wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 01:58 AM EDT

PDB ID	:	6DHH / pdb_00006dhh
Title	:	RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.2 Angstrom resolution
Authors	:	Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on	:	2018-05-20
Resolution	:	2.20 Å(reported)

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

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

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

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

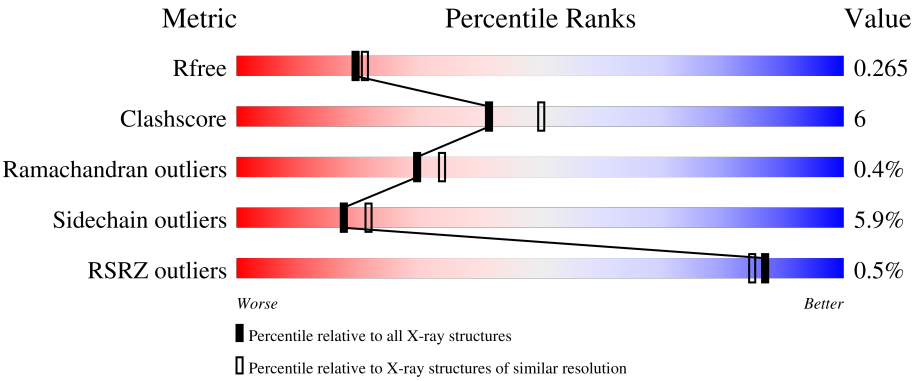
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0

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 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

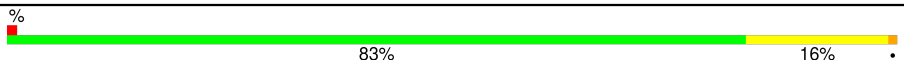
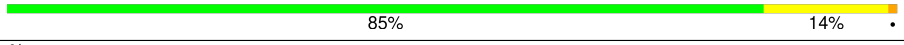
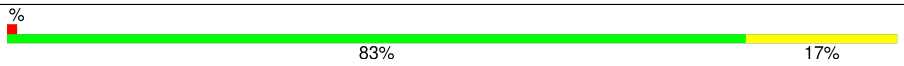
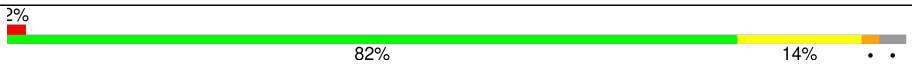
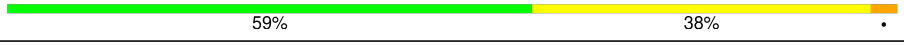
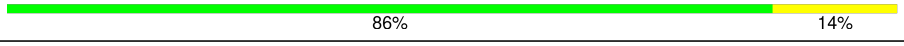
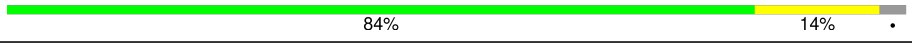
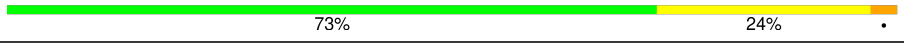
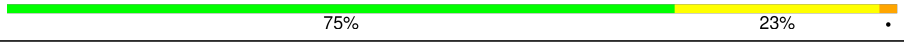
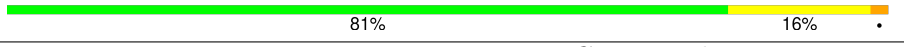
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	334	85% 15%

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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

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Mol	Chain	Length	Quality of chain
1	a	334	
2	B	505	
2	b	505	
3	C	451	
3	c	451	
4	D	341	
4	d	341	
5	E	82	
5	e	82	
6	F	34	
6	f	34	
7	H	65	
7	h	65	
8	I	36	
8	i	36	
9	J	36	
9	j	36	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	33	
12	m	33	
13	O	244	
13	o	244	

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Mol	Chain	Length	Quality of chain
14	T	30	80% 17%
14	t	30	3% 87% 10%
15	U	97	78% 21%
15	u	97	% 89% 10%
16	V	137	79% 18%
16	v	137	77% 23%
17	Y	30	7% 57% 20% 13% 10%
17	y	30	60% 30% 10%
18	X	38	76% 21%
18	x	38	74% 24%
19	Z	62	3% 63% 32% 5%
19	z	62	3% 65% 27% 8%
20	R	34	3% 71% 26%
20	r	34	9% 53% 29% 9% 9%

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
35	HEC	V	201	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 103673 atoms, of which 51476 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 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7849	2631	3845	666	694	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7789	2610	3811	665	690	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	0	0
			6752	2244	3335	570	590	13			
3	c	451	Total	C	H	N	O	S	0	1	0
			6901	2286	3407	587	608	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5330	1800	2613	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5342	1804	2619	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	S	0	0	0
			1030	338	523	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	80	83	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			516	172	261	40	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	1	0
			620	209	318	46	47			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	S	0	0	0
			620	202	316	48	53	1			
11	l	36	Total	C	H	N	O		0	0	0
			600	197	304	47	52				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	S	0	0	0
			525	171	269	37	47	1			
12	m	32	Total	C	H	N	O	S	0	0	0
			518	168	267	36	46	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1	0
			3730	1174	1850	317	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3718	1170	1844	317	383	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
14	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	Y	27	Total	C	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	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	H	N	O	0	0	0
			569	184	298	47	40			
20	r	31	Total	C	H	N	O	0	0	0
			461	154	234	40	33			

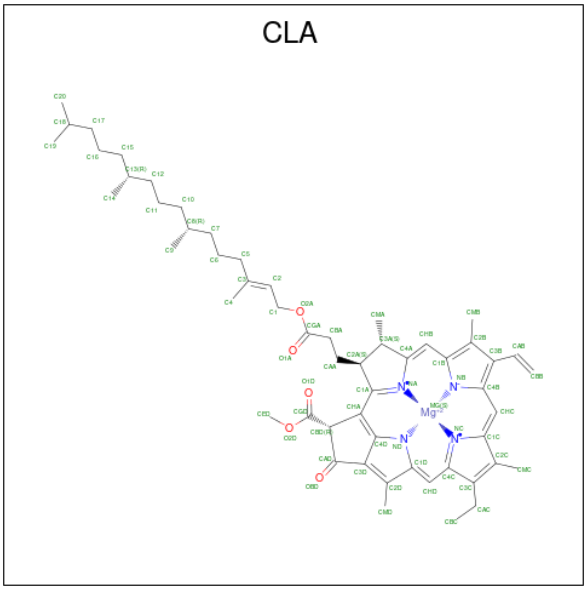
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is 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 H Mg N O 137 55 72 1 4 5	0	0
23	A	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	A	1	Total C H Mg N O 102 44 48 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0
23	B	1	Total C H Mg N O 137 55 72 1 4 5	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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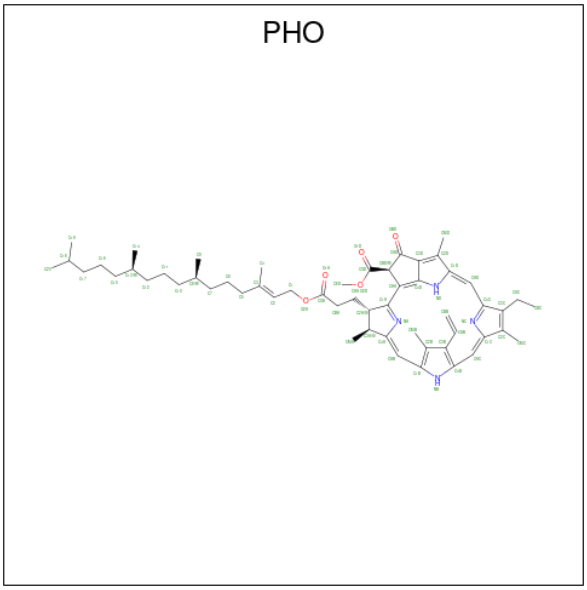
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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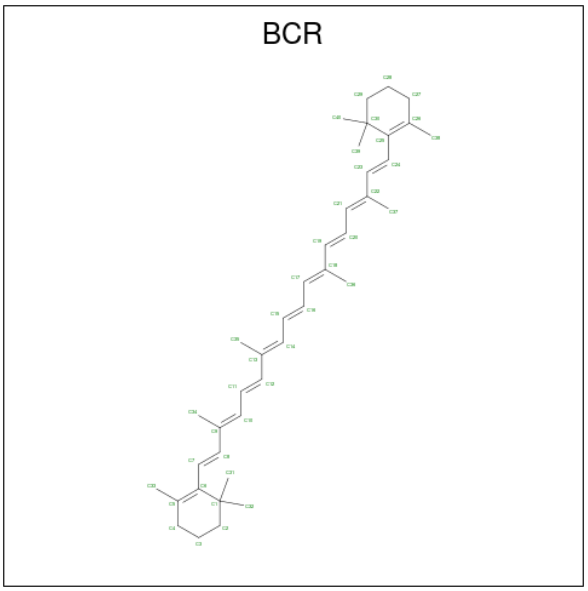
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	h	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- 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	H	N	O	0	0
			138	55	74	4	5		
24	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

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



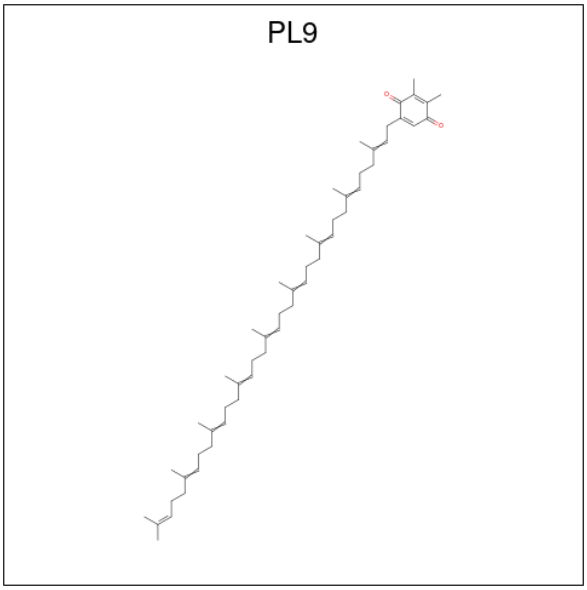
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	D	1	Total C H 96 40 56	0	0
25	H	1	Total C H 96 40 56	0	0
25	K	1	Total C H 96 40 56	0	0
25	T	1	Total C H 96 40 56	0	0
25	a	1	Total C H 96 40 56	0	0
25	b	1	Total C H 96 40 56	0	0
25	b	1	Total C H 96 40 56	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C H 96 40 56	0	0
25	c	1	Total C H 96 40 56	0	0
25	c	1	Total C H 96 40 56	0	0
25	c	1	Total C H 96 40 56	0	0
25	d	1	Total C H 96 40 56	0	0
25	h	1	Total C H 96 40 56	0	0
25	t	1	Total C H 96 40 56	0	0
25	y	1	Total C H 96 40 56	0	0

- Molecule 26 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: $C_{53}H_{80}O_2$).



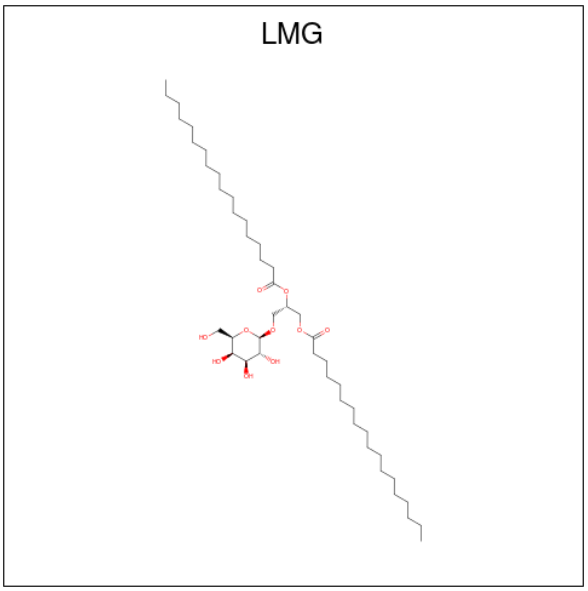
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C H O 135 53 80 2	0	0
26	D	1	Total C H O 135 53 80 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



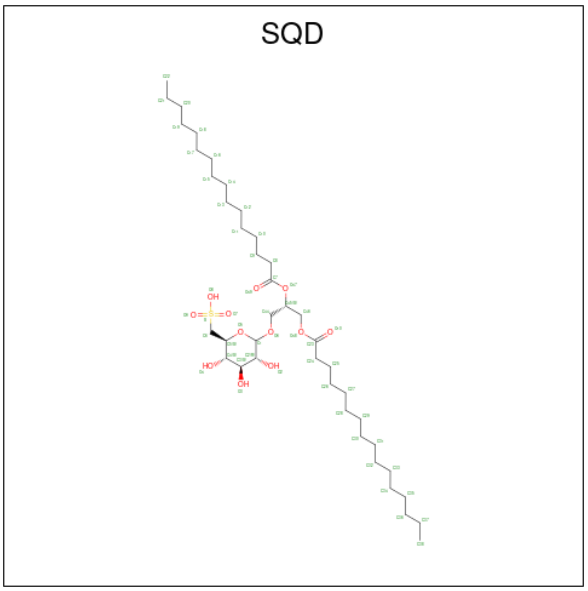
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			123	41	72	10		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			57	21	34	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C H O 81 27 44 10	0	0
27	c	1	Total C H O 117 38 69 10	0	0
27	d	1	Total C H O 102 34 58 10	0	0
27	m	1	Total C H O 123 41 72 10	0	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



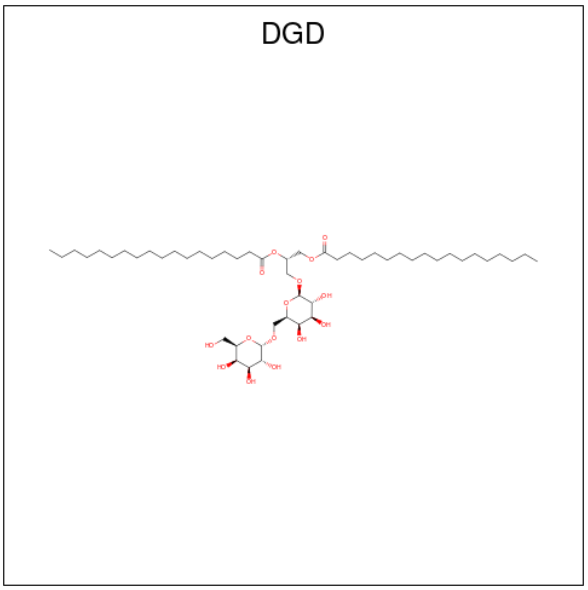
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C H O S 122 39 70 12 1	0	0
28	A	1	Total C H O 104 35 65 4	0	0
28	B	1	Total C H O S 132 41 78 12 1	0	0
28	F	1	Total C H O S 81 25 45 10 1	0	0
28	a	1	Total C H O S 132 41 78 12 1	0	0
28	a	1	Total C H O 92 31 56 5	0	0
28	b	1	Total C H O S 114 36 65 12 1	0	0

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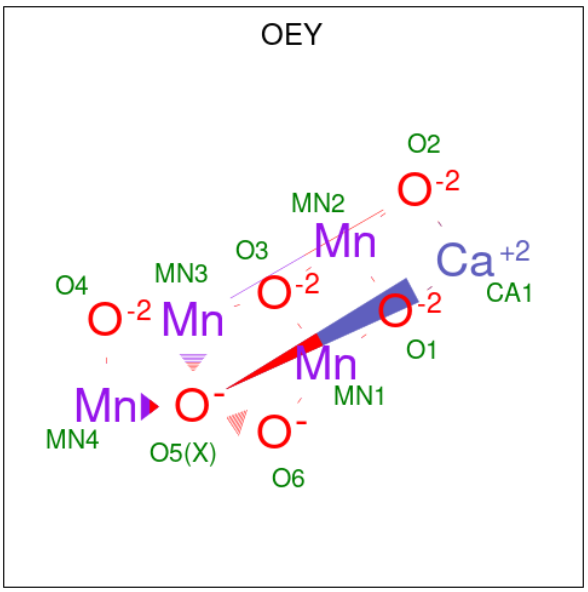
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	f	1	Total	C	H	O	S	0	0
			90	28	49	12	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



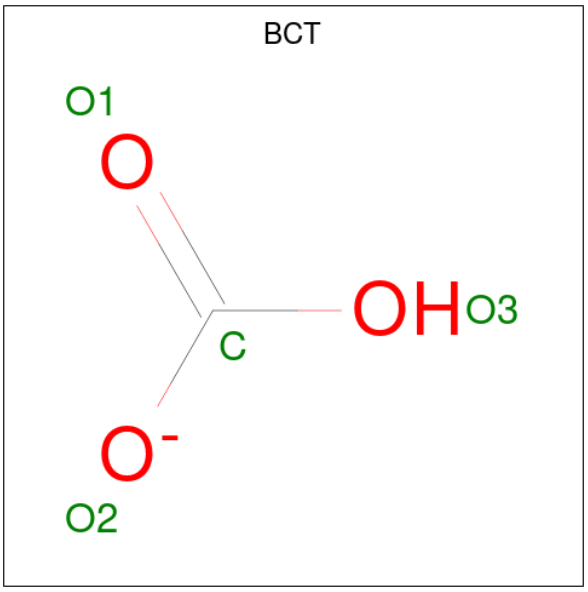
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	a	1	Total	C	H	O	0	0
			119	39	75	5		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 30 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: $CaMn_4O_6$).



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

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			5	1	1	3		

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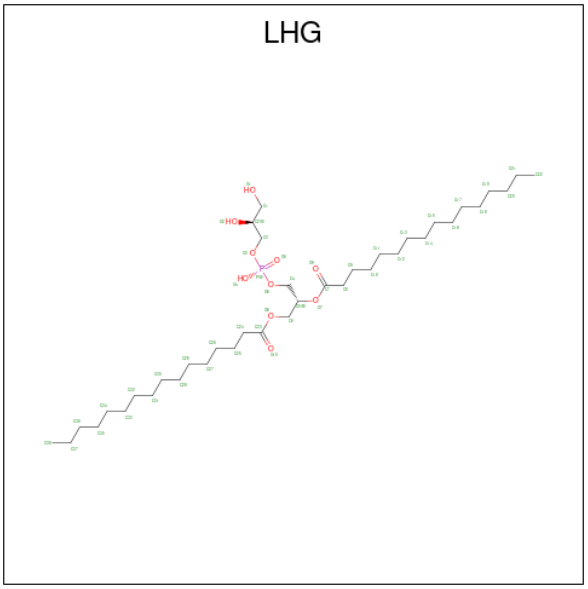
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	a	1	Total C H O 5 1 1 3	0	0

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

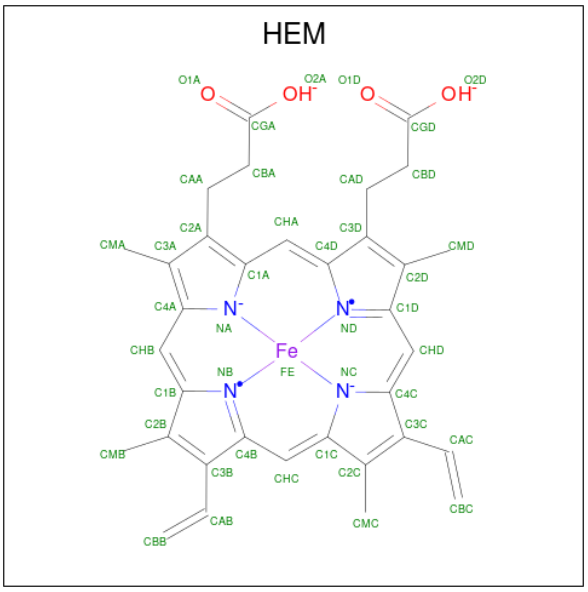
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	5	Total C H O 180 63 109 8	0	0
32	C	3	Total C H O 103 36 63 4	0	0
32	D	1	Total C H O 55 18 35 2	0	0
32	E	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	2	Total C H O 63 23 38 2	0	0
32	T	1	Total C H 44 15 29	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	5	Total C H O 223 76 141 6	0	0
32	c	2	Total C H O 83 28 51 4	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	l	1	Total C H 53 18 35	0	0
32	m	1	Total C H O 28 10 16 2	0	0
32	t	2	Total C H O 72 26 44 2	0	0
32	x	1	Total C H O 55 18 35 2	0	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



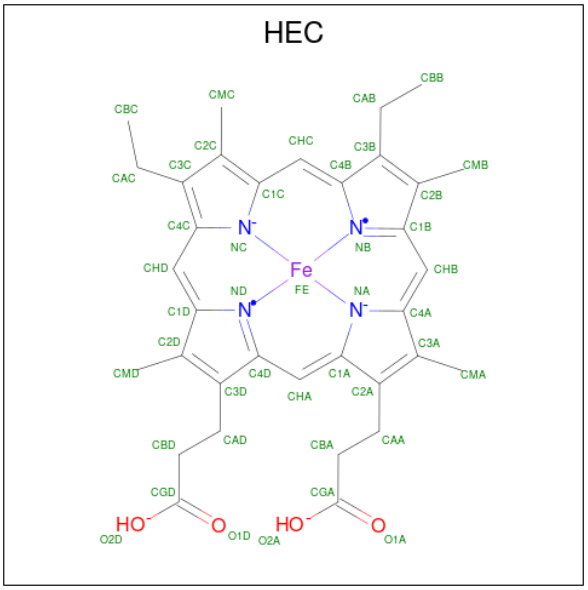
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	a	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
33	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
33	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
34	e	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	138	Total O 138 138	0	0
36	B	221	Total O 221 221	0	0
36	C	191	Total O 191 191	0	0
36	D	142	Total O 142 142	0	0
36	E	31	Total O 31 31	0	0
36	F	11	Total O 11 11	0	0
36	H	25	Total O 25 25	0	0
36	I	14	Total O 14 14	0	0
36	J	15	Total O 15 15	0	0
36	K	2	Total O 2 2	0	0
36	L	7	Total O 7 7	0	0
36	M	5	Total O 5 5	0	0
36	O	121	Total O 121 121	0	0
36	T	12	Total O 12 12	0	0
36	U	51	Total O 51 51	0	0
36	V	68	Total O 68 68	0	0
36	Y	5	Total O 5 5	0	0
36	X	8	Total O 8 8	0	0
36	Z	5	Total O 5 5	0	0
36	R	3	Total O 3 3	0	0
36	a	121	Total O 121 121	0	0

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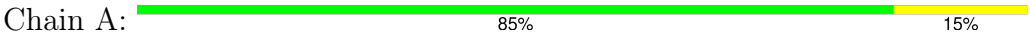
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	b	190	Total O 190 190	0	0
36	c	154	Total O 154 154	0	0
36	d	127	Total O 127 127	0	0
36	e	20	Total O 20 20	0	0
36	f	6	Total O 6 6	0	0
36	h	17	Total O 17 17	0	0
36	i	12	Total O 12 12	0	0
36	j	7	Total O 7 7	0	0
36	k	6	Total O 6 6	0	0
36	l	11	Total O 11 11	0	0
36	m	6	Total O 6 6	0	0
36	o	117	Total O 117 117	0	0
36	t	12	Total O 12 12	0	0
36	u	50	Total O 50 50	0	0
36	v	63	Total O 63 63	0	0
36	y	4	Total O 4 4	0	0
36	x	11	Total O 11 11	0	0
36	z	1	Total O 1 1	0	0
36	r	6	Total O 6 6	0	0

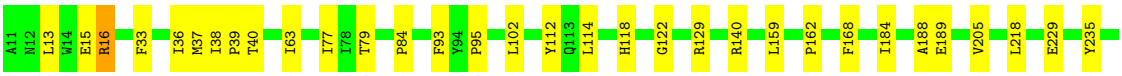
3 Residue-property plots (i)

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 1

Chain A:

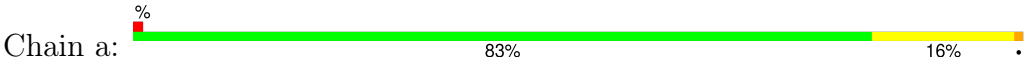


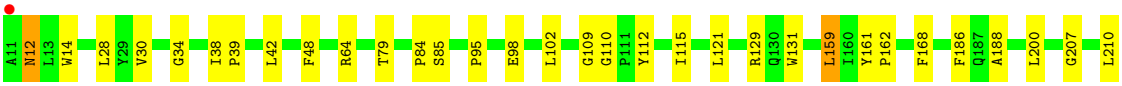


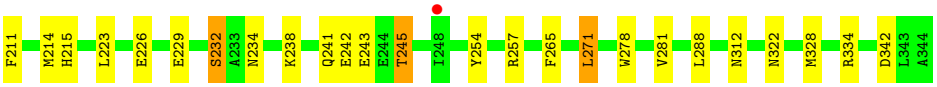


• Molecule 1: Photosystem II protein D1 1

Chain a:



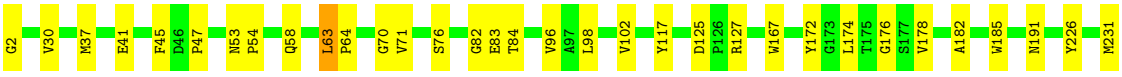




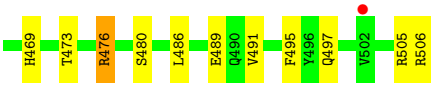
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:





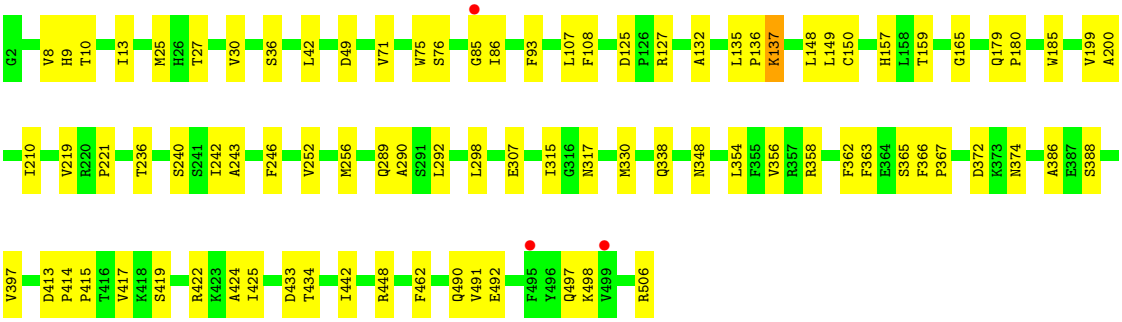




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

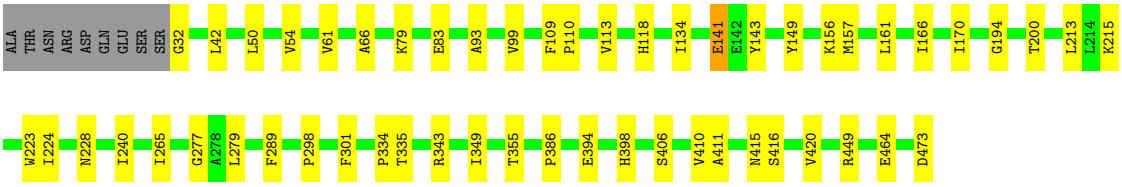




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

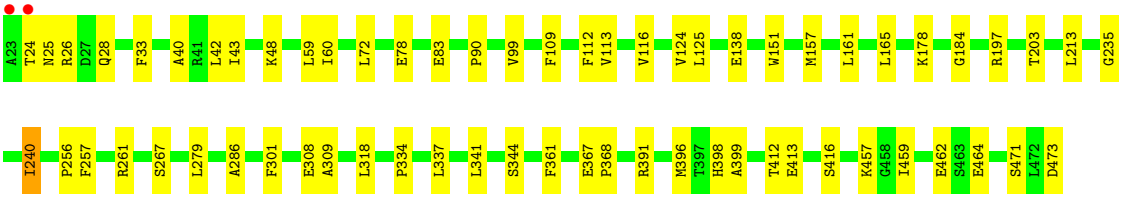




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

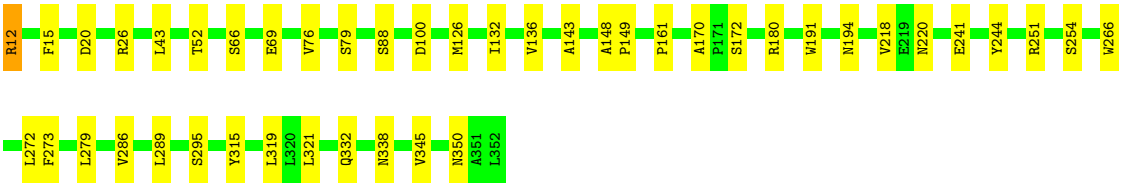




• Molecule 4: Photosystem II D2 protein

Chain D:

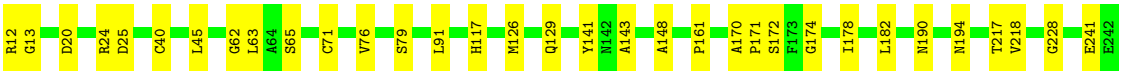




• Molecule 4: Photosystem II D2 protein

Chain d:



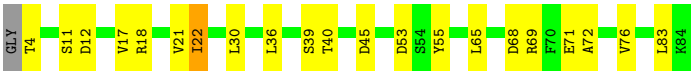




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:





• Molecule 5: Cytochrome b559 subunit alpha

Chain e:





• Molecule 6: Cytochrome b559 subunit beta

Chain F:

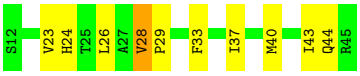




• Molecule 6: Cytochrome b559 subunit beta

Chain f:

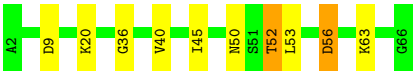




• Molecule 7: Photosystem II reaction center protein H

Chain H:

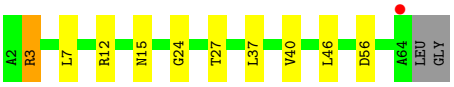




• Molecule 7: Photosystem II reaction center protein H

Chain h:

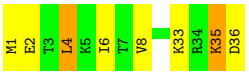




• Molecule 8: Photosystem II reaction center protein I

Chain I:





• Molecule 8: Photosystem II reaction center protein I

Chain i:

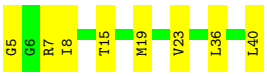




• Molecule 9: Photosystem II reaction center protein J

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:

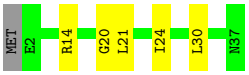




• Molecule 11: Photosystem II reaction center protein L

Chain l:

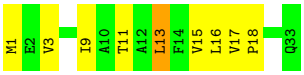




• Molecule 12: Photosystem II reaction center protein M

Chain M:





• Molecule 12: Photosystem II reaction center protein M

Chain m:

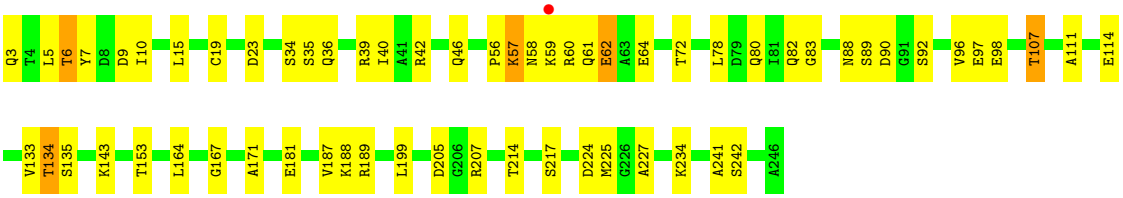




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

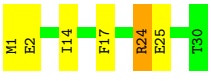




• Molecule 14: Photosystem II reaction center protein T

Chain T:

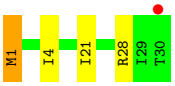




• Molecule 14: Photosystem II reaction center protein T

Chain t:

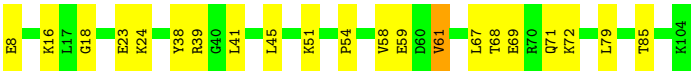




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

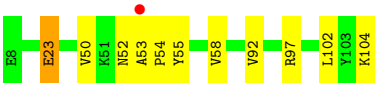




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:

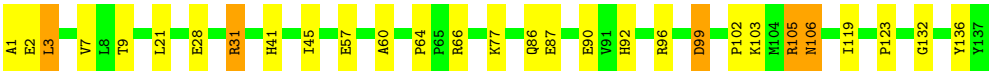




• Molecule 16: Cytochrome c-550

Chain V:





• Molecule 16: Cytochrome c-550

Chain v:

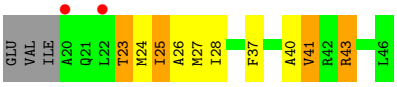




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:





• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:

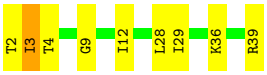




• Molecule 18: Photosystem II reaction center X protein

Chain X:

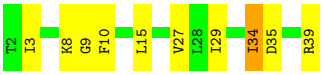




• Molecule 18: Photosystem II reaction center X protein

Chain x:





• Molecule 19: Photosystem II reaction center protein Z

Chain Z:

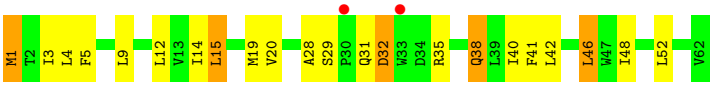




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

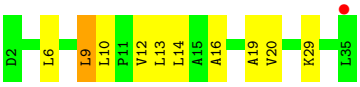




• Molecule 20: Photosystem II protein Y

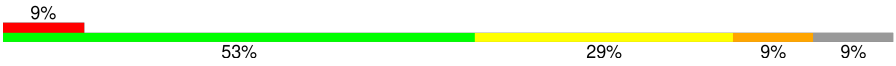
Chain R:

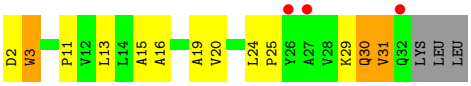




• Molecule 20: Photosystem II protein Y

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	117.69Å 222.53Å 308.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.85 – 2.20 30.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.85-2.20) 83.6 (30.85-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 2.20Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.193 , 0.264 0.194 , 0.265	Depositor DCC
R_{free} test set	3620 reflections (0.61%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	103673	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: OEY, UNL, BCR, SQD, FE2, BCT, HEC, LMG, HEM, FME, LHG, CL, DGD, PHO, CLA, PL9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.69	0/2707	0.76	0/3692
1	a	0.65	1/2704 (0.0%)	0.75	1/3688 (0.0%)
2	B	0.63	0/4160	0.71	0/5668
2	b	0.59	0/4118	0.69	0/5611
3	C	0.59	0/3530	0.67	0/4807
3	c	0.54	0/3610	0.69	0/4914
4	D	0.68	0/2812	0.74	0/3832
4	d	0.62	0/2821	0.72	0/3844
5	E	0.50	0/684	0.67	0/935
5	e	0.44	0/683	0.61	0/932
6	F	0.54	0/284	0.65	0/387
6	f	0.41	0/284	0.64	0/387
7	H	0.62	0/520	0.71	0/709
7	h	0.54	0/511	0.69	0/697
8	I	0.60	0/293	0.73	0/396
8	i	0.64	0/293	0.69	0/396
9	J	0.49	0/263	0.65	0/356
9	j	0.47	0/261	0.66	0/353
10	K	0.45	0/314	0.67	0/427
10	k	0.42	0/303	0.56	0/416
11	L	0.68	0/311	0.77	0/422
11	l	0.60	0/303	0.68	0/412
12	M	0.62	0/249	0.74	0/341
12	m	0.63	0/244	0.75	0/334
13	O	0.57	0/1914	0.69	0/2596
13	o	0.58	0/1905	0.72	0/2583
14	T	0.64	0/257	0.81	0/349
14	t	0.64	0/255	0.70	0/346
15	U	0.55	0/785	0.67	0/1064
15	u	0.55	0/785	0.70	0/1064
16	V	0.55	0/1085	0.63	0/1473
16	v	0.51	0/1085	0.67	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	Y	0.44	0/197	0.68	0/264
17	y	0.36	0/219	0.49	0/294
18	X	0.53	0/284	0.68	0/384
18	x	0.43	0/284	0.58	0/384
19	Z	0.44	0/490	0.60	0/669
19	z	0.38	0/488	0.55	0/666
20	R	0.38	0/277	0.65	0/380
20	r	0.32	0/233	0.56	0/323
All	All	0.59	1/42805 (0.0%)	0.70	1/58268 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	u	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	110	GLY	CA-C	-5.54	1.47	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	110	GLY	O-C-N	-8.77	117.91	121.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	u	52	ASN	Peptide

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	2622	2508	2519	36	0
1	a	2619	2499	2510	37	0
2	B	4004	3845	3864	47	0
2	b	3978	3811	3836	46	0
3	C	3417	3335	3348	35	0
3	c	3494	3407	3420	37	0
4	D	2717	2613	2621	33	0
4	d	2723	2619	2627	34	0
5	E	662	647	648	13	0
5	e	664	647	648	18	0
6	F	275	281	282	3	0
6	f	275	281	282	8	0
7	H	507	523	523	5	0
7	h	498	518	518	8	0
8	I	296	311	311	3	0
8	i	296	311	311	6	0
9	J	257	268	268	6	0
9	j	255	261	261	3	0
10	K	302	318	318	13	0
10	k	293	305	305	9	0
11	L	304	316	316	4	0
11	l	296	304	304	2	0
12	M	256	269	269	4	0
12	m	251	267	267	3	0
13	O	1880	1850	1852	42	0
13	o	1874	1844	1846	28	0
14	T	258	261	261	3	0
14	t	256	256	256	3	0
15	U	774	772	773	10	0
15	u	774	772	773	7	0
16	V	1064	1070	1073	19	0
16	v	1064	1070	1073	19	0
17	Y	196	208	217	6	0
17	y	218	241	241	8	0
18	X	281	312	312	5	0
18	x	281	312	312	8	0
19	Z	479	509	516	11	0
19	z	477	509	509	12	0
20	R	271	298	298	4	0
20	r	227	234	224	10	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	2	0	0	0	0
23	A	184	192	192	3	0
23	B	1035	1139	1139	13	0
23	C	839	922	922	7	0
23	D	195	216	216	4	0
23	a	195	216	216	1	0
23	b	970	1067	1067	19	0
23	c	839	919	919	13	0
23	d	195	216	216	1	0
23	h	65	72	72	5	0
24	A	64	74	74	1	0
24	D	64	74	74	1	0
24	a	64	74	74	0	0
24	d	64	74	74	1	0
25	A	40	56	56	1	0
25	B	120	168	168	6	0
25	C	120	168	168	4	0
25	D	40	56	56	2	0
25	H	40	56	56	2	0
25	K	40	56	56	3	0
25	T	40	56	56	2	0
25	a	40	56	56	2	0
25	b	120	168	168	8	0
25	c	120	168	168	8	0
25	d	40	56	56	2	0
25	h	40	56	56	3	0
25	t	40	56	56	4	0
25	y	40	56	56	1	0
26	A	55	80	80	3	0
26	D	55	80	80	1	0
26	a	55	80	80	2	0
26	d	55	80	80	1	0
27	A	48	66	66	1	0
27	B	51	72	72	3	0
27	C	48	66	66	0	0
27	D	112	157	157	3	0
27	a	49	68	68	2	0
27	b	78	120	120	0	0
27	c	85	113	113	1	0
27	d	44	58	57	0	0
27	m	51	72	72	1	0
28	A	91	135	134	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	54	78	78	2	0
28	F	36	45	45	0	0
28	a	90	134	133	3	0
28	b	49	65	64	0	0
28	f	41	49	49	2	0
29	A	66	96	96	2	0
29	C	186	246	243	0	0
29	H	62	82	80	1	0
29	a	44	75	75	2	0
29	c	186	246	240	0	0
29	h	62	82	82	0	0
30	A	11	0	0	1	0
30	a	11	0	0	1	0
31	A	4	1	1	0	0
31	a	4	1	1	0	0
32	B	71	109	0	0	0
32	C	40	63	0	0	0
32	D	20	35	0	0	0
32	E	12	16	0	0	0
32	H	18	35	0	0	0
32	I	15	26	0	0	0
32	J	12	16	0	0	0
32	M	25	38	0	0	0
32	T	15	29	0	0	0
32	a	12	16	0	0	0
32	b	82	141	0	0	0
32	c	32	51	0	0	0
32	d	17	26	0	0	0
32	j	12	16	0	0	0
32	l	18	35	0	0	0
32	m	12	16	0	0	0
32	t	28	44	0	0	0
32	x	20	35	0	0	0
33	B	49	74	74	1	0
33	D	96	141	141	4	0
33	E	49	74	74	1	0
33	L	49	74	74	2	0
33	a	49	74	74	3	0
33	d	88	125	125	2	0
33	e	42	57	57	1	0
33	l	49	74	74	1	0
34	E	43	30	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	e	43	30	30	3	0
35	V	43	30	30	1	0
35	v	43	30	30	0	0
36	A	138	0	0	8	0
36	B	221	0	0	13	0
36	C	191	0	0	9	0
36	D	142	0	0	5	0
36	E	31	0	0	1	0
36	F	11	0	0	0	0
36	H	25	0	0	3	0
36	I	14	0	0	0	0
36	J	15	0	0	1	0
36	K	2	0	0	0	0
36	L	7	0	0	0	0
36	M	5	0	0	0	0
36	O	121	0	0	13	1
36	R	3	0	0	0	0
36	T	12	0	0	0	0
36	U	51	0	0	3	0
36	V	68	0	0	6	0
36	X	8	0	0	1	0
36	Y	5	0	0	0	0
36	Z	5	0	0	0	0
36	a	121	0	0	6	0
36	b	190	0	0	7	0
36	c	154	0	0	4	0
36	d	127	0	0	6	0
36	e	20	0	0	0	0
36	f	6	0	0	0	0
36	h	17	0	0	5	0
36	i	12	0	0	2	0
36	j	7	0	0	0	0
36	k	6	0	0	2	0
36	l	11	0	0	1	0
36	m	6	0	0	1	0
36	o	117	0	0	6	1
36	r	6	0	0	1	0
36	t	12	0	0	0	0
36	u	50	0	0	1	0
36	v	63	0	0	3	0
36	x	11	0	0	2	0
36	y	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	z	1	0	0	0	0
All	All	52197	51476	50844	648	1

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 648 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)
13:O:90:ASP:OD1	36:O:301:HOH:O	1.60	1.15
4:D:332:GLN:O	36:D:501:HOH:O	1.79	0.99
2:b:358:ARG:O	36:b:701:HOH:O	1.83	0.96
1:a:243:GLU:OE1	36:a:501:HOH:O	1.86	0.93
2:B:2:GLY:N	36:B:701:HOH:O	2.04	0.91

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:362:HOH:O	36:o:304:HOH:O[1_655]	1.86	0.34

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	332/334 (99%)	322 (97%)	10 (3%)	0	100	100
1	a	332/334 (99%)	322 (97%)	10 (3%)	0	100	100
2	B	508/505 (101%)	490 (96%)	18 (4%)	0	100	100
2	b	503/505 (100%)	481 (96%)	20 (4%)	2 (0%)	30	34
3	C	440/451 (98%)	426 (97%)	13 (3%)	1 (0%)	43	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	c	450/451 (100%)	431 (96%)	18 (4%)	1 (0%)	43 51
4	D	339/341 (99%)	331 (98%)	7 (2%)	1 (0%)	36 42
4	d	340/341 (100%)	329 (97%)	10 (3%)	1 (0%)	36 42
5	E	80/82 (98%)	79 (99%)	1 (1%)	0	100 100
5	e	80/82 (98%)	77 (96%)	3 (4%)	0	100 100
6	F	32/34 (94%)	30 (94%)	2 (6%)	0	100 100
6	f	32/34 (94%)	30 (94%)	2 (6%)	0	100 100
7	H	63/65 (97%)	55 (87%)	8 (13%)	0	100 100
7	h	61/65 (94%)	56 (92%)	5 (8%)	0	100 100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100 100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100 100
9	J	34/36 (94%)	28 (82%)	6 (18%)	0	100 100
9	j	34/36 (94%)	29 (85%)	5 (15%)	0	100 100
10	K	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	3 2
10	k	35/37 (95%)	35 (100%)	0	0	100 100
11	L	35/37 (95%)	35 (100%)	0	0	100 100
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100 100
12	M	31/33 (94%)	31 (100%)	0	0	100 100
12	m	30/33 (91%)	29 (97%)	1 (3%)	0	100 100
13	O	243/244 (100%)	222 (91%)	19 (8%)	2 (1%)	16 16
13	o	242/244 (99%)	225 (93%)	14 (6%)	3 (1%)	10 8
14	T	28/30 (93%)	28 (100%)	0	0	100 100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100 100
15	U	95/97 (98%)	91 (96%)	4 (4%)	0	100 100
15	u	95/97 (98%)	92 (97%)	3 (3%)	0	100 100
16	V	135/137 (98%)	128 (95%)	7 (5%)	0	100 100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100 100
17	Y	25/30 (83%)	17 (68%)	5 (20%)	3 (12%)	0 0
17	y	28/30 (93%)	25 (89%)	1 (4%)	2 (7%)	1 0
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100 100
18	x	36/38 (95%)	34 (94%)	2 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100 100
19	z	60/62 (97%)	51 (85%)	6 (10%)	3 (5%)	1 0
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
20	r	29/34 (85%)	25 (86%)	2 (7%)	2 (7%)	1 0
All	All	5235/5326 (98%)	4988 (95%)	225 (4%)	22 (0%)	30 34

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	60	ARG
13	O	62	GLU
17	Y	41	VAL

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	270/270 (100%)	263 (97%)	7 (3%)	40 55
1	a	269/270 (100%)	254 (94%)	15 (6%)	19 24
2	B	407/403 (101%)	386 (95%)	21 (5%)	21 26
2	b	402/403 (100%)	385 (96%)	17 (4%)	26 36
3	C	344/352 (98%)	333 (97%)	11 (3%)	34 47
3	c	353/352 (100%)	338 (96%)	15 (4%)	26 36
4	D	276/276 (100%)	270 (98%)	6 (2%)	45 61
4	d	277/276 (100%)	270 (98%)	7 (2%)	42 56
5	E	72/72 (100%)	63 (88%)	9 (12%)	4 4
5	e	71/72 (99%)	62 (87%)	9 (13%)	4 4
6	F	28/28 (100%)	26 (93%)	2 (7%)	13 16
6	f	28/28 (100%)	25 (89%)	3 (11%)	6 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	H	53/54 (98%)	48 (91%)	5 (9%)	8 9
7	h	53/54 (98%)	47 (89%)	6 (11%)	5 5
8	I	32/32 (100%)	28 (88%)	4 (12%)	4 4
8	i	32/32 (100%)	32 (100%)	0	100 100
9	J	24/24 (100%)	23 (96%)	1 (4%)	26 36
9	j	23/24 (96%)	21 (91%)	2 (9%)	9 10
10	K	31/30 (103%)	30 (97%)	1 (3%)	34 47
10	k	30/30 (100%)	23 (77%)	7 (23%)	1 0
11	L	35/35 (100%)	34 (97%)	1 (3%)	37 51
11	l	34/35 (97%)	32 (94%)	2 (6%)	18 22
12	M	28/29 (97%)	25 (89%)	3 (11%)	6 6
12	m	28/29 (97%)	27 (96%)	1 (4%)	31 42
13	O	208/207 (100%)	188 (90%)	20 (10%)	8 8
13	o	207/207 (100%)	193 (93%)	14 (7%)	14 17
14	T	26/26 (100%)	23 (88%)	3 (12%)	5 5
14	t	25/26 (96%)	25 (100%)	0	100 100
15	U	84/84 (100%)	77 (92%)	7 (8%)	10 11
15	u	84/84 (100%)	82 (98%)	2 (2%)	43 58
16	V	117/117 (100%)	108 (92%)	9 (8%)	12 13
16	v	117/117 (100%)	111 (95%)	6 (5%)	21 27
17	Y	19/23 (83%)	15 (79%)	4 (21%)	1 1
17	y	22/23 (96%)	19 (86%)	3 (14%)	3 3
18	X	31/31 (100%)	27 (87%)	4 (13%)	4 4
18	x	31/31 (100%)	28 (90%)	3 (10%)	8 8
19	Z	52/52 (100%)	42 (81%)	10 (19%)	1 1
19	z	51/52 (98%)	42 (82%)	9 (18%)	2 1
20	R	28/29 (97%)	22 (79%)	6 (21%)	1 1
20	r	19/29 (66%)	17 (90%)	2 (10%)	6 6
All	All	4321/4348 (99%)	4064 (94%)	257 (6%)	18 22

5 of 257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	242	SER
16	v	109	GLU
15	U	59	GLU
15	U	8	GLU
18	x	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	73	GLN
13	o	58	ASN
2	b	409	GLN
13	o	155	ASN
4	d	255	GLN

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	$\#\|Z\| > 2$
12	FME	m	1	12	8,9,10	0.96	0	8,9,11	1.02	1 (12%)
14	FME	T	1	14	8,9,10	1.06	1 (12%)	8,9,11	1.99	2 (25%)
14	FME	t	1	14	8,9,10	0.98	1 (12%)	8,9,11	0.97	1 (12%)
8	FME	i	1	8	8,9,10	0.99	0	8,9,11	1.01	1 (12%)
12	FME	M	1	12	8,9,10	1.18	1 (12%)	8,9,11	1.38	2 (25%)
8	FME	I	1	8	8,9,10	1.02	0	8,9,11	1.40	1 (12%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
14	FME	t	1	14	-	4/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-2.65	1.42	1.46
14	T	1	FME	CA-N	-2.60	1.42	1.46
14	t	1	FME	CA-N	-2.06	1.43	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	CA-N-CN	-3.99	116.68	122.82
8	I	1	FME	C-CA-N	3.05	115.38	109.50
8	i	1	FME	C-CA-N	2.55	114.42	109.50
14	T	1	FME	O1-CN-N	-2.37	119.20	125.32
12	M	1	FME	C-CA-N	-2.31	105.05	109.50

