wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 07:20 AM JST

PDB ID	:	5GTH / pdb_00005gth
Title	:	Native XFEL structure of photosystem II (dark dataset)
Authors	:	Suga, M.; Shen, J.R.
Deposited on	:	2016-08-20
Resolution	:	2.50 Å(reported)

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

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

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

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

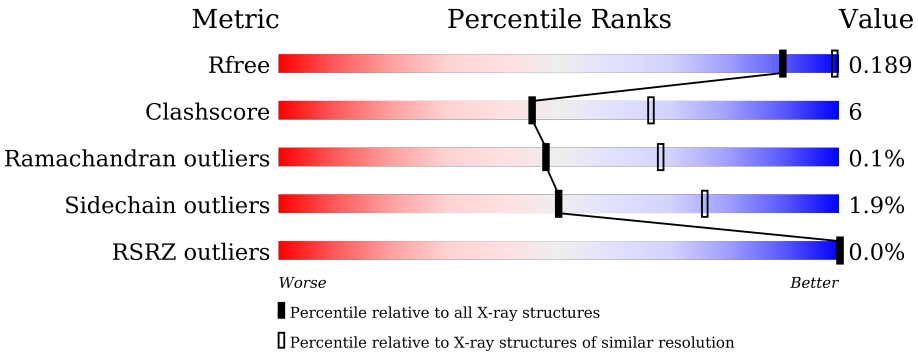
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	344	87% 10% •
1	a	344	86% 11% •
2	B	505	89% 10% •
2	b	505	89% 10% •
3	C	455	89% 9% ••
3	c	455	90% 10% •

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Mol	Chain	Length	Quality of chain
4	D	342	93% 7%
4	d	342	93% 7%
5	E	84	80% 17%
5	e	84	79% 13% 6%
6	F	44	61% 16% 23%
6	f	44	64% 7% 30%
7	H	65	2% 92% 6%
7	h	65	85% 15%
8	I	38	82% 18%
8	i	38	76% 21%
9	J	39	85% 10%
9	j	39	85% 15%
10	K	37	84% 14%
10	k	37	70% 22% 8%
11	L	37	86% 11%
11	l	37	92% 5%
12	M	36	72% 19% 8%
12	m	36	69% 22% 6%
13	O	244	85% 14%
13	o	244	86% 13%
14	T	32	81% 6% 6% 6%
14	t	32	81% 9% 6%
15	U	104	78% 14% 8%
15	u	104	90% 7%
16	V	137	94% 6%

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Mol	Chain	Length	Quality of chain
16	v	137	93% 6%
17	X	40	90% 5% 5%
17	x	40	82% 12% 5%
18	Y	30	73% 20%
18	y	30	70% 27%
19	Z	62	85% 13%
19	z	62	85% 13%
20	R	34	85% 15%

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
40	HEC	V	202	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 52773 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 protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	5	0
			2639	1732	431	461	15			

- 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 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	5	0
			3537	2317	589	618	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	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total 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	65	Total 511	C 341	N 82	O 86	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total 314	C 211	N 48	O 54	S 1	0	0	0
8	i	38	Total 314	C 211	N 48	O 54	S 1	0	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total 272	C 182	N 42	O 47	S 1	0	0	0
9	j	39	Total 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 (CCD ID: FE2) (formula: Fe).

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

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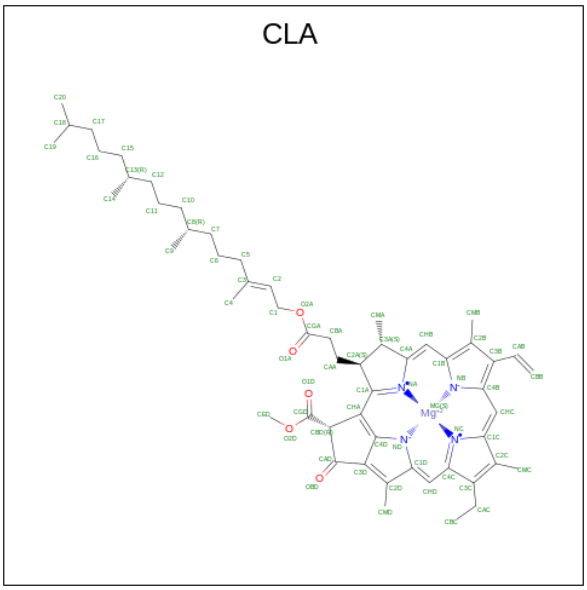
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	a	1	Total Fe 1 1	0	0

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

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

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



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

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

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

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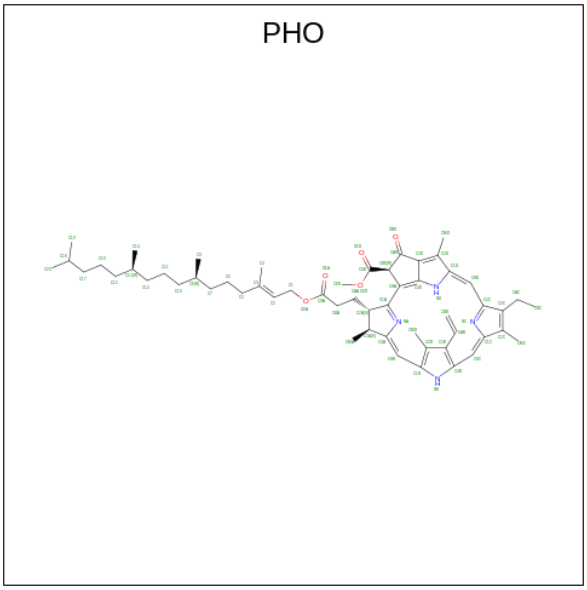
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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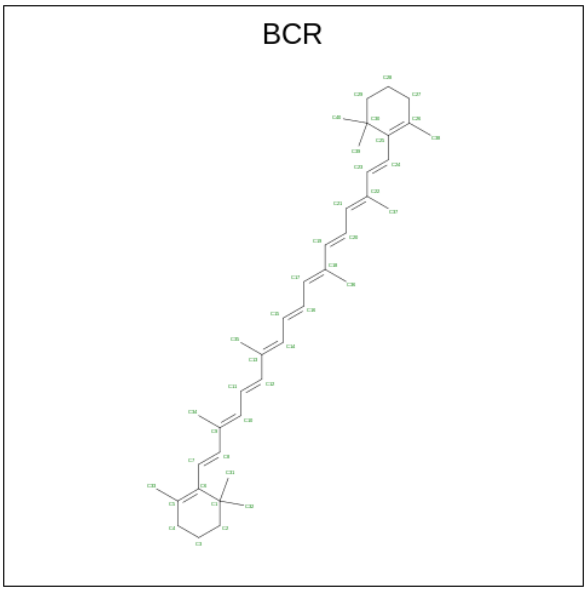
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



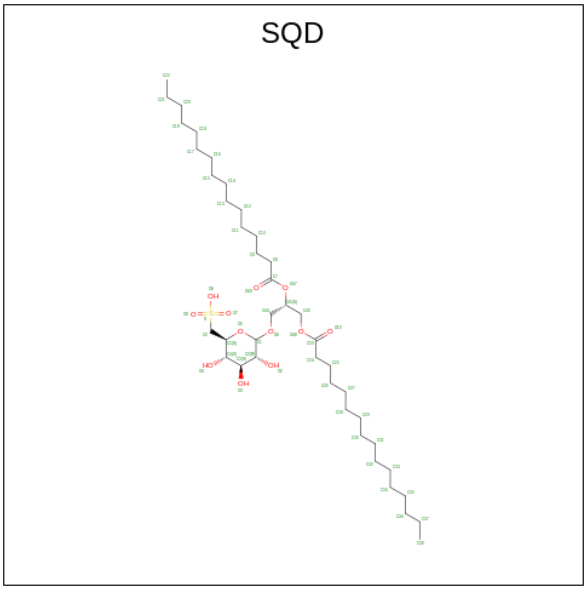
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



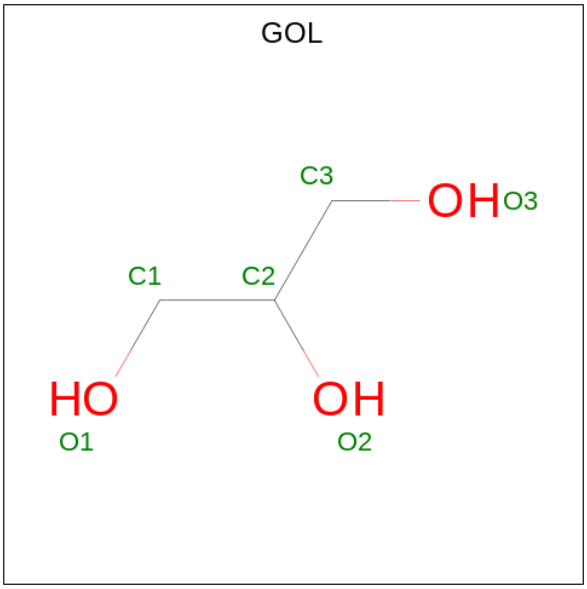
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	D	1	Total C O S 43 30 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0
26	a	1	Total C O S 54 41 12 1	0	0
26	a	1	Total C O S 54 41 12 1	0	0
26	f	1	Total C O S 43 30 12 1	0	0

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



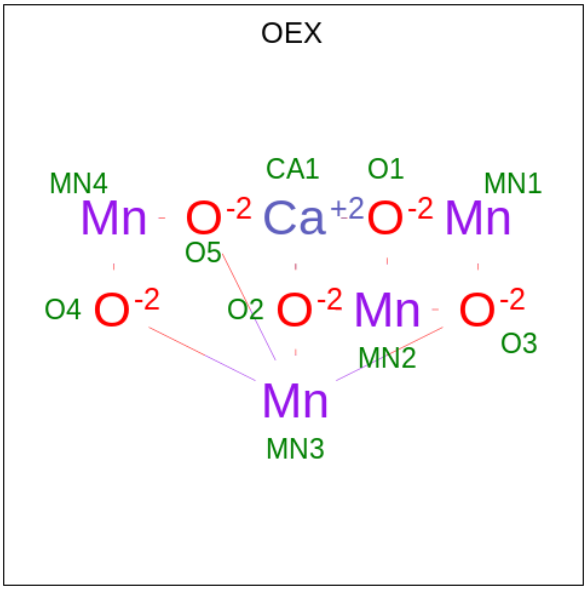
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	b	1	Total C O 6 3 3	0	0

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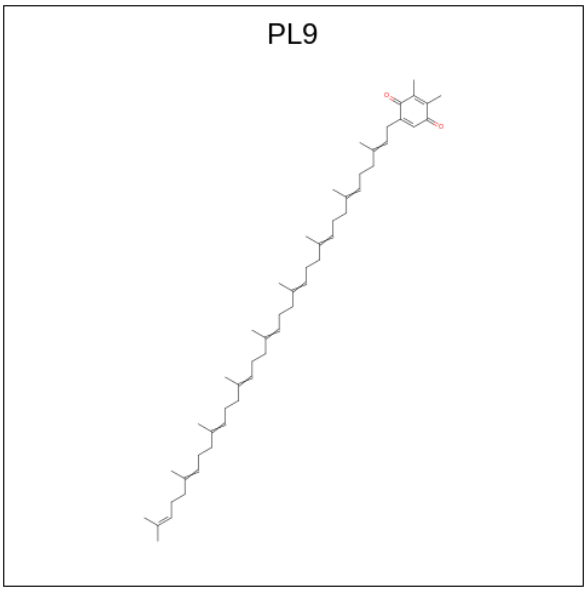
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	d	1	Total C O 6 3 3	0	0

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

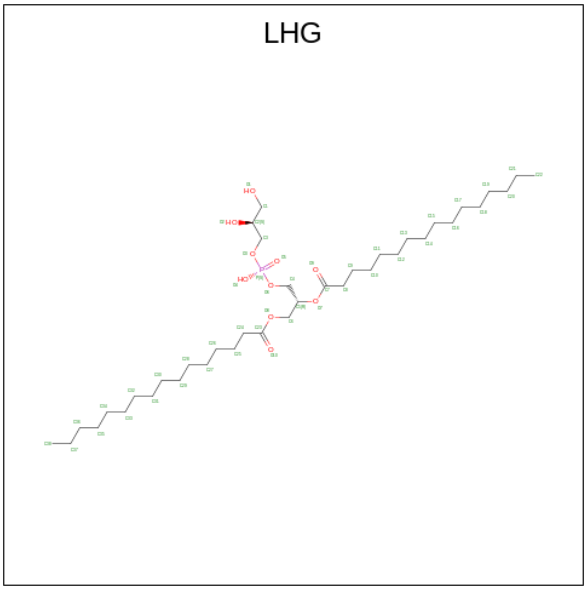
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 28 23 5	0	0
30	B	1	Total C O 33 28 5	0	0
30	D	2	Total C O 57 51 6	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 10 10	0	0
30	K	1	Total C O 34 29 5	0	0
30	M	1	Total C 10 10	0	0
30	X	1	Total C O 18 16 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a	1	Total C O 30 25 5	0	0
30	b	2	Total C O 69 59 10	0	0
30	c	1	Total C O 32 27 5	0	0
30	d	1	Total C O 17 16 1	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



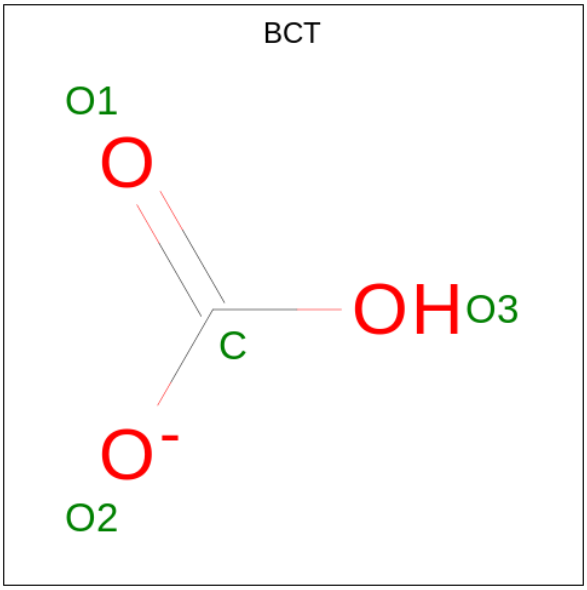
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O P 49 38 10 1	0	0
31	A	1	Total C O P 49 38 10 1	0	0
31	D	1	Total C O P 49 38 10 1	0	0

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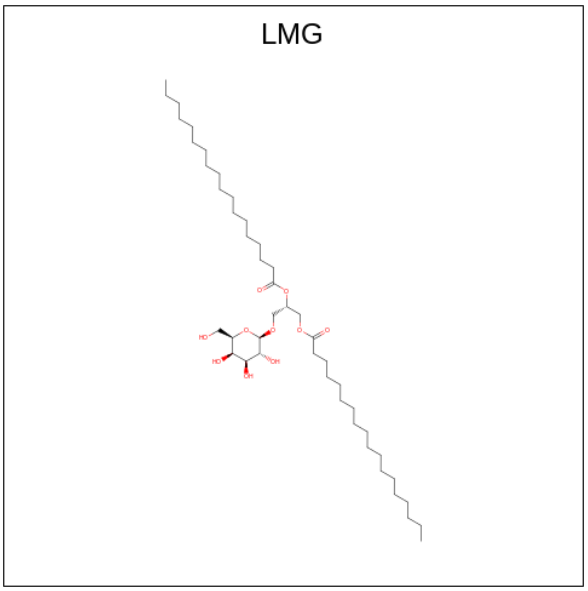
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		
31	l	1	Total	C	O	P	0	0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

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



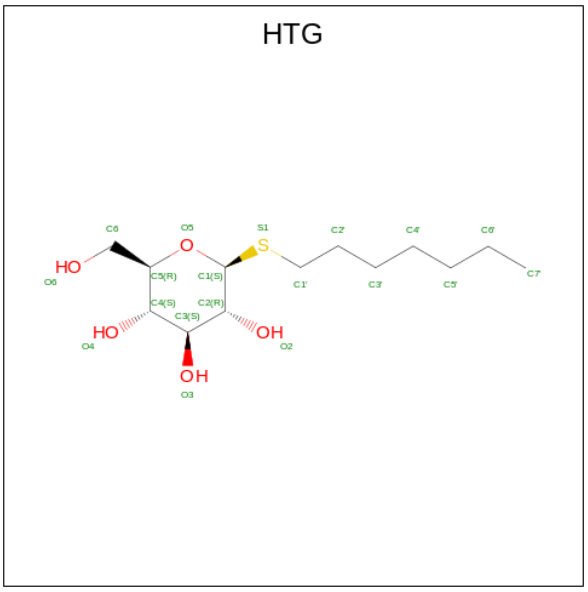
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

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



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

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



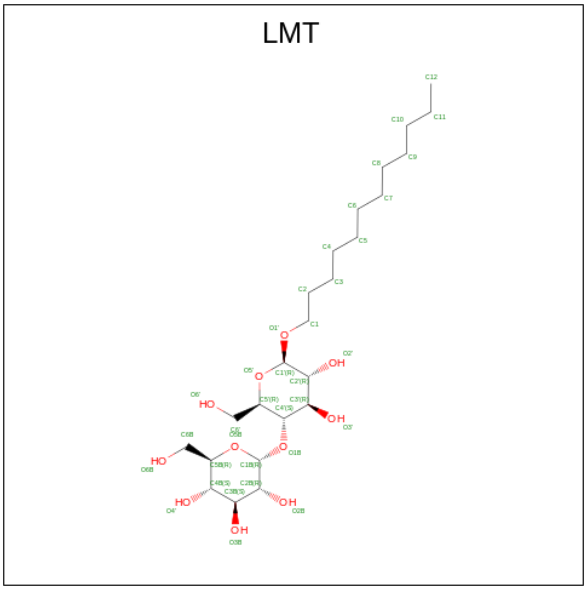
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	D	1	Total C O S 16 10 5 1	0	0
34	V	1	Total C O 11 6 5	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	c	1	Total C O S 19 13 5 1	0	0
34	c	1	Total C O S 19 13 5 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	d	1	Total C O S 16 10 5 1	0	0

- Molecule 35 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



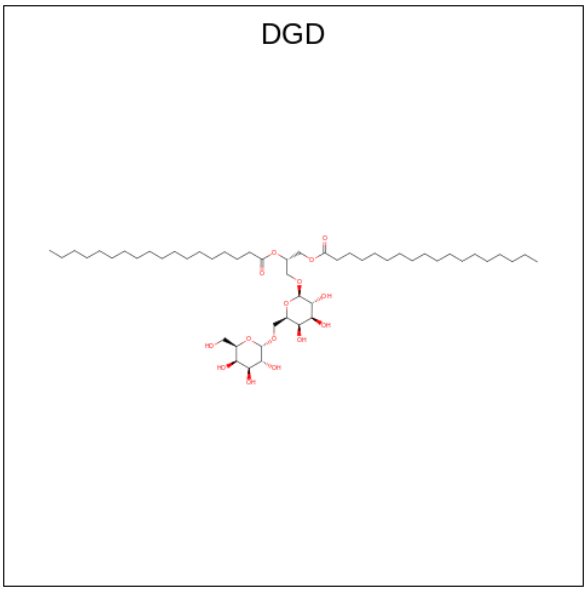
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	B	1	Total C O 25 19 6	0	0
35	B	1	Total C O 35 24 11	0	0
35	B	1	Total C O 26 19 7	0	0
35	D	1	Total C O 35 24 11	0	0
35	D	1	Total C O 35 24 11	0	0
35	E	1	Total C O 35 24 11	0	0
35	I	1	Total C O 35 24 11	0	0
35	M	1	Total C O 35 24 11	0	0
35	M	1	Total C O 35 24 11	0	0
35	a	1	Total C O 35 24 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	b	1	Total C O 25 19 6	0	0
35	b	1	Total C O 25 19 6	0	0
35	e	1	Total C O 35 24 11	0	0
35	m	1	Total C O 35 24 11	0	0

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



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

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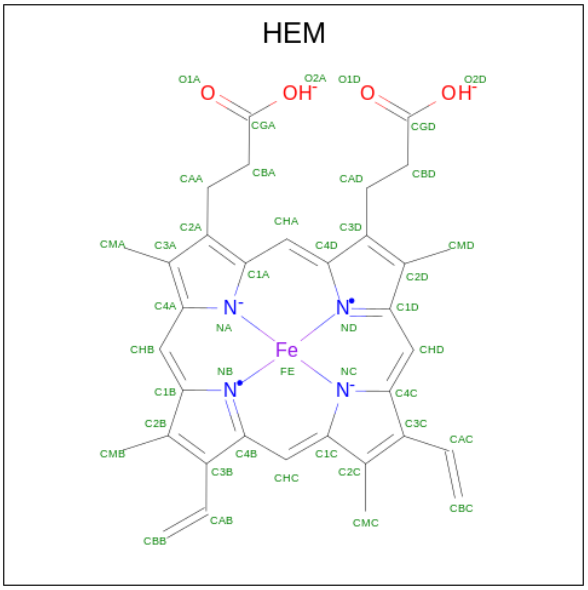
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	h	1	Total C O 62 47 15	0	0

- Molecule 37 is CALCIUM ION (CCD ID: 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	c	2	Total Ca 2 2	0	0
37	o	1	Total Ca 1 1	0	0

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

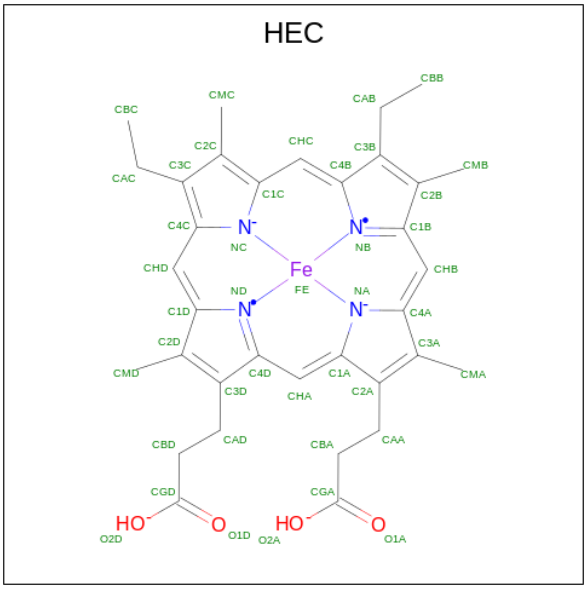


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	E	1	Total C Fe N O 43 34 1 4 4	0	0
38	e	1	Total C Fe N O 43 34 1 4 4	0	0

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

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

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	127	Total O 127 127	0	0
41	B	175	Total O 175 175	0	0
41	C	148	Total O 148 148	0	0
41	D	111	Total O 111 111	0	0
41	E	18	Total O 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	F	5	Total O 5 5	0	0
41	H	19	Total O 19 19	0	0
41	I	6	Total O 6 6	0	0
41	J	5	Total O 5 5	0	0
41	K	6	Total O 6 6	0	0
41	L	9	Total O 9 9	0	0
41	M	14	Total O 14 14	0	0
41	O	100	Total O 100 100	0	0
41	T	10	Total O 10 10	0	0
41	U	46	Total O 46 46	0	0
41	V	78	Total O 79 79	0	1
41	X	3	Total O 3 3	0	0
41	Y	1	Total O 1 1	0	0
41	a	130	Total O 130 130	0	0
41	b	192	Total O 192 192	0	0
41	c	136	Total O 136 136	0	0
41	d	108	Total O 108 108	0	0
41	e	15	Total O 15 15	0	0
41	f	5	Total O 5 5	0	0
41	h	28	Total O 28 28	0	0
41	i	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	j	3	Total O 3 3	0	0
41	k	4	Total O 4 4	0	0
41	l	7	Total O 7 7	0	0
41	m	11	Total O 11 11	0	0
41	o	109	Total O 109 109	0	0
41	t	7	Total O 7 7	0	0
41	u	64	Total O 64 64	0	0
41	v	71	Total O 71 71	0	0
41	x	4	Total O 4 4	0	0
41	y	2	Total O 2 2	0	0

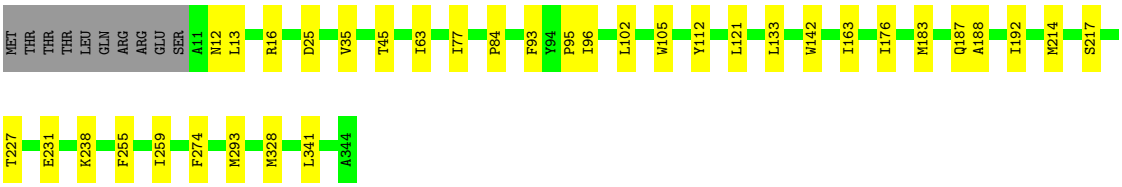
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

Chain A:

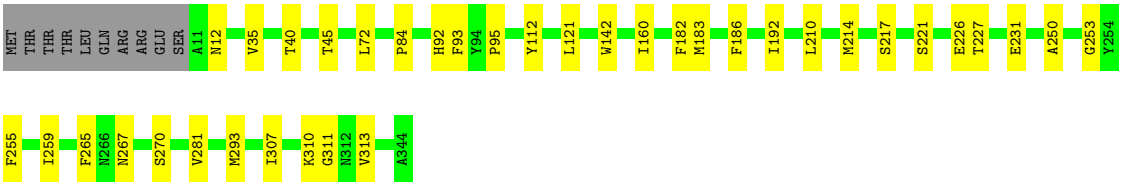




• Molecule 1: Photosystem II protein D1

Chain a:

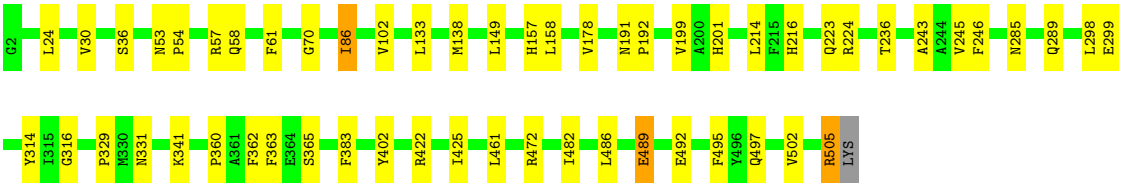




• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:

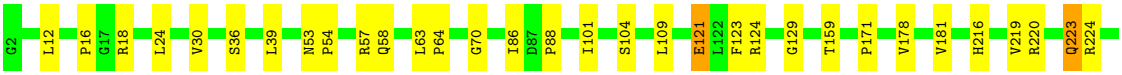




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



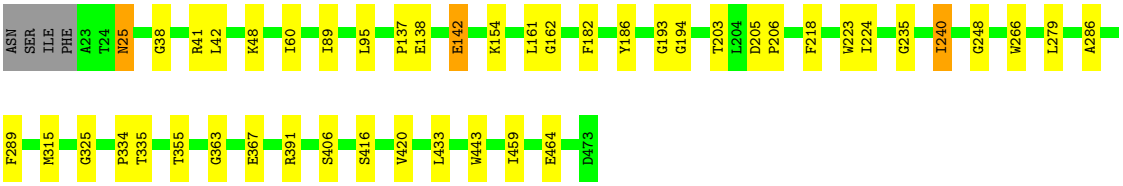




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

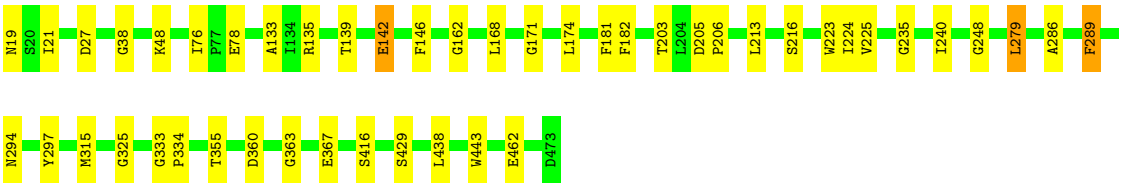




• Molecule 3: Photosystem II CP43 reaction center protein

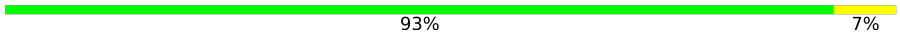
Chain c:





• Molecule 4: Photosystem II D2 protein

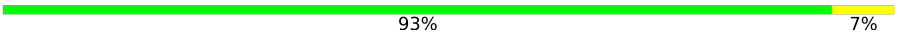
Chain D:

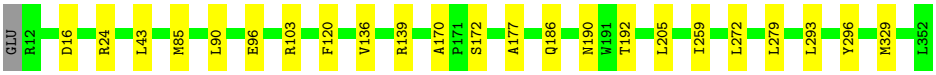




• Molecule 4: Photosystem II D2 protein

Chain d:

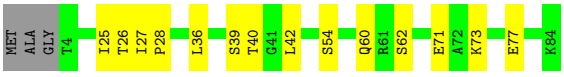




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

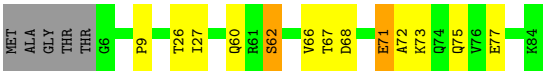




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:





• Molecule 6: Cytochrome b559 subunit beta

Chain F:





• Molecule 6: Cytochrome b559 subunit beta

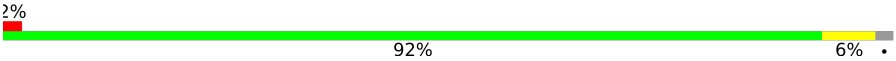
Chain f:

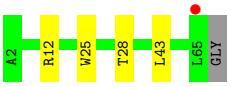




• Molecule 7: Photosystem II reaction center protein H

Chain H:

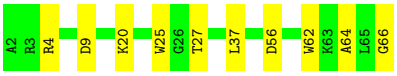




• Molecule 7: Photosystem II reaction center protein H

Chain h:





• Molecule 8: Photosystem II reaction center protein I

Chain I:





• Molecule 8: Photosystem II reaction center protein I

Chain i:

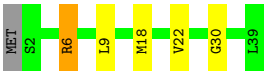




• Molecule 9: Photosystem II reaction center protein J

Chain J:

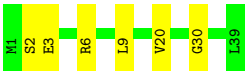




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

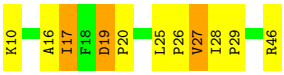




• Molecule 10: Photosystem II reaction center protein K

Chain k:

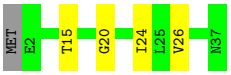




• Molecule 11: Photosystem II reaction center protein L

Chain L:

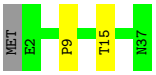




• Molecule 11: Photosystem II reaction center protein L

Chain l:

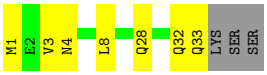




• Molecule 12: Photosystem II reaction center protein M

Chain M:





• Molecule 12: Photosystem II reaction center protein M

Chain m:

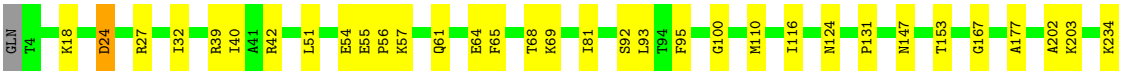




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:







• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

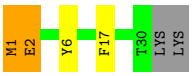




• Molecule 14: Photosystem II reaction center protein T

Chain T:

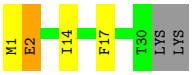




• Molecule 14: Photosystem II reaction center protein T

Chain t:

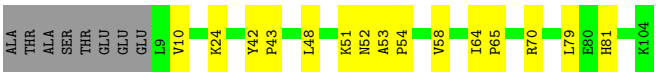




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

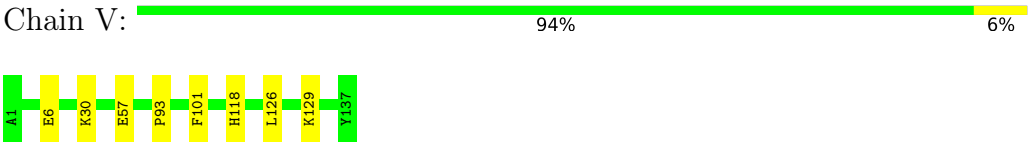
Chain u:





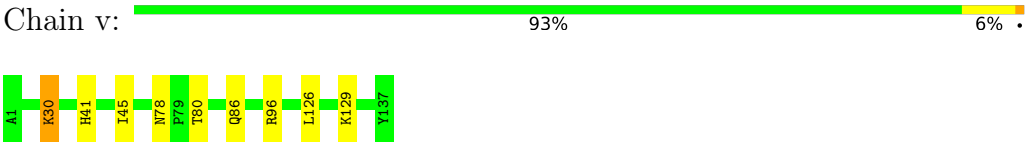
• Molecule 16: Cytochrome c-550

Chain V:



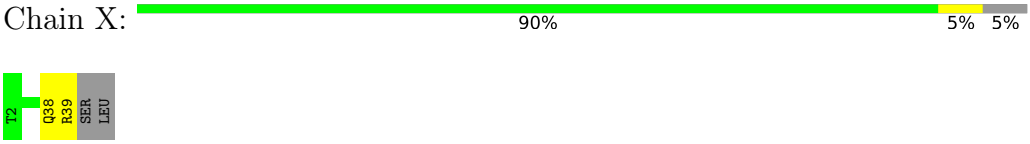
• Molecule 16: Cytochrome c-550

Chain v:



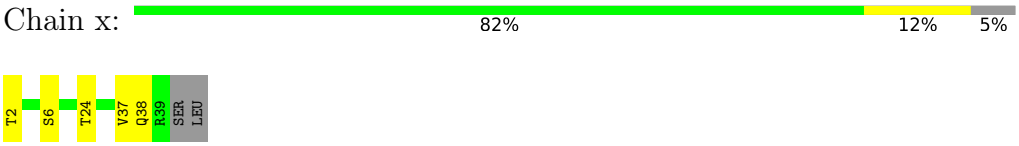
• Molecule 17: Photosystem II reaction center protein X

Chain X:



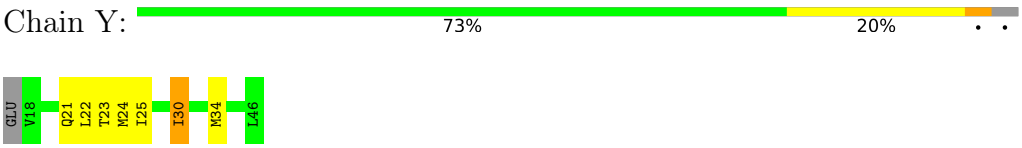
• Molecule 17: Photosystem II reaction center protein X

Chain x:



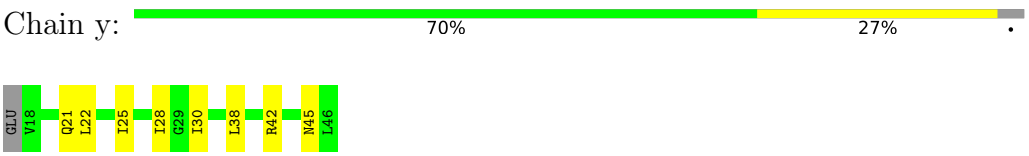
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



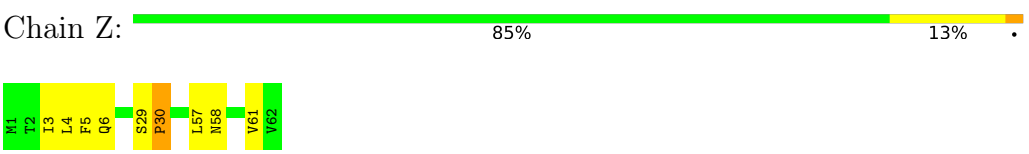
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



• Molecule 19: Photosystem II reaction center protein Z

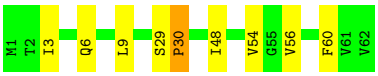
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:

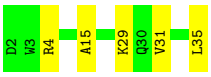




• Molecule 20: Photosystem II protein Y

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	126.52Å 231.23Å 287.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.50) 99.7 (19.98-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.139 , 0.186 0.145 , 0.189	Depositor DCC
R_{free} test set	14615 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	71.5	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.2	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	0.98	EDS
Total number of atoms	52773	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: OEX, HEM, HTG, CA, CLA, LHG, GOL, HEC, FE2, CL, LMT, DGD, PHO, BCT, LMG, BCR, UNL, FME, SQD, PL9, MG

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	0.57	0/2728	0.86	2/3719 (0.1%)
1	a	0.57	0/2739	0.84	1/3735 (0.0%)
2	B	0.52	0/4171	0.82	0/5683
2	b	0.52	0/4138	0.82	0/5640
3	C	0.50	1/3626 (0.0%)	0.84	1/4936 (0.0%)
3	c	0.51	0/3670	0.83	4/4996 (0.1%)
4	D	0.56	0/2827	0.84	4/3852 (0.1%)
4	d	0.56	0/2818	0.82	2/3840 (0.1%)
5	E	0.46	0/687	0.84	0/936
5	e	0.43	0/667	0.80	0/908
6	F	0.51	0/284	0.75	0/387
6	f	0.45	0/257	0.77	0/349
7	H	0.47	0/530	0.80	0/723
7	h	0.42	0/524	0.78	0/713
8	I	0.46	0/311	0.79	0/419
8	i	0.47	0/311	0.80	0/419
9	J	0.43	0/278	0.74	0/376
9	j	0.48	0/283	0.78	0/383
10	K	0.49	0/303	0.85	0/416
10	k	0.47	0/303	0.91	0/416
11	L	0.50	0/311	0.71	0/423
11	l	0.46	0/311	0.73	0/423
12	M	0.59	0/261	0.85	0/357
12	m	0.56	0/262	0.99	2/357 (0.6%)
13	O	0.46	0/1935	0.82	2/2623 (0.1%)
13	o	0.45	0/1910	0.82	2/2589 (0.1%)
14	T	0.58	0/257	0.75	0/349
14	t	0.58	0/257	0.80	0/349
15	U	0.48	0/776	0.81	0/1052
15	u	0.50	0/785	0.78	0/1064
16	V	0.51	0/1085	0.80	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.48	0/1085	0.81	0/1473
17	X	0.45	0/284	0.80	0/384
17	x	0.40	0/284	0.82	0/384
18	Y	0.42	0/216	0.78	0/289
18	y	0.44	0/216	0.83	0/289
19	Z	0.45	0/490	0.84	1/669 (0.1%)
19	z	0.42	0/490	0.85	0/669
20	R	0.44	0/279	0.75	0/383
All	All	0.51	1/42949 (0.0%)	0.82	21/58445 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	ILE	CA-CB	5.02	1.56	1.54

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	m	17	VAL	CA-C-N	-6.40	112.41	119.19
12	m	17	VAL	C-N-CA	-6.40	112.41	119.19
1	A	142	TRP	N-CA-C	6.33	120.62	113.02
3	C	193	GLY	N-CA-C	-6.25	104.77	112.33
3	c	333	GLY	CA-C-N	6.25	126.72	119.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2634	0	2546	24	0
1	a	2639	0	2554	26	0
2	B	4007	0	3879	42	0
2	b	3986	0	3855	44	0
3	C	3501	0	3428	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3537	0	3471	31	0
4	D	2729	0	2632	18	0
4	d	2720	0	2626	17	0
5	E	665	0	653	11	0
5	e	648	0	634	14	0
6	F	275	0	282	6	0
6	f	250	0	261	2	0
7	H	514	0	542	4	0
7	h	511	0	532	11	0
8	I	314	0	328	3	0
8	i	314	0	328	4	0
9	J	272	0	279	3	0
9	j	277	0	284	4	0
10	K	293	0	305	4	0
10	k	293	0	305	8	0
11	L	301	0	315	3	0
11	l	301	0	315	2	0
12	M	265	0	286	4	0
12	m	269	0	288	7	0
13	O	1889	0	1871	22	0
13	o	1873	0	1852	18	0
14	T	258	0	261	5	0
14	t	258	0	261	3	0
15	U	765	0	767	7	0
15	u	774	0	773	2	0
16	V	1064	0	1073	5	0
16	v	1064	0	1073	5	0
17	X	281	0	312	2	0
17	x	281	0	312	6	0
18	Y	215	0	246	5	0
18	y	215	0	246	4	0
19	Z	479	0	516	4	0
19	z	479	0	516	4	0
20	R	273	0	305	5	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	12	0
23	B	1040	0	1152	40	0
23	C	845	0	936	42	0
23	D	130	0	144	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	195	0	216	9	0
23	b	1040	0	1152	37	0
23	c	845	0	936	45	0
23	d	195	0	216	12	0
24	A	64	0	74	2	0
24	D	64	0	74	1	0
24	a	128	0	148	4	0
25	A	40	0	56	1	0
25	B	120	0	168	8	0
25	C	80	0	112	5	0
25	D	40	0	56	2	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0
25	T	40	0	56	5	0
25	Y	40	0	56	2	0
25	a	40	0	56	1	0
25	b	120	0	168	7	0
25	c	80	0	112	10	0
25	d	40	0	56	5	0
25	h	40	0	56	5	0
25	k	40	0	56	2	0
25	t	40	0	56	3	0
25	y	40	0	56	1	0
26	A	108	0	156	6	0
26	B	54	0	78	2	0
26	D	43	0	53	1	0
26	L	54	0	78	5	0
26	a	108	0	156	4	0
26	f	43	0	53	0	0
27	A	6	0	8	0	0
27	B	12	0	16	2	0
27	C	6	0	8	1	0
27	a	6	0	8	1	0
27	b	6	0	8	0	0
27	d	6	0	8	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	6	0
29	D	55	0	80	3	0
29	a	55	0	80	4	0
29	d	55	0	80	0	0
30	A	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	33	0	0	0	0
30	D	57	0	0	1	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	34	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	69	0	0	0	0
30	c	32	0	0	0	0
30	d	17	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	98	0	148	5	0
31	D	98	0	148	6	0
31	E	42	0	57	1	0
31	d	147	0	222	10	0
31	e	42	0	57	2	0
31	l	49	0	74	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	51	0	72	1	0
33	C	102	0	144	7	0
33	J	51	0	72	3	0
33	Z	88	0	116	3	0
33	a	51	0	72	4	0
33	b	51	0	72	1	0
33	c	102	0	144	2	0
33	j	51	0	72	2	0
33	z	39	0	48	1	0
34	B	76	0	104	6	0
34	C	38	0	52	1	0
34	D	16	0	17	0	0
34	V	11	0	10	0	0
34	b	76	0	104	4	0
34	c	38	0	52	2	0
34	d	16	0	17	1	0
35	B	86	0	116	4	0
35	D	70	0	92	4	0
35	E	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	I	35	0	46	1	0
35	M	70	0	92	3	0
35	a	35	0	46	0	0
35	b	50	0	70	1	0
35	e	35	0	46	0	0
35	m	35	0	46	0	0
36	C	186	0	246	8	0
36	H	62	0	82	1	0
36	c	186	0	246	8	0
36	h	62	0	82	0	0
37	C	1	0	0	0	0
37	O	1	0	0	0	0
37	V	1	0	0	0	0
37	c	2	0	0	0	0
37	o	1	0	0	0	0
38	E	43	0	30	3	0
38	e	43	0	30	3	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	127	0	0	2	0
41	B	175	0	0	1	0
41	C	148	0	0	1	0
41	D	111	0	0	0	0
41	E	18	0	0	1	0
41	F	5	0	0	0	0
41	H	19	0	0	0	0
41	I	6	0	0	1	0
41	J	5	0	0	1	0
41	K	6	0	0	0	0
41	L	9	0	0	0	0
41	M	14	0	0	1	0
41	O	100	0	0	1	0
41	T	10	0	0	0	0
41	U	46	0	0	0	0
41	V	79	0	0	1	0
41	X	3	0	0	0	0
41	Y	1	0	0	0	0
41	a	130	0	0	2	0
41	b	192	0	0	5	0
41	c	136	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	d	108	0	0	1	0
41	e	15	0	0	0	0
41	f	5	0	0	0	0
41	h	28	0	0	0	0
41	i	4	0	0	0	0
41	j	3	0	0	0	0
41	k	4	0	0	0	0
41	l	7	0	0	0	0
41	m	11	0	0	1	0
41	o	109	0	0	0	0
41	t	7	0	0	1	0
41	u	64	0	0	0	0
41	v	71	0	0	2	0
41	x	4	0	0	0	0
41	y	2	0	0	0	0
All	All	52773	0	52080	604	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 604 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:604:CLA:H42	23:B:605:CLA:H2	1.46	0.95
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.52	0.91
2:b:224:ARG:HH11	35:b:621:LMT:H12	1.41	0.84
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.27	0.81
34:B:622:HTG:H1	35:B:630:LMT:H21	1.60	0.81

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	335/344 (97%)	328 (98%)	6 (2%)	1 (0%)	36 55
1	a	337/344 (98%)	330 (98%)	6 (2%)	1 (0%)	36 55
2	B	510/505 (101%)	504 (99%)	6 (1%)	0	100 100
2	b	506/505 (100%)	499 (99%)	7 (1%)	0	100 100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	30 49
3	c	458/455 (101%)	445 (97%)	11 (2%)	2 (0%)	30 49
4	D	341/342 (100%)	332 (97%)	9 (3%)	0	100 100
4	d	340/342 (99%)	334 (98%)	6 (2%)	0	100 100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100 100
5	e	77/84 (92%)	75 (97%)	2 (3%)	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	63/65 (97%)	60 (95%)	3 (5%)	0	100 100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100 100
8	i	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4 6
9	J	36/39 (92%)	36 (100%)	0	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%)	31 (97%)	1 (3%)	0	100 100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100 100
13	O	246/244 (101%)	238 (97%)	8 (3%)	0	100 100
13	o	243/244 (100%)	234 (96%)	9 (4%)	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%)	91 (97%)	3 (3%)	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%)	128 (95%)	7 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	26 (96%)	1 (4%)	0	100 100
18	y	27/30 (90%)	24 (89%)	3 (11%)	0	100 100
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	7 13
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7 13
20	R	32/34 (94%)	32 (100%)	0	0	100 100
All	All	5255/5384 (98%)	5126 (98%)	120 (2%)	9 (0%)	48 63

5 of 9 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	272/279 (98%)	270 (99%)	2 (1%)	76 89
1	a	274/279 (98%)	272 (99%)	2 (1%)	76 89
2	B	410/403 (102%)	401 (98%)	9 (2%)	45 73
2	b	406/403 (101%)	398 (98%)	8 (2%)	48 75
3	C	356/356 (100%)	350 (98%)	6 (2%)	53 78
3	c	361/356 (101%)	351 (97%)	10 (3%)	38 66
4	D	278/277 (100%)	277 (100%)	1 (0%)	84 93
4	d	277/277 (100%)	274 (99%)	3 (1%)	65 84
5	E	73/73 (100%)	71 (97%)	2 (3%)	39 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	e	70/73 (96%)	68 (97%)	2 (3%)	37 65
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	25/38 (66%)	24 (96%)	1 (4%)	28 54
7	H	55/54 (102%)	53 (96%)	2 (4%)	31 58
7	h	54/54 (100%)	54 (100%)	0	100 100
8	I	34/34 (100%)	33 (97%)	1 (3%)	37 65
8	i	34/34 (100%)	32 (94%)	2 (6%)	18 37
9	J	26/27 (96%)	24 (92%)	2 (8%)	12 25
9	j	26/27 (96%)	24 (92%)	2 (8%)	12 25
10	K	30/30 (100%)	26 (87%)	4 (13%)	4 8
10	k	30/30 (100%)	26 (87%)	4 (13%)	4 8
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	35/35 (100%)	35 (100%)	0	100 100
12	M	30/32 (94%)	29 (97%)	1 (3%)	33 61
12	m	30/32 (94%)	28 (93%)	2 (7%)	15 31
13	O	211/207 (102%)	208 (99%)	3 (1%)	59 81
13	o	208/207 (100%)	205 (99%)	3 (1%)	59 81
14	T	26/28 (93%)	25 (96%)	1 (4%)	29 56
14	t	26/28 (93%)	25 (96%)	1 (4%)	29 56
15	U	83/89 (93%)	81 (98%)	2 (2%)	43 70
15	u	84/89 (94%)	83 (99%)	1 (1%)	63 83
16	V	117/117 (100%)	116 (99%)	1 (1%)	70 87
16	v	117/117 (100%)	116 (99%)	1 (1%)	70 87
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%)	24 49
18	y	22/23 (96%)	20 (91%)	2 (9%)	9 19
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29 56
19	z	52/52 (100%)	50 (96%)	2 (4%)	29 56
20	R	29/29 (100%)	29 (100%)	0	100 100
All	All	4360/4403 (99%)	4274 (98%)	86 (2%)	50 75

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	355	THR
10	k	17	ILE
3	c	462[B]	GLU
6	f	15	ILE
12	m	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	201	ASN
15	u	81	HIS
5	e	60	GLN
12	m	5	GLN
19	z	58	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	$\#\|Z\| > 2$
14	FME	T	1	14	8,9,10	0.62	0	7,9,11	1.31	1 (14%)
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.37	1 (14%)
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	1.85	3 (42%)
8	FME	I	1	8	8,9,10	0.59	0	7,9,11	1.09	1 (14%)
12	FME	m	1	12	8,9,10	0.58	0	7,9,11	1.38	2 (28%)
12	FME	M	1	12	8,9,10	0.58	0	7,9,11	1.50	2 (28%)

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
14	FME	T	1	14	-	4/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	3/7/9/11	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	O-C-CA	-2.73	117.62	124.78
14	t	1	FME	CA-N-CN	-2.63	118.77	122.82
12	M	1	FME	CA-N-CN	-2.31	119.27	122.82
8	I	1	FME	O-C-CA	-2.29	118.77	124.78
14	T	1	FME	O-C-CA	-2.25	118.88	124.78

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 214 ligands modelled in this entry, 14 are monoatomic and 18 are unknown - leaving 182 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	$\#\|Z\|>2$
36	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
23	CLA	B	613	2	69,73,73	2.05	20 (28%)	83,113,113	2.79	31 (37%)
23	CLA	a	405	41	69,73,73	2.03	20 (28%)	83,113,113	2.85	32 (38%)
34	HTG	b	622	-	19,19,19	0.96	1 (5%)	23,24,24	1.52	3 (13%)
23	CLA	c	513	3	69,73,73	2.09	20 (28%)	83,113,113	2.90	29 (34%)
35	LMT	B	631	-	26,26,36	0.50	0	31,31,47	0.81	1 (3%)
35	LMT	b	627	-	25,25,36	0.56	1 (4%)	30,30,47	1.07	3 (10%)
23	CLA	b	604	2	69,73,73	2.00	18 (26%)	83,113,113	2.82	29 (34%)
23	CLA	b	601	41	69,73,73	2.10	20 (28%)	83,113,113	2.77	29 (34%)
25	BCR	C	515	-	41,41,41	1.06	1 (2%)	56,56,56	1.58	9 (16%)
32	BCT	a	418	21	2,3,3	0.61	0	2,3,3	1.00	0
35	LMT	M	103	-	36,36,36	0.47	0	47,47,47	0.77	1 (2%)
23	CLA	B	614	2	69,73,73	2.03	21 (30%)	83,113,113	2.89	33 (39%)
31	LHG	e	101	-	41,41,48	1.03	2 (4%)	44,47,54	0.95	2 (4%)
24	PHO	A	407	-	58,69,69	2.82	14 (24%)	56,99,99	2.97	18 (32%)
23	CLA	a	408	1	69,73,73	2.06	20 (28%)	83,113,113	2.82	34 (40%)
35	LMT	a	417	-	36,36,36	0.46	0	47,47,47	0.77	1 (2%)
23	CLA	C	504	3	69,73,73	2.02	18 (26%)	83,113,113	2.88	28 (33%)
31	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	0.96	3 (5%)
23	CLA	B	616	2	69,73,73	2.06	20 (28%)	83,113,113	2.84	27 (32%)
23	CLA	b	605	2	69,73,73	2.05	22 (31%)	83,113,113	2.84	29 (34%)
36	DGD	h	102	-	63,63,67	0.89	3 (4%)	77,77,81	1.03	5 (6%)
23	CLA	c	509	3	69,73,73	2.11	20 (28%)	83,113,113	2.79	29 (34%)
36	DGD	c	517	-	63,63,67	0.91	3 (4%)	77,77,81	0.99	6 (7%)
25	BCR	a	409	-	41,41,41	0.95	1 (2%)	56,56,56	1.51	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	B	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.39	10 (17%)
26	SQD	A	410	-	53,54,54	0.97	3 (5%)	62,65,65	1.86	12 (19%)
26	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.10	6 (9%)
38	HEM	e	103	5,6	50,50,50	1.50	7 (14%)	66,82,82	1.75	11 (16%)
34	HTG	c	521	-	19,19,19	0.91	1 (5%)	23,24,24	1.51	1 (4%)
23	CLA	C	503	3	69,73,73	2.05	19 (27%)	83,113,113	2.70	28 (33%)
27	GOL	A	411	-	5,5,5	0.40	0	5,5,5	0.29	0
28	OEX	A	413	1,41,3	0,14,14	-	-	-		
36	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.00	6 (7%)
23	CLA	C	505	41	69,73,73	2.05	20 (28%)	83,113,113	2.81	32 (38%)
29	PL9	A	414	-	55,55,55	0.65	2 (3%)	68,69,69	1.95	21 (30%)
35	LMT	D	403	-	36,36,36	0.44	0	47,47,47	1.32	7 (14%)
23	CLA	c	511	3	69,73,73	2.10	21 (30%)	83,113,113	2.89	29 (34%)
34	HTG	B	623	-	19,19,19	0.84	1 (5%)	23,24,24	1.67	1 (4%)
36	DGD	c	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.16	6 (7%)
35	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.07	3 (6%)
23	CLA	c	506	3	69,73,73	2.05	20 (28%)	83,113,113	2.74	32 (38%)
35	LMT	m	102	-	36,36,36	0.51	0	47,47,47	0.92	2 (4%)
23	CLA	b	616	2	69,73,73	2.07	19 (27%)	83,113,113	2.88	31 (37%)
23	CLA	D	404	4	69,73,73	2.00	20 (28%)	83,113,113	2.87	30 (36%)
23	CLA	C	514	3	69,73,73	2.08	21 (30%)	83,113,113	2.89	29 (34%)
23	CLA	C	509	3	69,73,73	2.06	21 (30%)	83,113,113	2.78	28 (33%)
23	CLA	b	613	2	69,73,73	2.05	20 (28%)	83,113,113	2.75	31 (37%)
25	BCR	c	514	-	41,41,41	1.05	1 (2%)	56,56,56	1.79	13 (23%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.75	13 (23%)
33	LMG	b	620	-	51,51,55	0.86	2 (3%)	59,59,63	1.26	8 (13%)
26	SQD	L	101	-	53,54,54	1.02	3 (5%)	62,65,65	1.53	9 (14%)
23	CLA	B	605	2	69,73,73	2.07	20 (28%)	83,113,113	2.91	29 (34%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.52	11 (19%)
33	LMG	c	519	-	51,51,55	0.95	2 (3%)	59,59,63	1.02	3 (5%)
23	CLA	c	510	3	69,73,73	1.98	20 (28%)	83,113,113	2.88	34 (40%)
31	LHG	A	416	-	48,48,48	0.90	3 (6%)	51,54,54	1.10	4 (7%)
35	LMT	b	621	-	25,25,36	0.46	0	30,30,47	0.66	0
36	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	6 (7%)
23	CLA	b	609	2	69,73,73	2.06	20 (28%)	83,113,113	2.81	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	603	2	69,73,73	2.09	20 (28%)	83,113,113	2.93	29 (34%)
23	CLA	c	508	3	69,73,73	2.07	20 (28%)	83,113,113	2.81	28 (33%)
23	CLA	c	512	3	69,73,73	2.05	19 (27%)	83,113,113	2.92	30 (36%)
23	CLA	B	607	41	69,73,73	2.04	20 (28%)	83,113,113	2.83	30 (36%)
25	BCR	d	405	-	41,41,41	1.09	1 (2%)	56,56,56	1.86	14 (25%)
34	HTG	B	622	-	19,19,19	1.01	1 (5%)	23,24,24	1.44	4 (17%)
23	CLA	B	603	2	69,73,73	2.03	19 (27%)	83,113,113	2.80	30 (36%)
40	HEC	V	202	16	50,50,50	1.73	10 (20%)	68,82,82	1.82	17 (25%)
25	BCR	b	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.69	13 (23%)
23	CLA	C	508	41	69,73,73	2.06	19 (27%)	83,113,113	2.80	29 (34%)
31	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	5 (9%)
31	LHG	d	408	-	48,48,48	0.89	2 (4%)	51,54,54	0.91	3 (5%)
25	BCR	c	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.70	17 (30%)
23	CLA	b	611	2	69,73,73	2.05	20 (28%)	83,113,113	2.78	28 (33%)
23	CLA	C	510	3	69,73,73	2.08	20 (28%)	83,113,113	2.83	30 (36%)
23	CLA	b	610	41	69,73,73	2.12	20 (28%)	83,113,113	2.82	30 (36%)
34	HTG	b	623	-	19,19,19	1.07	2 (10%)	23,24,24	1.81	3 (13%)
29	PL9	d	406	-	55,55,55	0.63	1 (1%)	68,69,69	1.82	20 (29%)
23	CLA	C	502	3	69,73,73	1.97	20 (28%)	83,113,113	2.86	31 (37%)
33	LMG	Z	101	-	51,51,55	0.99	2 (3%)	59,59,63	1.27	5 (8%)
36	DGD	c	518	-	63,63,67	0.86	3 (4%)	77,77,81	1.09	6 (7%)
35	LMT	D	402	-	36,36,36	0.64	1 (2%)	47,47,47	1.26	4 (8%)
34	HTG	D	412	-	16,16,19	1.04	2 (12%)	20,21,24	1.45	1 (5%)
23	CLA	b	607	41	69,73,73	1.96	19 (27%)	83,113,113	2.83	28 (33%)
23	CLA	B	601	41	69,73,73	2.09	20 (28%)	83,113,113	2.80	29 (34%)
34	HTG	V	203	-	11,11,19	0.25	0	15,15,24	1.12	2 (13%)
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.64	11 (19%)
31	LHG	d	409	-	48,48,48	0.97	2 (4%)	51,54,54	1.00	3 (5%)
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.10	4 (8%)
26	SQD	D	413	-	42,43,54	1.15	3 (7%)	51,54,65	1.78	12 (23%)
23	CLA	a	404	1	69,73,73	2.02	19 (27%)	83,113,113	2.81	32 (38%)
27	GOL	d	402	-	5,5,5	0.32	0	5,5,5	0.55	0
25	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.73	13 (23%)
27	GOL	C	523	-	5,5,5	0.40	0	5,5,5	0.25	0
23	CLA	b	606	2	69,73,73	2.01	19 (27%)	83,113,113	2.86	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.02	2 (4%)
23	CLA	B	610	41	69,73,73	2.08	20 (28%)	83,113,113	2.82	31 (37%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.68	11 (19%)
34	HTG	B	627	-	19,19,19	0.97	2 (10%)	23,24,24	1.40	2 (8%)
23	CLA	c	507	41	69,73,73	2.06	19 (27%)	83,113,113	2.75	30 (36%)
34	HTG	b	625	-	19,19,19	0.92	2 (10%)	23,24,24	1.72	3 (13%)
26	SQD	a	410	-	53,54,54	0.96	3 (5%)	62,65,65	1.73	12 (19%)
23	CLA	d	403	4	69,73,73	2.04	19 (27%)	83,113,113	2.77	31 (37%)
26	SQD	a	412	-	53,54,54	1.06	3 (5%)	62,65,65	1.24	7 (11%)
23	CLA	C	506	3	69,73,73	2.01	20 (28%)	83,113,113	2.83	31 (37%)
33	LMG	j	101	39	51,51,55	0.88	2 (3%)	59,59,63	1.07	5 (8%)
23	CLA	c	501	3	69,73,73	2.06	20 (28%)	83,113,113	2.77	29 (34%)
34	HTG	B	624	-	19,19,19	1.00	1 (5%)	23,24,24	1.74	3 (13%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.58	12 (21%)
40	HEC	v	201	16	50,50,50	1.69	10 (20%)	68,82,82	1.80	19 (27%)
24	PHO	a	406	-	58,69,69	2.73	12 (20%)	56,99,99	2.88	17 (30%)
23	CLA	B	604	2	69,73,73	2.00	19 (27%)	83,113,113	2.75	30 (36%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
23	CLA	C	511	3	69,73,73	2.04	20 (28%)	83,113,113	2.86	31 (37%)
27	GOL	a	411	-	5,5,5	0.38	0	5,5,5	0.41	0
25	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.73	16 (28%)
35	LMT	B	630	-	36,36,36	0.52	1 (2%)	47,47,47	0.94	2 (4%)
31	LHG	A	417	-	48,48,48	0.94	2 (4%)	51,54,54	1.08	2 (3%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	4 (6%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.67	13 (23%)
23	CLA	b	608	2	69,73,73	2.06	20 (28%)	83,113,113	2.78	27 (32%)
25	BCR	b	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.39	8 (14%)
28	OEX	a	413	1,41,3	0,14,14	-	-	-		
32	BCT	A	418	21	2,3,3	0.60	0	2,3,3	0.99	0
23	CLA	B	611	2	69,73,73	2.04	20 (28%)	83,113,113	2.75	30 (36%)
24	PHO	a	407	-	58,69,69	2.81	12 (20%)	56,99,99	2.80	14 (25%)
25	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
33	LMG	Z	102	-	37,37,55	1.01	3 (8%)	45,45,63	1.64	9 (20%)
23	CLA	b	602	2	69,73,73	2.08	20 (28%)	83,113,113	2.83	34 (40%)
23	CLA	C	513	3	69,73,73	2.05	20 (28%)	83,113,113	2.79	34 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	SQD	f	101	-	42,43,54	1.19	3 (7%)	51,54,65	1.38	7 (13%)
23	CLA	A	405	41	69,73,73	2.07	20 (28%)	83,113,113	2.95	32 (38%)
23	CLA	B	606	2	69,73,73	2.06	18 (26%)	83,113,113	2.89	29 (34%)
33	LMG	J	101	39	51,51,55	0.91	2 (3%)	59,59,63	0.98	5 (8%)
25	BCR	B	617	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	10 (17%)
25	BCR	D	406	-	41,41,41	1.04	1 (2%)	56,56,56	1.81	14 (25%)
23	CLA	b	615	2	69,73,73	2.00	18 (26%)	83,113,113	2.83	28 (33%)
23	CLA	c	502	3	69,73,73	2.03	20 (28%)	83,113,113	2.74	30 (36%)
23	CLA	B	602	2	69,73,73	2.10	21 (30%)	83,113,113	2.81	33 (39%)
23	CLA	c	503	3	69,73,73	2.05	20 (28%)	83,113,113	2.88	29 (34%)
35	LMT	E	102	-	36,36,36	0.53	1 (2%)	47,47,47	0.84	0
31	LHG	D	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.10	4 (7%)
23	CLA	c	504	41	69,73,73	2.06	20 (28%)	83,113,113	2.89	32 (38%)
35	LMT	e	102	-	36,36,36	0.50	0	47,47,47	0.81	2 (4%)
27	GOL	B	625	-	5,5,5	0.37	0	5,5,5	0.37	0
33	LMG	a	416	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	3 (5%)
34	HTG	c	522	-	19,19,19	0.96	2 (10%)	23,24,24	1.49	3 (13%)
23	CLA	A	406	41	69,73,73	2.06	20 (28%)	83,113,113	2.93	33 (39%)
26	SQD	B	620	-	53,54,54	1.07	4 (7%)	62,65,65	1.48	10 (16%)
27	GOL	B	626	-	5,5,5	0.52	0	5,5,5	0.40	0
33	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.17	4 (6%)
23	CLA	C	512	3	69,73,73	2.06	20 (28%)	83,113,113	2.87	31 (37%)
25	BCR	K	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.42	9 (16%)
23	CLA	c	505	3	69,73,73	2.05	19 (27%)	83,113,113	2.76	30 (36%)
24	PHO	D	401	-	58,69,69	2.74	13 (22%)	56,99,99	3.02	18 (32%)
23	CLA	A	408	1	69,73,73	2.06	21 (30%)	83,113,113	2.91	29 (34%)
23	CLA	C	507	3	69,73,73	2.07	21 (30%)	83,113,113	2.79	33 (39%)
34	HTG	C	521	-	19,19,19	0.92	1 (5%)	23,24,24	1.44	3 (13%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.07	5 (6%)
29	PL9	a	414	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	20 (29%)
23	CLA	D	405	4	69,73,73	2.06	18 (26%)	83,113,113	2.97	32 (38%)
25	BCR	C	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.57	10 (17%)
23	CLA	B	615	2	69,73,73	2.01	18 (26%)	83,113,113	2.78	29 (34%)
23	CLA	b	612	2	69,73,73	2.07	20 (28%)	83,113,113	2.71	27 (32%)
29	PL9	D	407	-	55,55,55	0.65	1 (1%)	68,69,69	1.74	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	HEM	E	103	5,6	50,50,50	1.54	7 (14%)	66,82,82	1.79	17 (25%)
35	LMT	B	629	-	25,25,36	0.46	0	30,30,47	0.70	0
23	CLA	A	404	1	69,73,73	2.09	21 (30%)	83,113,113	2.81	34 (40%)
31	LHG	l	101	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
31	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.11	5 (11%)
34	HTG	b	628	-	19,19,19	1.01	1 (5%)	23,24,24	1.83	4 (17%)
23	CLA	B	608	2	69,73,73	1.99	19 (27%)	83,113,113	2.85	30 (36%)
23	CLA	b	614	2	69,73,73	2.00	20 (28%)	83,113,113	2.86	31 (37%)
34	HTG	C	522	-	19,19,19	1.05	2 (10%)	23,24,24	1.89	5 (21%)
33	LMG	c	520	-	51,51,55	0.97	3 (5%)	59,59,63	1.24	6 (10%)
25	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	13 (23%)
23	CLA	B	612	2	69,73,73	2.00	20 (28%)	83,113,113	2.75	30 (36%)
34	HTG	d	411	-	16,16,19	1.12	2 (12%)	20,21,24	1.50	1 (5%)
23	CLA	d	401	41	69,73,73	2.07	20 (28%)	83,113,113	2.95	33 (39%)
23	CLA	d	404	4	69,73,73	2.08	20 (28%)	83,113,113	2.89	34 (40%)
27	GOL	b	624	-	5,5,5	0.33	0	5,5,5	0.45	0
23	CLA	B	609	2	69,73,73	2.03	18 (26%)	83,113,113	2.78	28 (33%)

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
36	DGD	C	518	-	-	13/51/91/95	0/2/2/2
23	CLA	B	613	2	-	6/39/115/115	-
23	CLA	a	405	41	-	7/39/115/115	-
34	HTG	b	622	-	-	2/10/30/30	0/1/1/1
23	CLA	c	513	3	-	2/39/115/115	-
35	LMT	B	631	-	-	7/17/38/61	0/1/1/2
35	LMT	b	627	-	-	6/17/37/61	0/1/1/2
23	CLA	b	604	2	-	15/39/115/115	-
23	CLA	b	601	41	-	17/39/115/115	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
35	LMT	M	103	-	-	11/21/61/61	0/2/2/2
23	CLA	B	614	2	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	e	101	-	-	14/46/46/53	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
23	CLA	a	408	1	-	10/39/115/115	-
35	LMT	a	417	-	-	4/21/61/61	0/2/2/2
23	CLA	C	504	3	-	2/39/115/115	-
31	LHG	D	408	-	-	15/53/53/53	-
23	CLA	B	616	2	-	10/39/115/115	-
23	CLA	b	605	2	-	10/39/115/115	-
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
23	CLA	c	509	3	-	12/39/115/115	-
36	DGD	c	517	-	-	14/51/91/95	0/2/2/2
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	SQD	A	410	-	-	13/49/69/69	0/1/1/1
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
38	HEM	e	103	5,6	-	8/14/54/54	-
34	HTG	c	521	-	-	7/10/30/30	0/1/1/1
23	CLA	C	503	3	-	9/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
36	DGD	H	102	-	-	14/51/91/95	0/2/2/2
23	CLA	C	505	41	-	7/39/115/115	-
29	PL9	A	414	-	-	11/53/73/73	0/1/1/1
35	LMT	D	403	-	-	9/21/61/61	0/2/2/2
23	CLA	c	511	3	-	3/39/115/115	-
34	HTG	B	623	-	-	6/10/30/30	0/1/1/1
36	DGD	c	516	-	-	13/51/91/95	0/2/2/2
35	LMT	I	101	-	-	10/21/61/61	0/2/2/2
23	CLA	c	506	3	-	8/39/115/115	-
35	LMT	m	102	-	-	7/21/61/61	0/2/2/2
23	CLA	b	616	2	-	15/39/115/115	-
23	CLA	D	404	4	-	2/39/115/115	-
23	CLA	C	514	3	-	13/39/115/115	-
23	CLA	C	509	3	-	5/39/115/115	-
23	CLA	b	613	2	-	10/39/115/115	-
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
33	LMG	b	620	-	-	14/46/66/70	0/1/1/1
26	SQD	L	101	-	-	23/49/69/69	0/1/1/1
23	CLA	B	605	2	-	9/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
33	LMG	c	519	-	-	13/46/66/70	0/1/1/1
23	CLA	c	510	3	-	10/39/115/115	-
31	LHG	A	416	-	-	11/53/53/53	-
35	LMT	b	621	-	-	7/17/37/61	0/1/1/2
36	DGD	C	519	-	-	15/51/91/95	0/2/2/2
23	CLA	b	609	2	-	6/39/115/115	-
23	CLA	b	603	2	-	12/39/115/115	-
23	CLA	c	508	3	-	6/39/115/115	-
23	CLA	c	512	3	-	12/39/115/115	-
23	CLA	B	607	41	-	4/39/115/115	-
40	HEC	V	202	16	1/1/3/7	4/14/54/54	-
25	BCR	d	405	-	-	6/29/63/63	0/2/2/2
23	CLA	B	603	2	-	6/39/115/115	-
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
23	CLA	C	508	41	-	8/39/115/115	-
31	LHG	d	407	-	-	14/53/53/53	-
31	LHG	d	408	-	-	20/53/53/53	-
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
23	CLA	b	611	2	-	6/39/115/115	-
23	CLA	C	510	3	-	6/39/115/115	-
23	CLA	b	610	41	-	5/39/115/115	-
34	HTG	b	623	-	-	3/10/30/30	0/1/1/1
29	PL9	d	406	-	-	6/53/73/73	0/1/1/1
23	CLA	C	502	3	-	8/39/115/115	-
33	LMG	Z	101	-	-	9/46/66/70	0/1/1/1
36	DGD	c	518	-	-	5/51/91/95	0/2/2/2
35	LMT	D	402	-	-	6/21/61/61	0/2/2/2
34	HTG	D	412	-	-	0/7/27/30	0/1/1/1
23	CLA	b	607	41	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	601	41	-	13/39/115/115	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
25	BCR	y	101	-	-	7/29/63/63	0/2/2/2
31	LHG	d	409	-	-	16/53/53/53	-
33	LMG	z	101	-	-	6/34/54/70	0/1/1/1
26	SQD	D	413	-	-	14/38/58/69	0/1/1/1
23	CLA	a	404	1	-	10/39/115/115	-
27	GOL	d	402	-	-	2/4/4/4	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	GOL	C	523	-	-	2/4/4/4	-
23	CLA	b	606	2	-	12/39/115/115	-
35	LMT	M	101	-	-	2/21/61/61	0/2/2/2
23	CLA	B	610	41	-	8/39/115/115	-
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
34	HTG	B	627	-	-	2/10/30/30	0/1/1/1
23	CLA	c	507	41	-	9/39/115/115	-
34	HTG	b	625	-	-	6/10/30/30	0/1/1/1
26	SQD	a	410	-	-	12/49/69/69	0/1/1/1
23	CLA	d	403	4	-	5/39/115/115	-
26	SQD	a	412	-	-	11/49/69/69	0/1/1/1
23	CLA	C	506	3	-	10/39/115/115	-
33	LMG	j	101	39	-	12/46/66/70	0/1/1/1
23	CLA	c	501	3	-	6/39/115/115	-
34	HTG	B	624	-	-	4/10/30/30	0/1/1/1
25	BCR	A	409	-	-	2/29/63/63	0/2/2/2
40	HEC	v	201	16	1/1/3/7	4/14/54/54	-
24	PHO	a	406	-	-	2/37/103/103	0/5/6/6
23	CLA	B	604	2	-	11/39/115/115	-
33	LMG	C	520	-	-	15/46/66/70	0/1/1/1
23	CLA	C	511	3	-	14/39/115/115	-
27	GOL	a	411	-	-	2/4/4/4	-
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
35	LMT	B	630	-	-	7/21/61/61	0/2/2/2
31	LHG	A	417	-	-	21/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	B	621	-	-	13/46/66/70	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	608	2	-	4/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	B	611	2	-	3/39/115/115	-
24	PHO	a	407	-	-	3/37/103/103	0/5/6/6
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
33	LMG	Z	102	-	-	14/31/51/70	0/1/1/1
23	CLA	b	602	2	-	6/39/115/115	-
23	CLA	C	513	3	-	10/39/115/115	-
26	SQD	f	101	-	-	16/38/58/69	0/1/1/1
23	CLA	A	405	41	-	7/39/115/115	-
23	CLA	B	606	2	-	7/39/115/115	-
33	LMG	J	101	39	-	9/46/66/70	0/1/1/1
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	BCR	D	406	-	-	7/29/63/63	0/2/2/2
23	CLA	b	615	2	-	6/39/115/115	-
23	CLA	c	502	3	-	8/39/115/115	-
23	CLA	B	602	2	-	8/39/115/115	-
23	CLA	c	503	3	-	2/39/115/115	-
35	LMT	E	102	-	-	11/21/61/61	0/2/2/2
31	LHG	D	409	-	-	15/53/53/53	-
23	CLA	c	504	41	-	7/39/115/115	-
35	LMT	e	102	-	-	9/21/61/61	0/2/2/2
27	GOL	B	625	-	-	3/4/4/4	-
33	LMG	a	416	-	-	15/46/66/70	0/1/1/1
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
23	CLA	A	406	41	-	13/39/115/115	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
27	GOL	B	626	-	-	3/4/4/4	-
33	LMG	C	501	-	-	9/46/66/70	0/1/1/1
23	CLA	C	512	3	-	4/39/115/115	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	c	505	3	-	10/39/115/115	-
24	PHO	D	401	-	-	7/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	408	1	-	13/39/115/115	-
23	CLA	C	507	3	-	15/39/115/115	-
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
29	PL9	a	414	-	-	13/53/73/73	0/1/1/1
23	CLA	D	405	4	-	11/39/115/115	-
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
23	CLA	B	615	2	-	12/39/115/115	-
23	CLA	b	612	2	-	8/39/115/115	-
29	PL9	D	407	-	-	11/53/73/73	0/1/1/1
38	HEM	E	103	5,6	-	6/14/54/54	-
35	LMT	B	629	-	-	10/17/37/61	0/1/1/2
23	CLA	A	404	1	-	6/39/115/115	-
31	LHG	l	101	-	-	19/53/53/53	-
31	LHG	E	101	-	-	20/46/46/53	-
34	HTG	b	628	-	-	6/10/30/30	0/1/1/1
23	CLA	B	608	2	-	5/39/115/115	-
23	CLA	b	614	2	-	16/39/115/115	-
34	HTG	C	522	-	-	2/10/30/30	0/1/1/1
33	LMG	c	520	-	-	7/46/66/70	0/1/1/1
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	612	2	-	9/39/115/115	-
34	HTG	d	411	-	-	3/7/27/30	0/1/1/1
23	CLA	d	401	41	-	6/39/115/115	-
23	CLA	d	404	4	-	14/39/115/115	-
27	GOL	b	624	-	-	1/4/4/4	-
23	CLA	B	609	2	-	6/39/115/115	-

The worst 5 of 1614 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	PHO	C1D-C2D	9.58	1.50	1.39
24	a	407	PHO	C1D-C2D	9.19	1.49	1.39
24	A	407	PHO	C1D-C2D	9.14	1.49	1.39
24	A	407	PHO	C1B-C2B	8.96	1.49	1.39
24	a	406	PHO	C1D-C2D	8.75	1.49	1.39

The worst 5 of 2878 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	401	PHO	C2D-C1D-ND	12.21	117.96	109.53
24	a	406	PHO	C2D-C1D-ND	12.16	117.92	109.53
24	A	407	PHO	C2D-C1D-ND	11.63	117.56	109.53
24	a	407	PHO	C2D-C1D-ND	10.64	116.87	109.53
23	B	605	CLA	C1D-ND-C4D	-10.55	98.84	106.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	202	HEC	NA
40	v	201	HEC	NA

5 of 1400 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

151 monomers are involved in 343 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	C	518	DGD	2	0
23	B	613	CLA	2	0
23	a	405	CLA	2	0
34	b	622	HTG	2	0
23	c	513	CLA	7	0
23	b	604	CLA	5	0
23	b	601	CLA	2	0
25	C	515	BCR	2	0
35	M	103	LMT	1	0
23	B	614	CLA	4	0
31	e	101	LHG	2	0
24	A	407	PHO	2	0
23	a	408	CLA	3	0
23	C	504	CLA	5	0
31	D	408	LHG	2	0
23	B	616	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	605	CLA	7	0
23	c	509	CLA	5	0
36	c	517	DGD	3	0
25	a	409	BCR	1	0
25	B	619	BCR	3	0
26	A	410	SQD	3	0
26	A	412	SQD	3	0
38	e	103	HEM	3	0
34	c	521	HTG	1	0
23	C	503	CLA	2	0
36	H	102	DGD	1	0
23	C	505	CLA	1	0
29	A	414	PL9	6	0
35	D	403	LMT	2	0
23	c	511	CLA	3	0
34	B	623	HTG	2	0
36	c	516	DGD	3	0
35	I	101	LMT	1	0
23	c	506	CLA	5	0
23	b	616	CLA	3	0
23	D	404	CLA	3	0
23	C	514	CLA	7	0
23	C	509	CLA	3	0
23	b	613	CLA	3	0
25	c	514	BCR	6	0
25	T	101	BCR	5	0
33	b	620	LMG	1	0
26	L	101	SQD	5	0
23	B	605	CLA	6	0
25	b	617	BCR	2	0
33	c	519	LMG	1	0
23	c	510	CLA	3	0
31	A	416	LHG	3	0
35	b	621	LMT	1	0
36	C	519	DGD	1	0
23	b	609	CLA	5	0
23	b	603	CLA	3	0
23	c	508	CLA	7	0
23	c	512	CLA	6	0
23	B	607	CLA	1	0
25	d	405	BCR	5	0
34	B	622	HTG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	603	CLA	1	0
25	b	619	BCR	2	0
23	C	508	CLA	5	0
31	d	408	LHG	3	0
25	c	515	BCR	4	0
23	b	611	CLA	1	0
23	C	510	CLA	1	0
23	b	610	CLA	1	0
23	C	502	CLA	3	0
33	Z	101	LMG	2	0
36	c	518	DGD	3	0
35	D	402	LMT	2	0
23	B	601	CLA	2	0
25	y	101	BCR	1	0
31	d	409	LHG	7	0
33	z	101	LMG	1	0
26	D	413	SQD	1	0
23	a	404	CLA	4	0
25	H	101	BCR	3	0
27	C	523	GOL	1	0
35	M	101	LMT	2	0
23	B	610	CLA	1	0
25	Y	101	BCR	2	0
23	c	507	CLA	4	0
34	b	625	HTG	1	0
26	a	410	SQD	4	0
23	d	403	CLA	4	0
23	C	506	CLA	8	0
33	j	101	LMG	2	0
23	c	501	CLA	3	0
25	A	409	BCR	1	0
24	a	406	PHO	1	0
23	B	604	CLA	4	0
27	a	411	GOL	1	0
25	t	101	BCR	3	0
35	B	630	LMT	3	0
31	A	417	LHG	2	0
33	B	621	LMG	1	0
25	B	618	BCR	4	0
23	b	608	CLA	2	0
25	b	618	BCR	3	0
23	B	611	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	407	PHO	3	0
25	h	101	BCR	5	0
33	Z	102	LMG	1	0
23	b	602	CLA	1	0
23	C	513	CLA	5	0
23	A	405	CLA	2	0
23	B	606	CLA	3	0
33	J	101	LMG	3	0
25	B	617	BCR	1	0
25	D	406	BCR	2	0
23	b	615	CLA	3	0
23	c	502	CLA	3	0
23	B	602	CLA	5	0
23	c	503	CLA	3	0
35	E	102	LMT	1	0
31	D	409	LHG	4	0
23	c	504	CLA	2	0
27	B	625	GOL	1	0
33	a	416	LMG	4	0
34	c	522	HTG	1	0
23	A	406	CLA	2	0
26	B	620	SQD	2	0
27	B	626	GOL	1	0
33	C	501	LMG	7	0
23	C	512	CLA	2	0
25	K	102	BCR	1	0
23	c	505	CLA	5	0
24	D	401	PHO	1	0
23	A	408	CLA	6	0
23	C	507	CLA	9	0
34	C	521	HTG	1	0
36	C	517	DGD	5	0
29	a	414	PL9	4	0
25	C	516	BCR	3	0
23	B	615	CLA	3	0
23	b	612	CLA	4	0
29	D	407	PL9	3	0
38	E	103	HEM	3	0
35	B	629	LMT	1	0
23	A	404	CLA	2	0
31	E	101	LHG	1	0
34	b	628	HTG	1	0

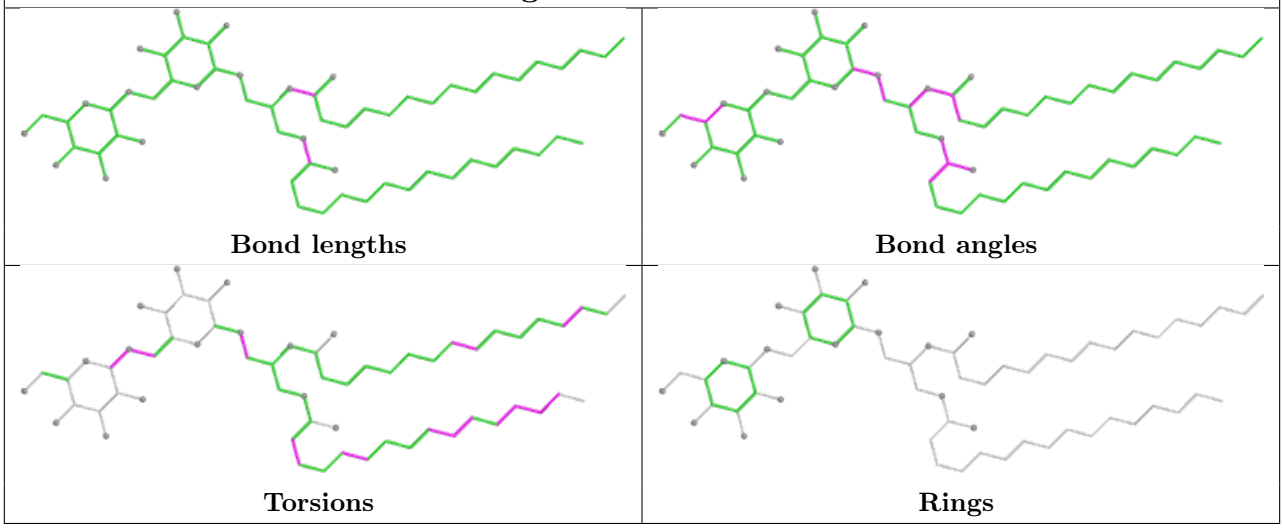
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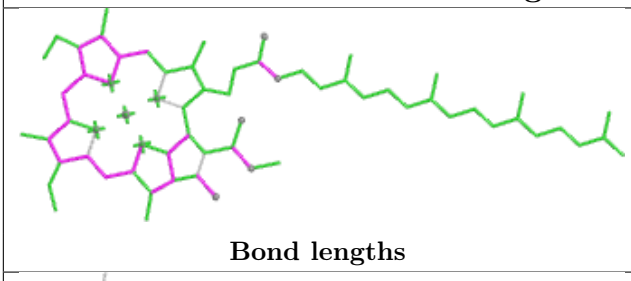
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	608	CLA	1	0
23	b	614	CLA	3	0
33	c	520	LMG	1	0
25	k	101	BCR	2	0
23	B	612	CLA	1	0
34	d	411	HTG	1	0
23	d	401	CLA	4	0
23	d	404	CLA	4	0
23	B	609	CLA	4	0

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

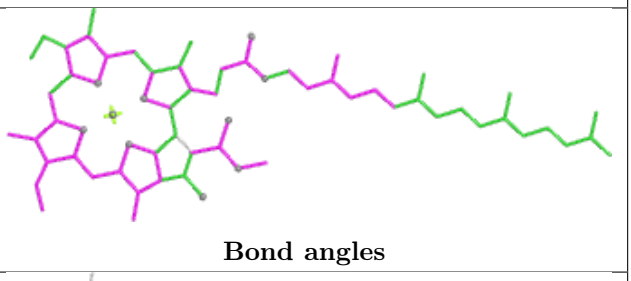
Ligand DGD C 518



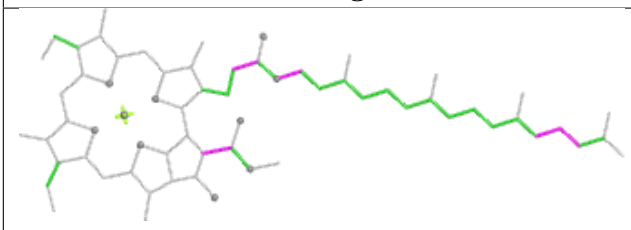
Ligand CLA B 613



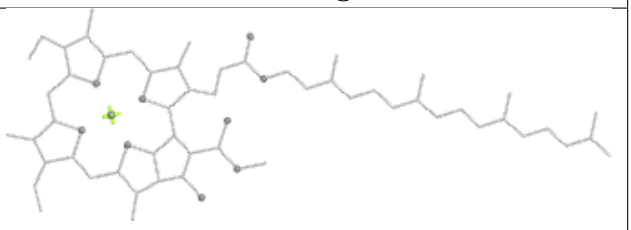
Bond lengths



Bond angles

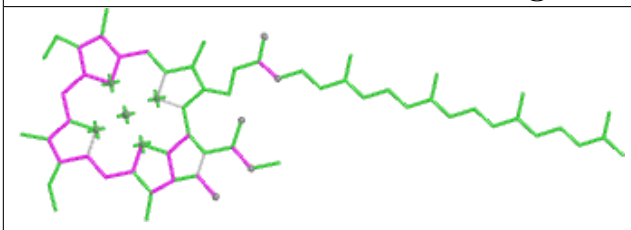


Torsions

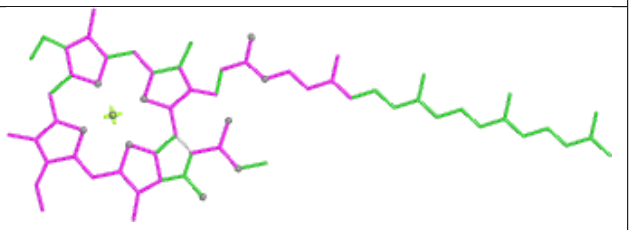


Rings

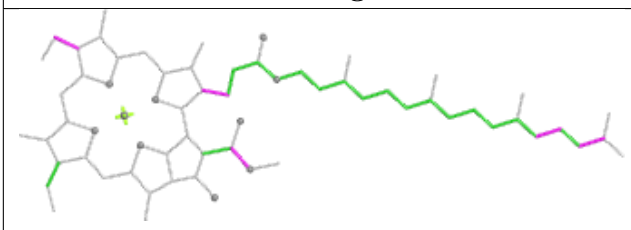
Ligand CLA a 405



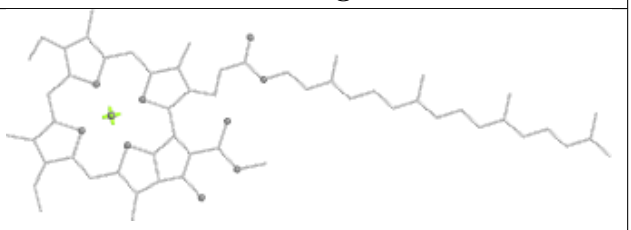
Bond lengths



Bond angles

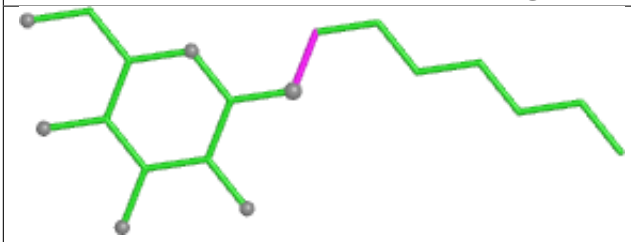


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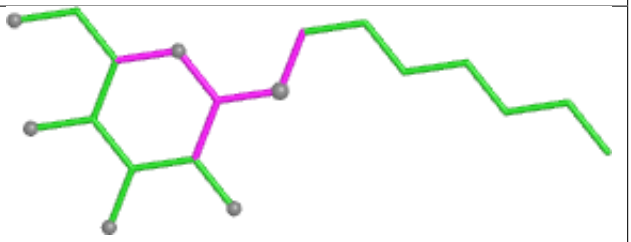


Rings

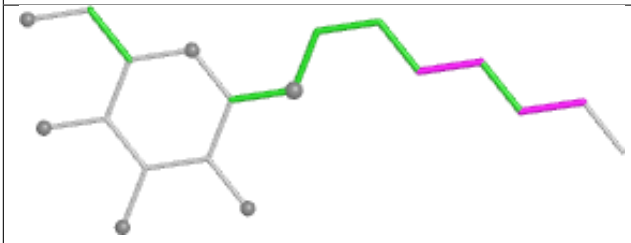
Ligand HTG b 622



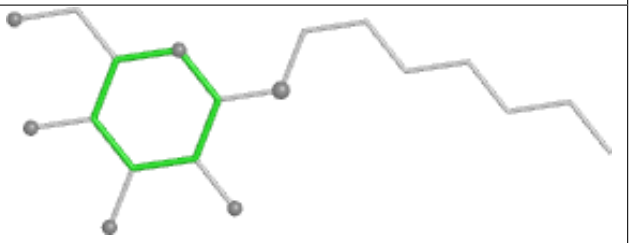
Bond lengths



Bond angles

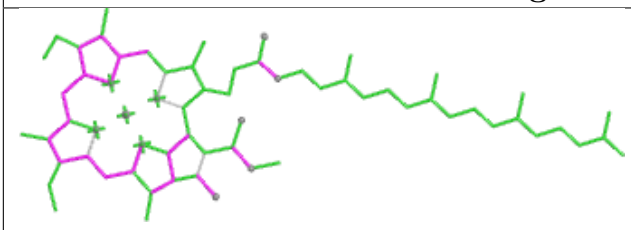


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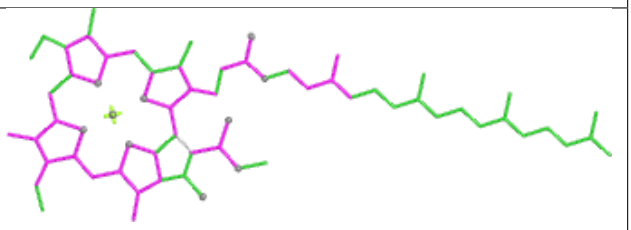


Rings

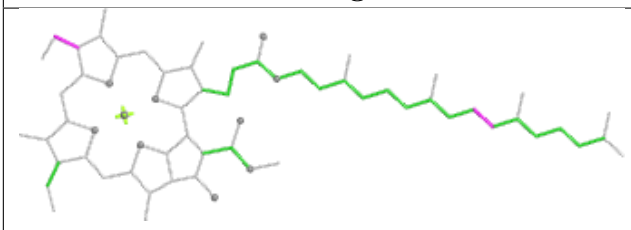
Ligand CLA c 513



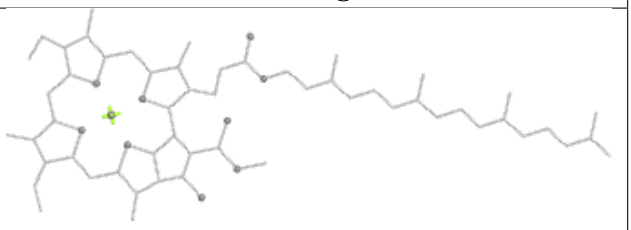
Bond lengths



Bond angles

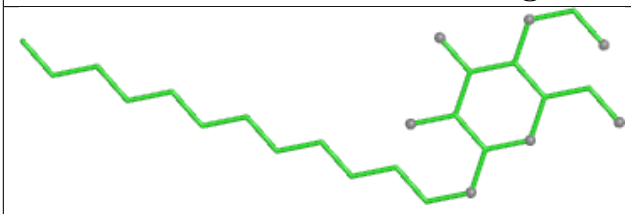


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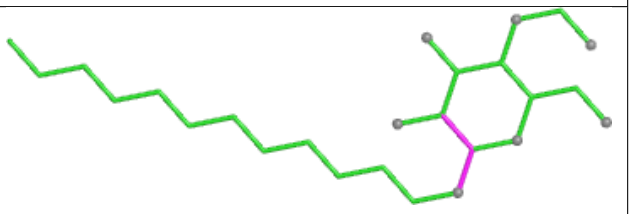


Rings

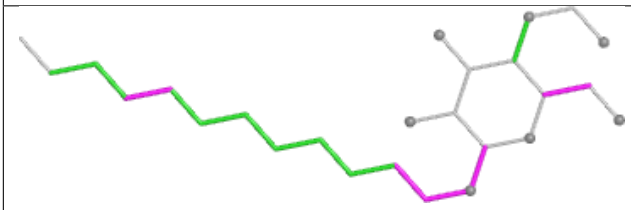
Ligand LMT B 631



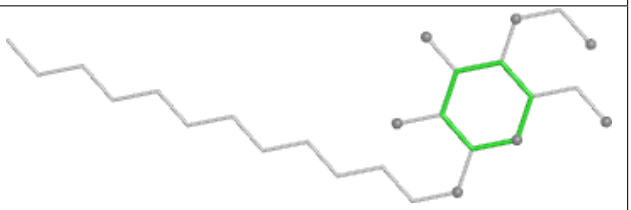
Bond lengths



Bond angles

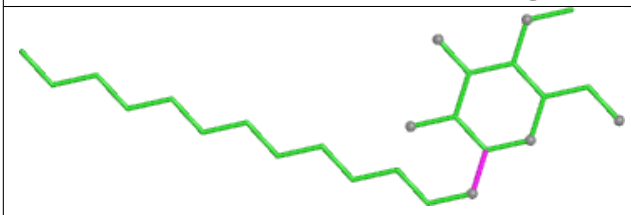


Torsions

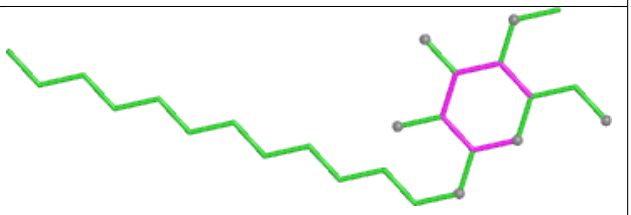


Rings

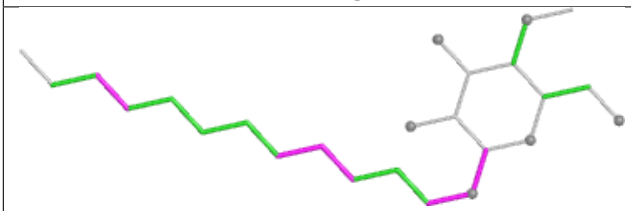
Ligand LMT b 627



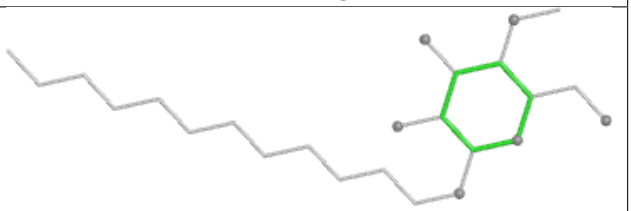
Bond lengths



Bond angles

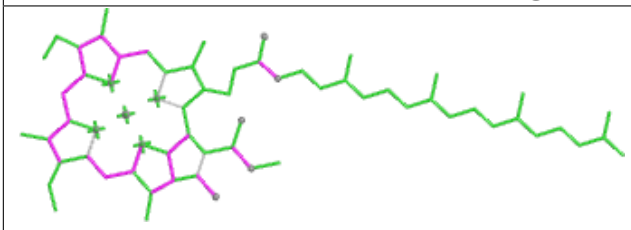


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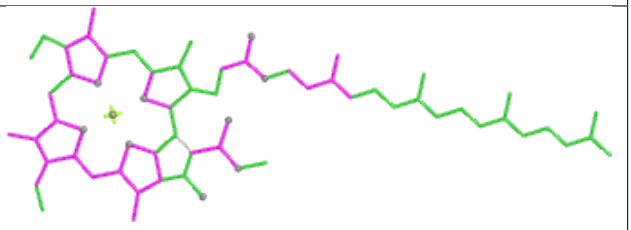


