wwPDB X-ray Structure Validation Summary Report (i)

Nov 25, 2024 – 08:03 PM EST

PDB ID	:	5WS6
Title	:	Native XFEL structure of Photosystem II (preflash two-flash dataset
Authors	:	Suga, M.; Shen, J.R.
Deposited on	:	2016-12-05
Resolution	:	2.35 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:

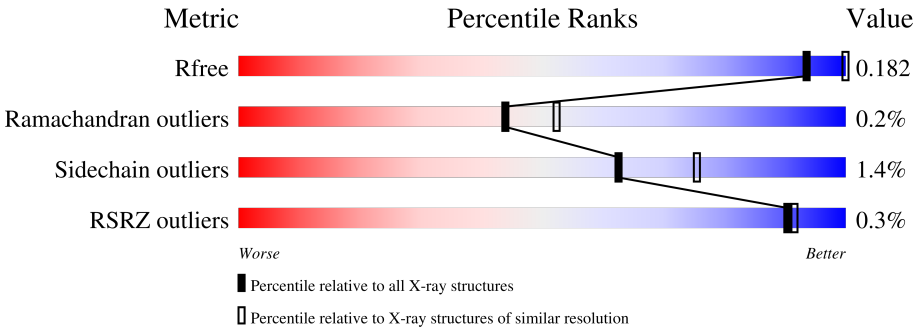
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.35 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}	164625	1460 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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%

Mol	Chain	Length	Quality of chain
1	A	344	97%
1	a	344	97%
2	B	505	99%
2	b	505	98%
3	C	455	98%
3	c	455	98%
4	D	342	100%

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Mol	Chain	Length	Quality of chain
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	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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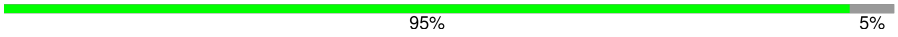
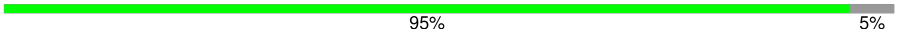
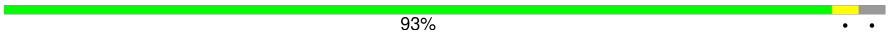
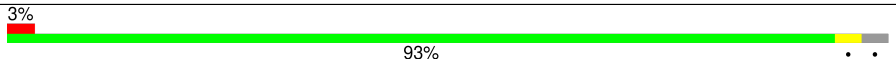
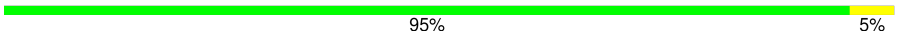
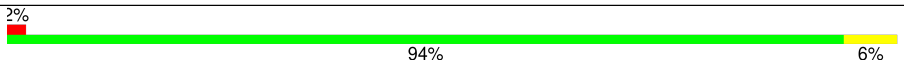
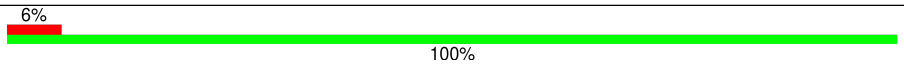
Mol	Chain	Length	Quality of chain
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
19	Z	62	
19	z	62	
20	R	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	404	X	-	-	-
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	350	X	-	-	-
24	CLA	a	403	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 53280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II D1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	29	0
			2850	1865	467	502	16			
1	a	334	Total	C	N	O	S	0	29	0
			2852	1867	466	503	16			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	10	0
			3542	2315	590	624	13			
3	c	455	Total	C	N	O	S	0	10	0
			3577	2340	595	629	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	3	0
			2748	1819	450	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2739	1814	449	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total 665	C 434	N 107	O 124	0	1	0
5	e	79	Total 648	C 424	N 105	O 119	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	31	Total 250	C 170	N 42	O 37	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	64	Total 514	C 344	N 84	O 84	S 2	0	1	0
7	h	64	Total 506	C 339	N 81	O 84	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 277	C 185	N 43	O 48	S 1	0	0	0

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

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

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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	36	Total 301	C 202	N 47	O 52	0	1	0
11	l	36	Total 301	C 202	N 47	O 52	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total 265	C 178	N 38	O 48	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 1889	C 1182	N 315	O 387	S 5	0	5	0
13	o	243	Total 1873	C 1171	N 315	O 382	S 5	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total 258	C 181	N 36	O 39	S 2	0	0	0
14	t	30	Total 258	C 181	N 36	O 39	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total 765	C 486	N 128	O 151	0	0	0
15	u	97	Total 774	C 491	N 129	O 154	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	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 X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

- 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 (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		

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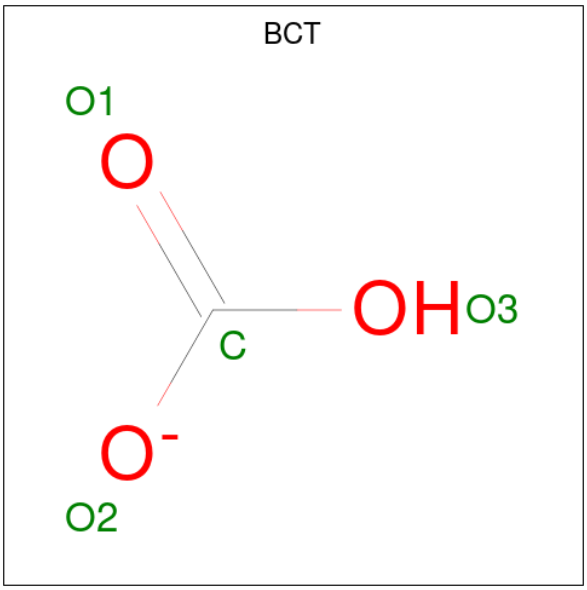
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	a	1	Total Fe 2 2	0	1

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

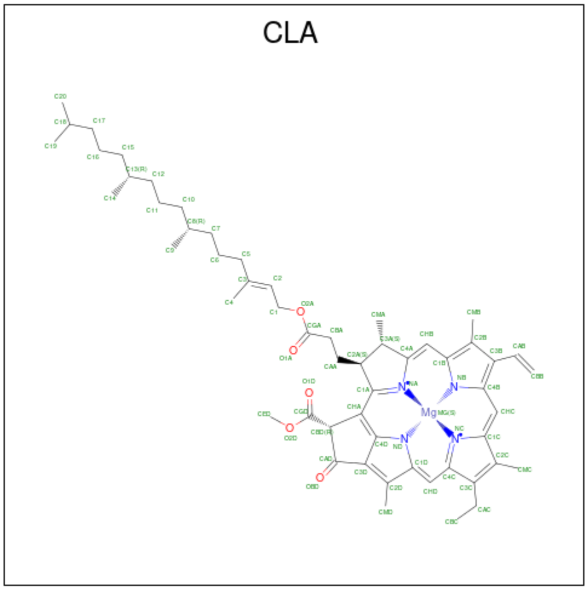
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	2	Total Cl 2 2	0	0
22	a	2	Total Cl 2 2	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 8 2 6	0	1
23	a	1	Total C O 8 2 6	0	1

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



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

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

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

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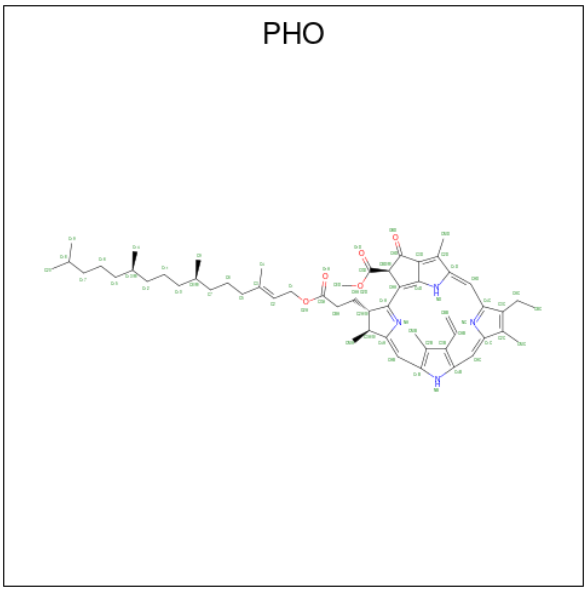
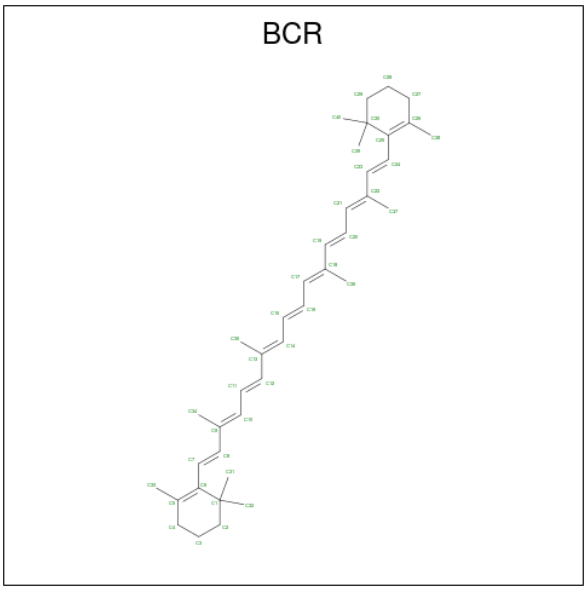
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4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

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



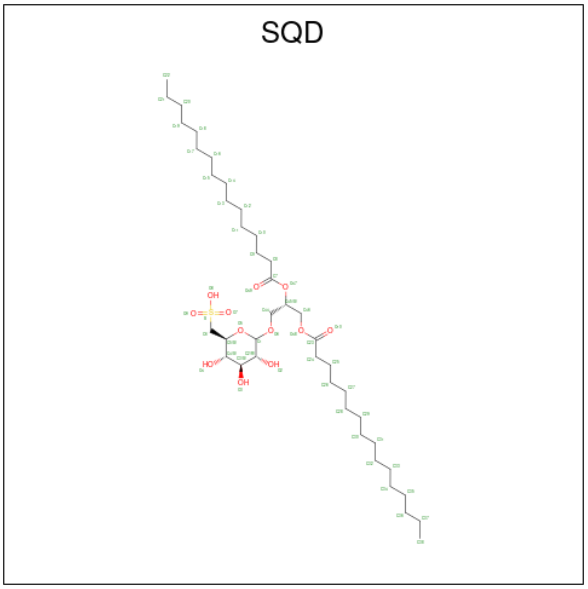
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



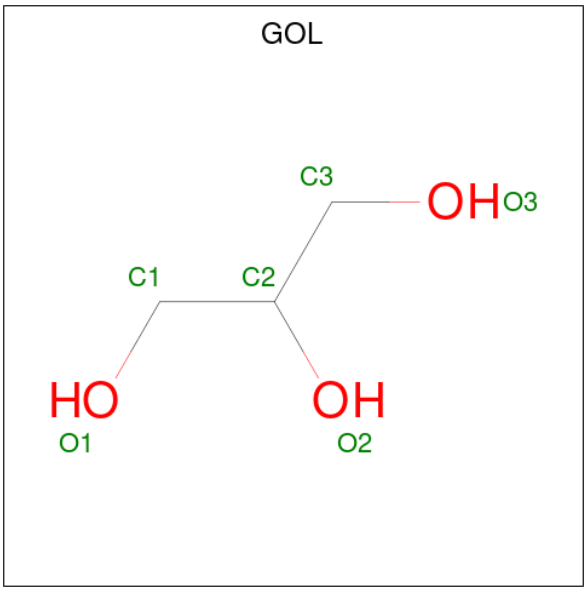
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total 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 (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



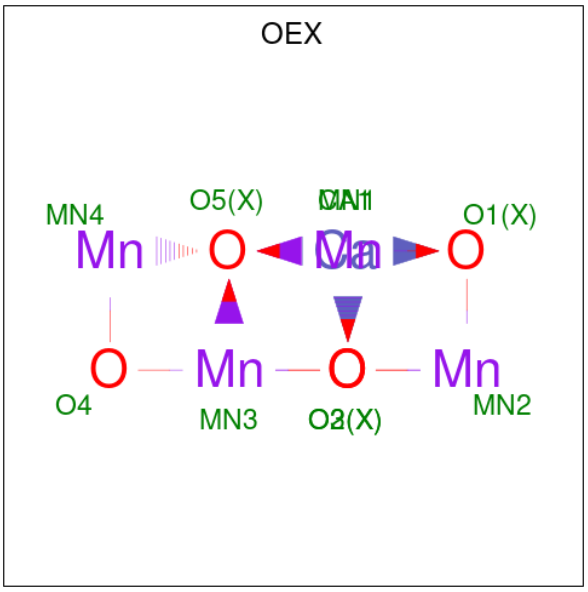
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0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

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



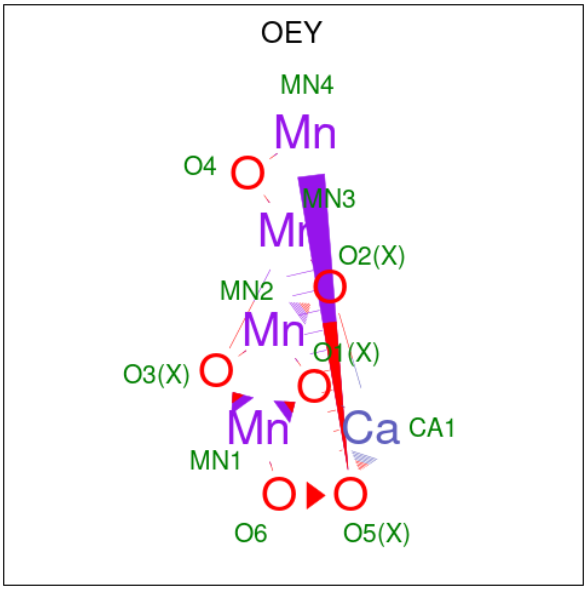
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



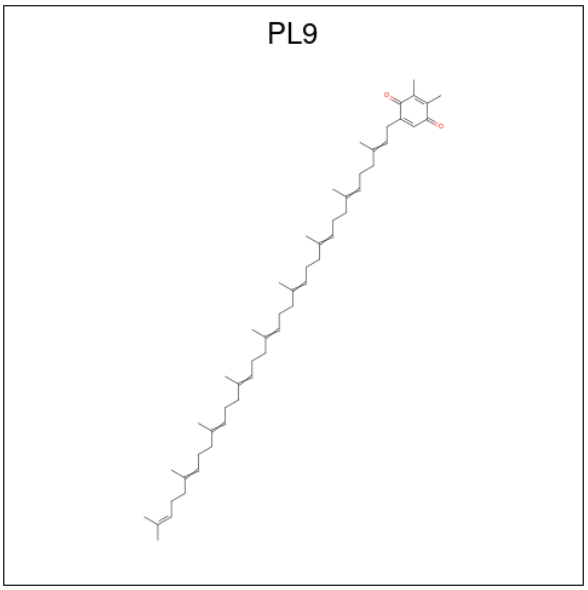
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: $CaMn_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
30	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 31 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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 110 106 4	0	1
31	D	1	Total C O 55 53 2	0	0
31	a	1	Total C O 110 106 4	0	1
31	d	1	Total C O 55 53 2	0	0

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 28 23 5	0	0
32	B	1	Total C O 33 28 5	0	0
32	D	2	Total C O 57 51 6	0	0
32	I	1	Total C O 40 35 5	0	0
32	J	1	Total C 10 10	0	0

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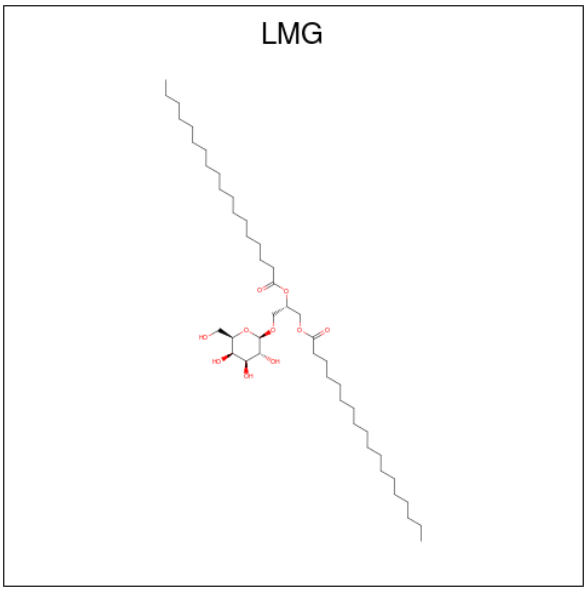
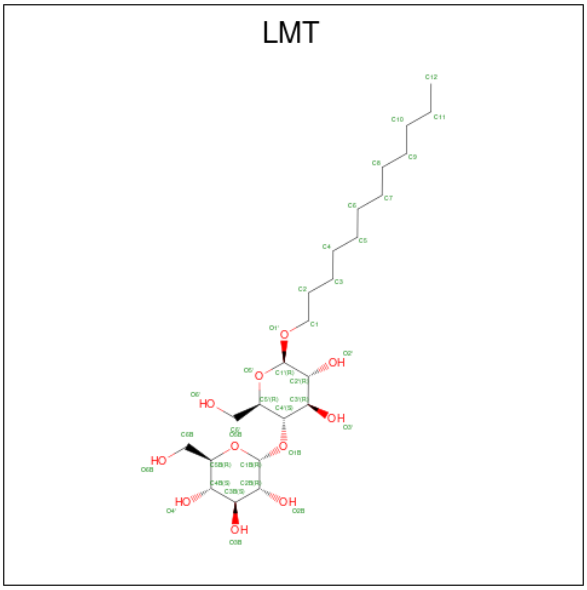
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	K	1	Total C O 34 29 5	0	0
32	M	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	2	Total C O 53 47 6	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	0	0
32	x	1	Total C O 18 16 2	0	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



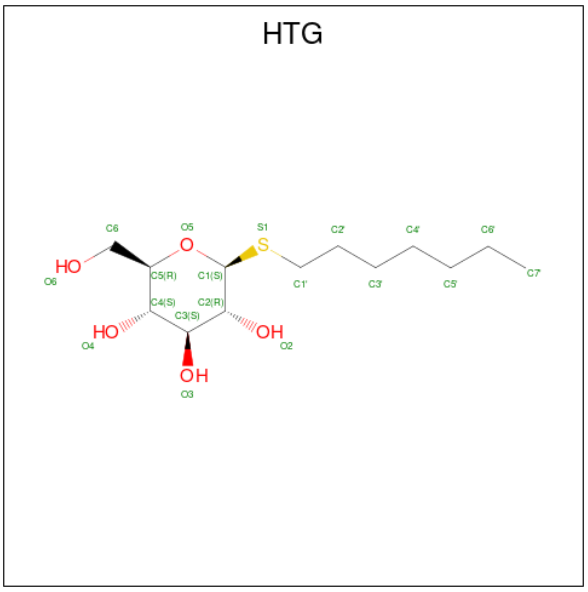
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			51	41	10		
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total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

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			35	24	11		
34	B	1	Total	C	O	0	0
			35	24	11		
34	B	1	Total	C	O	0	0
			25	19	6		
34	E	1	Total	C	O	0	0
			35	24	11		
34	I	1	Total	C	O	0	0
			35	24	11		
34	M	1	Total	C	O	0	0
			35	24	11		
34	M	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	b	1	Total	C	O	0	0
			25	19	6		
34	b	1	Total	C	O	0	0
			25	19	6		
34	e	1	Total	C	O	0	0
			35	24	11		
34	m	1	Total	C	O	0	0
			35	24	11		
34	t	1	Total	C	O	0	0
			26	19	7		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	B	1	Total C O S 19 13 5 1	0	0
35	B	1	Total C O S 19 13 5 1	0	0
35	B	1	Total C O S 19 13 5 1	0	0
35	B	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	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
35	V	1	Total C O 11 6 5	0	0
35	b	1	Total C O S 19 13 5 1	0	0
35	b	1	Total C O S 19 13 5 1	0	0
35	b	1	Total C O S 19 13 5 1	0	0
35	b	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	c	1	Total C O S 19 13 5 1	0	0

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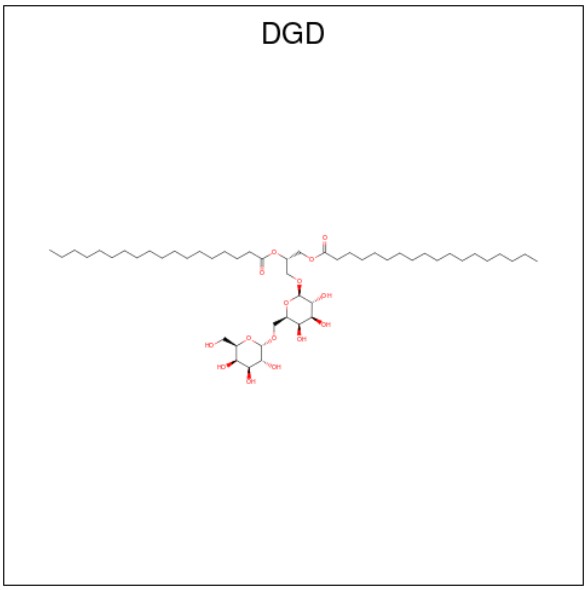
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	h	1	Total C O S 16 10 5 1	0	0

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

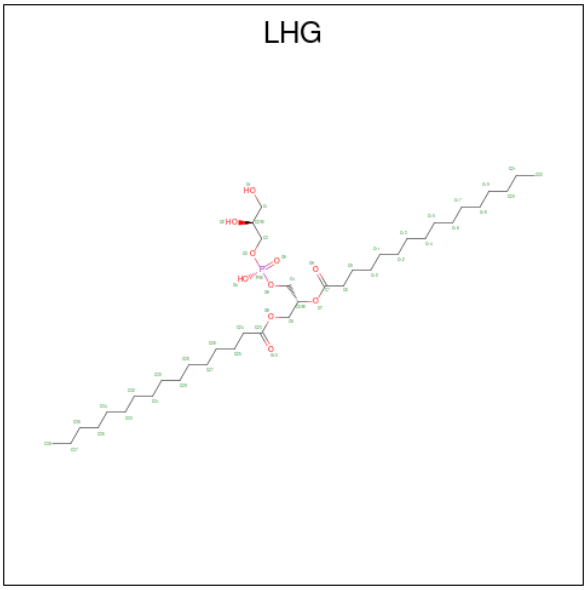


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	C	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	V	1	Total Ca 1 1	0	0
37	b	1	Total Ca 1 1	0	0
37	c	2	Total Ca 2 2	0	0
37	o	1	Total Ca 1 1	0	0
37	v	1	Total Ca 1 1	0	0

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



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

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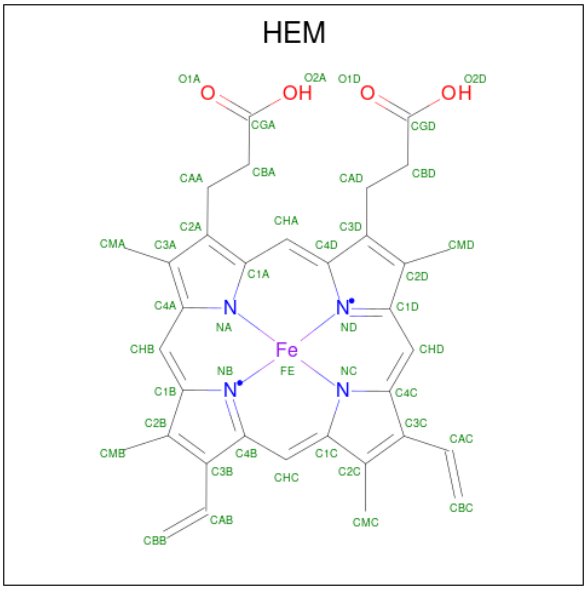
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	L	1	Total C O P 49 38 10 1	0	0
38	a	1	Total C O P 42 31 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0
38	d	1	Total C O P 49 38 10 1	0	0
38	l	1	Total C O P 49 38 10 1	0	0

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



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

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	J	1	Total Mg 1 1	0	0

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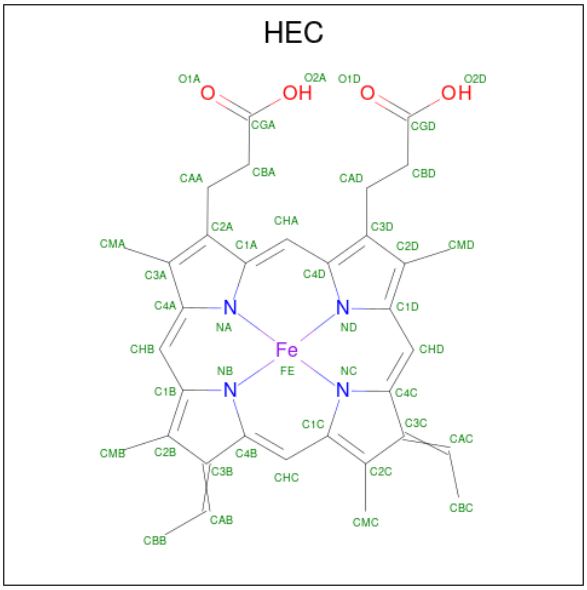
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	j	1	Total Mg 1 1	0	0

- Molecule 41 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	A	125	Total O 130 130	0	5
42	B	164	Total O 164 164	0	0
42	C	147	Total O 147 147	0	0
42	D	112	Total O 112 112	0	0
42	E	14	Total O 14 14	0	0
42	F	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	H	20	Total O 20 20	0	0
42	I	6	Total O 6 6	0	0
42	J	4	Total O 4 4	0	0
42	K	7	Total O 7 7	0	0
42	L	4	Total O 4 4	0	0
42	M	7	Total O 7 7	0	0
42	O	74	Total O 74 74	0	0
42	T	8	Total O 8 8	0	0
42	U	33	Total O 33 33	0	0
42	V	65	Total O 65 65	0	0
42	X	2	Total O 2 2	0	0
42	Y	1	Total O 1 1	0	0
42	a	128	Total O 133 133	0	5
42	b	185	Total O 185 185	0	0
42	c	122	Total O 122 122	0	0
42	d	109	Total O 109 109	0	0
42	e	7	Total O 7 7	0	0
42	f	3	Total O 3 3	0	0
42	h	14	Total O 14 14	0	0
42	i	3	Total O 3 3	0	0
42	j	2	Total O 2 2	0	0

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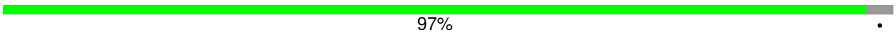
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	k	3	Total O 3 3	0	0
42	l	6	Total O 6 6	0	0
42	m	11	Total O 11 11	0	0
42	o	78	Total O 78 78	0	0
42	t	5	Total O 5 5	0	0
42	u	47	Total O 47 47	0	0
42	v	49	Total O 49 49	0	0
42	x	4	Total O 4 4	0	0
42	y	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

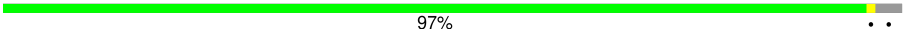
• Molecule 1: Photosystem II D1 protein

Chain A:



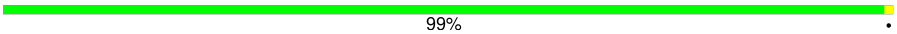
• Molecule 1: Photosystem II D1 protein

Chain a:



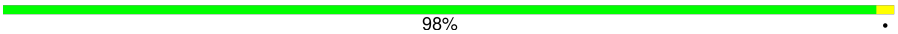
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



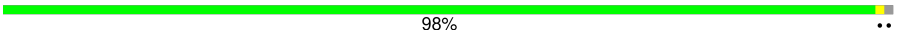
• Molecule 2: Photosystem II CP47 reaction center protein

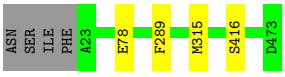
Chain b:



• Molecule 3: Photosystem II CP43 chlorophyll protein

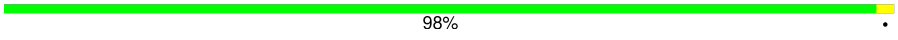
Chain C:





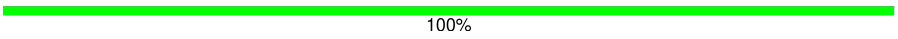
• Molecule 3: Photosystem II CP43 chlorophyll protein

Chain c:



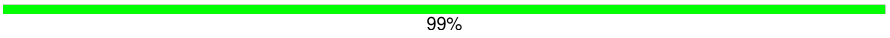
• Molecule 4: Photosystem II D2 protein

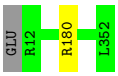
Chain D:



• Molecule 4: Photosystem II D2 protein

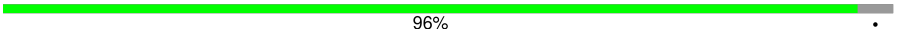
Chain d:

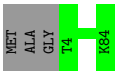




• Molecule 5: Cytochrome b559 subunit alpha

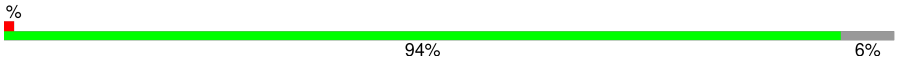
Chain E:

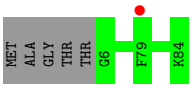




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



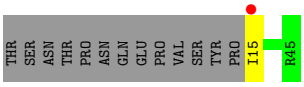


• Molecule 6: Cytochrome b559 subunit beta

Chain F:

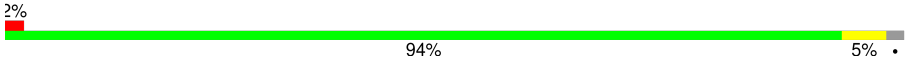
• Molecule 6: Cytochrome b559 subunit beta

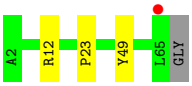
Chain f:



• Molecule 7: Photosystem II reaction center protein H

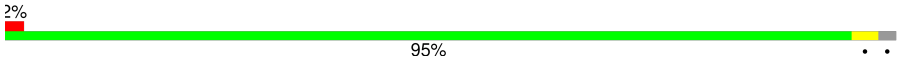
Chain H:

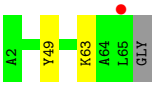




• Molecule 7: Photosystem II reaction center protein H

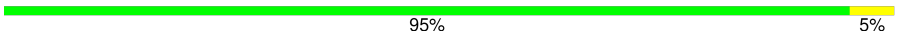
Chain h:





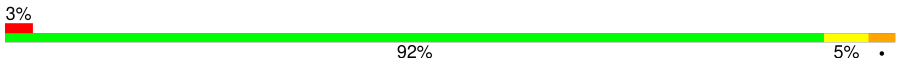
• Molecule 8: Photosystem II reaction center protein I

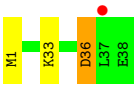
Chain I:



• Molecule 8: Photosystem II reaction center protein I

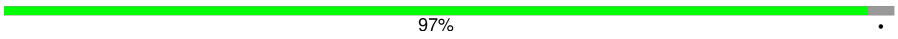
Chain i:





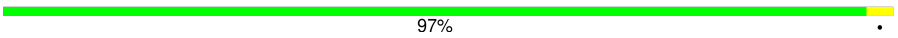
• Molecule 9: Photosystem II reaction center protein J

Chain J:



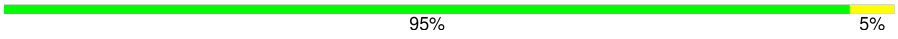
• Molecule 9: Photosystem II reaction center protein J

Chain j:



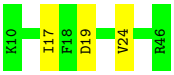
• Molecule 10: Photosystem II reaction center protein K

Chain K:



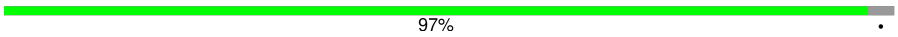
• Molecule 10: Photosystem II reaction center protein K

Chain k:



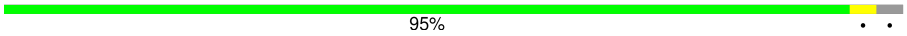
• Molecule 11: Photosystem II reaction center protein L

Chain L:



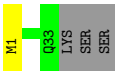
• Molecule 11: Photosystem II reaction center protein L

Chain l:



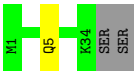
• Molecule 12: Photosystem II reaction center protein M

Chain M:



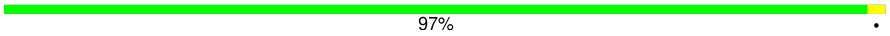
• Molecule 12: Photosystem II reaction center protein M

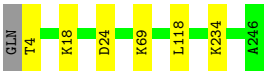
Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

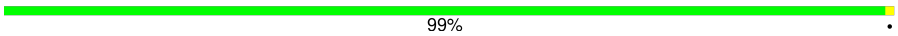
Chain O:

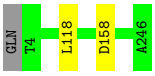




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



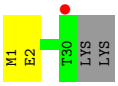


• Molecule 14: Photosystem II reaction center protein T

Chain T:

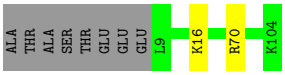
• Molecule 14: Photosystem II reaction center protein T

Chain t:



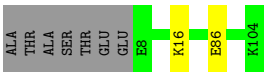
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



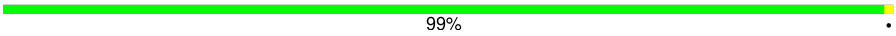
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



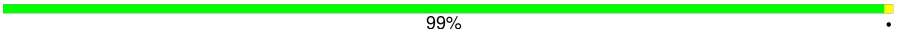
• Molecule 16: Cytochrome c-550

Chain V:



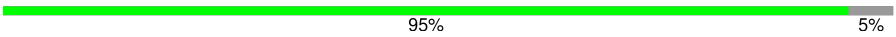
• Molecule 16: Cytochrome c-550

Chain v:



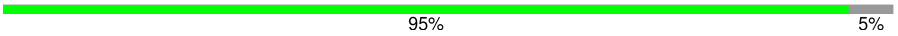
• Molecule 17: Photosystem II reaction center protein X

Chain X:



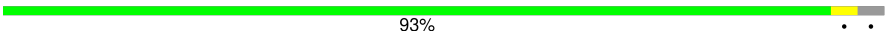
• Molecule 17: Photosystem II reaction center protein X

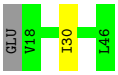
Chain x:



• Molecule 18: Photosystem II reaction center protein Ycf12

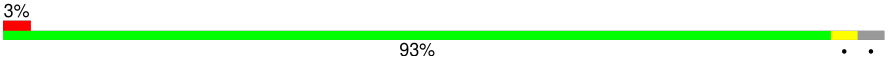
Chain Y:





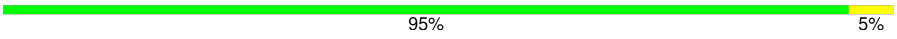
• Molecule 18: Photosystem II reaction center protein Ycf12

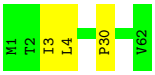
Chain y:



• Molecule 19: Photosystem II reaction center protein Z

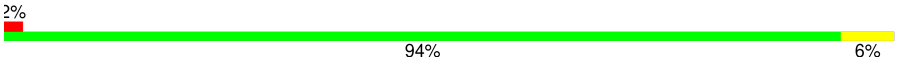
Chain Z:

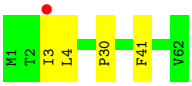




• Molecule 19: Photosystem II reaction center protein Z

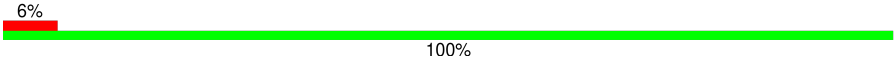
Chain z:

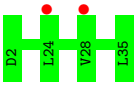




• Molecule 20: Photosystem II protein Y

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	124.96Å 230.22Å 286.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 99.8 (20.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.129 , 0.175 0.140 , 0.182	Depositor DCC
R_{free} test set	17097 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 91.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	53280	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: HTG, UNL, MG, SQD, CLA, PL9, FME, OEY, CA, FE2, DGD, OEX, HEM, CL, BCT, LMG, LHG, HEC, BCR, PHO, LMT, GOL

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	0.50	0/2952	0.59	0/4019
1	a	0.43	0/2957	0.55	0/4027
2	B	0.43	0/4171	0.54	0/5683
2	b	0.41	0/4138	0.53	0/5640
3	C	0.42	0/3667	0.53	0/4992
3	c	0.38	0/3703	0.50	0/5041
4	D	0.46	0/2847	0.56	0/3878
4	d	0.43	0/2838	0.53	0/3866
5	E	0.36	0/687	0.50	0/936
5	e	0.35	0/667	0.47	0/908
6	F	0.42	0/284	0.50	0/387
6	f	0.38	0/257	0.53	0/349
7	H	0.37	0/530	0.57	0/723
7	h	0.33	0/519	0.50	0/708
8	I	0.37	0/311	0.48	0/419
8	i	0.34	0/311	0.49	0/419
9	J	0.34	0/278	0.46	0/376
9	j	0.32	0/283	0.46	0/383
10	K	0.37	0/303	0.51	0/416
10	k	0.34	0/303	0.49	0/416
11	L	0.43	0/311	0.47	0/423
11	l	0.41	0/311	0.49	0/423
12	M	0.45	0/261	0.61	0/357
12	m	0.42	0/262	0.59	0/357
13	O	0.39	0/1935	0.56	0/2623
13	o	0.39	0/1910	0.57	1/2589 (0.0%)
14	T	0.49	0/257	0.55	0/349
14	t	0.47	0/257	0.51	0/349
15	U	0.38	0/776	0.54	0/1052
15	u	0.37	0/785	0.54	0/1064
16	V	0.38	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
16	v	0.34	0/1085	0.48	0/1473
17	X	0.33	0/284	0.46	0/384
17	x	0.31	0/284	0.45	0/384
18	Y	0.29	0/216	0.44	0/289
18	y	0.30	0/216	0.47	0/289
19	Z	0.31	0/490	0.44	0/669
19	z	0.29	0/490	0.39	0/669
20	R	0.28	0/279	0.39	0/383
All	All	0.41	0/43500	0.53	1/59185 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	o	158	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	359/344 (104%)	355 (99%)	3 (1%)	1 (0%)	37	43
1	a	360/344 (105%)	355 (99%)	4 (1%)	1 (0%)	37	43
2	B	510/505 (101%)	506 (99%)	4 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	30 34
3	c	463/455 (102%)	449 (97%)	12 (3%)	2 (0%)	30 34
4	D	343/342 (100%)	333 (97%)	10 (3%)	0	100 100
4	d	342/342 (100%)	336 (98%)	6 (2%)	0	100 100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100 100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100 100
6	F	32/44 (73%)	32 (100%)	0	0	100 100
6	f	29/44 (66%)	29 (100%)	0	0	100 100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100 100
7	h	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	8 6
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100 100
8	i	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4 2
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	35/37 (95%)	35 (100%)	0	0	100 100
11	l	35/37 (95%)	35 (100%)	0	0	100 100
12	M	32/36 (89%)	32 (100%)	0	0	100 100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100 100
13	O	246/244 (101%)	237 (96%)	9 (4%)	0	100 100
13	o	243/244 (100%)	238 (98%)	5 (2%)	0	100 100
14	T	28/32 (88%)	28 (100%)	0	0	100 100
14	t	28/32 (88%)	28 (100%)	0	0	100 100
15	U	94/104 (90%)	92 (98%)	2 (2%)	0	100 100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100 100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100 100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100 100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100 100
17	x	36/40 (90%)	36 (100%)	0	0	100 100
18	Y	27/30 (90%)	27 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	y	27/30 (90%)	27 (100%)	0	0	100 100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7 6
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7 6
20	R	32/34 (94%)	32 (100%)	0	0	100 100
All	All	5316/5384 (99%)	5202 (98%)	104 (2%)	10 (0%)	44 52

5 of 10 Ramachandran outliers are listed below:

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

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	295/279 (106%)	295 (100%)	0	100 100
1	a	296/279 (106%)	295 (100%)	1 (0%)	91 95
2	B	410/403 (102%)	405 (99%)	5 (1%)	67 80
2	b	406/403 (101%)	398 (98%)	8 (2%)	50 63
3	C	360/356 (101%)	357 (99%)	3 (1%)	79 88
3	c	364/356 (102%)	358 (98%)	6 (2%)	58 71
4	D	280/277 (101%)	279 (100%)	1 (0%)	89 94
4	d	279/277 (101%)	278 (100%)	1 (0%)	89 94
5	E	73/73 (100%)	73 (100%)	0	100 100
5	e	70/73 (96%)	70 (100%)	0	100 100
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	25/38 (66%)	24 (96%)	1 (4%)	27 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	H	55/54 (102%)	51 (93%)	4 (7%)	11 12
7	h	54/54 (100%)	53 (98%)	1 (2%)	52 65
8	I	34/34 (100%)	33 (97%)	1 (3%)	37 48
8	i	34/34 (100%)	32 (94%)	2 (6%)	16 18
9	J	26/27 (96%)	26 (100%)	0	100 100
9	j	26/27 (96%)	25 (96%)	1 (4%)	28 37
10	K	30/30 (100%)	28 (93%)	2 (7%)	13 14
10	k	30/30 (100%)	27 (90%)	3 (10%)	6 5
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	35/35 (100%)	34 (97%)	1 (3%)	37 48
12	M	30/32 (94%)	30 (100%)	0	100 100
12	m	30/32 (94%)	29 (97%)	1 (3%)	33 42
13	O	211/207 (102%)	205 (97%)	6 (3%)	38 49
13	o	208/207 (100%)	207 (100%)	1 (0%)	86 93
14	T	26/28 (93%)	26 (100%)	0	100 100
14	t	26/28 (93%)	25 (96%)	1 (4%)	28 37
15	U	83/89 (93%)	81 (98%)	2 (2%)	44 55
15	u	84/89 (94%)	82 (98%)	2 (2%)	44 55
16	V	117/117 (100%)	116 (99%)	1 (1%)	75 85
16	v	117/117 (100%)	116 (99%)	1 (1%)	75 85
17	X	31/33 (94%)	31 (100%)	0	100 100
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	23 29
18	y	22/23 (96%)	21 (96%)	1 (4%)	23 29
19	Z	52/52 (100%)	50 (96%)	2 (4%)	28 37
19	z	52/52 (100%)	49 (94%)	3 (6%)	17 19
20	R	29/29 (100%)	29 (100%)	0	100 100
All	All	4416/4403 (100%)	4353 (99%)	63 (1%)	62 75

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	12	ASN

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Mol	Chain	Res	Type
14	t	2	GLU
2	b	485	GLU
13	o	118	LEU
18	y	45	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	223	GLN
3	c	201	ASN
13	o	130	GLN
2	b	331	ASN
4	d	83	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	0.69	0	8,9,11	1.12	1 (12%)
14	FME	t	1	14	8,9,10	0.71	0	8,9,11	1.47	2 (25%)
14	FME	T	1	14	8,9,10	0.65	0	8,9,11	1.73	1 (12%)
12	FME	m	1	12	8,9,10	0.60	0	8,9,11	1.22	0
8	FME	I	1	8	8,9,10	0.66	0	8,9,11	1.03	1 (12%)
12	FME	M	1	12	8,9,10	0.67	0	8,9,11	1.17	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	CB-CA-N	-3.36	104.40	110.52
14	t	1	FME	O-C-CA	-2.77	117.64	124.77
14	t	1	FME	C-CA-N	2.24	113.81	109.50
12	M	1	FME	O-C-CA	-2.13	119.30	124.77
8	I	1	FME	O-C-CA	-2.09	119.39	124.77

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 227 ligands modelled in this entry, 18 are monoatomic and 18 are unknown - leaving 191 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	$\#\|Z\| > 2$
24	CLA	b	609	2	63,73,73	2.05	17 (26%)	74,113,113	2.70	26 (35%)
28	GOL	A	412	-	5,5,5	0.41	0	5,5,5	0.39	0
36	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	6 (7%)
35	HTG	B	624	-	19,19,19	0.82	1 (5%)	23,24,24	1.24	1 (4%)
24	CLA	b	610	42	63,73,73	2.10	16 (25%)	74,113,113	2.74	29 (39%)
30	OEY	A	415[B]	1,42,3	0,16,16	-	-	-		
24	CLA	C	507	3	63,73,73	2.06	17 (26%)	74,113,113	2.68	31 (41%)
35	HTG	b	628	-	19,19,19	0.83	1 (5%)	23,24,24	1.23	3 (13%)
24	CLA	B	609	2	63,73,73	2.02	16 (25%)	74,113,113	2.72	25 (33%)
27	SQD	A	411	-	52,54,54	0.88	2 (3%)	62,65,65	1.78	12 (19%)
38	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.13	5 (9%)
24	CLA	B	602	2	63,73,73	2.10	16 (25%)	74,113,113	2.72	30 (40%)
24	CLA	C	513	3	63,73,73	2.07	16 (25%)	74,113,113	2.69	27 (36%)
24	CLA	B	606	2	63,73,73	1.95	15 (23%)	74,113,113	2.87	28 (37%)
24	CLA	C	504	3	63,73,73	2.01	16 (25%)	74,113,113	2.67	23 (31%)
24	CLA	b	607	42	63,73,73	1.99	15 (23%)	74,113,113	2.74	26 (35%)
38	LHG	D	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.00	3 (5%)
28	GOL	C	525	-	5,5,5	0.43	0	5,5,5	0.15	0
38	LHG	D	406	-	48,48,48	0.90	3 (6%)	51,54,54	1.00	3 (5%)
24	CLA	B	613	2	63,73,73	2.05	16 (25%)	74,113,113	2.72	31 (41%)
23	BCT	a	420[A]	21	3,3,3	0.53	0	2,3,3	0.95	0
24	CLA	b	601	42	63,73,73	2.12	16 (25%)	74,113,113	2.63	26 (35%)
24	CLA	A	409	1	63,73,73	2.03	17 (26%)	74,113,113	2.77	30 (40%)
24	CLA	C	506	3	63,73,73	2.03	16 (25%)	74,113,113	2.64	27 (36%)
26	BCR	a	408	-	41,41,41	0.98	1 (2%)	56,56,56	1.57	12 (21%)
26	BCR	h	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.12	5 (11%)
24	CLA	b	604	2	63,73,73	2.03	15 (23%)	74,113,113	2.67	27 (36%)
26	BCR	d	404	-	41,41,41	1.16	2 (4%)	56,56,56	1.85	13 (23%)
34	LMT	t	101	-	26,26,36	0.56	1 (3%)	31,31,47	1.15	2 (6%)
26	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.51	14 (25%)
33	LMG	C	521	-	51,51,55	1.00	3 (5%)	59,59,63	1.19	4 (6%)
24	CLA	b	605	2	63,73,73	1.97	16 (25%)	74,113,113	2.83	25 (33%)
31	PL9	A	416[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.02	24 (35%)
39	HEM	E	103	5,6	42,50,50	1.30	6 (14%)	46,82,82	1.85	13 (28%)
36	DGD	h	103	-	63,63,67	0.86	3 (4%)	77,77,81	0.96	3 (3%)
26	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.48	11 (19%)
38	LHG	a	419	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
24	CLA	B	603	2	63,73,73	2.04	16 (25%)	74,113,113	2.85	29 (39%)
24	CLA	B	608	2	63,73,73	2.02	15 (23%)	74,113,113	2.69	28 (37%)
33	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.10	4 (8%)
30	OEY	a	413[B]	1,42,3	0,16,16	-	-	-		
24	CLA	d	402	4	63,73,73	1.99	16 (25%)	74,113,113	2.63	30 (40%)
31	PL9	a	414[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
26	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.77	14 (25%)
33	LMG	A	418	-	51,51,55	0.91	2 (3%)	59,59,63	1.20	5 (8%)
24	CLA	C	505	42	63,73,73	2.02	16 (25%)	74,113,113	2.69	32 (43%)
34	LMT	a	359	-	36,36,36	0.51	1 (2%)	47,47,47	0.92	2 (4%)
24	CLA	B	612	2	63,73,73	2.00	17 (26%)	74,113,113	2.74	29 (39%)
34	LMT	B	630	-	25,25,36	0.43	0	30,30,47	0.72	1 (3%)
35	HTG	b	623	-	19,19,19	0.95	1 (5%)	23,24,24	1.46	3 (13%)
35	HTG	b	625	-	19,19,19	1.00	2 (10%)	23,24,24	1.57	3 (13%)
26	BCR	y	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.71	12 (21%)
24	CLA	c	509	42	63,73,73	2.06	16 (25%)	74,113,113	2.68	26 (35%)
27	SQD	a	411	-	52,54,54	0.99	3 (5%)	62,65,65	1.21	7 (11%)
35	HTG	D	410	-	16,16,19	0.99	2 (12%)	20,21,24	1.17	1 (5%)
24	CLA	c	510	3	63,73,73	2.08	16 (25%)	74,113,113	2.68	27 (36%)
26	BCR	A	410	-	41,41,41	1.03	1 (2%)	56,56,56	1.64	11 (19%)
27	SQD	B	620	-	52,54,54	0.96	2 (3%)	62,65,65	1.37	7 (11%)
38	LHG	d	407	-	48,48,48	0.89	3 (6%)	51,54,54	0.91	3 (5%)
24	CLA	c	506	42	63,73,73	2.08	17 (26%)	74,113,113	2.67	29 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	c	512	3	63,73,73	2.07	16 (25%)	74,113,113	2.66	28 (37%)
36	DGD	c	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	4 (5%)
26	BCR	C	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.51	8 (14%)
36	DGD	C	519	-	63,63,67	0.82	3 (4%)	77,77,81	0.95	4 (5%)
24	CLA	B	610	42	63,73,73	2.08	16 (25%)	74,113,113	2.70	29 (39%)
24	CLA	C	509	3	63,73,73	2.13	17 (26%)	74,113,113	2.66	29 (39%)
26	BCR	Y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.77	14 (25%)
34	LMT	A	359	-	36,36,36	0.56	1 (2%)	47,47,47	0.88	1 (2%)
28	GOL	c	502	-	5,5,5	0.42	0	5,5,5	0.32	0
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.11	3 (5%)
35	HTG	B	623	-	19,19,19	0.89	1 (5%)	23,24,24	1.34	4 (17%)
24	CLA	B	614	2	63,73,73	1.99	16 (25%)	74,113,113	2.87	29 (39%)
28	GOL	B	626	-	5,5,5	0.38	0	5,5,5	0.51	0
24	CLA	a	407	1	63,73,73	2.01	16 (25%)	74,113,113	2.65	30 (40%)
24	CLA	c	504	3	63,73,73	2.00	16 (25%)	74,113,113	2.68	26 (35%)
24	CLA	C	514	3	63,73,73	2.09	16 (25%)	74,113,113	2.66	26 (35%)
24	CLA	c	505	3	63,73,73	2.05	16 (25%)	74,113,113	2.62	25 (33%)
24	CLA	B	607	42	63,73,73	2.00	15 (23%)	74,113,113	2.75	28 (37%)
24	CLA	C	512	3	63,73,73	2.10	17 (26%)	74,113,113	2.58	26 (35%)
34	LMT	I	101	-	36,36,36	0.49	1 (2%)	47,47,47	1.09	3 (6%)
35	HTG	V	204	-	11,11,19	0.23	0	15,15,24	1.01	1 (6%)
23	BCT	A	403[B]	21	3,3,3	0.55	0	2,3,3	0.82	0
35	HTG	h	101	-	16,16,19	1.05	2 (12%)	20,21,24	1.45	2 (10%)
24	CLA	a	404	42	63,73,73	2.04	17 (26%)	74,113,113	2.71	28 (37%)
24	CLA	a	403	1	63,73,73	2.07	15 (23%)	74,113,113	2.71	33 (44%)
35	HTG	c	526	-	19,19,19	0.94	2 (10%)	23,24,24	1.37	3 (13%)
26	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.63	12 (21%)
26	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.64	12 (21%)
24	CLA	b	616	2	63,73,73	2.02	16 (25%)	74,113,113	2.73	28 (37%)
27	SQD	F	101	-	41,43,54	1.10	2 (4%)	51,54,65	1.63	8 (15%)
26	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.57	9 (16%)
35	HTG	C	523	-	19,19,19	0.97	1 (5%)	23,24,24	1.74	5 (21%)
24	CLA	A	405	42	63,73,73	2.03	15 (23%)	74,113,113	2.82	29 (39%)
24	CLA	B	604	2	63,73,73	2.03	16 (25%)	74,113,113	2.66	27 (36%)
24	CLA	b	612	2	63,73,73	2.05	16 (25%)	74,113,113	2.60	28 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	HTG	B	628	-	19,19,19	0.88	2 (10%)	23,24,24	1.22	3 (13%)
24	CLA	c	514	3	63,73,73	2.04	16 (25%)	74,113,113	2.69	30 (40%)
24	CLA	C	510	3	63,73,73	2.15	17 (26%)	74,113,113	2.69	29 (39%)
24	CLA	b	614	2	63,73,73	2.01	16 (25%)	74,113,113	2.73	27 (36%)
25	PHO	A	408	-	50,69,69	1.97	8 (16%)	48,99,99	2.15	11 (22%)
27	SQD	a	409	-	52,54,54	0.89	2 (3%)	62,65,65	1.76	12 (19%)
26	BCR	D	404	-	41,41,41	1.06	1 (2%)	56,56,56	1.87	16 (28%)
24	CLA	B	605	2	63,73,73	2.02	16 (25%)	74,113,113	2.78	26 (35%)
28	GOL	B	627	-	5,5,5	0.48	0	5,5,5	0.38	0
24	CLA	D	403	4	63,73,73	2.03	15 (23%)	74,113,113	2.72	29 (39%)
25	PHO	A	407	-	50,69,69	1.88	8 (16%)	48,99,99	1.93	11 (22%)
27	SQD	A	413	-	52,54,54	0.95	2 (3%)	62,65,65	1.07	5 (8%)
26	BCR	C	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.63	12 (21%)
24	CLA	b	615	2	63,73,73	2.05	16 (25%)	74,113,113	2.66	27 (36%)
24	CLA	c	515	3	63,73,73	2.09	17 (26%)	74,113,113	2.69	29 (39%)
24	CLA	C	511	3	63,73,73	2.08	16 (25%)	74,113,113	2.75	29 (39%)
34	LMT	b	622	-	25,25,36	0.46	0	30,30,47	0.70	0
33	LMG	J	101	40	51,51,55	0.89	3 (5%)	59,59,63	0.90	3 (5%)
29	OEX	A	414[A]	1,42,3	0,15,15	-	-	-		
24	CLA	c	507	3	63,73,73	2.00	16 (25%)	74,113,113	2.57	25 (33%)
26	BCR	b	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.45	15 (26%)
26	BCR	b	619	-	41,41,41	1.02	1 (2%)	56,56,56	1.66	12 (21%)
36	DGD	c	519	-	63,63,67	0.88	2 (3%)	77,77,81	0.95	4 (5%)
31	PL9	D	405	-	55,55,55	0.69	2 (3%)	68,69,69	1.76	21 (30%)
24	CLA	D	402	4	63,73,73	1.98	16 (25%)	74,113,113	2.77	29 (39%)
28	GOL	V	202	-	5,5,5	0.39	0	5,5,5	0.36	0
35	HTG	b	624	-	19,19,19	0.93	1 (5%)	23,24,24	1.19	1 (4%)
33	LMG	Z	101	-	37,37,55	1.00	3 (8%)	45,45,63	1.49	7 (15%)
28	GOL	b	627	-	5,5,5	0.34	0	5,5,5	0.40	0
38	LHG	D	357	-	48,48,48	0.89	2 (4%)	51,54,54	1.22	5 (9%)
39	HEM	e	102	5,6	42,50,50	1.27	6 (14%)	46,82,82	1.71	12 (26%)
34	LMT	m	102	-	36,36,36	0.42	0	47,47,47	0.88	1 (2%)
33	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.13	5 (8%)
25	PHO	a	406	-	50,69,69	1.95	8 (16%)	48,99,99	2.19	13 (27%)
24	CLA	C	508	42	63,73,73	2.03	16 (25%)	74,113,113	2.59	27 (36%)
26	BCR	c	517	-	41,41,41	1.05	1 (2%)	56,56,56	1.66	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	OEX	a	412[A]	1,42,3	0,15,15	-	-	-		
38	LHG	d	406	-	48,48,48	0.90	3 (6%)	51,54,54	1.11	5 (9%)
24	CLA	c	503	3	63,73,73	2.09	16 (25%)	74,113,113	2.67	27 (36%)
35	HTG	B	625	-	19,19,19	0.91	1 (5%)	23,24,24	1.43	3 (13%)
24	CLA	b	602	2	63,73,73	2.10	16 (25%)	74,113,113	2.77	30 (40%)
24	CLA	B	601	42	63,73,73	2.09	15 (23%)	74,113,113	2.66	28 (37%)
24	CLA	b	606	2	63,73,73	1.98	14 (22%)	74,113,113	2.73	30 (40%)
28	GOL	a	416	-	5,5,5	0.37	0	5,5,5	0.68	0
31	PL9	A	416[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.89	19 (27%)
34	LMT	B	622	-	36,36,36	0.41	0	47,47,47	1.07	3 (6%)
24	CLA	C	502	3	63,73,73	2.05	17 (26%)	74,113,113	2.74	28 (37%)
36	DGD	c	520	-	63,63,67	0.83	3 (4%)	77,77,81	1.09	4 (5%)
33	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.18	6 (10%)
34	LMT	e	101	-	36,36,36	0.48	1 (2%)	47,47,47	0.81	1 (2%)
24	CLA	b	613	2	63,73,73	2.08	15 (23%)	74,113,113	2.64	27 (36%)
28	GOL	a	410	-	5,5,5	0.37	0	5,5,5	0.37	0
24	CLA	C	503	3	63,73,73	2.05	15 (23%)	74,113,113	2.63	26 (35%)
33	LMG	j	101	40	51,51,55	0.88	2 (3%)	59,59,63	1.14	5 (8%)
24	CLA	A	406	42	63,73,73	2.04	16 (25%)	74,113,113	2.70	31 (41%)
38	LHG	l	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.12	4 (7%)
26	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.76	12 (21%)
34	LMT	E	102	-	36,36,36	0.48	0	47,47,47	0.83	0
31	PL9	a	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.91	21 (30%)
24	CLA	B	611	2	63,73,73	1.99	15 (23%)	74,113,113	2.80	30 (40%)
24	CLA	B	616	2	63,73,73	2.05	16 (25%)	74,113,113	2.71	26 (35%)
28	GOL	v	202	-	5,5,5	0.38	0	5,5,5	0.31	0
35	HTG	C	522	-	19,19,19	0.92	1 (5%)	23,24,24	1.28	2 (8%)
41	HEC	v	203	16	32,50,50	1.48	4 (12%)	30,82,82	1.63	7 (23%)
24	CLA	d	403	4	63,73,73	2.08	16 (25%)	74,113,113	2.73	30 (40%)
26	BCR	t	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.74	14 (25%)
34	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.85	0
27	SQD	f	101	-	41,43,54	1.10	2 (4%)	51,54,65	1.41	8 (15%)
24	CLA	c	511	3	63,73,73	2.10	16 (25%)	74,113,113	2.67	28 (37%)
33	LMG	b	621	-	51,51,55	0.87	2 (3%)	59,59,63	1.28	5 (8%)
24	CLA	a	350	42	63,73,73	2.04	15 (23%)	74,113,113	2.76	26 (35%)
33	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.14	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	A	404	1	63,73,73	2.07	16 (25%)	74,113,113	2.77	28 (37%)
23	BCT	a	420[B]	21	3,3,3	0.52	0	2,3,3	0.85	0
24	CLA	b	603	2	63,73,73	2.05	16 (25%)	74,113,113	2.75	27 (36%)
26	BCR	B	617	-	41,41,41	1.03	2 (4%)	56,56,56	1.55	10 (17%)
24	CLA	b	608	2	63,73,73	2.05	16 (25%)	74,113,113	2.68	32 (43%)
24	CLA	c	513	3	63,73,73	2.08	15 (23%)	74,113,113	2.70	28 (37%)
36	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.16	5 (6%)
41	HEC	V	203	16	32,50,50	1.45	4 (12%)	30,82,82	1.64	6 (20%)
36	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	0.94	4 (5%)
34	LMT	b	630	-	25,25,36	0.52	1 (4%)	30,30,47	0.86	0
35	HTG	c	523	-	19,19,19	0.89	1 (5%)	23,24,24	1.21	1 (4%)
24	CLA	b	611	2	63,73,73	2.02	16 (25%)	74,113,113	2.74	24 (32%)
24	CLA	B	615	2	63,73,73	1.97	14 (22%)	74,113,113	2.72	29 (39%)
31	PL9	d	405	-	55,55,55	0.63	2 (3%)	68,69,69	1.71	17 (25%)
24	CLA	c	508	3	63,73,73	2.10	15 (23%)	74,113,113	2.59	30 (40%)
34	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.10	3 (6%)
38	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.09	4 (7%)
23	BCT	A	403[A]	21	3,3,3	0.54	0	2,3,3	0.77	0
25	PHO	a	405	-	50,69,69	1.86	9 (18%)	48,99,99	2.08	12 (25%)
27	SQD	b	620	-	52,54,54	0.97	2 (3%)	62,65,65	1.45	9 (14%)
34	LMT	M	103	-	36,36,36	0.42	0	47,47,47	0.96	3 (6%)
26	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.58	14 (25%)
33	LMG	c	521	-	51,51,55	0.93	2 (3%)	59,59,63	1.08	5 (8%)

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
24	CLA	b	609	2	1/1/15/20	5/37/115/115	-
28	GOL	A	412	-	-	2/4/4/4	-
36	DGD	C	518	-	-	9/51/91/95	0/2/2/2
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1
24	CLA	b	610	42	1/1/15/20	6/37/115/115	-
24	CLA	C	507	3	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	b	628	-	-	4/10/30/30	0/1/1/1
24	CLA	B	609	2	1/1/15/20	4/37/115/115	-
27	SQD	A	411	-	-	15/49/69/69	0/1/1/1
38	LHG	d	408	-	-	11/53/53/53	-
24	CLA	B	602	2	1/1/15/20	4/37/115/115	-
24	CLA	C	513	3	1/1/15/20	6/37/115/115	-
24	CLA	B	606	2	1/1/15/20	5/37/115/115	-
24	CLA	C	504	3	-	3/37/115/115	-
24	CLA	b	607	42	1/1/15/20	1/37/115/115	-
38	LHG	D	407	-	-	9/53/53/53	-
28	GOL	C	525	-	-	2/4/4/4	-
38	LHG	D	406	-	-	16/53/53/53	-
24	CLA	B	613	2	1/1/15/20	6/37/115/115	-
24	CLA	b	601	42	1/1/15/20	15/37/115/115	-
24	CLA	A	409	1	-	10/37/115/115	-
24	CLA	C	506	3	1/1/15/20	7/37/115/115	-
26	BCR	a	408	-	-	0/29/63/63	0/2/2/2
26	BCR	h	102	-	-	2/29/63/63	0/2/2/2
38	LHG	E	101	-	-	15/46/46/53	-
24	CLA	b	604	2	1/1/15/20	6/37/115/115	-
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
34	LMT	t	101	-	-	5/17/38/61	0/1/1/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
33	LMG	C	521	-	-	10/46/66/70	0/1/1/1
24	CLA	b	605	2	1/1/15/20	5/37/115/115	-
31	PL9	A	416[A]	-	-	16/53/73/73	0/1/1/1
39	HEM	E	103	5,6	-	4/12/54/54	-
36	DGD	h	103	-	-	11/51/91/95	0/2/2/2
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2
38	LHG	a	419	-	-	8/46/46/53	-
24	CLA	B	603	2	1/1/15/20	4/37/115/115	-
24	CLA	B	608	2	-	4/37/115/115	-
33	LMG	z	101	-	-	6/34/54/70	0/1/1/1
24	CLA	d	402	4	1/1/15/20	4/37/115/115	-
31	PL9	a	414[A]	-	-	16/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	T	101	-	-	2/29/63/63	0/2/2/2
33	LMG	A	418	-	-	10/46/66/70	0/1/1/1
24	CLA	C	505	42	1/1/15/20	4/37/115/115	-
34	LMT	a	359	-	-	7/21/61/61	0/2/2/2
24	CLA	B	612	2	1/1/15/20	4/37/115/115	-
34	LMT	B	630	-	-	11/17/37/61	0/1/1/2
35	HTG	b	623	-	-	6/10/30/30	0/1/1/1
35	HTG	b	625	-	-	2/10/30/30	0/1/1/1
26	BCR	y	101	-	-	6/29/63/63	0/2/2/2
24	CLA	c	509	42	1/1/15/20	9/37/115/115	-
27	SQD	a	411	-	-	15/49/69/69	0/1/1/1
35	HTG	D	410	-	-	0/7/27/30	0/1/1/1
24	CLA	c	510	3	1/1/15/20	2/37/115/115	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
27	SQD	B	620	-	-	18/49/69/69	0/1/1/1
38	LHG	d	407	-	-	15/53/53/53	-
24	CLA	c	506	42	1/1/15/20	4/37/115/115	-
24	CLA	c	512	3	1/1/15/20	8/37/115/115	-
36	DGD	c	518	-	-	19/51/91/95	0/2/2/2
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
36	DGD	C	519	-	-	11/51/91/95	0/2/2/2
24	CLA	B	610	42	1/1/15/20	7/37/115/115	-
24	CLA	C	509	3	1/1/15/20	2/37/115/115	-
26	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
34	LMT	A	359	-	-	4/21/61/61	0/2/2/2
28	GOL	c	502	-	-	0/4/4/4	-
33	LMG	B	621	-	-	12/46/66/70	0/1/1/1
35	HTG	B	623	-	-	2/10/30/30	0/1/1/1
24	CLA	B	614	2	1/1/15/20	11/37/115/115	-
28	GOL	B	626	-	-	4/4/4/4	-
24	CLA	a	407	1	1/1/15/20	8/37/115/115	-
24	CLA	c	504	3	1/1/15/20	7/37/115/115	-
24	CLA	C	514	3	1/1/15/20	9/37/115/115	-
24	CLA	c	505	3	1/1/15/20	0/37/115/115	-
24	CLA	B	607	42	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	512	3	1/1/15/20	5/37/115/115	-
34	LMT	I	101	-	-	9/21/61/61	0/2/2/2
35	HTG	V	204	-	-	0/2/19/30	0/1/1/1
35	HTG	h	101	-	-	0/7/27/30	0/1/1/1
24	CLA	a	404	42	-	4/37/115/115	-
24	CLA	a	403	1	1/1/15/20	1/37/115/115	-
35	HTG	c	526	-	-	1/10/30/30	0/1/1/1
26	BCR	K	102	-	-	2/29/63/63	0/2/2/2
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
24	CLA	b	616	2	1/1/15/20	12/37/115/115	-
27	SQD	F	101	-	-	9/38/58/69	0/1/1/1
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
24	CLA	A	405	42	1/1/15/20	3/37/115/115	-
24	CLA	B	604	2	1/1/15/20	10/37/115/115	-
24	CLA	b	612	2	1/1/15/20	3/37/115/115	-
35	HTG	B	628	-	-	3/10/30/30	0/1/1/1
24	CLA	c	514	3	1/1/15/20	8/37/115/115	-
24	CLA	C	510	3	1/1/15/20	6/37/115/115	-
24	CLA	b	614	2	1/1/15/20	11/37/115/115	-
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
27	SQD	a	409	-	-	12/49/69/69	0/1/1/1
26	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	CLA	B	605	2	1/1/15/20	8/37/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
24	CLA	D	403	4	1/1/15/20	10/37/115/115	-
25	PHO	A	407	-	-	2/37/103/103	0/5/6/6
27	SQD	A	413	-	-	7/49/69/69	0/1/1/1
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
24	CLA	b	615	2	1/1/15/20	5/37/115/115	-
24	CLA	c	515	3	1/1/15/20	6/37/115/115	-
24	CLA	C	511	3	1/1/15/20	10/37/115/115	-
34	LMT	b	622	-	-	5/17/37/61	0/1/1/2
33	LMG	J	101	40	-	12/46/66/70	0/1/1/1
24	CLA	c	507	3	1/1/15/20	2/37/115/115	-
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
36	DGD	c	519	-	-	11/51/91/95	0/2/2/2
31	PL9	D	405	-	-	15/53/73/73	0/1/1/1
24	CLA	D	402	4	1/1/15/20	0/37/115/115	-
28	GOL	V	202	-	-	2/4/4/4	-
35	HTG	b	624	-	-	3/10/30/30	0/1/1/1
33	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
28	GOL	b	627	-	-	2/4/4/4	-
38	LHG	D	357	-	-	14/53/53/53	-
39	HEM	e	102	5,6	-	7/12/54/54	-
34	LMT	m	102	-	-	5/21/61/61	0/2/2/2
33	LMG	C	520	-	-	14/46/66/70	0/1/1/1
25	PHO	a	406	-	-	2/37/103/103	0/5/6/6
24	CLA	C	508	42	1/1/15/20	6/37/115/115	-
26	BCR	c	517	-	-	3/29/63/63	0/2/2/2
38	LHG	d	406	-	-	7/53/53/53	-
24	CLA	c	503	3	1/1/15/20	3/37/115/115	-
35	HTG	B	625	-	-	3/10/30/30	0/1/1/1
24	CLA	b	602	2	1/1/15/20	4/37/115/115	-
24	CLA	B	601	42	1/1/15/20	11/37/115/115	-
24	CLA	b	606	2	1/1/15/20	8/37/115/115	-
28	GOL	a	416	-	-	3/4/4/4	-
31	PL9	A	416[B]	-	-	18/53/73/73	0/1/1/1
34	LMT	B	622	-	-	8/21/61/61	0/2/2/2
24	CLA	C	502	3	1/1/15/20	6/37/115/115	-
36	DGD	c	520	-	-	11/51/91/95	0/2/2/2
33	LMG	a	417	-	-	13/46/66/70	0/1/1/1
34	LMT	e	101	-	-	6/21/61/61	0/2/2/2
24	CLA	b	613	2	1/1/15/20	7/37/115/115	-
28	GOL	a	410	-	-	4/4/4/4	-
24	CLA	C	503	3	1/1/15/20	8/37/115/115	-
33	LMG	j	101	40	-	9/46/66/70	0/1/1/1
24	CLA	A	406	42	1/1/15/20	4/37/115/115	-
38	LHG	l	101	-	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
34	LMT	E	102	-	-	9/21/61/61	0/2/2/2
31	PL9	a	414[B]	-	-	22/53/73/73	0/1/1/1
24	CLA	B	611	2	1/1/15/20	3/37/115/115	-
24	CLA	B	616	2	1/1/15/20	7/37/115/115	-
28	GOL	v	202	-	-	2/4/4/4	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
41	HEC	v	203	16	-	2/10/54/54	-
24	CLA	d	403	4	1/1/15/20	6/37/115/115	-
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
27	SQD	f	101	-	-	14/38/58/69	0/1/1/1
24	CLA	c	511	3	1/1/15/20	10/37/115/115	-
33	LMG	b	621	-	-	10/46/66/70	0/1/1/1
24	CLA	a	350	42	1/1/15/20	4/37/115/115	-
33	LMG	c	522	-	-	10/46/66/70	0/1/1/1
24	CLA	A	404	1	1/1/15/20	1/37/115/115	-
24	CLA	b	603	2	1/1/15/20	5/37/115/115	-
26	BCR	B	617	-	-	0/29/63/63	0/2/2/2
24	CLA	b	608	2	-	2/37/115/115	-
24	CLA	c	513	3	1/1/15/20	5/37/115/115	-
36	DGD	C	517	-	-	16/51/91/95	0/2/2/2
41	HEC	V	203	16	-	2/10/54/54	-
36	DGD	H	102	-	-	15/51/91/95	0/2/2/2
34	LMT	b	630	-	-	9/17/37/61	0/1/1/2
35	HTG	c	523	-	-	3/10/30/30	0/1/1/1
24	CLA	b	611	2	1/1/15/20	3/37/115/115	-
24	CLA	B	615	2	1/1/15/20	9/37/115/115	-
31	PL9	d	405	-	-	10/53/73/73	0/1/1/1
24	CLA	c	508	3	1/1/15/20	9/37/115/115	-
34	LMT	M	101	-	-	3/21/61/61	0/2/2/2
38	LHG	L	101	-	-	13/53/53/53	-
25	PHO	a	405	-	-	2/37/103/103	0/5/6/6
27	SQD	b	620	-	-	20/49/69/69	0/1/1/1
34	LMT	M	103	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
33	LMG	c	521	-	-	8/46/66/70	0/1/1/1

The worst 5 of 1315 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C3B-C2B	7.14	1.50	1.40
24	B	613	CLA	C3B-C2B	6.77	1.49	1.40
24	B	612	CLA	C3B-C2B	6.68	1.49	1.40
25	A	408	PHO	C3B-C2B	6.62	1.49	1.40
24	A	404	CLA	C3B-C2B	6.62	1.49	1.40

The worst 5 of 2695 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	405	PHO	O2D-CGD-CBD	10.45	122.43	110.95
24	a	404	CLA	C1D-ND-C4D	-10.20	99.15	106.31
24	b	605	CLA	C1D-ND-C4D	-10.11	99.22	106.31
24	c	513	CLA	C1D-ND-C4D	-10.07	99.24	106.31
24	B	614	CLA	C1D-ND-C4D	-10.05	99.26	106.31

5 of 65 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	404	CLA	ND
24	A	405	CLA	ND
24	A	406	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND

5 of 1174 torsion outliers are listed below:

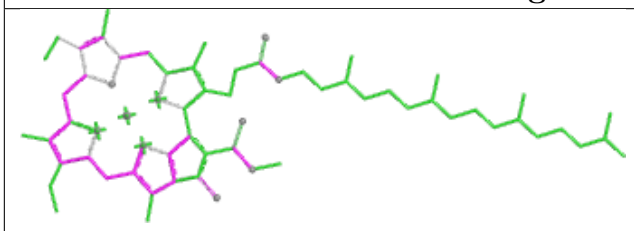
Mol	Chain	Res	Type	Atoms
24	B	601	CLA	CAD-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

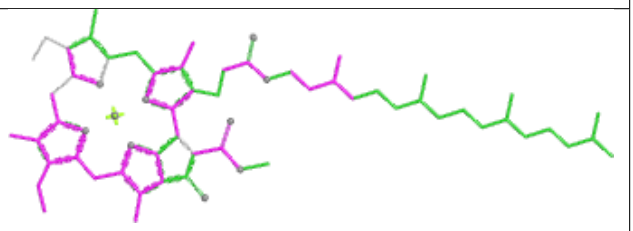
No monomer is involved in short contacts.