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	C-CA-CB-CG
12	M	1	FME	CB-CA-N-CN
14	t	1	FME	C-CA-CB-CG
14	t	1	FME	CB-CG-SD-CE
14	t	1	FME	N-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 186 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 149 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	$\#\|Z\| > 2$
27	LMG	b	622	-	55,55,55	1.08	4 (7%)	63,63,63	1.46	10 (15%)
25	BCR	D	405	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	8 (14%)
25	BCR	c	521	-	41,41,41	0.94	2 (4%)	56,56,56	1.15	4 (7%)
23	CLA	C	502	3	69,73,73	1.46	10 (14%)	82,113,113	1.31	8 (9%)
29	DGD	C	516	-	63,63,67	1.40	11 (17%)	77,77,81	1.37	9 (11%)
33	LHG	a	410	-	48,48,48	0.80	1 (2%)	51,54,54	1.38	6 (11%)
23	CLA	B	612	2	69,73,73	1.04	4 (5%)	82,113,113	1.58	13 (15%)
23	CLA	B	607	36	69,73,73	1.31	9 (13%)	82,113,113	1.19	7 (8%)
27	LMG	m	101	-	51,51,55	0.92	2 (3%)	59,59,63	1.57	14 (23%)
23	CLA	b	604	2	69,73,73	1.55	13 (18%)	82,113,113	1.58	11 (13%)
33	LHG	B	622	-	48,48,48	0.92	2 (4%)	51,54,54	1.44	7 (13%)
28	SQD	a	411	-	52,54,54	1.01	5 (9%)	62,65,65	1.81	15 (24%)
27	LMG	D	410	-	31,31,55	1.16	4 (12%)	33,33,63	1.14	3 (9%)
23	CLA	b	608	36	69,73,73	1.13	7 (10%)	82,113,113	1.25	5 (6%)
23	CLA	c	505	3	69,73,73	1.26	7 (10%)	82,113,113	1.31	12 (14%)
25	BCR	B	619	-	41,41,41	1.27	3 (7%)	56,56,56	1.37	11 (19%)
25	BCR	C	520	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	2 (3%)
23	CLA	b	603	2	69,73,73	1.25	7 (10%)	82,113,113	1.37	13 (15%)
23	CLA	b	610	2	69,73,73	1.37	8 (11%)	82,113,113	1.32	9 (10%)
25	BCR	K	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.22	5 (8%)
33	LHG	L	101	-	48,48,48	0.96	2 (4%)	51,54,54	1.19	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LHG	e	101	-	41,41,48	0.83	2 (4%)	44,47,54	1.30	5 (11%)
23	CLA	B	608	2	69,73,73	1.31	9 (13%)	82,113,113	1.38	8 (9%)
23	CLA	c	507	36	69,73,73	1.37	7 (10%)	82,113,113	1.32	10 (12%)
23	CLA	c	510	3	69,73,73	1.24	5 (7%)	82,113,113	1.43	12 (14%)
23	CLA	D	402	36	69,73,73	1.32	10 (14%)	82,113,113	1.46	11 (13%)
23	CLA	B	602	2	69,73,73	1.46	10 (14%)	82,113,113	1.61	14 (17%)
24	PHO	A	406	-	58,69,69	1.99	15 (25%)	55,99,99	1.79	13 (23%)
26	PL9	d	406	-	55,55,55	1.32	8 (14%)	68,69,69	1.66	20 (29%)
28	SQD	f	101	-	39,41,54	1.10	4 (10%)	49,52,65	1.81	10 (20%)
23	CLA	b	613	2	69,73,73	1.50	10 (14%)	82,113,113	1.41	11 (13%)
25	BCR	C	515	-	41,41,41	1.28	4 (9%)	56,56,56	1.40	7 (12%)
31	BCT	a	417	21	3,3,3	1.32	0	2,3,3	2.83	2 (100%)
23	CLA	c	502	3	69,73,73	1.71	8 (11%)	82,113,113	1.41	8 (9%)
23	CLA	C	507	36	69,73,73	1.22	10 (14%)	82,113,113	1.20	5 (6%)
23	CLA	c	512	3	69,73,73	1.45	10 (14%)	82,113,113	1.39	10 (12%)
29	DGD	c	517	-	63,63,67	1.28	11 (17%)	77,77,81	1.53	10 (12%)
25	BCR	B	618	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	7 (12%)
23	CLA	C	503	3	69,73,73	1.31	10 (14%)	82,113,113	1.56	12 (14%)
23	CLA	B	609	2	69,73,73	1.69	11 (15%)	82,113,113	1.19	7 (8%)
23	CLA	c	513	3	69,73,73	1.23	11 (15%)	82,113,113	1.14	6 (7%)
27	LMG	c	519	-	37,37,55	1.10	4 (10%)	45,45,63	1.21	3 (6%)
33	LHG	D	409	-	46,46,48	1.03	4 (8%)	49,52,54	1.35	4 (8%)
23	CLA	b	605	2	69,73,73	1.58	10 (14%)	82,113,113	1.74	15 (18%)
27	LMG	D	407	-	51,51,55	1.07	2 (3%)	59,59,63	1.27	5 (8%)
23	CLA	B	613	2	69,73,73	1.57	12 (17%)	82,113,113	1.43	13 (15%)
23	CLA	a	407	1	69,73,73	1.45	11 (15%)	82,113,113	1.30	14 (17%)
23	CLA	b	616	2	69,73,73	1.85	13 (18%)	82,113,113	1.46	15 (18%)
27	LMG	a	414	-	49,49,55	0.88	2 (4%)	57,57,63	1.27	4 (7%)
27	LMG	d	409	-	44,44,55	1.17	3 (6%)	52,52,63	1.42	9 (17%)
29	DGD	A	413	-	67,67,67	1.29	10 (14%)	81,81,81	1.36	7 (8%)
23	CLA	b	609	2	69,73,73	1.24	7 (10%)	82,113,113	1.58	11 (13%)
33	LHG	d	407	-	48,48,48	0.91	3 (6%)	51,54,54	1.21	4 (7%)
26	PL9	a	409	-	55,55,55	1.38	6 (10%)	68,69,69	1.39	8 (11%)
25	BCR	T	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.40	7 (12%)
24	PHO	d	401	-	58,69,69	2.24	10 (17%)	55,99,99	1.71	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	SQD	B	623	-	52,54,54	0.91	3 (5%)	62,65,65	1.86	14 (22%)
34	HEM	E	102	5,6	50,50,50	1.44	4 (8%)	67,82,82	1.23	6 (8%)
35	HEC	v	201	16	50,50,50	1.37	4 (8%)	68,82,82	1.32	8 (11%)
23	CLA	C	511	3	69,73,73	1.63	10 (14%)	82,113,113	1.45	8 (9%)
25	BCR	C	514	-	41,41,41	1.20	2 (4%)	56,56,56	1.40	9 (16%)
23	CLA	C	501	3	69,73,73	2.14	9 (13%)	82,113,113	1.62	9 (10%)
23	CLA	a	404	1	69,73,73	1.66	9 (13%)	82,113,113	1.61	12 (14%)
28	SQD	F	101	-	34,36,54	1.06	3 (8%)	42,45,65	1.79	10 (23%)
29	DGD	H	102	-	63,63,67	1.65	10 (15%)	77,77,81	1.64	15 (19%)
23	CLA	d	403	4	69,73,73	1.24	10 (14%)	82,113,113	1.17	6 (7%)
23	CLA	B	604	2	69,73,73	1.41	10 (14%)	82,113,113	1.72	9 (10%)
23	CLA	B	601	36	69,73,73	1.53	10 (14%)	82,113,113	1.65	9 (10%)
28	SQD	A	411	-	50,52,54	1.07	4 (8%)	60,63,65	2.10	10 (16%)
25	BCR	b	620	-	41,41,41	1.02	3 (7%)	56,56,56	1.33	7 (12%)
23	CLA	C	506	3	69,73,73	1.65	12 (17%)	82,113,113	1.19	5 (6%)
23	CLA	B	603	2	69,73,73	1.24	9 (13%)	82,113,113	1.45	11 (13%)
27	LMG	C	519	-	48,48,55	1.12	5 (10%)	56,56,63	1.35	6 (10%)
25	BCR	h	102	-	41,41,41	1.25	2 (4%)	56,56,56	1.34	9 (16%)
23	CLA	C	509	3	69,73,73	1.90	7 (10%)	82,113,113	1.31	6 (7%)
23	CLA	D	404	4	69,73,73	1.85	8 (11%)	82,113,113	1.17	9 (10%)
34	HEM	e	102	5,6	50,50,50	1.46	7 (14%)	67,82,82	1.24	8 (11%)
23	CLA	B	611	2	69,73,73	1.13	7 (10%)	82,113,113	1.34	10 (12%)
33	LHG	l	101	-	48,48,48	0.85	3 (6%)	51,54,54	1.21	4 (7%)
33	LHG	D	408	-	48,48,48	1.15	5 (10%)	51,54,54	1.20	4 (7%)
23	CLA	C	505	3	69,73,73	1.43	8 (11%)	82,113,113	1.32	7 (8%)
23	CLA	c	511	3	69,73,73	1.52	11 (15%)	82,113,113	1.28	5 (6%)
25	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.37	6 (10%)
24	PHO	D	401	-	58,69,69	2.18	10 (17%)	55,99,99	1.46	8 (14%)
28	SQD	A	412	-	38,38,54	1.16	4 (10%)	40,40,65	1.06	1 (2%)
23	CLA	b	614	2	69,73,73	1.23	9 (13%)	82,113,113	1.38	11 (13%)
23	CLA	A	405	36	69,73,73	1.17	7 (10%)	82,113,113	1.34	13 (15%)
23	CLA	C	508	3	69,73,73	1.35	8 (11%)	82,113,113	1.48	12 (14%)
23	CLA	c	509	3	69,73,73	1.69	10 (14%)	82,113,113	1.66	12 (14%)
25	BCR	c	515	-	41,41,41	1.19	4 (9%)	56,56,56	1.46	11 (19%)
25	BCR	d	405	-	41,41,41	1.16	2 (4%)	56,56,56	1.33	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	610	36	69,73,73	1.52	12 (17%)	82,113,113	1.50	12 (14%)
23	CLA	b	617	2	64,68,73	1.26	10 (15%)	76,107,113	1.64	10 (13%)
30	OEY	A	414	36,1,3	0,16,16	-	-	-		
23	CLA	b	612	2	69,73,73	1.66	11 (15%)	82,113,113	1.51	13 (15%)
23	CLA	c	508	3	68,72,73	1.32	8 (11%)	80,111,113	1.25	8 (10%)
23	CLA	b	606	2	69,73,73	1.28	6 (8%)	82,113,113	1.55	13 (15%)
23	CLA	D	403	4	69,73,73	1.58	11 (15%)	82,113,113	1.59	8 (9%)
26	PL9	D	406	-	55,55,55	1.42	7 (12%)	68,69,69	1.50	11 (16%)
23	CLA	C	504	36	63,67,73	1.24	6 (9%)	74,105,113	1.41	12 (16%)
23	CLA	C	513	3	69,73,73	1.33	7 (10%)	82,113,113	1.50	9 (10%)
23	CLA	d	404	4	69,73,73	1.80	10 (14%)	82,113,113	1.12	6 (7%)
23	CLA	a	405	36	69,73,73	1.36	7 (10%)	82,113,113	1.22	9 (10%)
25	BCR	a	408	-	41,41,41	1.19	4 (9%)	56,56,56	1.46	7 (12%)
23	CLA	h	101	36	69,73,73	1.34	11 (15%)	82,113,113	1.38	10 (12%)
25	BCR	t	101	-	41,41,41	1.10	4 (9%)	56,56,56	1.30	7 (12%)
33	LHG	d	408	-	38,38,48	0.91	1 (2%)	41,44,54	1.10	4 (9%)
29	DGD	c	516	-	63,63,67	1.30	10 (15%)	77,77,81	1.59	14 (18%)
23	CLA	b	607	2	69,73,73	1.47	5 (7%)	82,113,113	1.63	9 (10%)
27	LMG	c	522	-	48,48,55	1.27	8 (16%)	56,56,63	1.46	7 (12%)
31	BCT	A	415	21	3,3,3	1.22	0	2,3,3	2.87	1 (50%)
23	CLA	c	503	3	69,73,73	1.15	5 (7%)	82,113,113	1.45	9 (10%)
27	LMG	b	623	-	21,21,55	1.03	1 (4%)	20,20,63	0.90	0
29	DGD	a	413	-	43,43,67	1.19	3 (6%)	45,45,81	1.43	6 (13%)
23	CLA	B	605	2	69,73,73	1.72	12 (17%)	82,113,113	1.54	15 (18%)
29	DGD	h	103	-	63,63,67	1.00	4 (6%)	77,77,81	1.60	17 (22%)
24	PHO	a	406	-	58,69,69	2.12	11 (18%)	55,99,99	1.42	9 (16%)
23	CLA	B	606	2	69,73,73	1.65	9 (13%)	82,113,113	1.47	10 (12%)
30	OEY	a	416	36,1,3	0,16,16	-	-	-		
25	BCR	b	618	-	41,41,41	1.19	4 (9%)	56,56,56	1.43	11 (19%)
29	DGD	C	518	-	63,63,67	1.13	6 (9%)	77,77,81	1.49	10 (12%)
35	HEC	V	201	16	50,50,50	1.49	8 (16%)	68,82,82	1.05	4 (5%)
23	CLA	C	512	3	69,73,73	1.79	12 (17%)	82,113,113	1.29	8 (9%)
27	LMG	D	411	-	26,26,55	1.04	2 (7%)	26,26,63	1.24	3 (11%)
23	CLA	A	404	1	69,73,73	1.32	9 (13%)	82,113,113	1.53	15 (18%)
23	CLA	c	501	3	69,73,73	1.31	10 (14%)	82,113,113	1.55	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	A	408	-	41,41,41	0.99	2 (4%)	56,56,56	1.41	8 (14%)
25	BCR	H	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.43	10 (17%)
27	LMG	B	620	-	51,51,55	0.94	3 (5%)	59,59,63	1.55	12 (20%)
29	DGD	C	517	-	63,63,67	1.28	7 (11%)	77,77,81	1.55	10 (12%)
23	CLA	c	504	36	64,68,73	1.84	11 (17%)	76,107,113	1.50	11 (14%)
28	SQD	b	601	-	47,49,54	1.00	2 (4%)	57,60,65	2.33	16 (28%)
23	CLA	c	506	3	69,73,73	1.44	8 (11%)	82,113,113	1.55	15 (18%)
23	CLA	b	615	2	69,73,73	1.59	8 (11%)	82,113,113	1.51	12 (14%)
23	CLA	C	510	3	69,73,73	1.62	10 (14%)	82,113,113	1.57	6 (7%)
29	DGD	c	518	-	63,63,67	1.25	9 (14%)	77,77,81	1.46	14 (18%)
23	CLA	A	407	1	58,62,73	1.64	10 (17%)	68,99,113	1.70	15 (22%)
25	BCR	b	619	-	41,41,41	1.28	2 (4%)	56,56,56	1.33	7 (12%)
23	CLA	d	402	36	69,73,73	1.47	7 (10%)	82,113,113	1.57	8 (9%)
28	SQD	a	412	-	35,35,54	1.14	2 (5%)	37,37,65	1.34	5 (13%)
25	BCR	y	101	-	41,41,41	1.15	4 (9%)	56,56,56	1.25	5 (8%)
23	CLA	B	615	2	69,73,73	1.48	11 (15%)	82,113,113	1.39	10 (12%)
23	CLA	B	616	2	64,68,73	1.78	14 (21%)	76,107,113	1.46	10 (13%)
33	LHG	E	101	-	48,48,48	1.05	5 (10%)	51,54,54	1.17	3 (5%)
23	CLA	b	611	36	69,73,73	1.24	8 (11%)	82,113,113	1.55	11 (13%)
27	LMG	A	410	-	48,48,55	1.03	2 (4%)	56,56,63	1.24	5 (8%)
26	PL9	A	409	-	55,55,55	0.93	1 (1%)	68,69,69	1.62	12 (17%)
25	BCR	B	617	-	41,41,41	1.19	3 (7%)	56,56,56	1.40	8 (14%)
23	CLA	B	614	2	69,73,73	1.49	8 (11%)	82,113,113	1.35	9 (10%)

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
27	LMG	b	622	-	-	24/50/70/70	0/1/1/1
25	BCR	D	405	-	-	12/29/63/63	0/2/2/2
25	BCR	c	521	-	-	4/29/63/63	0/2/2/2
23	CLA	C	502	3	-	9/39/115/115	-
29	DGD	C	516	-	-	21/51/91/95	0/2/2/2
33	LHG	a	410	-	-	19/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	612	2	-	10/39/115/115	-
23	CLA	B	607	36	-	11/39/115/115	-
27	LMG	m	101	-	-	19/46/66/70	0/1/1/1
23	CLA	b	604	2	-	10/39/115/115	-
33	LHG	B	622	-	-	11/53/53/53	-
28	SQD	a	411	-	-	18/49/69/69	0/1/1/1
27	LMG	D	410	-	-	17/33/33/70	-
23	CLA	b	608	36	-	14/39/115/115	-
23	CLA	c	505	3	-	14/39/115/115	-
25	BCR	B	619	-	-	3/29/63/63	0/2/2/2
25	BCR	C	520	-	-	10/29/63/63	0/2/2/2
23	CLA	b	603	2	-	4/39/115/115	-
23	CLA	b	610	2	-	4/39/115/115	-
25	BCR	K	101	-	-	9/29/63/63	0/2/2/2
33	LHG	L	101	-	-	21/53/53/53	-
33	LHG	e	101	-	-	23/46/46/53	-
23	CLA	B	608	2	-	3/39/115/115	-
23	CLA	c	507	36	-	14/39/115/115	-
23	CLA	c	510	3	-	18/39/115/115	-
23	CLA	D	402	36	-	0/39/115/115	-
23	CLA	B	602	2	-	4/39/115/115	-
24	PHO	A	406	-	-	9/37/103/103	0/5/6/6
26	PL9	d	406	-	-	21/53/73/73	0/1/1/1
28	SQD	f	101	-	-	12/36/56/69	0/1/1/1
23	CLA	b	613	2	-	11/39/115/115	-
25	BCR	C	515	-	-	4/29/63/63	0/2/2/2
23	CLA	c	502	3	-	6/39/115/115	-
23	CLA	C	507	36	-	12/39/115/115	-
23	CLA	c	512	3	-	18/39/115/115	-
29	DGD	c	517	-	-	20/51/91/95	0/2/2/2
25	BCR	B	618	-	-	11/29/63/63	0/2/2/2
23	CLA	C	503	3	-	9/39/115/115	-
23	CLA	B	609	2	-	10/39/115/115	-
23	CLA	c	513	3	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	c	519	-	-	10/31/51/70	0/1/1/1
33	LHG	D	409	-	-	24/51/51/53	-
23	CLA	b	605	2	-	12/39/115/115	-
27	LMG	D	407	-	-	19/46/66/70	0/1/1/1
23	CLA	B	613	2	-	9/39/115/115	-
23	CLA	a	407	1	-	9/39/115/115	-
23	CLA	b	616	2	-	5/39/115/115	-
27	LMG	a	414	-	-	28/44/64/70	0/1/1/1
27	LMG	d	409	-	-	11/39/59/70	0/1/1/1
29	DGD	A	413	-	-	31/55/95/95	0/2/2/2
23	CLA	b	609	2	-	7/39/115/115	-
33	LHG	d	407	-	-	23/53/53/53	-
26	PL9	a	409	-	-	26/53/73/73	0/1/1/1
25	BCR	T	101	-	-	14/29/63/63	0/2/2/2
24	PHO	d	401	-	-	3/37/103/103	0/5/6/6
28	SQD	B	623	-	-	19/49/69/69	0/1/1/1
34	HEM	E	102	5,6	-	2/14/54/54	-
35	HEC	v	201	16	1/1/7/7	6/14/54/54	-
23	CLA	C	511	3	-	3/39/115/115	-
25	BCR	C	514	-	-	15/29/63/63	0/2/2/2
23	CLA	C	501	3	-	4/39/115/115	-
23	CLA	a	404	1	-	10/39/115/115	-
28	SQD	F	101	-	-	14/28/48/69	0/1/1/1
29	DGD	H	102	-	-	17/51/91/95	0/2/2/2
23	CLA	d	403	4	-	10/39/115/115	-
23	CLA	B	604	2	-	10/39/115/115	-
23	CLA	B	601	36	-	17/39/115/115	-
28	SQD	A	411	-	-	19/47/67/69	0/1/1/1
25	BCR	b	620	-	-	5/29/63/63	0/2/2/2
23	CLA	C	506	3	-	14/39/115/115	-
23	CLA	B	603	2	-	16/39/115/115	-
27	LMG	C	519	-	-	19/43/63/70	0/1/1/1
25	BCR	h	102	-	-	6/29/63/63	0/2/2/2
23	CLA	C	509	3	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	404	4	-	9/39/115/115	-
34	HEM	e	102	5,6	-	3/14/54/54	-
23	CLA	B	611	2	-	10/39/115/115	-
33	LHG	l	101	-	-	19/53/53/53	-
33	LHG	D	408	-	-	24/53/53/53	-
23	CLA	C	505	3	-	8/39/115/115	-
23	CLA	c	511	3	-	12/39/115/115	-
25	BCR	c	514	-	-	11/29/63/63	0/2/2/2
24	PHO	D	401	-	-	4/37/103/103	0/5/6/6
28	SQD	A	412	-	-	17/39/39/69	-
23	CLA	b	614	2	-	5/39/115/115	-
23	CLA	A	405	36	-	2/39/115/115	-
23	CLA	C	508	3	-	7/39/115/115	-
23	CLA	c	509	3	-	10/39/115/115	-
25	BCR	c	515	-	-	8/29/63/63	0/2/2/2
25	BCR	d	405	-	-	13/29/63/63	0/2/2/2
23	CLA	B	610	36	-	6/39/115/115	-
23	CLA	b	617	2	-	8/33/109/115	-
23	CLA	b	612	2	-	9/39/115/115	-
23	CLA	c	508	3	-	9/38/114/115	-
23	CLA	b	606	2	-	5/39/115/115	-
23	CLA	D	403	4	-	12/39/115/115	-
26	PL9	D	406	-	-	11/53/73/73	0/1/1/1
23	CLA	C	504	36	-	8/32/108/115	-
23	CLA	C	513	3	-	14/39/115/115	-
23	CLA	d	404	4	-	7/39/115/115	-
23	CLA	a	405	36	-	10/39/115/115	-
25	BCR	a	408	-	-	2/29/63/63	0/2/2/2
23	CLA	h	101	36	-	17/39/115/115	-
25	BCR	t	101	-	-	4/29/63/63	0/2/2/2
33	LHG	d	408	-	-	14/43/43/53	-
29	DGD	c	516	-	-	24/51/91/95	0/2/2/2
23	CLA	b	607	2	-	9/39/115/115	-
27	LMG	c	522	-	-	21/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	503	3	-	12/39/115/115	-
27	LMG	b	623	-	-	12/17/17/70	-
29	DGD	a	413	-	-	21/45/45/95	-
23	CLA	B	605	2	-	9/39/115/115	-
29	DGD	h	103	-	-	15/51/91/95	0/2/2/2
24	PHO	a	406	-	-	5/37/103/103	0/5/6/6
23	CLA	B	606	2	-	13/39/115/115	-
25	BCR	b	618	-	-	4/29/63/63	0/2/2/2
35	HEC	V	201	16	1/1/7/7	6/14/54/54	-
29	DGD	C	518	-	-	16/51/91/95	0/2/2/2
23	CLA	C	512	3	-	11/39/115/115	-
27	LMG	D	411	-	-	13/22/22/70	-
23	CLA	A	404	1	-	4/39/115/115	-
23	CLA	c	501	3	-	6/39/115/115	-
25	BCR	A	408	-	-	5/29/63/63	0/2/2/2
25	BCR	H	101	-	-	7/29/63/63	0/2/2/2
27	LMG	B	620	-	-	21/46/66/70	0/1/1/1
29	DGD	C	517	-	-	18/51/91/95	0/2/2/2
23	CLA	c	504	36	-	10/33/109/115	-
28	SQD	b	601	-	-	20/44/64/69	0/1/1/1
23	CLA	c	506	3	-	17/39/115/115	-
23	CLA	b	615	2	-	14/39/115/115	-
23	CLA	C	510	3	-	8/39/115/115	-
29	DGD	c	518	-	-	20/51/91/95	0/2/2/2
23	CLA	A	407	1	-	2/26/102/115	-
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
23	CLA	d	402	36	-	5/39/115/115	-
28	SQD	a	412	-	-	21/37/37/69	-
25	BCR	y	101	-	-	8/29/63/63	0/2/2/2
23	CLA	B	615	2	-	9/39/115/115	-
23	CLA	B	616	2	-	8/33/109/115	-
33	LHG	E	101	-	-	27/53/53/53	-
23	CLA	b	611	36	-	8/39/115/115	-
27	LMG	A	410	-	-	20/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PL9	A	409	-	-	21/53/73/73	0/1/1/1
25	BCR	B	617	-	-	3/29/63/63	0/2/2/2
23	CLA	B	614	2	-	10/39/115/115	-

The worst 5 of 968 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	MG-NB	-11.83	1.82	2.05
23	D	404	CLA	MG-NB	-11.58	1.82	2.05
23	C	501	CLA	MG-ND	-11.02	1.83	2.05
24	d	401	PHO	C1B-C2B	10.83	1.51	1.39
24	D	401	PHO	C1B-C2B	9.97	1.50	1.39

The worst 5 of 1308 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C4A-NA-C1A	10.48	111.46	106.68
23	d	402	CLA	C4A-NA-C1A	10.08	111.28	106.68
28	b	601	SQD	O6-C1-C2	10.06	123.55	108.27
23	C	510	CLA	C4A-NA-C1A	9.86	111.18	106.68
23	b	607	CLA	C4A-NA-C1A	9.86	111.18	106.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	V	201	HEC	NA
35	v	201	HEC	NA

5 of 1710 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	C2B-C3B-CAB-CBB
23	B	605	CLA	C4B-C3B-CAB-CBB
23	B	606	CLA	CBD-CGD-O2D-CED
23	B	609	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

96 monomers are involved in 151 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	D	405	BCR	2	0
25	c	521	BCR	4	0
33	a	410	LHG	3	0
23	B	612	CLA	1	0
23	B	607	CLA	1	0
27	m	101	LMG	1	0
23	b	604	CLA	3	0
33	B	622	LHG	1	0
28	a	411	SQD	1	0
23	c	505	CLA	3	0
25	B	619	BCR	1	0
25	C	520	BCR	1	0
23	b	610	CLA	2	0
25	K	101	BCR	3	0
33	L	101	LHG	2	0
33	e	101	LHG	1	0
23	B	608	CLA	1	0
23	c	510	CLA	1	0
23	D	402	CLA	1	0
23	B	602	CLA	1	0
24	A	406	PHO	1	0
26	d	406	PL9	1	0
28	f	101	SQD	2	0
23	b	613	CLA	1	0
25	C	515	BCR	3	0
23	c	502	CLA	1	0
23	c	512	CLA	2	0
25	B	618	BCR	1	0
27	c	519	LMG	1	0
27	D	407	LMG	3	0
23	B	613	CLA	1	0
23	b	616	CLA	5	0
27	a	414	LMG	2	0
29	A	413	DGD	2	0
33	d	407	LHG	1	0
26	a	409	PL9	2	0
25	T	101	BCR	2	0
24	d	401	PHO	1	0
28	B	623	SQD	2	0
34	E	102	HEM	2	0
23	C	511	CLA	1	0
23	a	404	CLA	1	0
29	H	102	DGD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	601	CLA	3	0
25	b	620	BCR	2	0
25	h	102	BCR	3	0
23	C	509	CLA	3	0
34	e	102	HEM	3	0
23	B	611	CLA	1	0
33	l	101	LHG	1	0
33	D	408	LHG	4	0
23	C	505	CLA	2	0
23	c	511	CLA	1	0
25	c	514	BCR	2	0
24	D	401	PHO	1	0
28	A	412	SQD	1	0
23	b	614	CLA	2	0
23	A	405	CLA	2	0
23	c	509	CLA	1	0
25	c	515	BCR	2	0
25	d	405	BCR	2	0
23	b	617	CLA	2	0
30	A	414	OEY	1	0
23	c	508	CLA	1	0
23	b	606	CLA	2	0
23	D	403	CLA	3	0
26	D	406	PL9	1	0
23	C	513	CLA	1	0
23	d	404	CLA	1	0
25	a	408	BCR	2	0
23	h	101	CLA	5	0
25	t	101	BCR	4	0
33	d	408	LHG	1	0
23	b	607	CLA	2	0
23	c	503	CLA	1	0
29	a	413	DGD	2	0
23	B	605	CLA	2	0
23	B	606	CLA	2	0
30	a	416	OEY	1	0
25	b	618	BCR	1	0
35	V	201	HEC	1	0
25	A	408	BCR	1	0
25	H	101	BCR	2	0
27	B	620	LMG	3	0
23	c	504	CLA	1	0