Rings

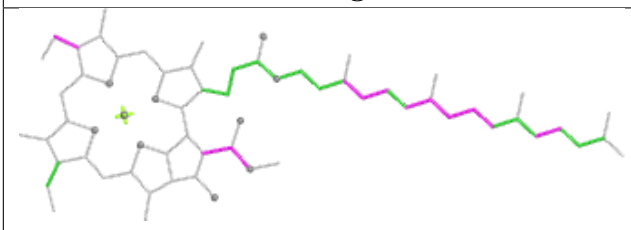
Ligand CLA b 604



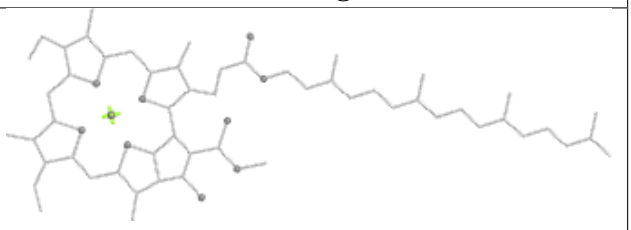
Bond lengths



Bond angles

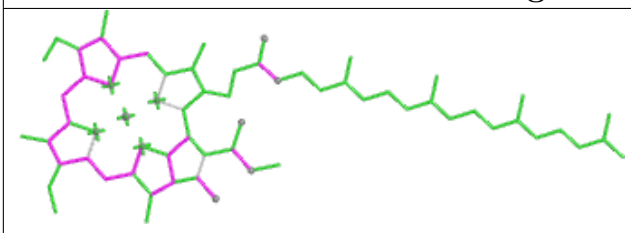


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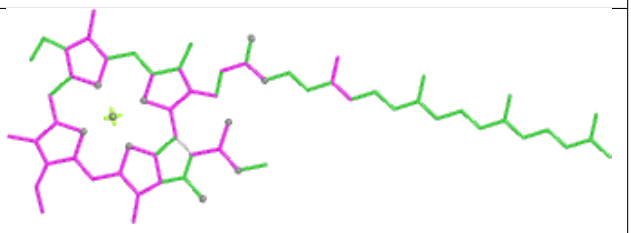


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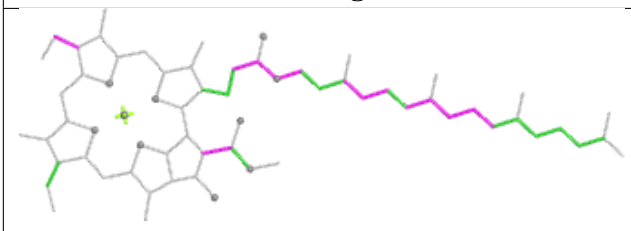
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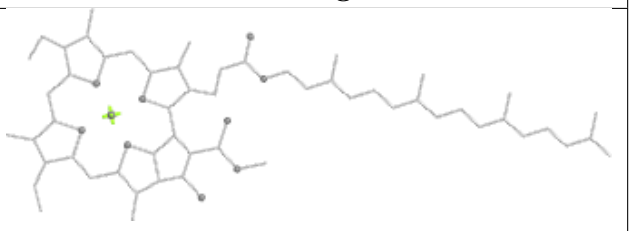
Bond lengths



Bond angles

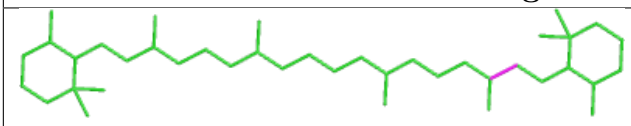


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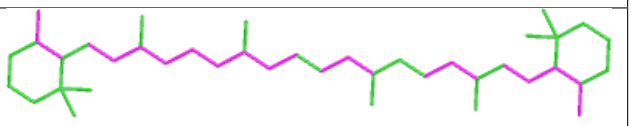


Rings

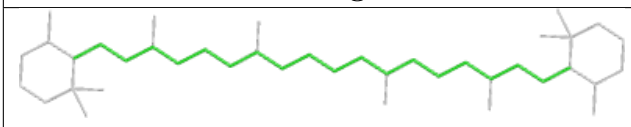
Ligand BCR C 515



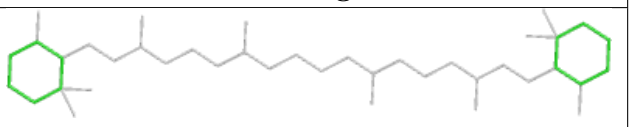
Bond lengths



Bond angles

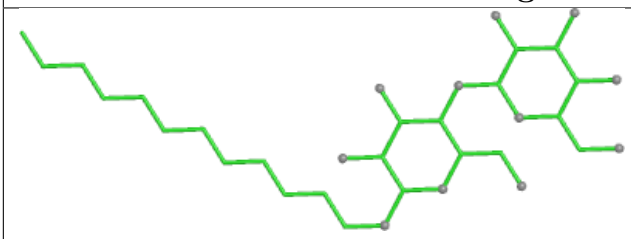


Torsions

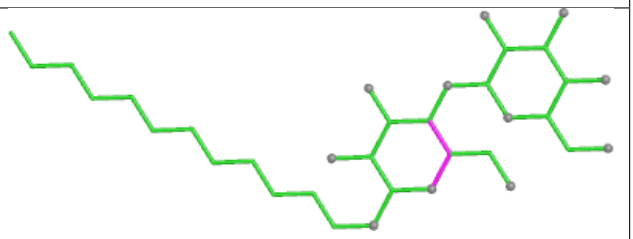


Rings

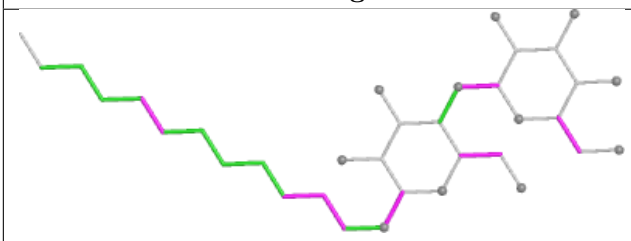
Ligand LMT M 103



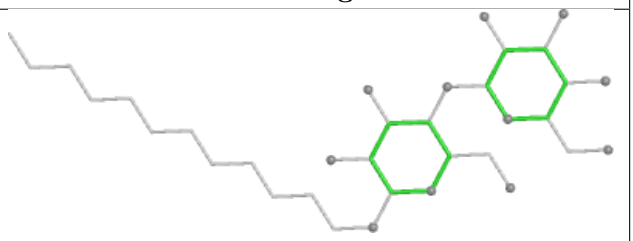
Bond lengths



Bond angles

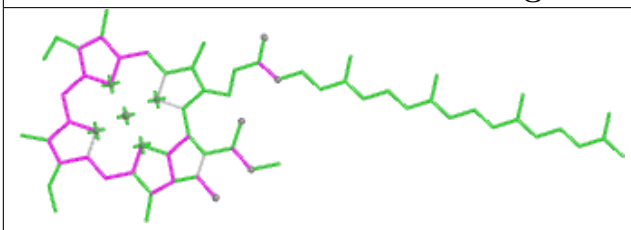


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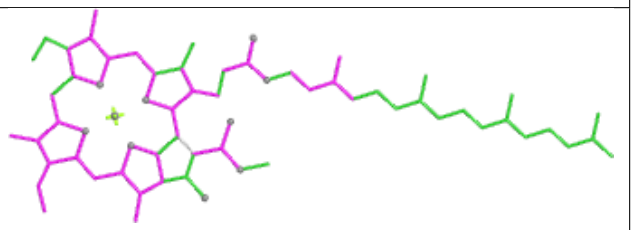


Rings

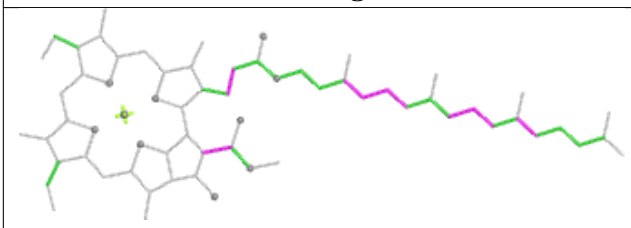
Ligand CLA B 614



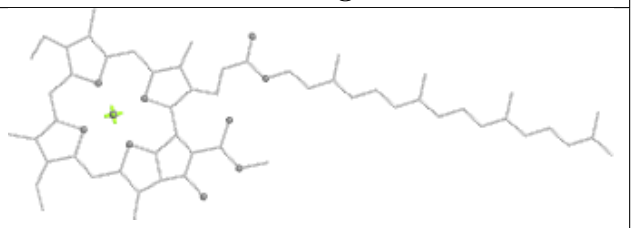
Bond lengths



Bond angles

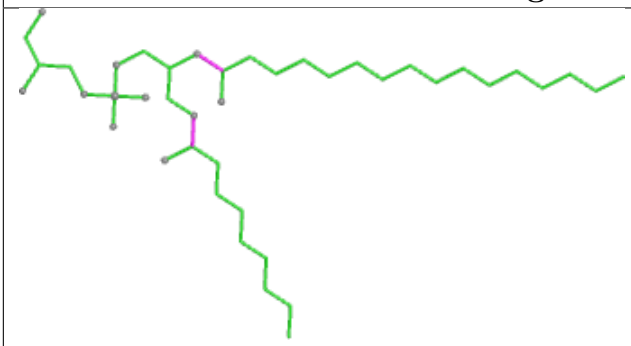


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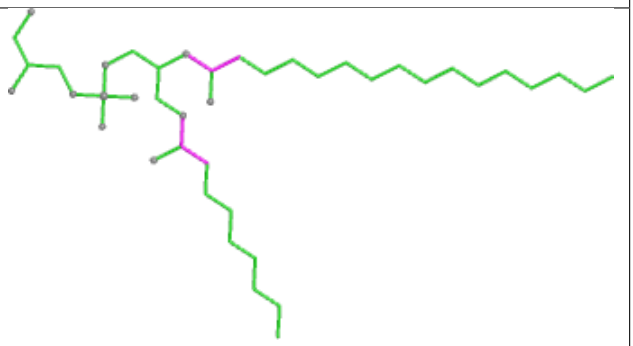


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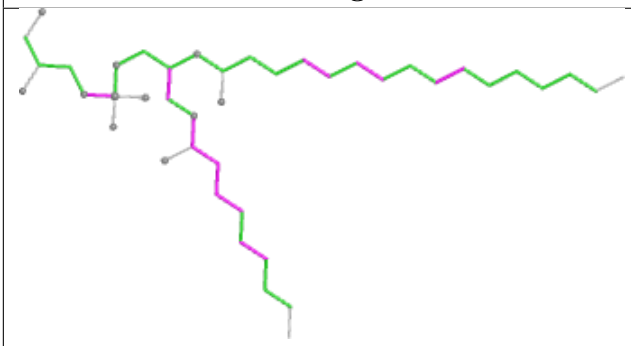
Ligand LHG e 101



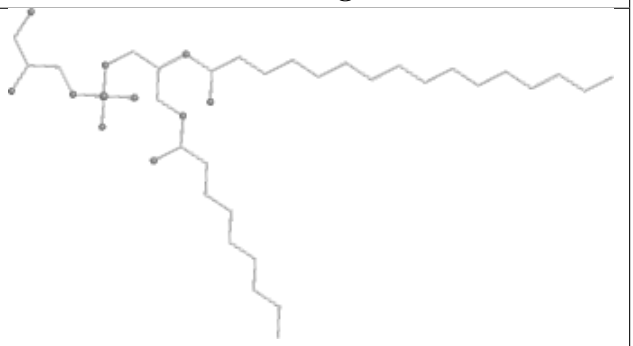
Bond lengths



Bond angles

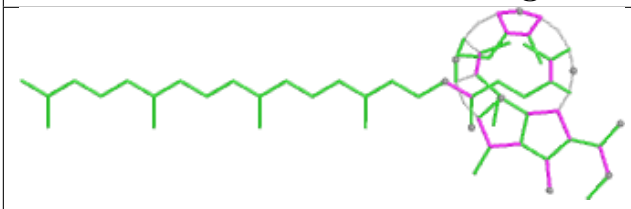


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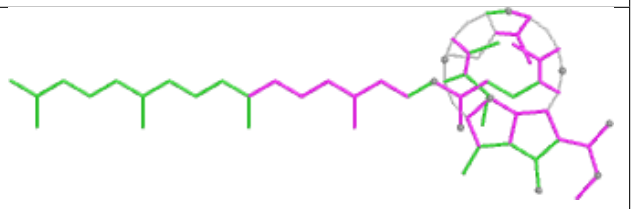


Rings

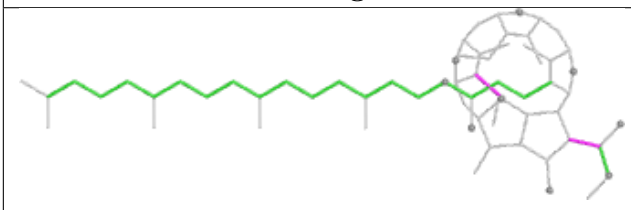
Ligand PHO A 407



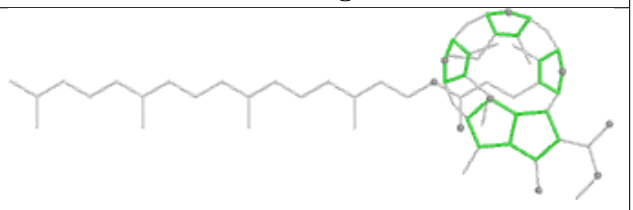
Bond lengths



Bond angles

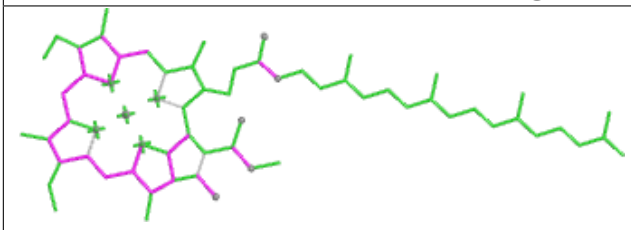


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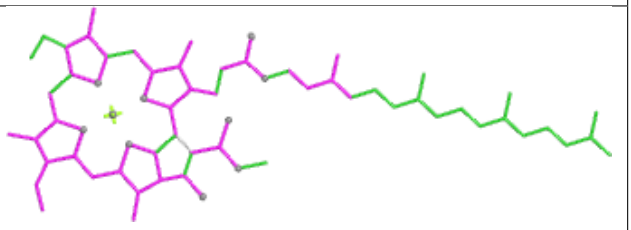


Rings

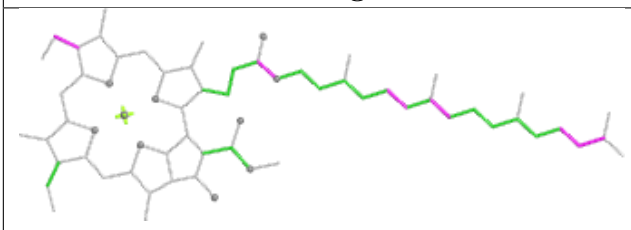
Ligand CLA a 408



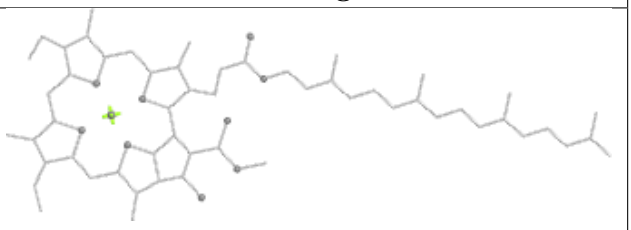
Bond lengths



Bond angles

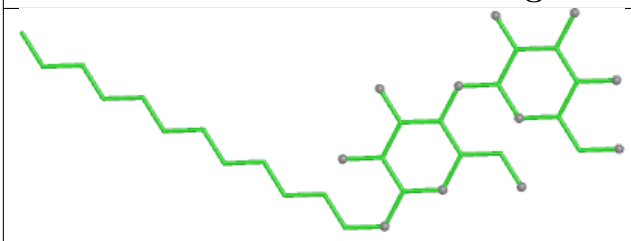


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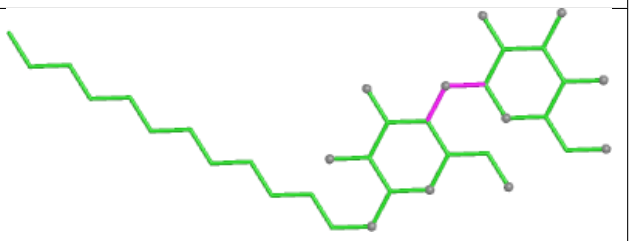


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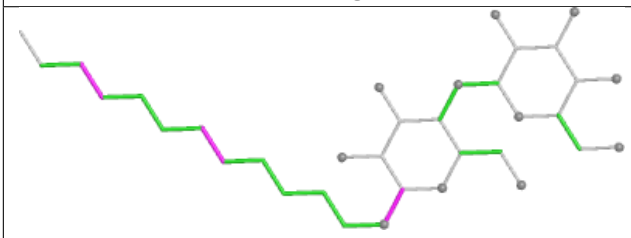
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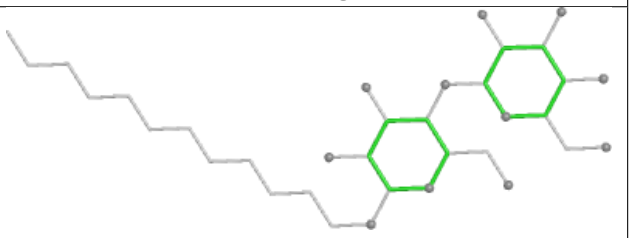
Bond lengths



Bond angles

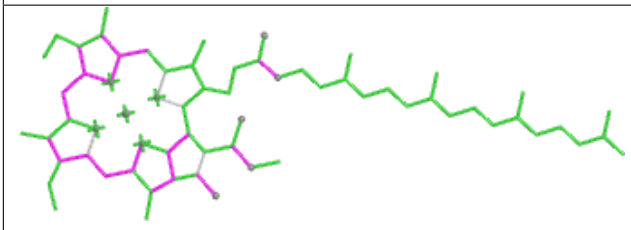


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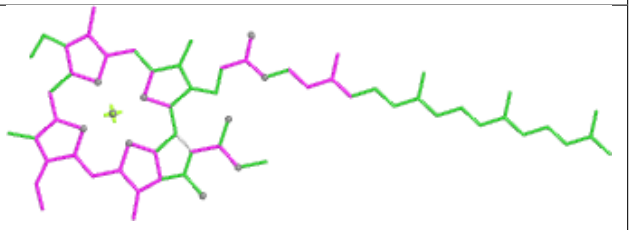


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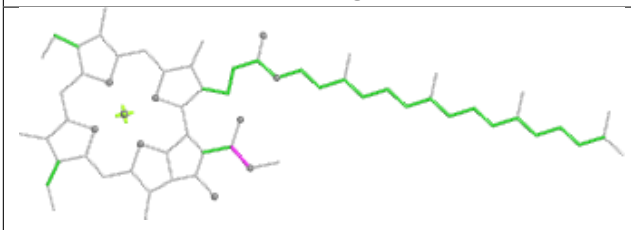
Ligand CLA C 504



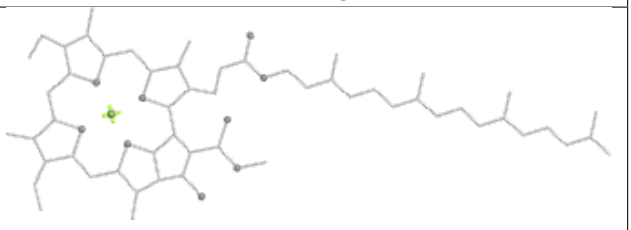
Bond lengths



Bond angles

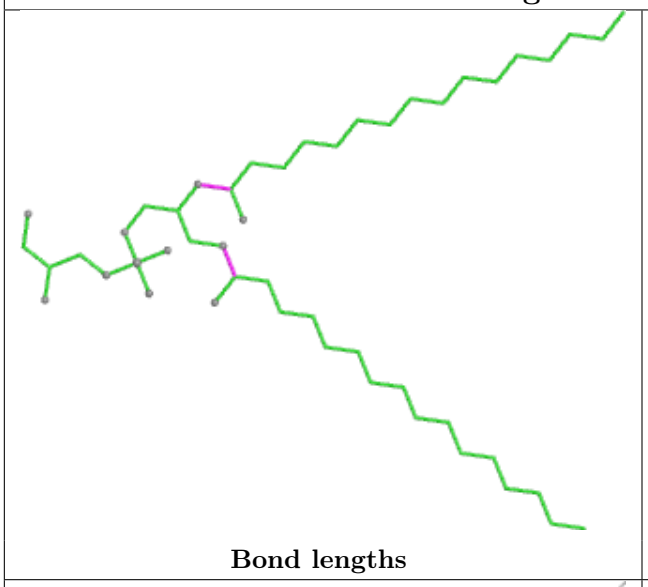


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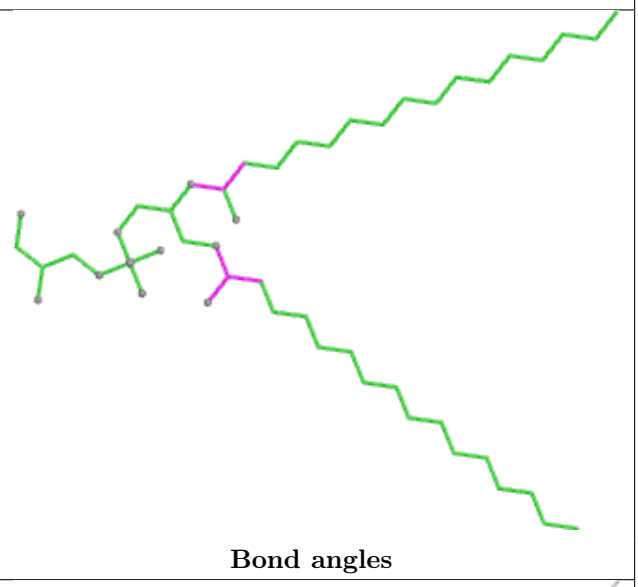


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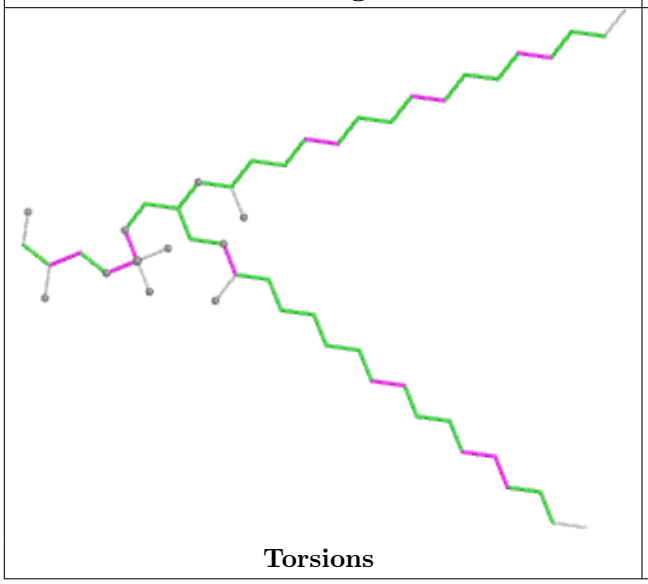
Ligand LHG D 408



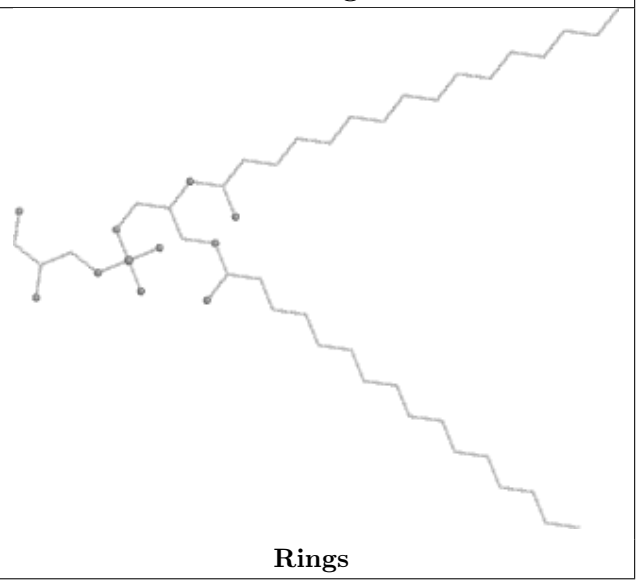
Bond lengths



Bond angles

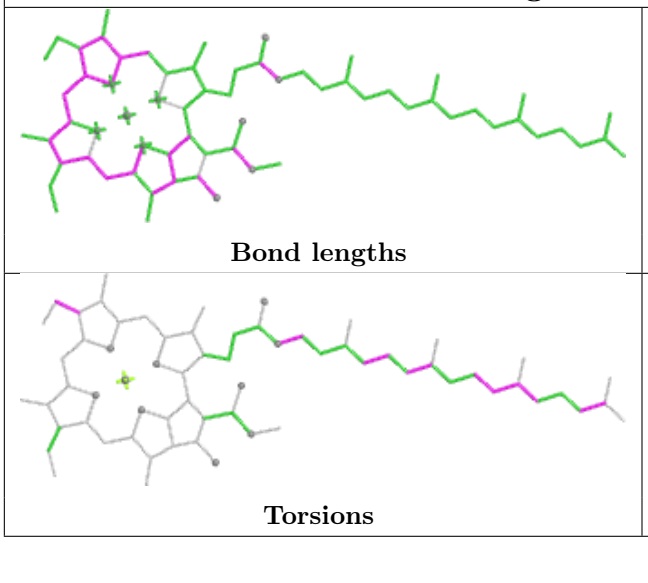


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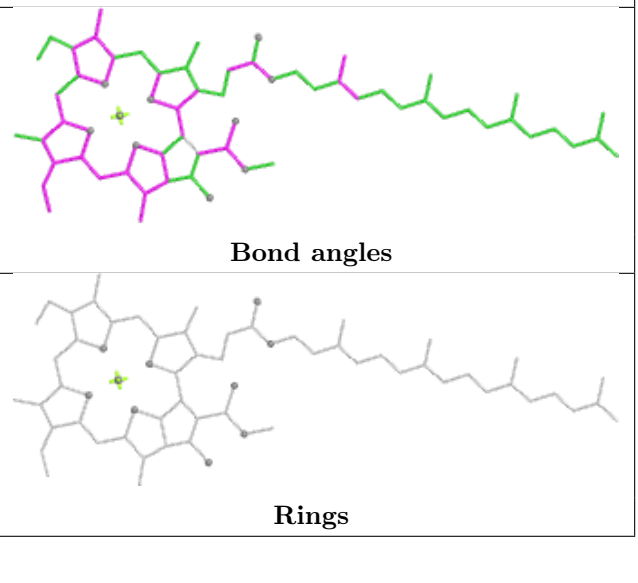


Rings

Ligand CLA B 616



Bond lengths

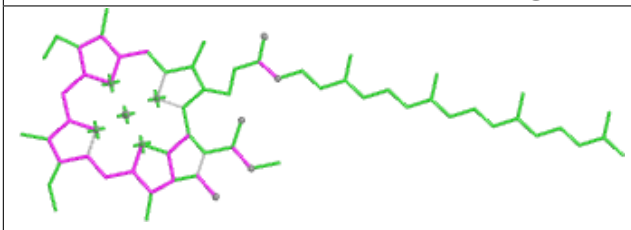


Bond angles

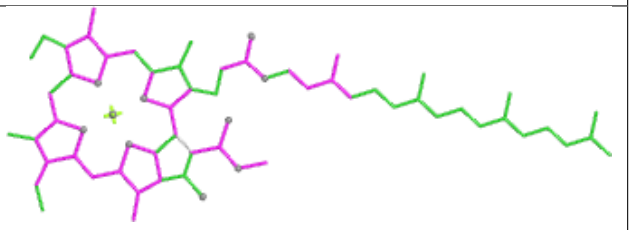
Torsions

Rings

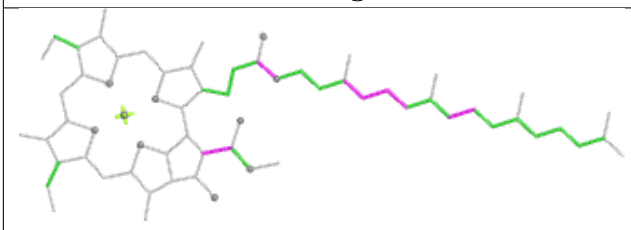
Ligand CLA b 605



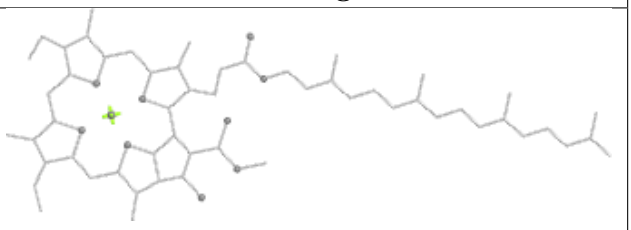
Bond lengths



Bond angles

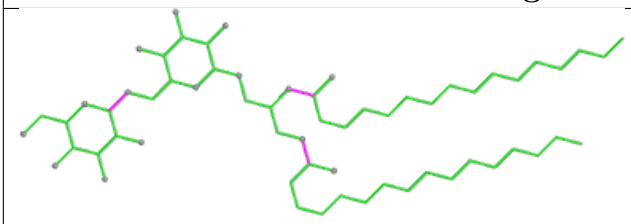


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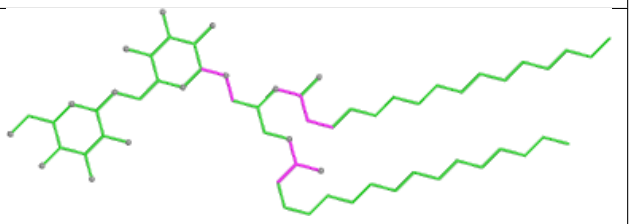


Rings

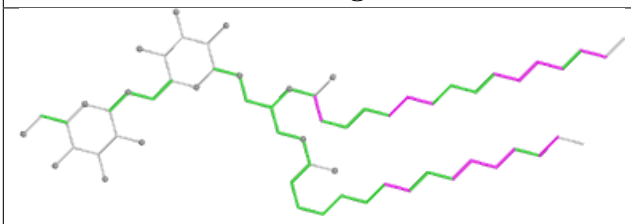
Ligand DGD h 102



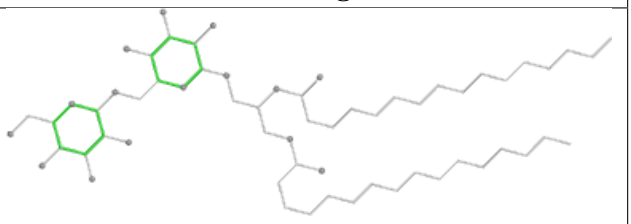
Bond lengths



Bond angles

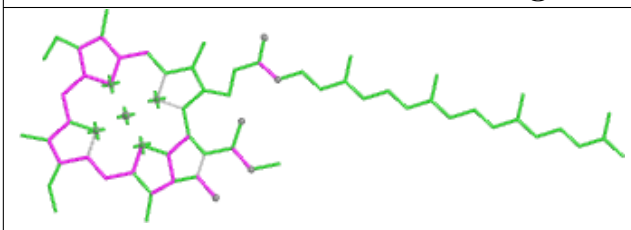


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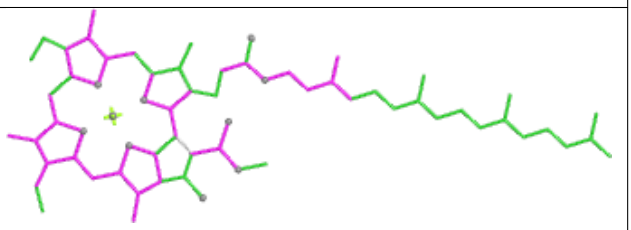


Rings

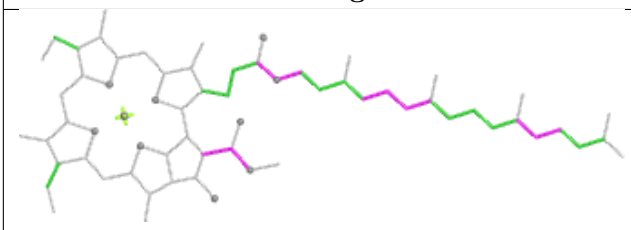
Ligand CLA c 509



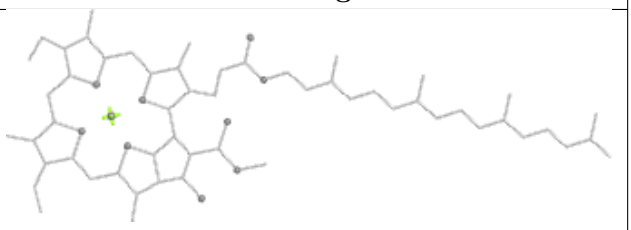
Bond lengths



Bond angles

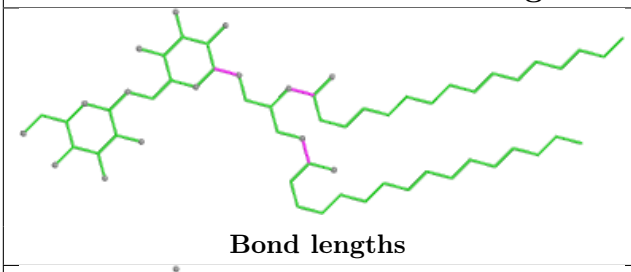


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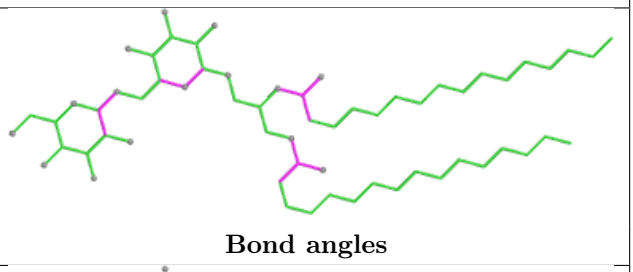


Rings

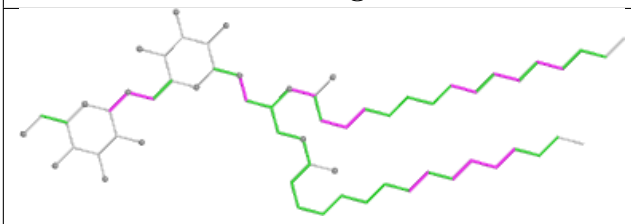
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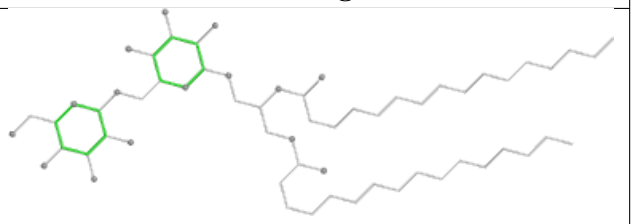
Bond lengths



Bond angles

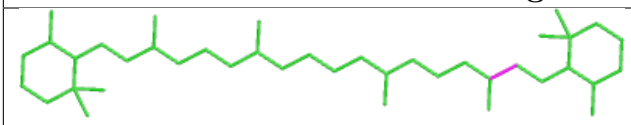


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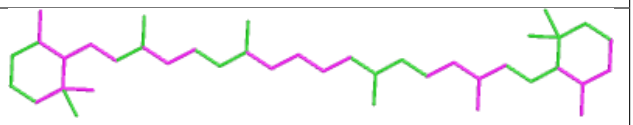


Rings

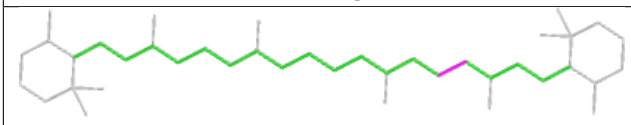
Ligand BCR a 409



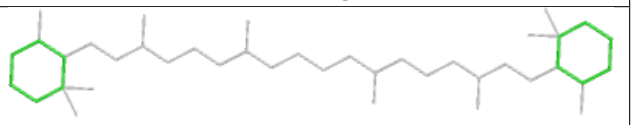
Bond lengths



Bond angles

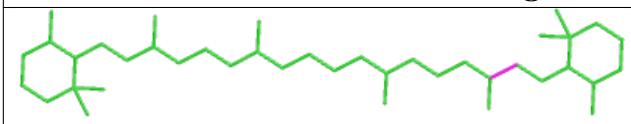


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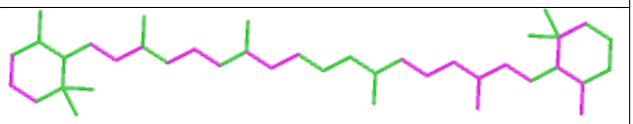


Rings

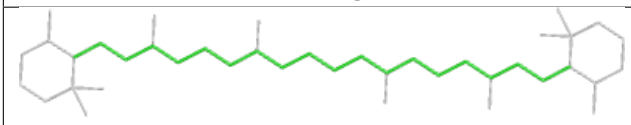
Ligand BCR B 619



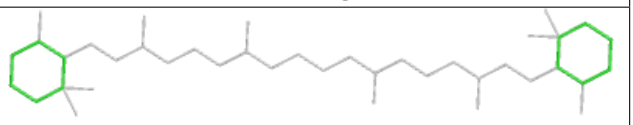
Bond lengths



Bond angles

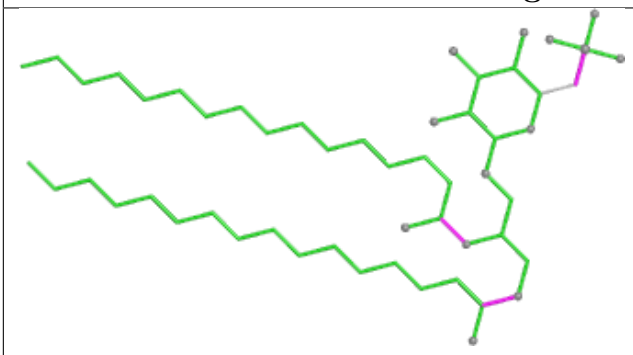


Torsions

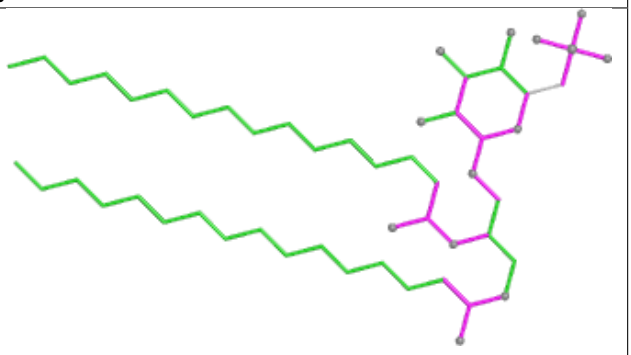


Rings

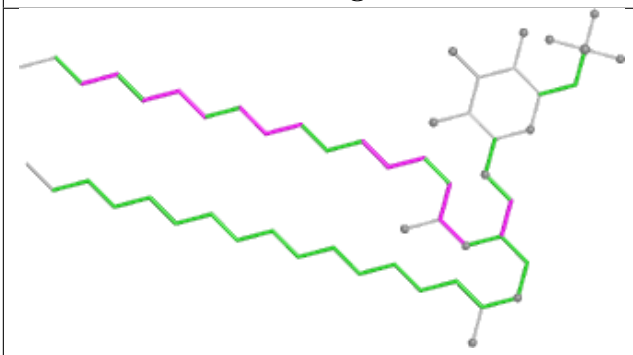
Ligand SQD A 410



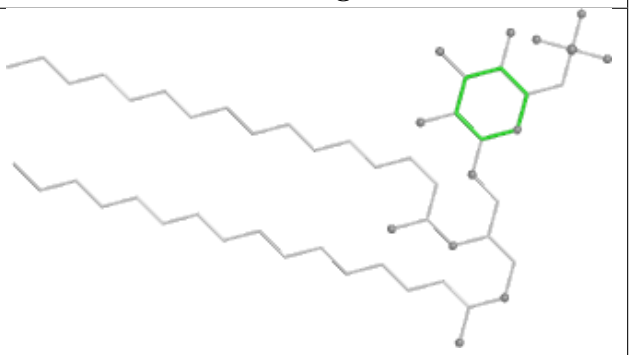
Bond lengths



Bond angles

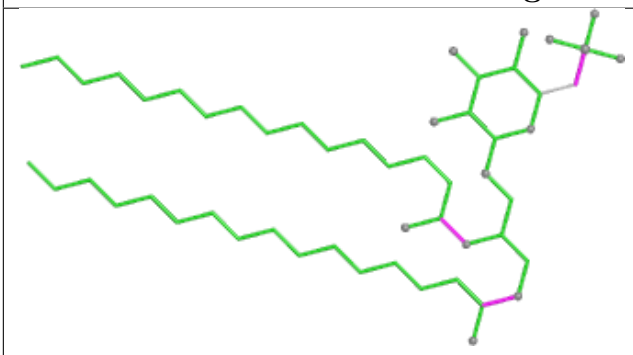


Torsions

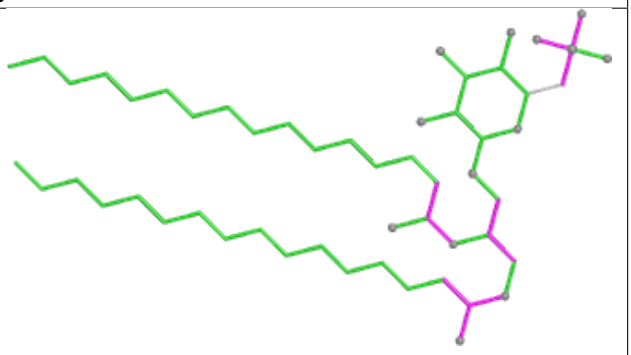


Rings

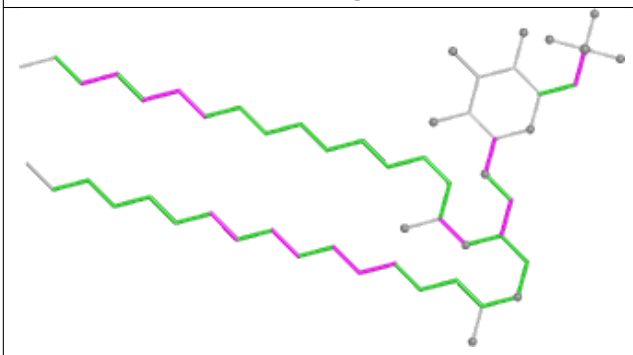
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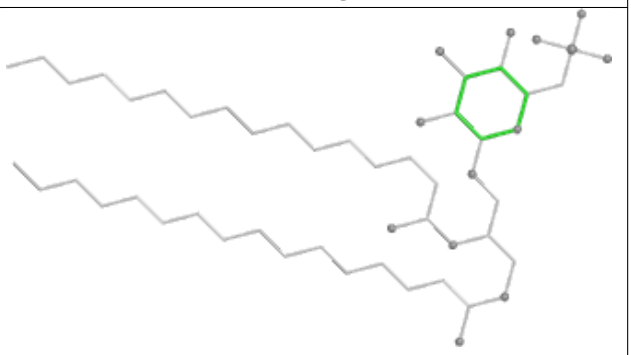
Bond lengths



Bond angles

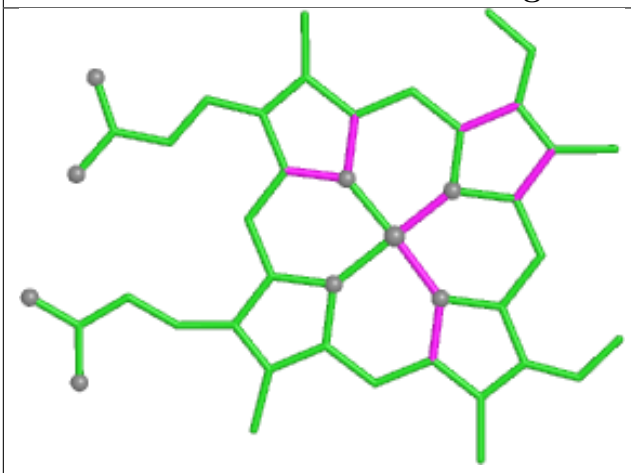


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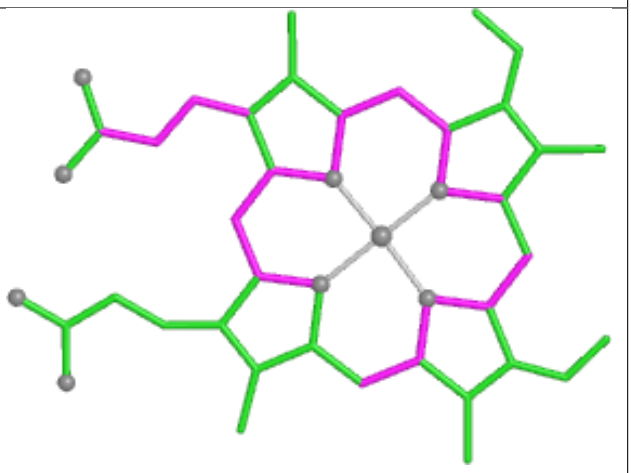


Rings

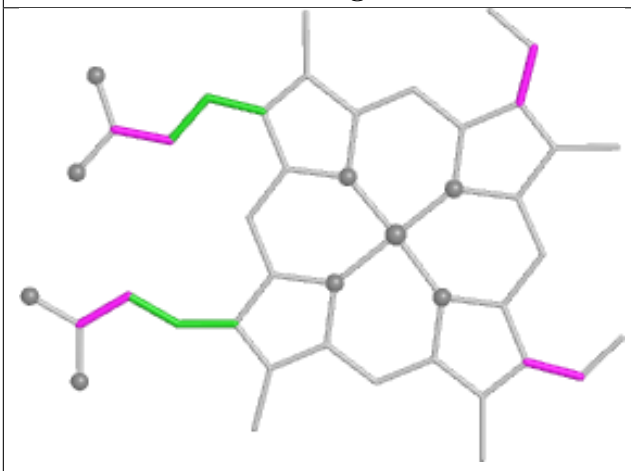
Ligand HEM e 103



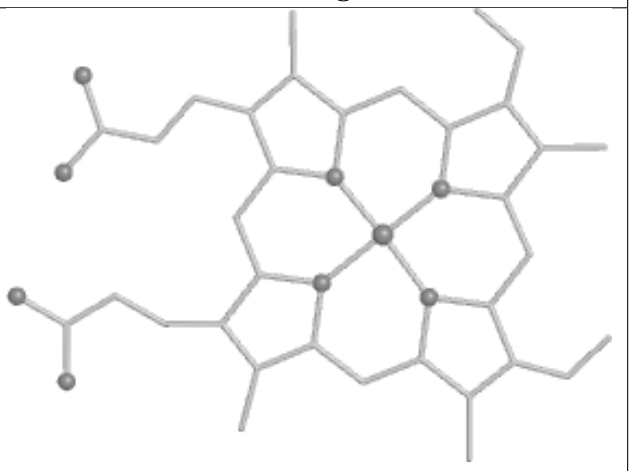
Bond lengths



Bond angles

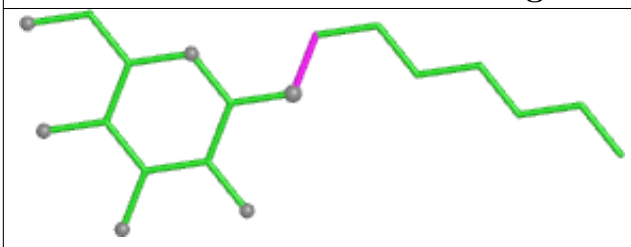


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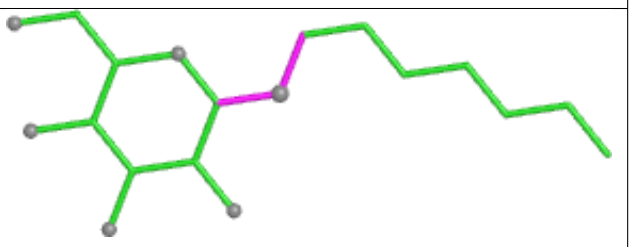


Rings

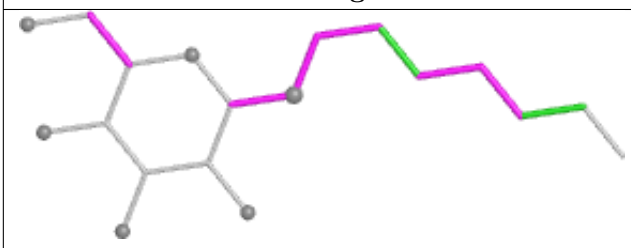
Ligand HTG c 521



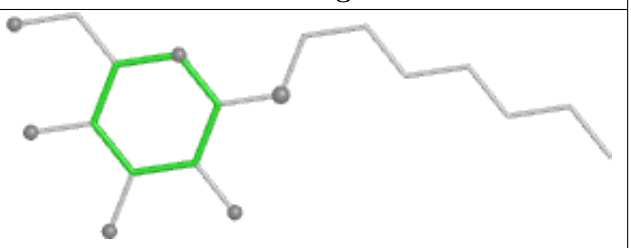
Bond lengths



Bond angles

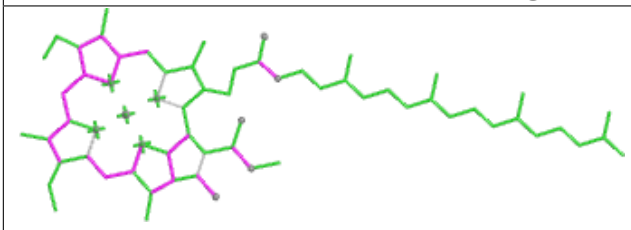


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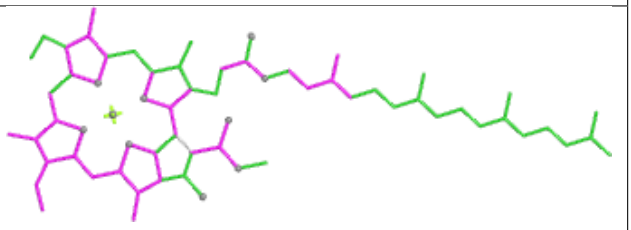


Rings

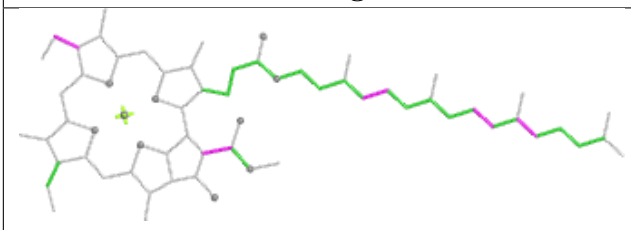
Ligand CLA C 503



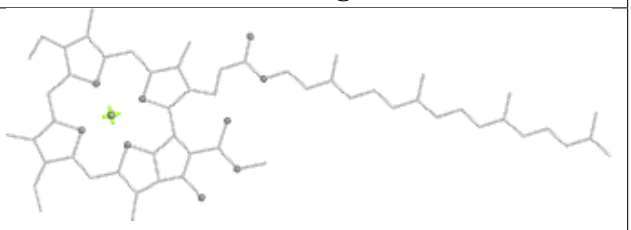
Bond lengths



Bond angles

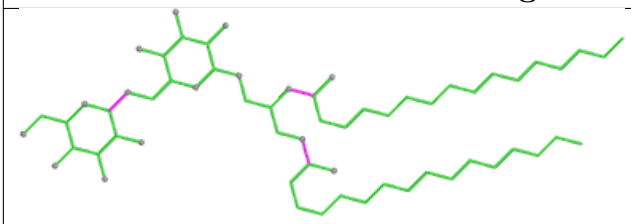


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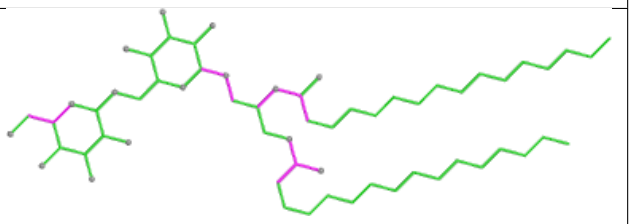


Rings

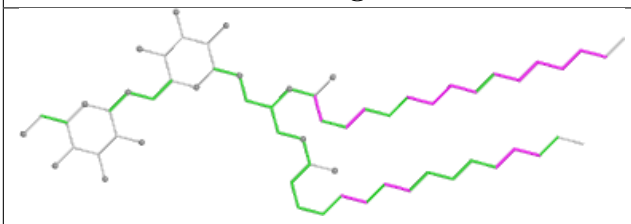
Ligand DGD H 102



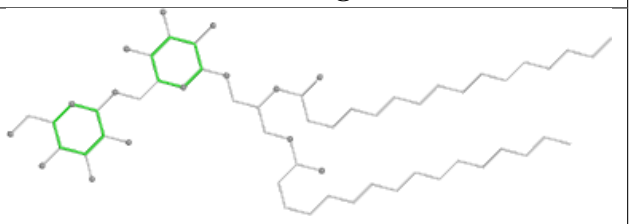
Bond lengths



Bond angles

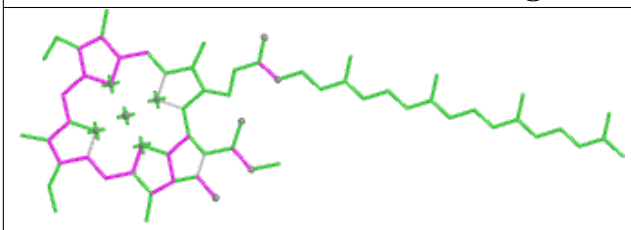


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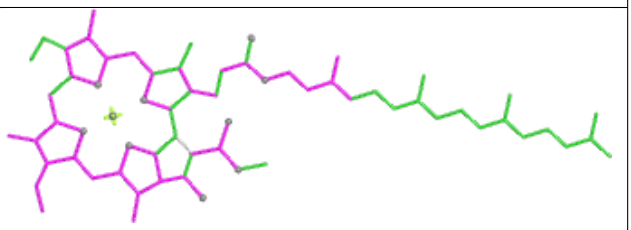


Rings

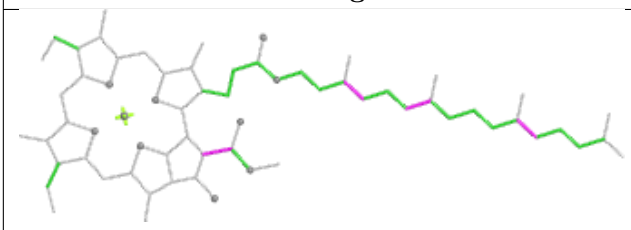
Ligand CLA C 505



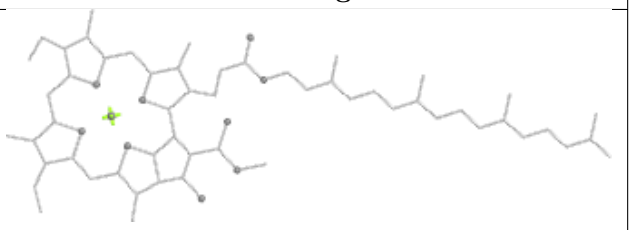
Bond lengths



Bond angles

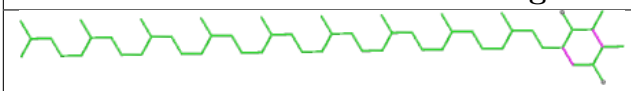


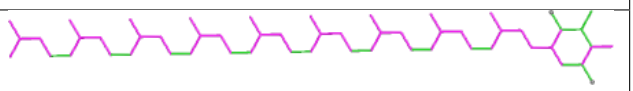
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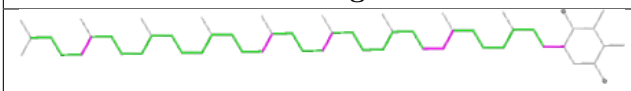


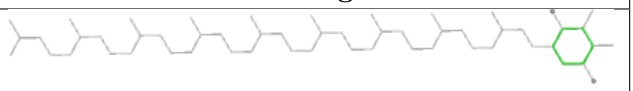
Rings

Ligand PL9 A 414

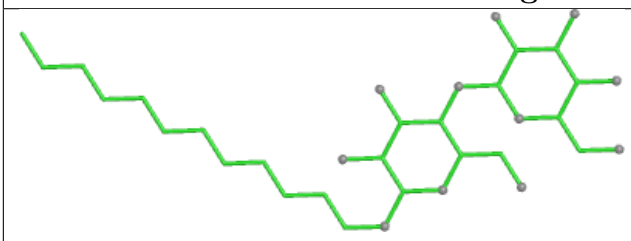

Bond lengths

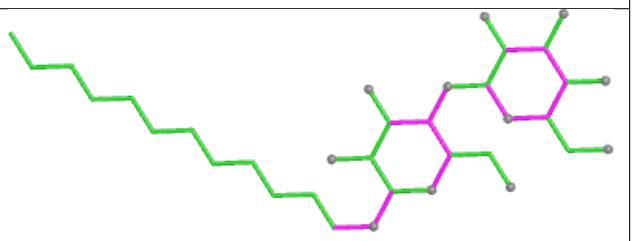

Bond angles

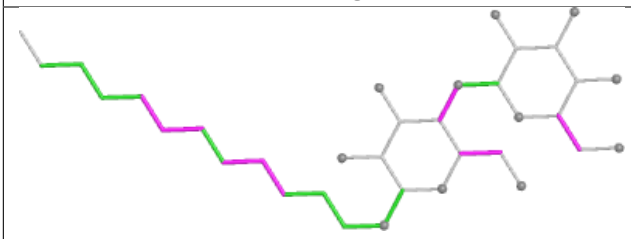

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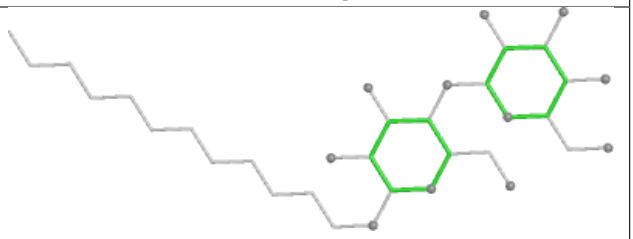

Rings

Ligand LMT D 403

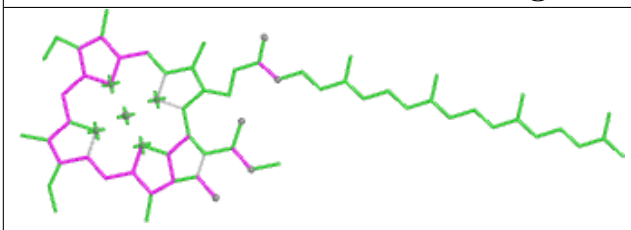

Bond lengths

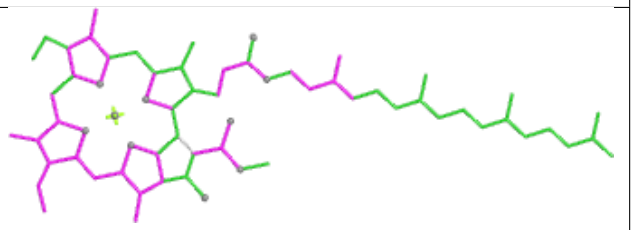

Bond angles

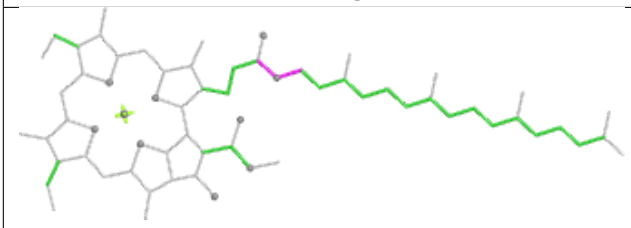

Torsions

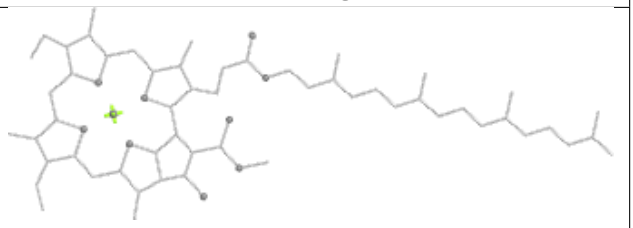

Rings

Ligand CLA c 511

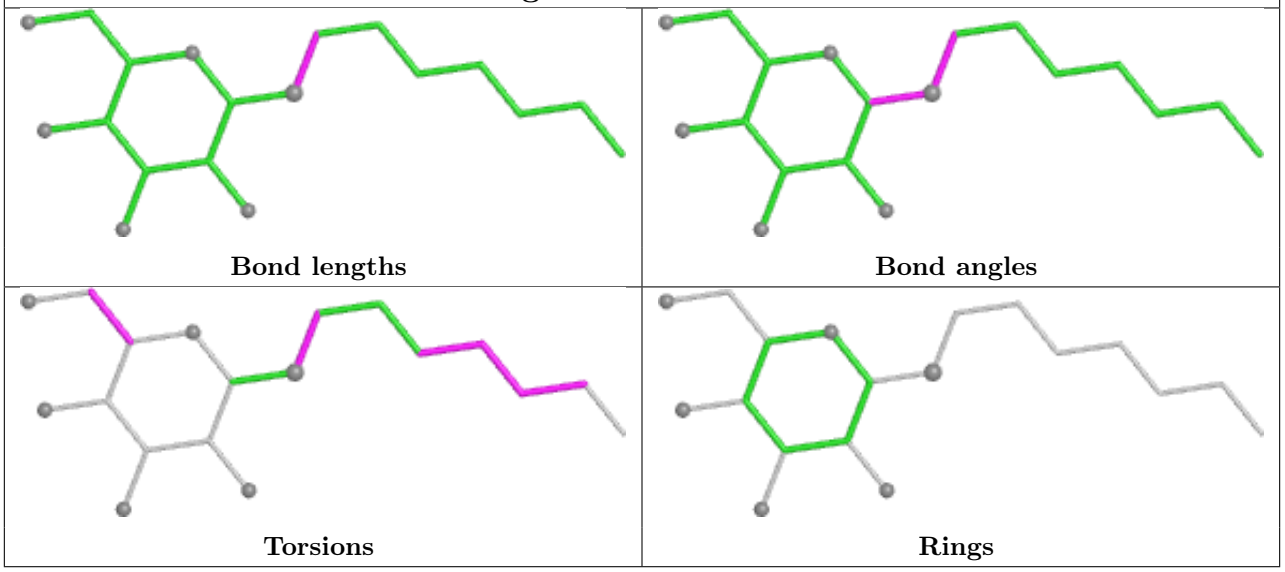

Bond lengths


Bond angles

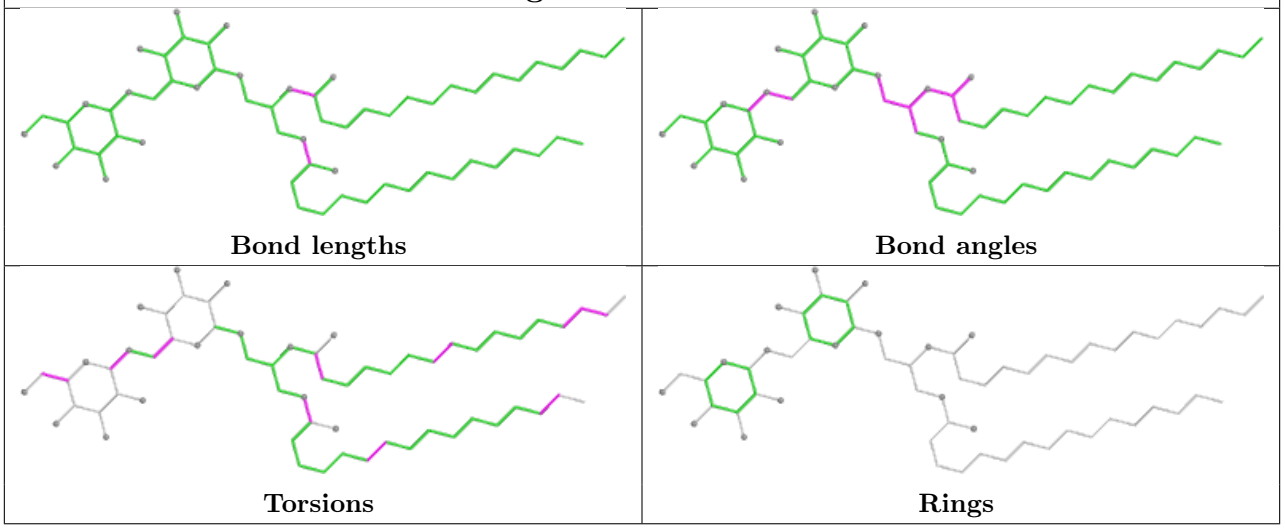

Torsions


Rings

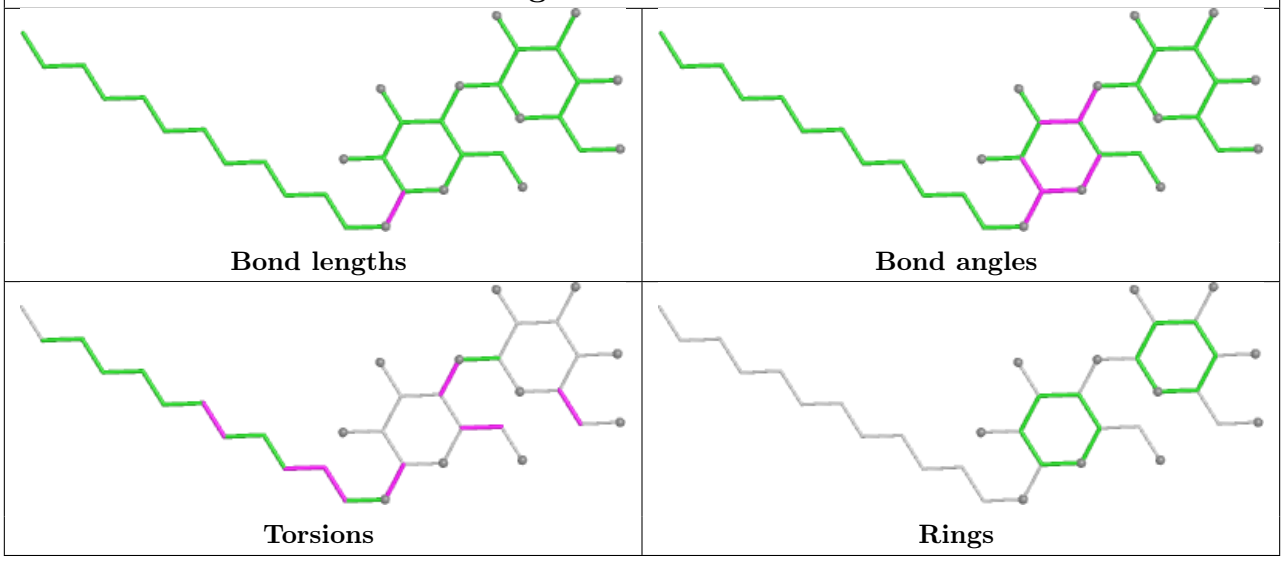
Ligand HTG B 623



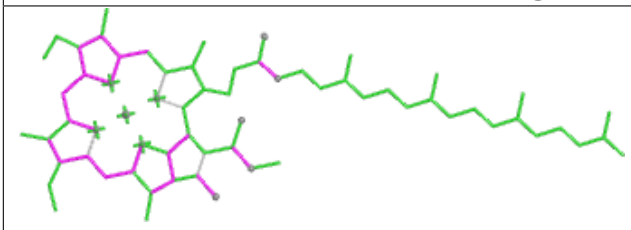
Ligand DGD c 516



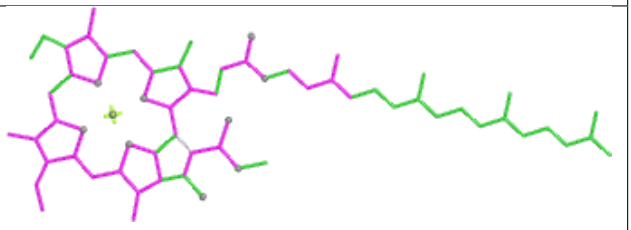
Ligand LMT I 101



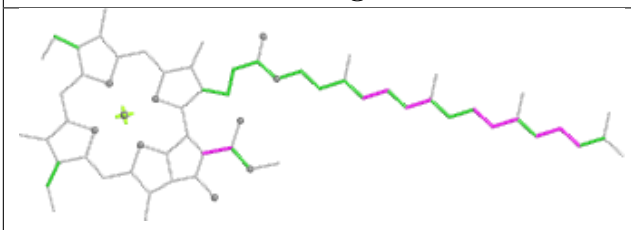
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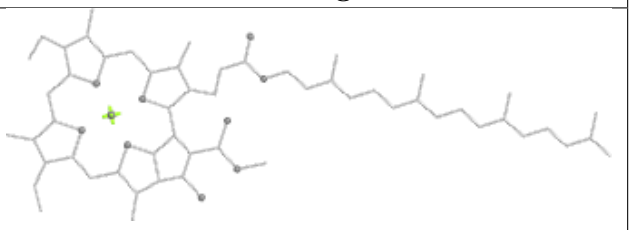
Bond lengths



Bond angles

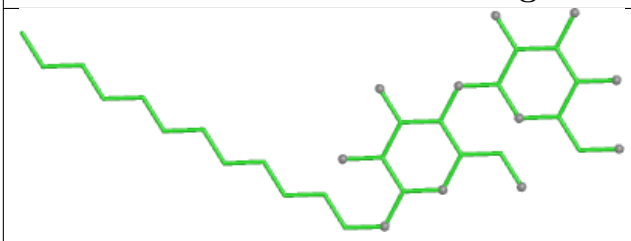


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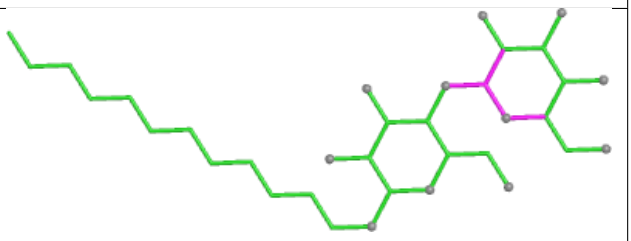


Rings

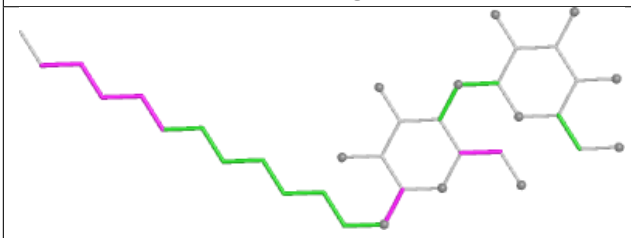
Ligand LMT m 102



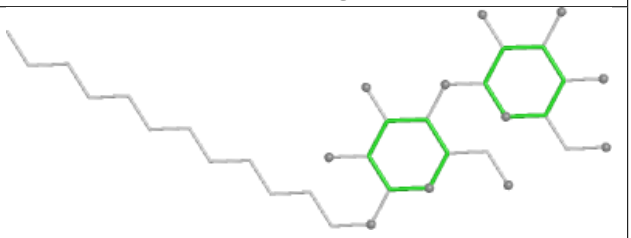
Bond lengths



Bond angles

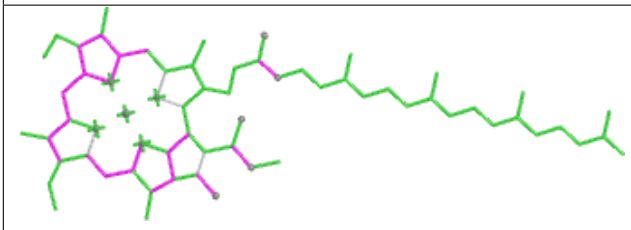


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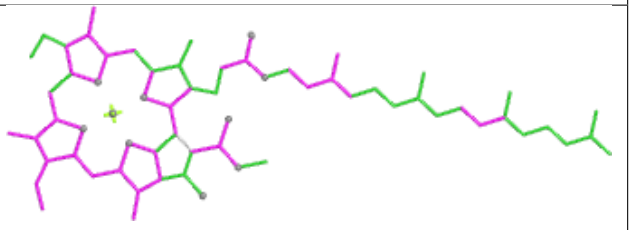


Rings

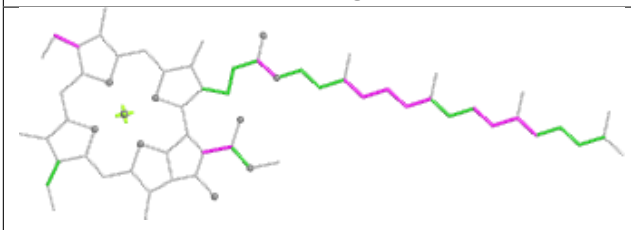
Ligand CLA b 616



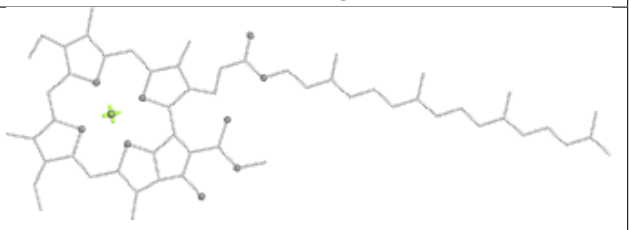
Bond lengths



Bond angles

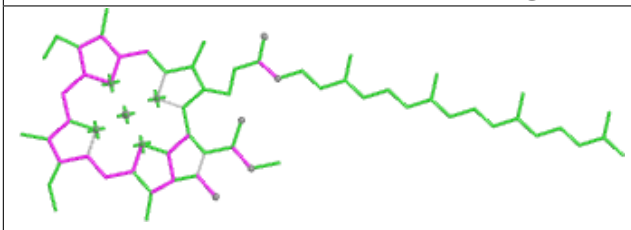


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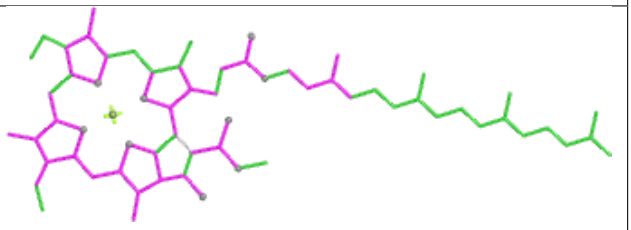


Rings

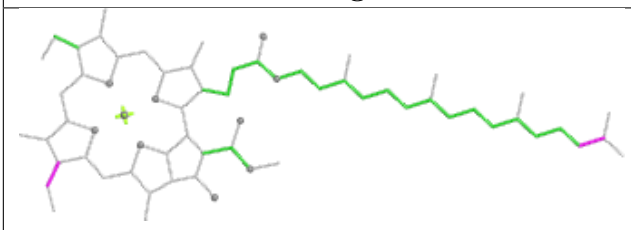
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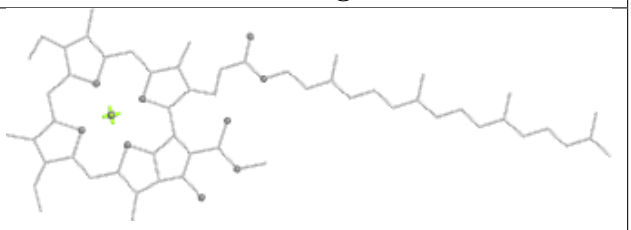
Bond lengths



Bond angles

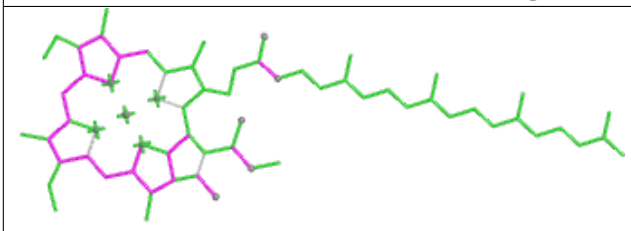


Torsions

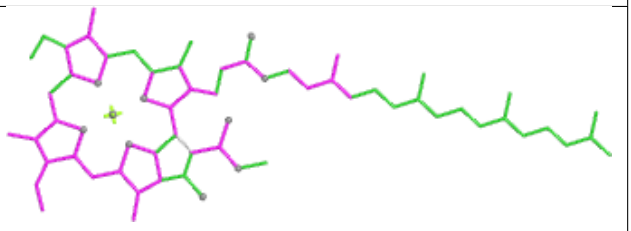


Rings

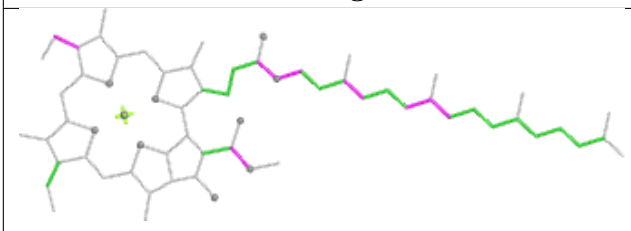
Ligand CLA C 514



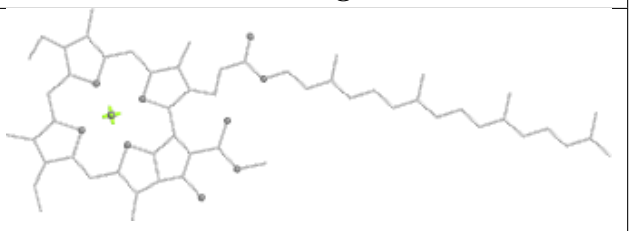
Bond lengths



Bond angles

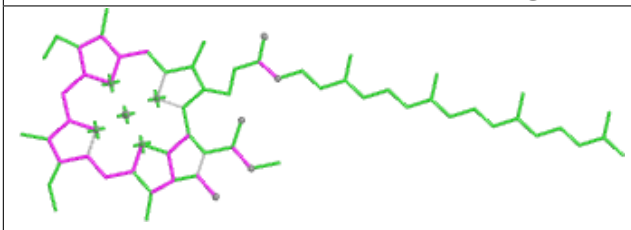


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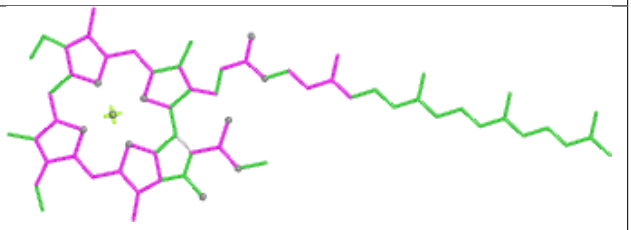


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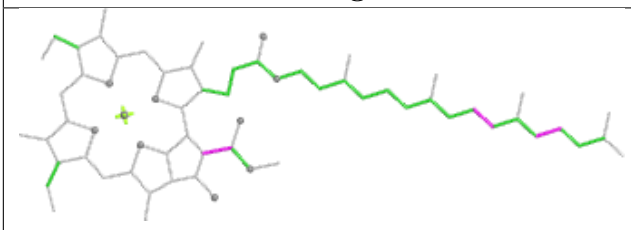
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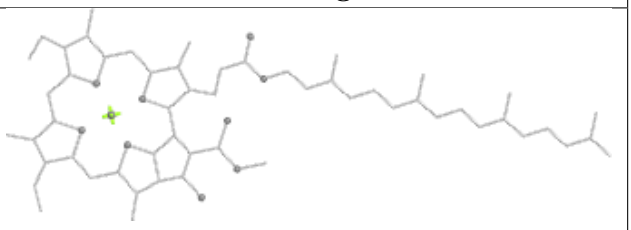
Bond lengths



Bond angles

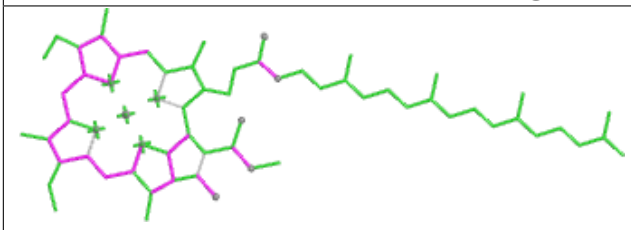


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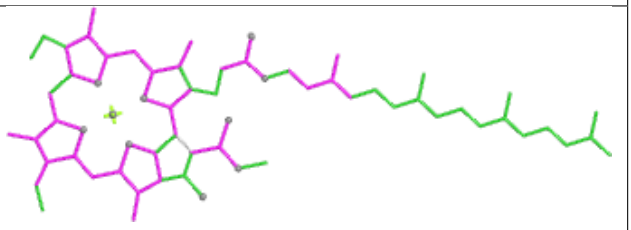


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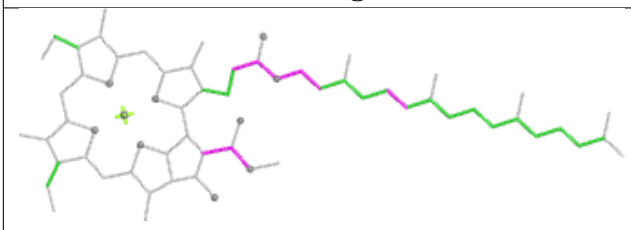
Ligand CLA b 613



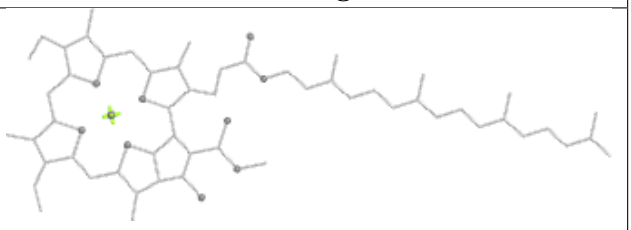
Bond lengths



Bond angles



Torsions

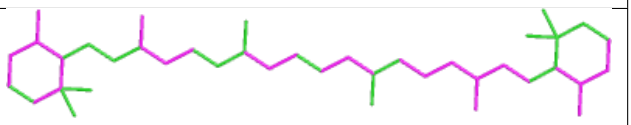


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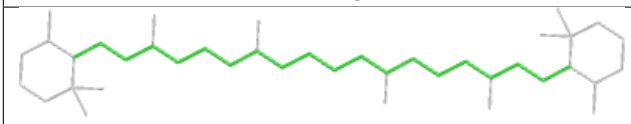
Ligand BCR c 514



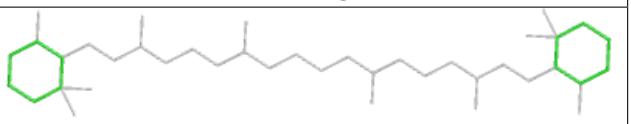
Bond lengths



Bond angles

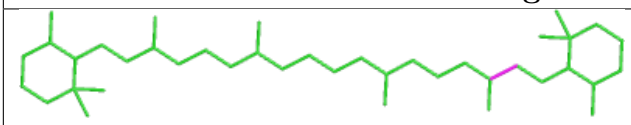


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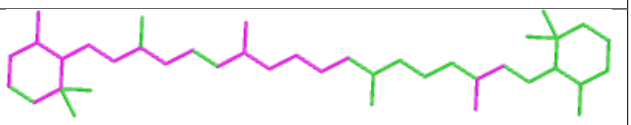


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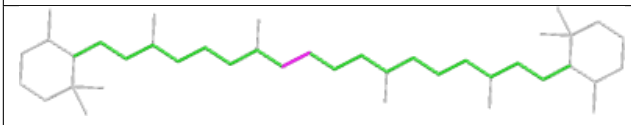
Ligand BCR T 101



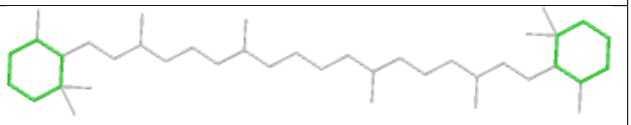
Bond lengths



Bond angles

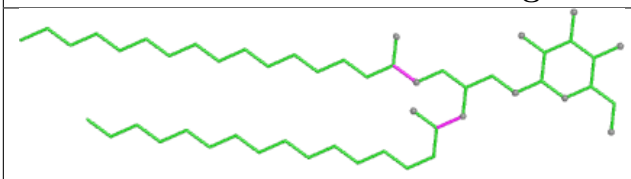


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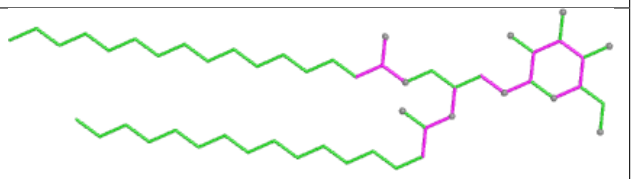


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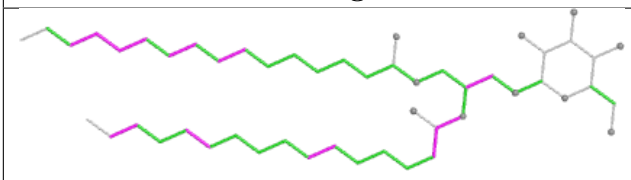
Ligand LMG b 620



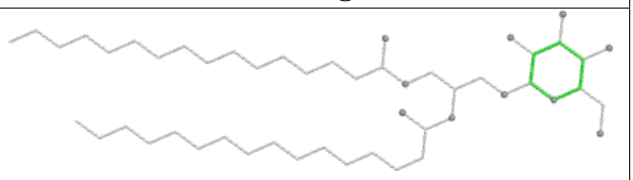
Bond lengths



Bond angles

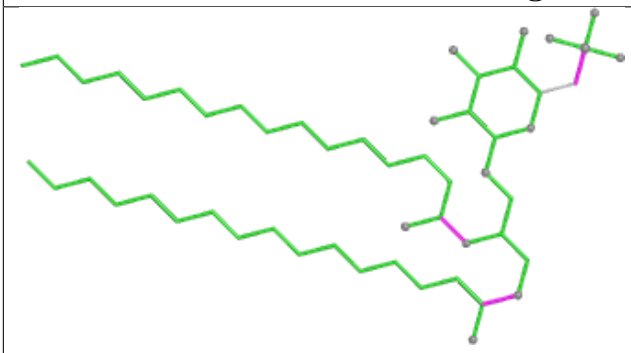


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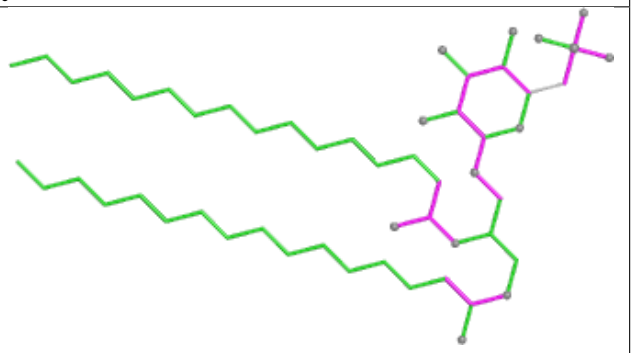


Rings

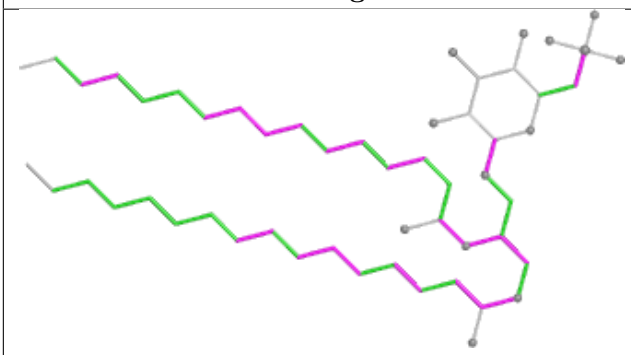
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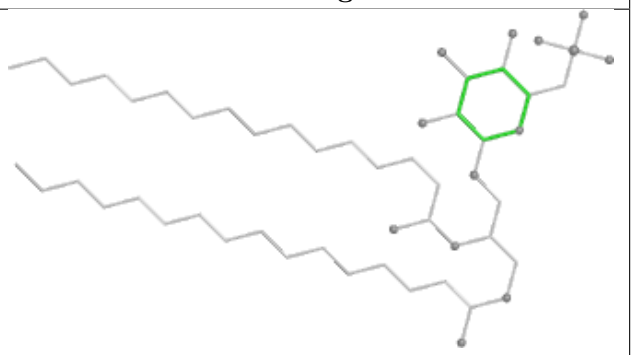
Bond lengths



Bond angles

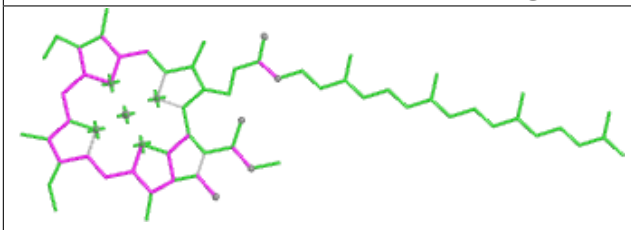


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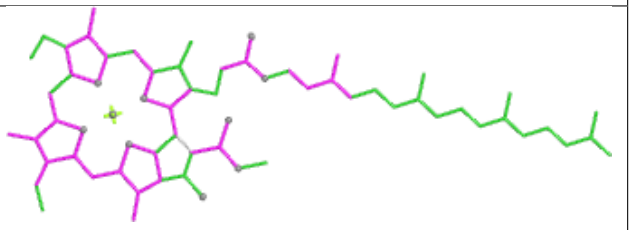


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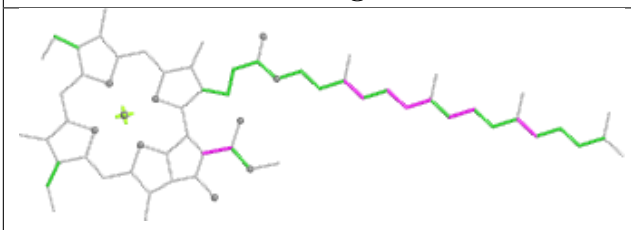
Ligand CLA B 605



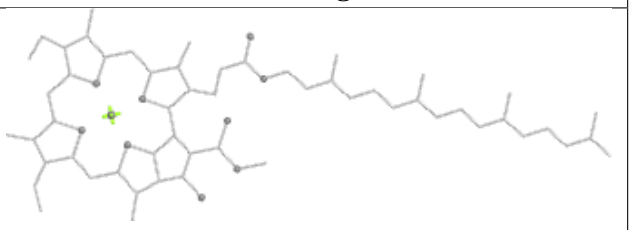
Bond lengths



Bond angles



Torsions

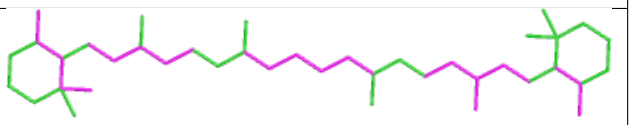


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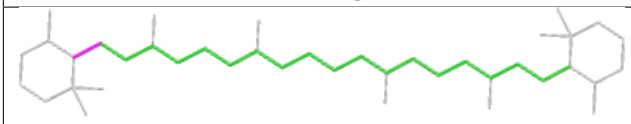
Ligand BCR b 617



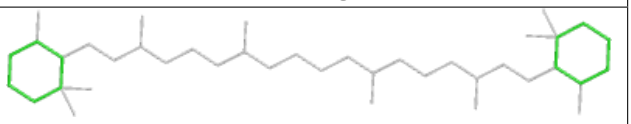
Bond lengths



Bond angles

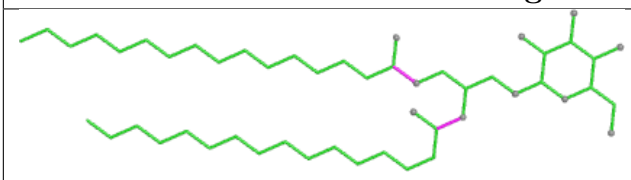


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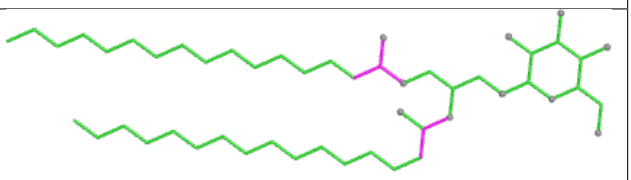


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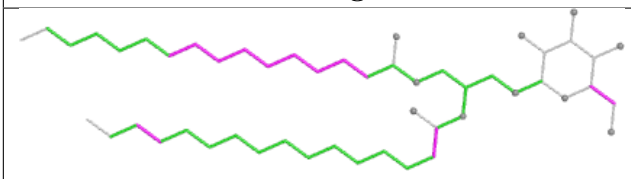
Ligand LMG c 519



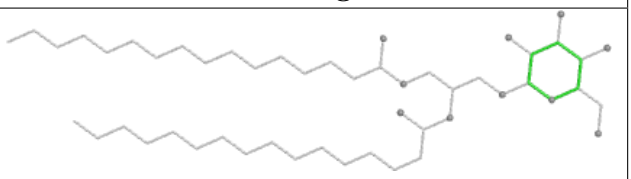
Bond lengths



Bond angles

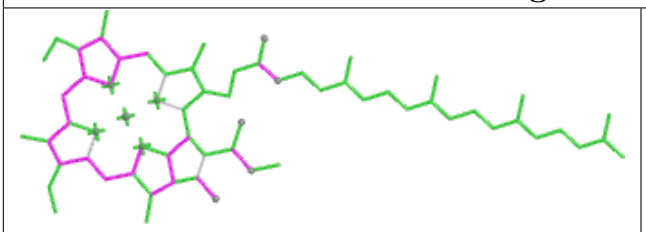


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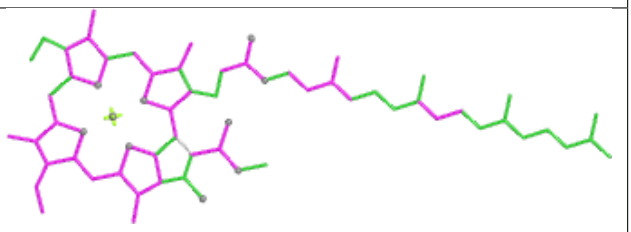


