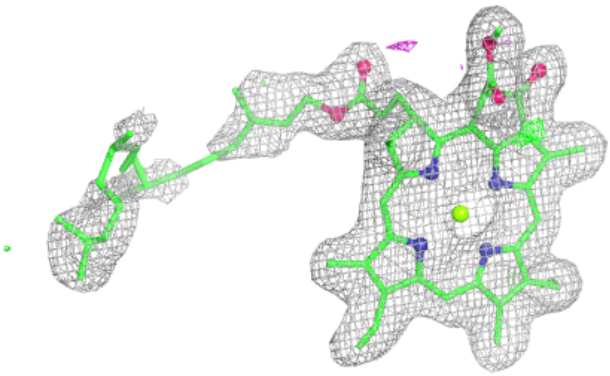
Electron density around CLA B 614:

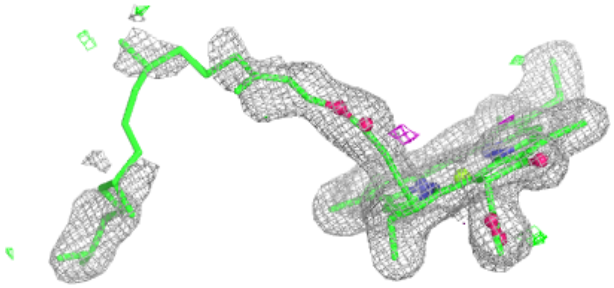
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

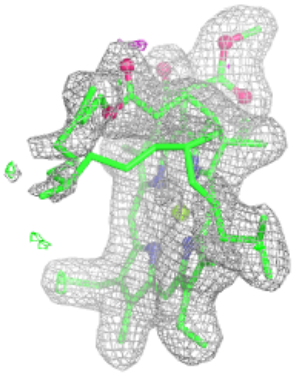


Electron density around CLA A 409:

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

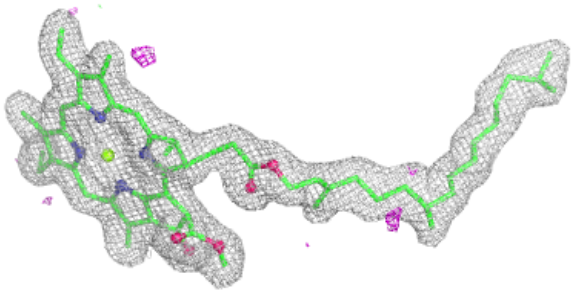


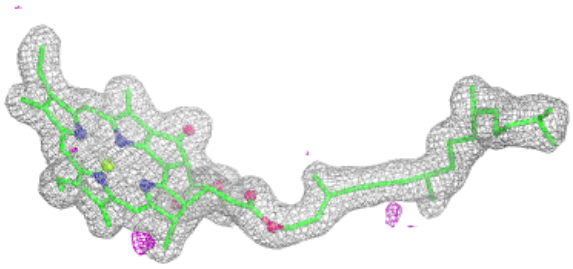


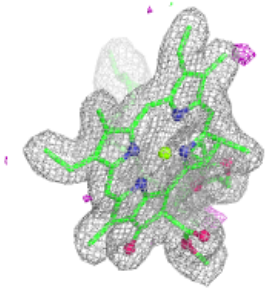


Electron density around CLA a 406:

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

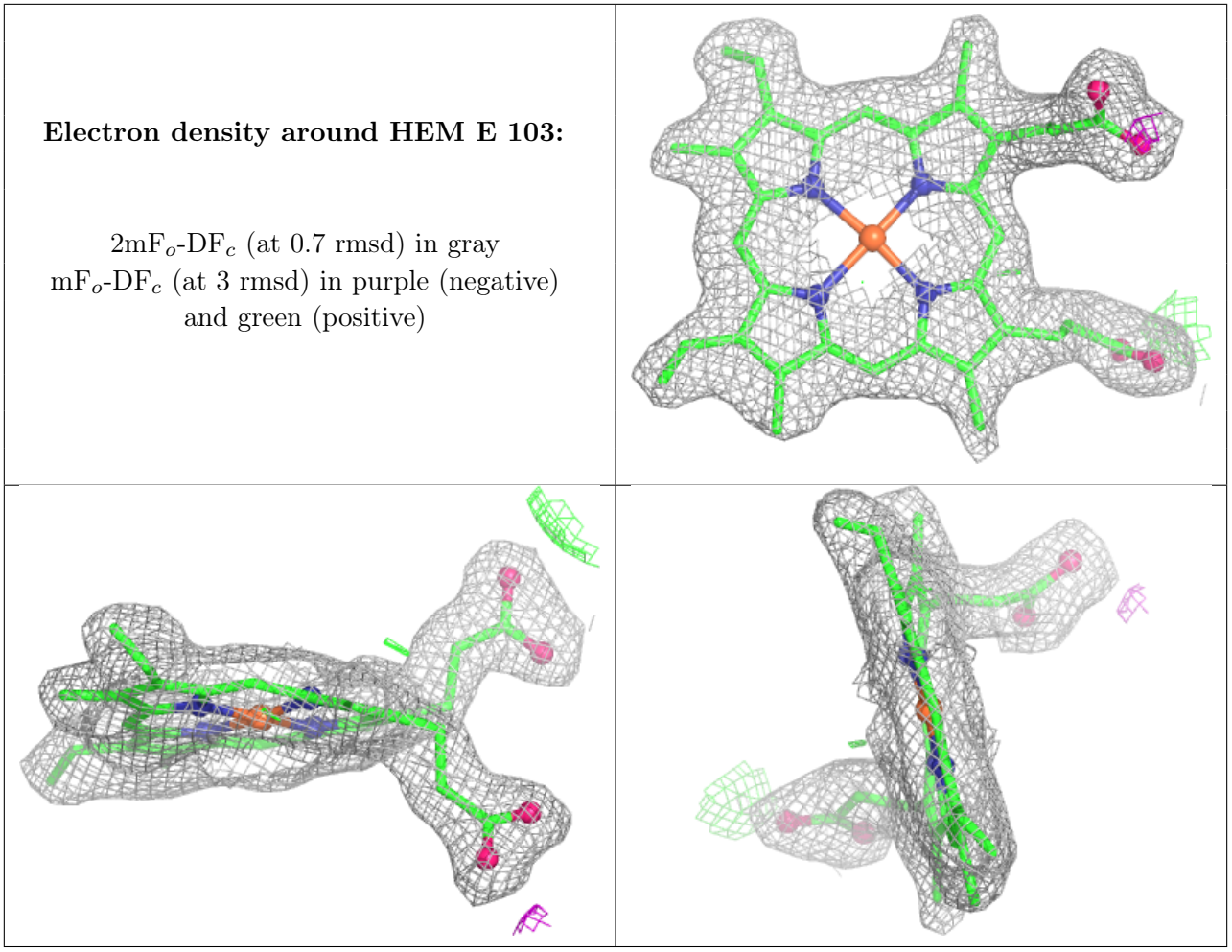






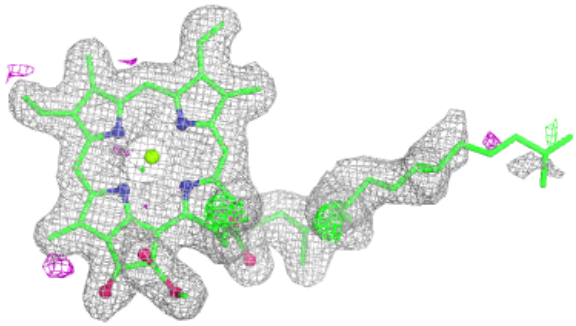
Electron density around HEM E 103:

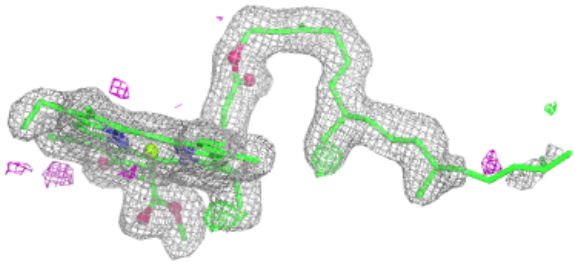
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

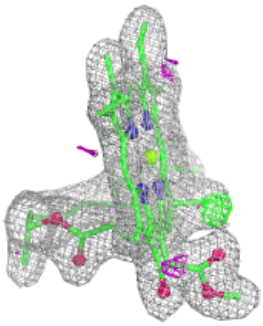


Electron density around CLA A 406:

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

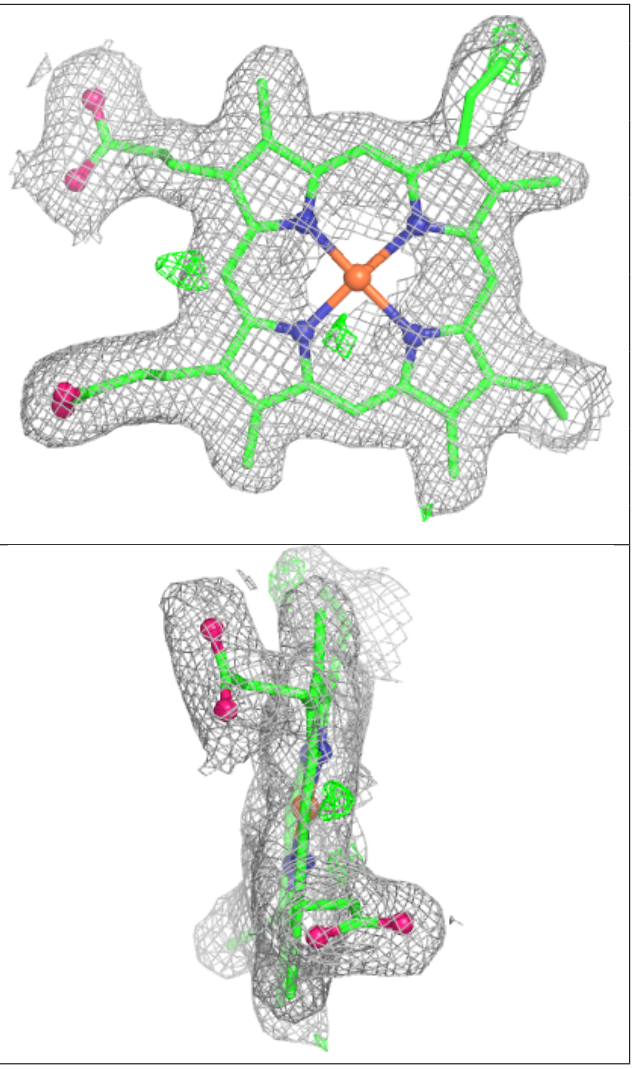






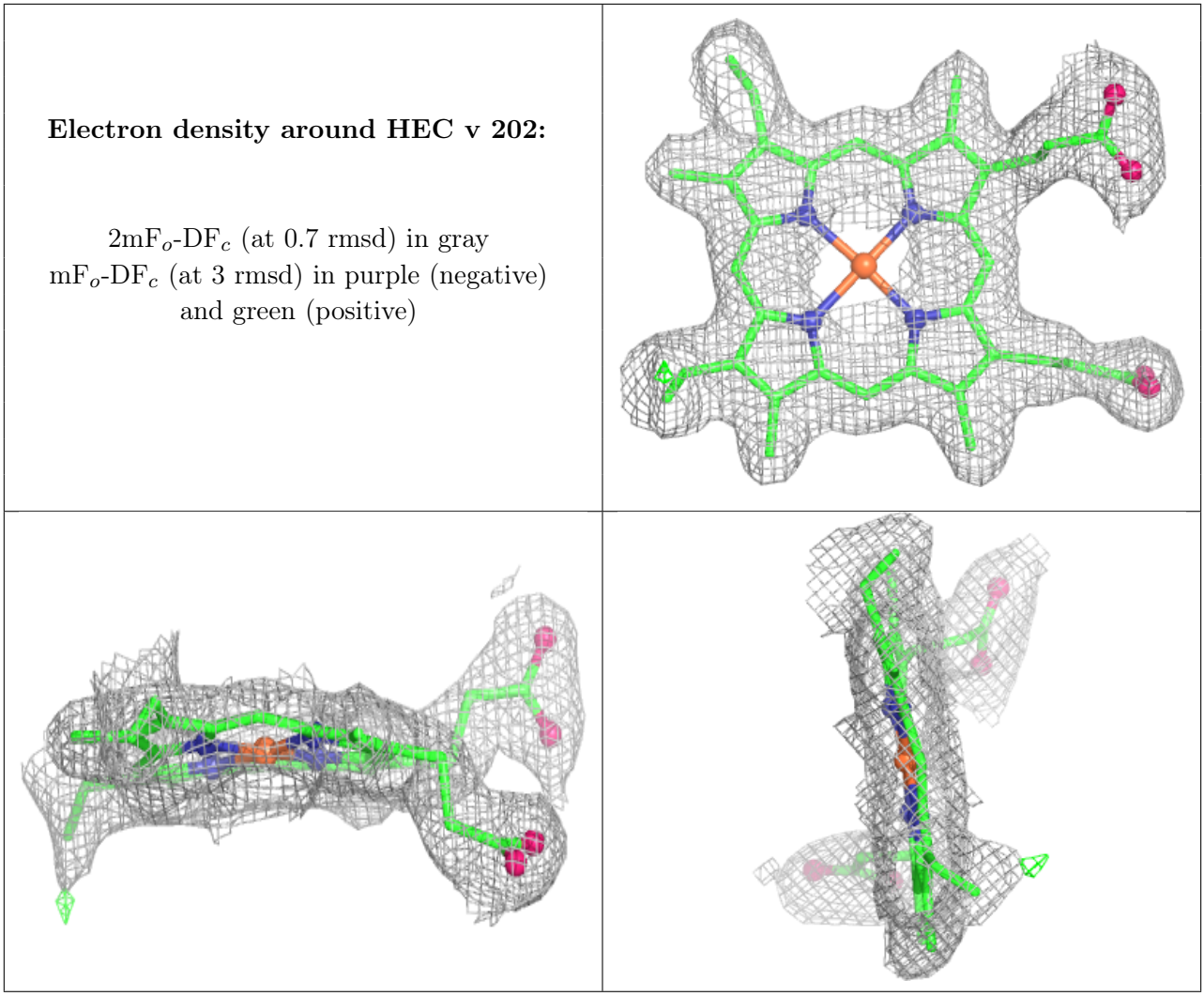
Electron density around HEC V 203:

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



Electron density around HEC v 202:

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



6.5 Other polymers

There are no such residues in this entry.