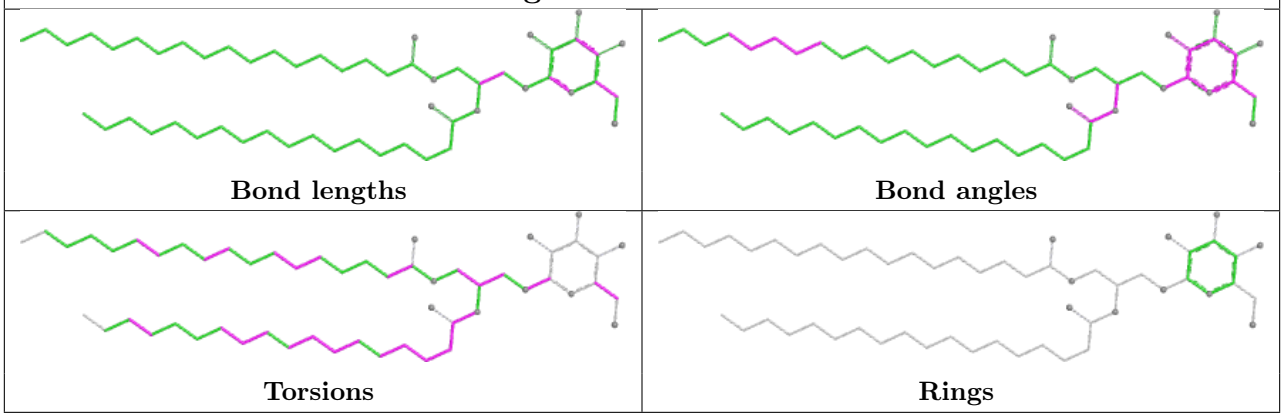
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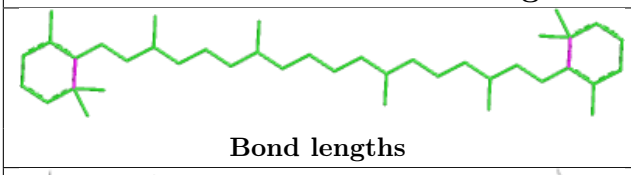
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	506	CLA	2	0
23	b	615	CLA	4	0
23	A	407	CLA	1	0
25	b	619	BCR	5	0
28	a	412	SQD	2	0
25	y	101	BCR	1	0
33	E	101	LHG	1	0
27	A	410	LMG	1	0
26	A	409	PL9	3	0
25	B	617	BCR	4	0
23	B	614	CLA	1	0

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

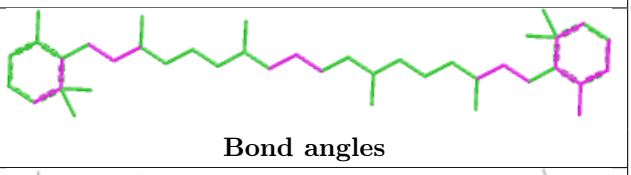
Ligand LMG b 622



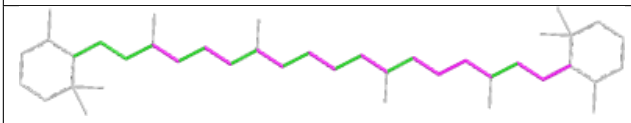
Ligand BCR D 405



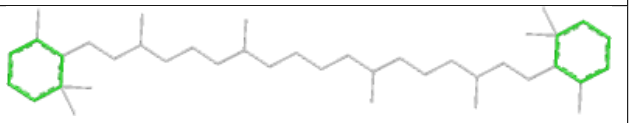
Bond lengths



Bond angles



Torsions

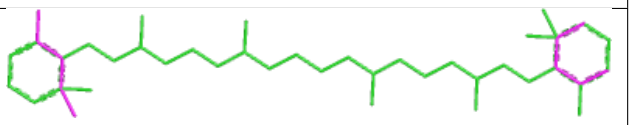


Rings

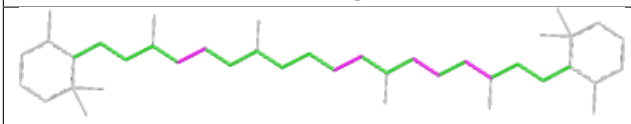
Ligand BCR c 521



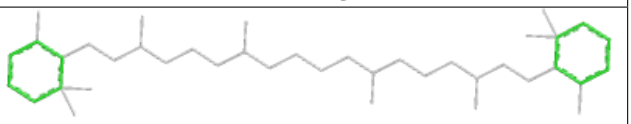
Bond lengths



Bond angles

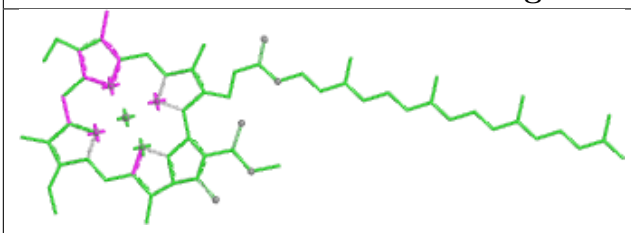


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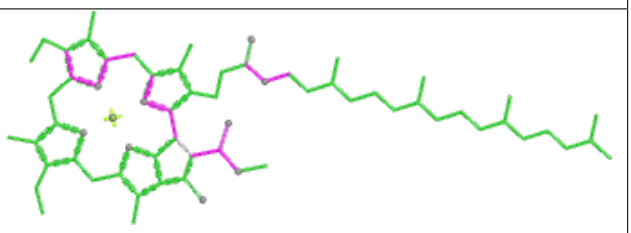


Rings

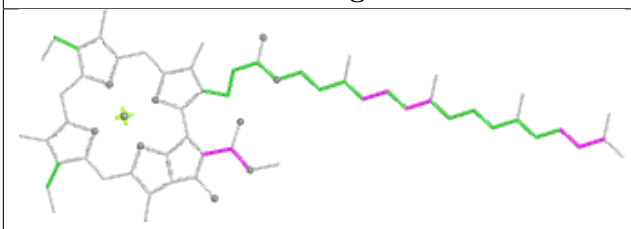
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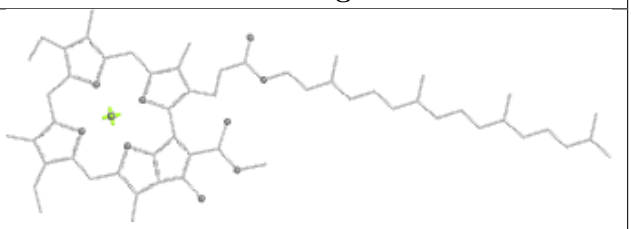
Bond lengths



Bond angles

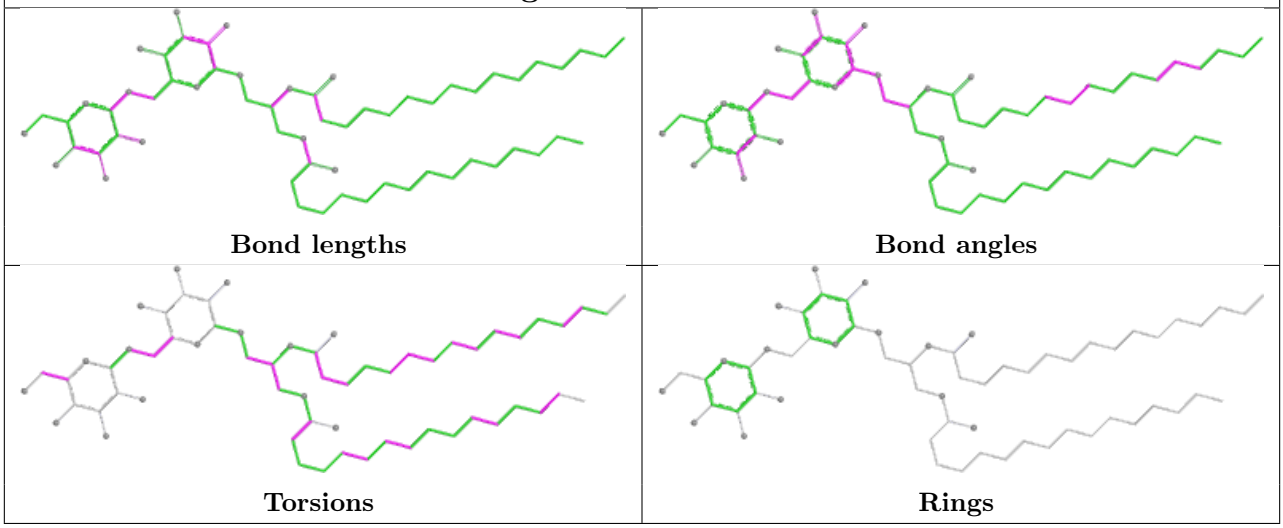


Torsions

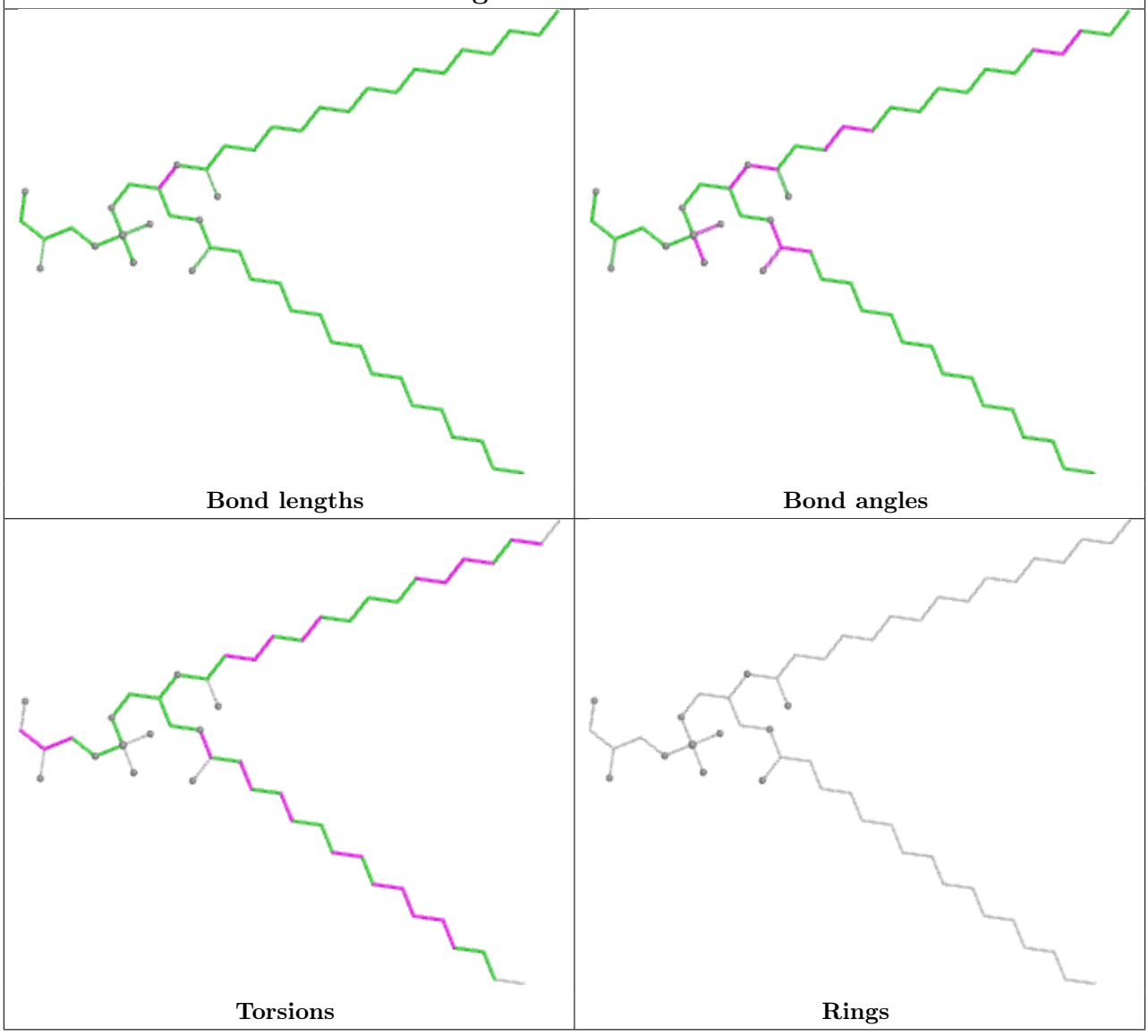


Rings

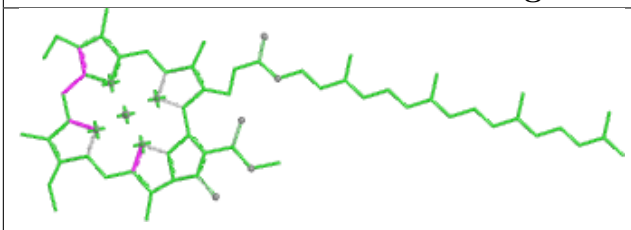
Ligand DGD C 516



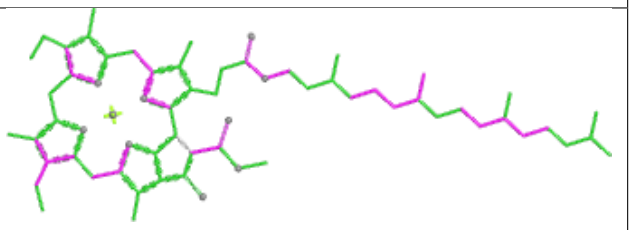
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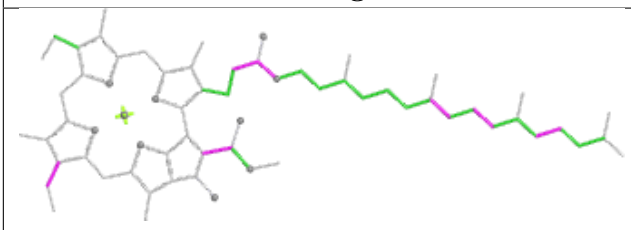
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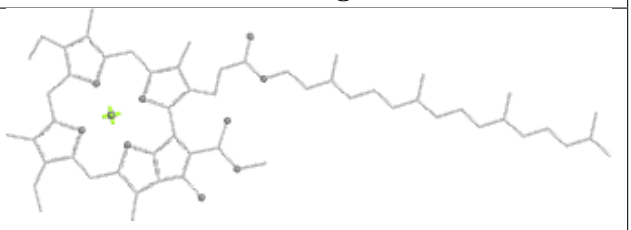
Bond lengths



Bond angles

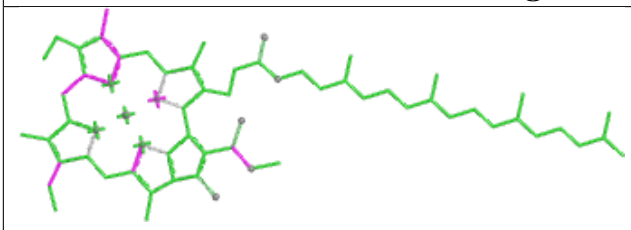


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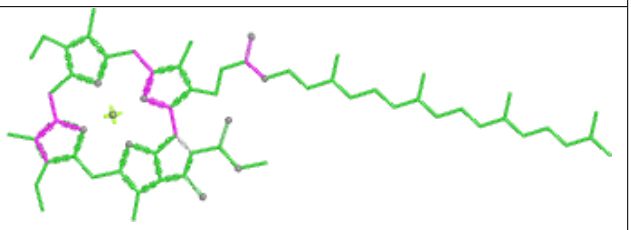


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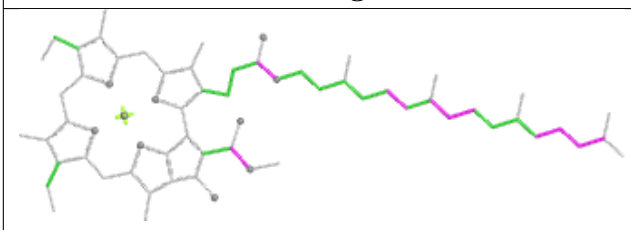
Ligand CLA B 607



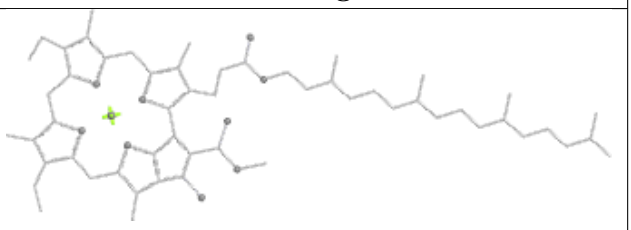
Bond lengths



Bond angles

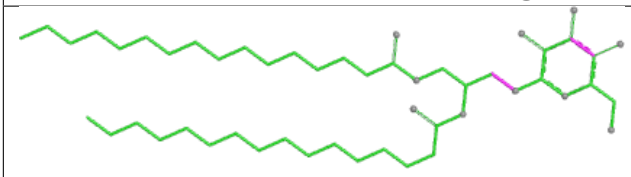


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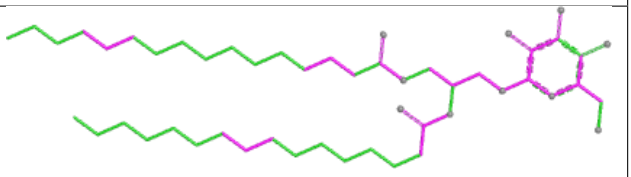


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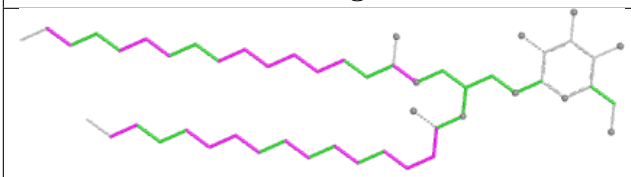
Ligand LMG m 101



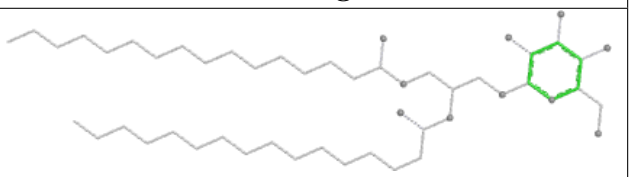
Bond lengths



Bond angles

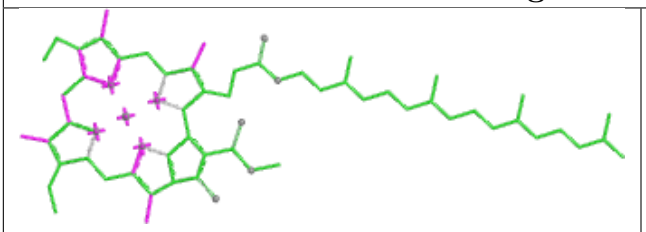


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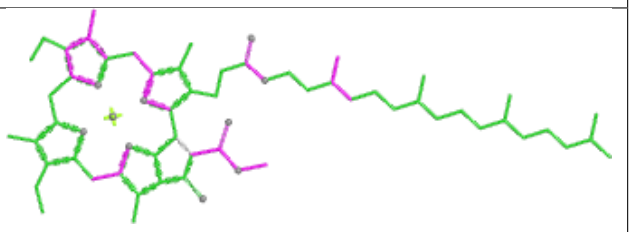


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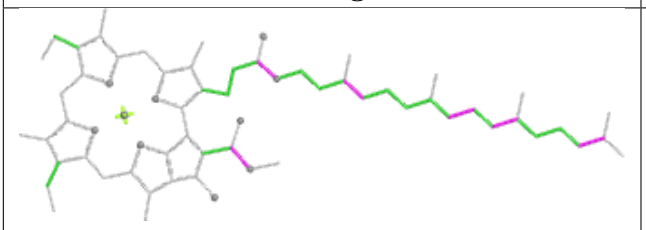
Ligand CLA b 604



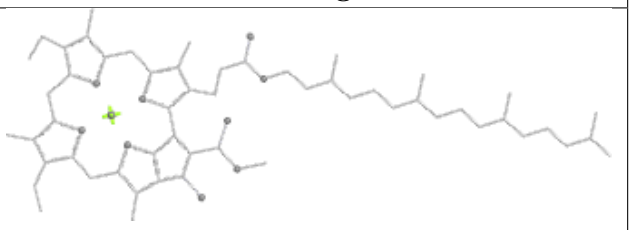
Bond lengths



Bond angles

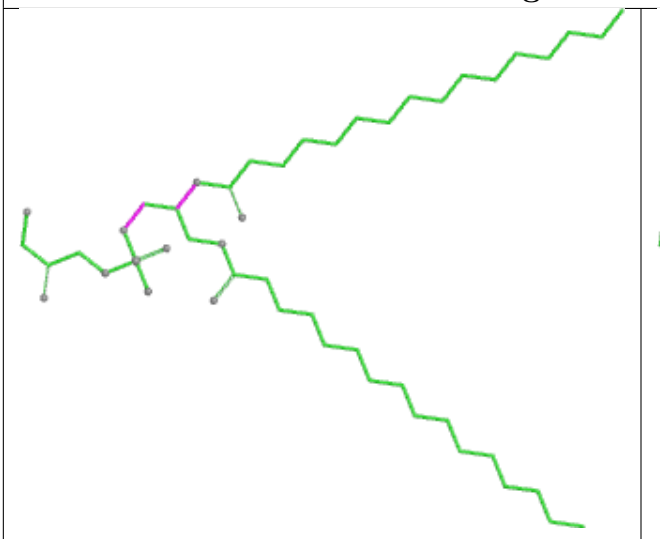


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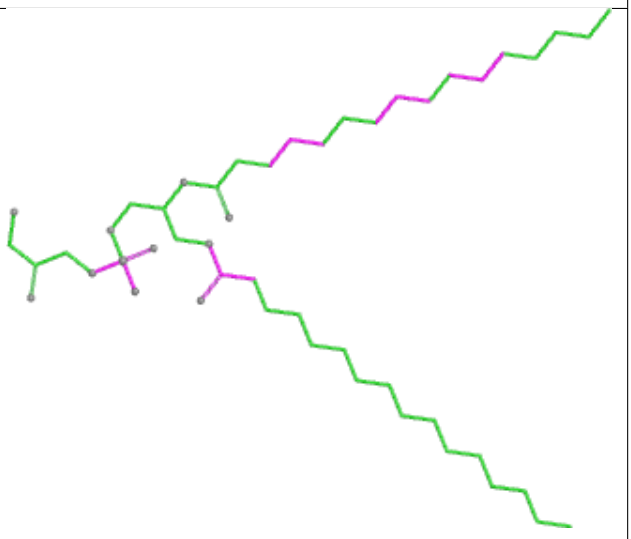


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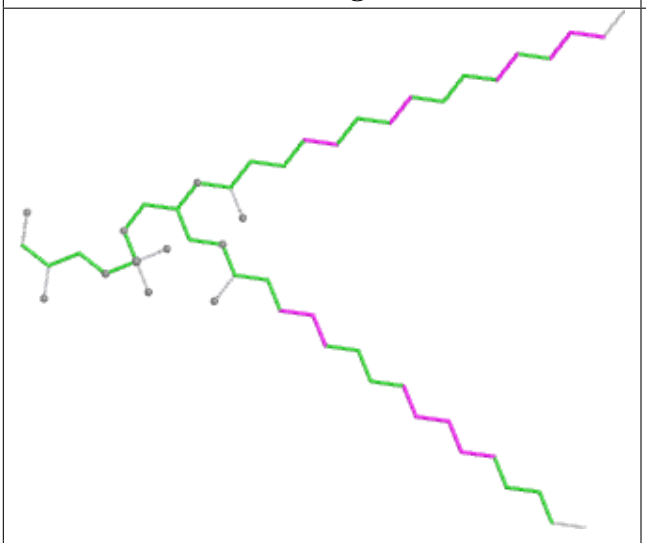
Ligand LHG B 622