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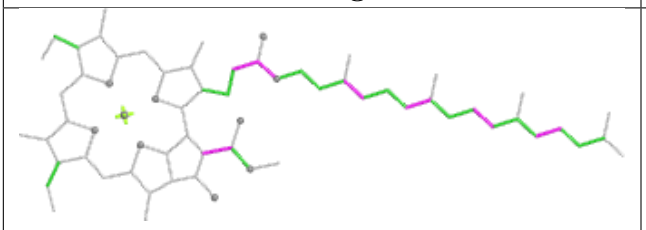
Ligand CLA c 510



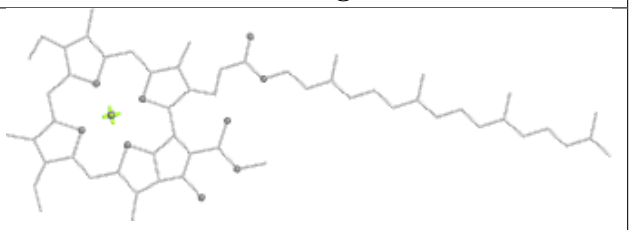
Bond lengths



Bond angles

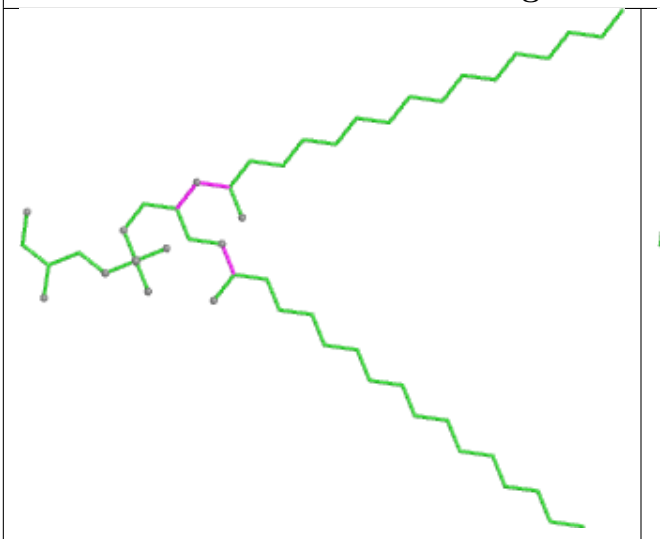


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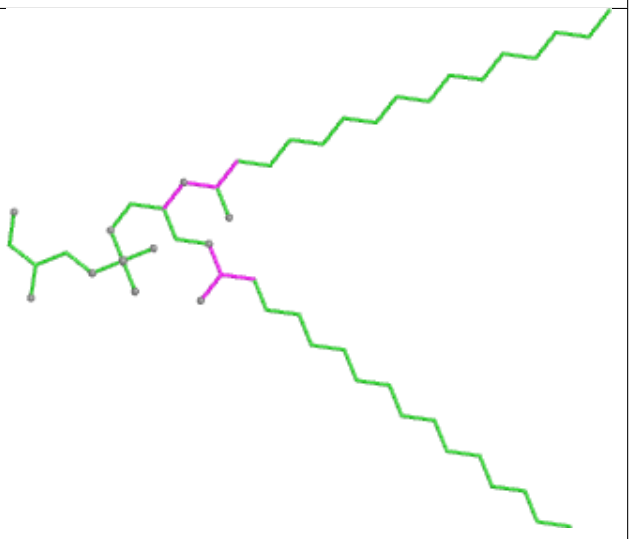


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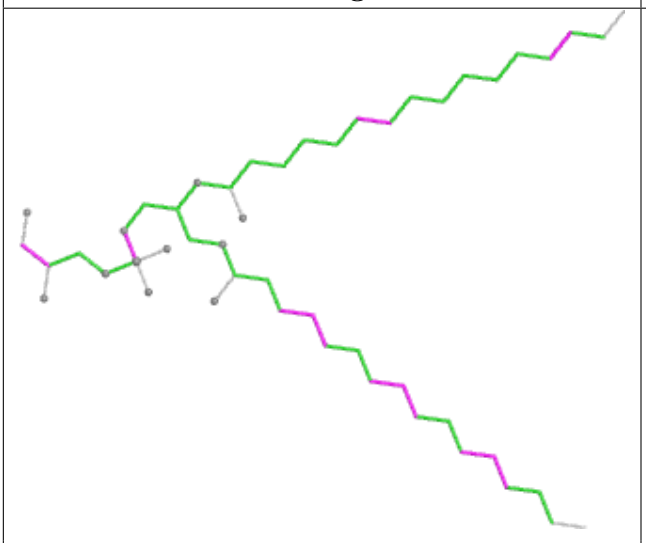
Ligand LHG A 416



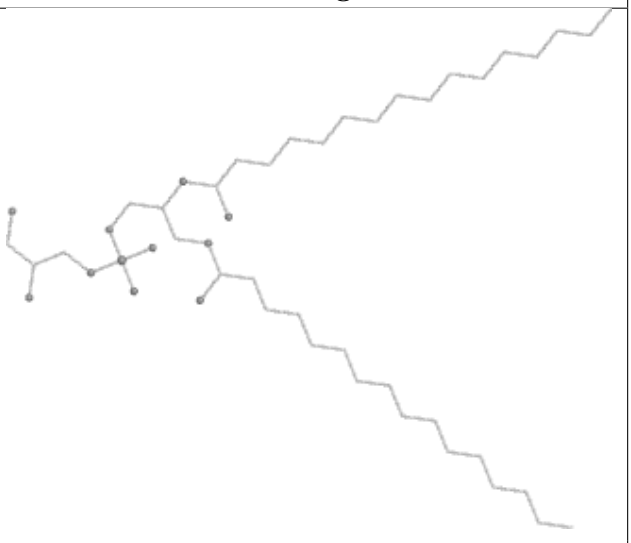
Bond lengths



Bond angles

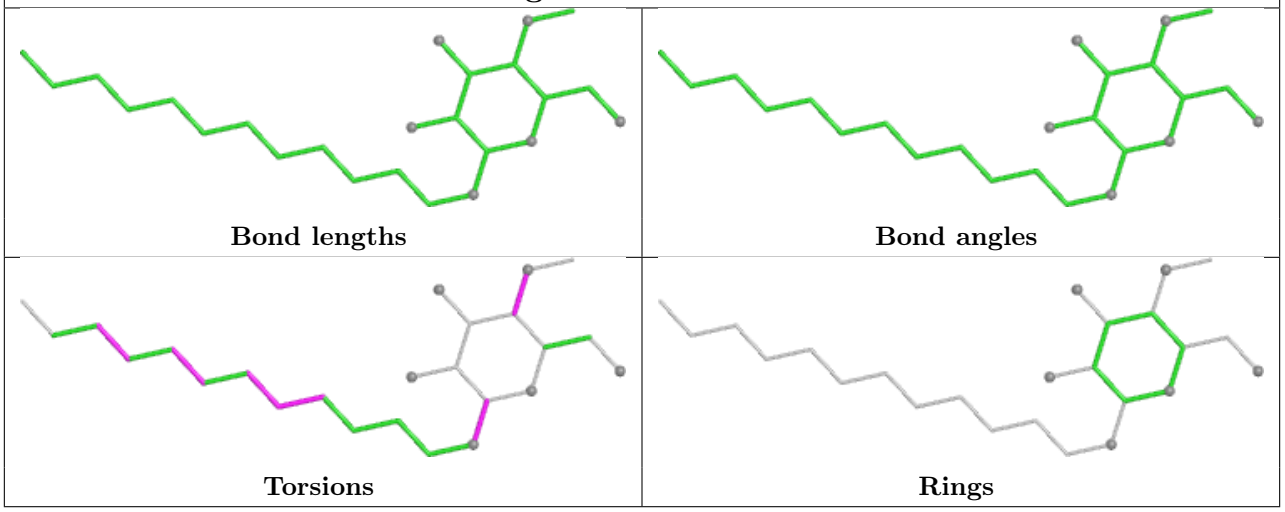


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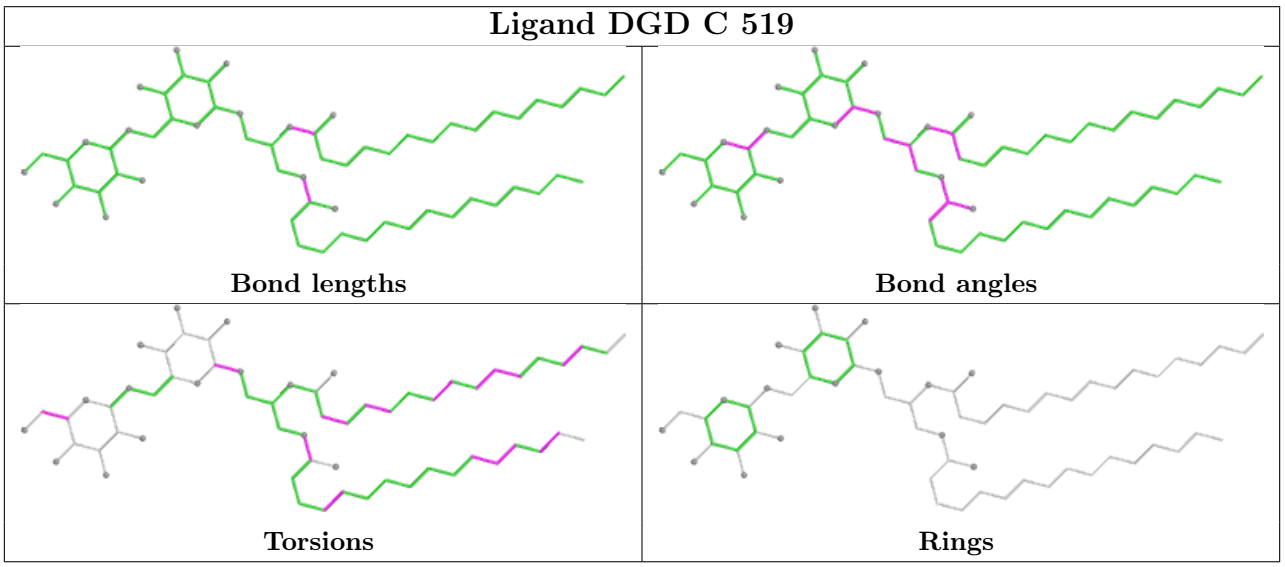


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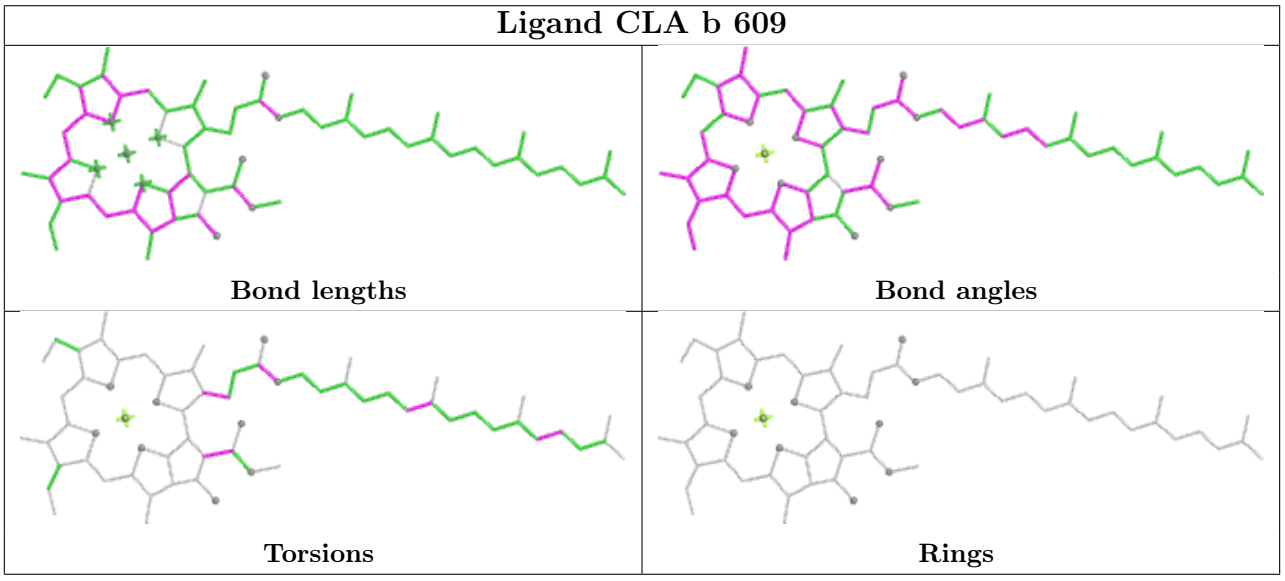
Ligand LMT b 621



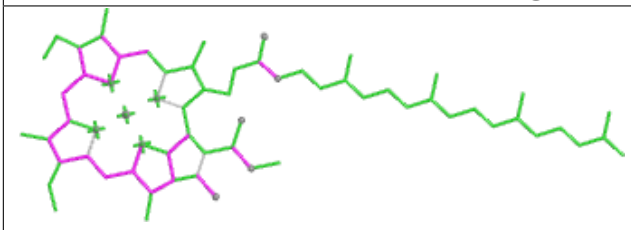
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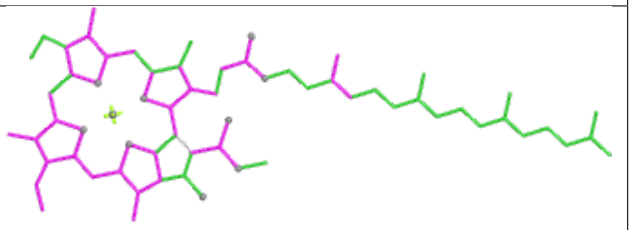
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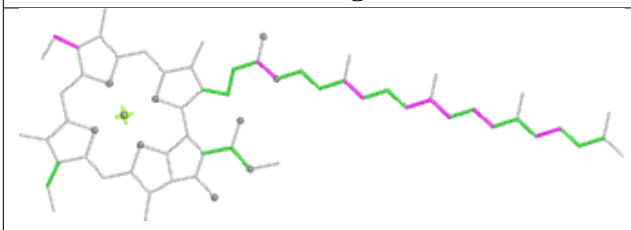
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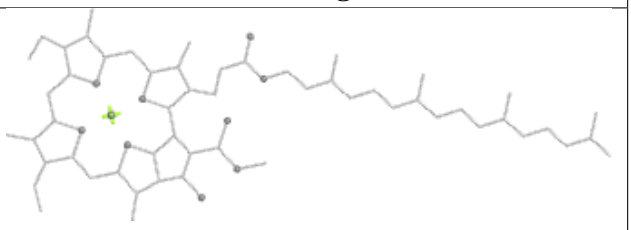
Bond lengths



Bond angles

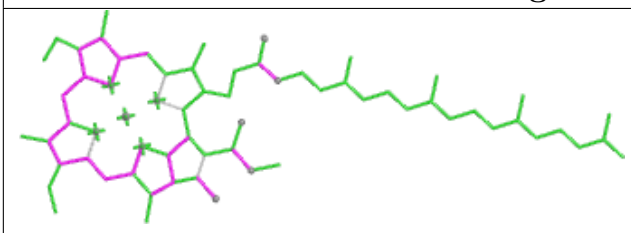


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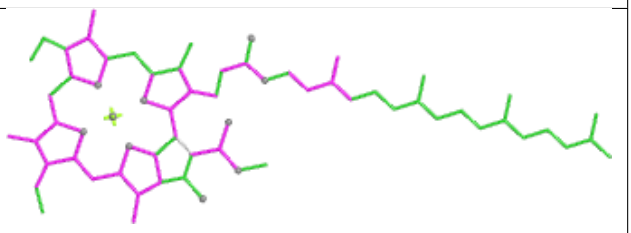


Rings

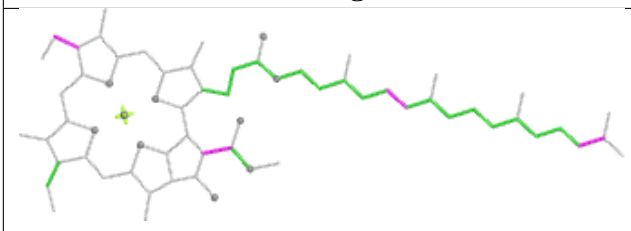
Ligand CLA c 508



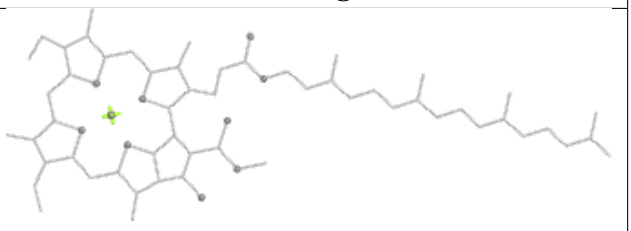
Bond lengths



Bond angles

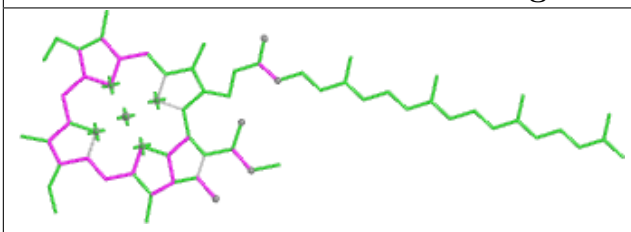


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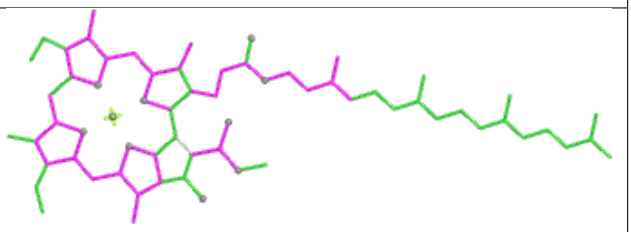


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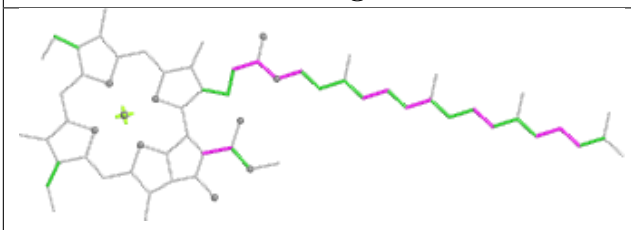
Ligand CLA c 512



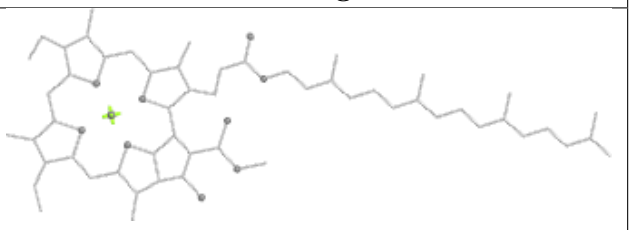
Bond lengths



Bond angles

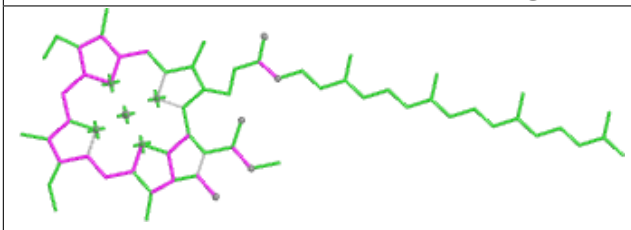


Torsions

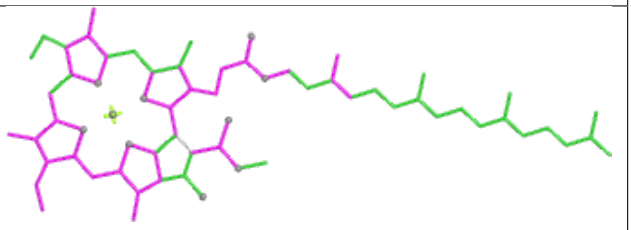


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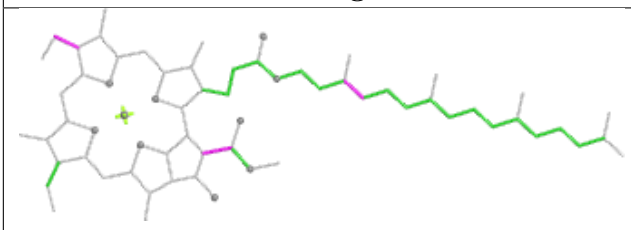
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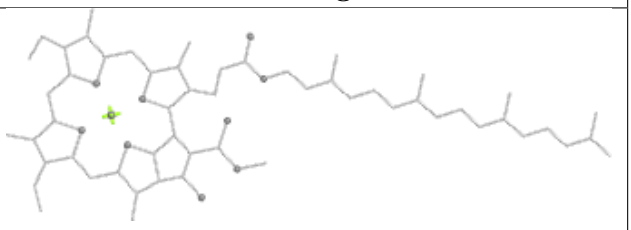
Bond lengths



Bond angles



Torsions

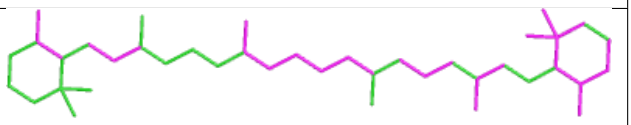


Rings

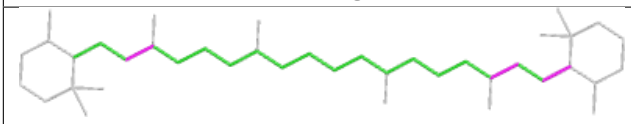
Ligand BCR d 405



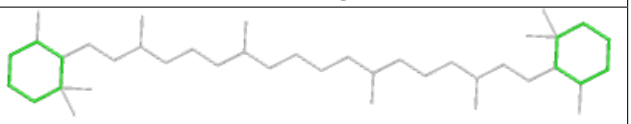
Bond lengths



Bond angles

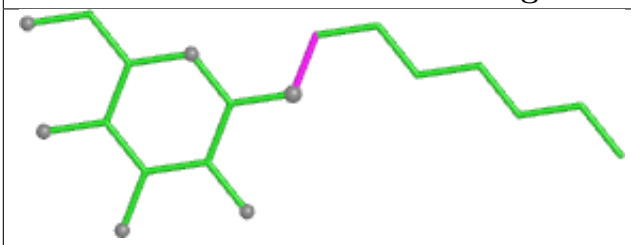


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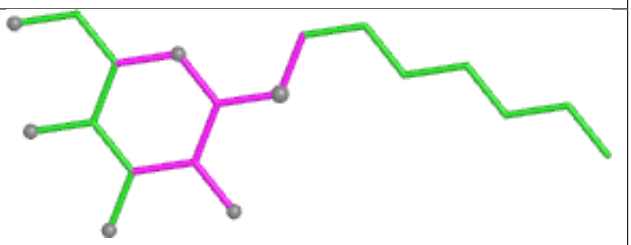


Rings

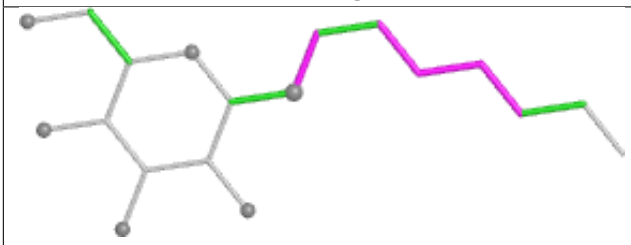
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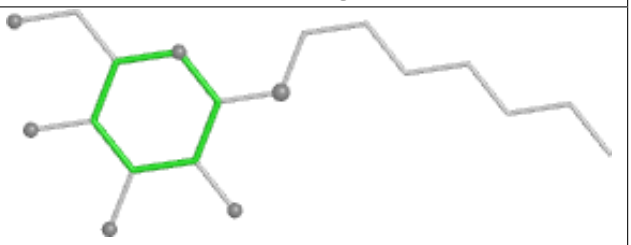
Bond lengths



Bond angles

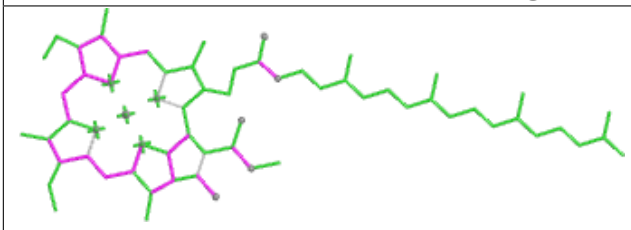


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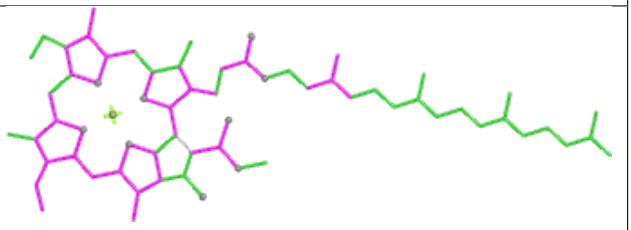


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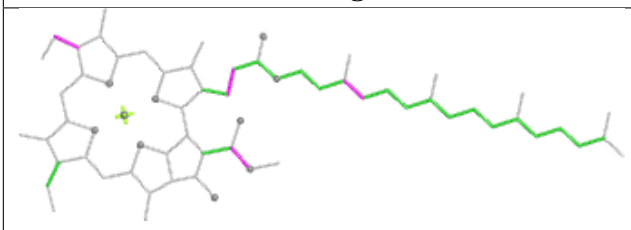
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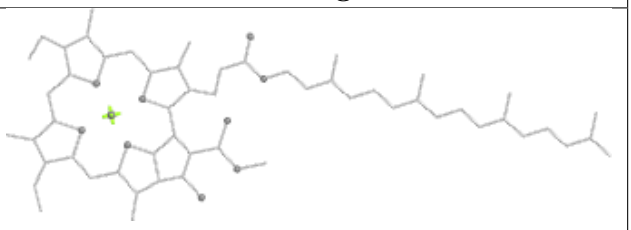
Bond lengths



Bond angles

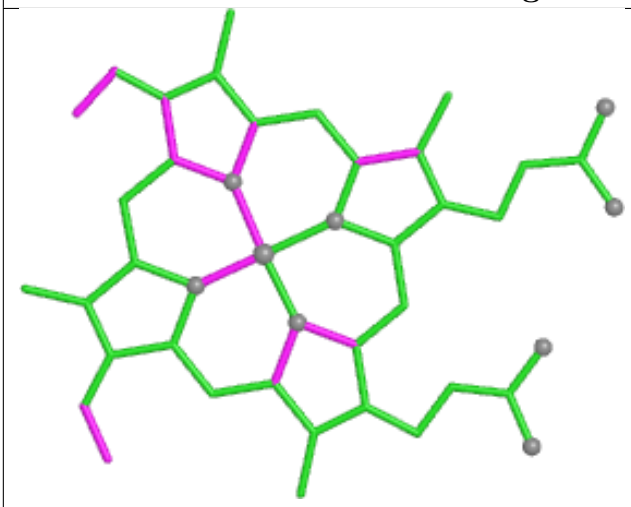


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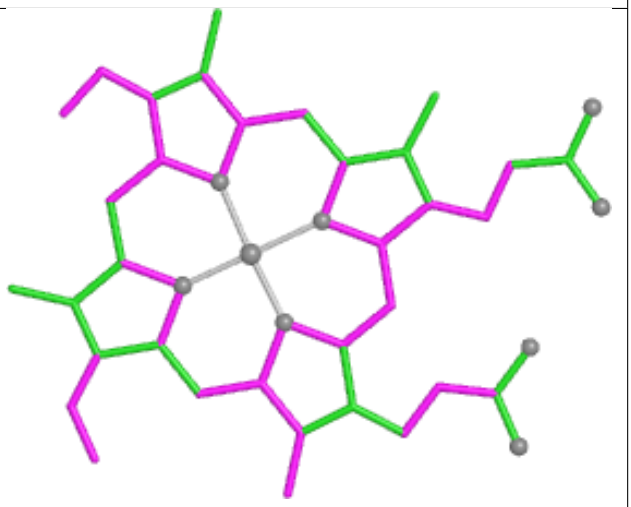


Rings

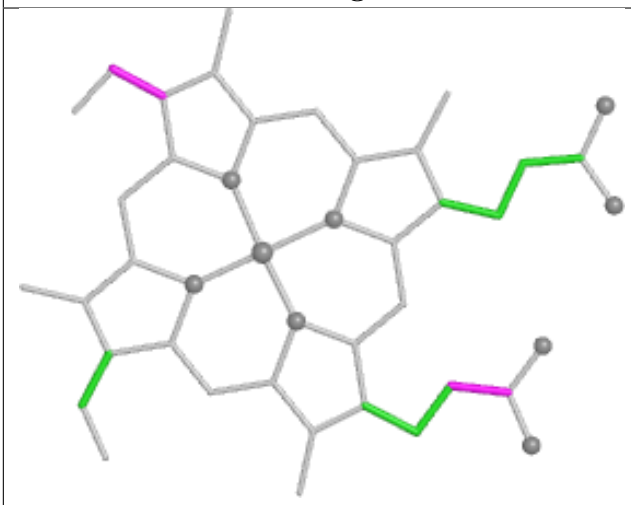
Ligand HEC V 202



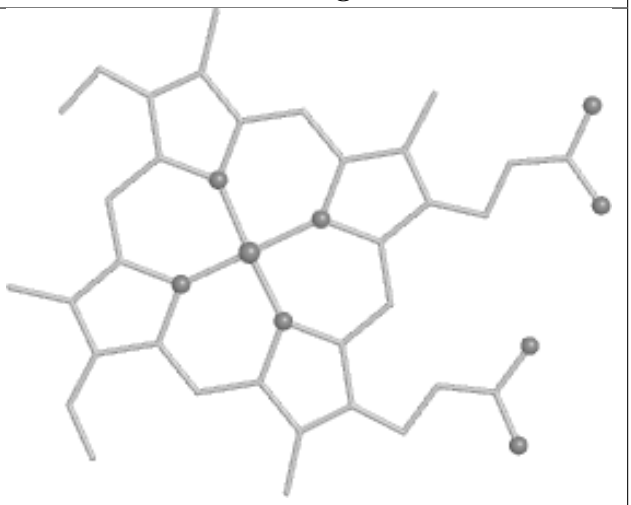
Bond lengths



Bond angles

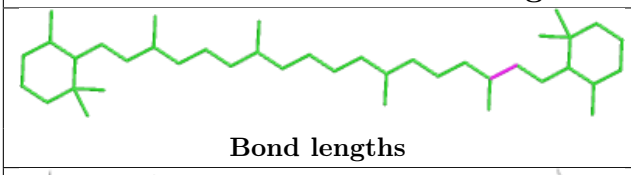


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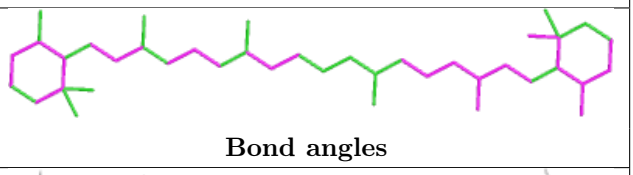


Rings

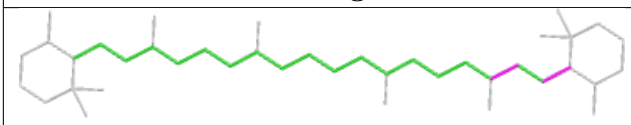
Ligand BCR b 619



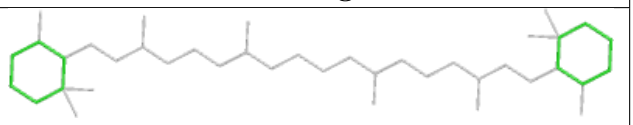
Bond lengths



Bond angles

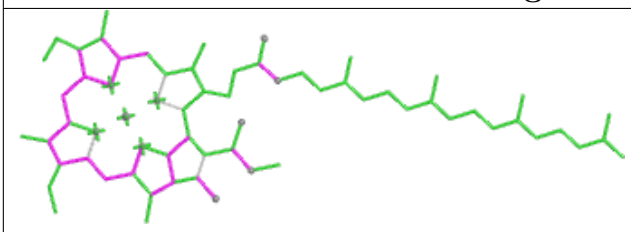


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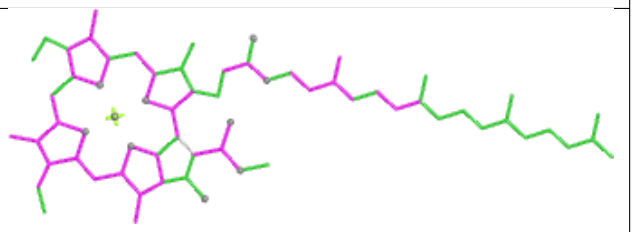


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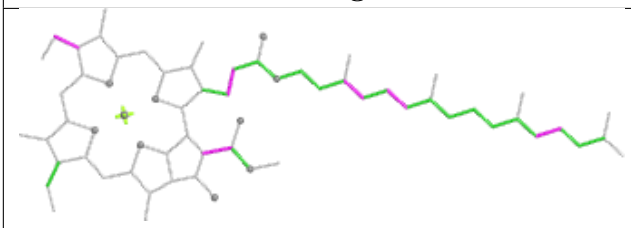
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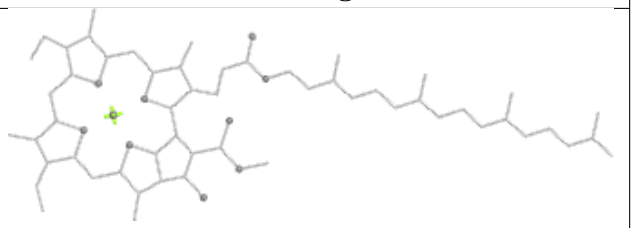
Bond lengths



Bond angles

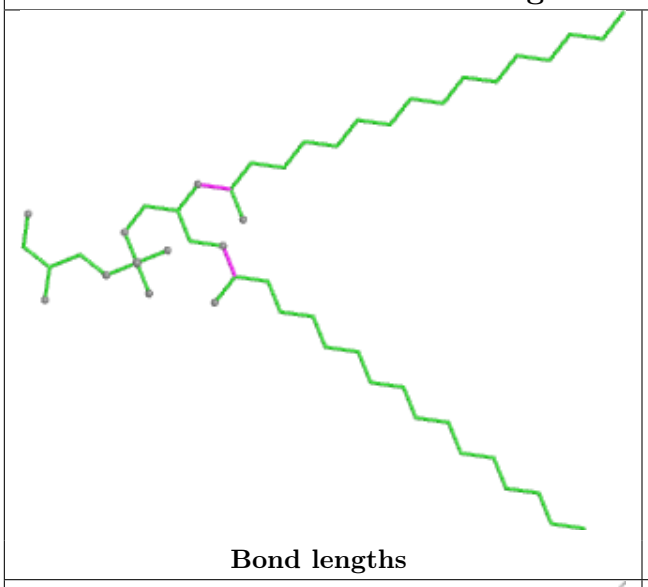


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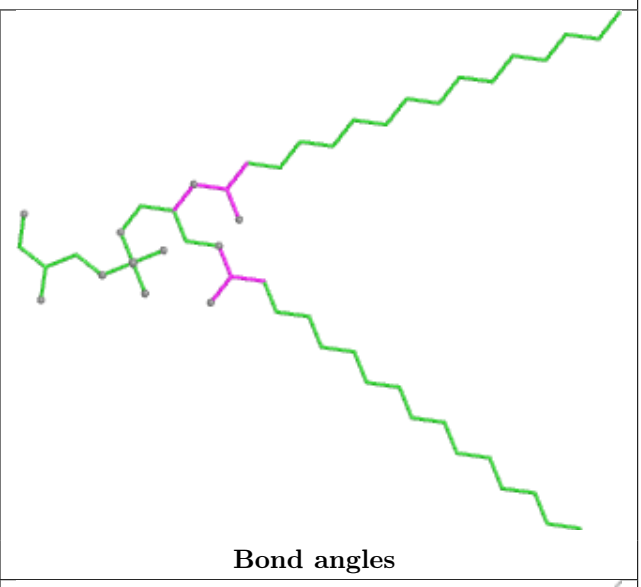


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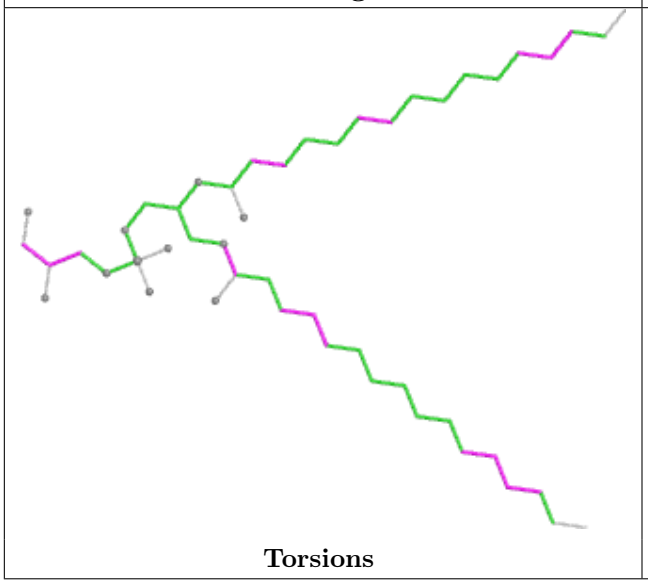
Ligand LHG d 407



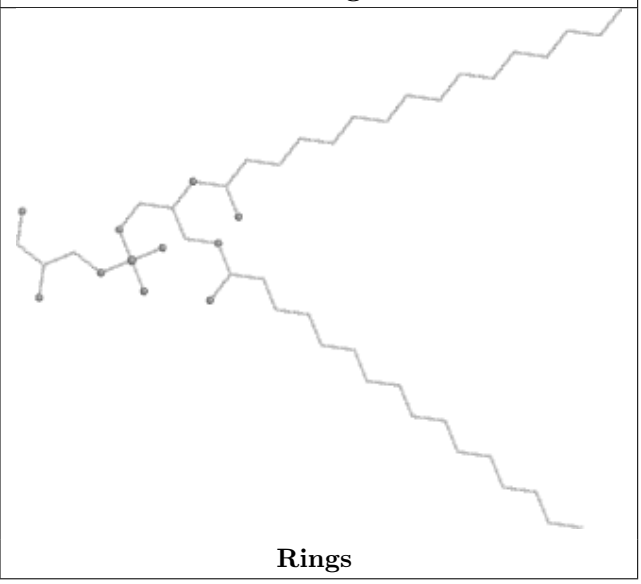
Bond lengths



Bond angles

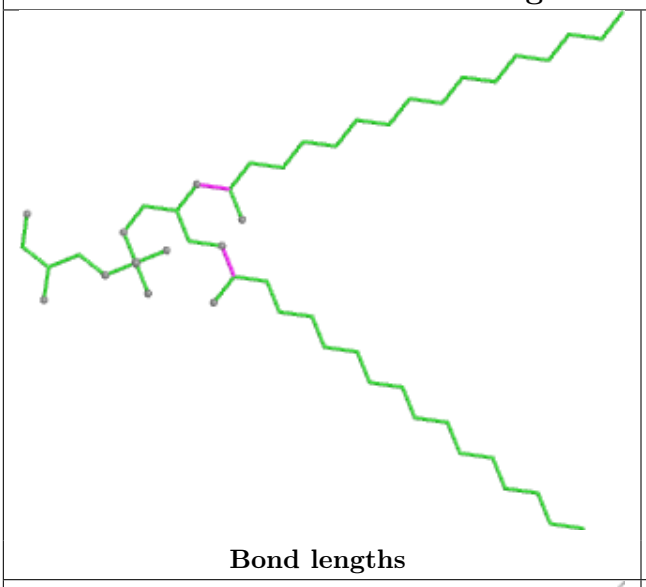


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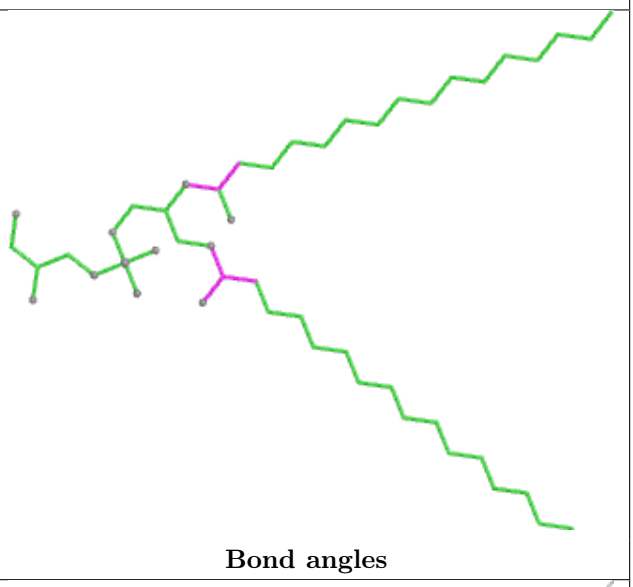


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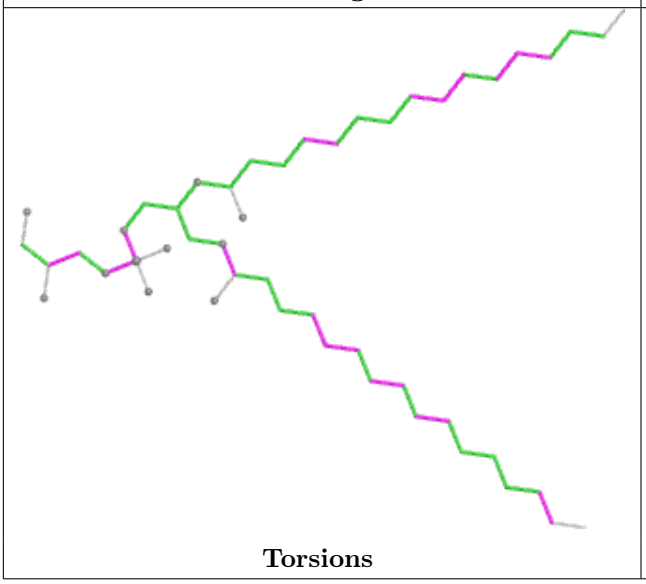
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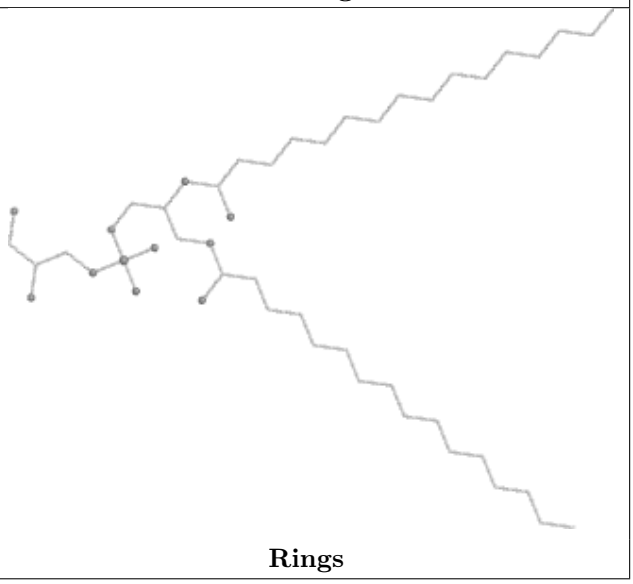
Bond lengths



Bond angles



Torsions

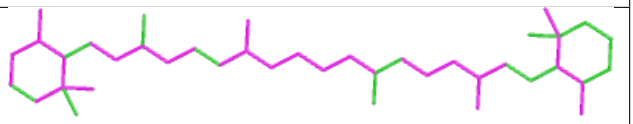


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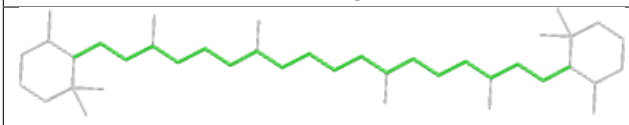
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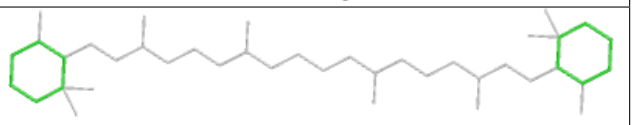
Bond lengths



Bond angles

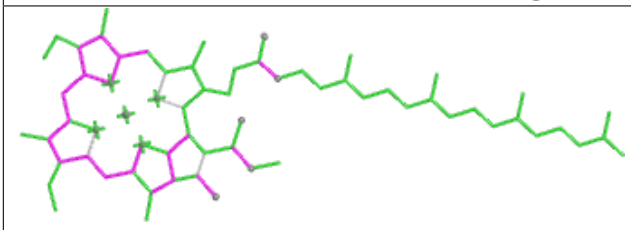


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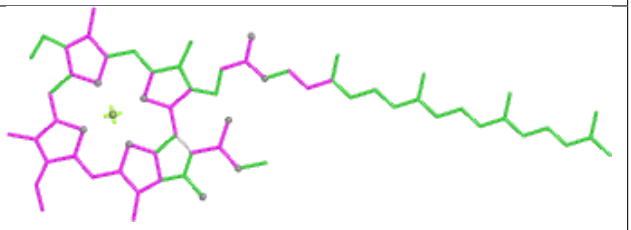


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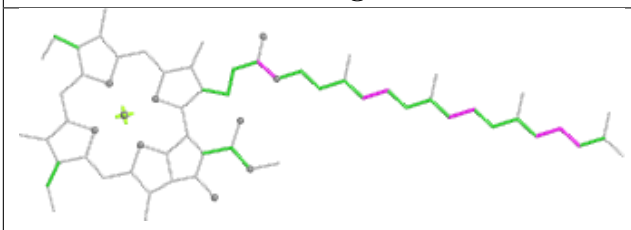
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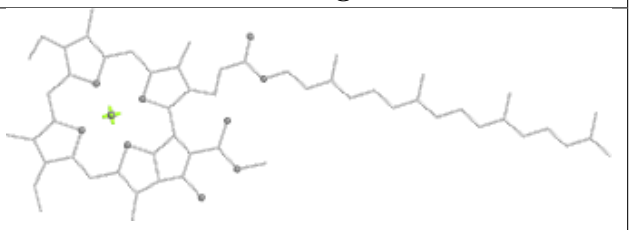
Bond lengths



Bond angles

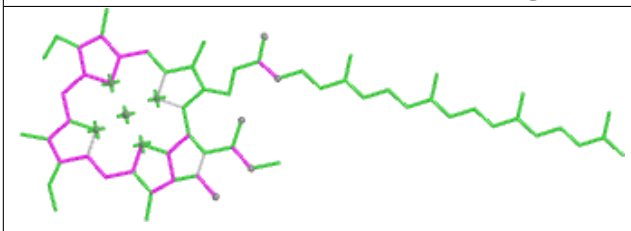


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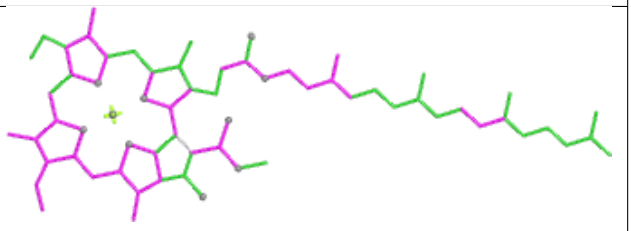


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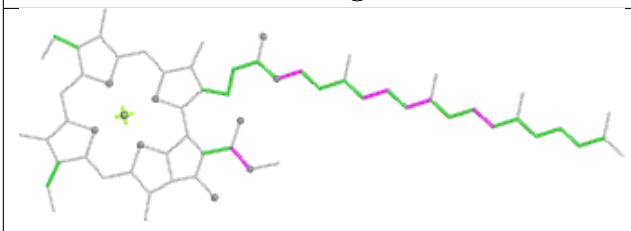
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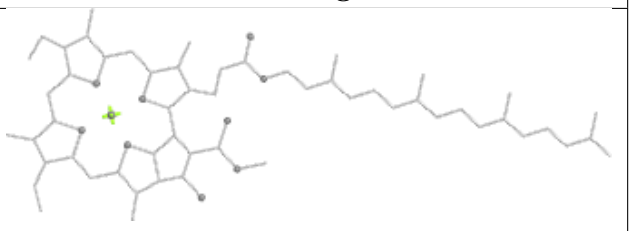
Bond lengths



Bond angles

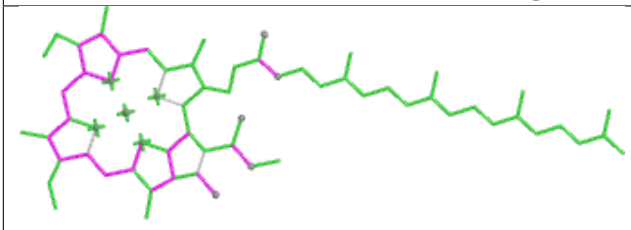


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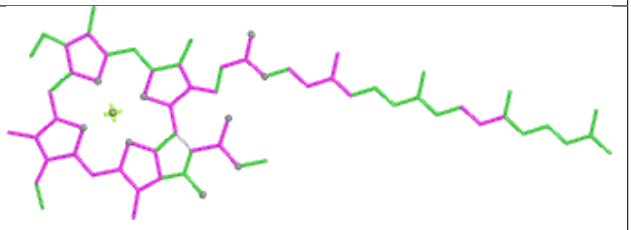


Rings

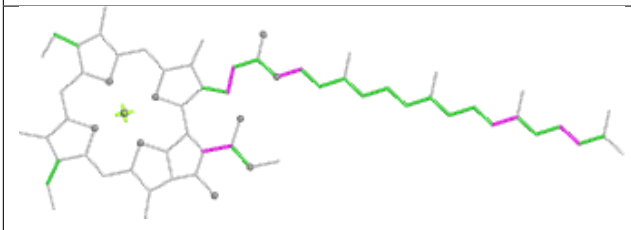
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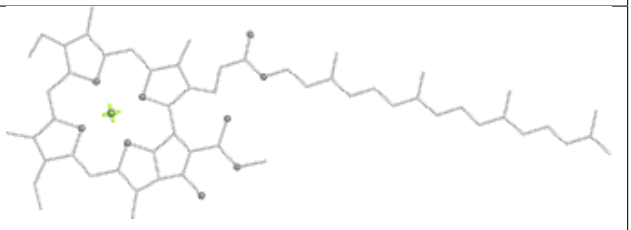
Bond lengths



Bond angles

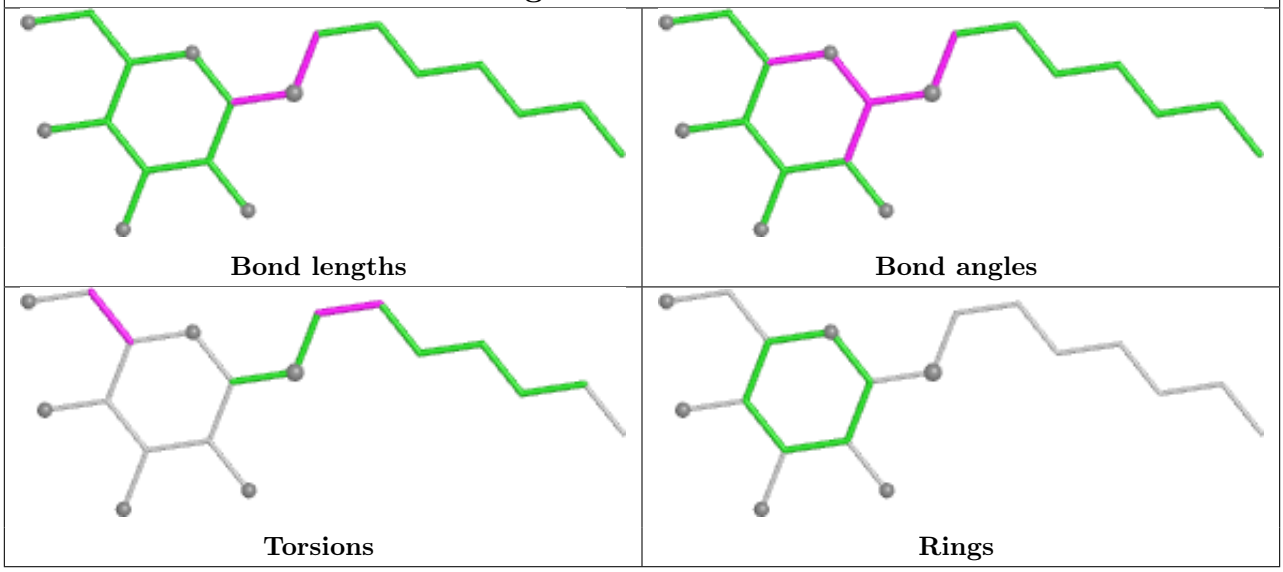


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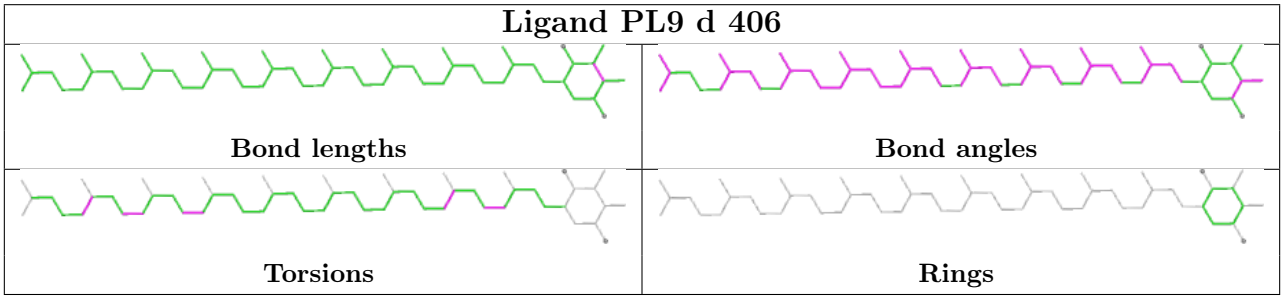


Rings

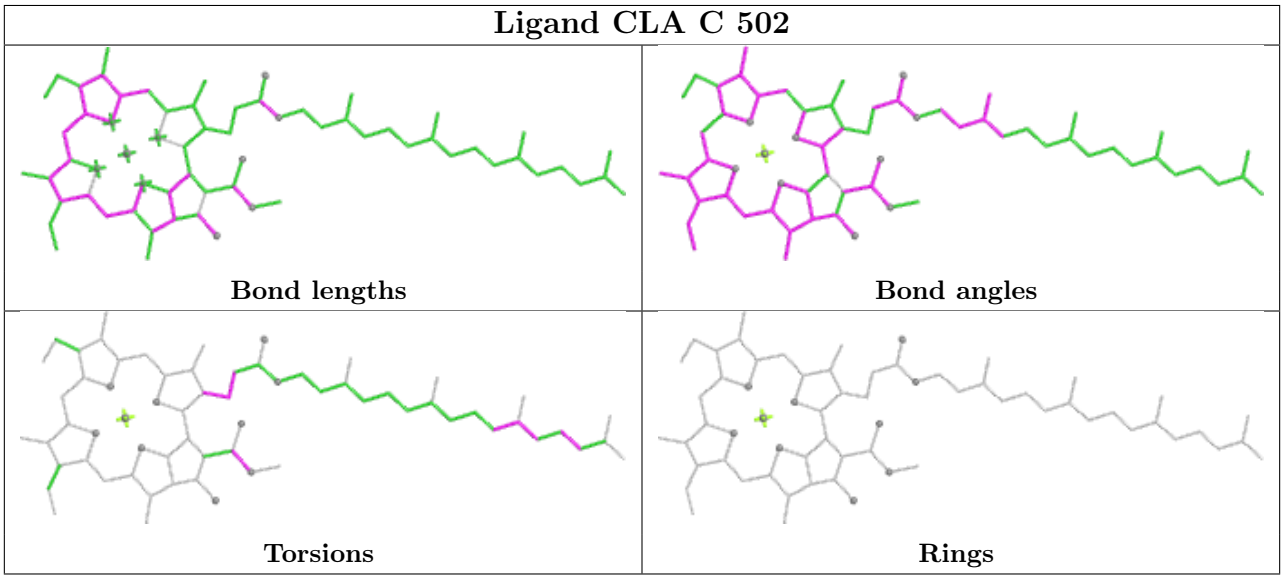
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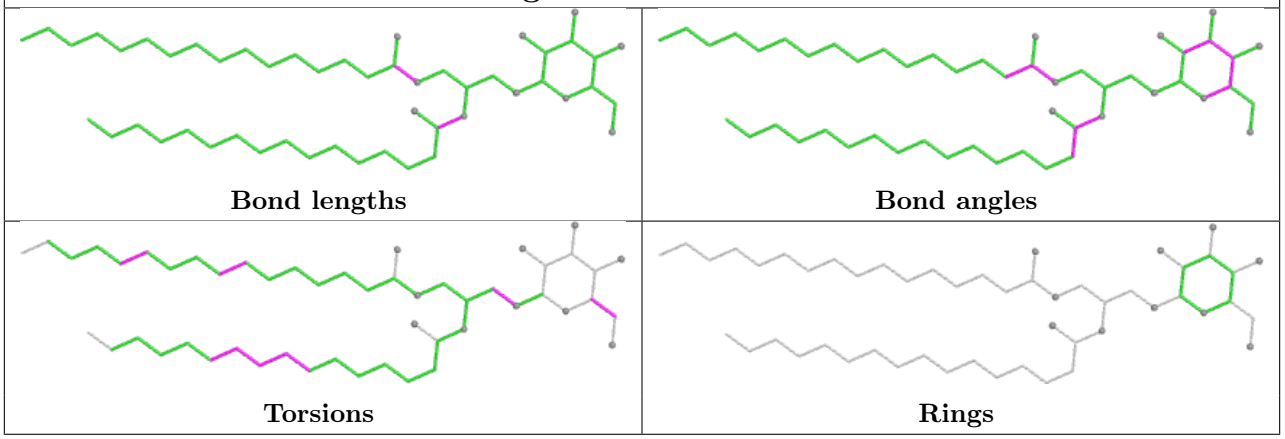
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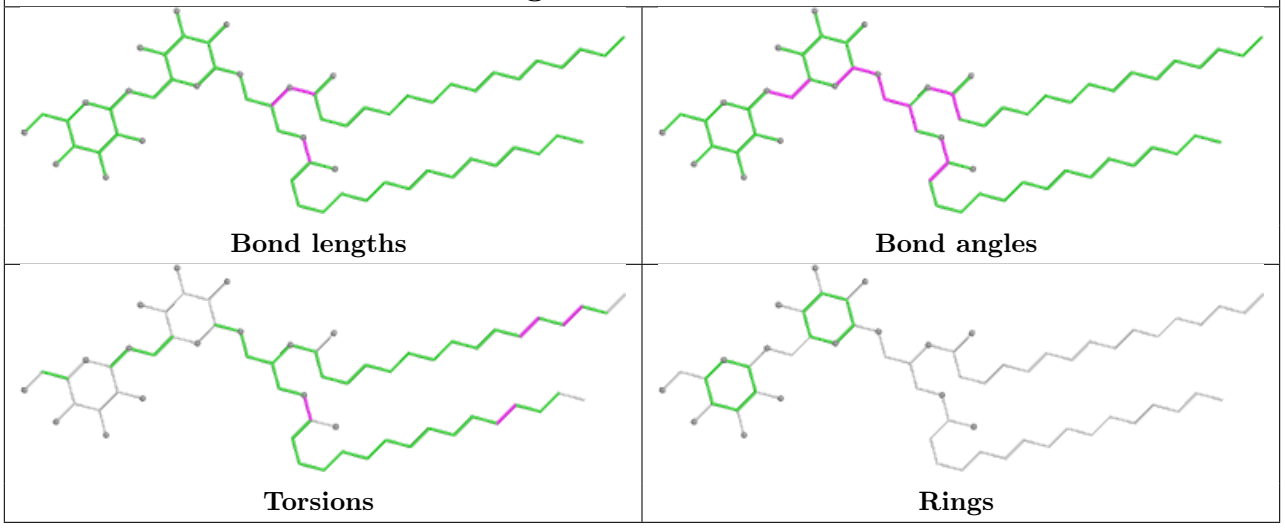
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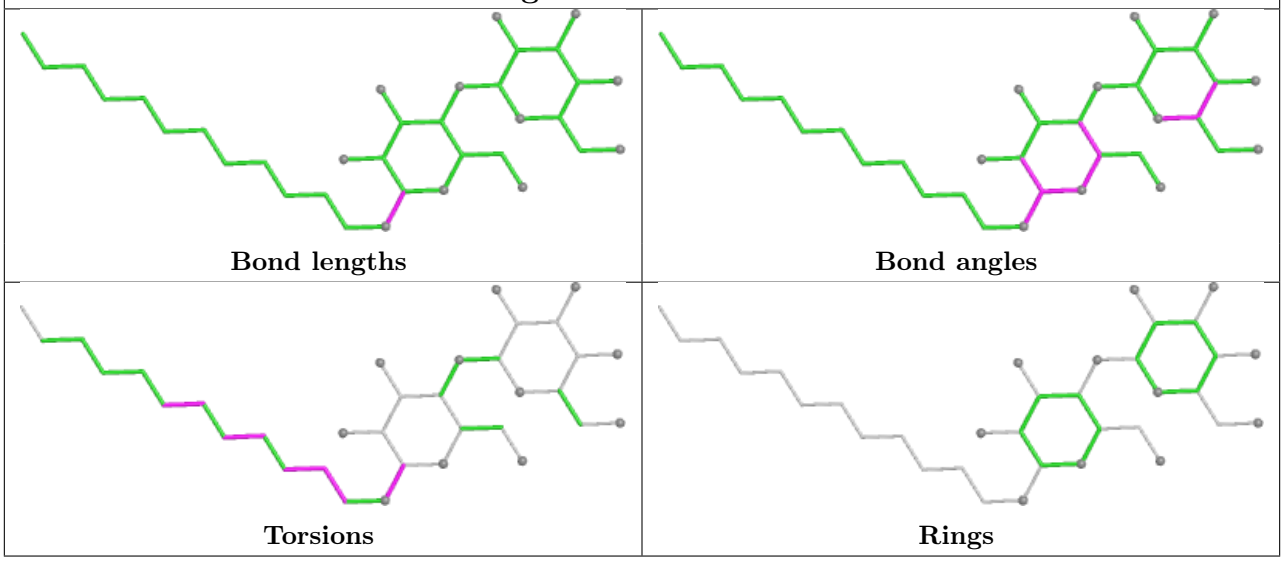
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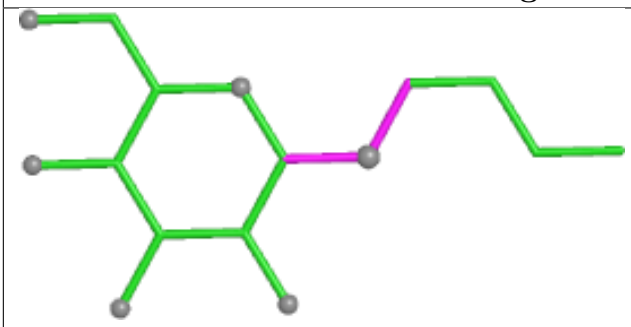
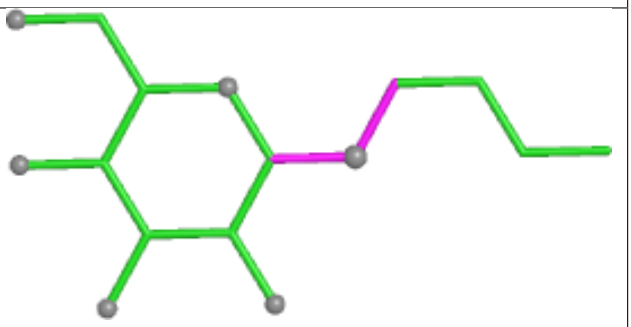
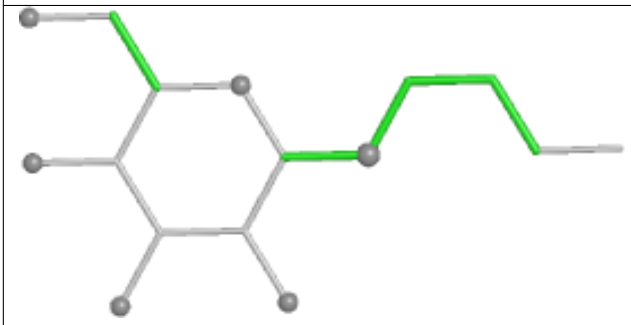
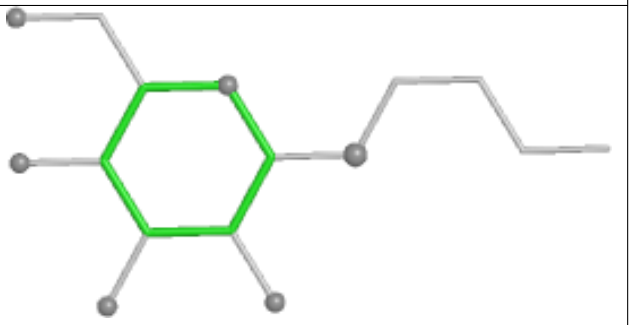


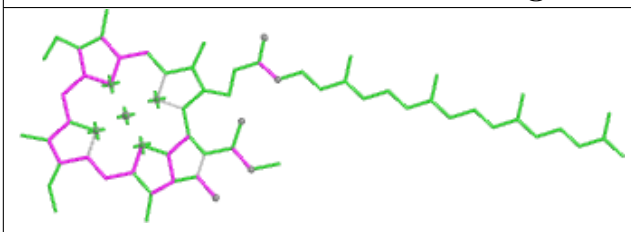
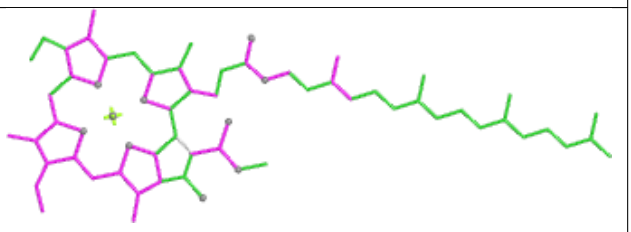
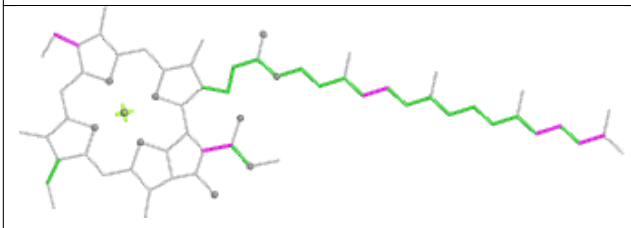
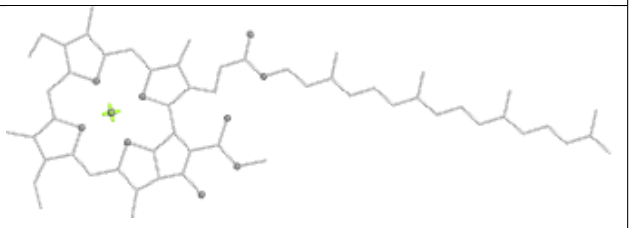
Ligand DGD c 518



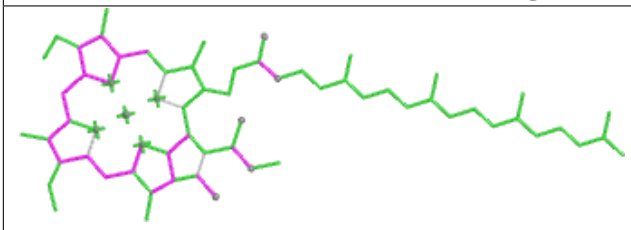
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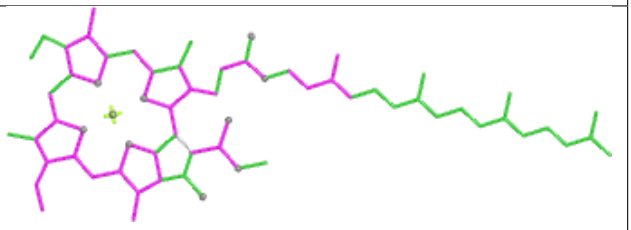
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

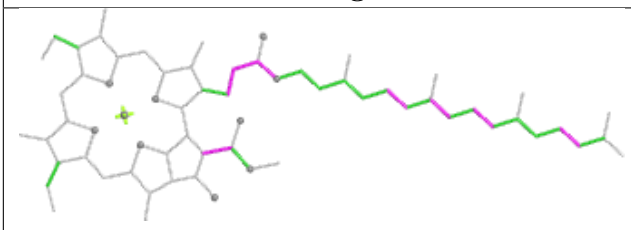
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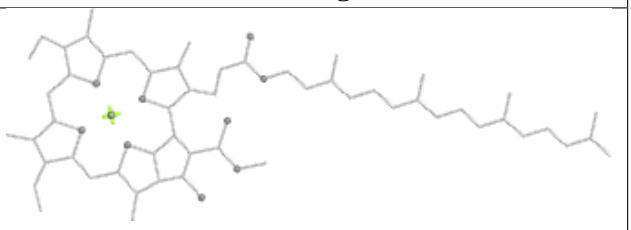
Bond lengths



Bond angles

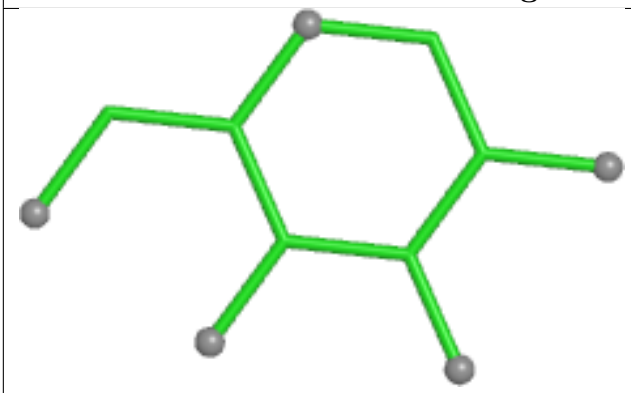


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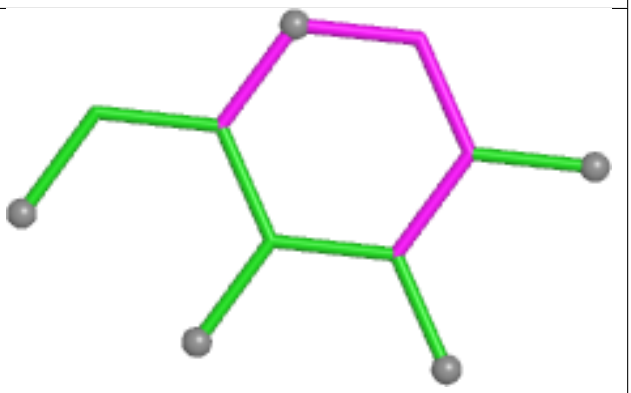


Rings

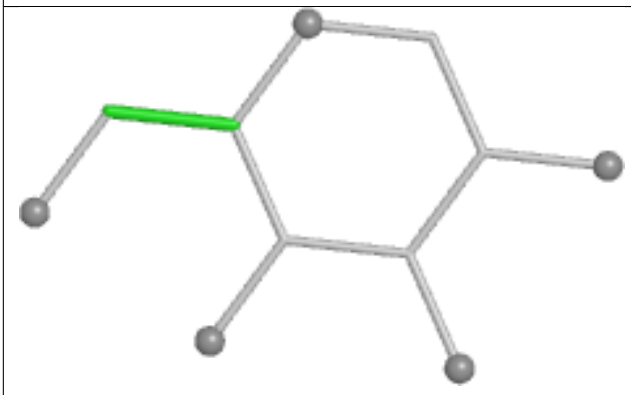
Ligand HTG V 203



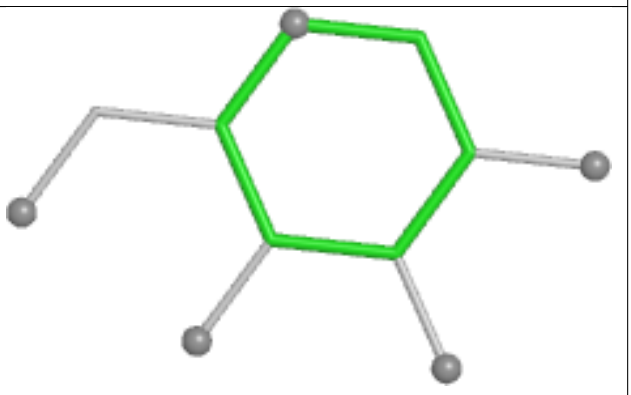
Bond lengths



Bond angles

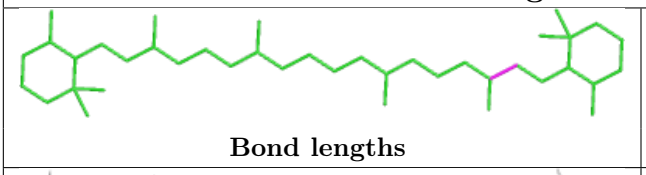


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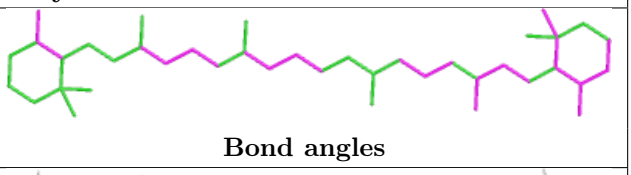


Rings

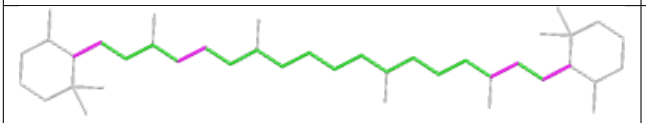
Ligand BCR y 101



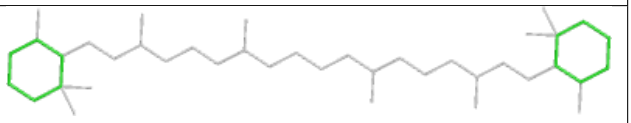
Bond lengths



Bond angles

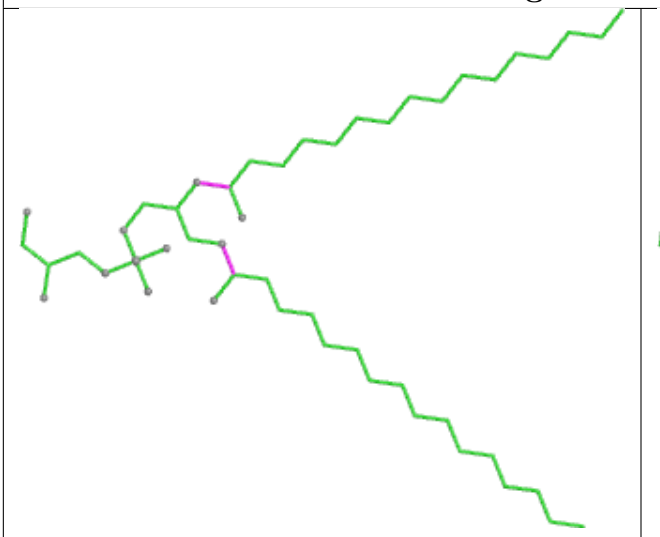


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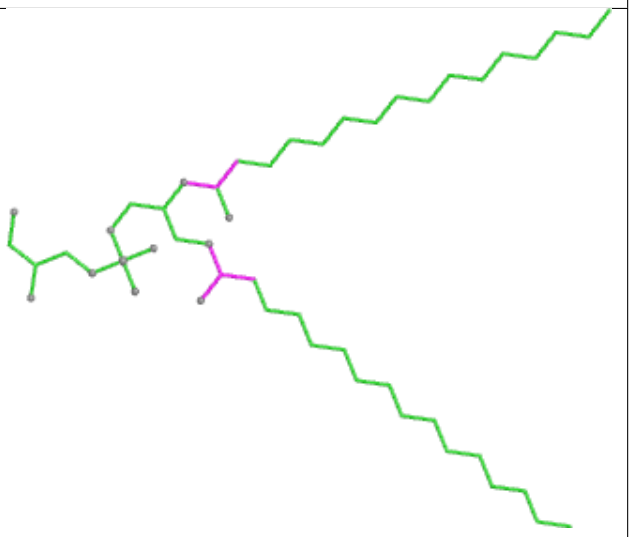


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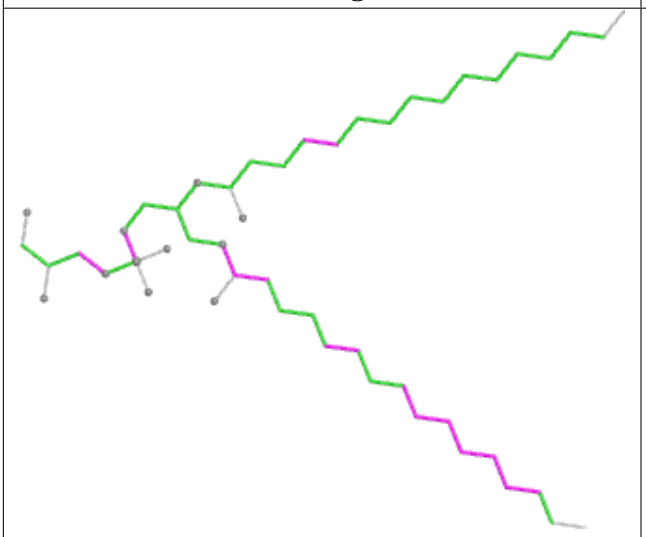
Ligand LHG d 409



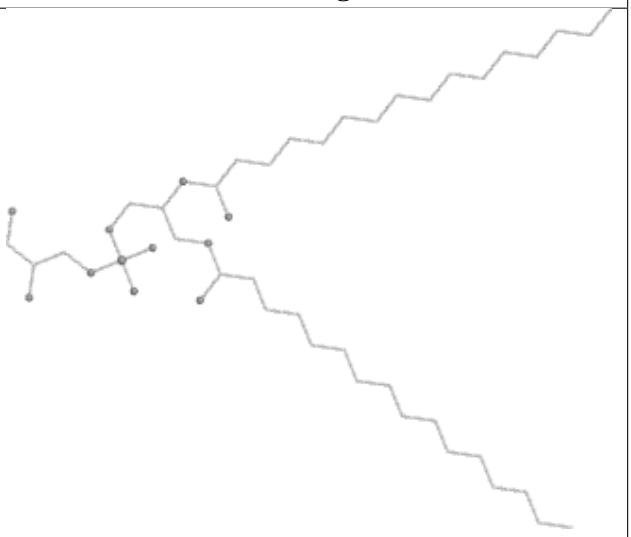
Bond lengths



Bond angles

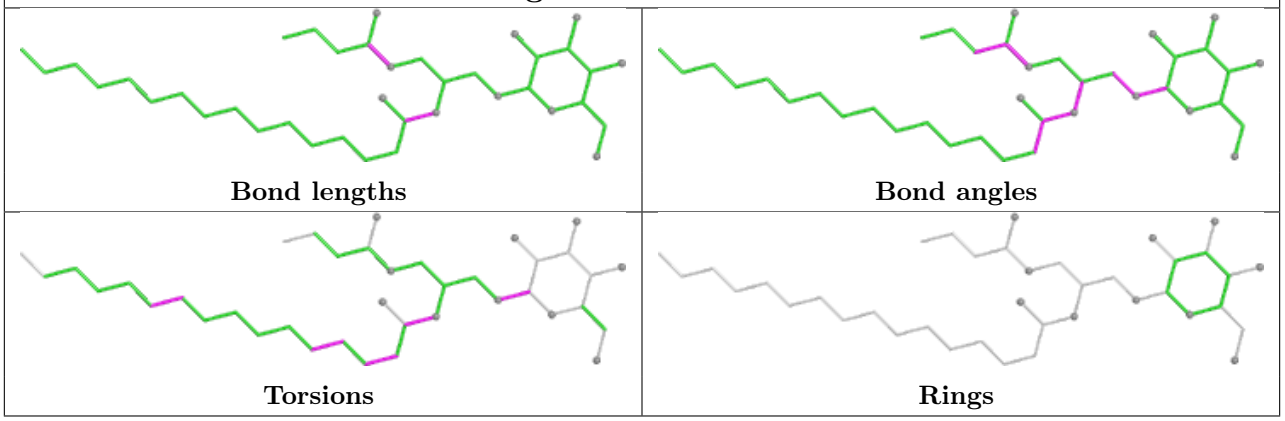


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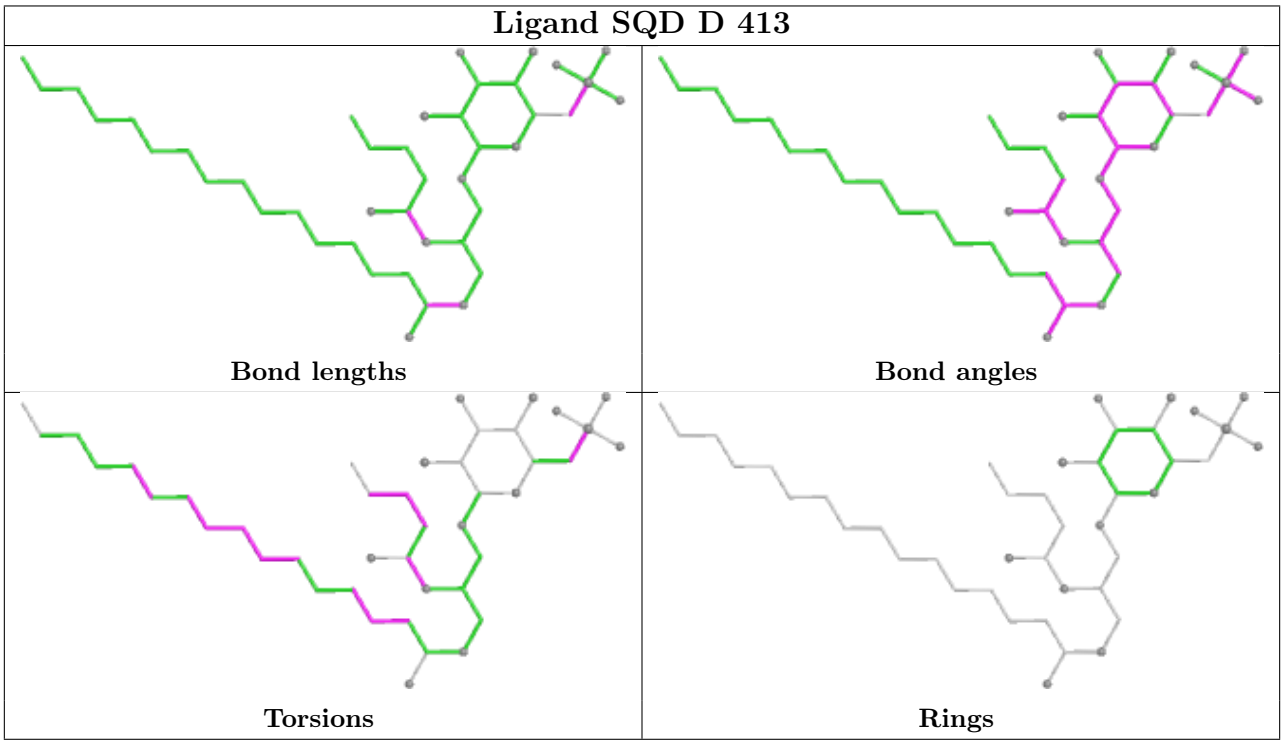


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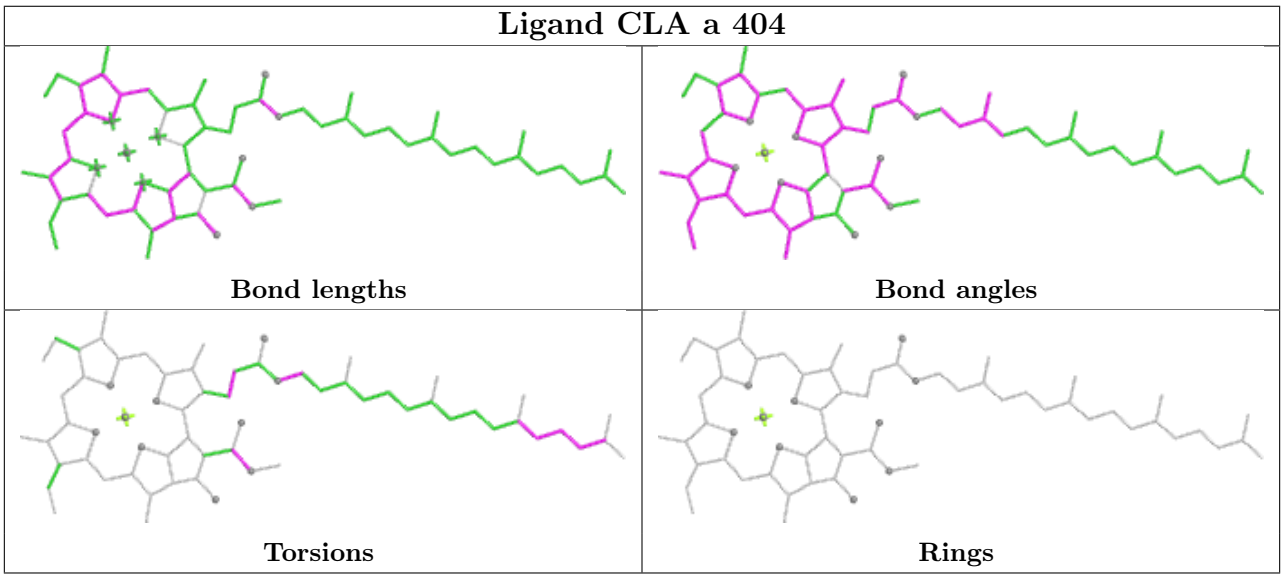
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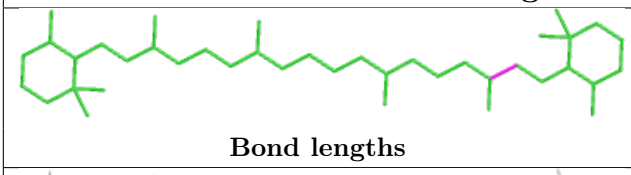
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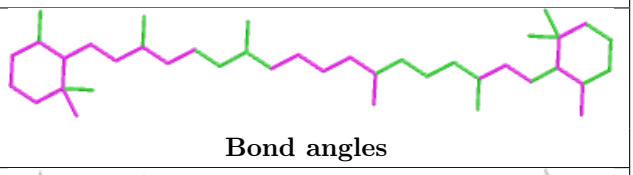
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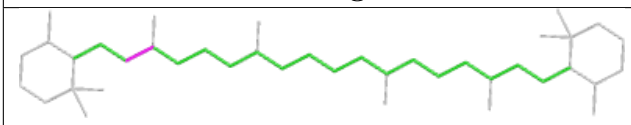
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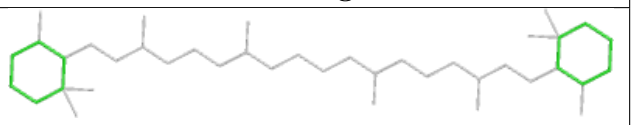
Bond lengths



Bond angles

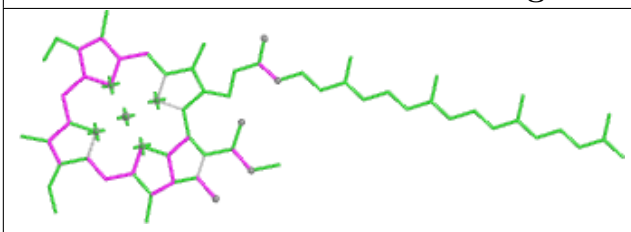


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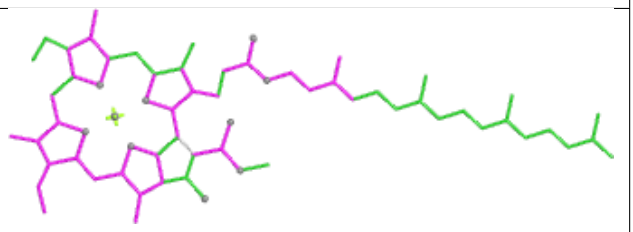


Rings

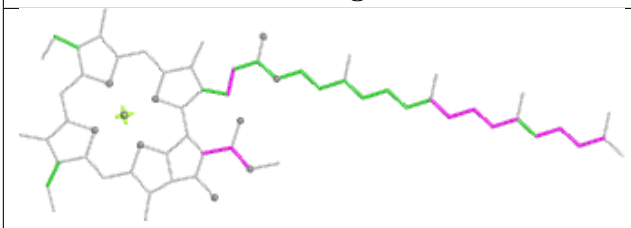
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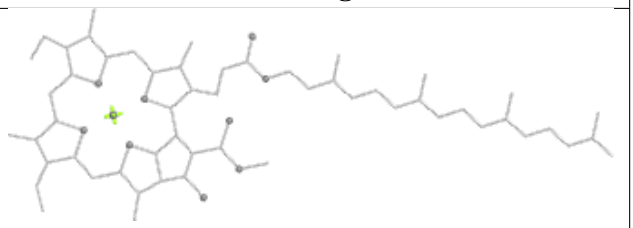
Bond lengths



Bond angles

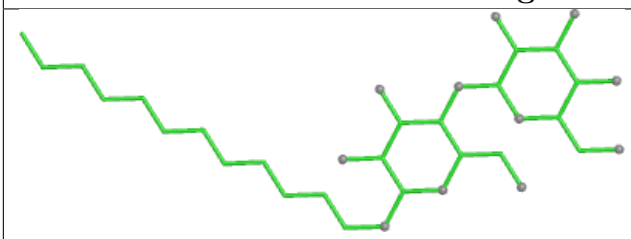


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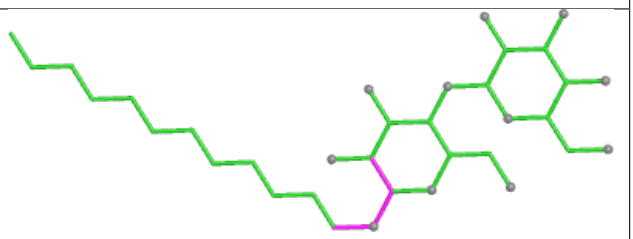


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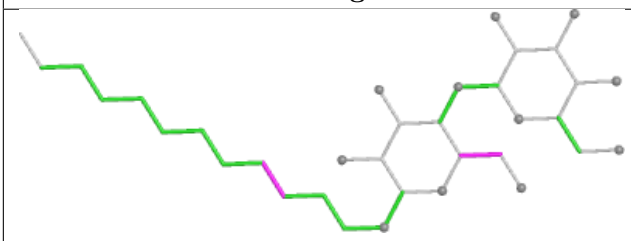
Ligand LMT M 101



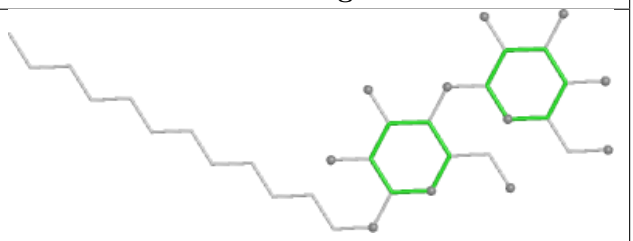
Bond lengths



Bond angles

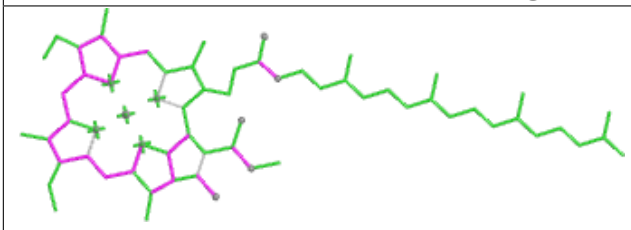


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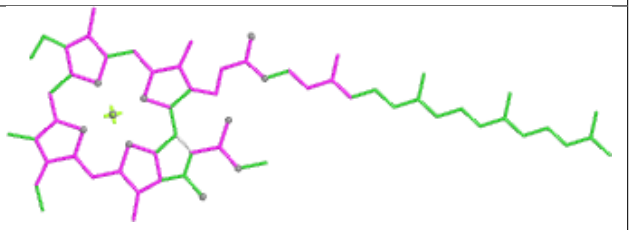


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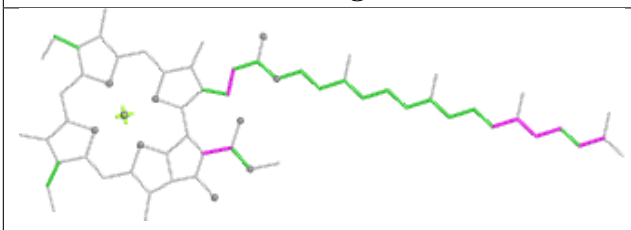
Ligand CLA B 610



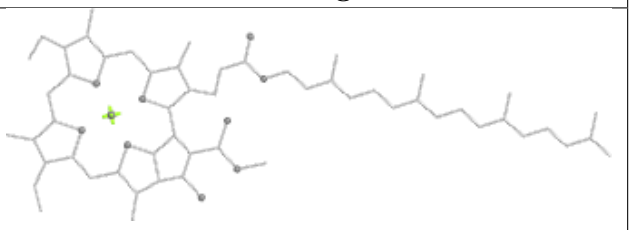
Bond lengths



Bond angles



Torsions



Rings

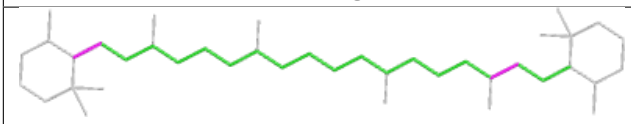
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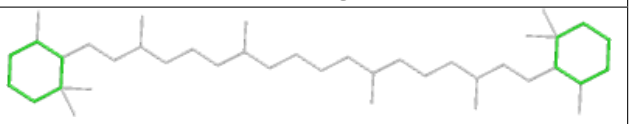
Bond lengths



Bond angles

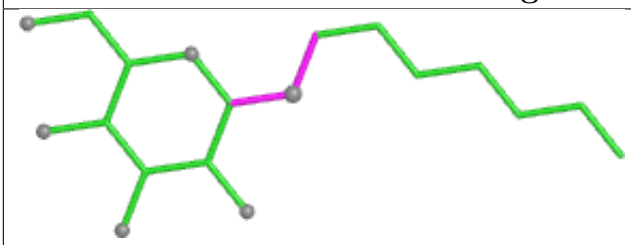


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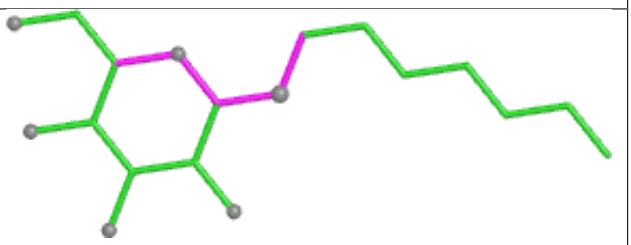