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

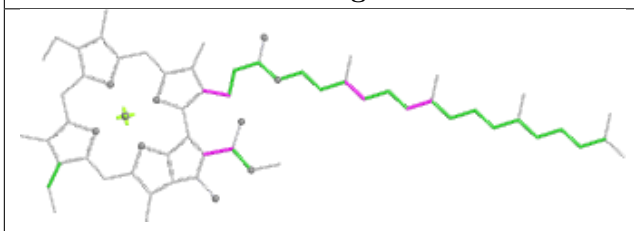
Ligand CLA b 609



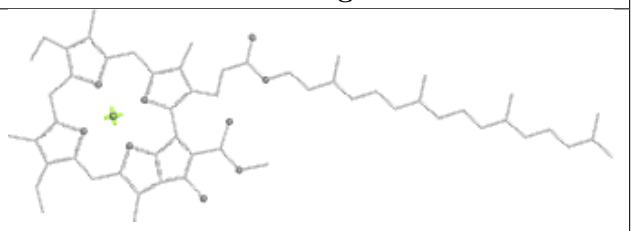
Bond lengths



Bond angles

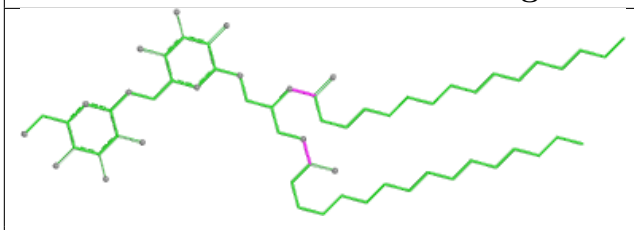


Torsions

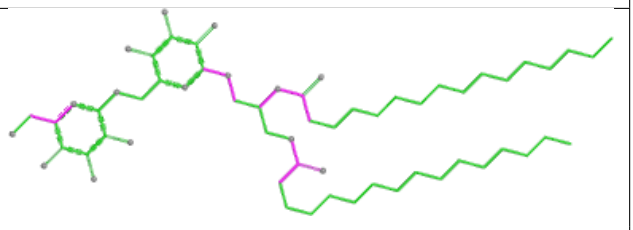


Rings

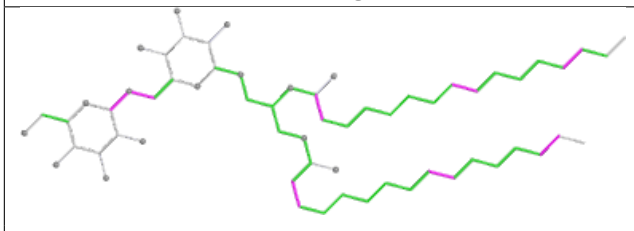
Ligand DGD C 518



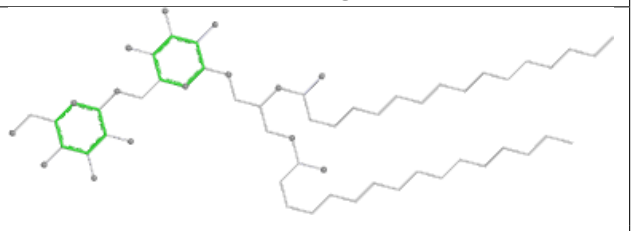
Bond lengths



Bond angles

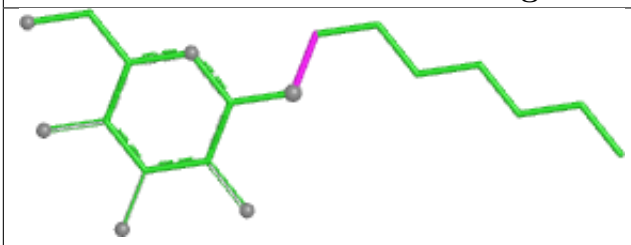


Torsions

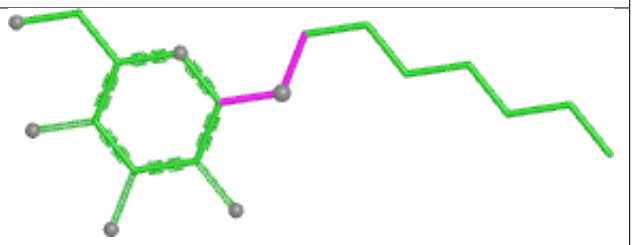


Rings

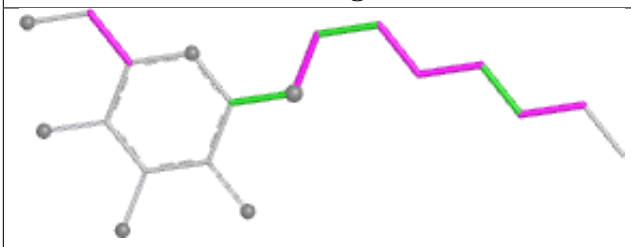
Ligand HTG B 624



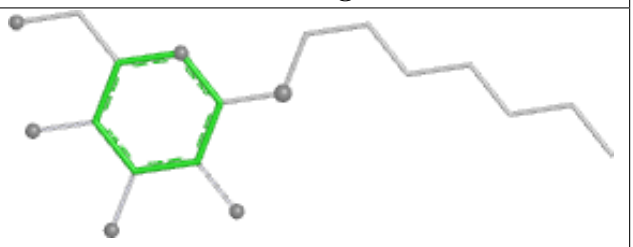
Bond lengths



Bond angles

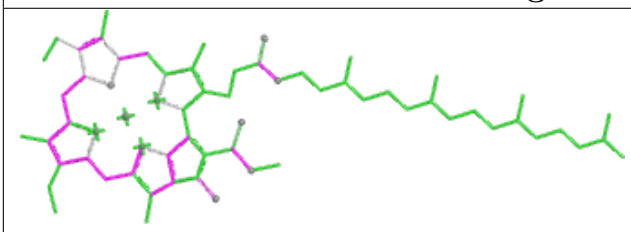


Torsions

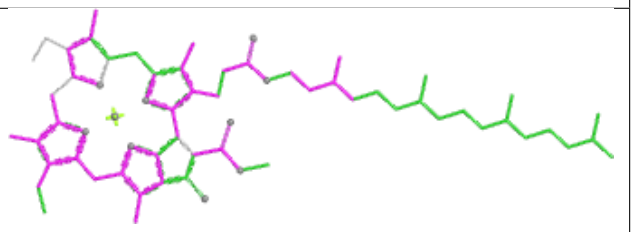


Rings

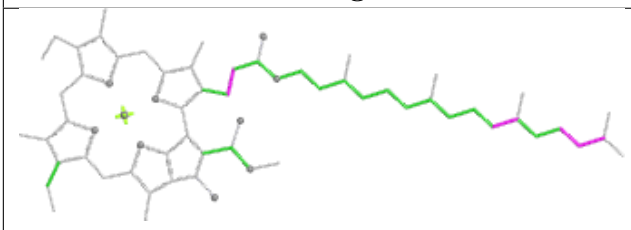
Ligand CLA b 610



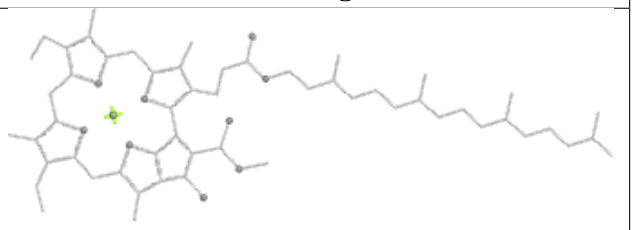
Bond lengths



Bond angles

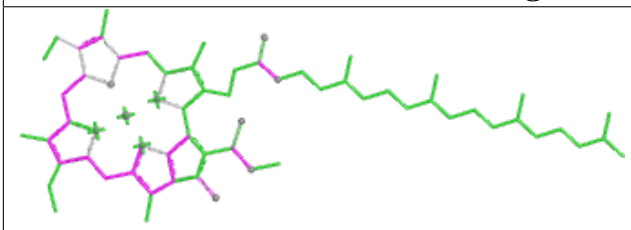


Torsions

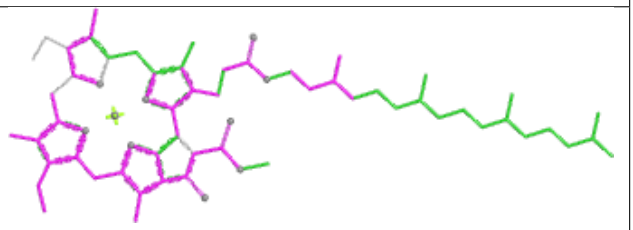


Rings

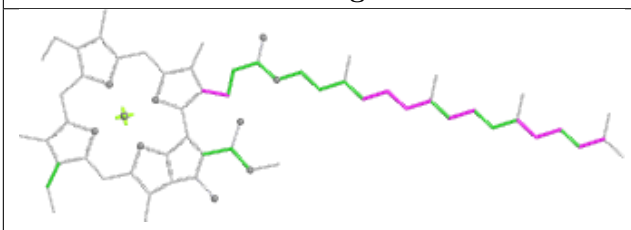
Ligand CLA C 507



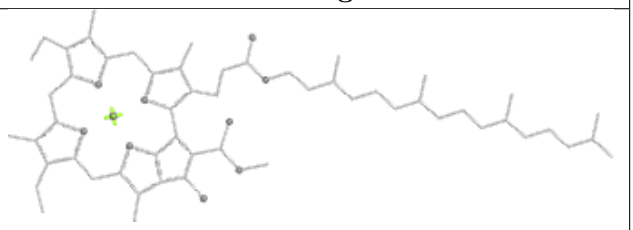
Bond lengths



Bond angles

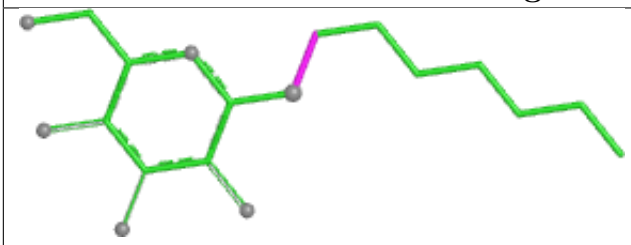


Torsions

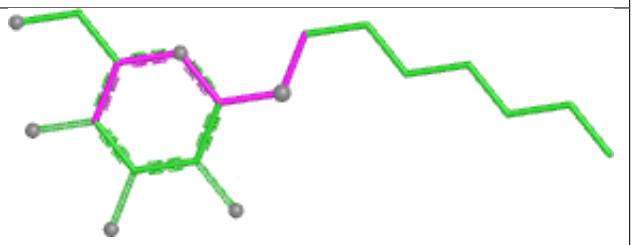


Rings

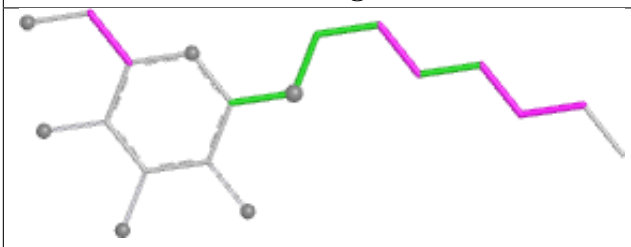
Ligand HTG b 628



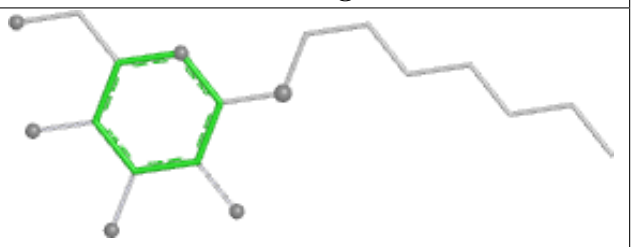
Bond lengths



Bond angles

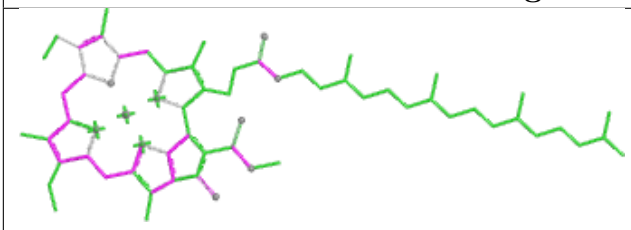


Torsions

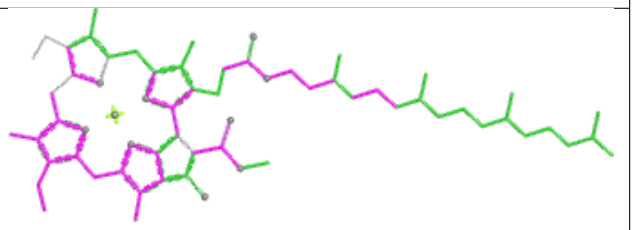


Rings

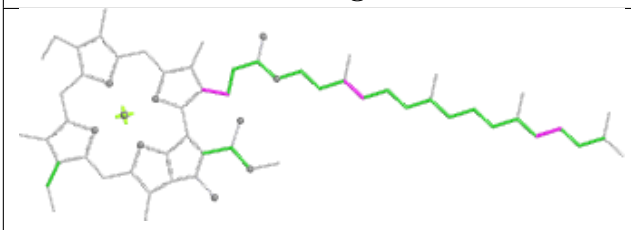
Ligand CLA B 609



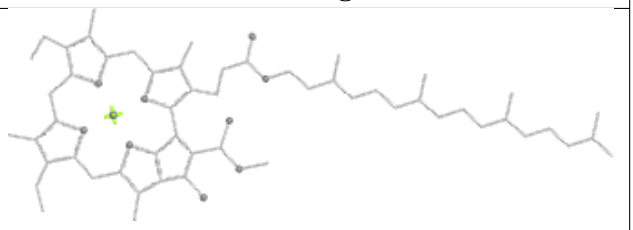
Bond lengths



Bond angles

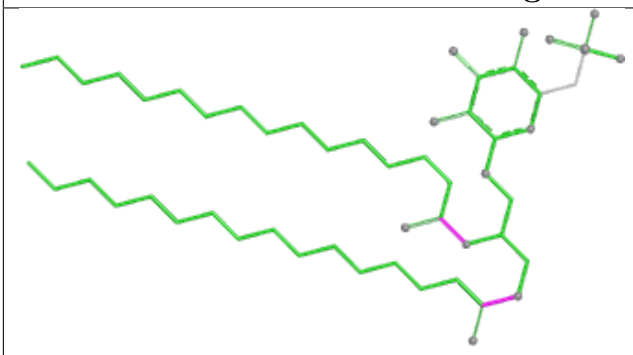


Torsions

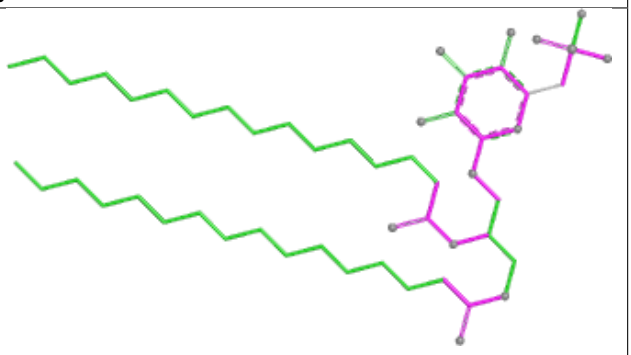


Rings

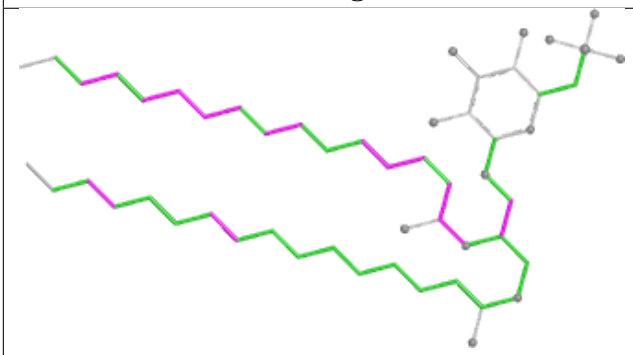
Ligand SQD A 411



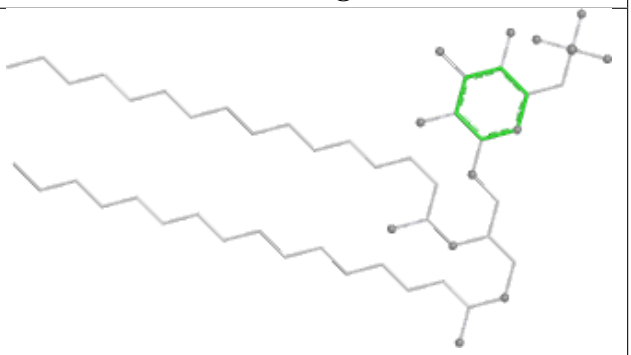
Bond lengths



Bond angles

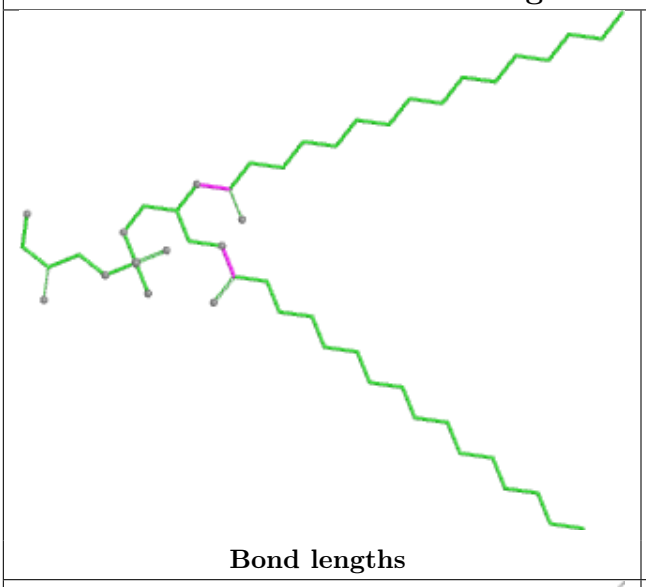


Torsions

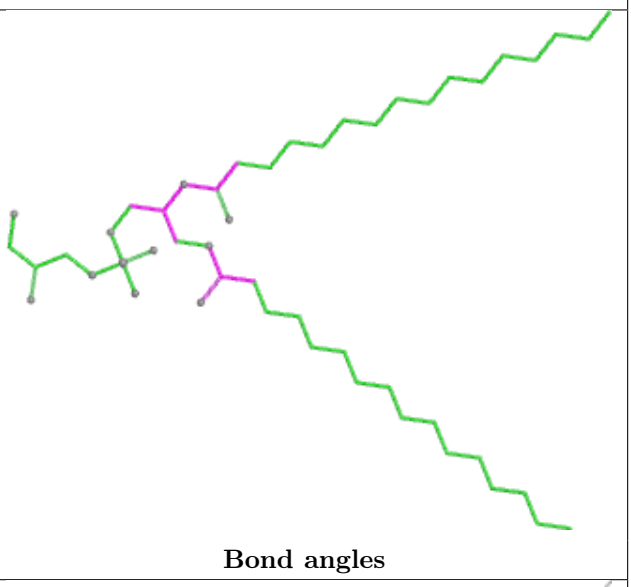


Rings

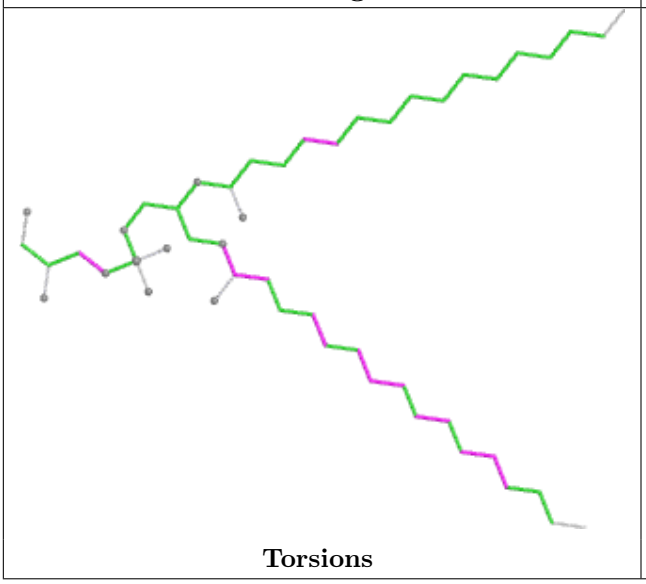
Ligand LHG d 408



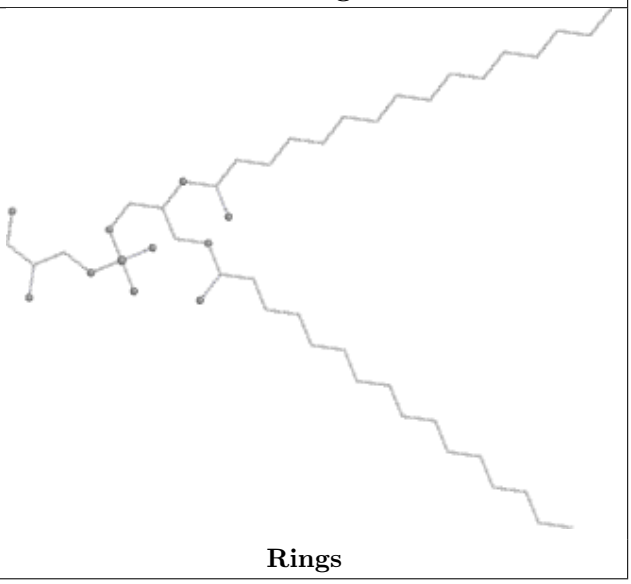
Bond lengths



Bond angles

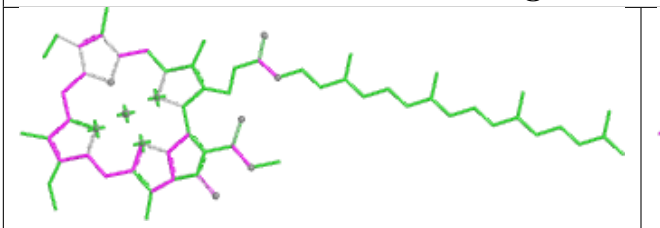


Torsions

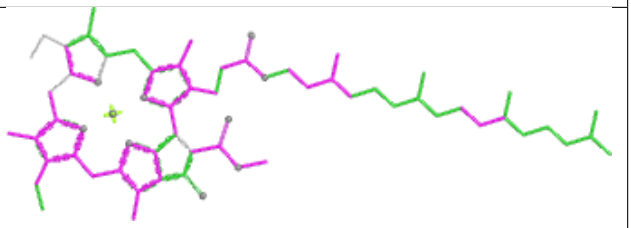


Rings

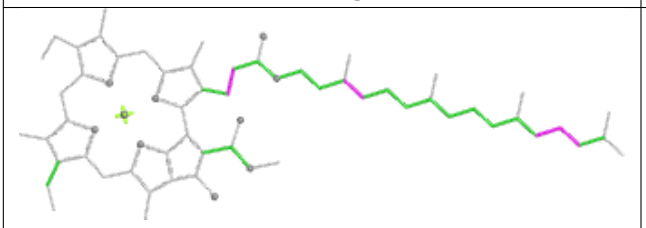
Ligand CLA B 602



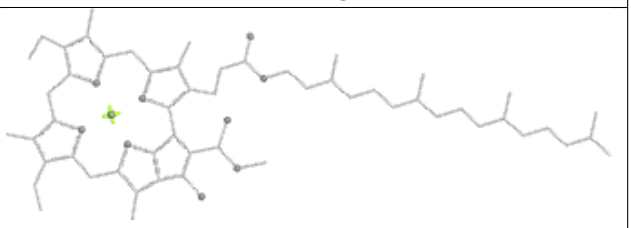
Bond lengths



Bond angles

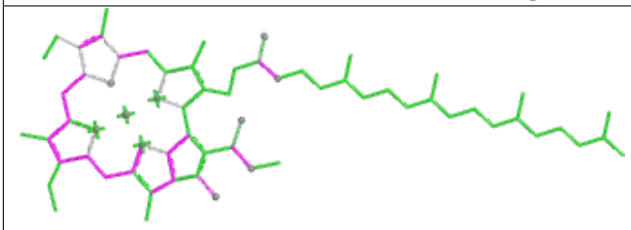


Torsions

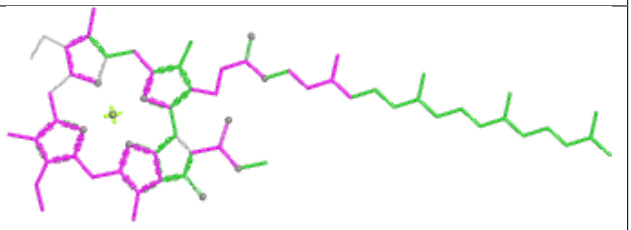


Rings

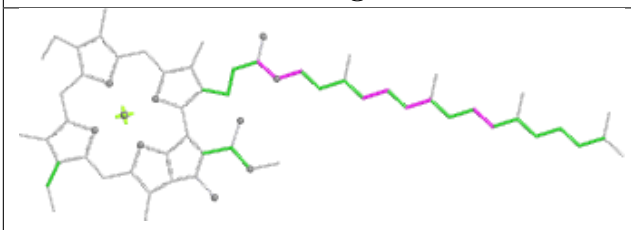
Ligand CLA C 513



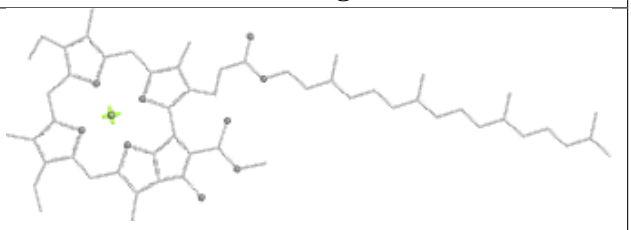
Bond lengths



Bond angles

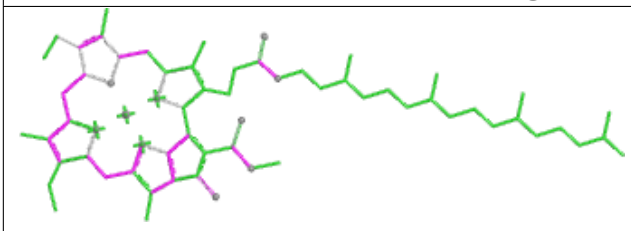


Torsions

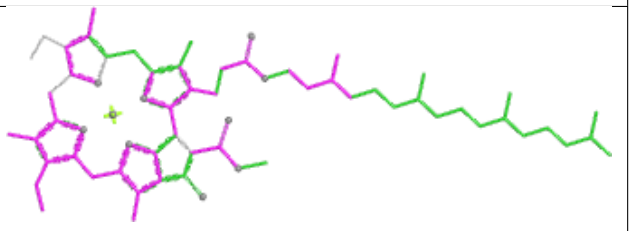


Rings

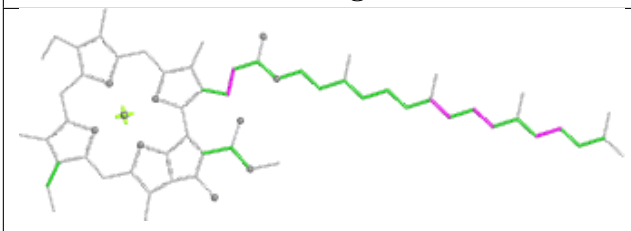
Ligand CLA B 606



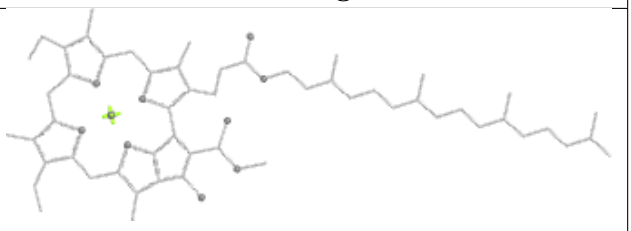
Bond lengths



Bond angles

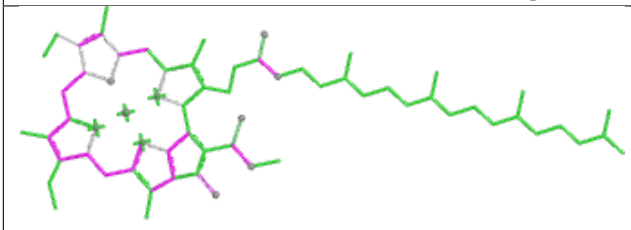


Torsions

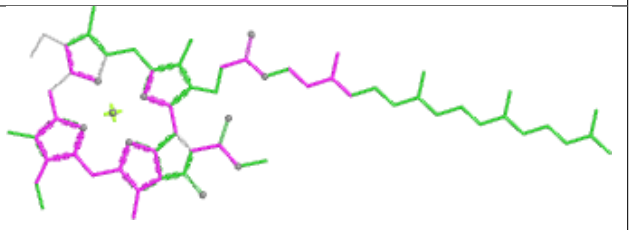


Rings

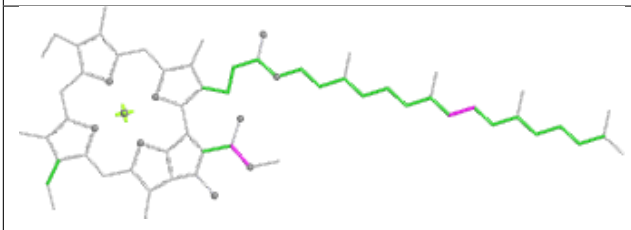
Ligand CLA C 504



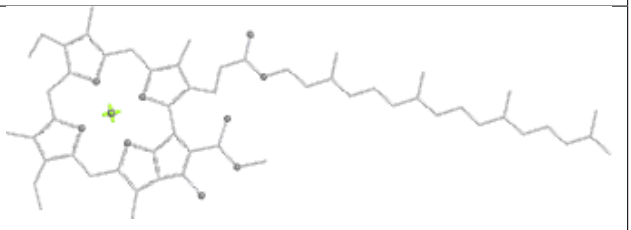
Bond lengths



Bond angles

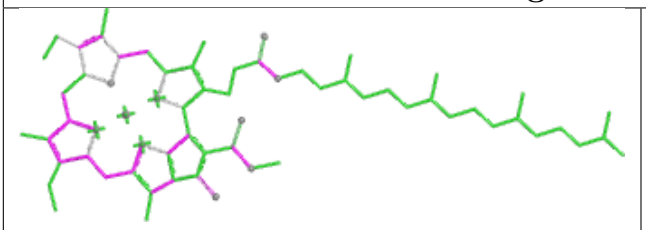


Torsions

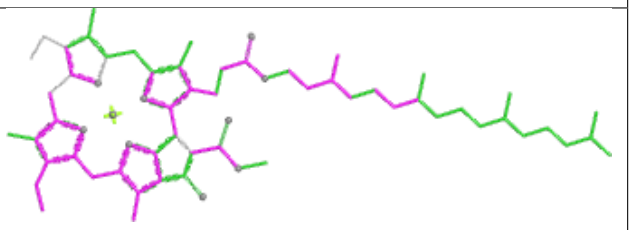


Rings

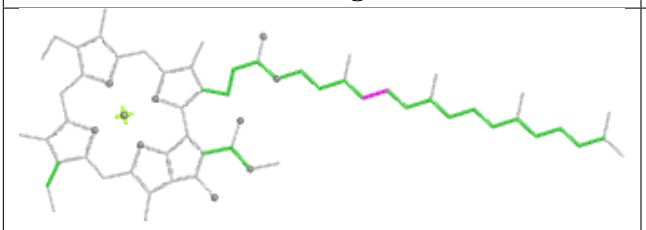
Ligand CLA b 607



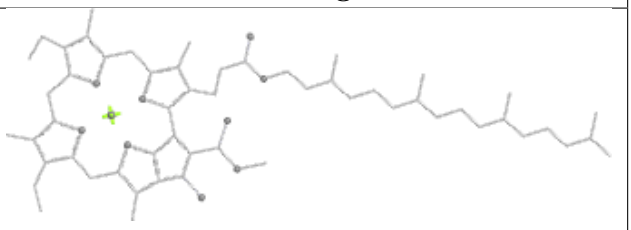
Bond lengths



Bond angles

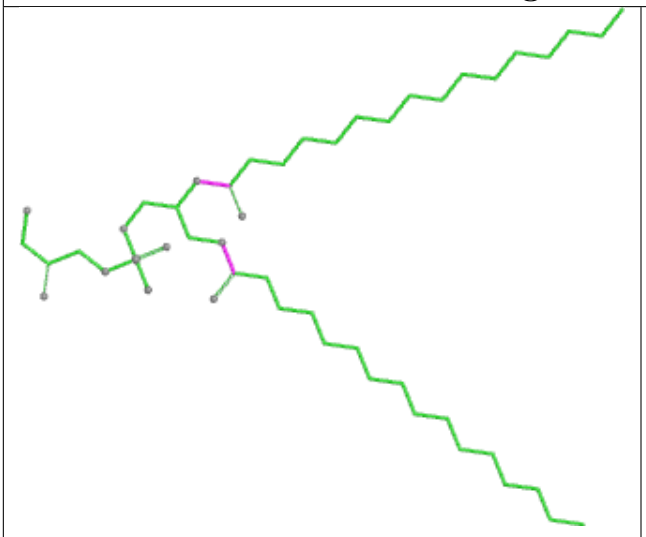


Torsions

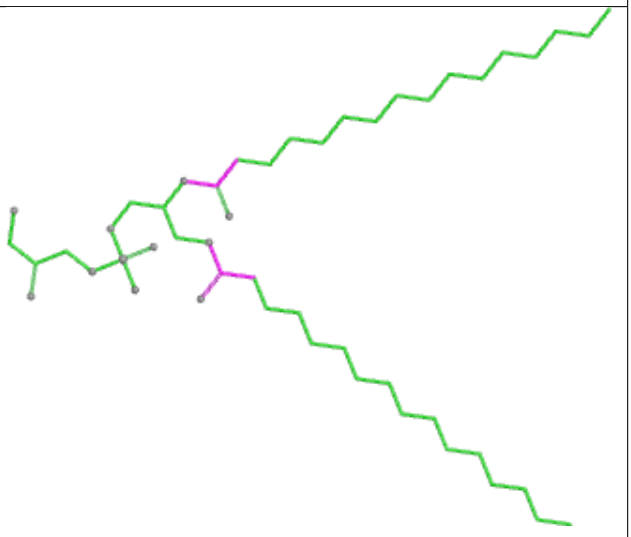


Rings

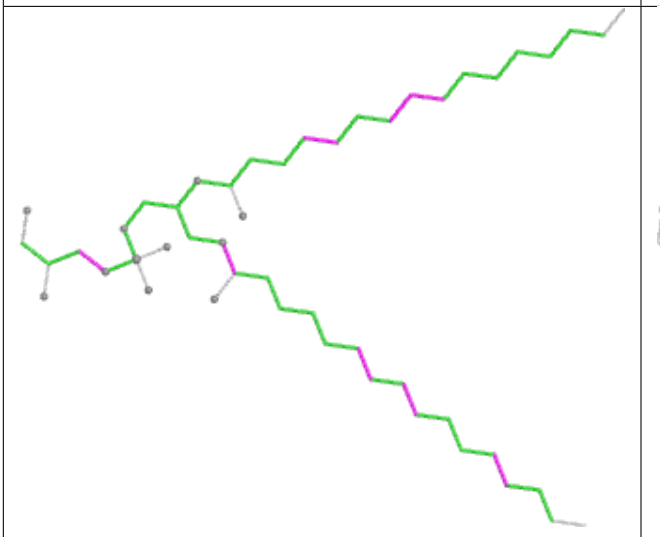
Ligand LHG D 407



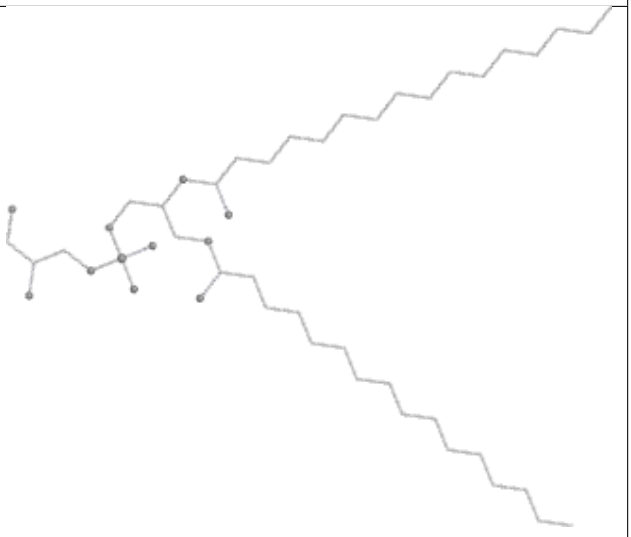
Bond lengths



Bond angles

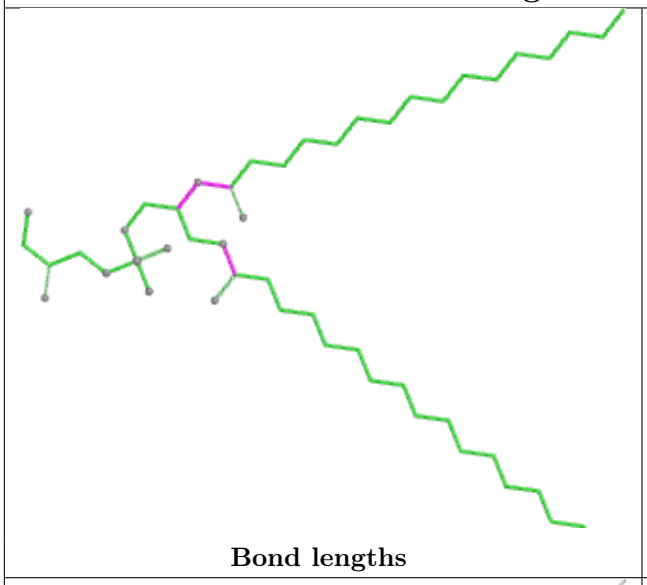


Torsions

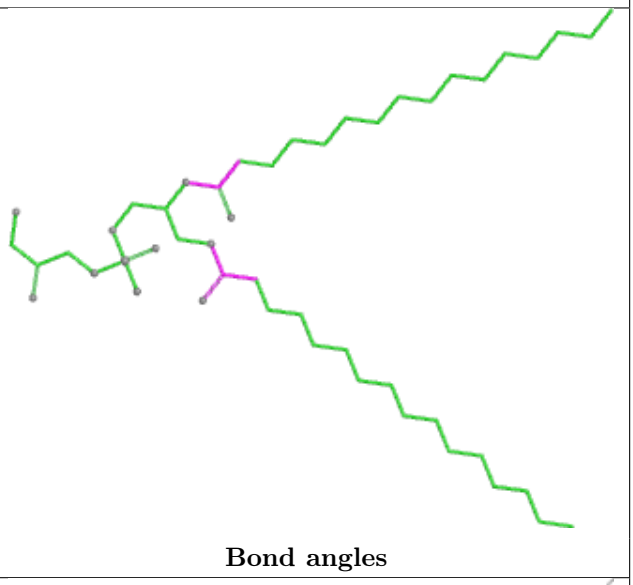


Rings

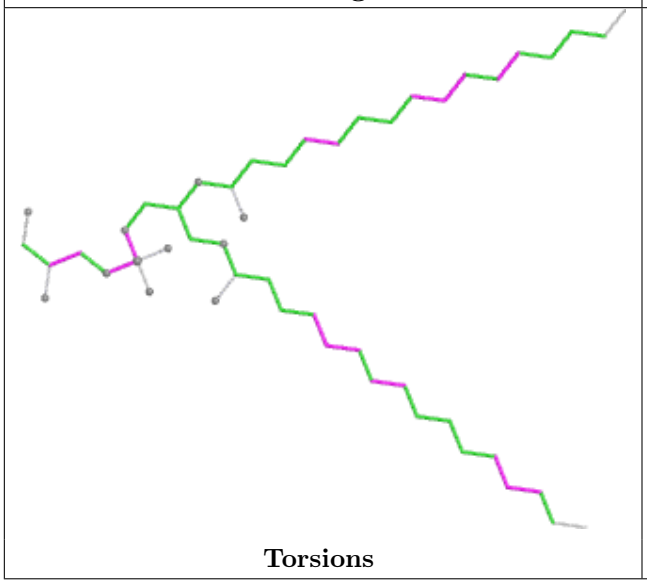
Ligand LHG D 406



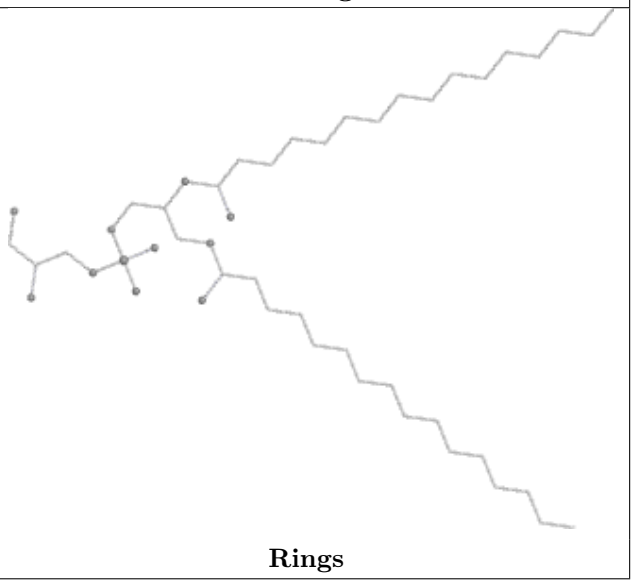
Bond lengths



Bond angles

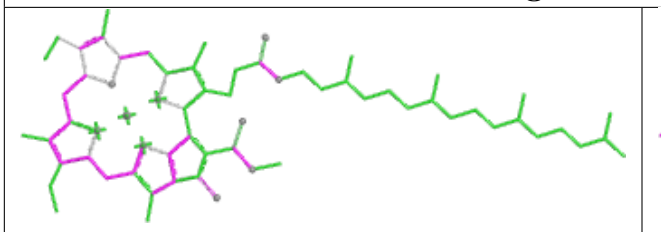


Torsions

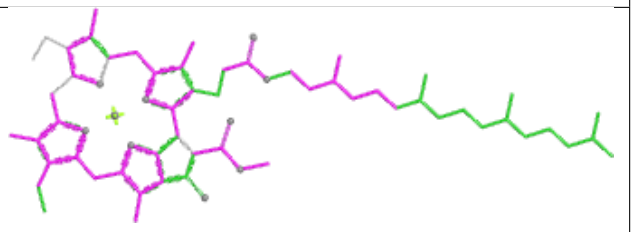


Rings

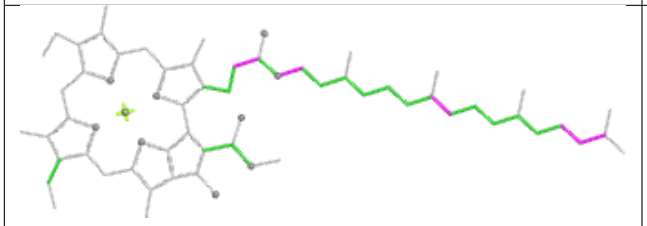
Ligand CLA B 613



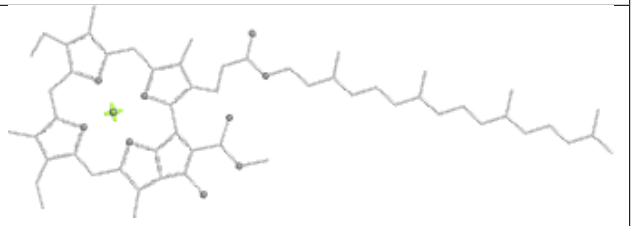
Bond lengths



Bond angles

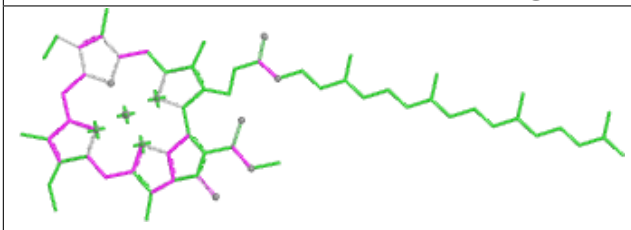


Torsions



Rings

Ligand CLA b 601



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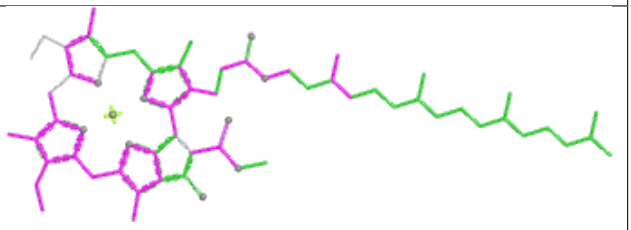
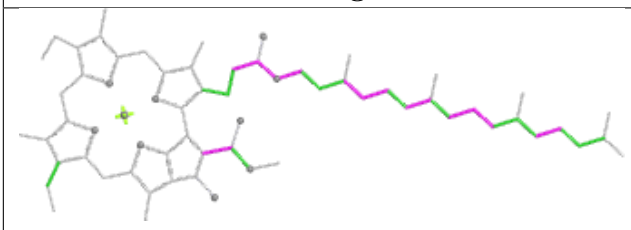
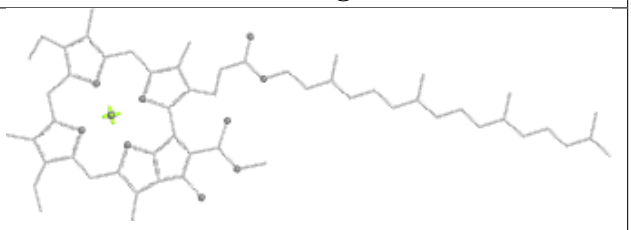


Bond angles

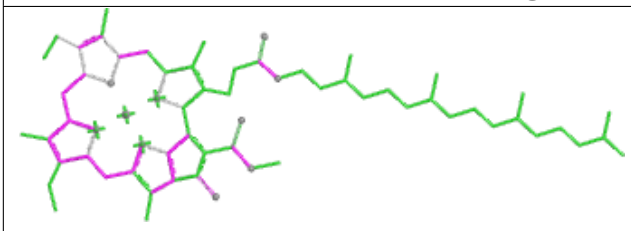


Torsions

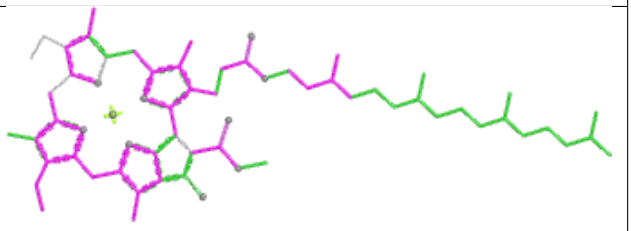


Rings

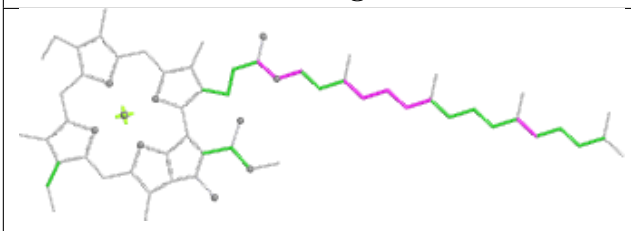
Ligand CLA A 409



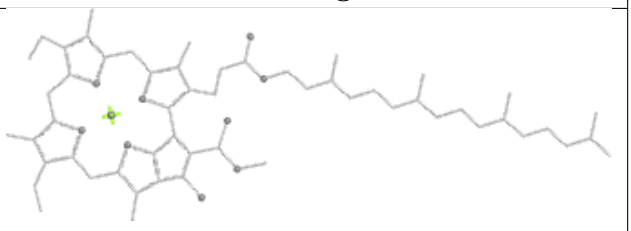
Bond lengths



Bond angles

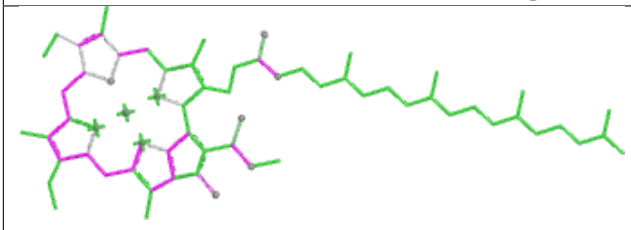


Torsions

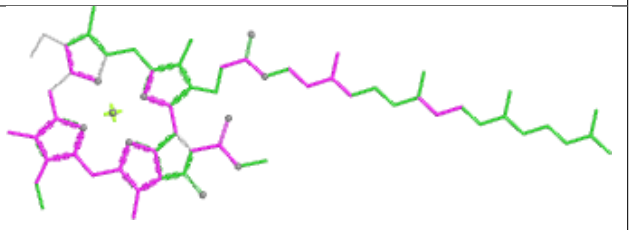


Rings

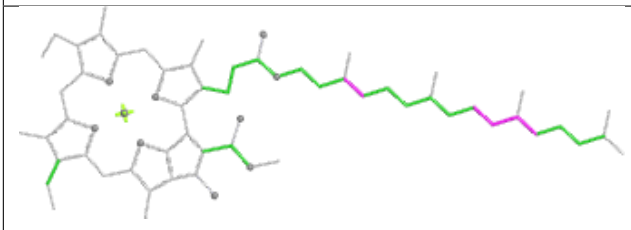
Ligand CLA C 506



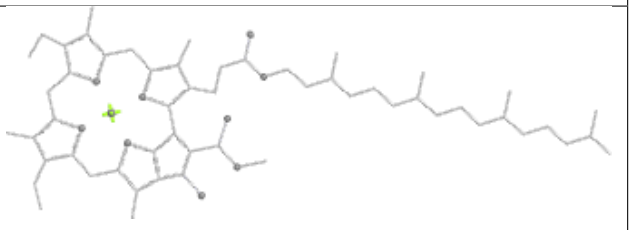
Bond lengths



Bond angles

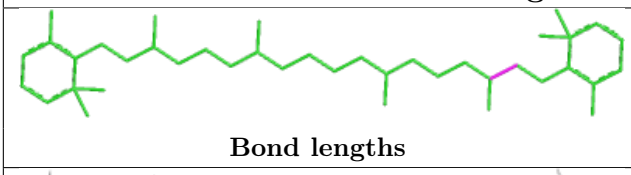


Torsions

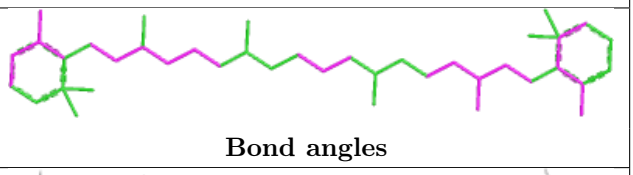


Rings

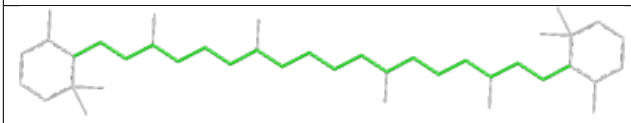
Ligand BCR a 408



Bond lengths



Bond angles



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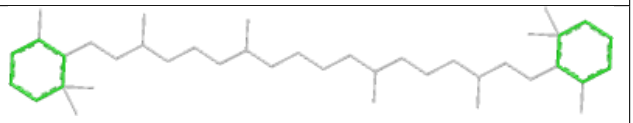
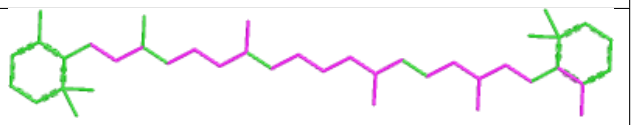


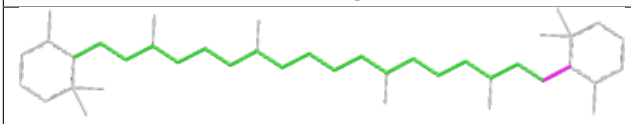
Rings

Ligand BCR h 102

Bond lengths



Bond angles



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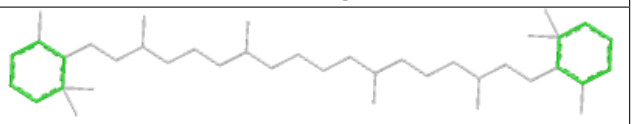
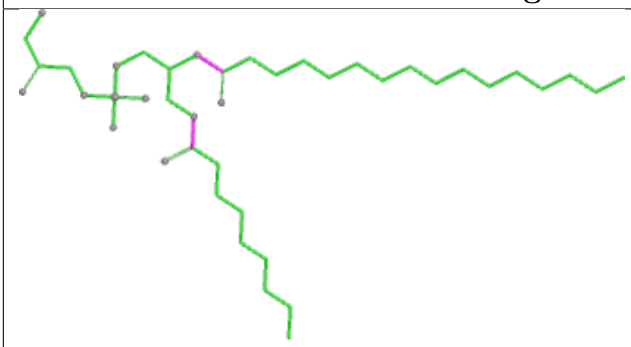
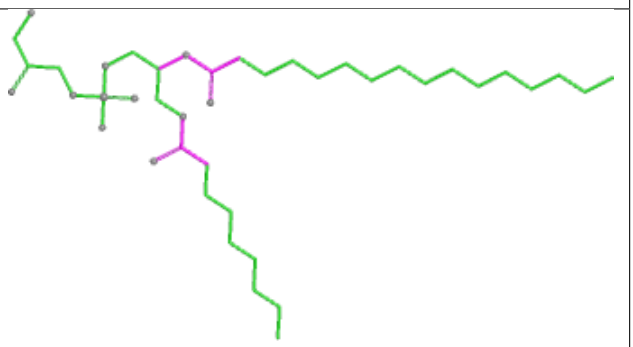


Rings

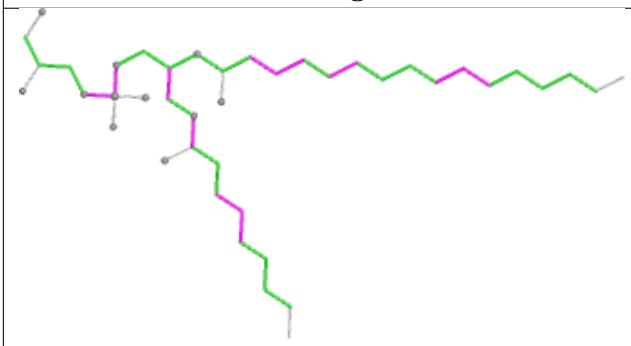
Ligand LHG E 101



Bond lengths



Bond angles



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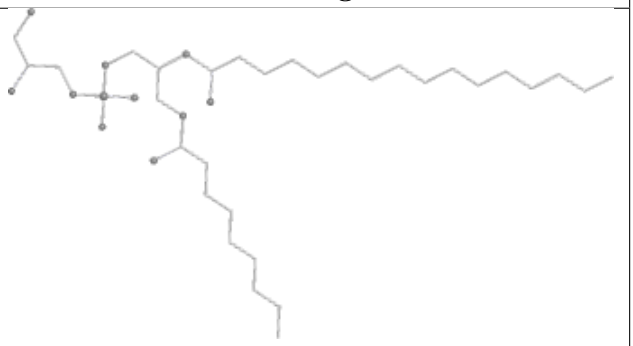
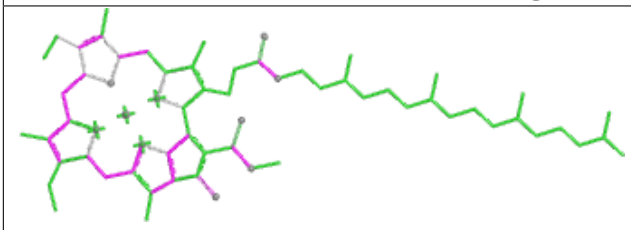
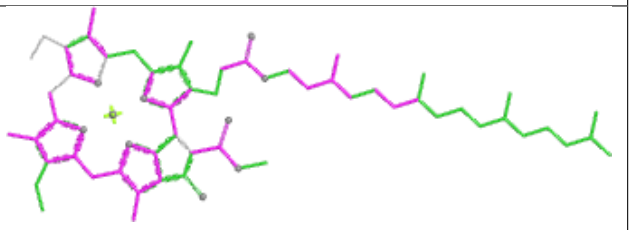


Rings

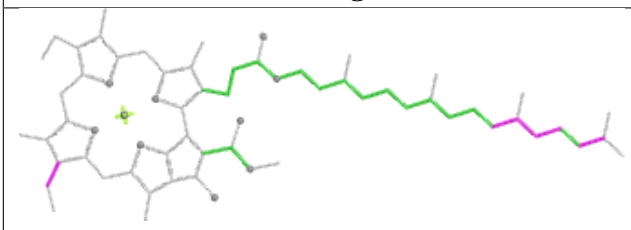
Ligand CLA b 604



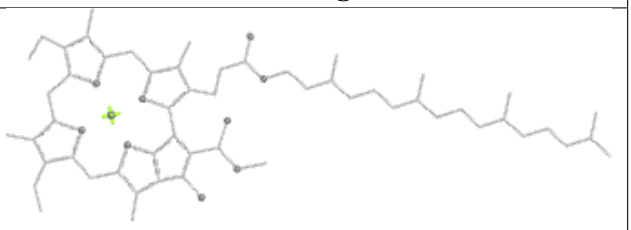
Bond lengths



Bond angles



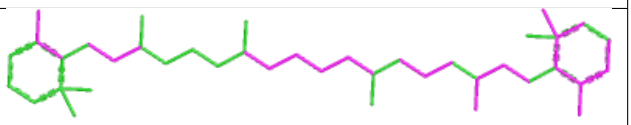
Torsions



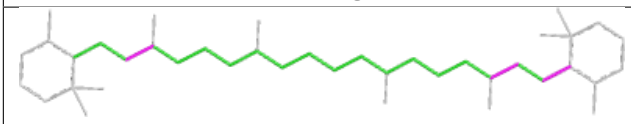
Rings

Ligand BCR d 404

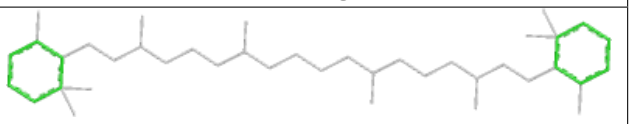
Bond lengths



Bond angles

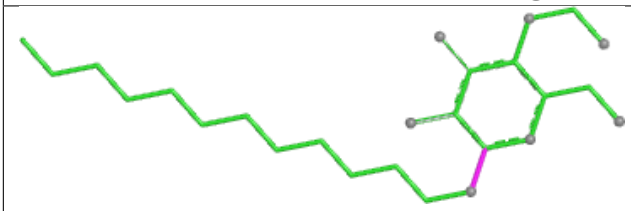


Torsions

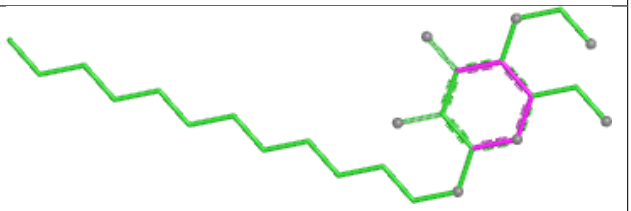


Rings

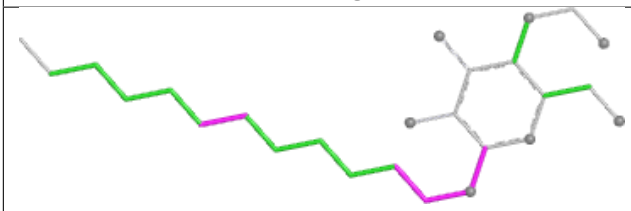
Ligand LMT t 101



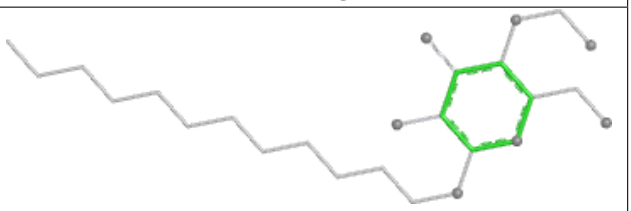
Bond lengths



Bond angles

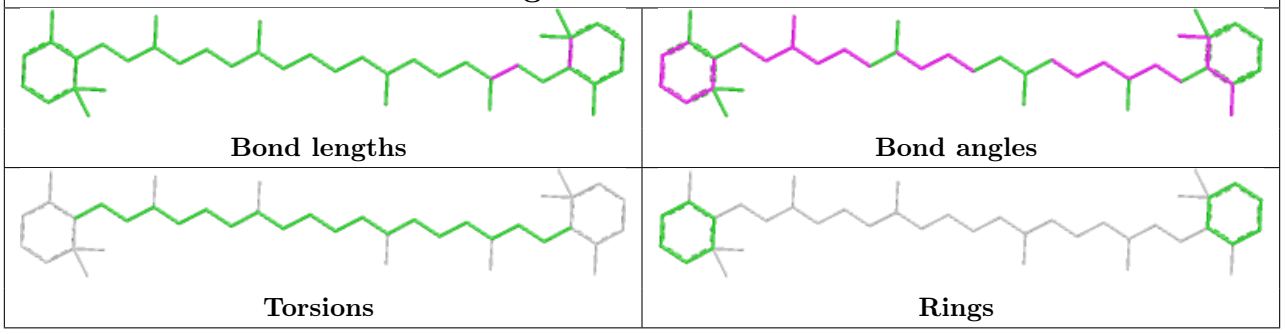


Torsions

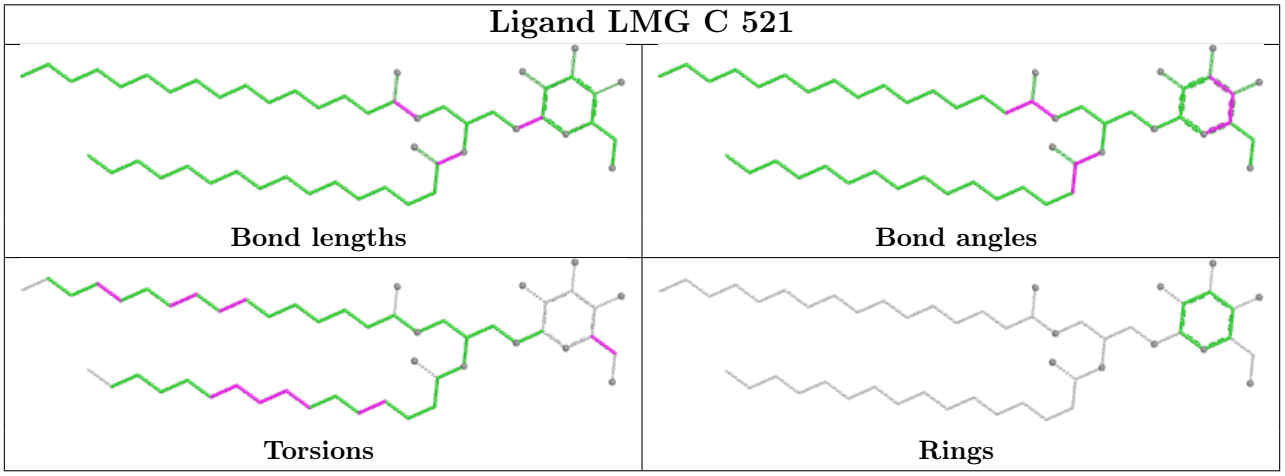


Rings

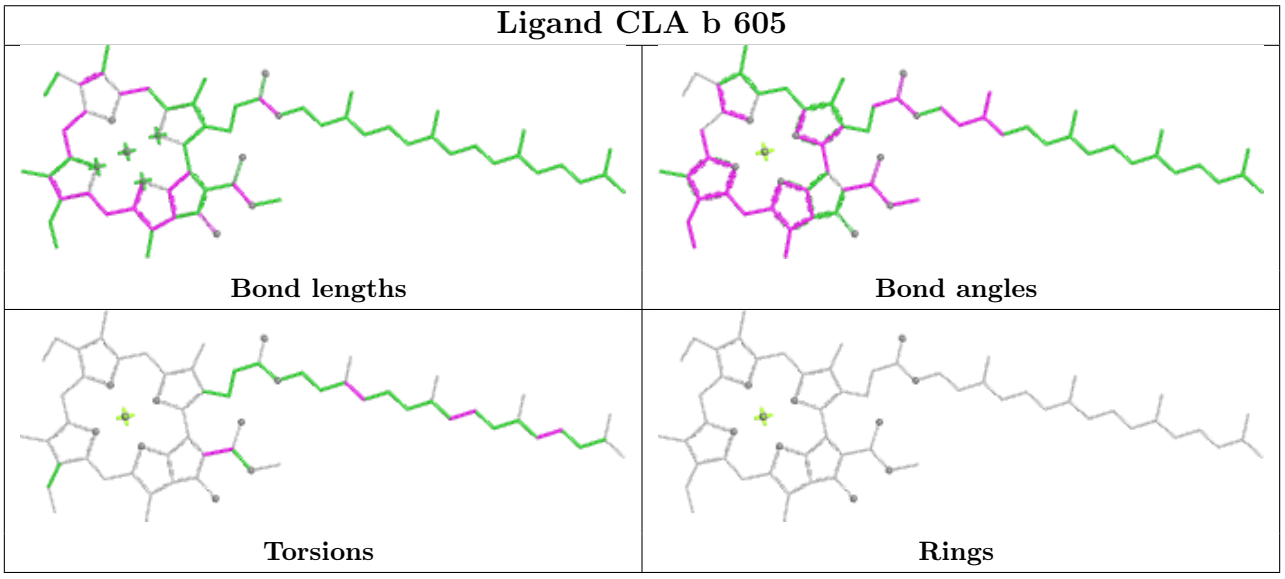
Ligand BCR B 619



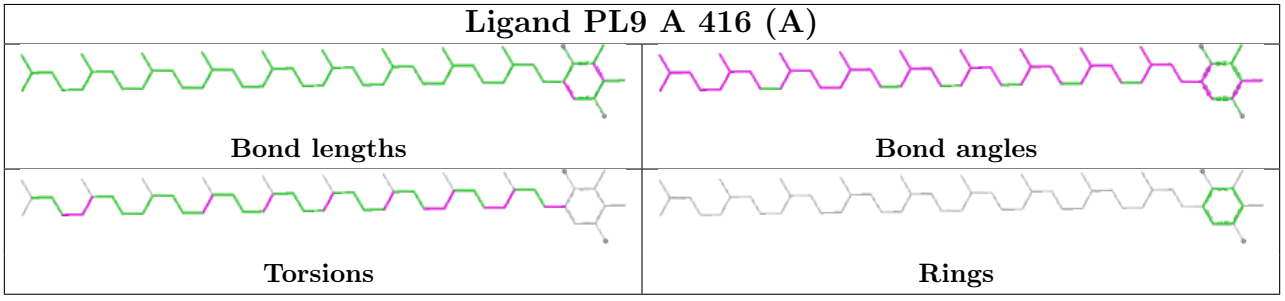
Ligand LMG C 521



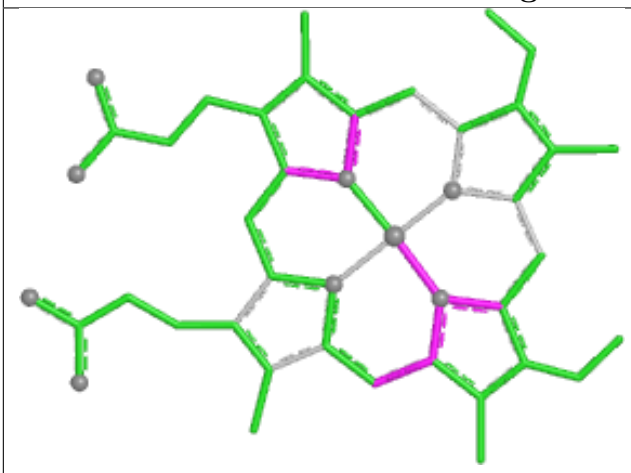
Ligand CLA b 605



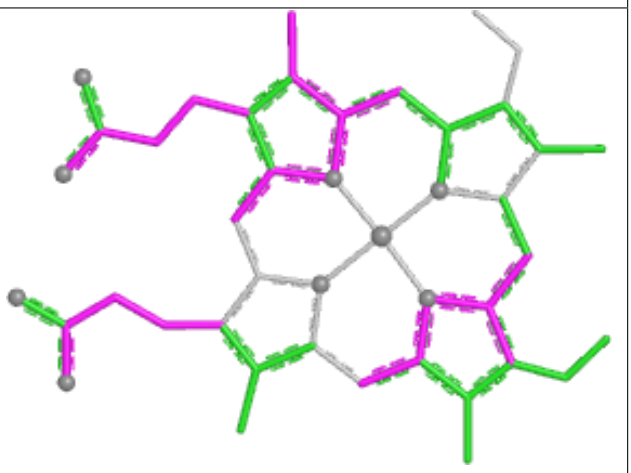
Ligand PL9 A 416 (A)



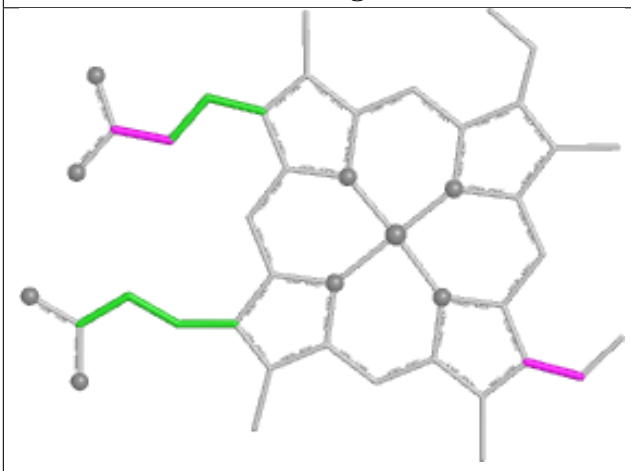
Ligand HEM E 103



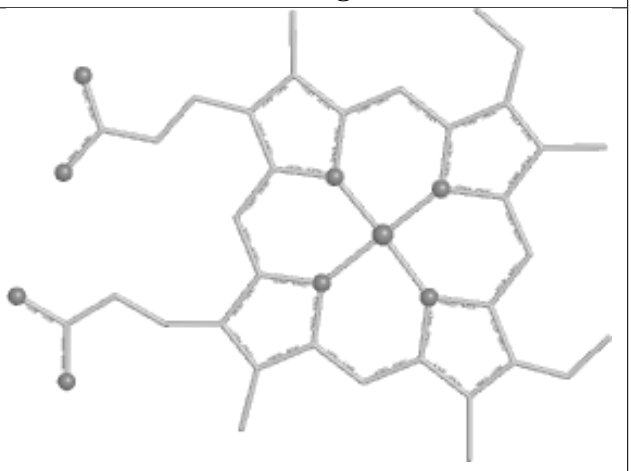
Bond lengths



Bond angles

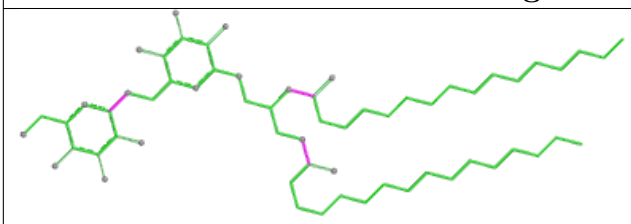


Torsions

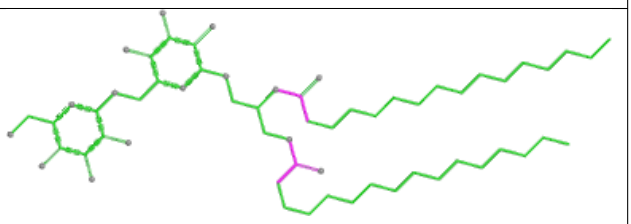


Rings

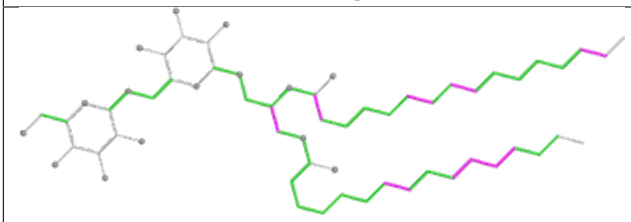
Ligand DGD h 103



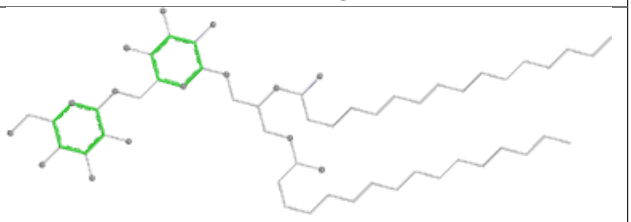
Bond lengths



Bond angles

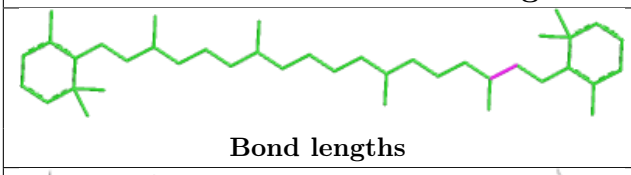


Torsions

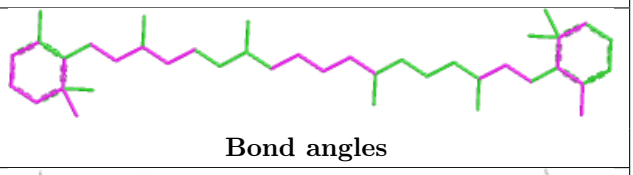


Rings

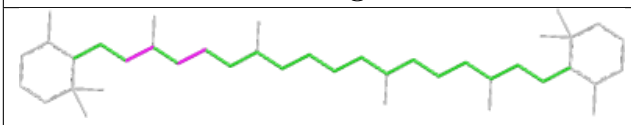
Ligand BCR H 101



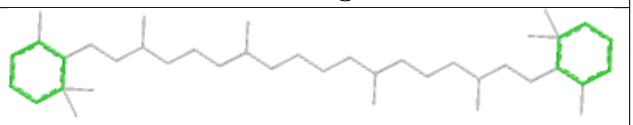
Bond lengths



Bond angles

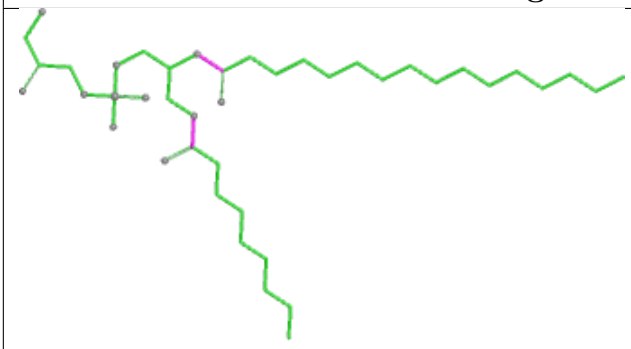


Torsions

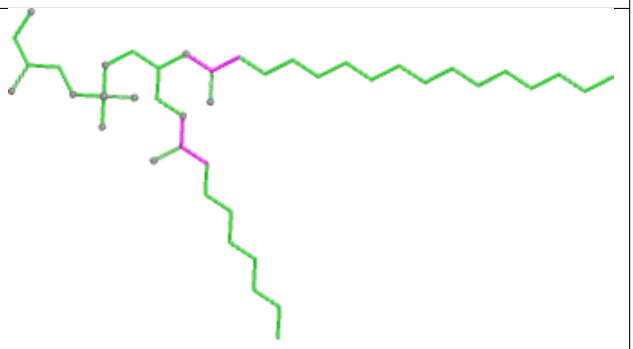


Rings

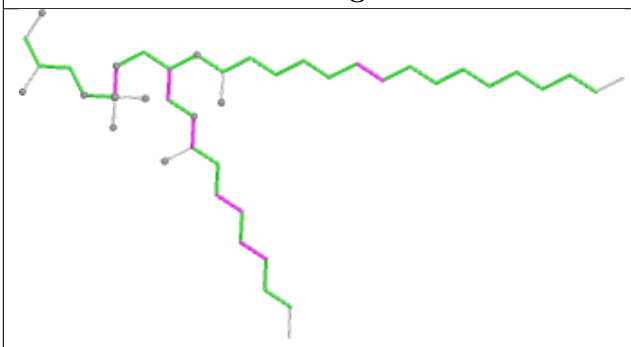
Ligand LHG a 419



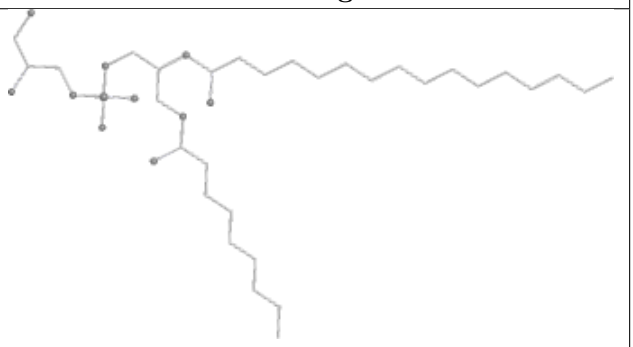
Bond lengths



Bond angles

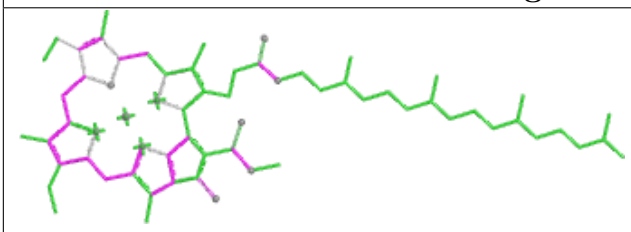


Torsions

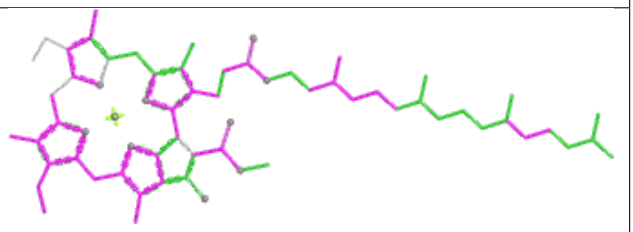


Rings

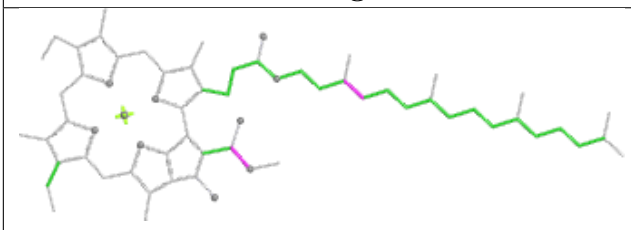
Ligand CLA B 603



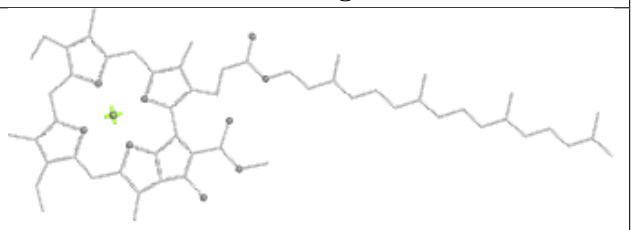
Bond lengths



Bond angles

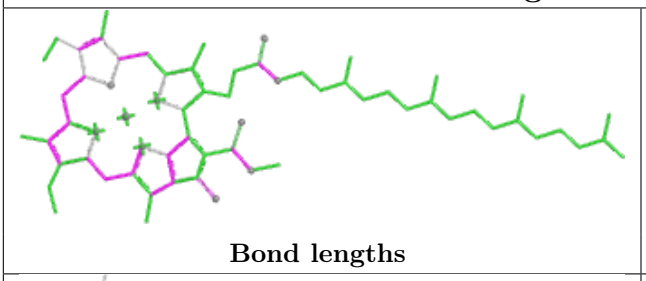


Torsions

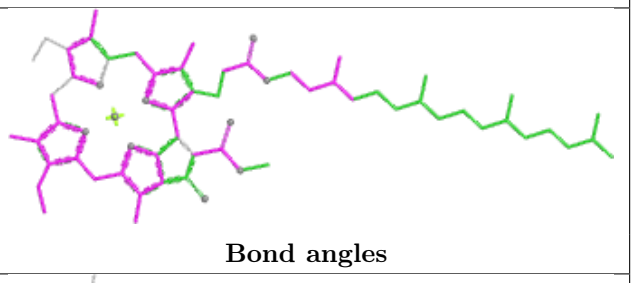


Rings

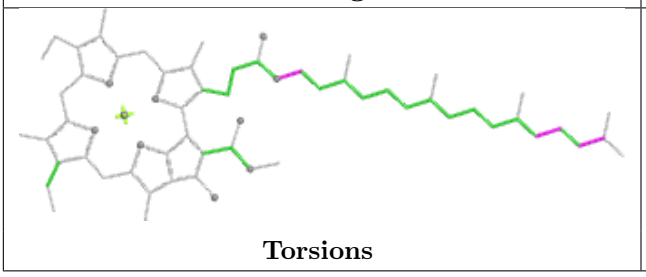
Ligand CLA B 608



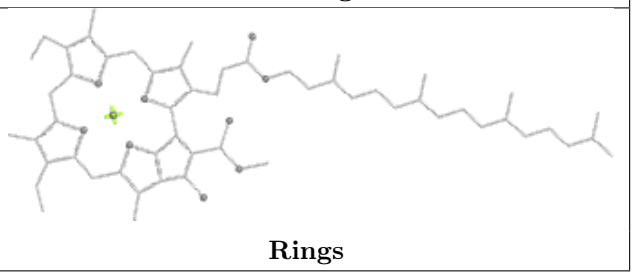
Bond lengths



Bond angles

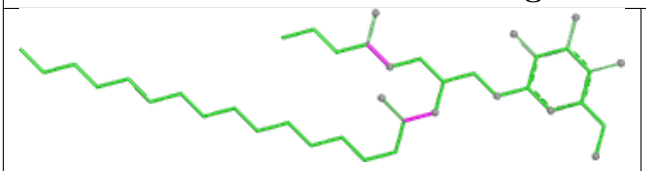


Torsions

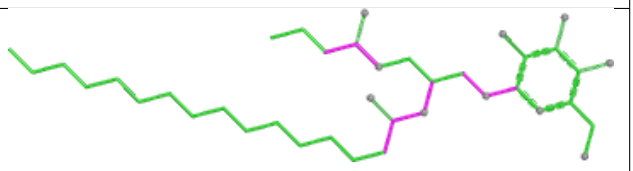


Rings

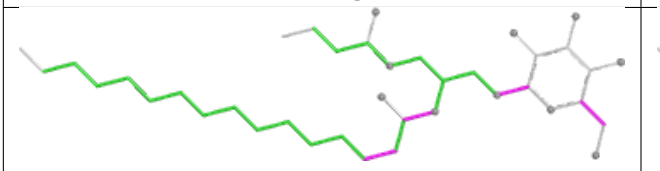
Ligand LMG z 101



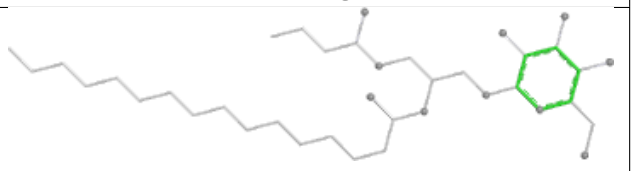
Bond lengths



Bond angles

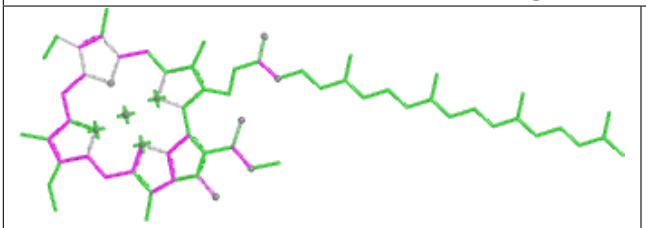


Torsions

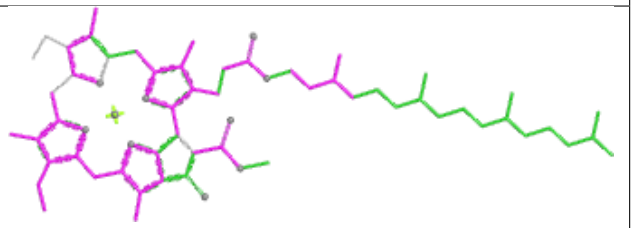


Rings

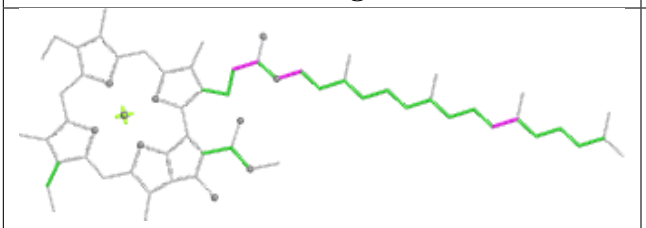
Ligand CLA d 402



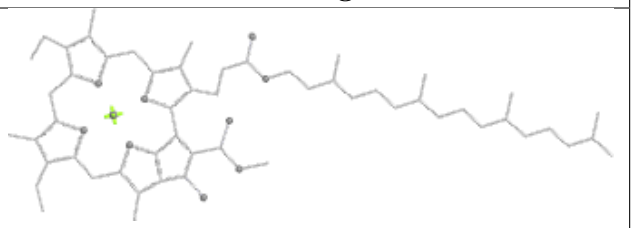
Bond lengths



Bond angles

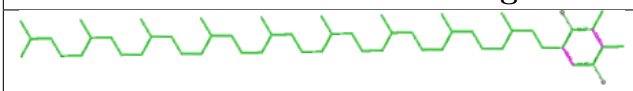


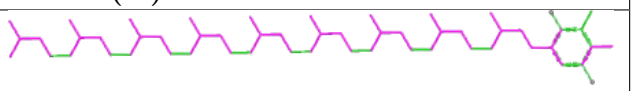
Torsions

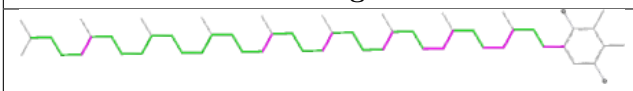


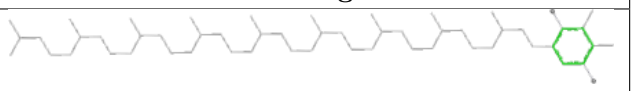
Rings

Ligand PL9 a 414 (A)

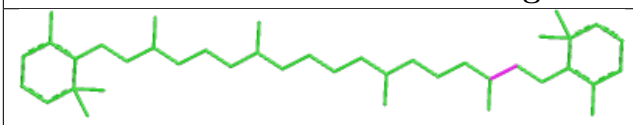

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR T 101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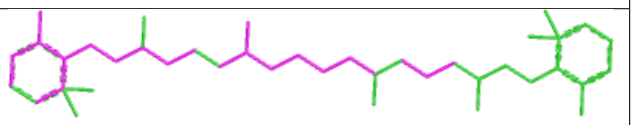
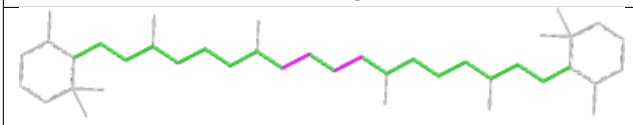
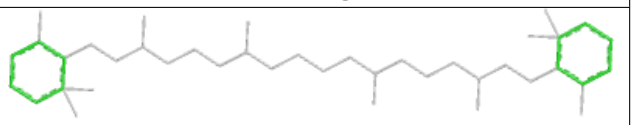
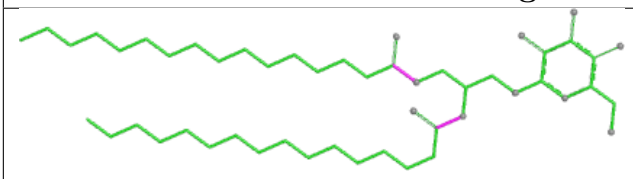
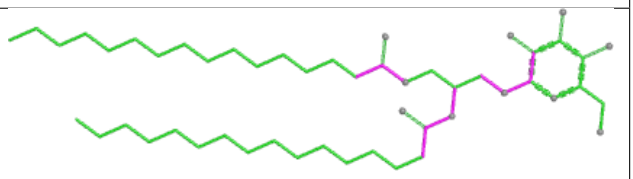

Bond angles

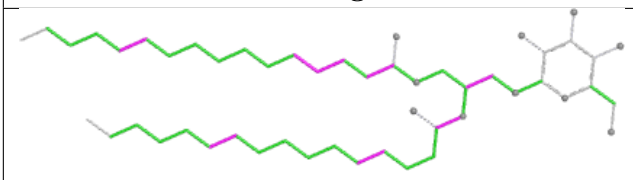

Torsions

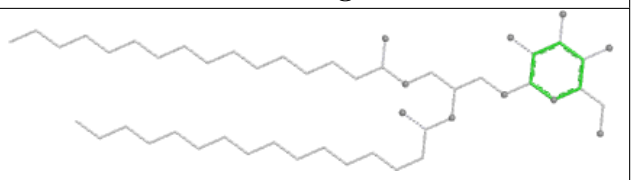

Rings

Ligand LMG A 418

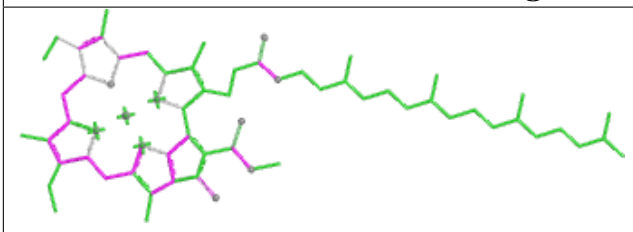

Bond lengths

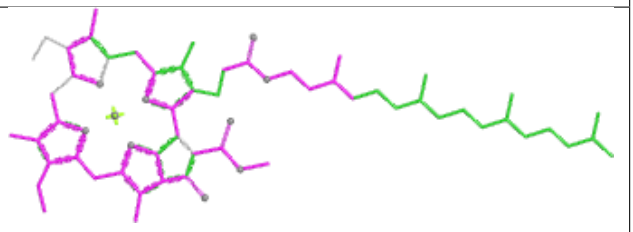

Bond angles

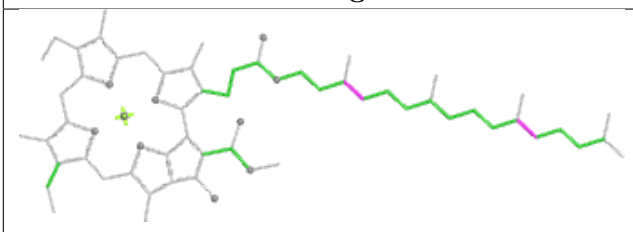

Torsions

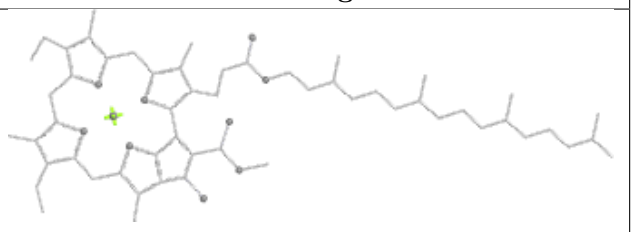

Rings

Ligand CLA C 505

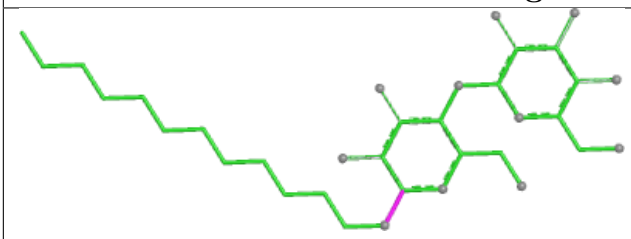

Bond lengths

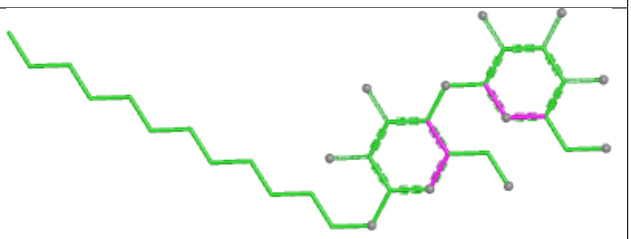

Bond angles

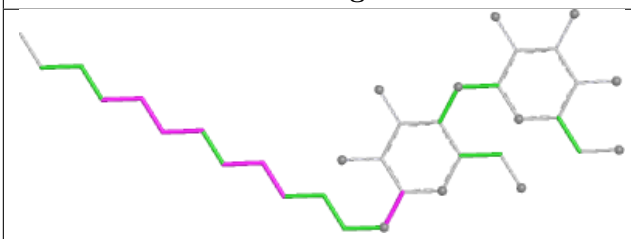

Torsions

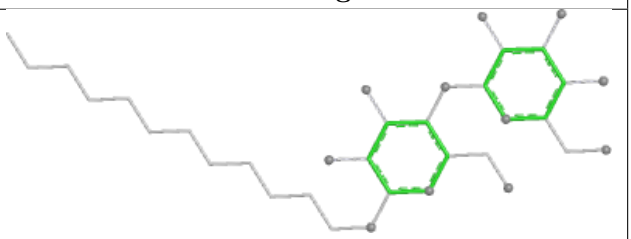

Rings

Ligand LMT a 359

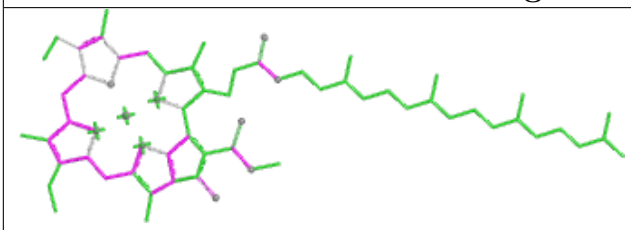

Bond lengths

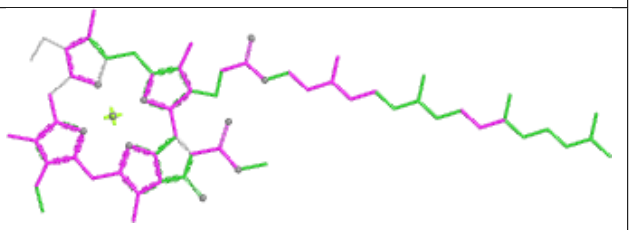

Bond angles

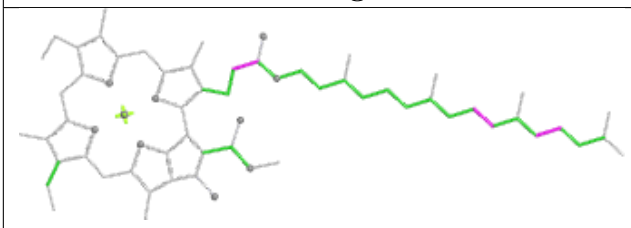

Torsions

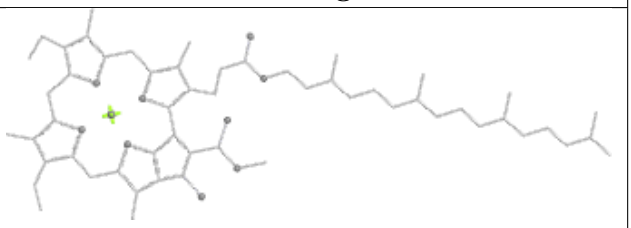

Rings

Ligand CLA B 612

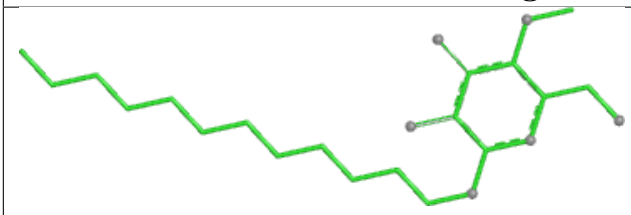

Bond lengths

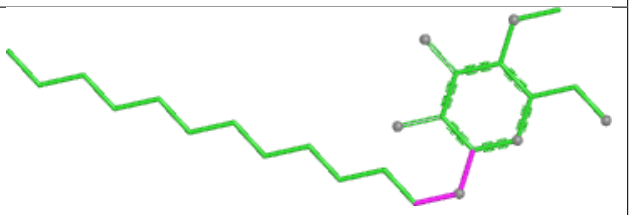

Bond angles

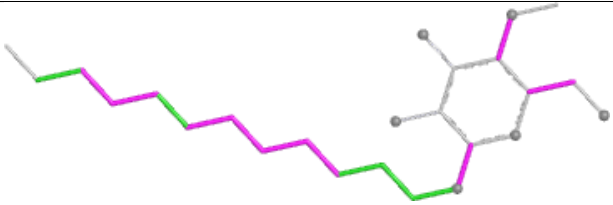

Torsions

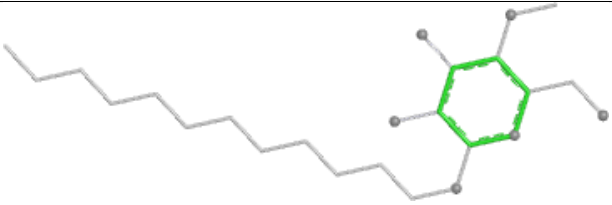

Rings

Ligand LMT B 630

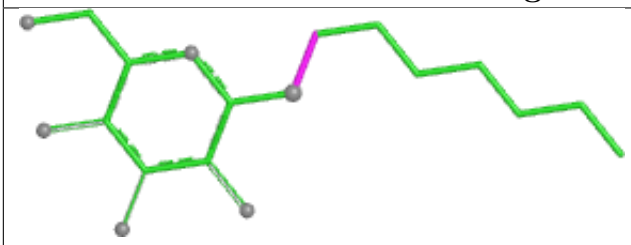

Bond lengths


Bond angles

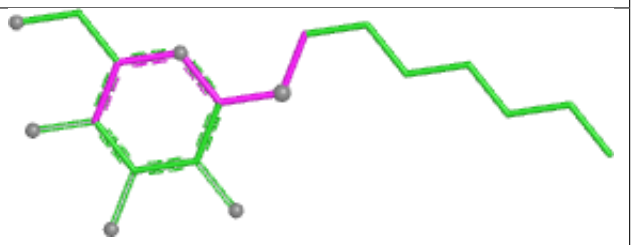

Torsions


Rings

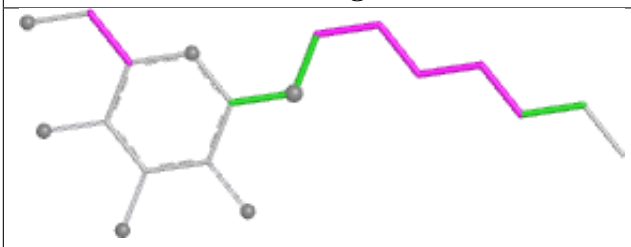
Ligand HTG b 623



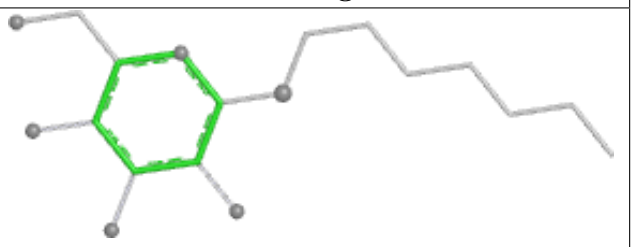
Bond lengths



Bond angles

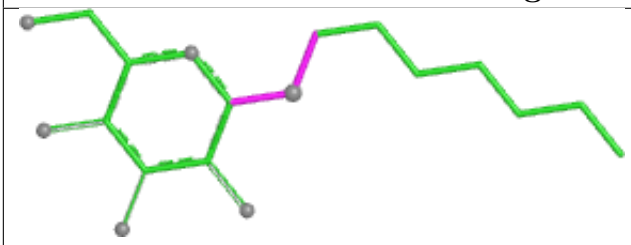


Torsions

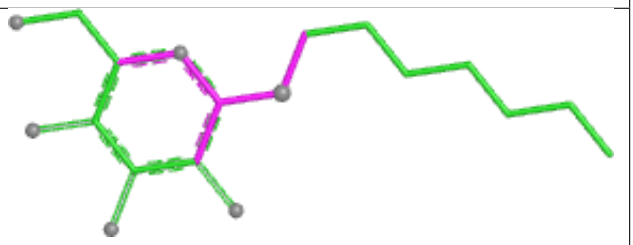


Rings

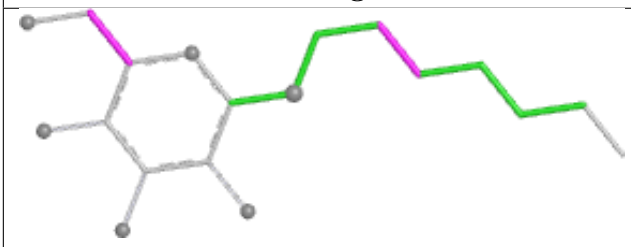
Ligand HTG b 625



Bond lengths



Bond angles



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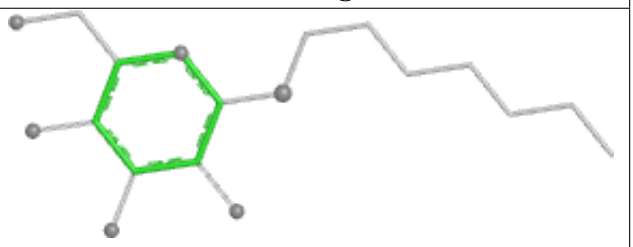
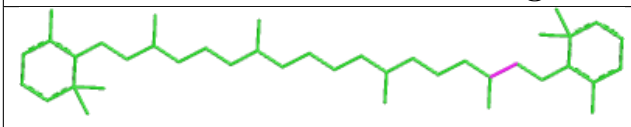
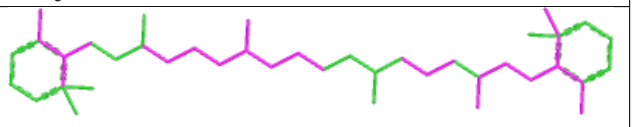


Rings

Ligand BCR y 101

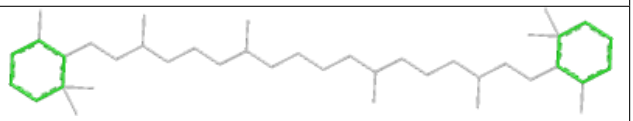


Bond lengths



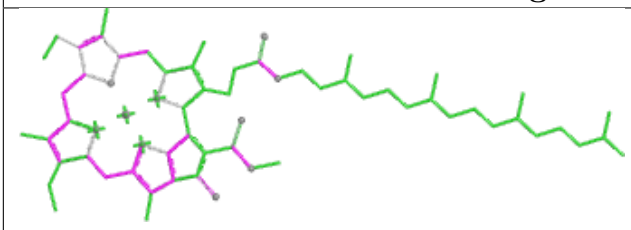
Bond angles

Torsions



Rings

Ligand CLA c 509



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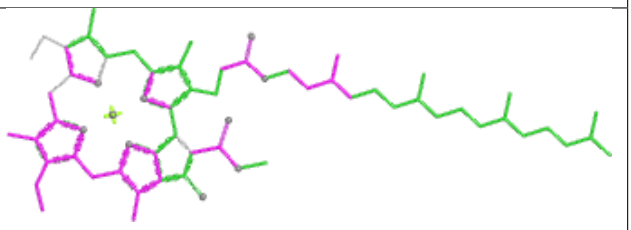
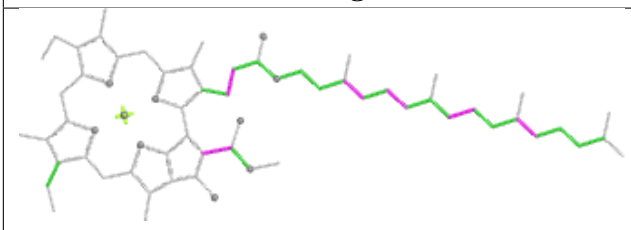


Bond angles



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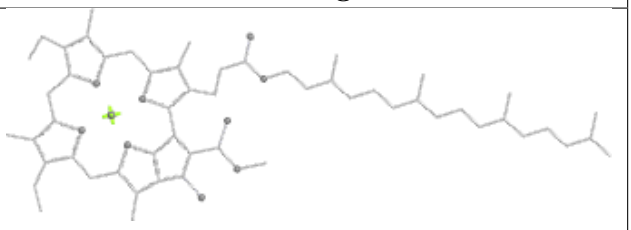
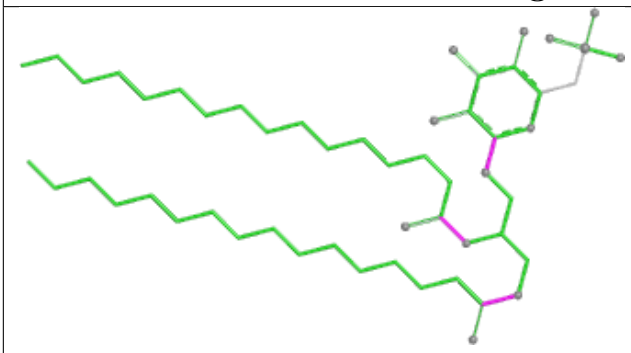
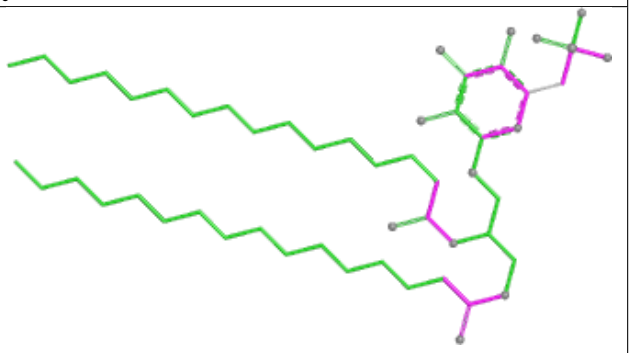


Rings

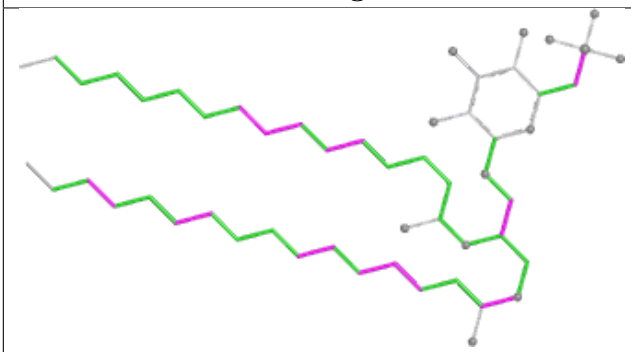
Ligand SQD a 411



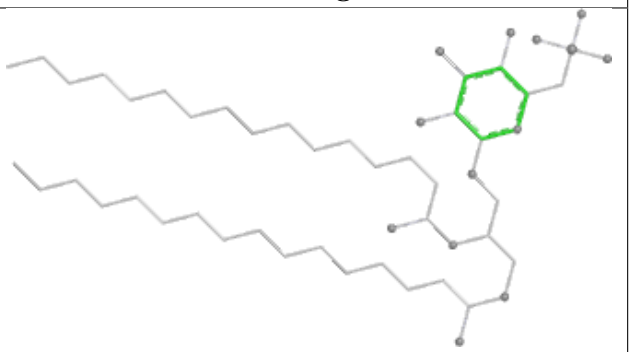
Bond lengths



Bond angles

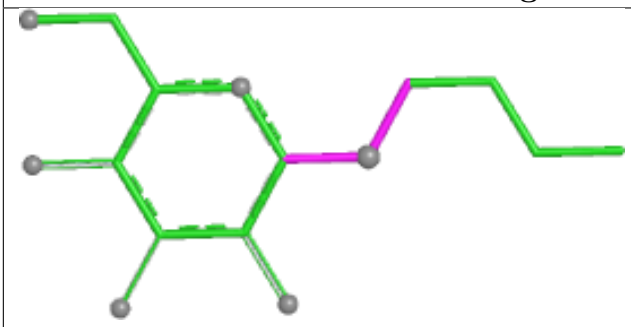


Torsions

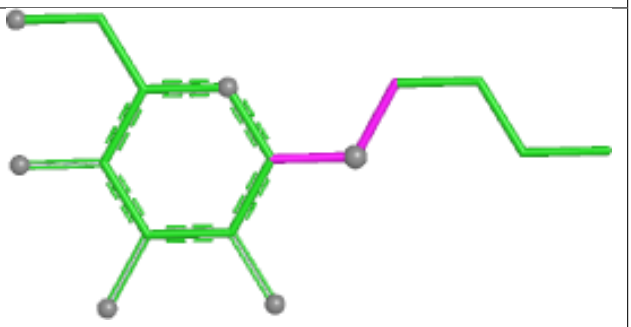


Rings

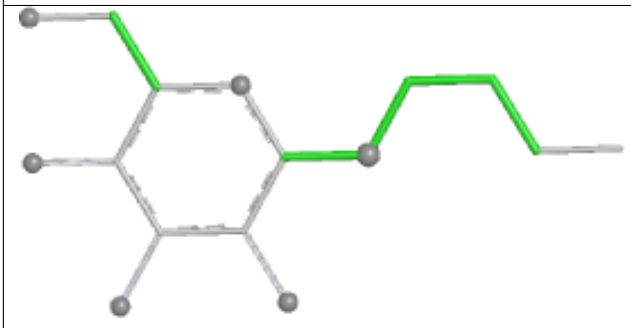
Ligand HTG D 410



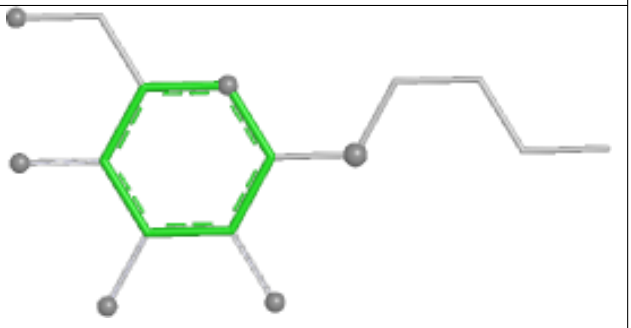
Bond lengths



Bond angles

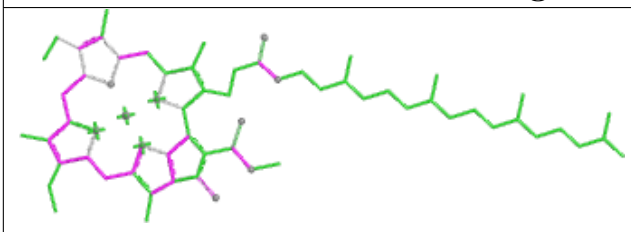


Torsions

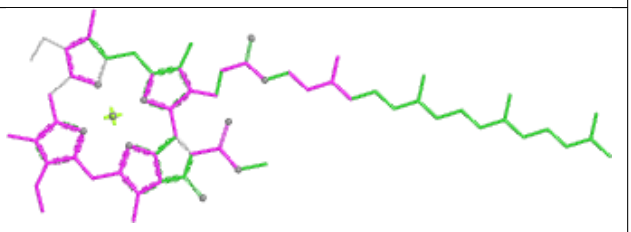


Rings

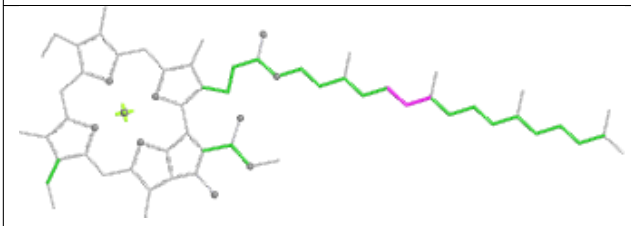
Ligand CLA c 510



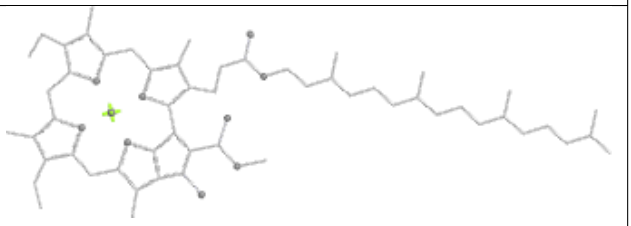
Bond lengths



Bond angles

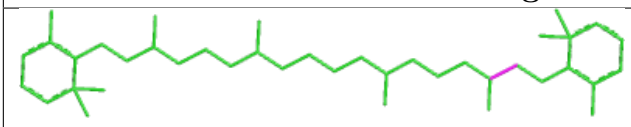


Torsions

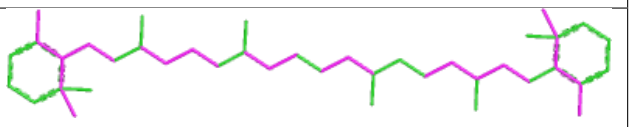


Rings

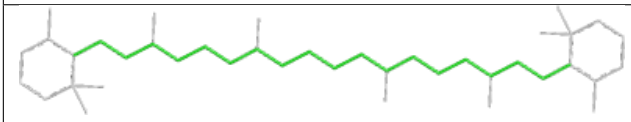
Ligand BCR A 410



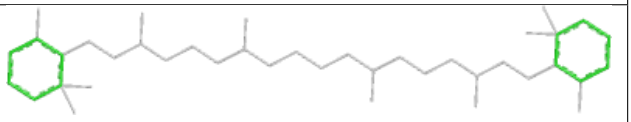
Bond lengths



Bond angles

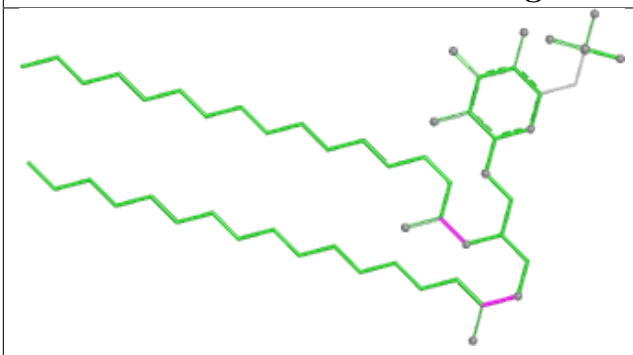


Torsions

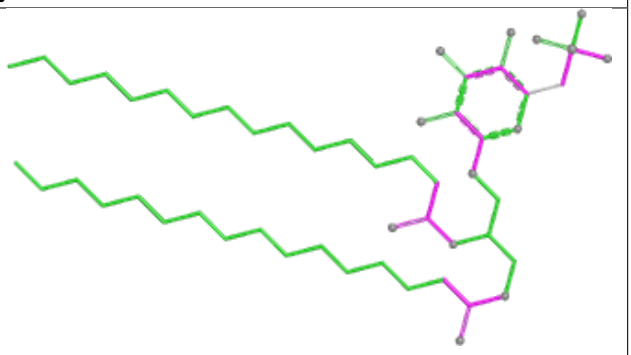


Rings

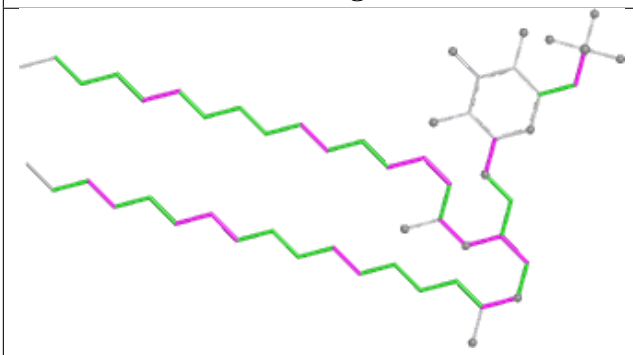
Ligand SQD B 620



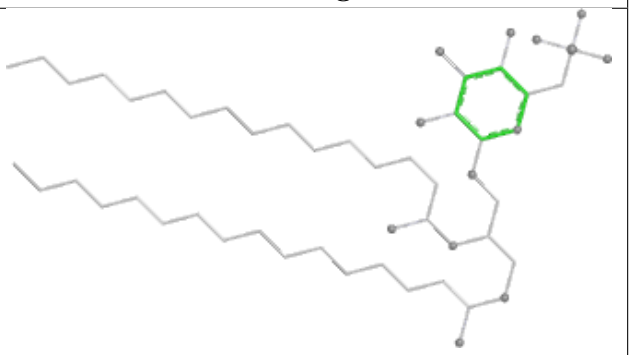
Bond lengths



Bond angles

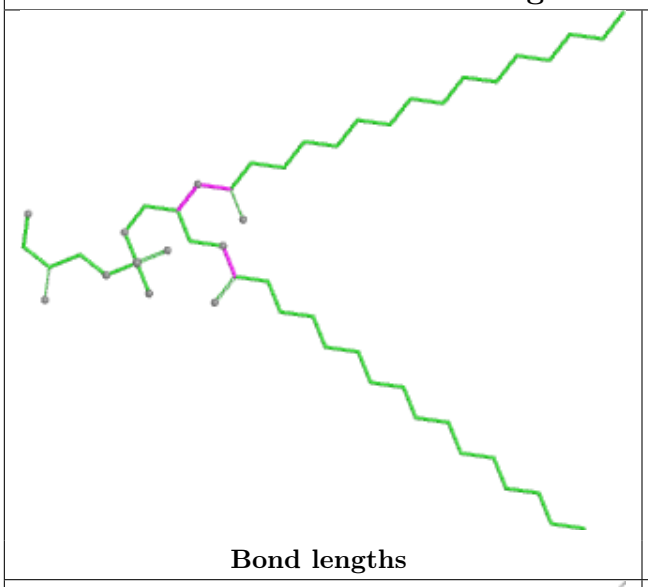


Torsions



Rings

Ligand LHG d 407



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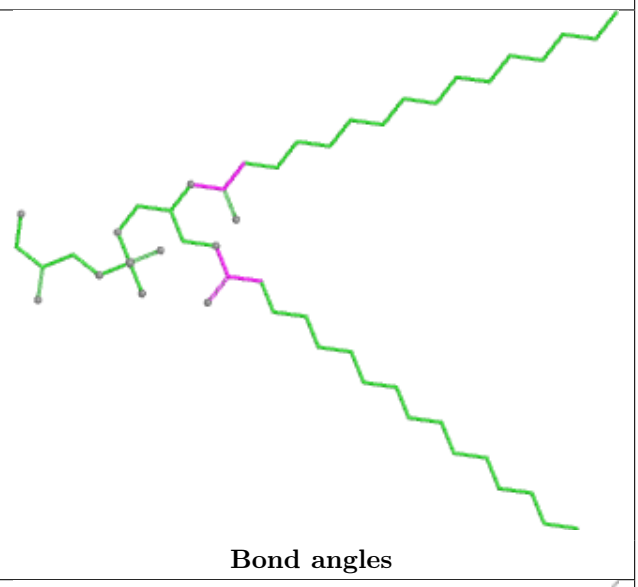
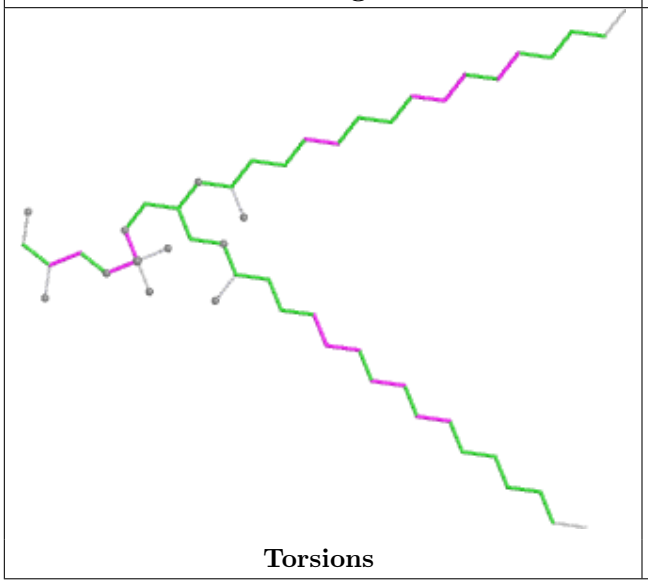
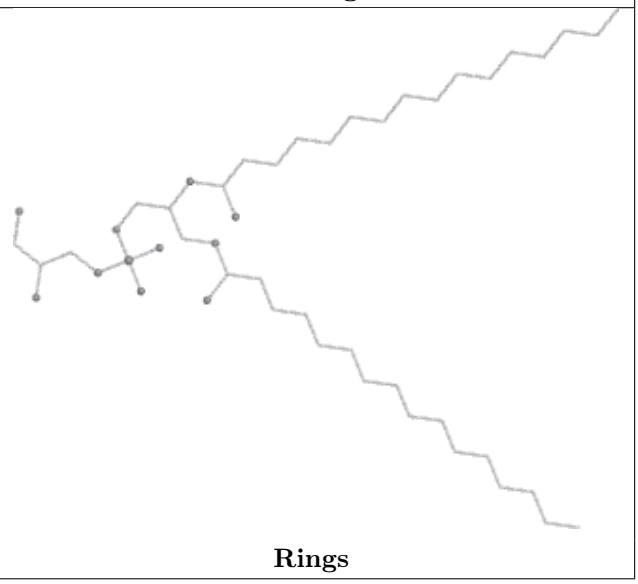