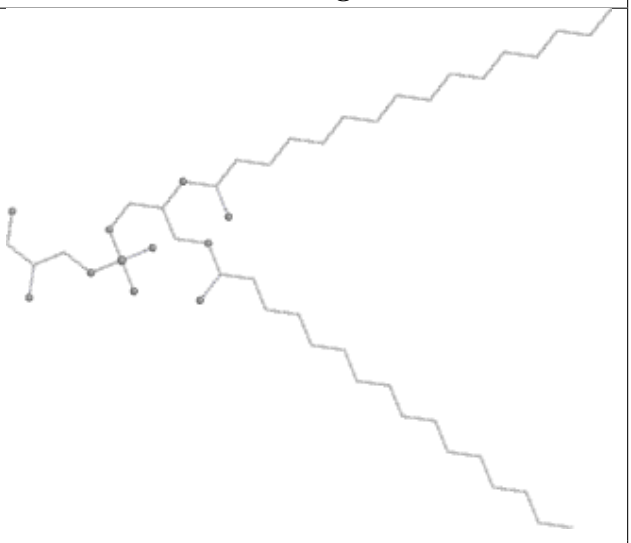
Bond lengths



Bond angles

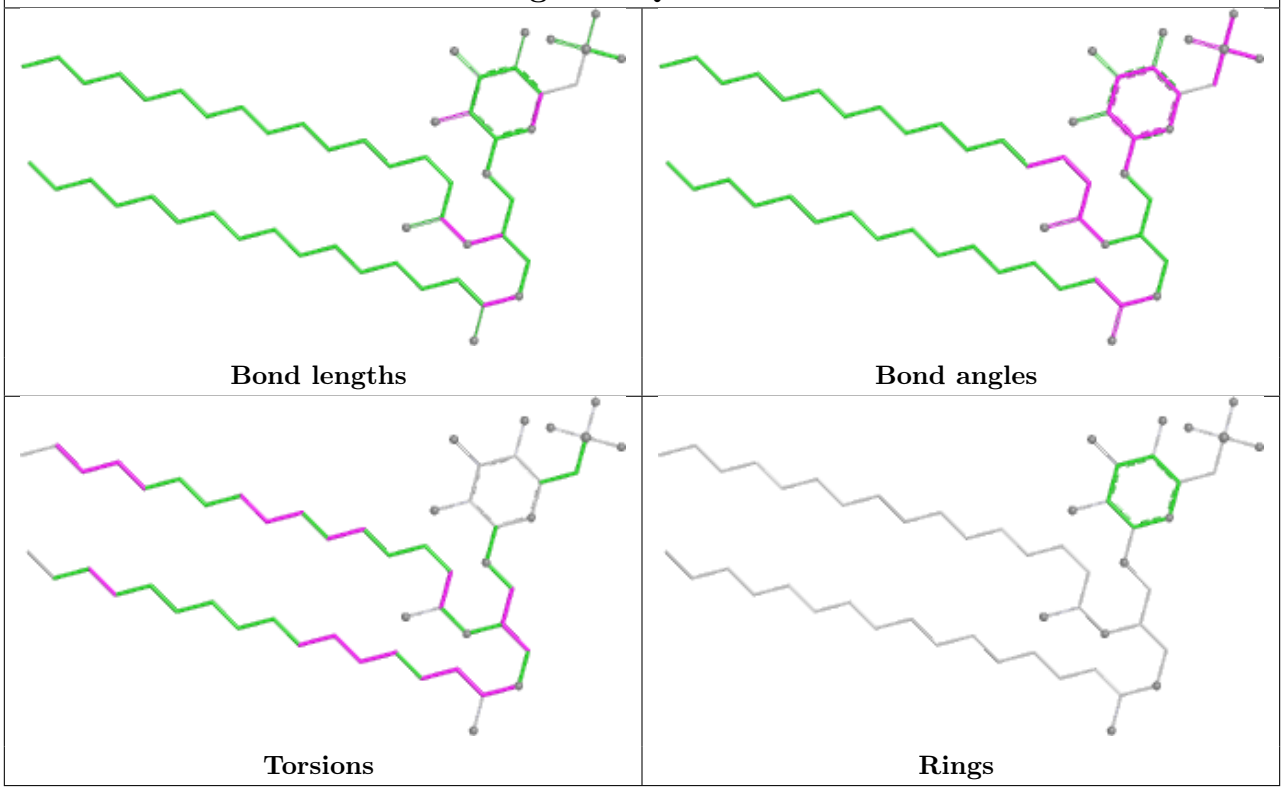


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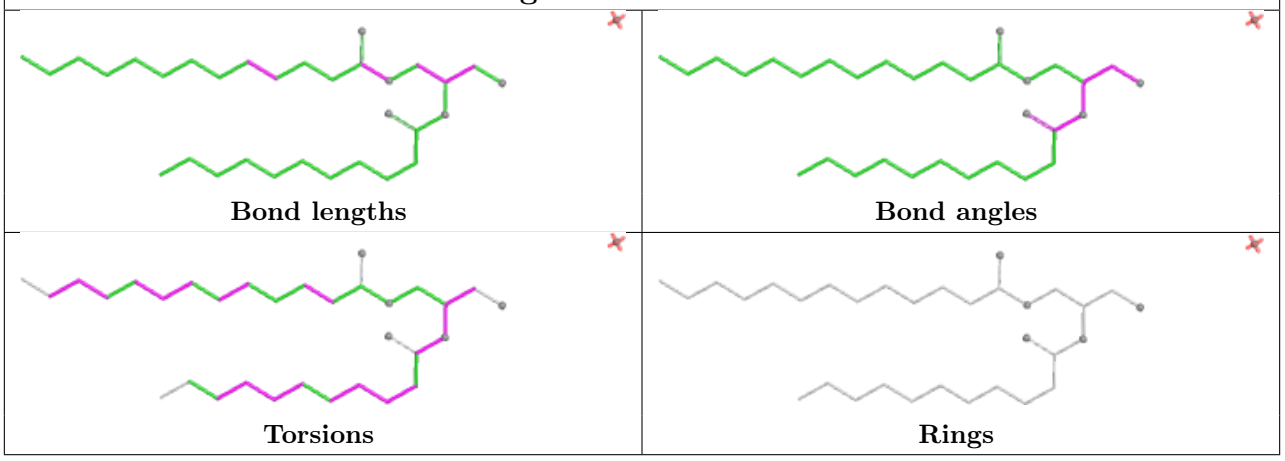


Rings

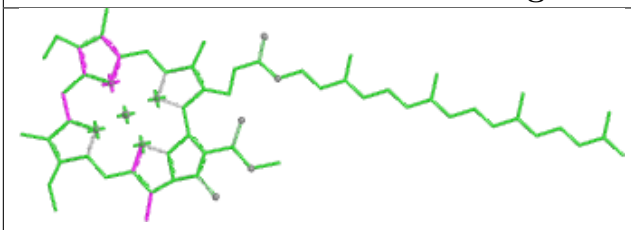
Ligand SQD a 411



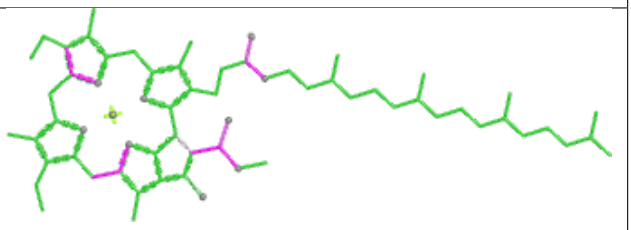
Ligand LMG D 410



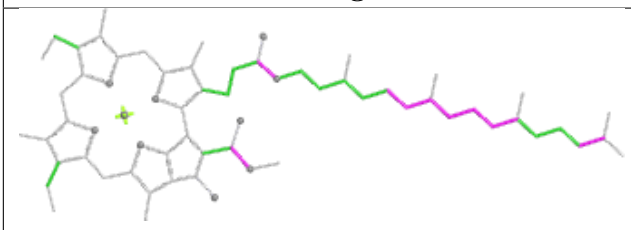
Ligand CLA b 608



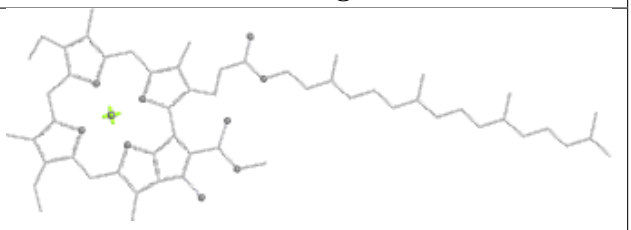
Bond lengths



Bond angles

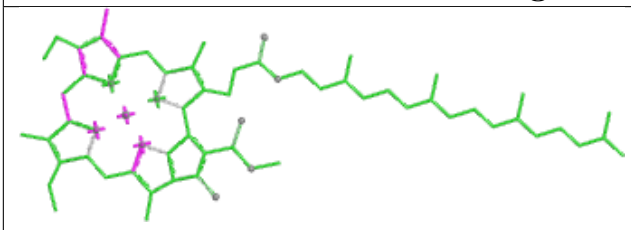


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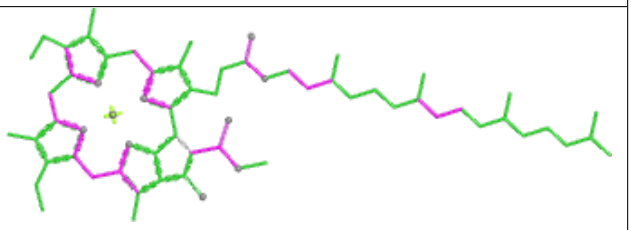


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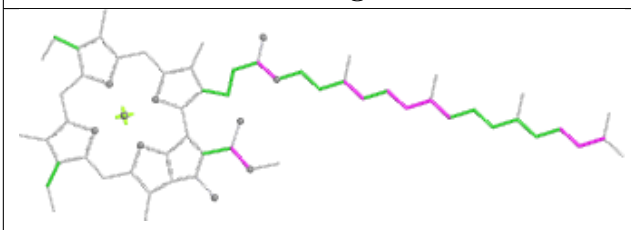
Ligand CLA c 505



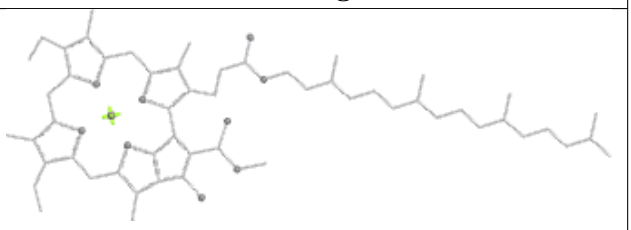
Bond lengths



Bond angles

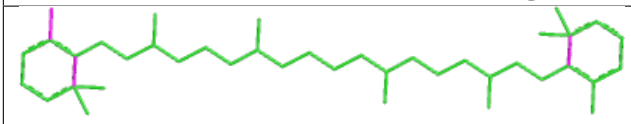


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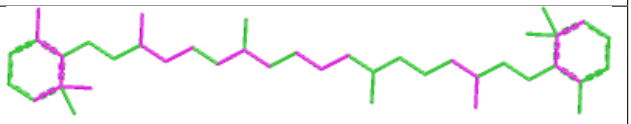


Rings

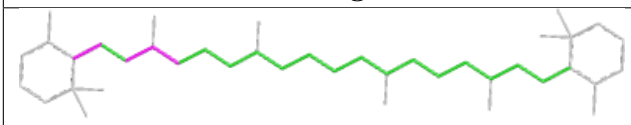
Ligand BCR B 619



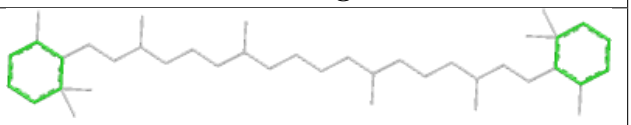
Bond lengths



Bond angles

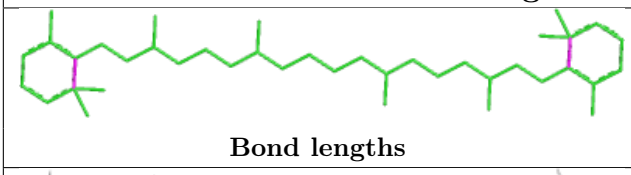


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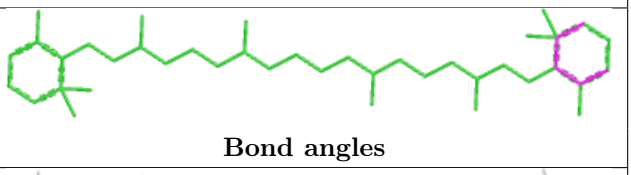


Rings

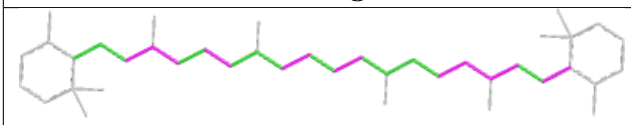
Ligand BCR C 520



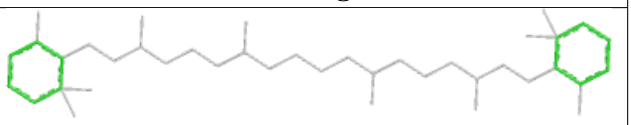
Bond lengths



Bond angles

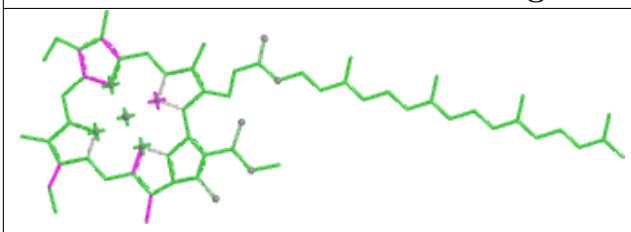


Torsions

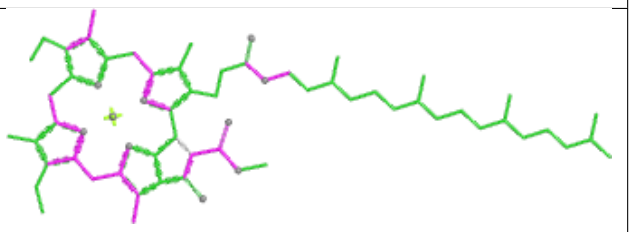


Rings

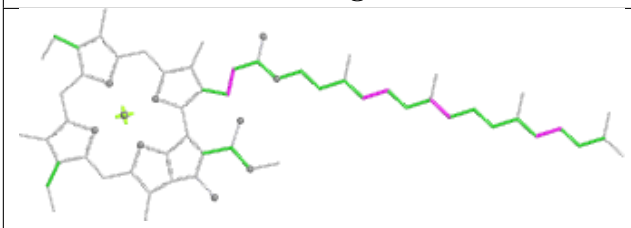
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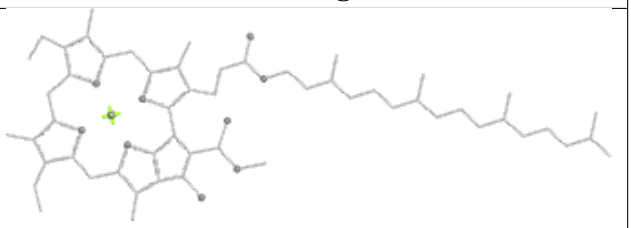
Bond lengths



Bond angles

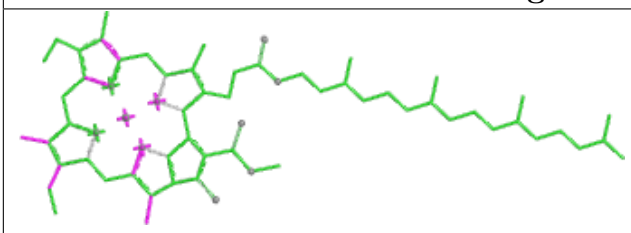


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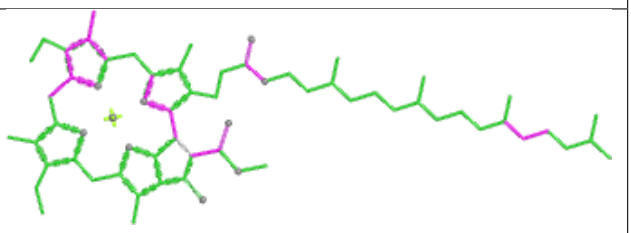


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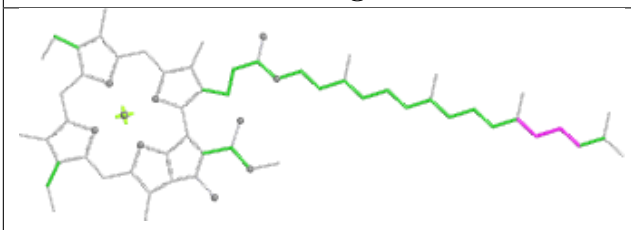
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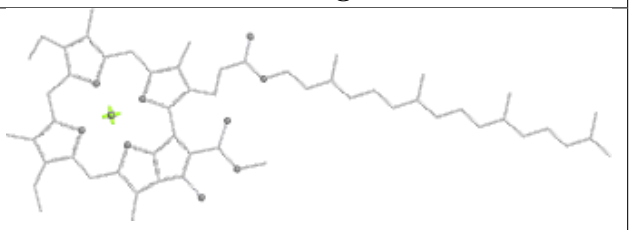
Bond lengths



Bond angles

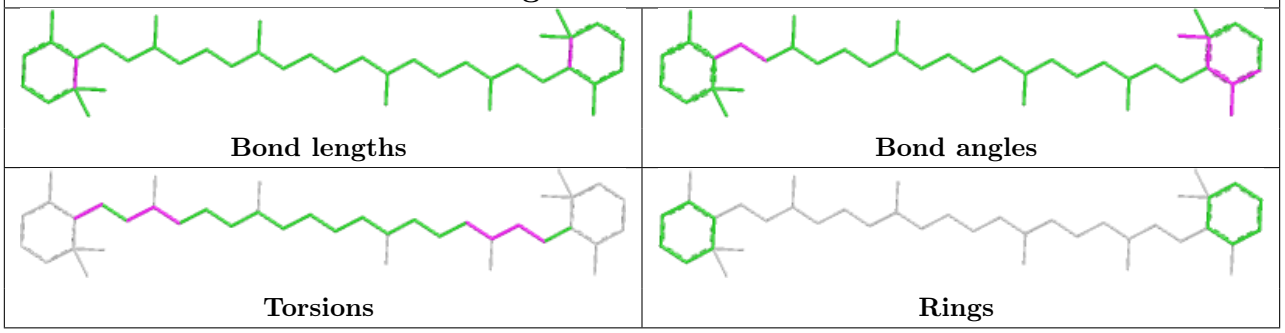


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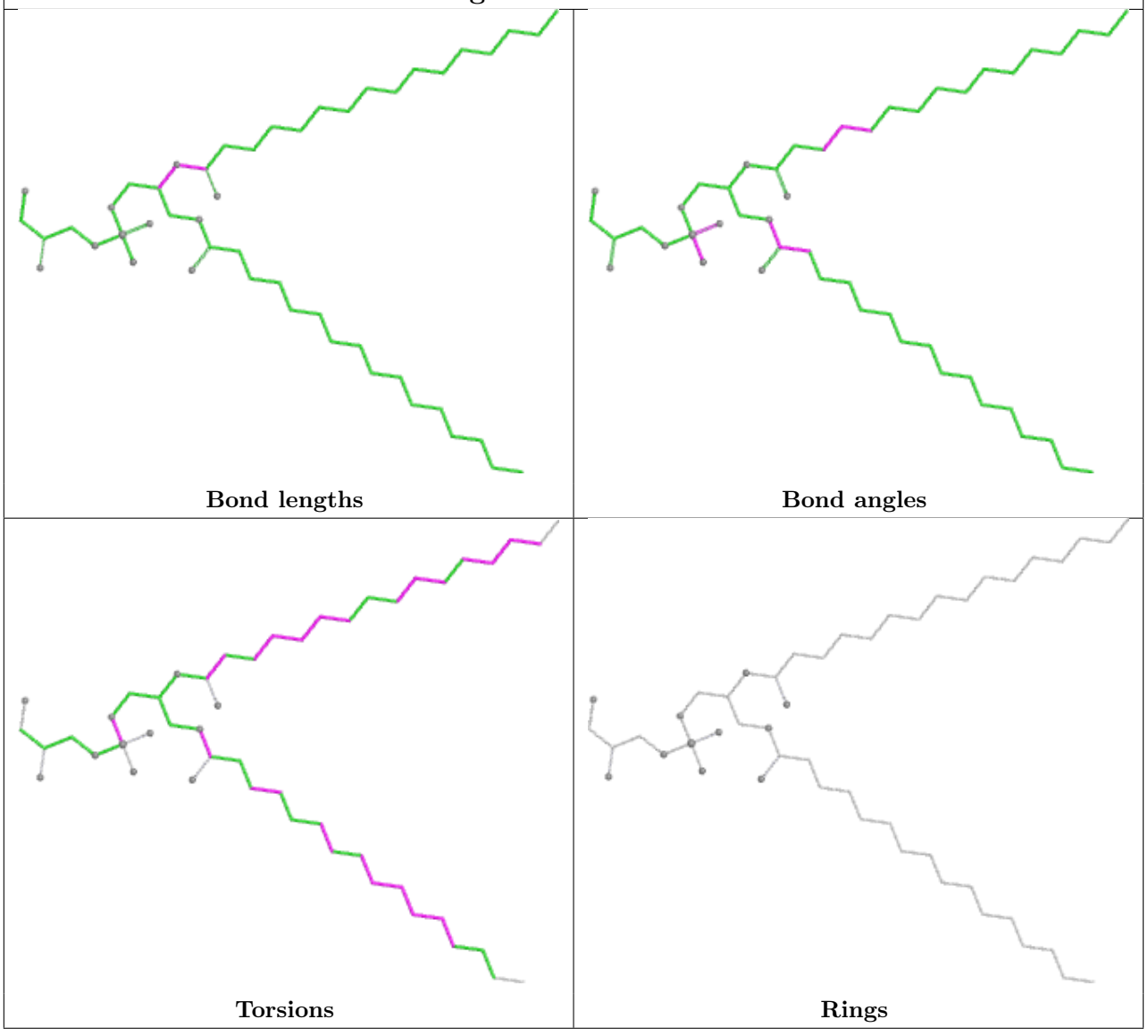


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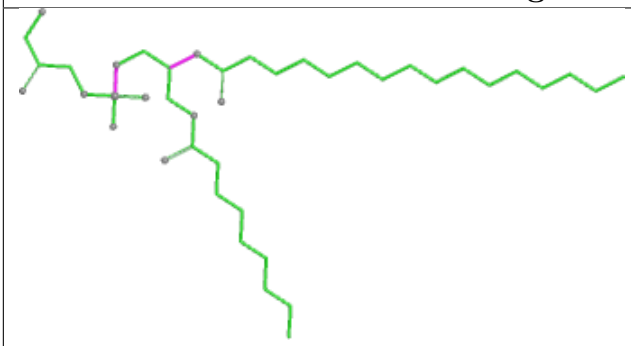
Ligand BCR K 101



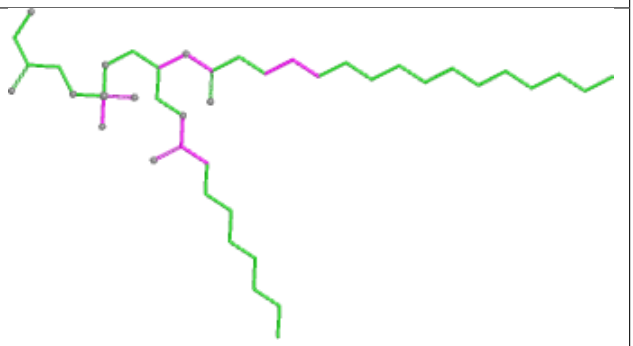
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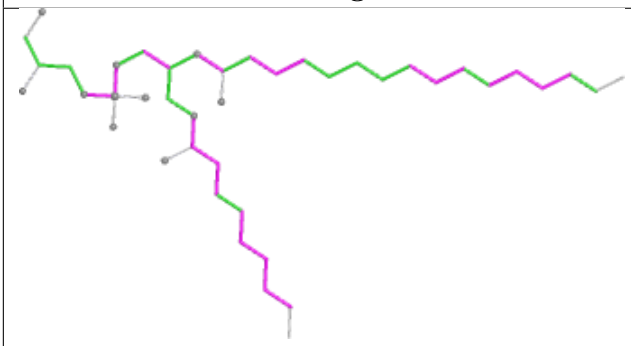
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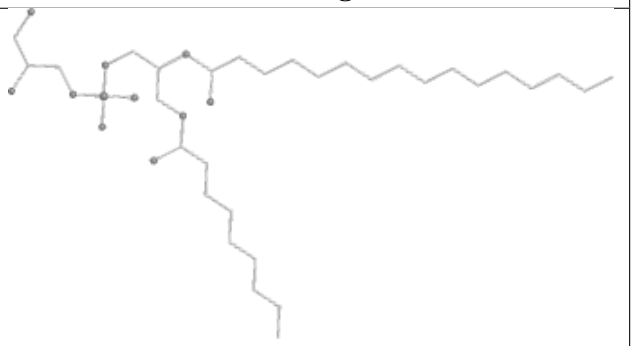
Bond lengths



Bond angles

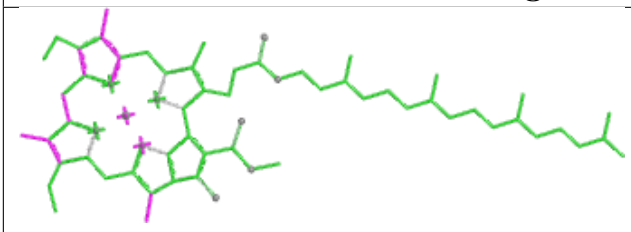


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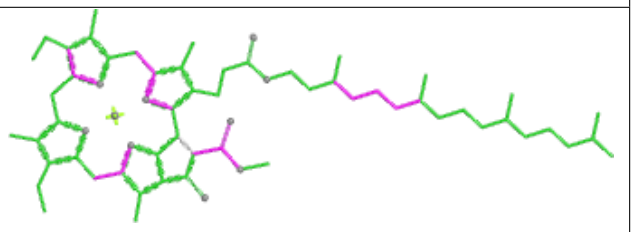


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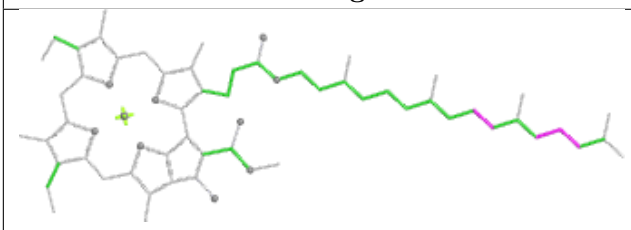
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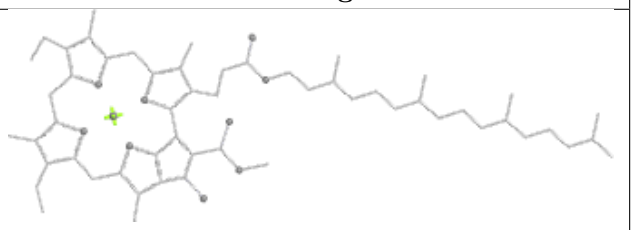
Bond lengths