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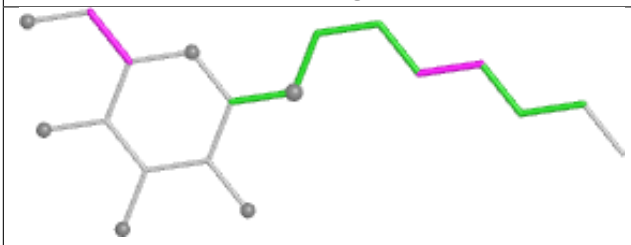
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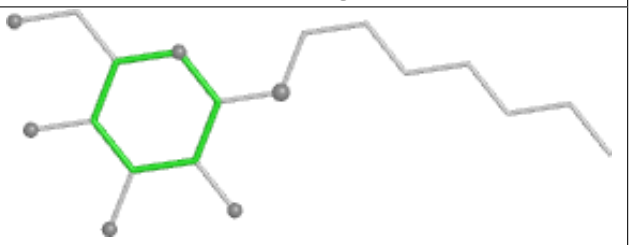
Bond lengths



Bond angles

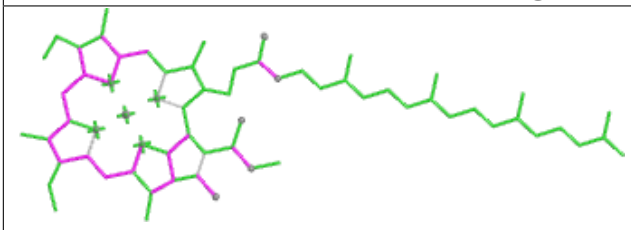


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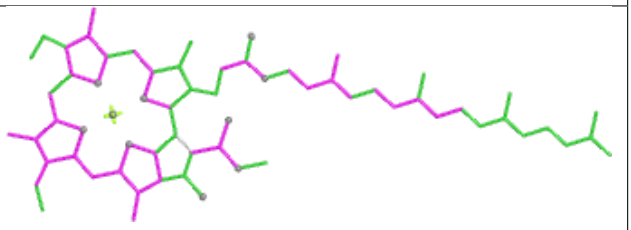


Rings

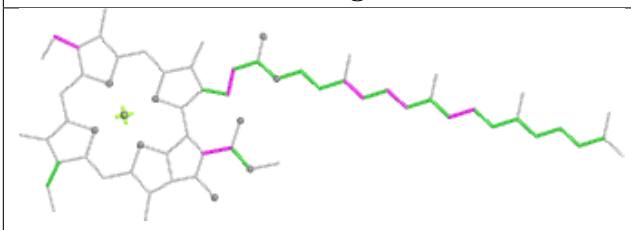
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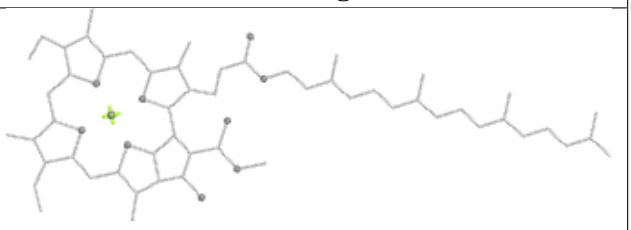
Bond lengths



Bond angles

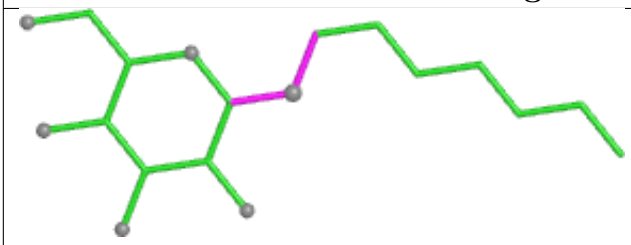


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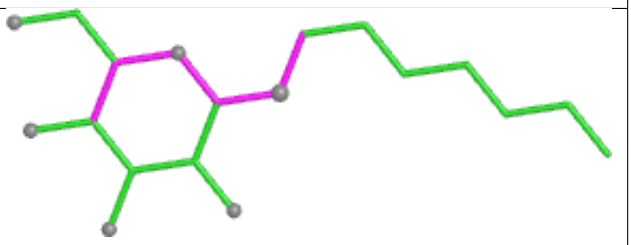


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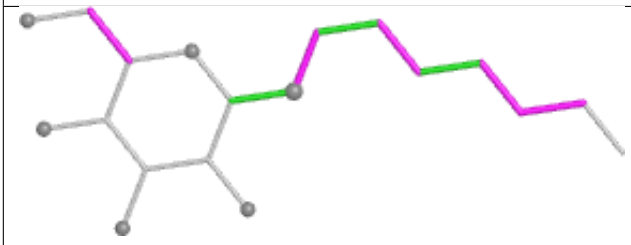
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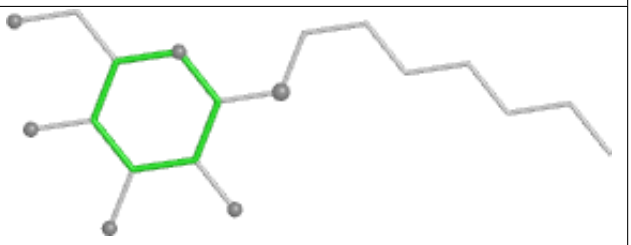
Bond lengths



Bond angles

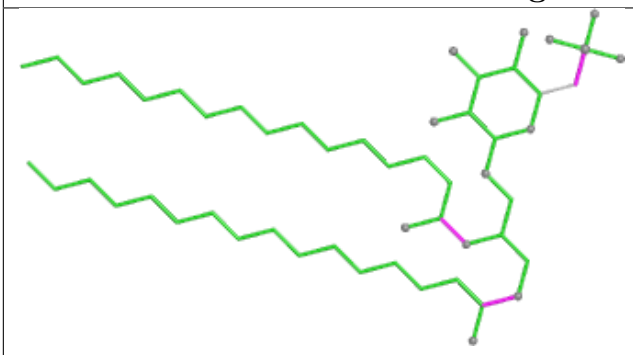


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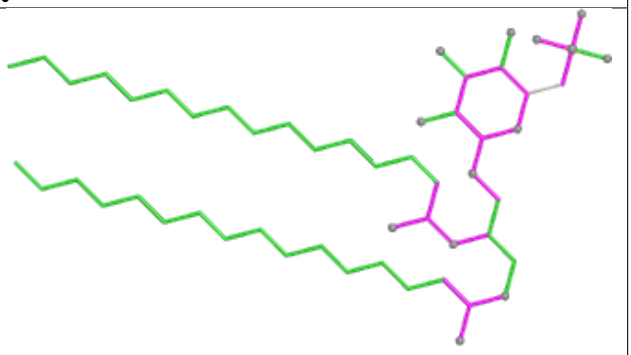


Rings

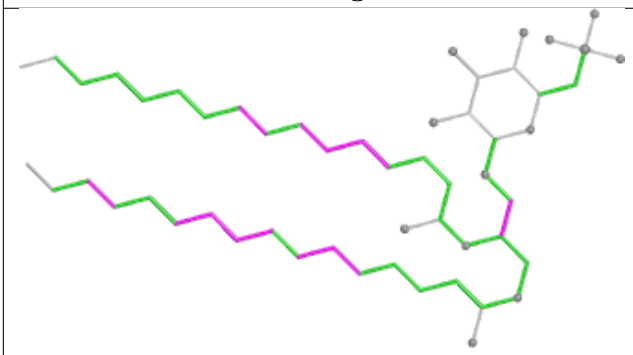
Ligand SQD a 410



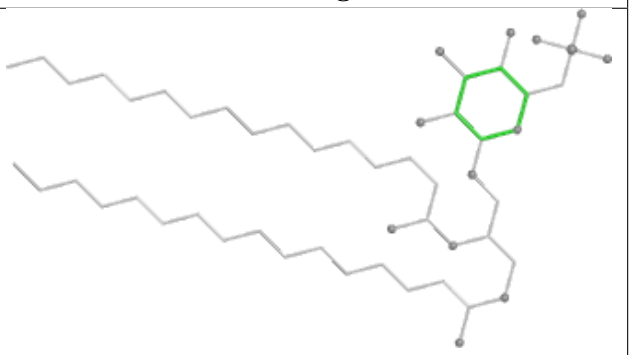
Bond lengths



Bond angles

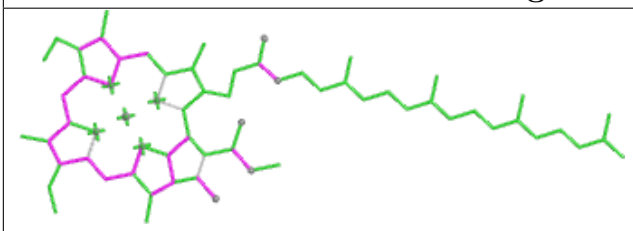


Torsions

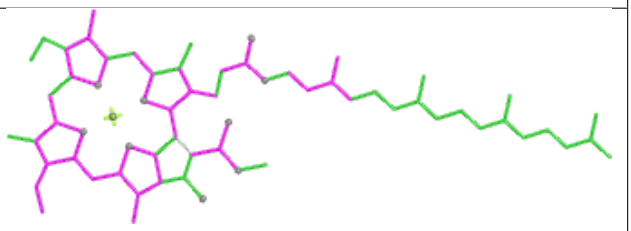


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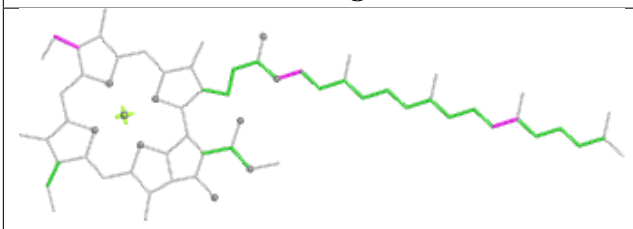
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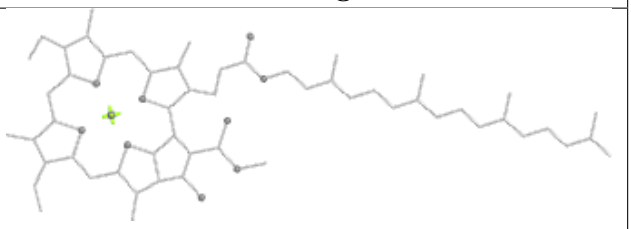
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Bond angles

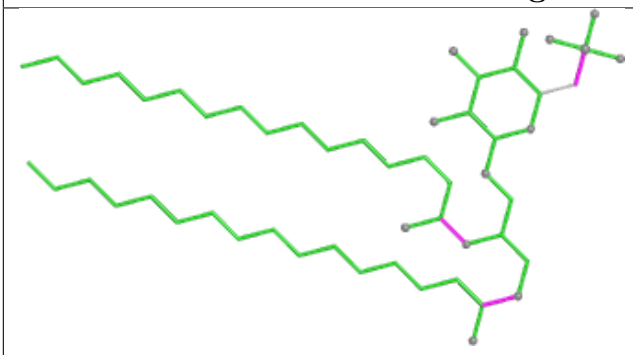


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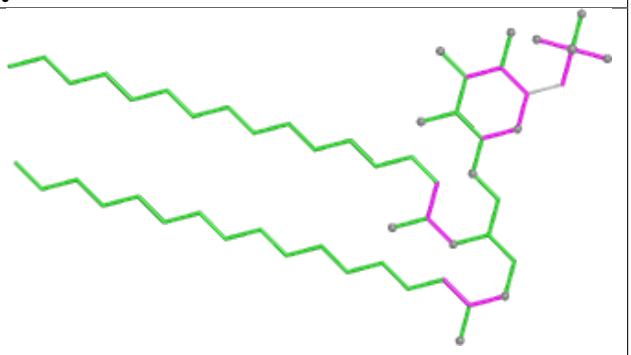


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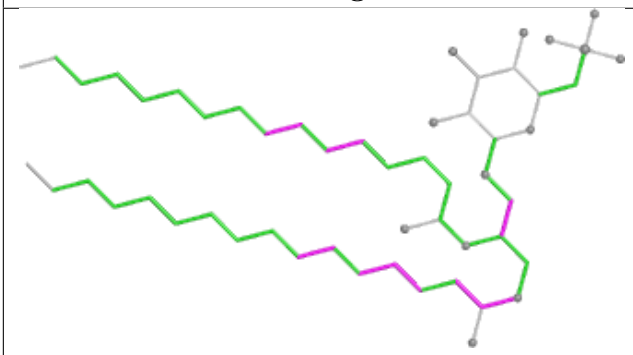
Ligand SQD a 412



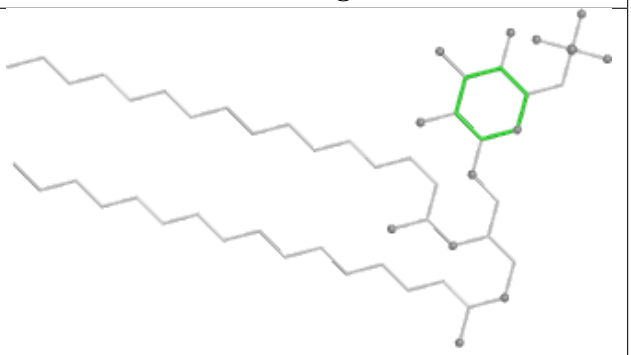
Bond lengths



Bond angles

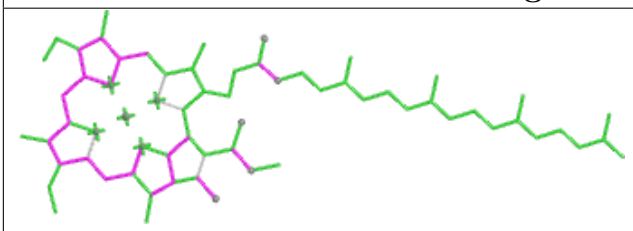


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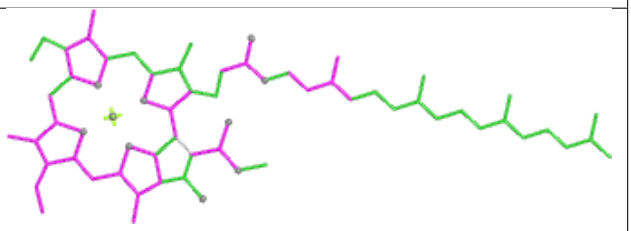


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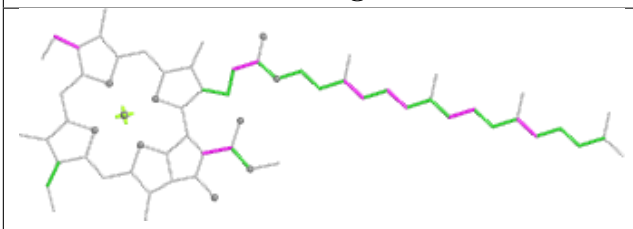
Ligand CLA C 506



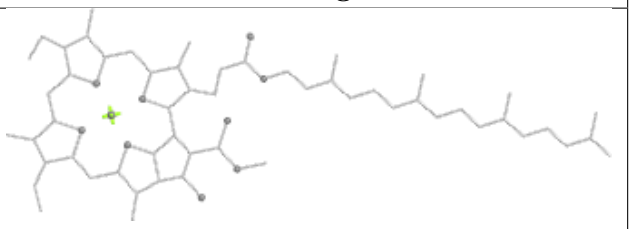
Bond lengths



Bond angles

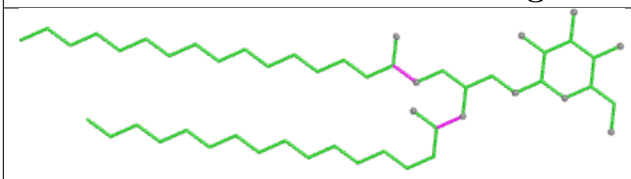


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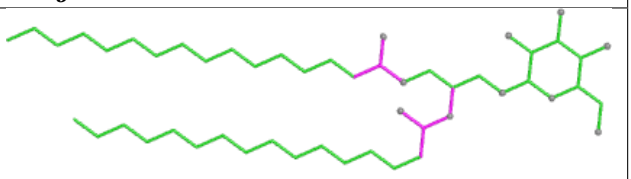


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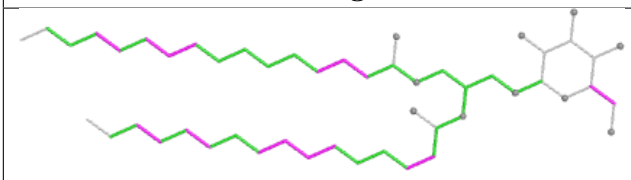
Ligand LMG j 101



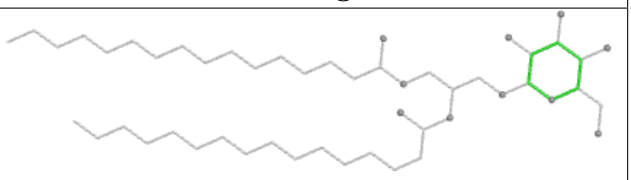
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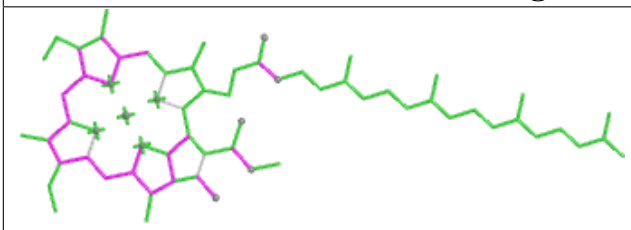


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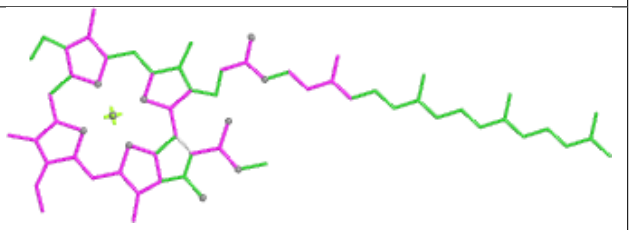


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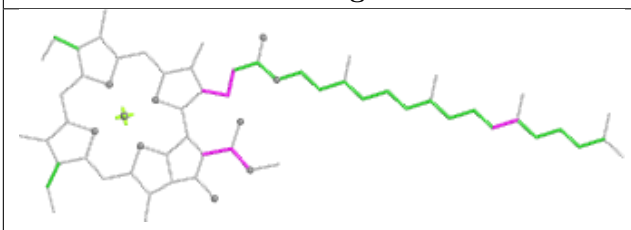
Ligand CLA c 501



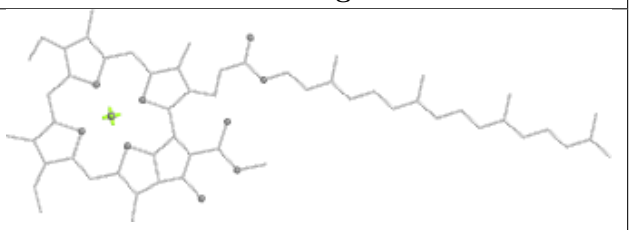
Bond lengths



Bond angles

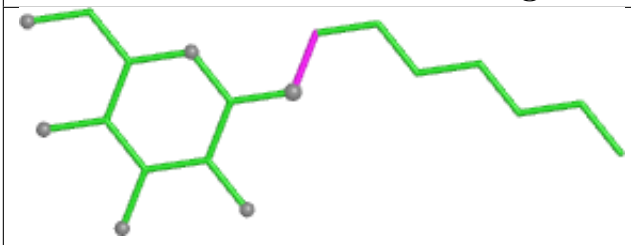


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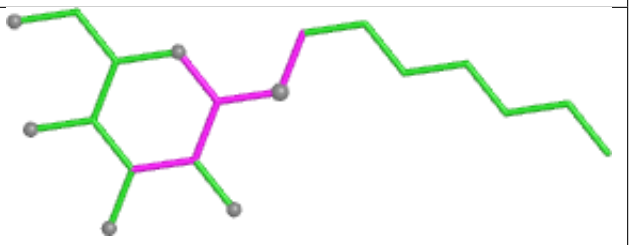


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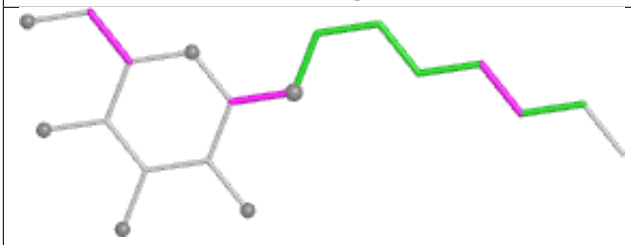
Ligand HTG B 624



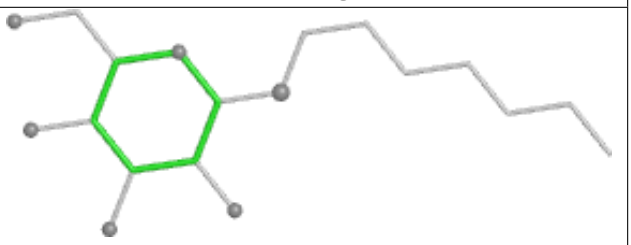
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Bond angles

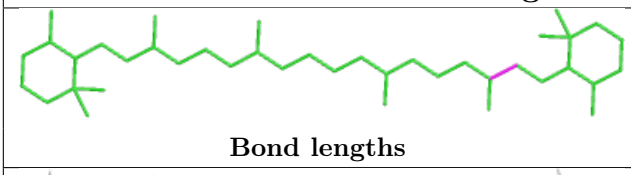


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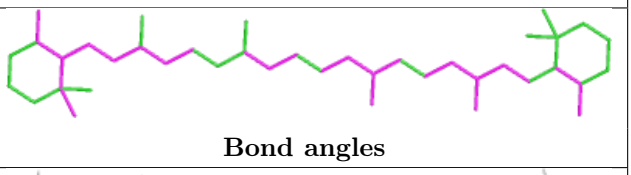


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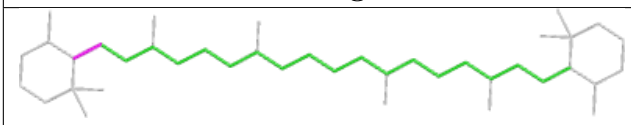
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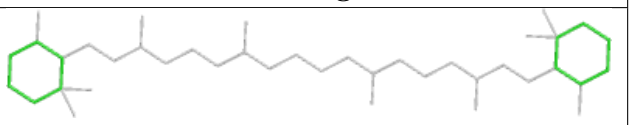
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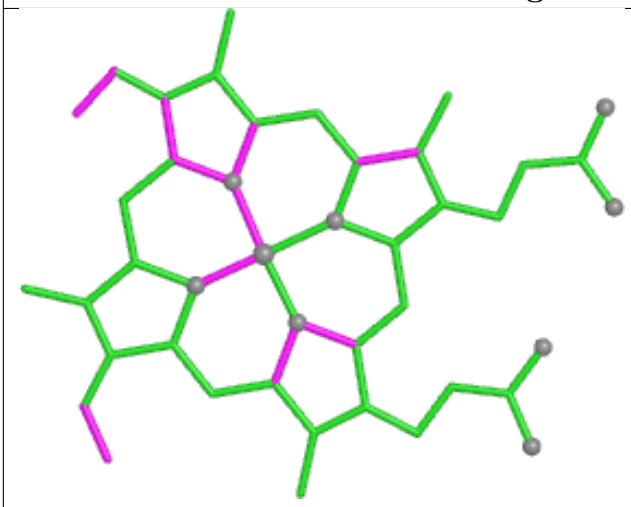


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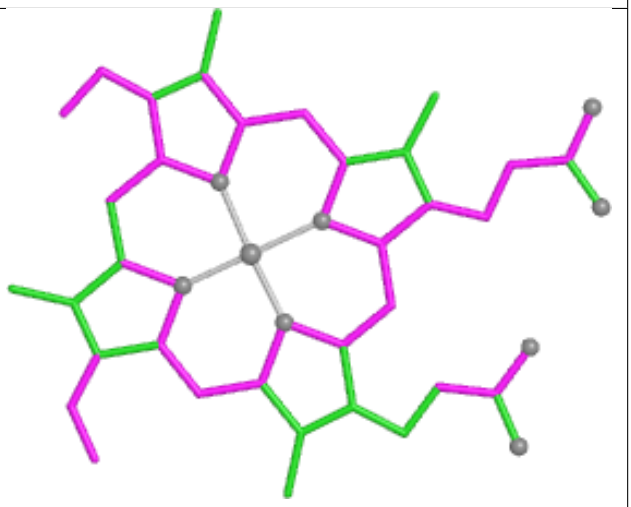


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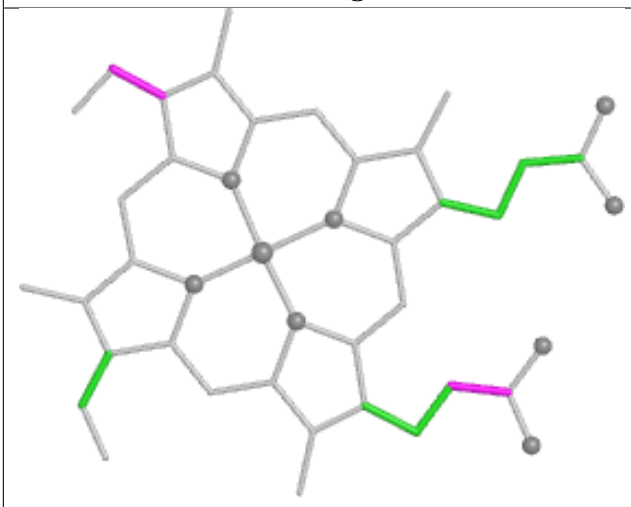
Ligand HEC v 201



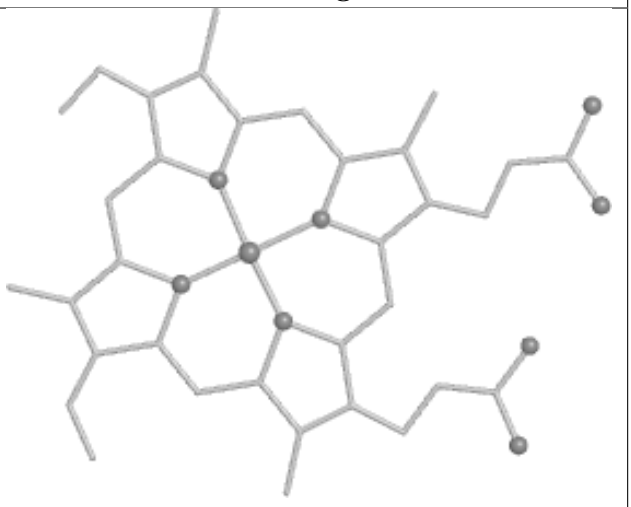
Bond lengths



Bond angles

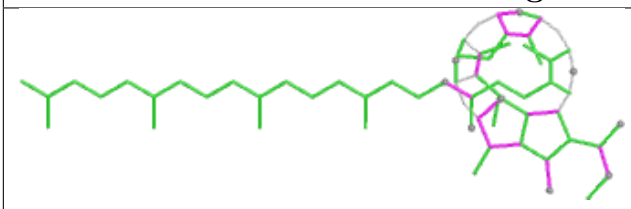


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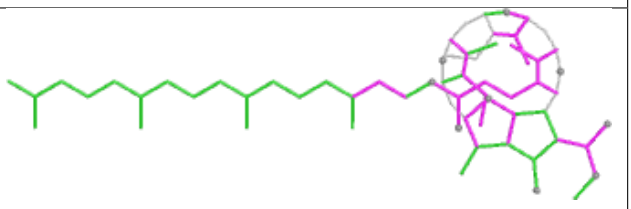


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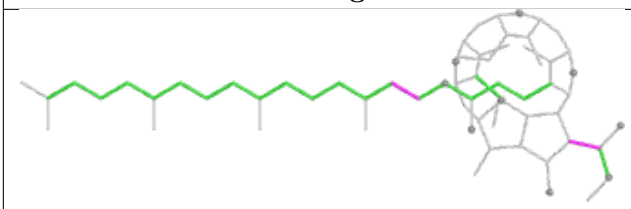
Ligand PHO a 406



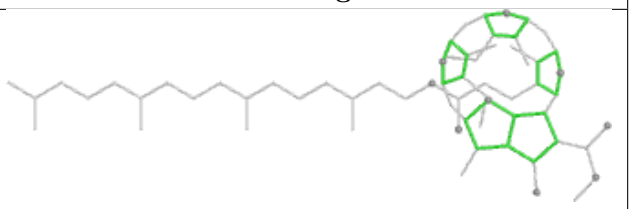
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Bond angles

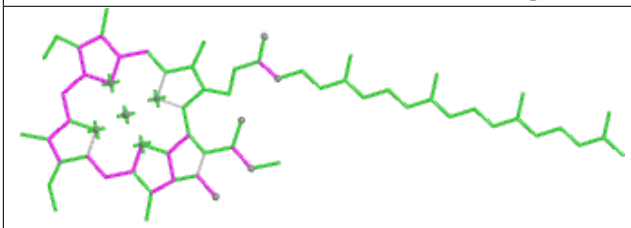


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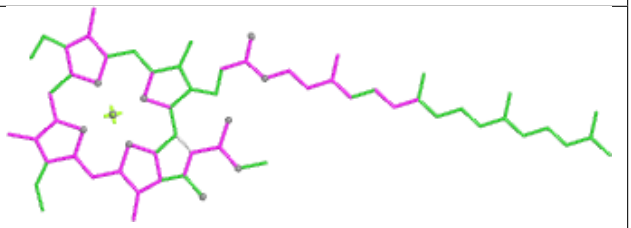


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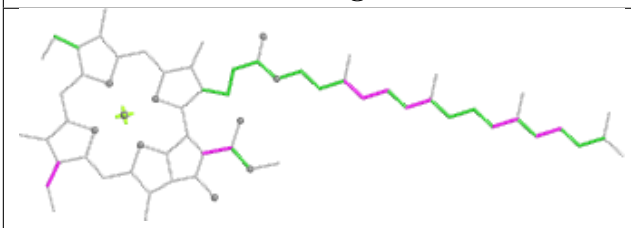
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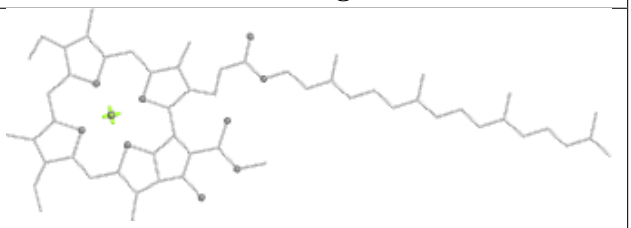
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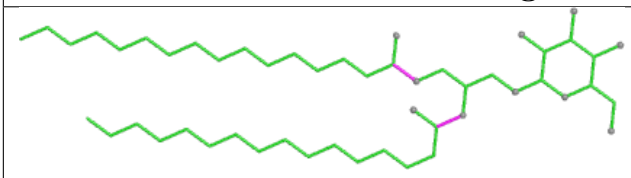


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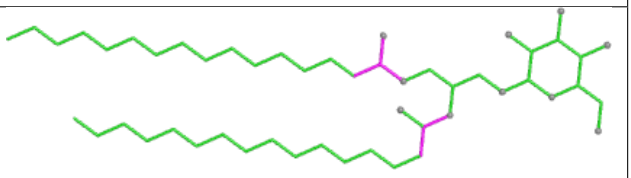


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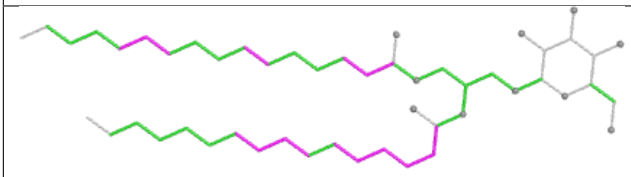
Ligand LMG C 520



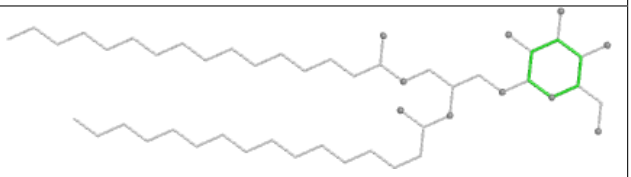
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Bond angles

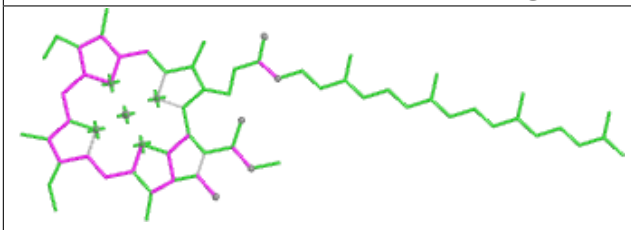


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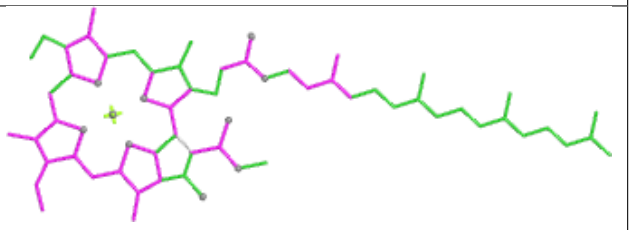


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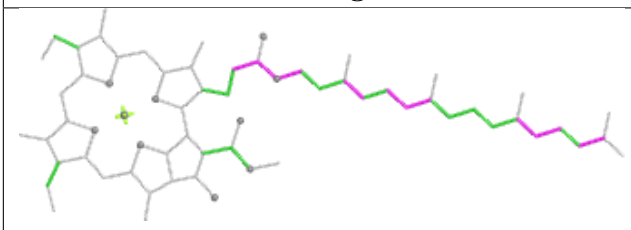
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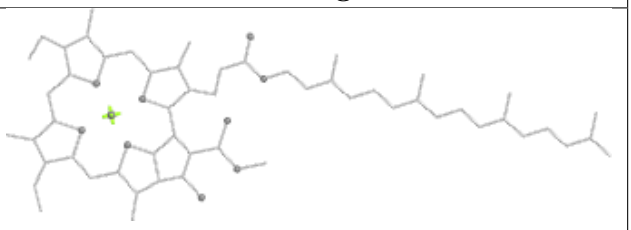
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Bond angles



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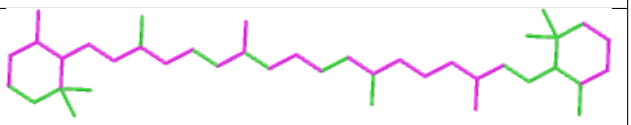


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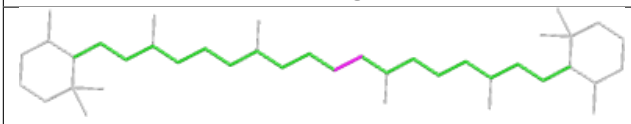
Ligand BCR t 101



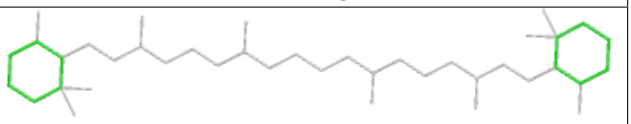
Bond lengths



Bond angles

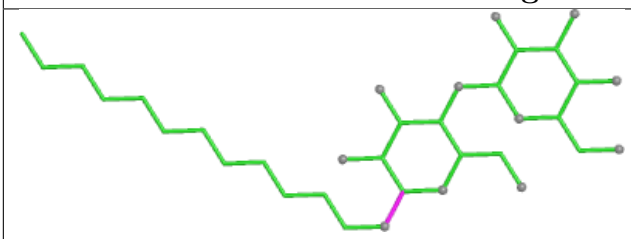


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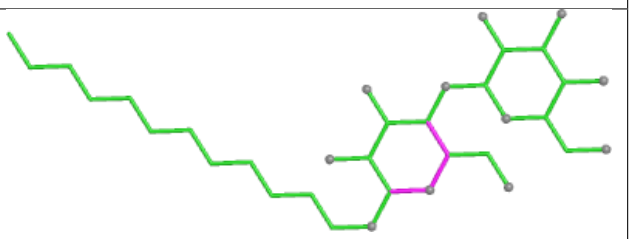


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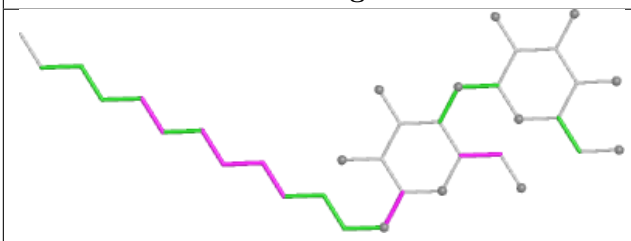
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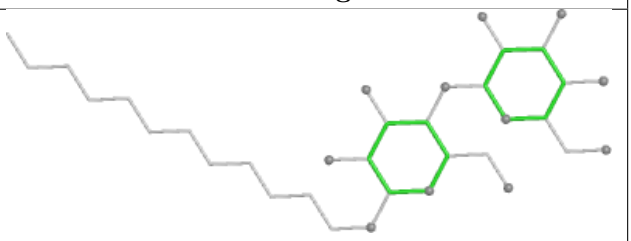
Bond lengths



Bond angles

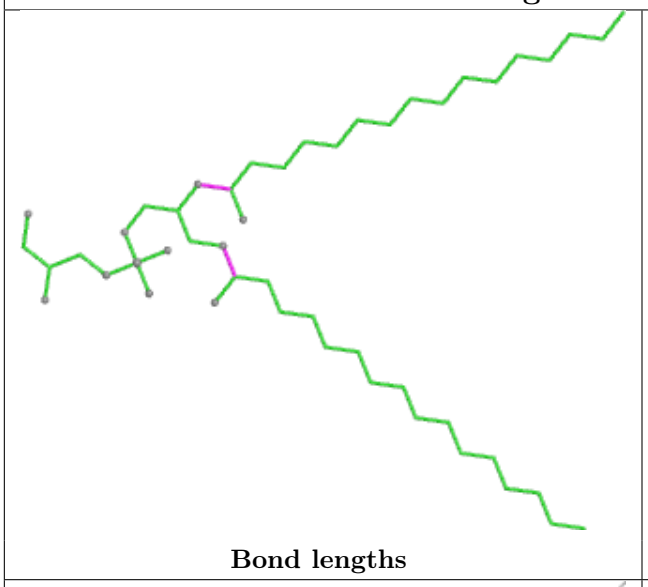


Torsions

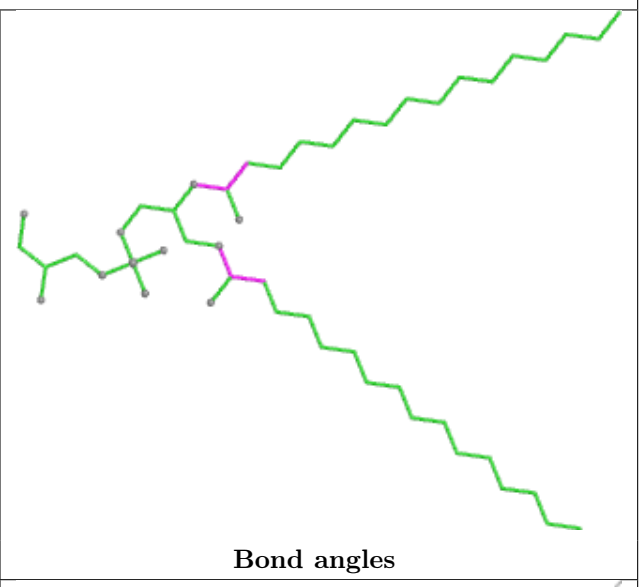


Rings

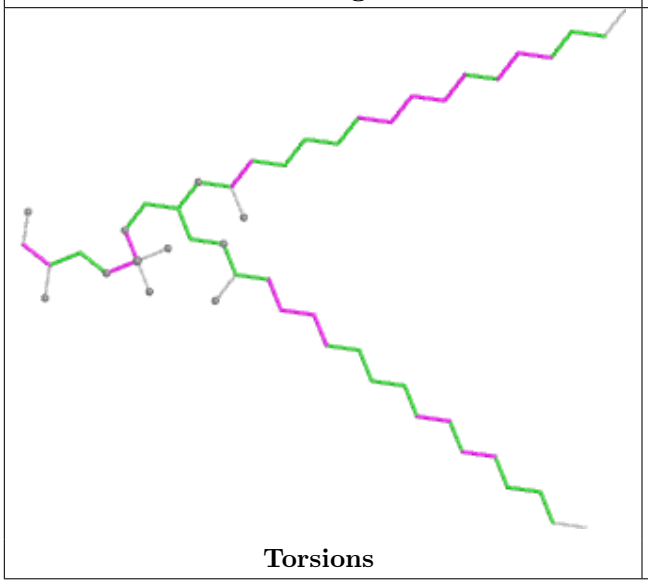
Ligand LHG A 417



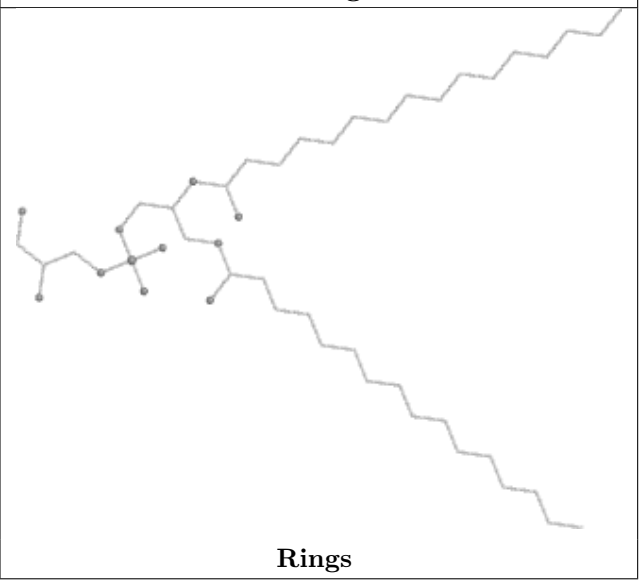
Bond lengths



Bond angles

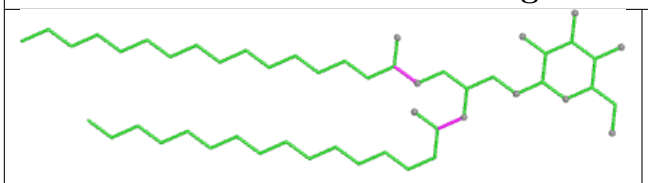


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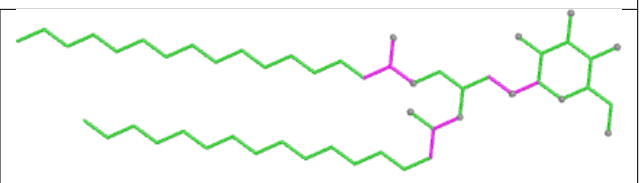


Rings

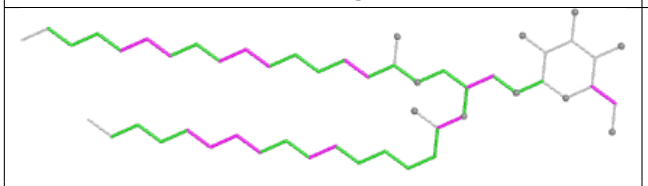
Ligand LMG B 621



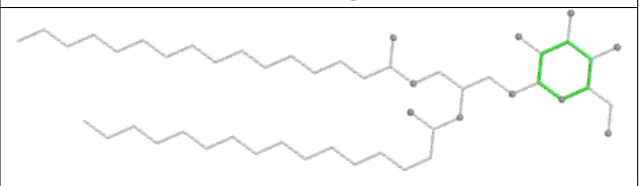
Bond lengths



Bond angles

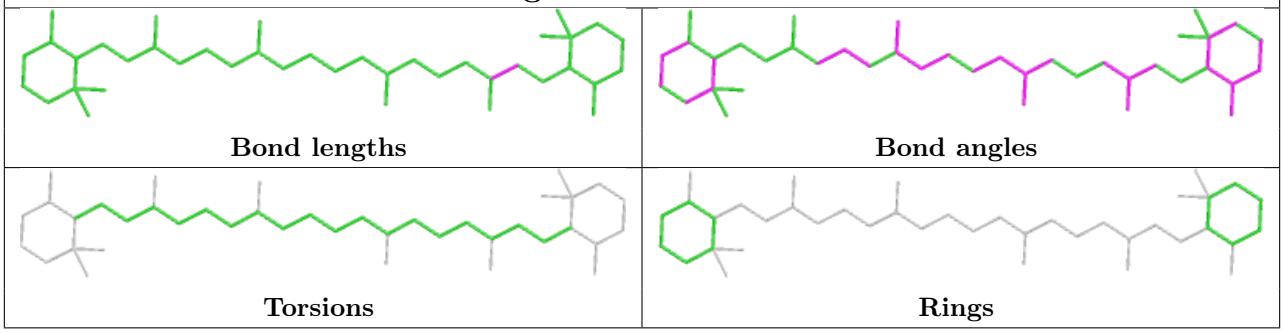


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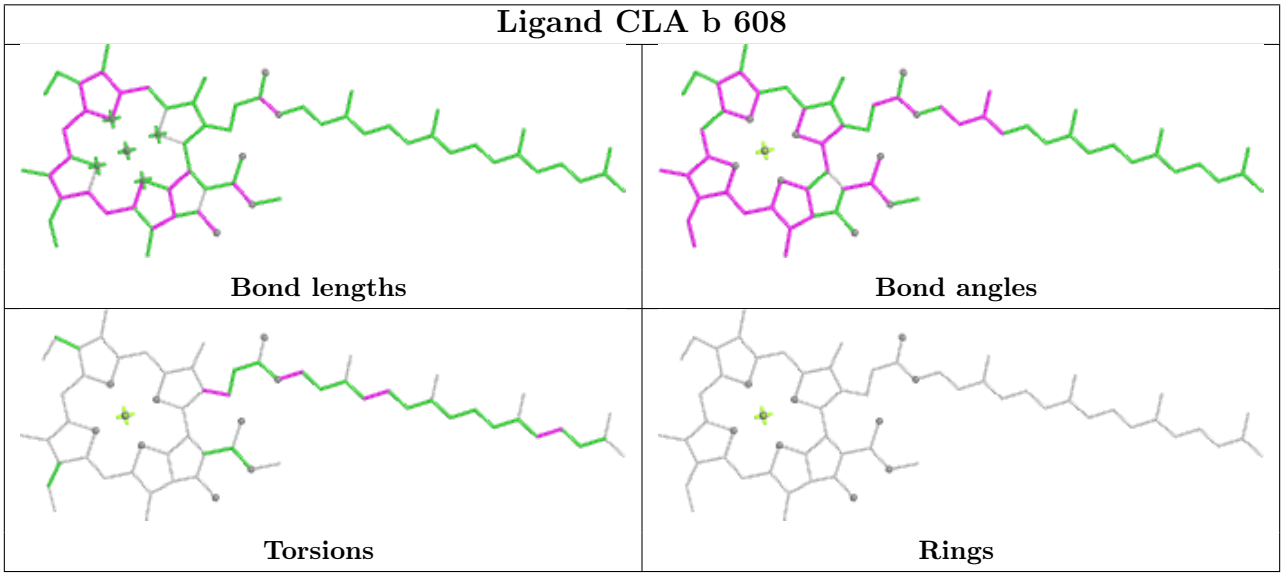


Rings

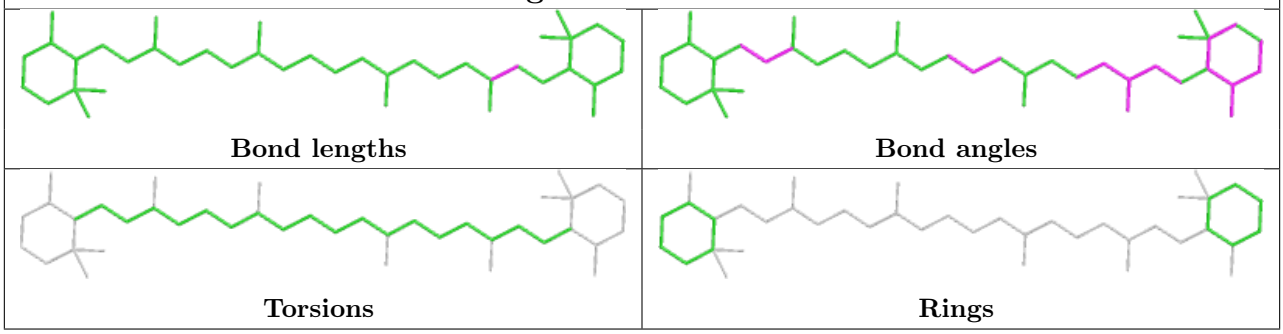
Ligand BCR B 618



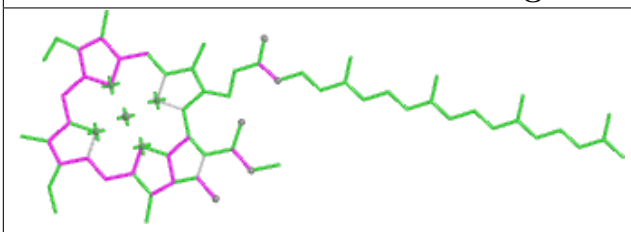
Ligand CLA b 608



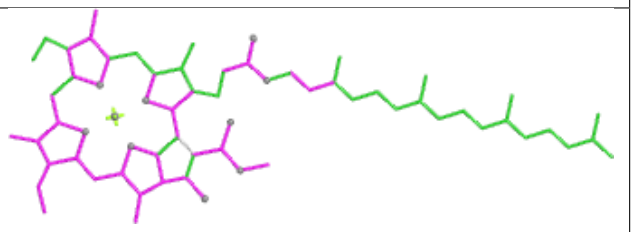
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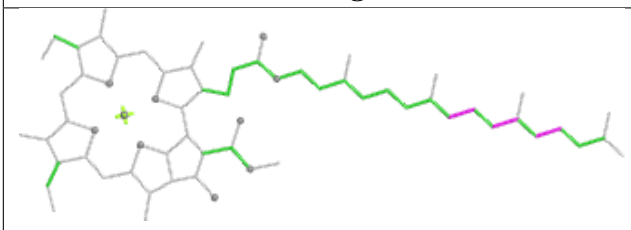
Ligand CLA B 611



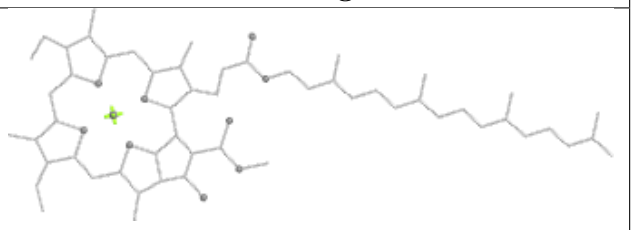
Bond lengths



Bond angles



Torsions

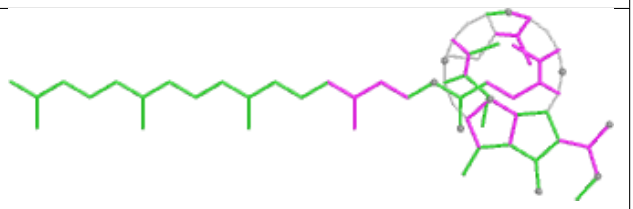


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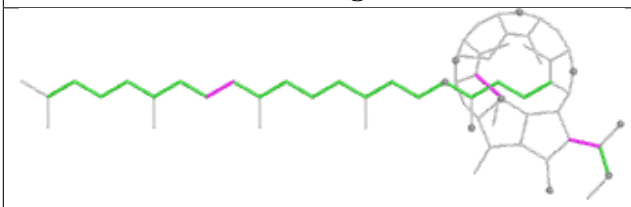
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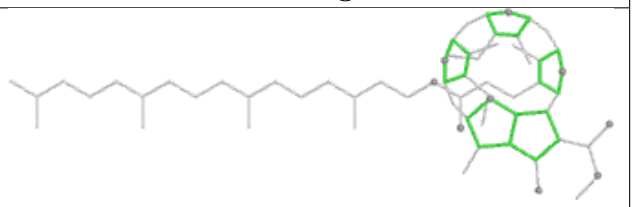
Bond lengths



Bond angles

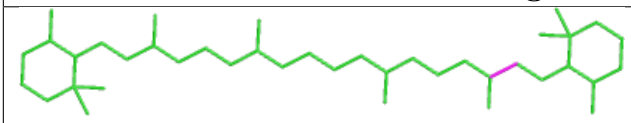


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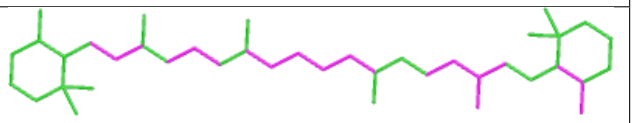


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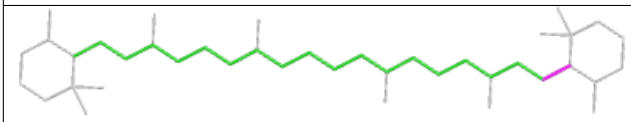
Ligand BCR h 101



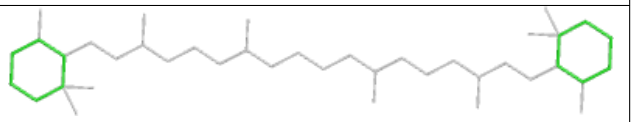
Bond lengths



Bond angles

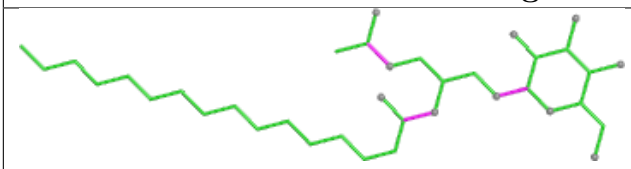


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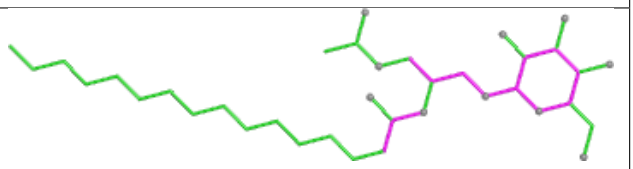


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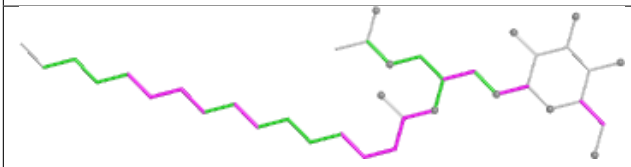
Ligand LMG Z 102



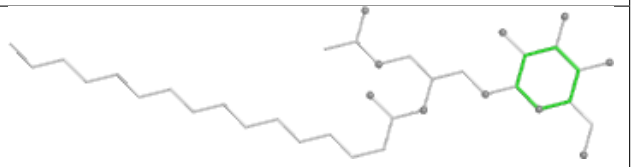
Bond lengths



Bond angles

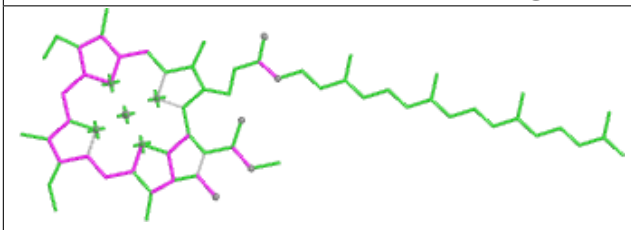


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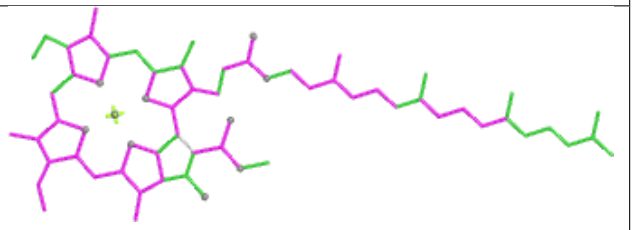


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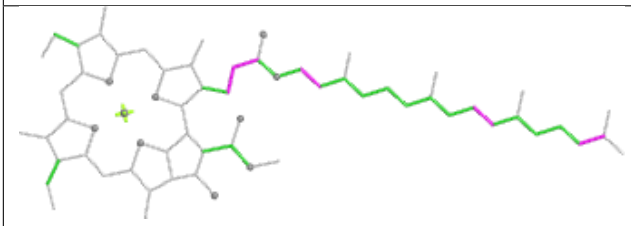
Ligand CLA b 602



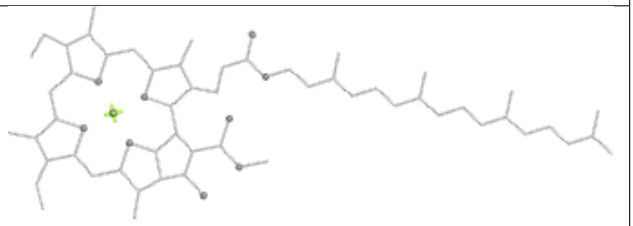
Bond lengths



Bond angles

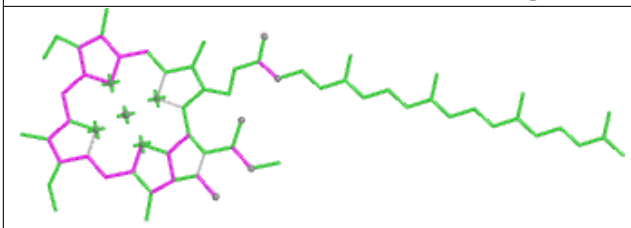


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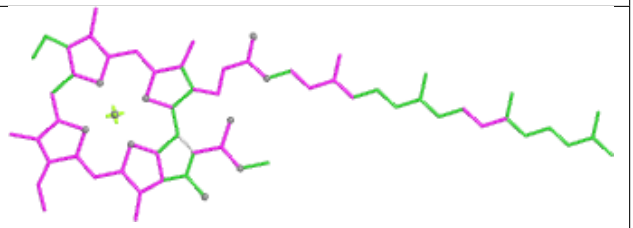


Rings

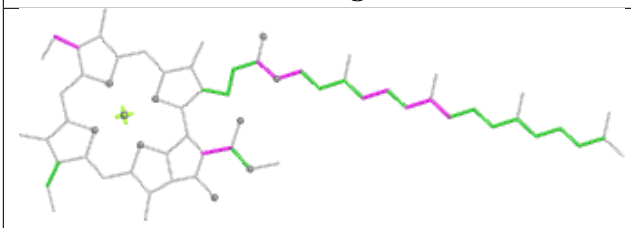
Ligand CLA C 513



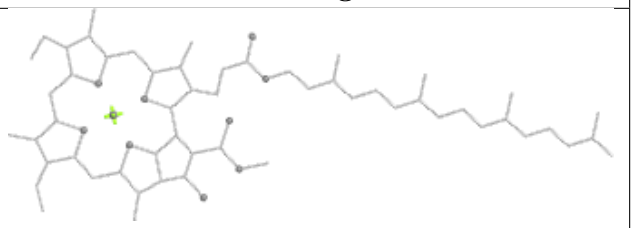
Bond lengths



Bond angles

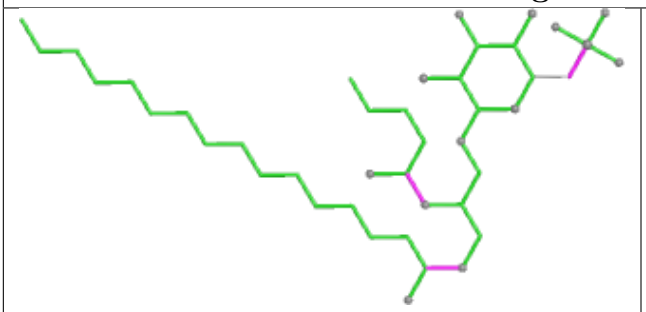


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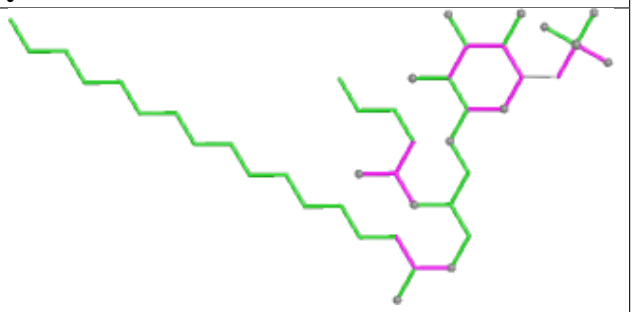


Rings

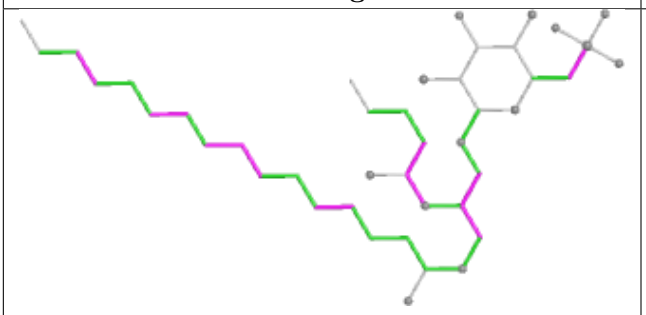
Ligand SQD f 101



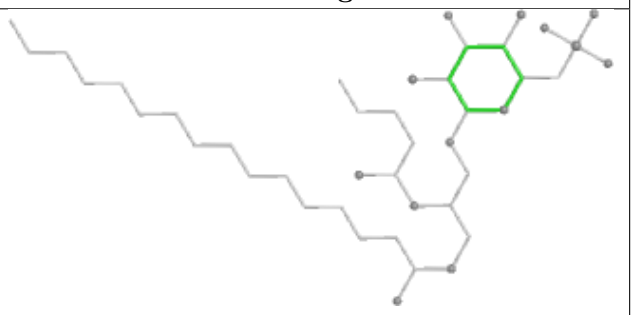
Bond lengths



Bond angles

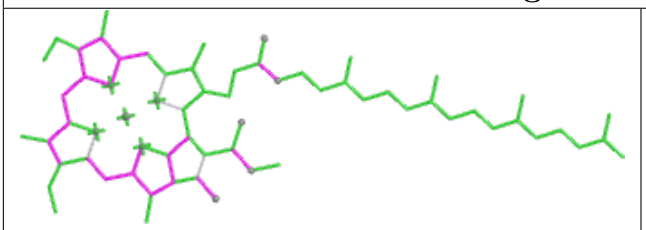


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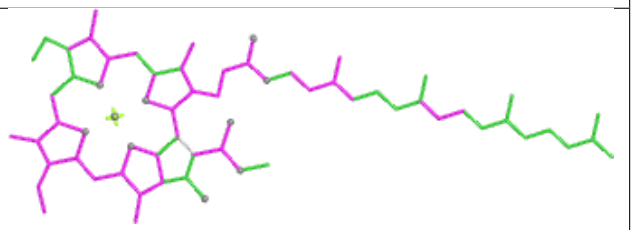


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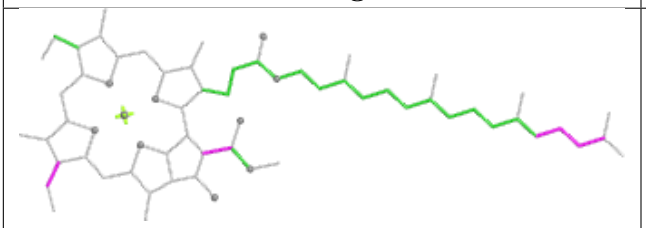
Ligand CLA A 405



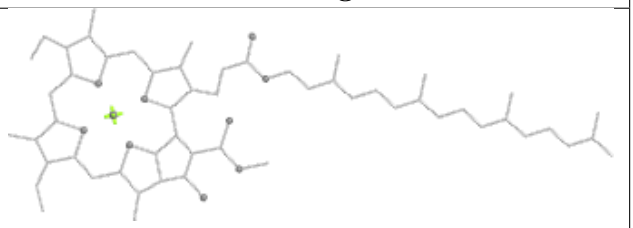
Bond lengths



Bond angles

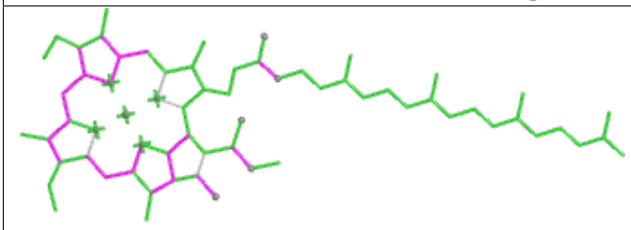


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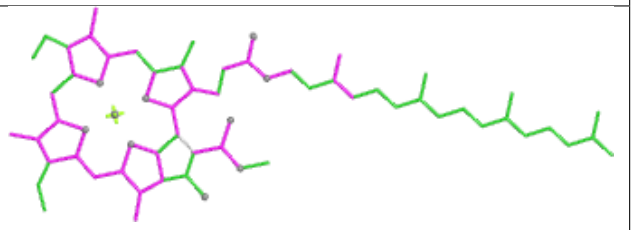


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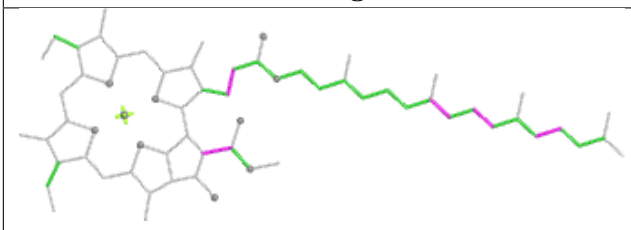
Ligand CLA B 606



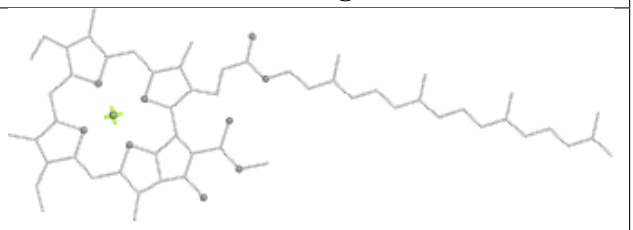
Bond lengths



Bond angles

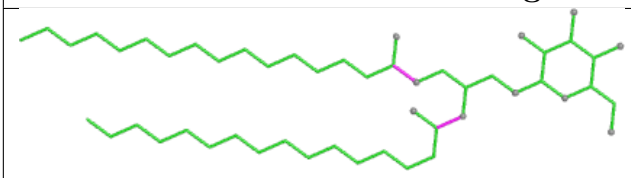


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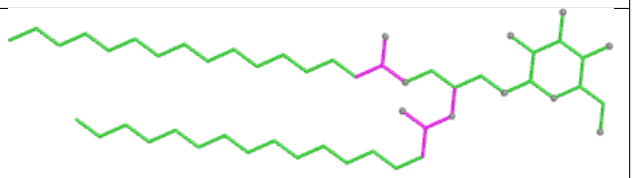


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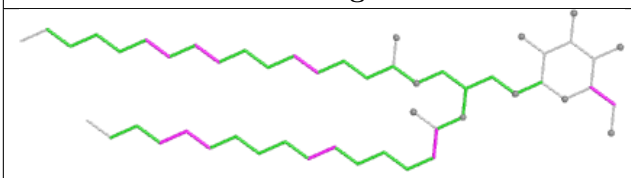
Ligand LMG J 101



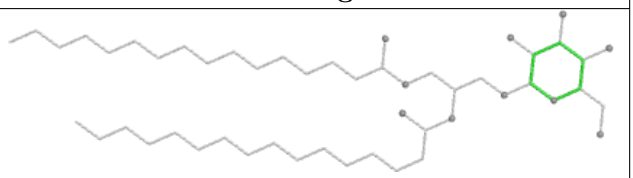
Bond lengths



Bond angles



Torsions



Rings

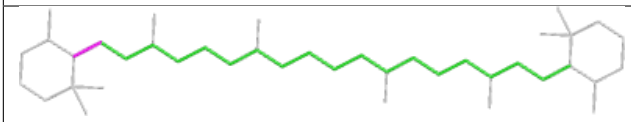
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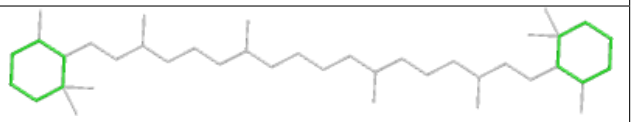
Bond lengths



Bond angles

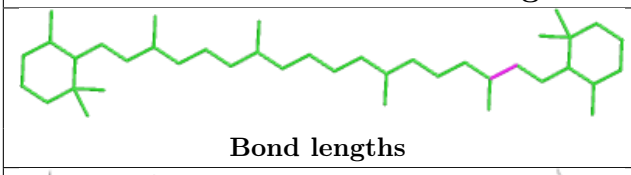


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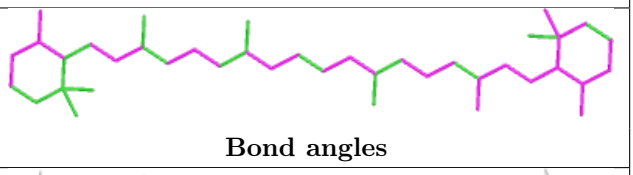


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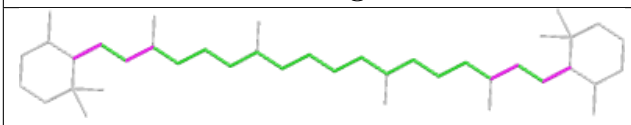
Ligand BCR D 406



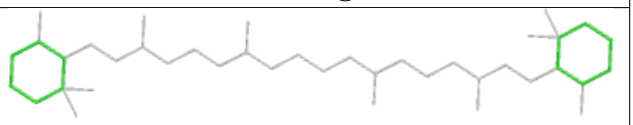
Bond lengths



Bond angles

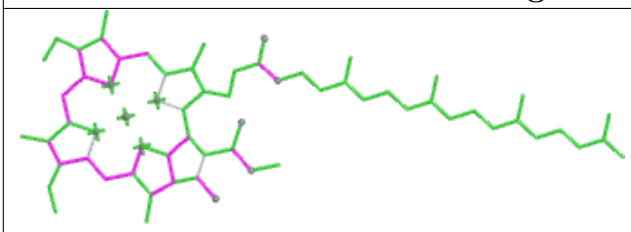


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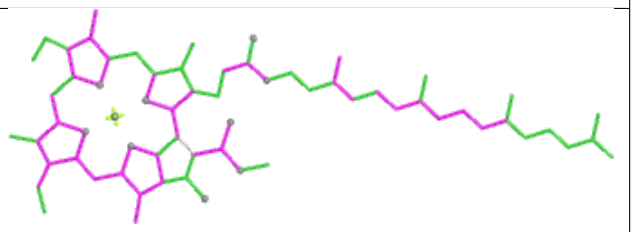


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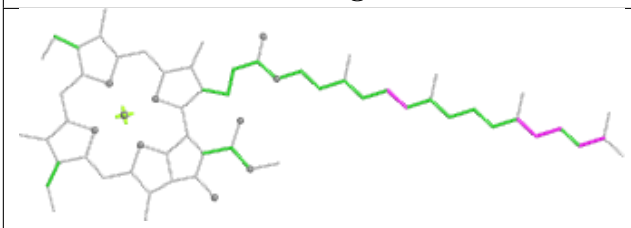
Ligand CLA b 615



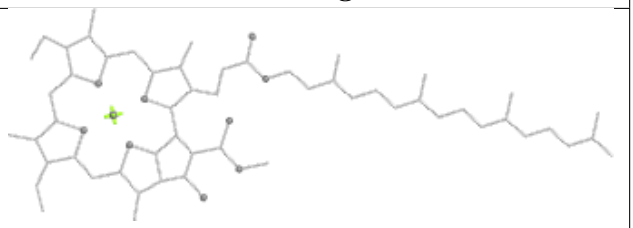
Bond lengths



Bond angles

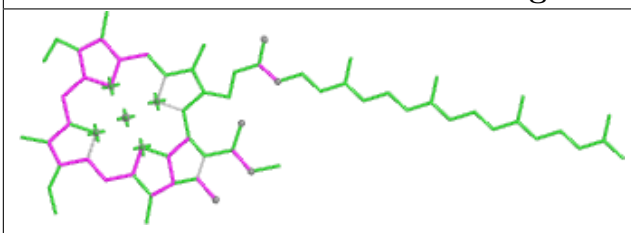


Torsions

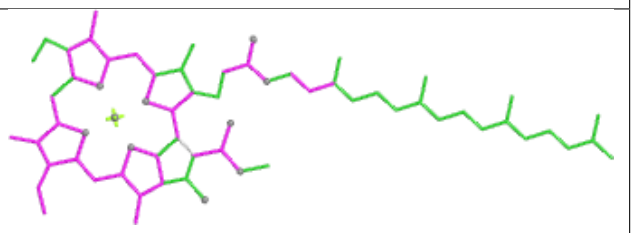


Rings

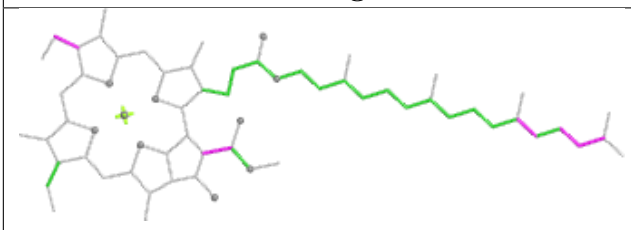
Ligand CLA c 502



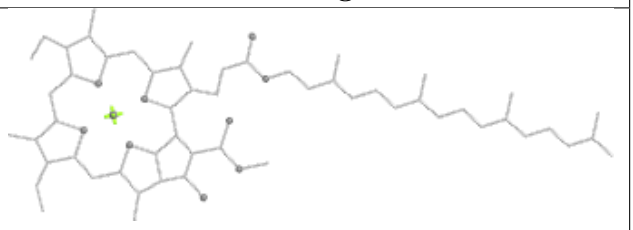
Bond lengths



Bond angles

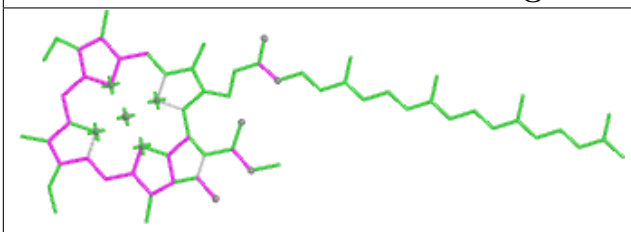


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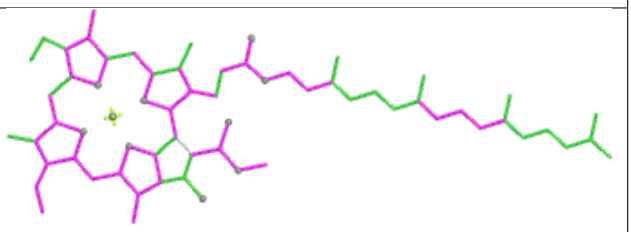


Rings

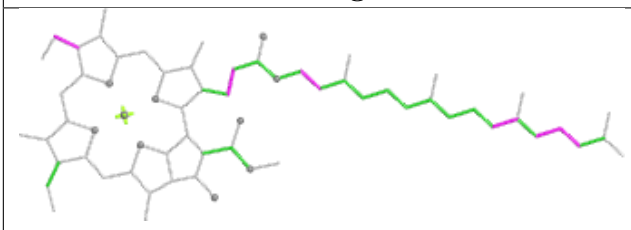
Ligand CLA B 602



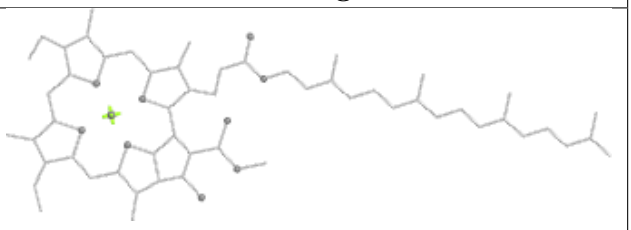
Bond lengths



Bond angles

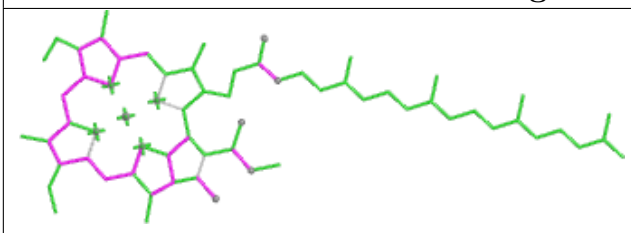


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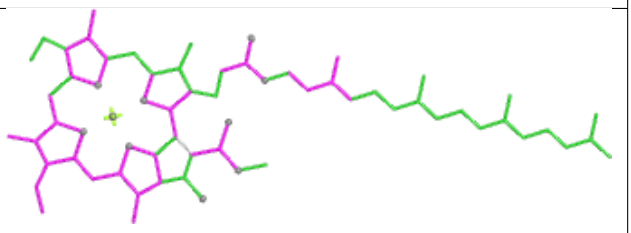


Rings

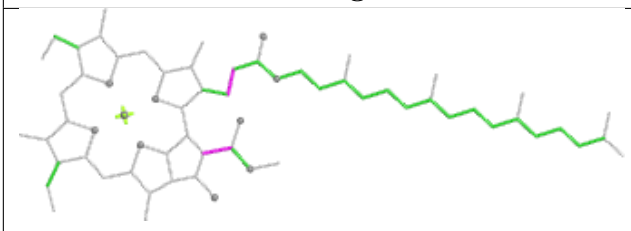
Ligand CLA c 503



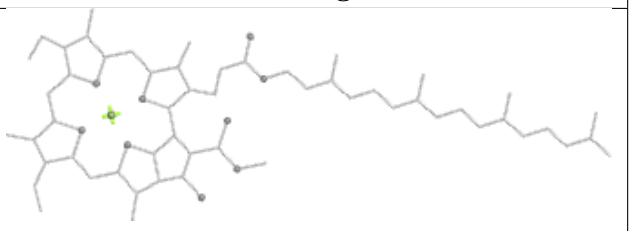
Bond lengths



Bond angles

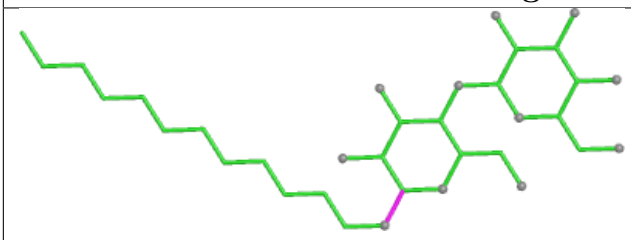


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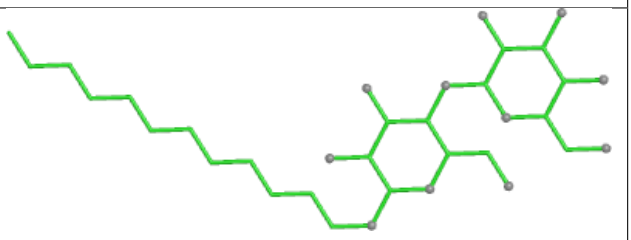


Rings

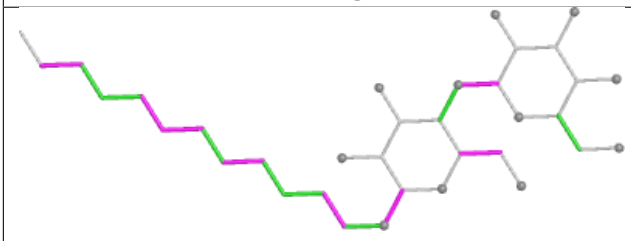
Ligand LMT E 102



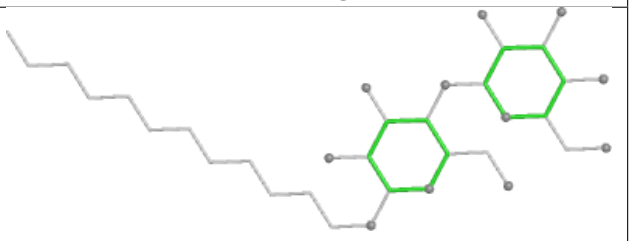
Bond lengths



Bond angles

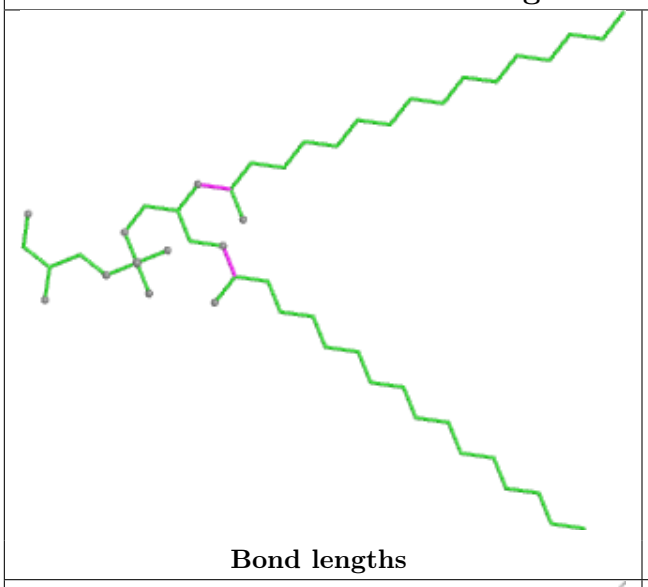


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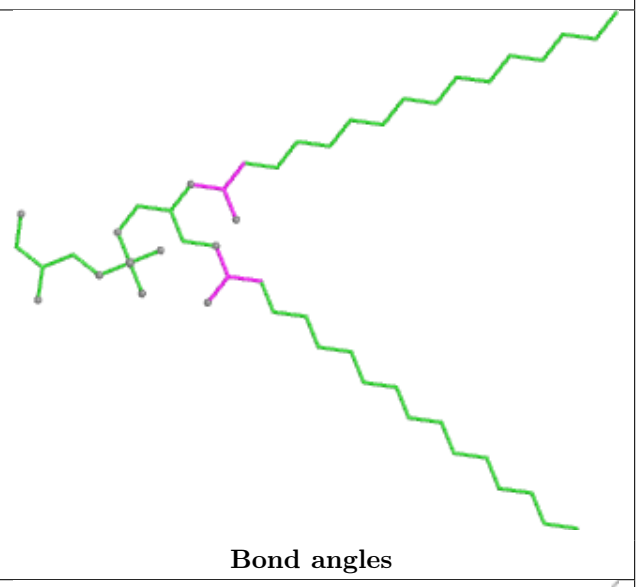


Rings

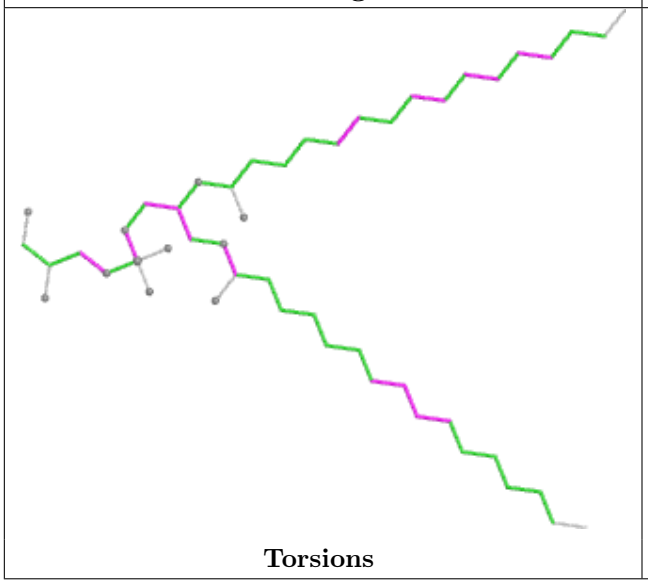
Ligand LHG D 409



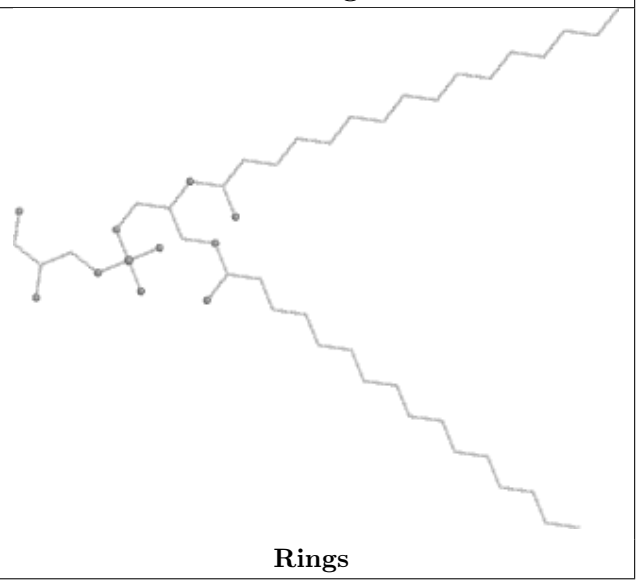
Bond lengths



Bond angles

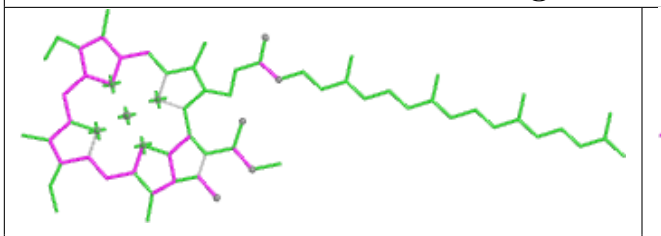


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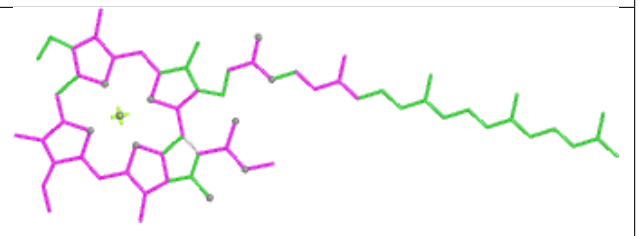


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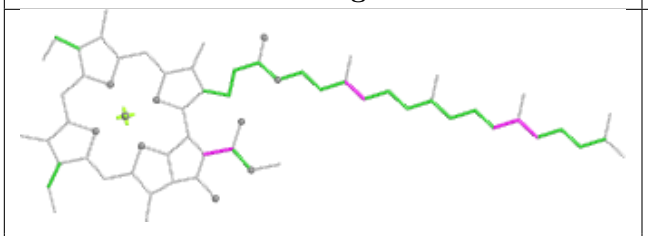
Ligand CLA c 504



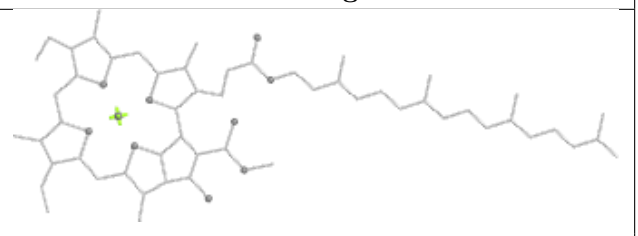
Bond lengths



Bond angles

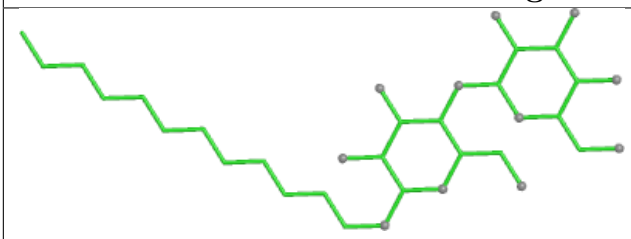


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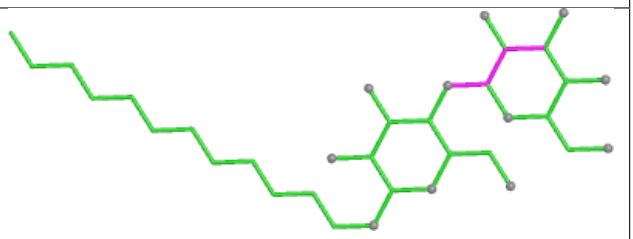


Rings

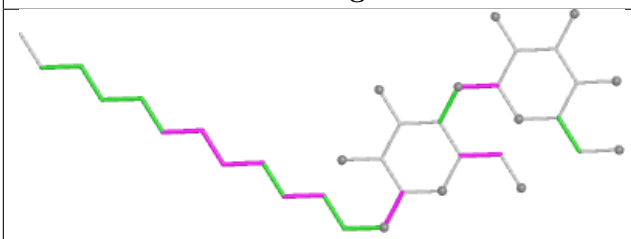
Ligand LMT e 102



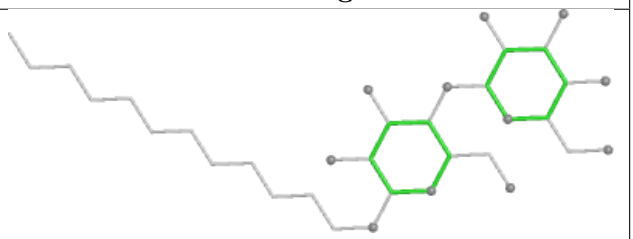
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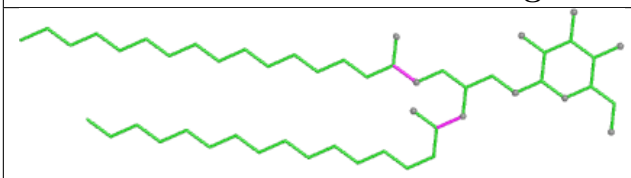


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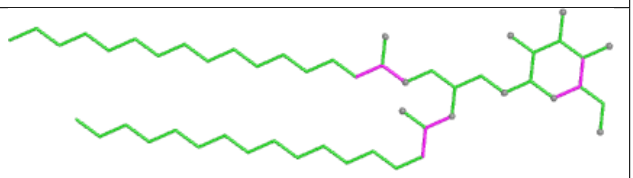


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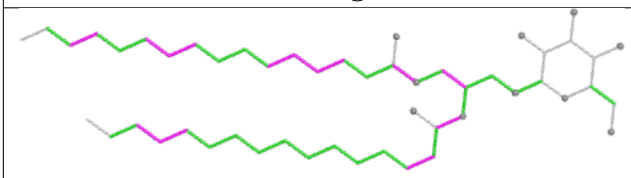
Ligand LMG a 416



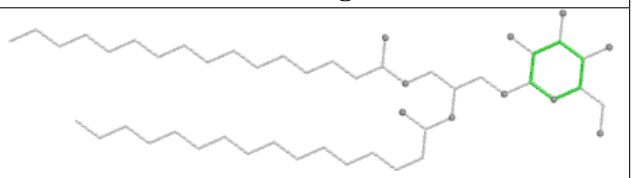
Bond lengths



Bond angles

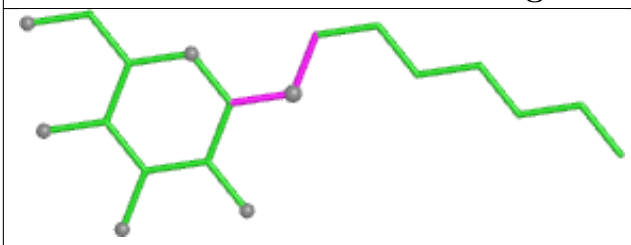


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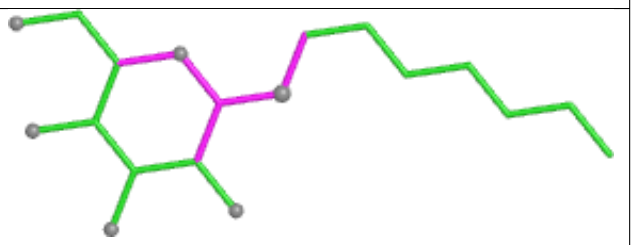


Rings

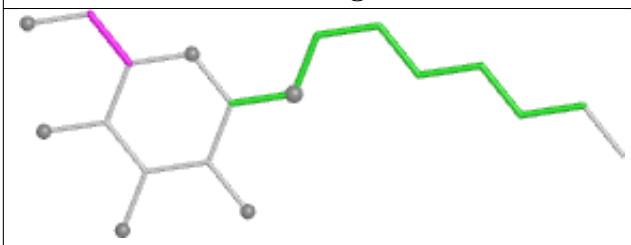
Ligand HTG c 522



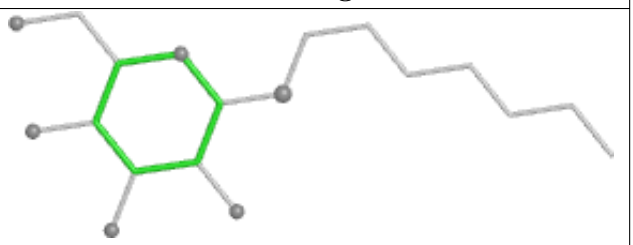
Bond lengths



Bond angles

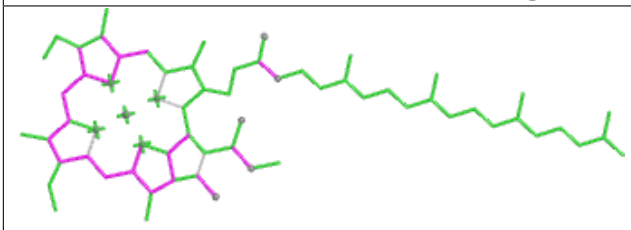


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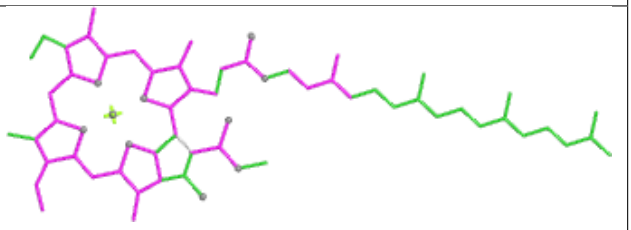


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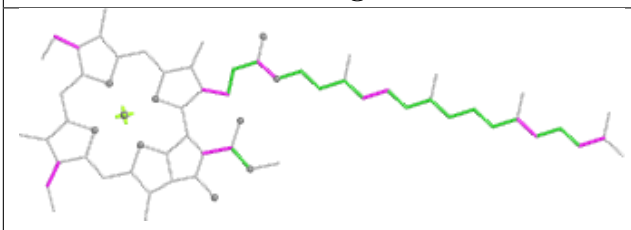
Ligand CLA A 406