Bond angles

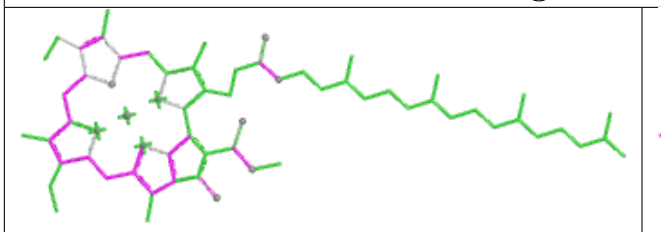


Torsions

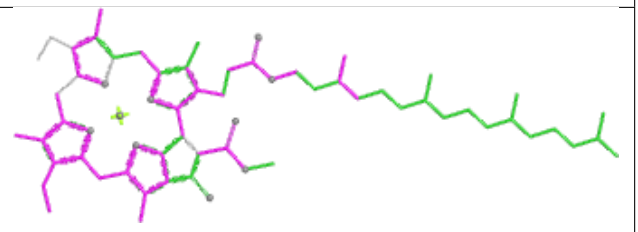


Rings

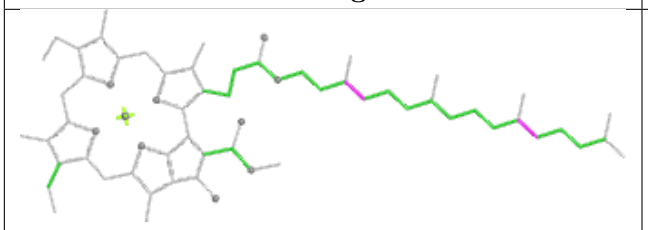
Ligand CLA c 506



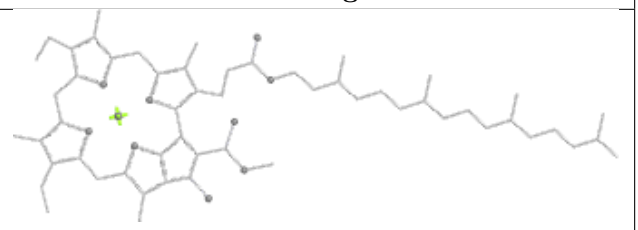
Bond lengths



Bond angles

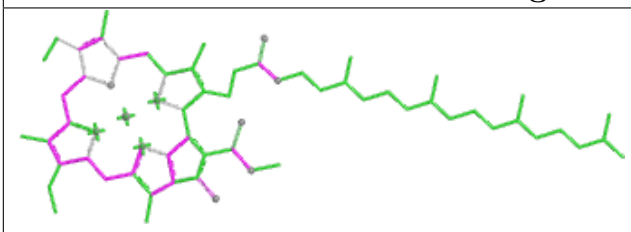


Torsions

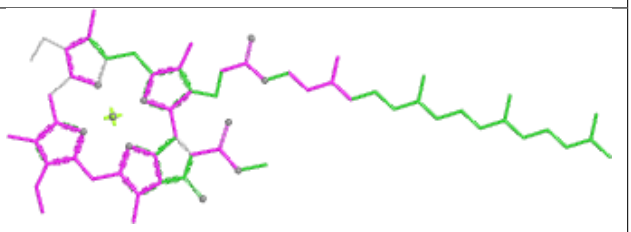


Rings

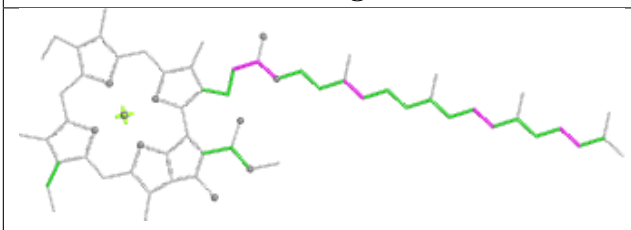
Ligand CLA c 512



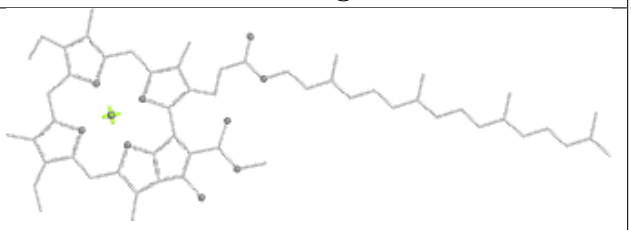
Bond lengths



Bond angles

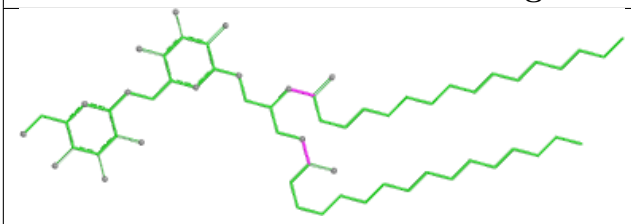


Torsions

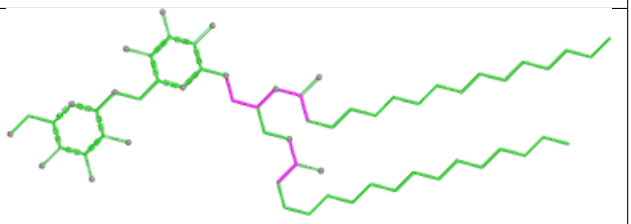


Rings

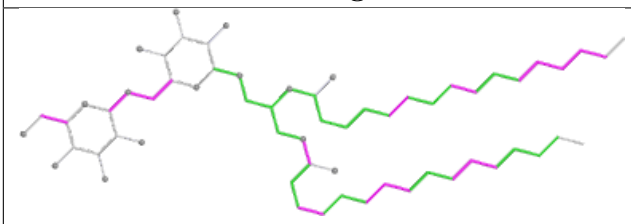
Ligand DGD c 518



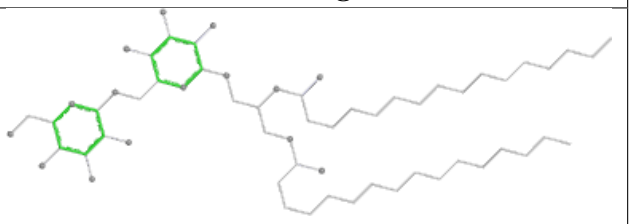
Bond lengths



Bond angles

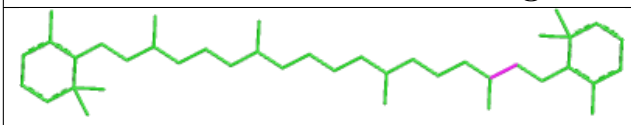


Torsions

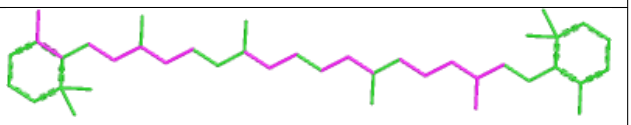


Rings

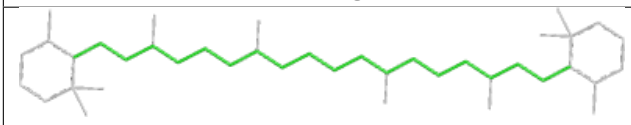
Ligand BCR C 515



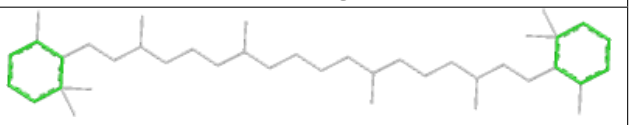
Bond lengths



Bond angles

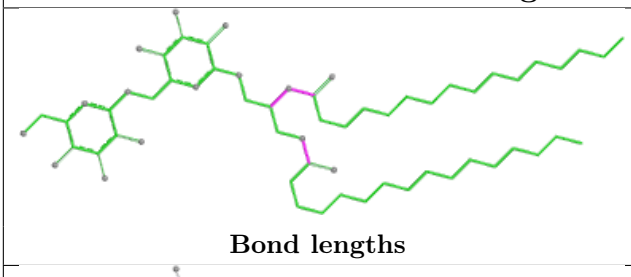


Torsions

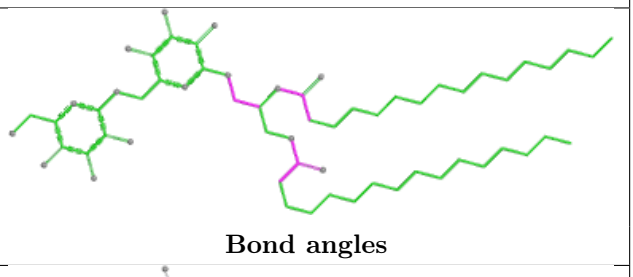


Rings

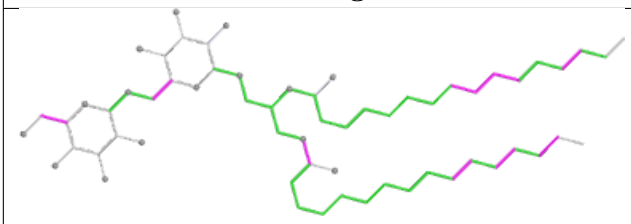
Ligand DGD C 519



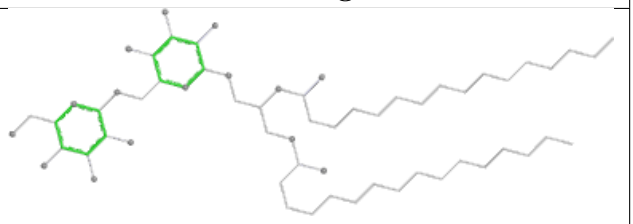
Bond lengths



Bond angles

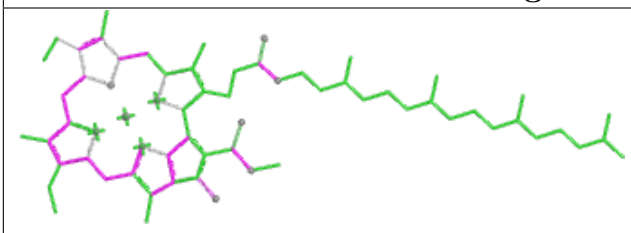


Torsions

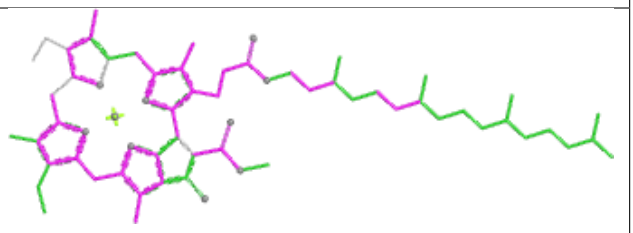


Rings

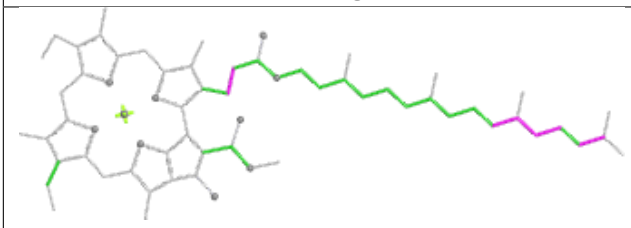
Ligand CLA B 610



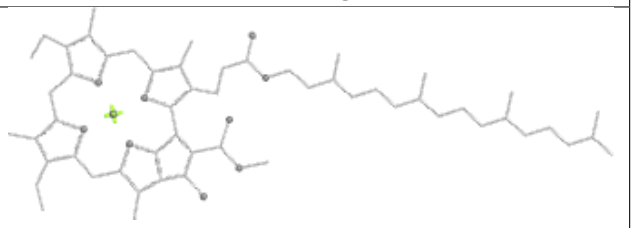
Bond lengths



Bond angles

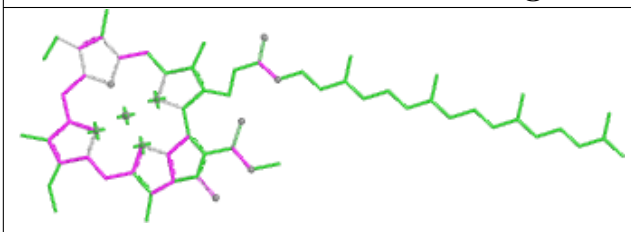


Torsions

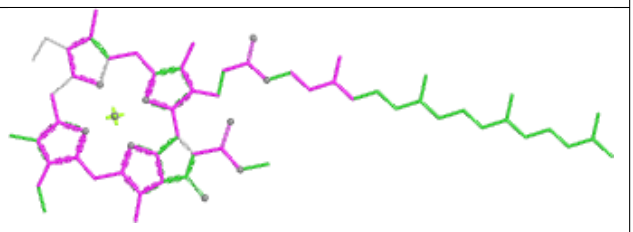


Rings

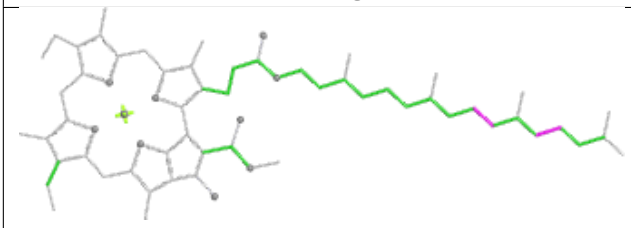
Ligand CLA C 509



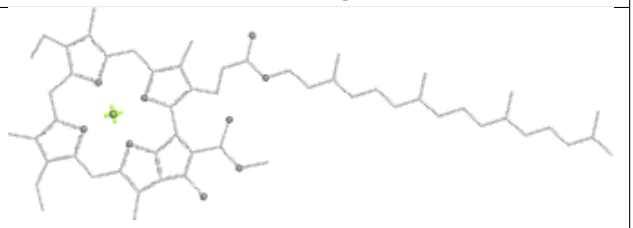
Bond lengths



Bond angles

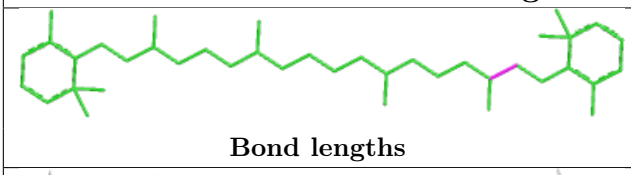


Torsions

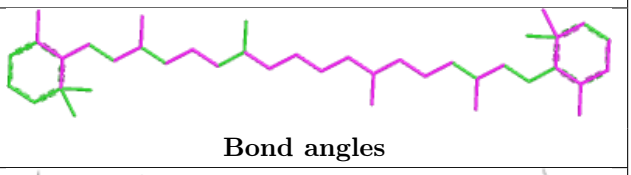


Rings

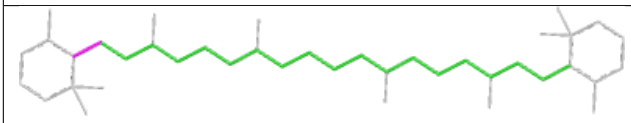
Ligand BCR Y 101



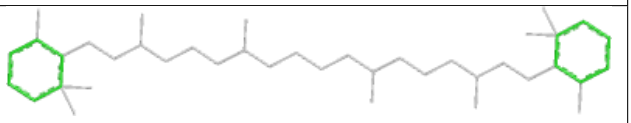
Bond lengths



Bond angles

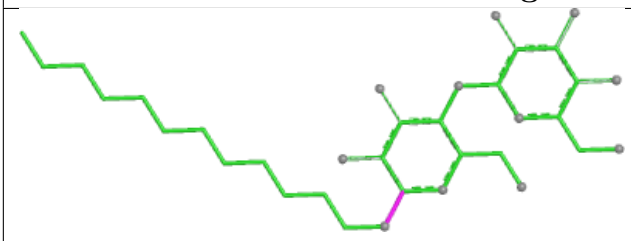


Torsions

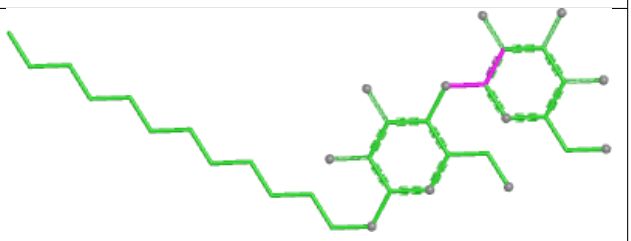


Rings

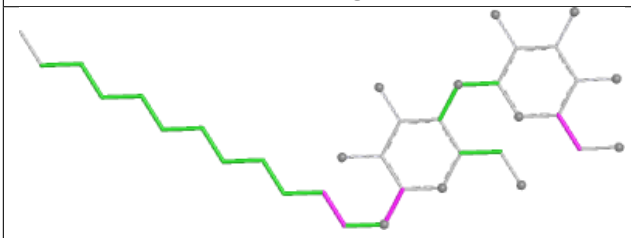
Ligand LMT A 359



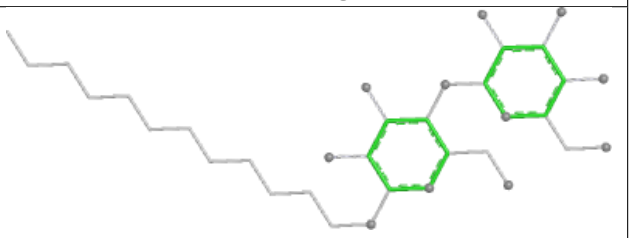
Bond lengths



Bond angles

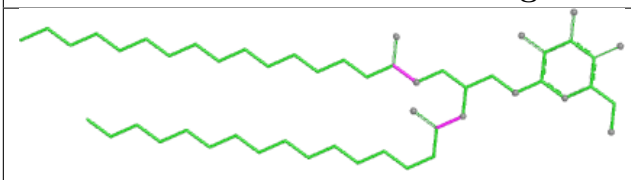


Torsions

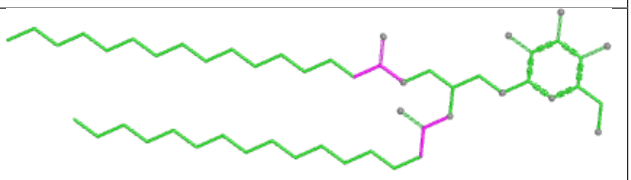


Rings

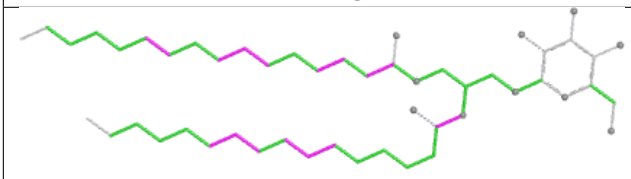
Ligand LMG B 621



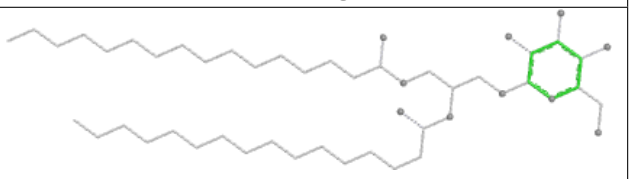
Bond lengths



Bond angles

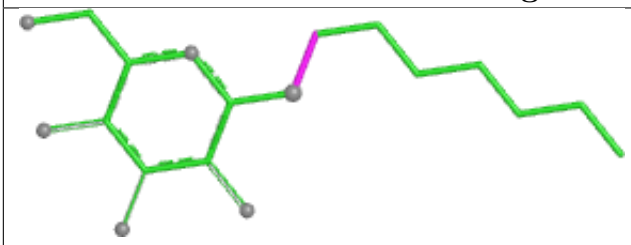


Torsions

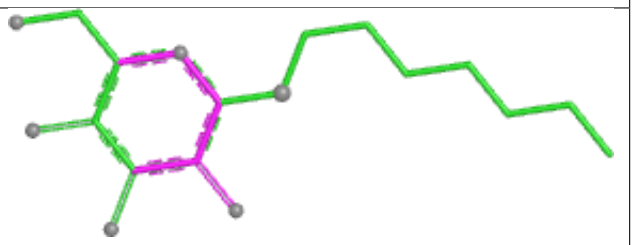


Rings

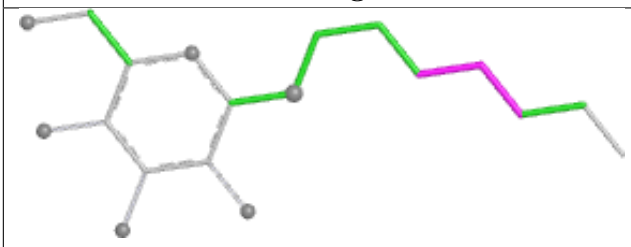
Ligand HTG B 623



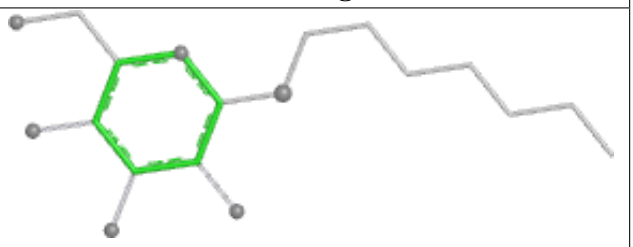
Bond lengths



Bond angles

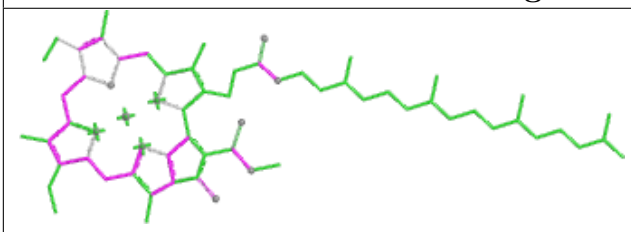


Torsions

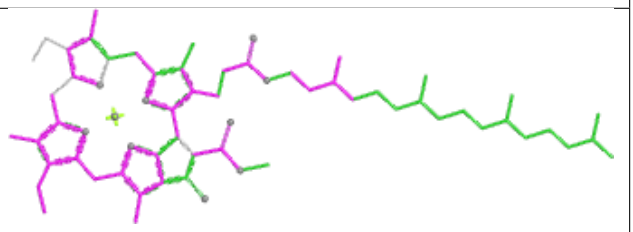


Rings

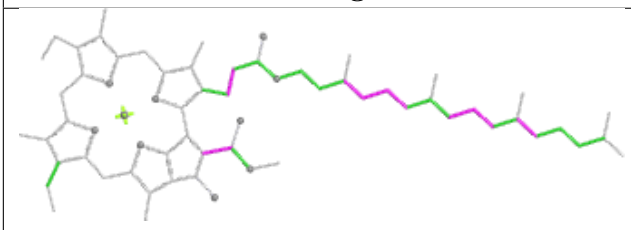
Ligand CLA B 614



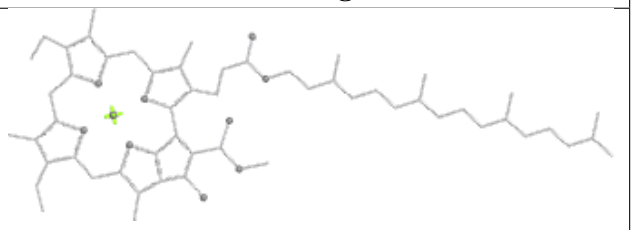
Bond lengths



Bond angles

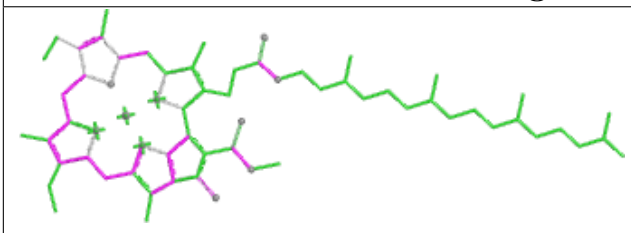


Torsions

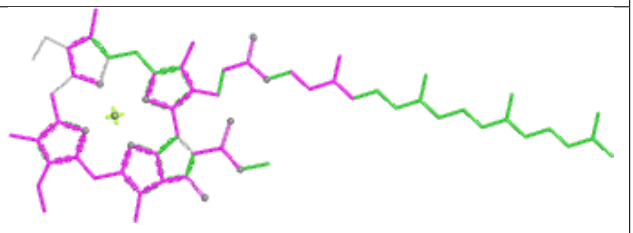


Rings

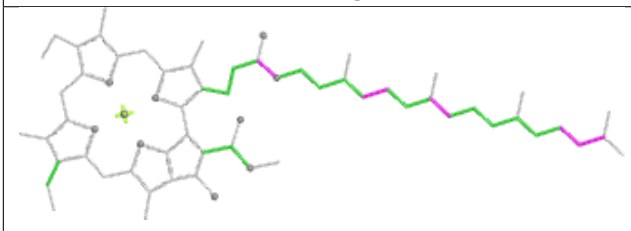
Ligand CLA a 407



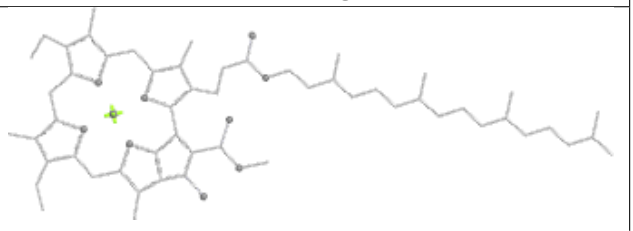
Bond lengths



Bond angles

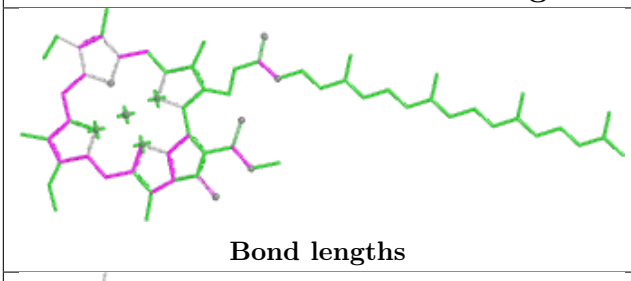


Torsions

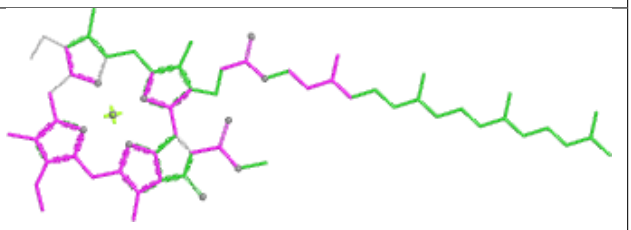


Rings

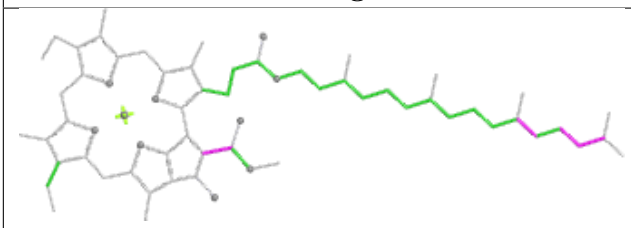
Ligand CLA c 504



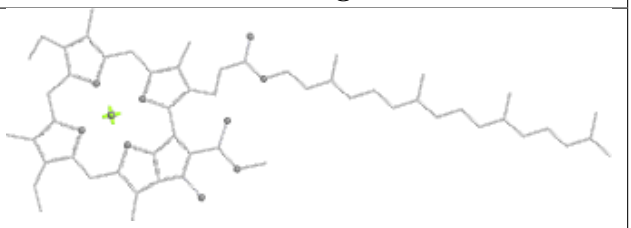
Bond lengths



Bond angles

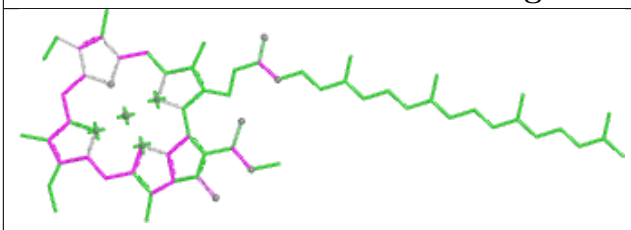


Torsions

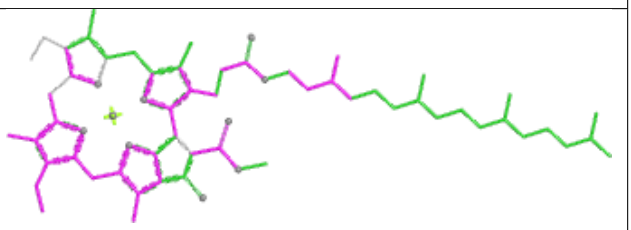


Rings

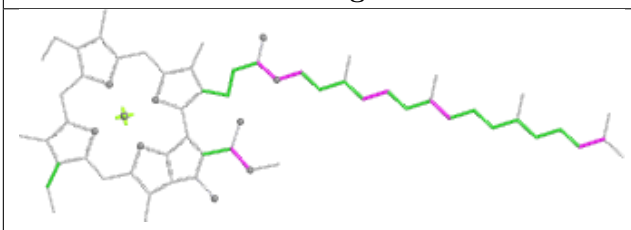
Ligand CLA C 514



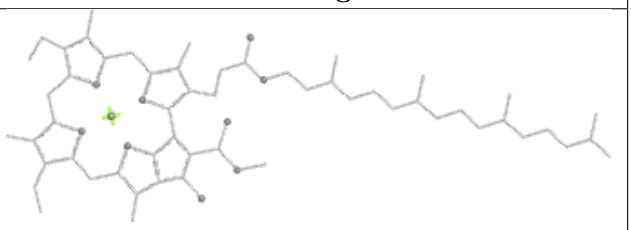
Bond lengths



Bond angles

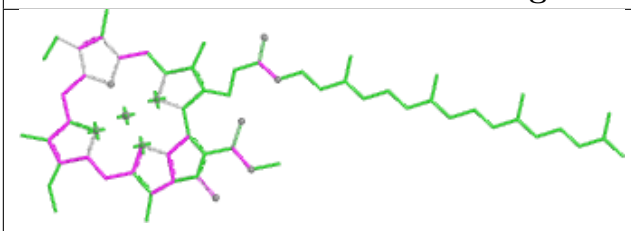


Torsions

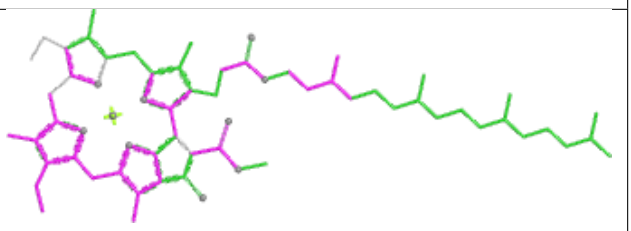


Rings

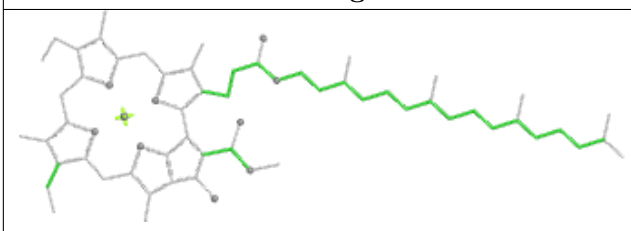
Ligand CLA c 505



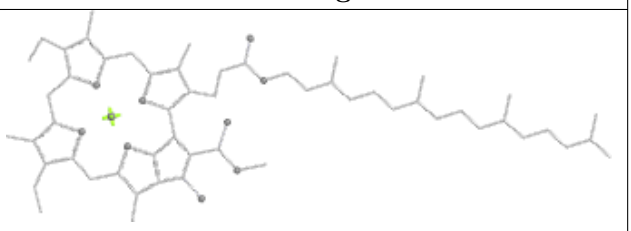
Bond lengths



Bond angles

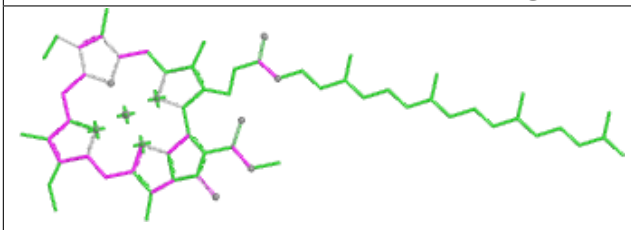


Torsions

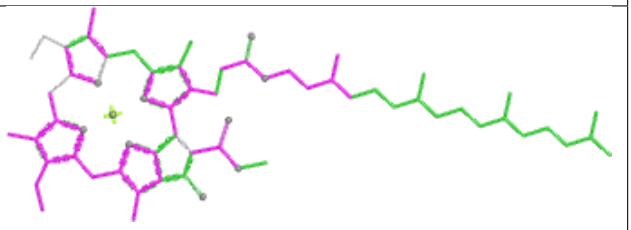


Rings

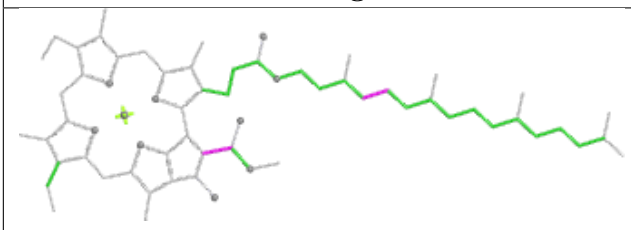
Ligand CLA B 607



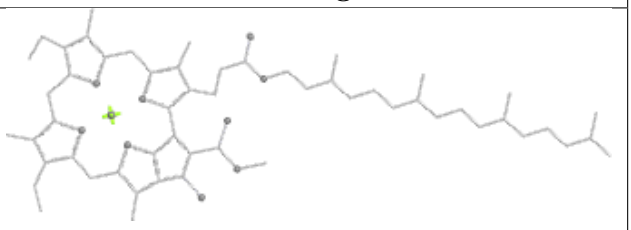
Bond lengths



Bond angles

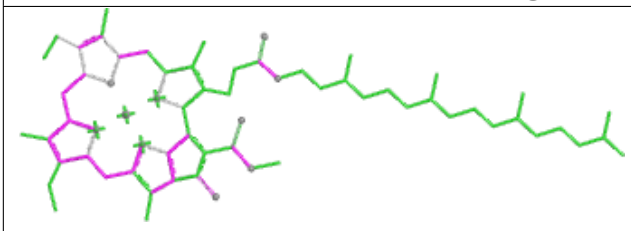


Torsions

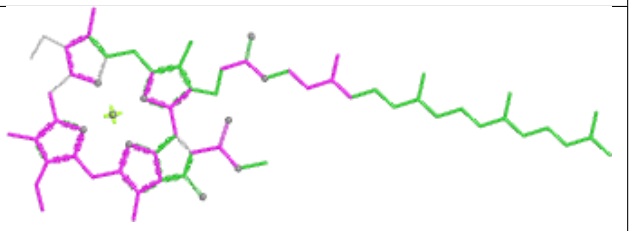


Rings

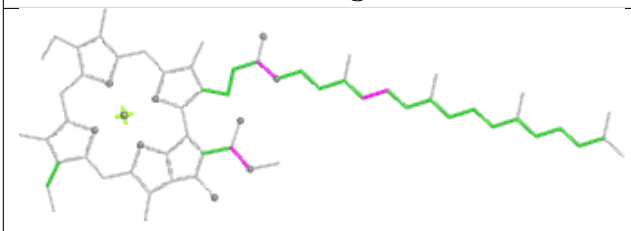
Ligand CLA C 512



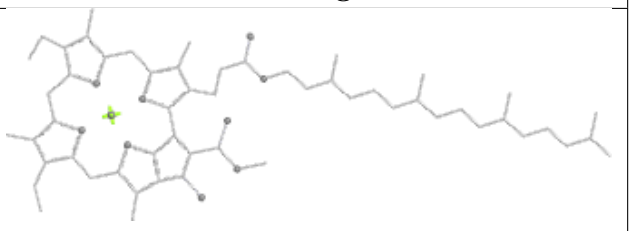
Bond lengths



Bond angles

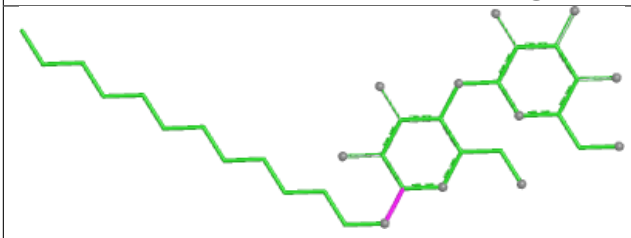


Torsions



Rings

Ligand LMT I 101



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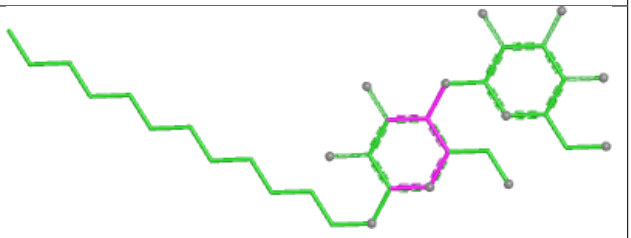
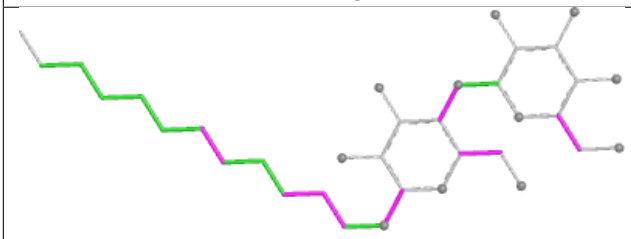
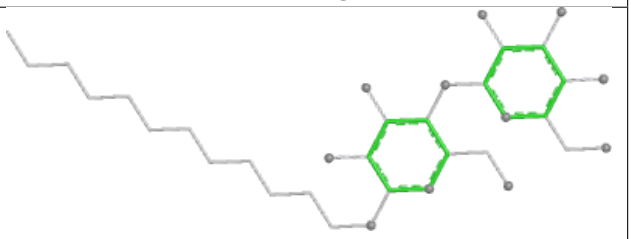


Bond angles

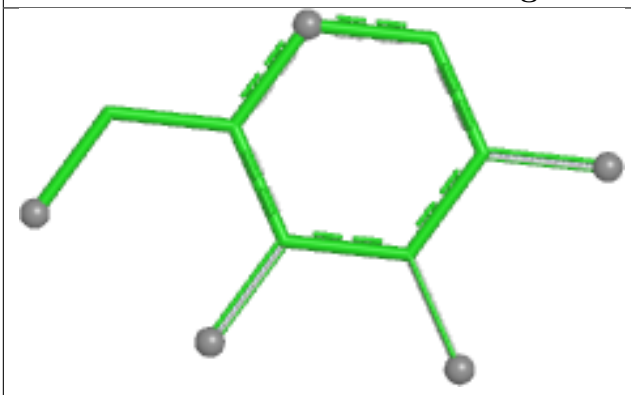


Torsions

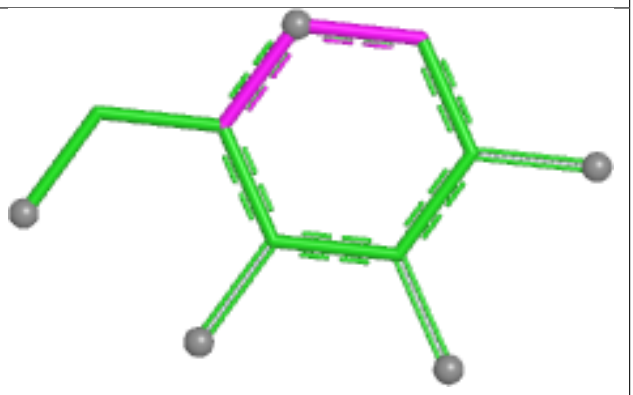


Rings

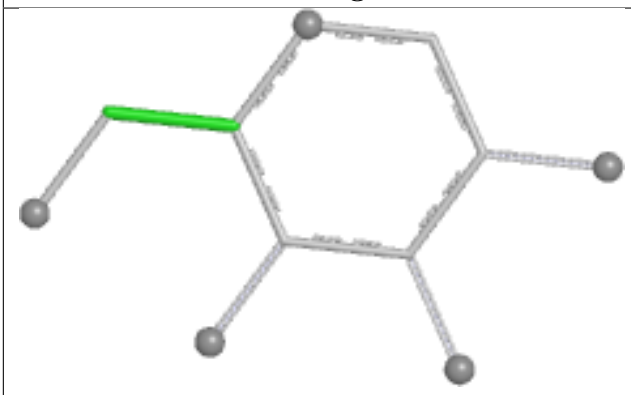
Ligand HTG V 204



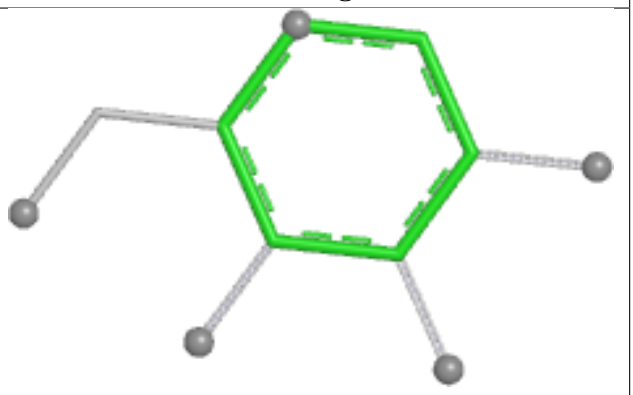
Bond lengths



Bond angles

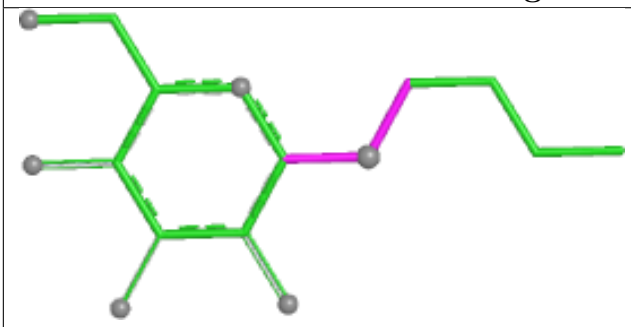


Torsions



Rings

Ligand HTG h 101



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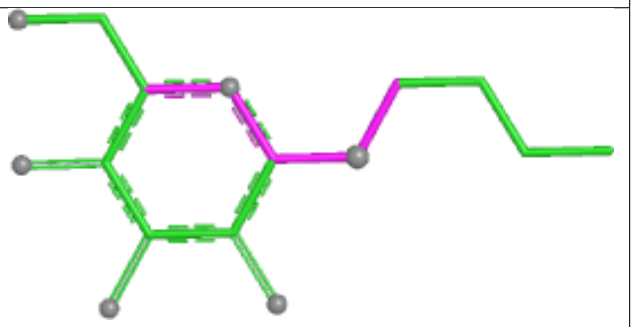
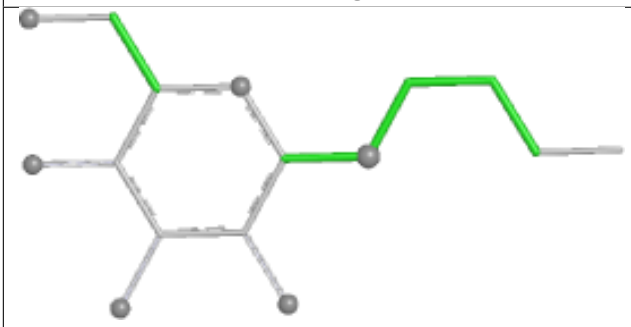
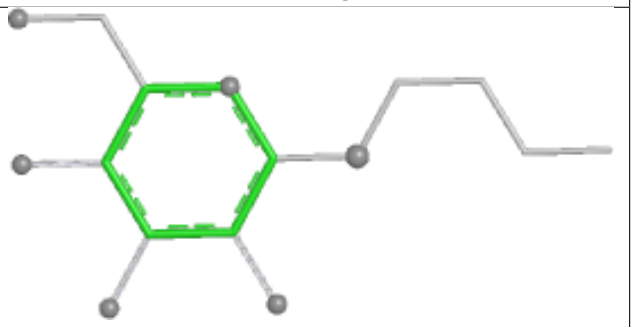


Bond angles

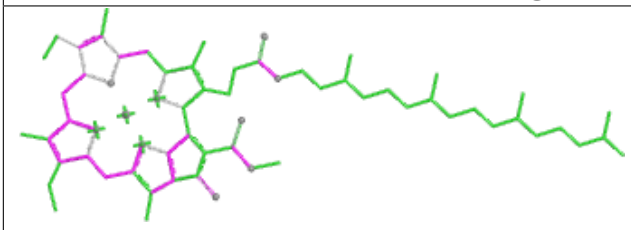


Torsions

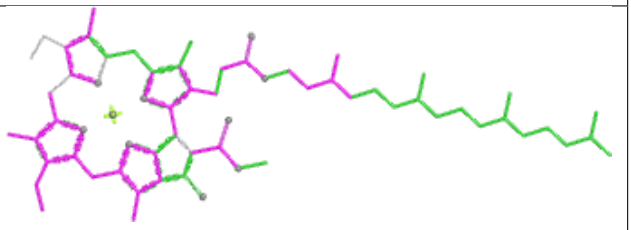


Rings

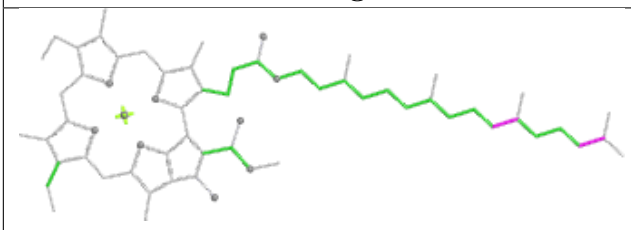
Ligand CLA a 404



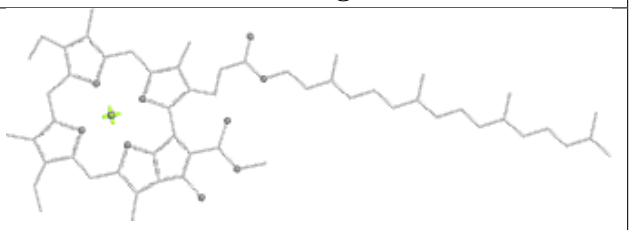
Bond lengths



Bond angles

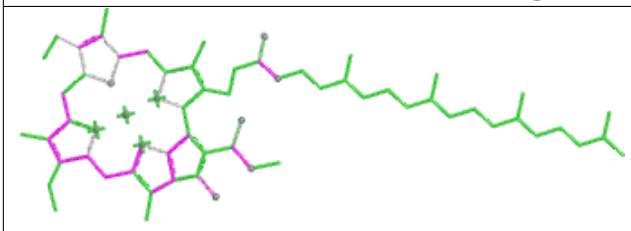


Torsions

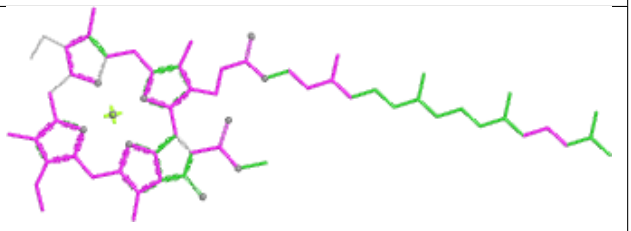


Rings

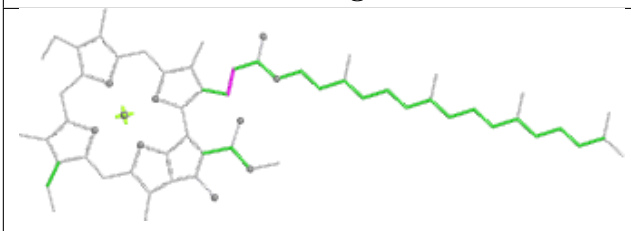
Ligand CLA a 403



Bond lengths



Bond angles



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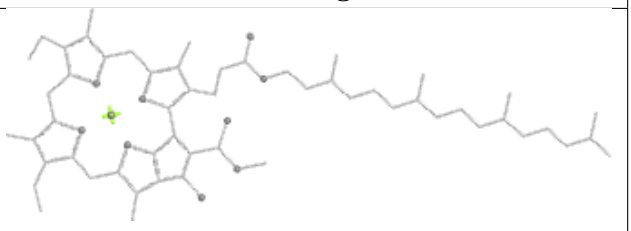
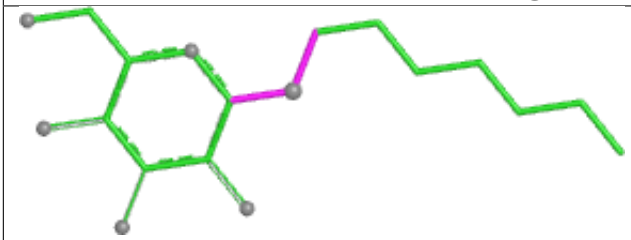
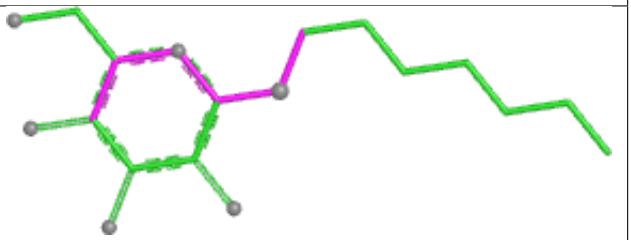


Rings

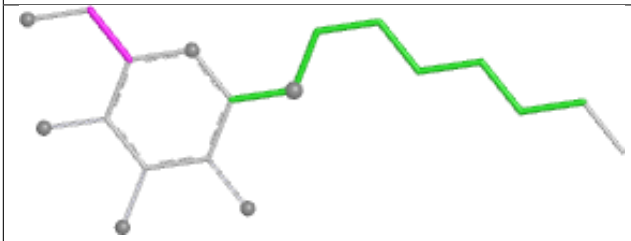
Ligand HTG c 526



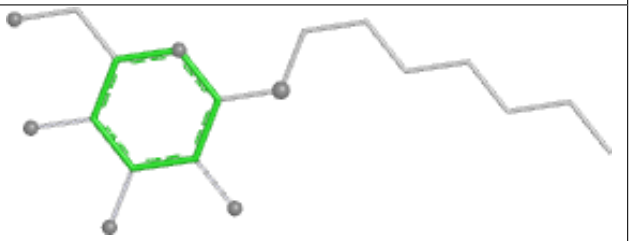
Bond lengths



Bond angles

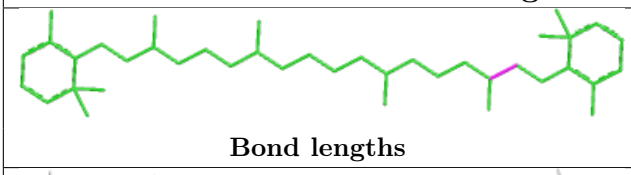


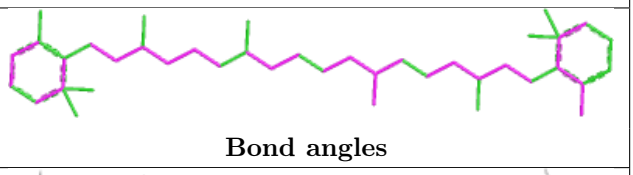
Torsions

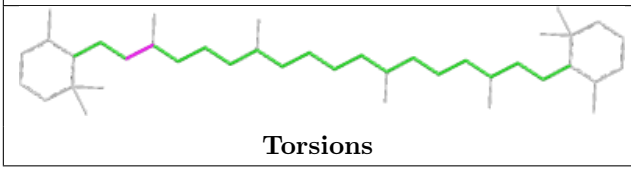


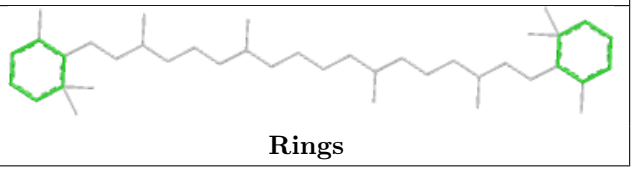
Rings

Ligand BCR K 102

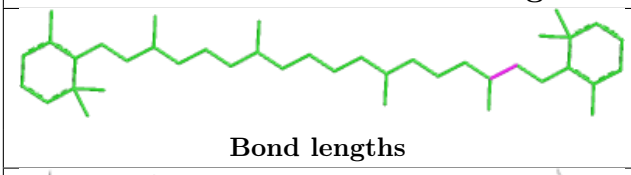

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR k 101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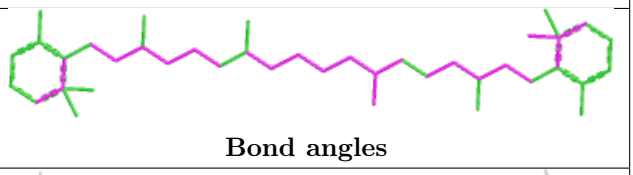
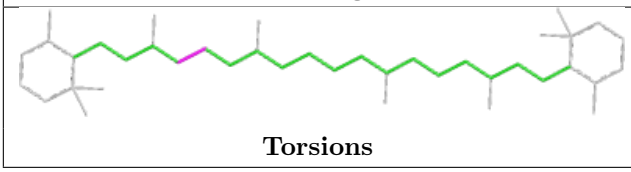
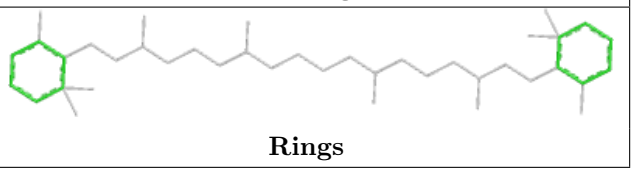
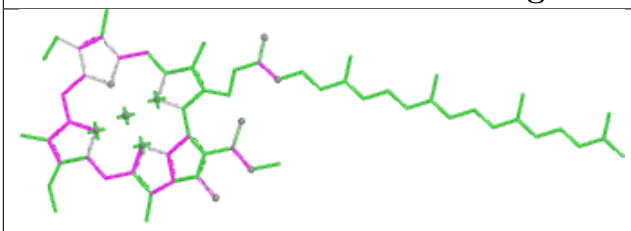
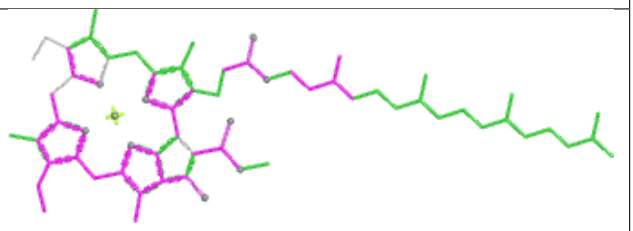

Bond angles

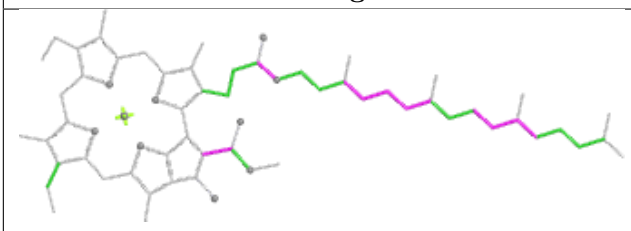

Torsions

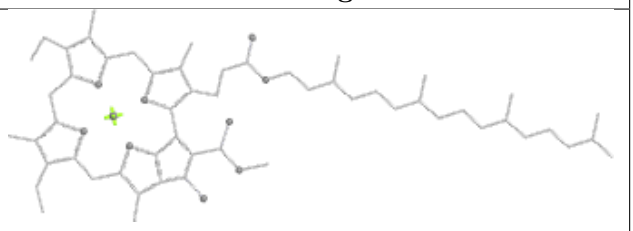

Rings

Ligand CLA b 616

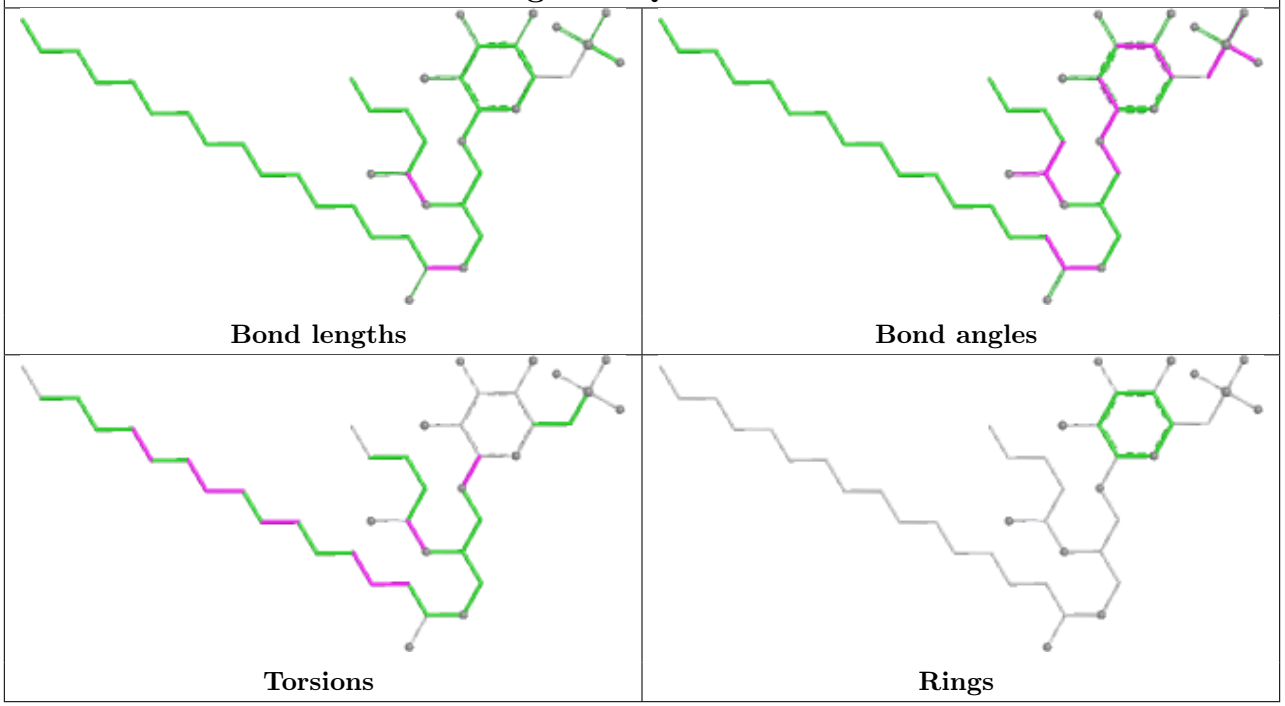

Bond lengths


Bond angles

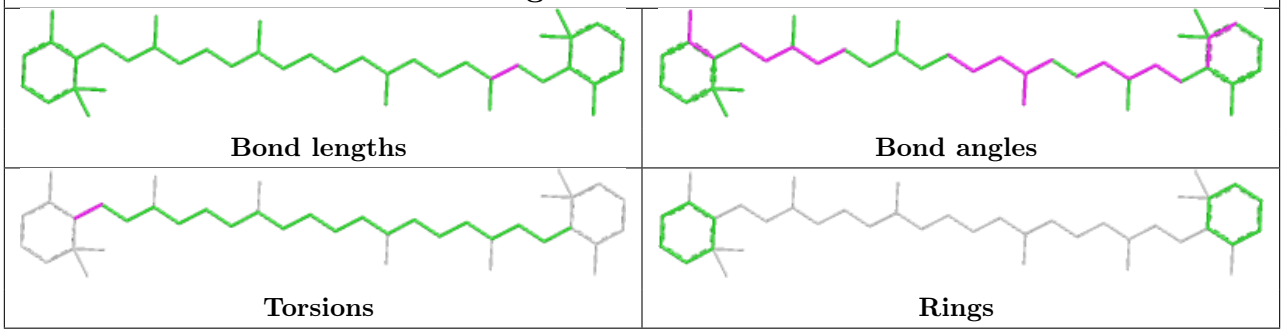

Torsions


Rings

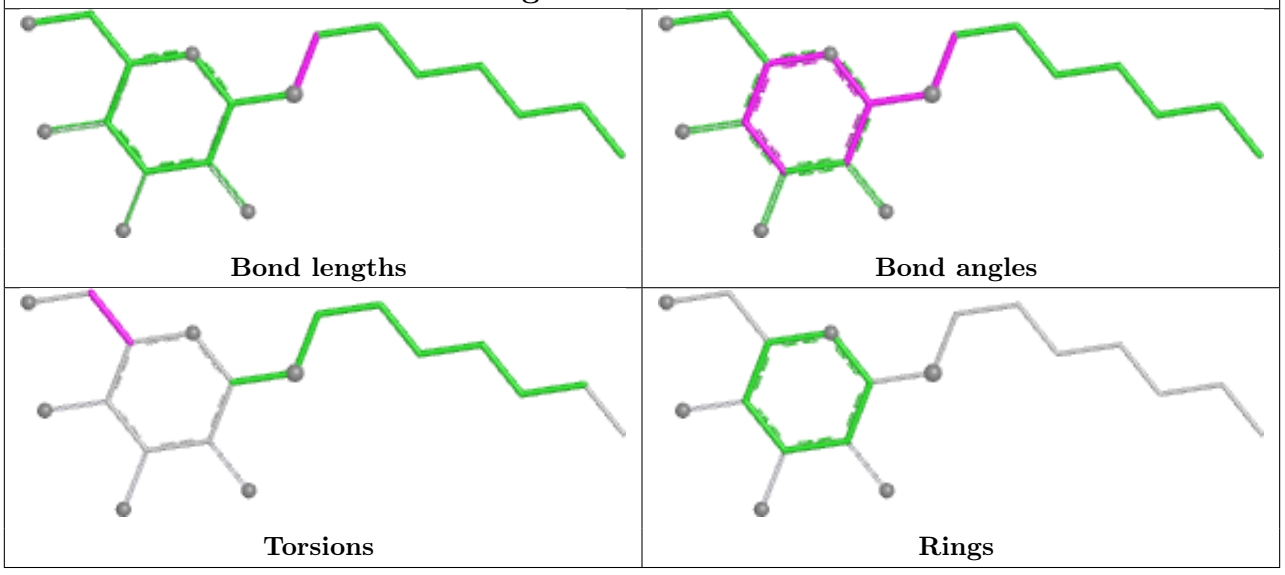
Ligand SQD F 101



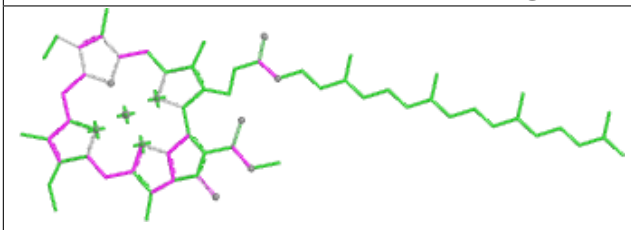
Ligand BCR b 617



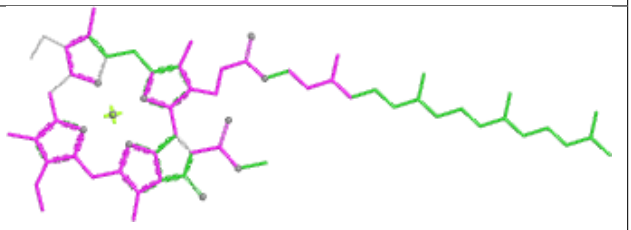
Ligand HTG C 523



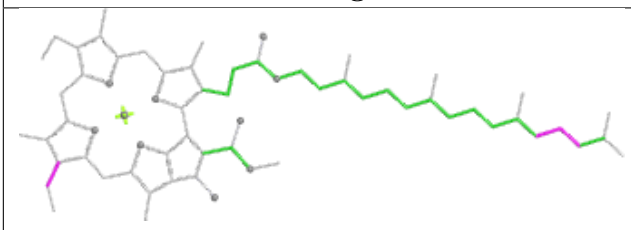
Ligand CLA A 405



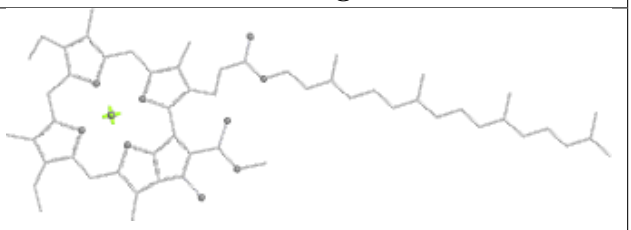
Bond lengths



Bond angles

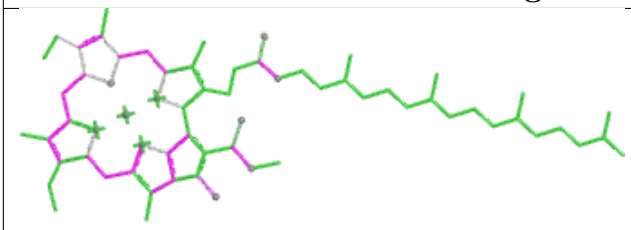


Torsions

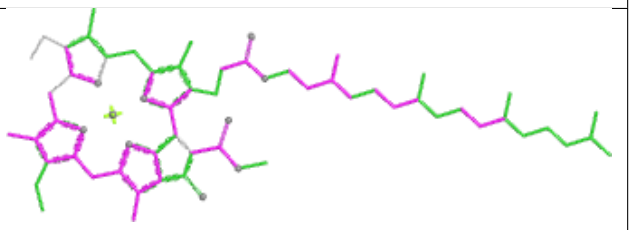


Rings

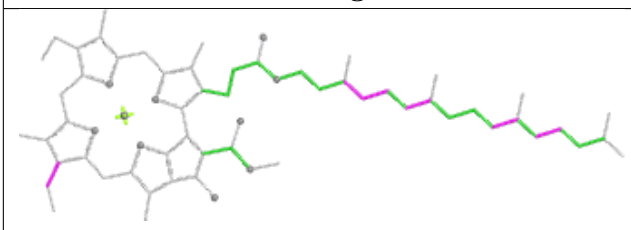
Ligand CLA B 604



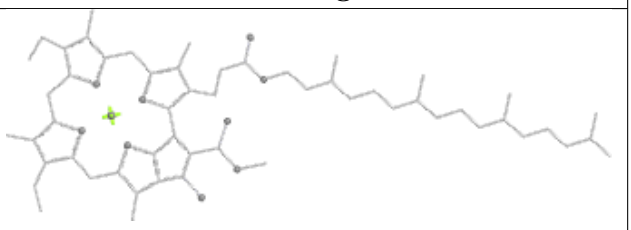
Bond lengths



Bond angles

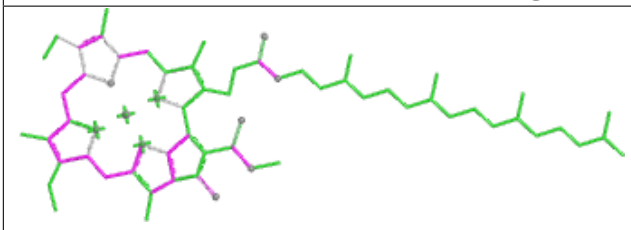


Torsions

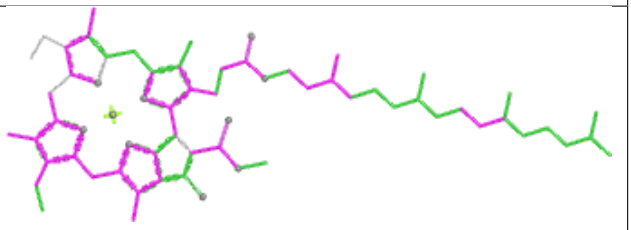


Rings

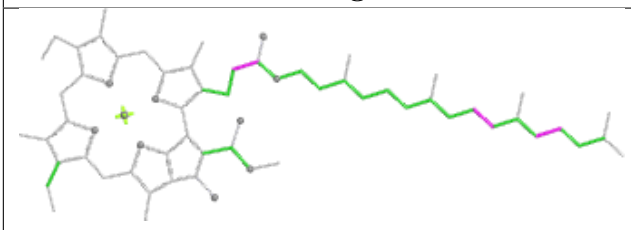
Ligand CLA b 612



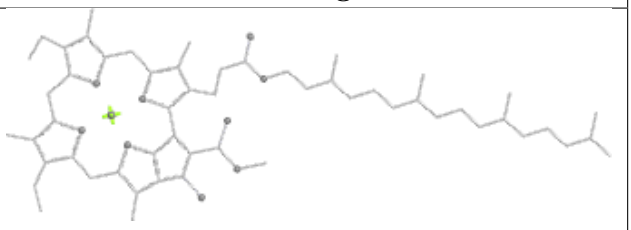
Bond lengths



Bond angles

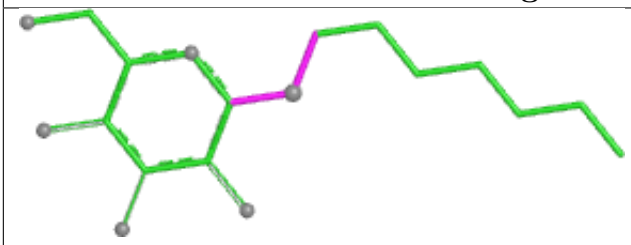


Torsions

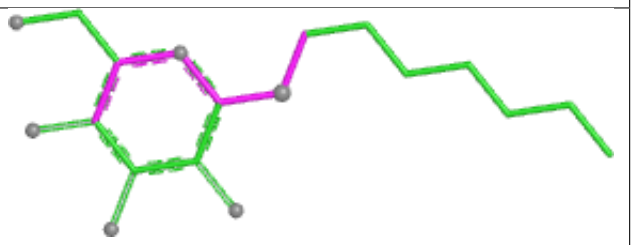


Rings

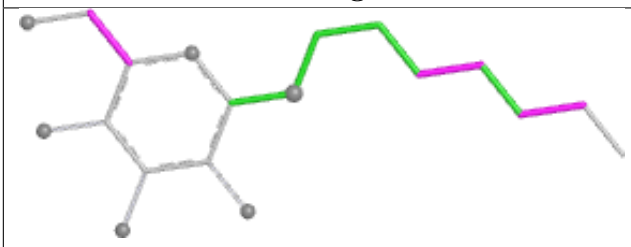
Ligand HTG B 628



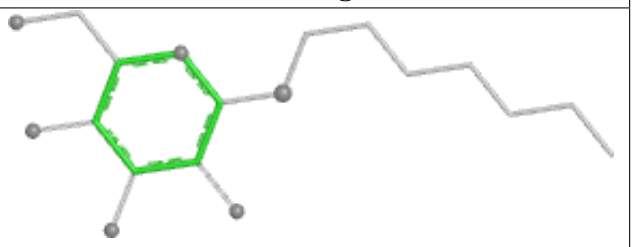
Bond lengths



Bond angles

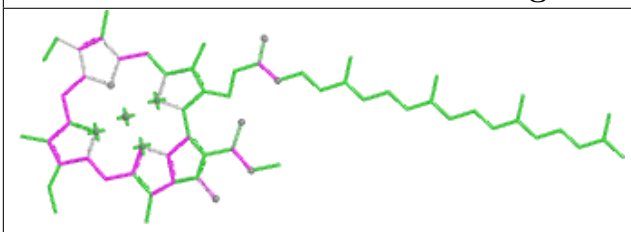


Torsions

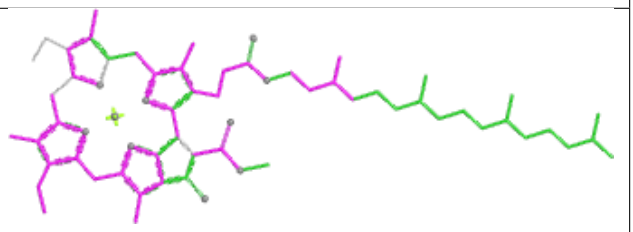


Rings

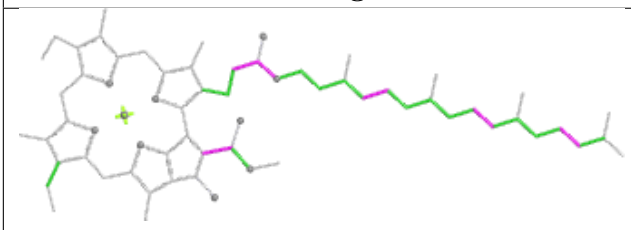
Ligand CLA c 514



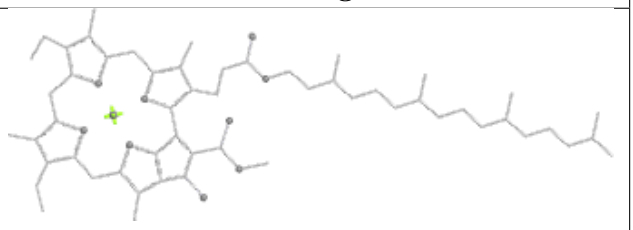
Bond lengths



Bond angles

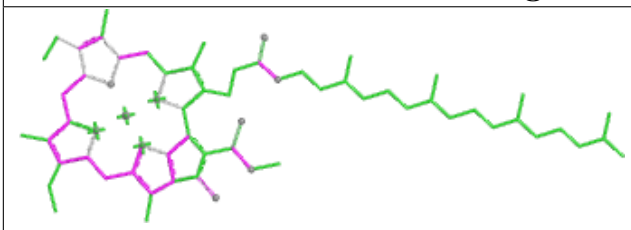


Torsions

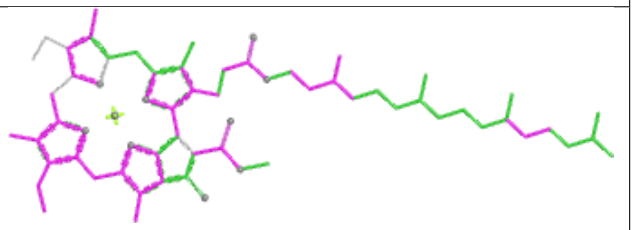


Rings

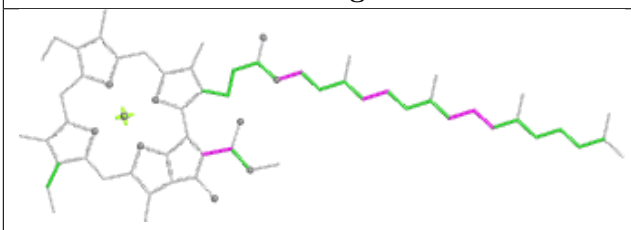
Ligand CLA C 510



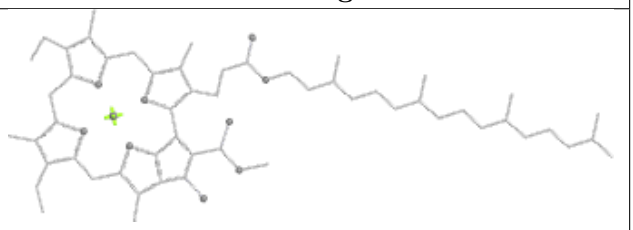
Bond lengths



Bond angles

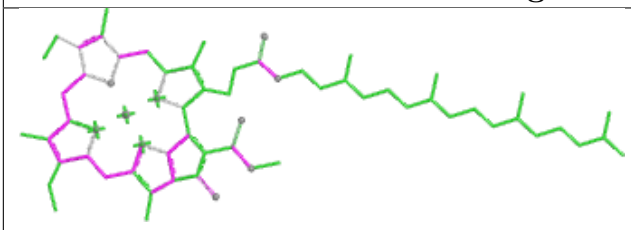


Torsions

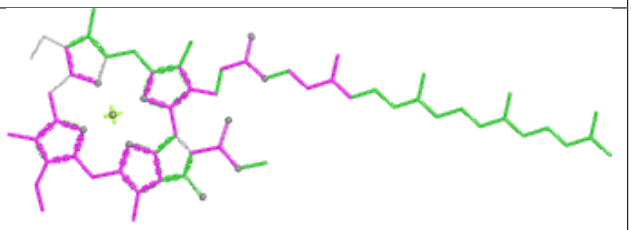


Rings

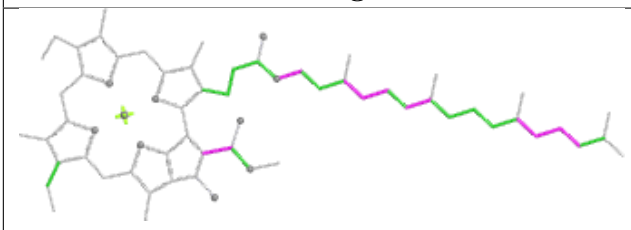
Ligand CLA b 614



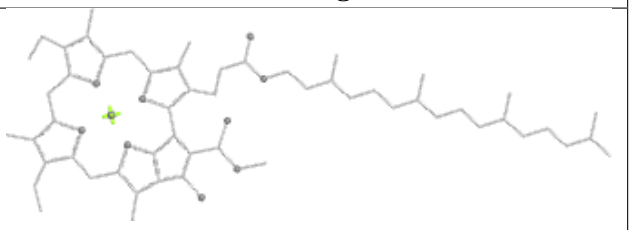
Bond lengths



Bond angles

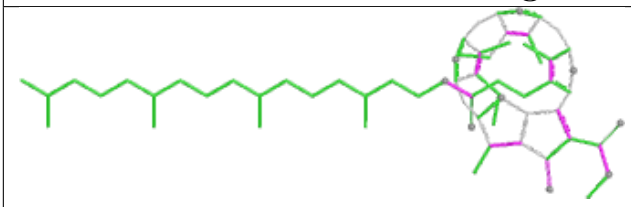


Torsions

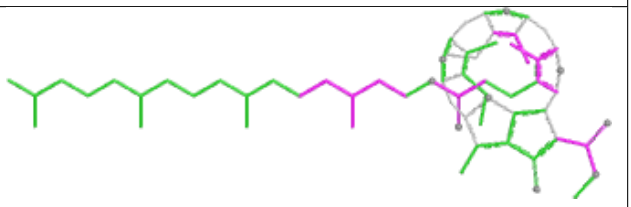


Rings

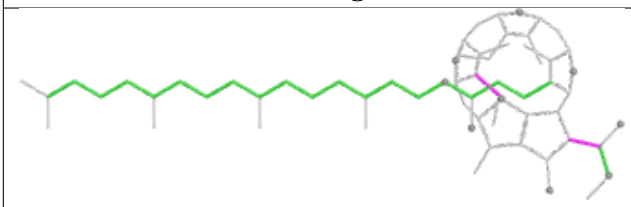
Ligand PHO A 408



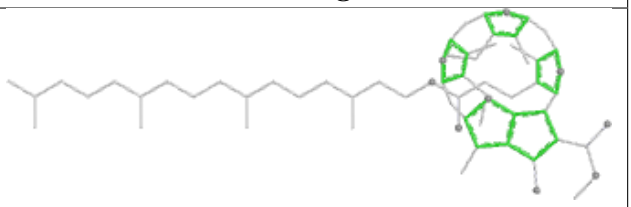
Bond lengths



Bond angles

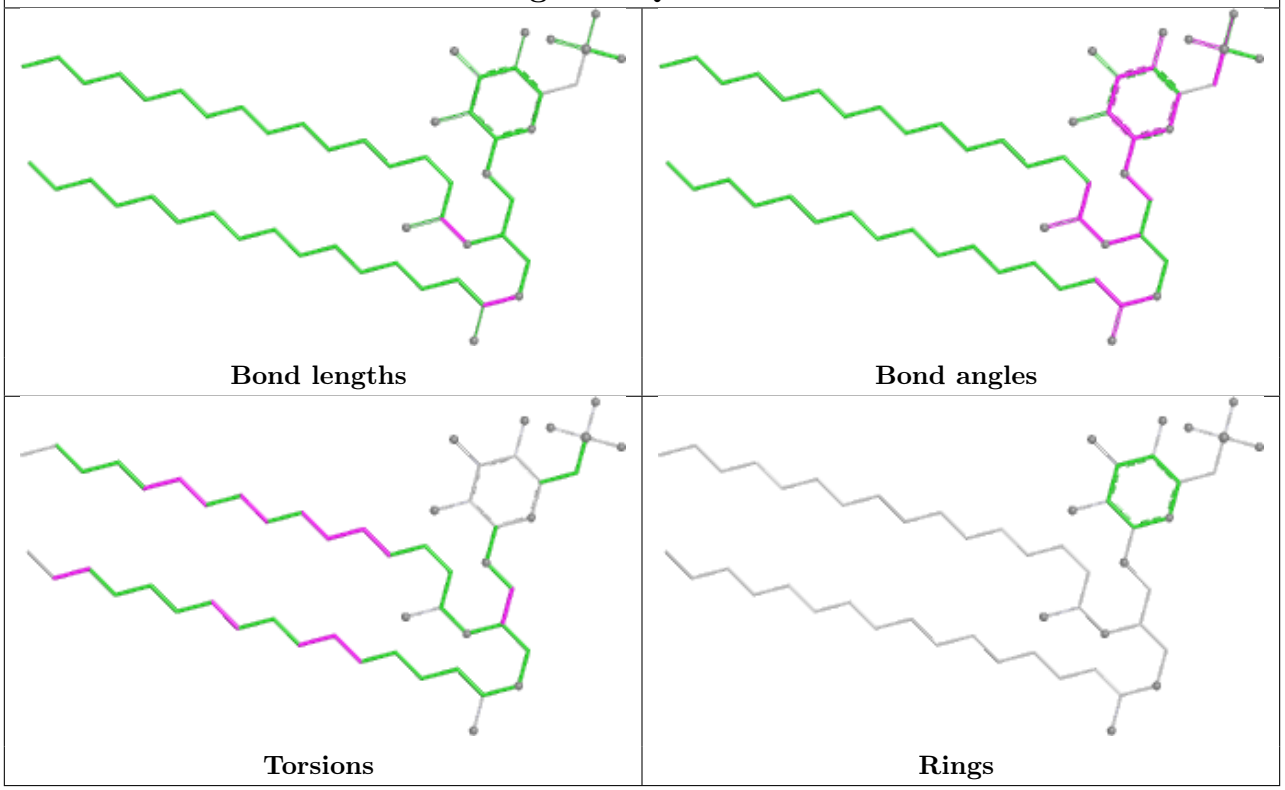


Torsions

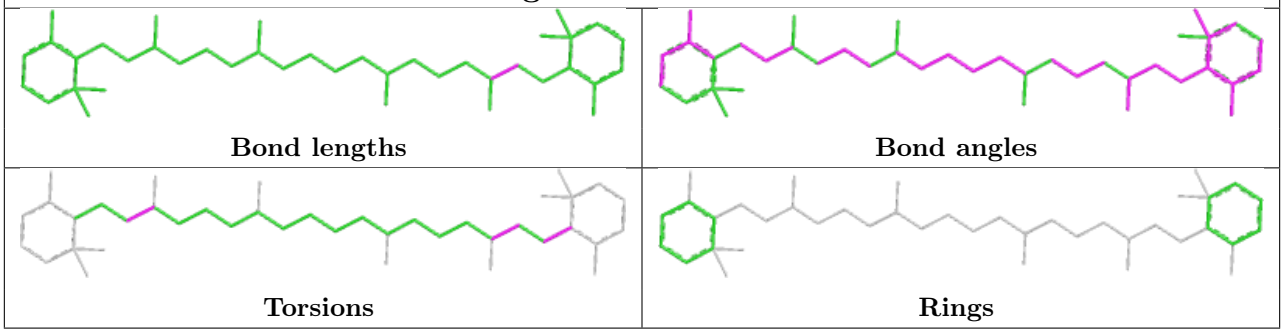


Rings

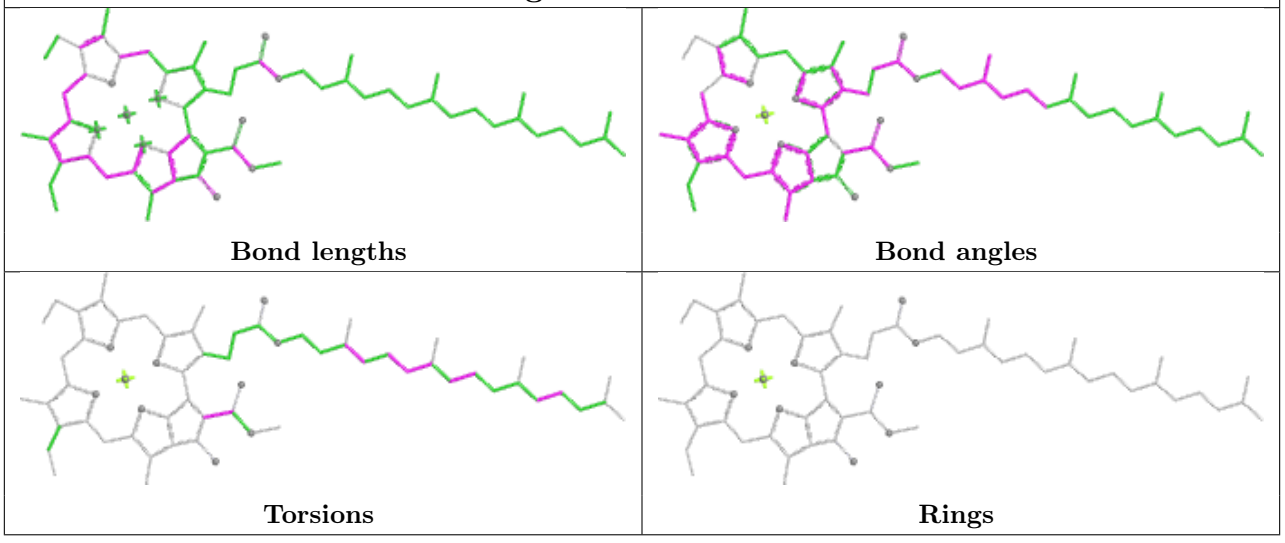
Ligand SQD a 409



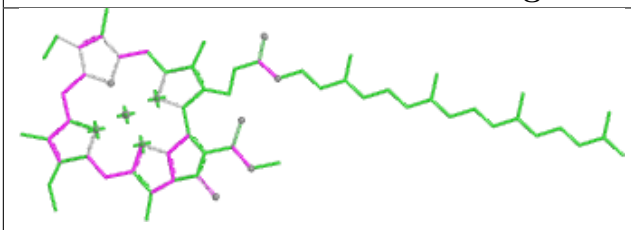
Ligand BCR D 404



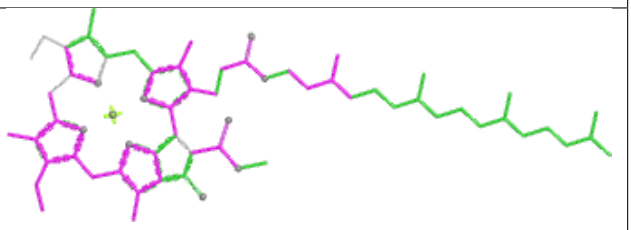
Ligand CLA B 605



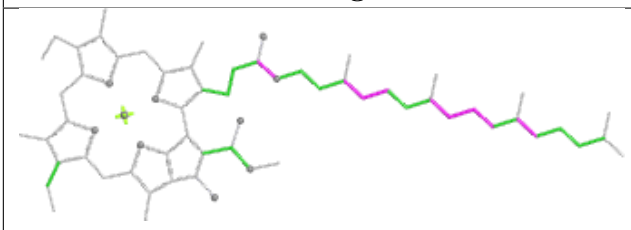
Ligand CLA D 403



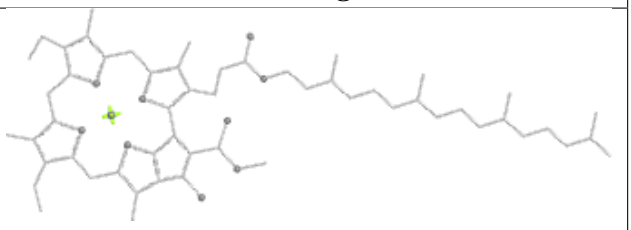
Bond lengths



Bond angles

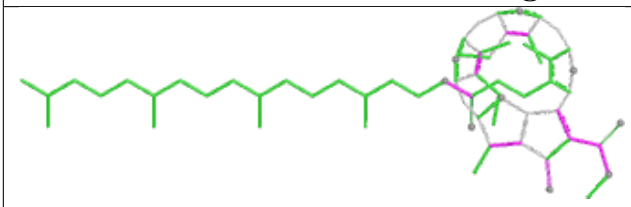


Torsions

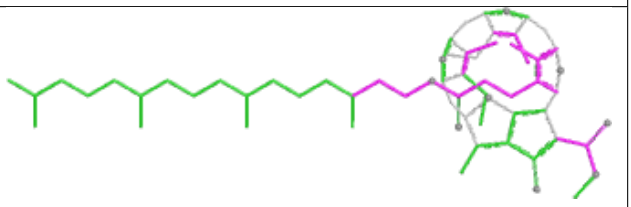


Rings

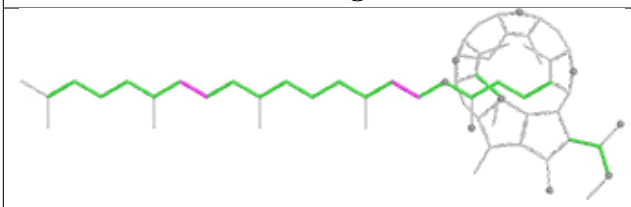
Ligand PHO A 407



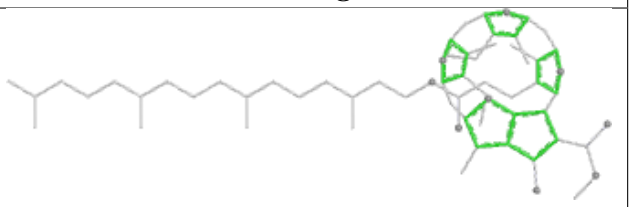
Bond lengths



Bond angles

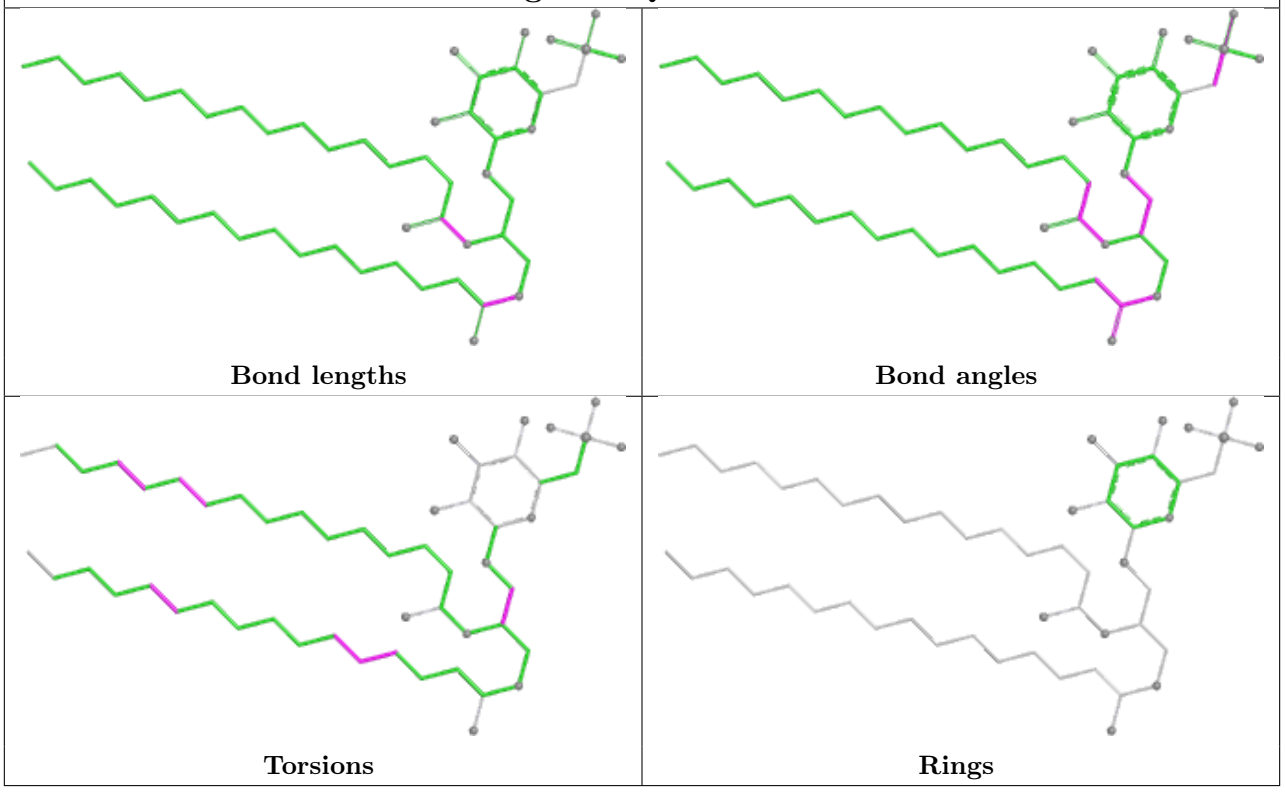


Torsions

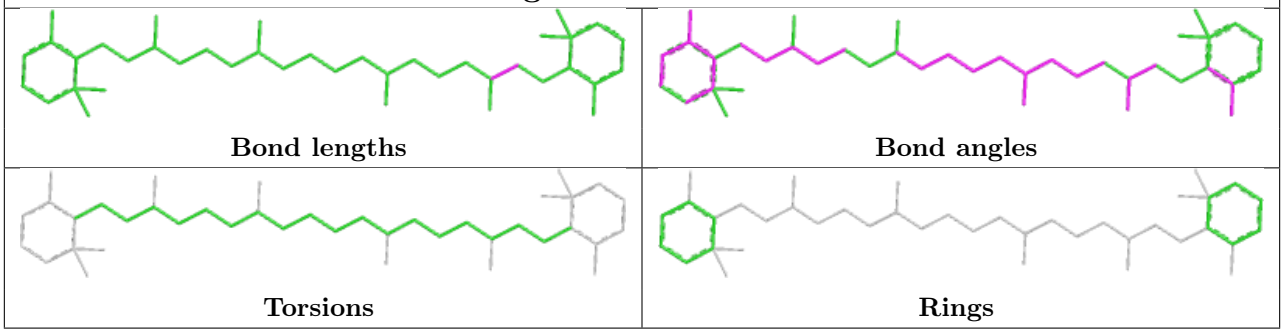


Rings

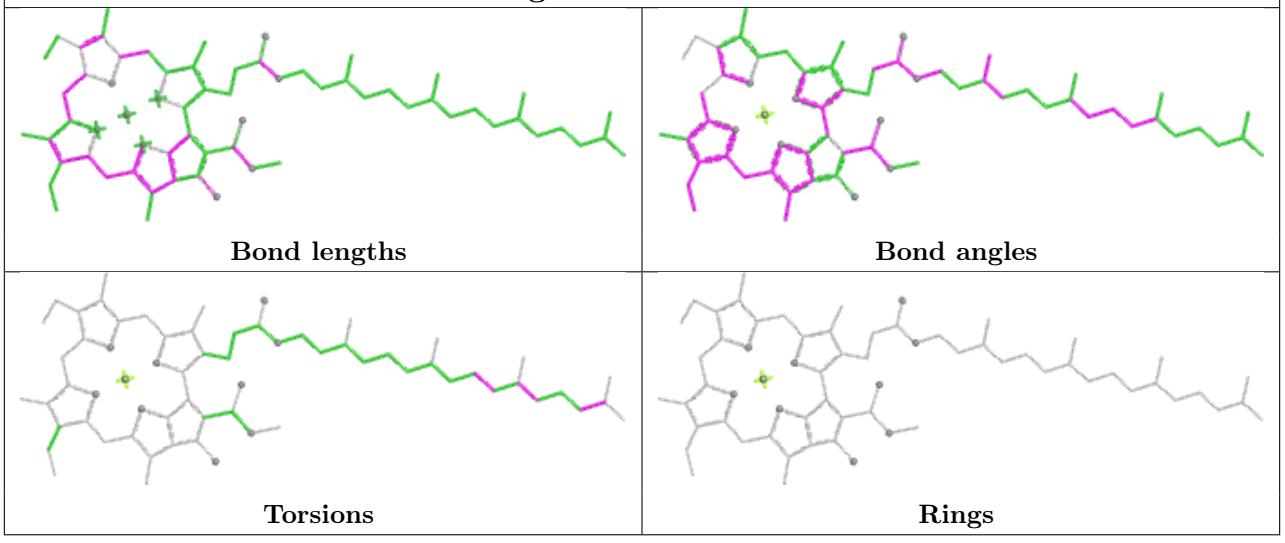
Ligand SQD A 413



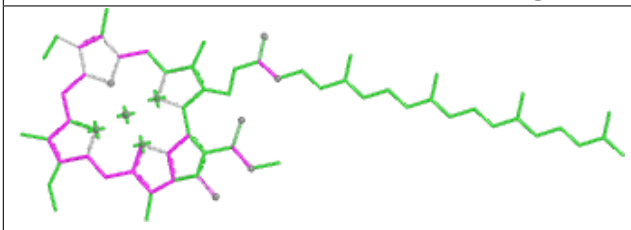
Ligand BCR C 516



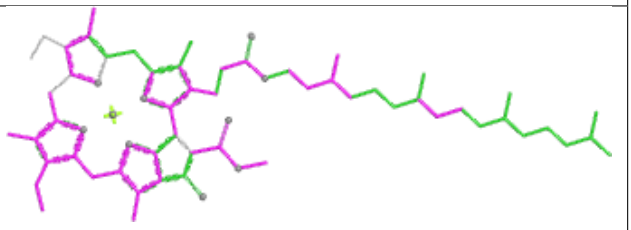
Ligand CLA b 615



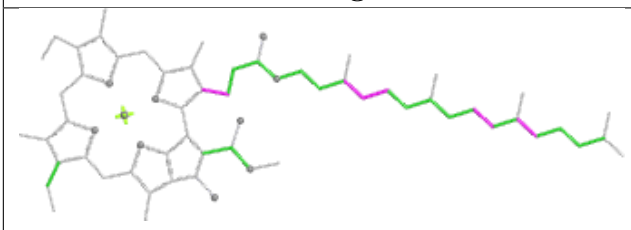
Ligand CLA c 515



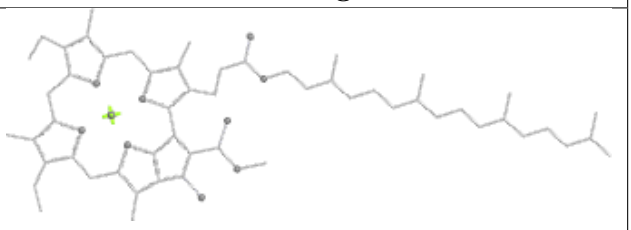
Bond lengths



Bond angles

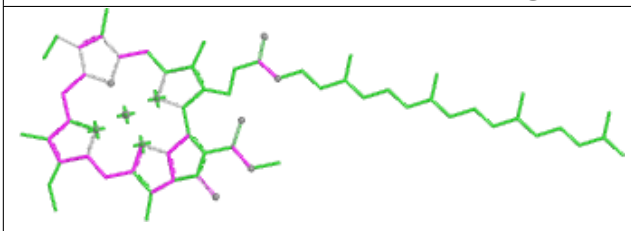


Torsions

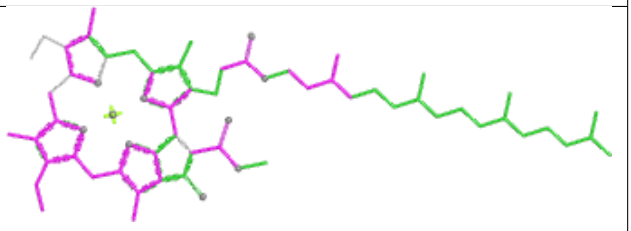


Rings

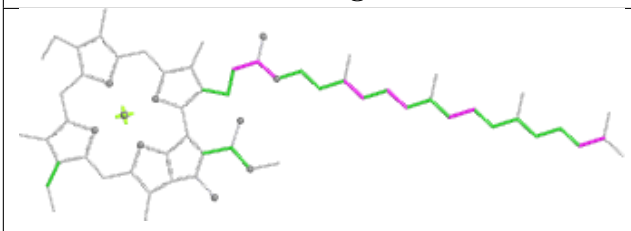
Ligand CLA C 511



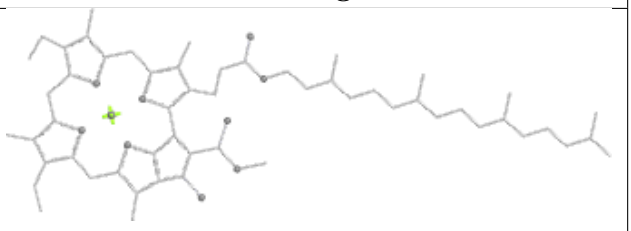
Bond lengths



Bond angles

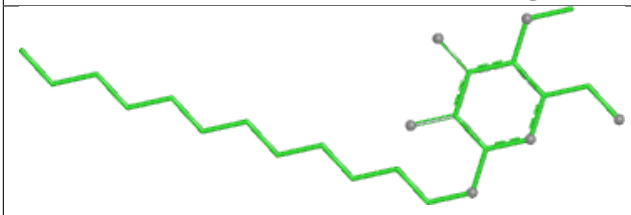


Torsions

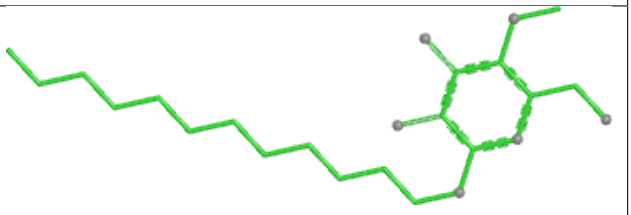


Rings

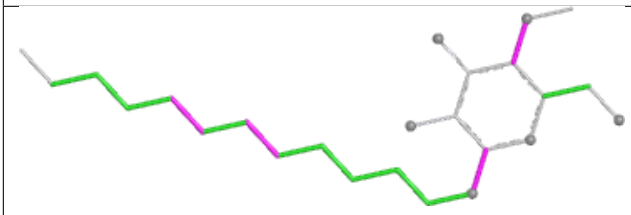
Ligand LMT b 622



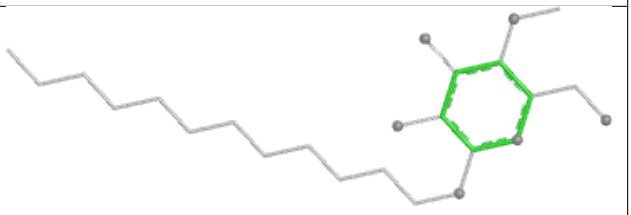
Bond lengths



Bond angles

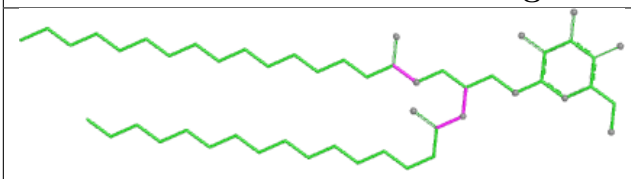


Torsions

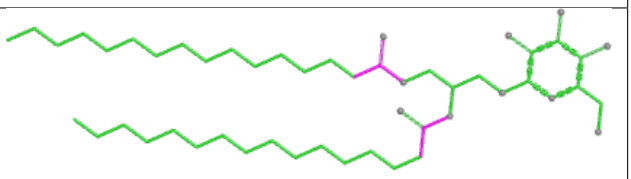


Rings

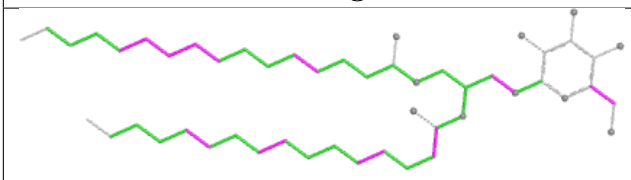
Ligand LMG J 101



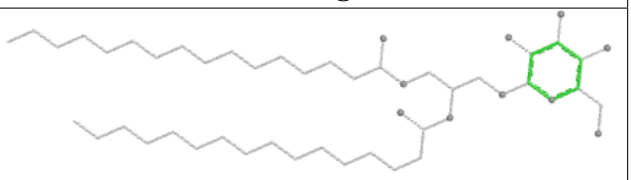
Bond lengths



Bond angles

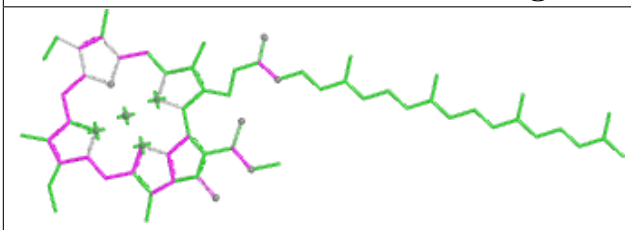


Torsions

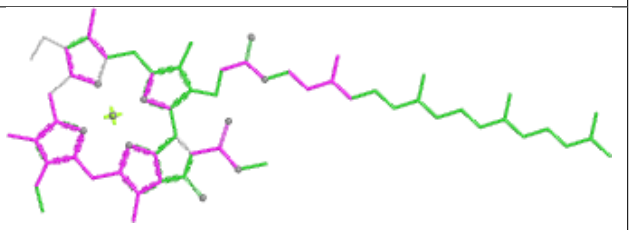


Rings

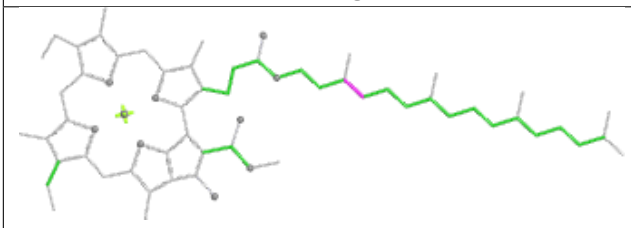
Ligand CLA c 507



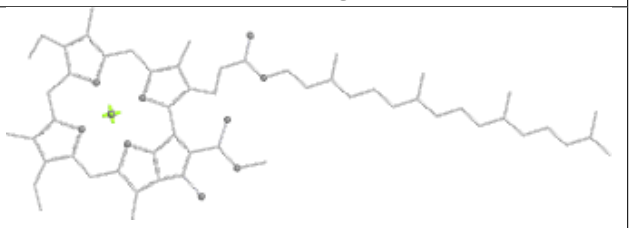
Bond lengths



Bond angles



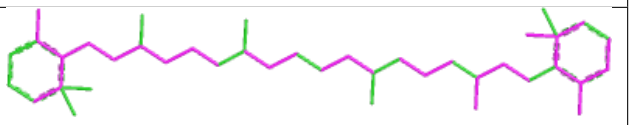
Torsions



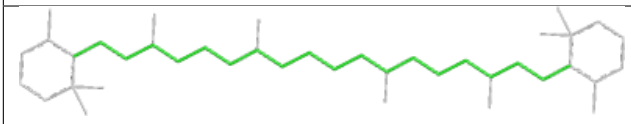
Rings

Ligand BCR b 618

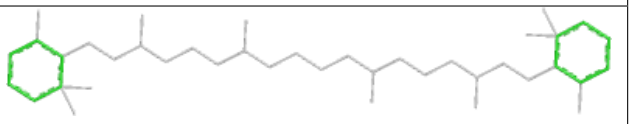
Bond lengths



Bond angles

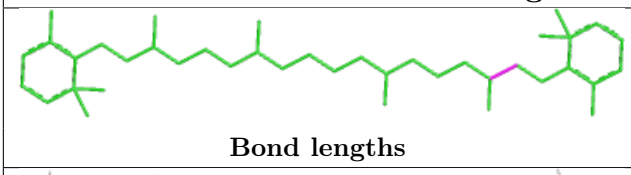


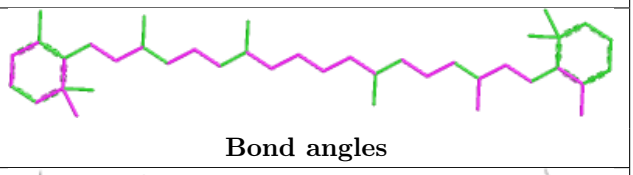
Torsions

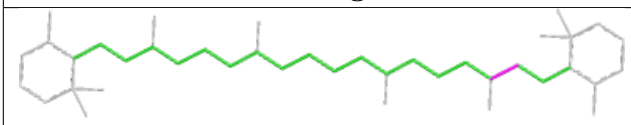


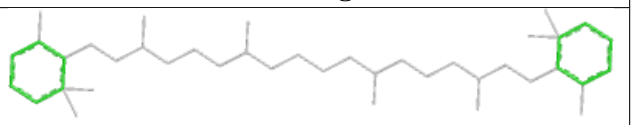
Rings

Ligand BCR b 619

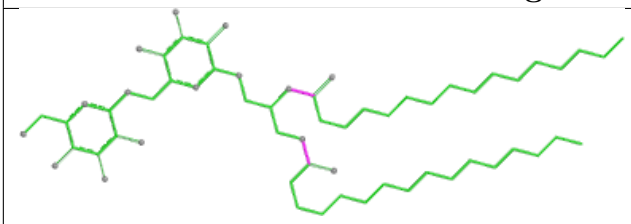

Bond lengths

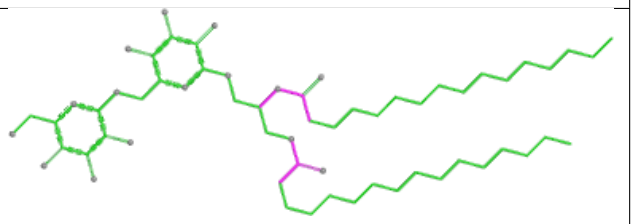

Bond angles

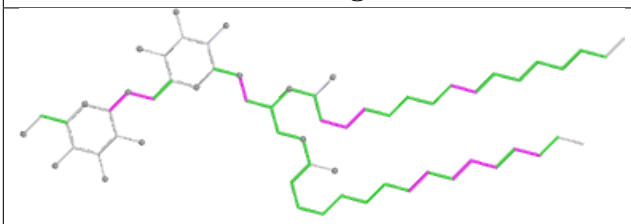

Torsions

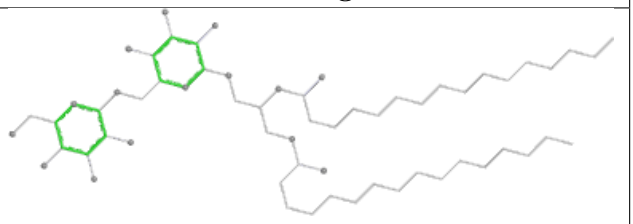

Rings

Ligand DGD c 519

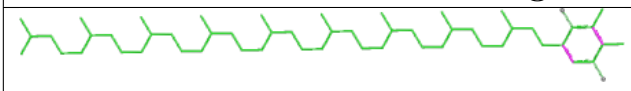

Bond lengths

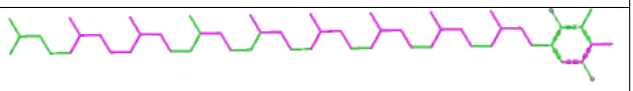

Bond angles

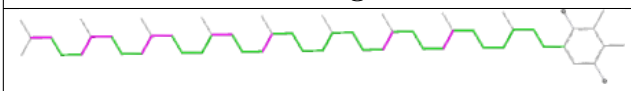

Torsions


Rings

Ligand PL9 D 405


Bond lengths


Bond angles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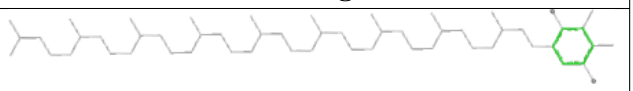
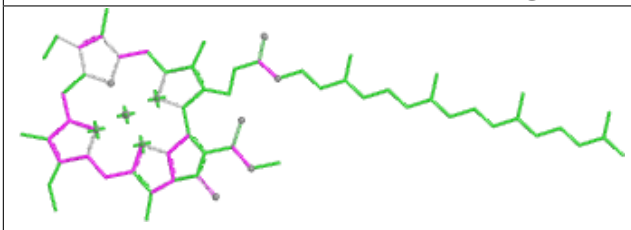