Bond angles

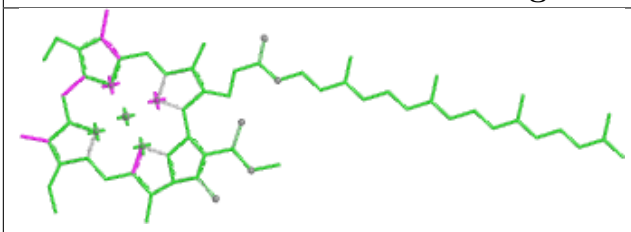


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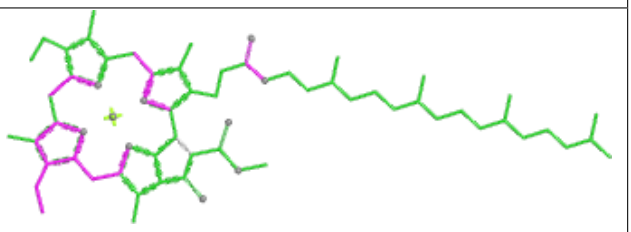


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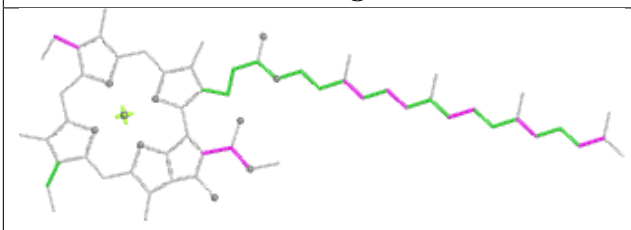
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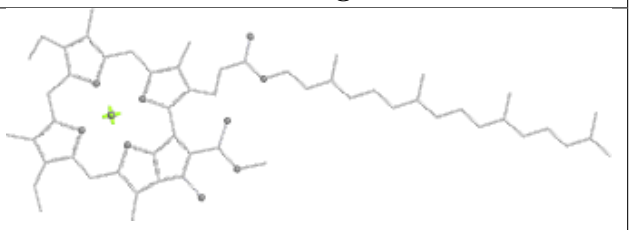
Bond lengths



Bond angles

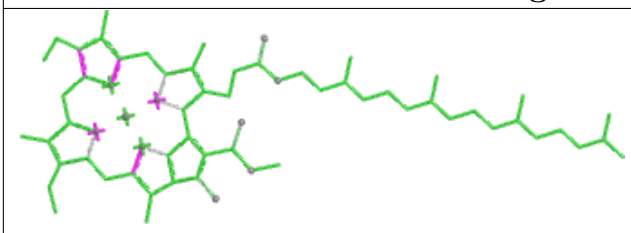


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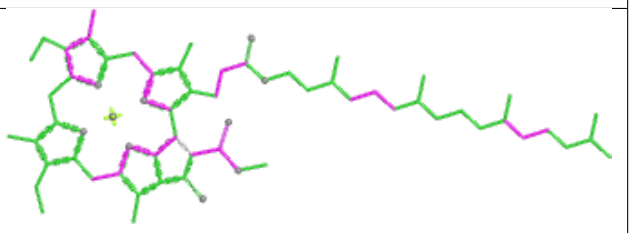


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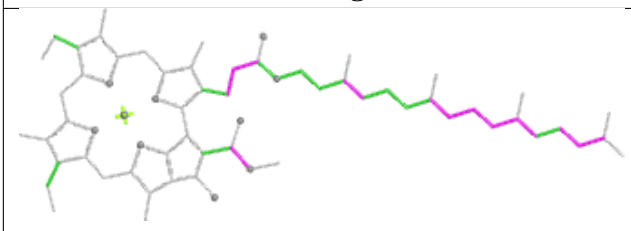
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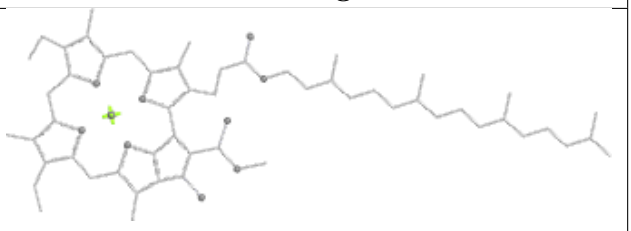
Bond lengths



Bond angles

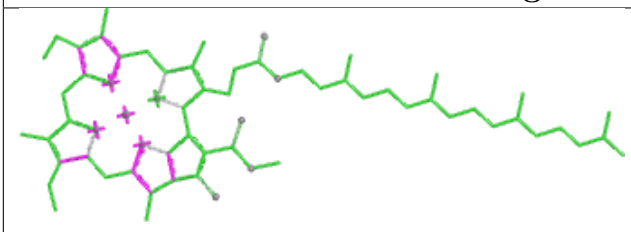


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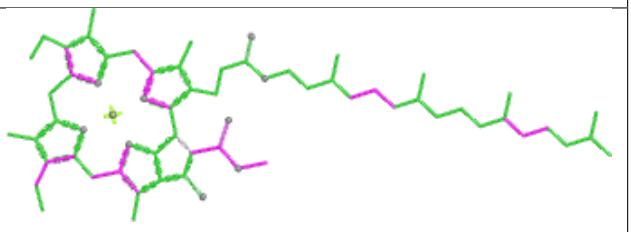


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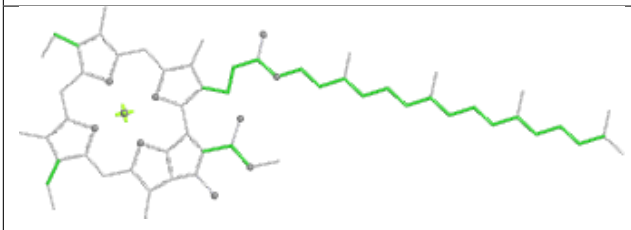
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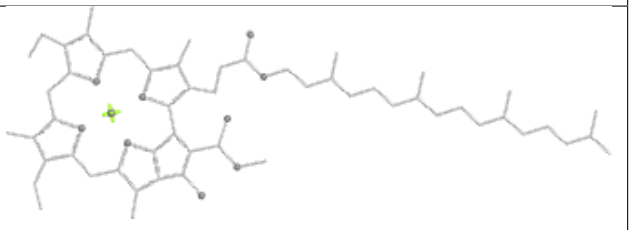
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Bond angles

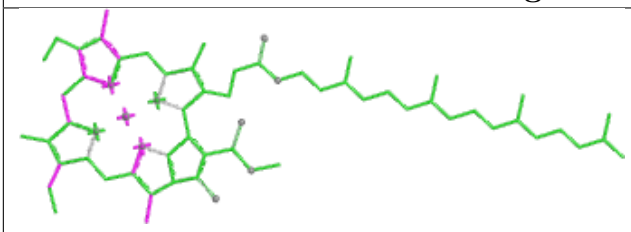


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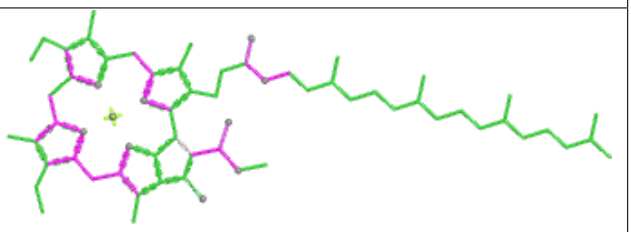


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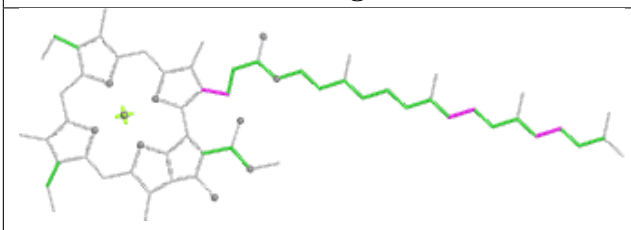
Ligand CLA B 602



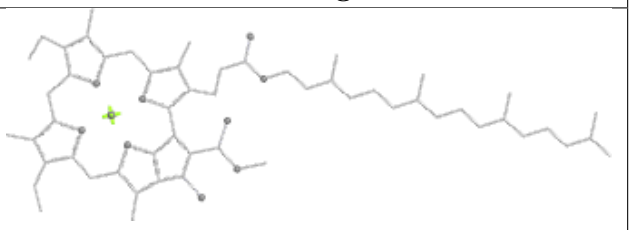
Bond lengths



Bond angles



Torsions



Rings

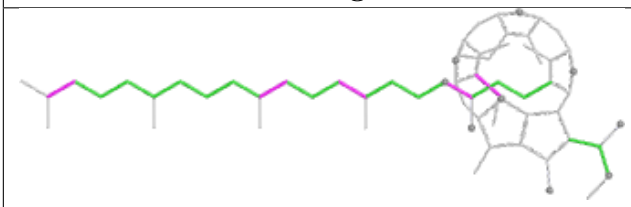
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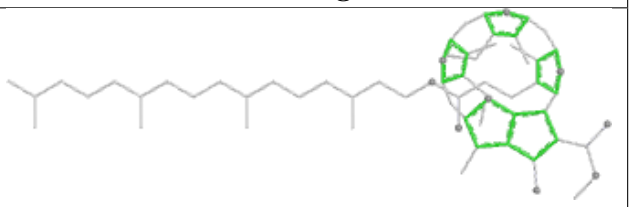
Bond lengths



Bond angles

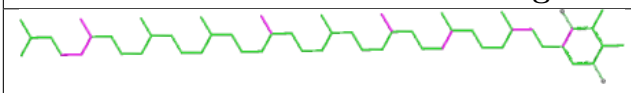


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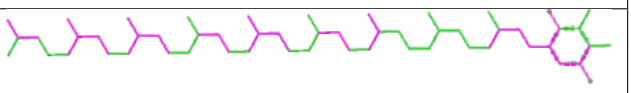


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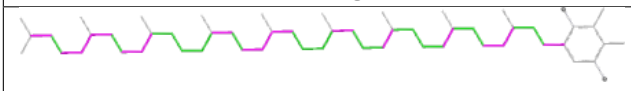
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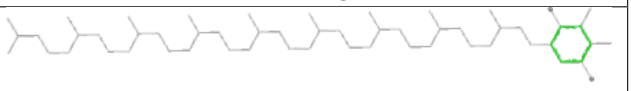
Bond lengths



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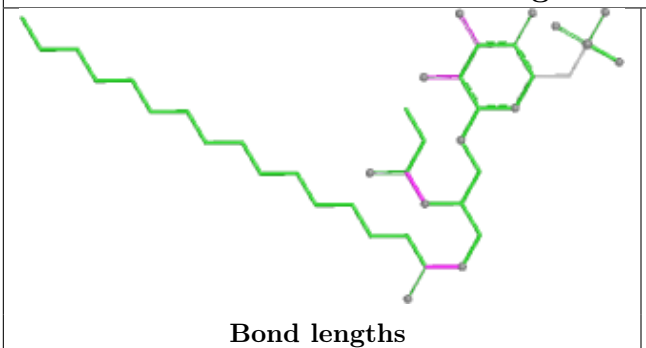


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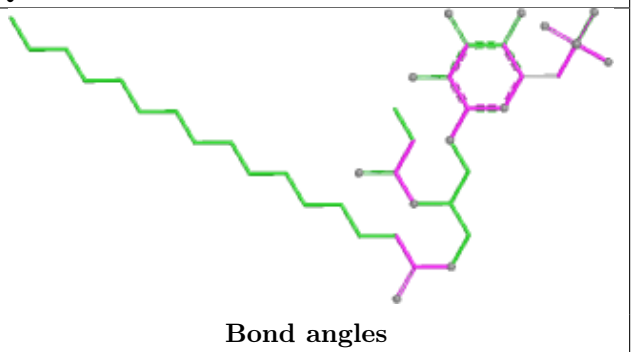


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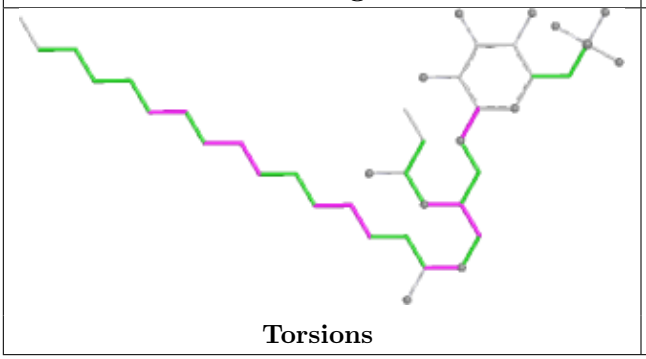
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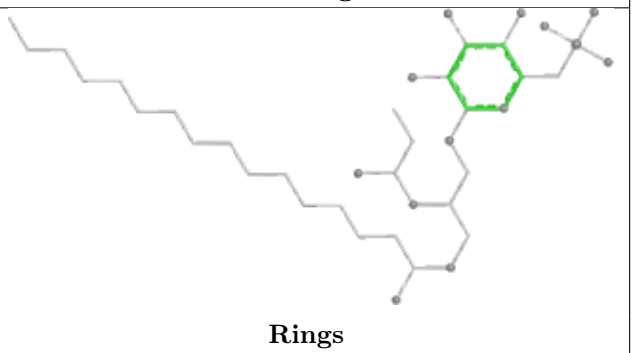
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Bond angles

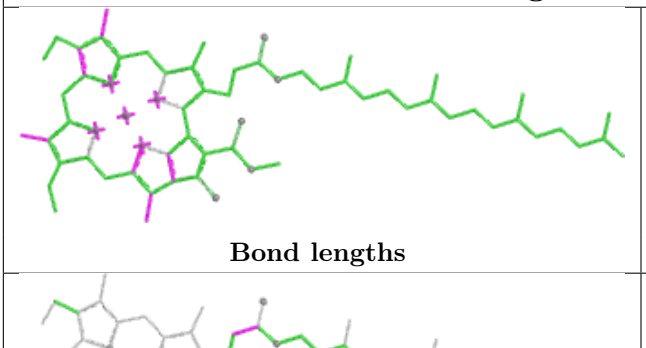


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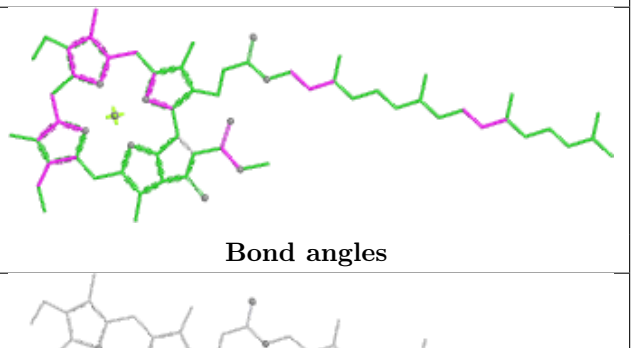


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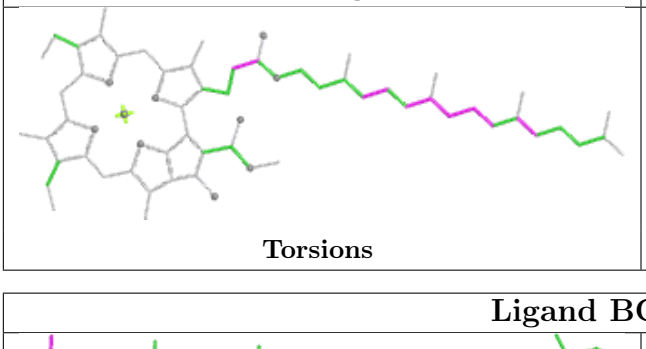
Ligand CLA b 613



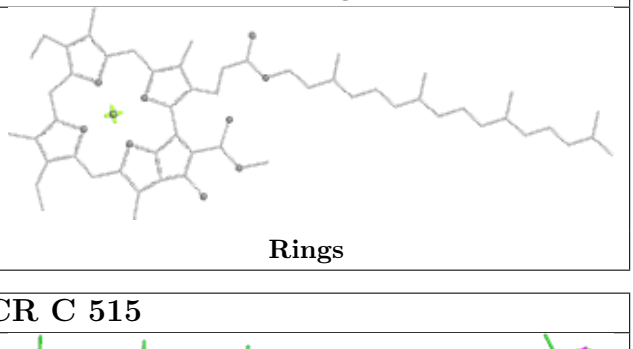
Bond lengths



Bond angles

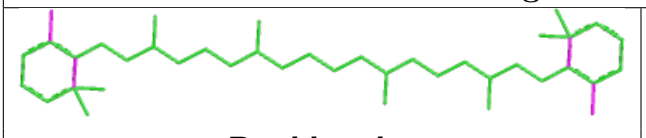


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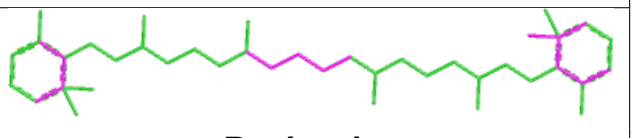


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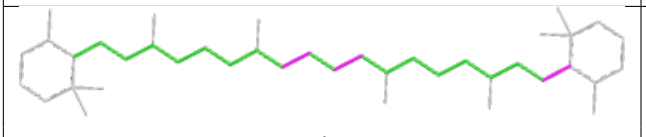
Ligand BCR C 515



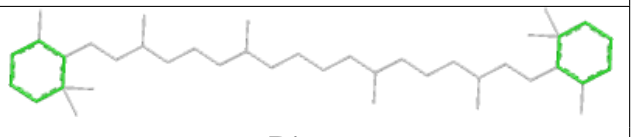
Bond lengths



Bond angles

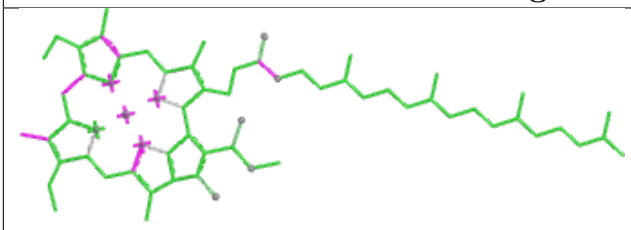


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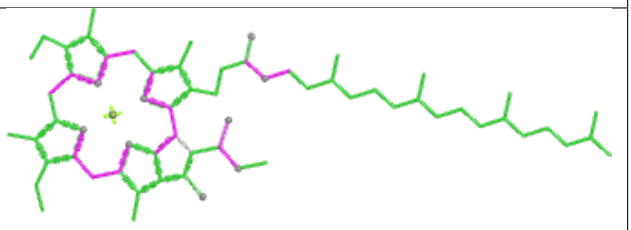


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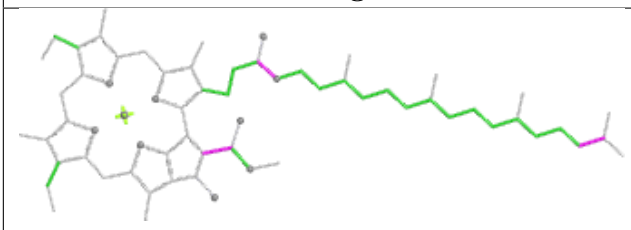
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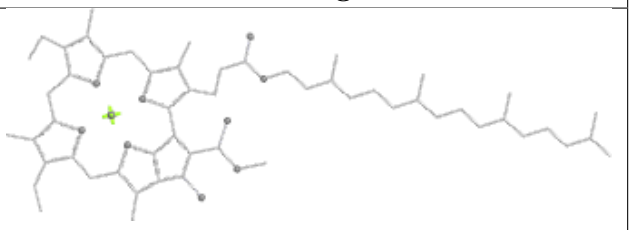
Bond lengths



Bond angles

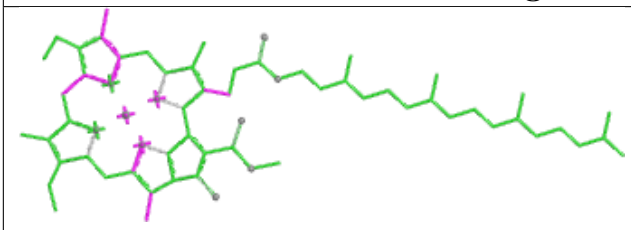


Torsions

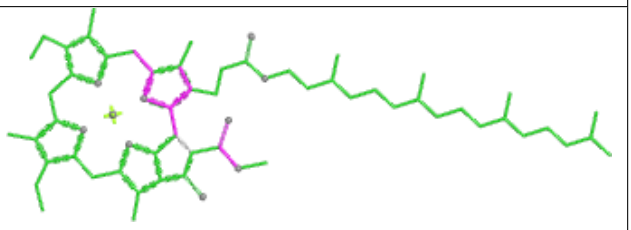


Rings

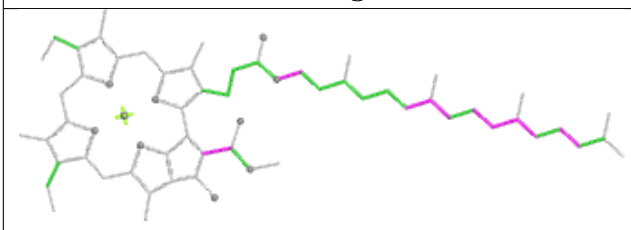
Ligand CLA C 507



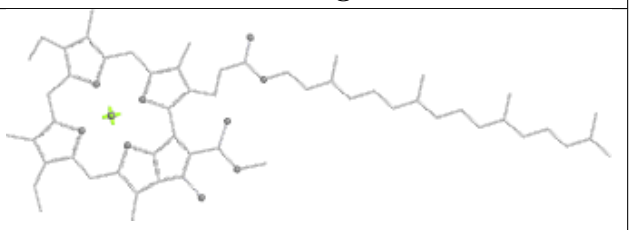
Bond lengths



Bond angles

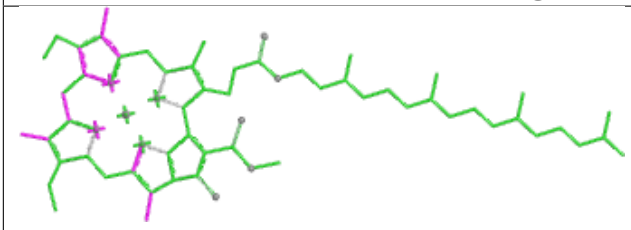


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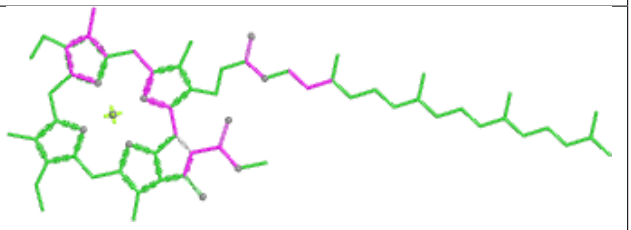


Rings

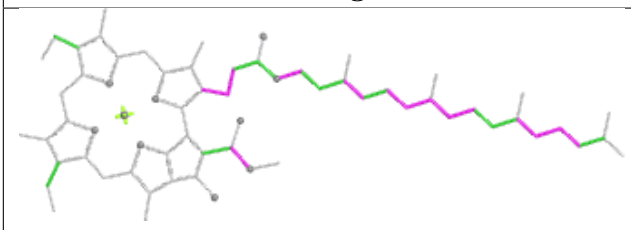
Ligand CLA c 512



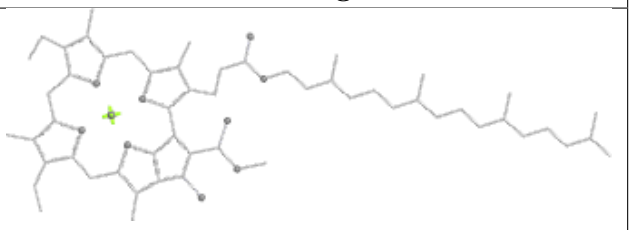
Bond lengths



Bond angles

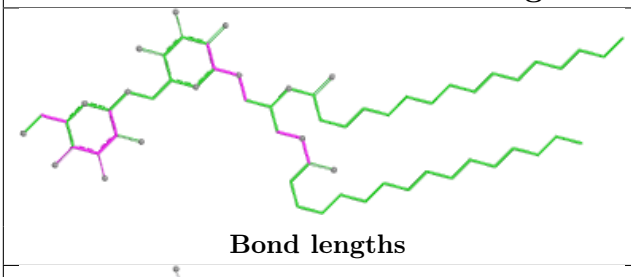


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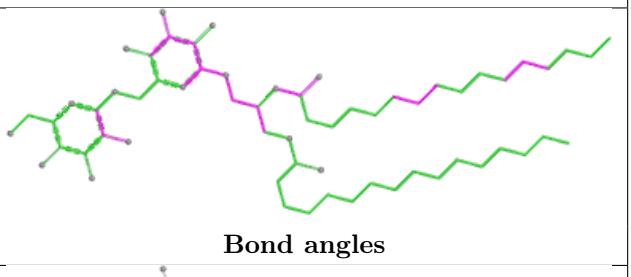


Rings

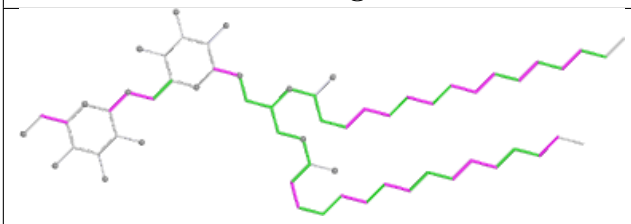
Ligand DGD c 517



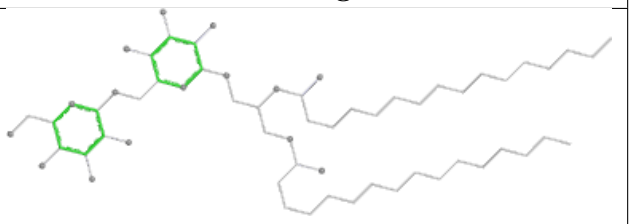
Bond lengths



Bond angles

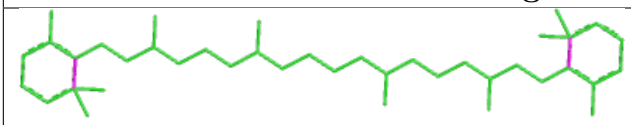


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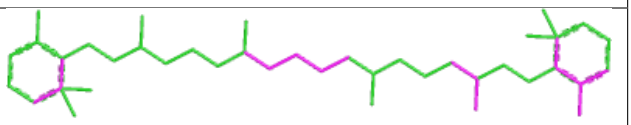