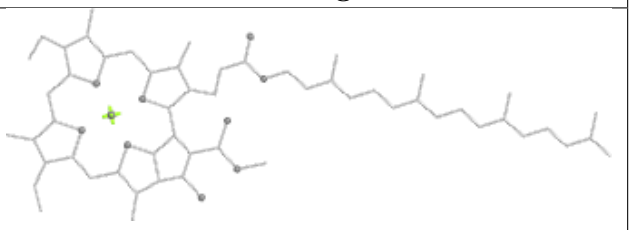
Bond lengths



Bond angles

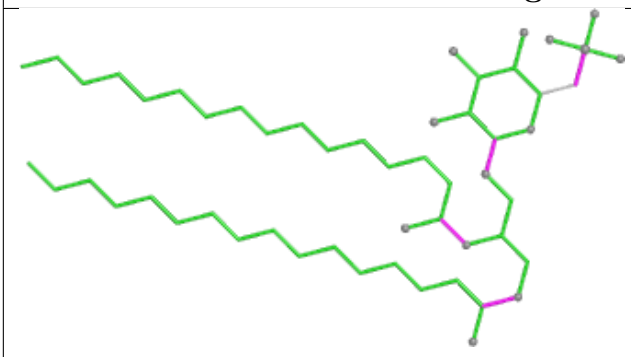


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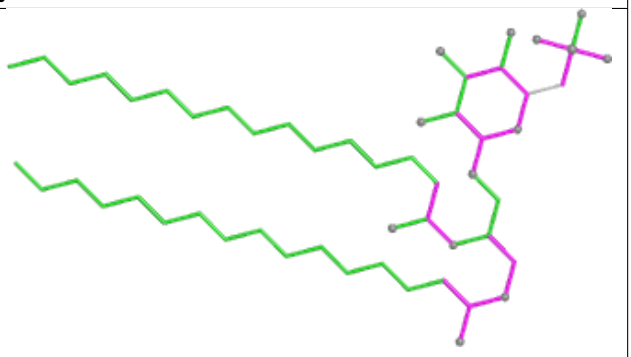


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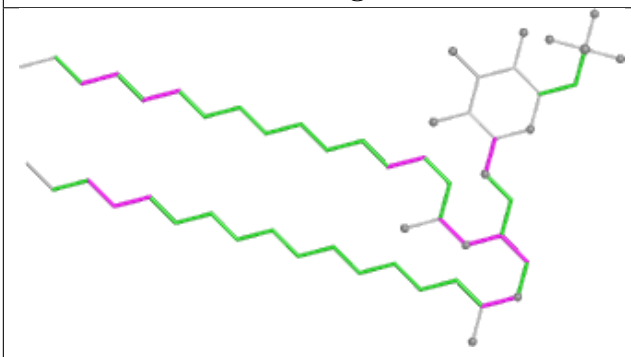
Ligand SQD B 620



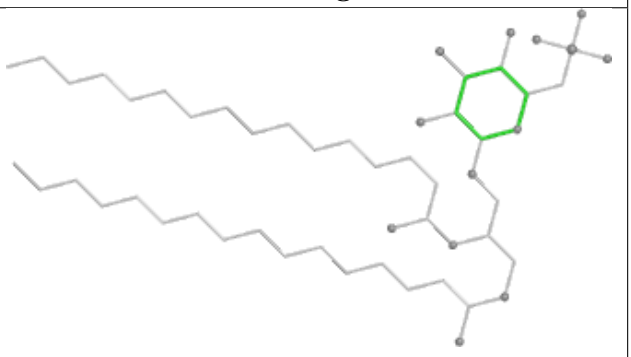
Bond lengths



Bond angles

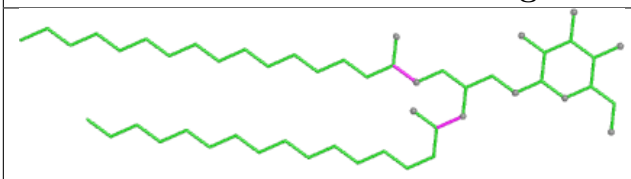


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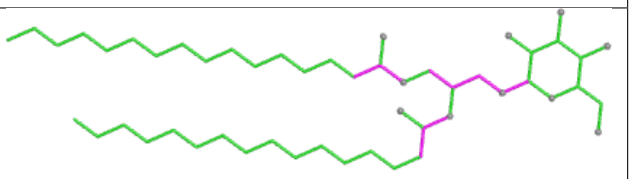


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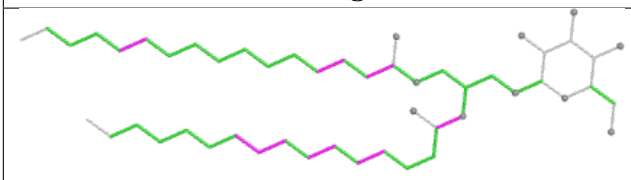
Ligand LMG C 501



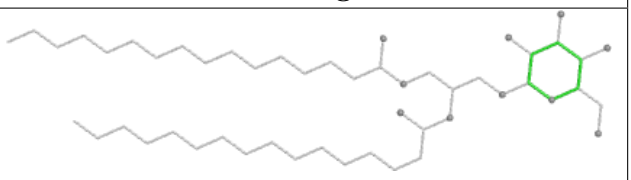
Bond lengths



Bond angles

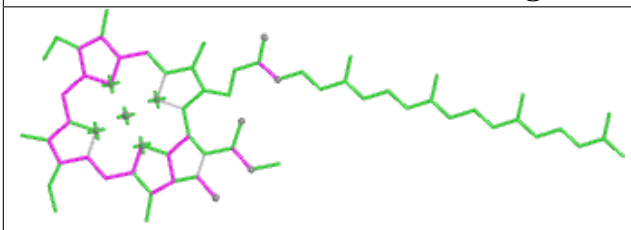


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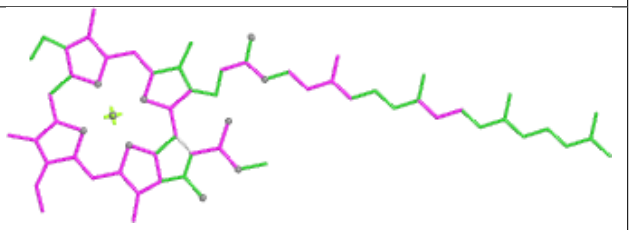


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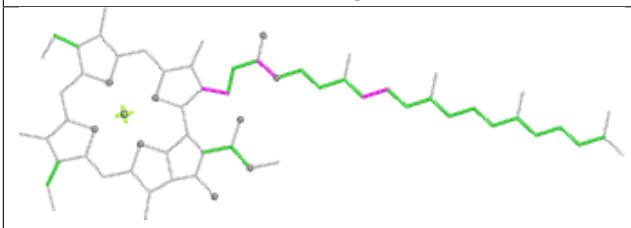
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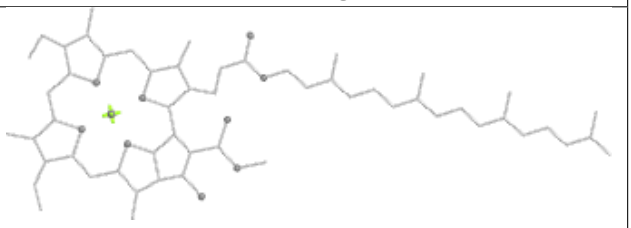
Bond lengths



Bond angles



Torsions

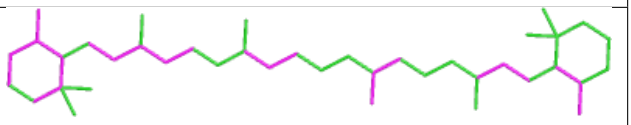


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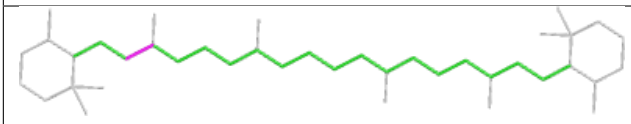
Ligand BCR K 102



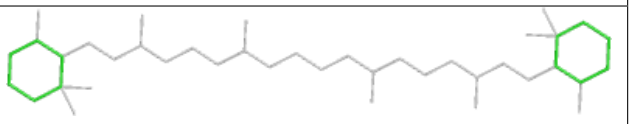
Bond lengths



Bond angles

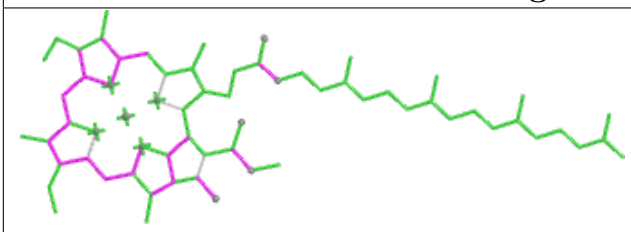


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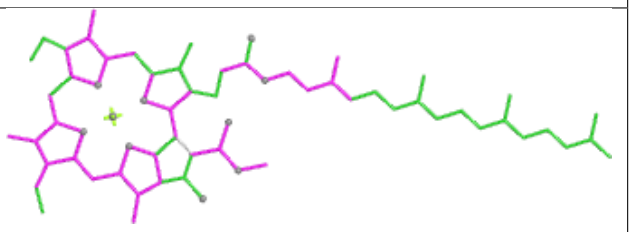


Rings

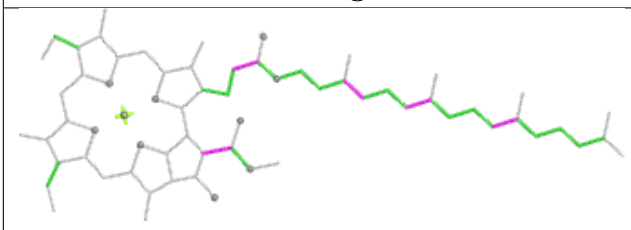
Ligand CLA c 505



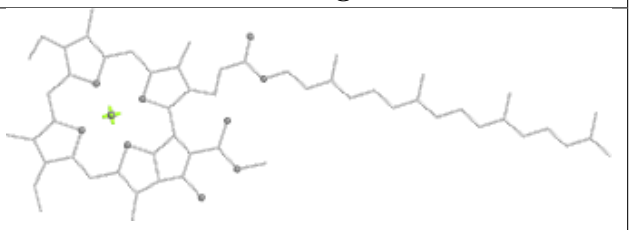
Bond lengths



Bond angles



Torsions

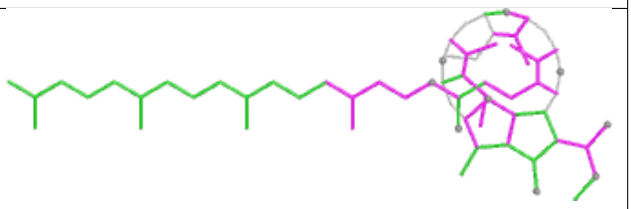


Rings

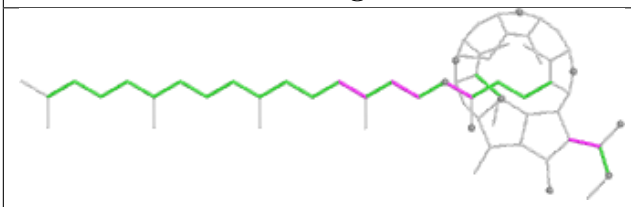
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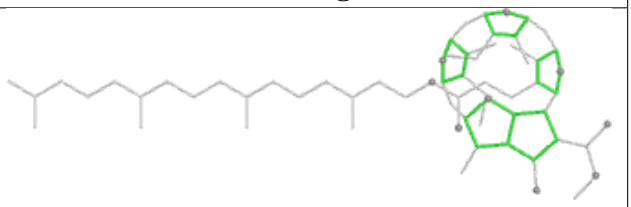
Bond lengths



Bond angles

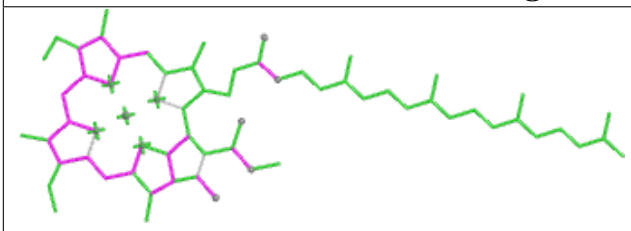


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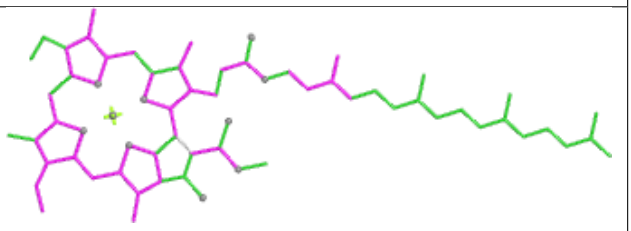


Rings

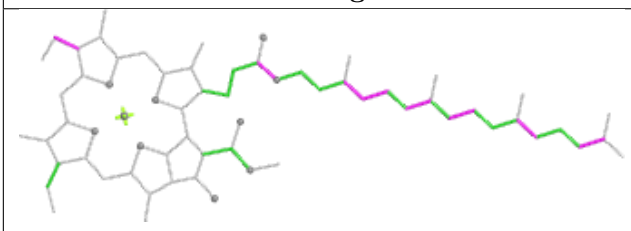
Ligand CLA A 408



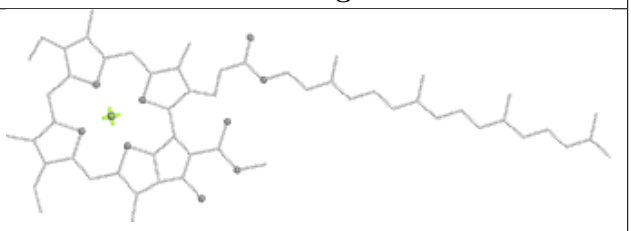
Bond lengths



Bond angles

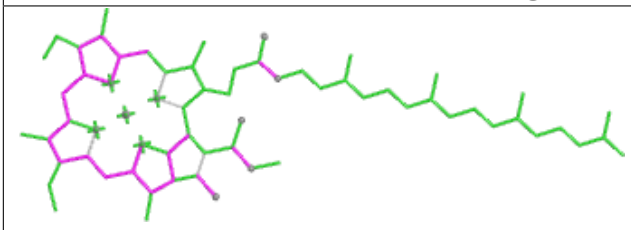


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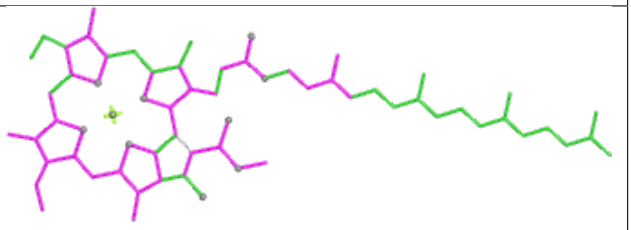


Rings

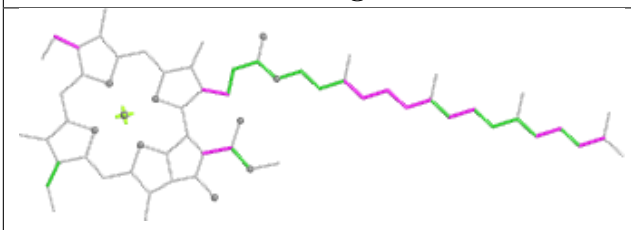
Ligand CLA C 507



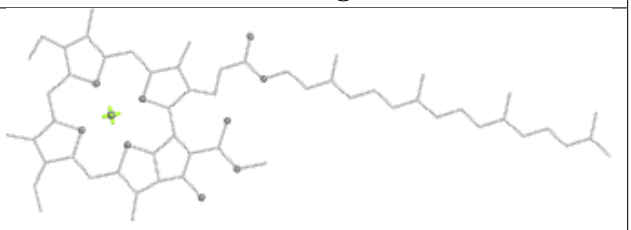
Bond lengths



Bond angles

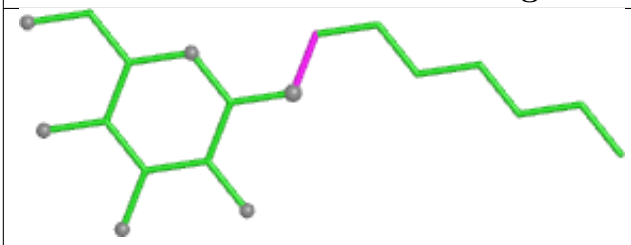


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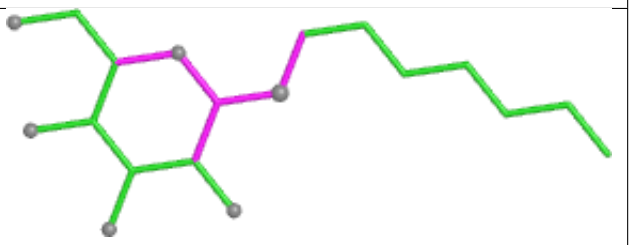


Rings

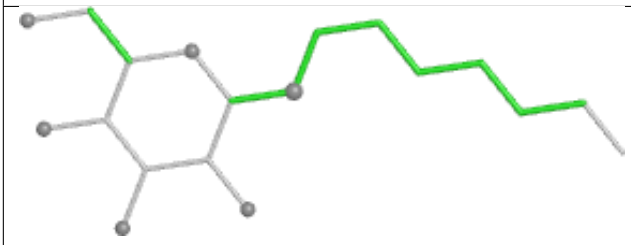
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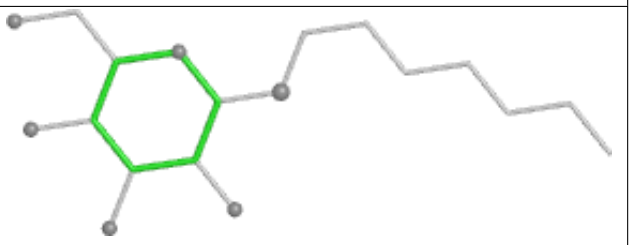
Bond lengths



Bond angles

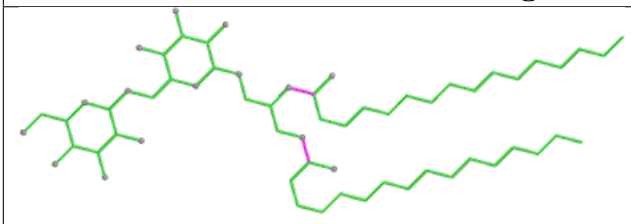


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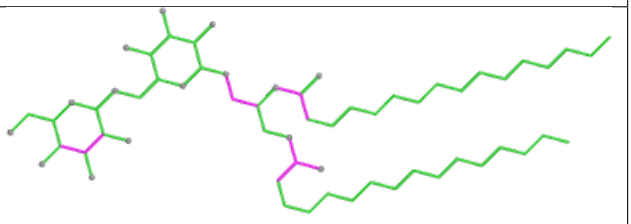


Rings

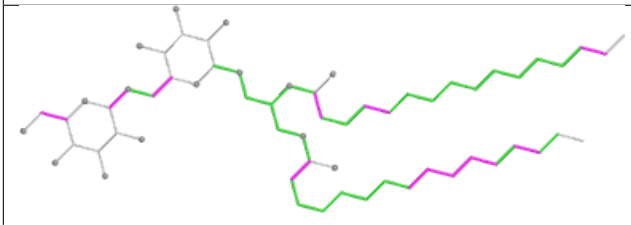
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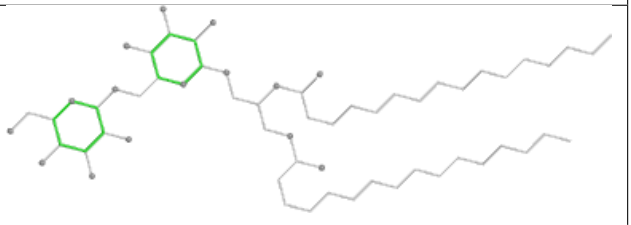
Bond lengths



Bond angles

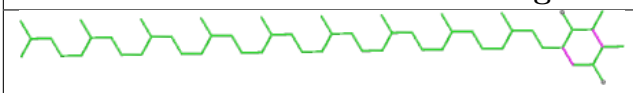


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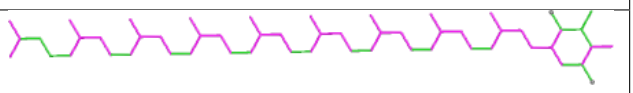


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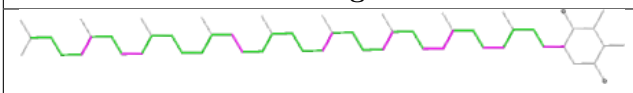
Ligand PL9 a 414



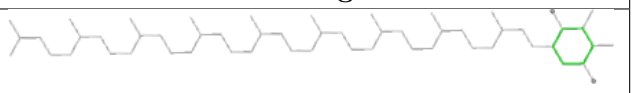
Bond lengths



Bond angles

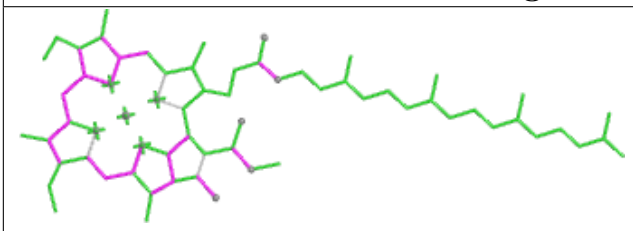


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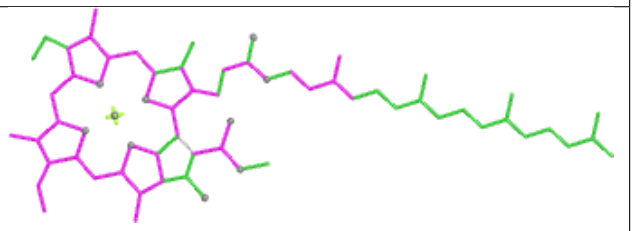


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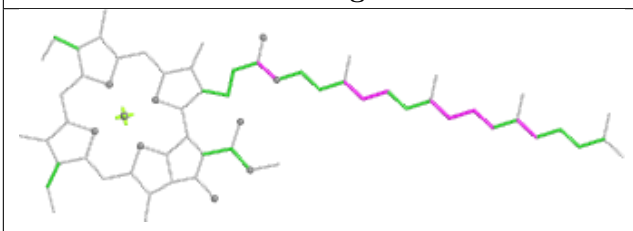
Ligand CLA D 405



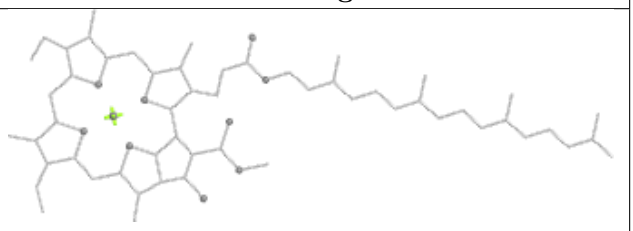
Bond lengths



Bond angles



Torsions

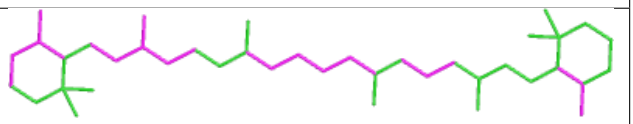


Rings

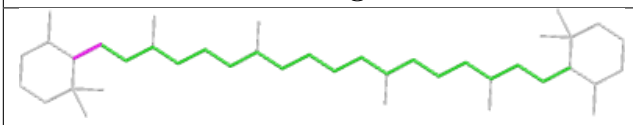
Ligand BCR C 516



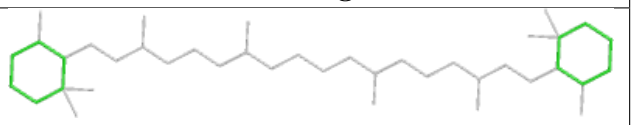
Bond lengths



Bond angles

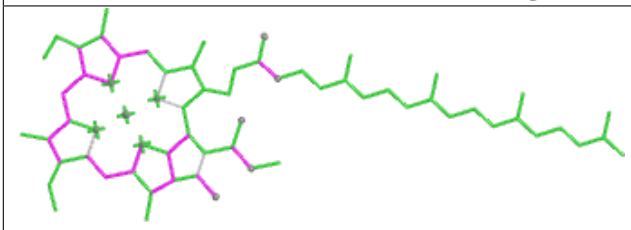


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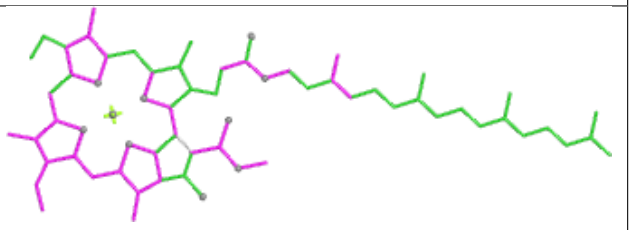


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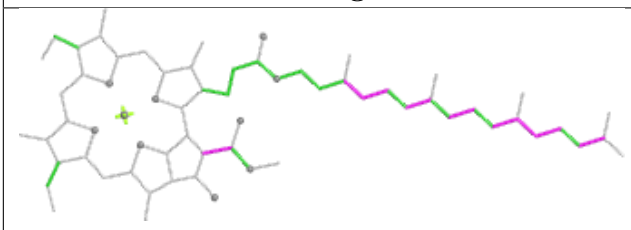
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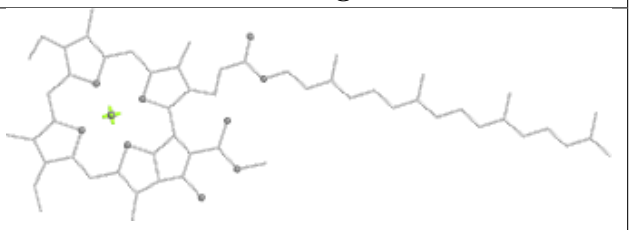
Bond lengths



Bond angles

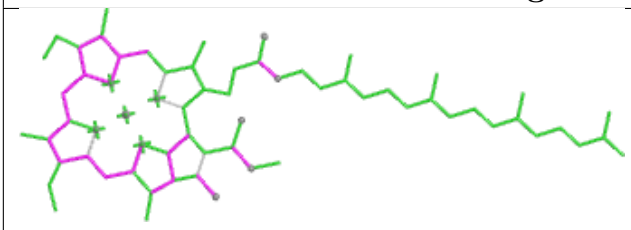


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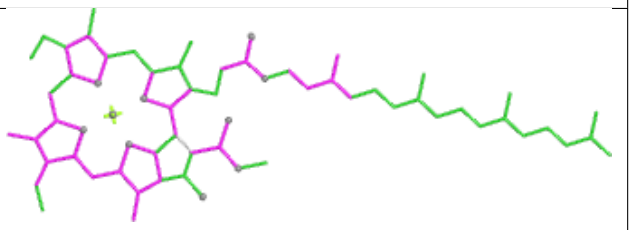


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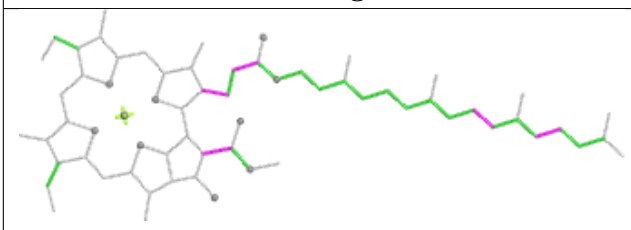
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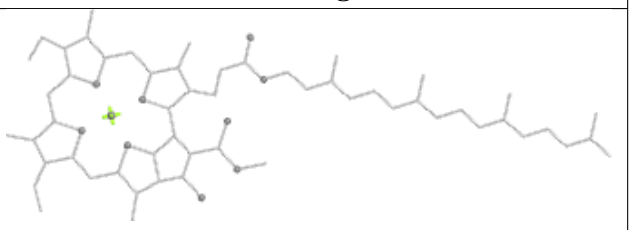
Bond lengths



Bond angles

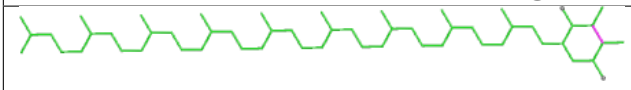


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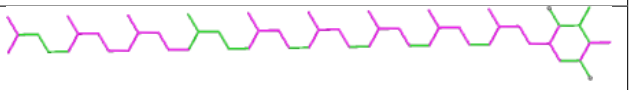


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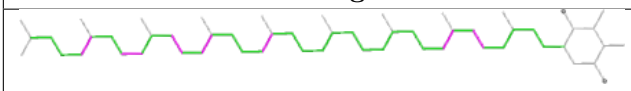
Ligand PL9 D 407



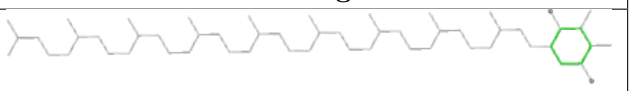
Bond lengths



Bond angles

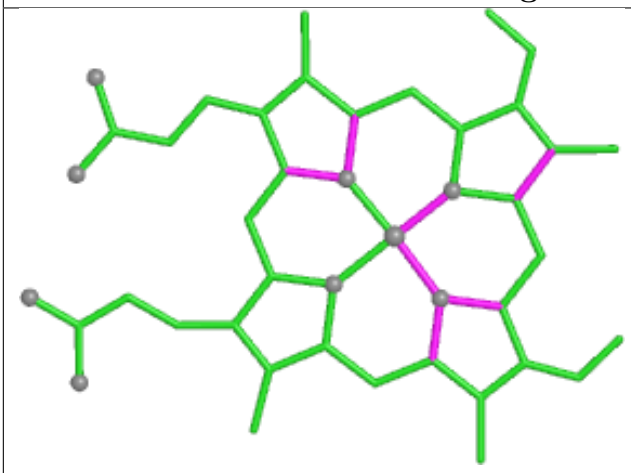


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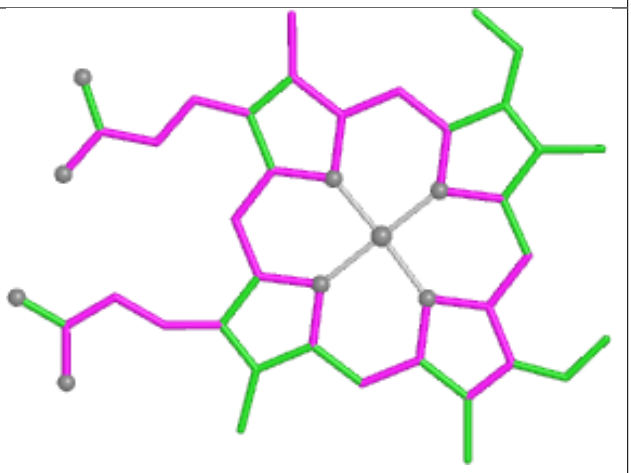


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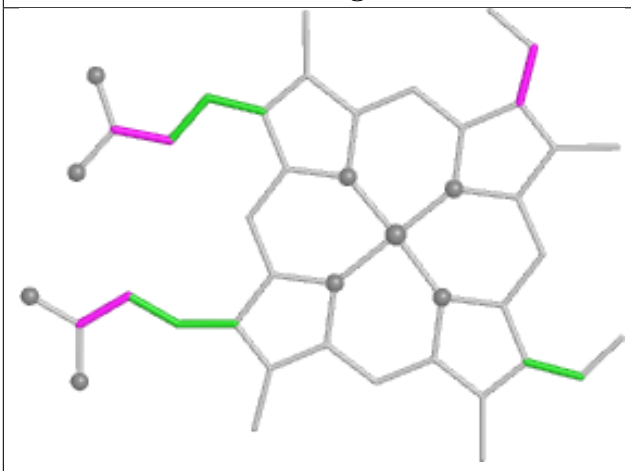
Ligand HEM E 103



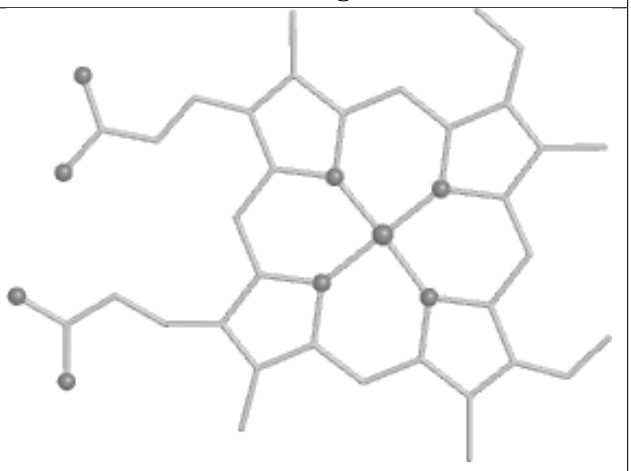
Bond lengths



Bond angles

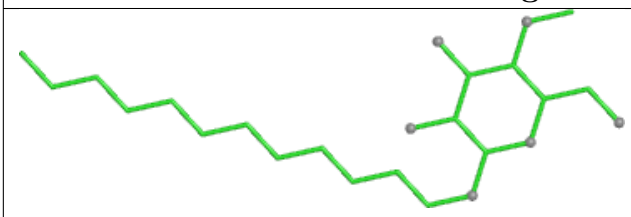


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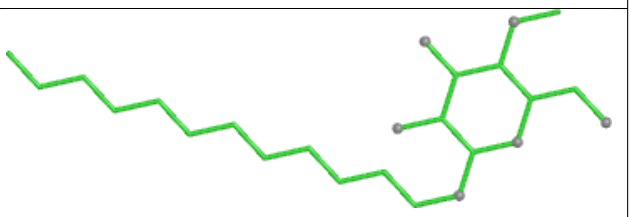


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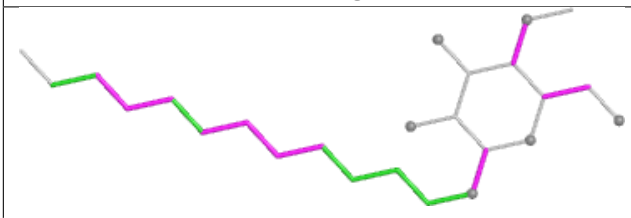
Ligand LMT B 629



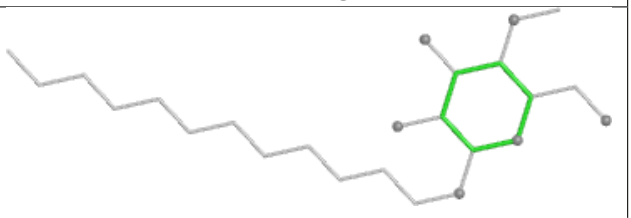
Bond lengths



Bond angles

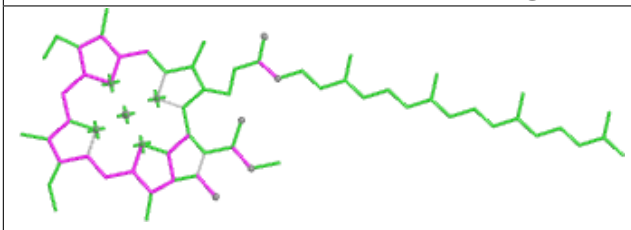


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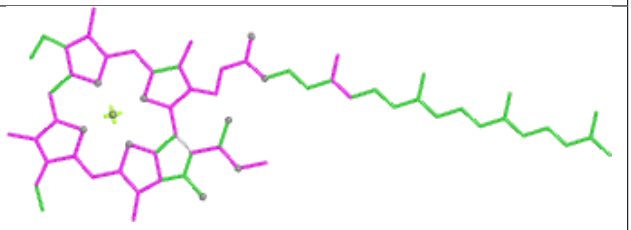


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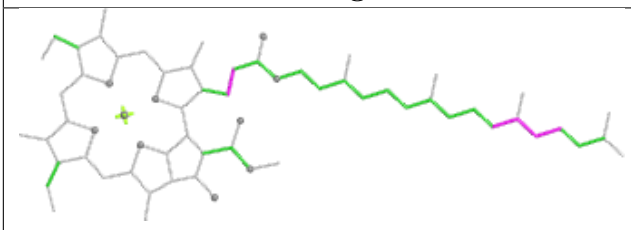
Ligand CLA A 404



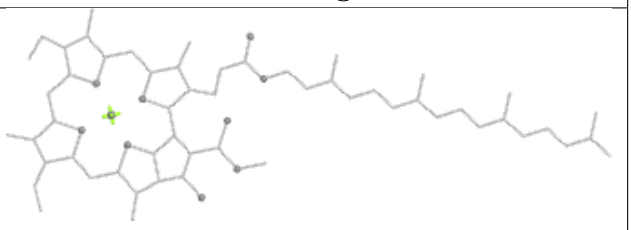
Bond lengths



Bond angles

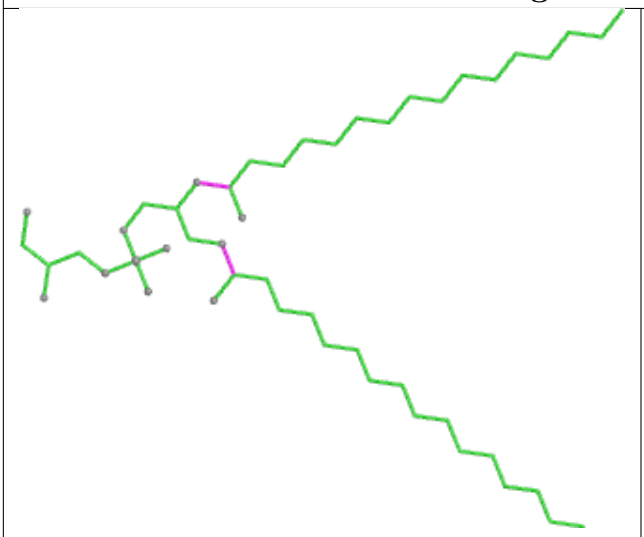


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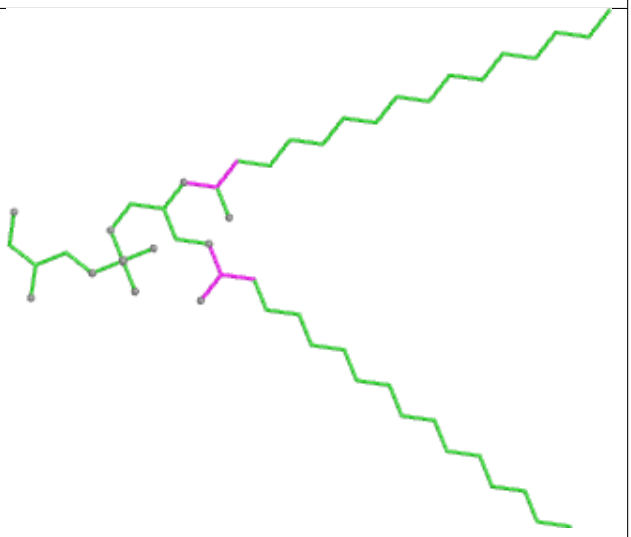


Rings

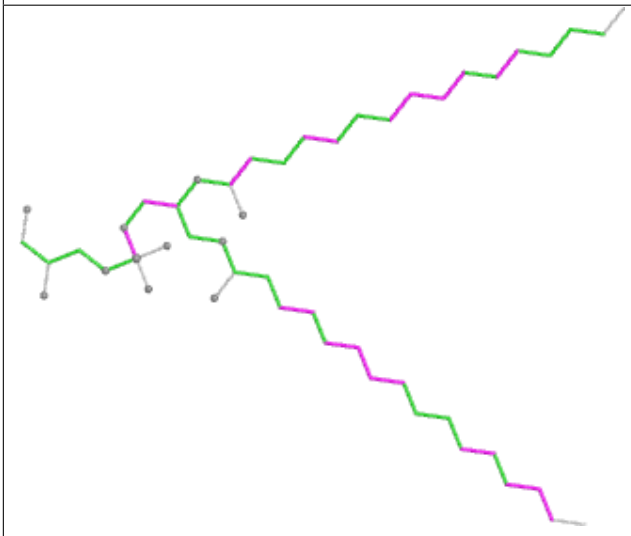
Ligand LHG l 101



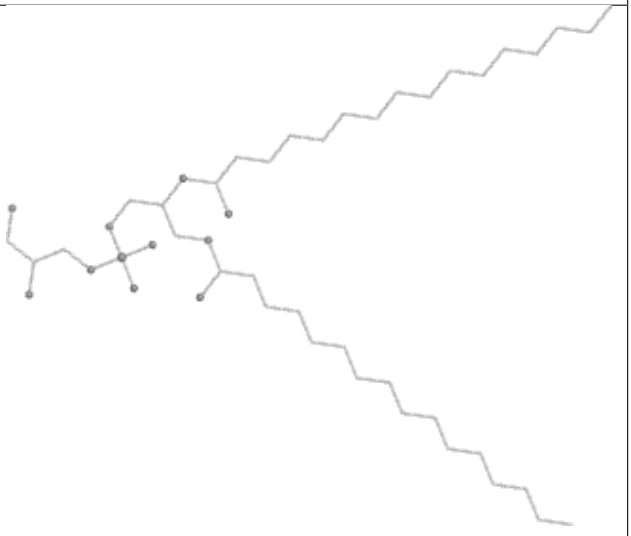
Bond lengths



Bond angles

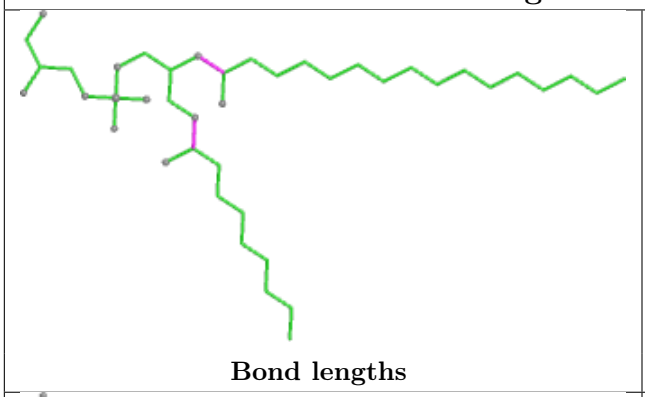


Torsions

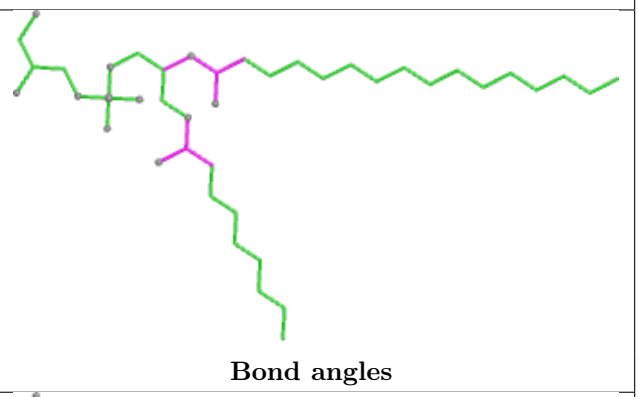


Rings

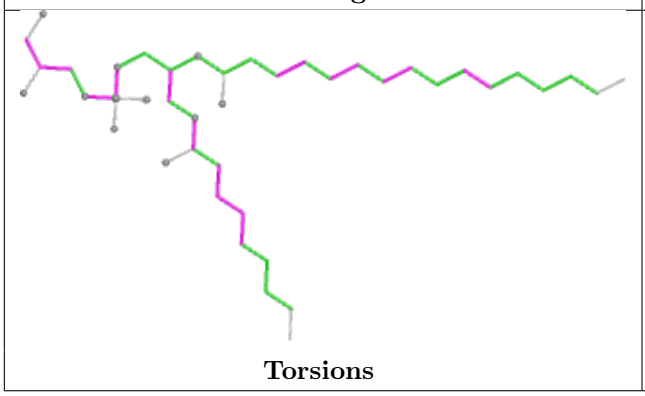
Ligand LHG E 101



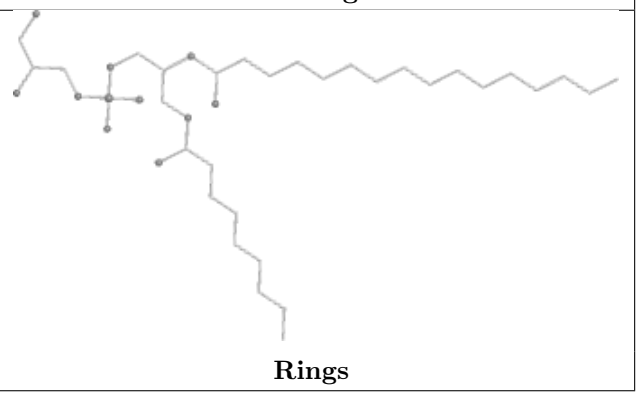
Bond lengths



Bond angles

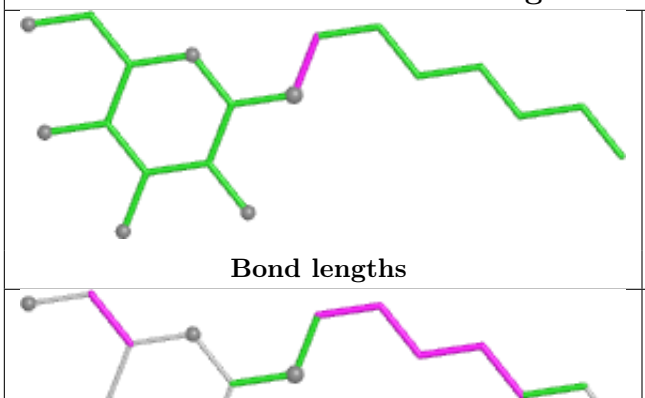


Torsions

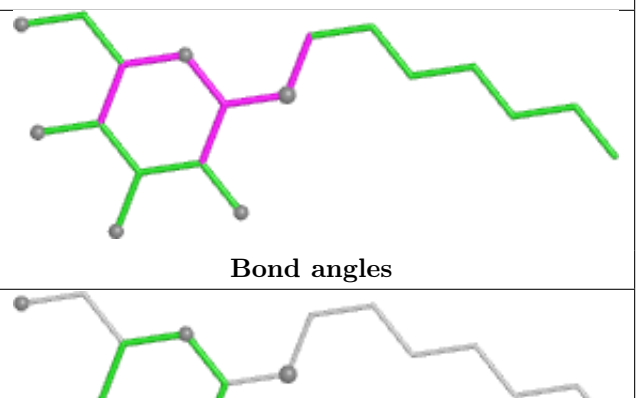


Rings

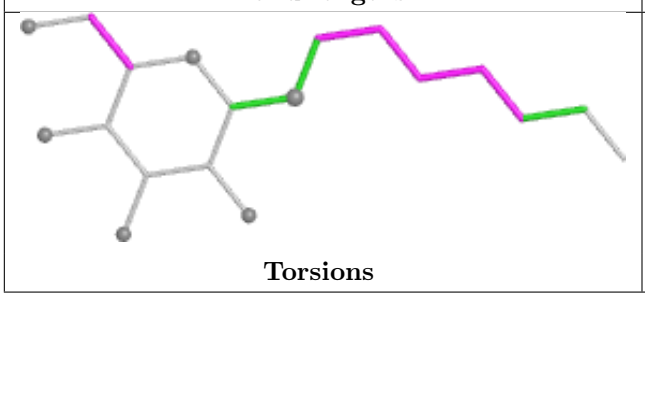
Ligand HTG b 628



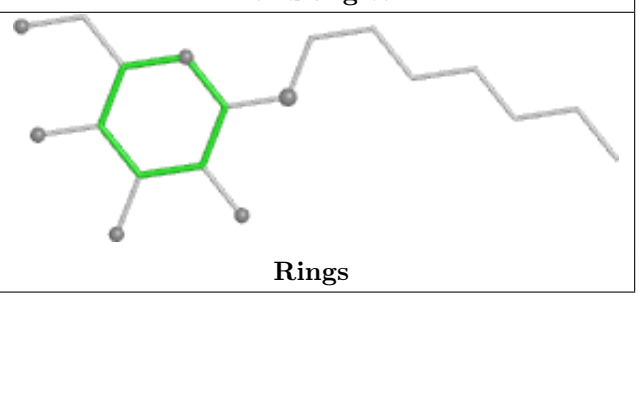
Bond lengths



Bond angles

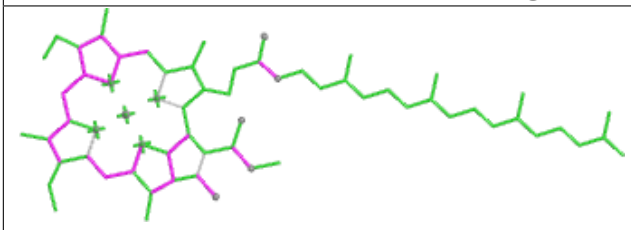


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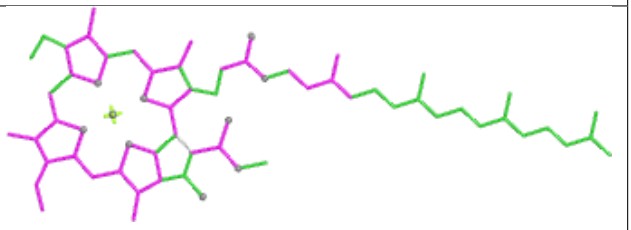


Rings

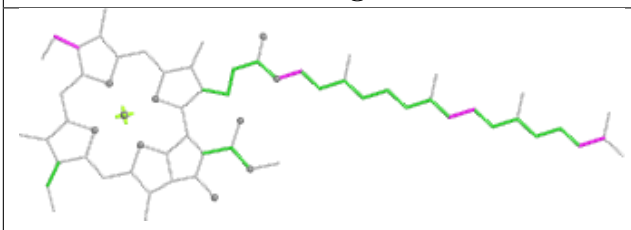
Ligand CLA B 608



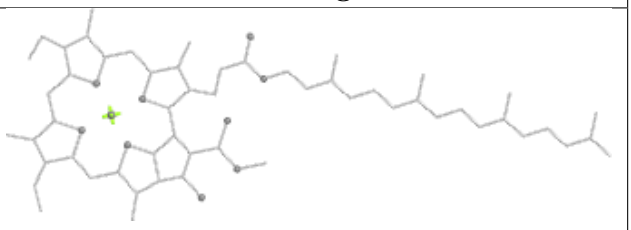
Bond lengths



Bond angles

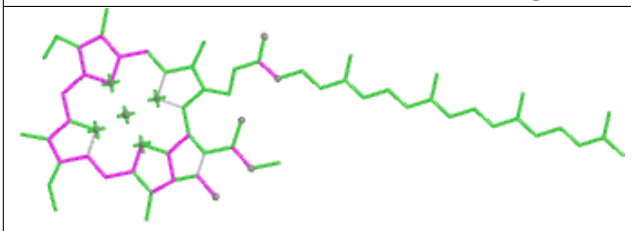


Torsions

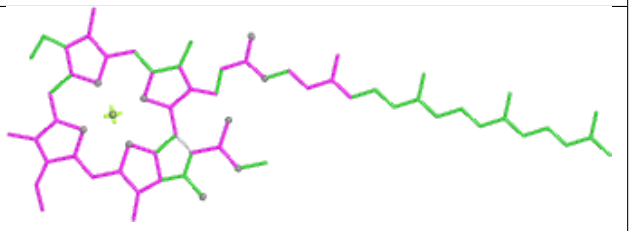


Rings

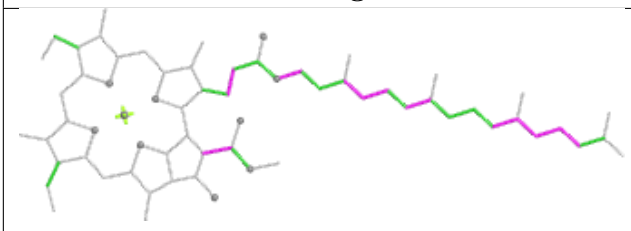
Ligand CLA b 614



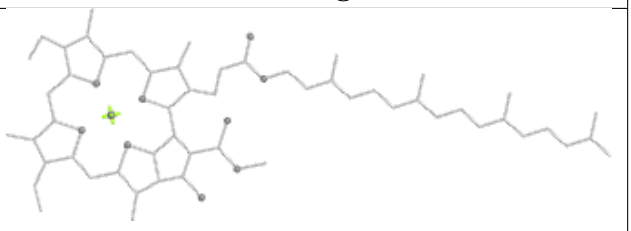
Bond lengths



Bond angles

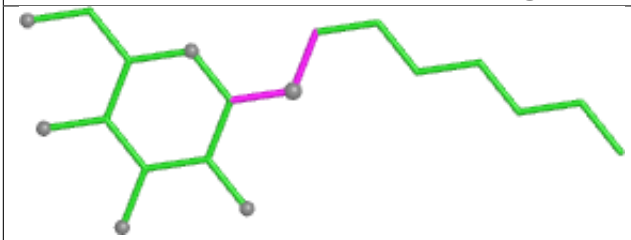


Torsions

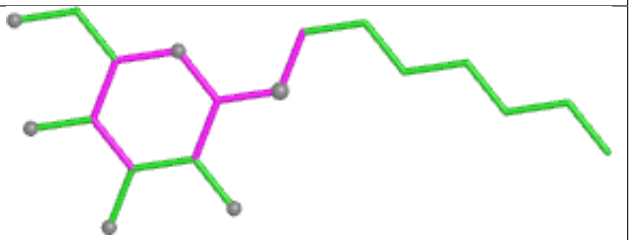


Rings

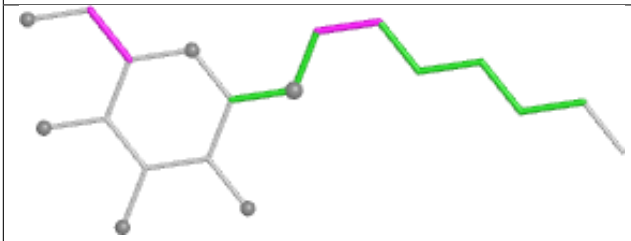
Ligand HTG C 522



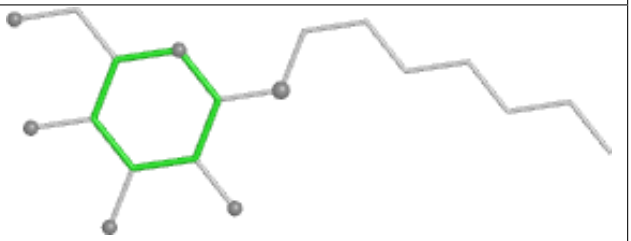
Bond lengths



Bond angles

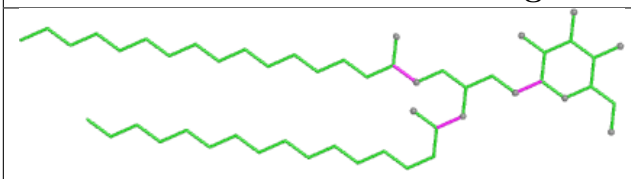


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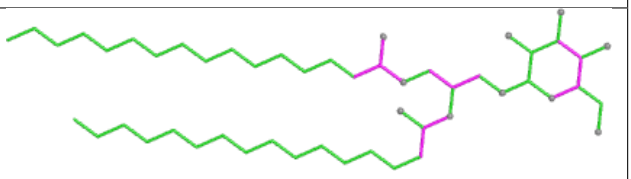


Rings

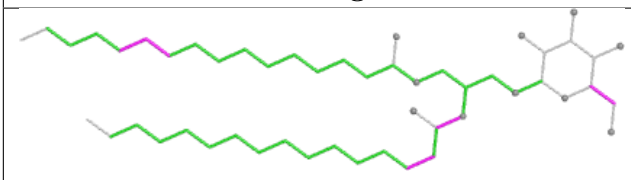
Ligand LMG c 520



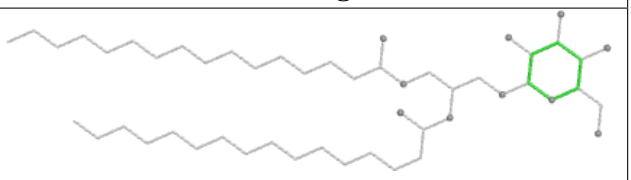
Bond lengths



Bond angles

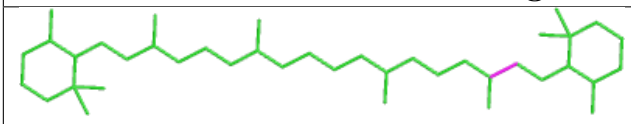


Torsions

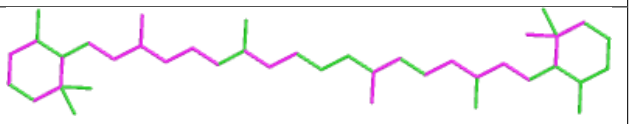


Rings

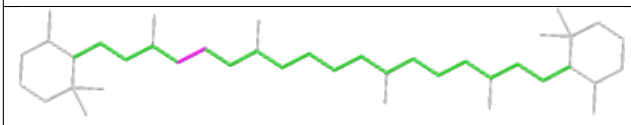
Ligand BCR k 101



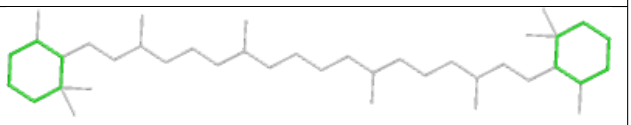
Bond lengths



Bond angles

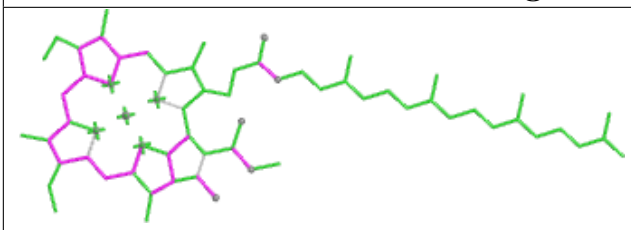


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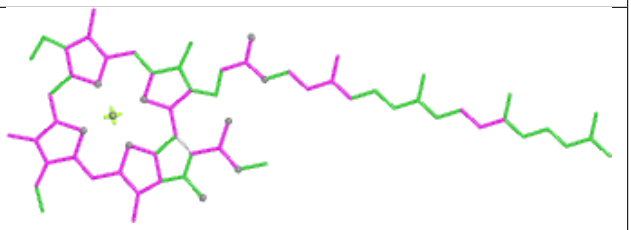


Rings

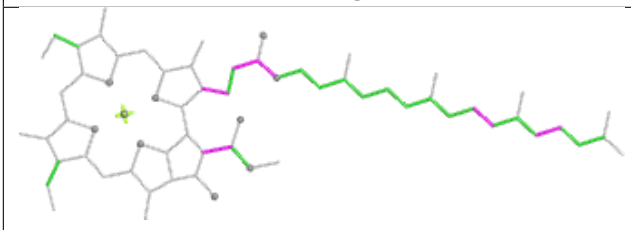
Ligand CLA B 612



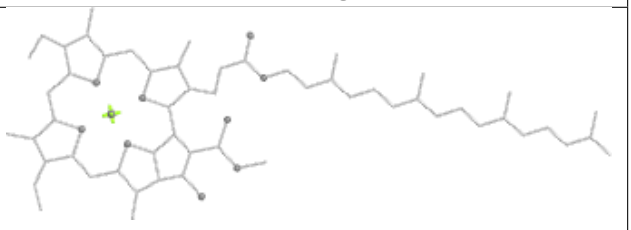
Bond lengths



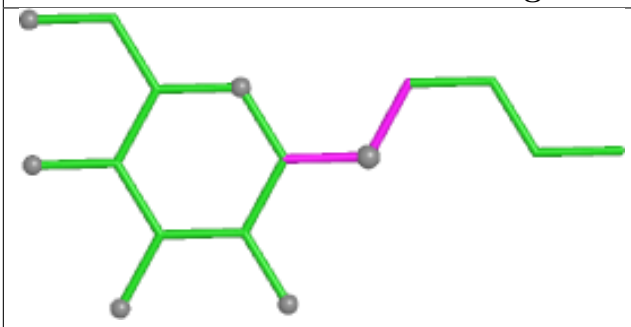
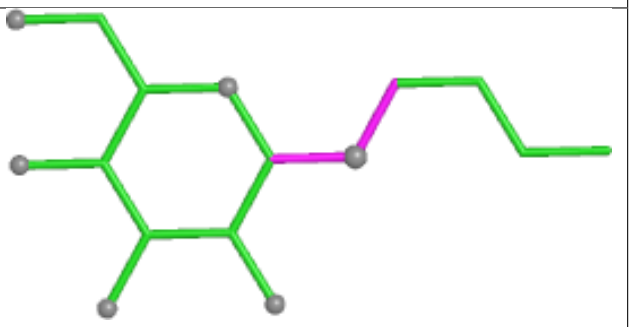
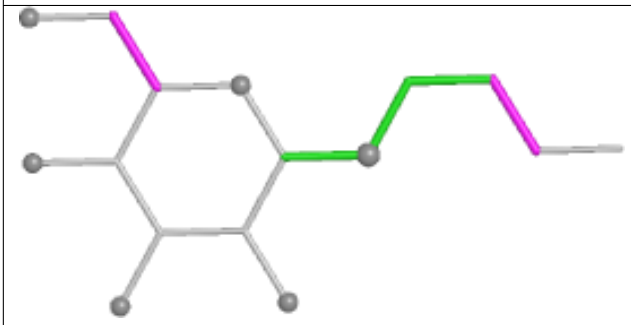
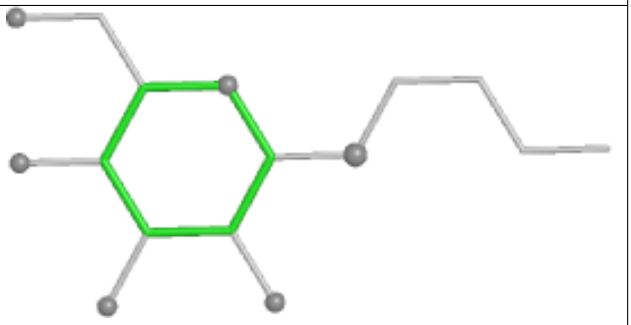
Bond angles

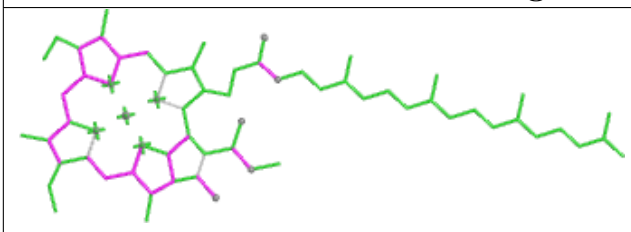
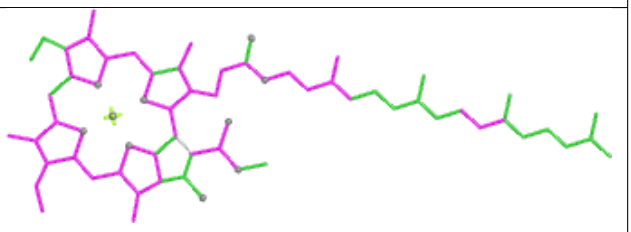
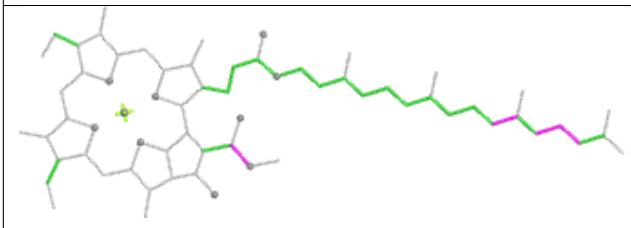
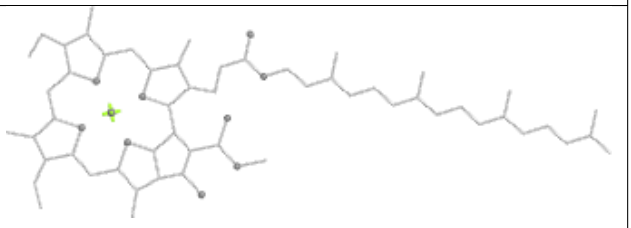


Torsions

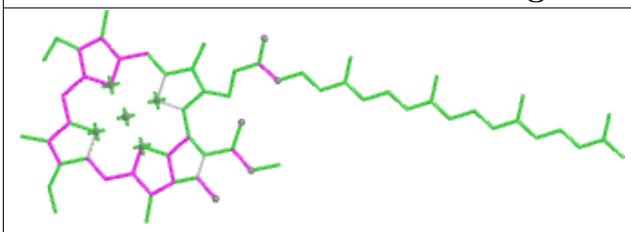


Rings

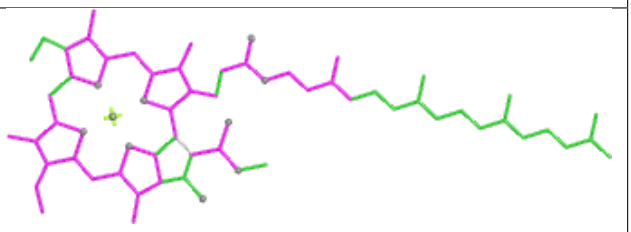
Ligand HTG d 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

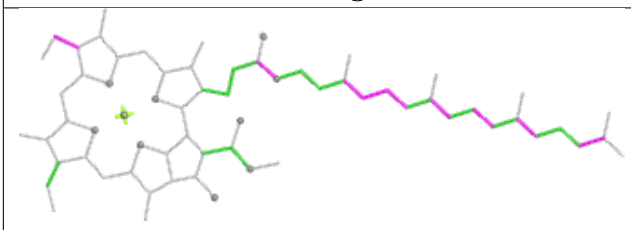
Ligand CLA d 404



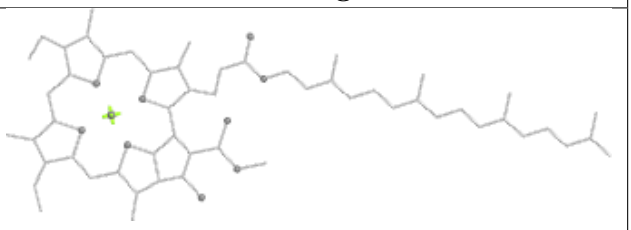
Bond lengths



Bond angles

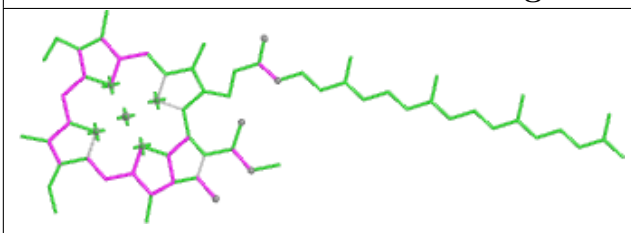


Torsions

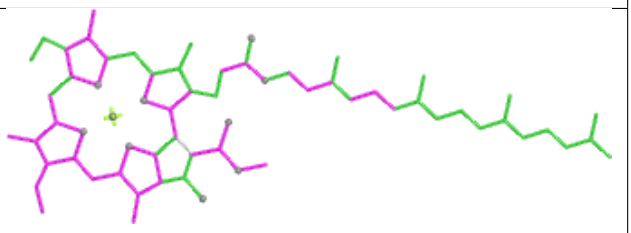


Rings

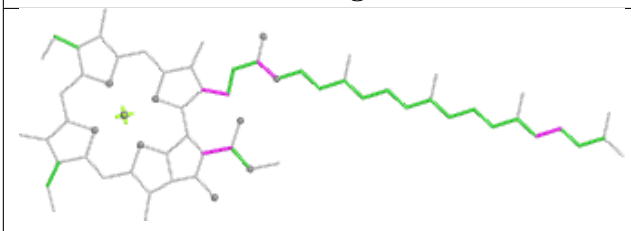
Ligand CLA B 609



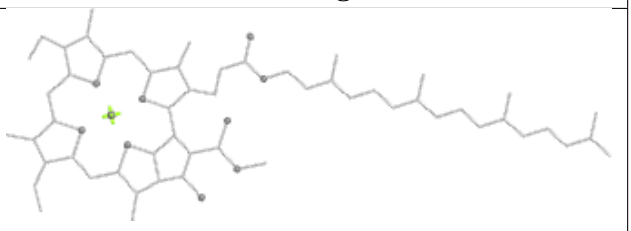
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-1.12	0	100	100	20, 31, 53, 100	3 (0%)
1	a	334/344 (97%)	-1.11	0	100	100	22, 33, 62, 108	5 (1%)
2	B	504/505 (99%)	-1.08	0	100	100	17, 36, 65, 109	8 (1%)
2	b	504/505 (99%)	-1.03	0	100	100	20, 37, 74, 118	4 (0%)
3	C	451/455 (99%)	-1.01	0	100	100	24, 45, 67, 117	4 (0%)
3	c	455/455 (100%)	-0.99	0	100	100	27, 48, 69, 109	5 (1%)
4	D	342/342 (100%)	-1.12	0	100	100	18, 32, 53, 108	1 (0%)
4	d	341/342 (99%)	-1.14	0	100	100	20, 36, 54, 123	1 (0%)
5	E	81/84 (96%)	-0.87	0	100	100	35, 54, 82, 120	1 (1%)
5	e	79/84 (94%)	-0.85	0	100	100	42, 58, 97, 120	0
6	F	34/44 (77%)	-0.97	0	100	100	38, 46, 78, 92	0
6	f	31/44 (70%)	-0.87	0	100	100	44, 50, 86, 122	0
7	H	64/65 (98%)	-0.85	1 (1%)	70	67	26, 47, 68, 101	1 (1%)
7	h	65/65 (100%)	-0.97	0	100	100	37, 51, 74, 141	0
8	I	37/38 (97%)	-0.88	0	100	100	37, 46, 88, 130	0
8	i	37/38 (97%)	-0.78	0	100	100	38, 46, 93, 135	0
9	J	38/39 (97%)	-0.98	0	100	100	32, 52, 106, 147	0
9	j	39/39 (100%)	-0.81	0	100	100	40, 51, 107, 129	0
10	K	37/37 (100%)	-1.05	0	100	100	44, 53, 76, 91	0
10	k	37/37 (100%)	-1.06	0	100	100	47, 54, 78, 93	0
11	L	36/37 (97%)	-1.16	0	100	100	15, 26, 89, 129	1 (2%)
11	l	36/37 (97%)	-1.12	0	100	100	17, 28, 87, 128	1 (2%)
12	M	32/36 (88%)	-1.12	0	100	100	16, 29, 49, 117	1 (3%)
12	m	33/36 (91%)	-1.09	0	100	100	24, 29, 72, 116	0

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Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.99	0	100	100	22, 45, 100, 157	5 (2%)
13	o	243/244 (99%)	-1.00	0	100	100	24, 46, 99, 144	2 (0%)
14	T	29/32 (90%)	-1.11	0	100	100	23, 28, 60, 96	0
14	t	29/32 (90%)	-1.12	0	100	100	23, 29, 61, 97	0
15	U	96/104 (92%)	-1.08	0	100	100	31, 40, 66, 84	0
15	u	97/104 (93%)	-1.14	0	100	100	32, 43, 68, 101	0
16	V	137/137 (100%)	-1.02	0	100	100	29, 43, 70, 100	0
16	v	137/137 (100%)	-1.02	0	100	100	34, 50, 74, 101	0
17	X	38/40 (95%)	-0.77	0	100	100	44, 56, 82, 110	0
17	x	38/40 (95%)	-0.55	0	100	100	47, 58, 83, 112	0
18	Y	29/30 (96%)	-0.50	0	100	100	56, 71, 112, 114	0
18	y	29/30 (96%)	-0.77	0	100	100	58, 70, 110, 114	0
19	Z	62/62 (100%)	-0.80	0	100	100	57, 72, 117, 152	0
19	z	62/62 (100%)	-0.55	0	100	100	60, 74, 117, 153	0
20	R	34/34 (100%)	0.41	0	100	100	89, 108, 128, 135	0
All	All	5284/5384 (98%)	-1.01	1 (0%)	100	100	15, 41, 82, 157	43 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.1

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
8	FME	I	1	10/11	0.97	0.04	31,47,56,62	0
14	FME	T	1	10/11	0.97	0.05	18,32,46,47	0
14	FME	t	1	10/11	0.97	0.04	21,32,41,71	0
8	FME	i	1	10/11	0.98	0.03	37,49,57,62	0
12	FME	m	1	10/11	0.98	0.04	30,42,63,78	0
12	FME	M	1	10/11	0.98	0.06	18,38,70,79	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	A	415	28/-	0.65	0.14	67,87,108,112	0
30	UNL	i	101	40/-	0.67	0.13	48,88,140,147	0
35	LMT	E	102	35/35	0.68	0.14	78,120,147,150	0
30	UNL	m	101	10/-	0.69	0.12	40,50,55,56	0
34	HTG	B	624	19/19	0.71	0.10	57,104,140,144	0
30	UNL	J	102	10/-	0.72	0.15	55,64,89,90	0
34	HTG	D	412	16/19	0.73	0.10	48,115,128,130	0
35	LMT	B	630	35/35	0.73	0.12	33,105,126,134	0
35	LMT	D	402	35/35	0.73	0.11	31,97,113,115	0
33	LMG	Z	101	51/55	0.73	0.11	46,105,140,150	0
34	HTG	B	623	19/19	0.75	0.14	60,84,110,115	0
34	HTG	b	622	19/19	0.75	0.14	74,95,125,130	0
34	HTG	c	521	19/19	0.75	0.10	68,112,134,140	0
30	UNL	a	415	30/-	0.76	0.11	72,90,111,118	0
30	UNL	K	101	34/-	0.77	0.10	55,96,114,125	0
35	LMT	a	417	35/35	0.77	0.11	78,114,130,131	0
35	LMT	e	102	35/35	0.77	0.12	76,134,147,156	0
26	SQD	f	101	43/54	0.78	0.11	85,111,157,164	0
30	UNL	D	411	40/-	0.78	0.11	40,77,117,122	0
35	LMT	I	101	35/35	0.79	0.10	74,108,131,141	0
35	LMT	D	403	35/35	0.79	0.09	48,91,116,117	0
35	LMT	b	621	25/35	0.79	0.10	60,99,144,148	0
34	HTG	C	521	19/19	0.79	0.10	66,101,116,120	0
35	LMT	M	103	35/35	0.80	0.10	40,120,148,154	0
34	HTG	c	522	19/19	0.80	0.11	79,124,142,146	0
30	UNL	M	102	10/-	0.80	0.10	33,52,59,69	0
34	HTG	V	203	11/19	0.80	0.09	71,92,107,108	0
33	LMG	c	520	51/55	0.81	0.09	51,102,132,138	0
34	HTG	b	623	19/19	0.81	0.10	71,109,141,169	0
34	HTG	d	411	16/19	0.81	0.11	81,112,121,122	0
30	UNL	I	102	40/-	0.82	0.11	40,85,135,142	0
30	UNL	b	629	36/-	0.83	0.09	49,80,131,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	b	626	33/-	0.83	0.10	44,78,131,135	0
30	UNL	c	525	32/-	0.84	0.10	71,97,113,119	0
30	UNL	B	628	33/-	0.84	0.10	29,76,136,139	0
30	UNL	j	102	10/-	0.84	0.11	60,75,88,89	0
34	HTG	C	522	19/19	0.84	0.09	58,139,157,179	0
29	PL9	A	414	55/55	0.85	0.13	41,88,105,119	0
35	LMT	M	101	35/35	0.85	0.08	39,80,103,109	0
33	LMG	Z	102	37/55	0.85	0.10	47,97,129,137	0
26	SQD	a	412	54/54	0.86	0.08	44,73,125,133	0
31	LHG	E	101	42/49	0.86	0.09	41,93,108,124	0
31	LHG	e	101	42/49	0.86	0.09	81,118,142,148	0
35	LMT	m	102	35/35	0.86	0.09	34,78,102,109	0
35	LMT	B	629	25/35	0.87	0.10	34,68,124,125	0
27	GOL	a	411	6/6	0.87	0.11	52,60,62,66	0
26	SQD	A	412	54/54	0.87	0.07	39,65,102,118	0
29	PL9	a	414	55/55	0.87	0.12	57,93,112,120	0
34	HTG	b	628	19/19	0.88	0.10	34,65,115,119	0
26	SQD	B	620	54/54	0.89	0.08	41,73,108,113	0
27	GOL	b	624	6/6	0.89	0.08	58,76,78,86	0
34	HTG	B	627	19/19	0.89	0.07	45,63,74,75	0
27	GOL	d	402	6/6	0.89	0.21	33,50,65,68	0
33	LMG	z	101	39/55	0.89	0.10	63,112,140,147	0
33	LMG	C	501	51/55	0.90	0.08	35,74,98,102	0
26	SQD	D	413	43/54	0.90	0.09	64,97,112,116	0
30	UNL	D	410	17/-	0.90	0.08	44,56,91,100	0
30	UNL	x	101	18/-	0.90	0.09	44,63,91,92	0
26	SQD	L	101	54/54	0.90	0.07	47,71,116,121	0
27	GOL	B	626	6/6	0.90	0.12	38,51,55,62	0
25	BCR	D	406	40/40	0.91	0.07	32,42,87,90	0
33	LMG	a	416	51/55	0.91	0.07	41,77,102,118	0
33	LMG	c	519	51/55	0.91	0.08	43,77,114,124	0
35	LMT	b	627	25/35	0.91	0.08	29,61,134,139	0
27	GOL	C	523	6/6	0.91	0.10	44,54,59,60	0
25	BCR	y	101	40/40	0.91	0.07	44,54,70,72	0
35	LMT	B	631	26/35	0.92	0.08	52,80,105,109	0
23	CLA	b	601	65/65	0.92	0.07	43,69,99,126	0
27	GOL	A	411	6/6	0.92	0.07	50,58,65,79	0
33	LMG	C	520	51/55	0.92	0.08	37,69,104,121	0
34	HTG	B	622	19/19	0.93	0.07	34,61,127,132	0
25	BCR	d	405	40/40	0.93	0.07	40,50,74,81	0
23	CLA	c	513	65/65	0.93	0.07	52,73,115,119	0
23	CLA	B	601	65/65	0.93	0.07	39,57,88,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LMG	J	101	51/55	0.93	0.07	30,51,88,99	0
33	LMG	j	101	51/55	0.93	0.07	37,53,102,123	0
27	GOL	B	625	6/6	0.93	0.09	48,76,85,89	0
36	DGD	c	517	62/66	0.93	0.06	38,53,112,129	0
37	CA	V	201	1/1	0.93	0.05	93,93,93,93	0
26	SQD	a	410	54/54	0.94	0.07	41,64,98,105	0
25	BCR	K	102	40/40	0.94	0.07	39,47,62,65	0
25	BCR	Y	101	40/40	0.94	0.07	37,49,59,62	0
23	CLA	c	504	65/65	0.94	0.07	37,50,89,111	0
30	UNL	d	410	17/-	0.94	0.06	42,57,85,90	0
33	LMG	b	620	51/55	0.94	0.06	29,50,88,106	0
23	CLA	C	514	65/65	0.94	0.07	46,64,87,95	0
34	HTG	b	625	19/19	0.94	0.06	43,56,83,93	0
26	SQD	A	410	54/54	0.94	0.07	38,62,99,105	0
25	BCR	B	619	40/40	0.94	0.06	28,42,63,67	0
25	BCR	C	515	40/40	0.94	0.07	46,61,72,73	0
23	CLA	C	507	65/65	0.94	0.07	39,55,102,106	0
36	DGD	c	516	62/66	0.94	0.06	33,43,73,95	0
25	BCR	H	101	40/40	0.94	0.06	33,42,63,67	0
30	UNL	X	101	18/-	0.94	0.08	40,53,83,90	0
29	PL9	d	406	55/55	0.95	0.06	23,30,41,58	0
25	BCR	k	101	40/40	0.95	0.07	47,55,79,81	0
25	BCR	t	101	40/40	0.95	0.05	19,42,59,62	0
23	CLA	b	616	65/65	0.95	0.07	31,46,98,105	0
23	CLA	C	513	65/65	0.95	0.07	43,59,94,101	0
23	CLA	c	506	65/65	0.95	0.06	44,58,90,111	0
23	CLA	c	507	65/65	0.95	0.07	41,53,65,68	0
25	BCR	T	101	40/40	0.95	0.05	20,36,45,53	0
31	LHG	A	416	49/49	0.95	0.06	26,44,61,77	0
31	LHG	D	409	49/49	0.95	0.07	29,47,107,124	0
23	CLA	C	505	65/65	0.95	0.06	30,41,79,104	0
36	DGD	C	518	62/66	0.95	0.06	29,46,103,110	0
25	BCR	c	514	40/40	0.95	0.06	52,65,76,79	0
33	LMG	B	621	51/55	0.95	0.06	32,49,79,105	0
36	DGD	c	518	62/66	0.95	0.05	36,46,77,96	0
23	CLA	B	606	65/65	0.95	0.06	26,35,76,99	0
37	CA	c	523	1/1	0.95	0.07	68,68,68,68	0
25	BCR	b	617	40/40	0.96	0.04	20,34,41,44	0
25	BCR	b	618	40/40	0.96	0.04	21,34,49,55	0
25	BCR	b	619	40/40	0.96	0.05	32,45,61,69	0
31	LHG	d	407	49/49	0.96	0.06	25,44,72,87	0
31	LHG	d	409	49/49	0.96	0.07	33,50,98,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	PL9	D	407	55/55	0.96	0.05	20,31,45,54	0
31	LHG	l	101	49/49	0.96	0.05	25,38,55,60	0
23	CLA	B	614	65/65	0.96	0.06	21,31,82,100	0
25	BCR	c	515	40/40	0.96	0.05	37,52,65,75	0
23	CLA	B	616	65/65	0.96	0.07	30,45,113,124	0
25	BCR	h	101	40/40	0.96	0.06	39,50,64,77	0
23	CLA	c	508	65/65	0.96	0.06	35,48,107,118	0
23	CLA	c	511	65/65	0.96	0.07	43,56,74,82	0
23	CLA	c	512	65/65	0.96	0.06	48,64,90,96	0
23	CLA	D	405	65/65	0.96	0.07	31,46,99,111	0
23	CLA	d	404	65/65	0.96	0.07	38,48,98,109	0
24	PHO	a	407	64/64	0.96	0.05	28,35,50,52	0
25	BCR	A	409	40/40	0.96	0.05	22,34,46,49	0
25	BCR	B	618	40/40	0.96	0.04	21,36,54,69	0
23	CLA	a	405	65/65	0.96	0.06	27,36,105,111	0
23	CLA	a	408	65/65	0.96	0.08	28,40,107,115	0
36	DGD	C	517	62/66	0.96	0.05	27,36,81,92	0
25	BCR	C	516	40/40	0.96	0.05	36,48,66,73	0
36	DGD	C	519	62/66	0.96	0.05	28,44,71,95	0
23	CLA	B	602	65/65	0.96	0.05	29,37,55,67	0
23	CLA	b	606	65/65	0.96	0.05	27,42,77,106	0
23	CLA	A	408	65/65	0.96	0.06	26,36,101,109	0
23	CLA	c	501	65/65	0.96	0.05	38,49,64,71	0
23	CLA	C	509	65/65	0.96	0.06	30,43,102,115	0
23	CLA	b	608	65/65	0.97	0.04	32,41,60,68	0
25	BCR	a	409	40/40	0.97	0.04	24,35,45,49	0
23	CLA	b	609	65/65	0.97	0.05	36,44,63,82	0
23	CLA	b	611	65/65	0.97	0.04	25,34,49,61	0
23	CLA	b	612	65/65	0.97	0.05	25,35,48,59	0
23	CLA	b	614	65/65	0.97	0.05	23,34,76,89	0
23	CLA	b	615	65/65	0.97	0.05	29,40,66,81	0
23	CLA	B	609	65/65	0.97	0.05	29,39,53,63	0
23	CLA	C	506	65/65	0.97	0.05	31,40,71,78	0
23	CLA	c	502	65/65	0.97	0.05	37,48,68,73	0
23	CLA	c	503	65/65	0.97	0.05	40,51,63,78	0
23	CLA	B	610	65/65	0.97	0.06	27,36,52,69	0
23	CLA	c	505	65/65	0.97	0.05	32,45,68,86	0
23	CLA	C	508	65/65	0.97	0.05	36,47,60,70	0
23	CLA	B	611	65/65	0.97	0.04	23,30,41,45	0
23	CLA	C	510	65/65	0.97	0.06	36,47,67,69	0
31	LHG	A	417	49/49	0.97	0.05	23,37,55,66	0
31	LHG	D	408	49/49	0.97	0.06	22,34,51,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	c	509	65/65	0.97	0.06	43,52,66,73	0
23	CLA	c	510	65/65	0.97	0.05	39,47,62,66	0
23	CLA	C	511	65/65	0.97	0.04	33,44,57,61	0
31	LHG	d	408	49/49	0.97	0.05	24,35,53,70	0
23	CLA	C	512	65/65	0.97	0.06	36,52,73,84	0
23	CLA	B	613	65/65	0.97	0.04	21,29,68,78	0
23	CLA	B	603	65/65	0.97	0.05	26,39,52,57	0
24	PHO	A	407	64/64	0.97	0.05	23,31,46,51	0
23	CLA	D	404	65/65	0.97	0.05	20,26,46,52	0
23	CLA	B	615	65/65	0.97	0.04	27,34,61,68	0
25	BCR	B	617	40/40	0.97	0.04	22,31,46,49	0
23	CLA	A	406	65/65	0.97	0.05	22,29,80,89	0
23	CLA	C	502	65/65	0.97	0.05	34,41,60,77	0
23	CLA	C	503	65/65	0.97	0.06	31,42,55,73	0
36	DGD	H	102	62/66	0.97	0.05	26,40,58,66	0
23	CLA	b	602	65/65	0.97	0.05	32,44,60,68	0
23	CLA	b	603	65/65	0.97	0.05	30,40,53,74	0
23	CLA	b	604	65/65	0.97	0.05	23,31,85,96	0
36	DGD	h	102	62/66	0.97	0.05	31,46,62,73	0
23	CLA	C	504	65/65	0.97	0.05	36,44,65,75	0
23	CLA	b	607	65/65	0.97	0.05	20,31,53,63	0
23	CLA	B	604	65/65	0.98	0.05	21,29,92,104	0
23	CLA	B	612	65/65	0.98	0.05	24,29,42,51	0
23	CLA	B	605	65/65	0.98	0.04	22,30,44,48	0
23	CLA	b	605	65/65	0.98	0.05	24,34,52,97	0
23	CLA	d	401	65/65	0.98	0.04	23,26,48,75	0
23	CLA	d	403	65/65	0.98	0.05	25,29,49,62	0
23	CLA	A	405	65/65	0.98	0.04	19,23,41,47	0
23	CLA	B	607	65/65	0.98	0.04	18,27,54,66	0
24	PHO	D	401	64/64	0.98	0.04	21,27,35,45	0
24	PHO	a	406	64/64	0.98	0.04	22,31,40,51	0
23	CLA	a	404	65/65	0.98	0.05	25,30,50,60	0
23	CLA	B	608	65/65	0.98	0.03	27,37,51,55	0
23	CLA	b	610	65/65	0.98	0.04	30,42,51,60	0
22	CL	a	403	1/1	0.98	0.04	34,34,34,34	0
23	CLA	A	404	65/65	0.98	0.04	20,23,41,58	0
37	CA	O	301	1/1	0.98	0.05	87,87,87,87	0
23	CLA	b	613	65/65	0.98	0.04	22,33,67,78	0
32	BCT	a	418	4/4	0.98	0.04	45,52,54,59	0
37	CA	o	301	1/1	0.98	0.02	85,85,85,85	0
38	HEM	E	103	43/43	0.98	0.06	40,54,66,73	0
38	HEM	e	103	43/43	0.98	0.07	48,73,98,105	0

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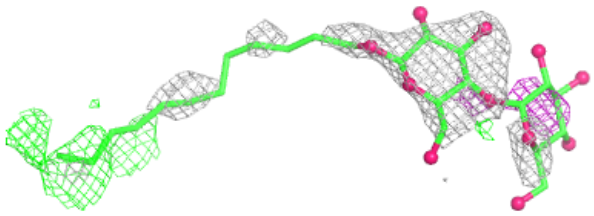
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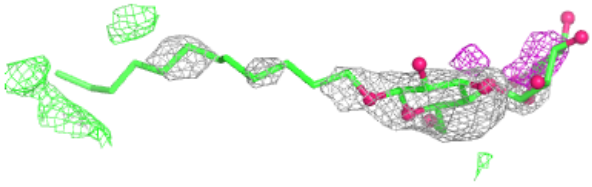
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
39	MG	j	103	1/1	0.98	0.07	51,51,51,51	0
40	HEC	v	201	43/43	0.98	0.05	40,50,59,66	0
22	CL	A	402	1/1	0.99	0.06	24,24,24,24	0
22	CL	A	403	1/1	0.99	0.01	27,27,27,27	0
37	CA	c	524	1/1	0.99	0.05	66,66,66,66	0
32	BCT	A	418	4/4	0.99	0.04	34,39,47,65	0
22	CL	a	402	1/1	0.99	0.04	31,31,31,31	0
21	FE2	A	401	1/1	0.99	0.03	42,42,42,42	0
39	MG	J	103	1/1	0.99	0.08	39,39,39,39	0
37	CA	C	524	1/1	0.99	0.08	62,62,62,62	0
40	HEC	V	202	43/43	0.99	0.04	30,33,44,53	0
21	FE2	a	401	1/1	0.99	0.05	45,45,45,45	0
28	OEX	a	413	10/10	1.00	0.02	27,34,45,53	0
28	OEX	A	413	10/10	1.00	0.02	22,30,43,45	0

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

Electron density around LMT 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)

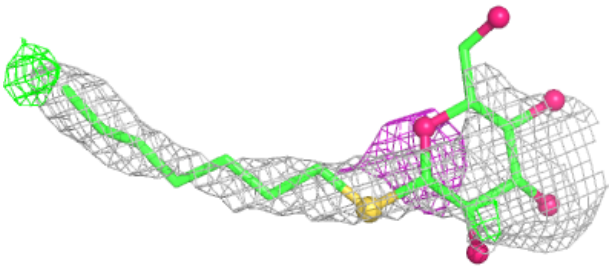


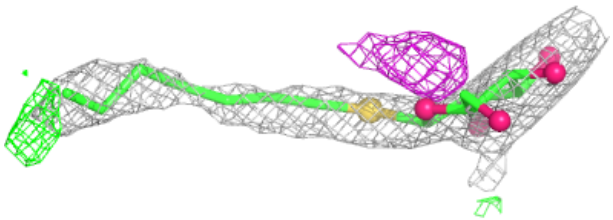


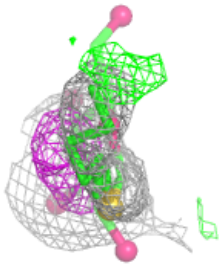


Electron density around HTG B 624:

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

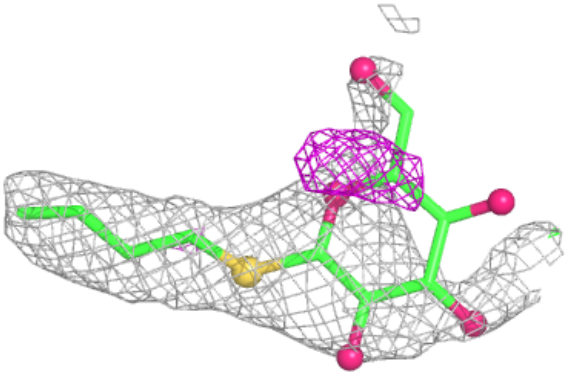


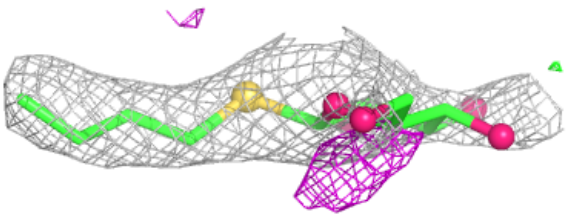


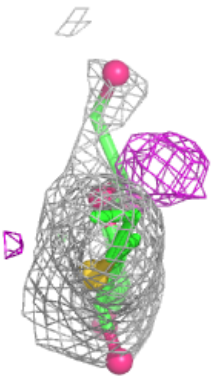


Electron density around HTG D 412:

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

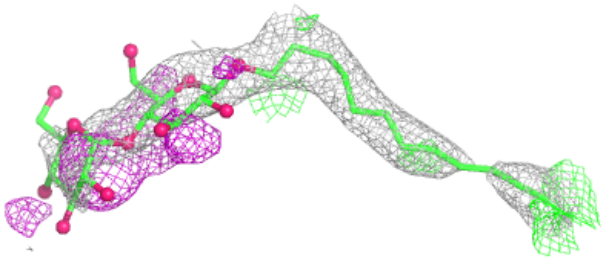


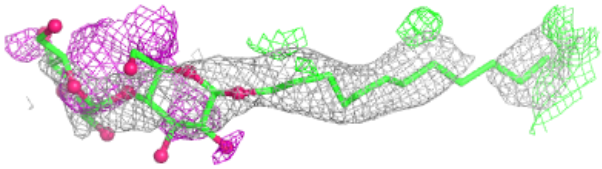


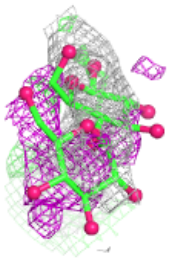


Electron density around LMT B 630:

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

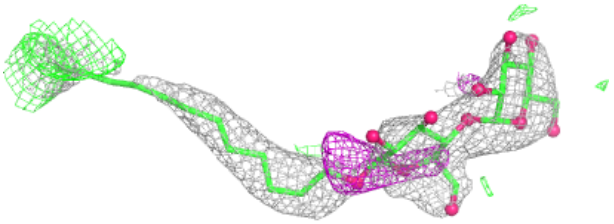


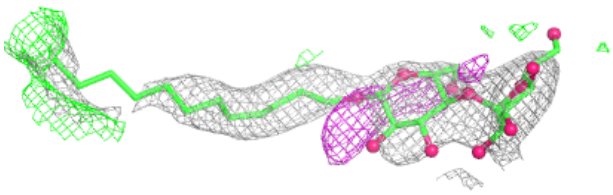


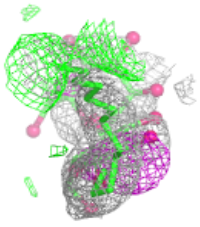


Electron density around LMT D 402:

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

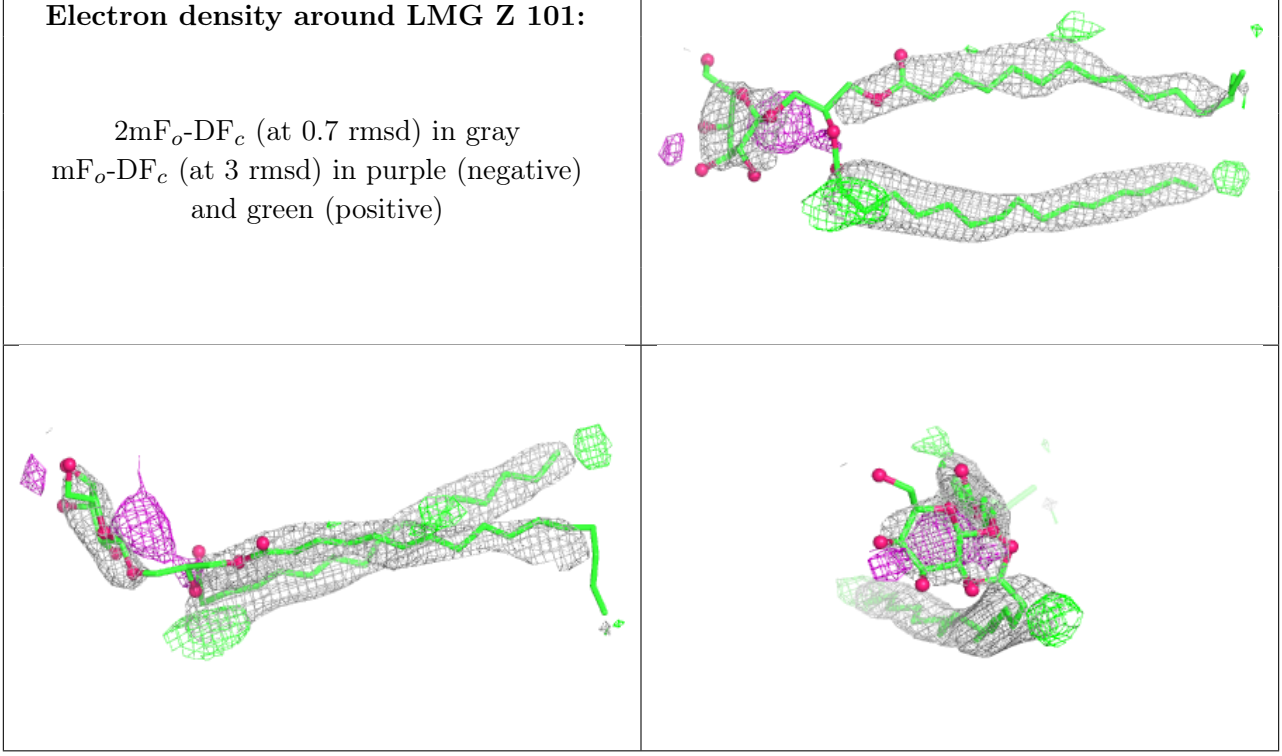






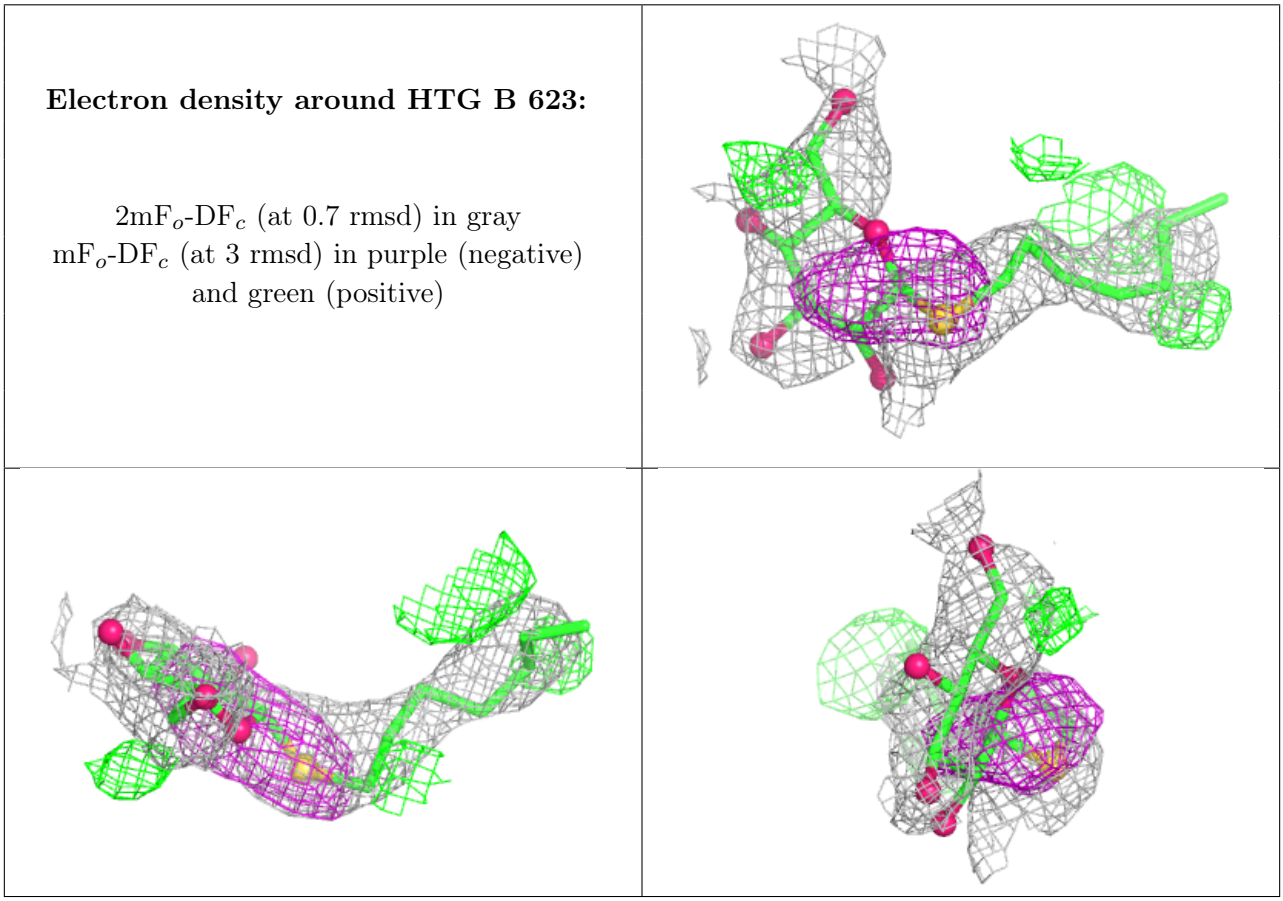
Electron density around LMG Z 101:

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



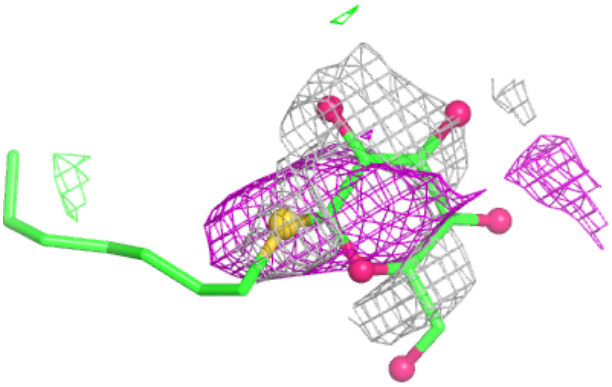
Electron density around HTG B 623:

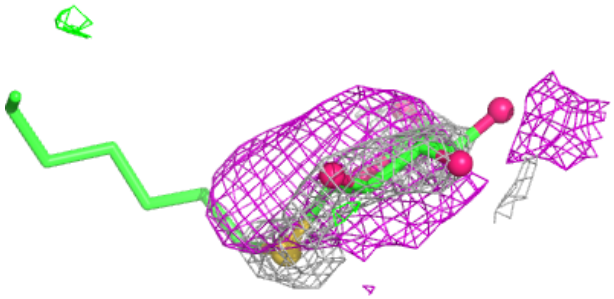
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

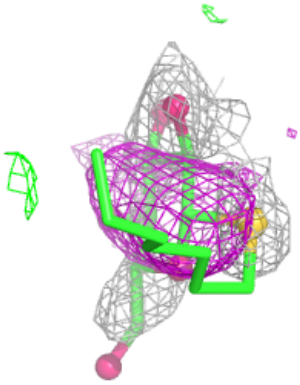


Electron density around HTG b 622:

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

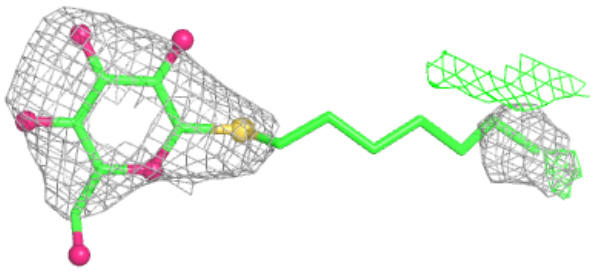


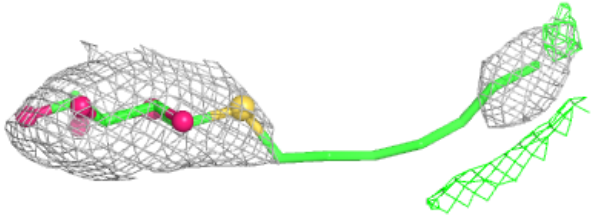


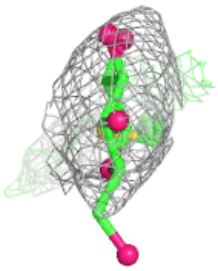


Electron density around HTG c 521:

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

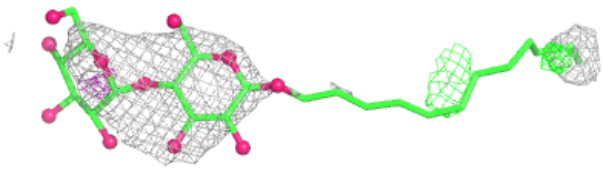


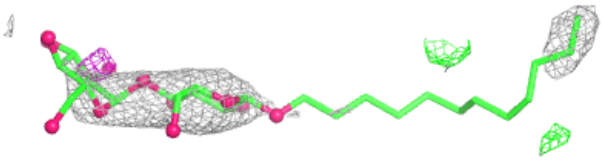


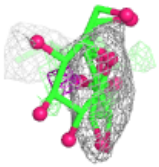


Electron density around LMT a 417:

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

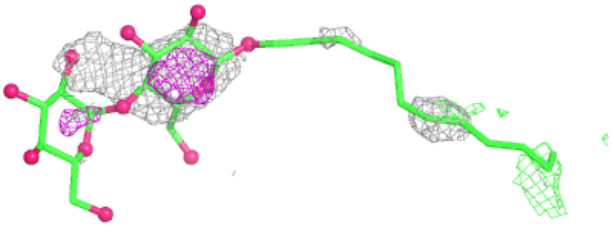


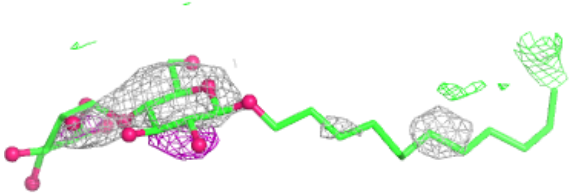


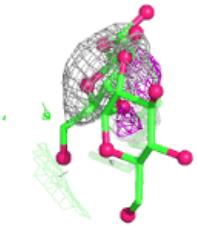


Electron density around LMT e 102:

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

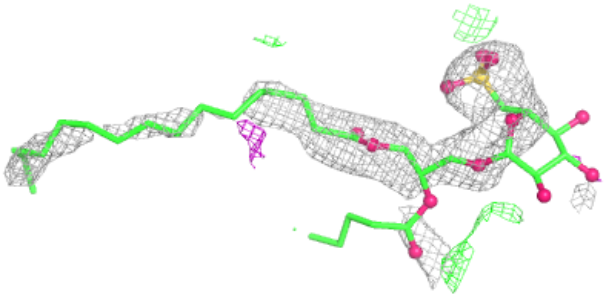


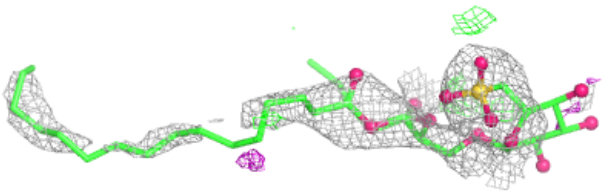




Electron density around SQD f 101:

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

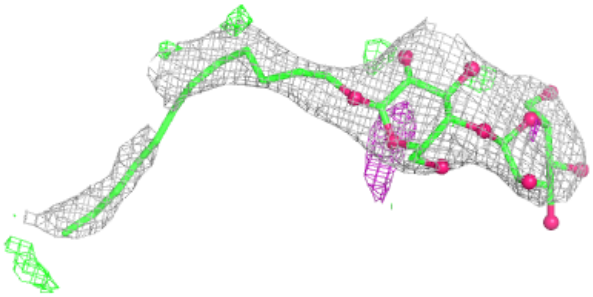


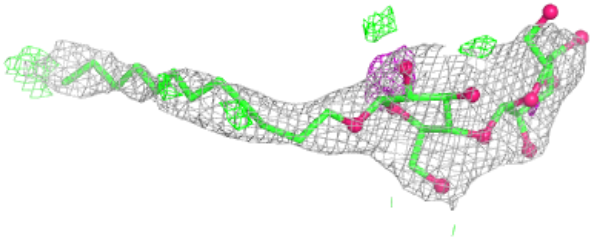


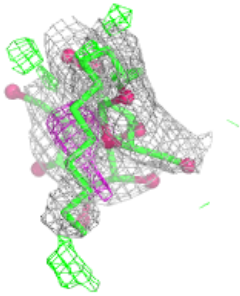


Electron density around LMT I 101:

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

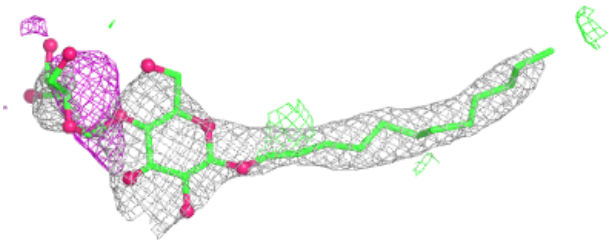


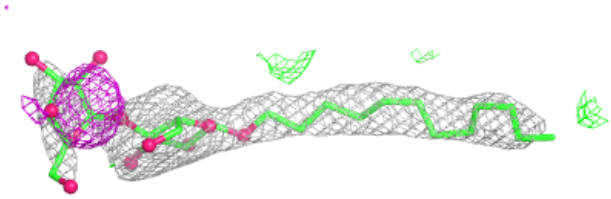


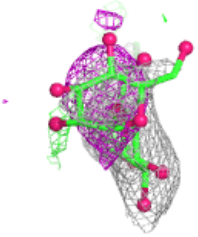


Electron density around LMT D 403:

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

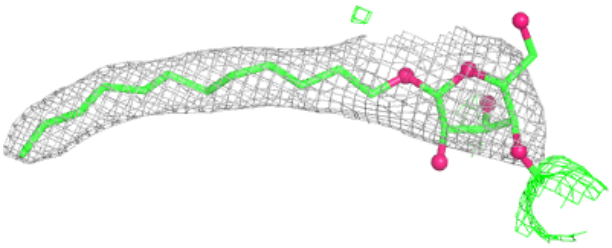


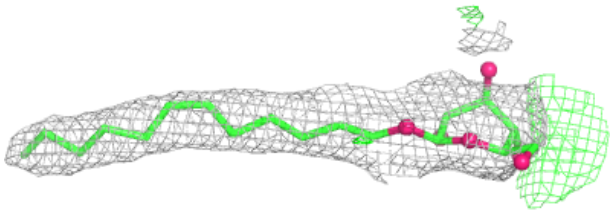


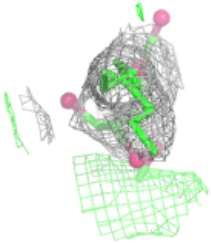


Electron density around LMT b 621:

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

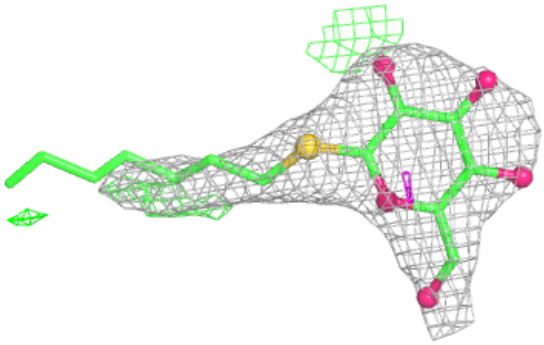


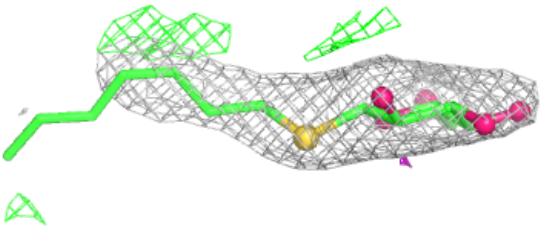


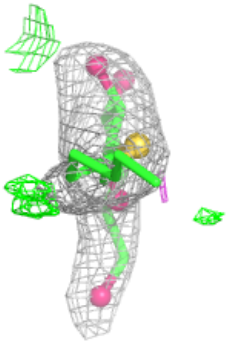


Electron density around HTG C 521:

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

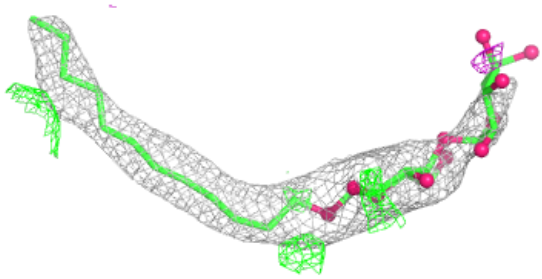


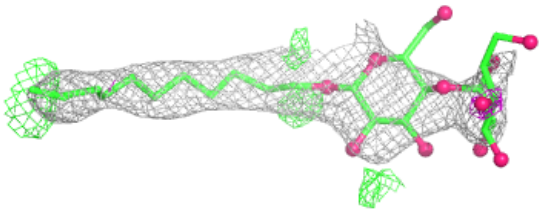


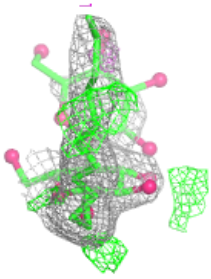


Electron density around LMT M 103:

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

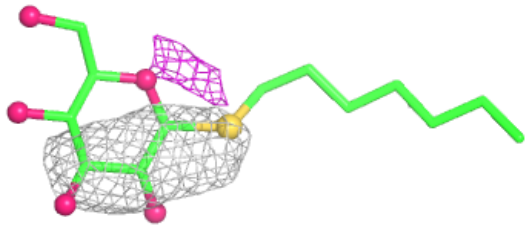


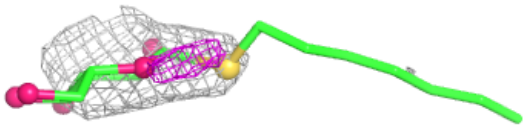


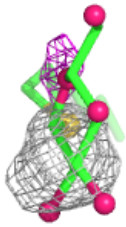


Electron density around HTG c 522:

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

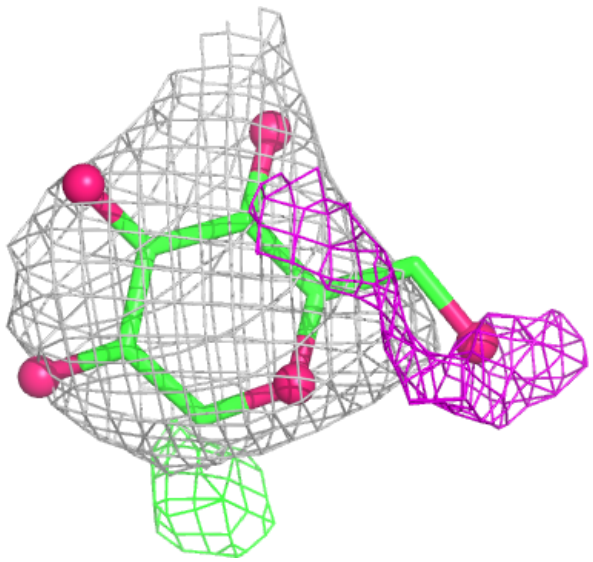


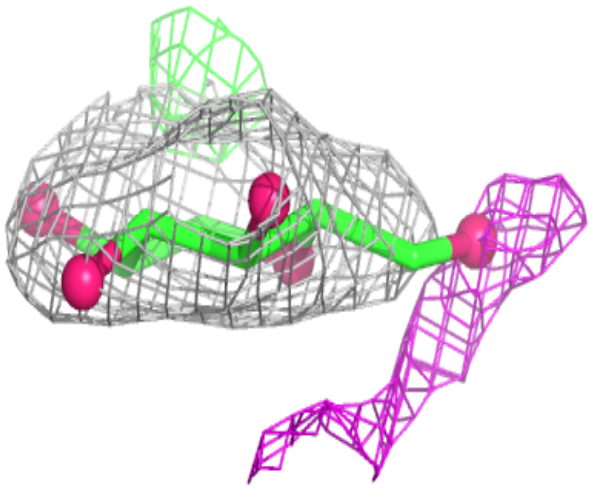


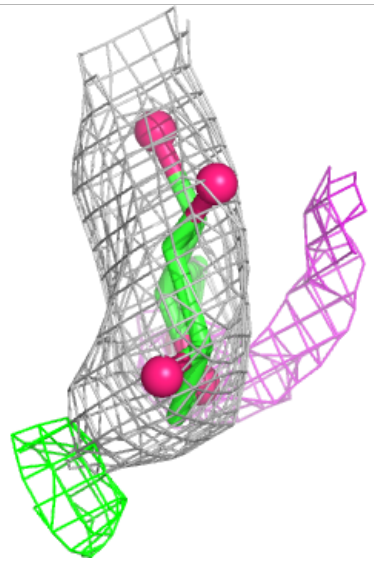


Electron density around HTG V 203:

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

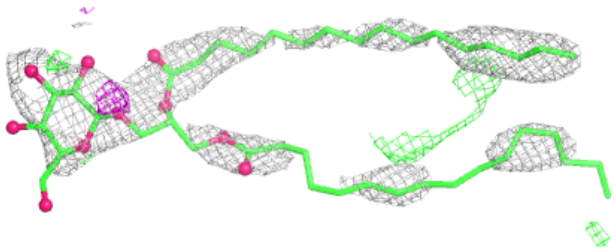


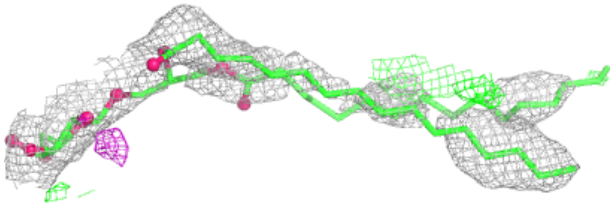


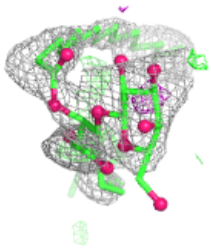


Electron density around LMG c 520:

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

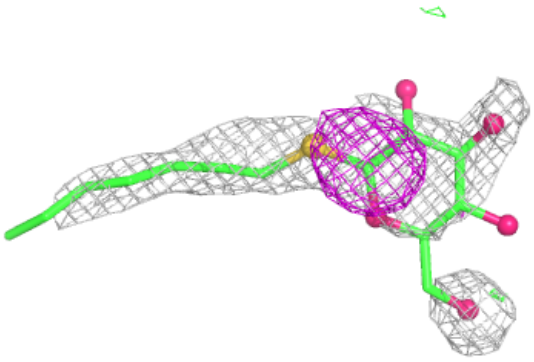


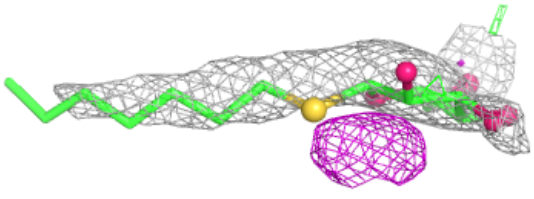


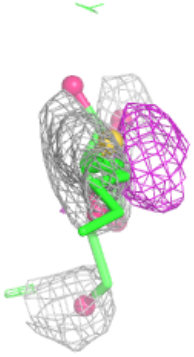


Electron density around HTG b 623:

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

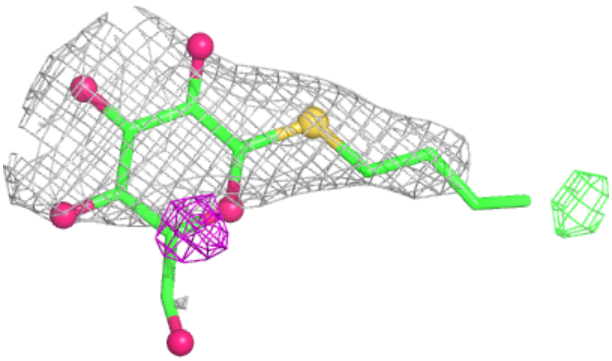


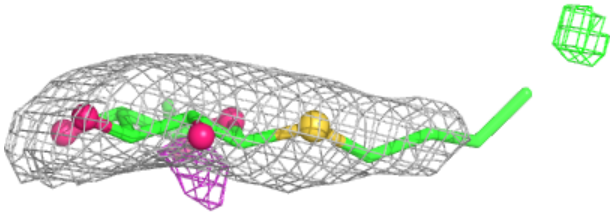


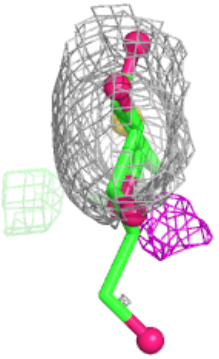


Electron density around HTG d 411:

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

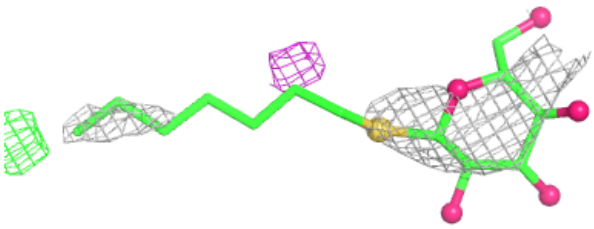


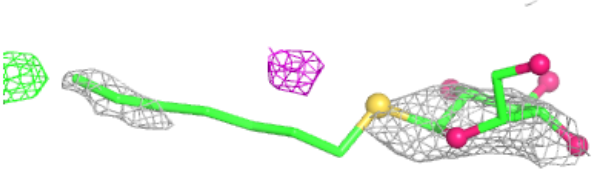


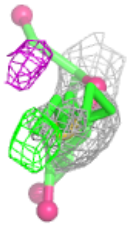


Electron density around HTG C 522:

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

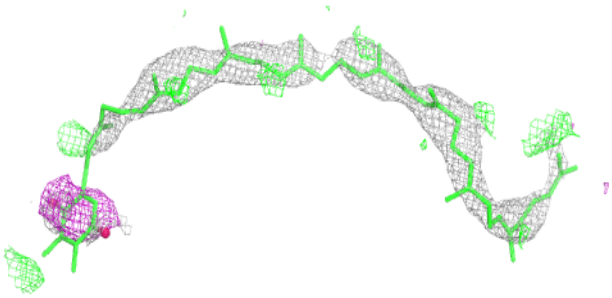


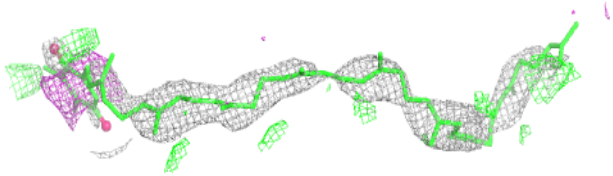


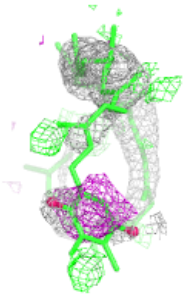


Electron density around PL9 A 414:

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

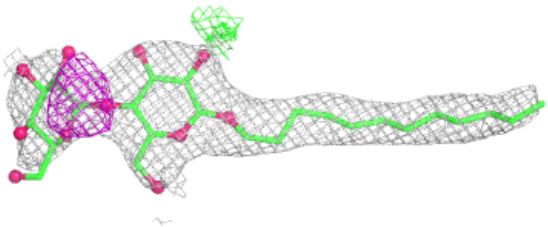


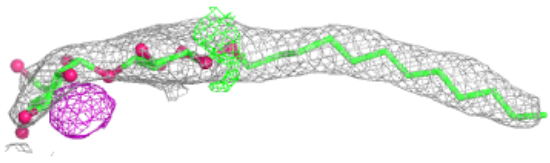


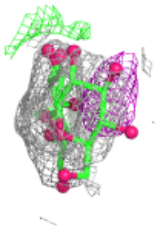


Electron density around LMT M 101:

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

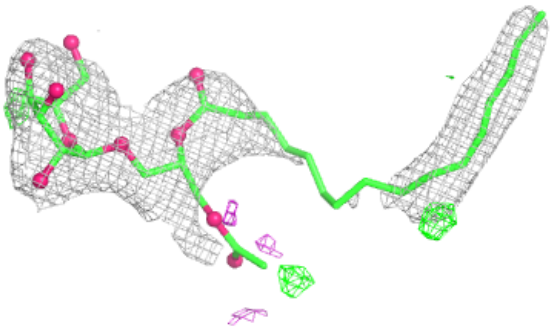


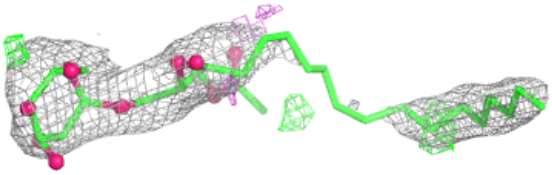


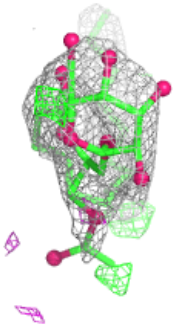


Electron density around LMG Z 102:

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

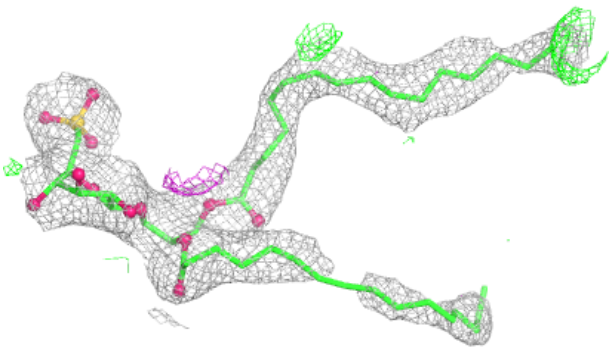


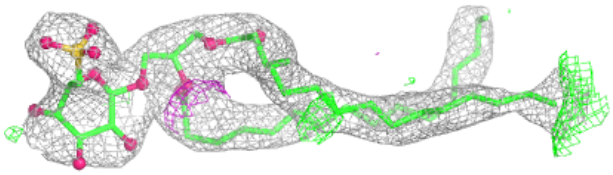


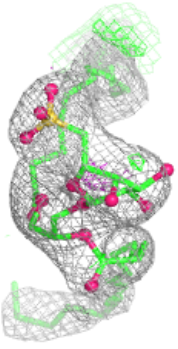


Electron density around SQD a 412:

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

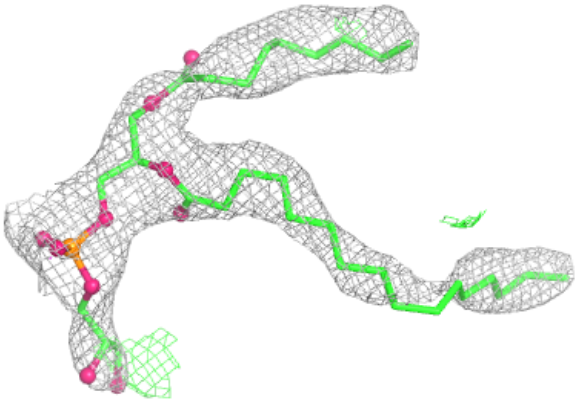


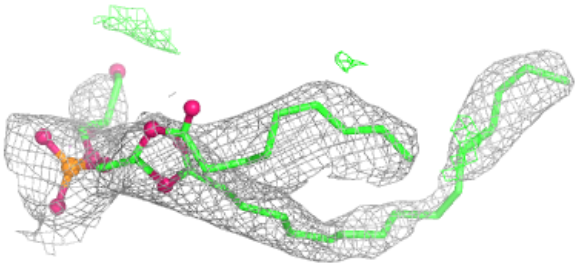


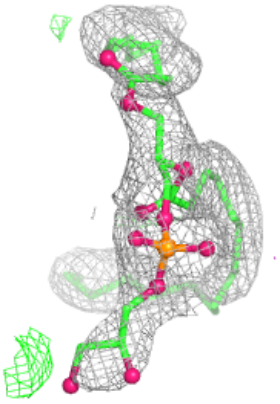


Electron density around LHG E 101:

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

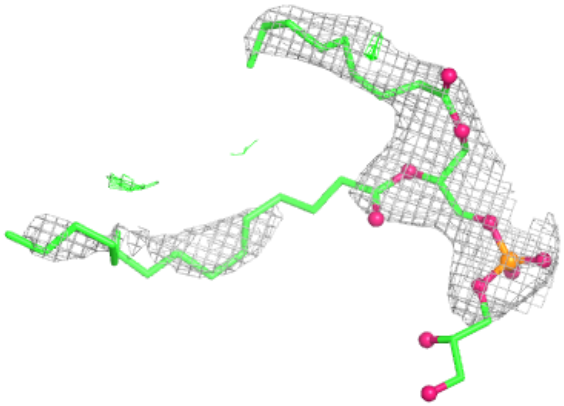


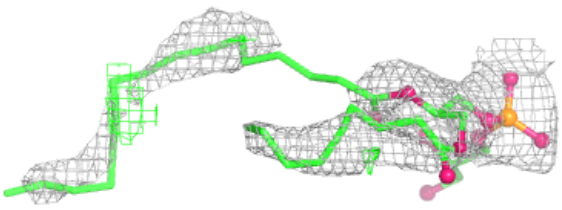


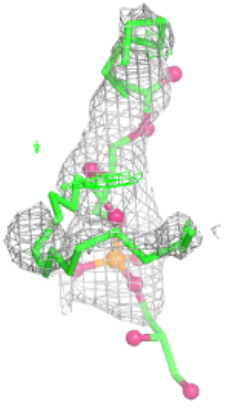


Electron density around LHG e 101:

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

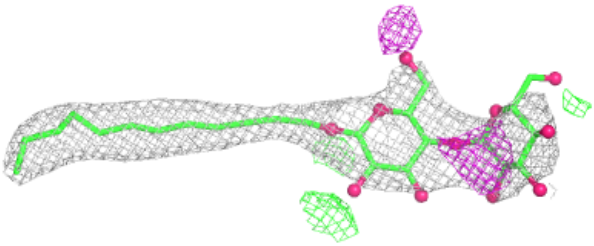


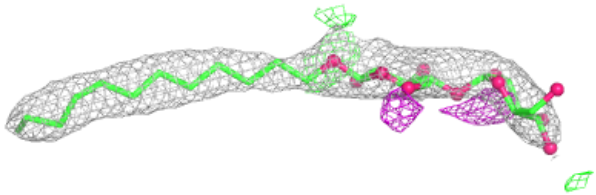


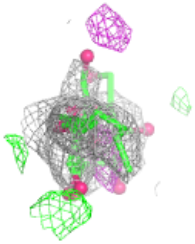


Electron density around LMT m 102:

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

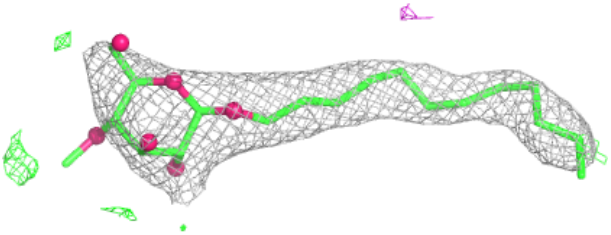


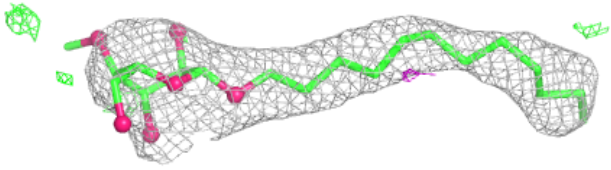


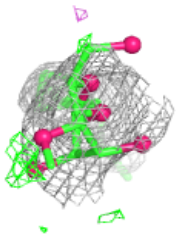


Electron density around LMT B 629:

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

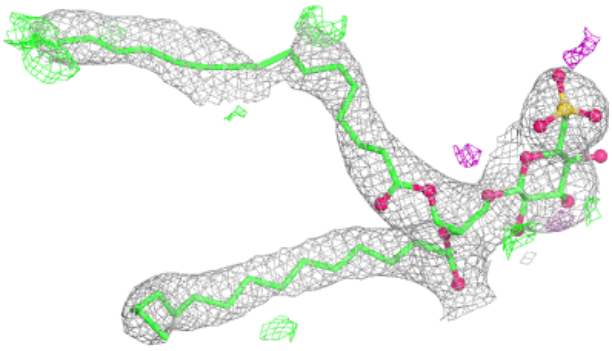


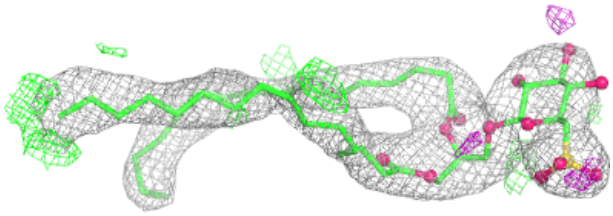


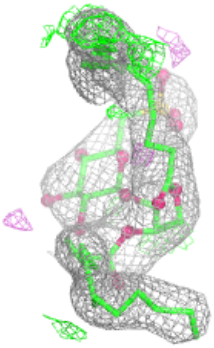


Electron density around SQD A 412:

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

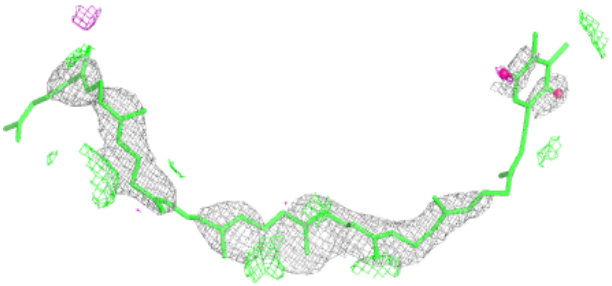


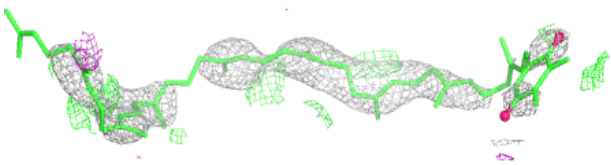


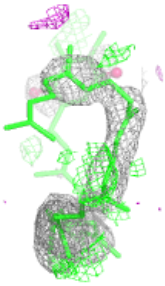


Electron density around PL9 a 414:

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

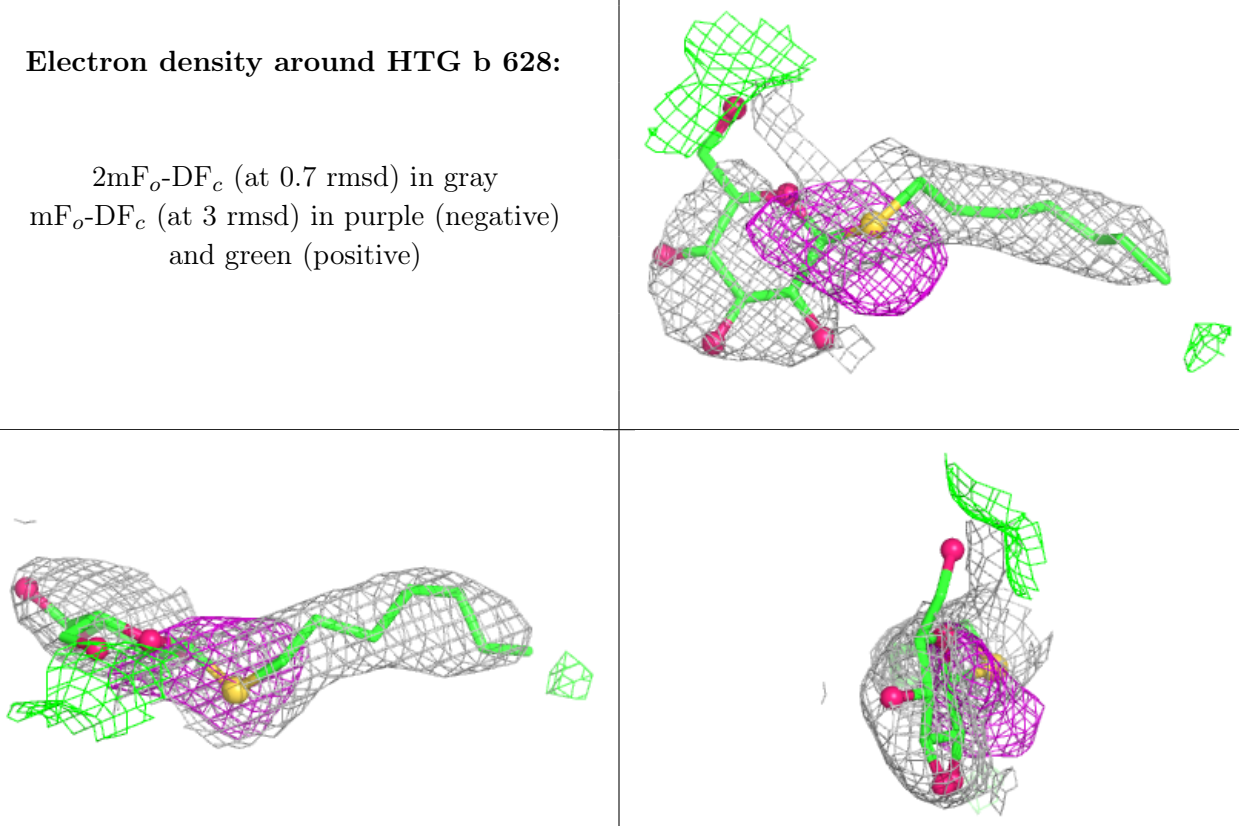






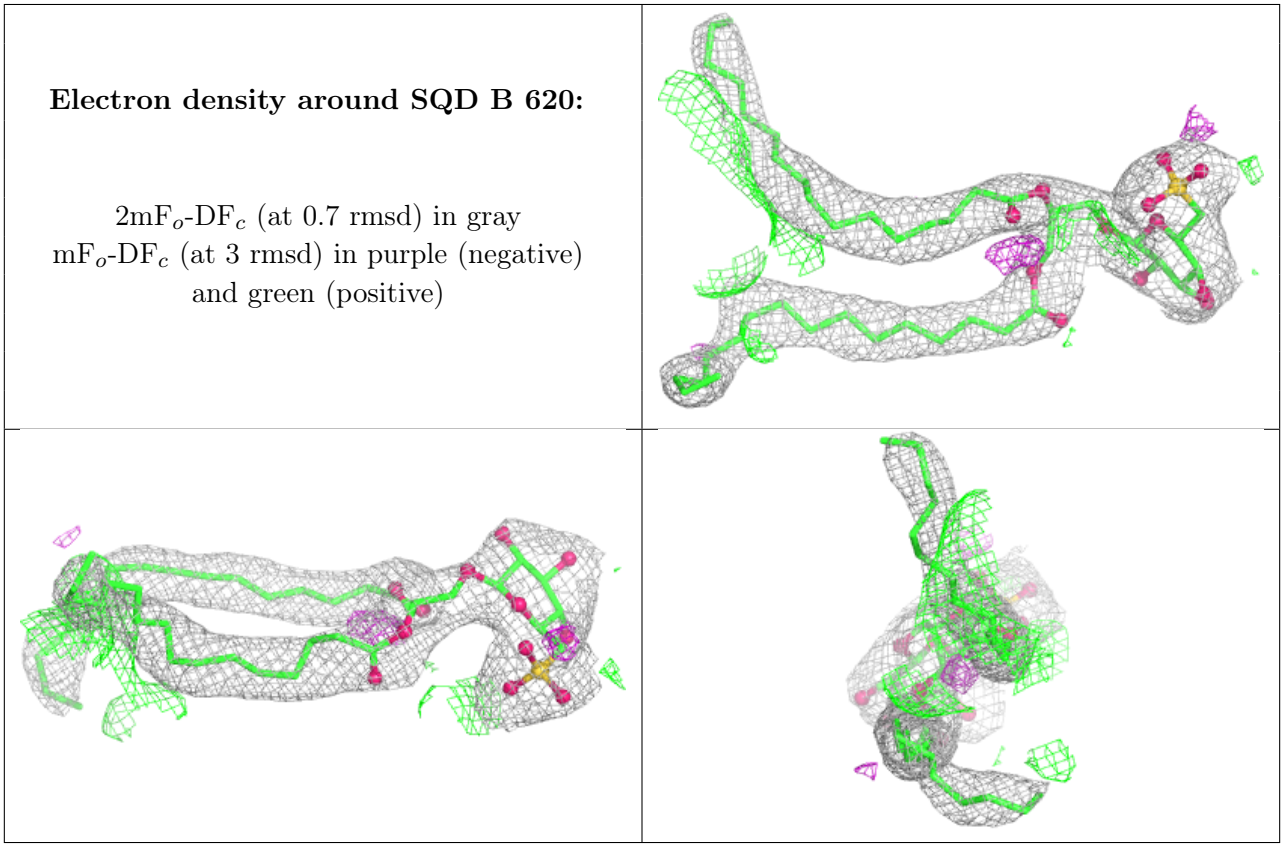
Electron density around HTG b 628:

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



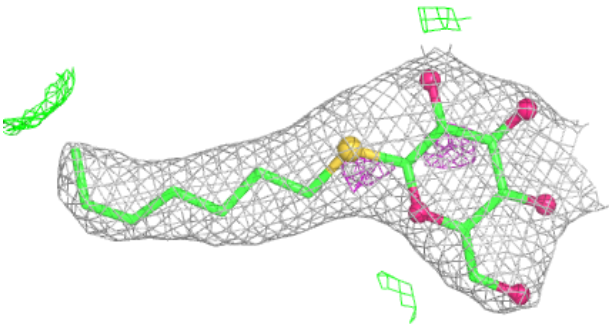
Electron density around SQD B 620:

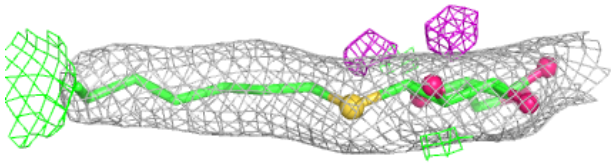
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

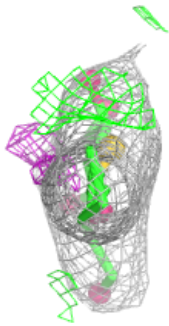


Electron density around HTG B 627:

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

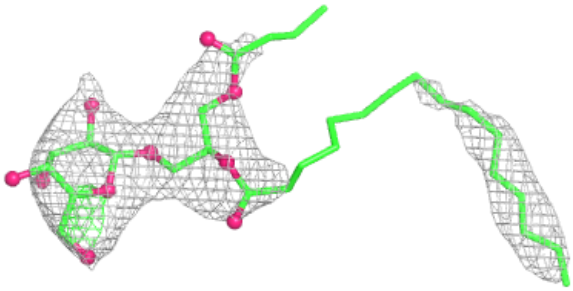


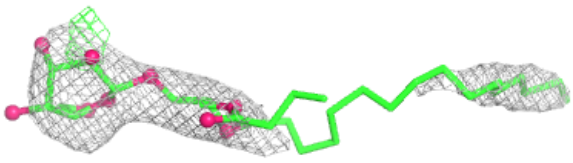


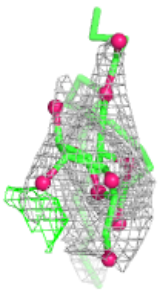


Electron density around LMG z 101:

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

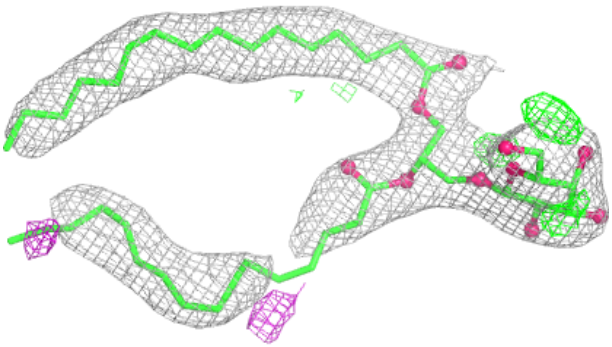


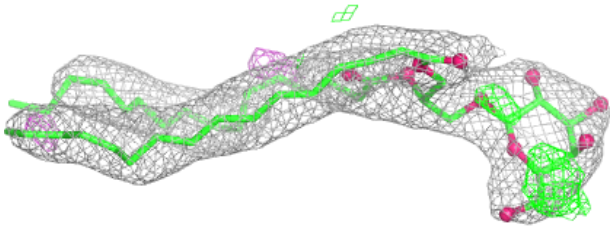


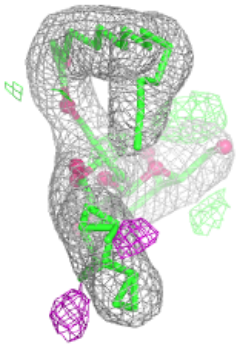


Electron density around LMG C 501:

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

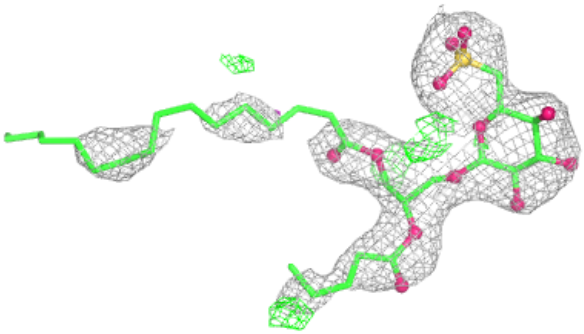


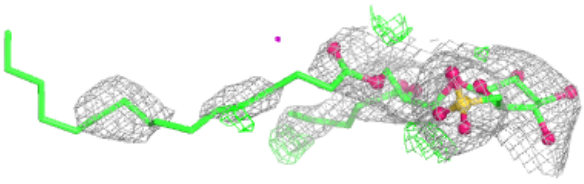


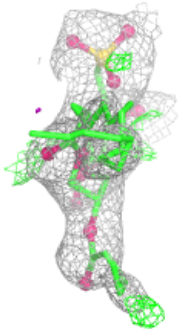


Electron density around SQD D 413:

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

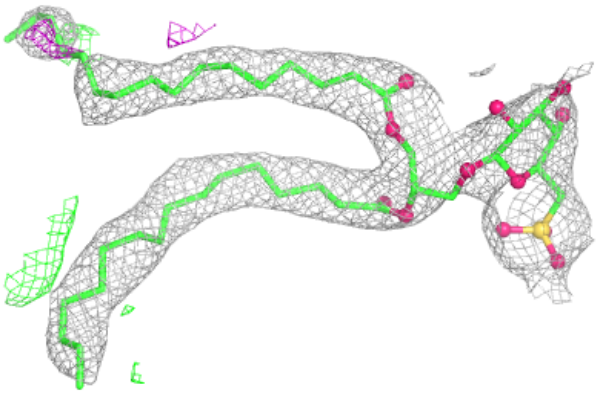


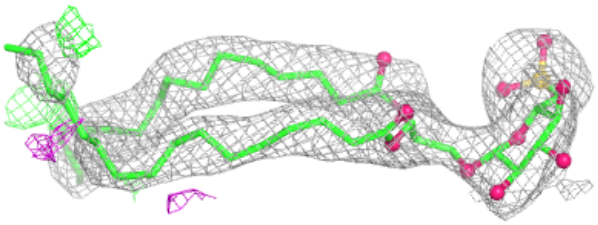


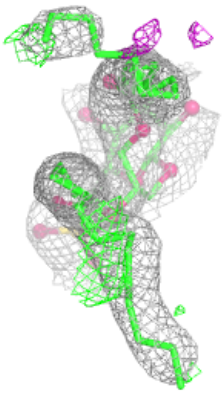


Electron density around SQD L 101:

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

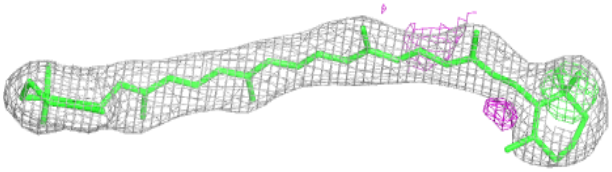


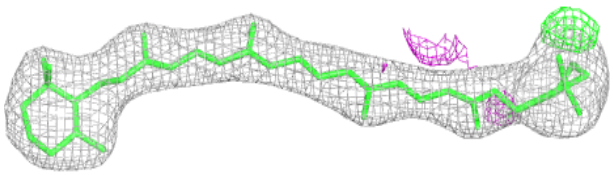


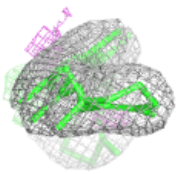


Electron density around BCR D 406:

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

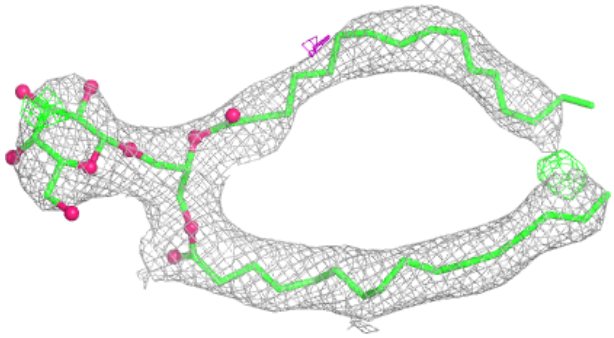


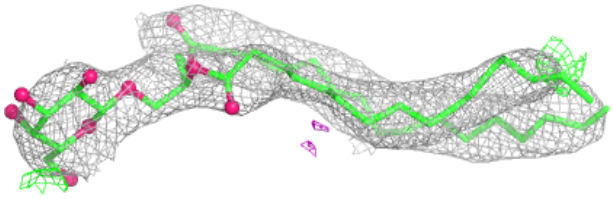


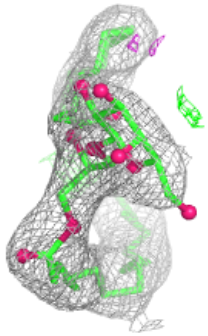


Electron density around LMG a 416:

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

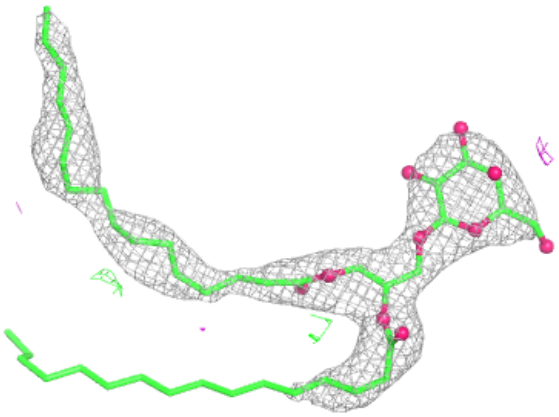


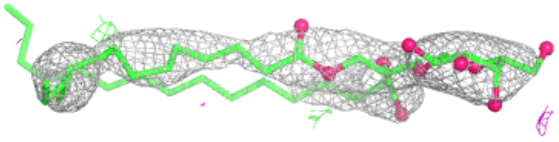


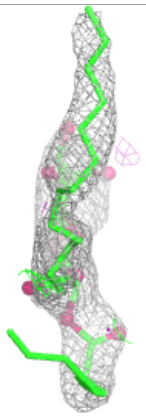


Electron density around LMG c 519:

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

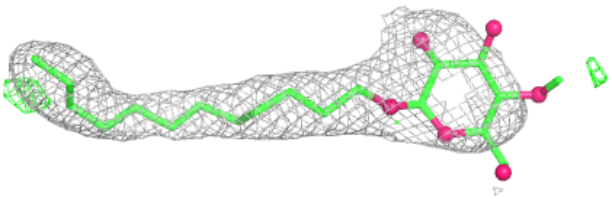


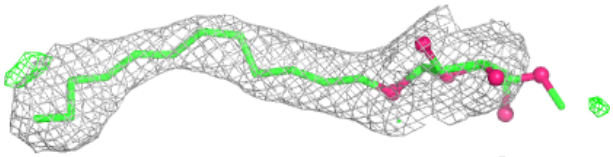


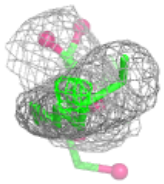


Electron density around LMT b 627:

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

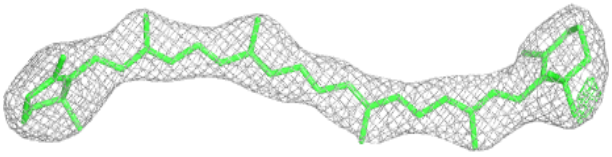


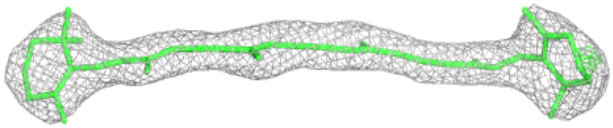


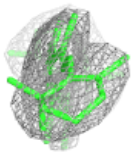


Electron density around BCR y 101:

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

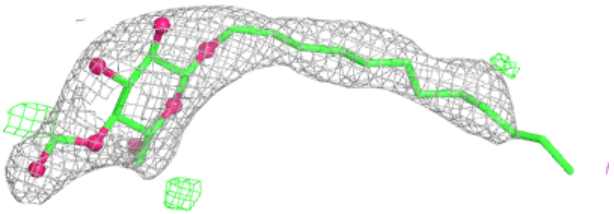


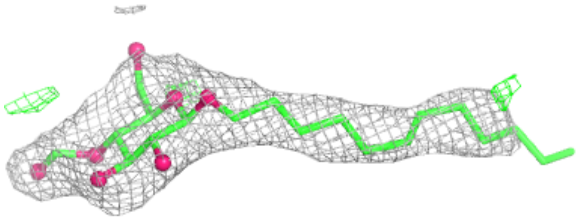


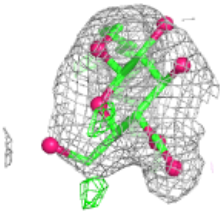


Electron density around LMT B 631:

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

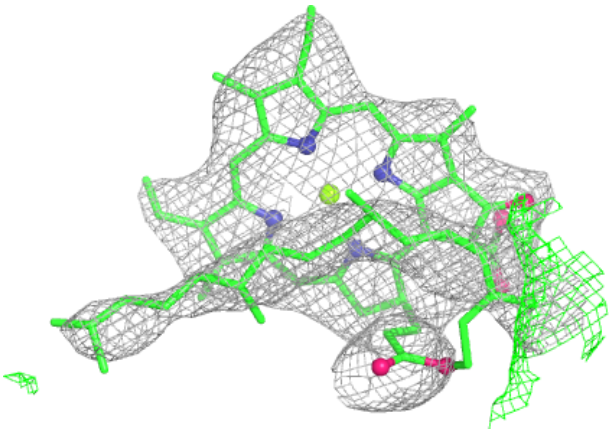


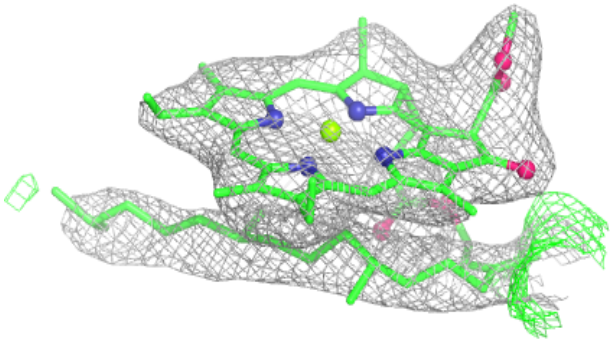


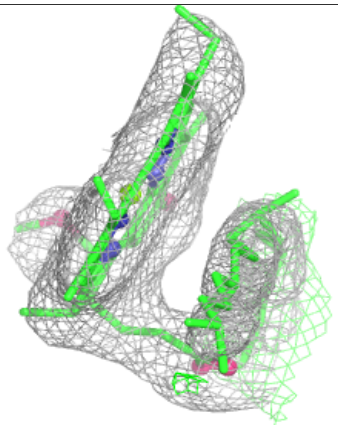


Electron density around CLA b 601:

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

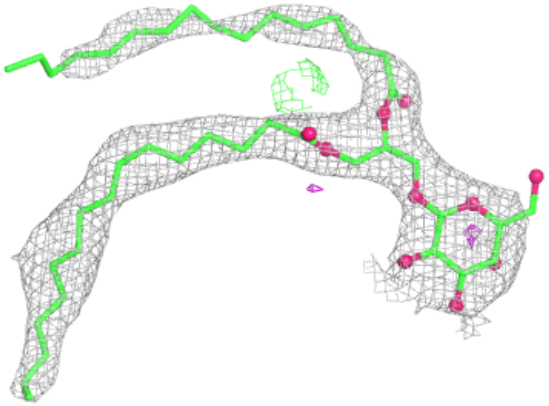


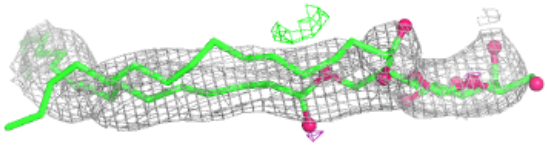




Electron density around LMG C 520:

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

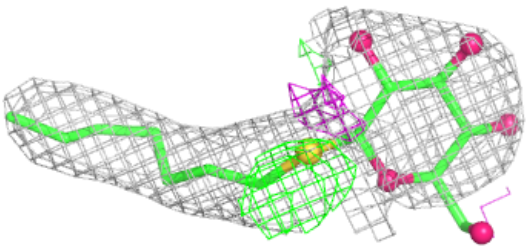


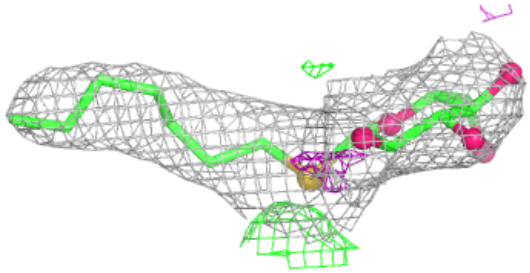


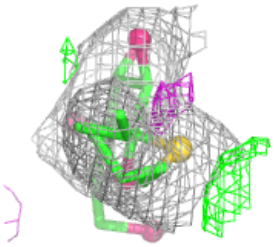


Electron density around HTG B 622:

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

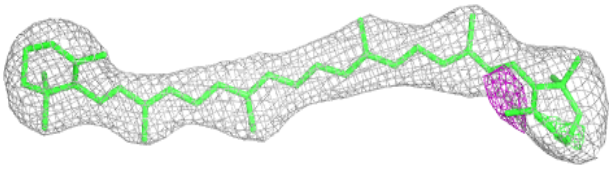


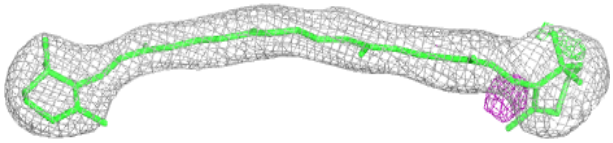


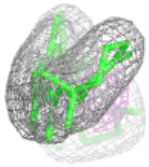


Electron density around BCR d 405:

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

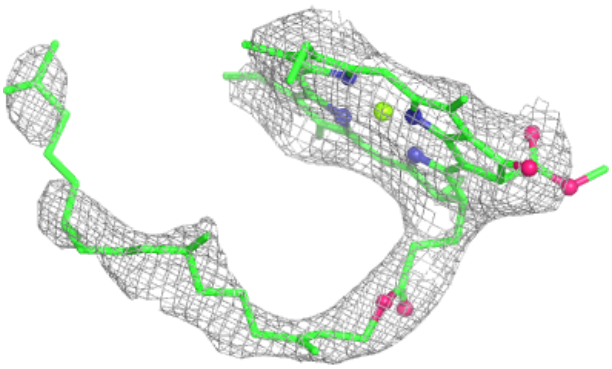


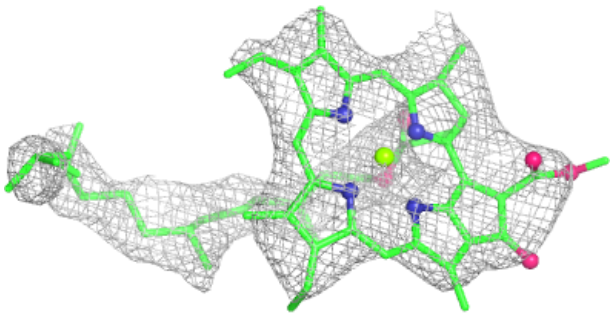




Electron density around CLA c 513:

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

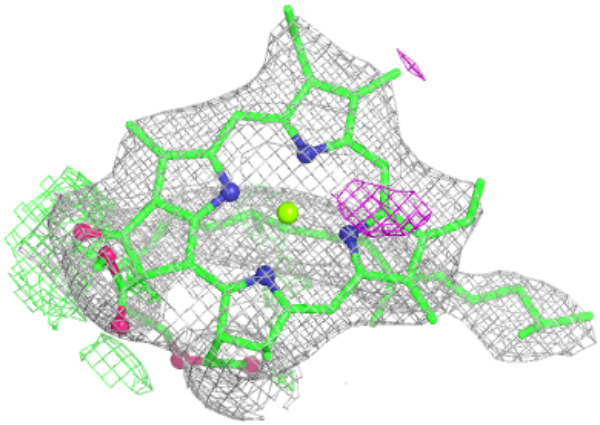


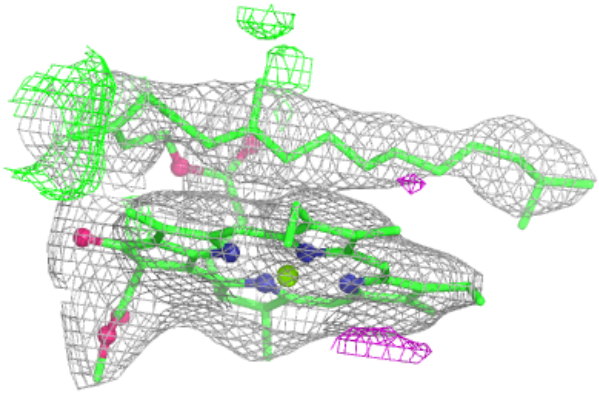


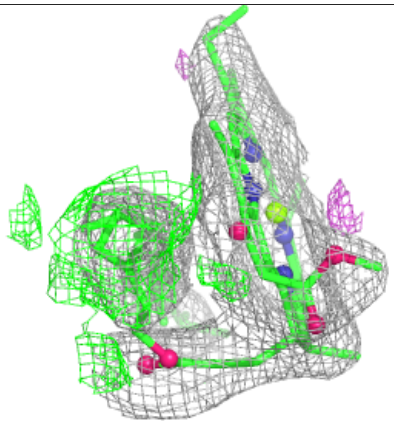


Electron density around CLA B 601:

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

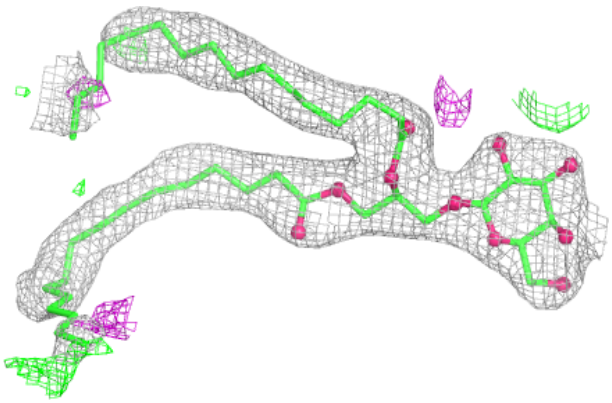


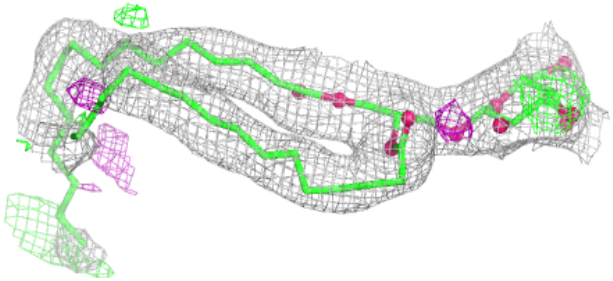




Electron density around LMG J 101:

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

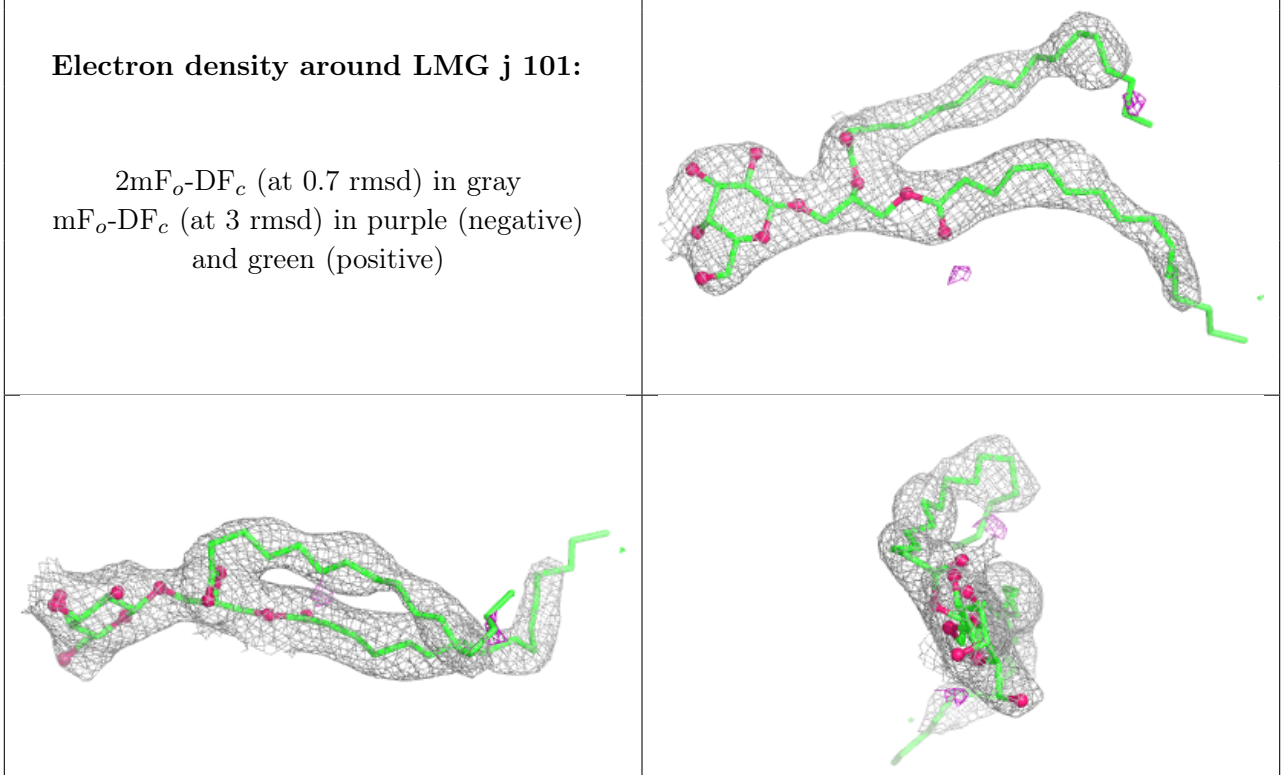






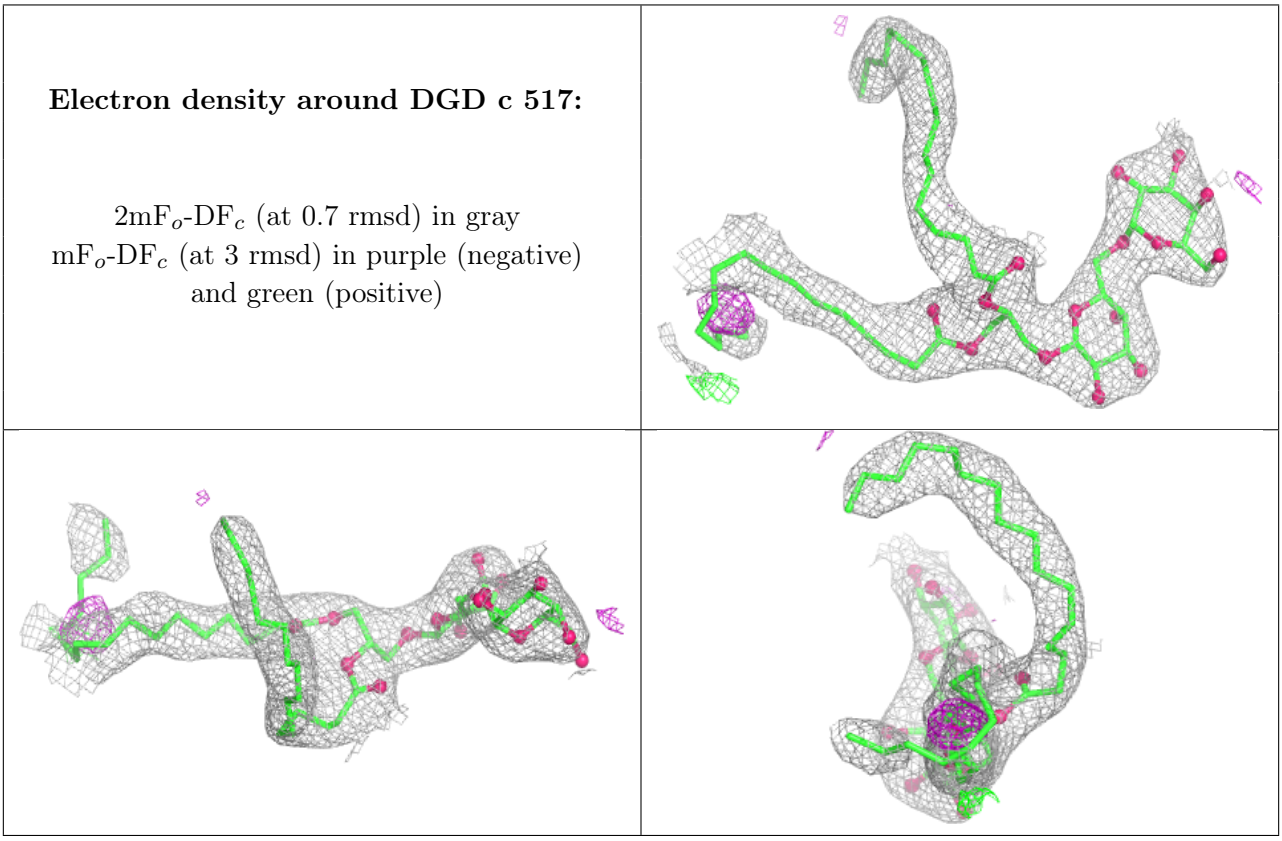
Electron density around LMG j 101:

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



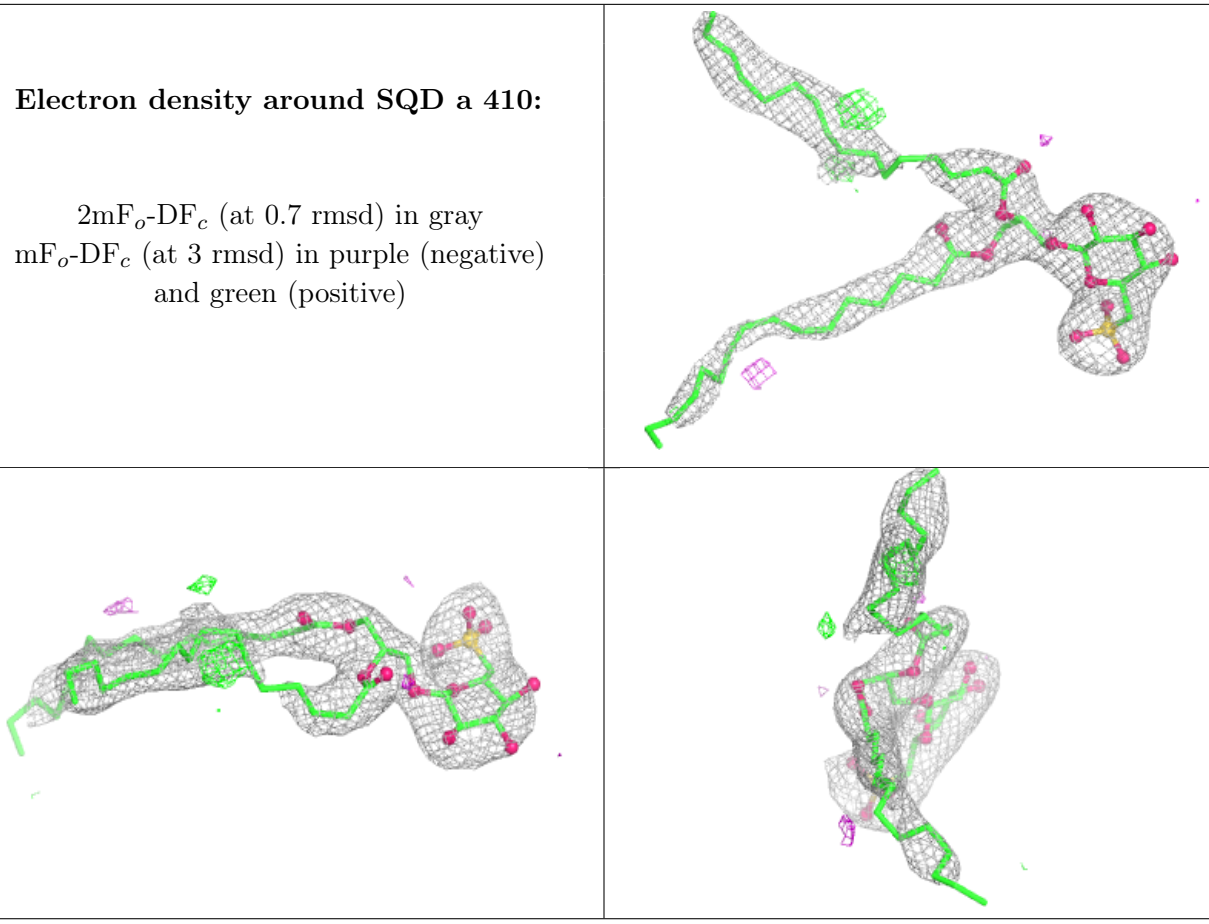
Electron density around DGD c 517:

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



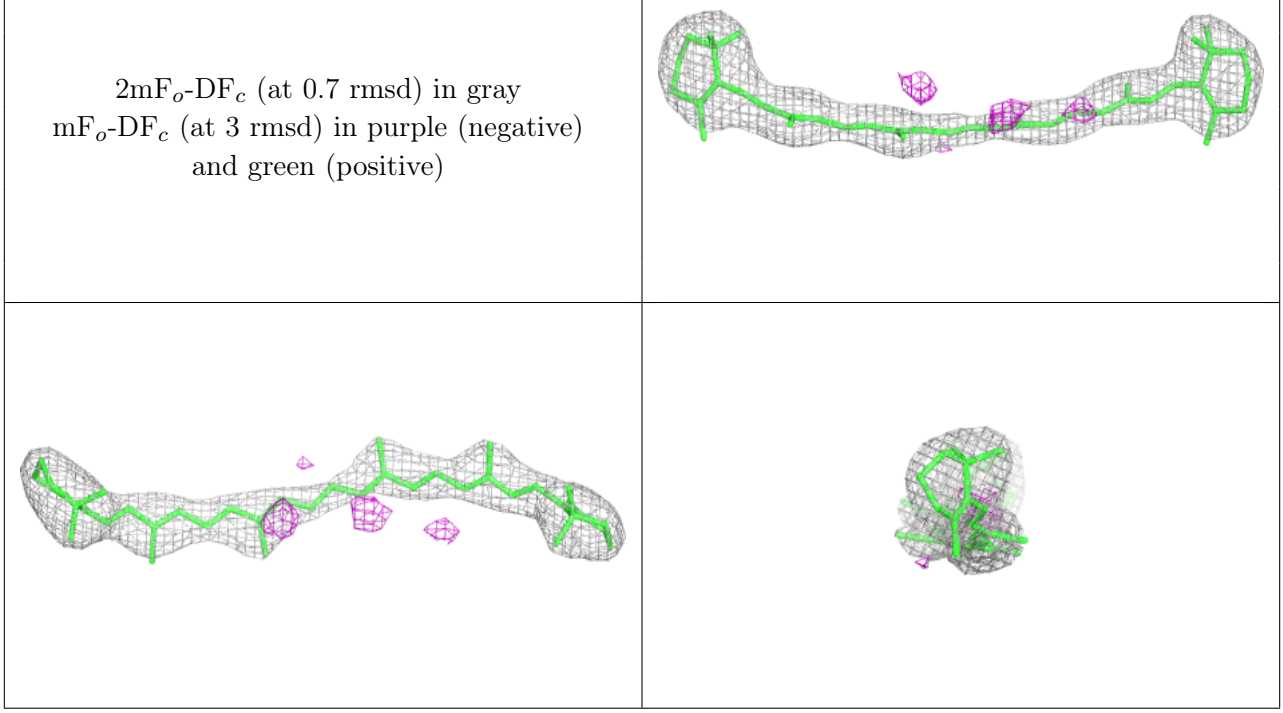
Electron density around SQD a 410:

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



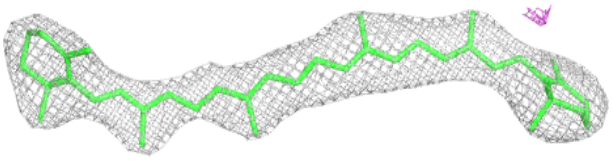
Electron density around BCR K 102:

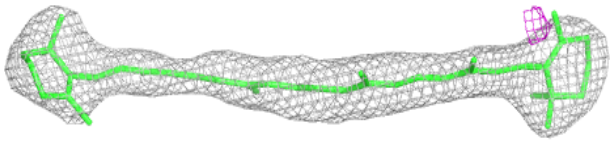
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

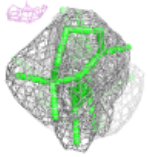


Electron density around BCR Y 101:

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

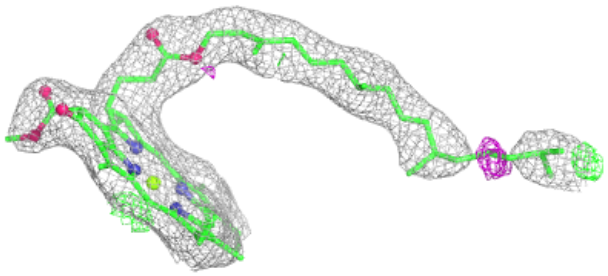


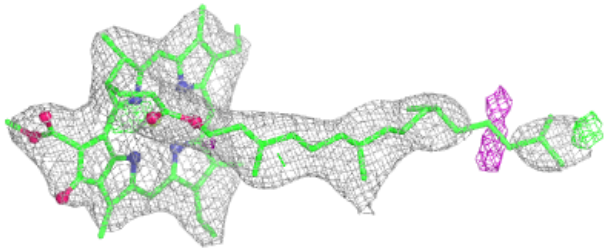


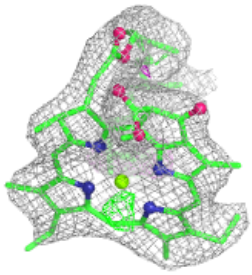


Electron density around CLA c 504:

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

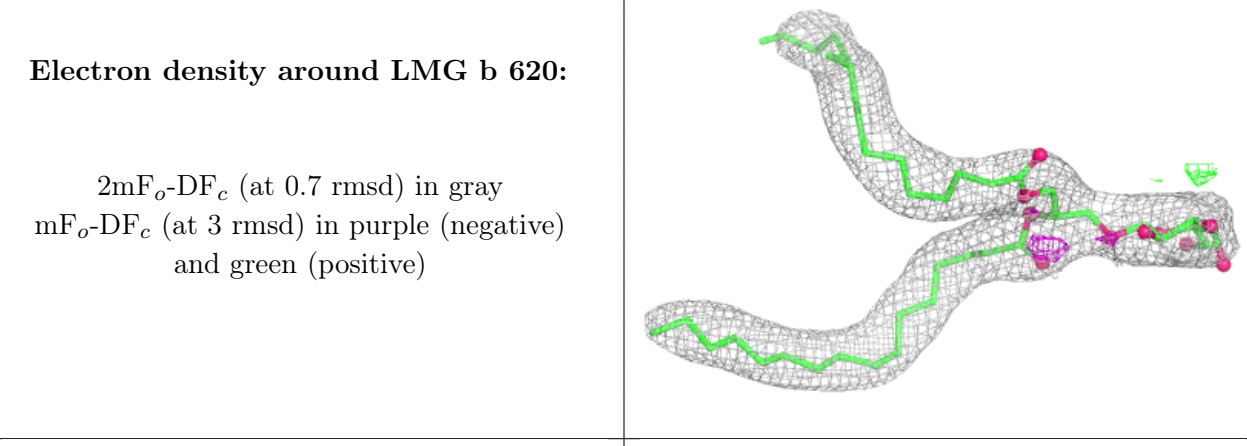






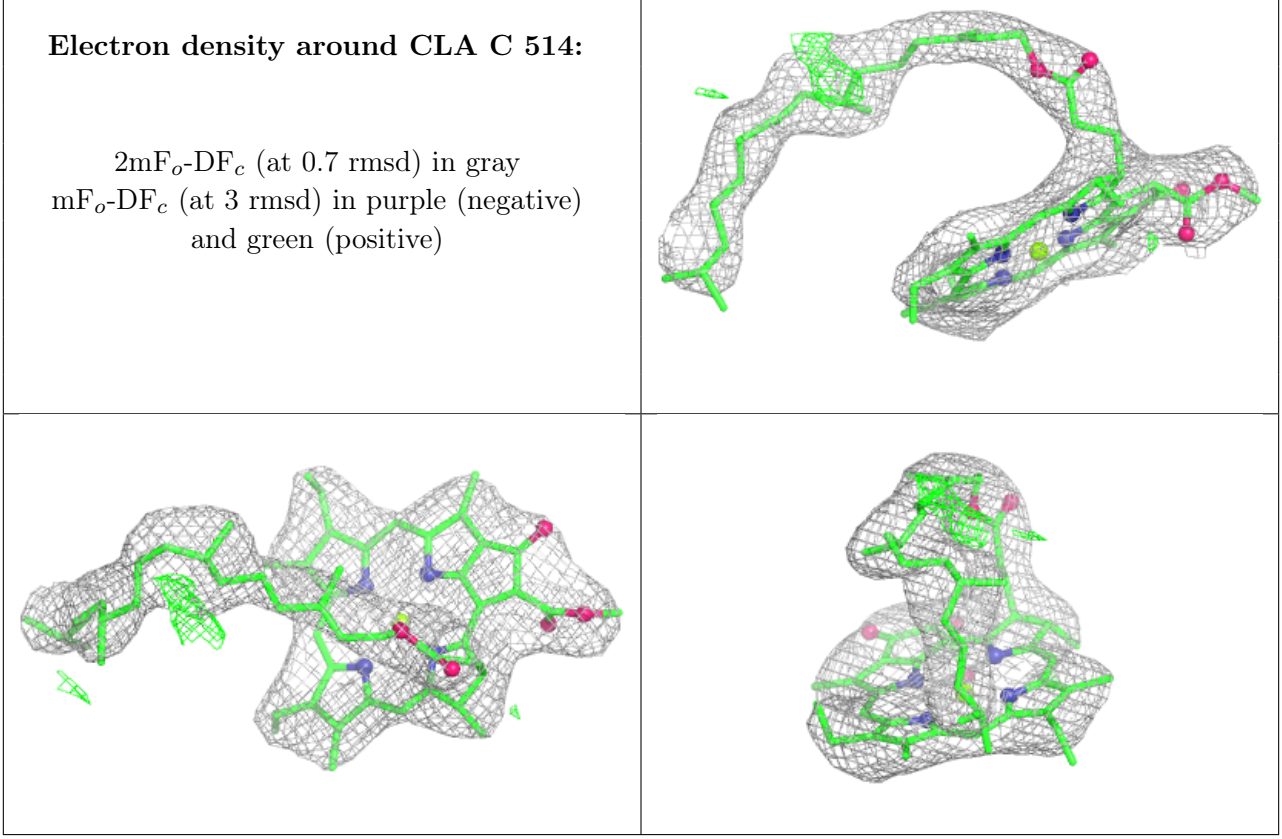
Electron density around LMG b 620:

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



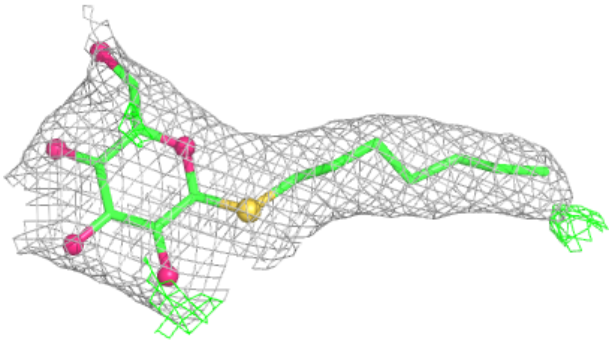
Electron density around CLA C 514:

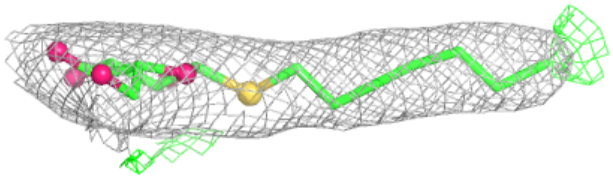
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

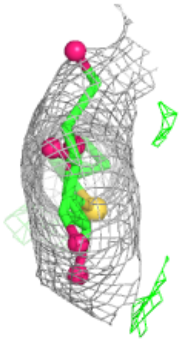


Electron density around HTG b 625:

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

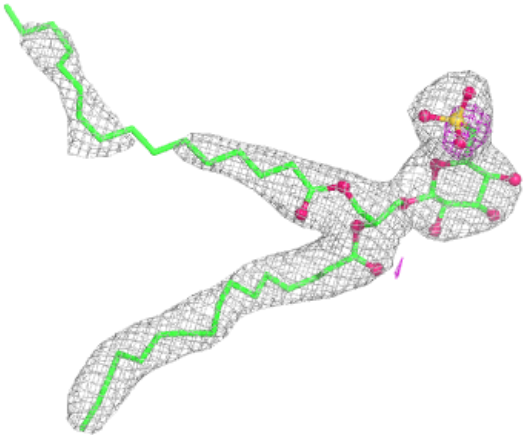


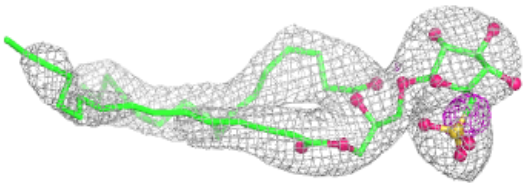


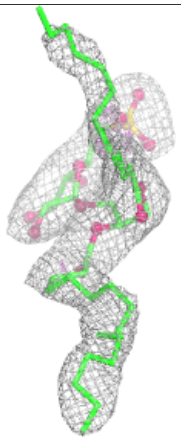


Electron density around SQD A 410:

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

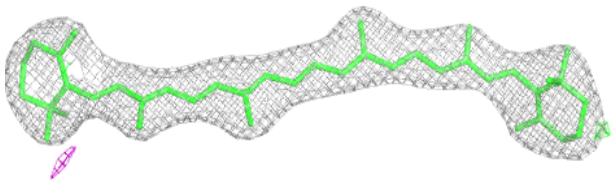


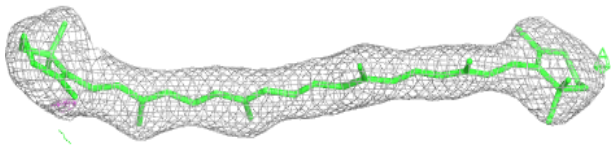


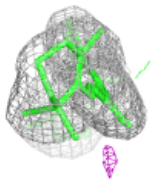


Electron density around BCR B 619:

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

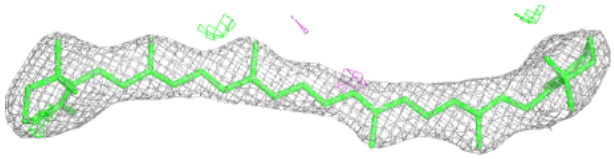


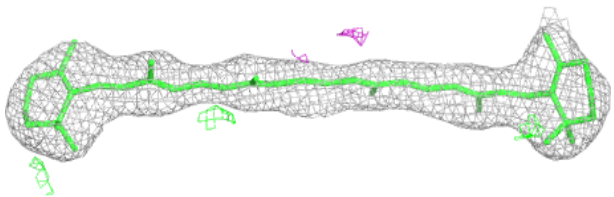


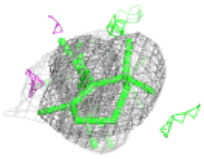


Electron density around BCR C 515:

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

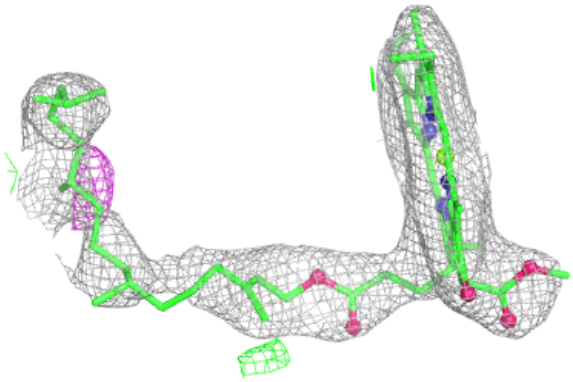


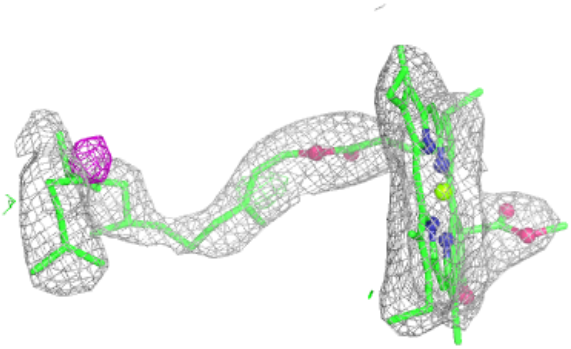


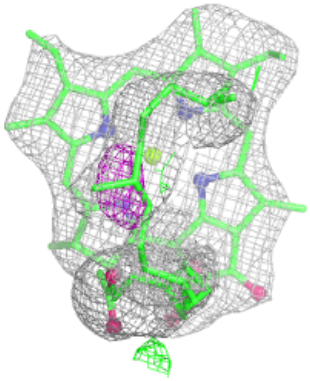


Electron density around CLA C 507:

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

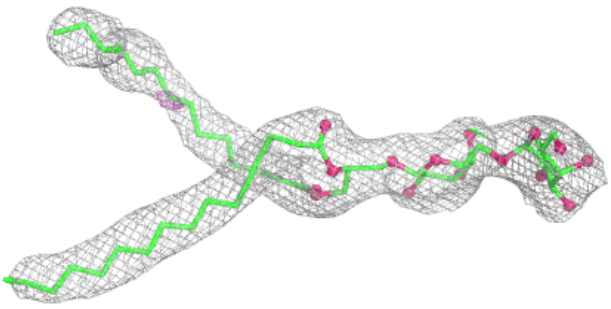


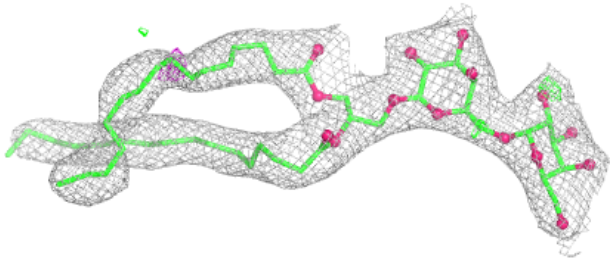




Electron density around DGD c 516:

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

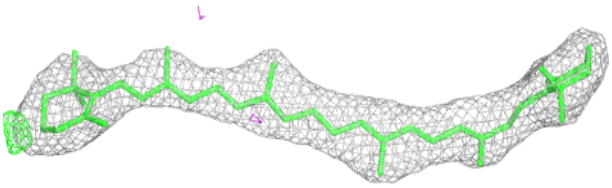


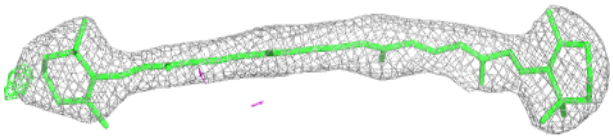


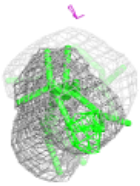


Electron density around BCR H 101:

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

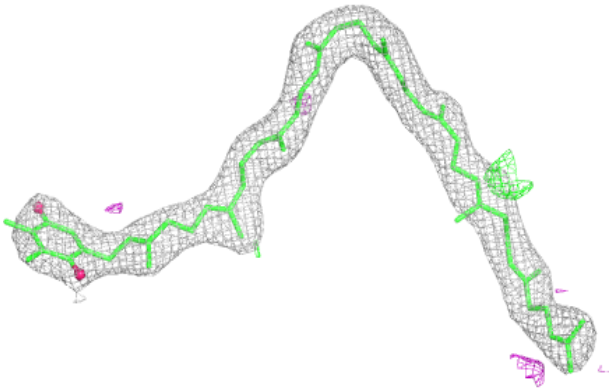


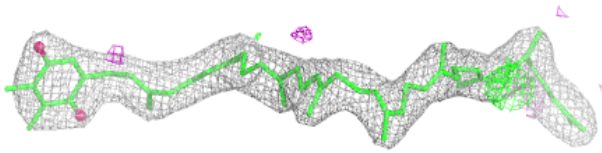




Electron density around PL9 d 406:

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

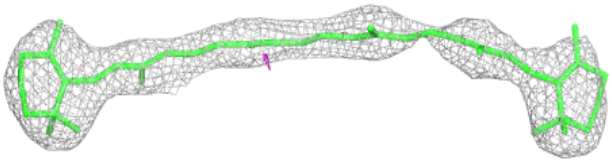


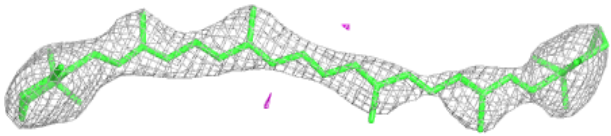


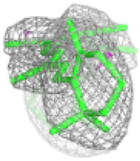


Electron density around BCR k 101:

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

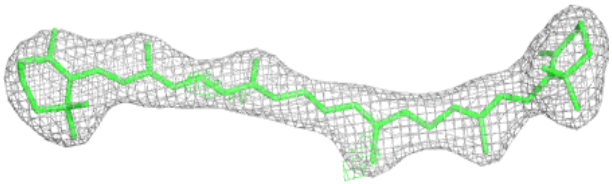


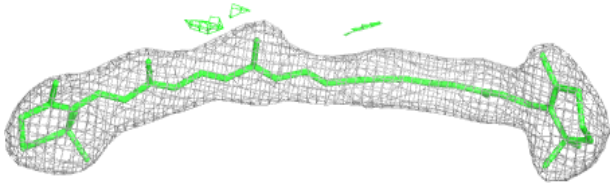


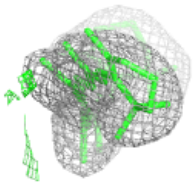


Electron density around BCR t 101:

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

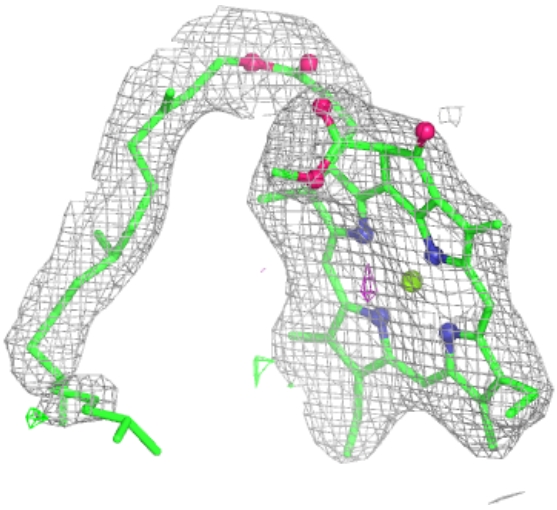


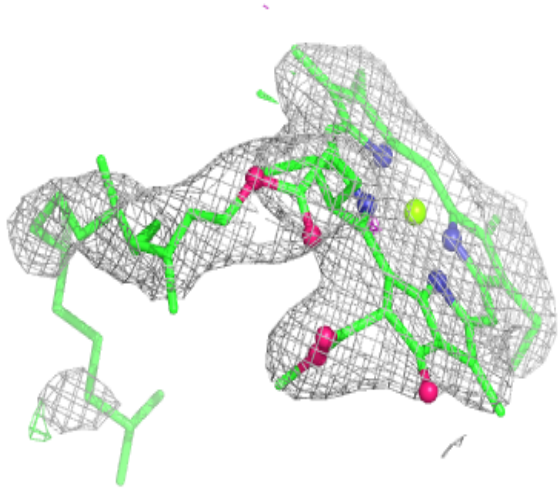


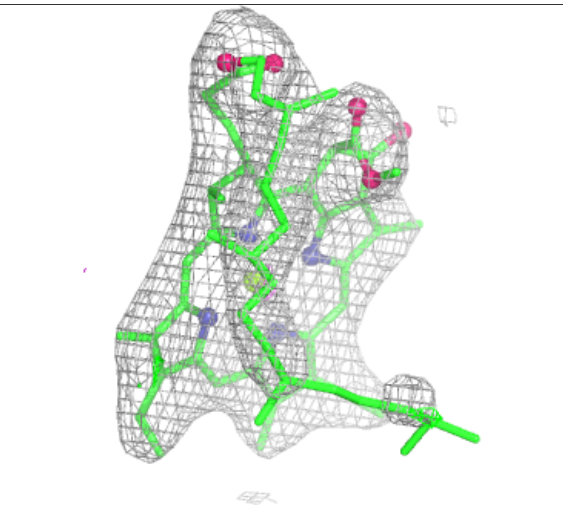


Electron density around CLA b 616:

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

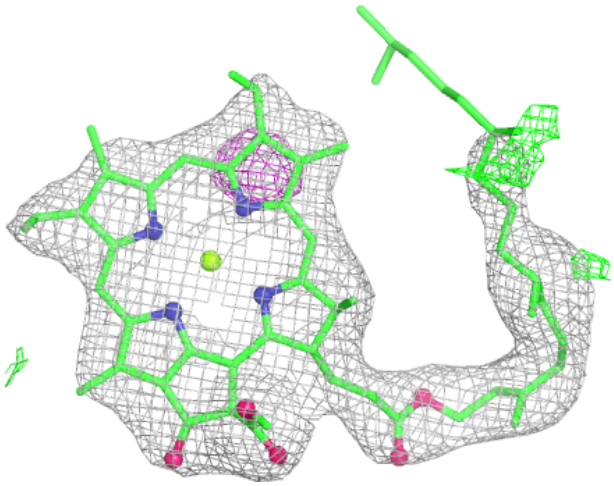


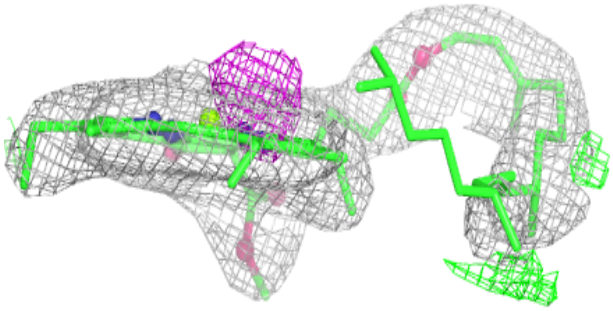


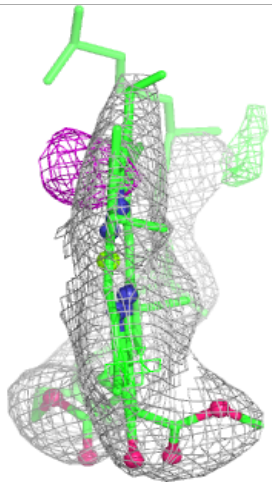


Electron density around CLA C 513:

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

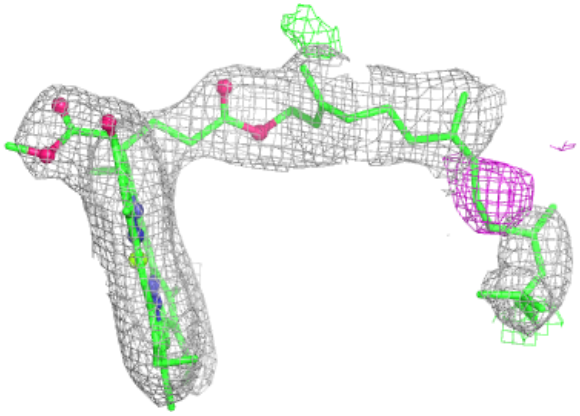


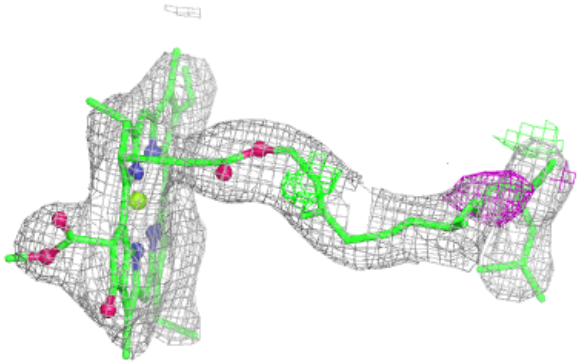


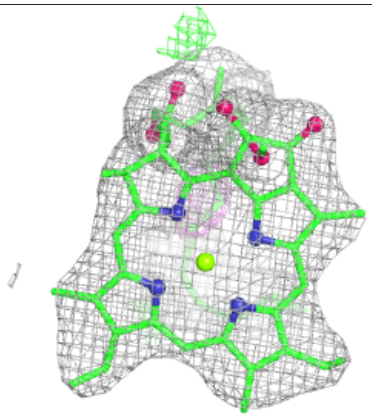


Electron density around CLA c 506:

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

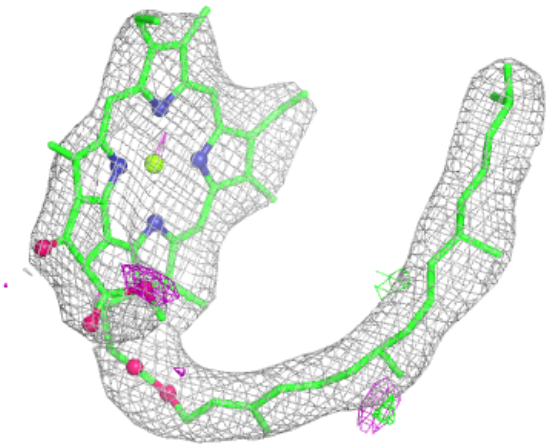


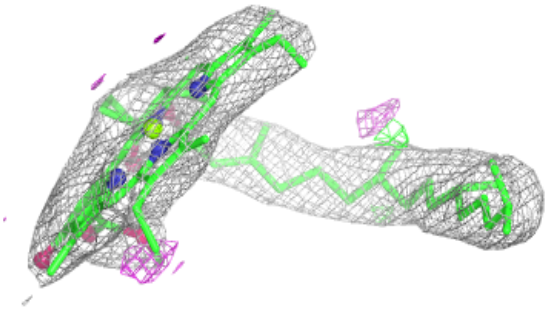


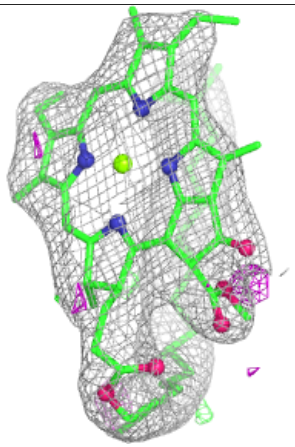


Electron density around CLA c 507:

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

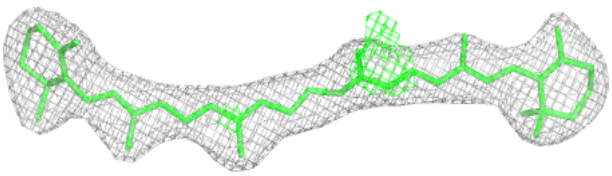


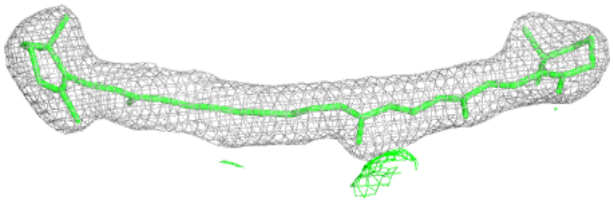


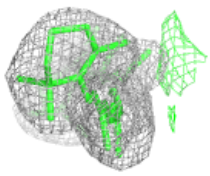


Electron density around BCR T 101:

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

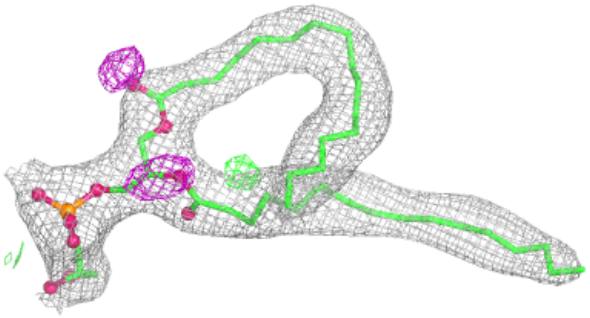


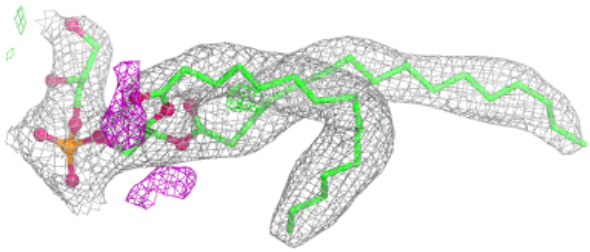


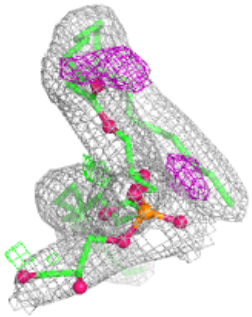


Electron density around LHG A 416:

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

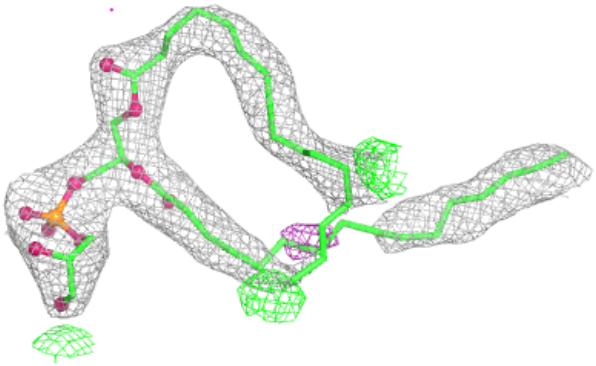


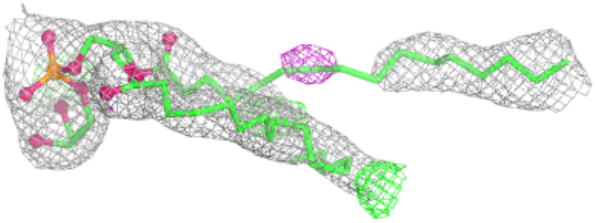


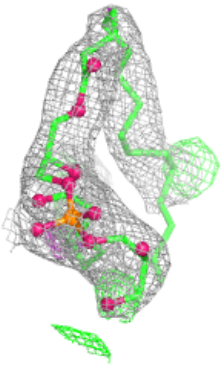


Electron density around LHG D 409:

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

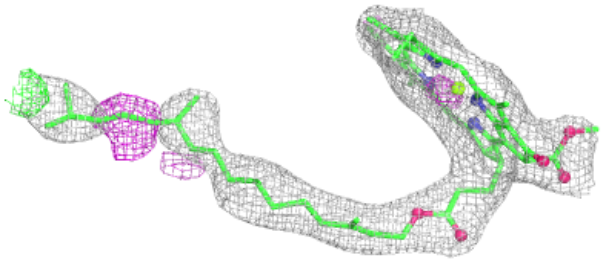


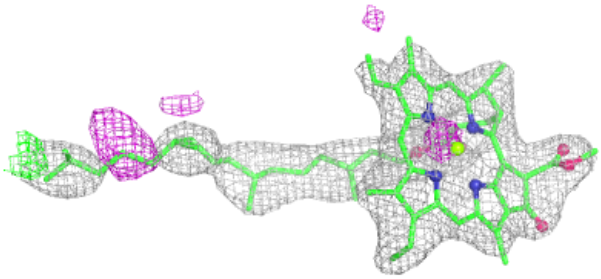


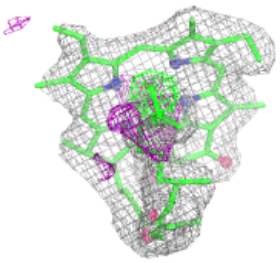


Electron density around CLA C 505:

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

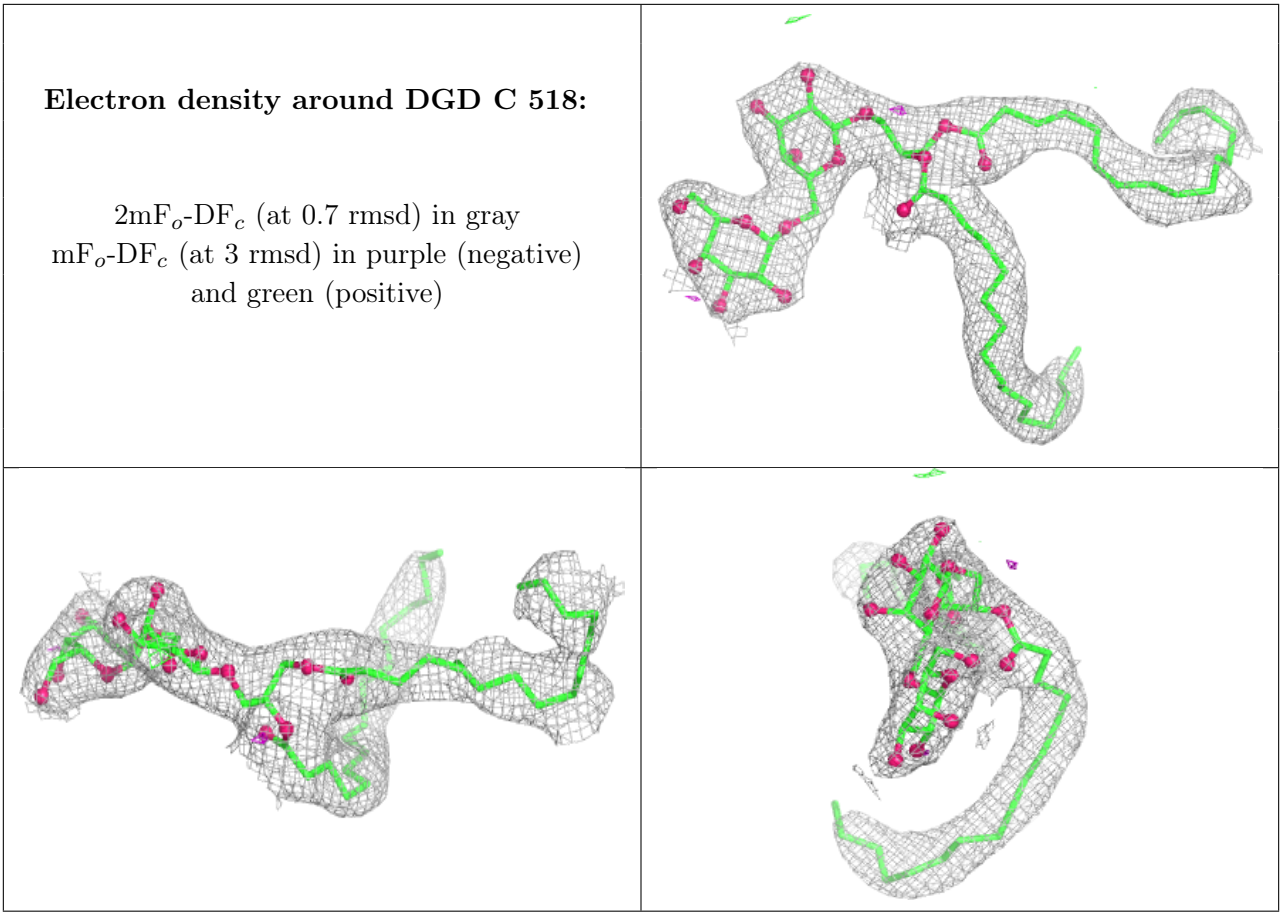






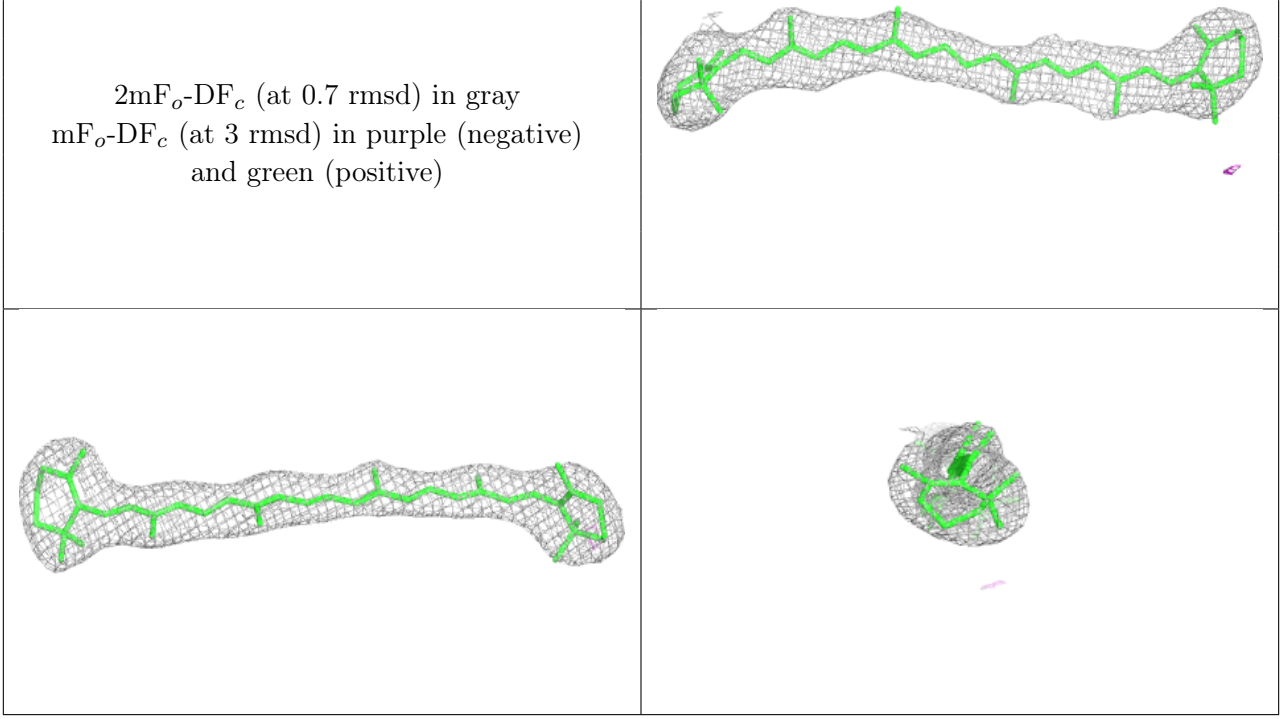
Electron density around DGD C 518:

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



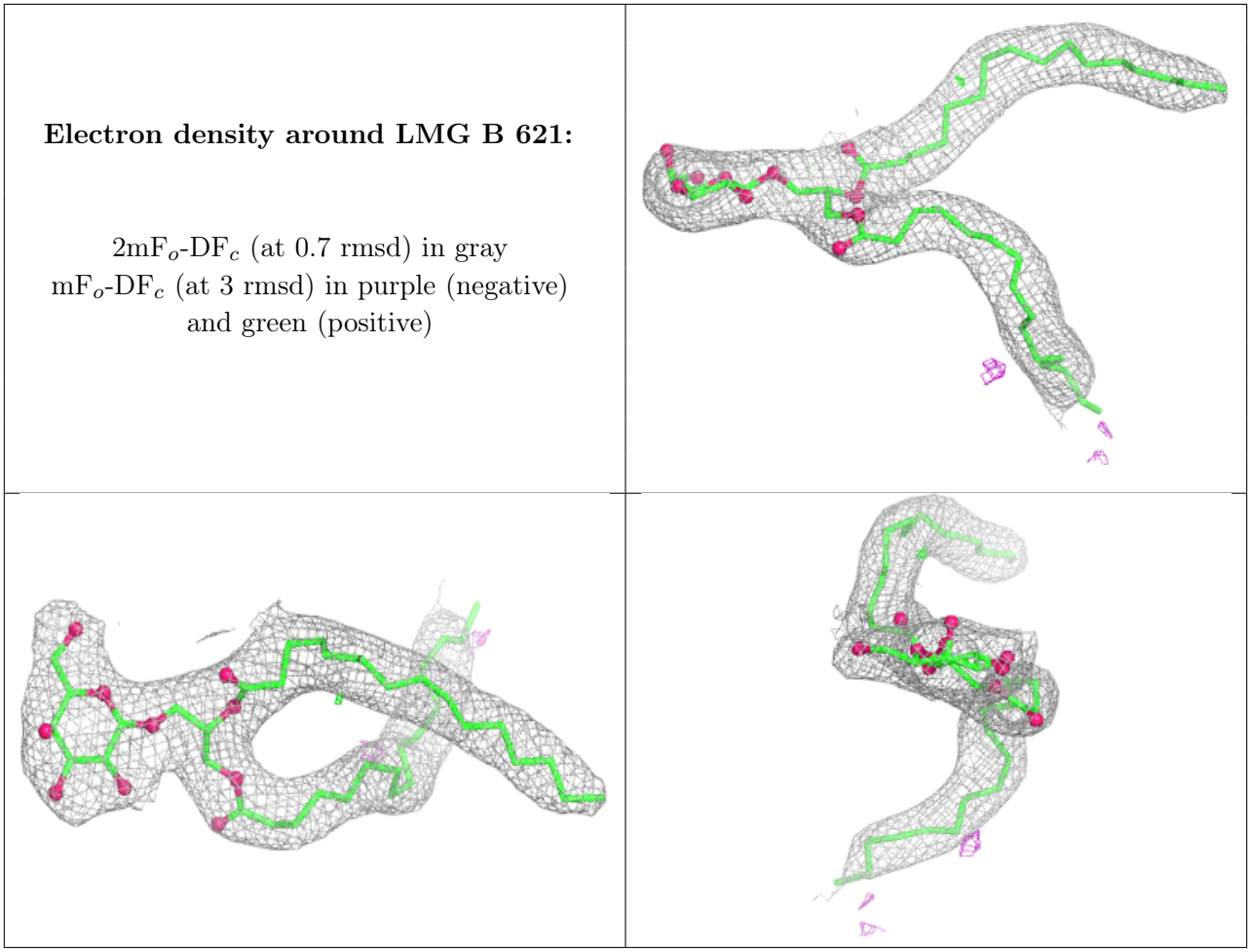
Electron density around BCR c 514:

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



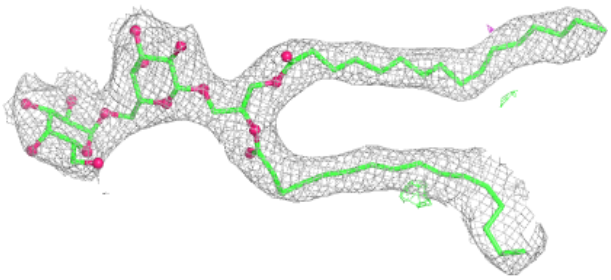
Electron density around LMG B 621:

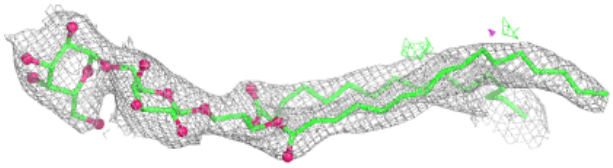
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

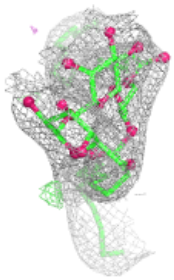


Electron density around DGD c 518:

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

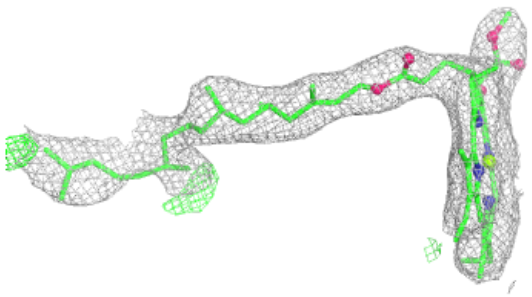


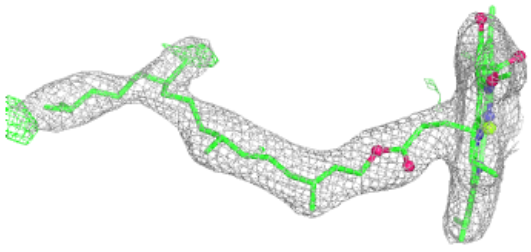


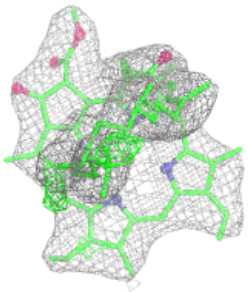


Electron density around CLA B 606:

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

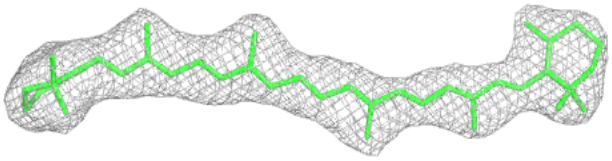


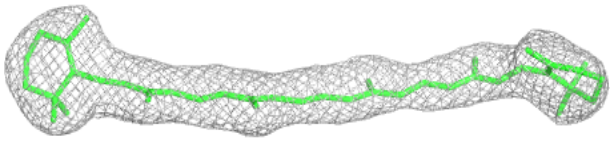


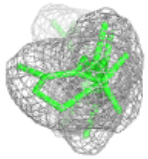


Electron density around BCR b 617:

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

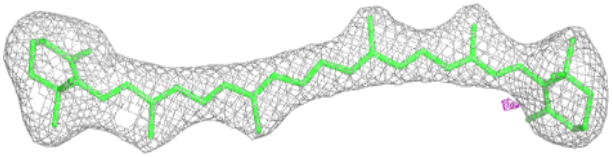


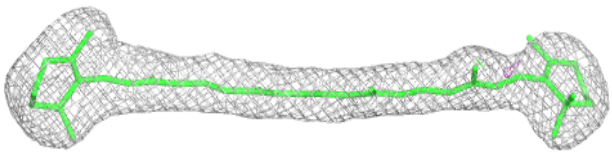


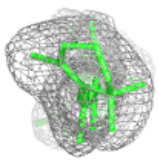


Electron density around BCR b 618:

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

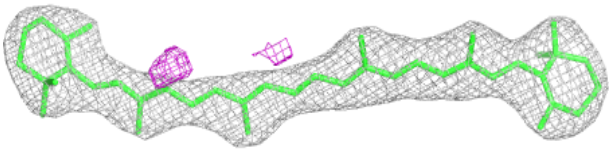




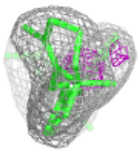


Electron density around BCR b 619:

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

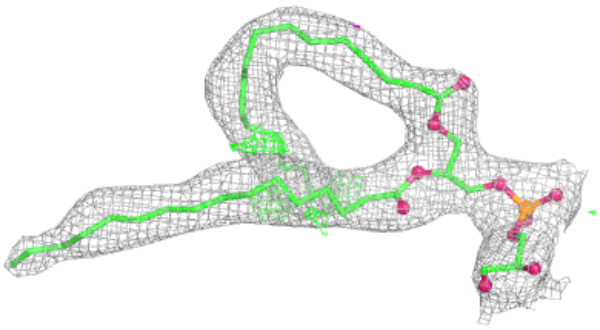


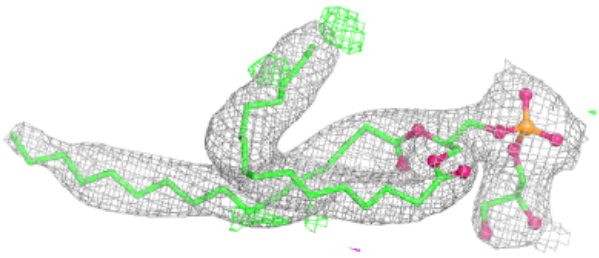


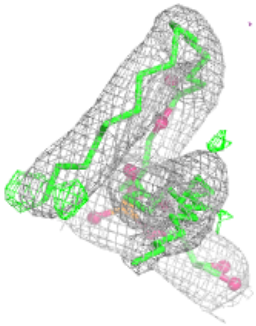


Electron density around LHG d 407:

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

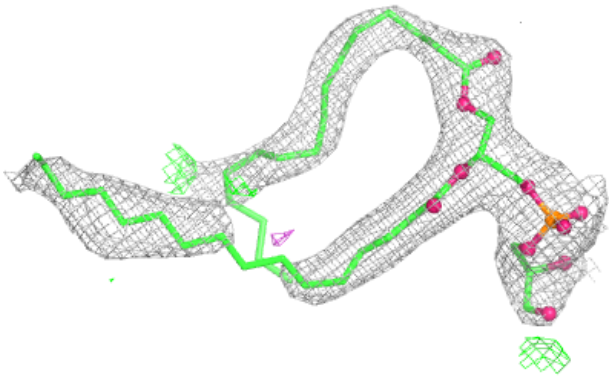


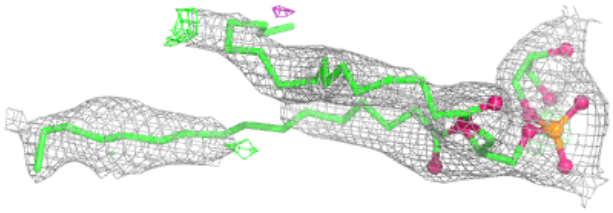


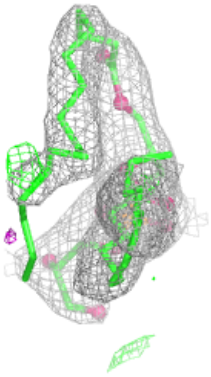


Electron density around LHG d 409:

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

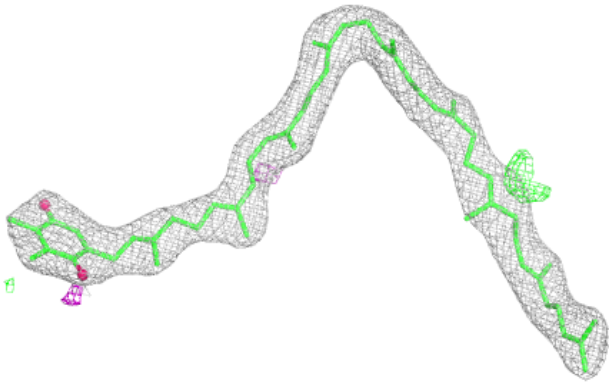


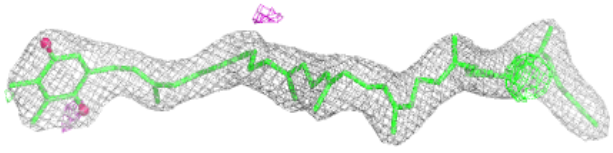


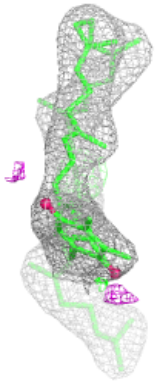


Electron density around PL9 D 407:

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

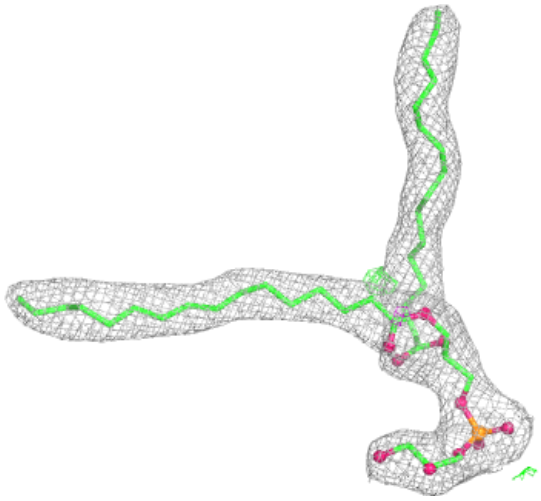


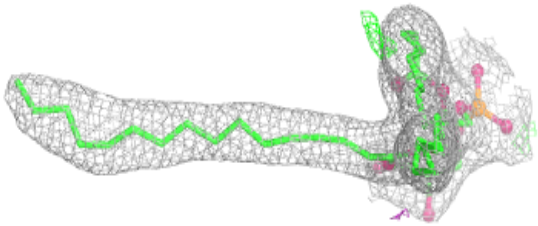


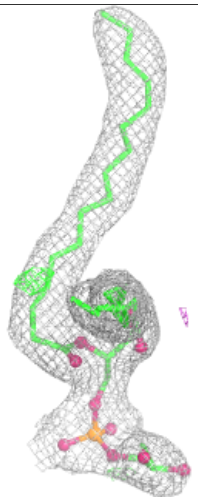


Electron density around LHG l 101:

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

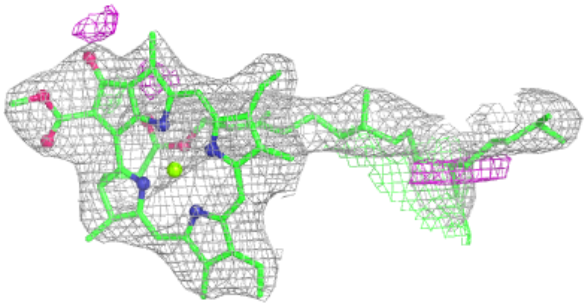


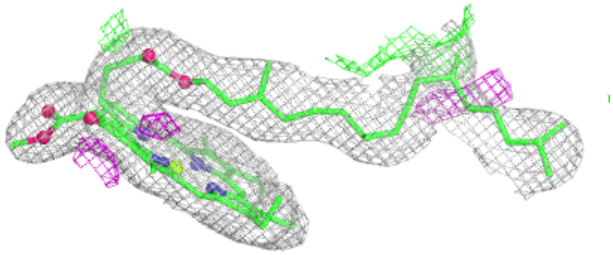


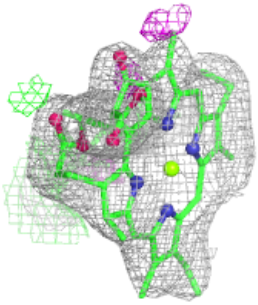


Electron density around CLA B 614:

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

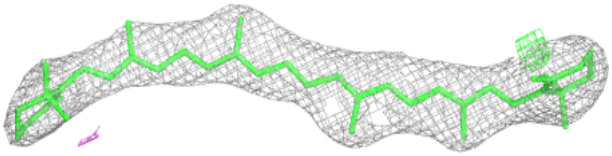


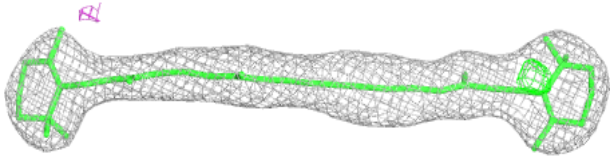


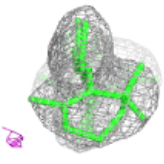


Electron density around BCR c 515:

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

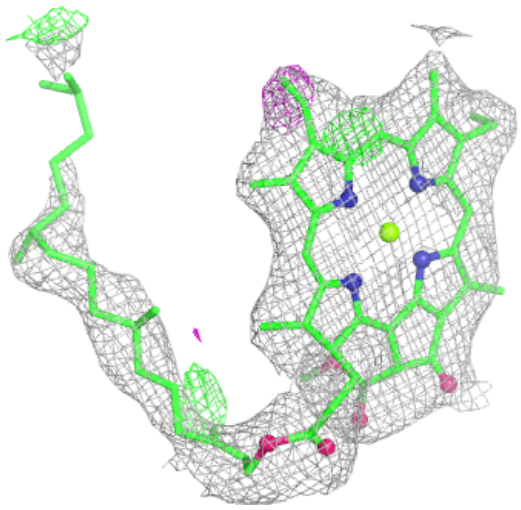


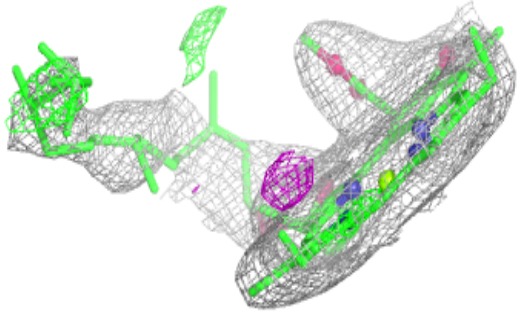


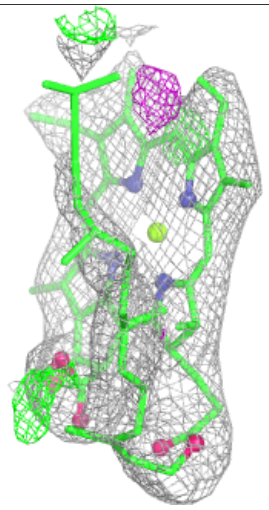


Electron density around CLA B 616:

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

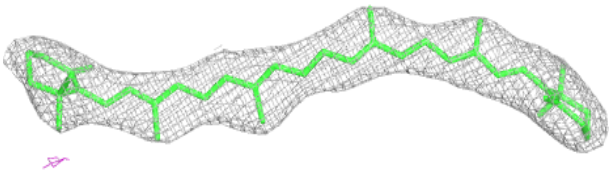


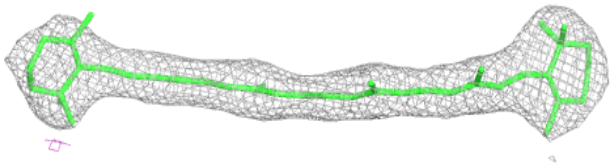


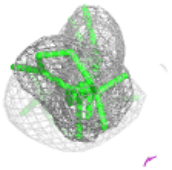


Electron density around BCR h 101:

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

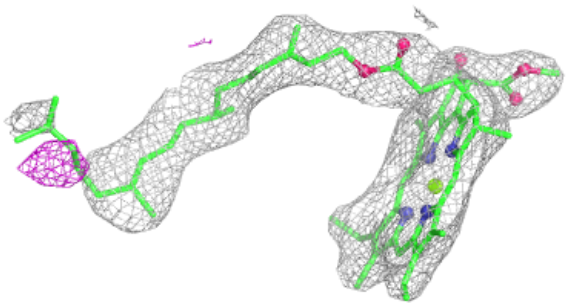


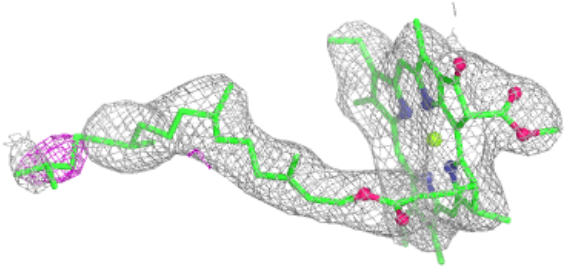


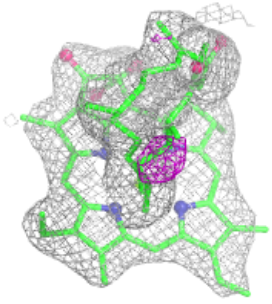


Electron density around CLA c 508:

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

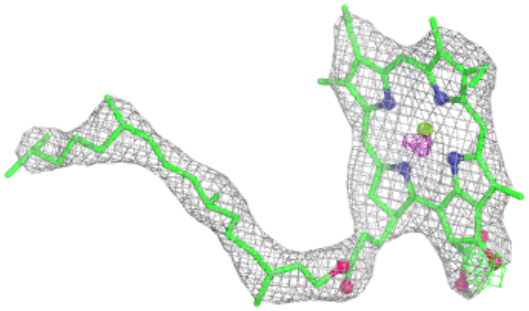


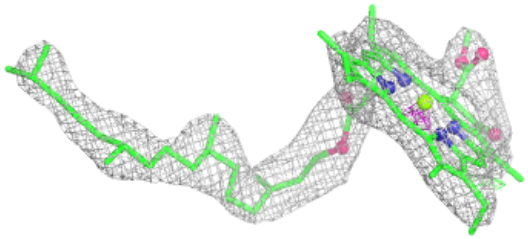


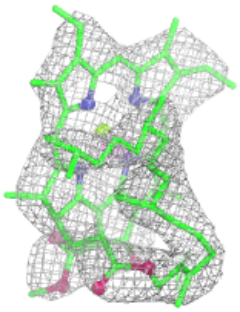


Electron density around CLA c 511:

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

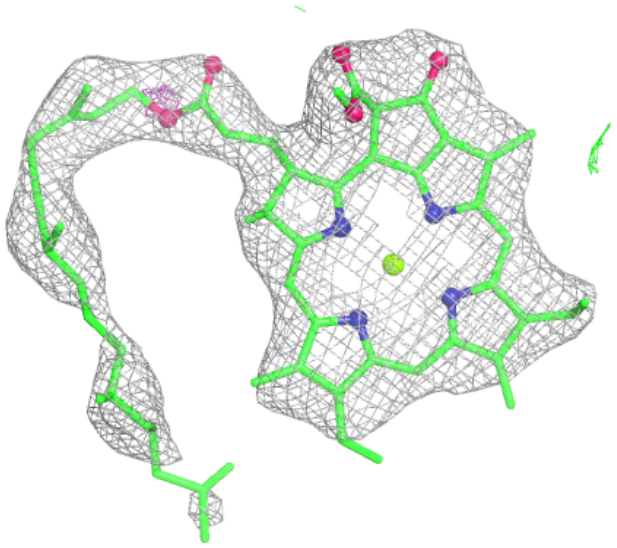


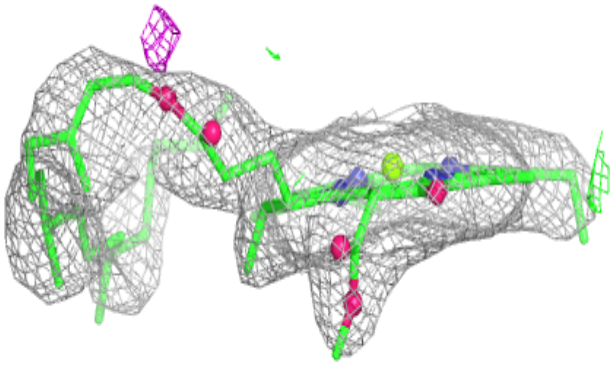


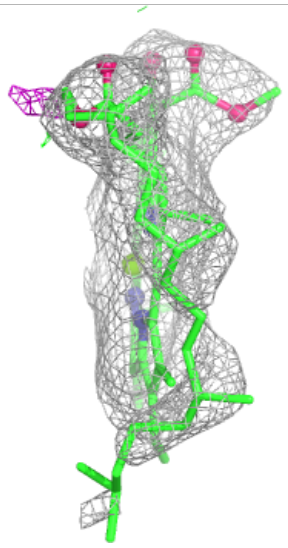


Electron density around CLA c 512:

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

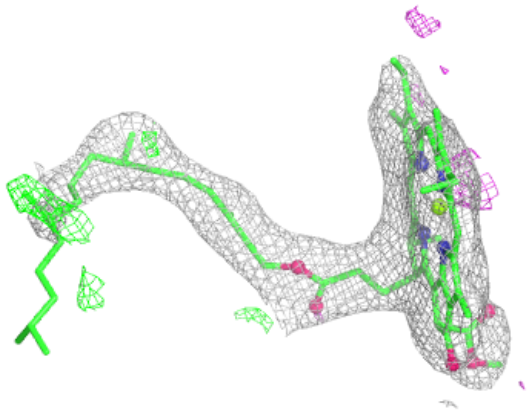


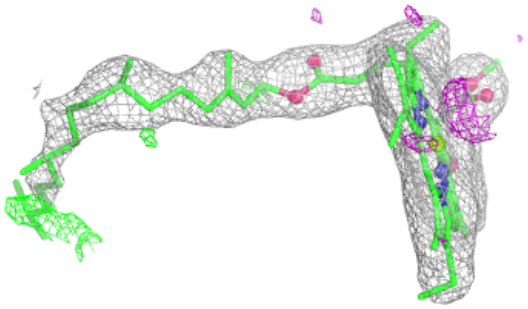


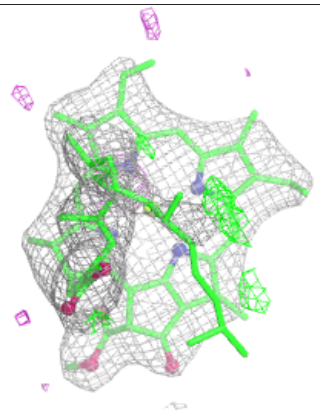


Electron density around CLA D 405:

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

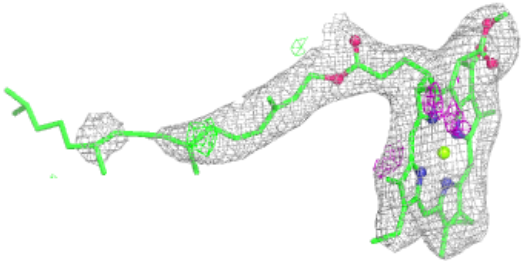


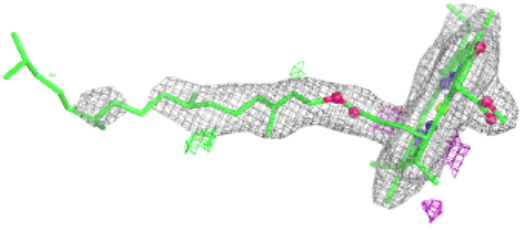


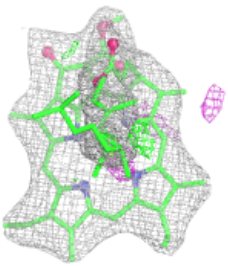


Electron density around CLA d 404:

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

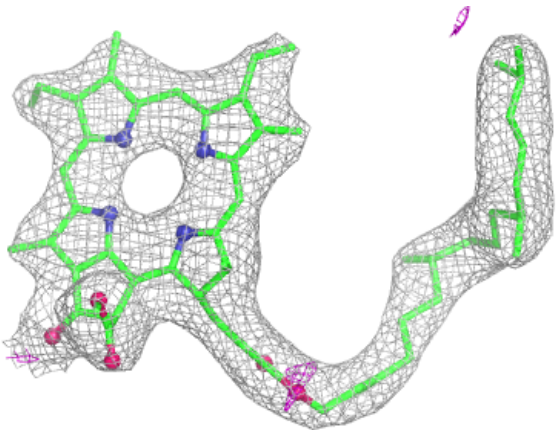


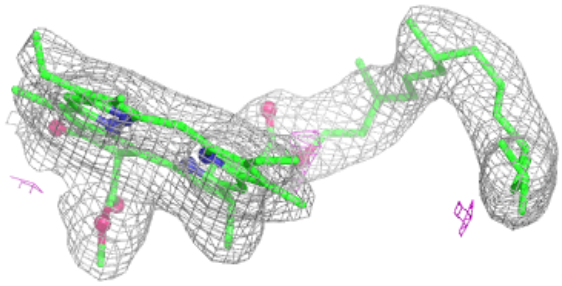


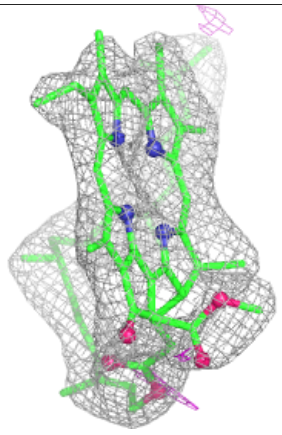


Electron density around PHO a 407:

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

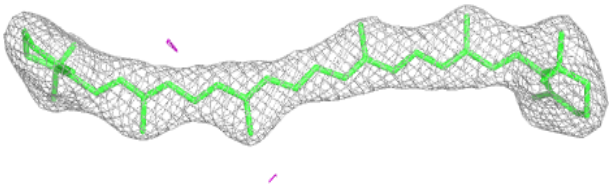


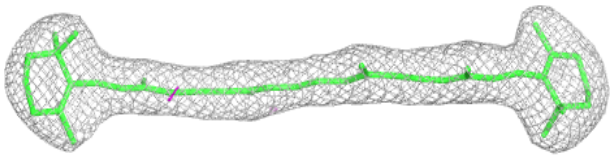


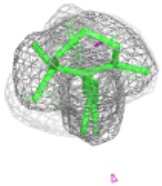


Electron density around BCR A 409:

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

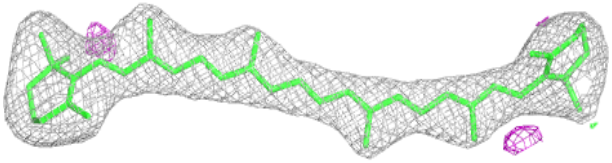


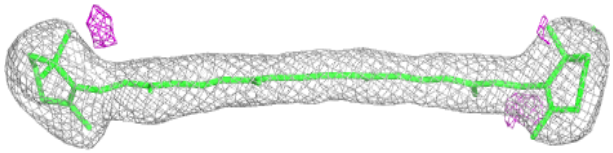


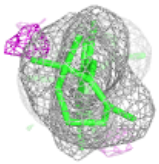


Electron density around BCR B 618:

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

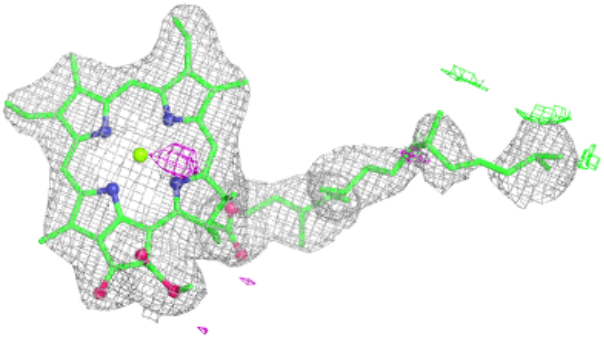


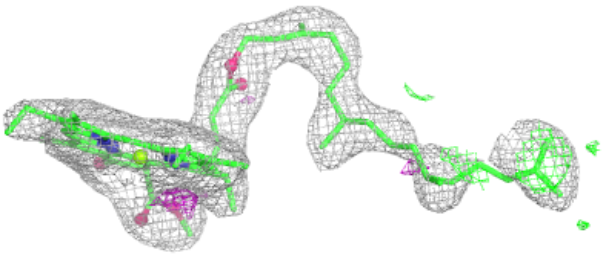


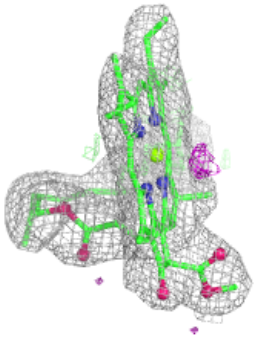


Electron density around CLA a 405:

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

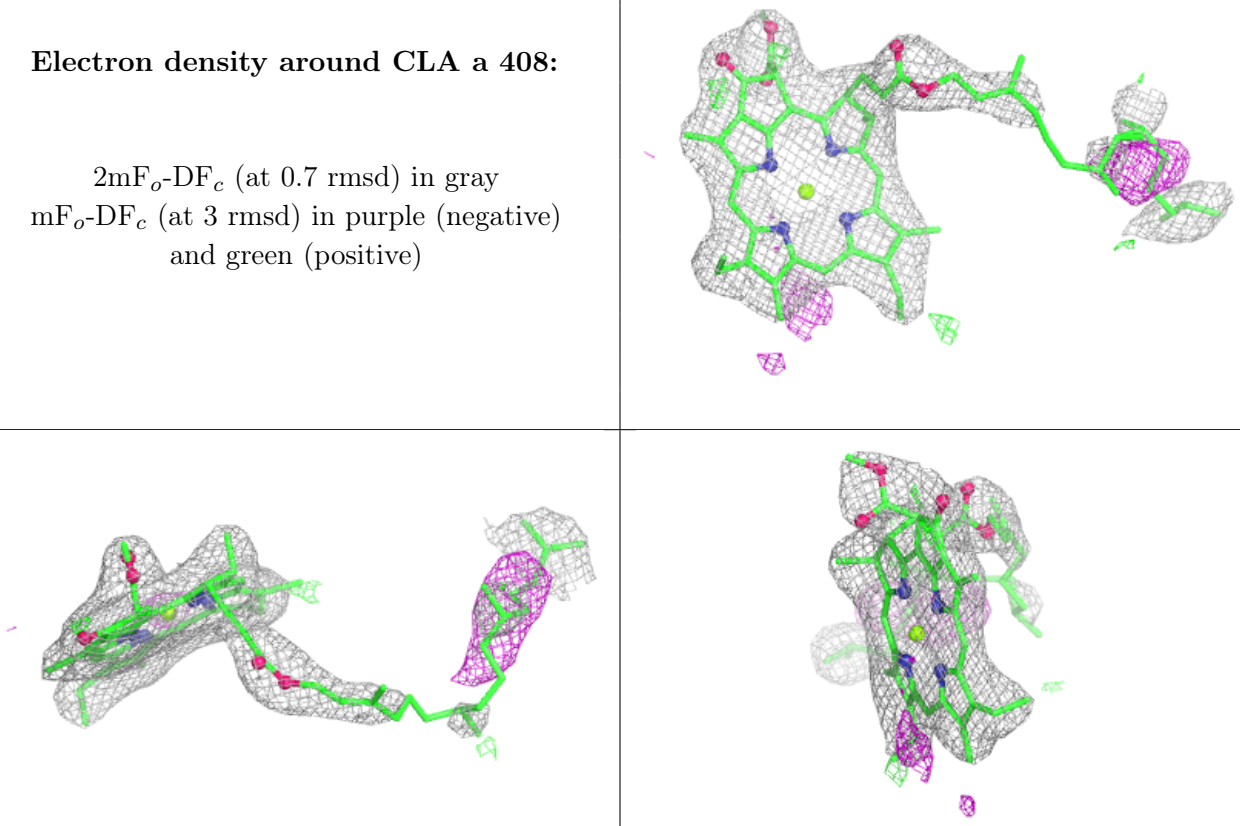






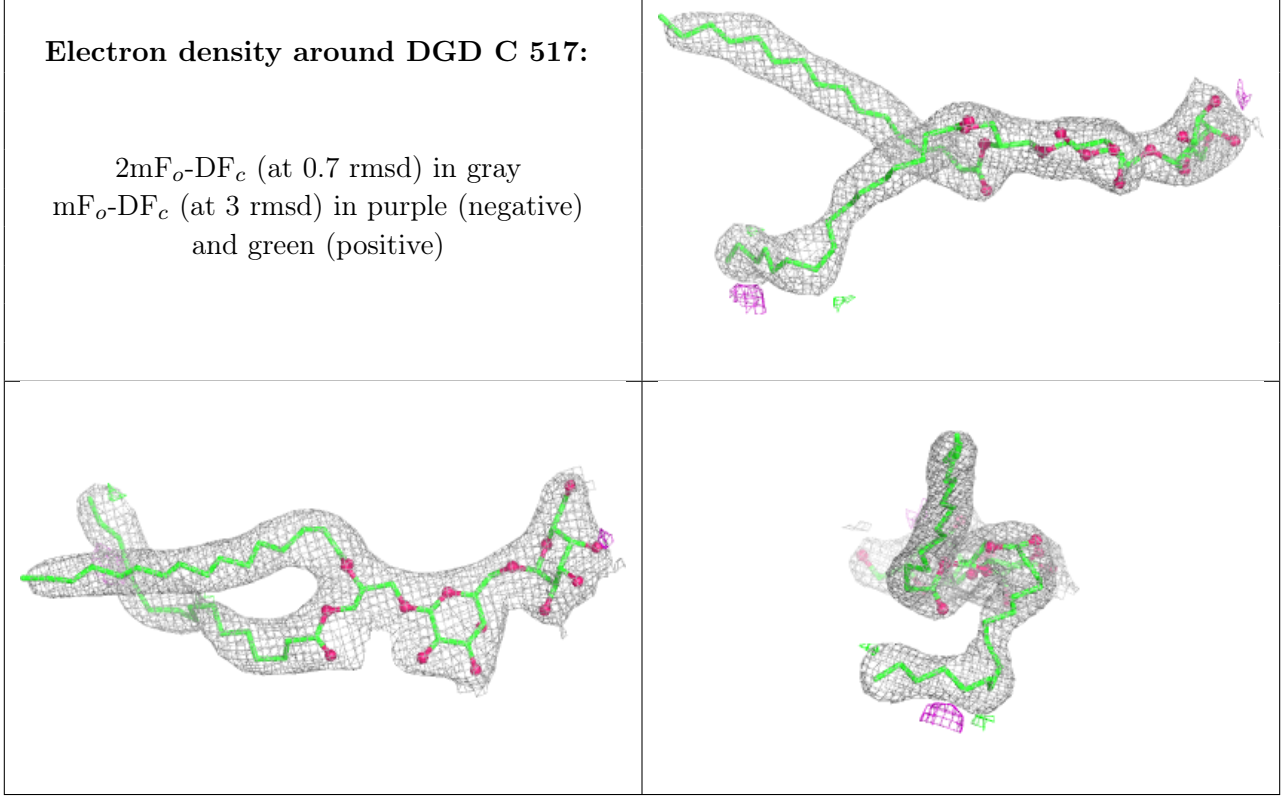
Electron density around CLA a 408:

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



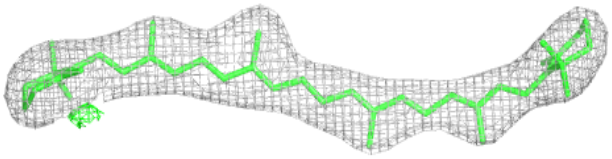
Electron density around DGD C 517:

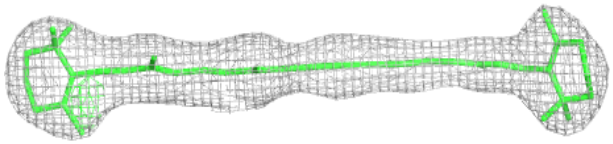
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

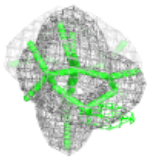


Electron density around BCR C 516:

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

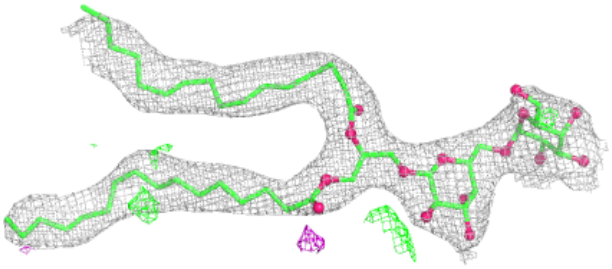


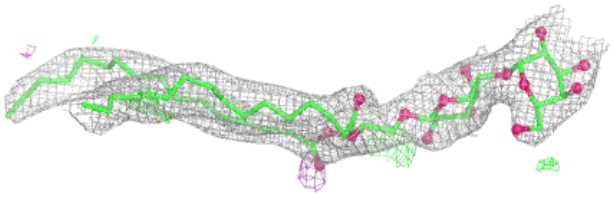


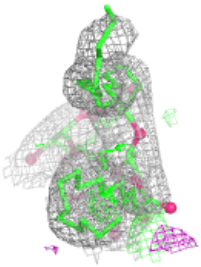


Electron density around DGD C 519:

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

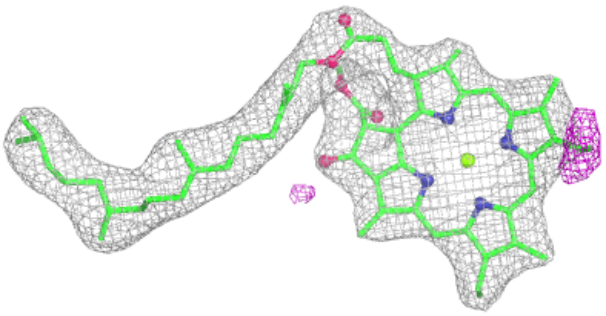


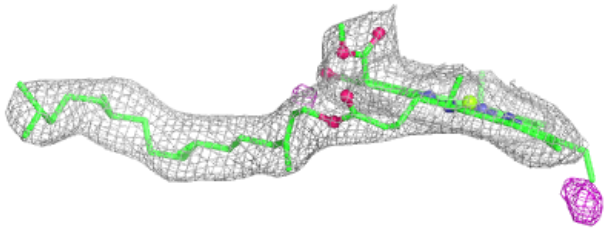


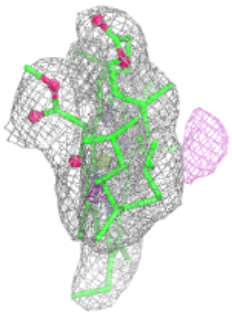


Electron density around CLA B 602:

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

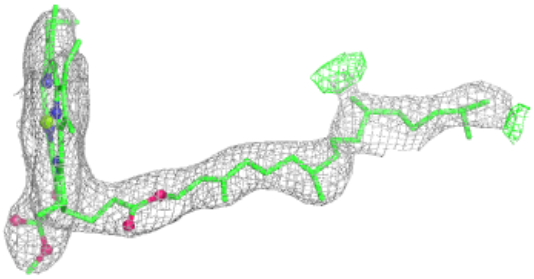


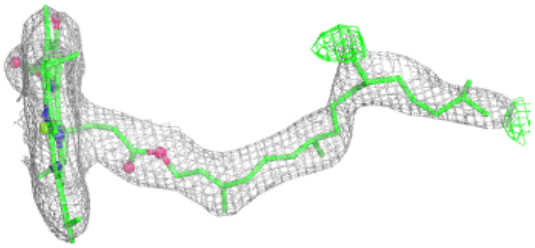


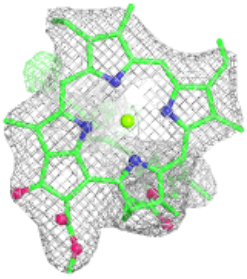


Electron density around CLA b 606:

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

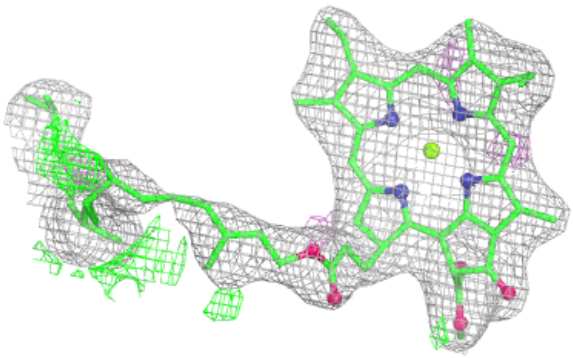


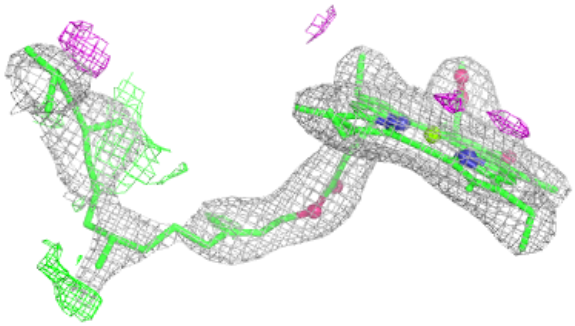


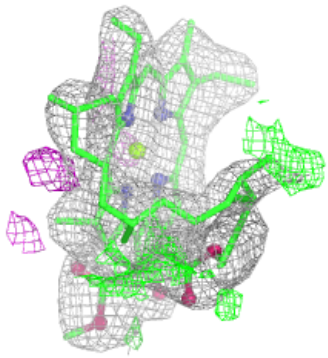


Electron density around CLA A 408:

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

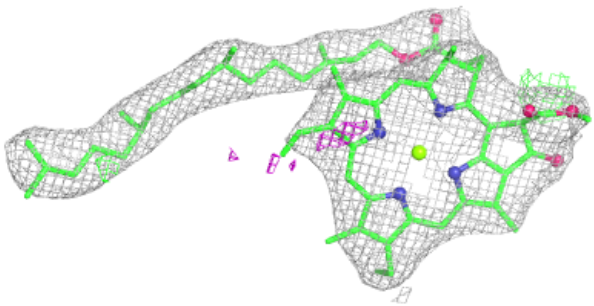


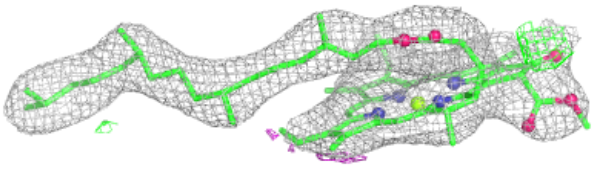


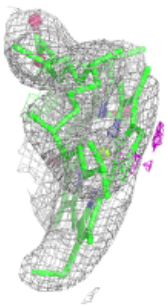


Electron density around CLA c 501:

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

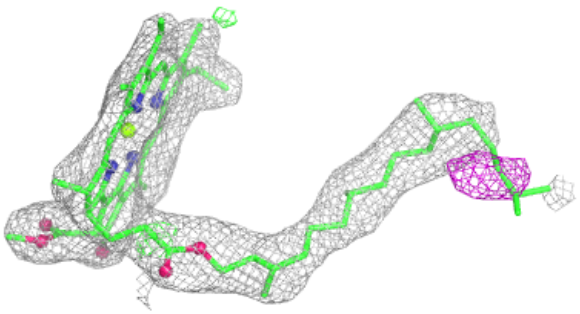


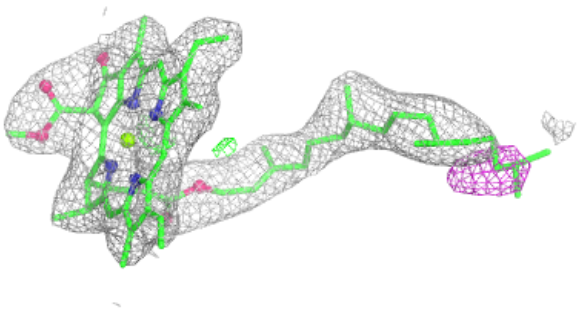


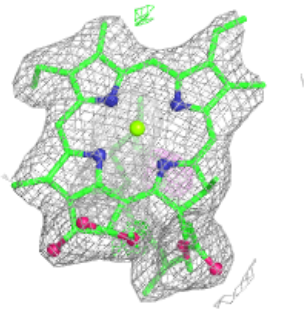


Electron density around CLA C 509:

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

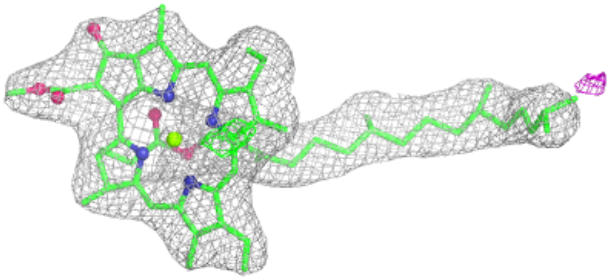


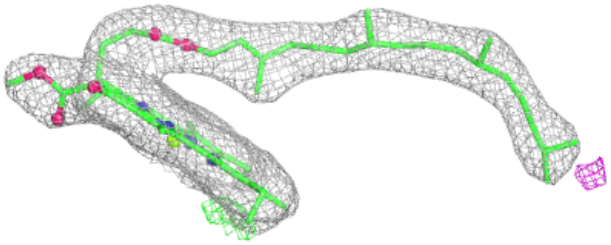


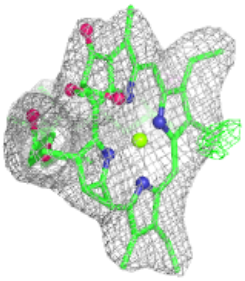


Electron density around CLA b 608:

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

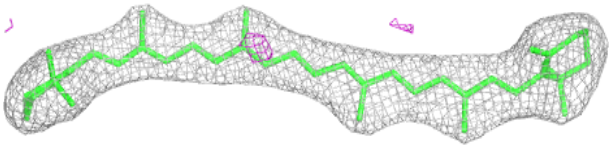


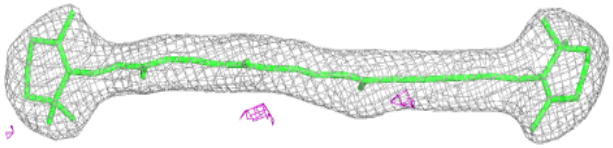


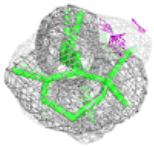


Electron density around BCR a 409:

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

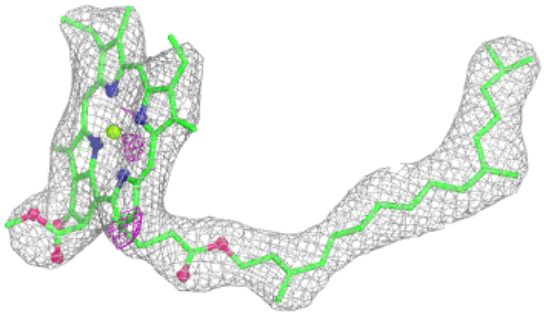


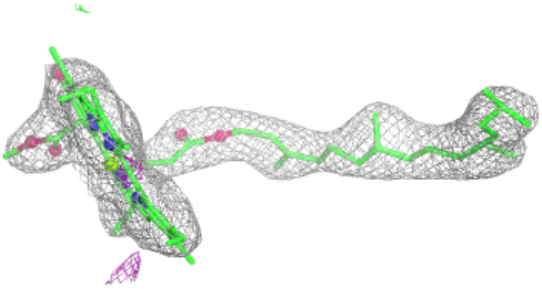


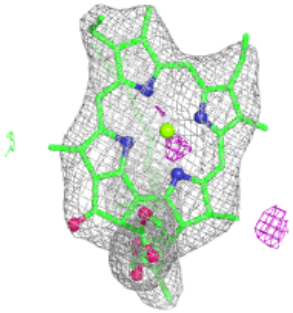


Electron density around CLA b 609:

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

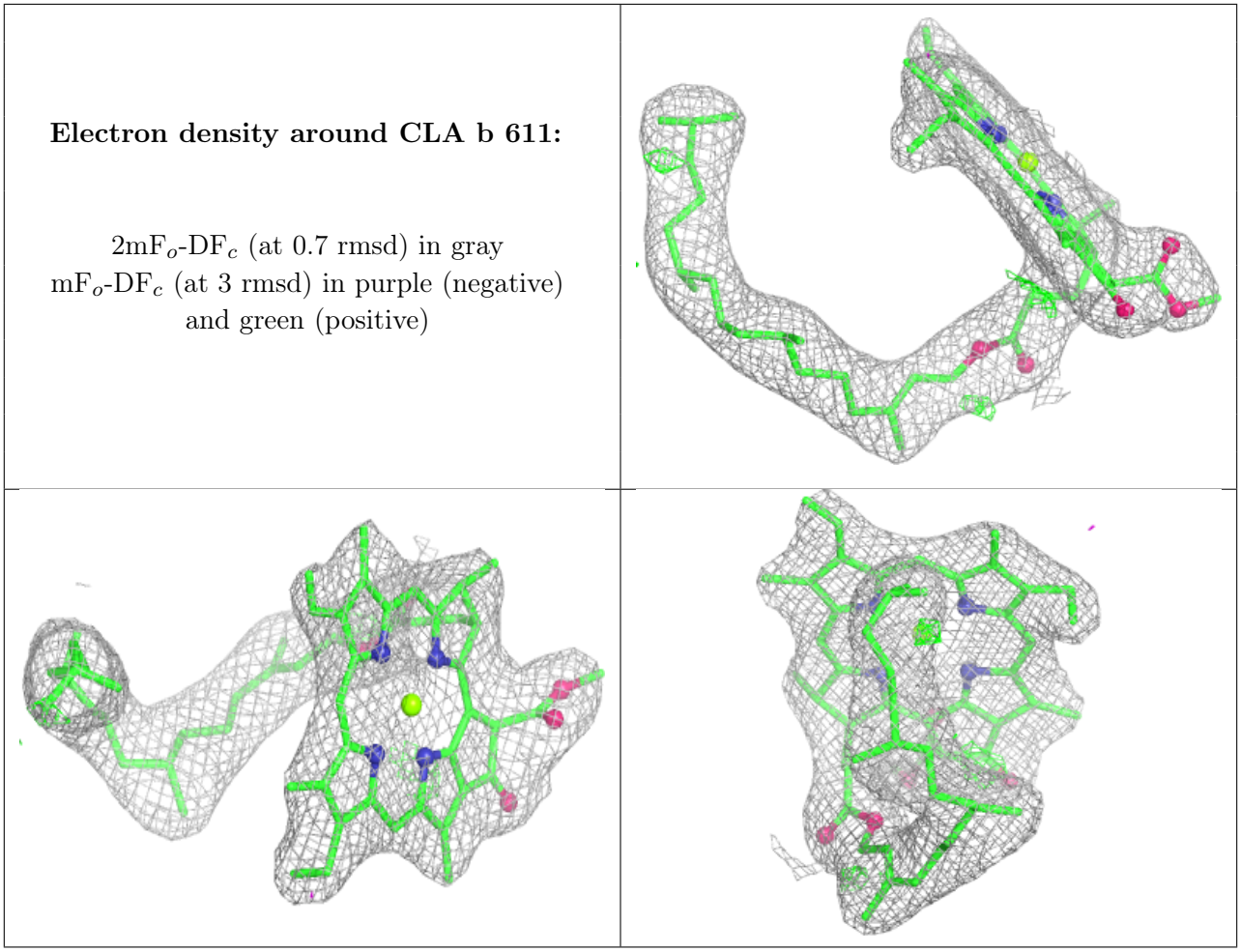






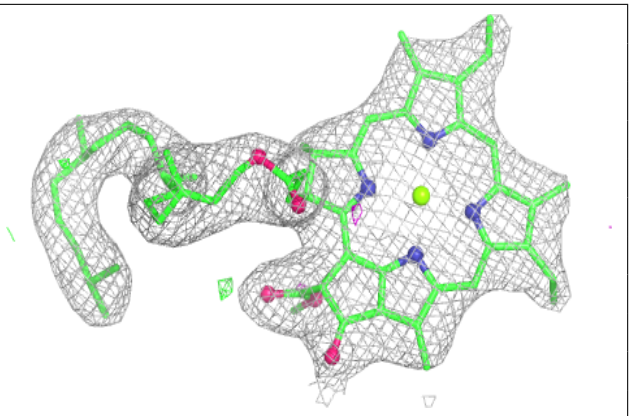
Electron density around CLA b 611:

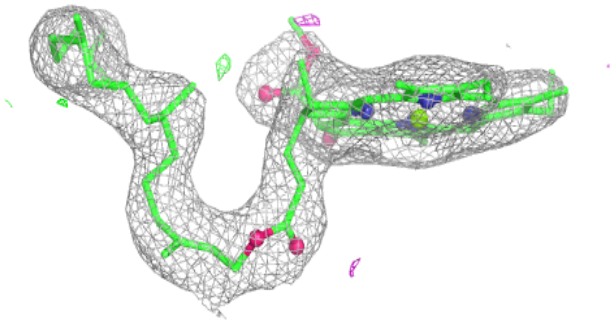
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

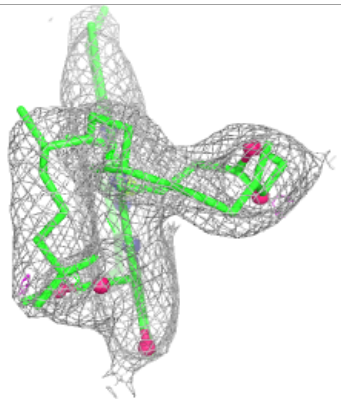


Electron density around CLA b 612:

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

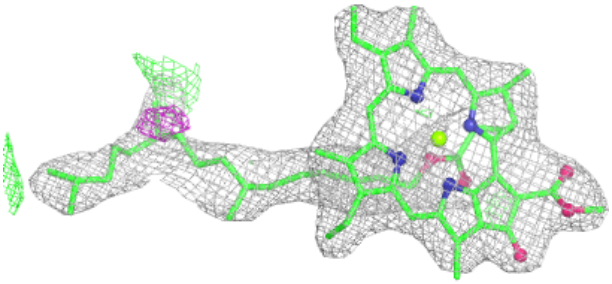


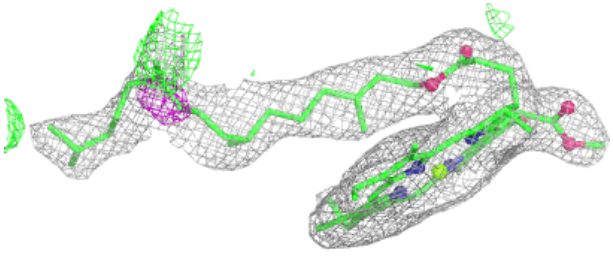


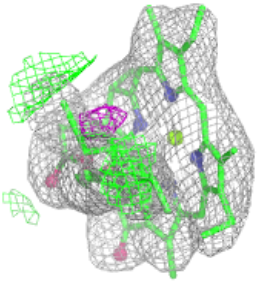


Electron density around CLA b 614:

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

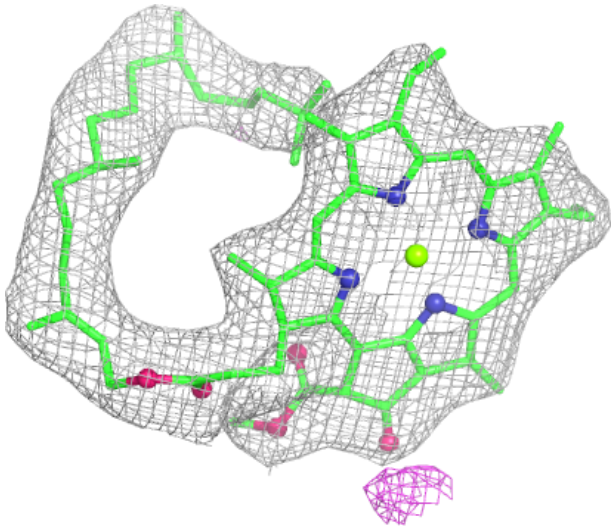


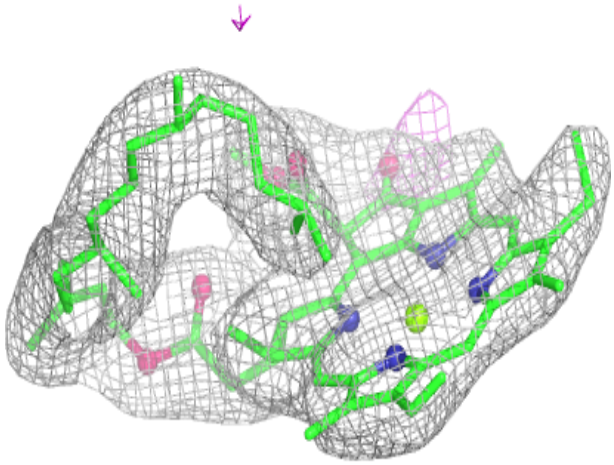


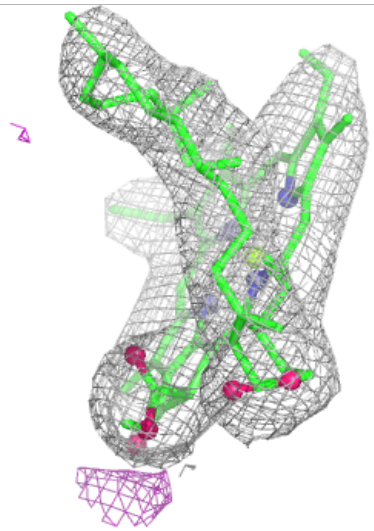


Electron density around CLA b 615:

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

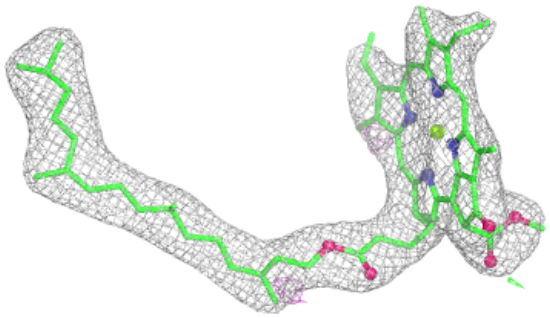


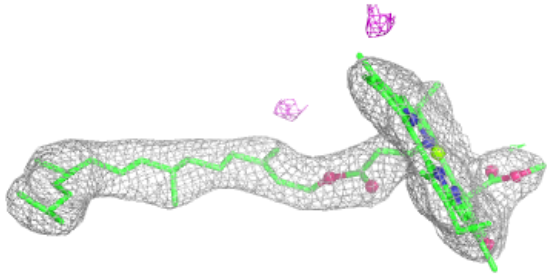


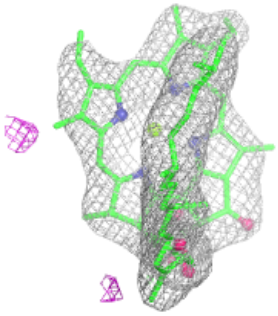


Electron density around CLA B 609:

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

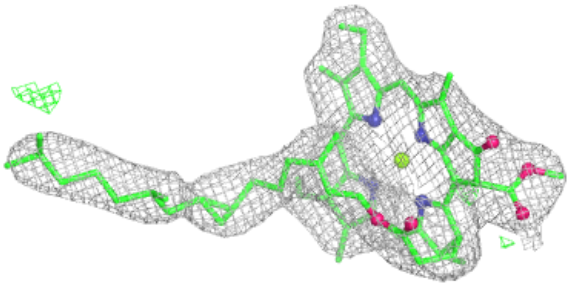


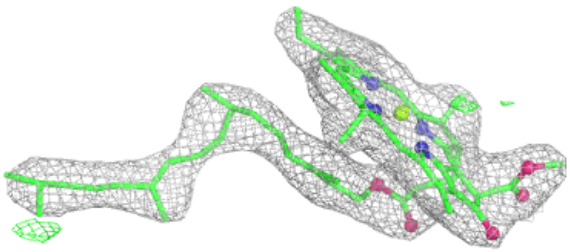


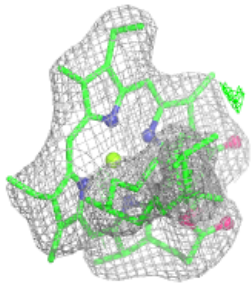


Electron density around CLA C 506:

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

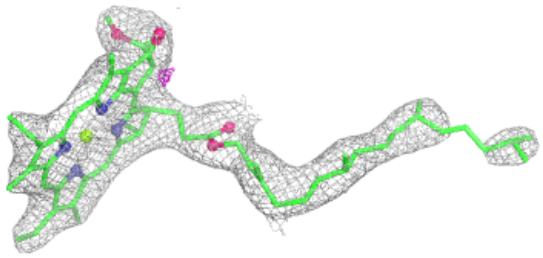


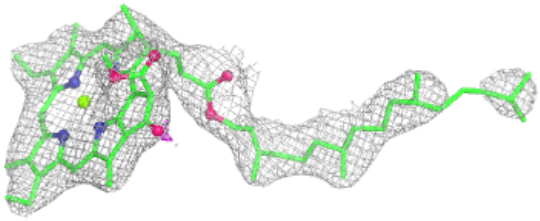


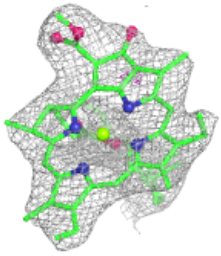


Electron density around CLA c 502:

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

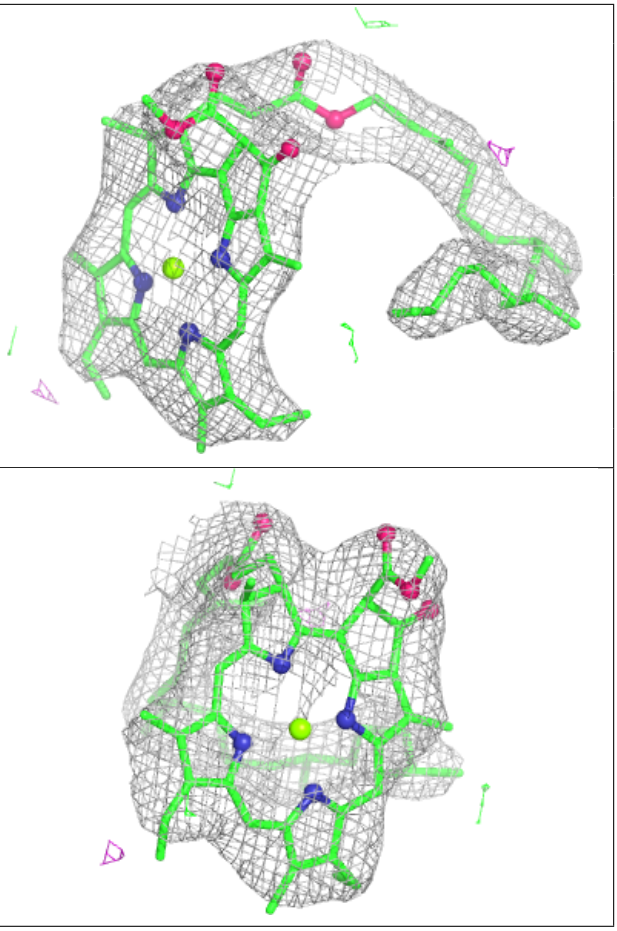


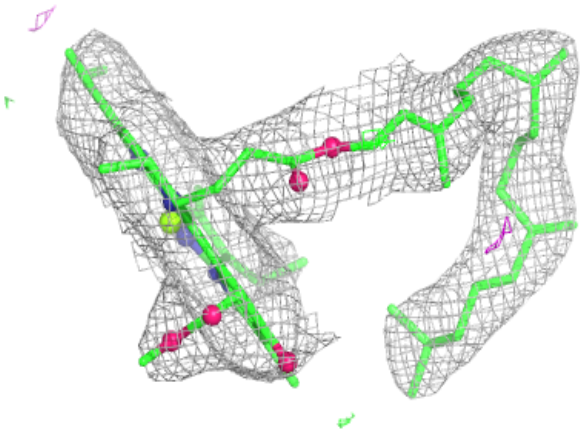




Electron density around CLA c 503:

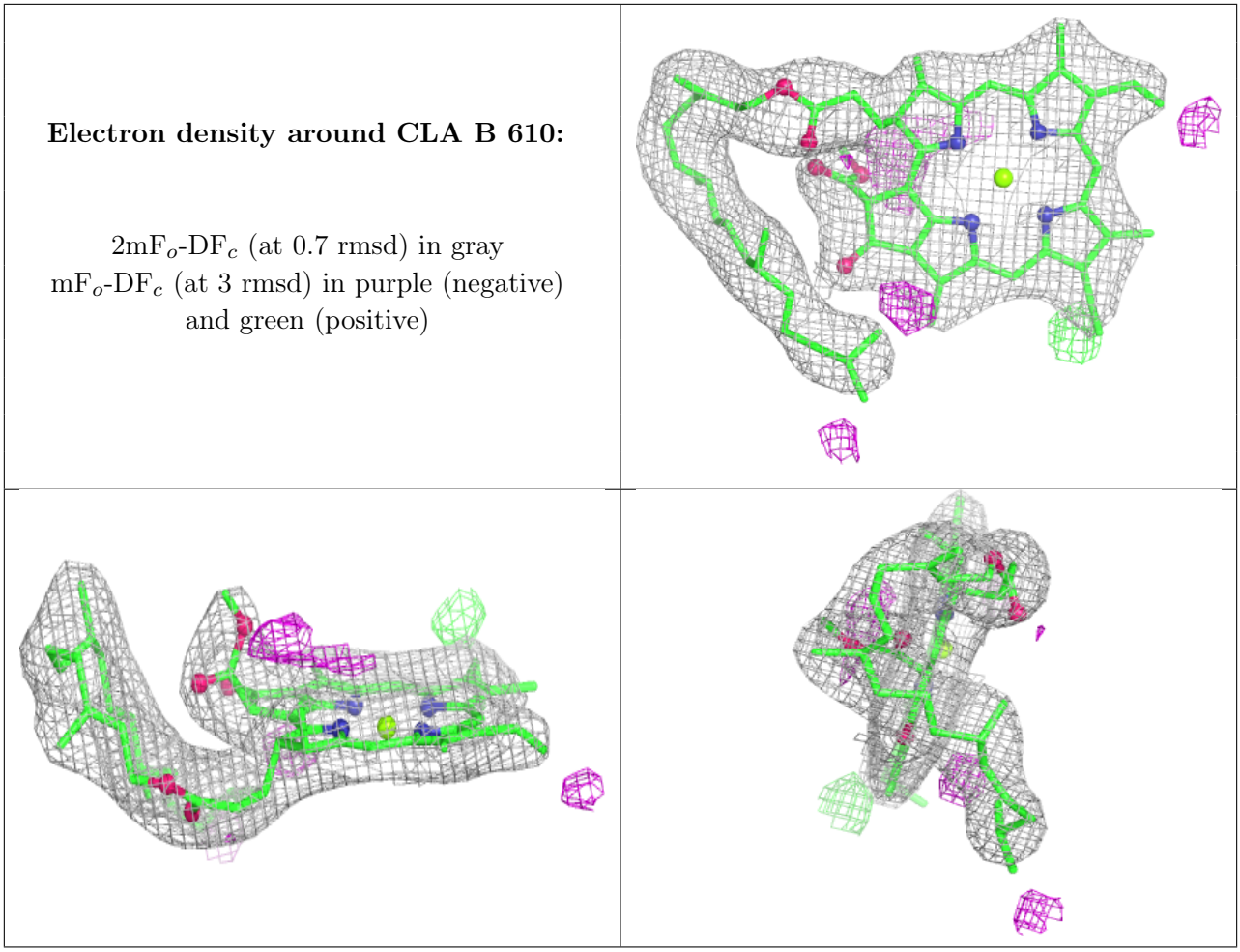
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