Rings

Ligand CLA D 402



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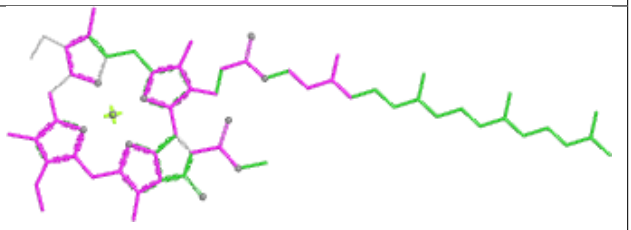

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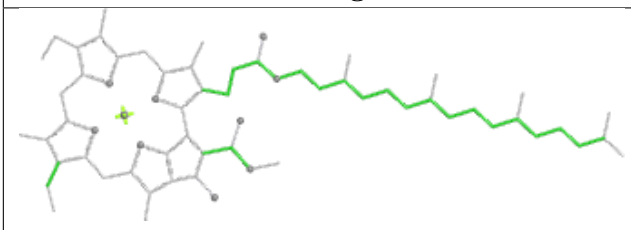

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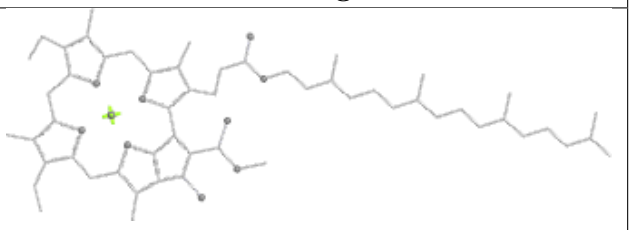
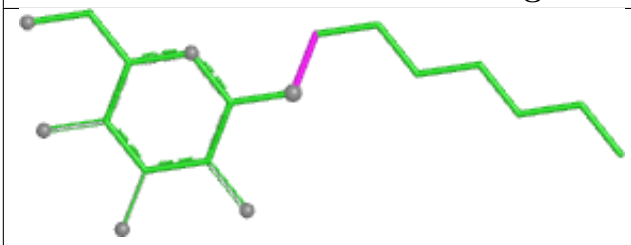
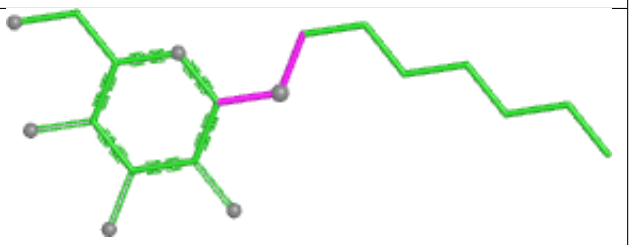


Rings

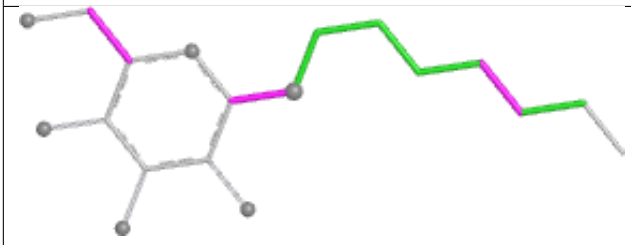
Ligand HTG b 624



Bond lengths



Bond angles



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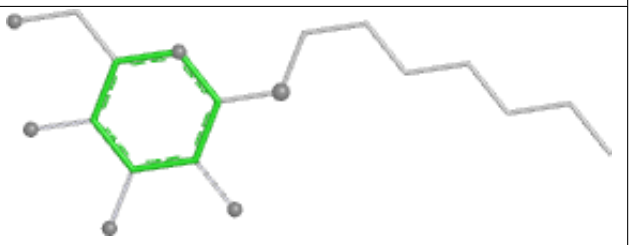
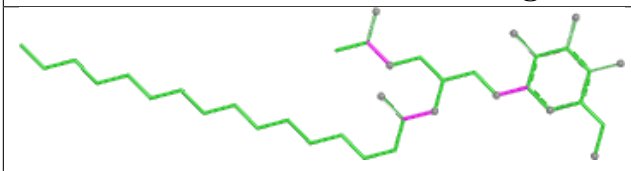


Rings

Ligand LMG Z 101



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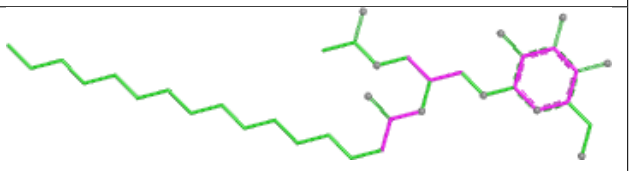
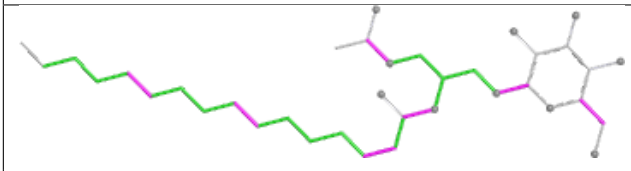


Bond angles



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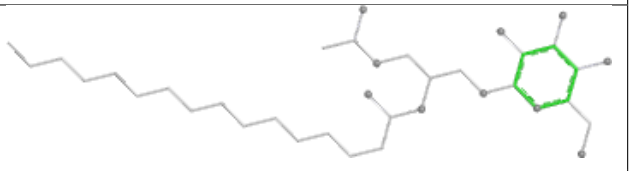
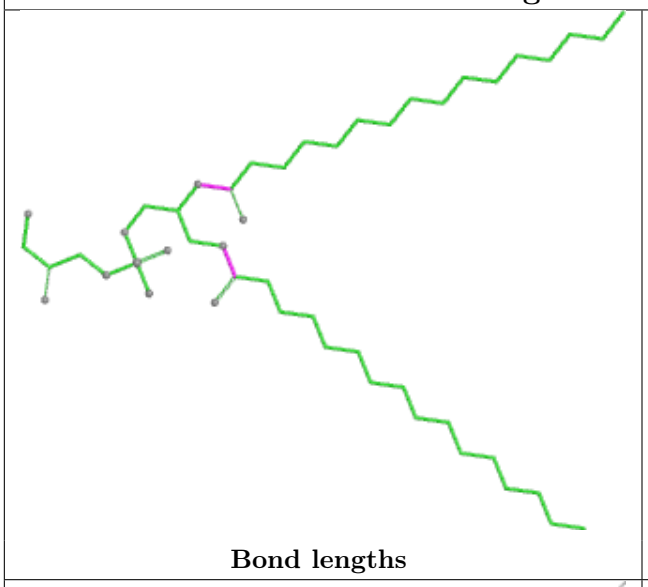


Rings

Ligand LHG D 357



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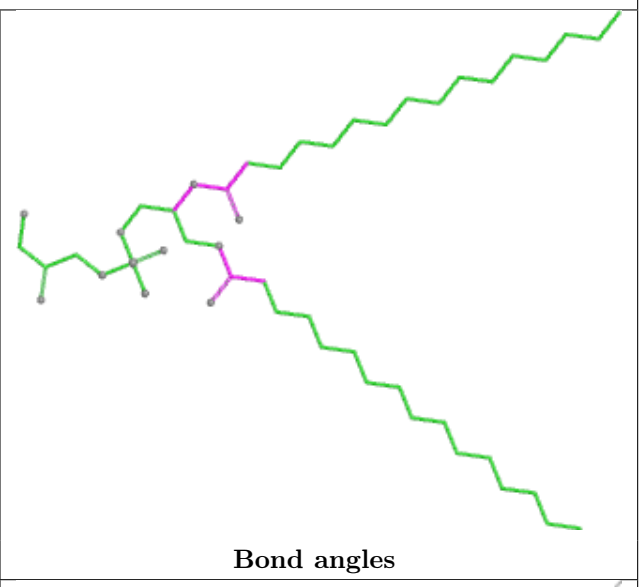
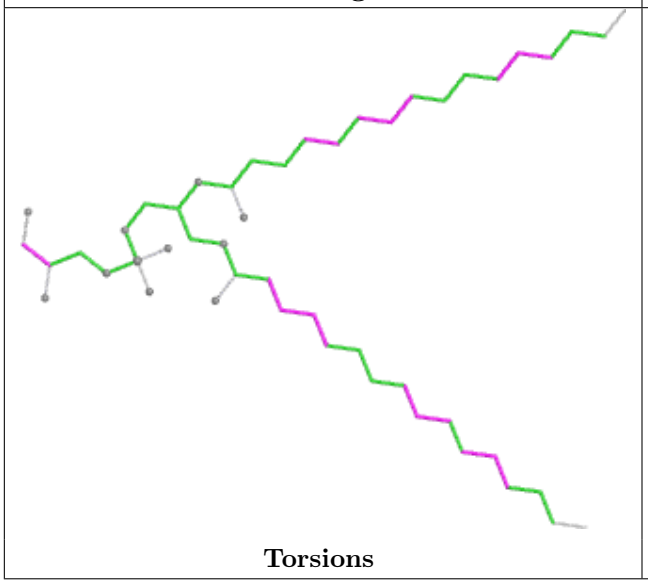


Bond angles



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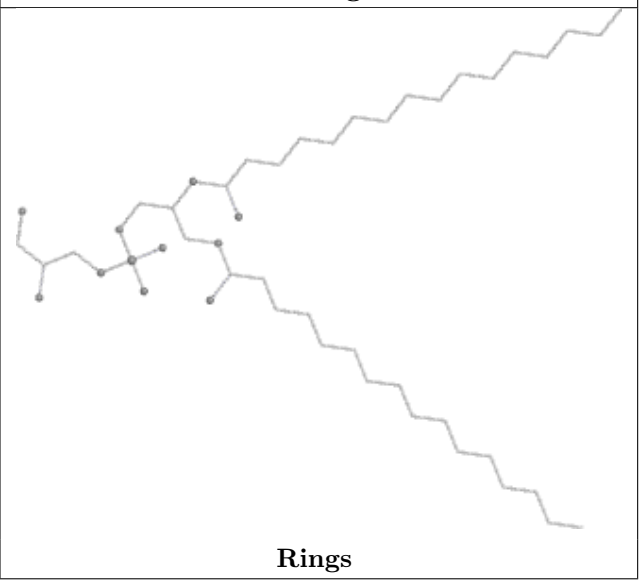
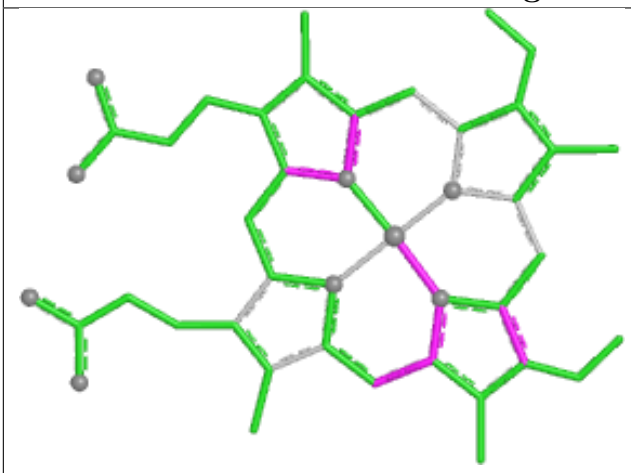


Rings

Ligand HEM e 102



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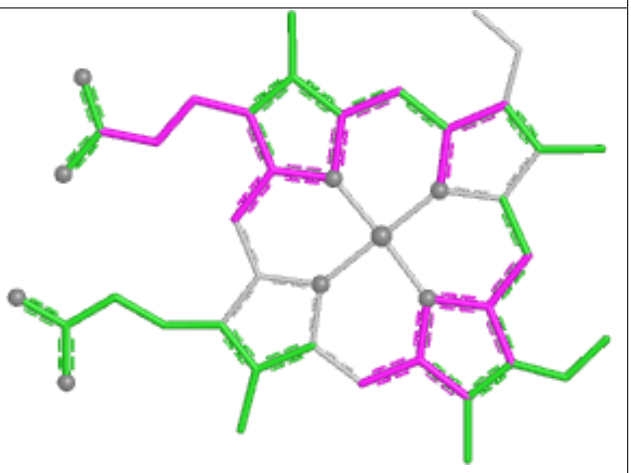
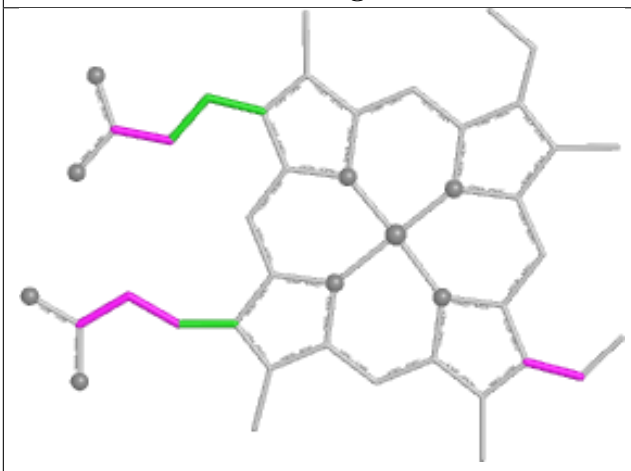


Bond angles



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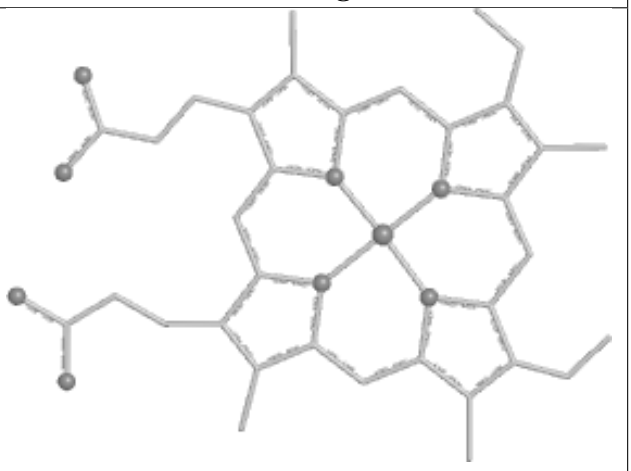
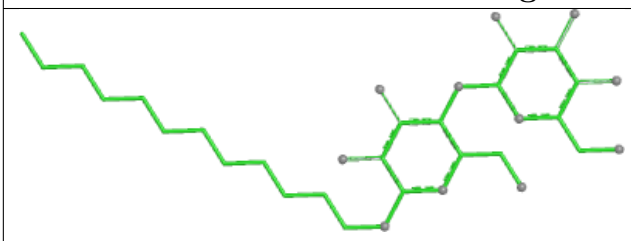
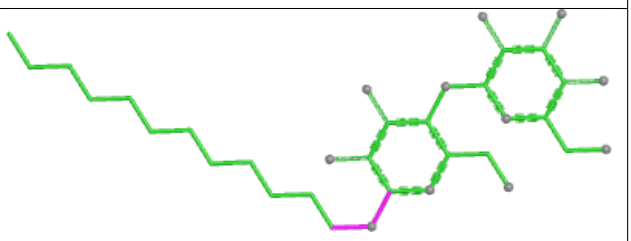


Rings

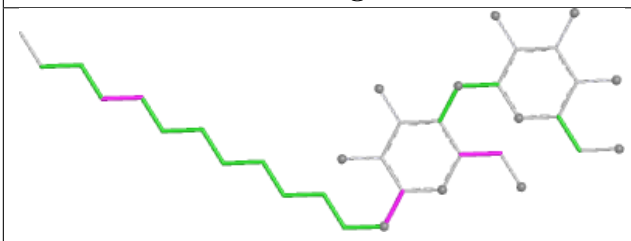
Ligand LMT m 102



Bond lengths



Bond angles



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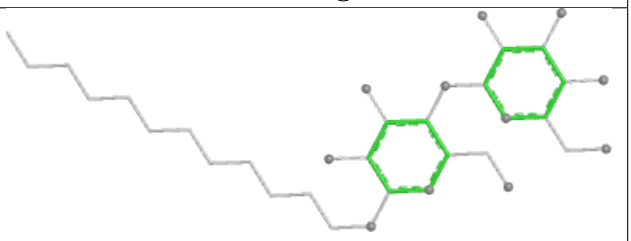
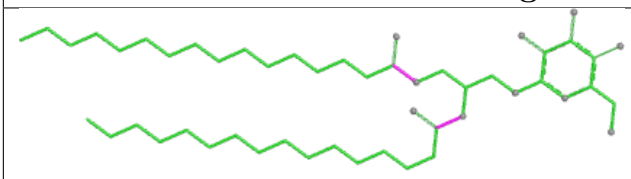


Rings

Ligand LMG C 520



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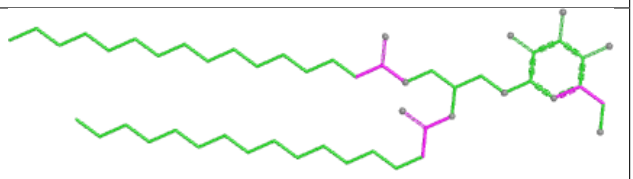
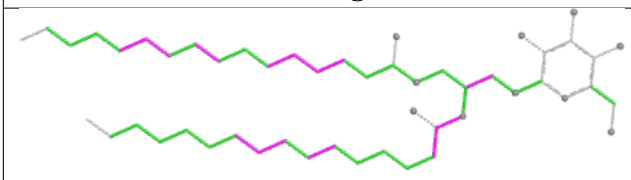
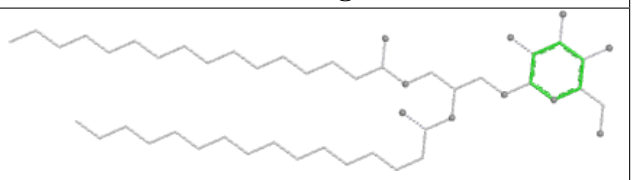


Bond angles

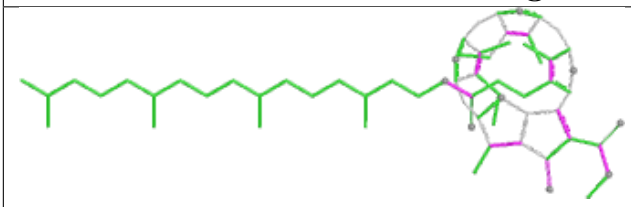


Torsions



Rings

Ligand PHO a 406



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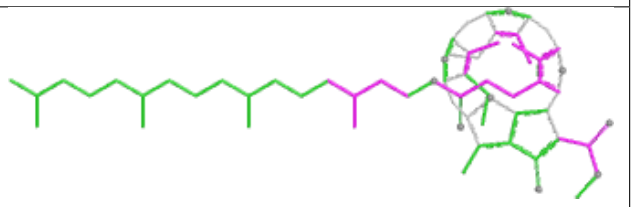
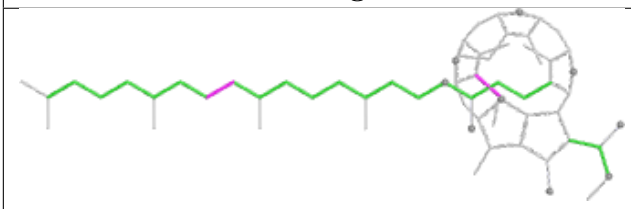
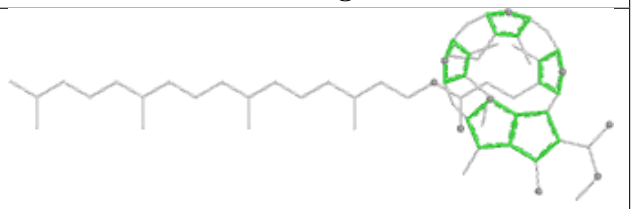


Bond angles

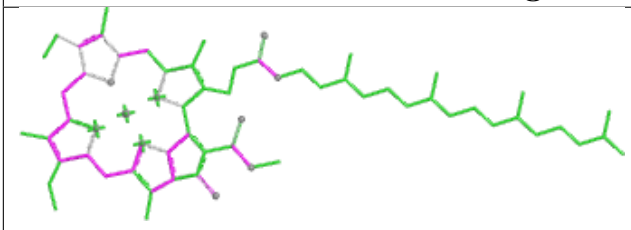


Torsions



Rings

Ligand CLA C 508



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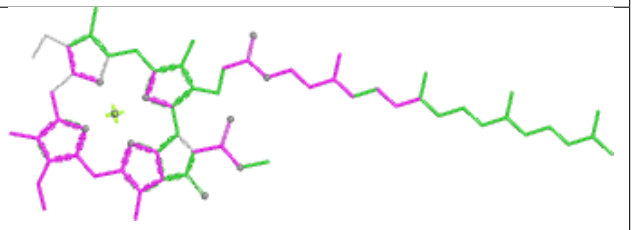
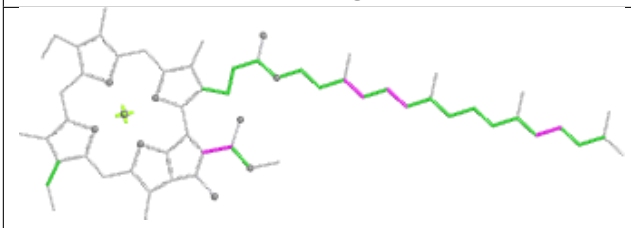
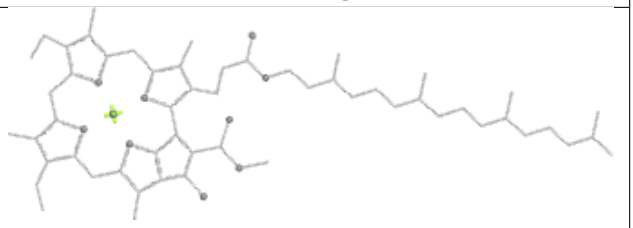


Bond angles

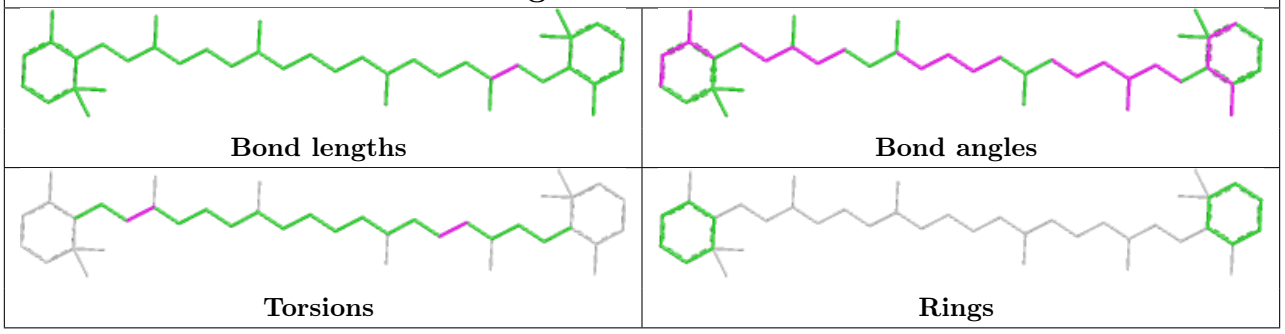


Torsions

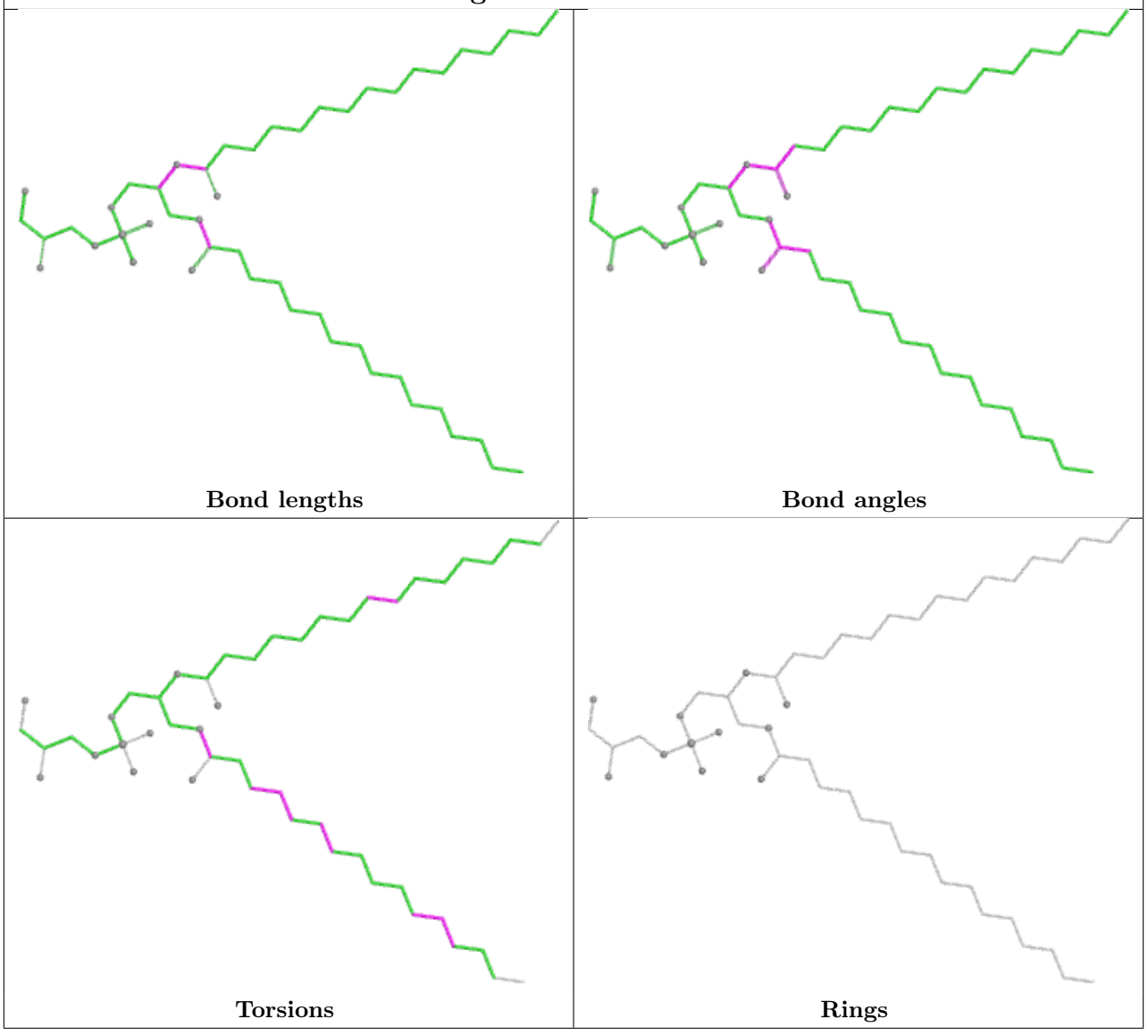


Rings

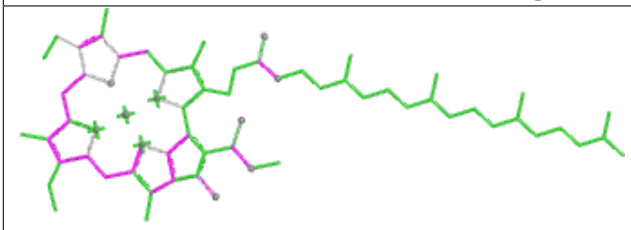
Ligand BCR c 517



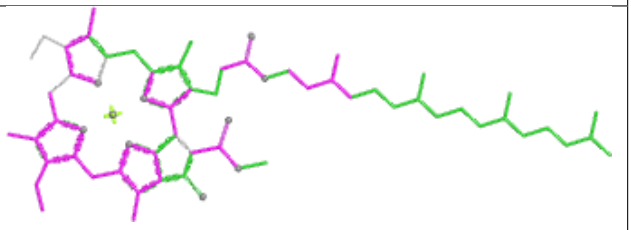
Ligand LHG d 406



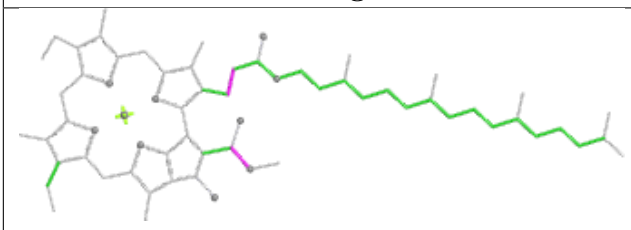
Ligand CLA c 503



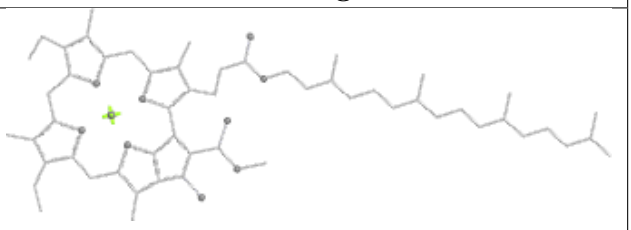
Bond lengths



Bond angles

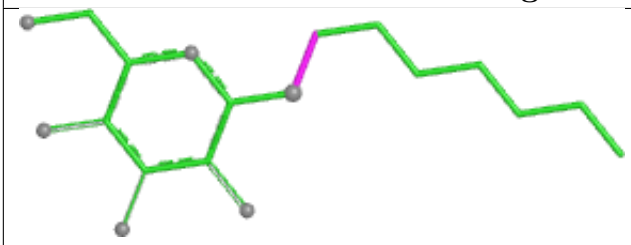


Torsions

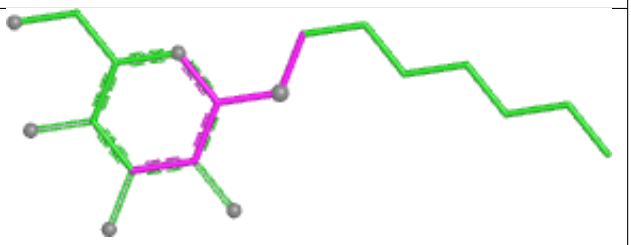


Rings

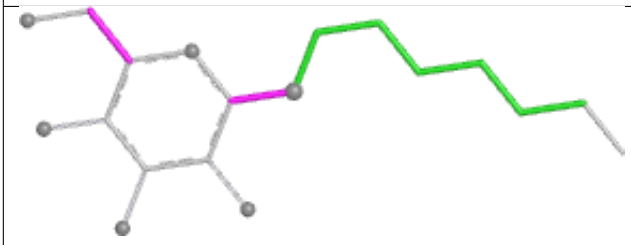
Ligand HTG B 625



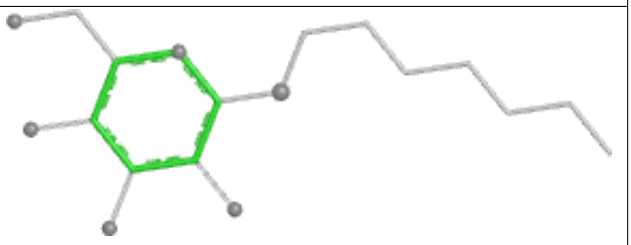
Bond lengths



Bond angles

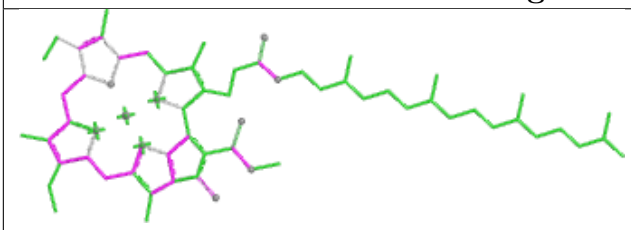


Torsions

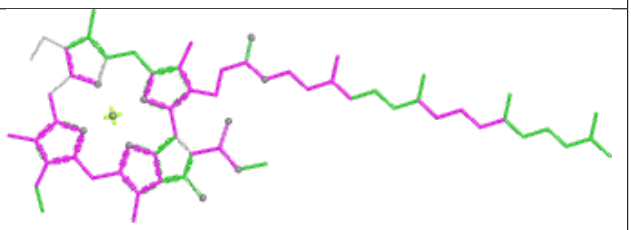


Rings

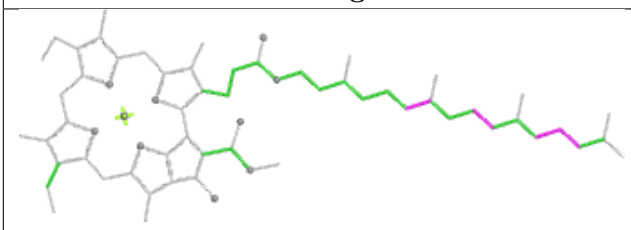
Ligand CLA b 602



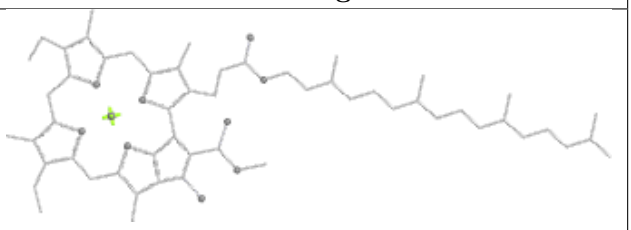
Bond lengths



Bond angles

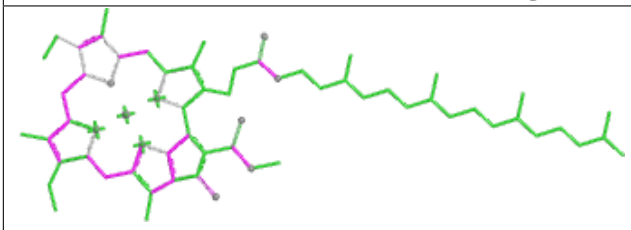


Torsions

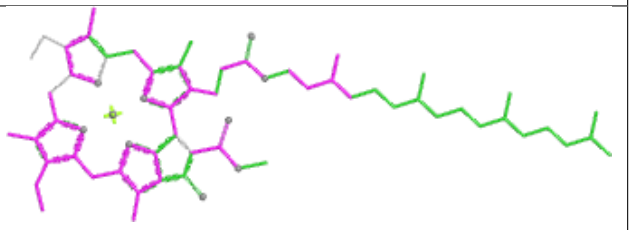


Rings

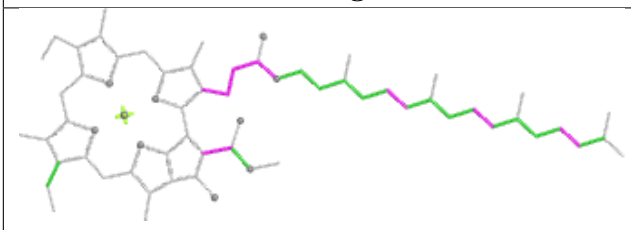
Ligand CLA B 601



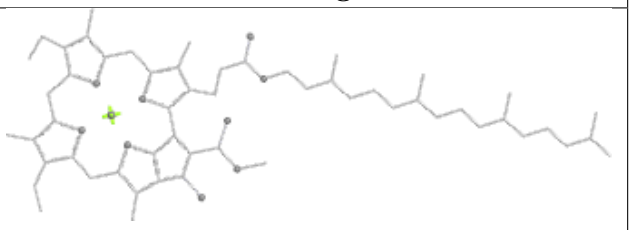
Bond lengths



Bond angles

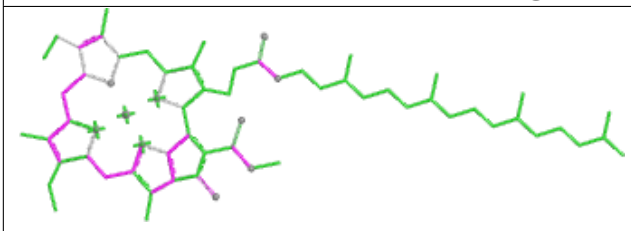


Torsions

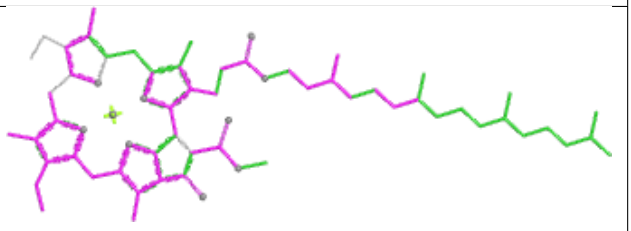


Rings

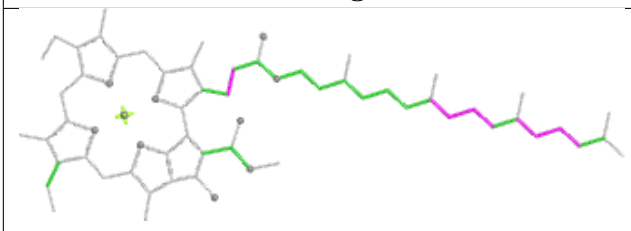
Ligand CLA b 606



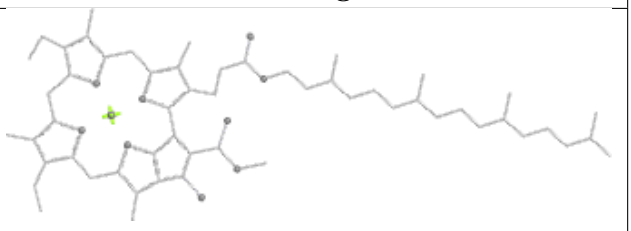
Bond lengths



Bond angles

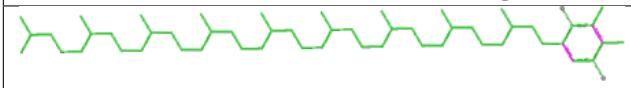


Torsions

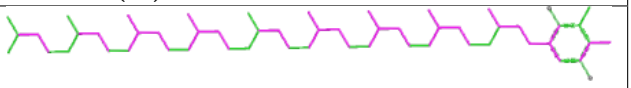


Rings

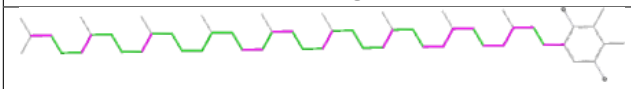
Ligand PL9 A 416 (B)



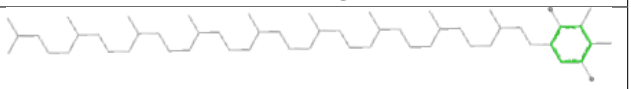
Bond lengths



Bond angles

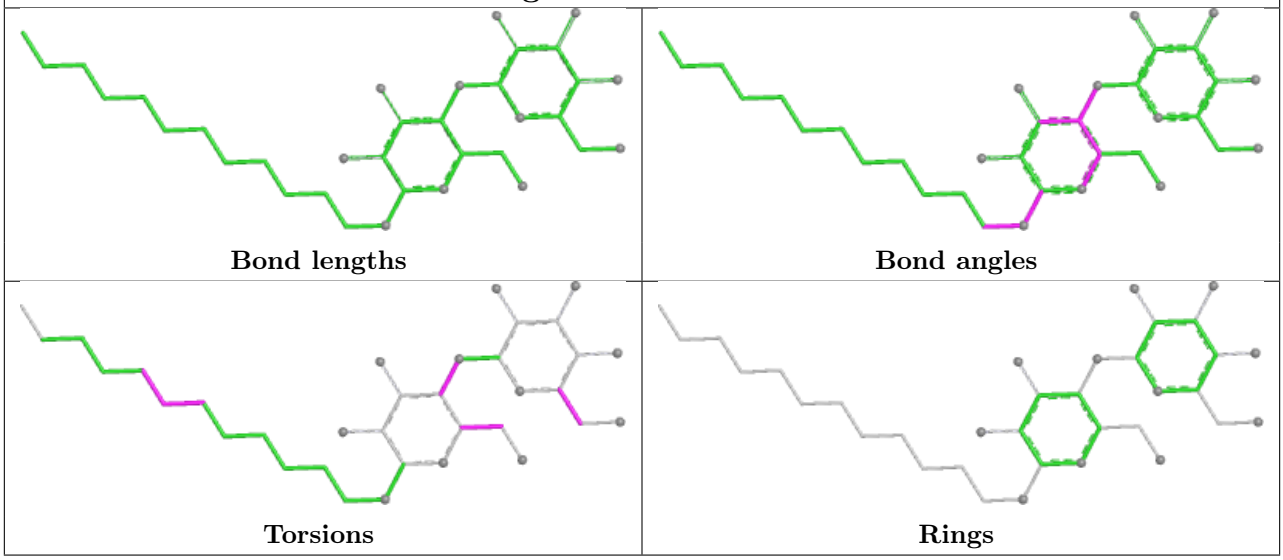


Torsions

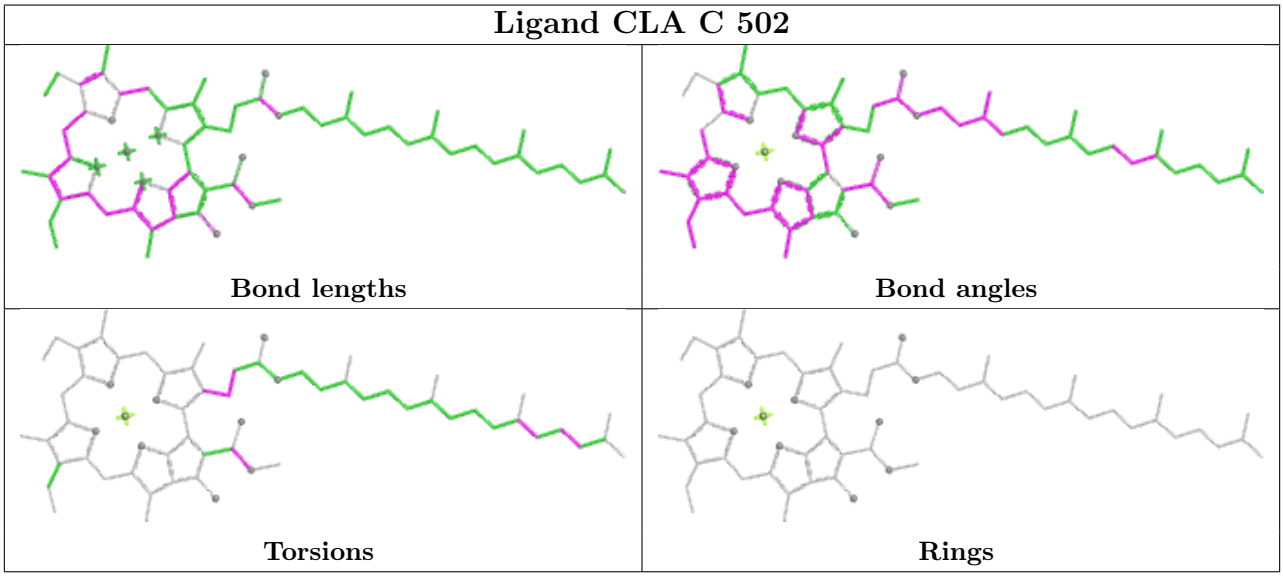


Rings

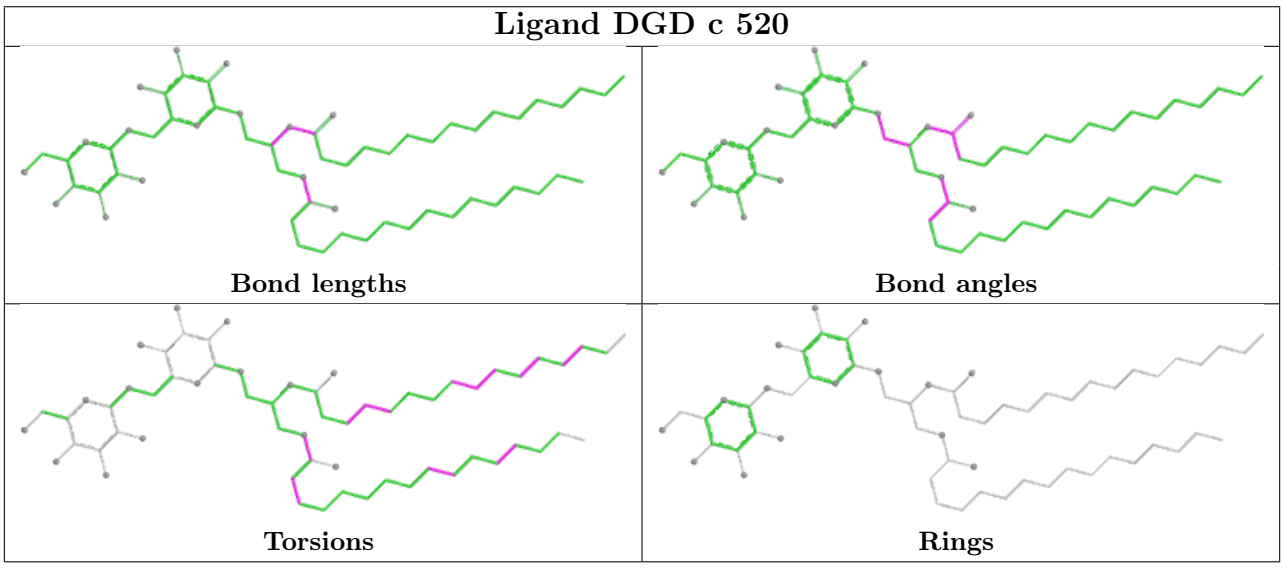
Ligand LMT B 622



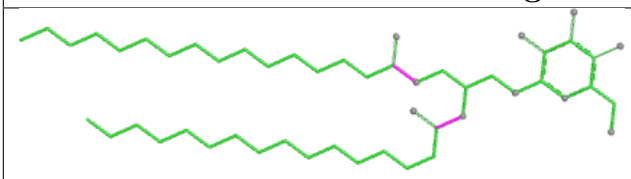
Ligand CLA C 502



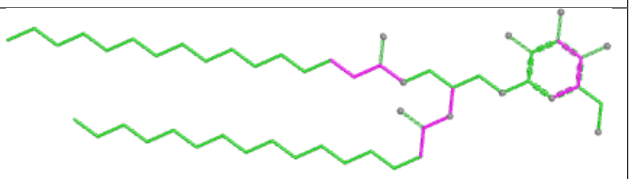
Ligand DGD c 520



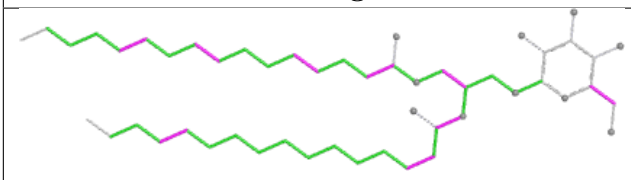
Ligand LMG a 417



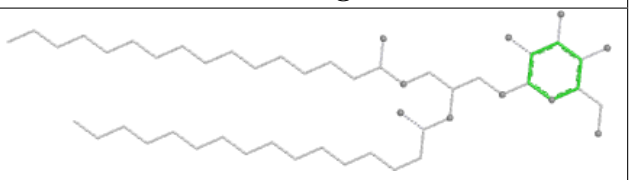
Bond lengths



Bond angles

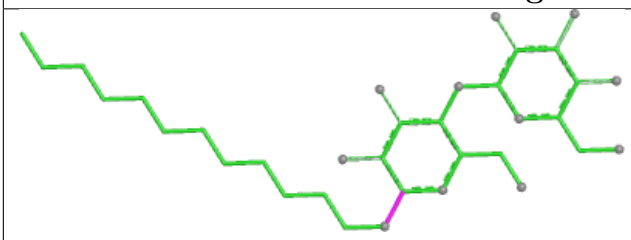


Torsions

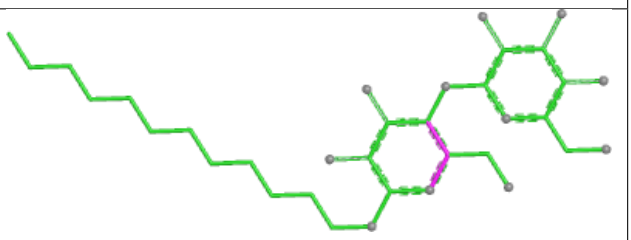


Rings

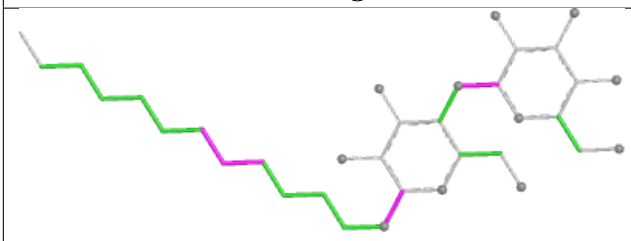
Ligand LMT e 101



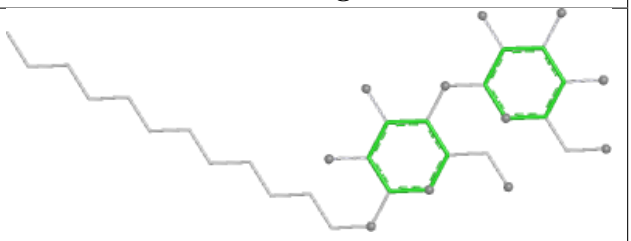
Bond lengths



Bond angles

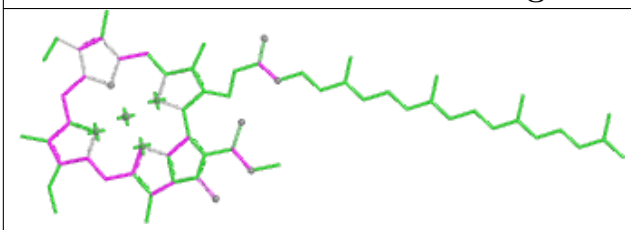


Torsions

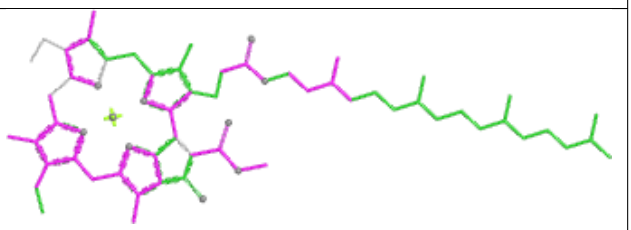


Rings

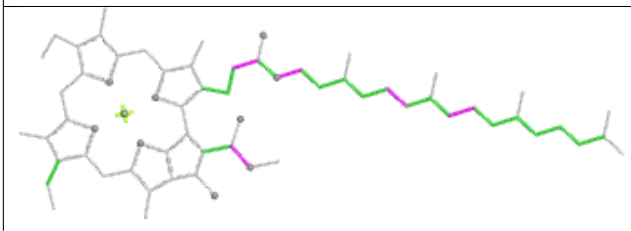
Ligand CLA b 613



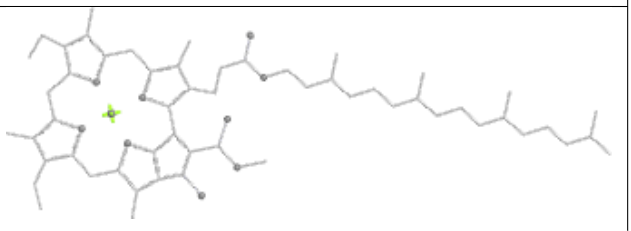
Bond lengths



Bond angles

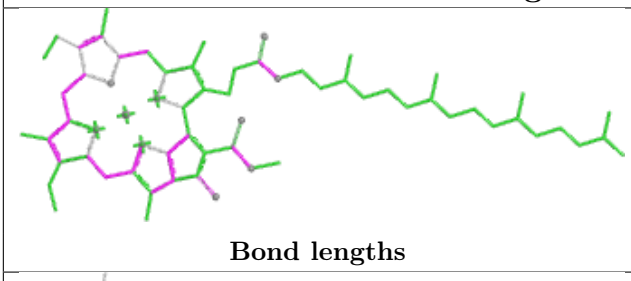


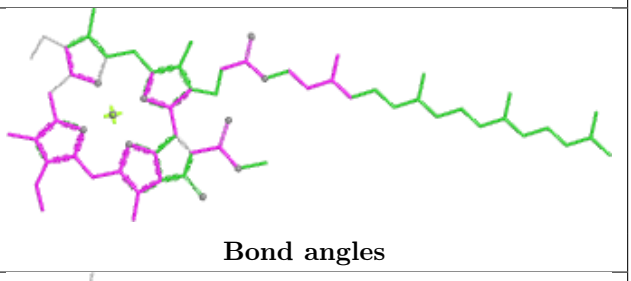
Torsions

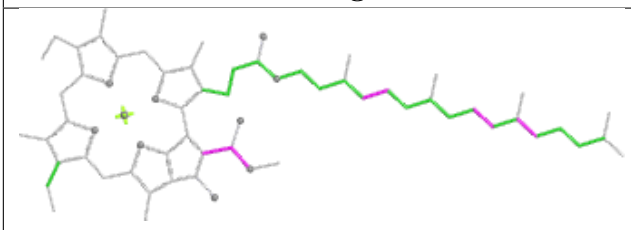


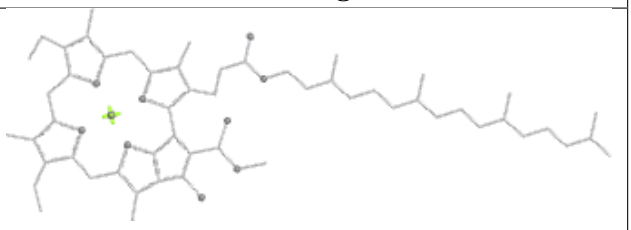
Rings

Ligand CLA C 503

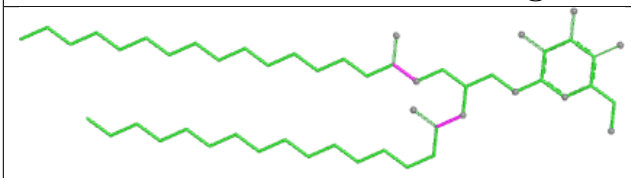

Bond lengths

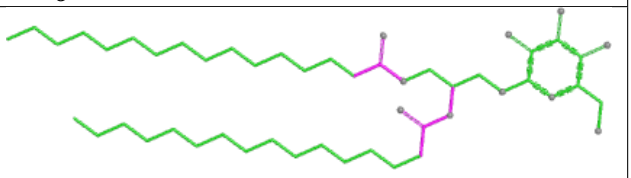

Bond angles

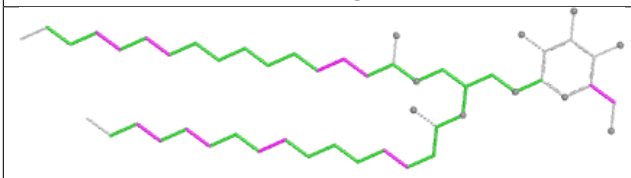

Torsions

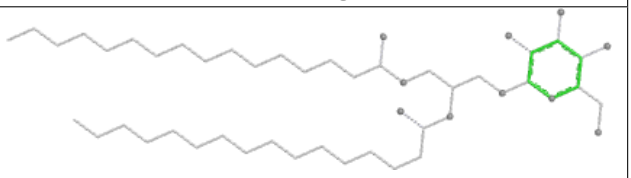

Rings

Ligand LMG j 101

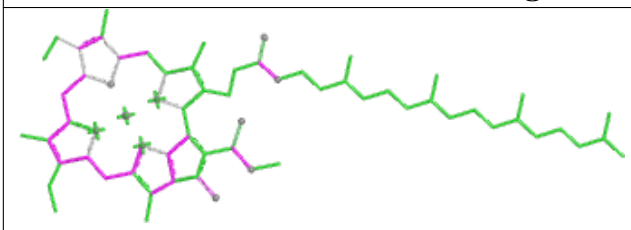

Bond lengths

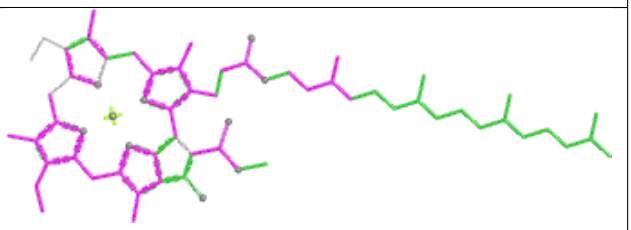

Bond angles

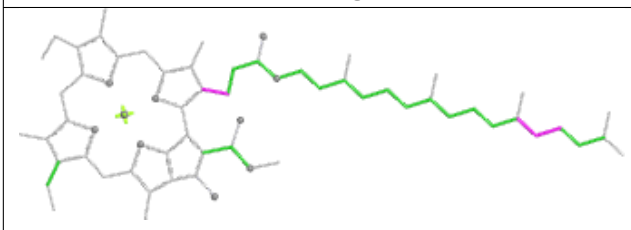

Torsions

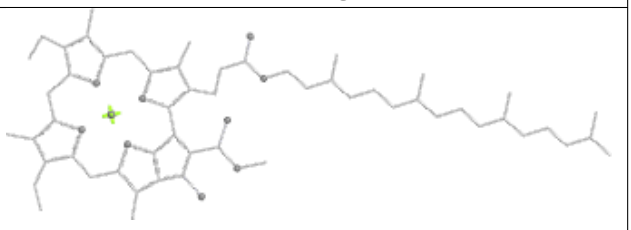

Rings

Ligand CLA A 406

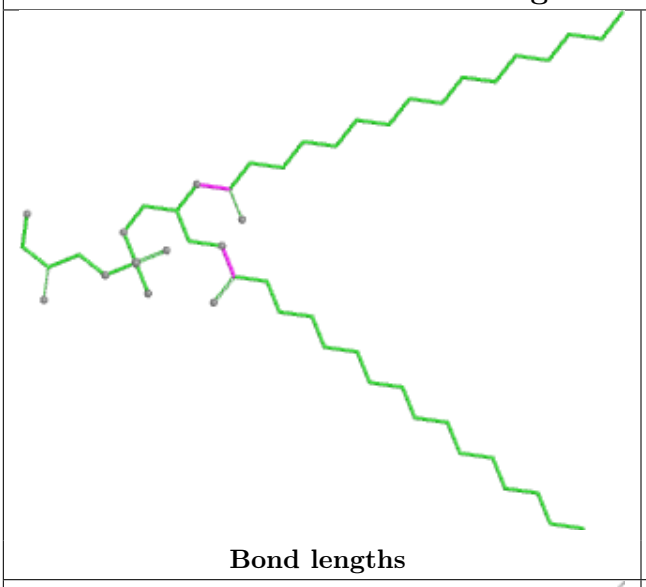

Bond lengths


Bond angles

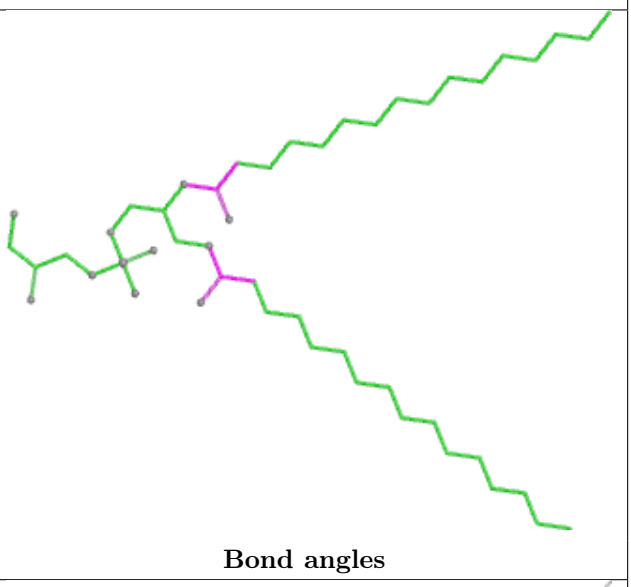

Torsions


Rings

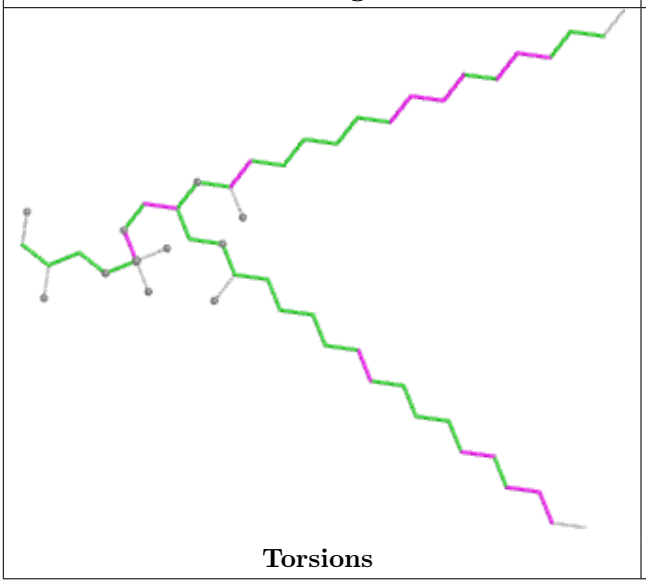
Ligand LHG l 101



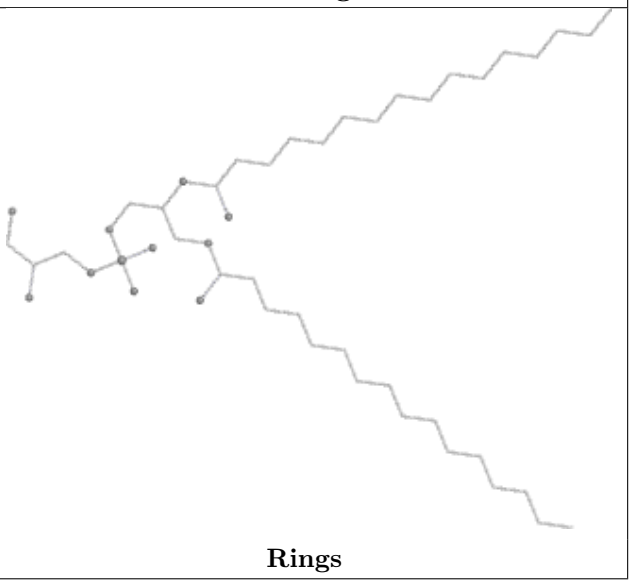
Bond lengths



Bond angles



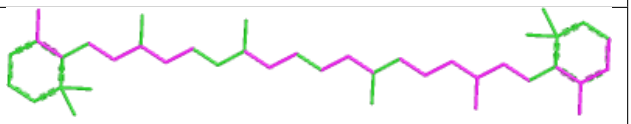
Torsions



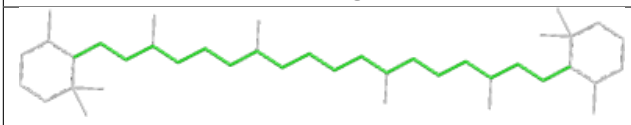
Rings

Ligand BCR c 516

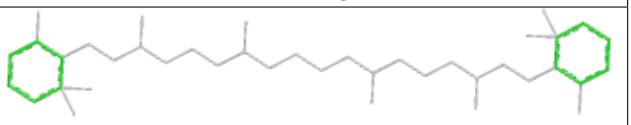
Bond lengths



Bond angles

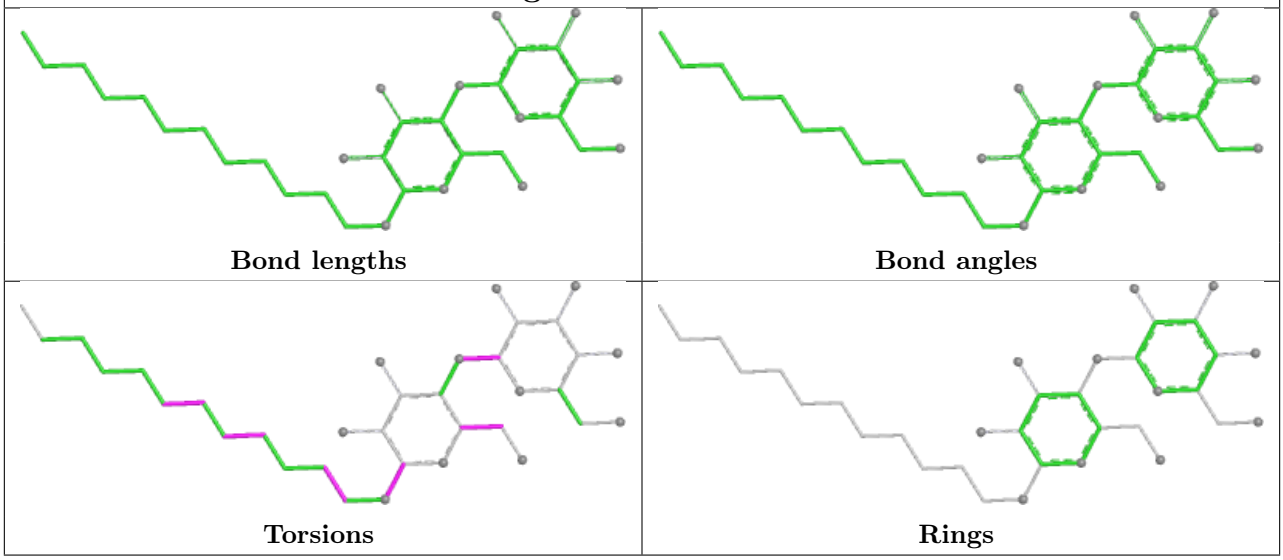


Torsions

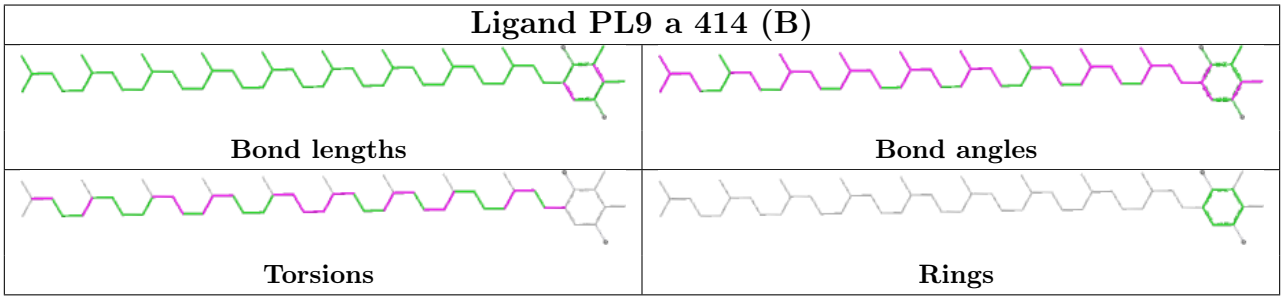


Rings

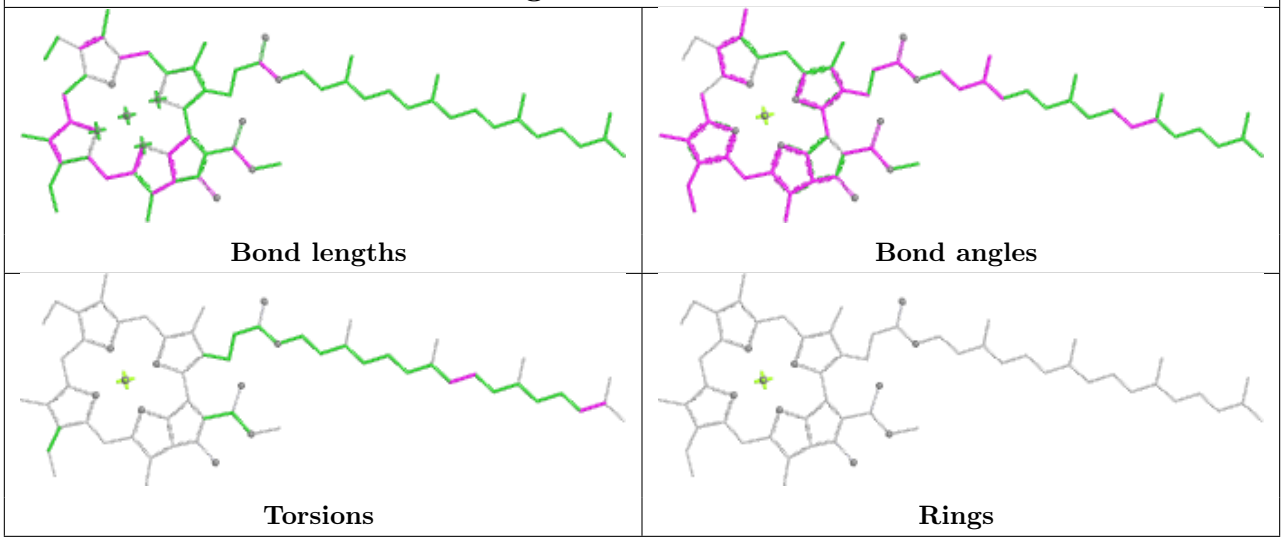
Ligand LMT E 102



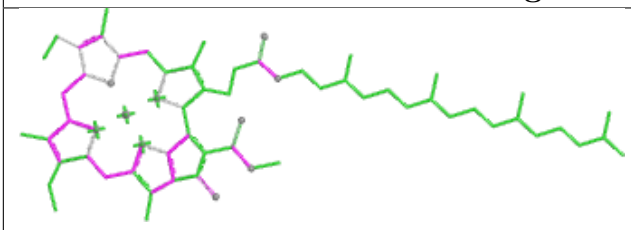
Ligand PL9 a 414 (B)



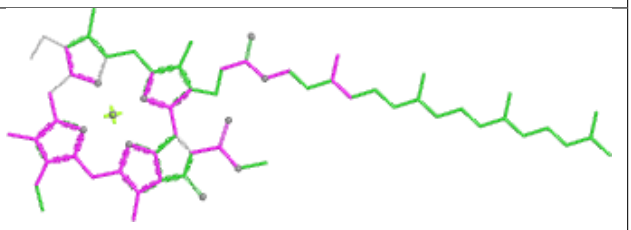
Ligand CLA B 611



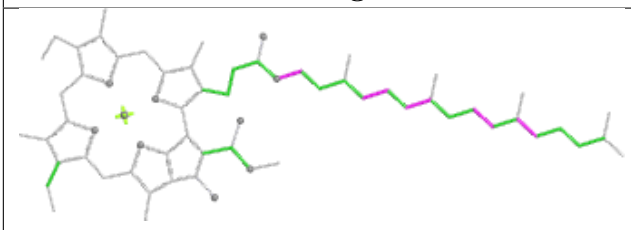
Ligand CLA B 616



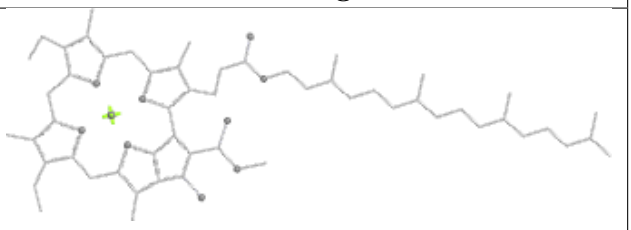
Bond lengths



Bond angles

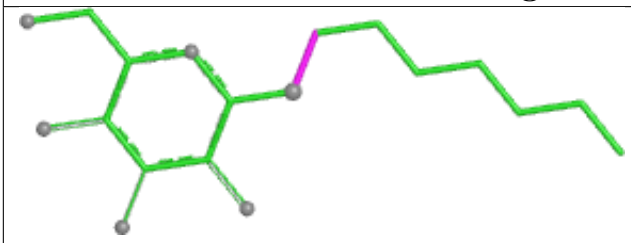


Torsions

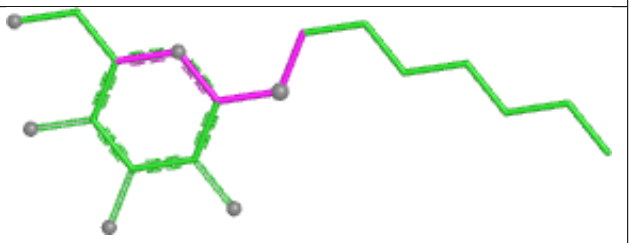


Rings

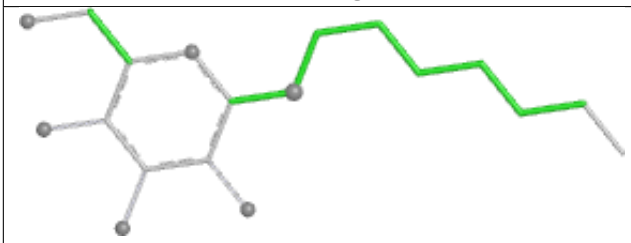
Ligand HTG C 522



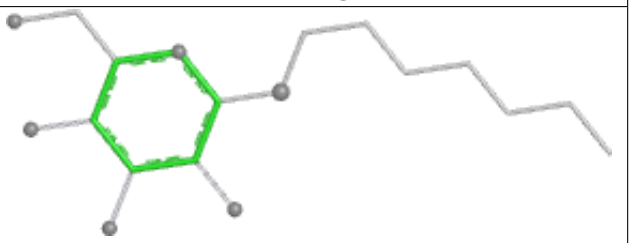
Bond lengths



Bond angles

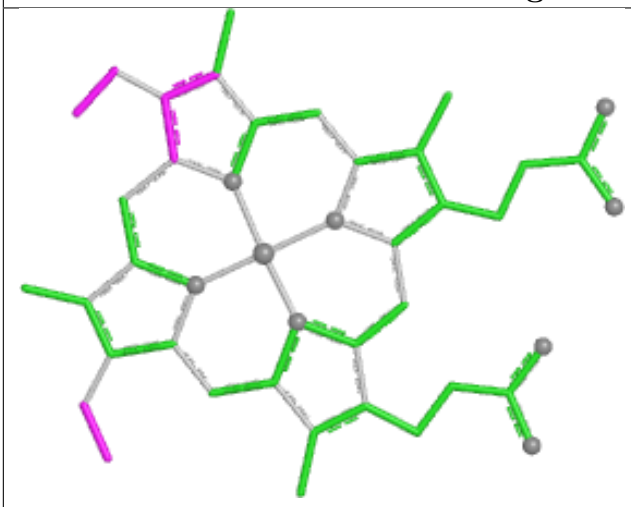


Torsions

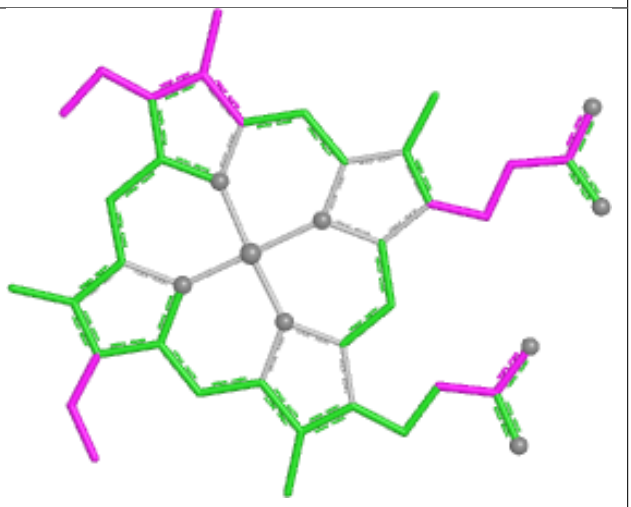


Rings

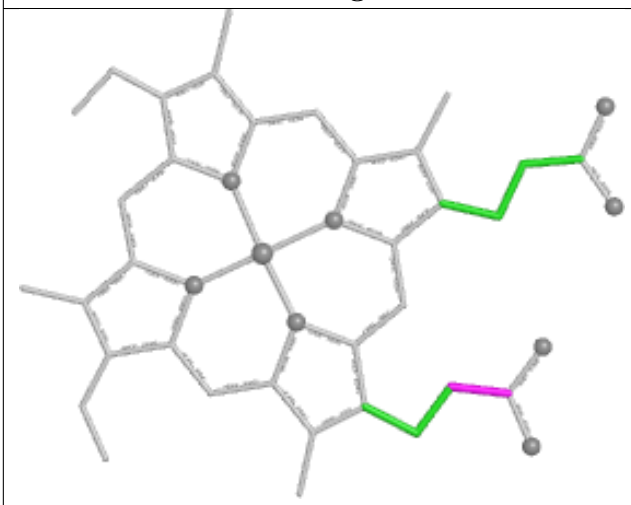
Ligand HEC v 203



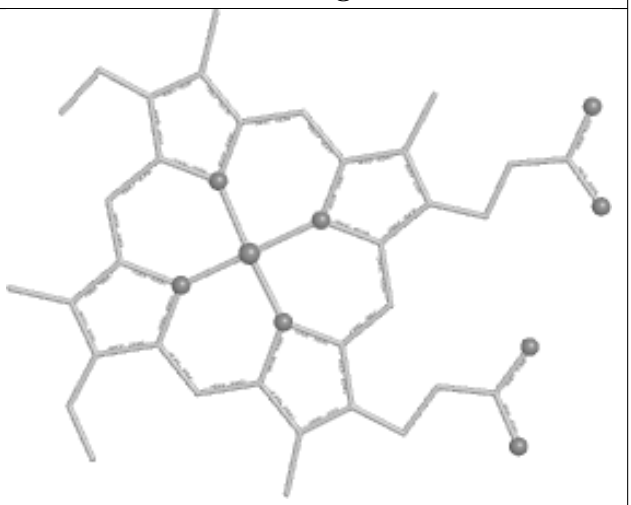
Bond lengths



Bond angles

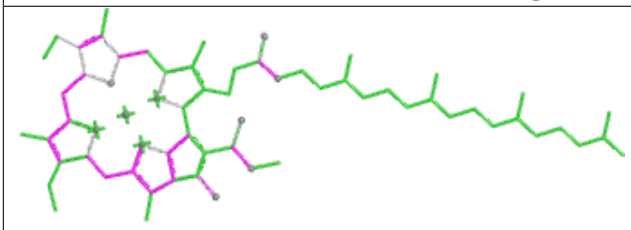


Torsions

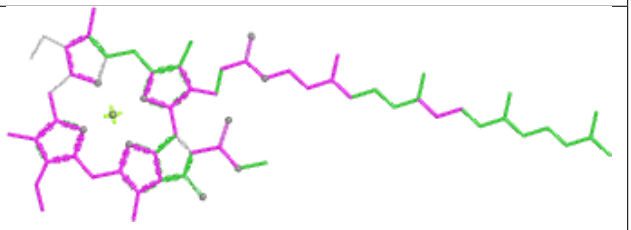


Rings

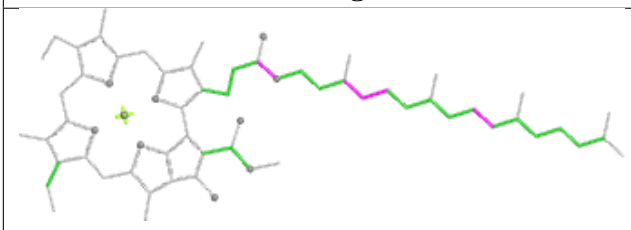
Ligand CLA d 403



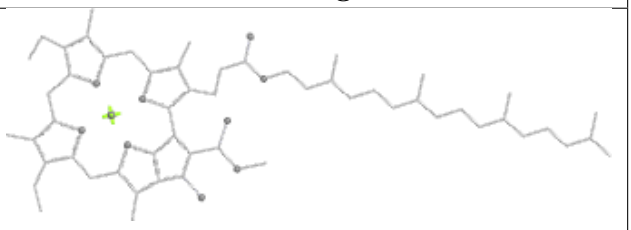
Bond lengths



Bond angles

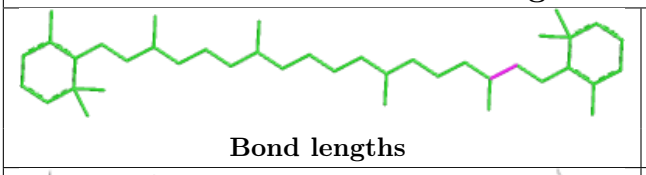


Torsions

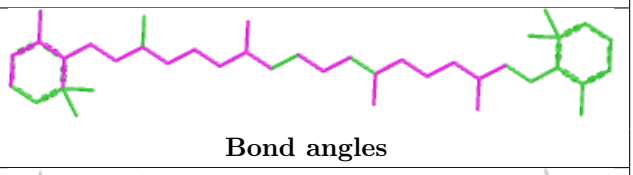


Rings

Ligand BCR t 102

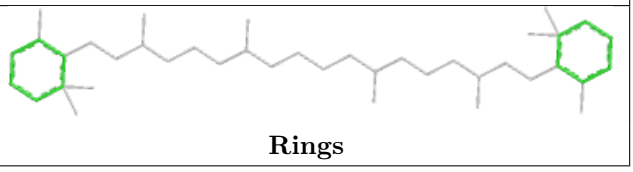


Bond lengths



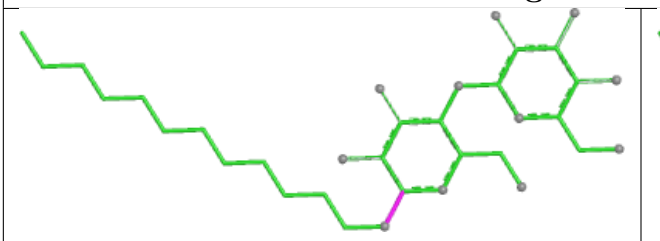
Bond angles

Torsions

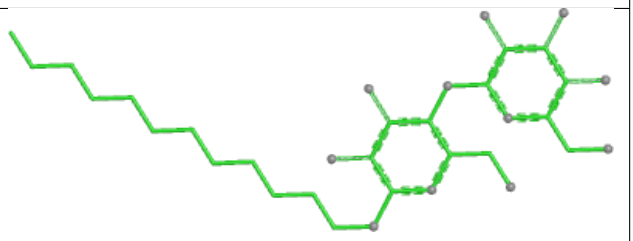


Rings

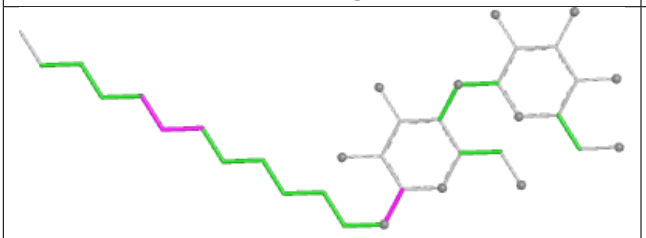
Ligand LMT a 418



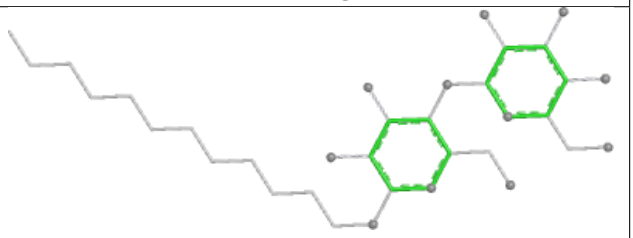
Bond lengths



Bond angles

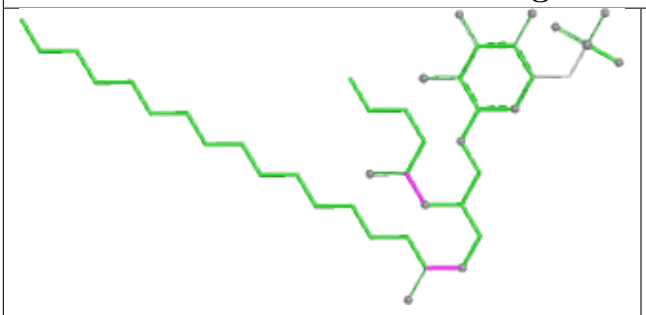


Torsions

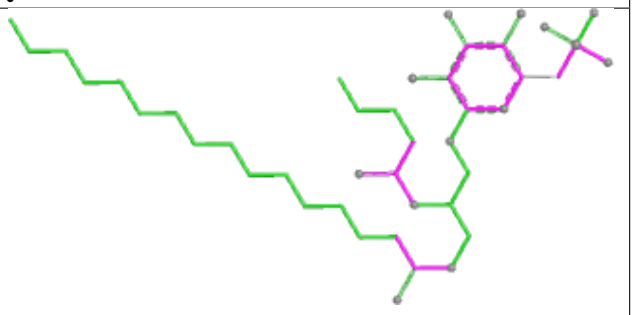


Rings

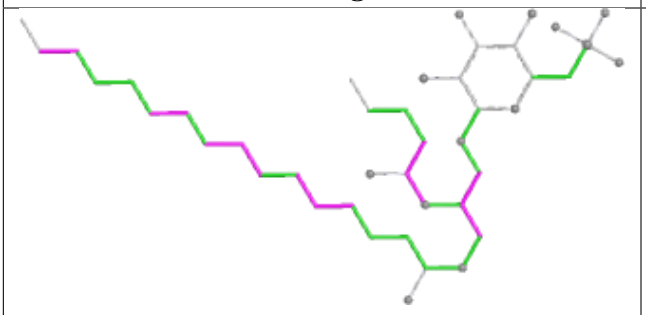
Ligand SQD f 101



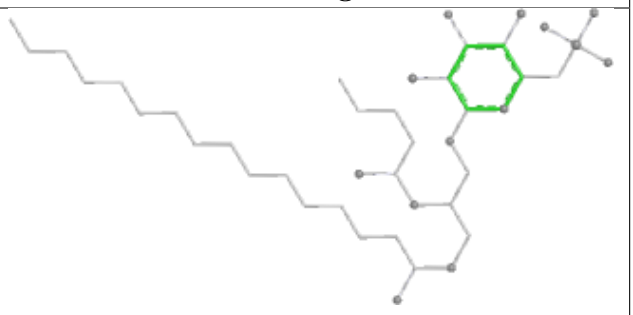
Bond lengths



Bond angles

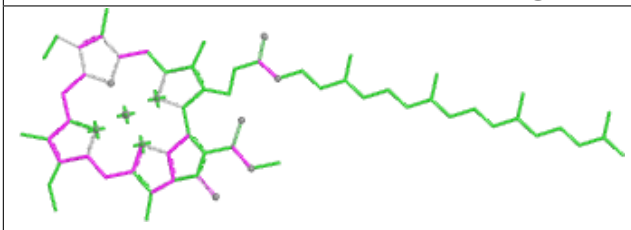


Torsions

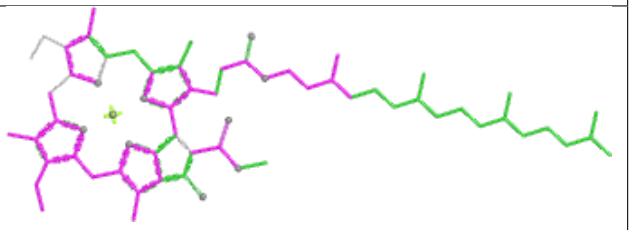


Rings

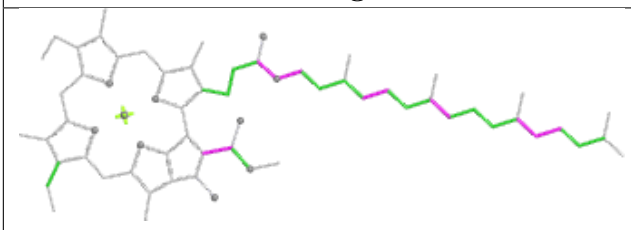
Ligand CLA c 511



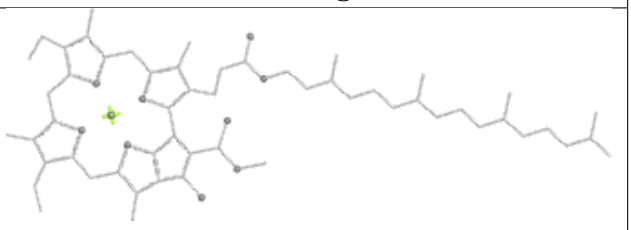
Bond lengths



Bond angles

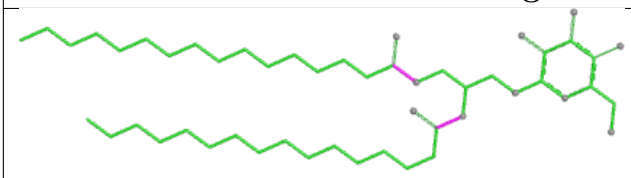


Torsions

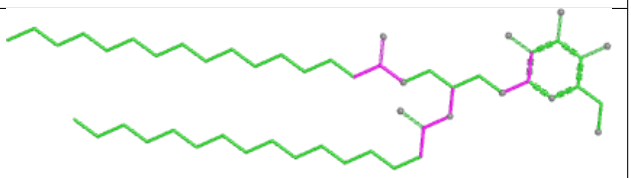


Rings

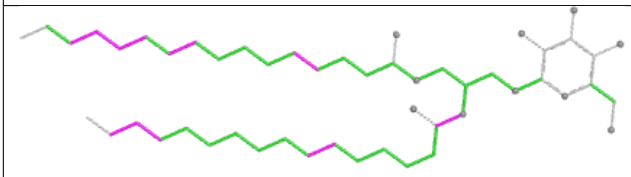
Ligand LMG b 621



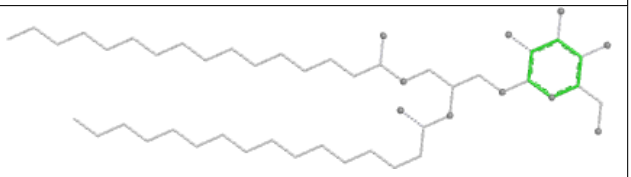
Bond lengths



Bond angles

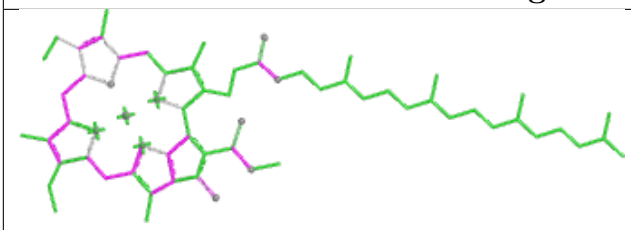


Torsions

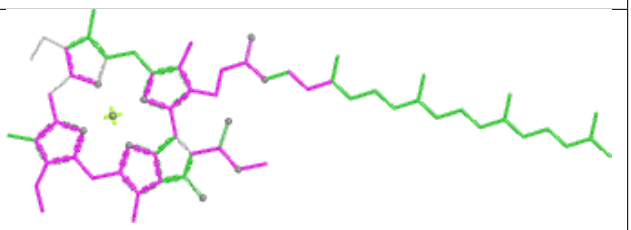


Rings

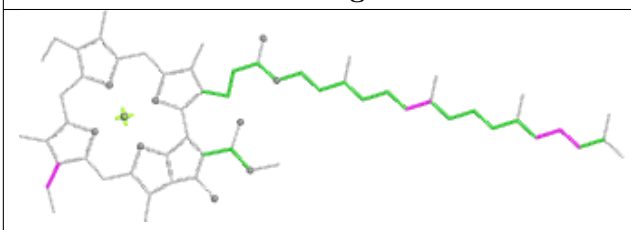
Ligand CLA a 350



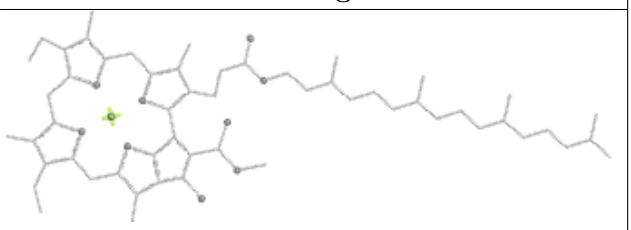
Bond lengths



Bond angles

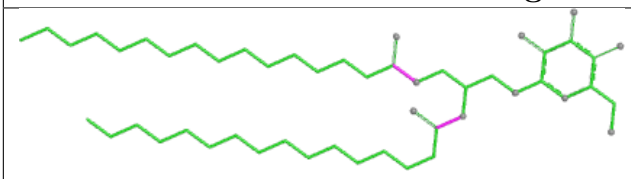


Torsions

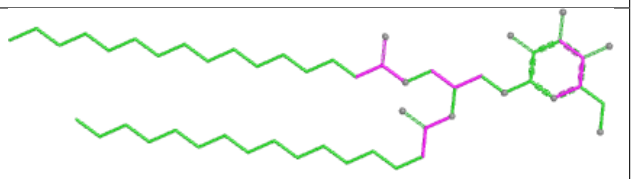


Rings

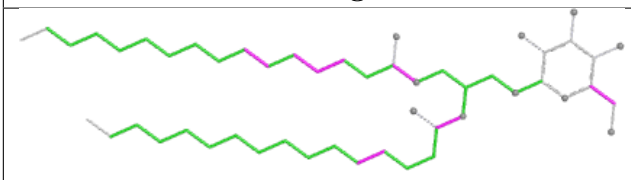
Ligand LMG c 522



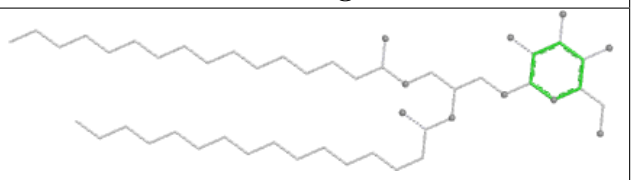
Bond lengths



Bond angles

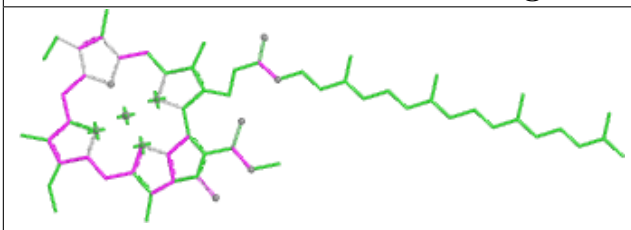


Torsions

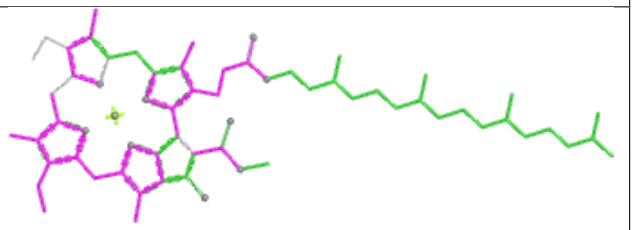


Rings

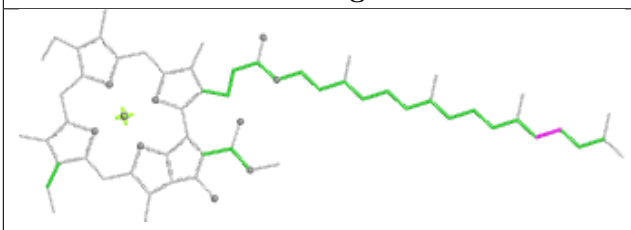
Ligand CLA A 404



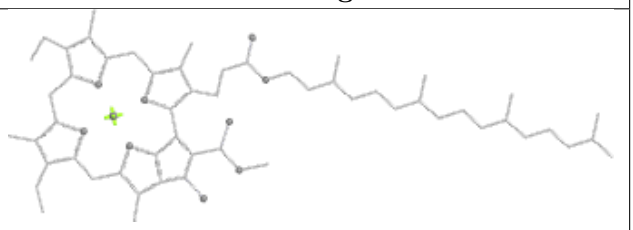
Bond lengths



Bond angles

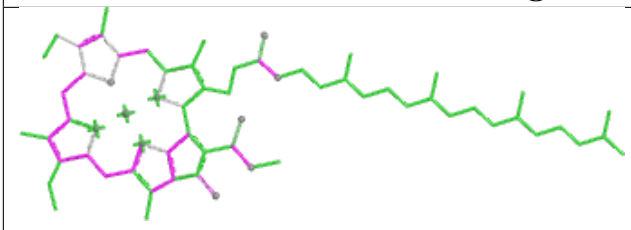


Torsions

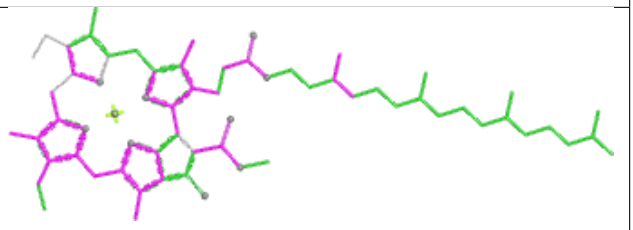


Rings

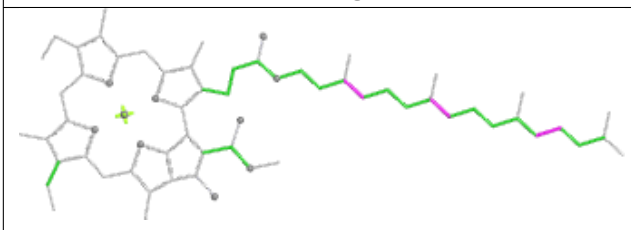
Ligand CLA b 603



Bond lengths



Bond angles



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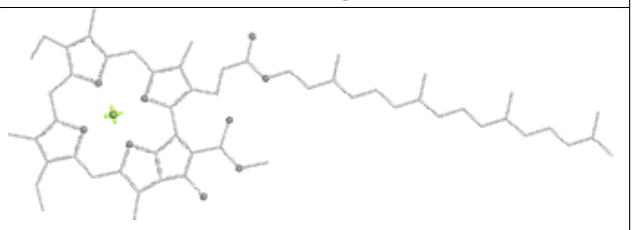
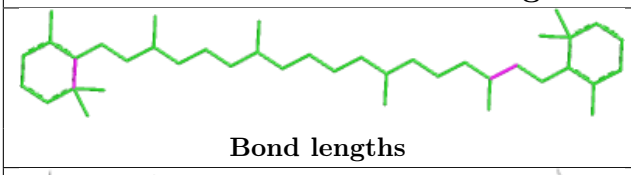
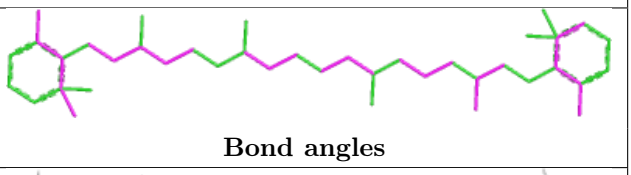