Rings

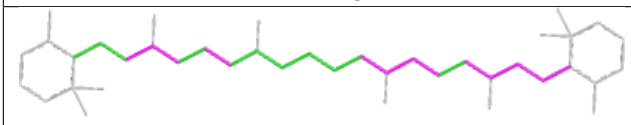
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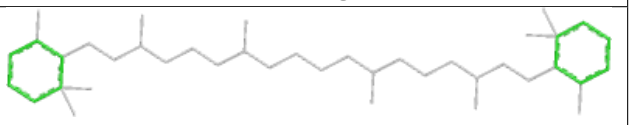
Bond lengths



Bond angles

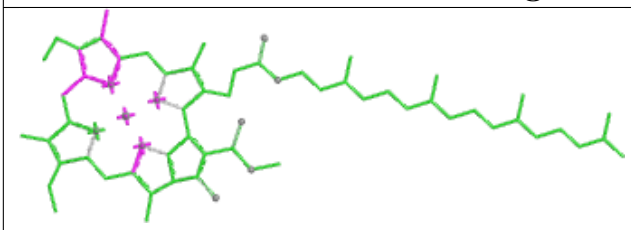


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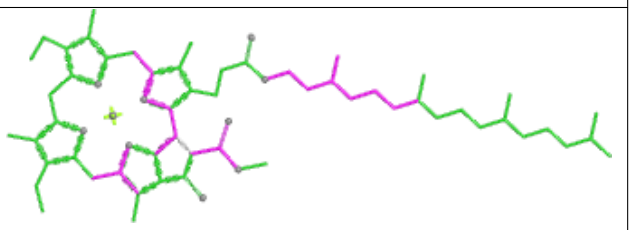


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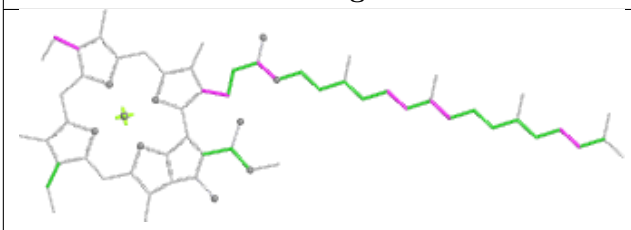
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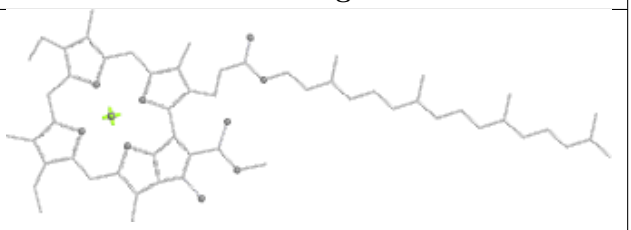
Bond lengths



Bond angles

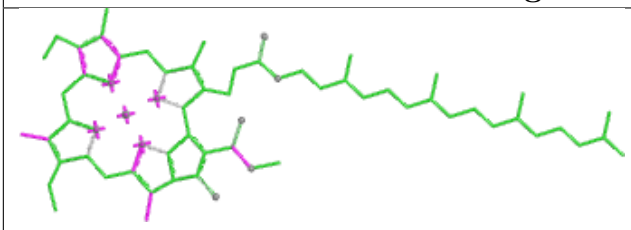


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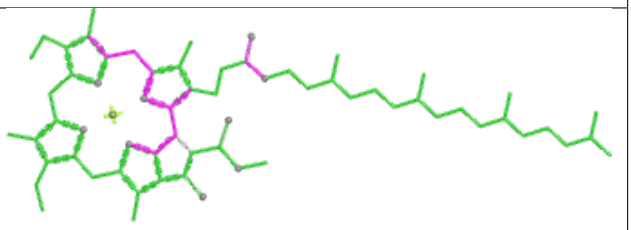


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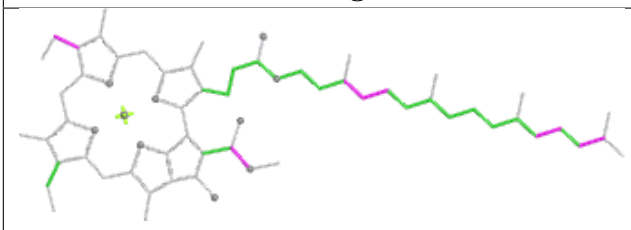
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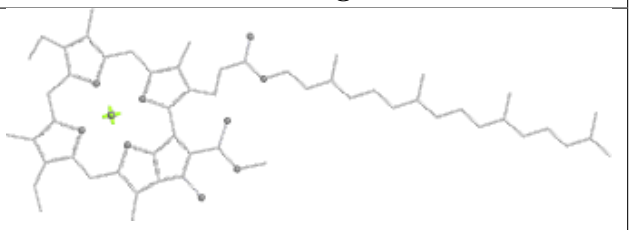
Bond lengths



Bond angles

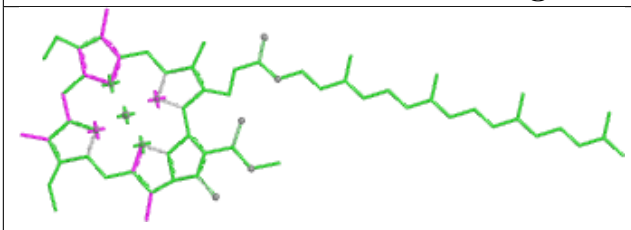


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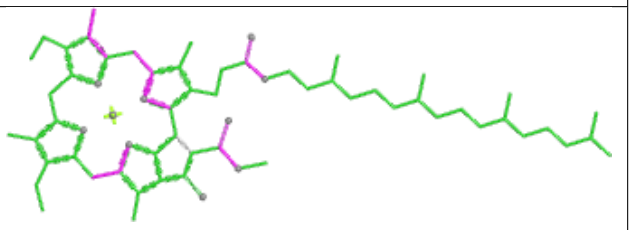


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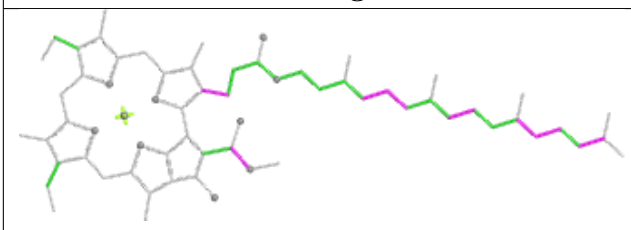
Ligand CLA c 513



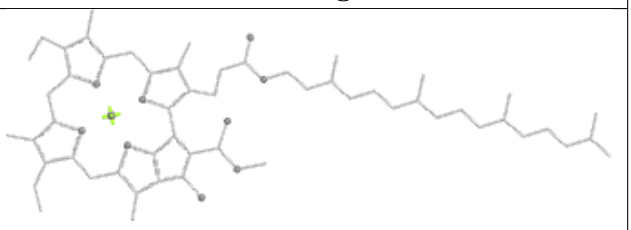
Bond lengths



Bond angles

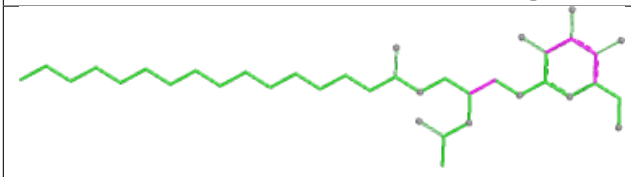


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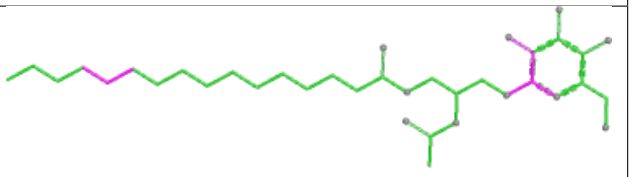


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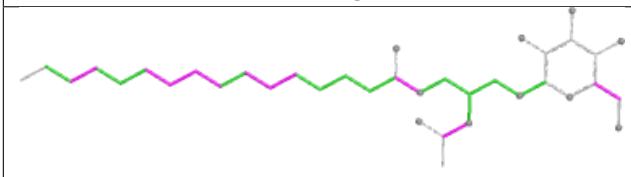
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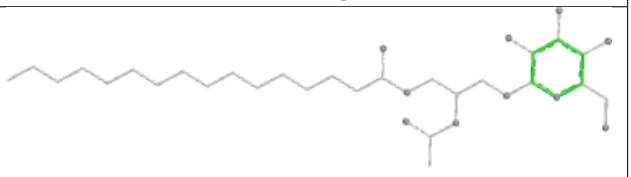
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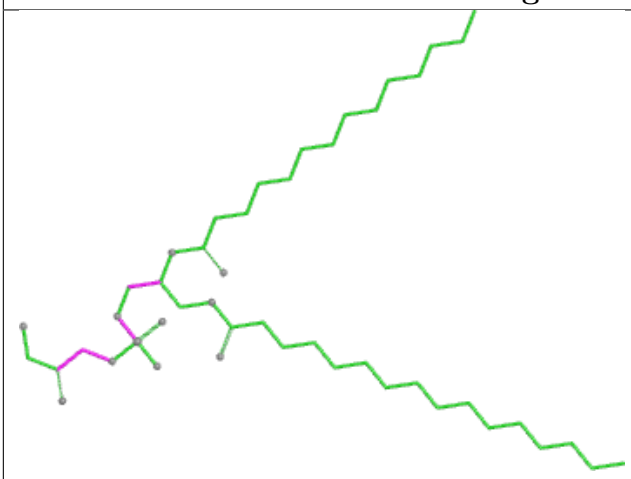


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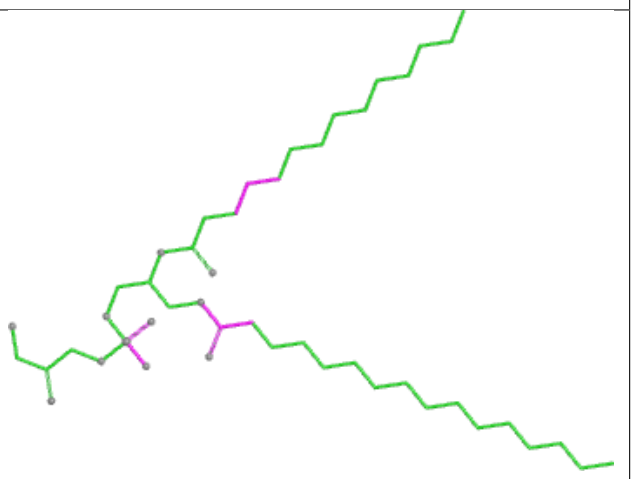


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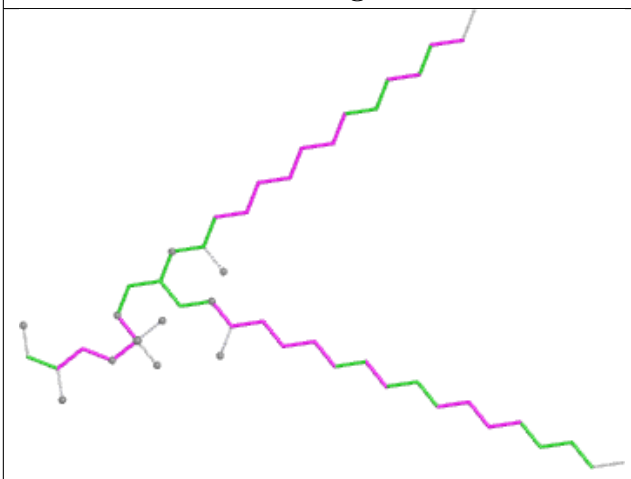
Ligand LHG D 409



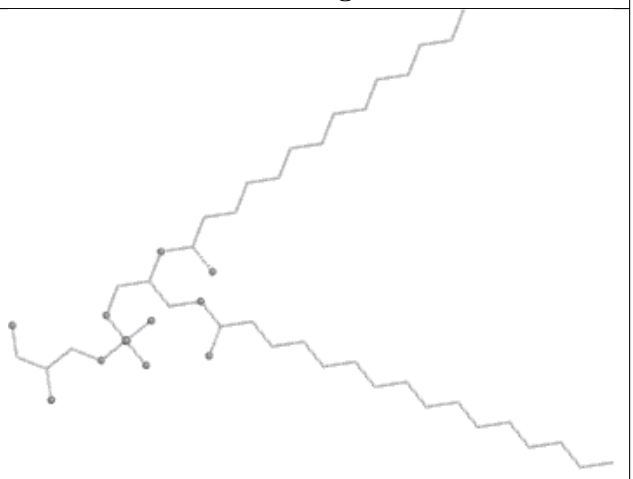
Bond lengths



Bond angles

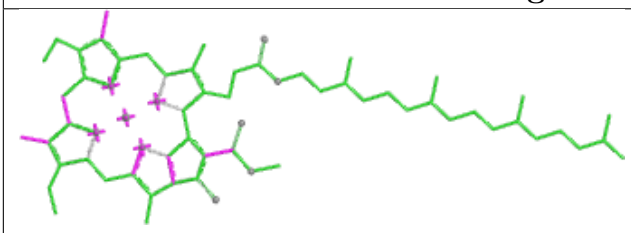


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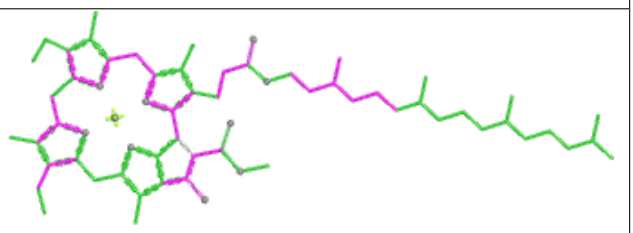


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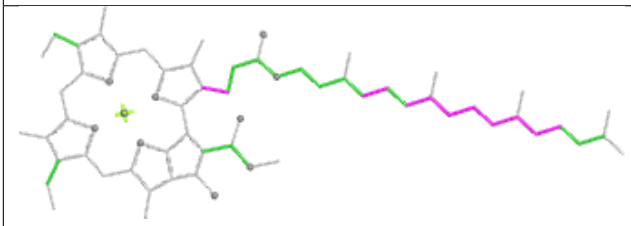
Ligand CLA b 605



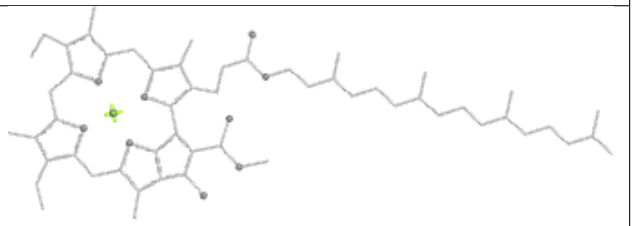
Bond lengths



Bond angles

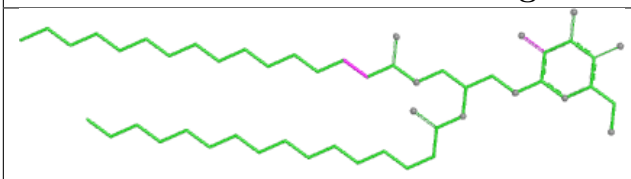


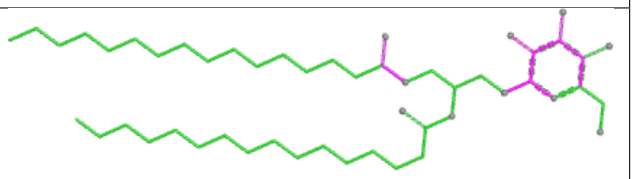
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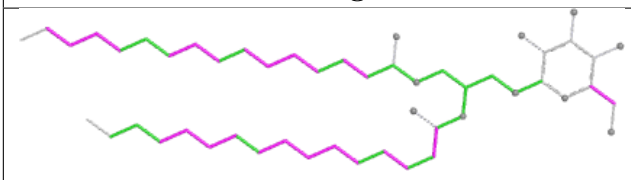


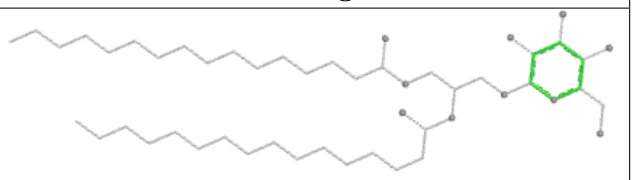
Rings

Ligand LMG D 407

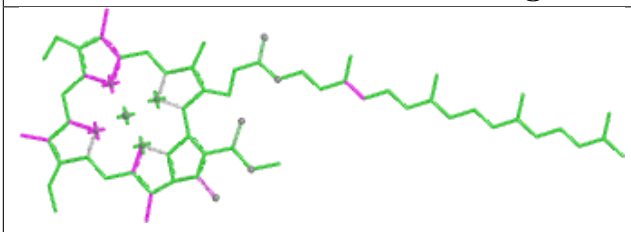

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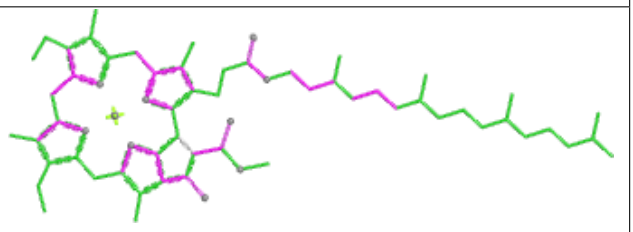

Bond angles

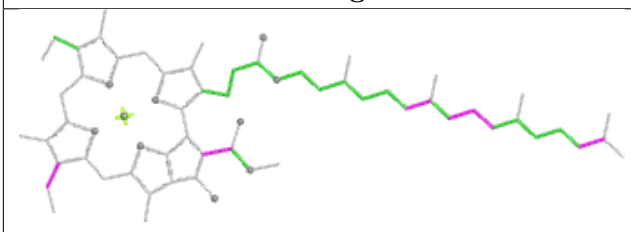

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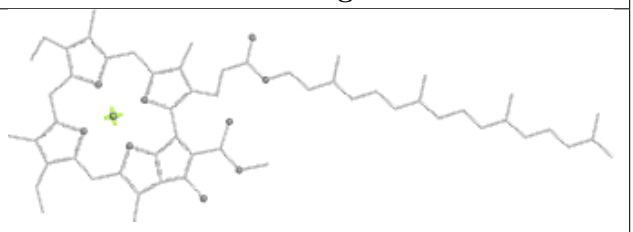

Rings

Ligand CLA B 613

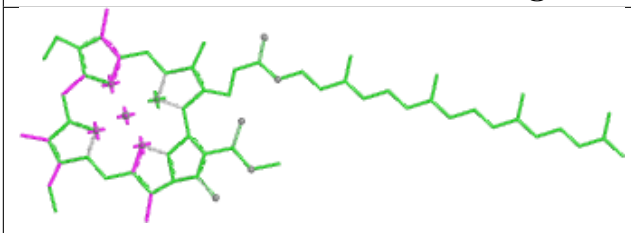

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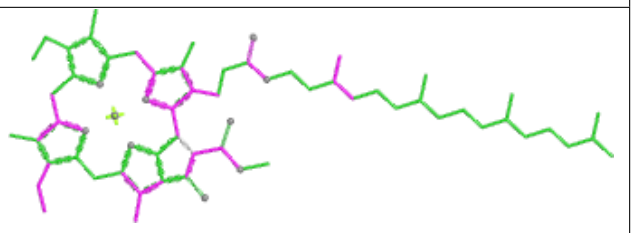

Bond angles

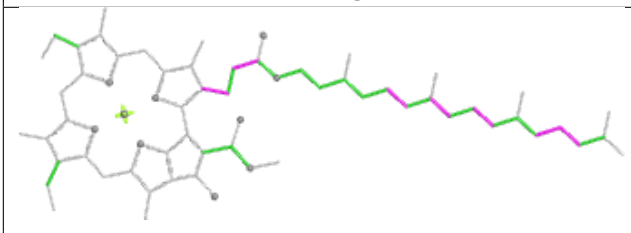

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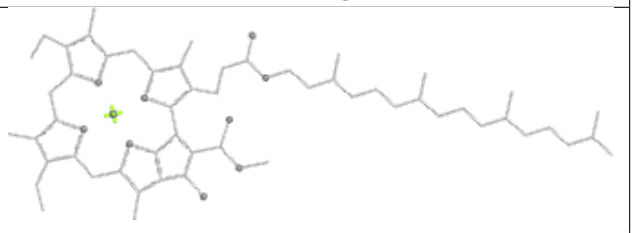

Rings

Ligand CLA a 407

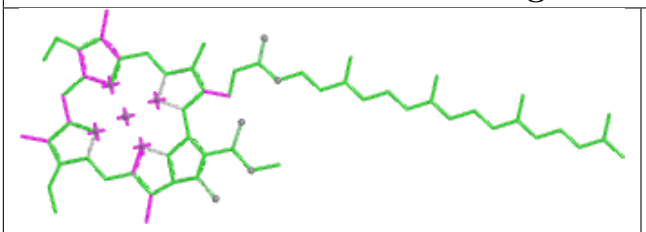

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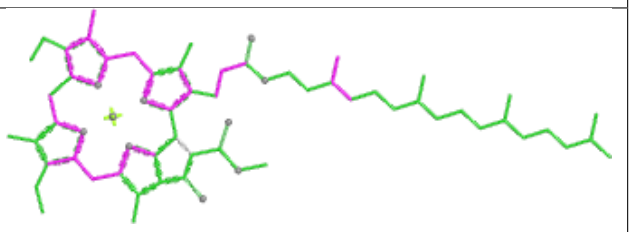

Bond angles

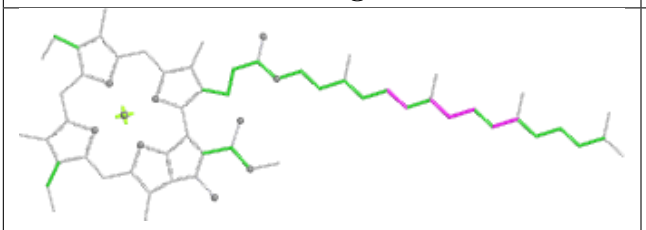

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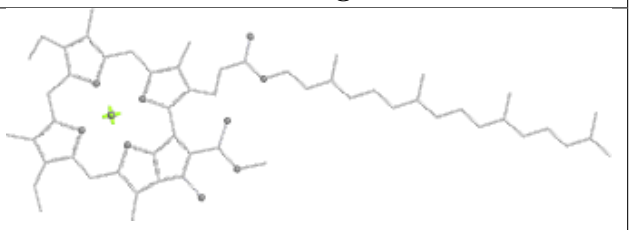

Rings

Ligand CLA b 616

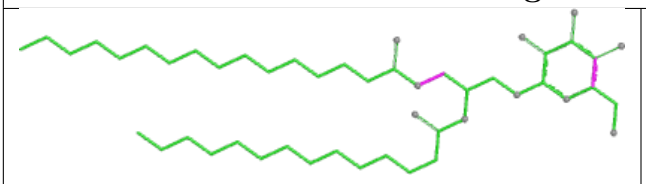

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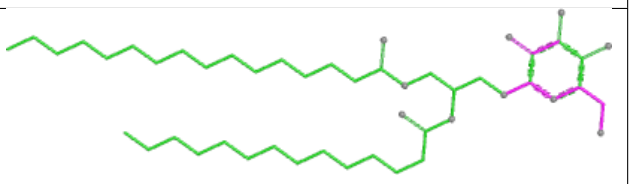

Bond angles

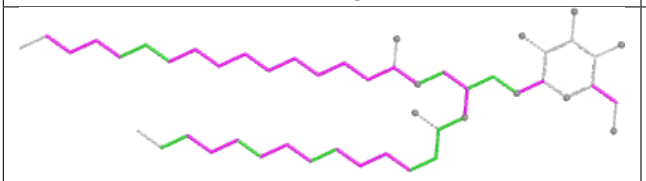

Torsions

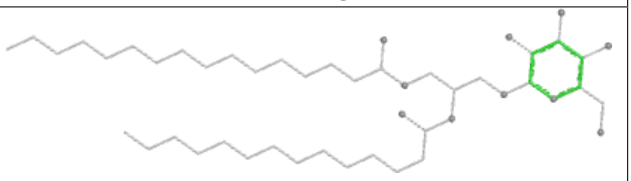

Rings

Ligand LMG a 414

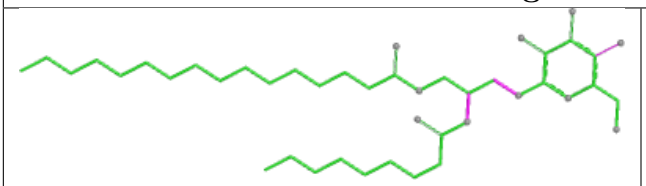

Bond lengths

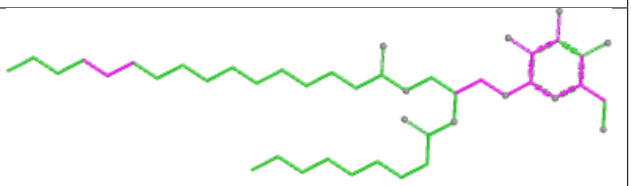

Bond angles

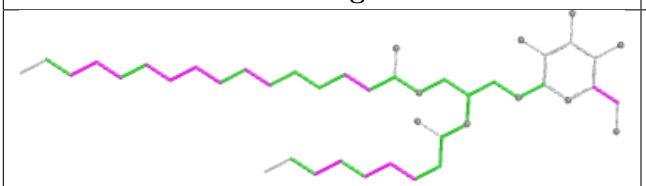

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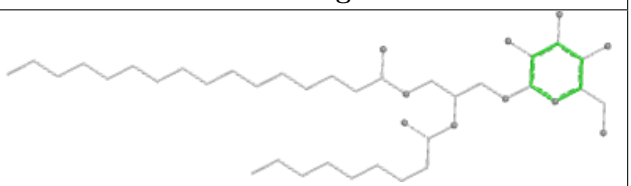