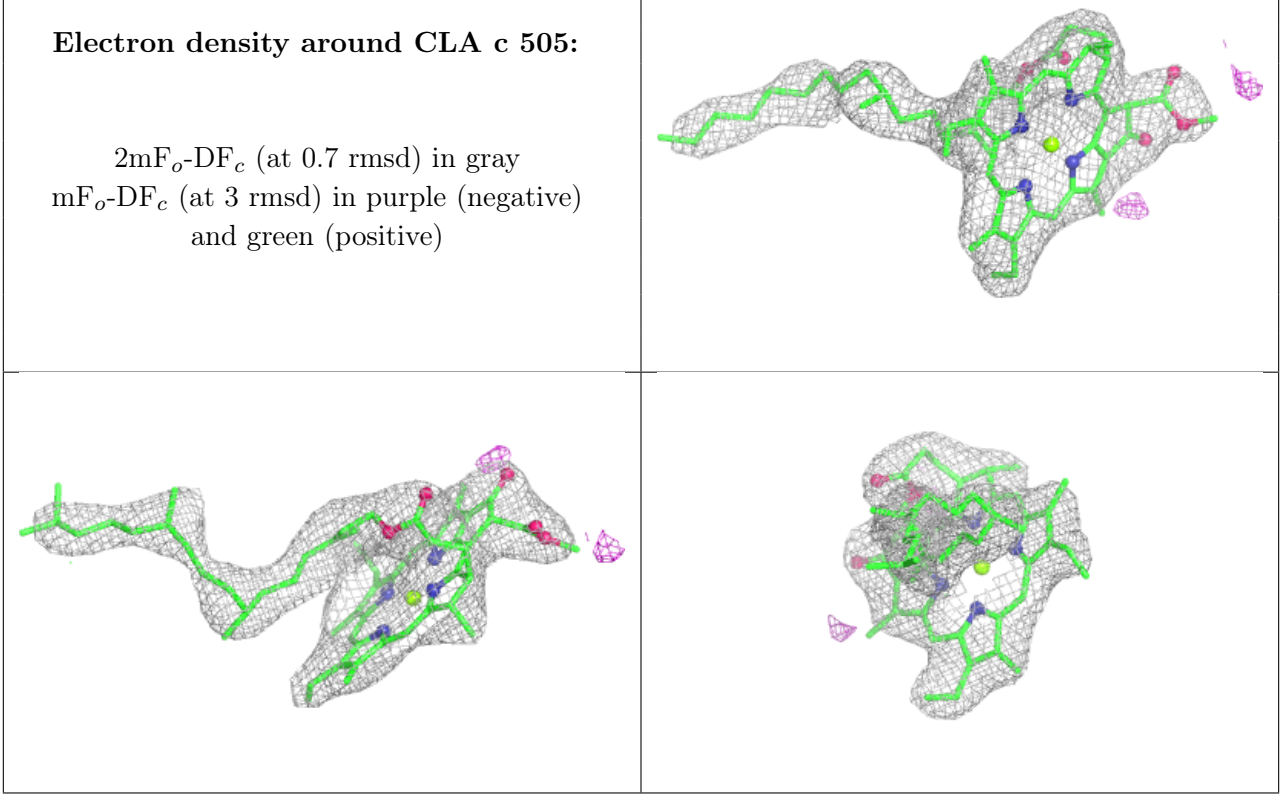
Electron density around CLA B 610:

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



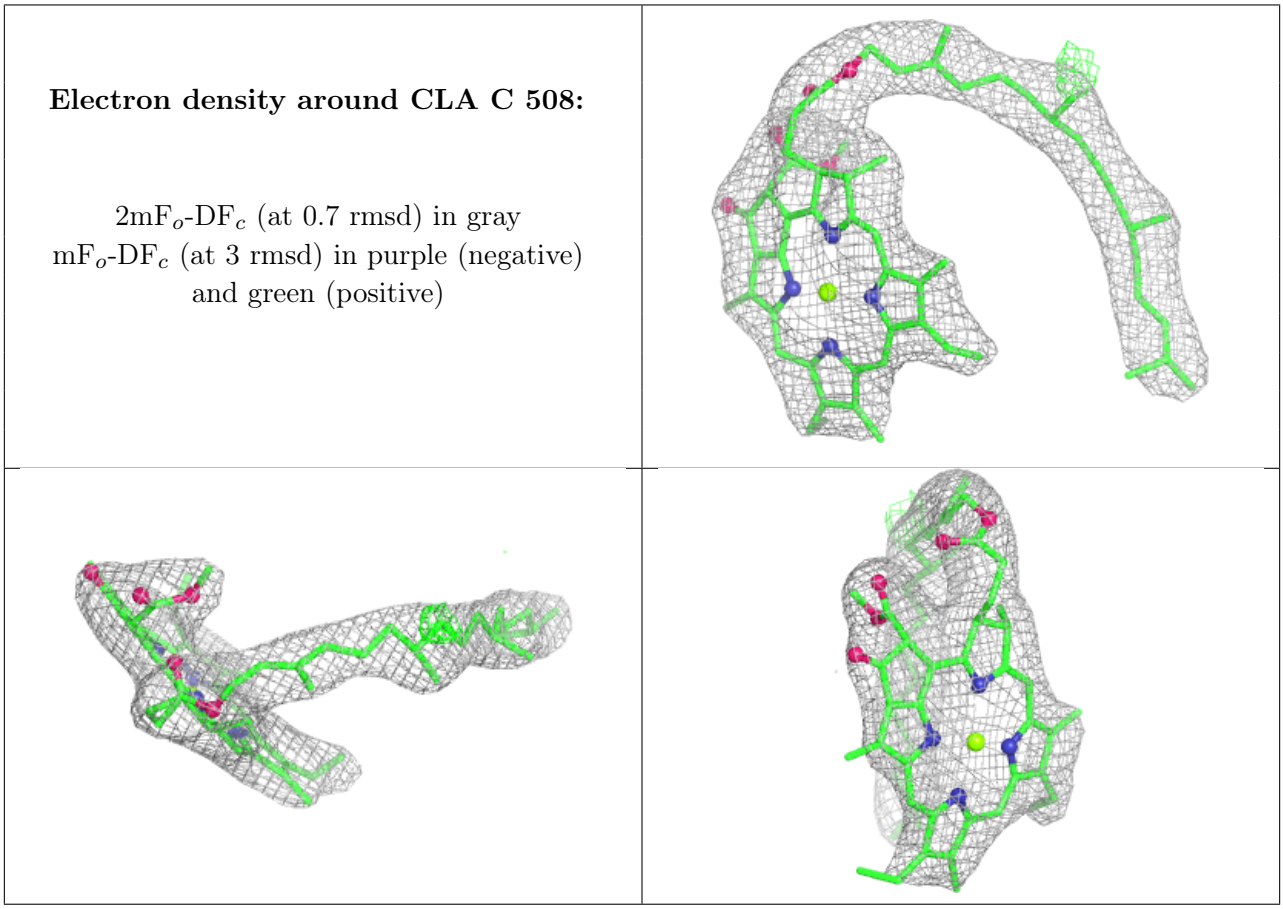
Electron density around CLA c 505:

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



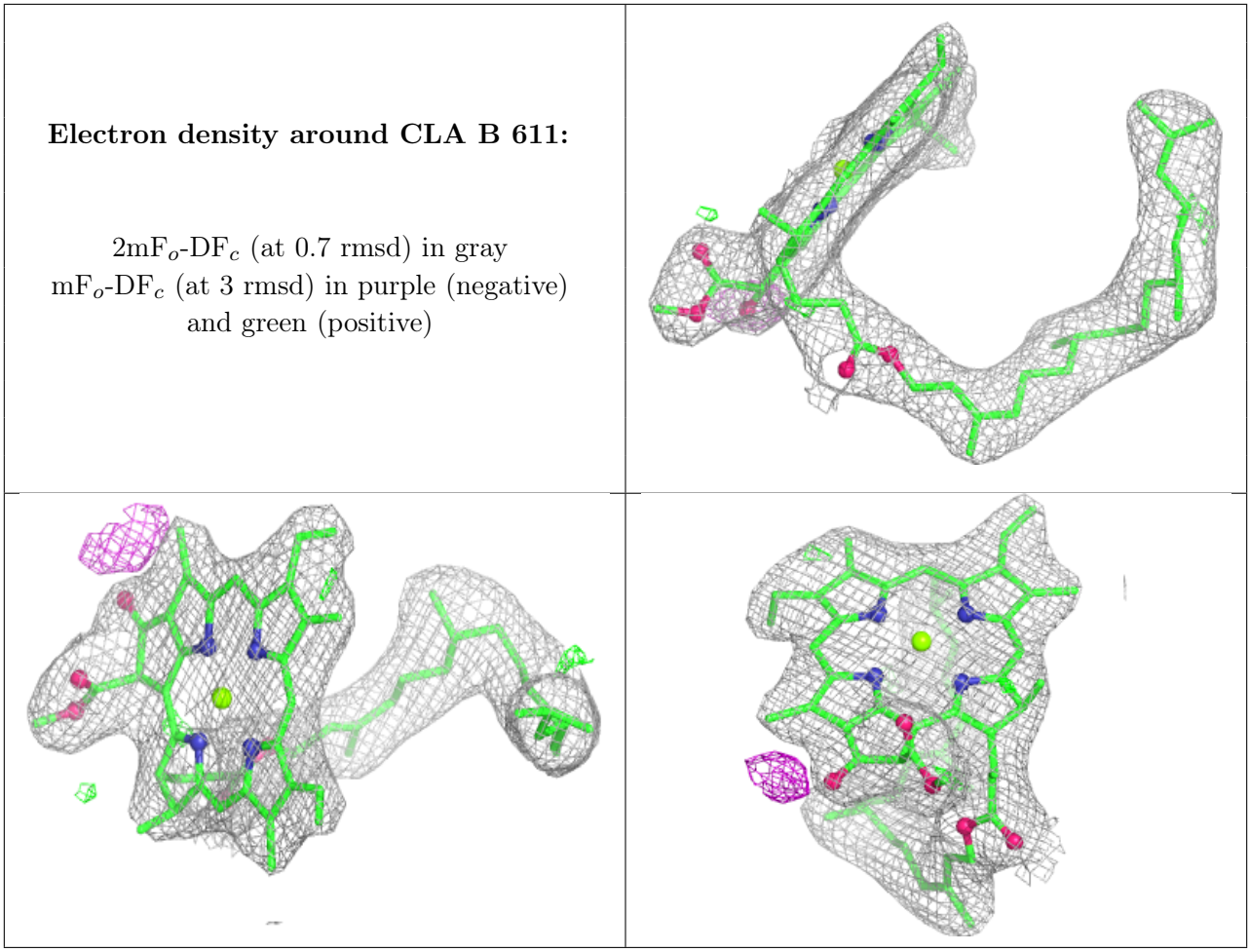
Electron density around CLA C 508:

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



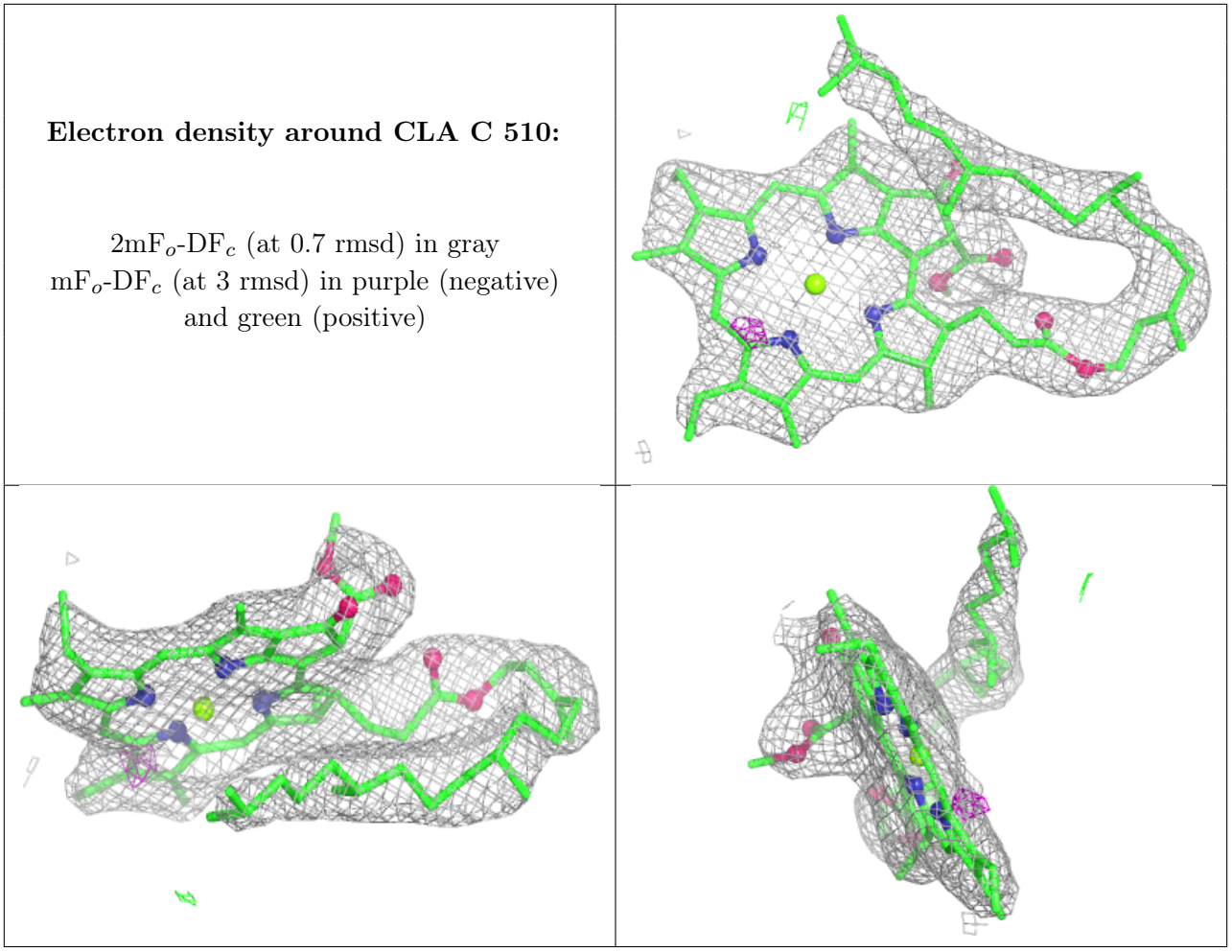
Electron density around CLA B 611:

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



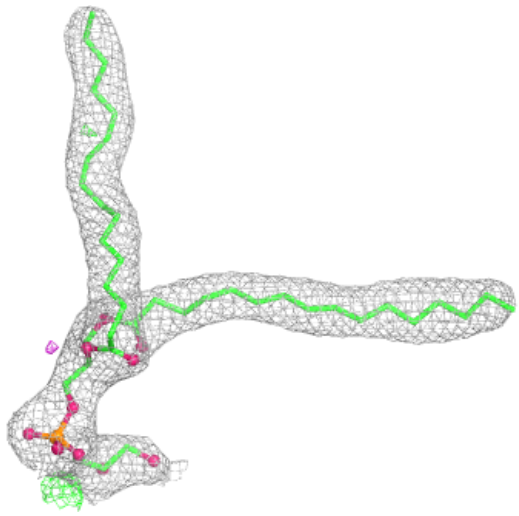
Electron density around CLA C 510:

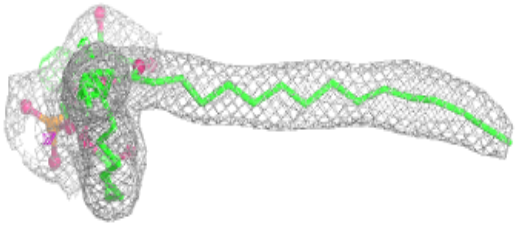
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

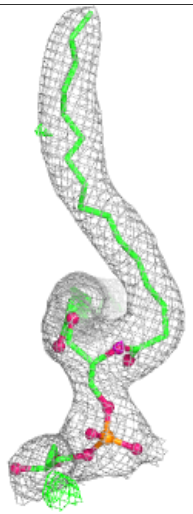


Electron density around LHG A 417:

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

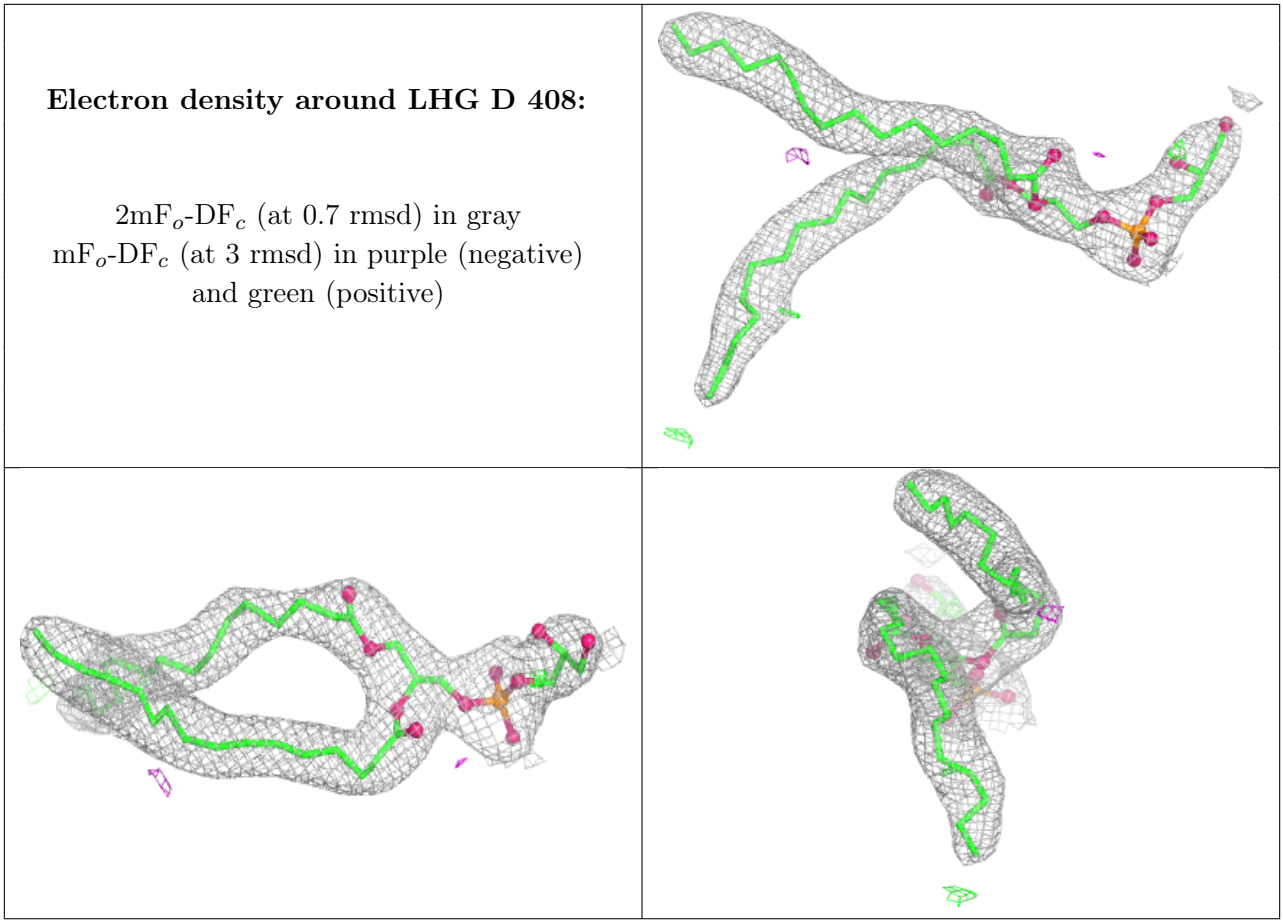






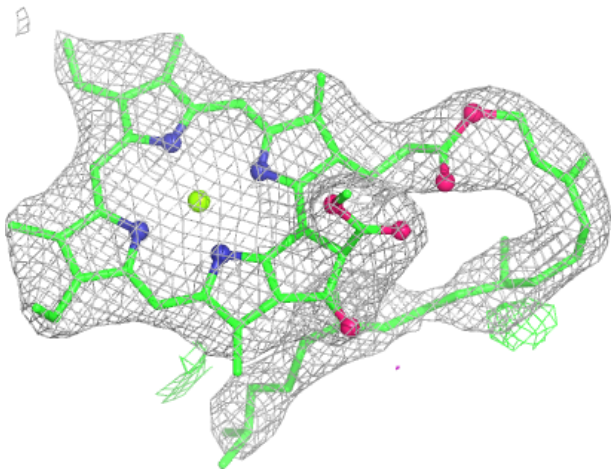
Electron density around LHG D 408:

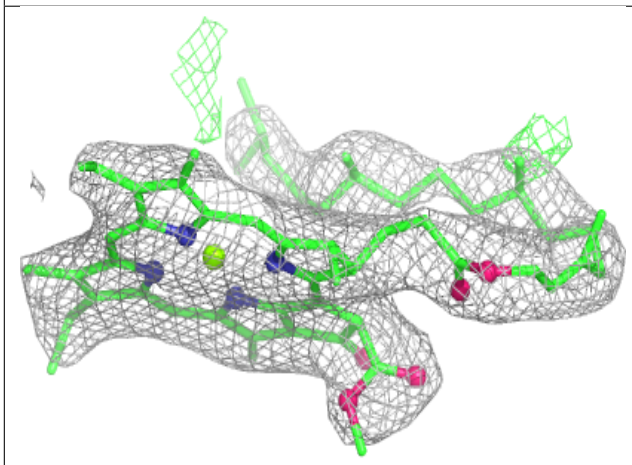
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

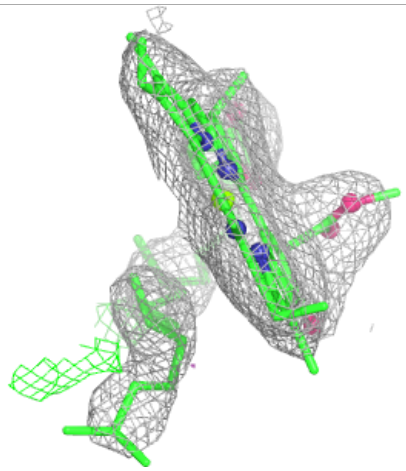


Electron density around CLA c 509:

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

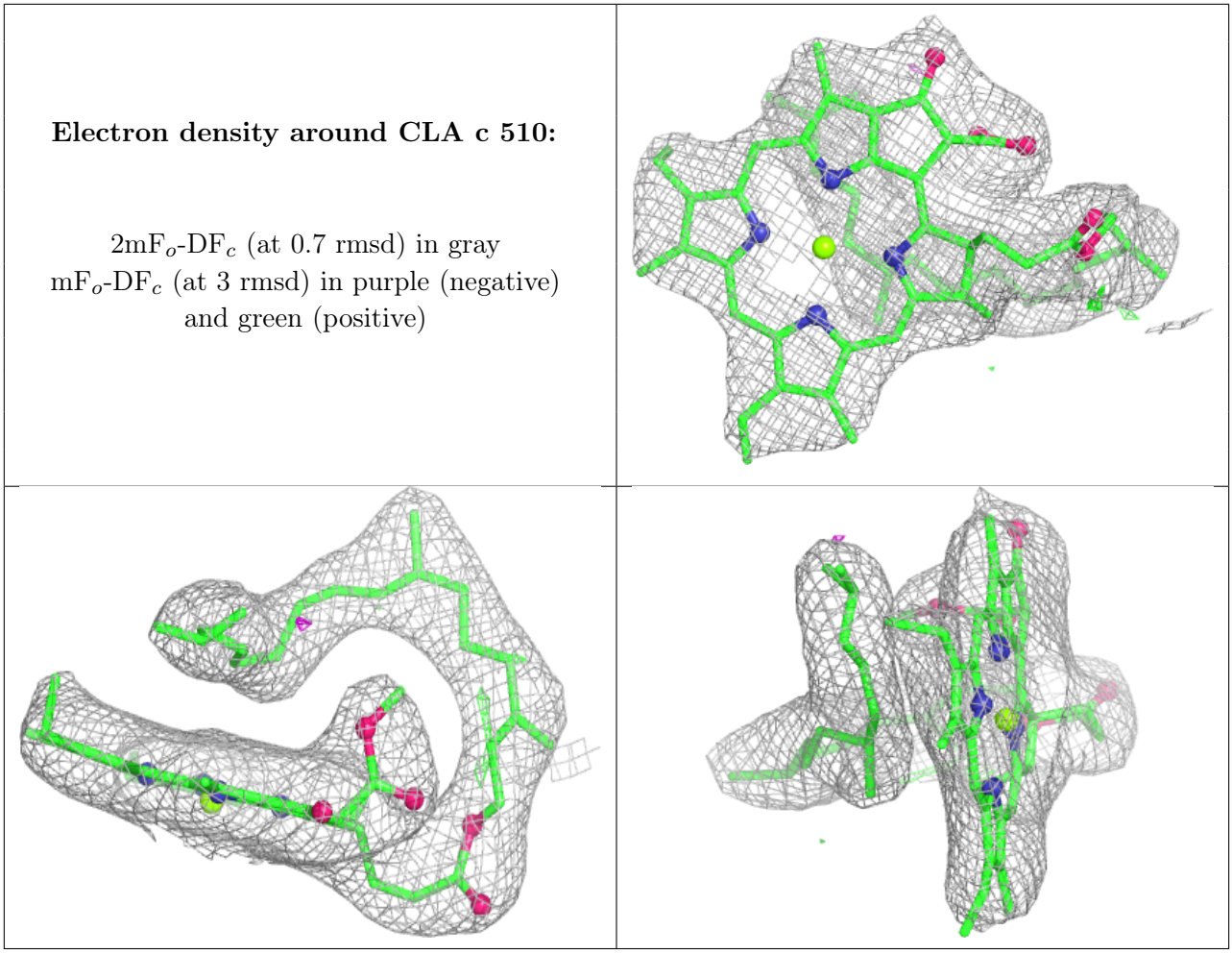






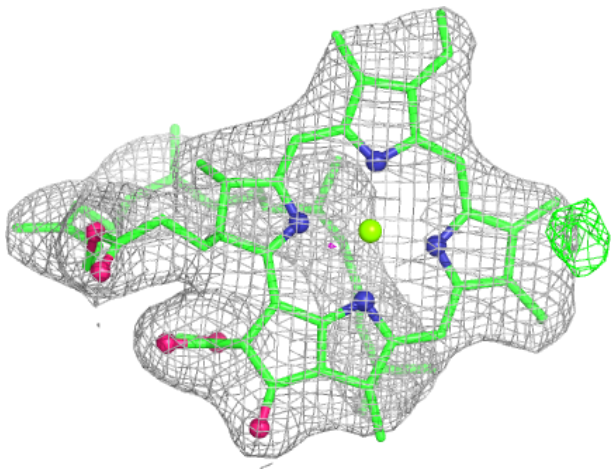
Electron density around CLA c 510:

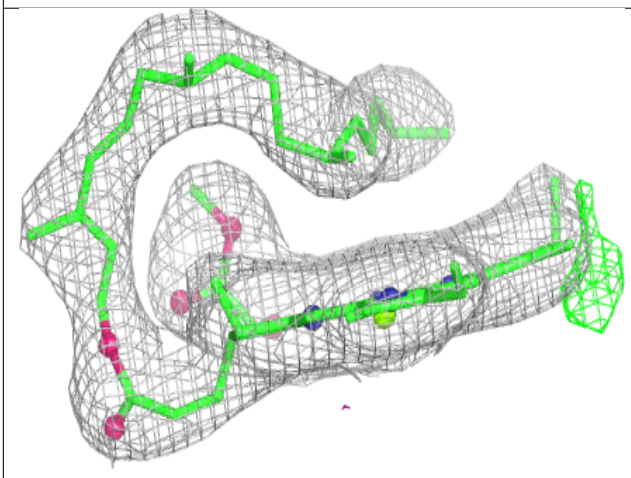
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

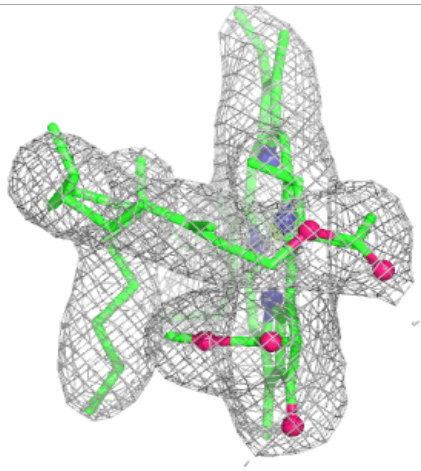


Electron density around CLA C 511:

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

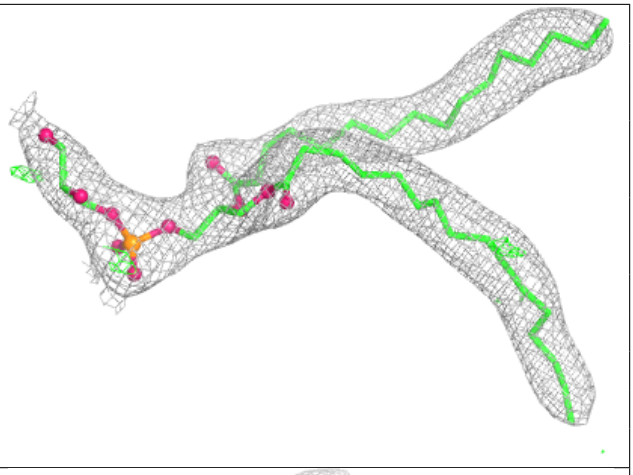


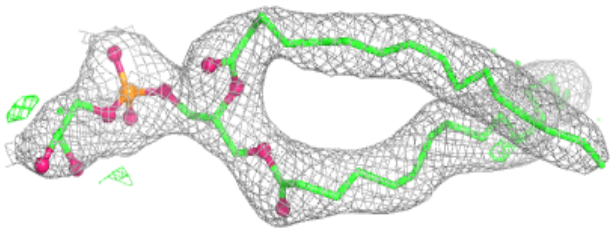


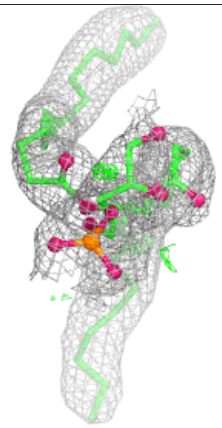


Electron density around LHG d 408:

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

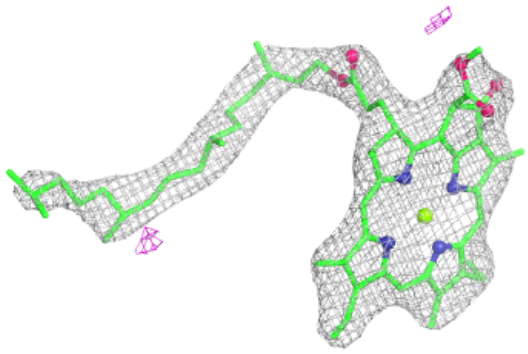


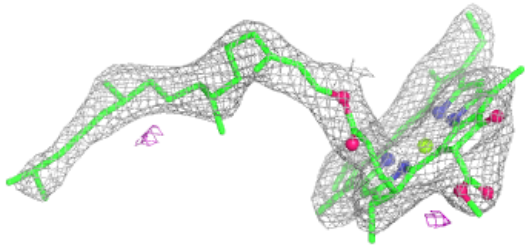


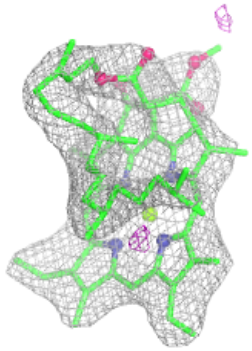


Electron density around CLA C 512:

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

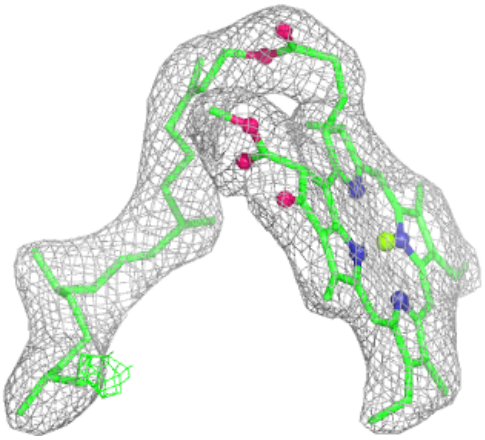


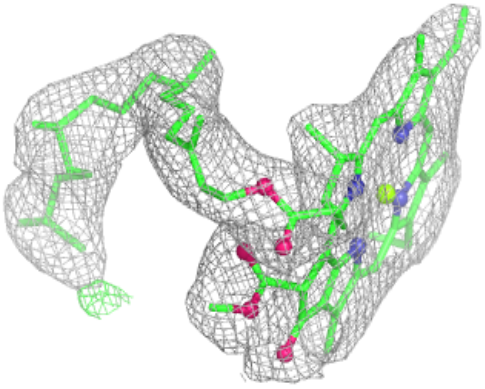


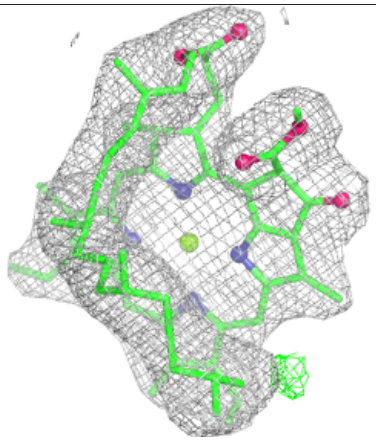


Electron density around CLA B 613:

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

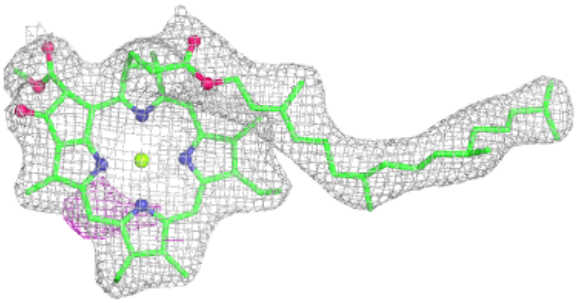


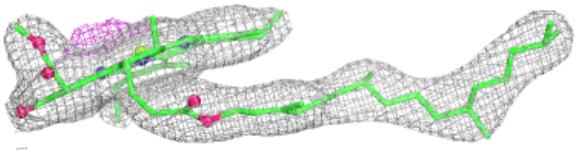


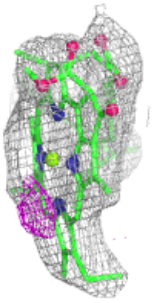


Electron density around CLA B 603:

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

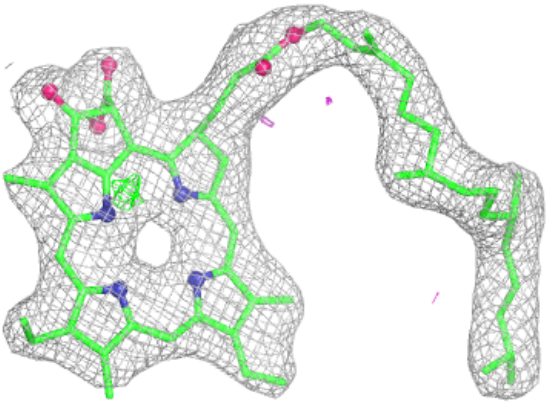


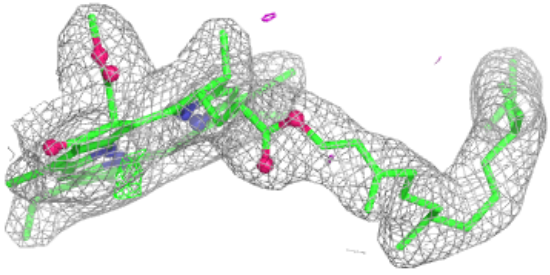


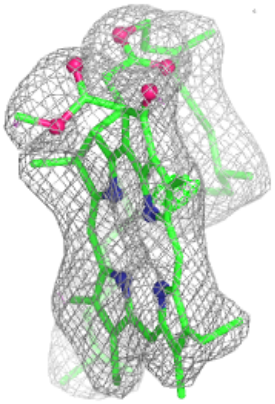


Electron density around PHO A 407:

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

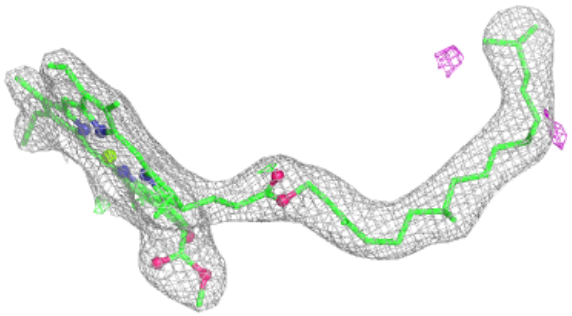


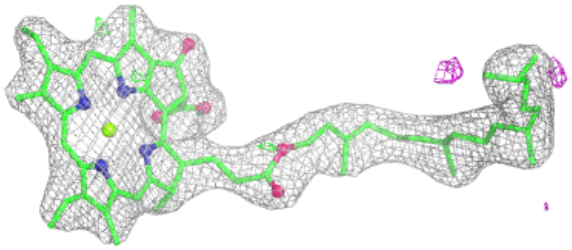


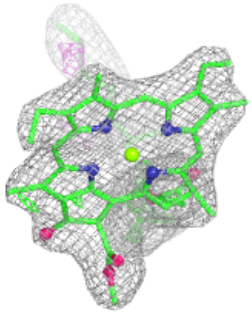


Electron density around CLA D 404:

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

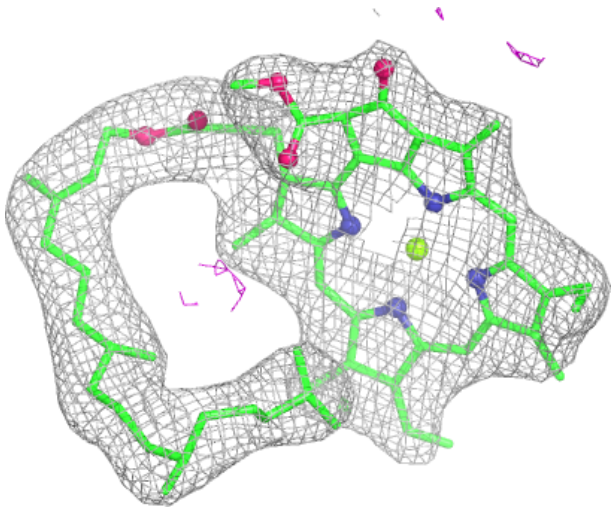


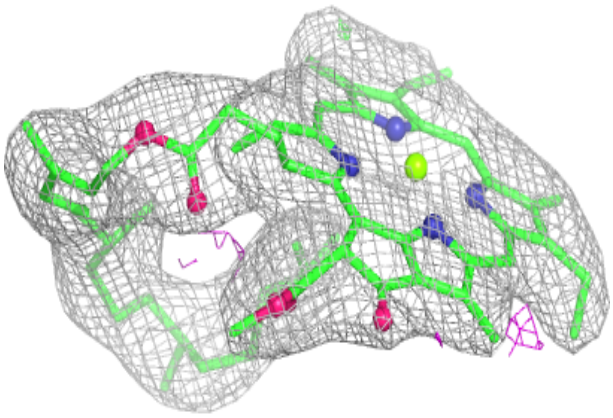


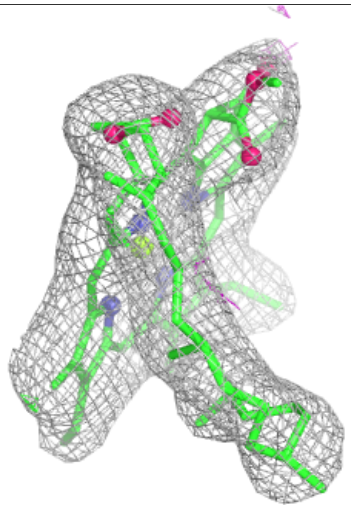


Electron density around CLA B 615:

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

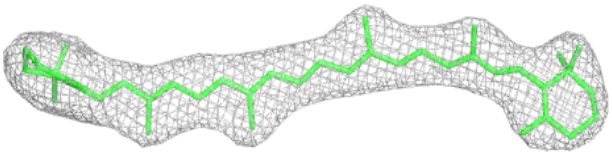


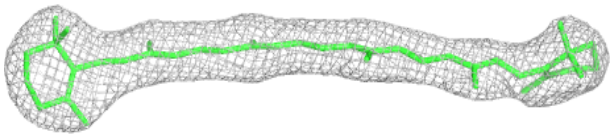


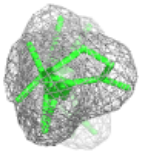


Electron density around BCR B 617:

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

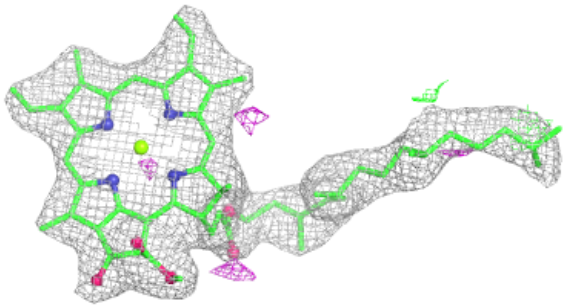


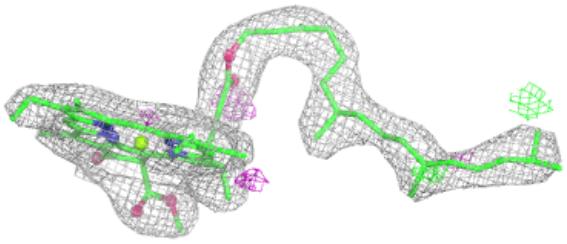


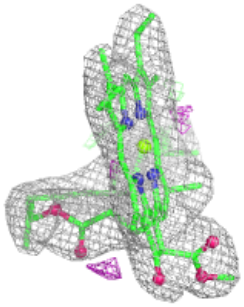


Electron density around CLA A 406:

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

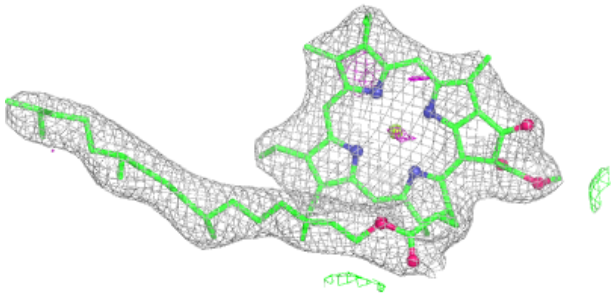


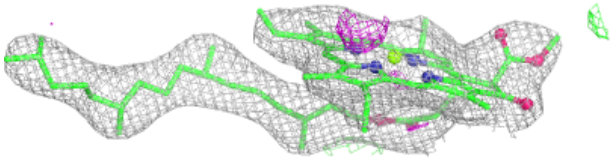


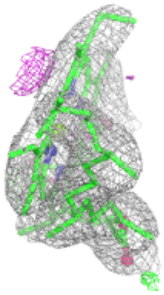


Electron density around CLA C 502:

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

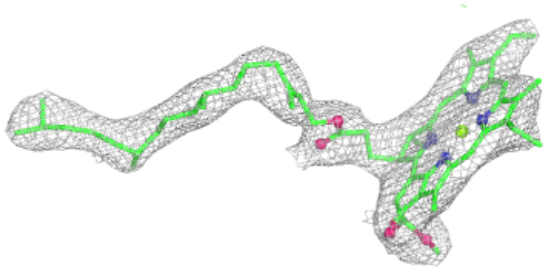


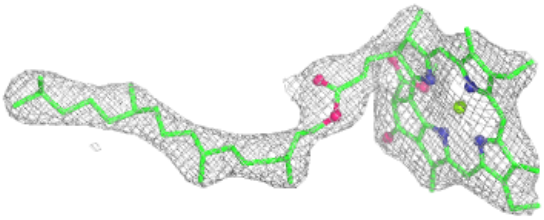


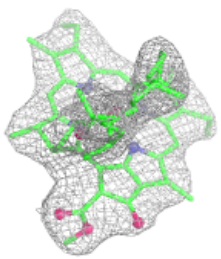


Electron density around CLA C 503:

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

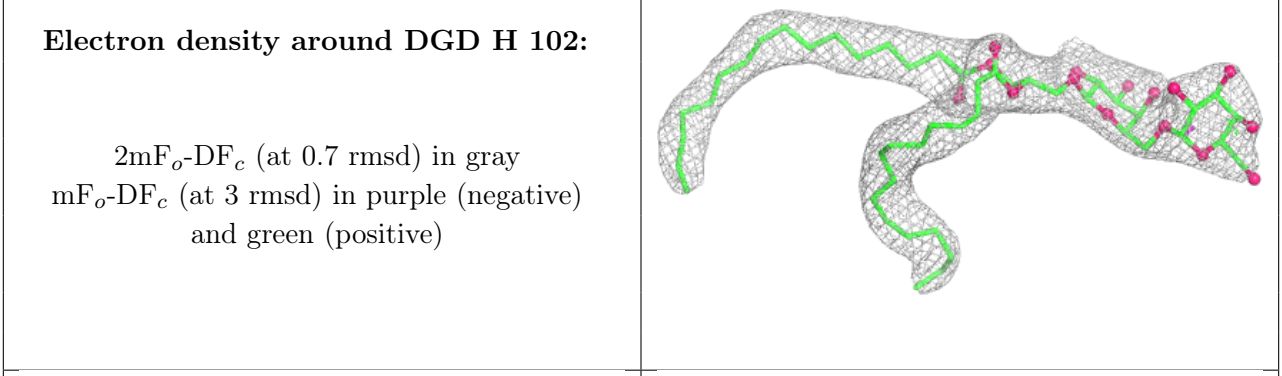


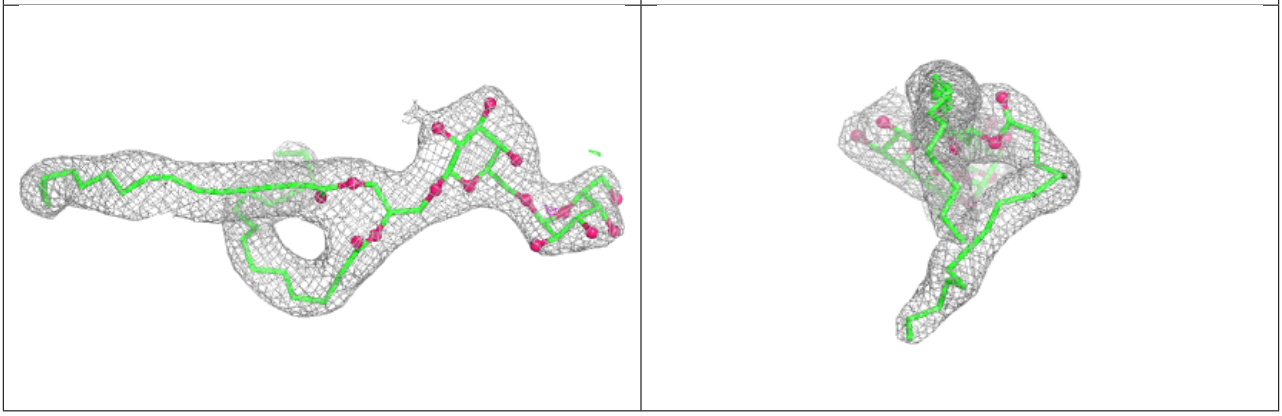




Electron density around DGD H 102:

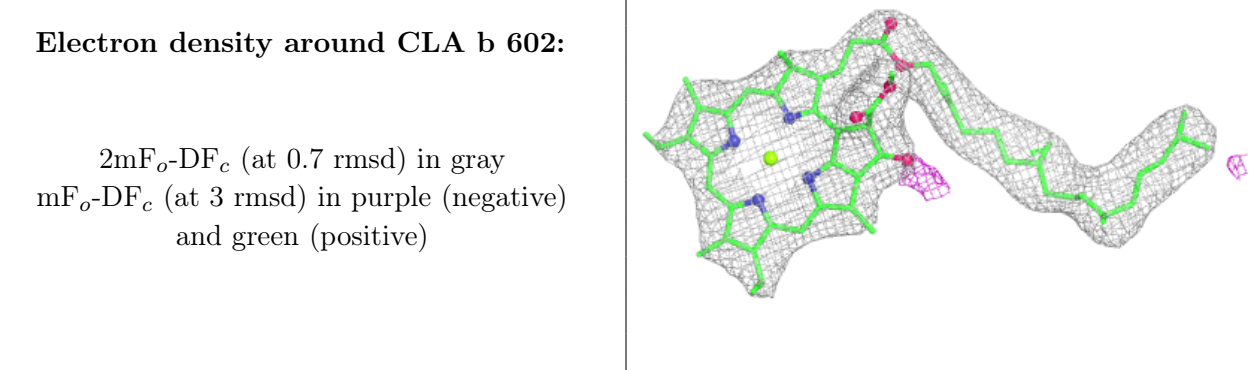
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

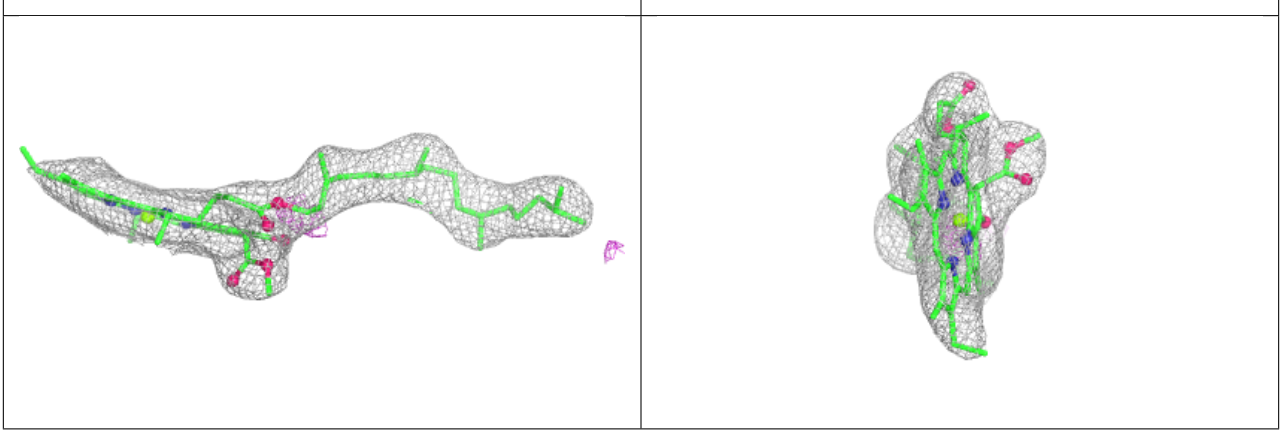




Electron density around CLA b 602:

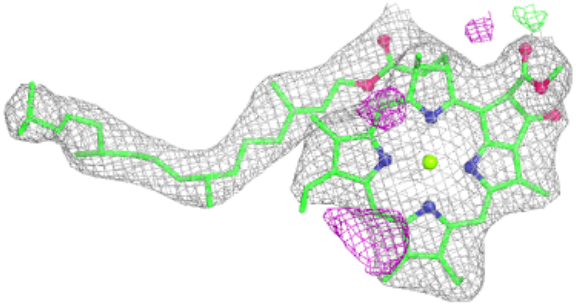
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

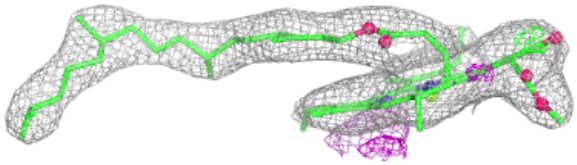


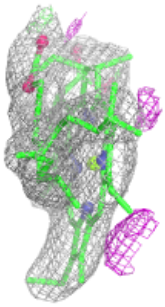


Electron density around CLA b 603:

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

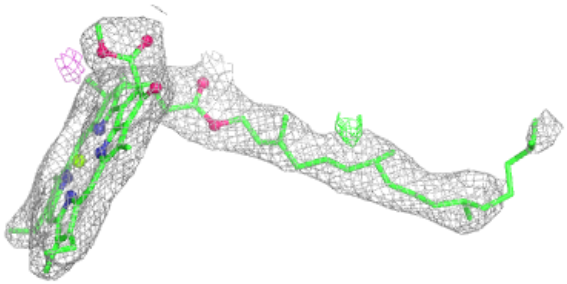


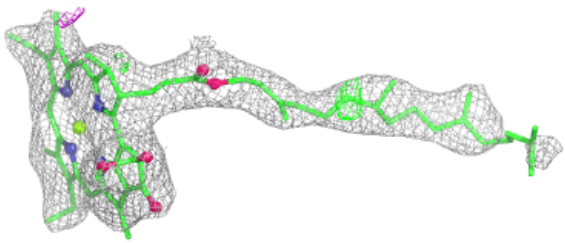


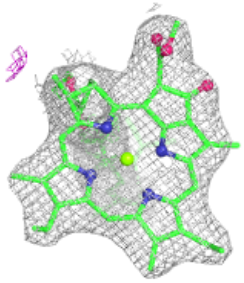


Electron density around CLA b 604:

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

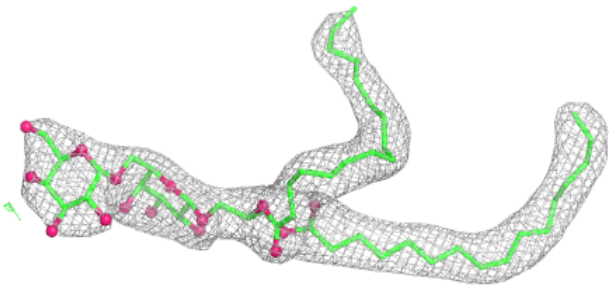


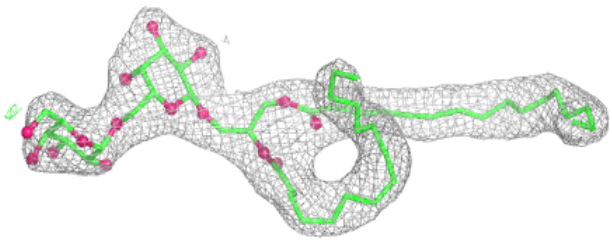




Electron density around DGD h 102:

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

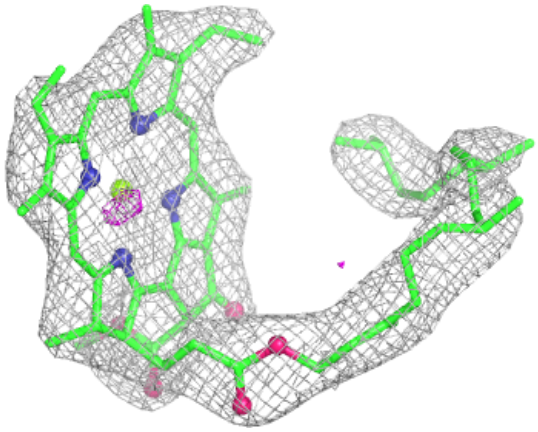


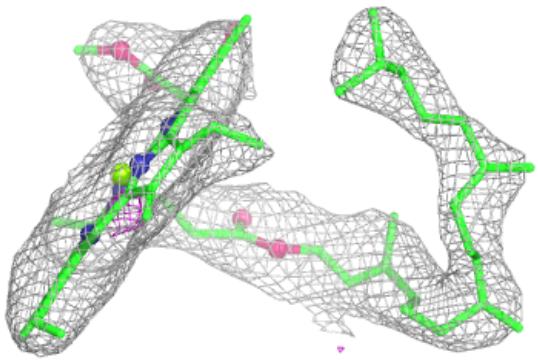


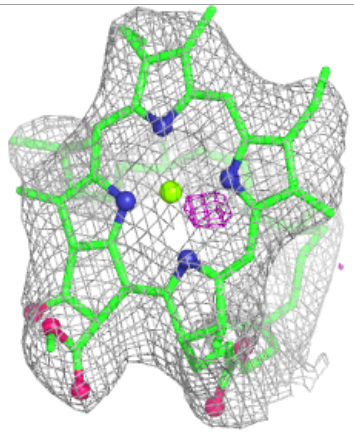


Electron density around CLA C 504:

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

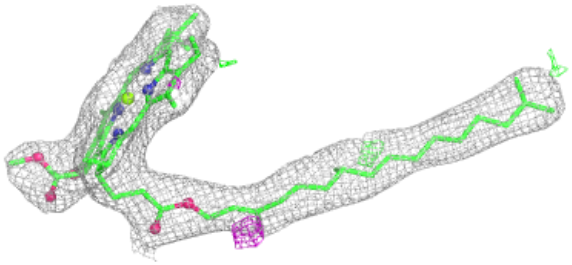


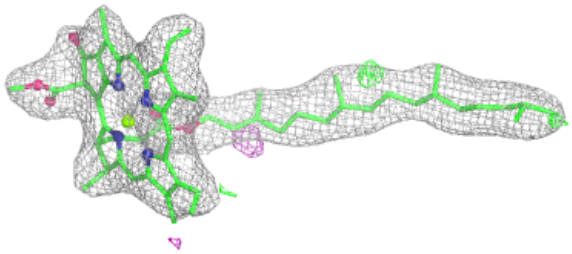


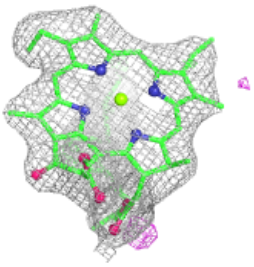


Electron density around CLA b 607:

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

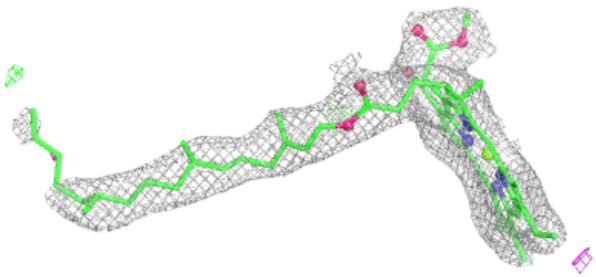


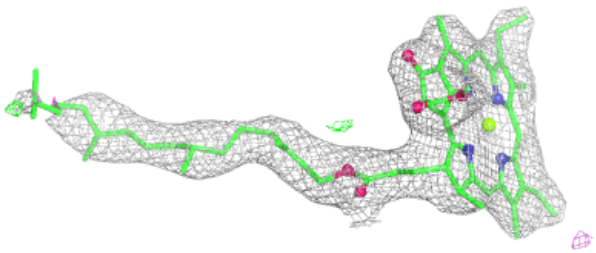


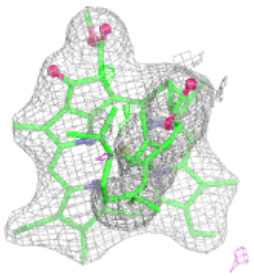


Electron density around CLA B 604:

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

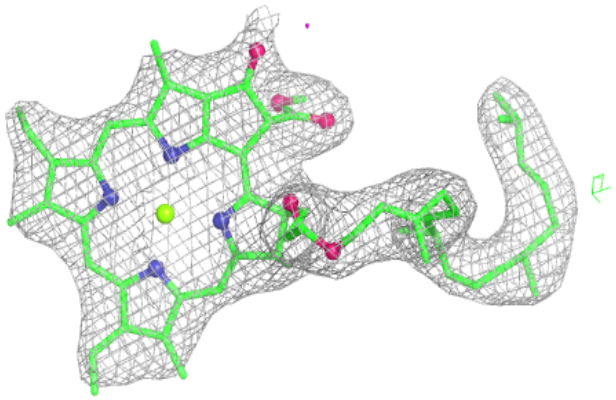


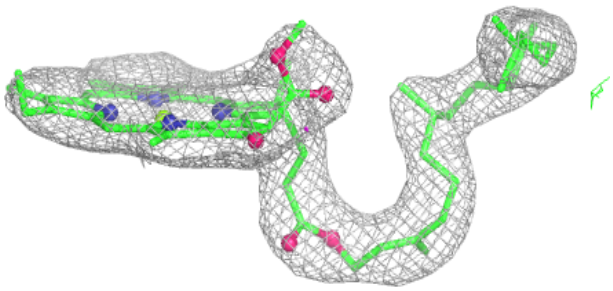


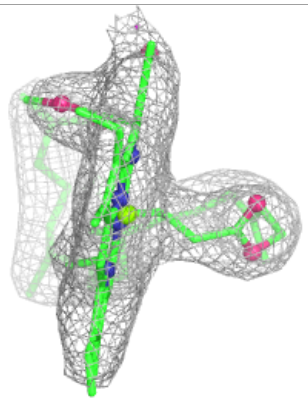


Electron density around CLA B 612:

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

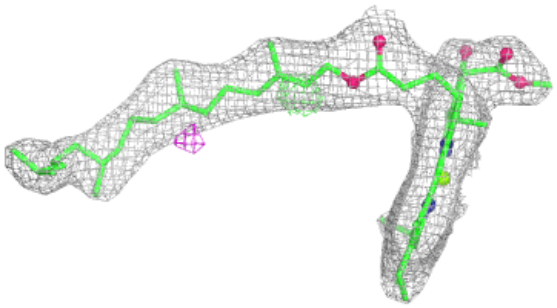


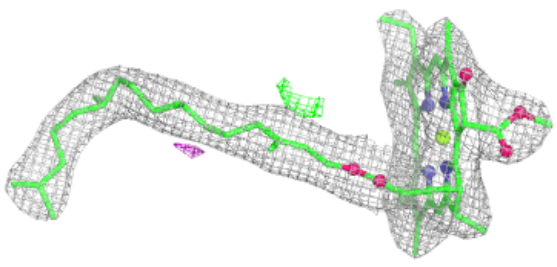


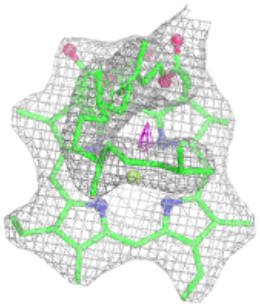


Electron density around CLA B 605:

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

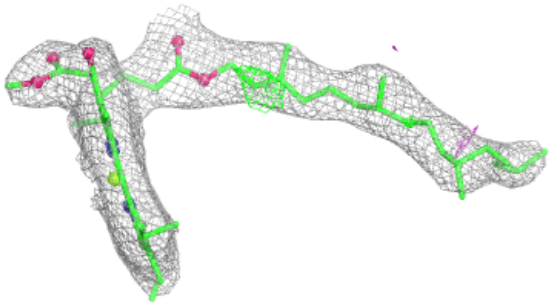


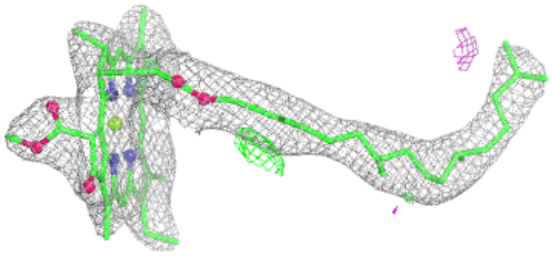


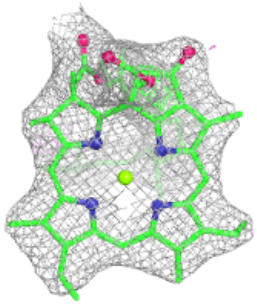


Electron density around CLA b 605:

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

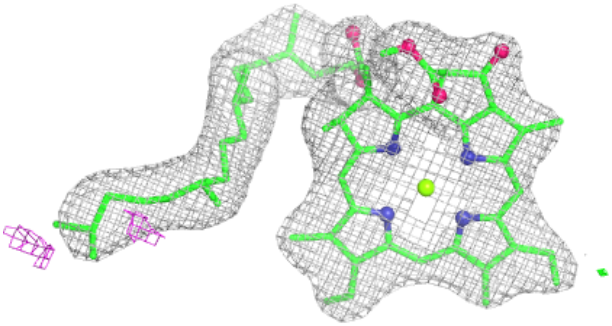


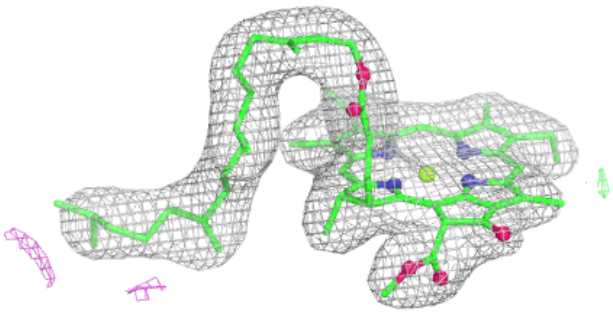




Electron density around CLA d 401:

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

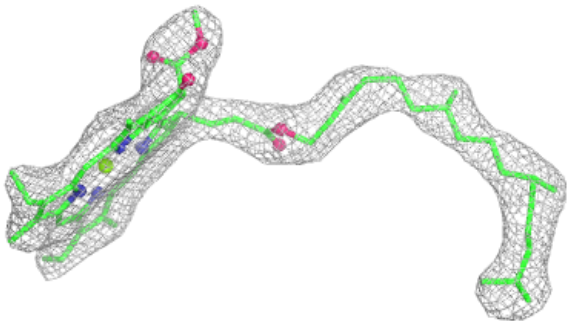


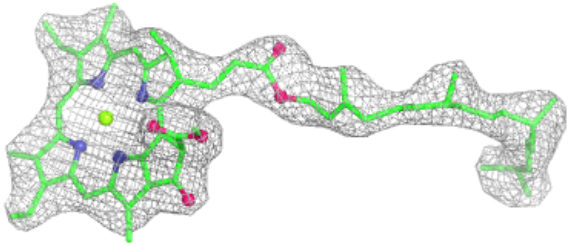


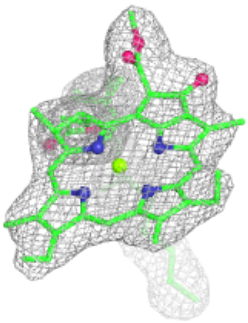


Electron density around CLA d 403:

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

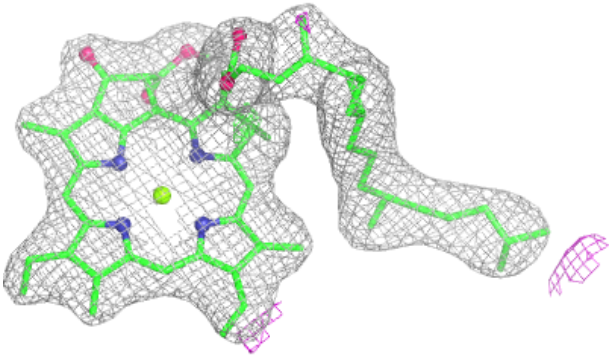


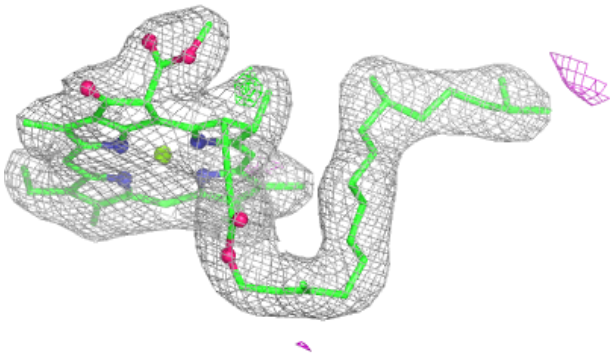


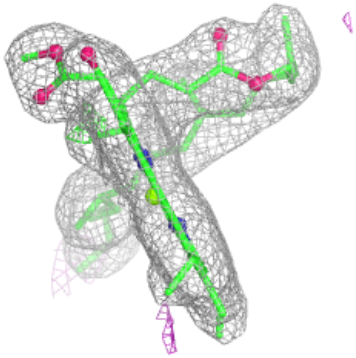


Electron density around CLA A 405:

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

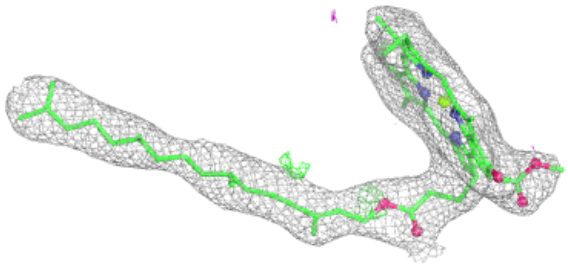


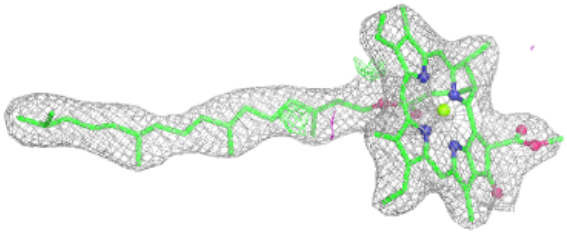


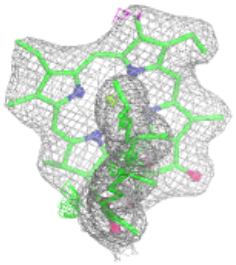


Electron density around CLA B 607:

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

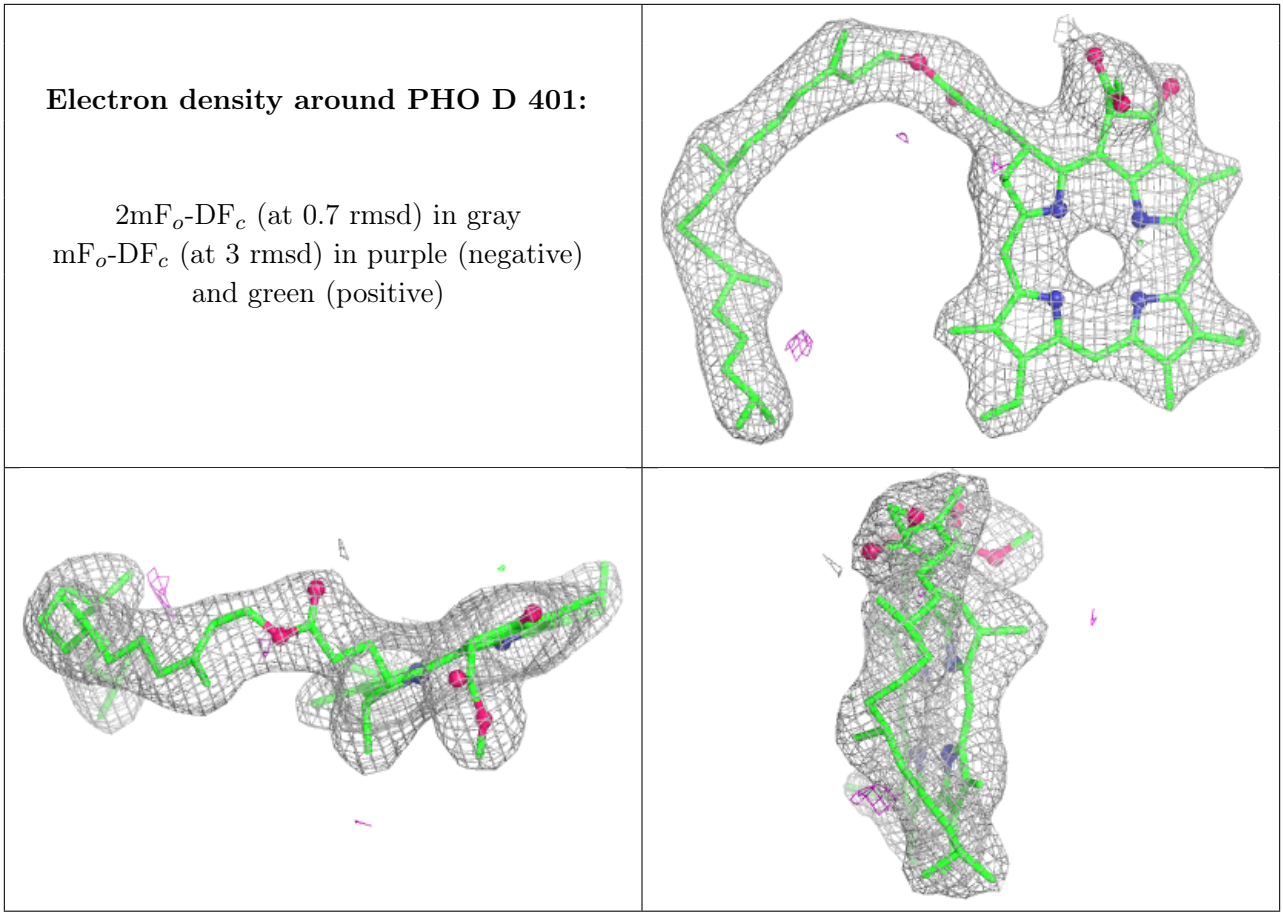






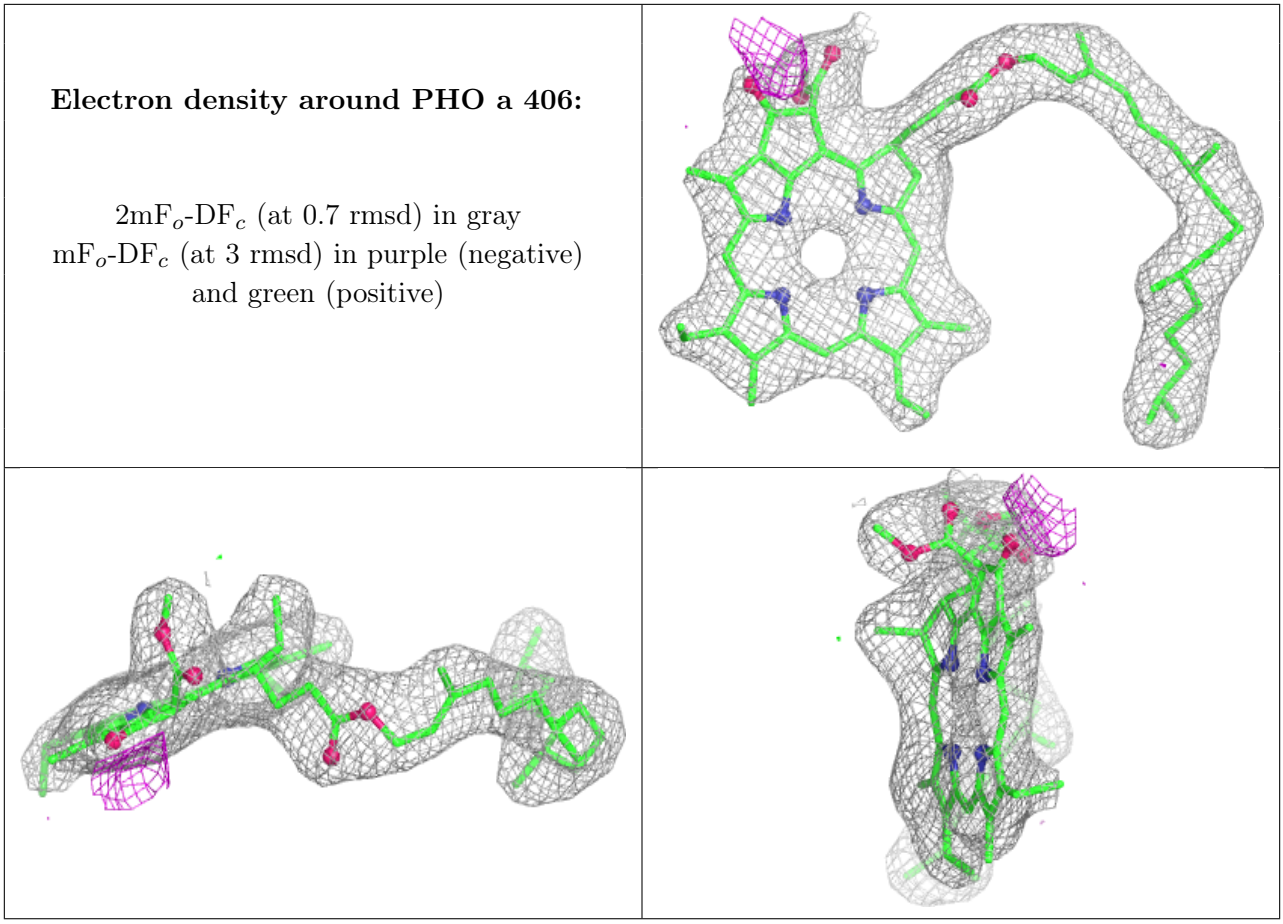
Electron density around PHO D 401:

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



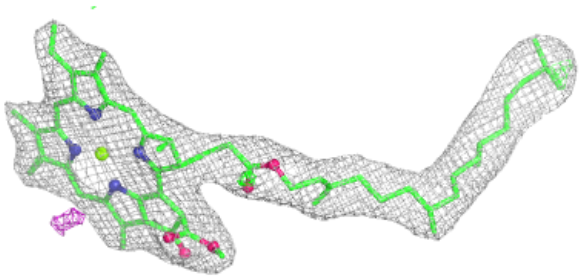
Electron density around PHO a 406:

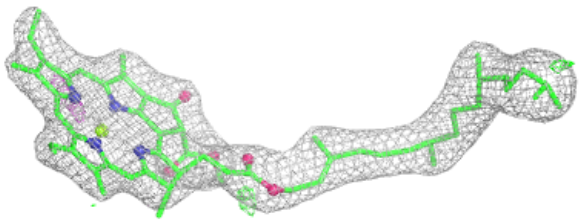
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 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)

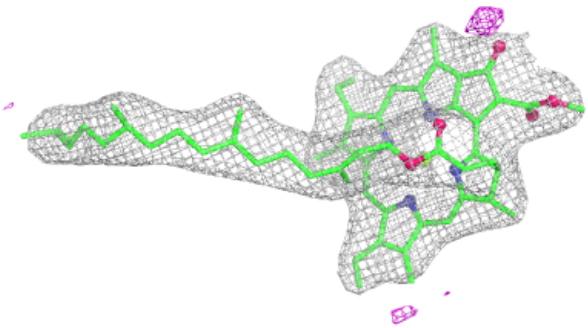


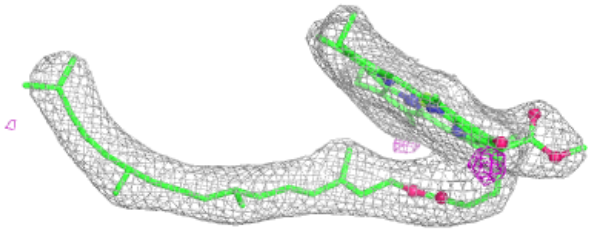


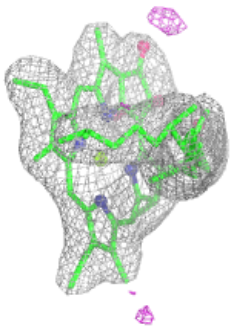


Electron density around CLA B 608:

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

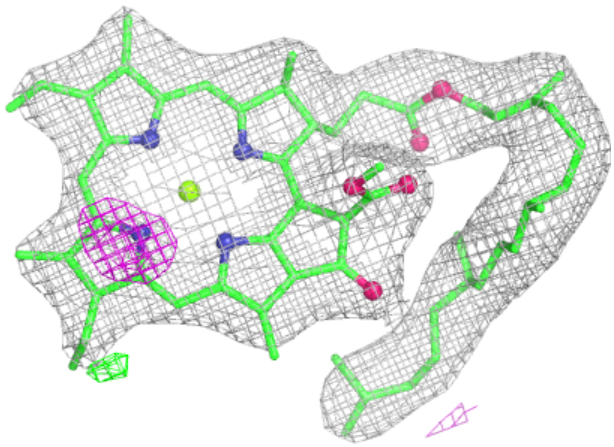


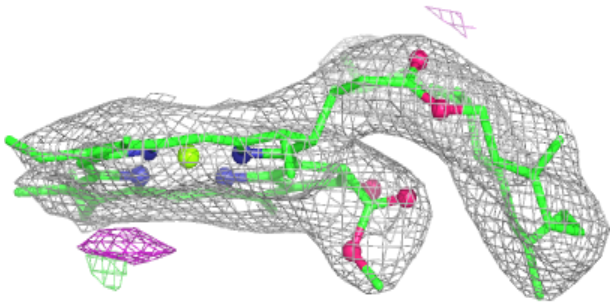


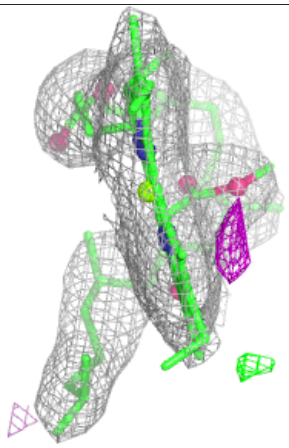


Electron density around CLA b 610:

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

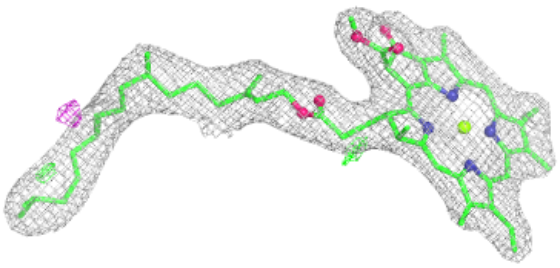


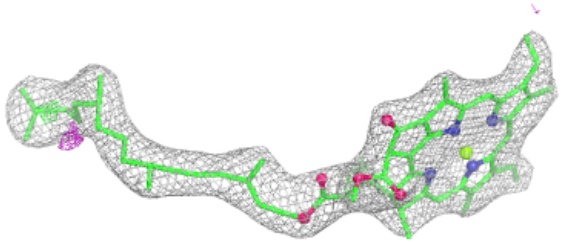




Electron density around CLA A 404:

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

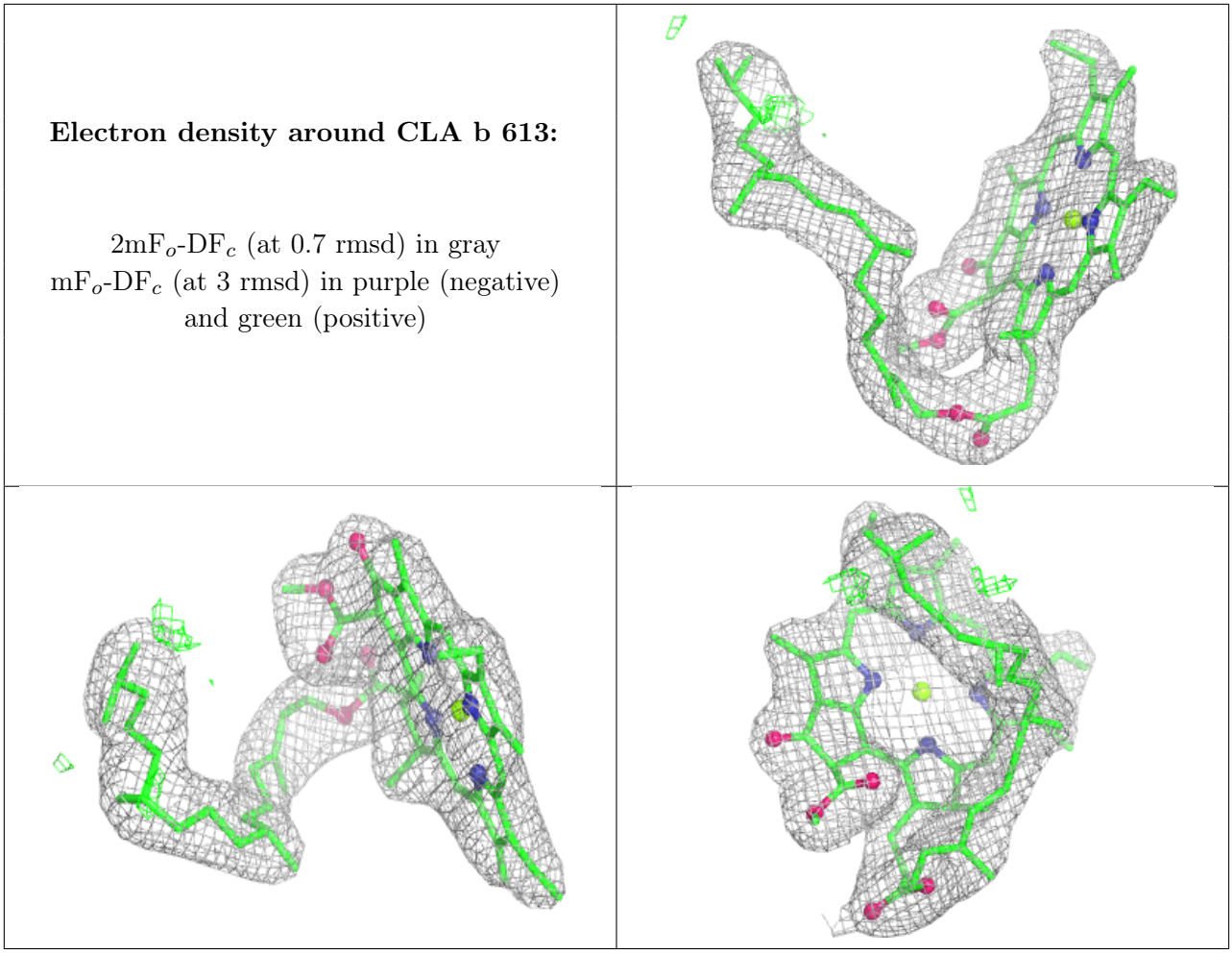






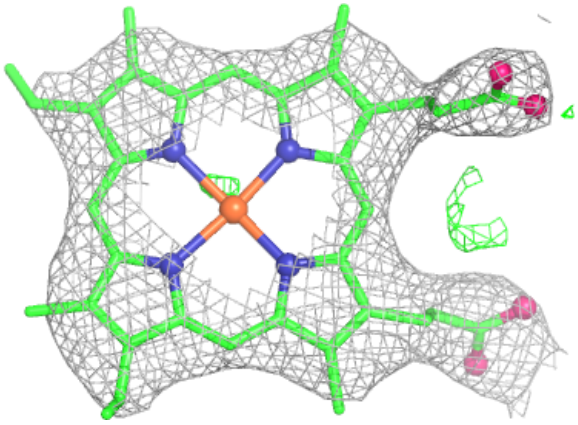
Electron density around CLA b 613:

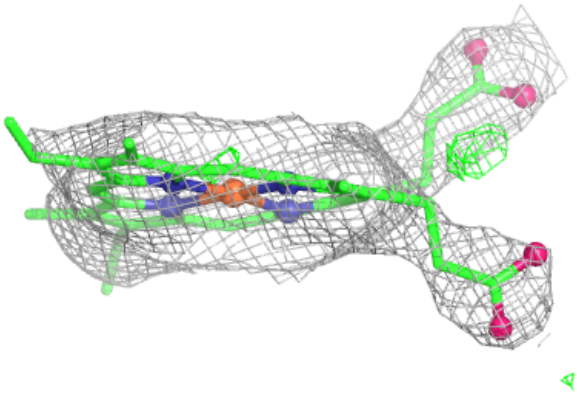
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

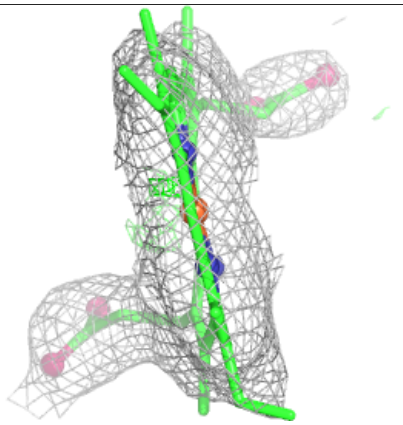


Electron density around HEM E 103:

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

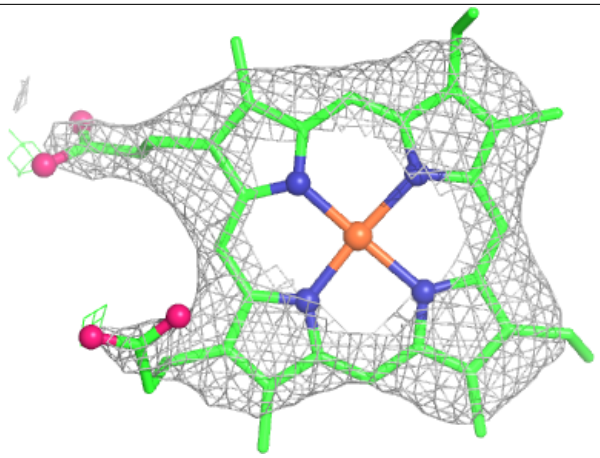


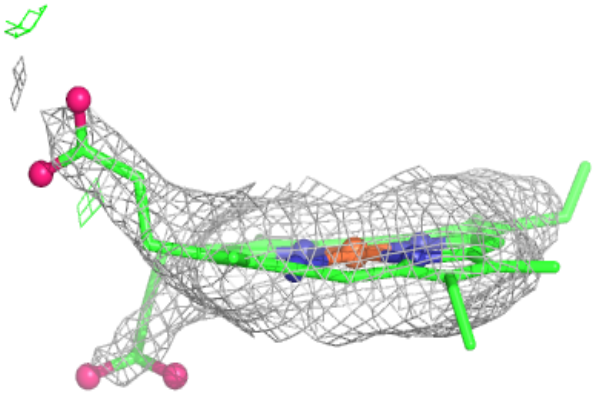


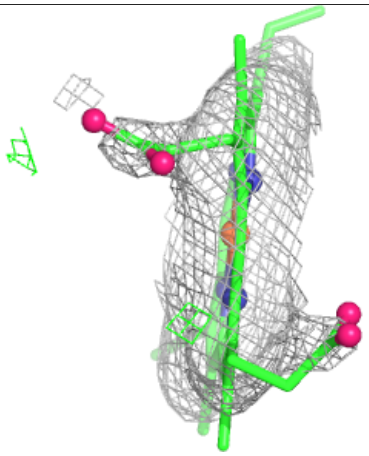


Electron density around HEM e 103:

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

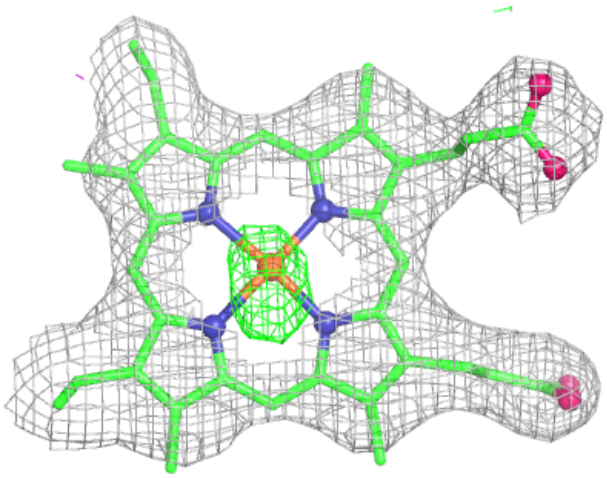


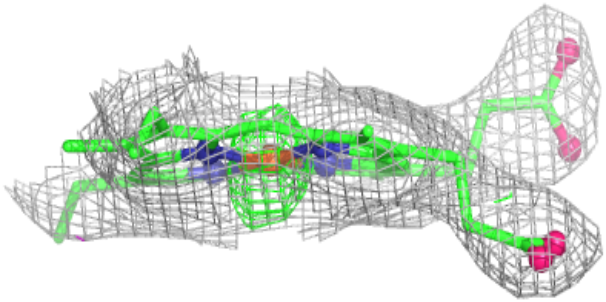


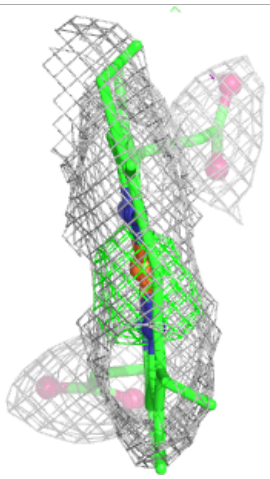


Electron density around HEC v 201:

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

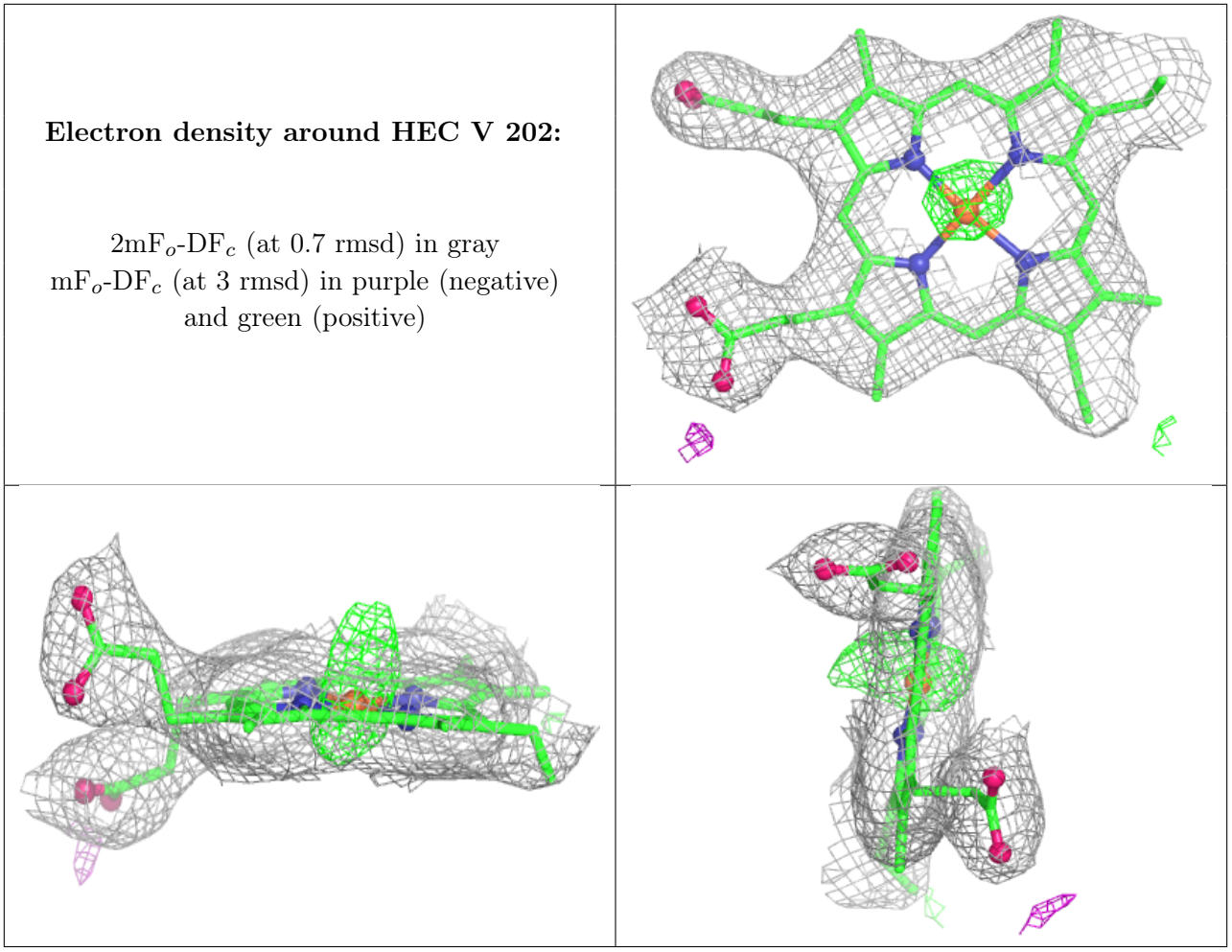






Electron density around HEC V 202:

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



6.5 Other polymers

There are no such residues in this entry.