Rings

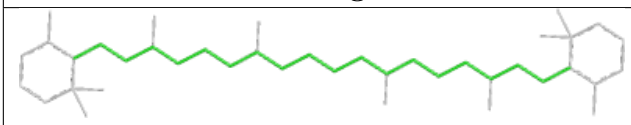
Ligand BCR B 617



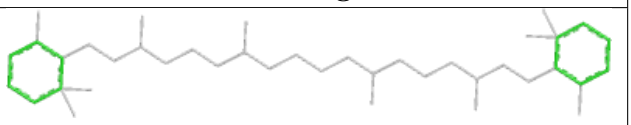
Bond lengths



Bond angles

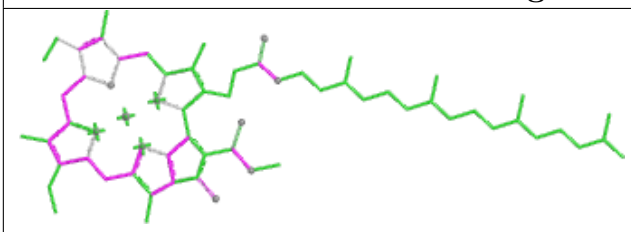


Torsions

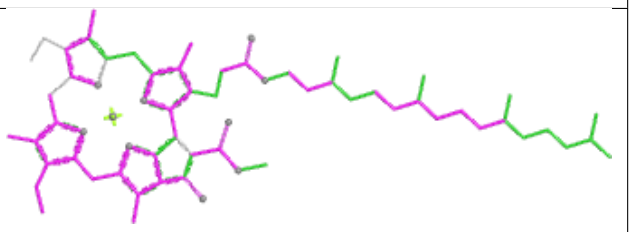


Rings

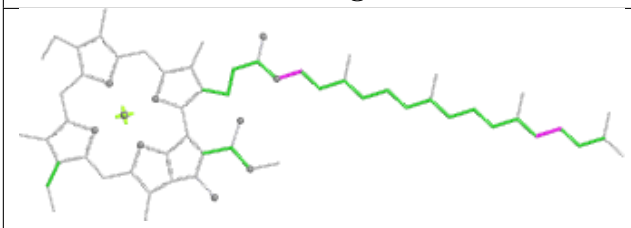
Ligand CLA b 608



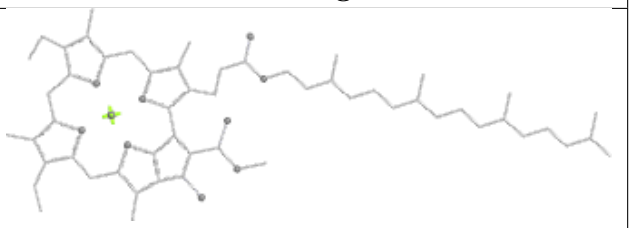
Bond lengths



Bond angles

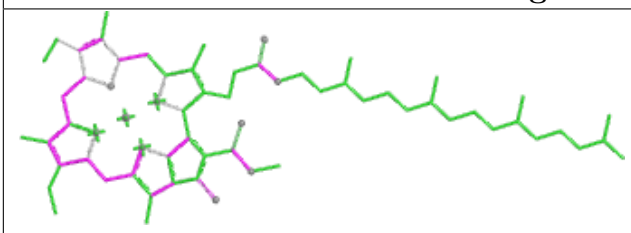


Torsions

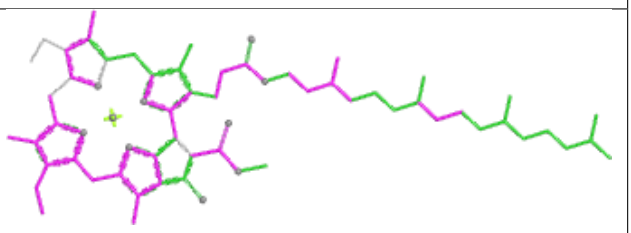


Rings

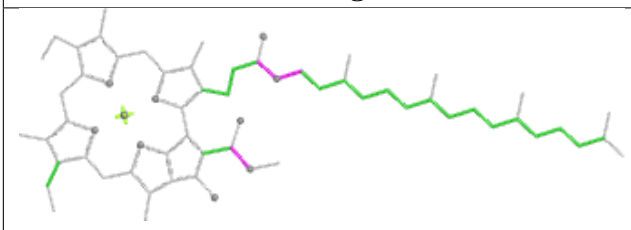
Ligand CLA c 513



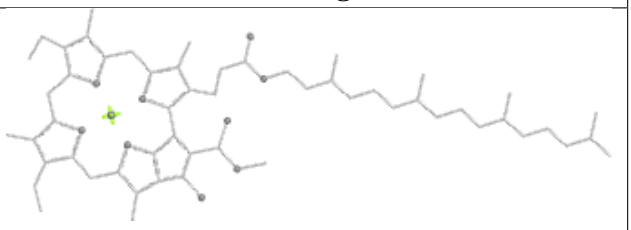
Bond lengths



Bond angles

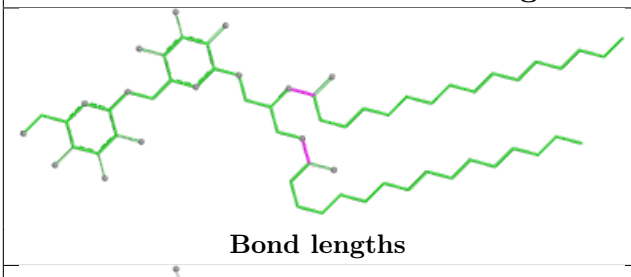


Torsions

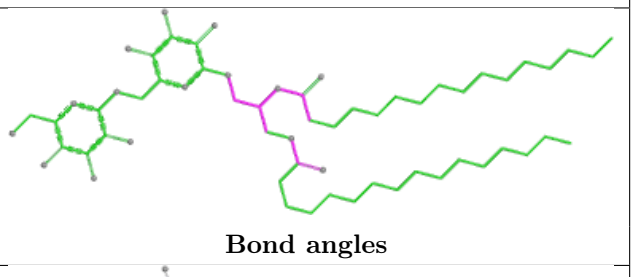


Rings

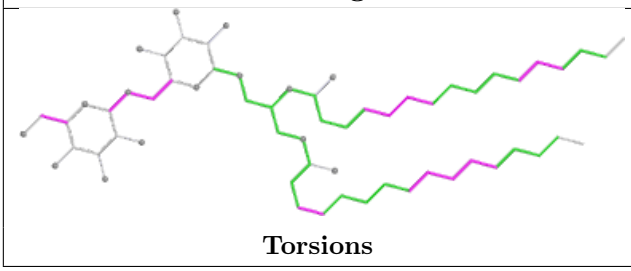
Ligand DGD C 517



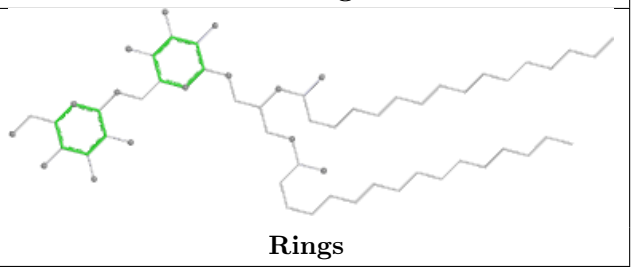
Bond lengths



Bond angles

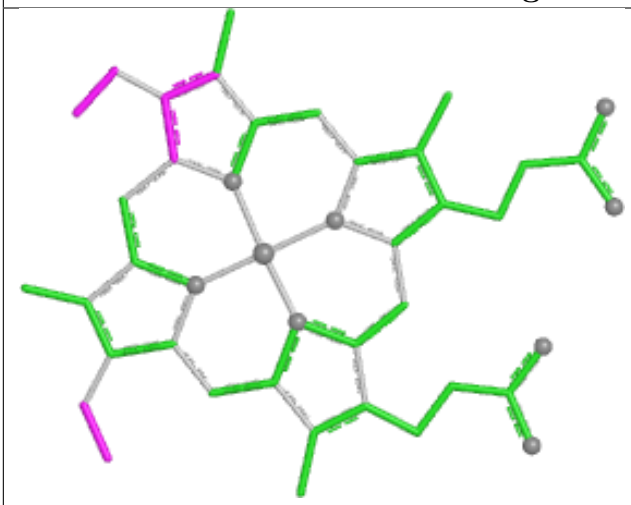


Torsions

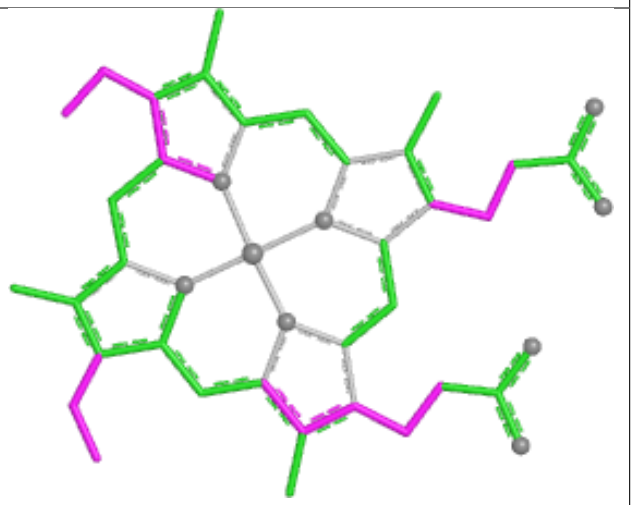


Rings

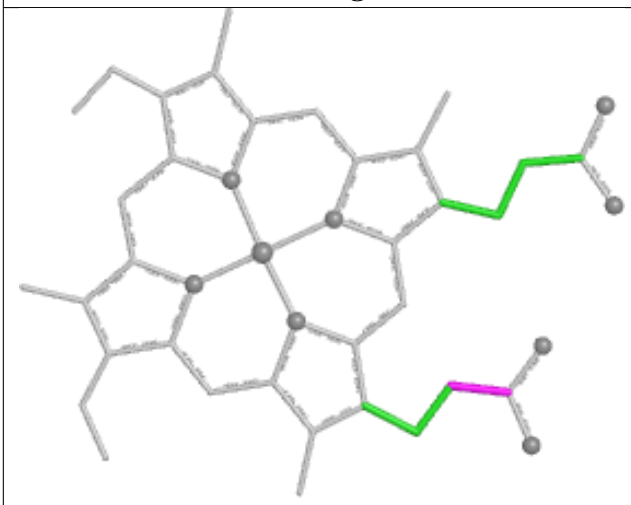
Ligand HEC V 203



Bond lengths



Bond angles



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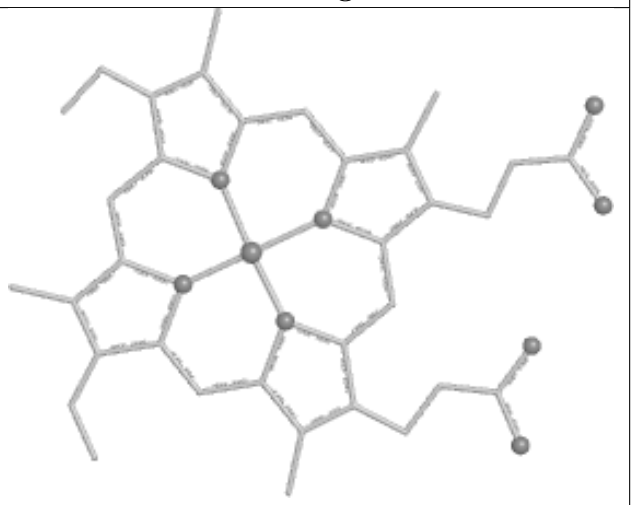
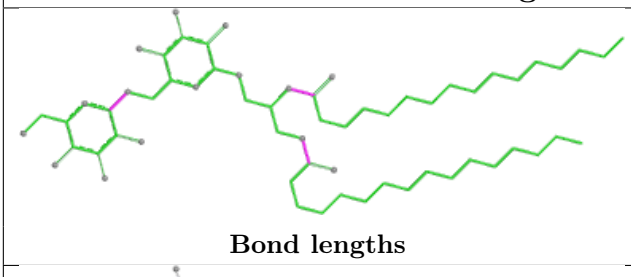
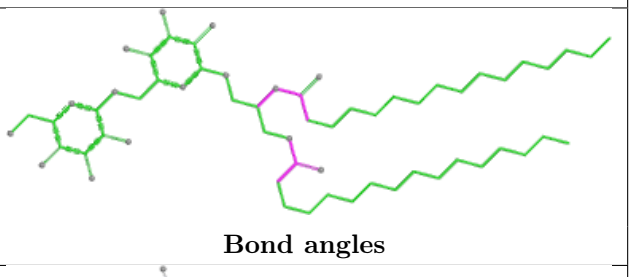


Rings

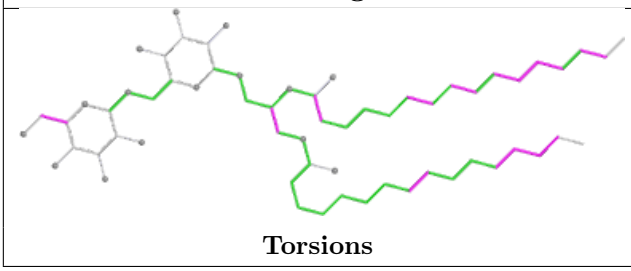
Ligand DGD H 102



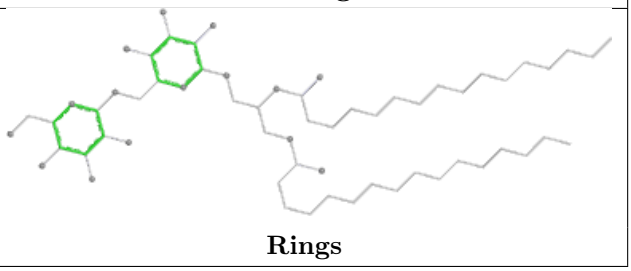
Bond lengths



Bond angles

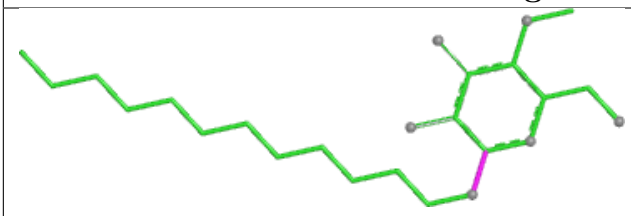


Torsions

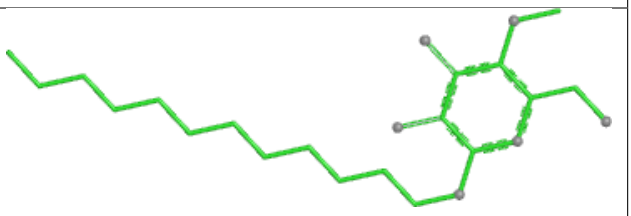


Rings

Ligand LMT b 630

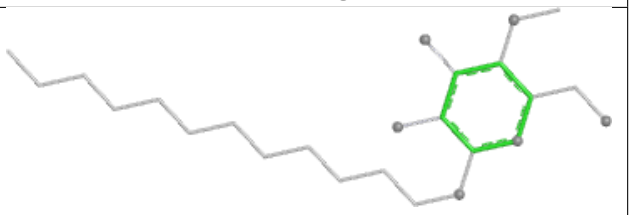


Bond lengths



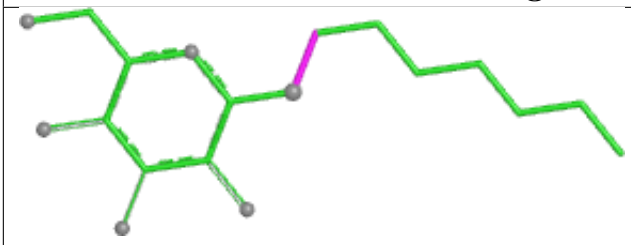
Bond angles

Torsions

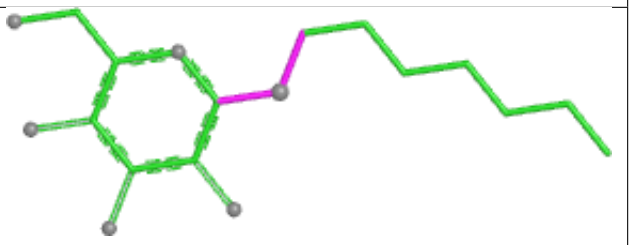


Rings

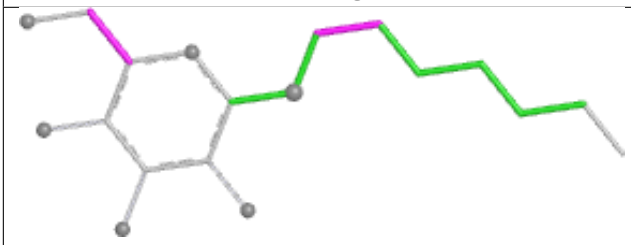
Ligand HTG c 523



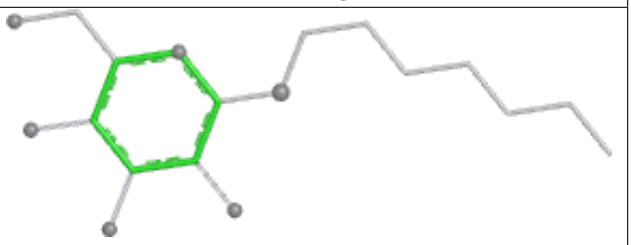
Bond lengths



Bond angles

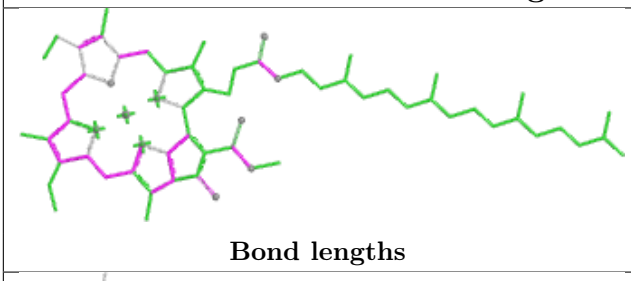


Torsions

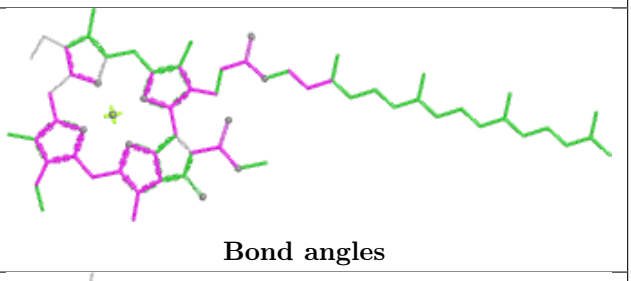


Rings

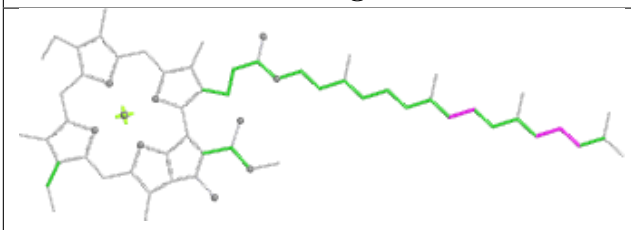
Ligand CLA b 611



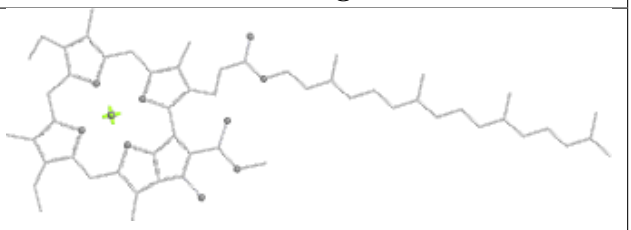
Bond lengths



Bond angles

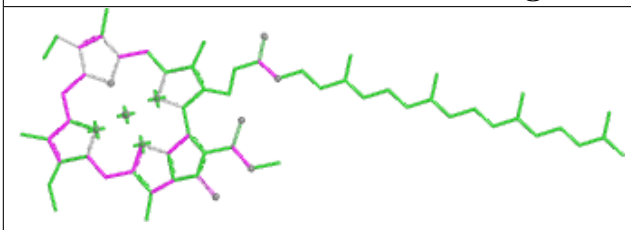


Torsions

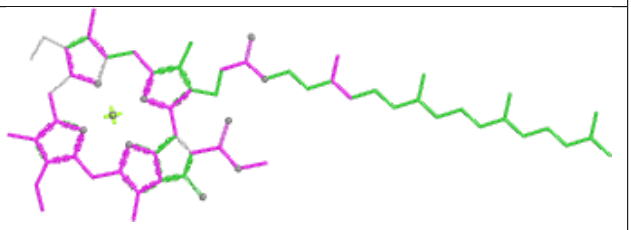


Rings

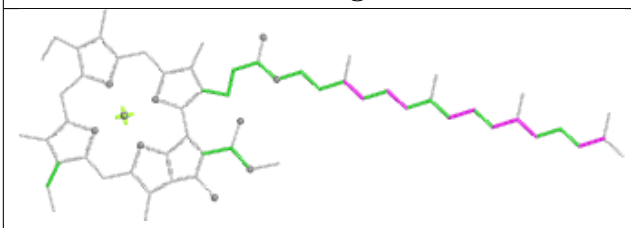
Ligand CLA B 615



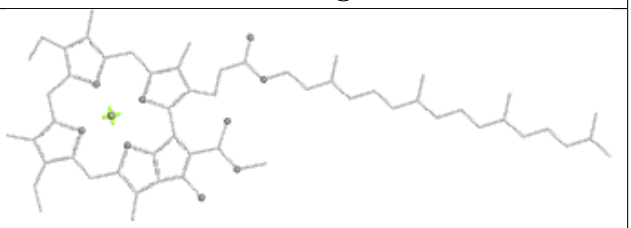
Bond lengths



Bond angles

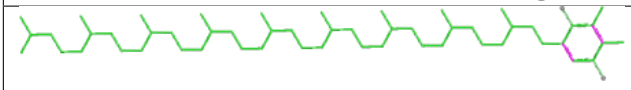


Torsions

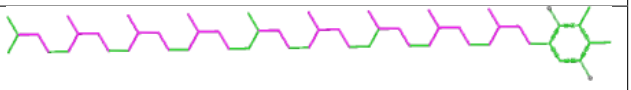


Rings

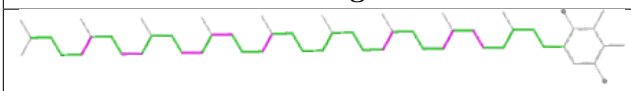
Ligand PL9 d 405



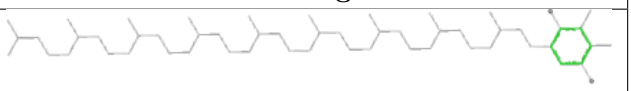
Bond lengths



Bond angles

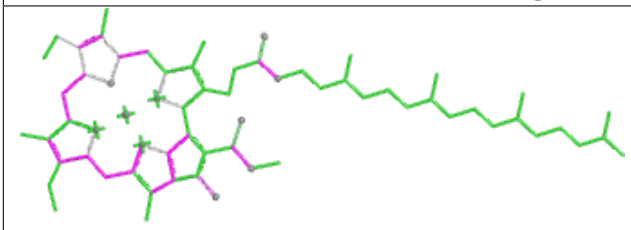


Torsions

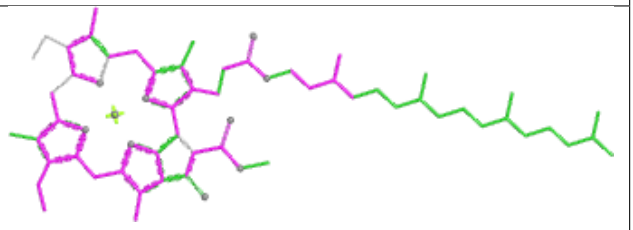


Rings

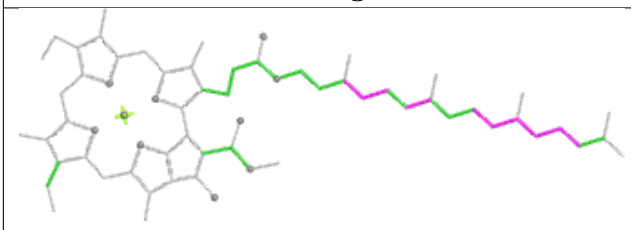
Ligand CLA c 508



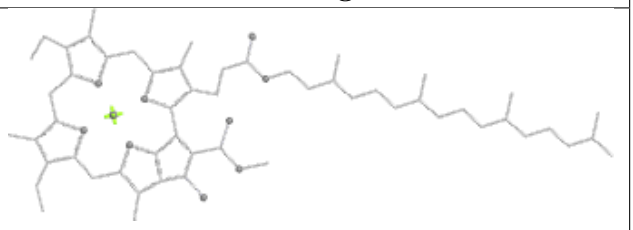
Bond lengths



Bond angles

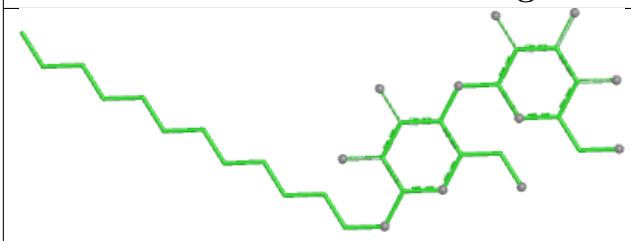


Torsions

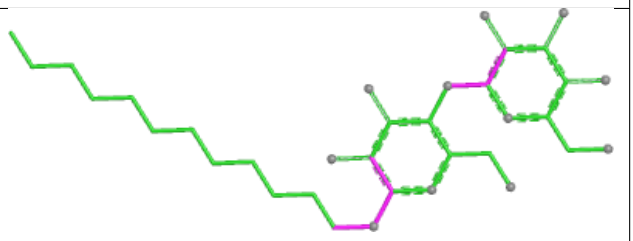


Rings

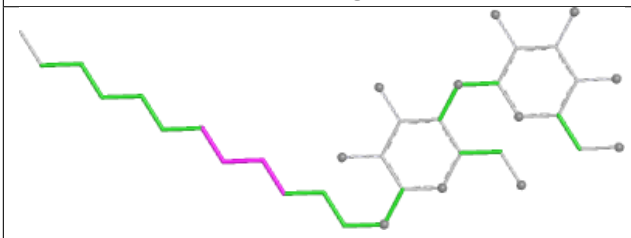
Ligand LMT M 101



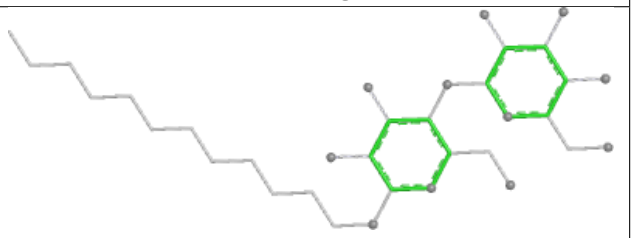
Bond lengths



Bond angles

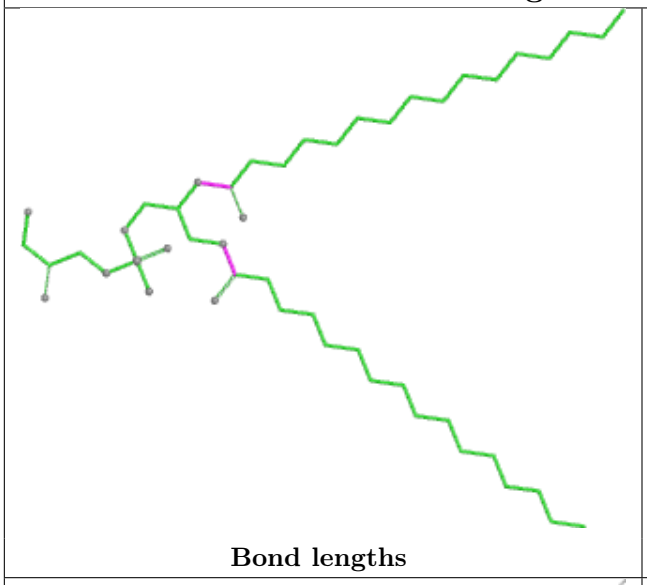


Torsions

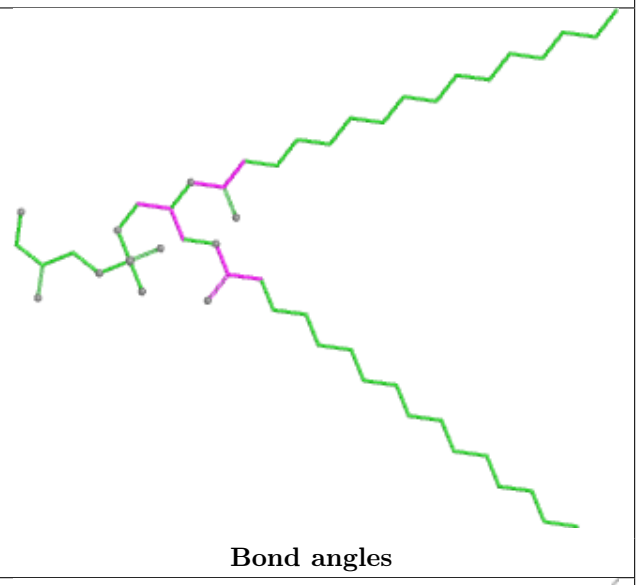


Rings

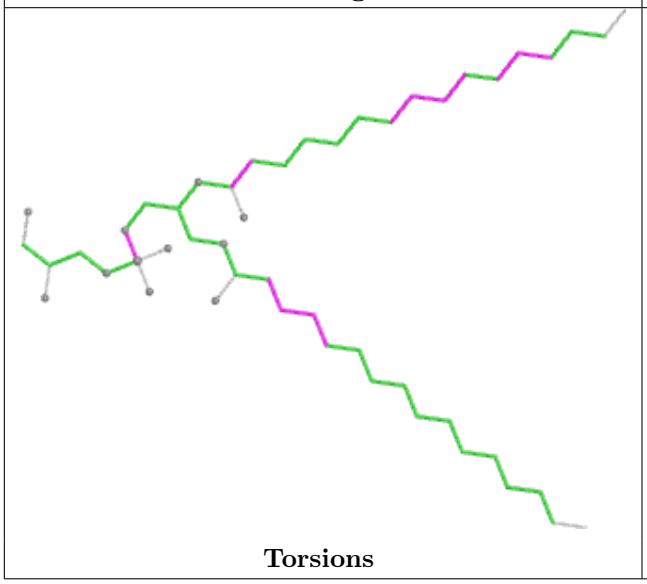
Ligand LHG L 101



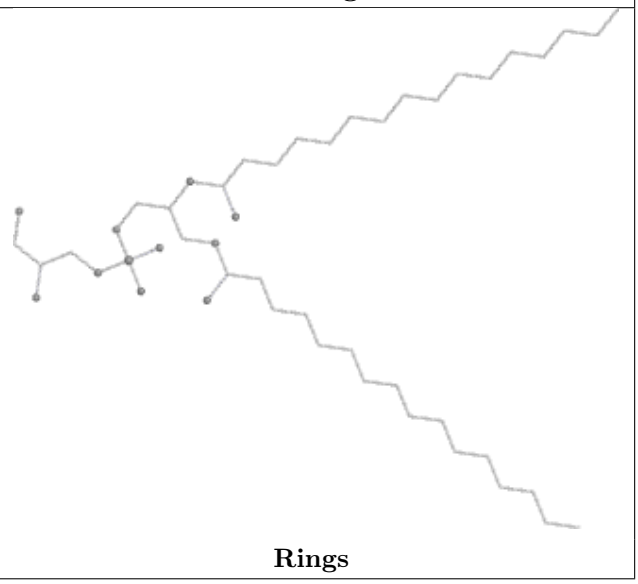
Bond lengths



Bond angles

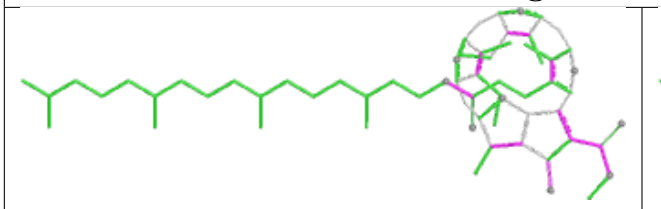


Torsions

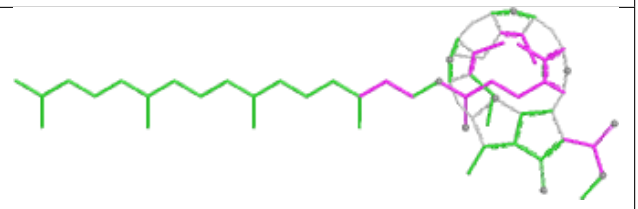


Rings

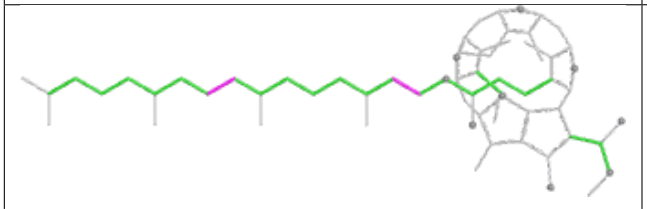
Ligand PHO a 405



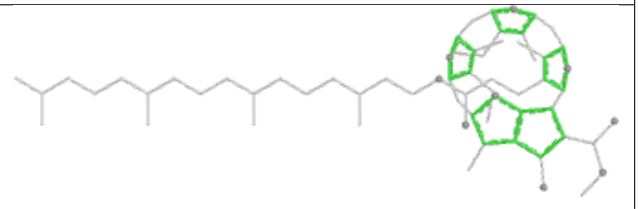
Bond lengths



Bond angles

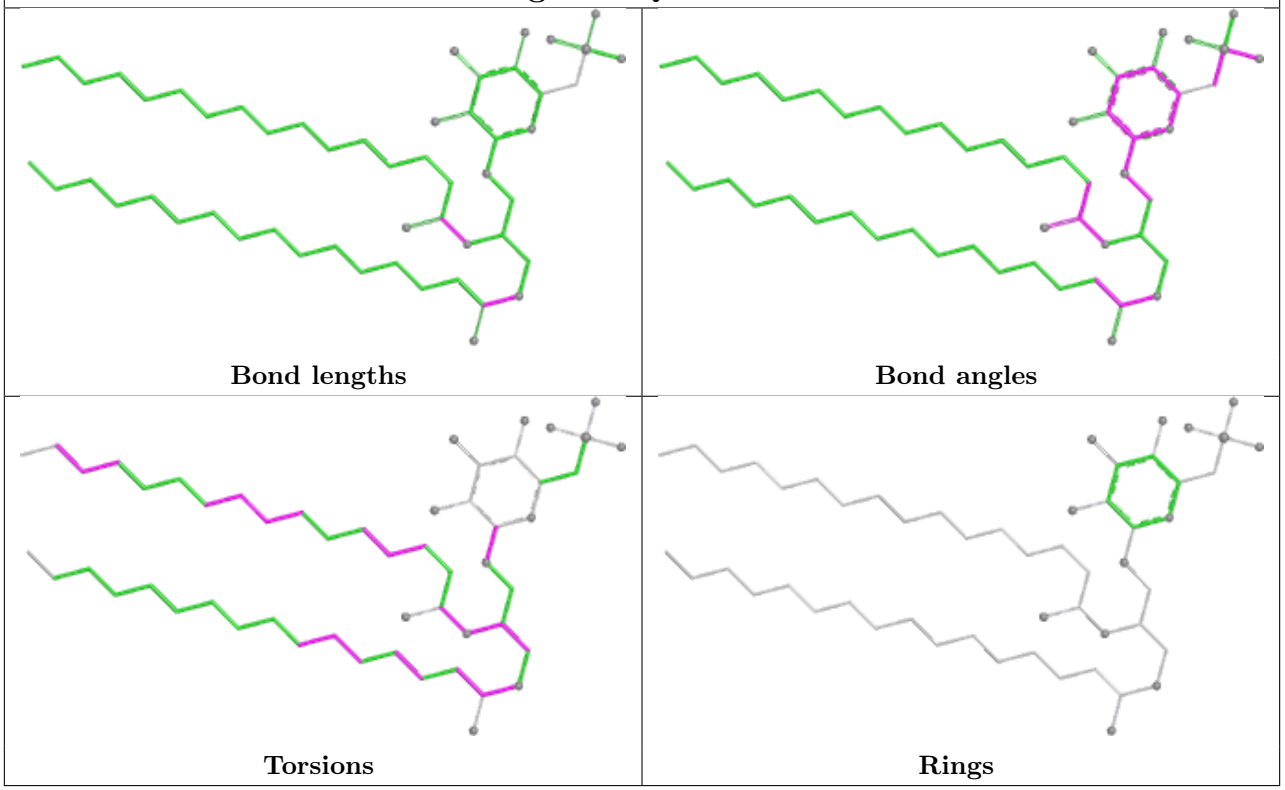


Torsions

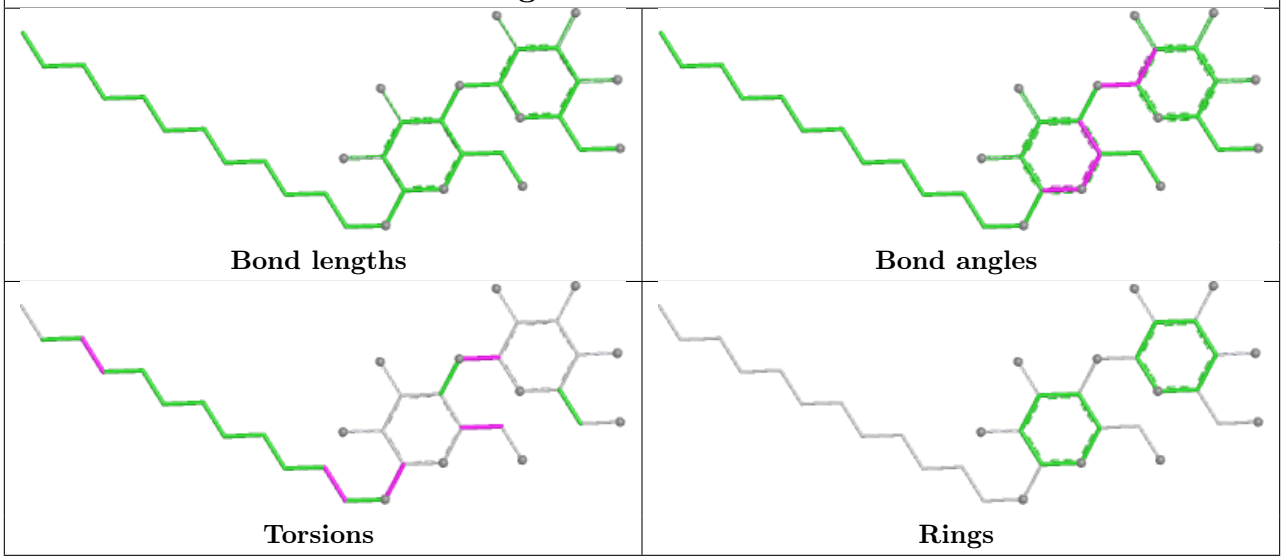


Rings

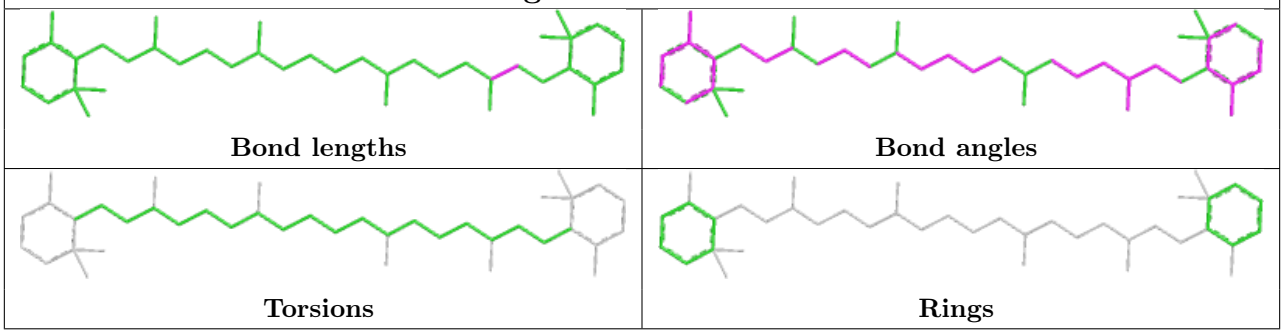
Ligand SQD b 620



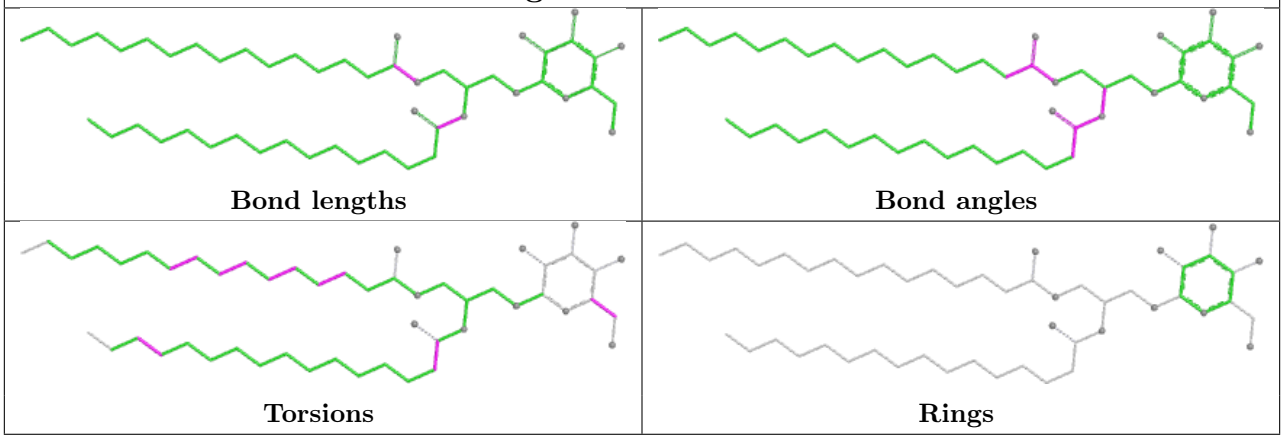
Ligand LMT M 103



Ligand BCR B 618



Ligand LMG c 521



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

Warning: The R factor obtained from EDS is 0.1949, which does not match the depositor's R factor of 0.1289. Please interpret the results in this section carefully.

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%)	-0.78	0 100 100	22, 47, 68, 120	29 (8%)
1	a	334/344 (97%)	-0.72	0 100 100	23, 51, 82, 120	29 (8%)
2	B	504/505 (99%)	-0.71	2 (0%) 89 90	30, 53, 83, 128	8 (1%)
2	b	504/505 (99%)	-0.64	2 (0%) 89 90	35, 57, 97, 149	4 (0%)
3	C	451/455 (99%)	-0.70	0 100 100	23, 59, 80, 142	10 (2%)
3	c	455/455 (100%)	-0.58	0 100 100	26, 67, 89, 129	10 (2%)
4	D	342/342 (100%)	-0.84	0 100 100	23, 49, 68, 139	3 (0%)
4	d	341/342 (99%)	-0.77	0 100 100	24, 55, 78, 147	3 (0%)
5	E	81/84 (96%)	-0.33	0 100 100	53, 70, 100, 151	1 (1%)
5	e	79/84 (94%)	-0.22	1 (1%) 74 79	62, 78, 122, 140	0
6	F	34/44 (77%)	-0.56	0 100 100	52, 63, 90, 117	0
6	f	31/44 (70%)	-0.32	1 (3%) 50 57	62, 68, 100, 140	0
7	H	64/65 (98%)	-0.54	1 (1%) 70 75	33, 62, 81, 129	1 (1%)
7	h	64/65 (98%)	-0.47	1 (1%) 70 75	58, 69, 95, 147	0
8	I	37/38 (97%)	-0.40	0 100 100	55, 62, 127, 147	0
8	i	37/38 (97%)	-0.34	1 (2%) 56 62	57, 66, 123, 138	0
9	J	38/39 (97%)	-0.30	0 100 100	51, 71, 129, 175	0
9	j	39/39 (100%)	-0.10	0 100 100	56, 80, 149, 175	0
10	K	37/37 (100%)	-0.54	0 100 100	60, 67, 89, 101	0
10	k	37/37 (100%)	-0.44	0 100 100	70, 77, 101, 117	0
11	L	36/37 (97%)	-0.70	0 100 100	27, 47, 109, 162	1 (2%)
11	l	36/37 (97%)	-0.74	0 100 100	28, 48, 103, 152	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
12	M	32/36 (88%)	-0.65	0 100 100	28, 49, 74, 134	1 (3%)
12	m	33/36 (91%)	-0.68	0 100 100	43, 50, 86, 140	0
13	O	243/244 (99%)	-0.57	0 100 100	36, 63, 115, 176	5 (2%)
13	o	243/244 (99%)	-0.55	0 100 100	34, 65, 121, 161	2 (0%)
14	T	29/32 (90%)	-0.74	1 (3%) 48 54	42, 49, 81, 115	0
14	t	29/32 (90%)	-0.74	1 (3%) 48 54	43, 50, 81, 130	0
15	U	96/104 (92%)	-0.73	0 100 100	47, 60, 90, 101	0
15	u	97/104 (93%)	-0.73	0 100 100	51, 62, 84, 121	0
16	V	137/137 (100%)	-0.77	0 100 100	46, 57, 82, 112	0
16	v	137/137 (100%)	-0.58	0 100 100	52, 71, 104, 137	0
17	X	38/40 (95%)	-0.33	0 100 100	59, 71, 96, 126	0
17	x	38/40 (95%)	-0.10	0 100 100	65, 78, 117, 154	0
18	Y	29/30 (96%)	0.17	0 100 100	73, 87, 140, 155	0
18	y	29/30 (96%)	0.08	1 (3%) 48 54	79, 97, 126, 136	0
19	Z	62/62 (100%)	-0.21	0 100 100	67, 84, 131, 173	0
19	z	62/62 (100%)	0.21	1 (1%) 70 75	83, 99, 148, 185	0
20	R	34/34 (100%)	1.06	2 (5%) 29 34	97, 125, 149, 154	0
All	All	5283/5384 (98%)	-0.61	15 (0%) 90 91	22, 59, 104, 185	108 (2%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	5.0
7	h	65	LEU	4.2
2	b	502	VAL	3.0
14	t	30	THR	2.6
2	B	494	GLY	2.6

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
14	FME	T	1	10/11	0.96	0.08	44,50,74,88	0
12	FME	m	1	10/11	0.96	0.08	47,60,91,103	0
12	FME	M	1	10/11	0.97	0.09	34,56,91,100	0
14	FME	t	1	10/11	0.97	0.07	43,51,75,84	0
8	FME	i	1	10/11	0.98	0.06	59,64,77,78	0
8	FME	I	1	10/11	0.98	0.06	46,65,76,76	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
35	HTG	c	523	19/19	0.74	0.14	118,144,148,169	0
34	LMT	e	101	35/35	0.75	0.15	121,166,181,186	0
34	LMT	a	418	35/35	0.78	0.15	113,136,151,151	0
32	UNL	i	101	40/-	0.78	0.15	77,109,164,165	0
35	HTG	C	522	19/19	0.78	0.14	112,123,133,150	0
34	LMT	A	359	35/35	0.78	0.15	73,134,144,148	0
35	HTG	c	526	19/19	0.78	0.13	114,161,170,200	0
34	LMT	E	102	35/35	0.79	0.15	119,145,171,173	0
32	UNL	a	415	30/-	0.79	0.16	98,115,136,146	0
32	UNL	K	101	34/-	0.80	0.14	83,119,134,150	0
27	SQD	f	101	43/54	0.80	0.14	118,136,170,175	0
32	UNL	A	417	28/-	0.80	0.16	98,110,128,144	0
32	UNL	j	102	10/-	0.80	0.15	87,106,117,118	0
32	UNL	m	101	10/-	0.80	0.12	69,78,80,84	0
32	UNL	J	102	10/-	0.80	0.16	77,81,99,104	0
32	UNL	c	527	32/-	0.81	0.15	93,125,140,143	0
35	HTG	b	624	19/19	0.81	0.18	114,128,145,170	0
34	LMT	a	359	35/35	0.81	0.15	65,144,151,154	0
34	LMT	I	101	35/35	0.81	0.14	110,145,160,162	0
37	CA	b	626	1/1	0.81	0.08	151,151,151,151	0
32	UNL	I	102	40/-	0.82	0.15	66,113,156,158	0
38	LHG	a	419	42/49	0.82	0.11	78,141,167,179	0
33	LMG	C	521	51/55	0.83	0.13	68,121,155,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	HTG	B	624	19/19	0.83	0.16	71,103,114,115	0
34	LMT	b	622	25/35	0.84	0.12	88,117,159,160	0
35	HTG	B	625	19/19	0.84	0.13	82,167,178,238	0
32	UNL	b	629	33/-	0.84	0.14	72,108,162,162	0
35	HTG	h	101	16/19	0.84	0.14	98,133,140,163	0
35	HTG	C	523	19/19	0.84	0.12	84,153,166,186	0
35	HTG	D	410	16/19	0.84	0.12	82,121,136,138	0
35	HTG	b	625	19/19	0.85	0.13	91,138,154,196	0
32	UNL	D	409	40/-	0.85	0.12	67,93,136,140	0
31	PL9	A	416[A]	55/55	0.86	0.14	66,93,107,111	55
34	LMT	M	103	35/35	0.86	0.11	68,146,169,171	0
33	LMG	c	522	51/55	0.86	0.11	80,127,154,158	0
31	PL9	A	416[B]	55/55	0.86	0.14	66,93,108,113	55
34	LMT	B	622	35/35	0.86	0.13	78,125,142,144	0
32	UNL	d	410	36/-	0.86	0.12	73,100,136,140	0
33	LMG	Z	101	37/55	0.87	0.13	77,129,150,151	0
33	LMG	z	101	39/55	0.88	0.12	84,133,148,153	0
28	GOL	a	410	6/6	0.88	0.12	79,81,90,95	0
34	LMT	t	101	26/35	0.88	0.11	71,110,152,153	0
27	SQD	a	411	54/54	0.88	0.10	72,95,139,149	0
38	LHG	E	101	42/49	0.88	0.11	72,118,132,132	0
27	SQD	F	101	43/54	0.88	0.12	81,114,134,137	0
35	HTG	V	204	11/19	0.89	0.12	104,117,122,125	0
28	GOL	c	502	6/6	0.89	0.19	68,70,71,75	0
32	UNL	B	629	33/-	0.89	0.12	57,103,166,173	0
35	HTG	B	623	19/19	0.89	0.12	70,88,128,128	0
28	GOL	v	202	6/6	0.89	0.11	75,86,94,96	0
33	LMG	A	418	51/55	0.89	0.11	61,97,118,121	0
32	UNL	M	102	10/-	0.89	0.09	62,72,86,92	0
34	LMT	B	630	25/35	0.89	0.12	54,89,147,148	0
34	LMT	b	630	25/35	0.89	0.12	57,81,151,153	0
28	GOL	B	627	6/6	0.90	0.14	58,77,85,87	0
27	SQD	B	620	54/54	0.90	0.10	65,93,132,134	0
28	GOL	a	416	6/6	0.90	0.21	55,82,84,86	0
28	GOL	b	627	6/6	0.90	0.12	97,106,113,116	0
27	SQD	b	620	54/54	0.90	0.10	68,93,144,152	0
27	SQD	A	413	54/54	0.90	0.10	63,91,128,137	0
28	GOL	A	412	6/6	0.91	0.12	80,82,86,98	0
24	CLA	B	601	65/65	0.91	0.10	53,77,112,132	0
33	LMG	a	417	51/55	0.91	0.10	76,100,122,129	0
24	CLA	c	515	65/65	0.91	0.10	70,91,134,138	0
34	LMT	m	102	35/35	0.91	0.11	63,95,117,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	CA	v	201	1/1	0.91	0.13	123,123,123,123	0
31	PL9	a	414[A]	55/55	0.91	0.16	97,107,120,124	55
31	PL9	a	414[B]	55/55	0.91	0.16	97,107,120,124	55
35	HTG	b	623	19/19	0.92	0.11	68,88,130,131	0
37	CA	V	201	1/1	0.92	0.14	141,141,141,141	0
34	LMT	M	101	35/35	0.92	0.10	61,99,123,126	0
24	CLA	b	601	65/65	0.92	0.10	58,85,115,130	0
33	LMG	c	521	51/55	0.92	0.09	68,101,145,156	0
33	LMG	C	520	51/55	0.92	0.09	56,90,127,140	0
28	GOL	V	202	6/6	0.93	0.11	64,74,85,92	0
37	CA	O	301	1/1	0.93	0.07	119,119,119,119	0
24	CLA	c	514	65/65	0.93	0.09	59,80,123,128	0
35	HTG	B	628	19/19	0.93	0.08	65,80,89,95	0
24	CLA	C	514	65/65	0.93	0.09	60,81,122,127	0
28	GOL	C	525	6/6	0.93	0.12	66,73,76,78	0
32	UNL	D	408	17/-	0.93	0.09	66,85,107,110	0
24	CLA	C	507	65/65	0.94	0.09	53,69,137,141	0
24	CLA	C	513	65/65	0.94	0.08	60,73,118,123	0
26	BCR	C	515	40/40	0.94	0.08	63,75,82,85	0
27	SQD	a	409	54/54	0.94	0.09	63,85,127,131	0
33	LMG	b	621	51/55	0.94	0.09	53,74,105,124	0
26	BCR	D	404	40/40	0.94	0.08	46,61,94,95	0
26	BCR	d	404	40/40	0.94	0.08	53,67,96,98	0
24	CLA	c	506	65/65	0.95	0.07	51,66,116,125	0
24	CLA	c	508	65/65	0.95	0.08	60,72,120,133	0
33	LMG	J	101	51/55	0.95	0.08	48,73,119,126	0
24	CLA	c	509	65/65	0.95	0.08	56,70,86,92	0
24	CLA	C	509	65/65	0.95	0.07	44,57,115,131	0
24	CLA	B	614	65/65	0.95	0.08	38,49,103,113	0
24	CLA	d	403	65/65	0.95	0.08	46,64,132,137	0
24	CLA	C	505	65/65	0.95	0.07	42,56,103,113	0
33	LMG	j	101	51/55	0.95	0.08	60,70,121,138	0
24	CLA	B	606	65/65	0.95	0.08	41,52,104,114	0
26	BCR	K	102	40/40	0.95	0.07	56,67,74,81	0
32	UNL	X	101	18/-	0.95	0.09	57,76,100,100	0
26	BCR	Y	101	40/40	0.95	0.07	57,68,74,81	0
35	HTG	b	628	19/19	0.95	0.08	61,82,106,112	0
24	CLA	b	606	65/65	0.95	0.08	45,58,114,129	0
26	BCR	h	102	40/40	0.95	0.07	56,70,80,81	0
26	BCR	t	102	40/40	0.95	0.07	45,60,76,80	0
36	DGD	C	518	62/66	0.95	0.08	48,67,127,131	0
36	DGD	c	519	62/66	0.95	0.08	56,73,136,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	y	101	40/40	0.95	0.08	58,74,88,88	0
27	SQD	A	411	54/54	0.95	0.08	55,86,123,126	0
24	CLA	b	614	65/65	0.95	0.07	41,49,116,120	0
37	CA	o	301	1/1	0.95	0.07	108,108,108,108	0
32	UNL	x	101	18/-	0.95	0.09	70,85,105,106	0
38	LHG	D	407	49/49	0.95	0.09	53,61,120,125	0
24	CLA	b	616	65/65	0.95	0.09	50,60,124,127	0
33	LMG	B	621	51/55	0.95	0.08	53,72,94,108	0
38	LHG	d	406	49/49	0.95	0.08	50,66,90,106	0
38	LHG	d	408	49/49	0.95	0.09	53,68,121,125	0
28	GOL	B	626	6/6	0.96	0.10	85,88,90,95	0
26	BCR	A	410	40/40	0.96	0.06	42,51,61,62	0
26	BCR	B	618	40/40	0.96	0.06	44,57,70,77	0
26	BCR	B	619	40/40	0.96	0.06	45,57,80,87	0
24	CLA	C	504	65/65	0.96	0.07	47,58,76,85	0
24	CLA	b	607	65/65	0.96	0.07	35,49,77,87	0
26	BCR	H	101	40/40	0.96	0.06	50,65,77,82	0
24	CLA	b	609	65/65	0.96	0.07	50,61,83,99	0
26	BCR	T	101	40/40	0.96	0.06	46,57,68,72	0
24	CLA	B	602	65/65	0.96	0.07	45,55,80,84	0
26	BCR	b	617	40/40	0.96	0.06	45,52,63,63	0
26	BCR	b	618	40/40	0.96	0.06	44,60,73,75	0
26	BCR	c	516	40/40	0.96	0.07	77,86,93,96	0
24	CLA	b	615	65/65	0.96	0.07	46,59,81,86	0
24	CLA	B	616	65/65	0.96	0.10	45,58,147,153	0
26	BCR	k	101	40/40	0.96	0.07	58,73,84,90	0
36	DGD	C	517	62/66	0.96	0.07	43,63,104,106	0
24	CLA	c	505	65/65	0.96	0.06	58,67,77,83	0
36	DGD	C	519	62/66	0.96	0.07	43,60,94,116	0
36	DGD	c	518	62/66	0.96	0.07	49,67,95,103	0
24	CLA	D	403	65/65	0.96	0.08	44,58,139,144	0
36	DGD	c	520	62/66	0.96	0.07	55,64,100,116	0
24	CLA	c	507	65/65	0.96	0.07	49,61,91,95	0
24	CLA	a	404	65/65	0.96	0.07	42,53,126,133	0
24	CLA	a	407	65/65	0.96	0.09	44,57,134,140	0
24	CLA	c	510	65/65	0.96	0.07	53,63,141,145	0
24	CLA	c	511	65/65	0.96	0.08	51,69,82,89	0
24	CLA	c	513	65/65	0.96	0.07	57,71,91,97	0
38	LHG	D	357	49/49	0.96	0.07	49,64,86,102	0
24	CLA	C	508	65/65	0.96	0.07	49,60,80,82	0
32	UNL	d	409	17/-	0.96	0.07	68,83,111,114	0
24	CLA	b	602	65/65	0.96	0.07	51,62,79,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	b	604	65/65	0.96	0.07	37,50,122,128	0
38	LHG	l	101	49/49	0.96	0.07	50,60,74,91	0
39	HEM	e	102	43/43	0.96	0.09	67,93,128,137	0
24	CLA	a	403	65/65	0.97	0.06	36,48,69,86	0
26	BCR	B	617	40/40	0.97	0.05	44,52,59,65	0
31	PL9	D	405	55/55	0.97	0.06	37,49,62,78	0
24	CLA	B	609	65/65	0.97	0.06	47,57,73,80	0
24	CLA	B	610	65/65	0.97	0.07	43,53,64,80	0
31	PL9	d	405	55/55	0.97	0.06	41,50,66,85	0
24	CLA	a	350	65/65	0.97	0.05	36,46,63,77	0
26	BCR	C	516	40/40	0.97	0.06	53,62,72,81	0
24	CLA	B	611	65/65	0.97	0.06	37,47,63,73	0
24	CLA	B	612	65/65	0.97	0.05	35,47,57,74	0
24	CLA	b	603	65/65	0.97	0.06	46,56,85,92	0
24	CLA	B	613	65/65	0.97	0.06	37,47,94,103	0
24	CLA	b	605	65/65	0.97	0.06	43,52,70,74	0
26	BCR	a	408	40/40	0.97	0.05	42,52,65,68	0
24	CLA	A	406	65/65	0.97	0.06	36,47,110,116	0
24	CLA	B	615	65/65	0.97	0.06	37,52,74,83	0
26	BCR	b	619	40/40	0.97	0.06	51,62,81,84	0
24	CLA	b	608	65/65	0.97	0.05	46,58,81,84	0
26	BCR	c	517	40/40	0.97	0.06	56,67,80,81	0
24	CLA	A	409	65/65	0.97	0.08	42,53,136,144	0
24	CLA	b	610	65/65	0.97	0.07	47,58,73,75	0
24	CLA	b	611	65/65	0.97	0.06	41,52,73,82	0
24	CLA	b	612	65/65	0.97	0.06	43,54,64,75	0
24	CLA	C	502	65/65	0.97	0.06	48,59,73,83	0
24	CLA	C	503	65/65	0.97	0.06	47,55,78,95	0
23	BCT	A	403[A]	4/4	0.97	0.07	58,60,60,69	4
36	DGD	H	102	62/66	0.97	0.07	46,63,76,78	0
24	CLA	c	503	65/65	0.97	0.07	56,66,79,86	0
24	CLA	c	504	65/65	0.97	0.06	45,65,86,89	0
23	BCT	A	403[B]	4/4	0.97	0.07	55,61,62,78	4
36	DGD	h	103	62/66	0.97	0.07	52,66,78,86	0
24	CLA	C	506	65/65	0.97	0.06	49,57,92,100	0
24	CLA	B	603	65/65	0.97	0.06	42,52,69,76	0
24	CLA	B	604	65/65	0.97	0.07	34,46,123,127	0
24	CLA	B	605	65/65	0.97	0.06	39,48,65,68	0
24	CLA	C	510	65/65	0.97	0.07	49,60,81,91	0
38	LHG	D	406	49/49	0.97	0.07	47,57,76,93	0
24	CLA	C	511	65/65	0.97	0.06	49,61,74,88	0
24	CLA	c	512	65/65	0.97	0.07	50,65,81,92	0

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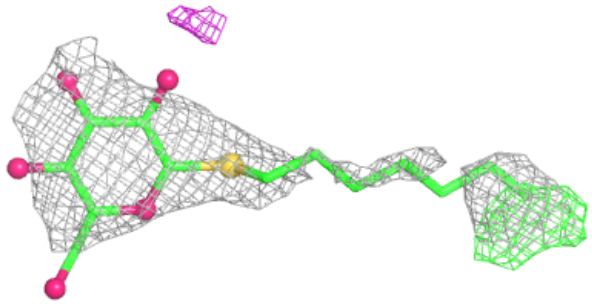
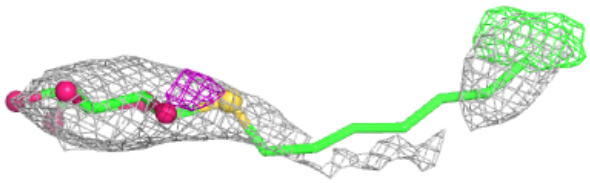
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	C	512	65/65	0.97	0.06	52,63,79,86	0
38	LHG	L	101	49/49	0.97	0.06	45,55,67,96	0
24	CLA	A	404	65/65	0.97	0.06	36,43,66,80	0
24	CLA	B	607	65/65	0.97	0.06	32,45,71,78	0
38	LHG	d	407	49/49	0.97	0.06	48,59,73,85	0
24	CLA	B	608	65/65	0.97	0.05	41,54,68,71	0
25	PHO	A	408	64/64	0.97	0.06	37,49,57,60	0
39	HEM	E	103	43/43	0.97	0.07	60,70,80,93	0
25	PHO	a	406	64/64	0.97	0.06	41,55,63,65	0
24	CLA	b	613	65/65	0.98	0.05	42,49,101,106	0
24	CLA	A	405	65/65	0.98	0.05	34,45,54,63	0
24	CLA	d	402	65/65	0.98	0.05	39,48,74,86	0
22	CL	a	347	1/1	0.98	0.09	53,53,53,53	0
37	CA	c	524	1/1	0.98	0.09	78,78,78,78	0
37	CA	c	525	1/1	0.98	0.04	92,92,92,92	0
25	PHO	A	407	64/64	0.98	0.05	35,45,54,58	0
24	CLA	D	402	65/65	0.98	0.05	31,45,68,82	0
25	PHO	a	405	64/64	0.98	0.05	41,49,56,64	0
22	CL	A	347	1/1	0.98	0.06	49,49,49,49	0
40	MG	J	103	1/1	0.98	0.06	61,61,61,61	0
40	MG	j	103	1/1	0.98	0.04	64,64,64,64	0
41	HEC	V	203	43/43	0.98	0.05	39,52,58,60	0
41	HEC	v	203	43/43	0.98	0.06	51,64,72,78	0
23	BCT	a	420[A]	4/4	0.99	0.05	58,63,63,68	4
23	BCT	a	420[B]	4/4	0.99	0.05	54,63,64,72	4
29	OEX	A	414[A]	10/10	0.99	0.05	44,48,55,59	10
29	OEX	a	412[A]	10/10	0.99	0.05	50,55,61,74	10
30	OEY	A	415[B]	11/11	0.99	0.05	43,49,55,56	11
30	OEY	a	413[B]	11/11	0.99	0.05	50,54,58,74	11
22	CL	a	402	1/1	0.99	0.02	51,51,51,51	0
21	FE2	A	401[B]	1/1	0.99	0.04	60,60,60,60	1
22	CL	A	402	1/1	0.99	0.04	44,44,44,44	0
37	CA	C	524	1/1	0.99	0.10	72,72,72,72	0
21	FE2	A	401[A]	1/1	0.99	0.04	62,62,62,62	1
21	FE2	a	401[B]	1/1	1.00	0.05	60,60,60,60	1
21	FE2	a	401[A]	1/1	1.00	0.05	60,60,60,60	1

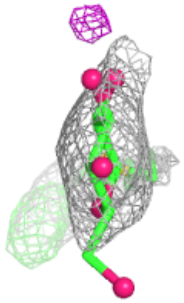
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG 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)

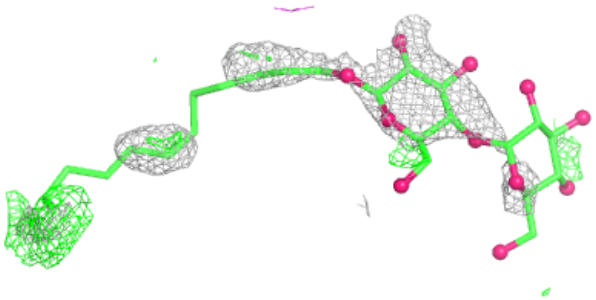


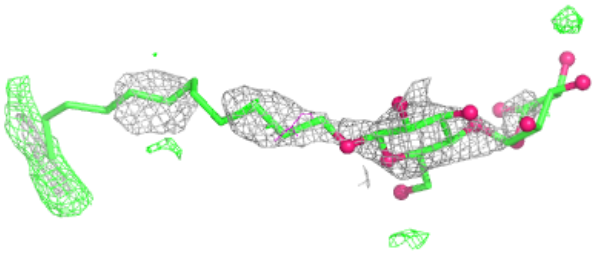


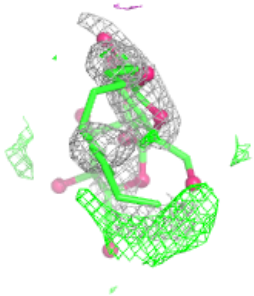


Electron density around LMT e 101:

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

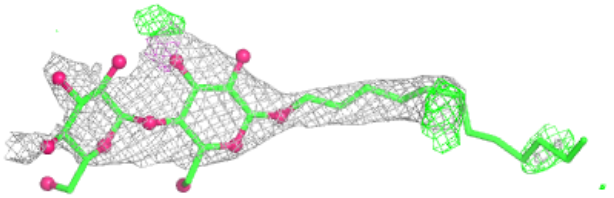


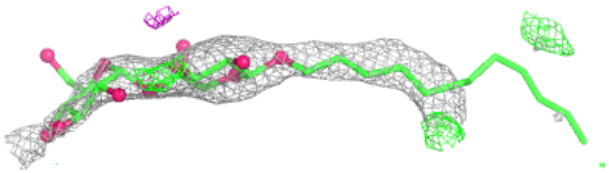


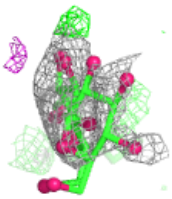


Electron density around LMT a 418:

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

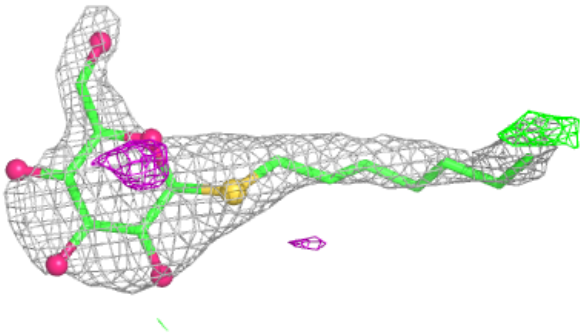


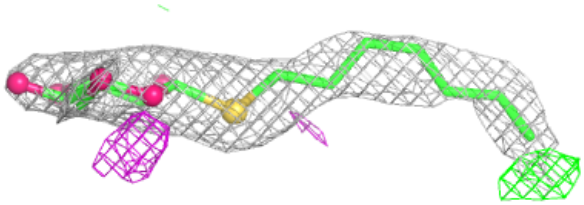


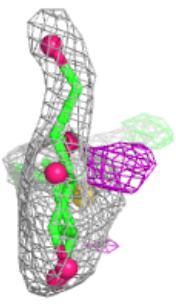


Electron density around HTG C 522:

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

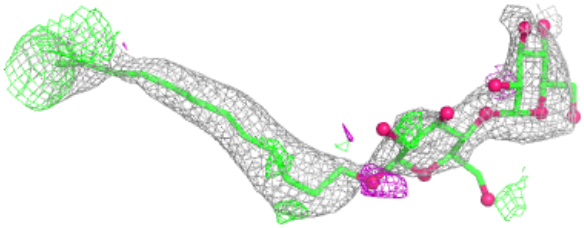


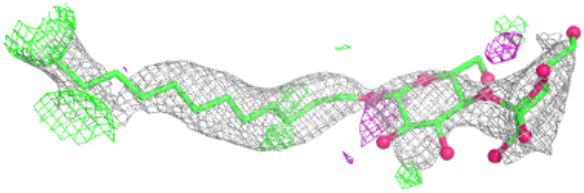


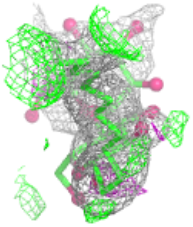


Electron density around LMT A 359:

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

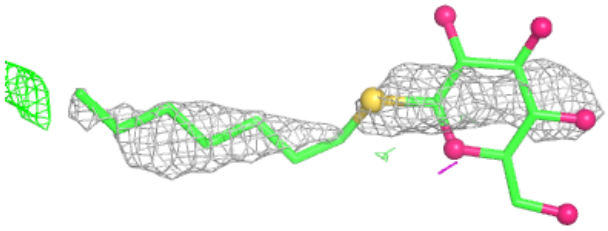


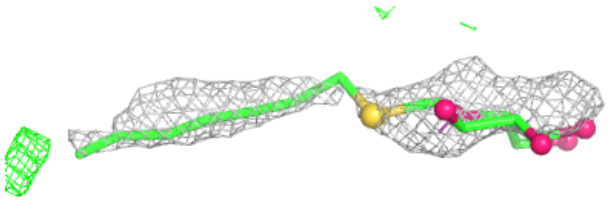


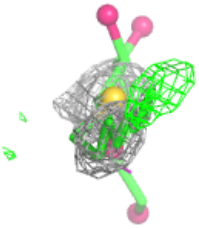


Electron density around HTG c 526:

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

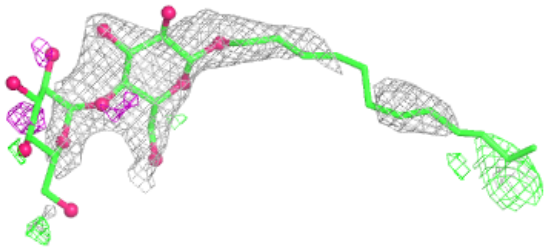


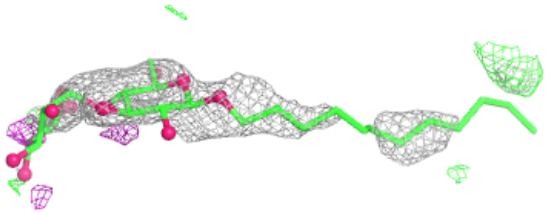


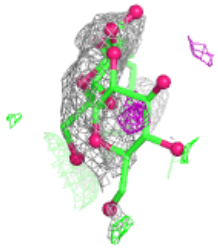


Electron density around LMT E 102:

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

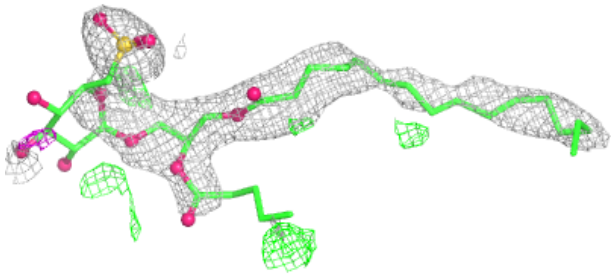


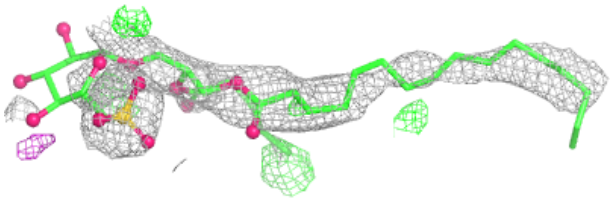


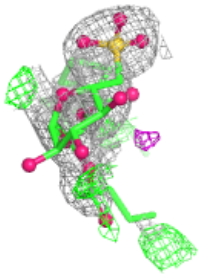


Electron density around SQD f 101:

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

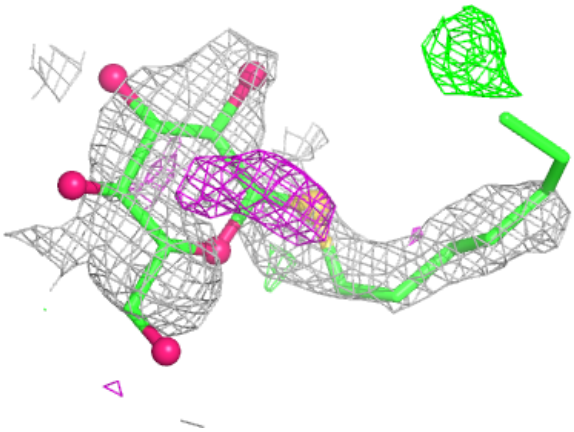


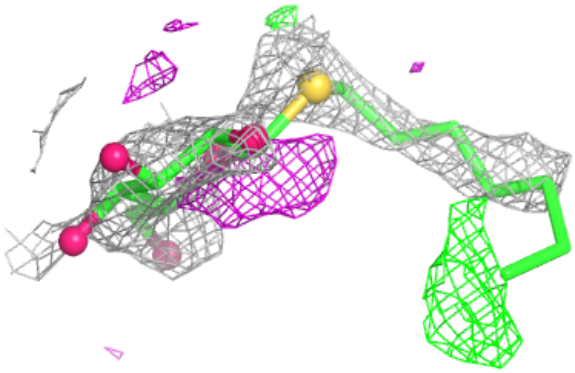


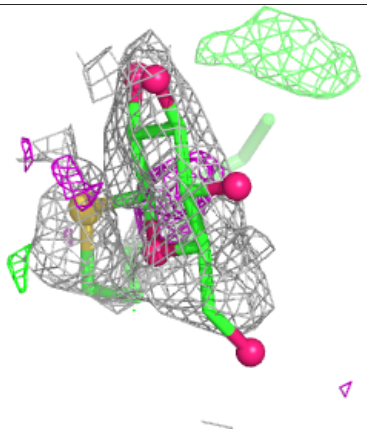


Electron density around HTG b 624:

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

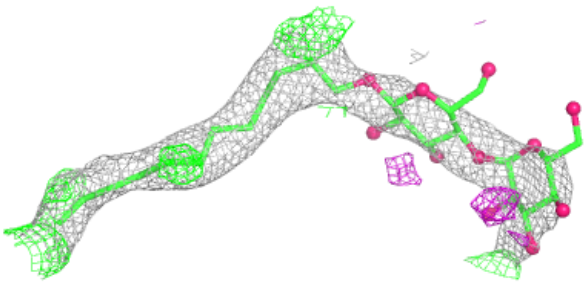


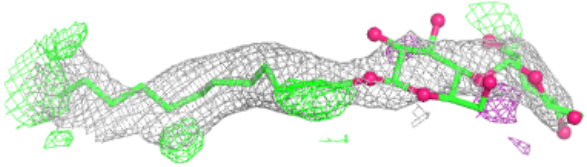


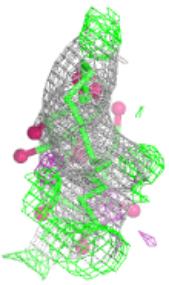


Electron density around LMT a 359:

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

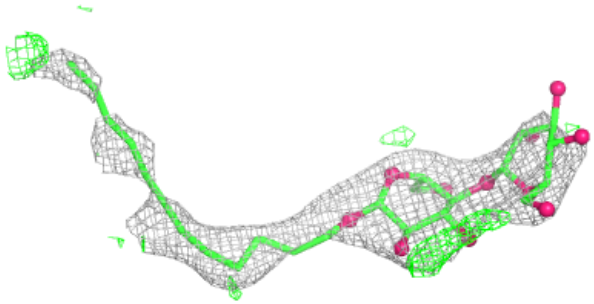


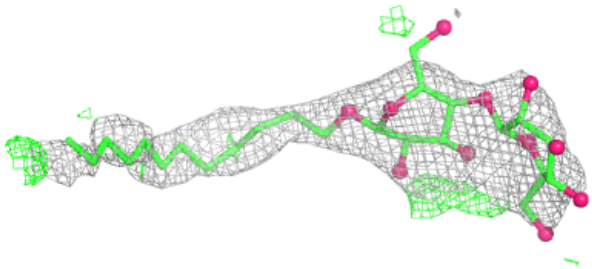


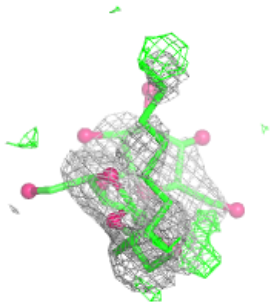


Electron density around LMT I 101:

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

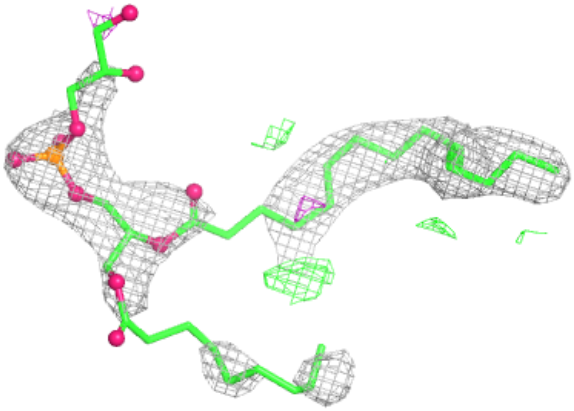


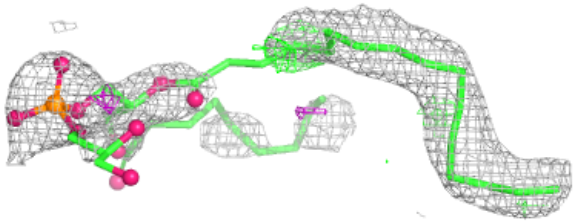


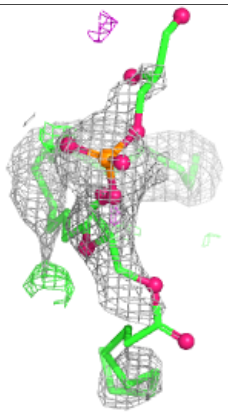


Electron density around LHG a 419:

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

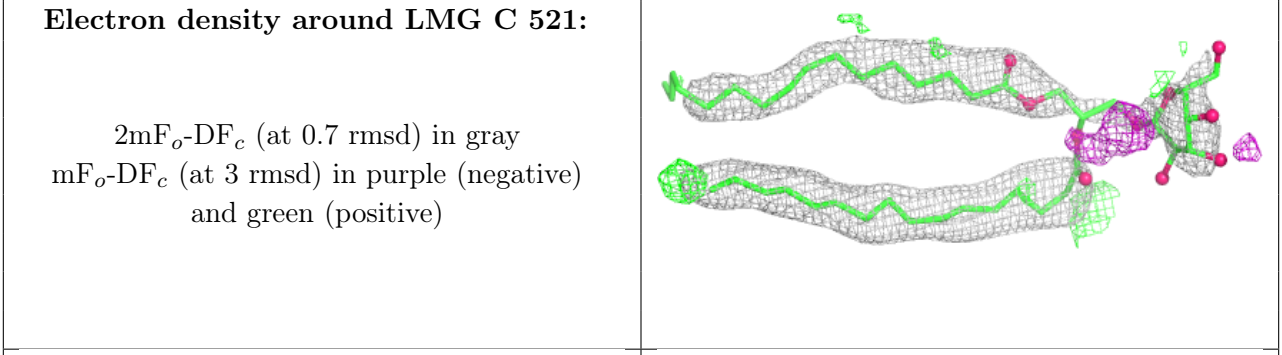


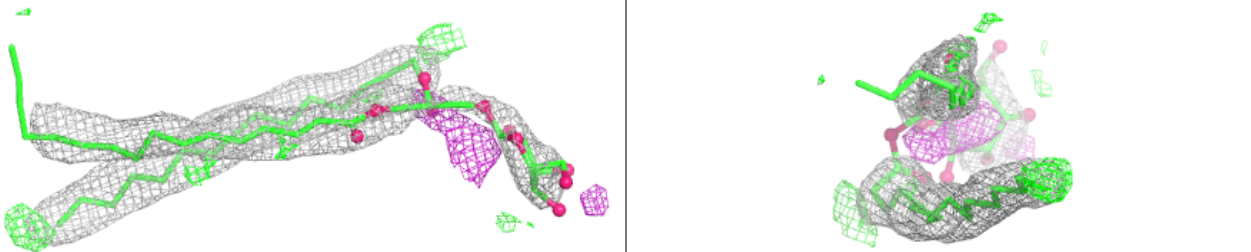




Electron density around LMG C 521:

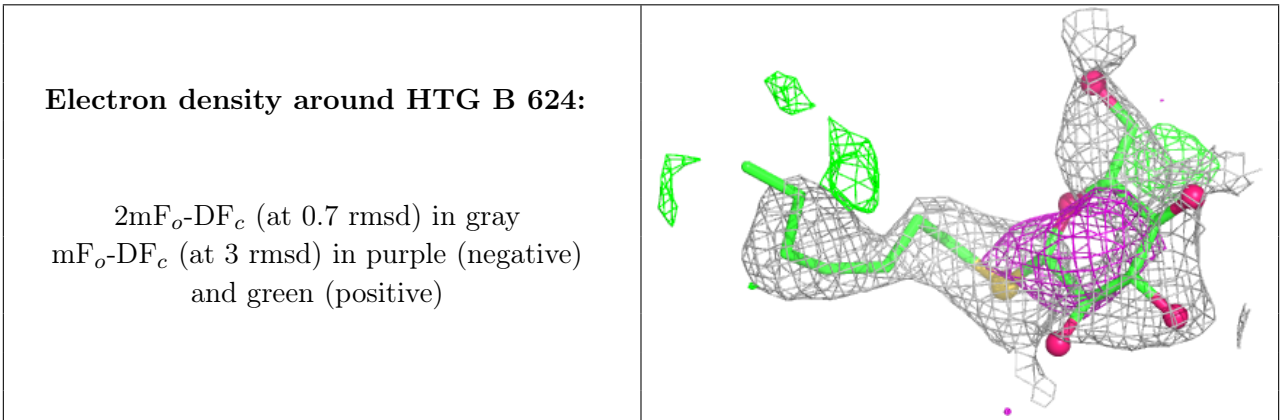
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

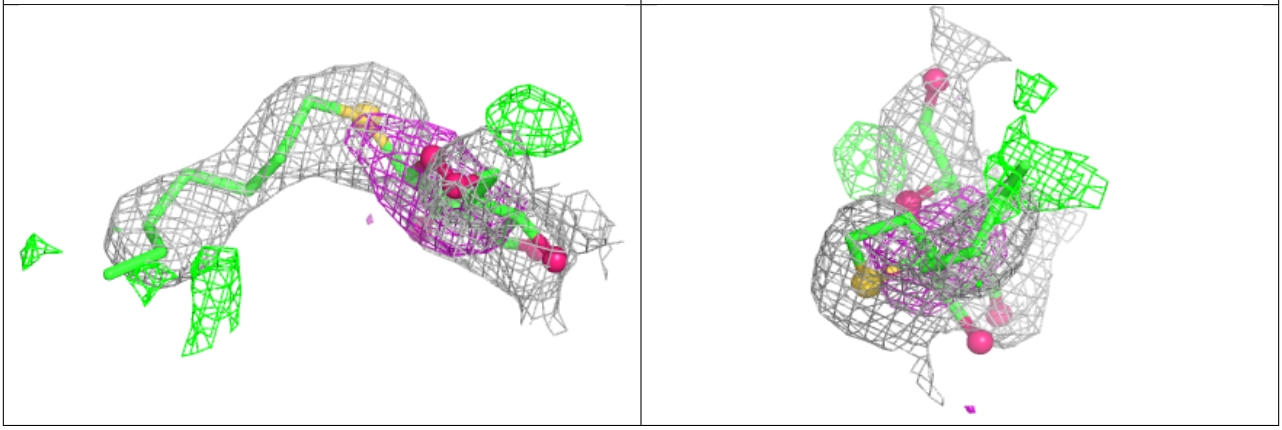




Electron density around HTG B 624:

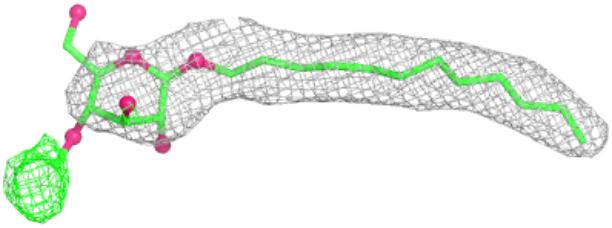
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

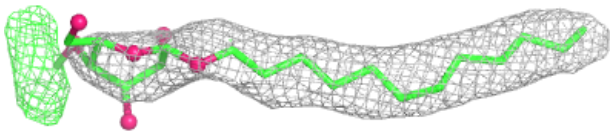


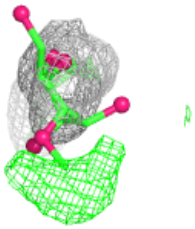


Electron density around LMT b 622:

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

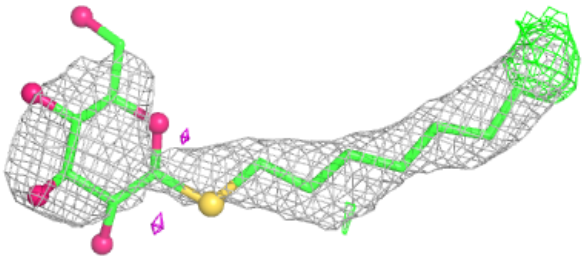


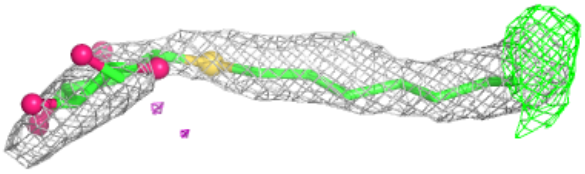


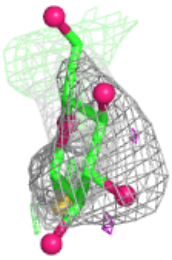


Electron density around HTG B 625:

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

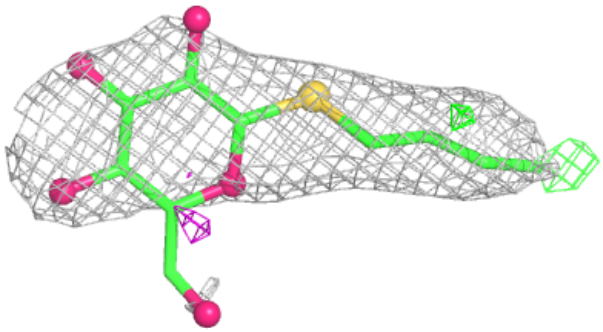


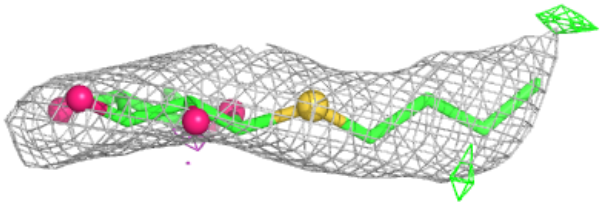


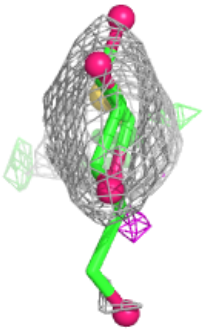


Electron density around HTG h 101:

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

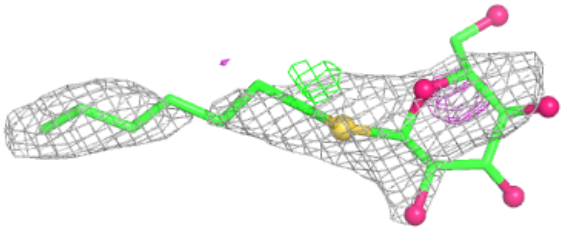


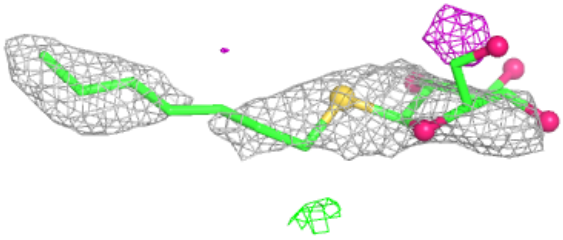


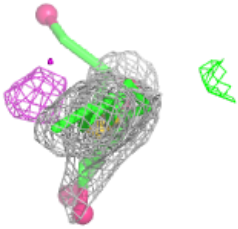


Electron density around HTG C 523:

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

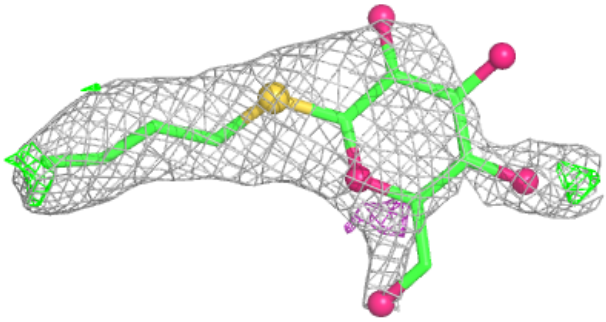


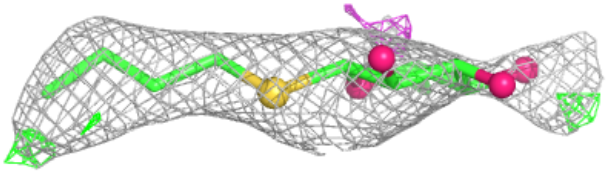


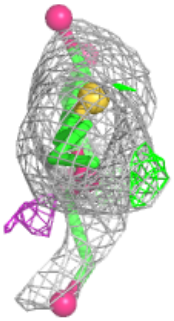


Electron density around HTG D 410:

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

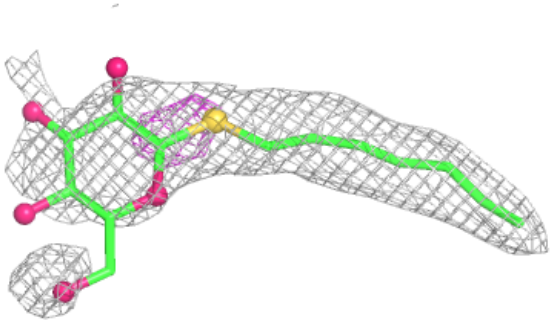


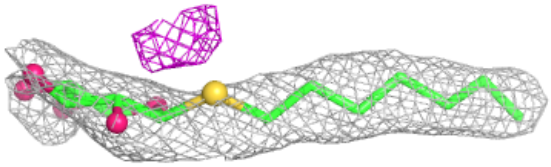


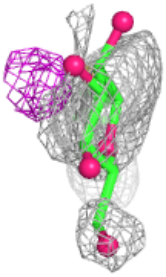


Electron density around HTG b 625:

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

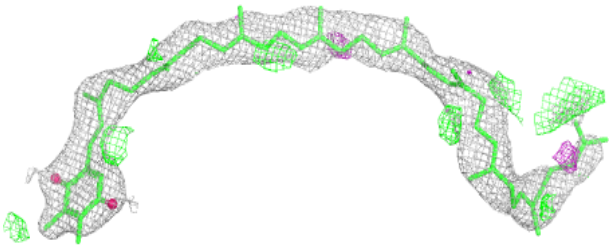


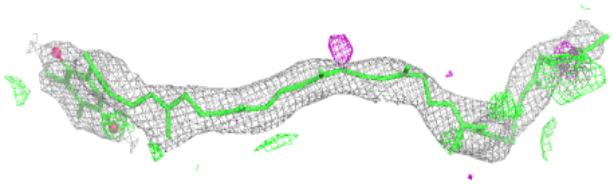


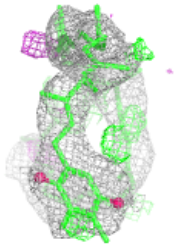


Electron density around PL9 A 416 (A):

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

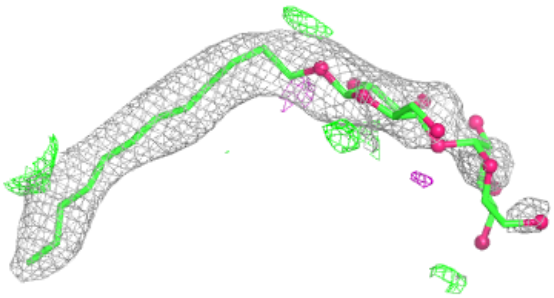


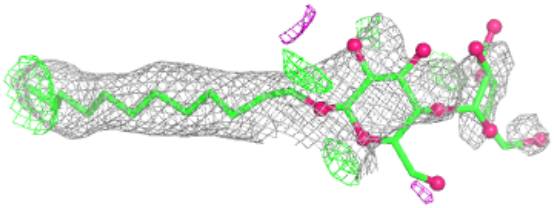


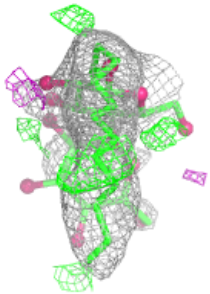


Electron density around LMT M 103:

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

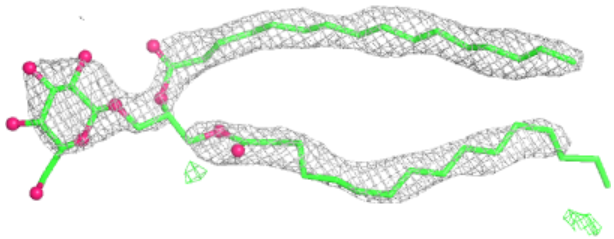


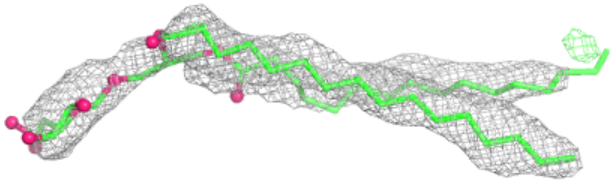


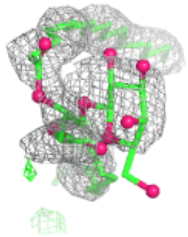


Electron density around LMG c 522:

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

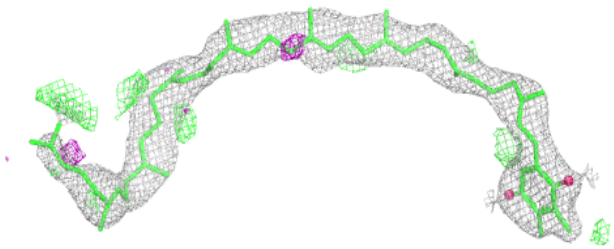


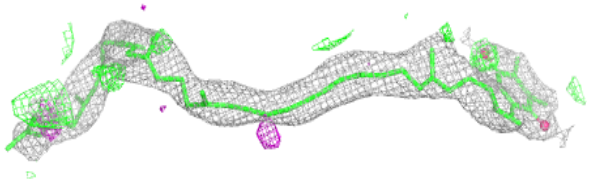


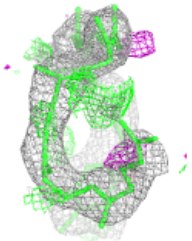


Electron density around PL9 A 416 (B):

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

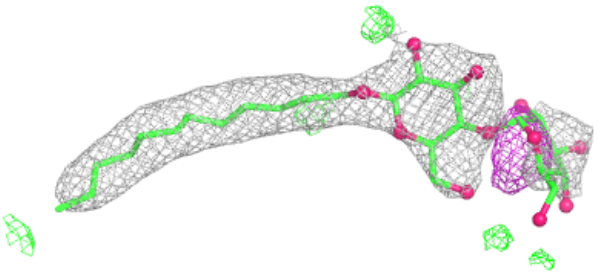


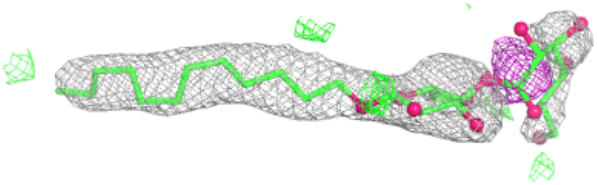


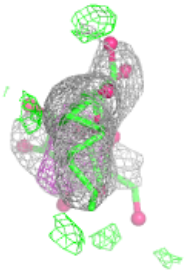


Electron density around LMT B 622:

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

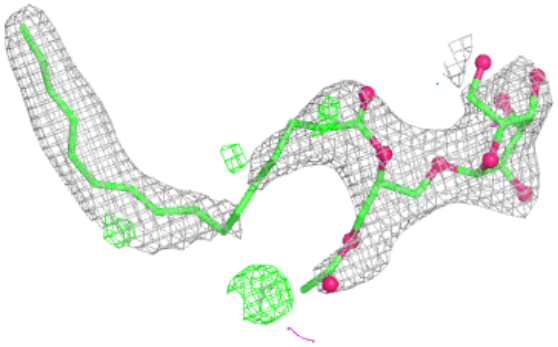


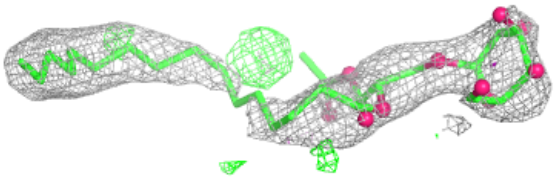


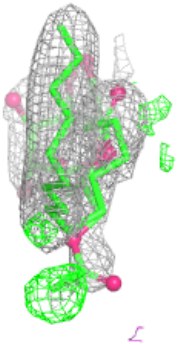


Electron density around LMG Z 101:

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

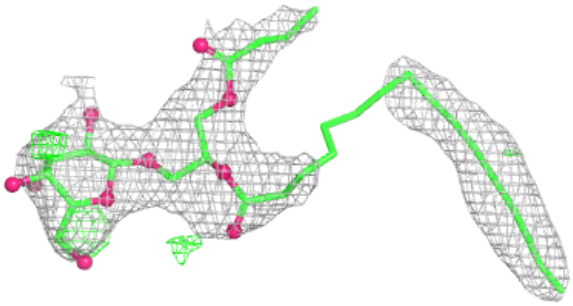


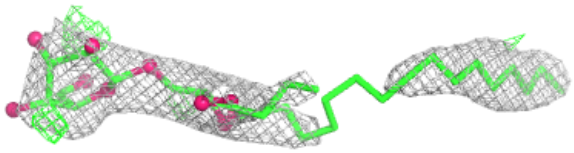


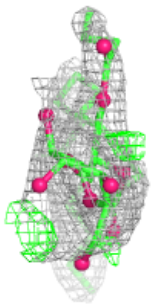


Electron density around LMG z 101:

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

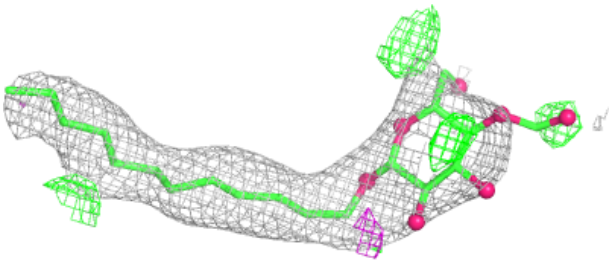


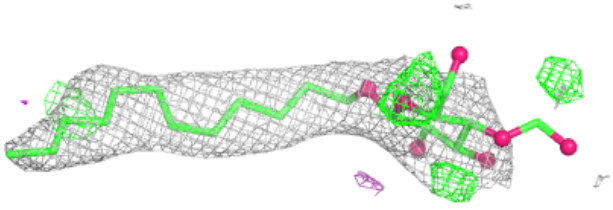


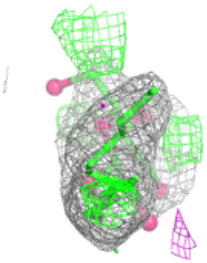


Electron density around LMT t 101:

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

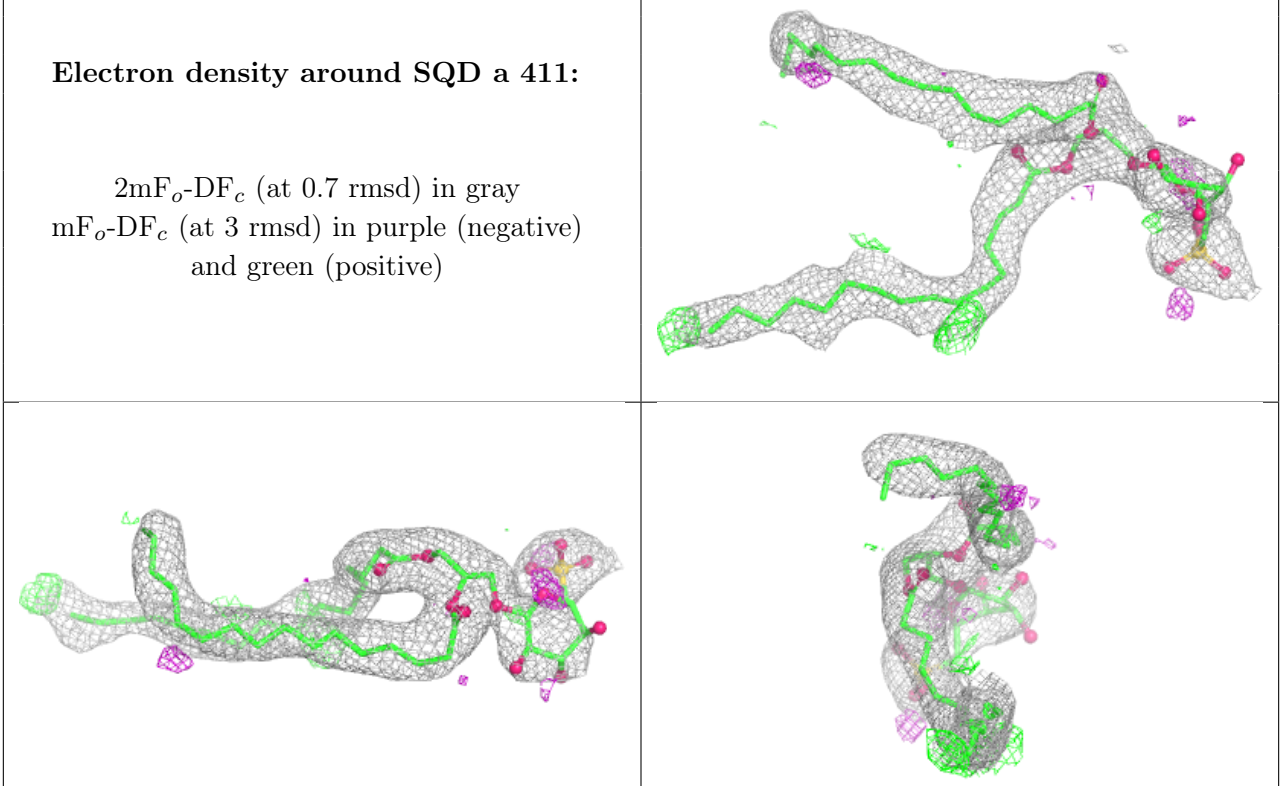






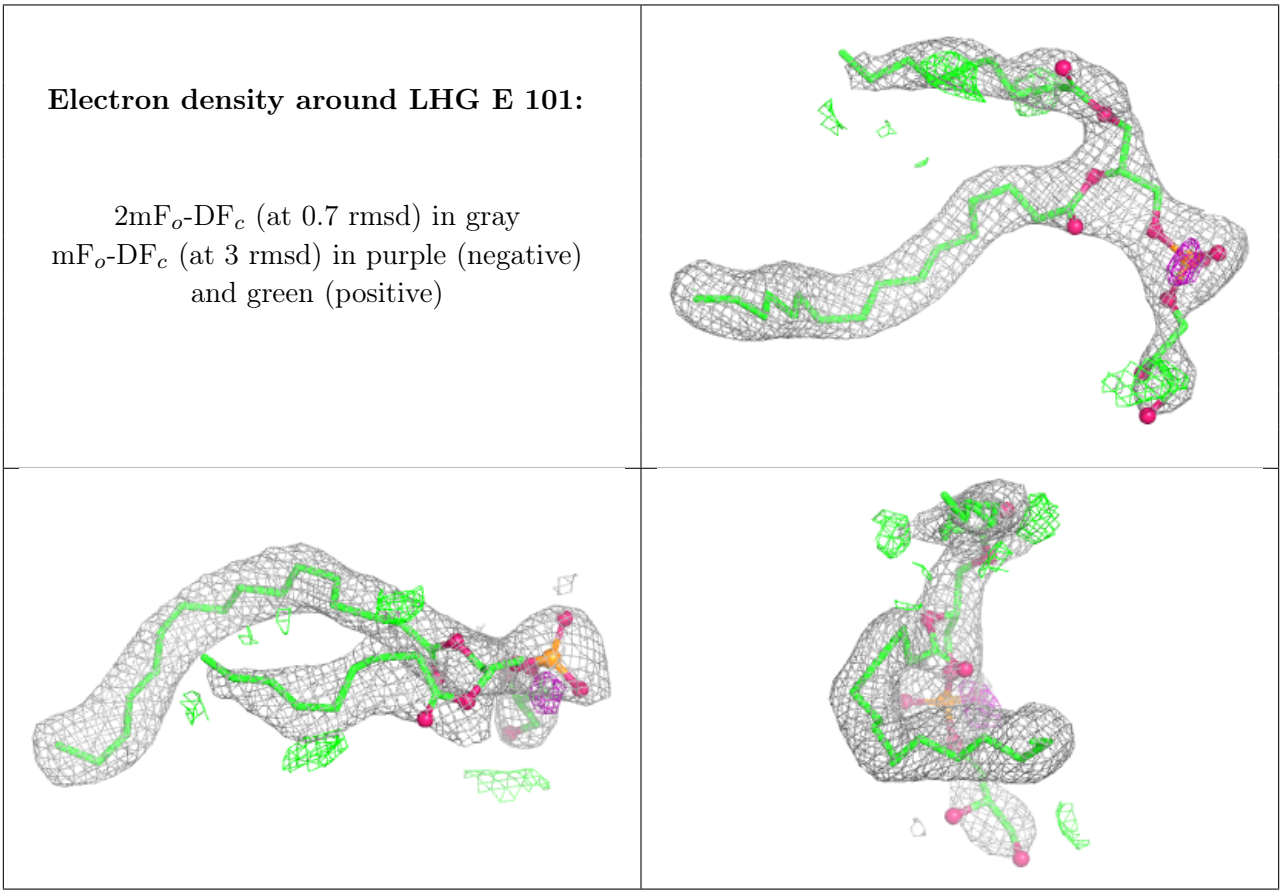
Electron density around SQD a 411:

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



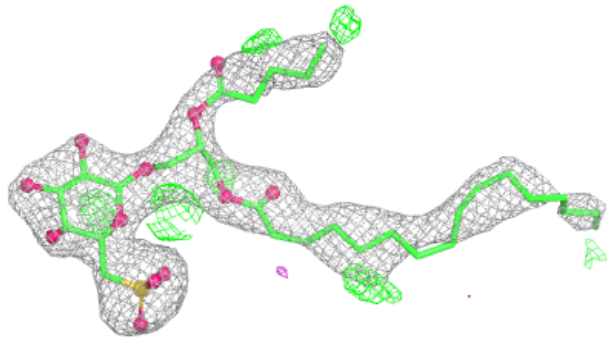
Electron density around LHG E 101:

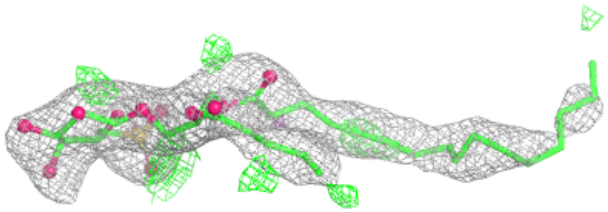
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

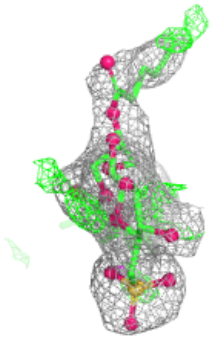


Electron density around SQD F 101:

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

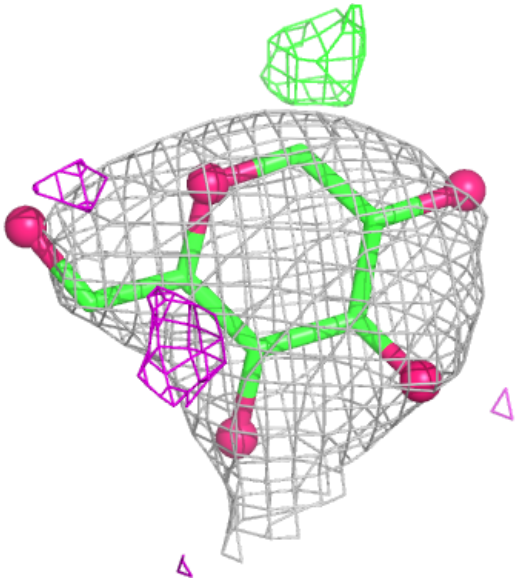


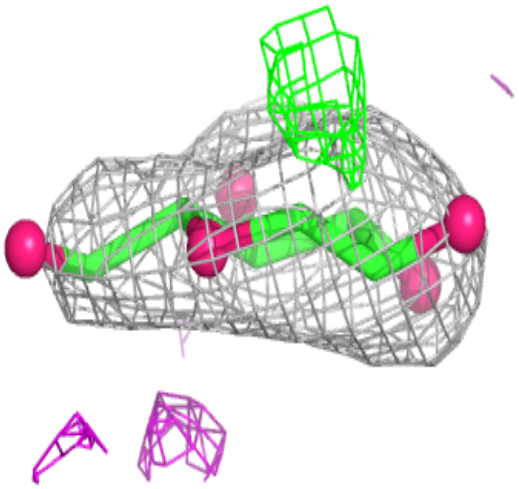


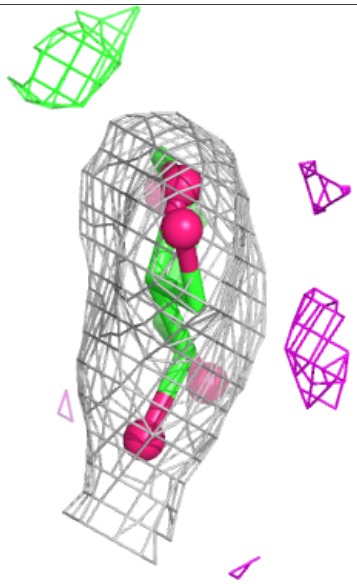


Electron density around HTG V 204:

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

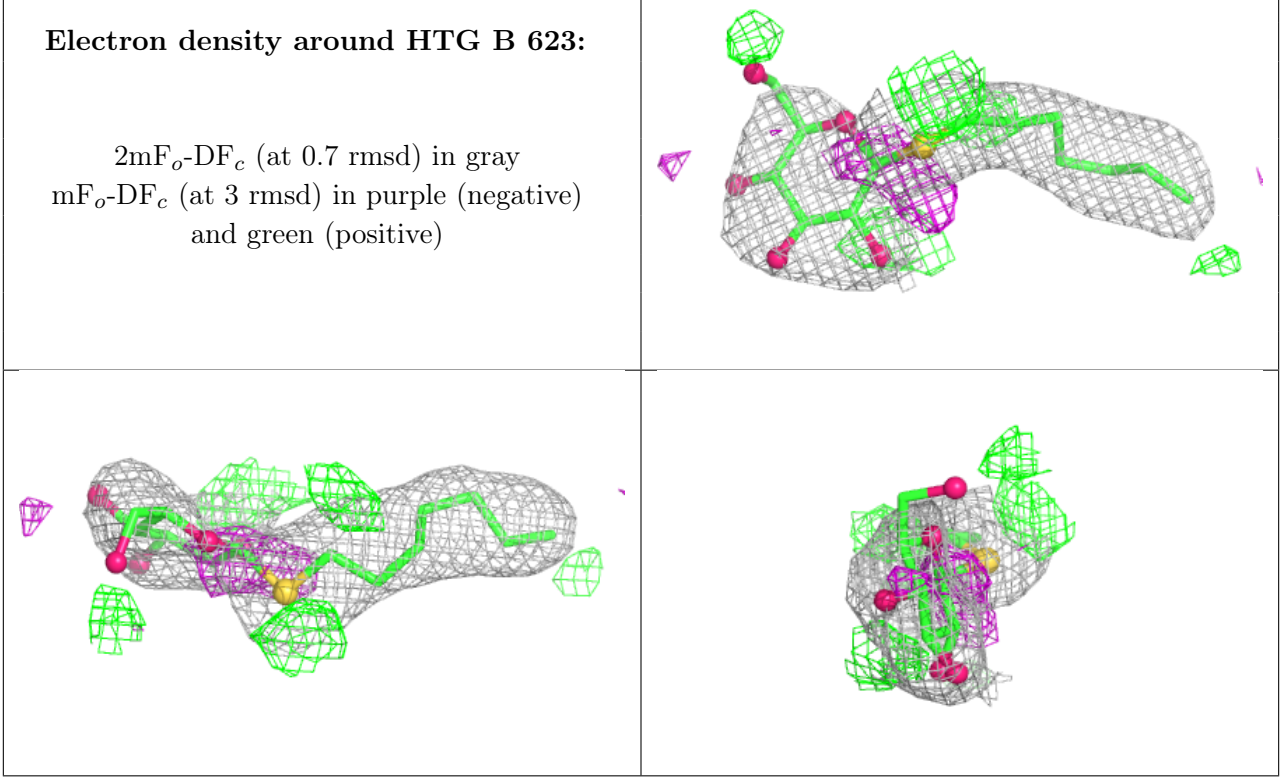






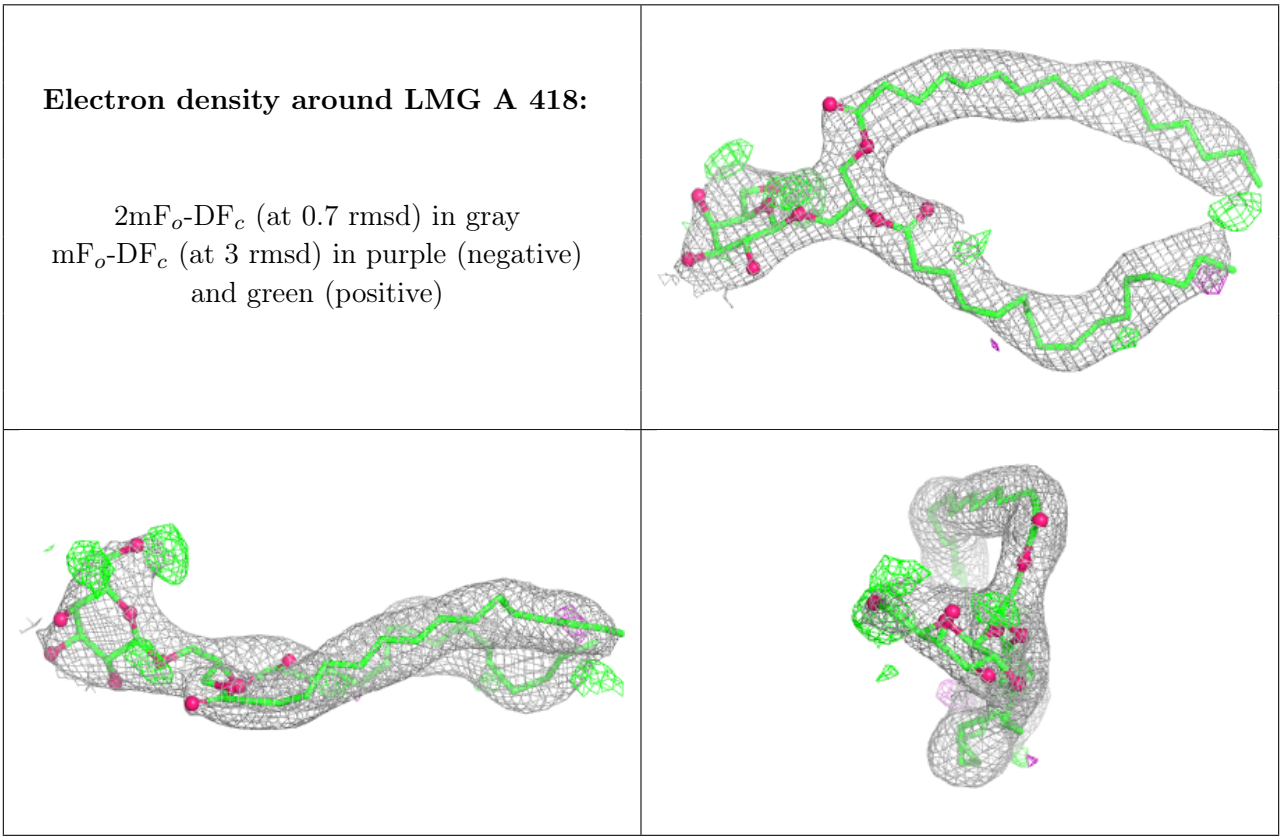
Electron density around HTG B 623:

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



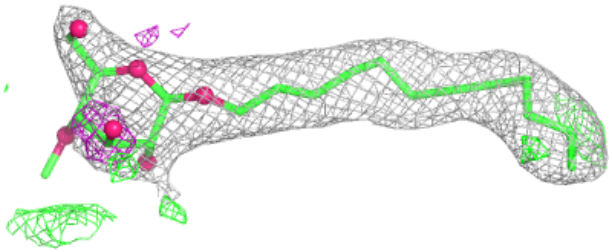
Electron density around LMG A 418:

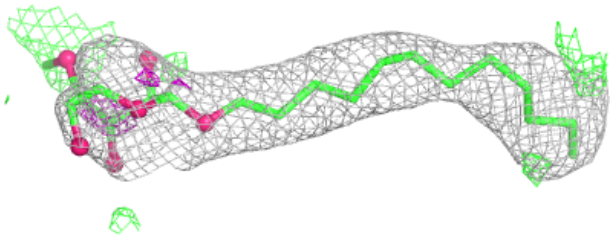
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

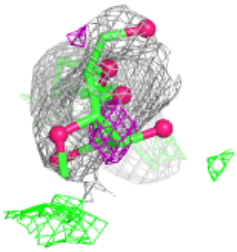


Electron density around LMT B 630:

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

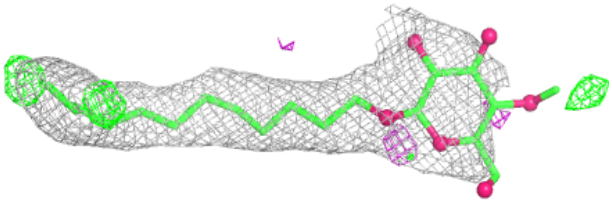


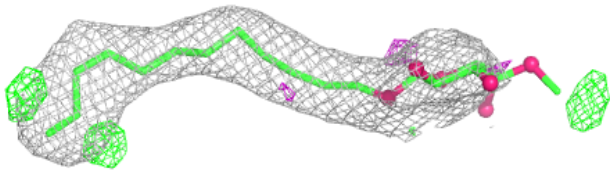


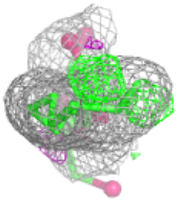


Electron density around LMT b 630:

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

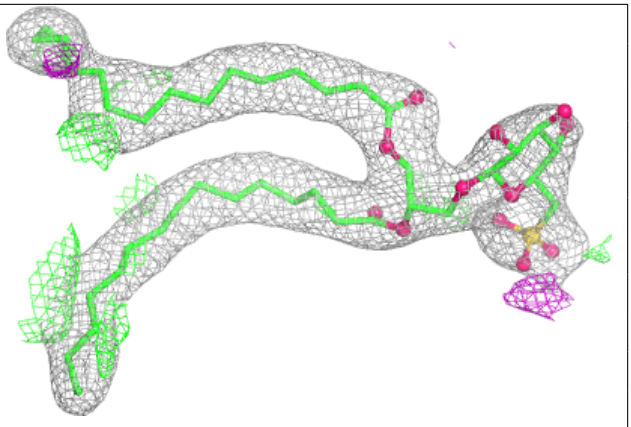


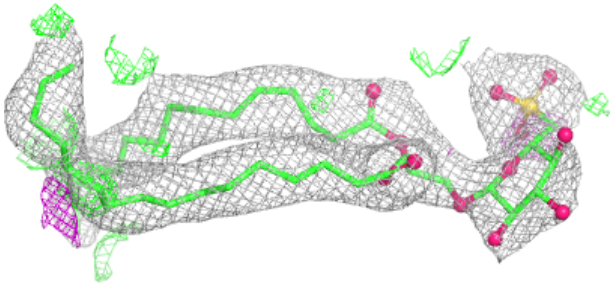


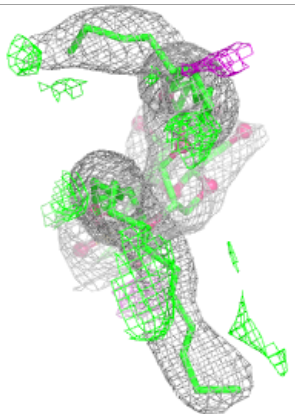


Electron density around SQD B 620:

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

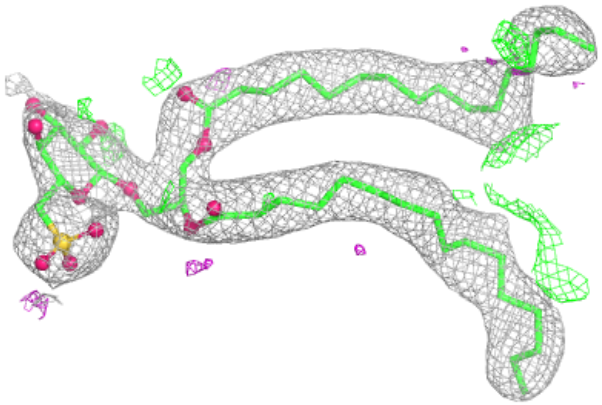


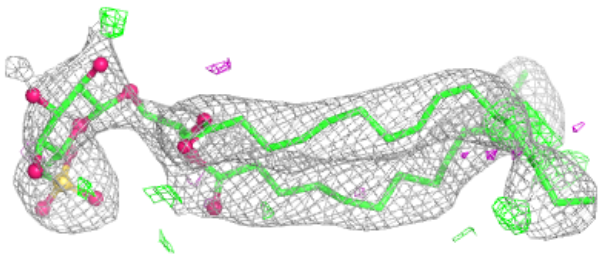




Electron density around SQD b 620:

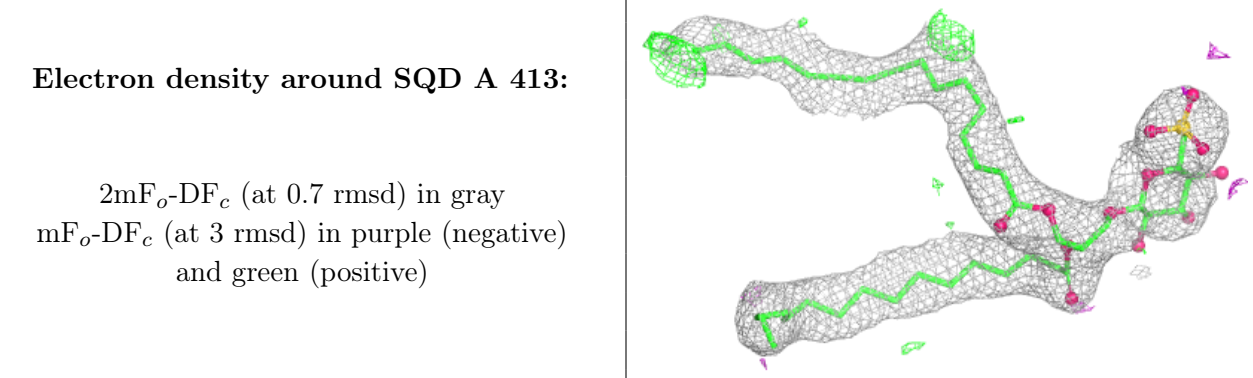
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





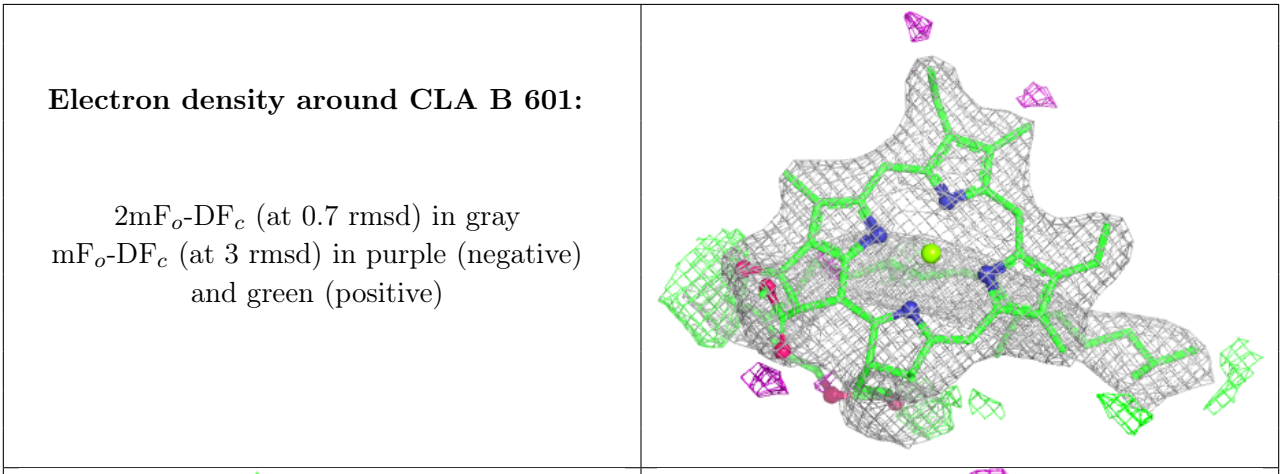
Electron density around SQD A 413:

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



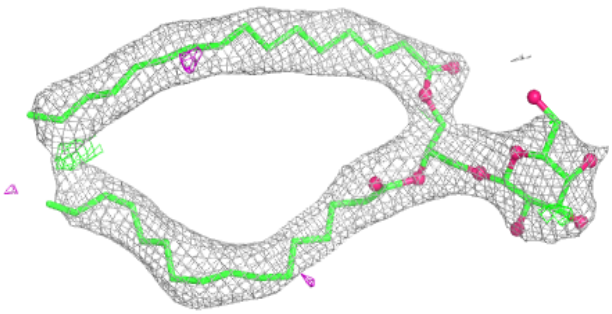
Electron density around CLA B 601:

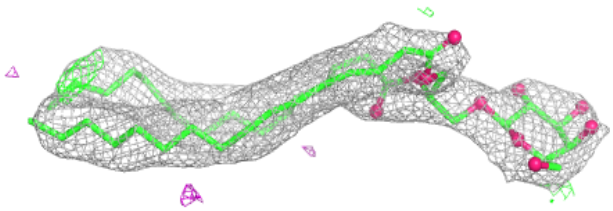
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

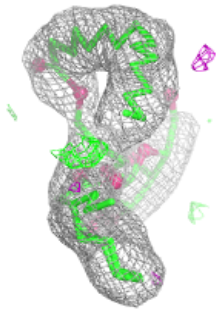


Electron density around LMG a 417:

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

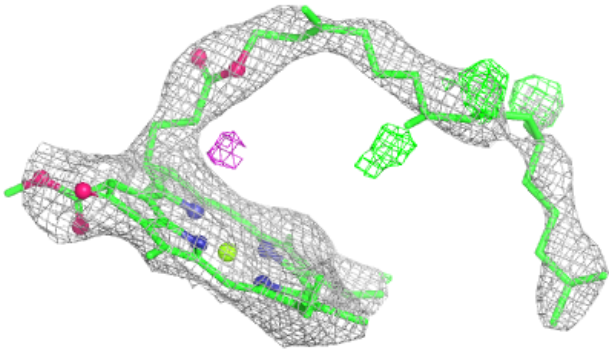


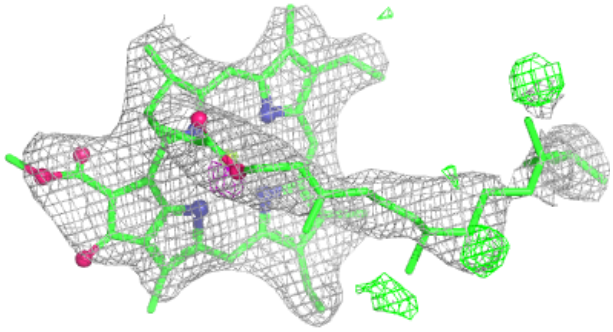


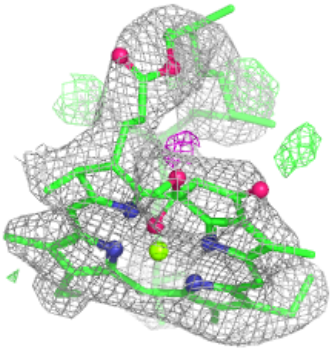


Electron density around CLA c 515:

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

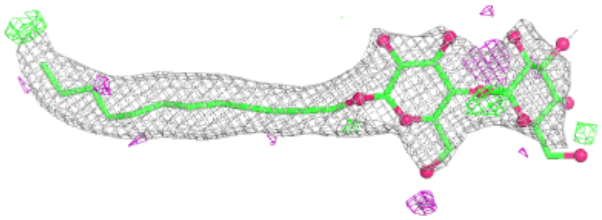


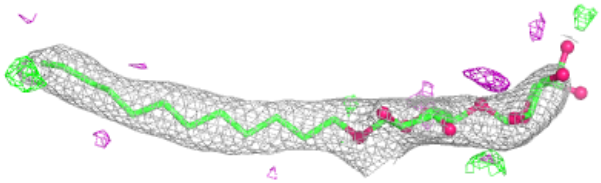


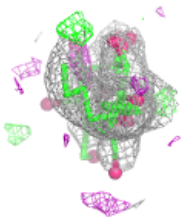


Electron density around LMT m 102:

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

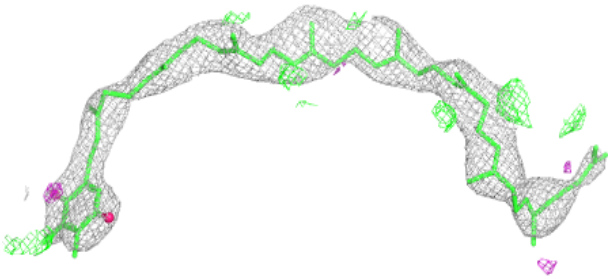


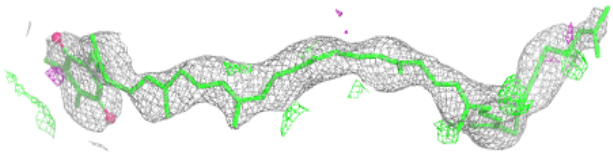


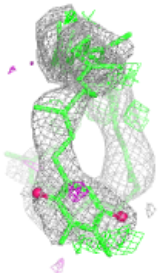


Electron density around PL9 a 414 (A):

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

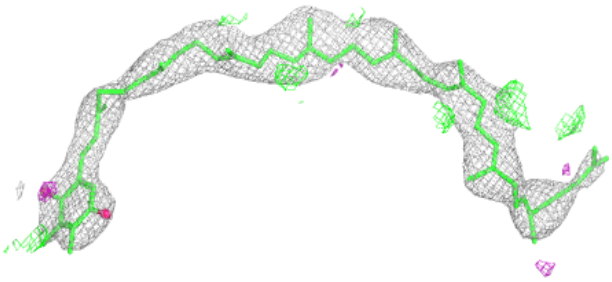


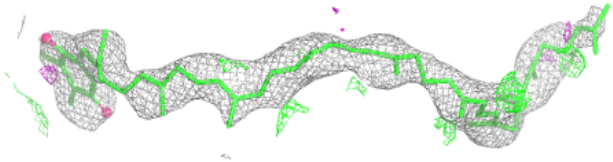


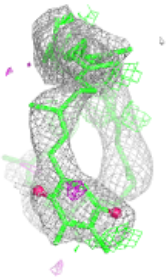


Electron density around PL9 a 414 (B):

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

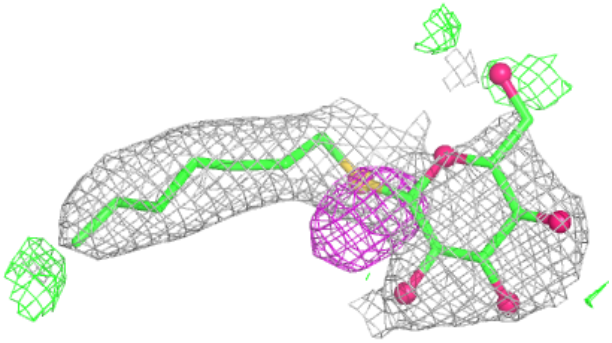


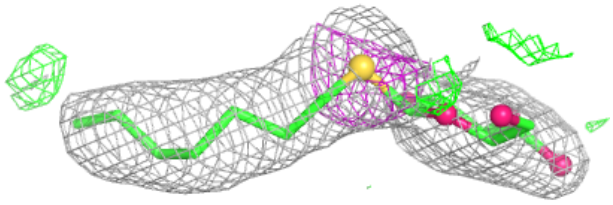


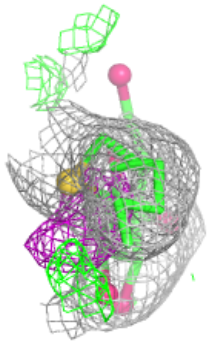


Electron density around HTG b 623:

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

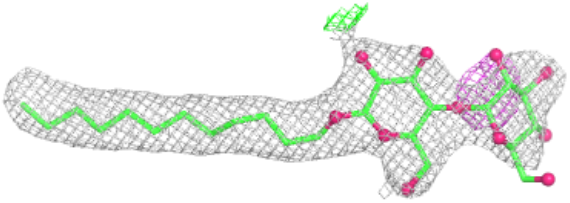


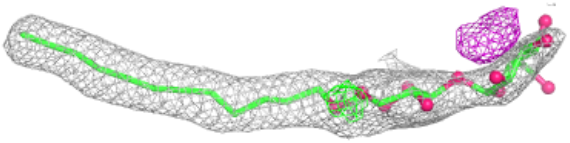


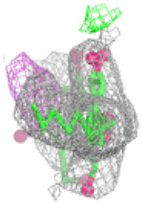


Electron density around LMT M 101:

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

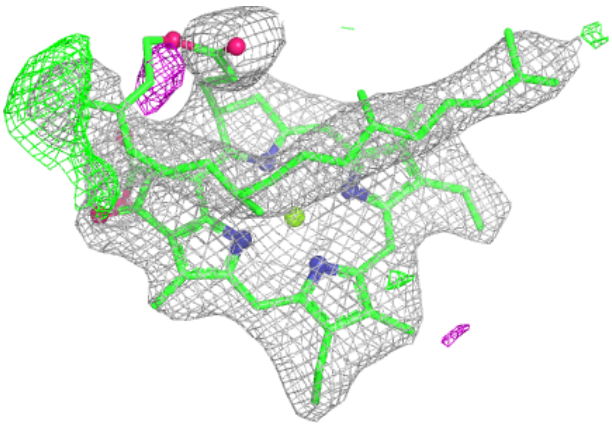


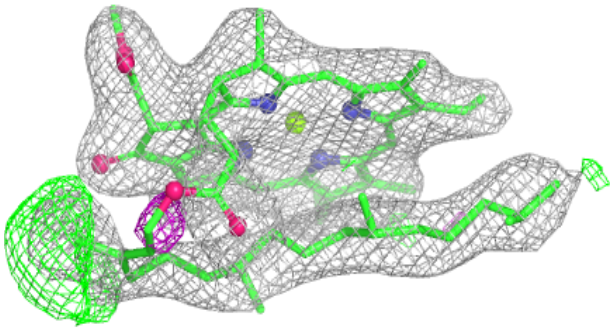


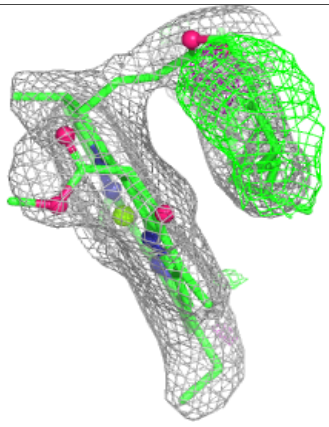


Electron density around CLA b 601:

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

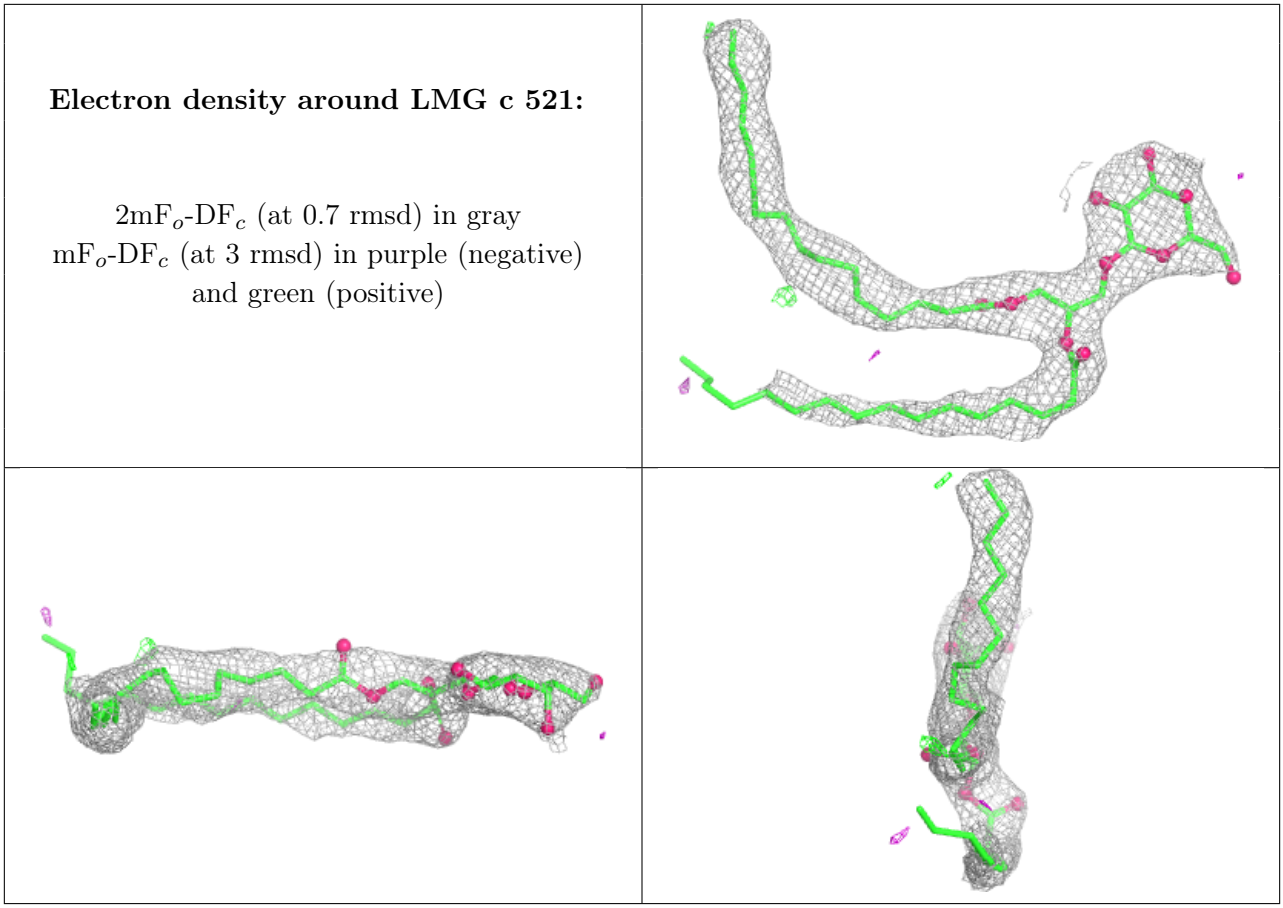






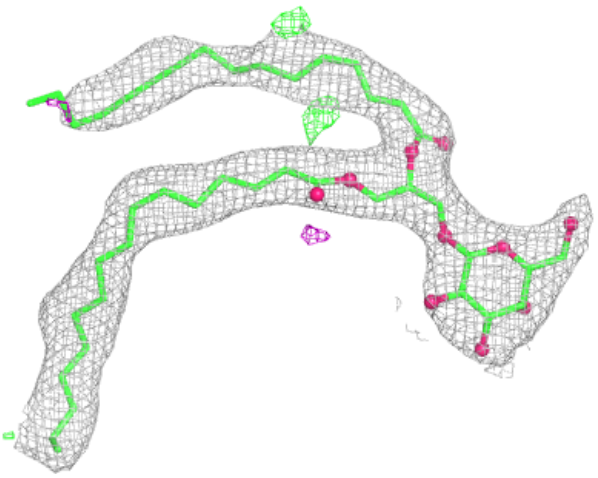
Electron density around LMG c 521:

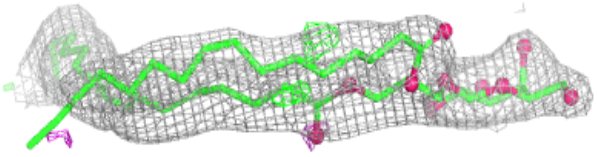
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

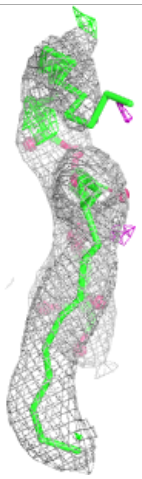


Electron density around LMG C 520:

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

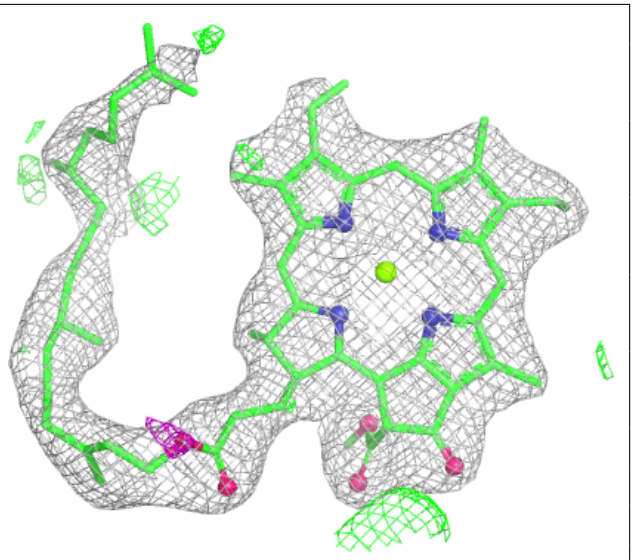


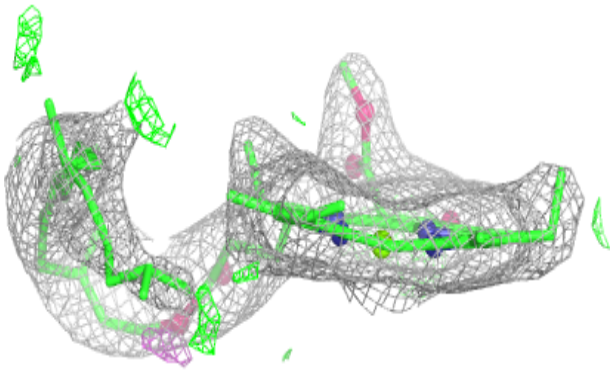


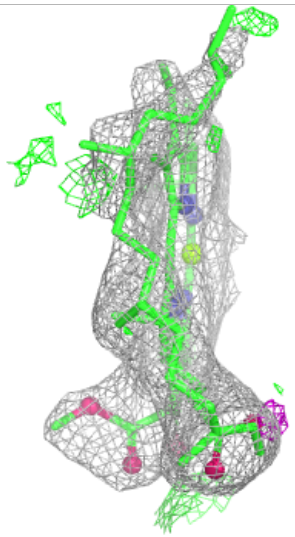


Electron density around CLA c 514:

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

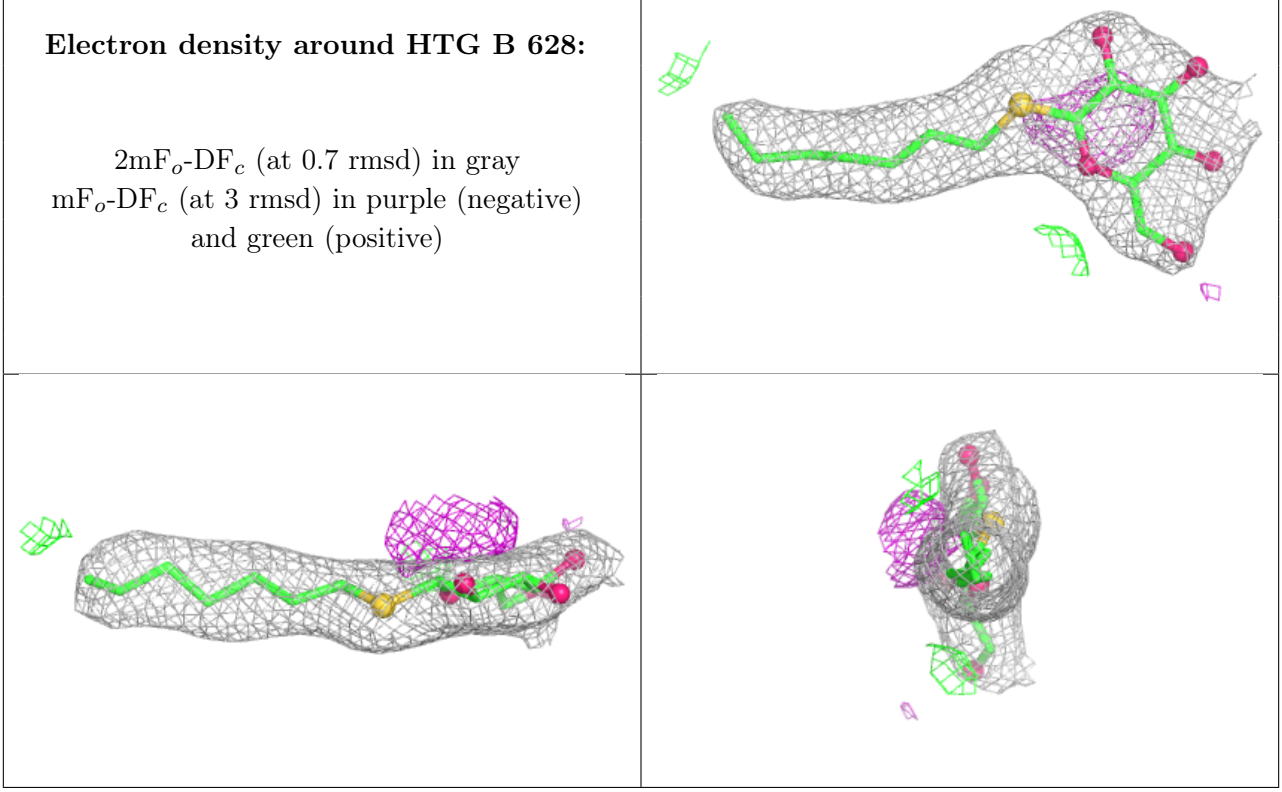






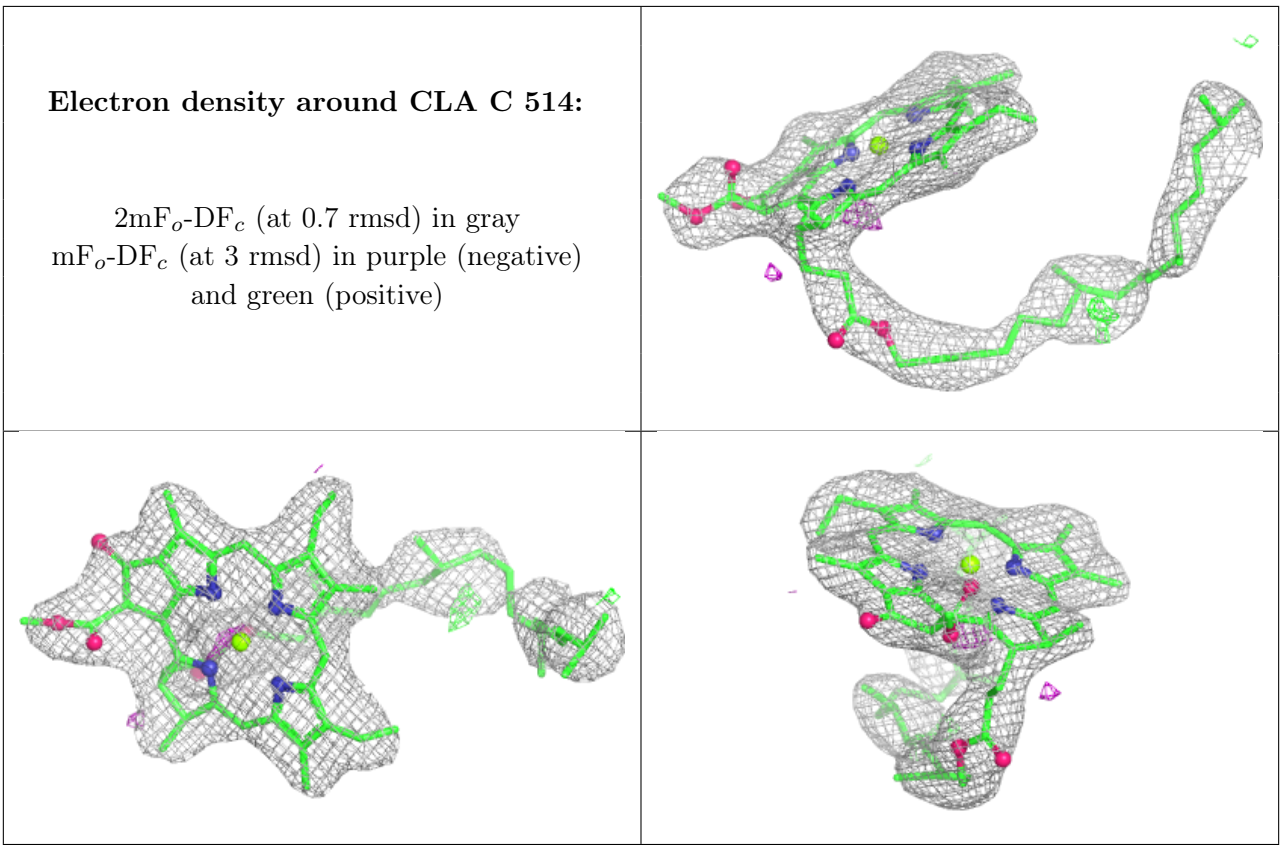
Electron density around HTG B 628:

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



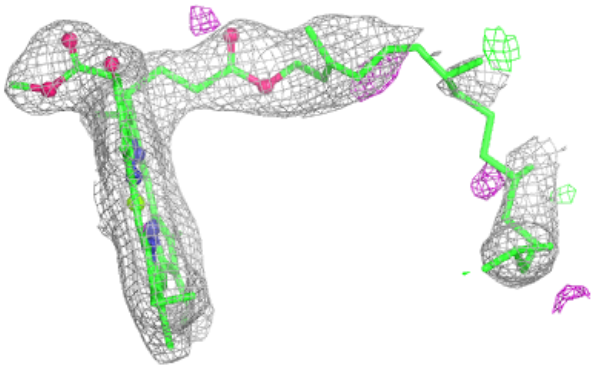
Electron density around CLA C 514:

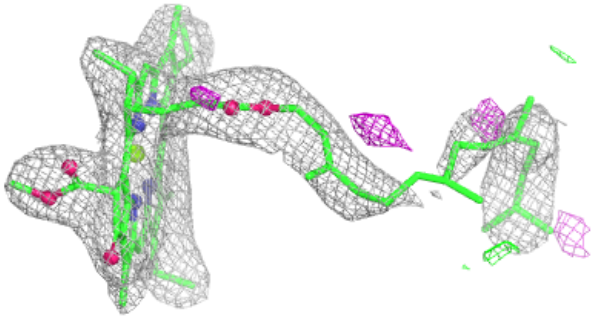
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

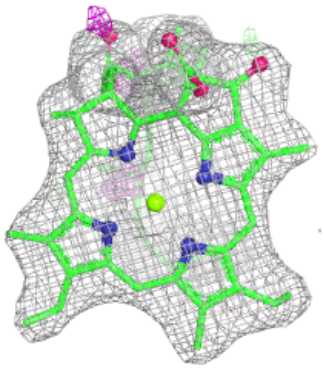


Electron density around CLA C 507:

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

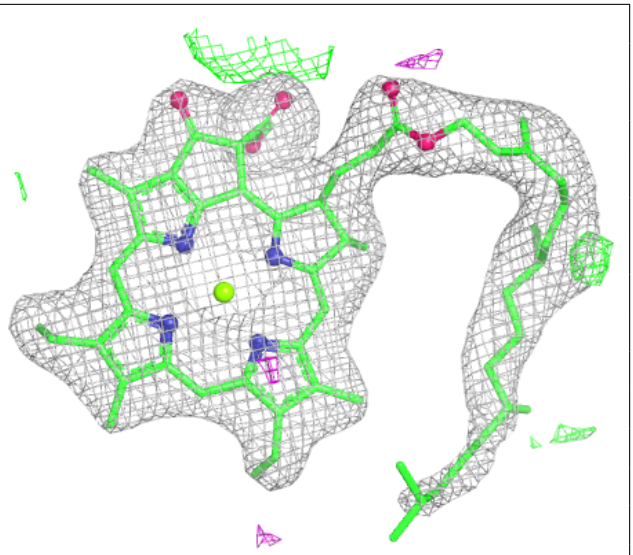


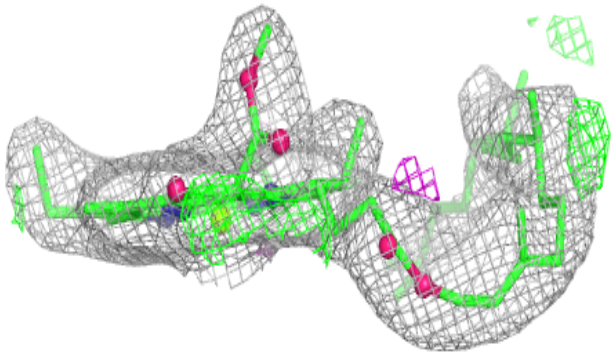


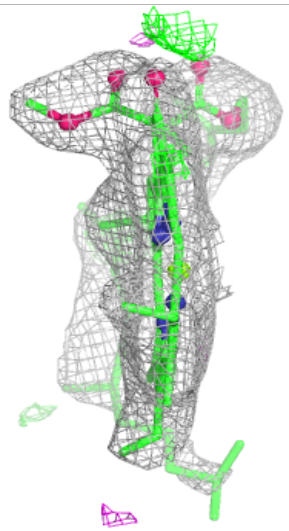


Electron density around CLA C 513:

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

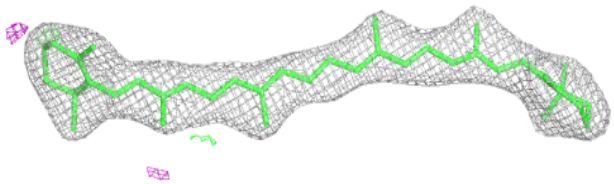


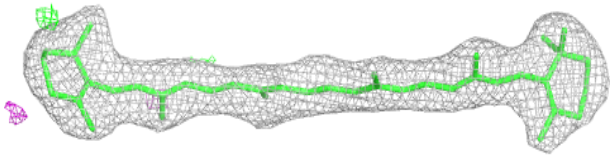


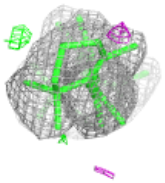


Electron density around BCR C 515:

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

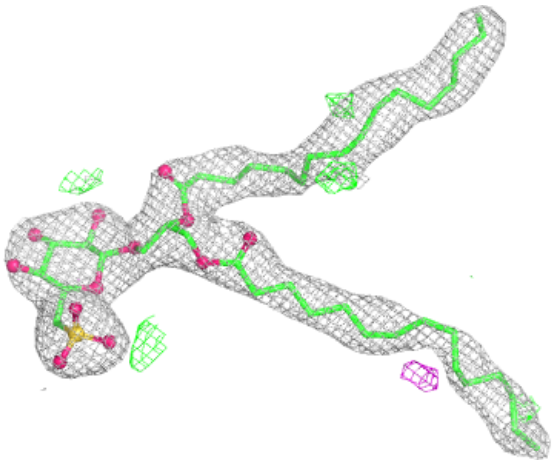


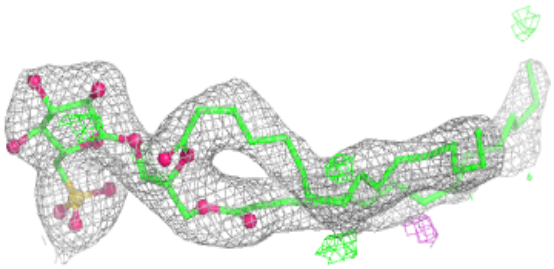


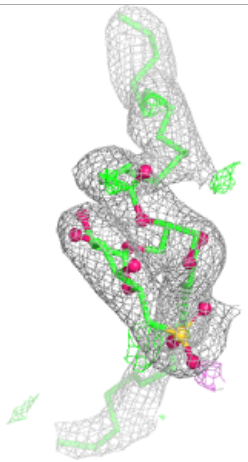


Electron density around SQD a 409:

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

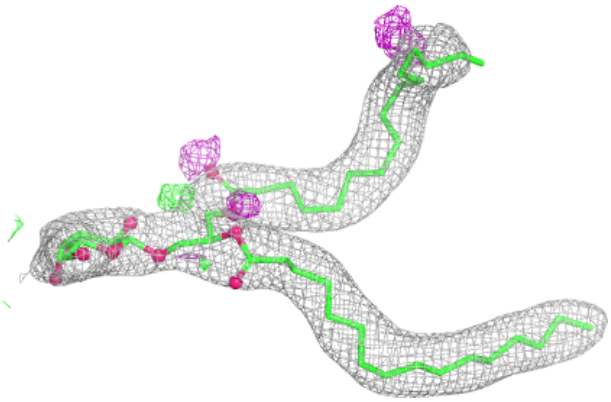


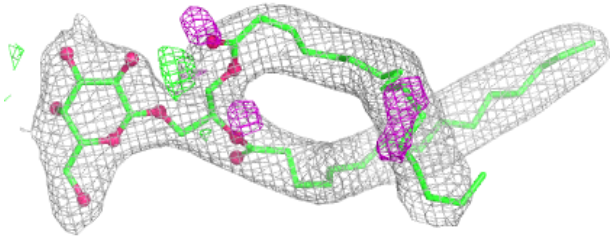


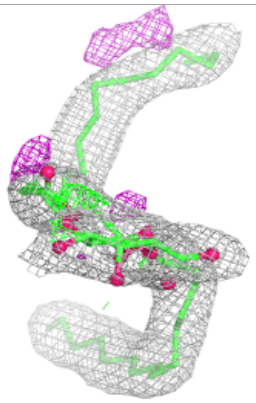


Electron density around LMG b 621:

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

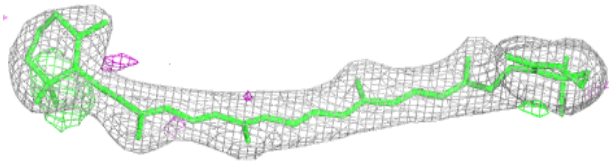


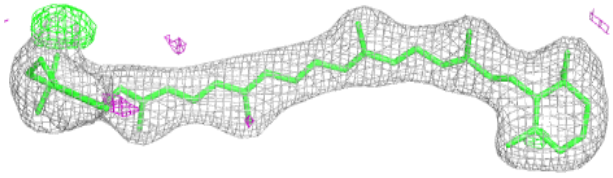


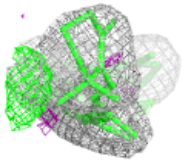


Electron density around BCR D 404:

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

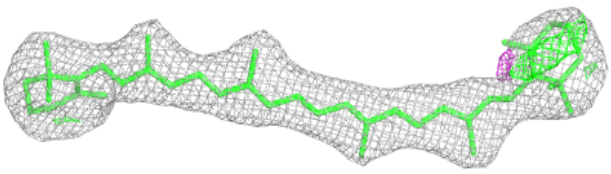


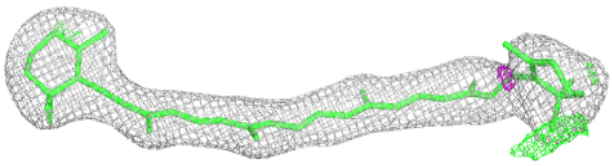


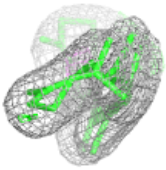


Electron density around BCR d 404:

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

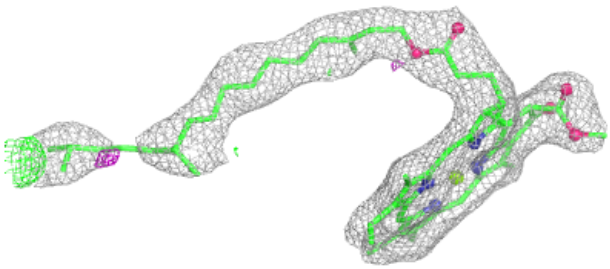


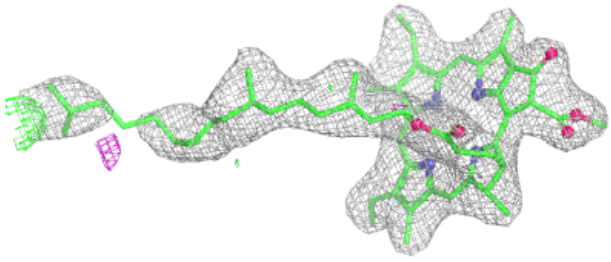


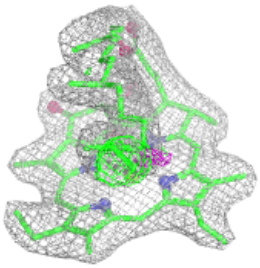


Electron density around CLA c 506:

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

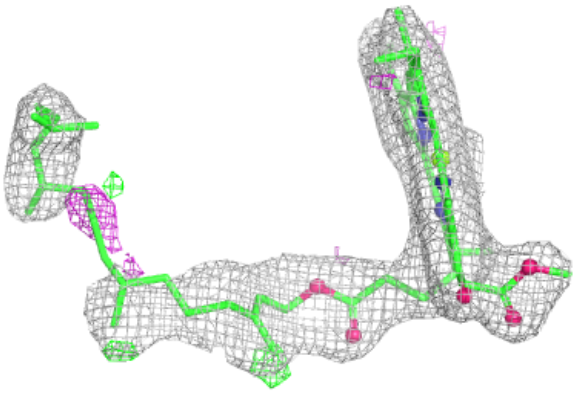


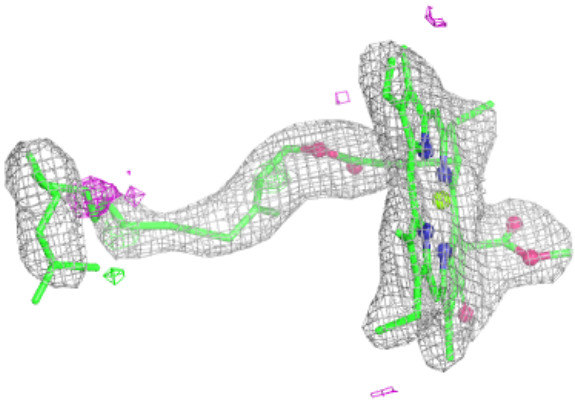


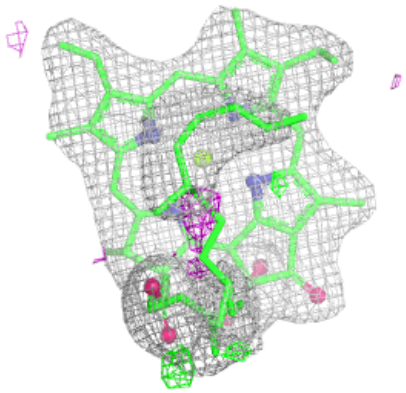


Electron density around CLA c 508:

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

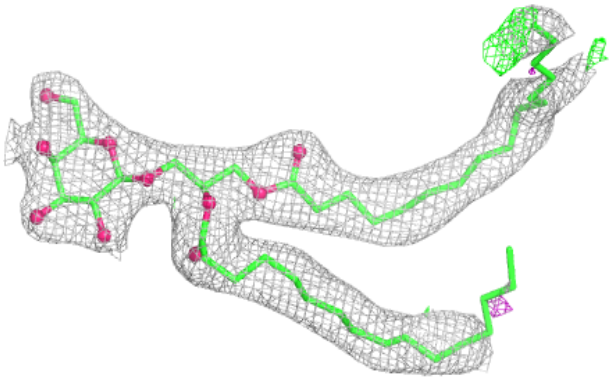


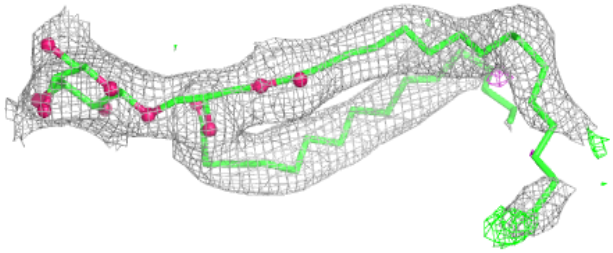




Electron density around LMG J 101:

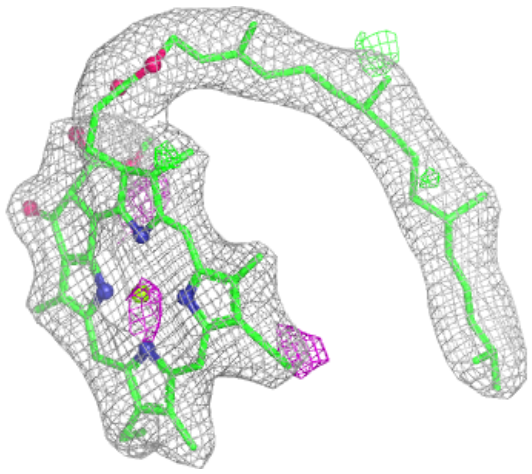
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

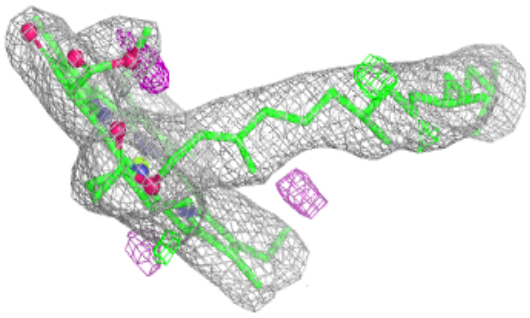


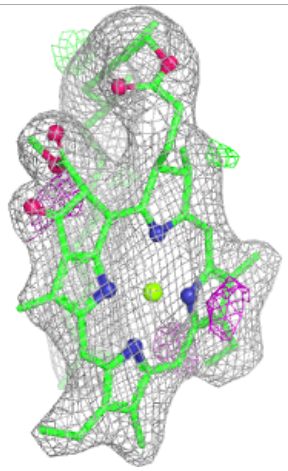


Electron density around CLA c 509:

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

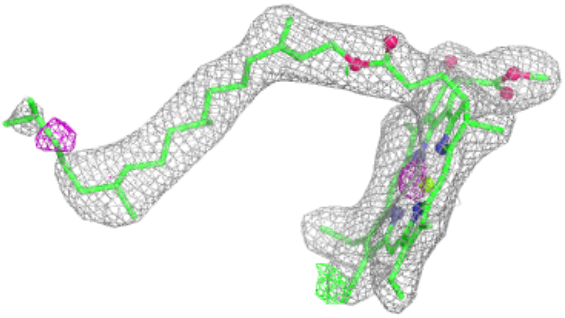


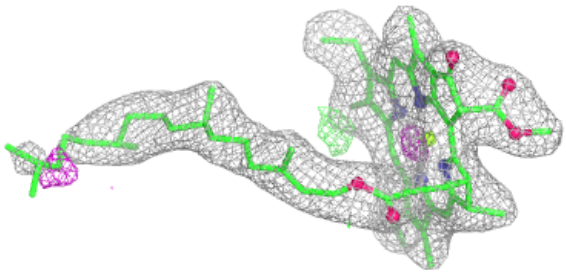


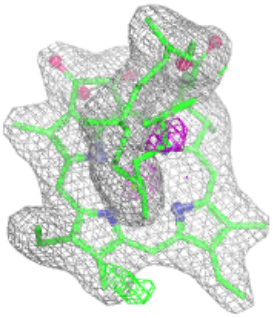


Electron density around CLA C 509:

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

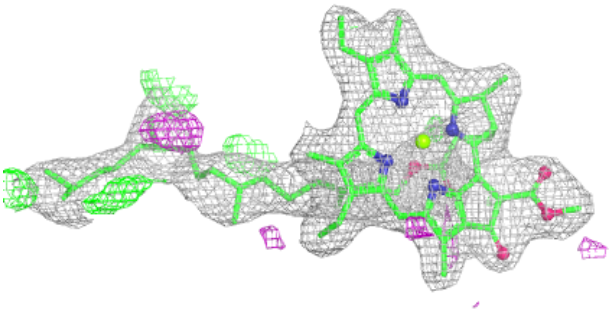


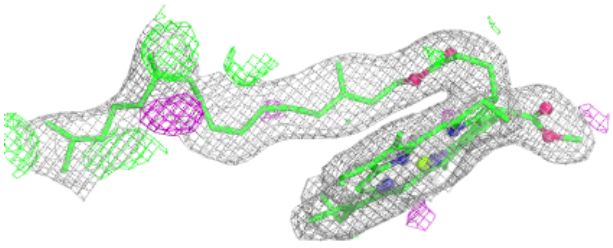


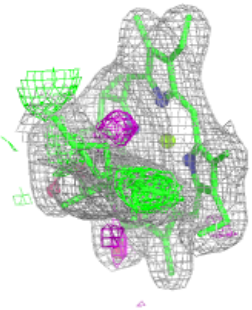


Electron density around CLA B 614:

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

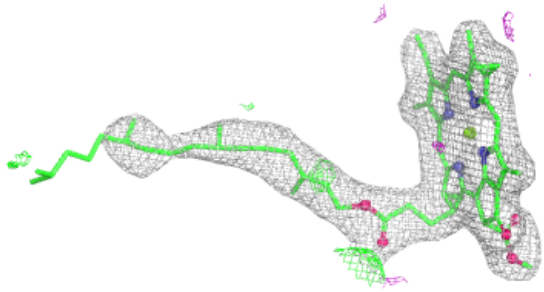


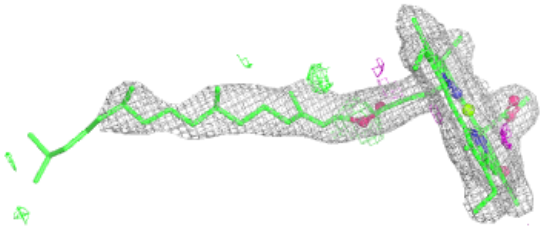


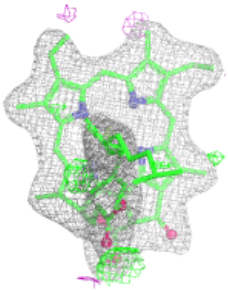


Electron density around CLA d 403:

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

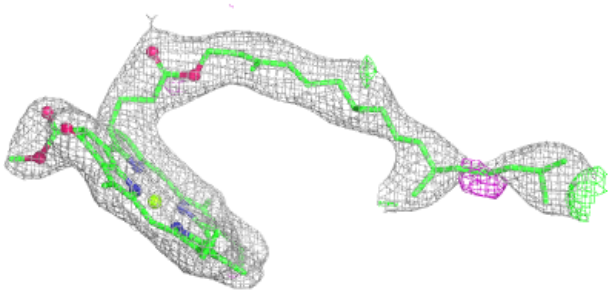


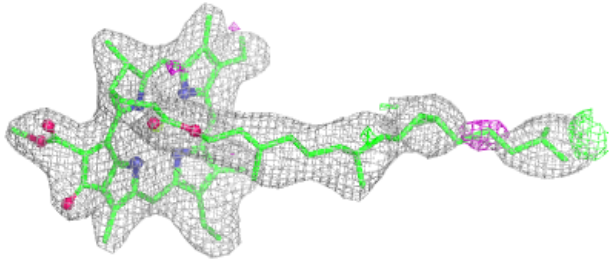


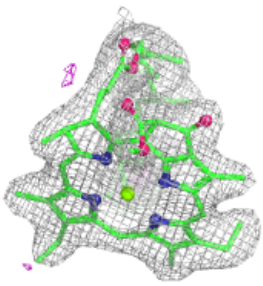


Electron density around CLA C 505:

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

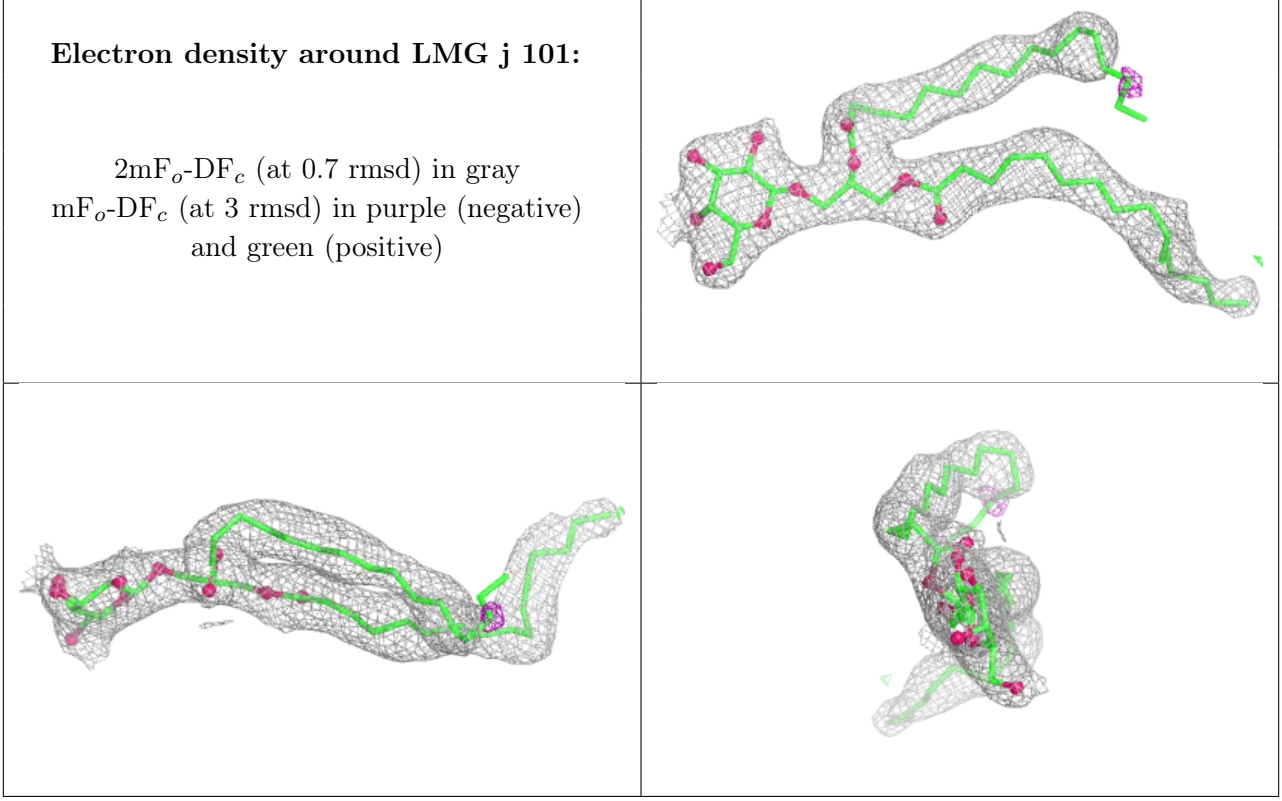






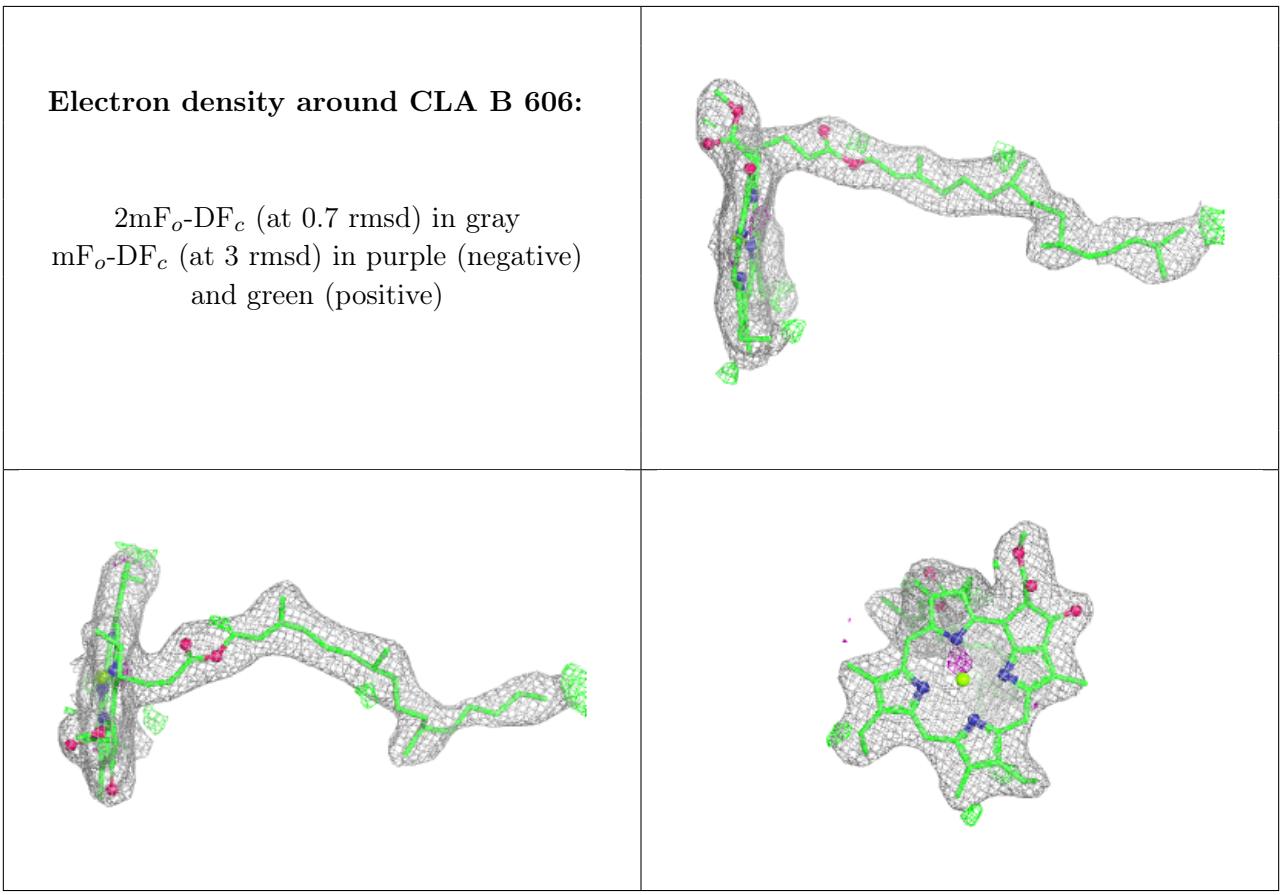
Electron density around LMG j 101:

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



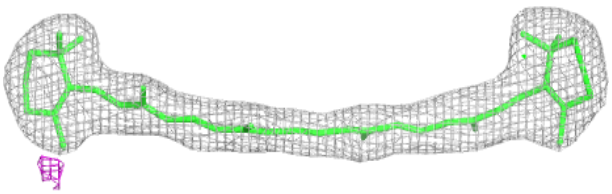
Electron density around CLA B 606:

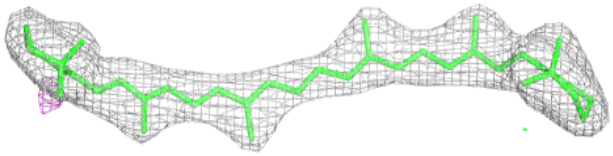
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

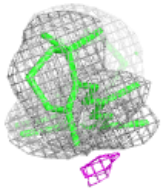


Electron density around BCR K 102:

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

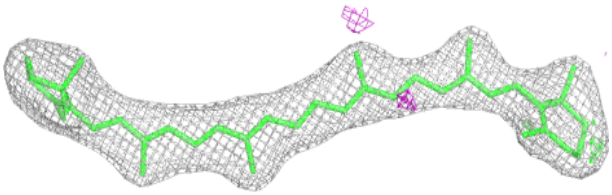


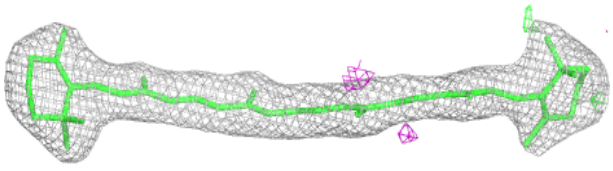


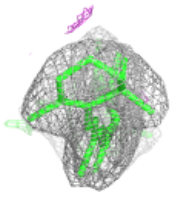


Electron density around BCR Y 101:

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

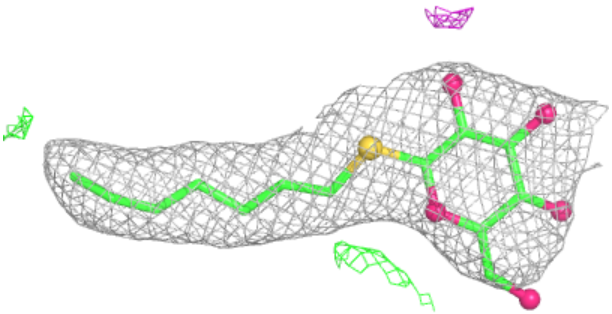


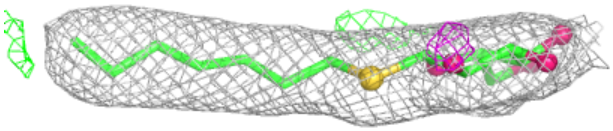


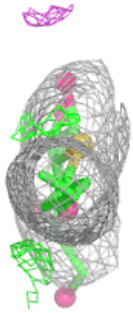


Electron density around HTG b 628:

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

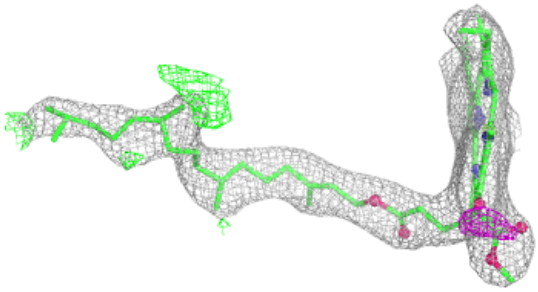


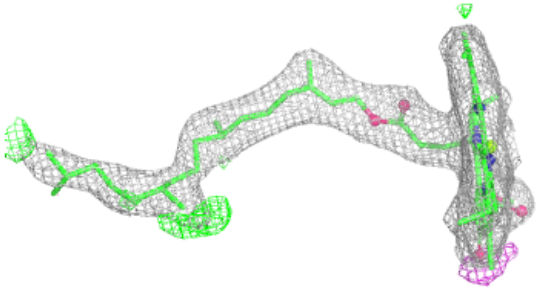


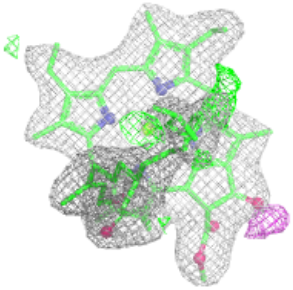


Electron density around CLA b 606:

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

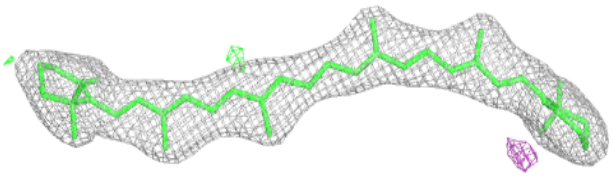


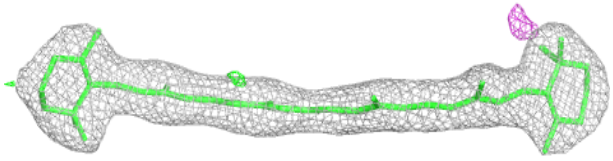


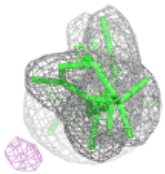


Electron density around BCR h 102:

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

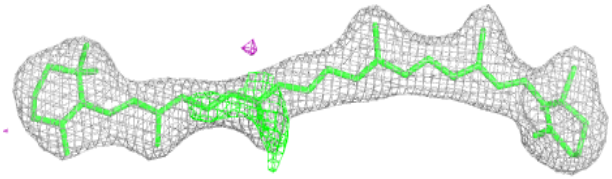


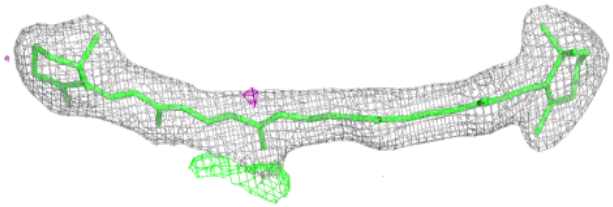


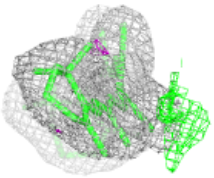


Electron density around BCR t 102:

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

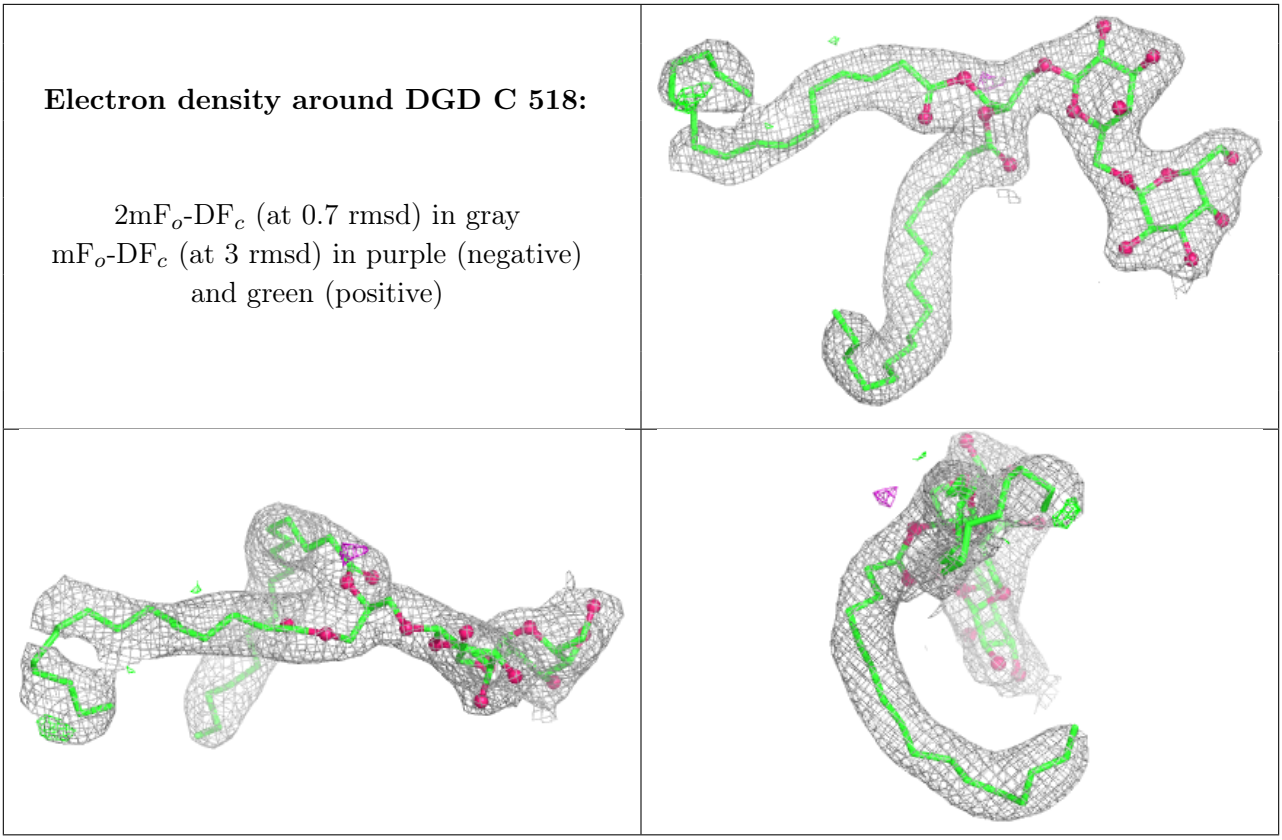






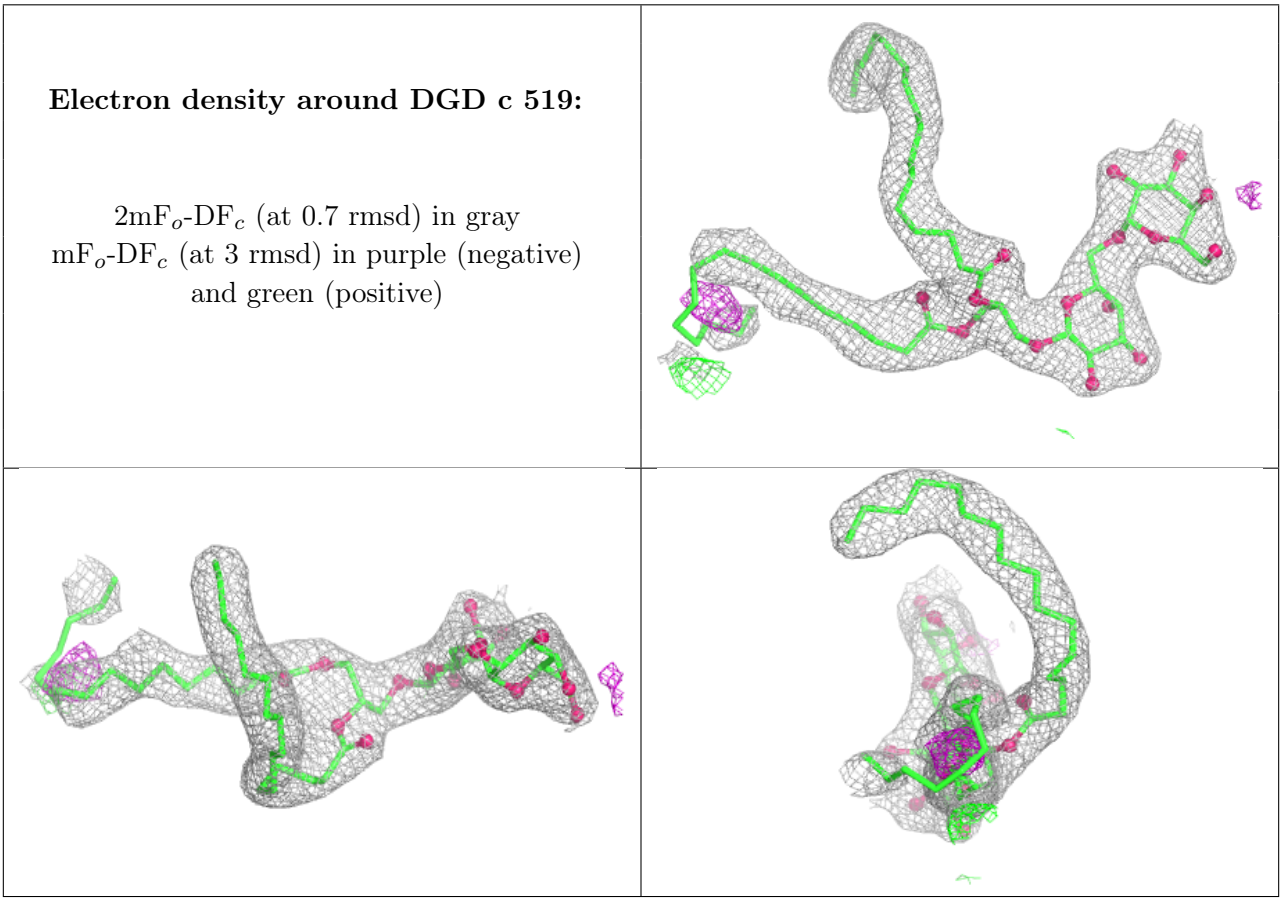
Electron density around DGD C 518:

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



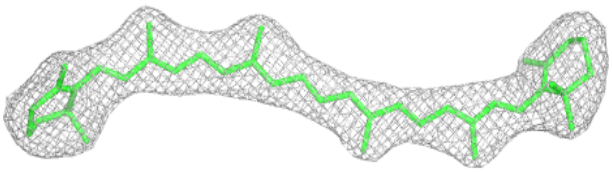
Electron density around DGD c 519:

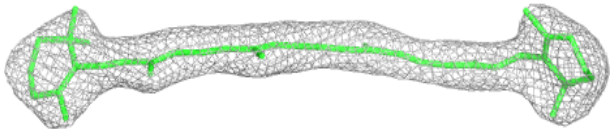
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

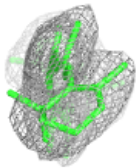


Electron density around BCR y 101:

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

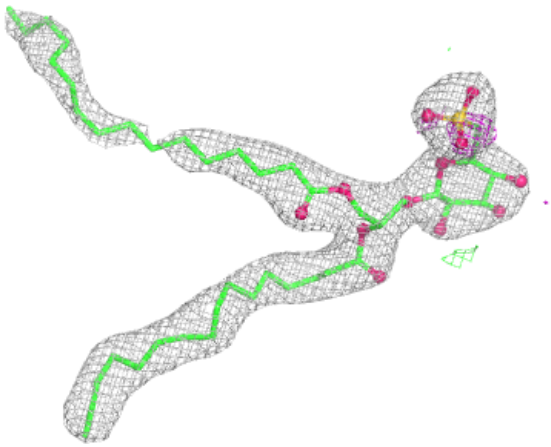


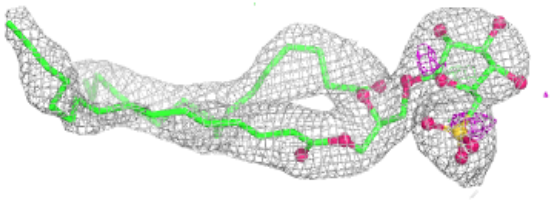


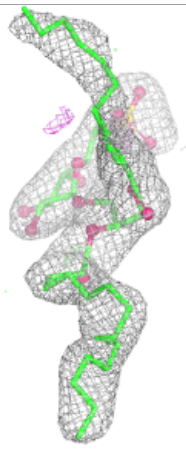


Electron density around SQD A 411:

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

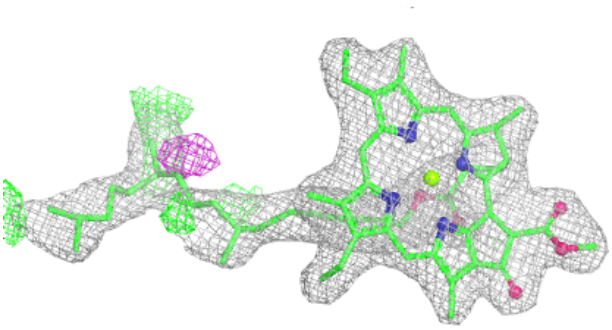


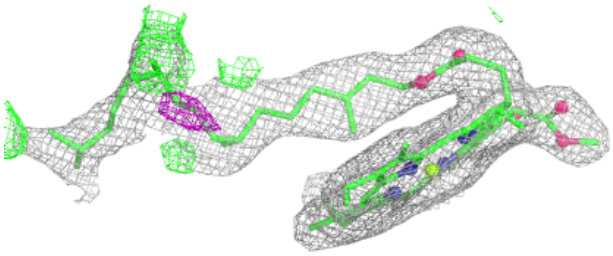




Electron density around CLA b 614:

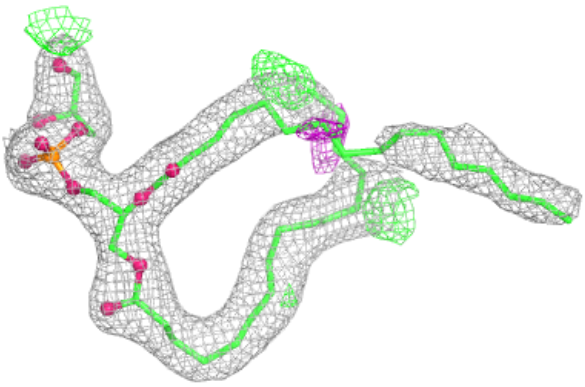
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

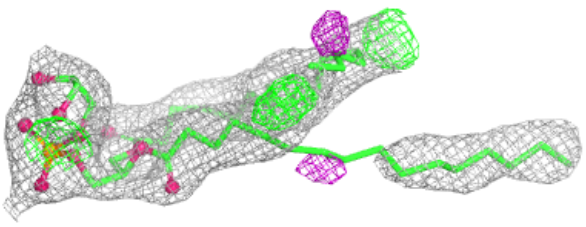


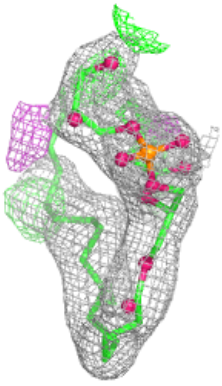


Electron density around LHG D 407:

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

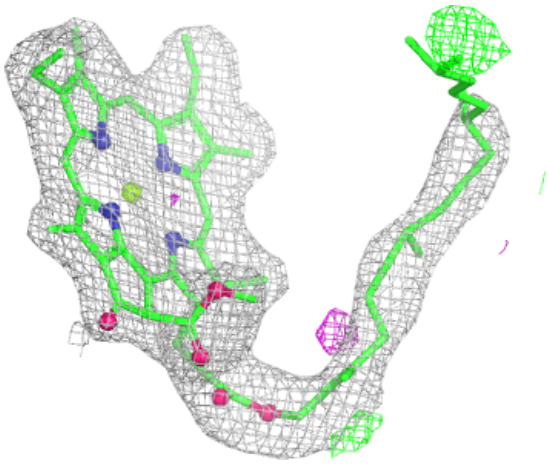


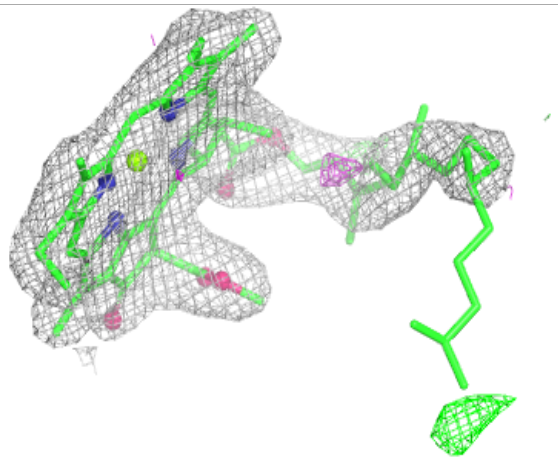


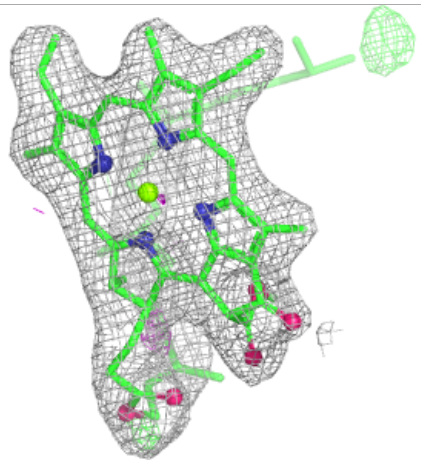


Electron density around CLA b 616:

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

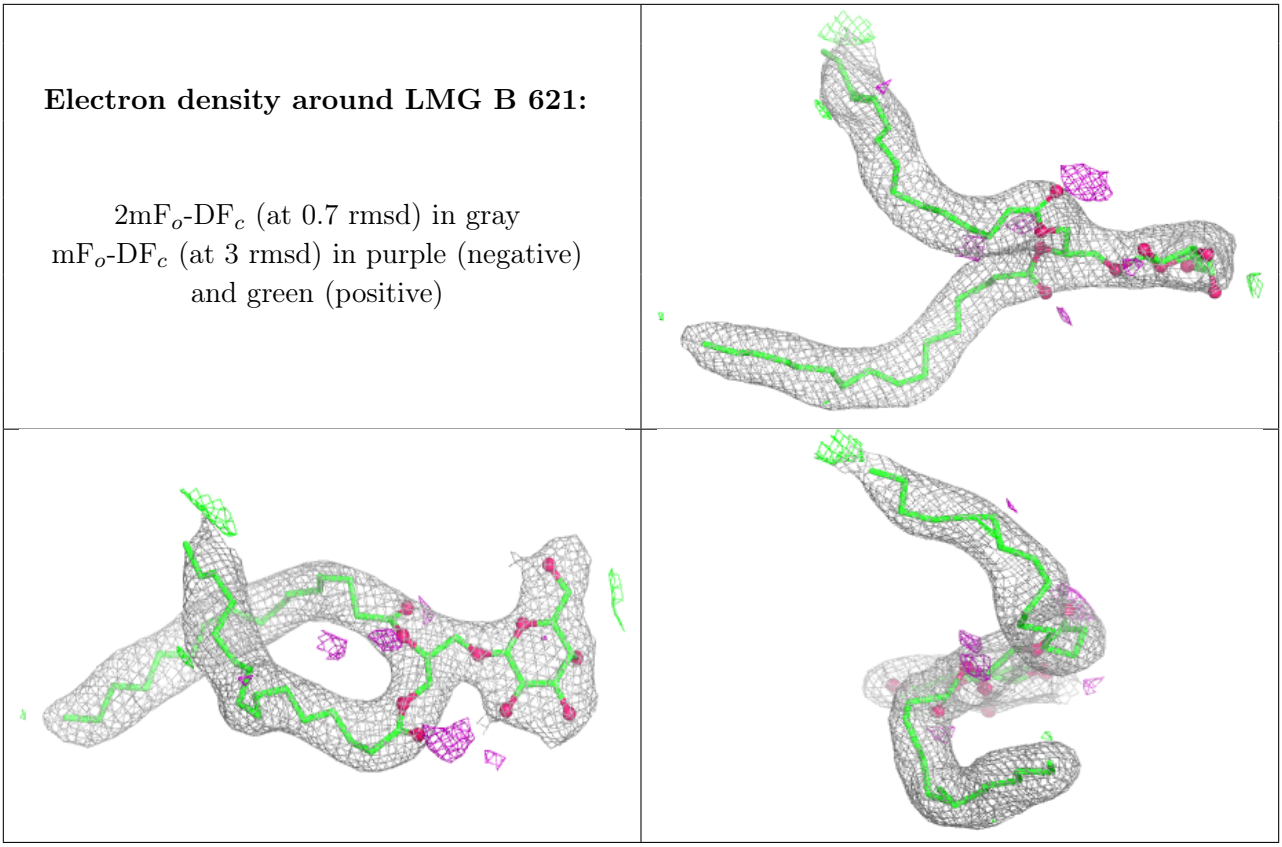






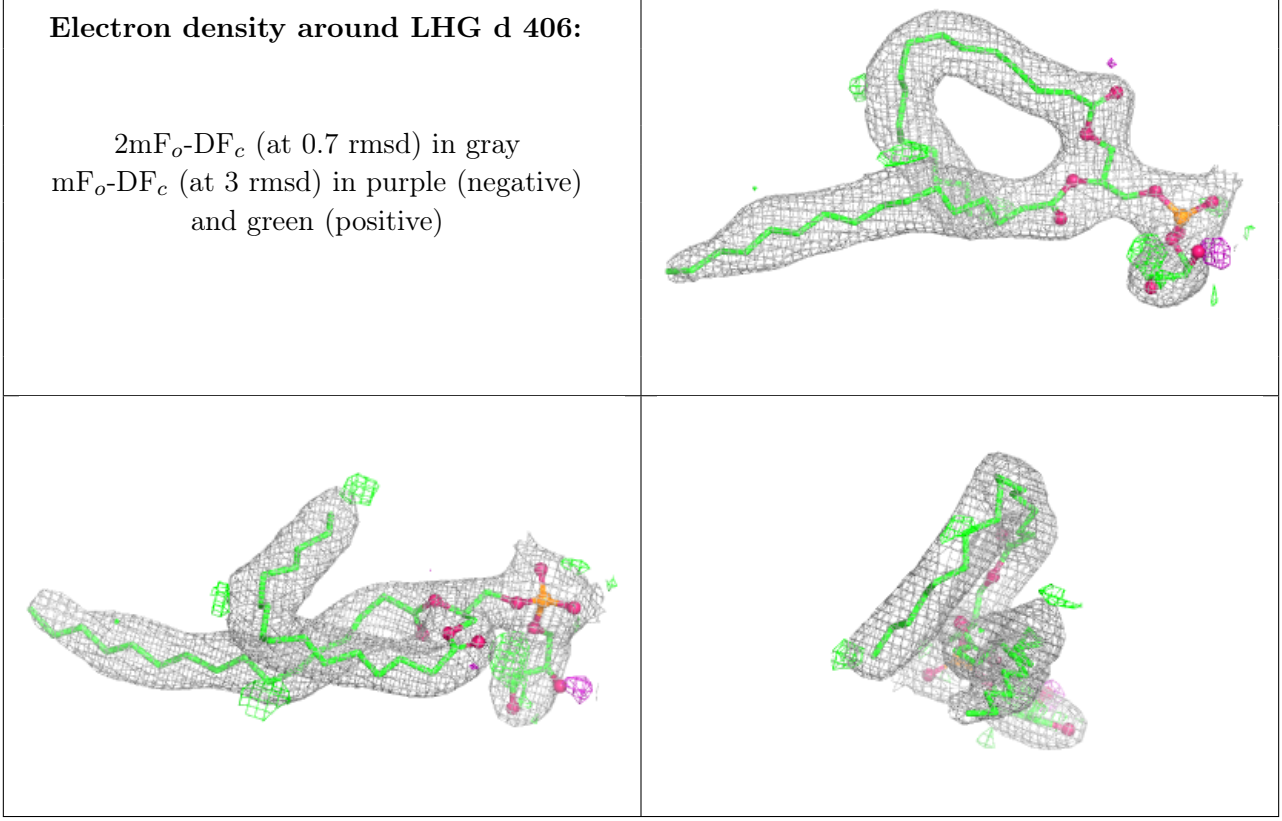
Electron density around LMG B 621:

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



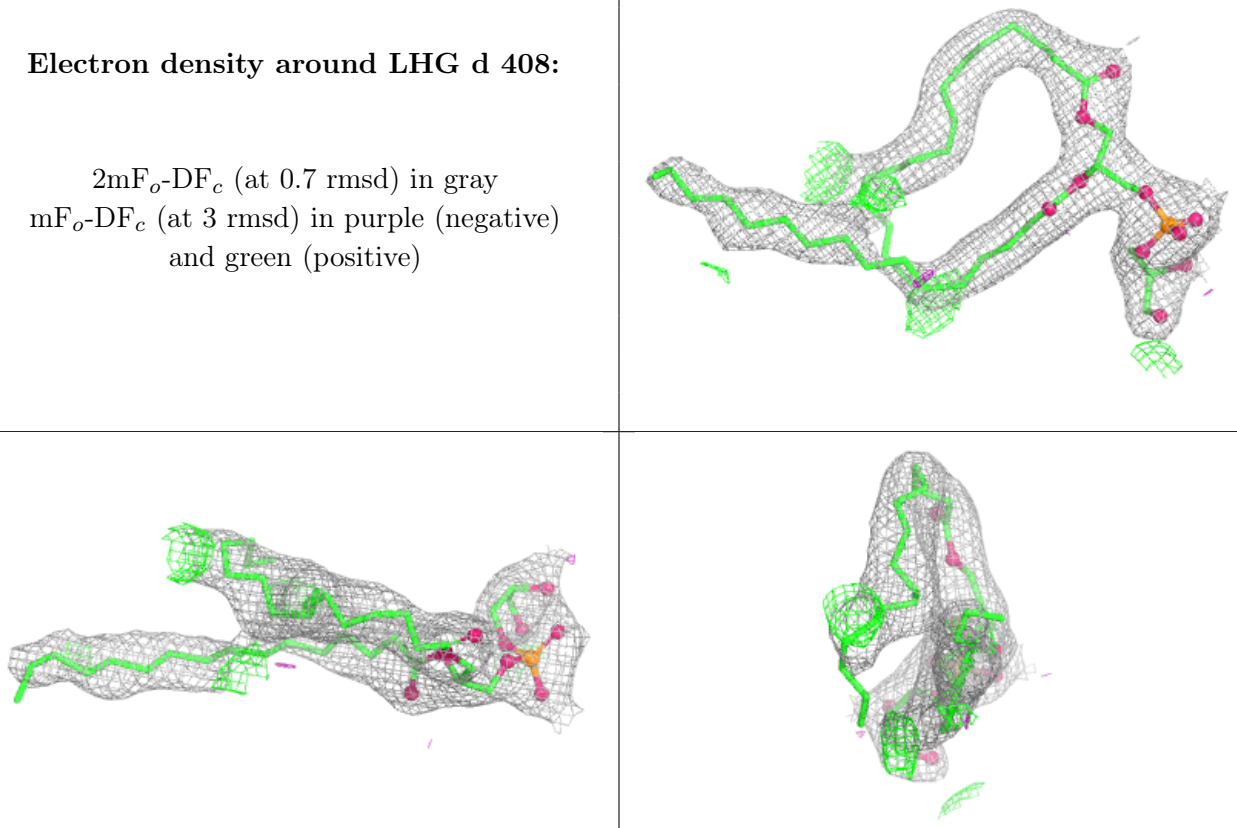
Electron density around LHG d 406:

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



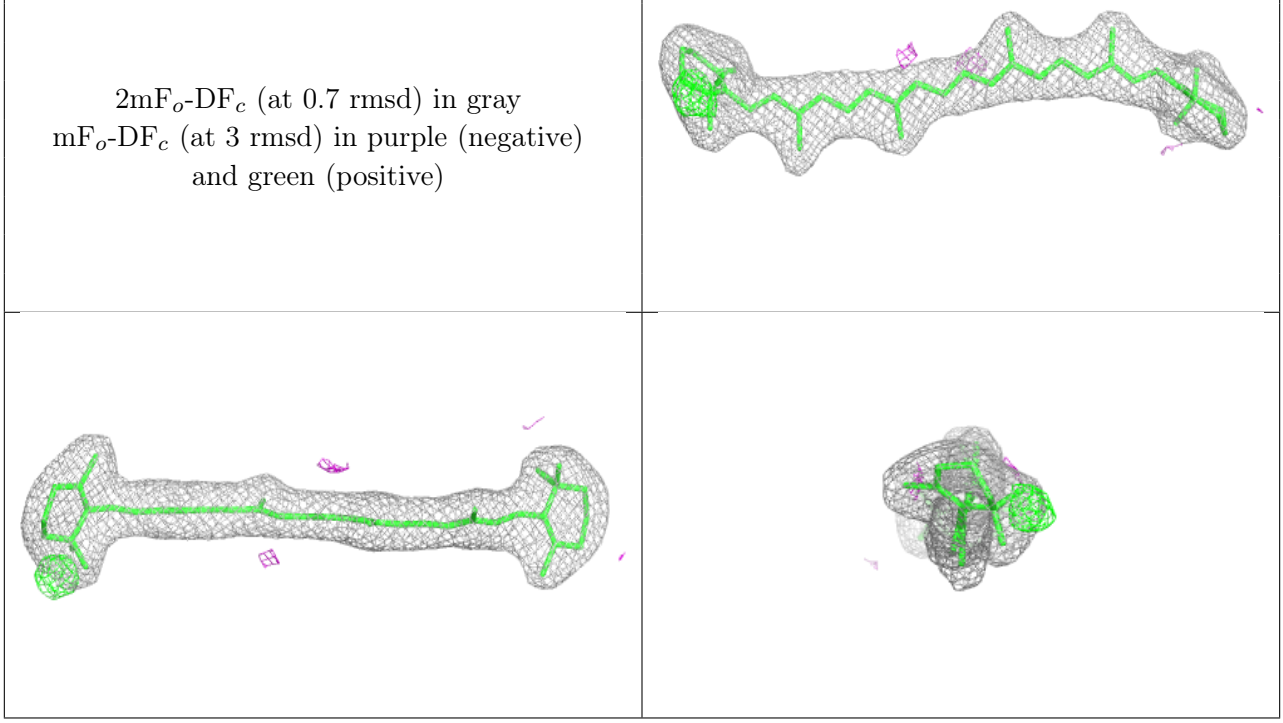
Electron density around LHG d 408:

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



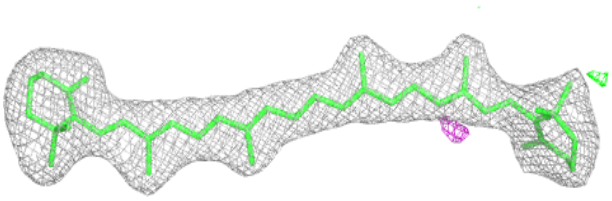
Electron density around BCR A 410:

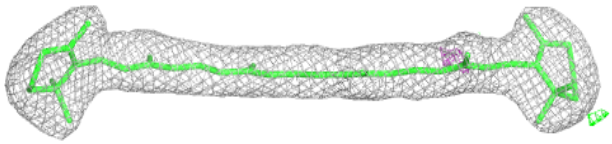
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

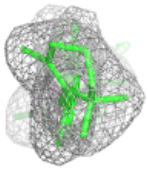


Electron density around BCR B 618:

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

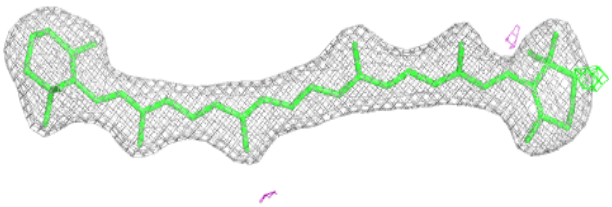


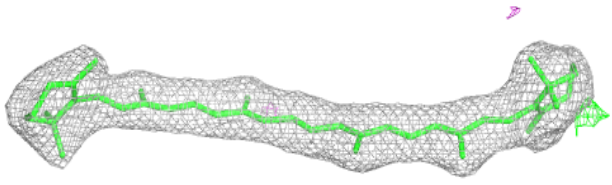


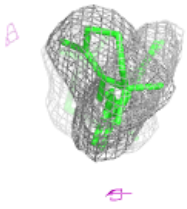


Electron density around BCR B 619:

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

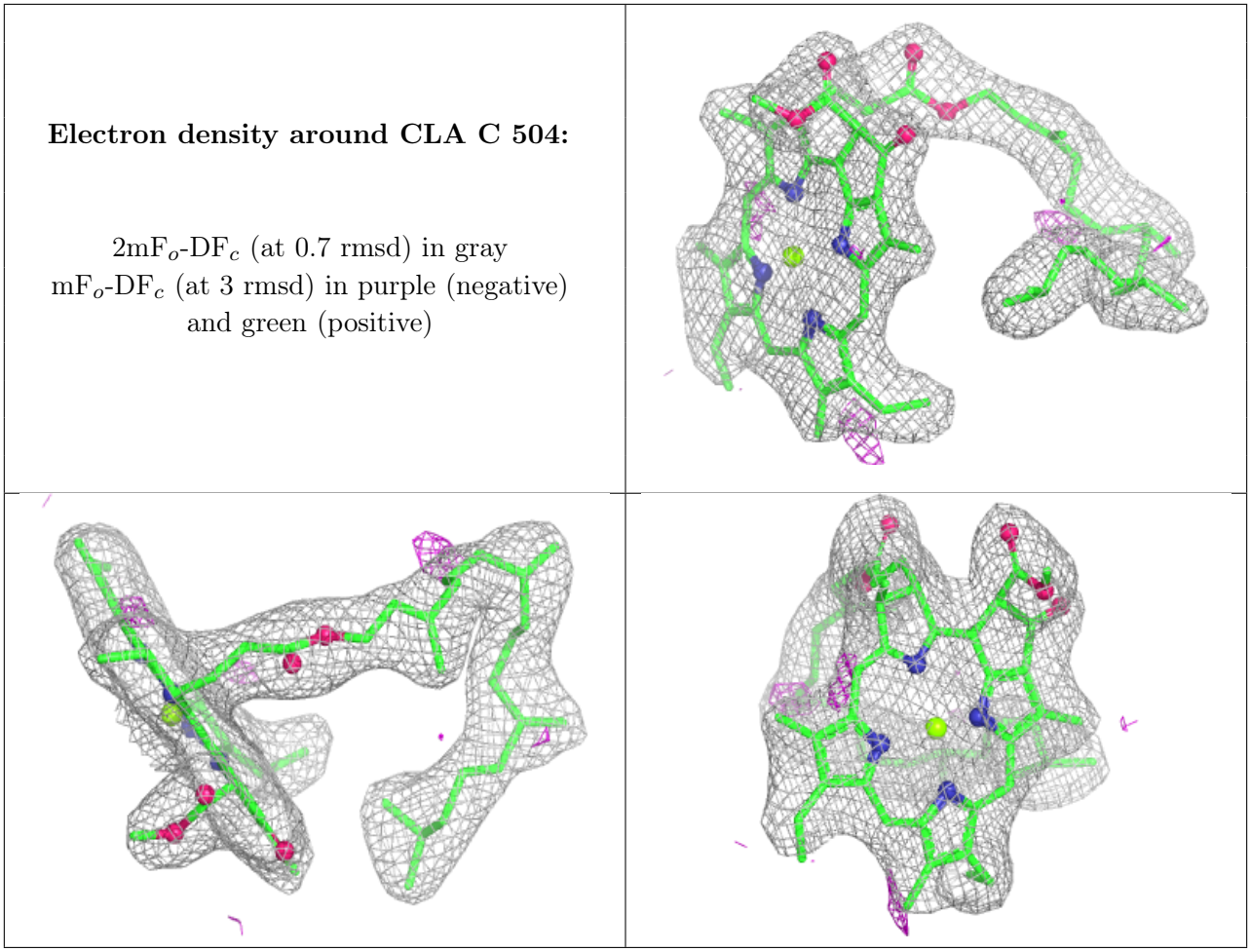






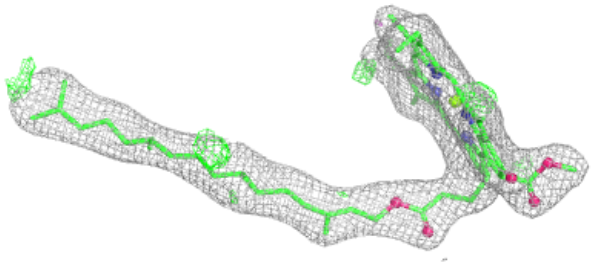
Electron density around CLA C 504:

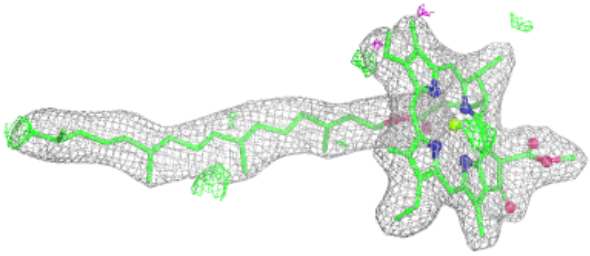
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

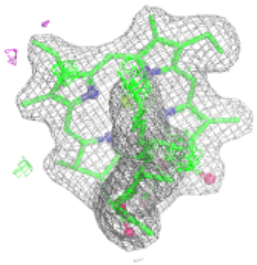


Electron density around CLA b 607:

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

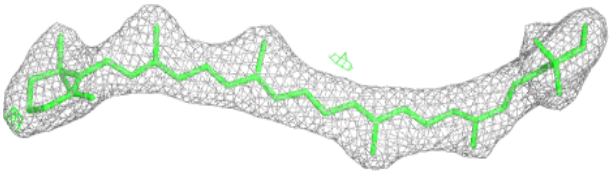


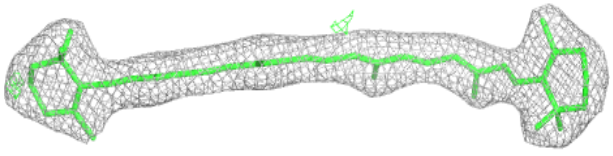


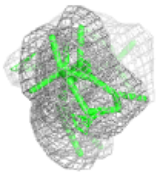


Electron density around BCR H 101:

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

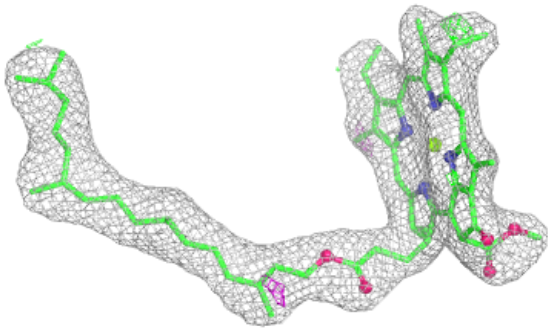


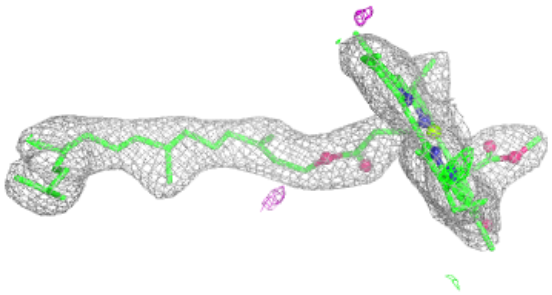


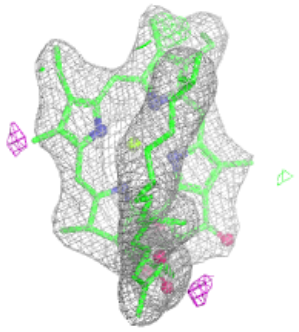


Electron density around CLA b 609:

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

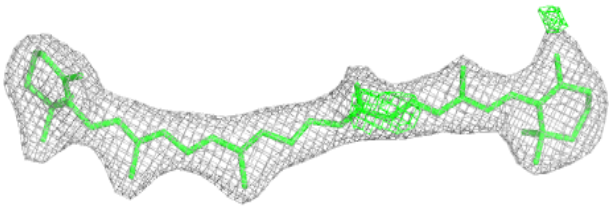


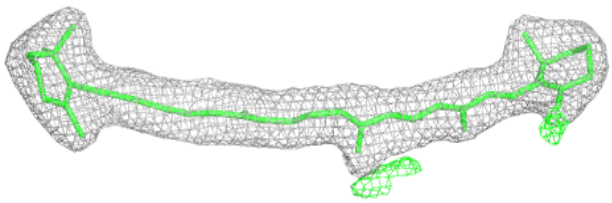


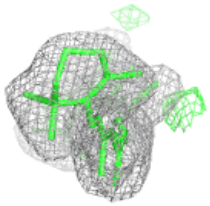


Electron density around BCR T 101:

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

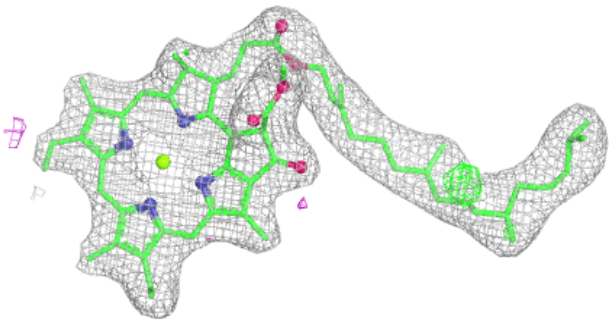


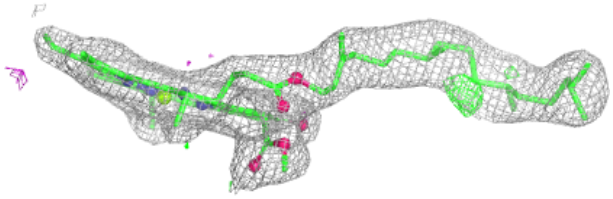


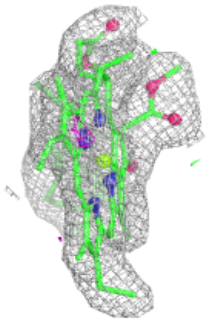


Electron density around CLA B 602:

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

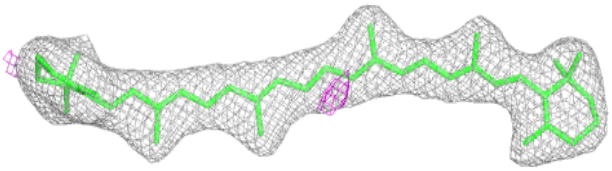


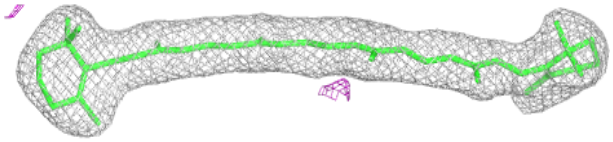


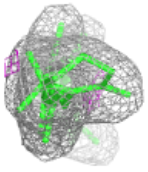


Electron density around BCR b 617:

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

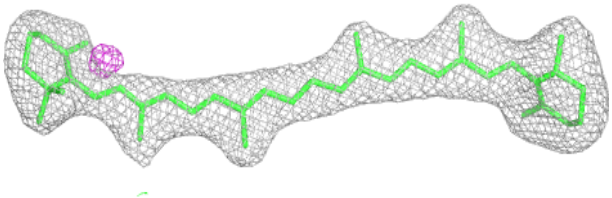


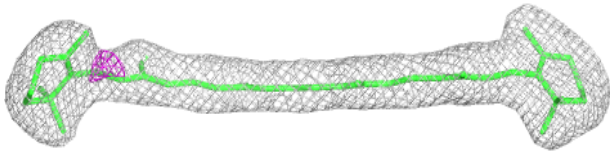


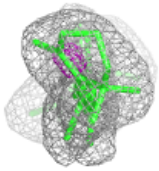


Electron density around BCR b 618:

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

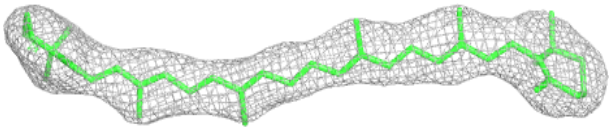


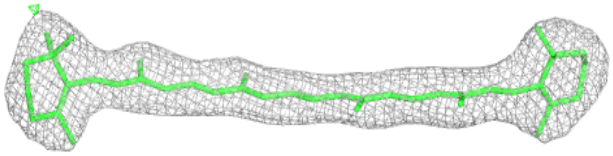


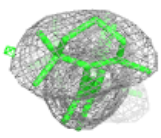


Electron density around BCR c 516:

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

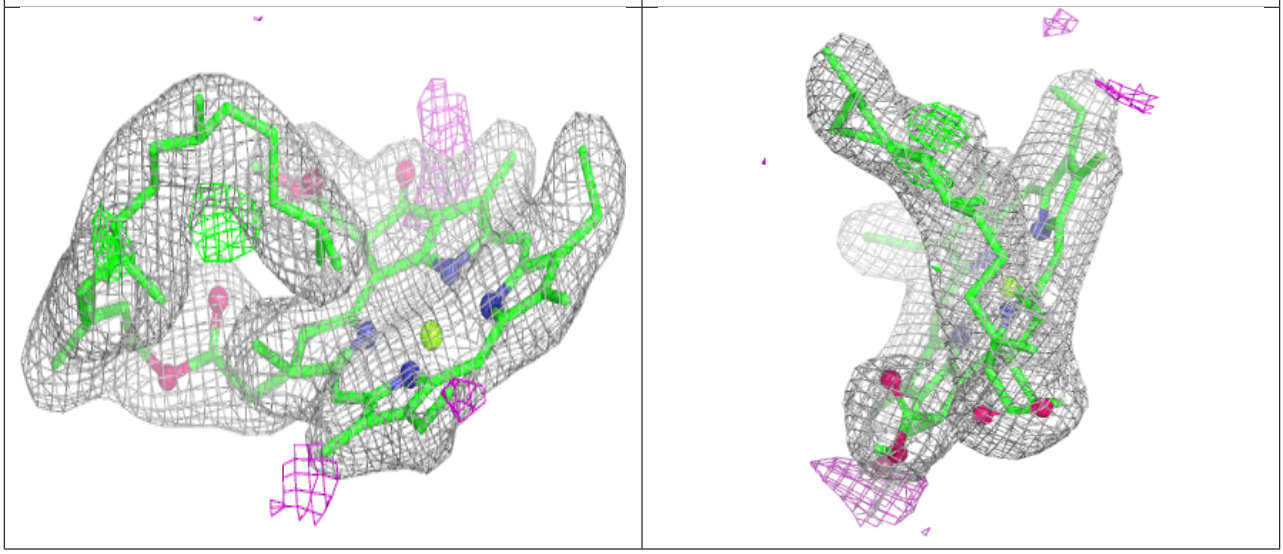






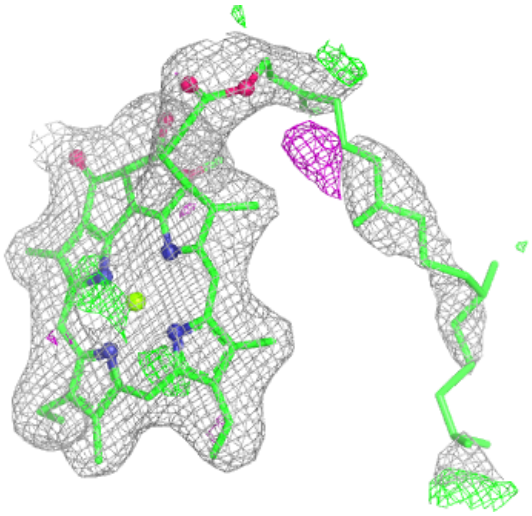
Electron density around CLA b 615:

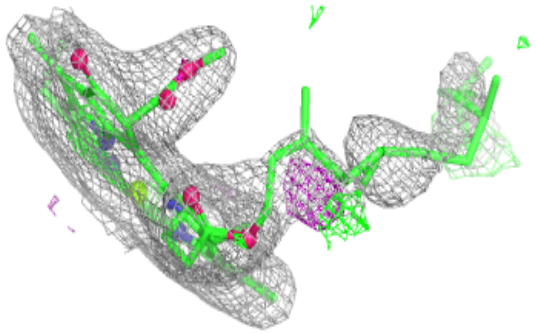
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

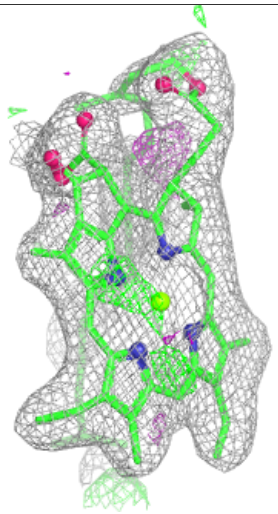


Electron density around CLA B 616:

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

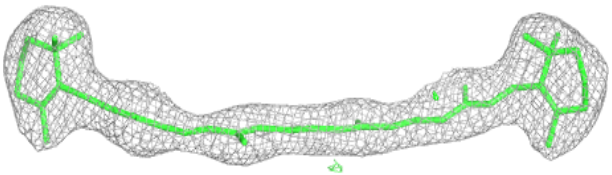


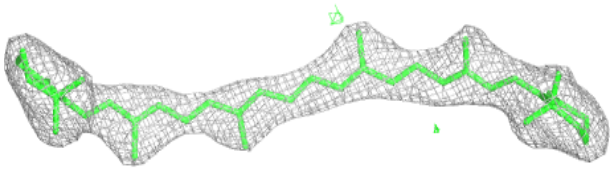


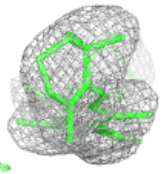


Electron density around BCR k 101:

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

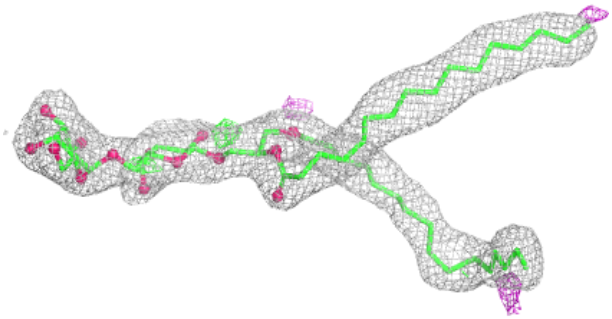


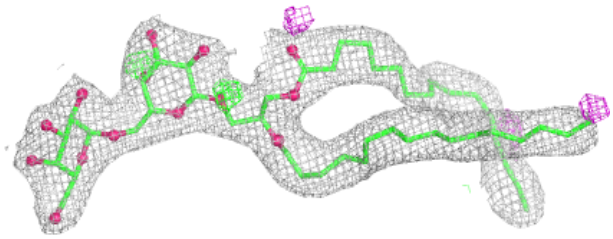


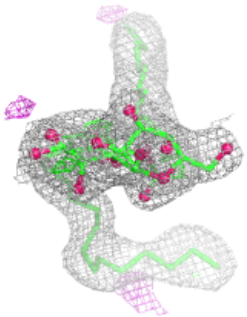


Electron density around DGD C 517:

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

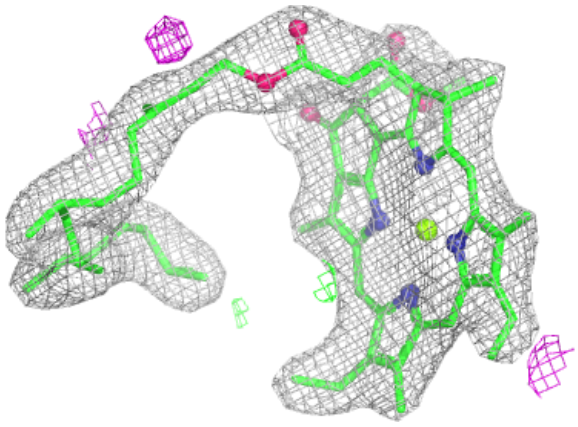


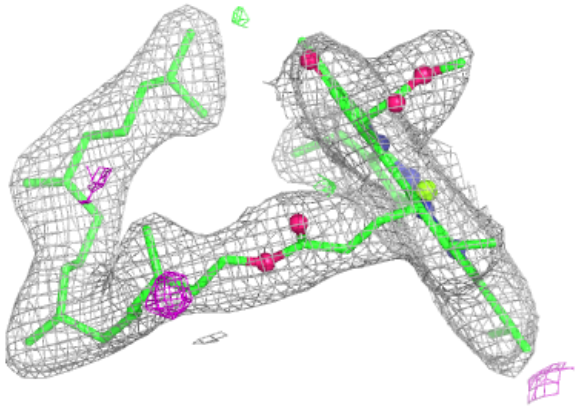


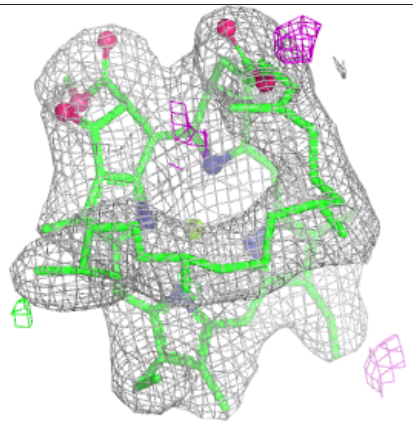


Electron density around CLA c 505:

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

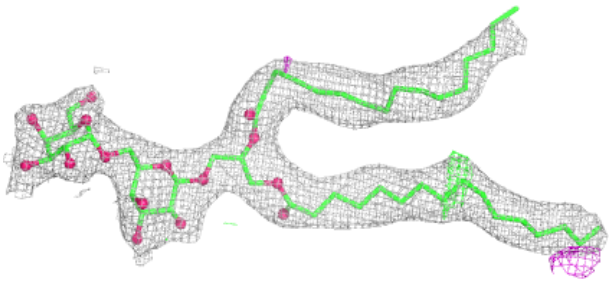


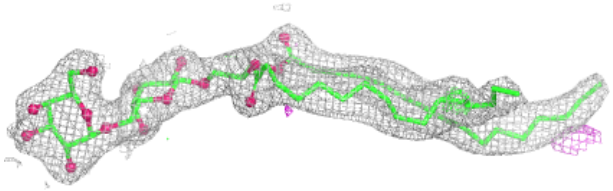


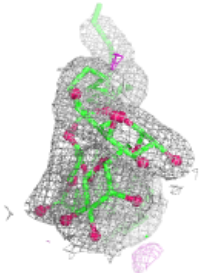


Electron density around DGD C 519:

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

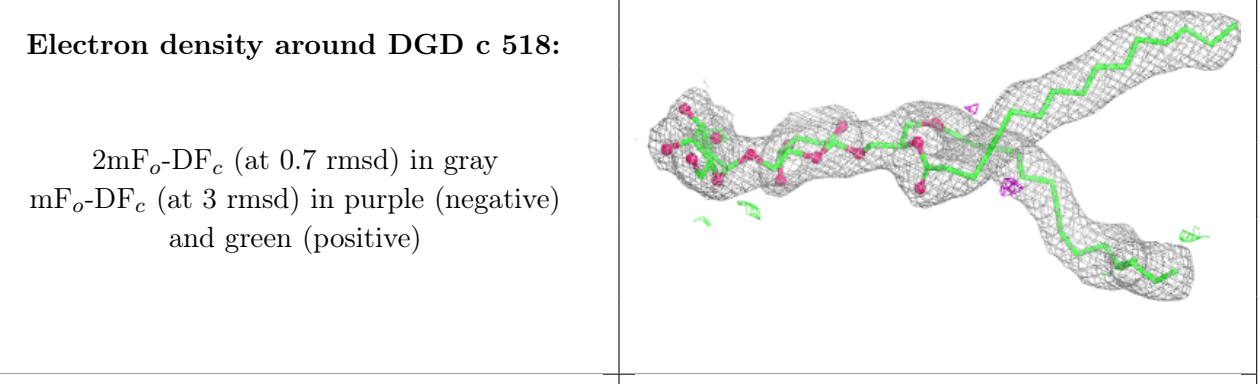






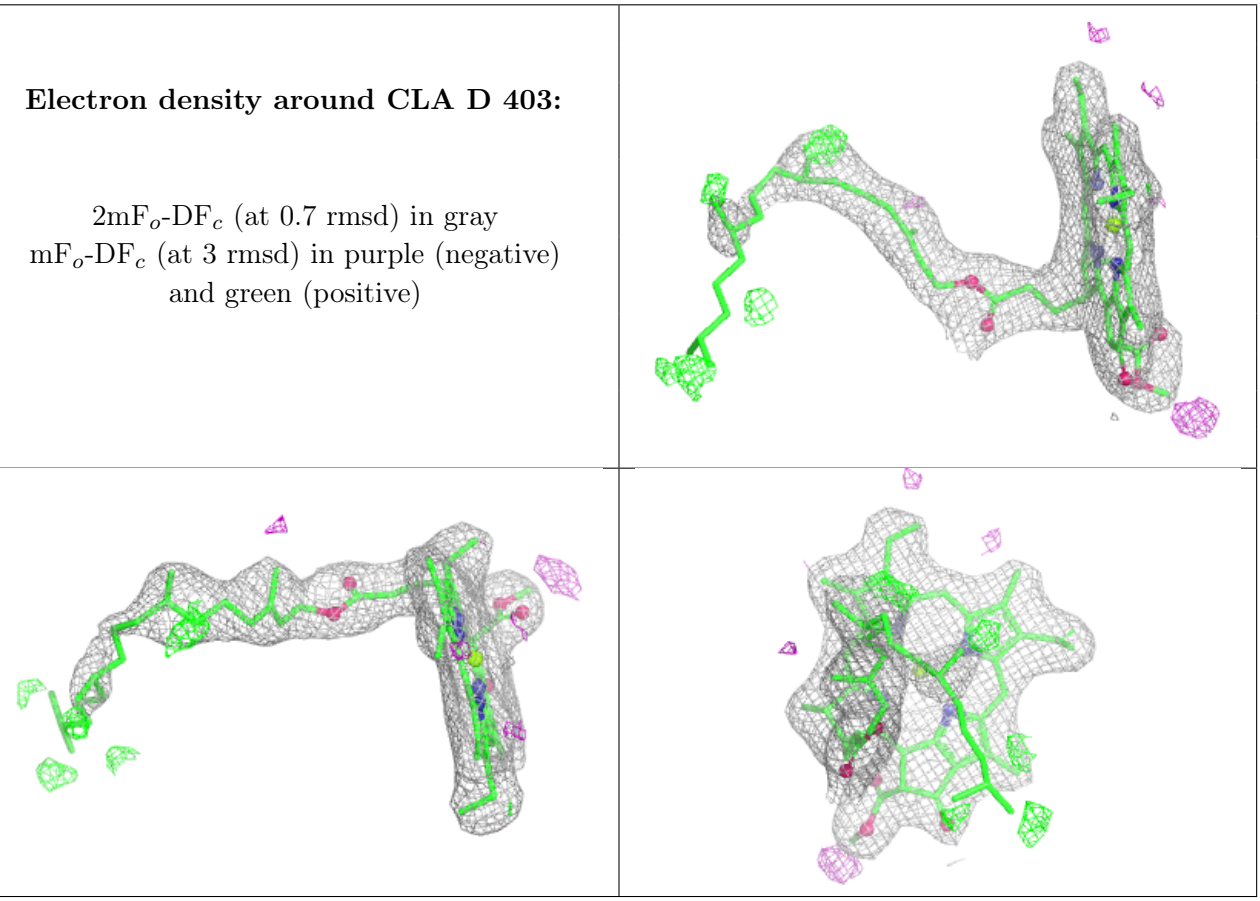
Electron density around DGD c 518:

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



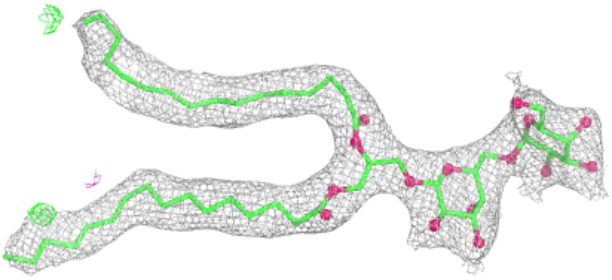
Electron density around CLA D 403:

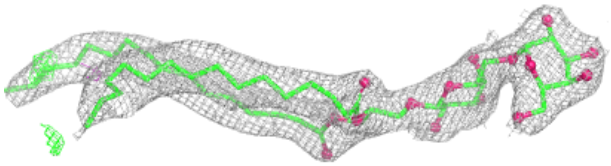
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

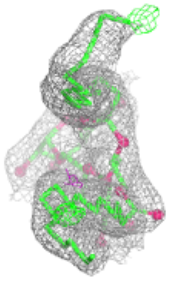


Electron density around DGD c 520:

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

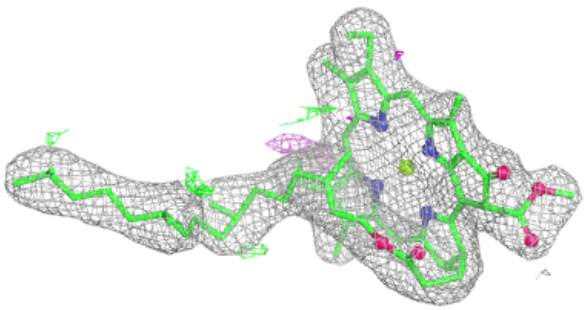


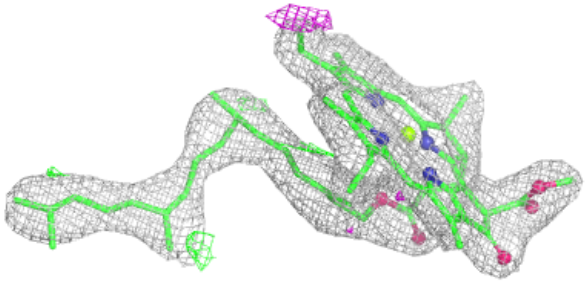


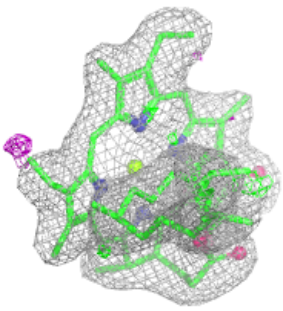


Electron density around CLA c 507:

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

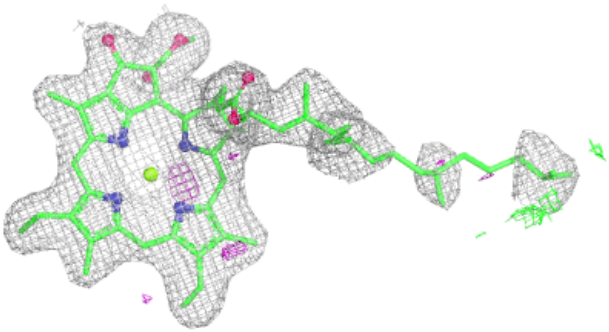


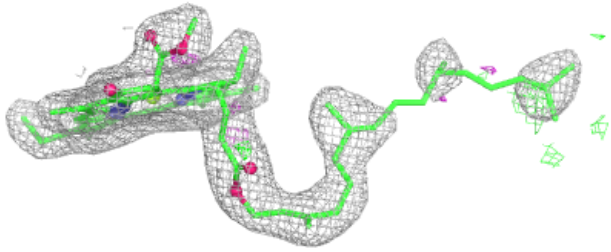




Electron density around CLA a 404:

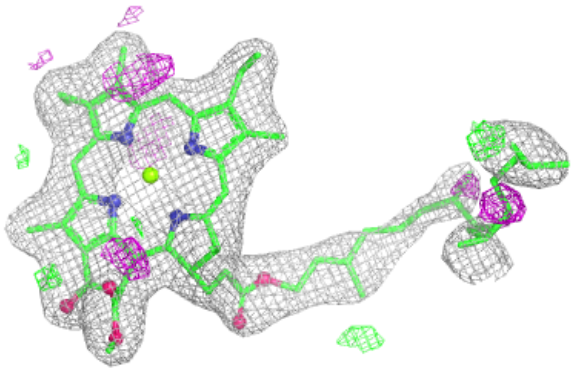
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

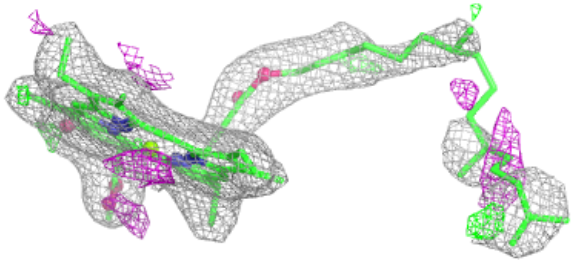


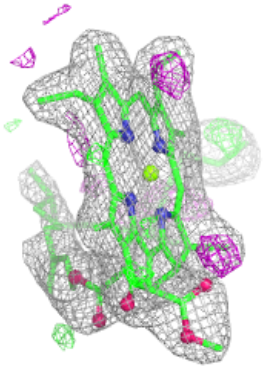


Electron density around CLA a 407:

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

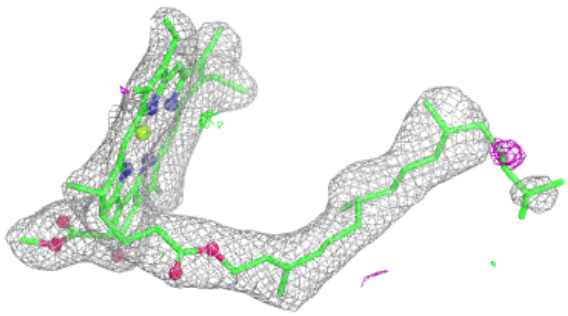


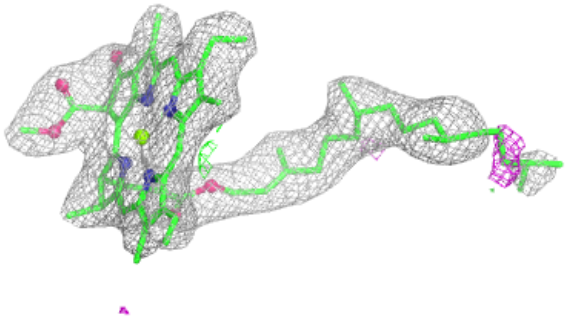


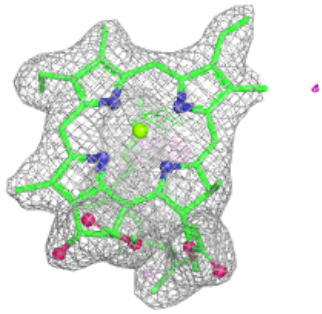


Electron density around CLA c 510:

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

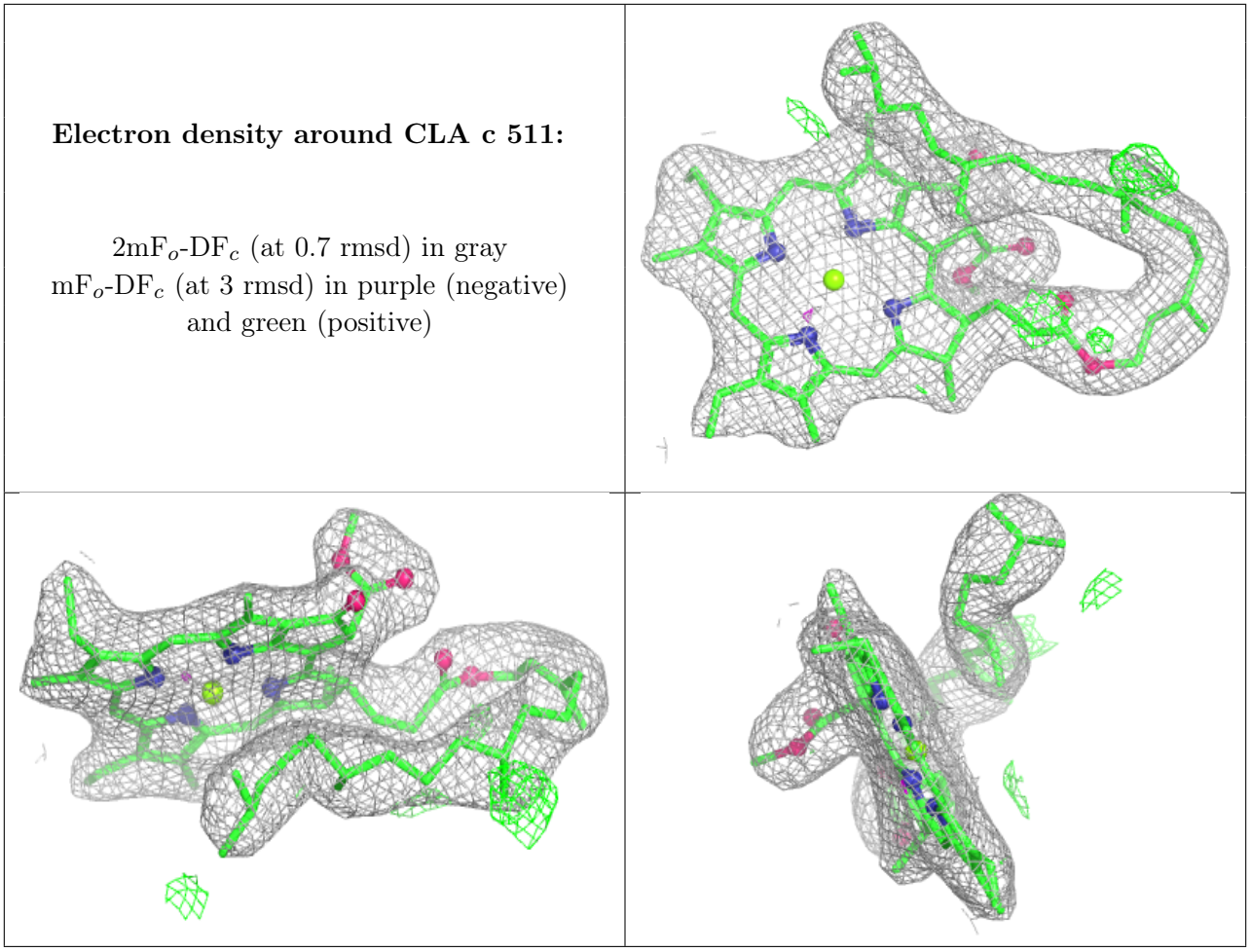






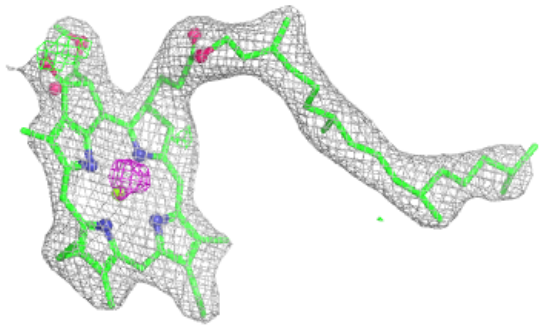
Electron density around CLA c 511:

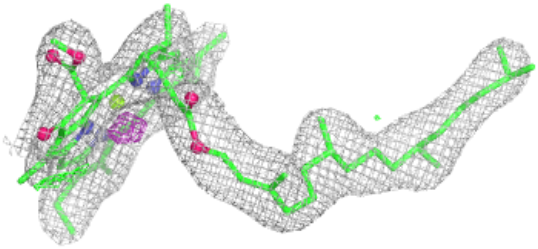
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

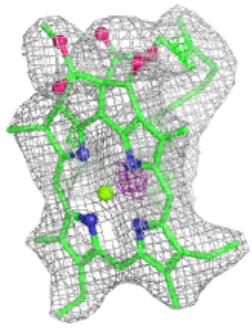


Electron density around CLA c 513:

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

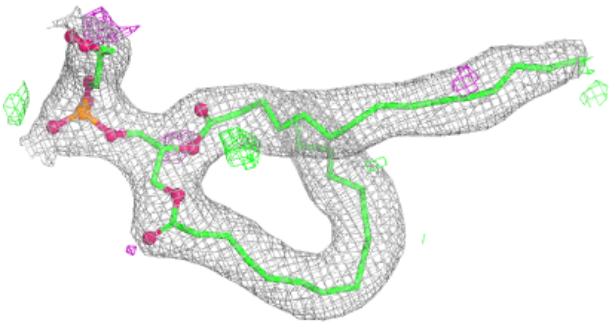


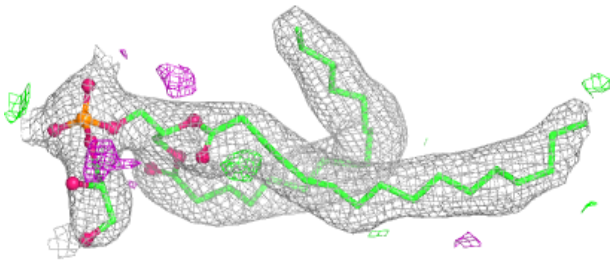


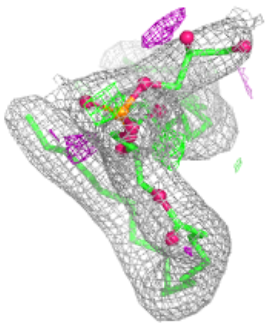


Electron density around LHG D 357:

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

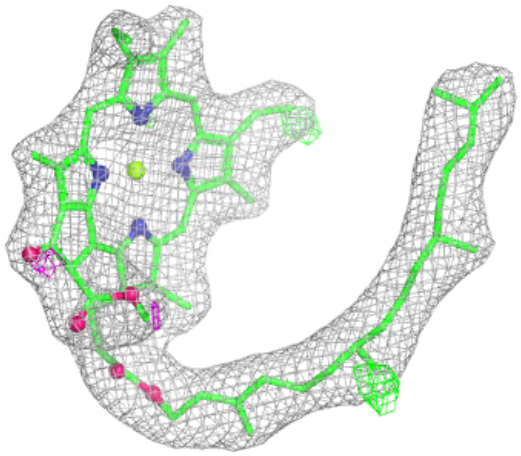


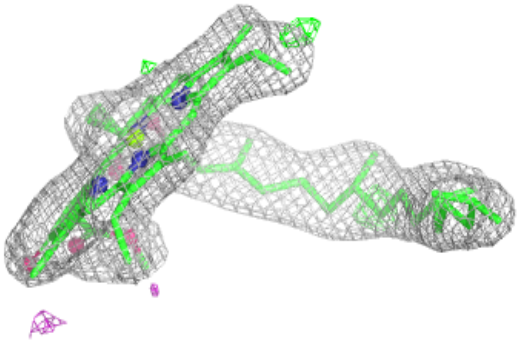


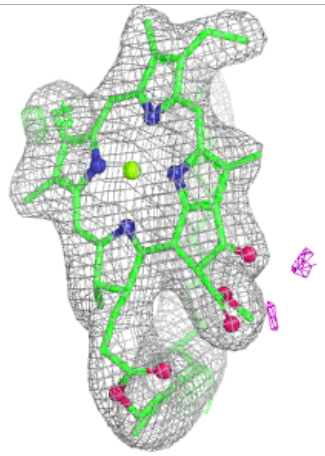


Electron density around CLA C 508:

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

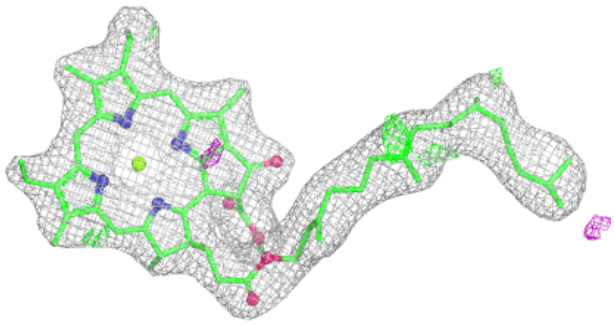


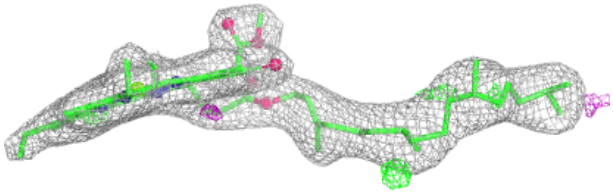


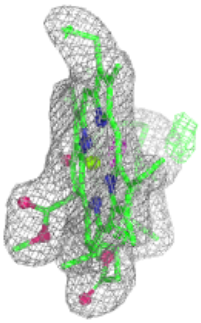


Electron density around CLA b 602:

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

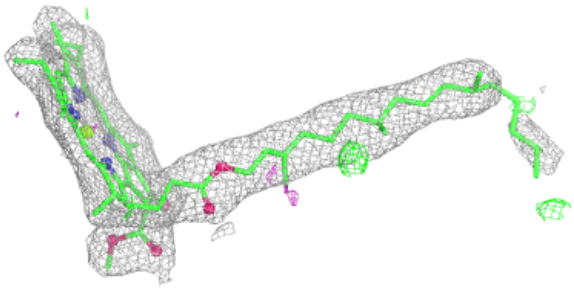


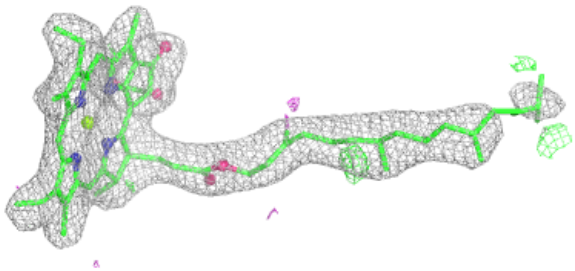


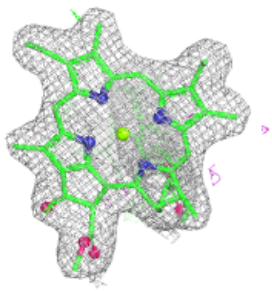


Electron density around CLA b 604:

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

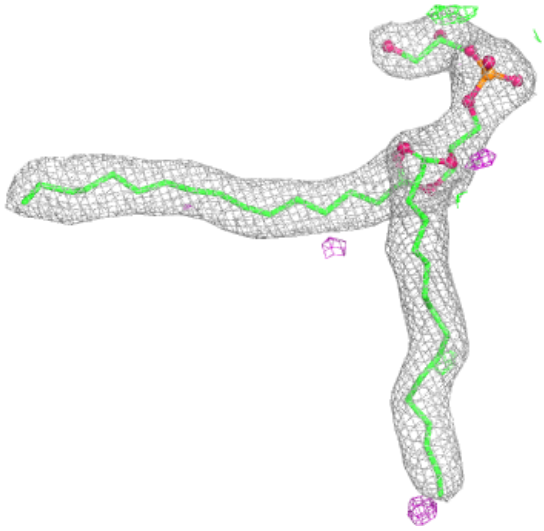


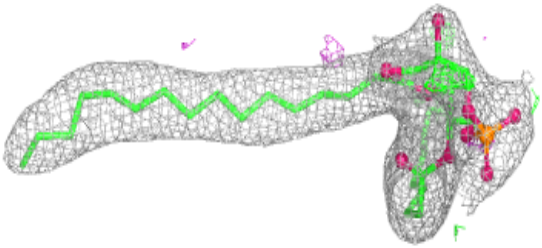


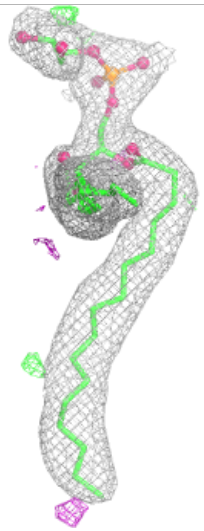


Electron density around LHG l 101:

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

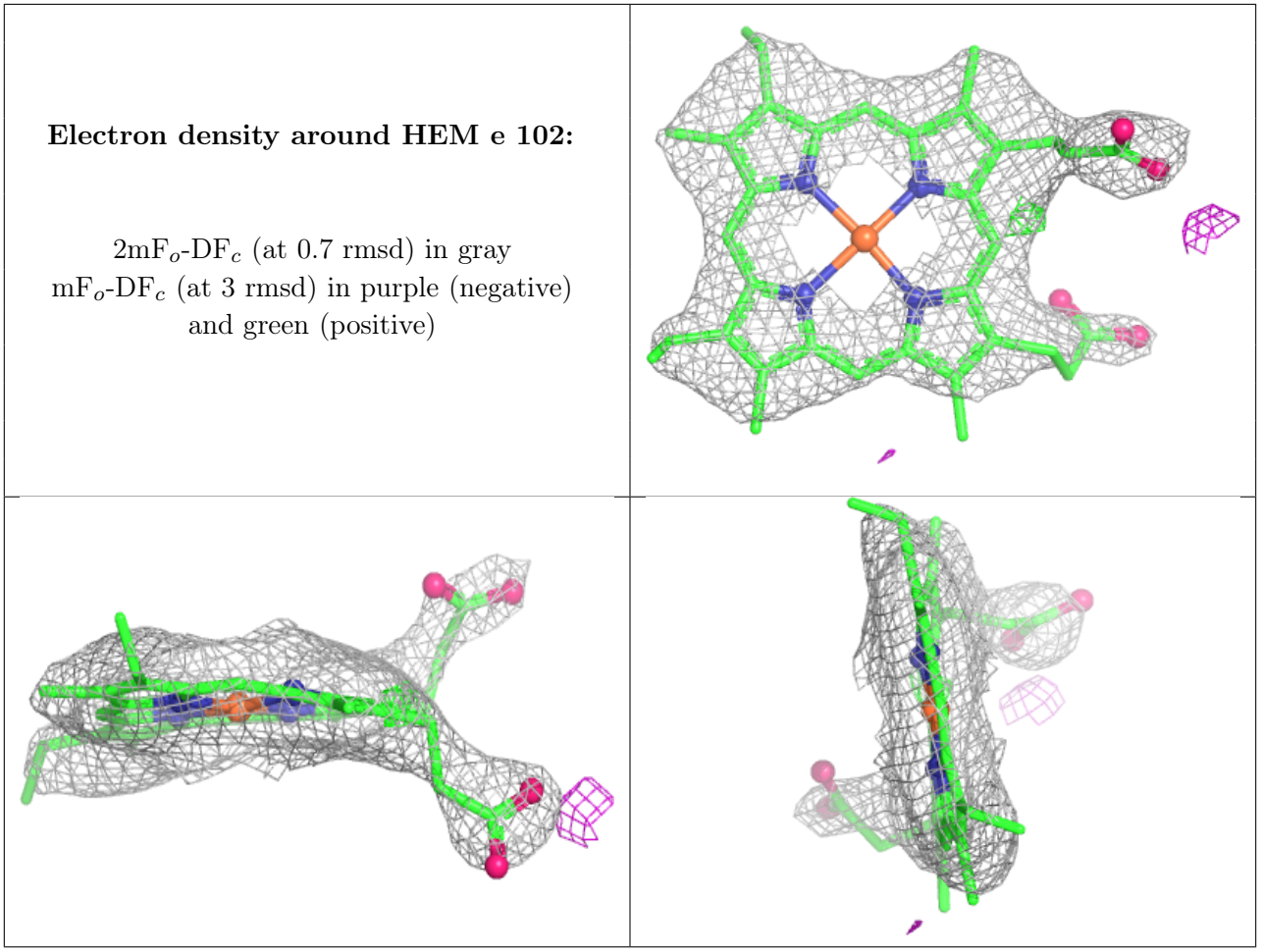






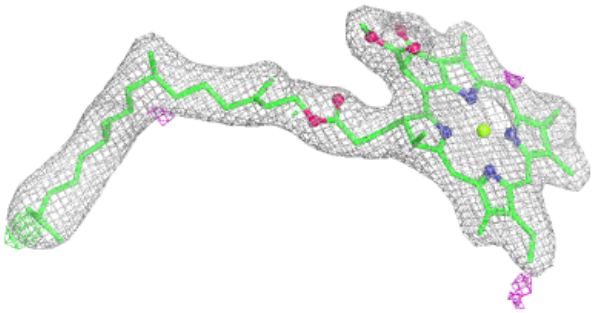
Electron density around HEM e 102:

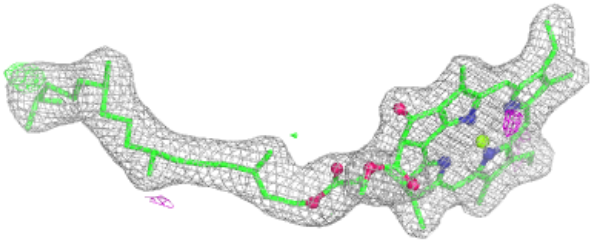
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

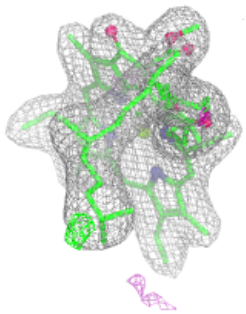


Electron density around CLA a 403:

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

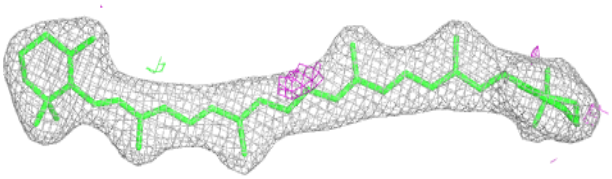


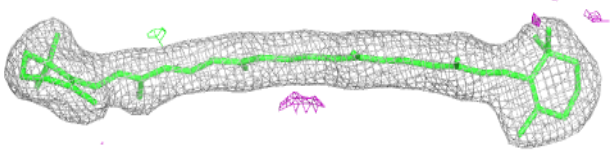


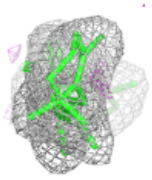


Electron density around BCR B 617:

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

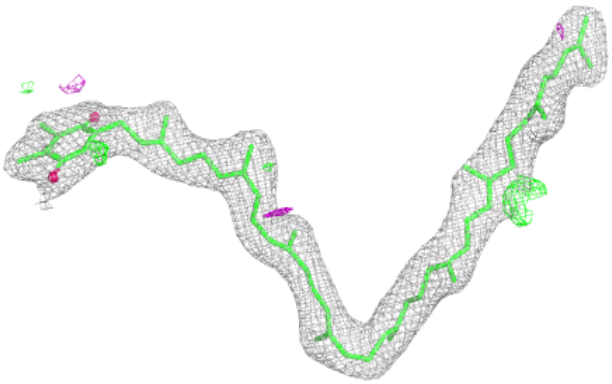


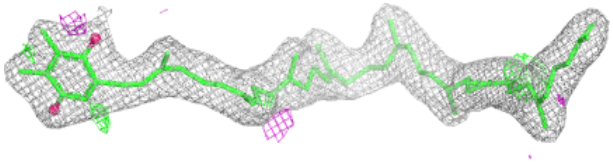


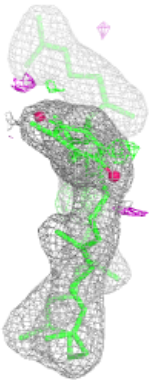


Electron density around PL9 D 405:

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

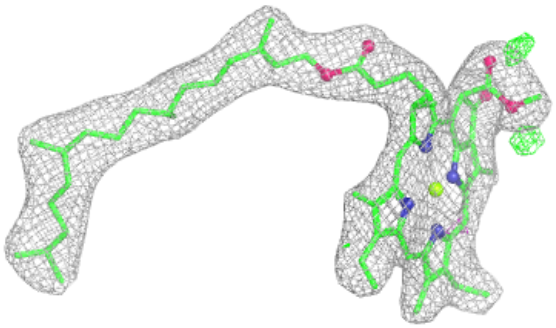


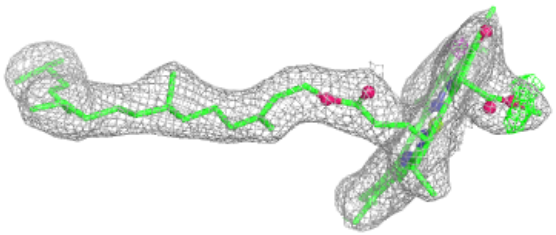


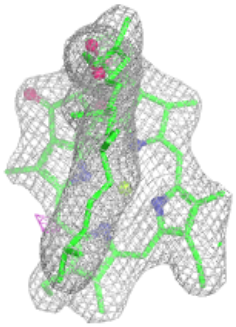


Electron density around CLA B 609:

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

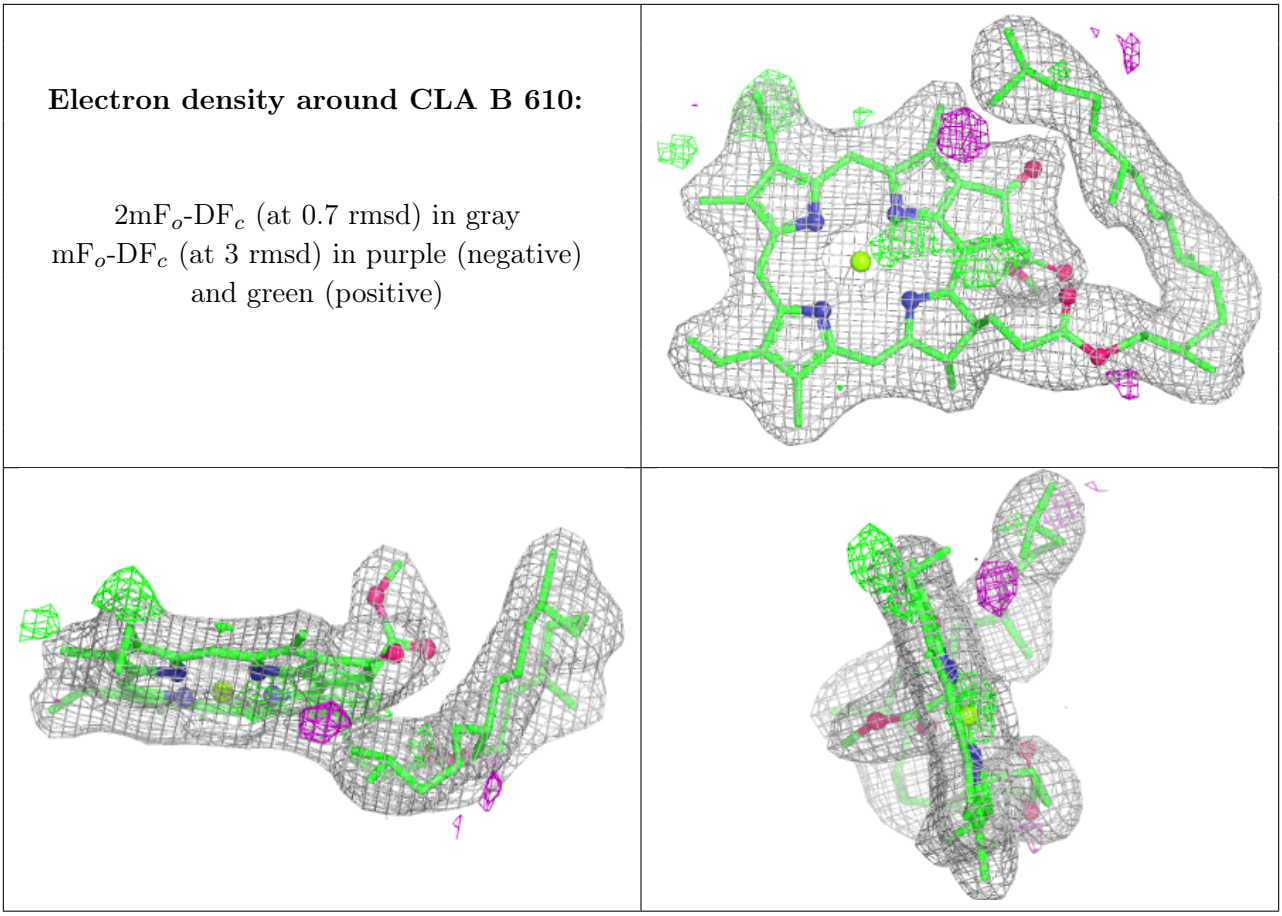






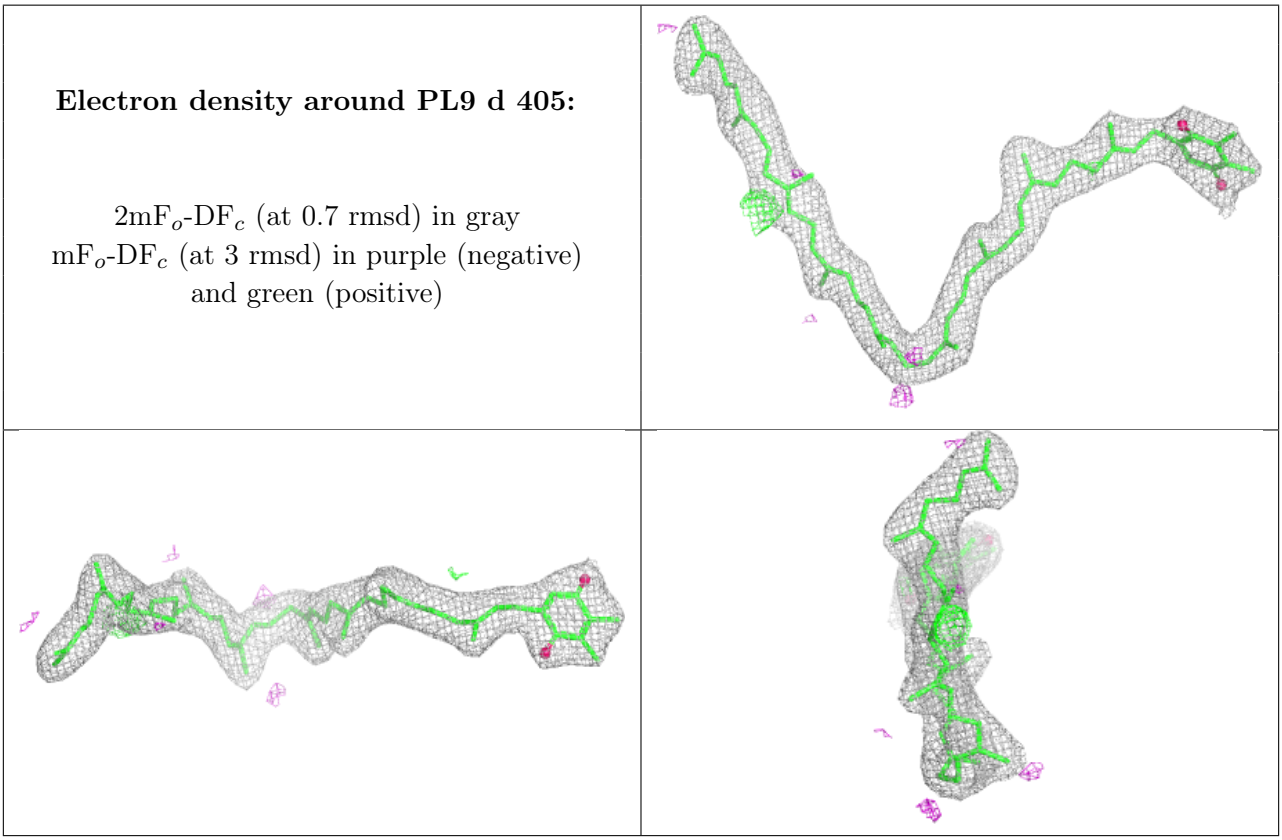
Electron density around CLA B 610:

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



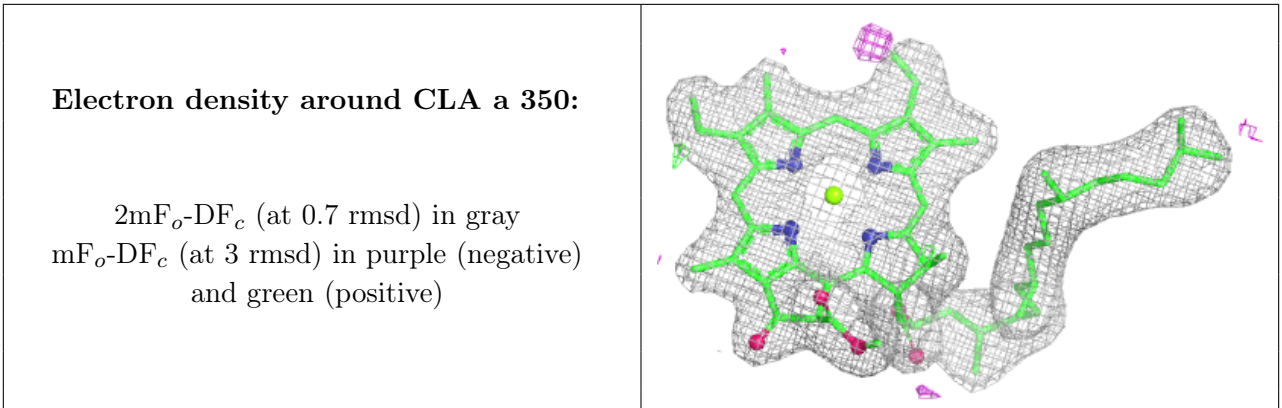
Electron density around PL9 d 405:

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



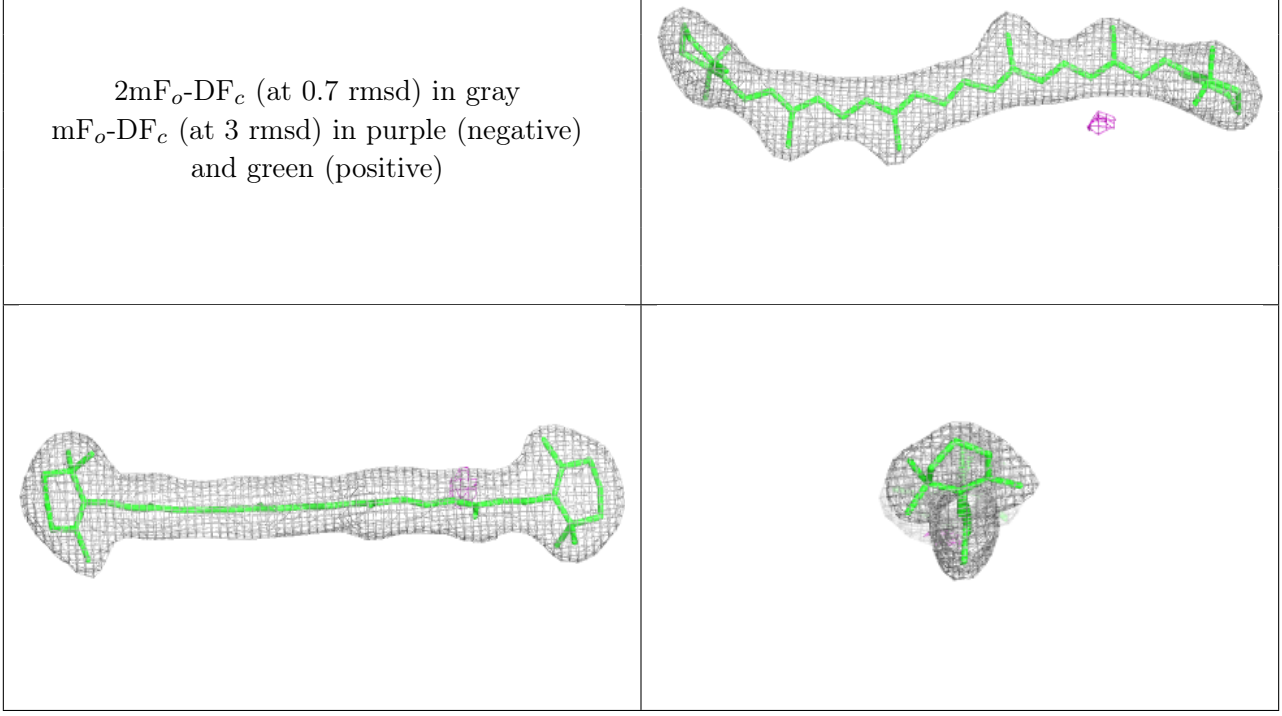
Electron density around CLA a 350:

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



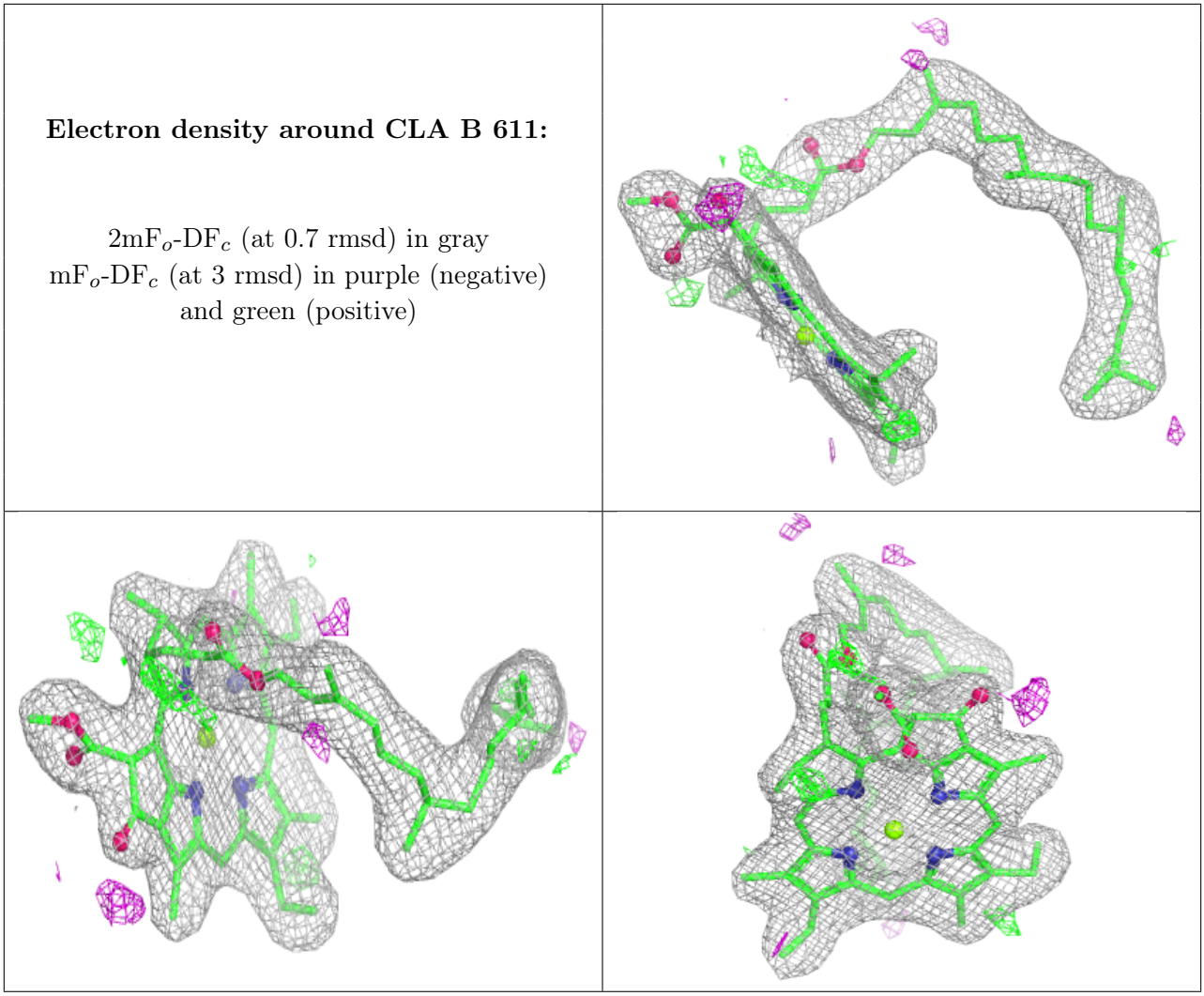
Electron density around BCR C 516:

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



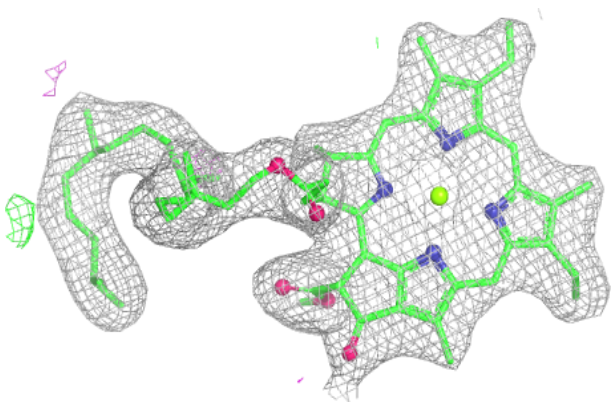
Electron density around CLA B 611:

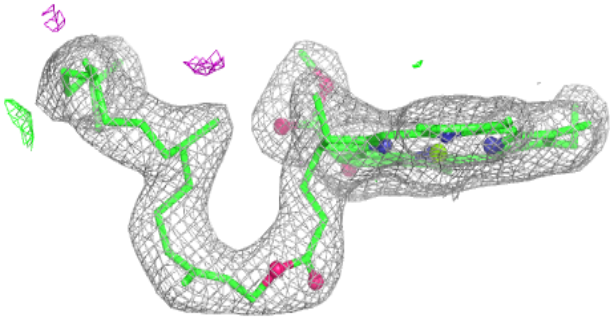
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

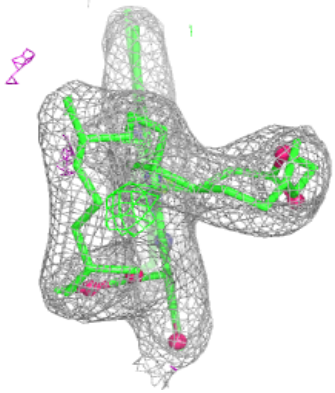


Electron density around CLA B 612:

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

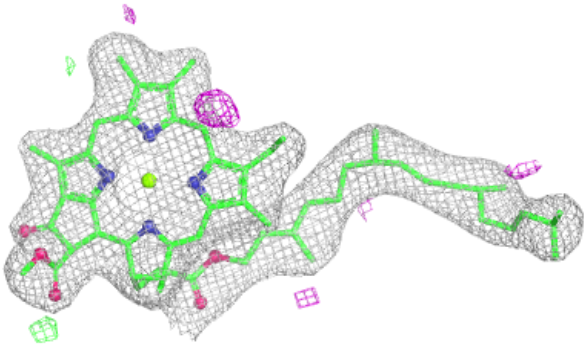


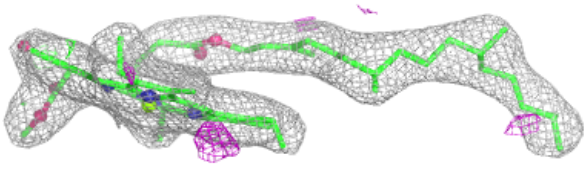


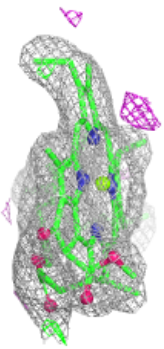


Electron density around CLA b 603:

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

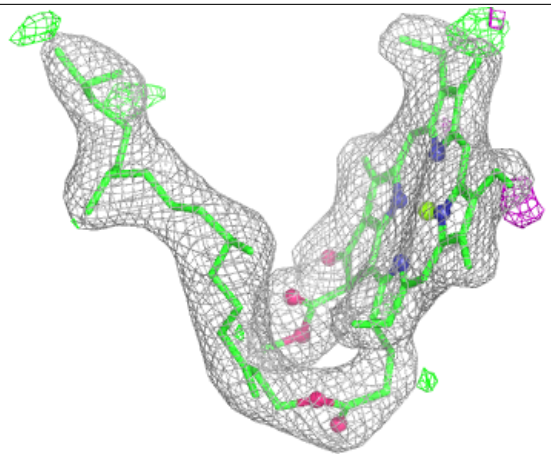


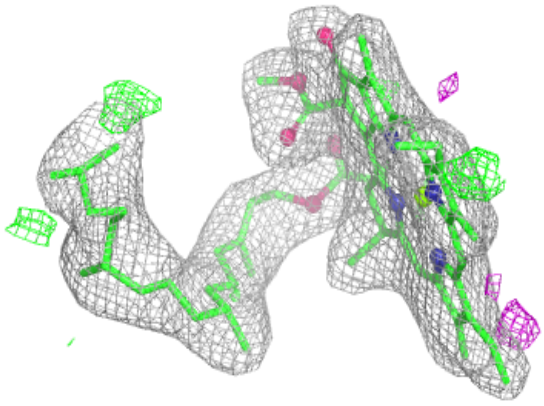


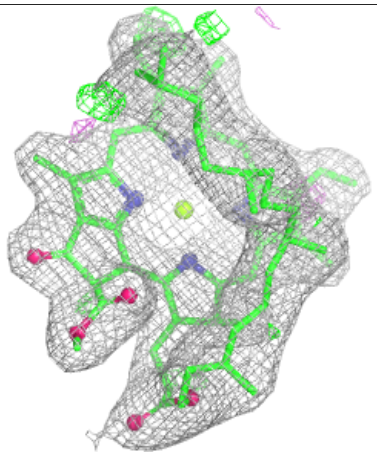


Electron density around CLA B 613:

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

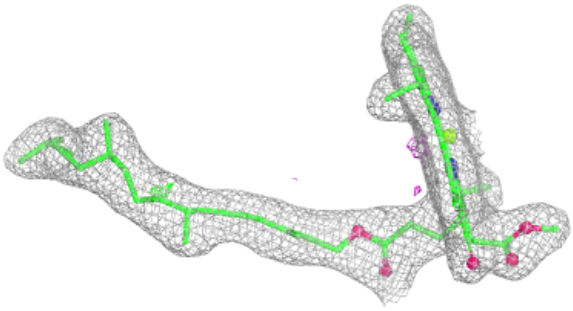


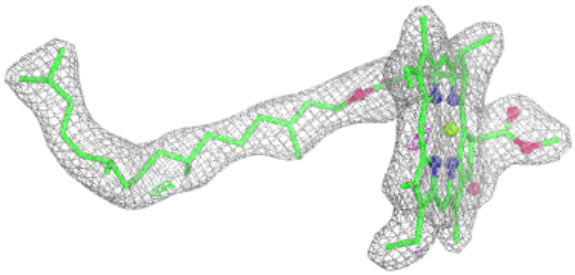


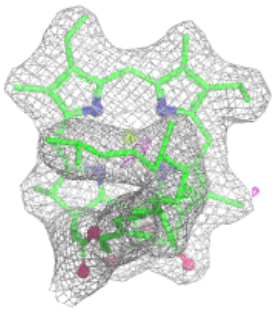


Electron density around CLA b 605:

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

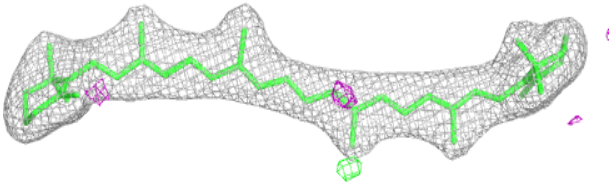


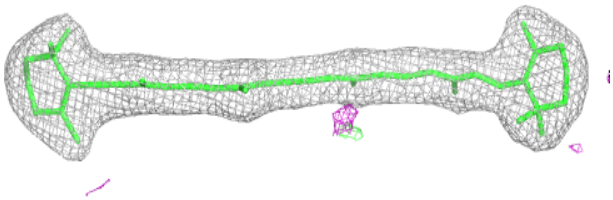


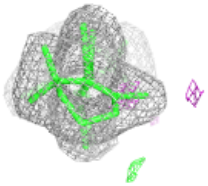


Electron density around BCR a 408:

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

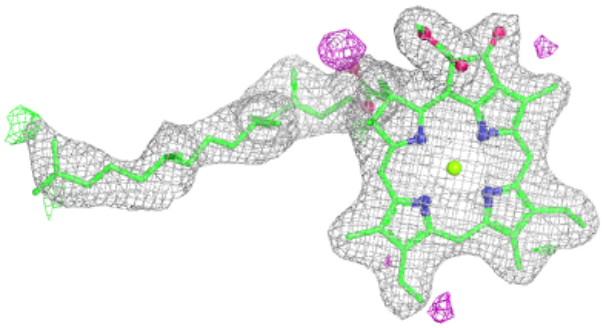


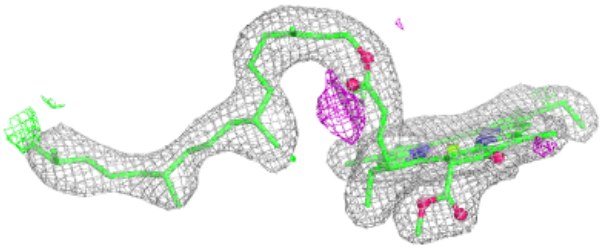


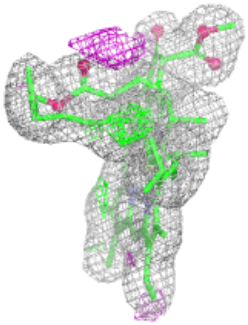


Electron density around CLA A 406:

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

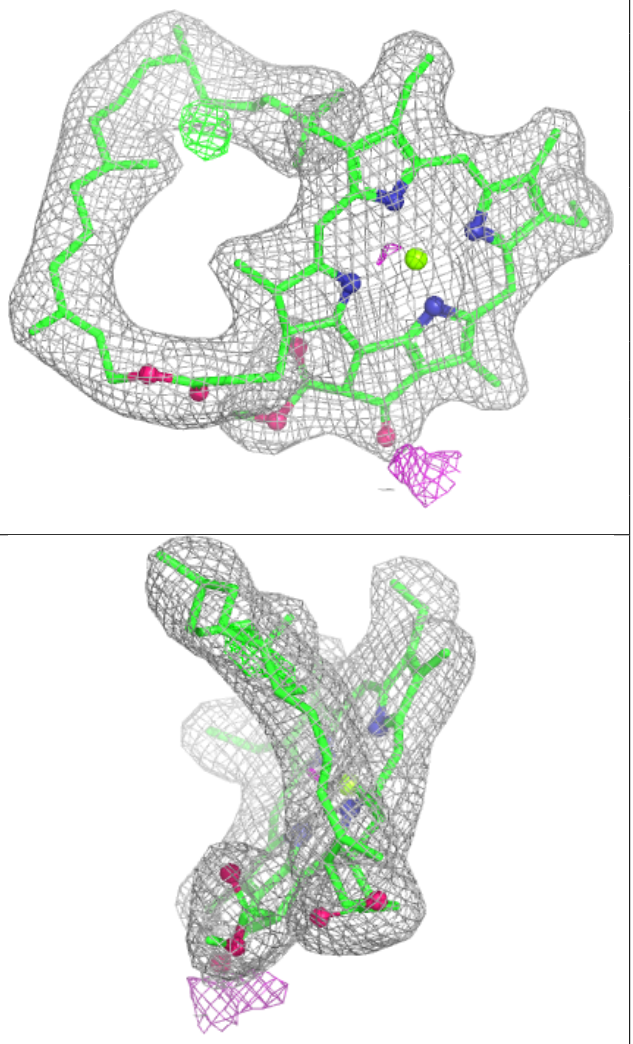






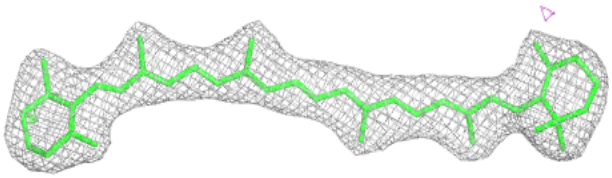
Electron density around CLA B 615:

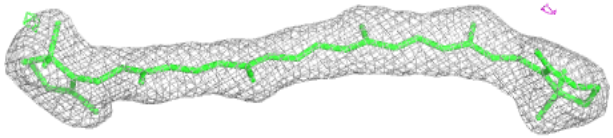
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

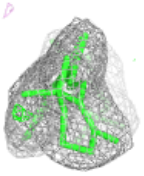


Electron density around BCR b 619:

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

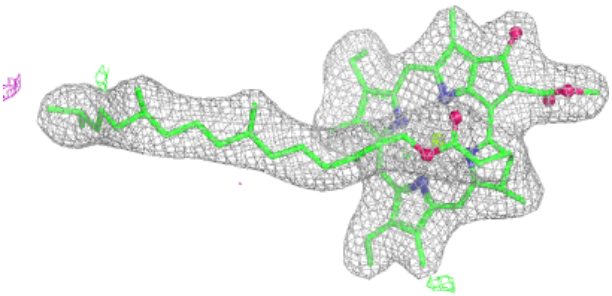


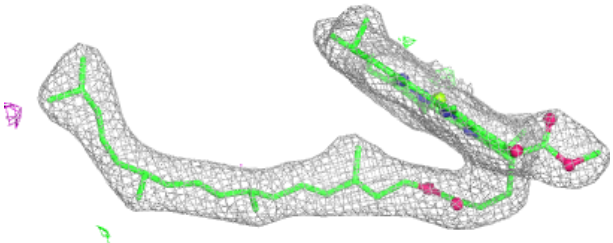


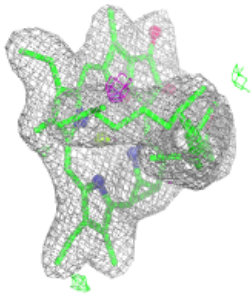


Electron density around CLA b 608:

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

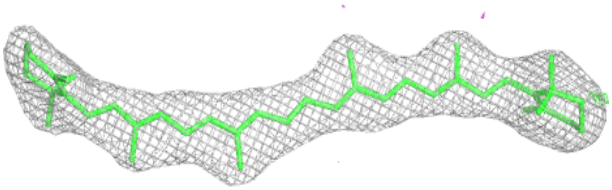


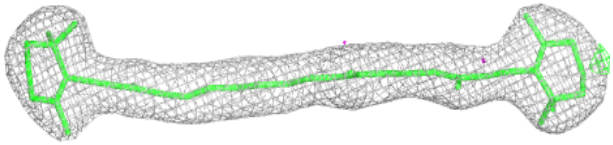


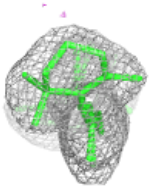


Electron density around BCR c 517:

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

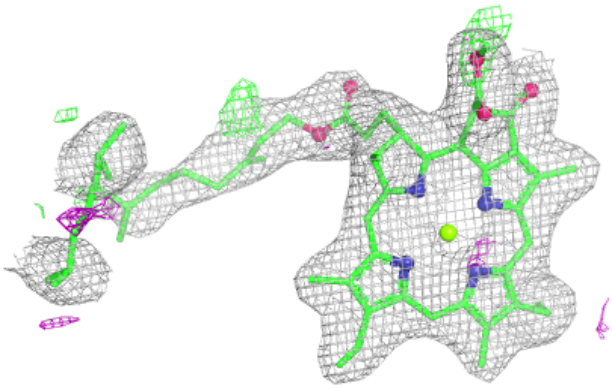


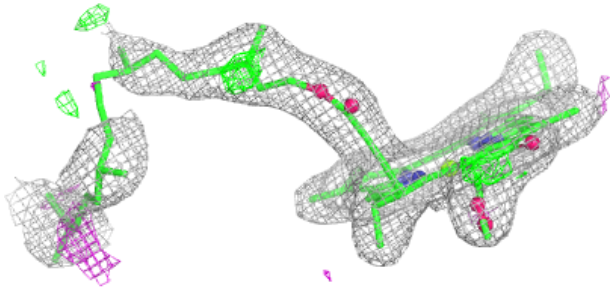


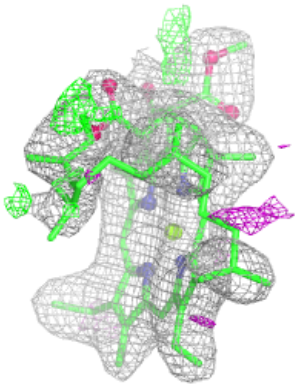


Electron density around CLA A 409:

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

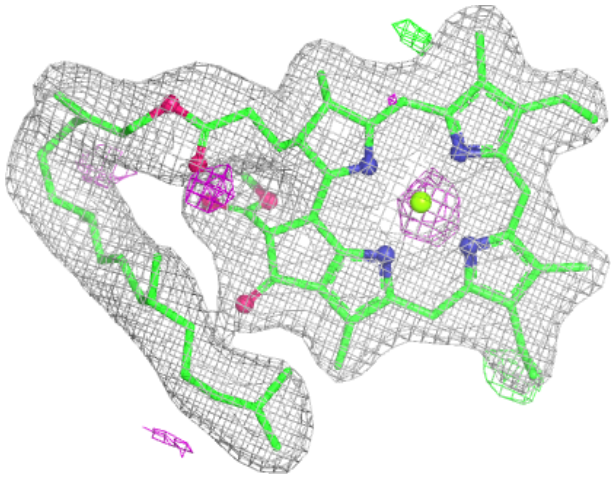


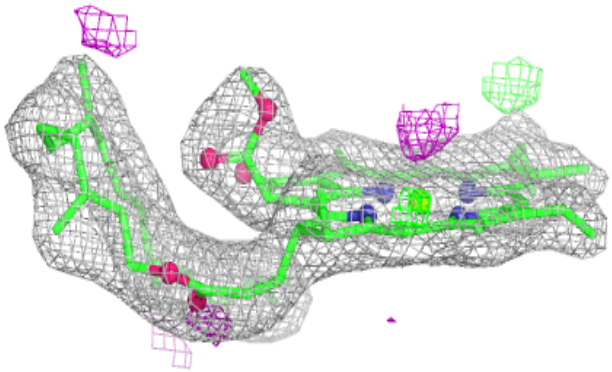


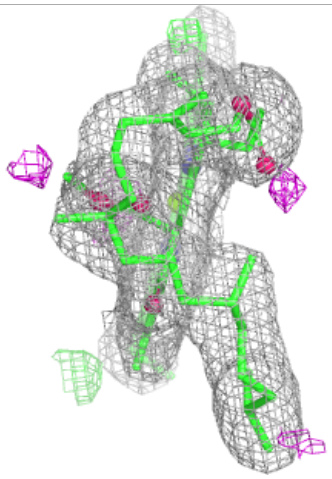


Electron density around CLA b 610:

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

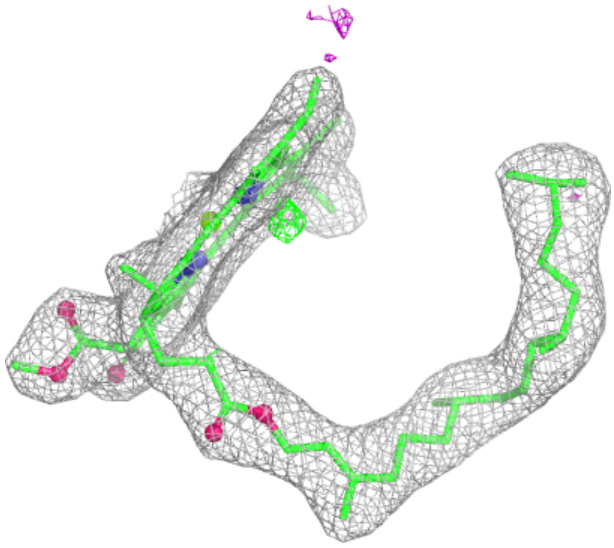


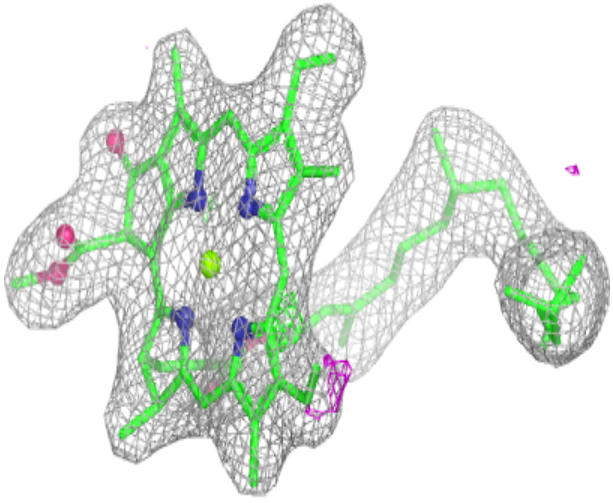


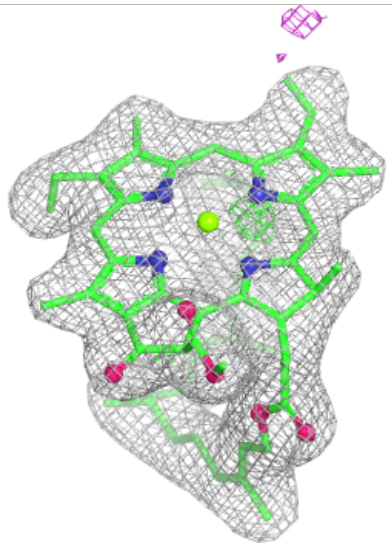


Electron density around CLA b 611:

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

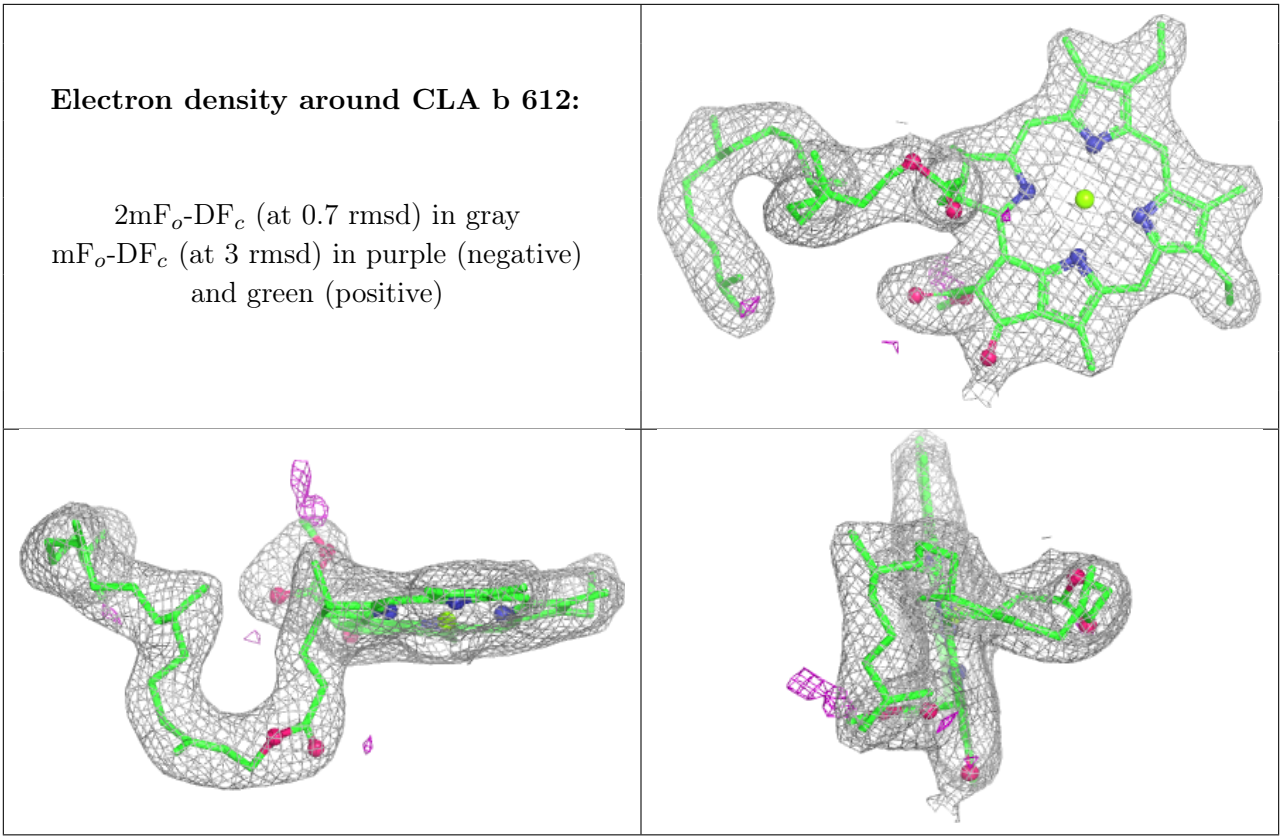






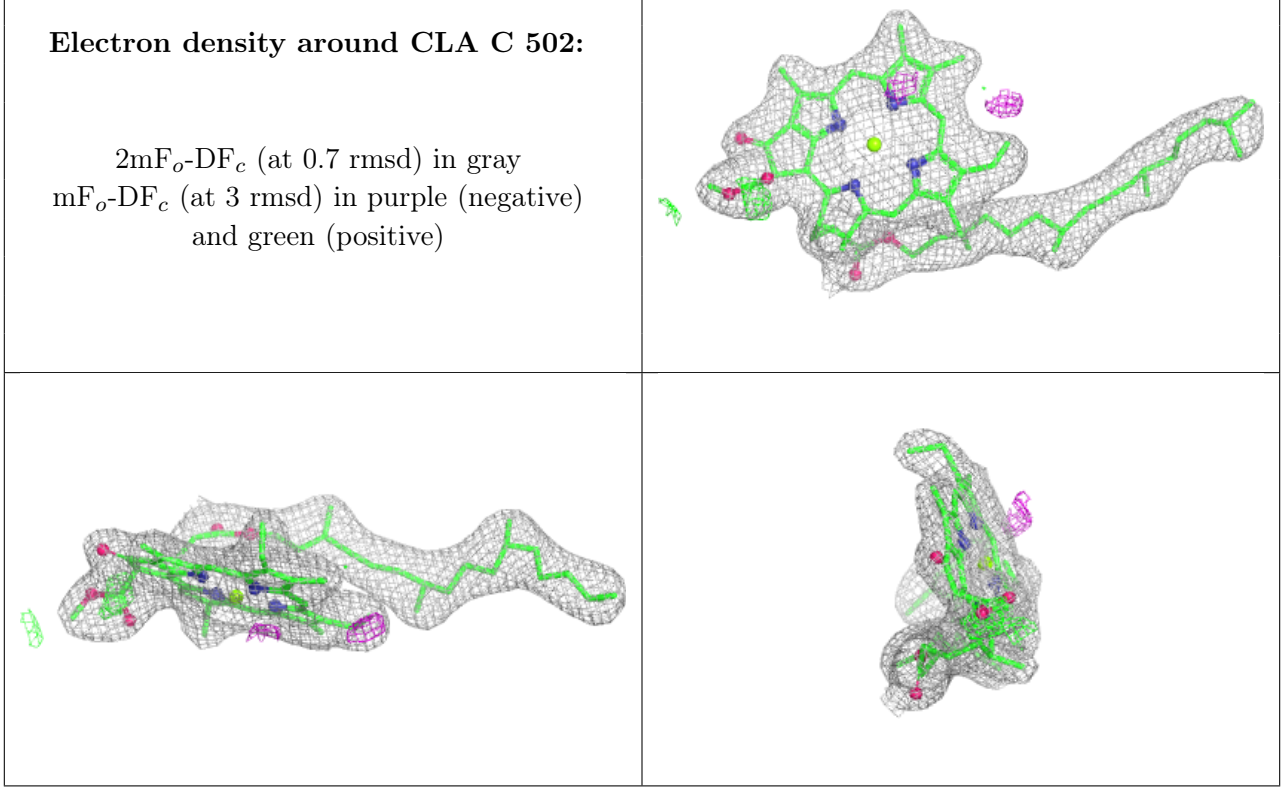
Electron density around CLA b 612:

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



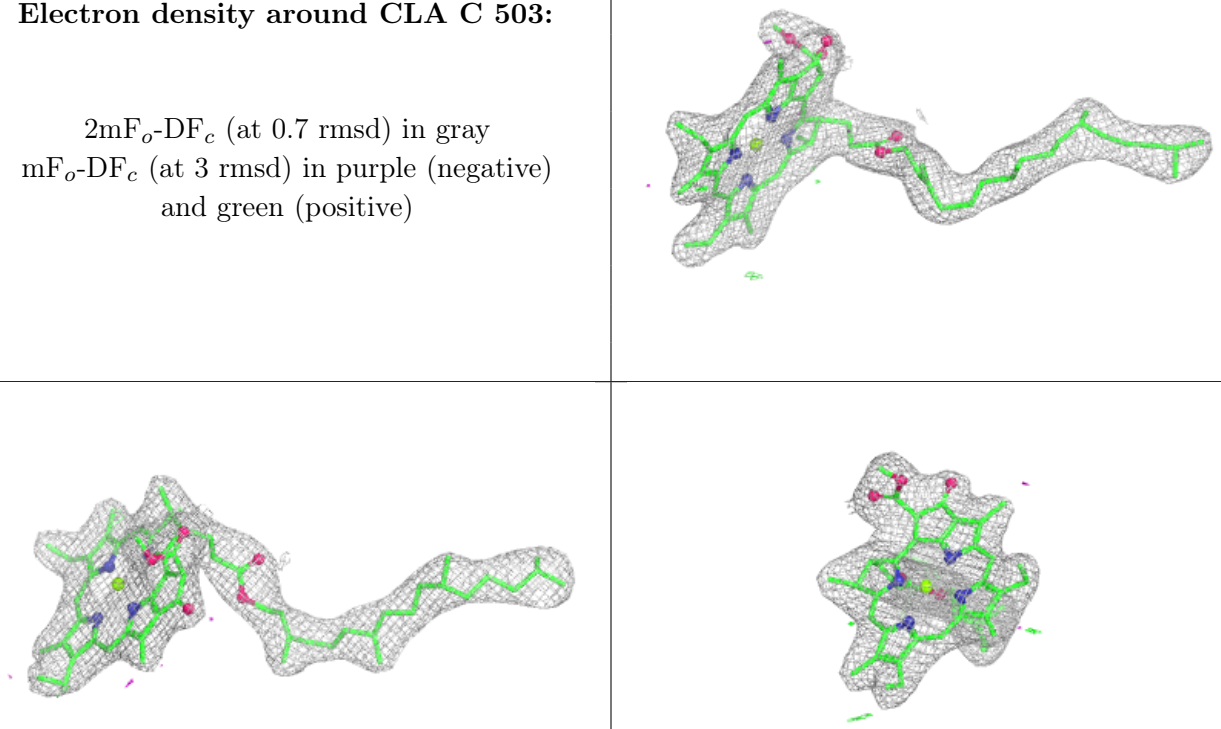
Electron density around CLA C 502:

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



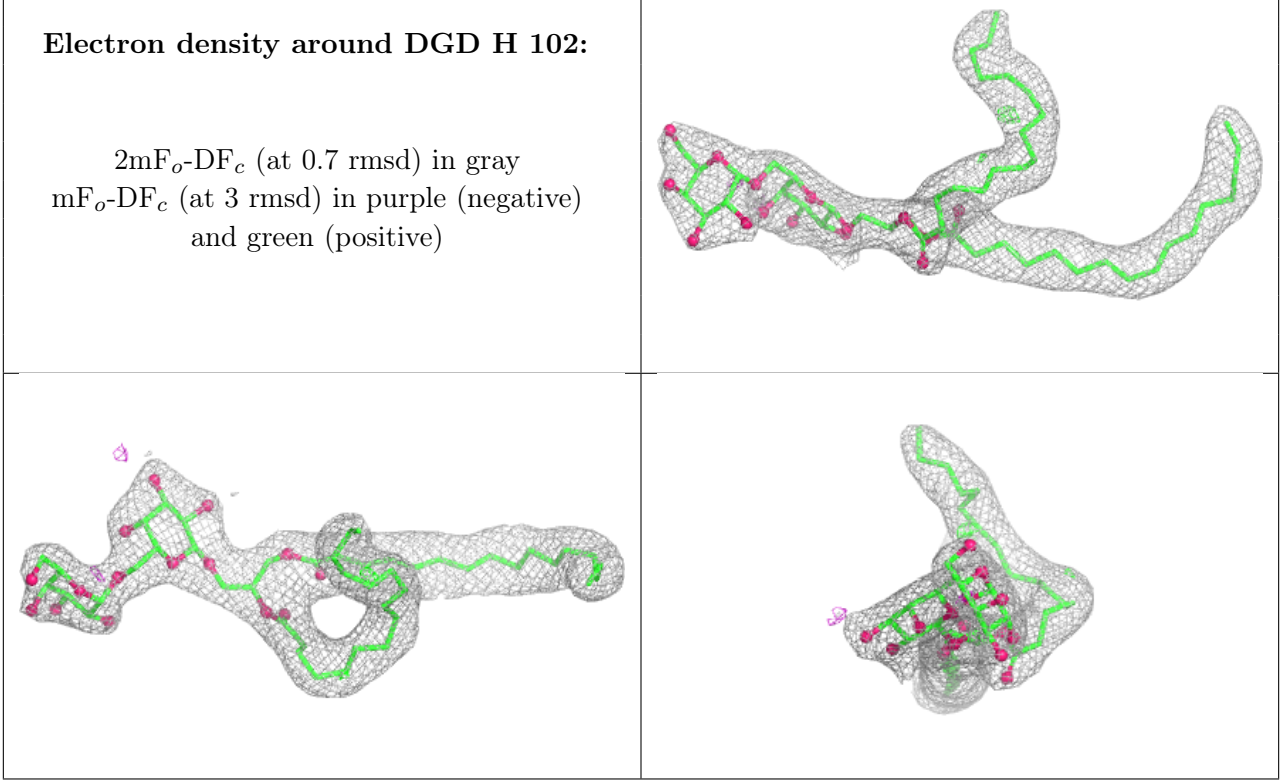
Electron density around CLA C 503:

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



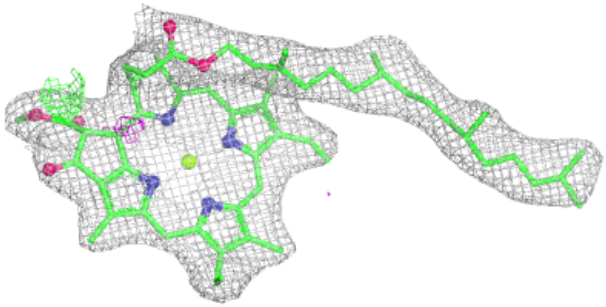
Electron density around DGD H 102:

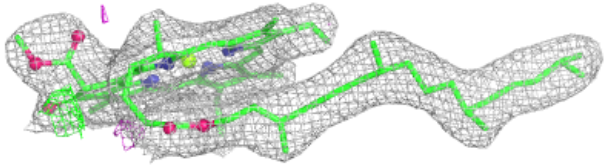
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

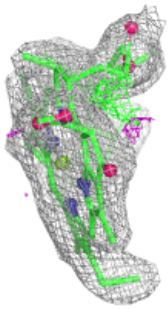


Electron density around CLA c 503:

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

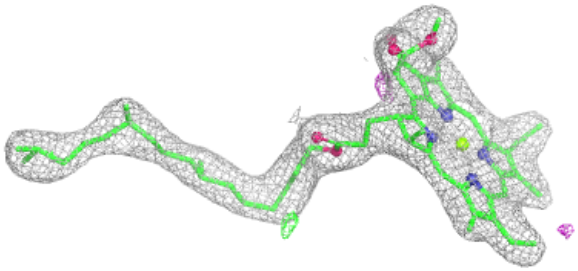


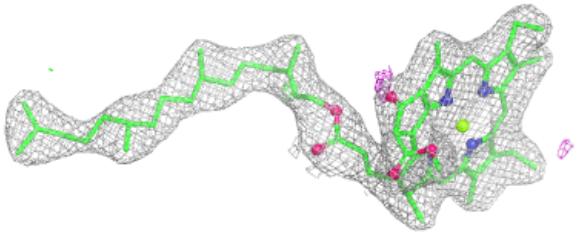


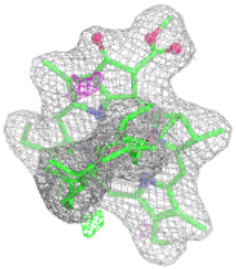


Electron density around CLA c 504:

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

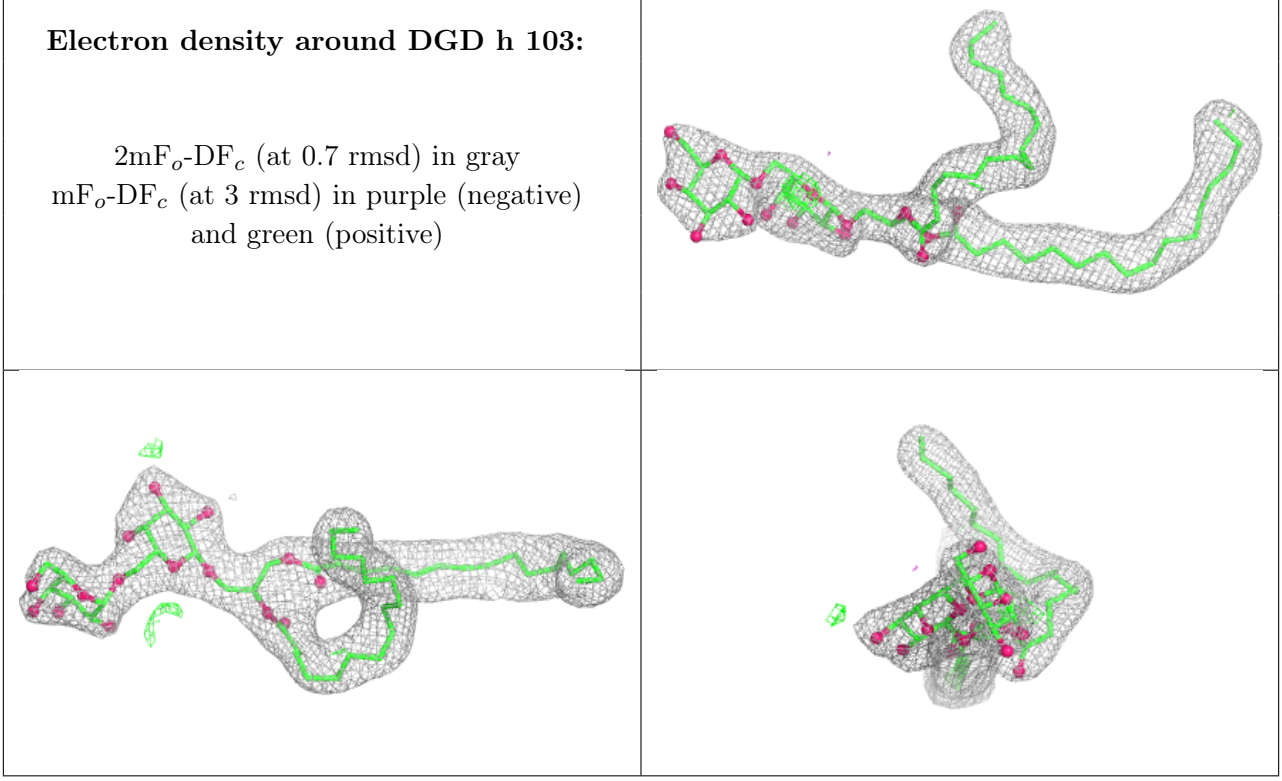






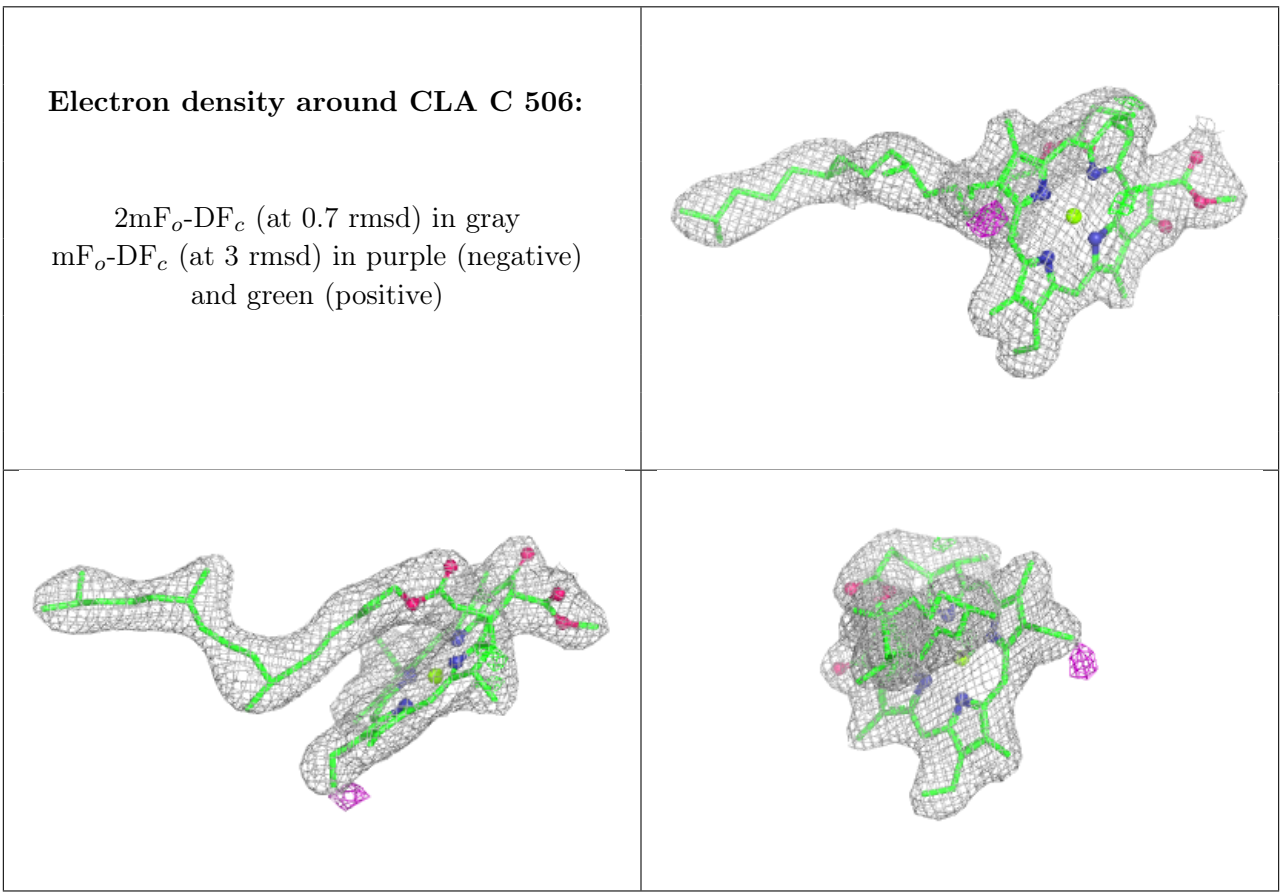
Electron density around DGD h 103:

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



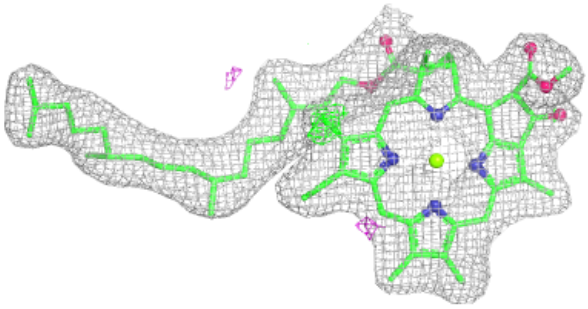
Electron density around CLA C 506:

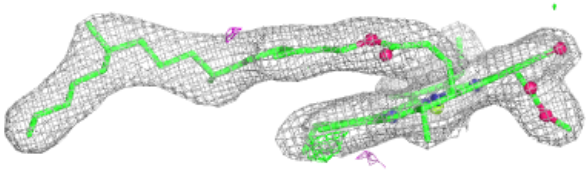
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

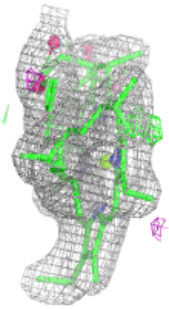


Electron density around CLA B 603:

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

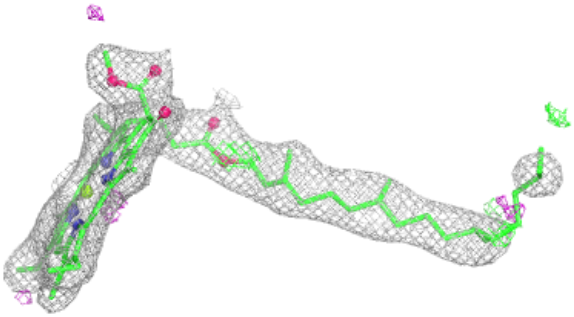


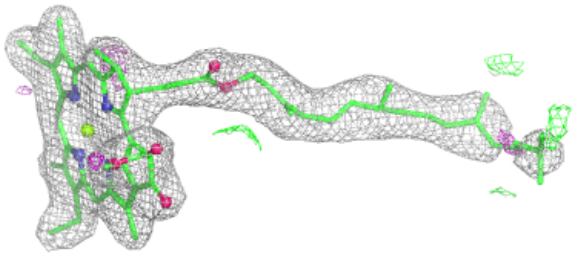


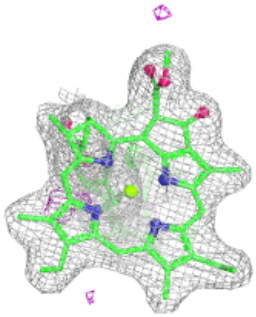


Electron density around CLA B 604:

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

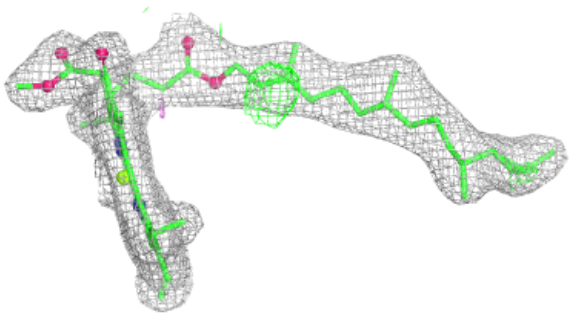


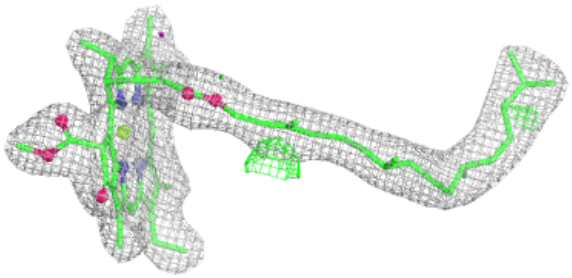


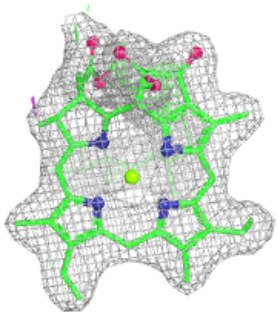


Electron density around CLA B 605:

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

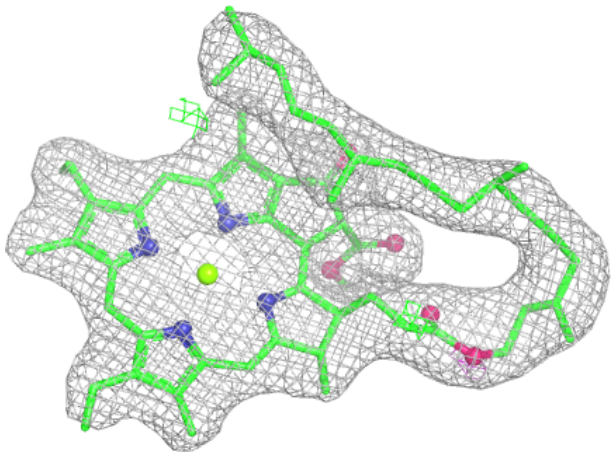


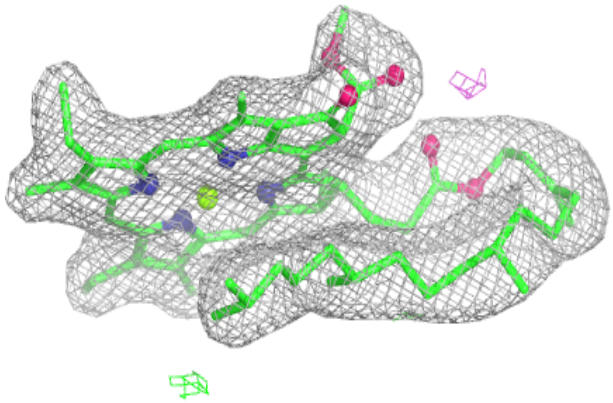


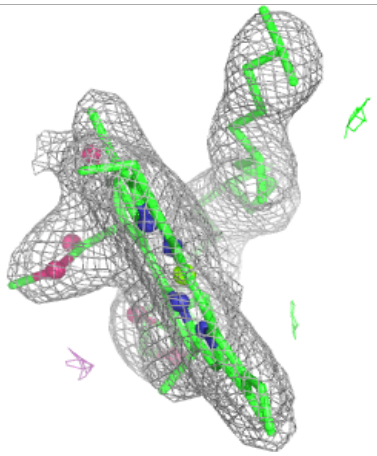


Electron density around CLA C 510:

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

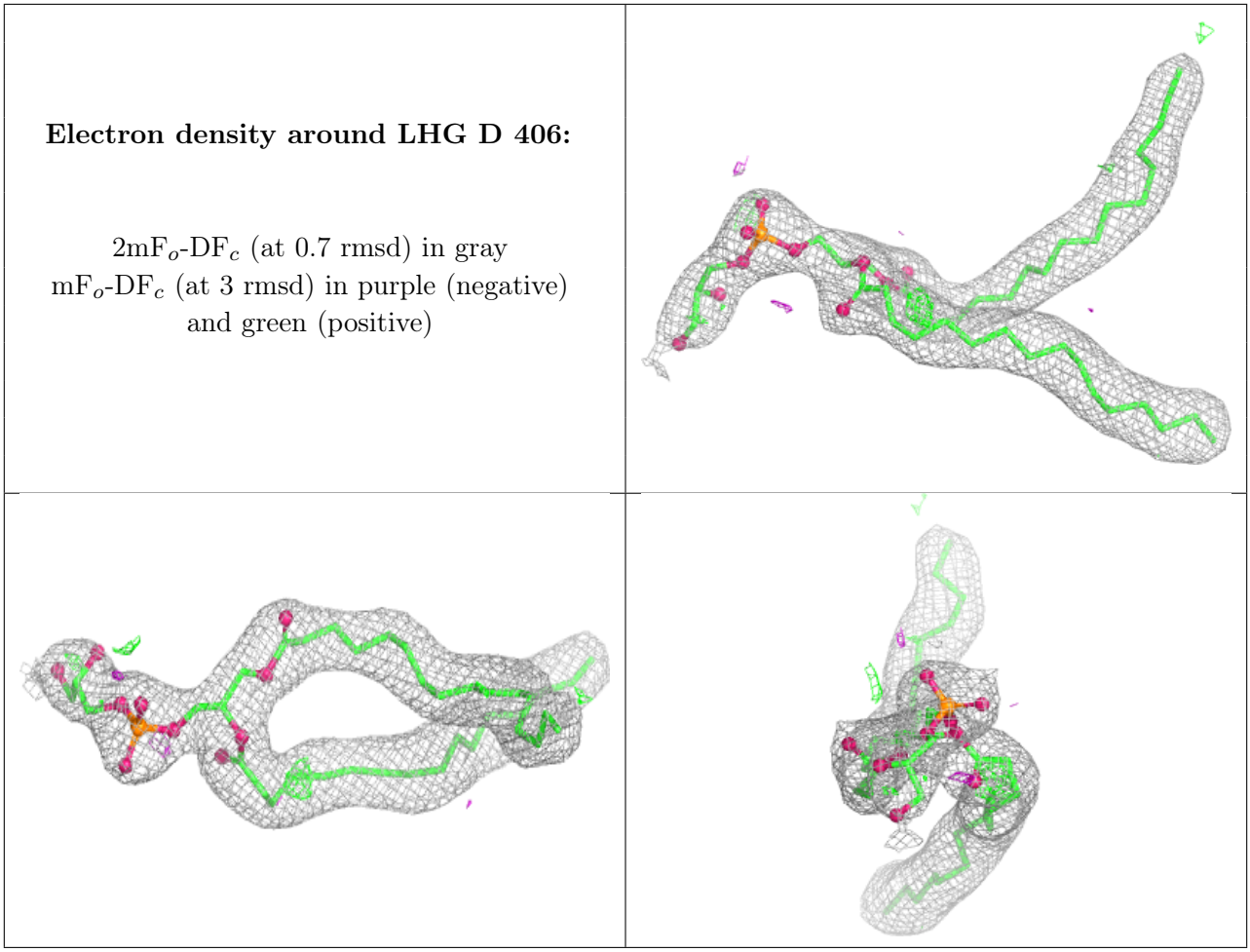






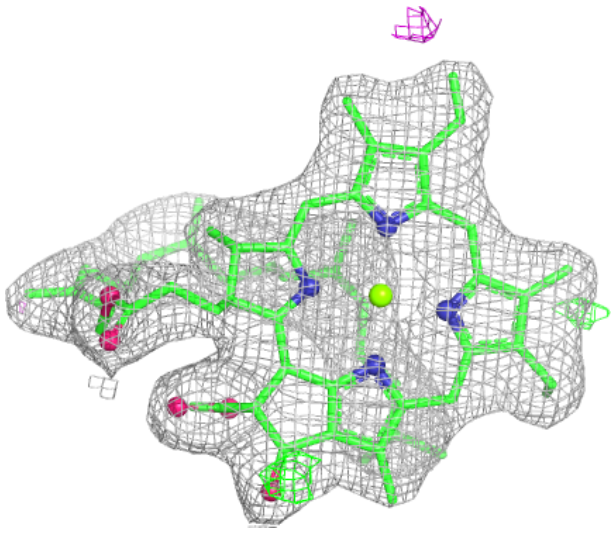
Electron density around LHG D 406:

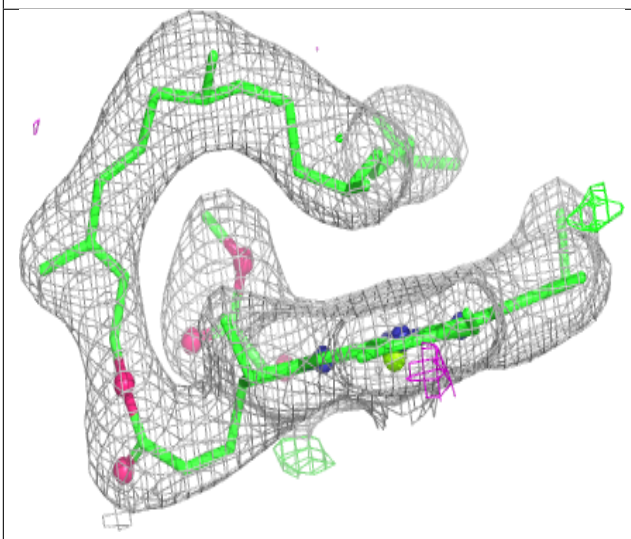
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

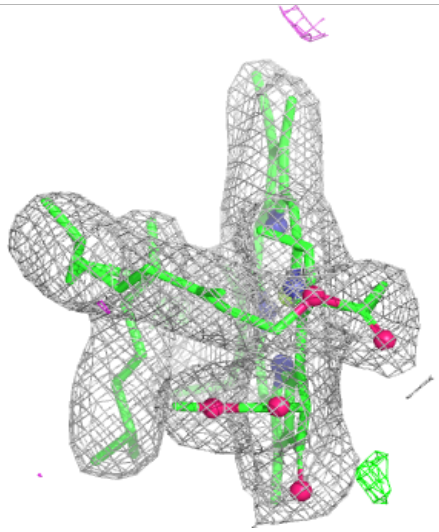


Electron density around CLA C 511:

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

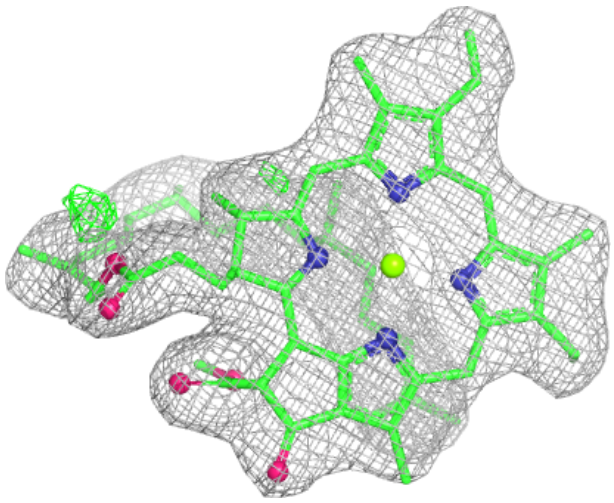


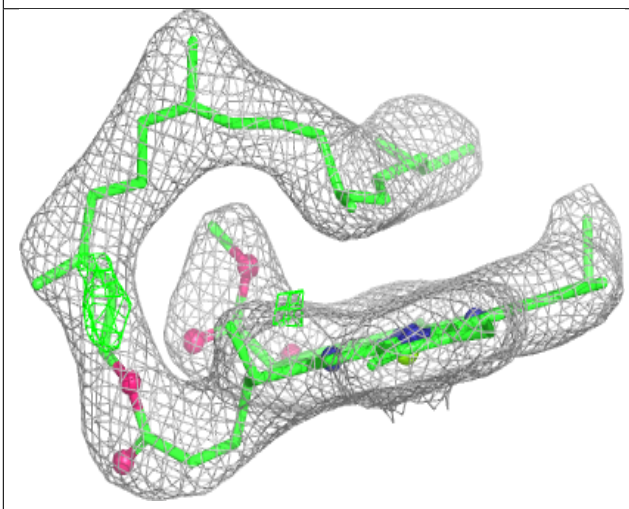


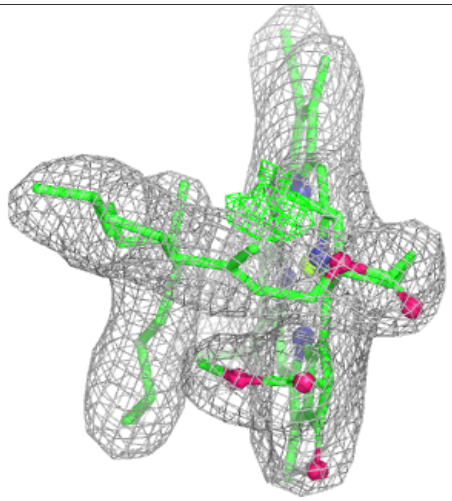


Electron density around CLA c 512:

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

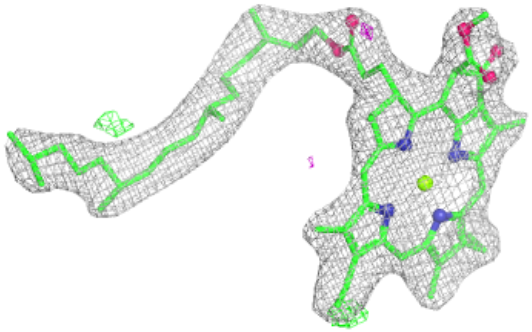


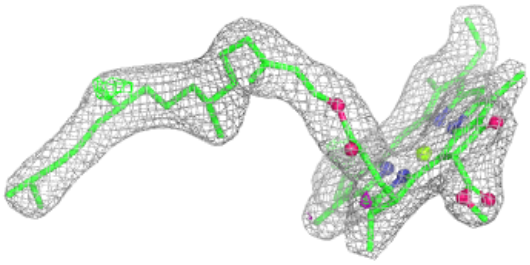


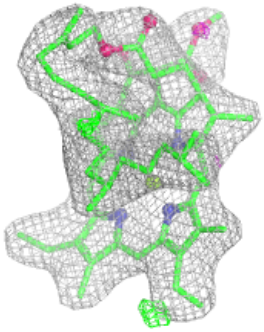


Electron density around CLA C 512:

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

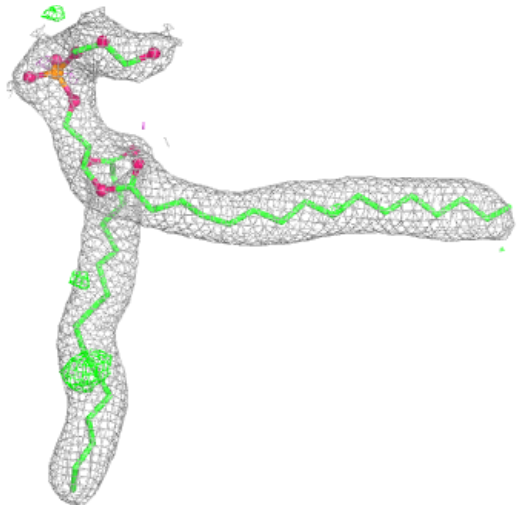


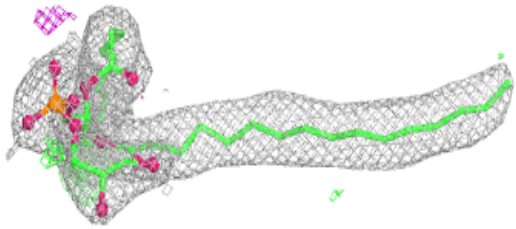


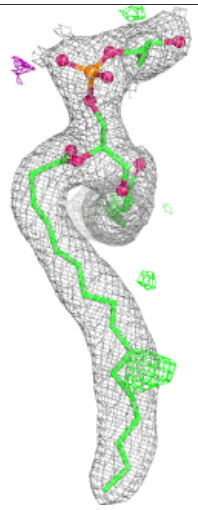


Electron density around LHG L 101:

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

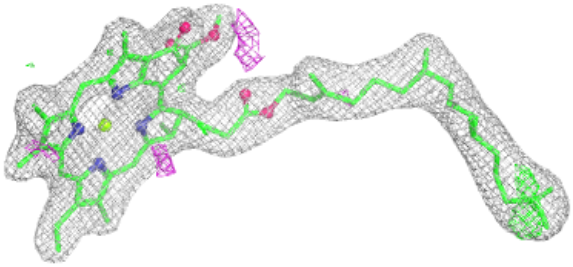


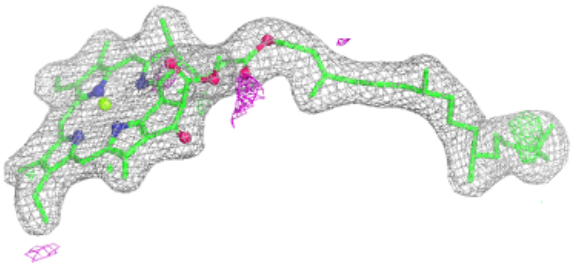


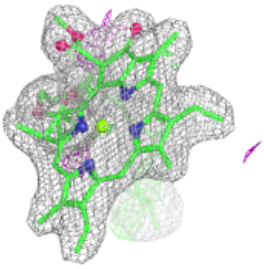


Electron density around CLA A 404:

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

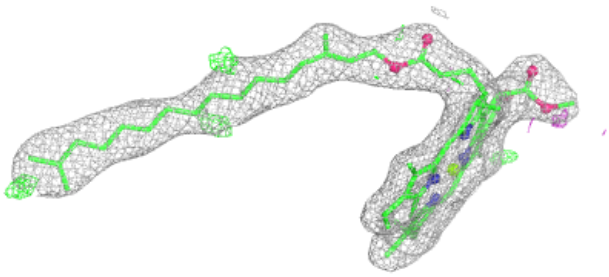


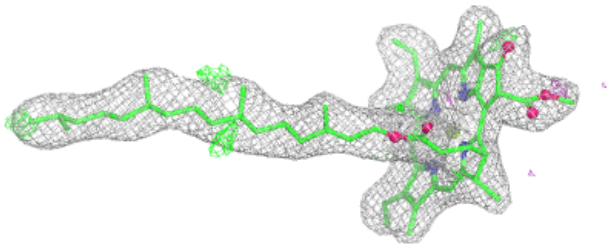


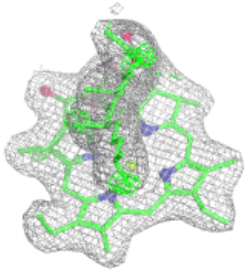


Electron density around CLA B 607:

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

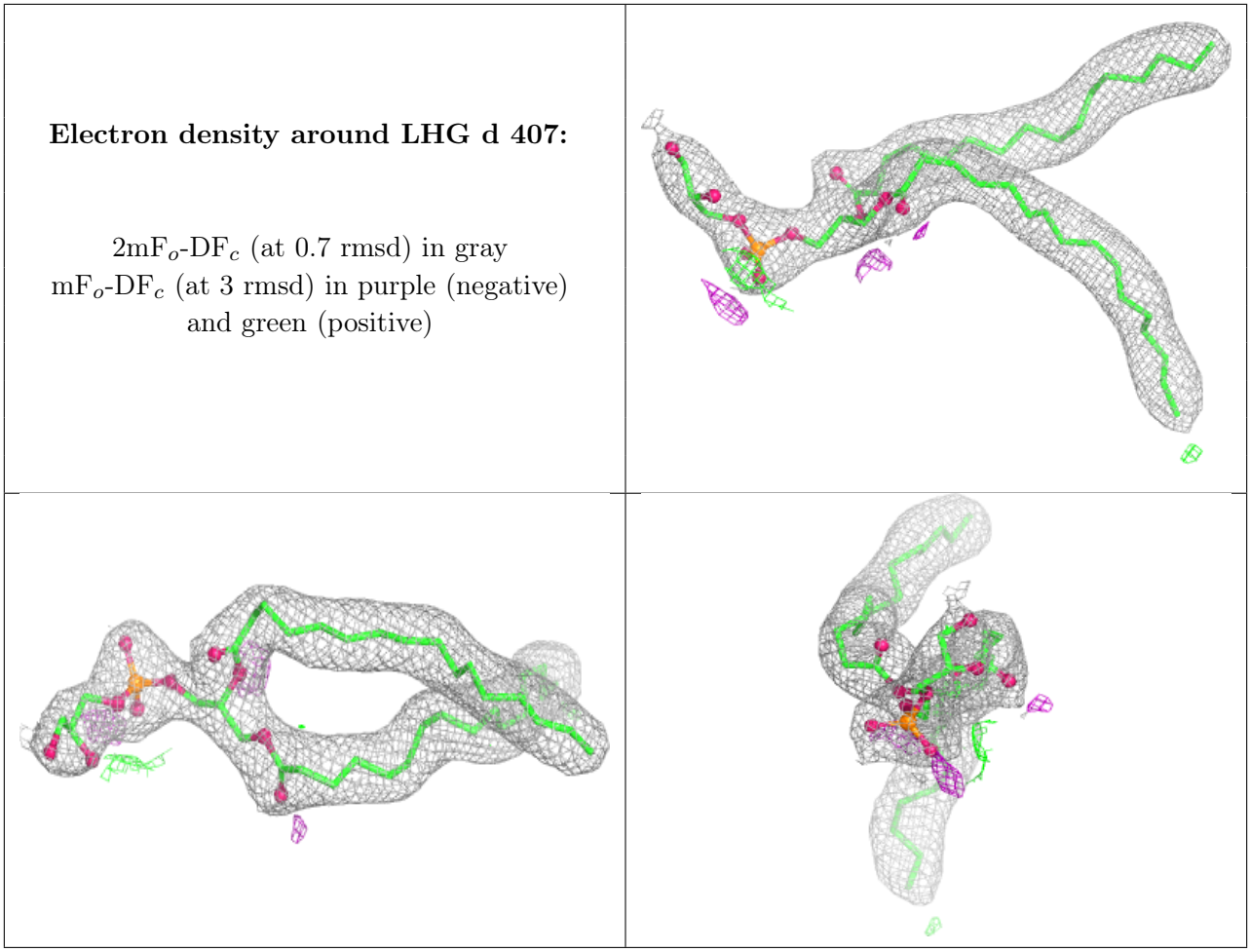






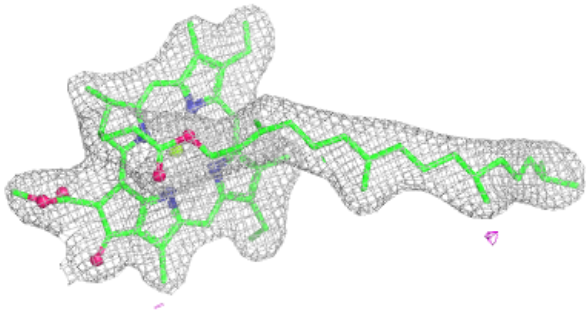
Electron density around LHG d 407:

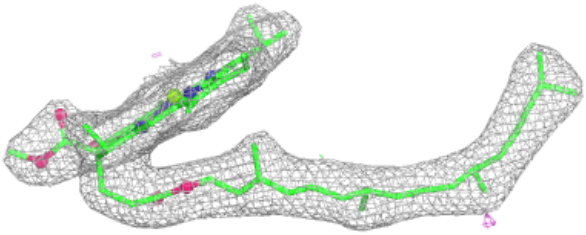
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

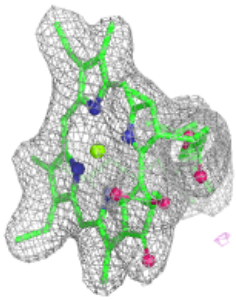


Electron density around CLA B 608:

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

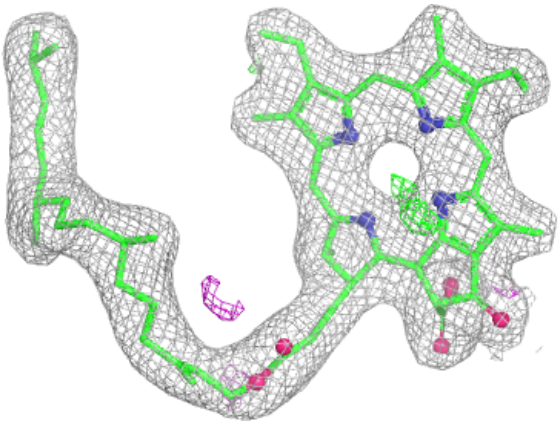


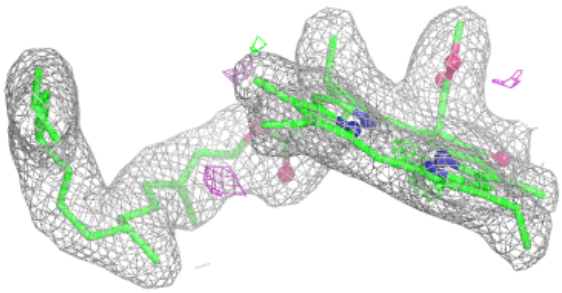


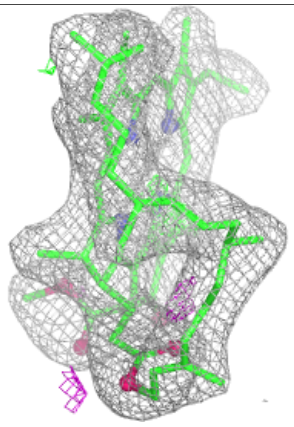


Electron density around PHO A 408:

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

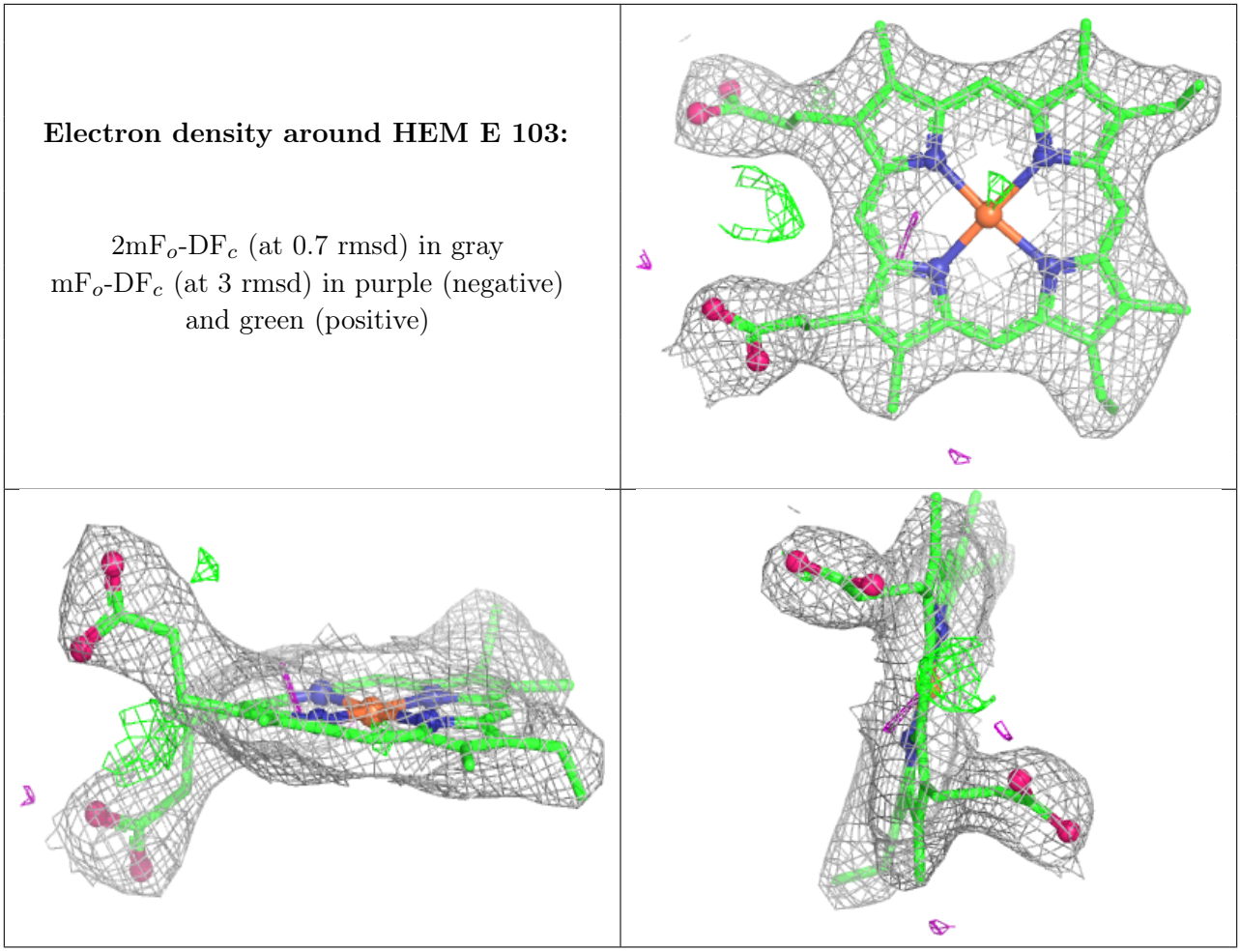






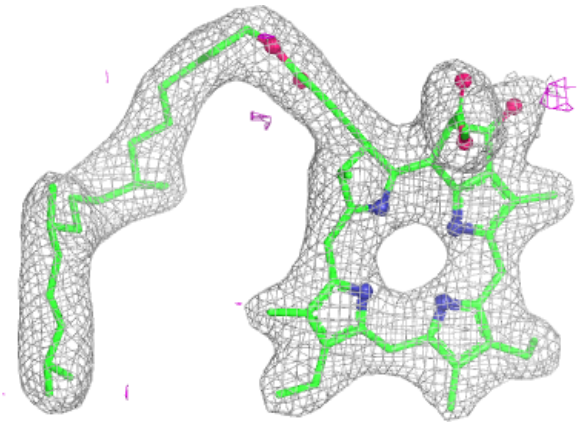
Electron density around HEM E 103:

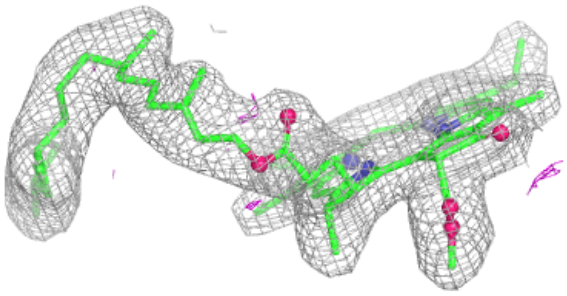
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

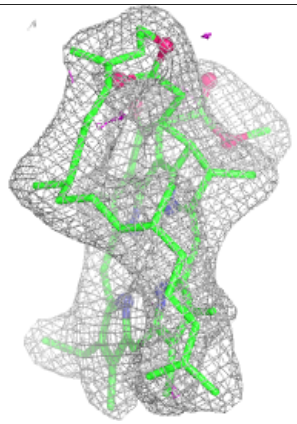


Electron density around PHO a 406:

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

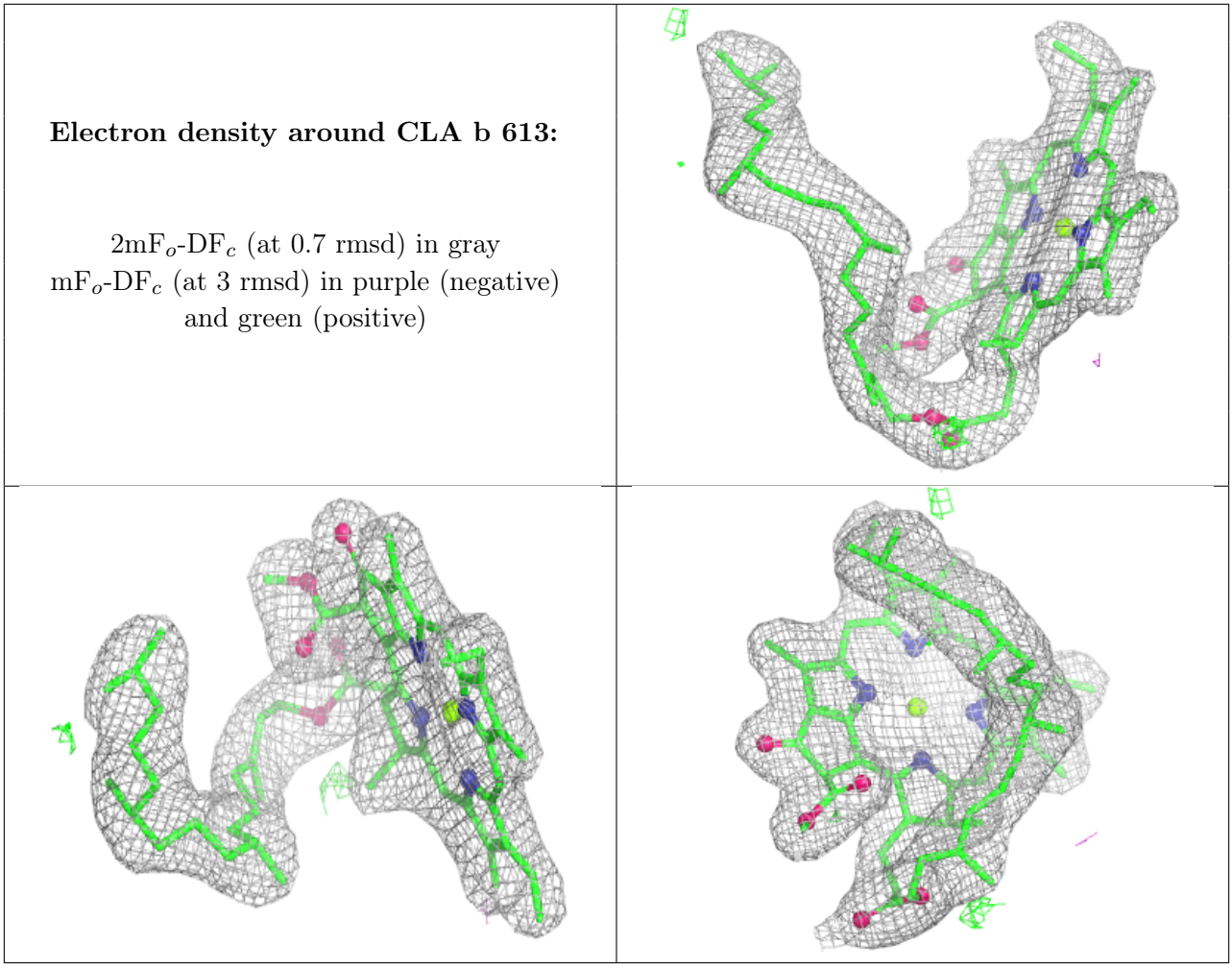






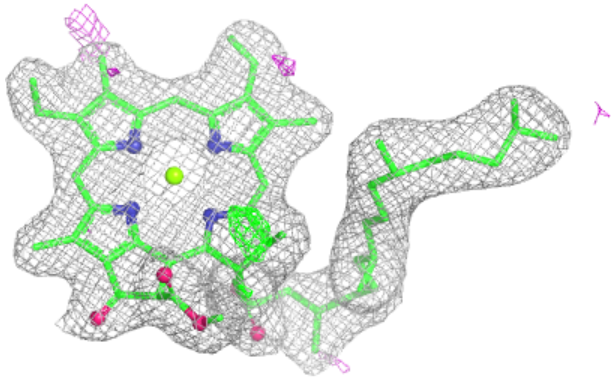
Electron density around CLA b 613:

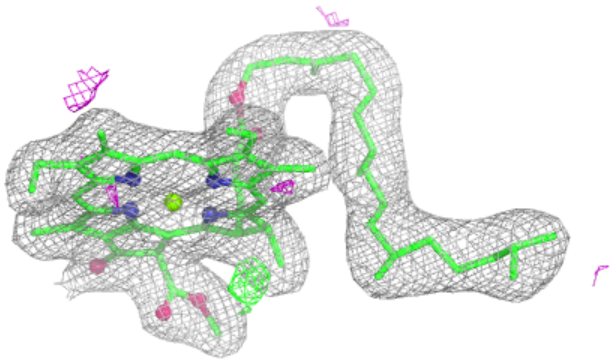
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

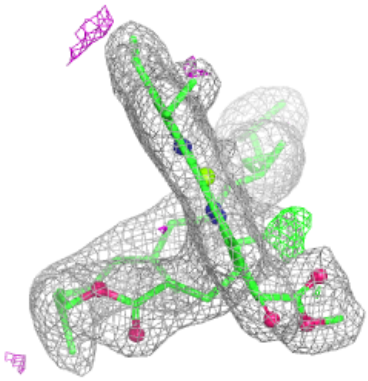


Electron density around CLA A 405:

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

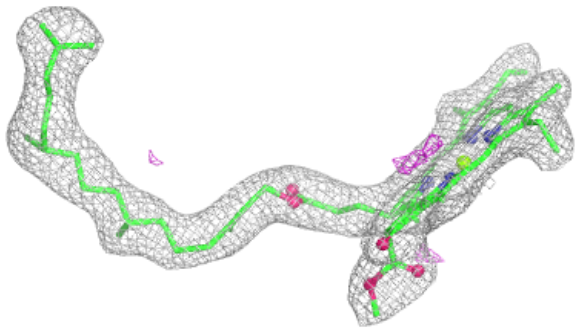


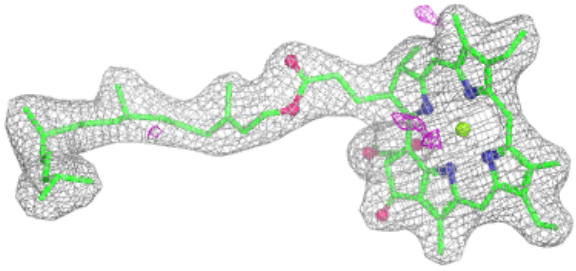


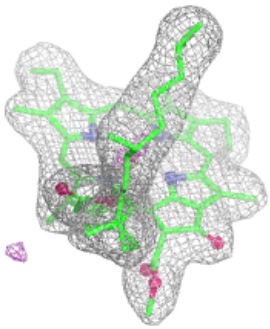


Electron density around CLA d 402:

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

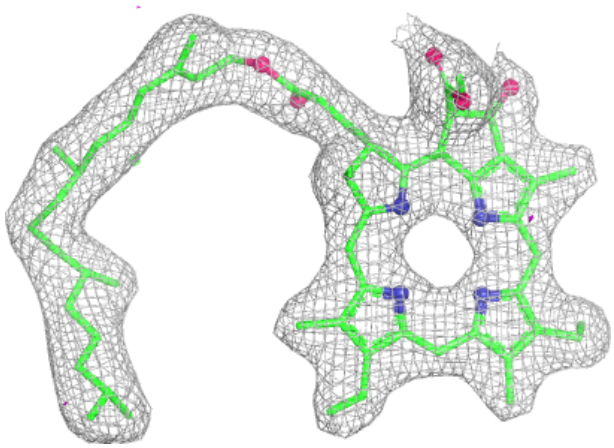


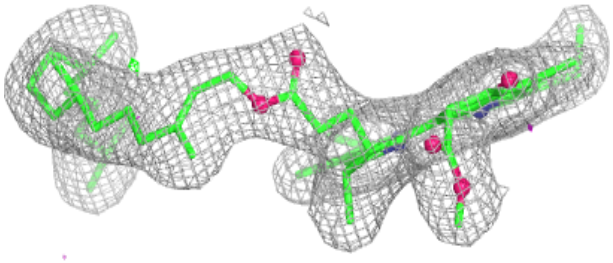


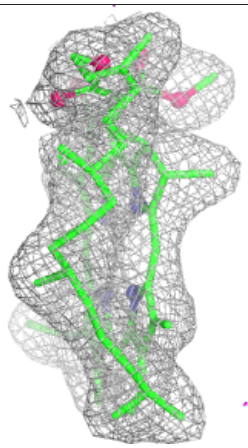


Electron density around PHO A 407:

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

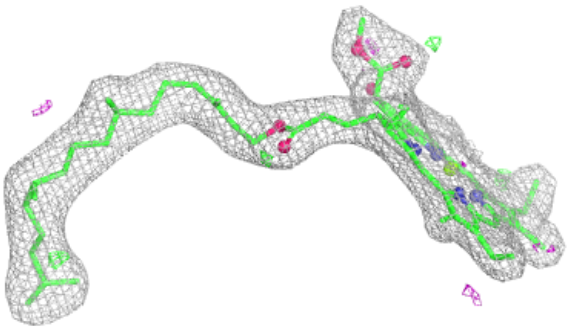


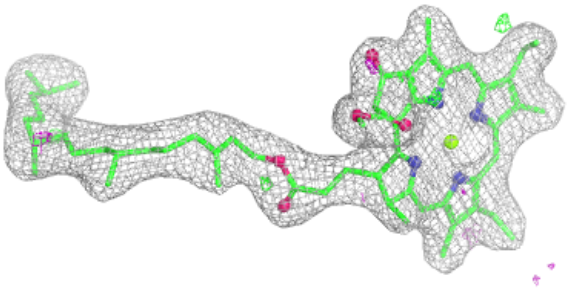




Electron density around CLA D 402:

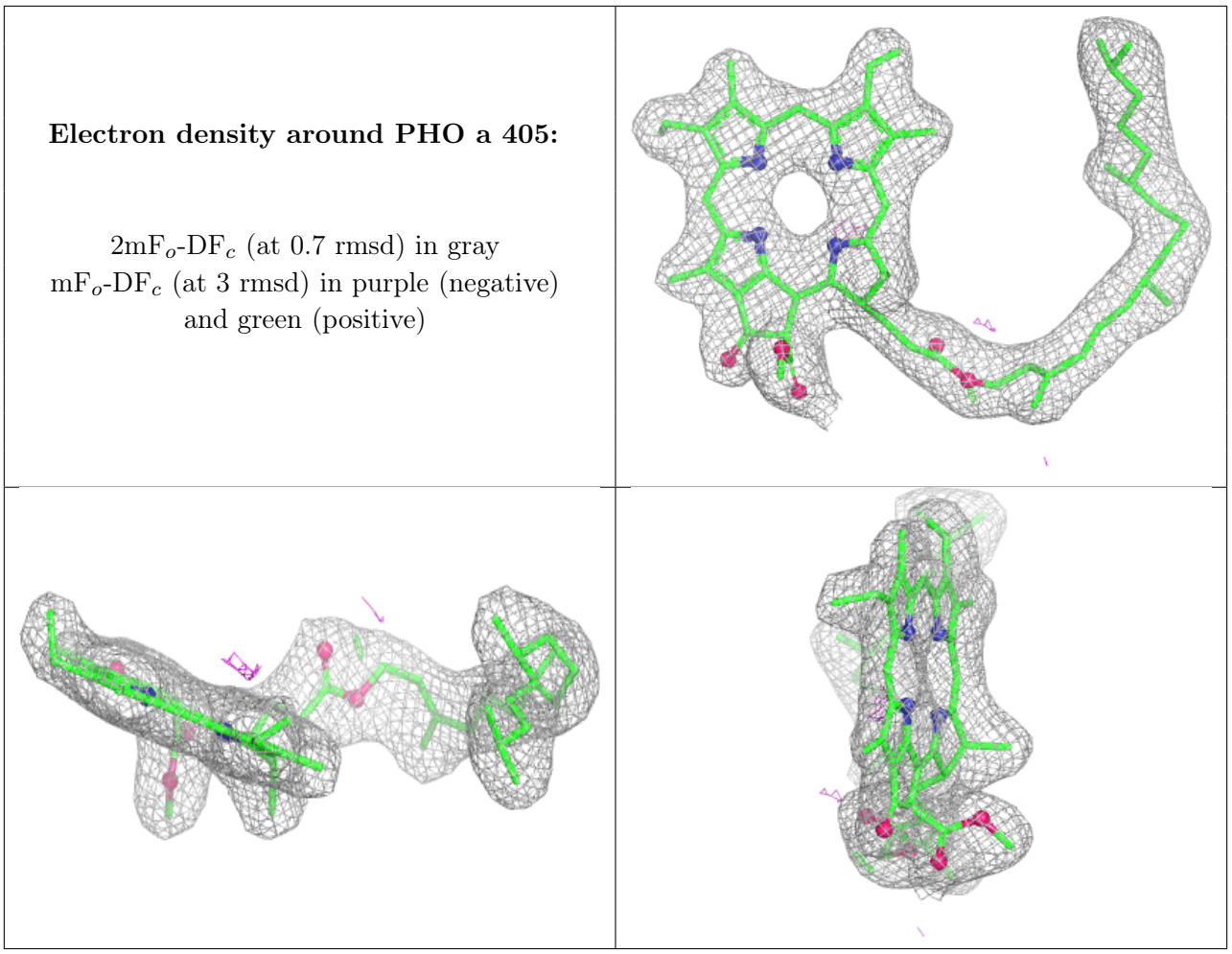
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





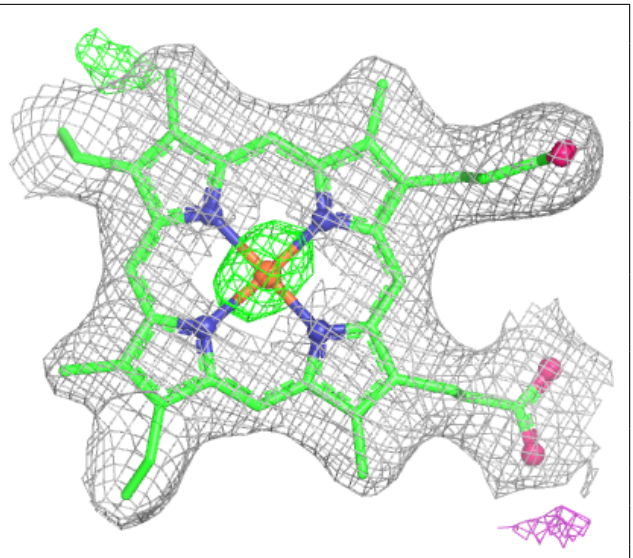
Electron density around PHO a 405:

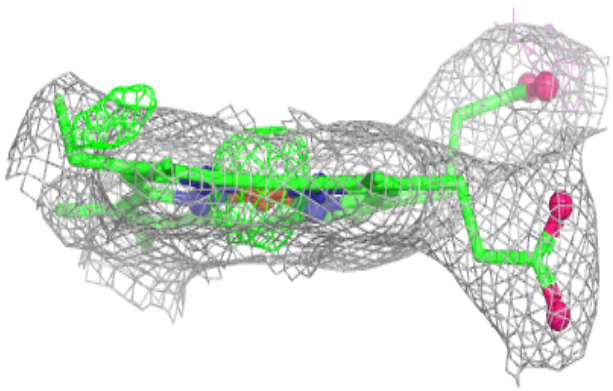
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

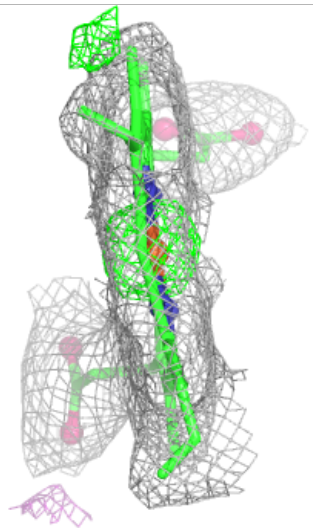


Electron density around HEC V 203:

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

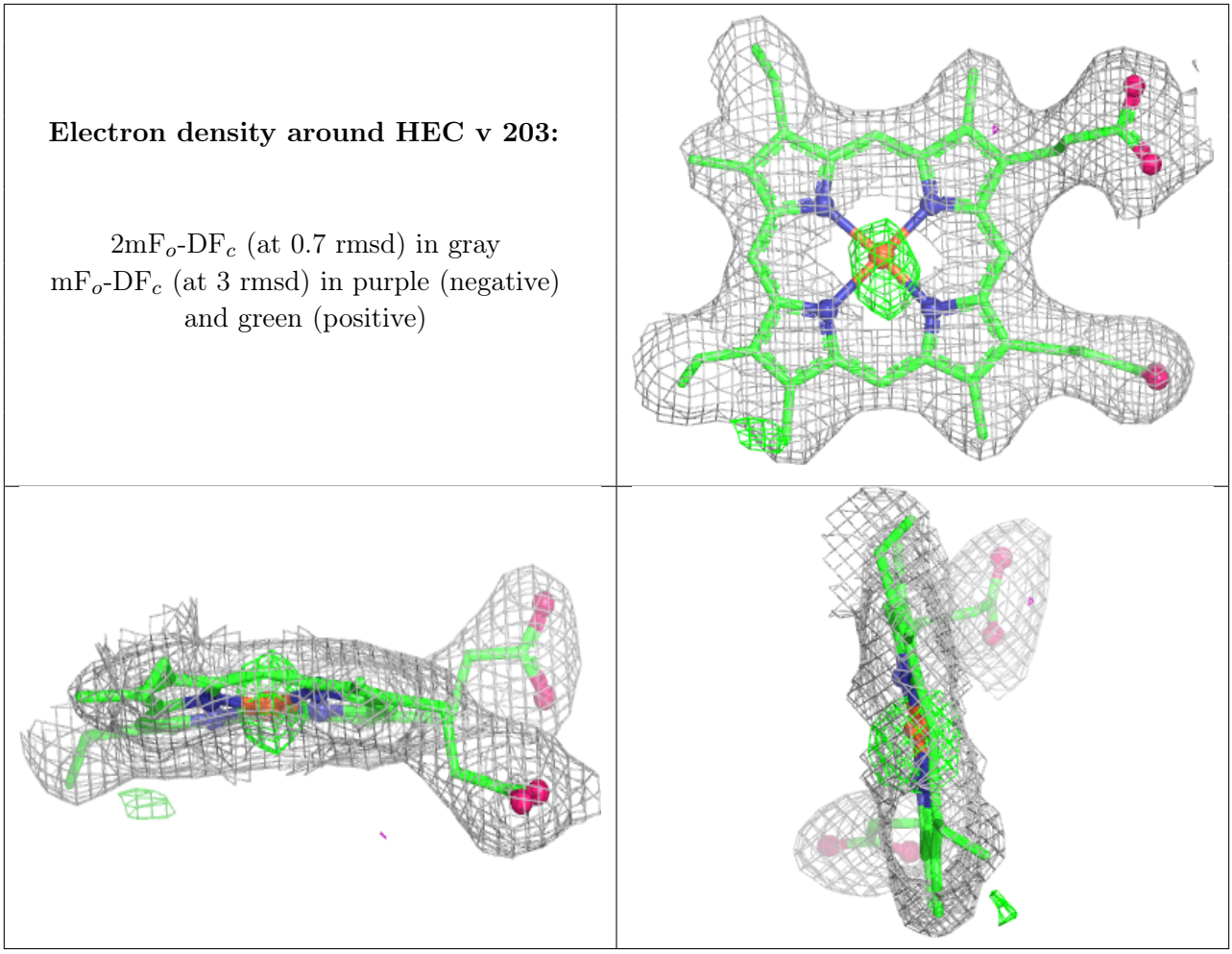






Electron density around HEC v 203:

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



6.5 Other polymers

There are no such residues in this entry.