Rings

Ligand LMG d 409

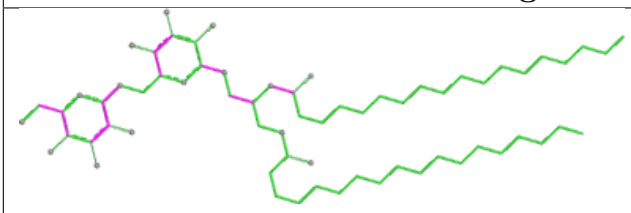

Bond lengths


Bond angles

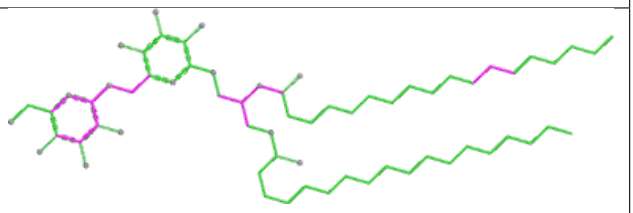

Torsions


Rings

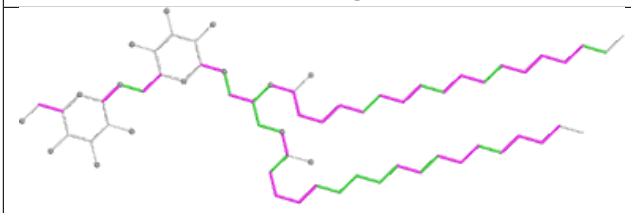
Ligand DGD A 413



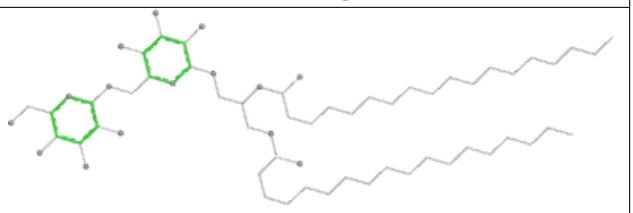
Bond lengths



Bond angles

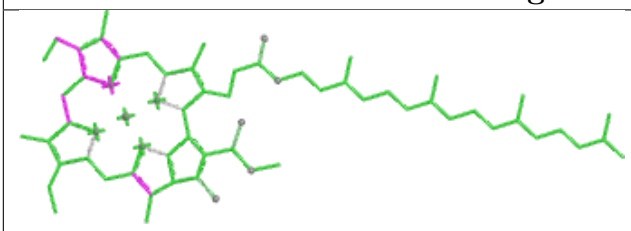


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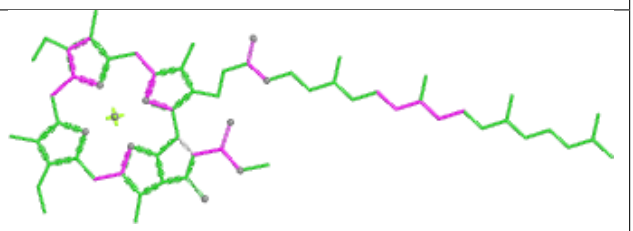


Rings

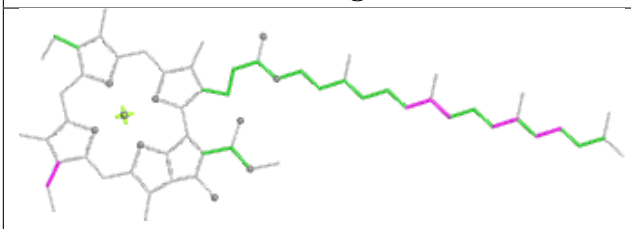
Ligand CLA b 609



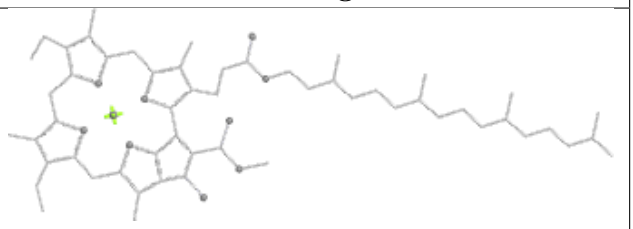
Bond lengths



Bond angles

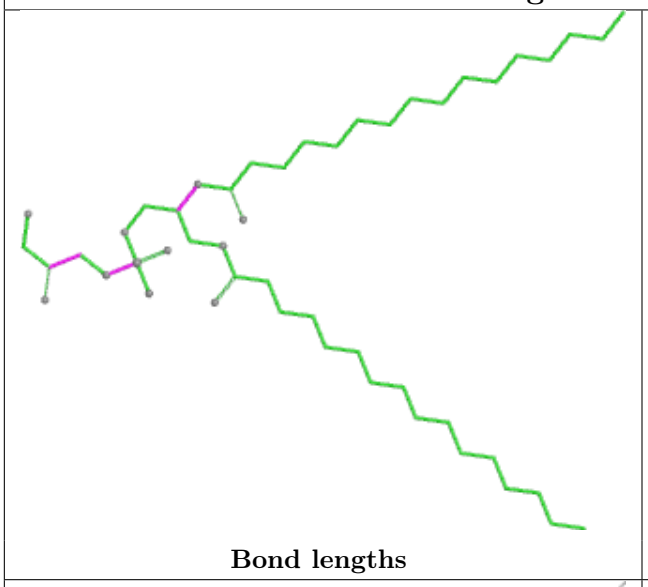


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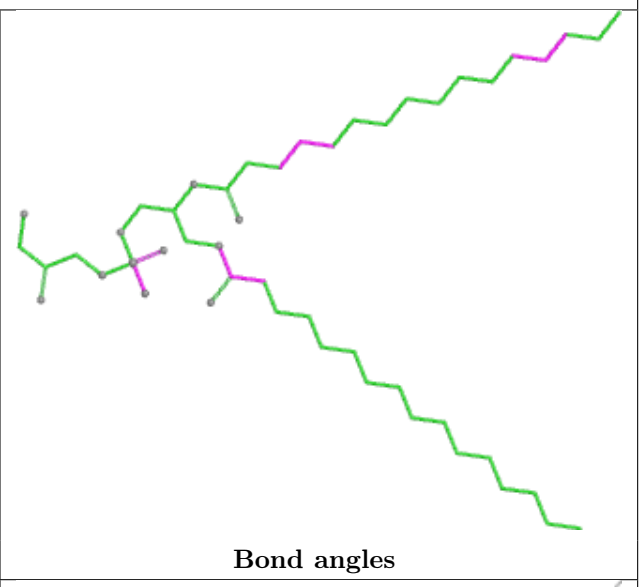


Rings

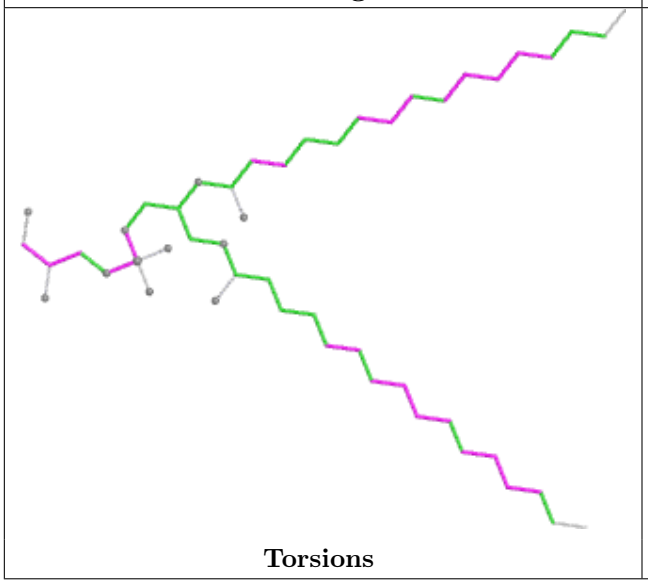
Ligand LHG d 407



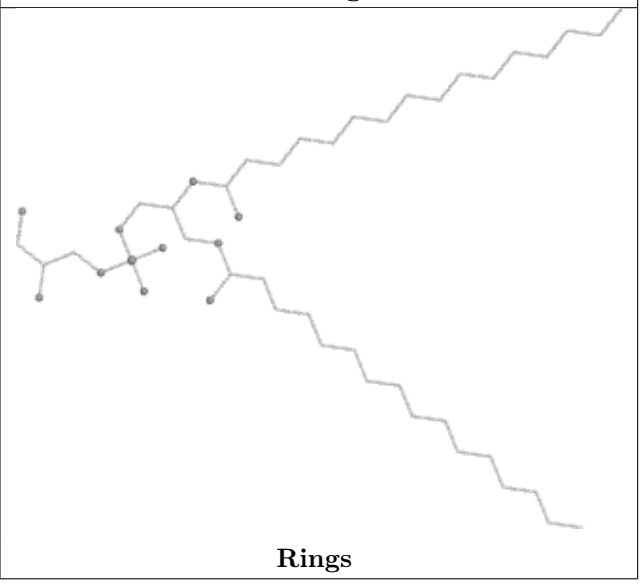
Bond lengths



Bond angles



Torsions



Rings

Ligand PL9 a 409



Bond lengths



Bond angles

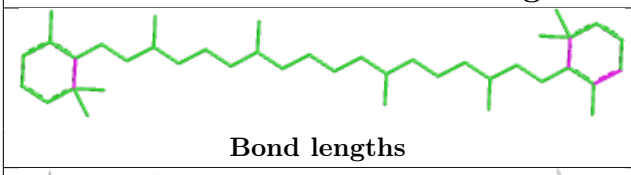


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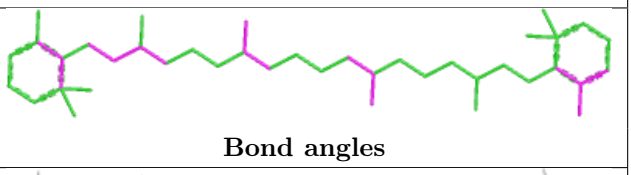


Rings

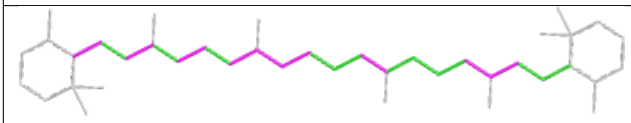
Ligand BCR T 101



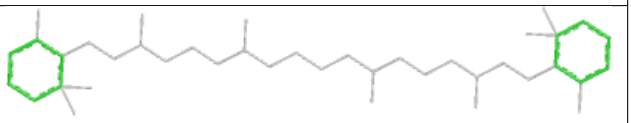
Bond lengths



Bond angles



Torsions

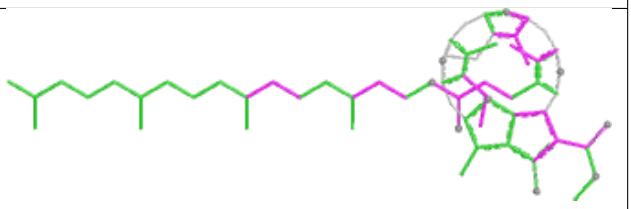


Rings

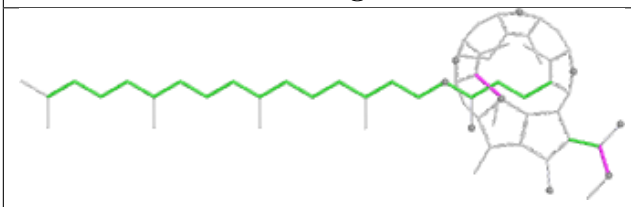
Ligand PHO d 401



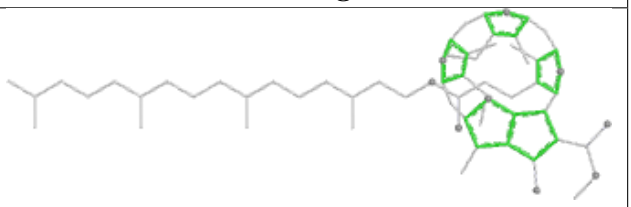
Bond lengths



Bond angles

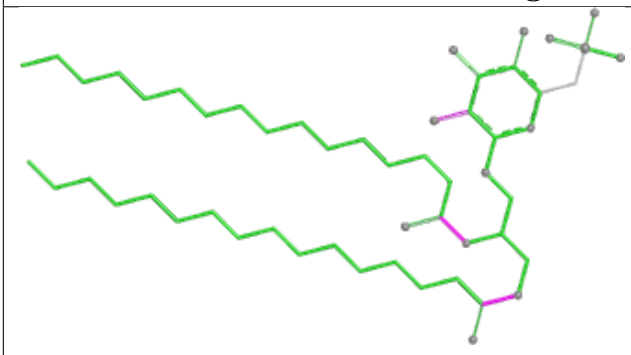


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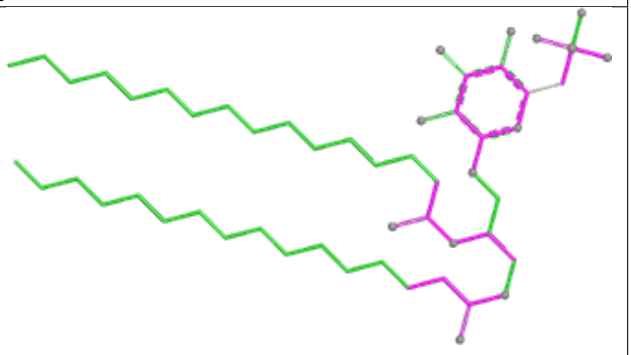


Rings

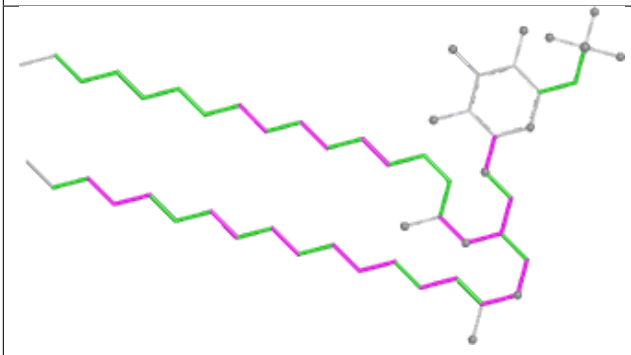
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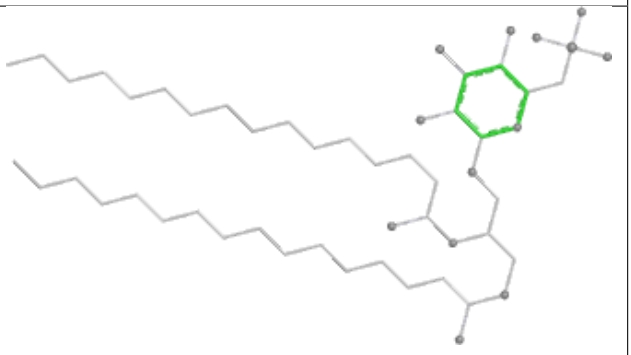
Bond lengths



Bond angles

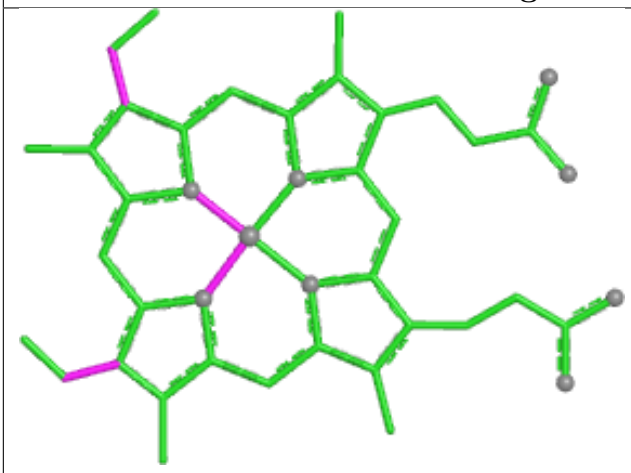


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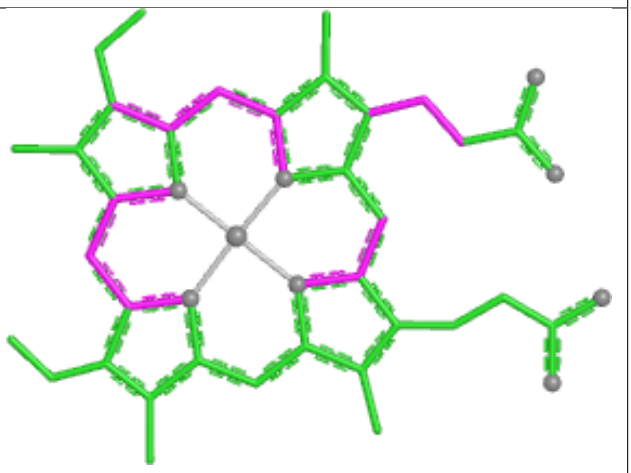


Rings

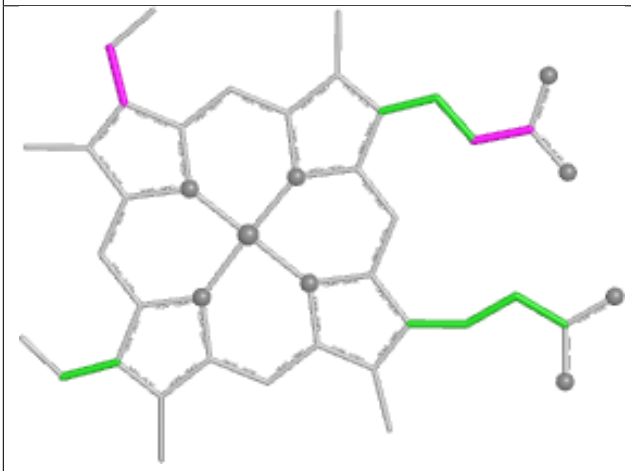
Ligand HEM E 102



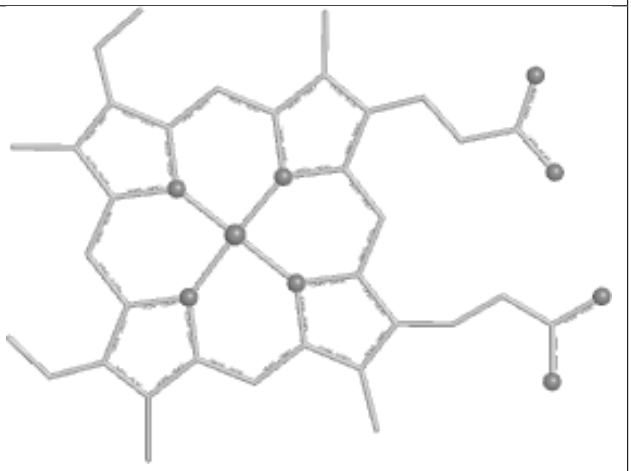
Bond lengths



Bond angles

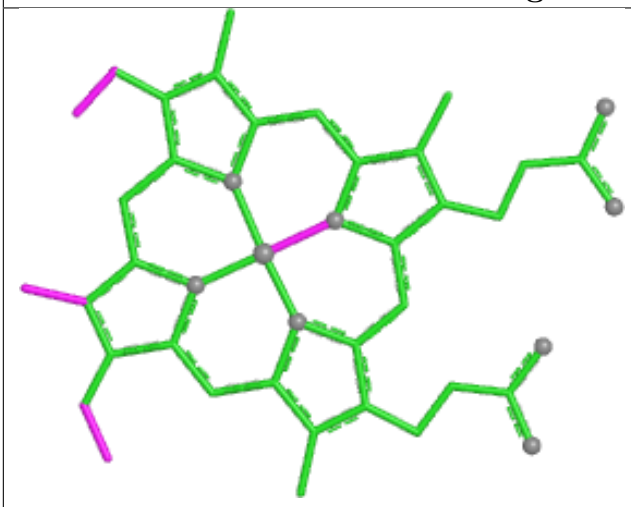


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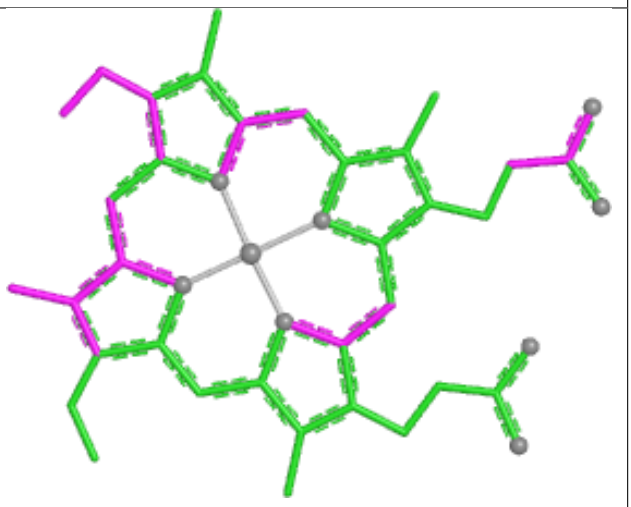


Rings

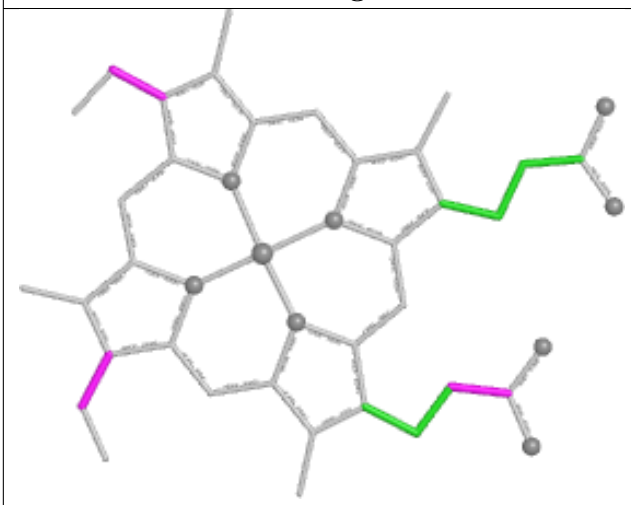
Ligand HEC v 201



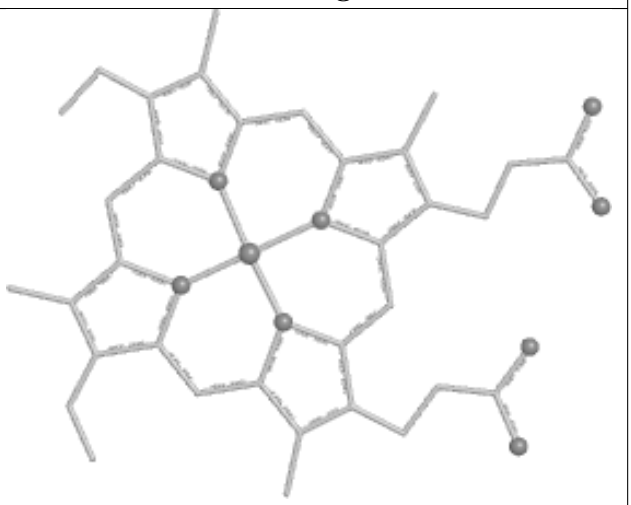
Bond lengths



Bond angles

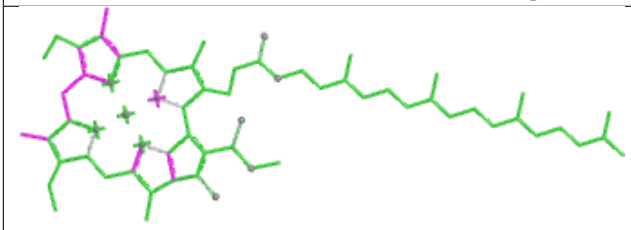


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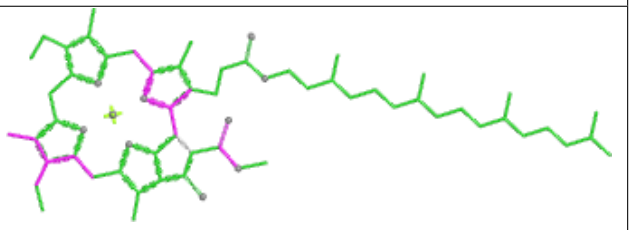


Rings

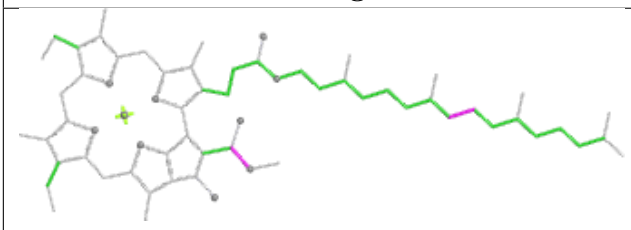
Ligand CLA C 511



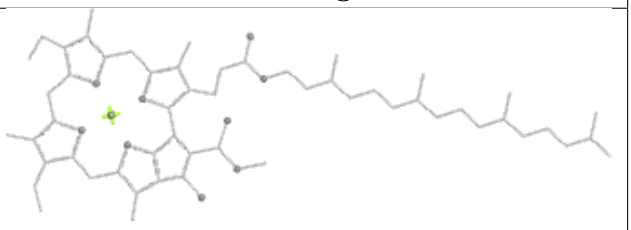
Bond lengths



Bond angles

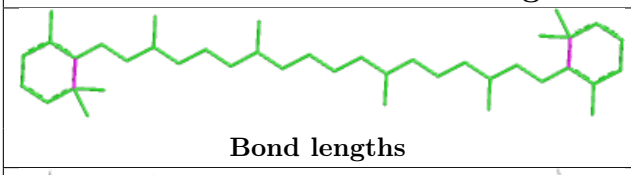


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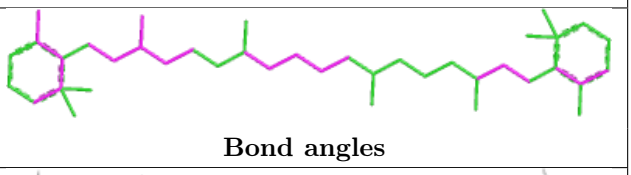


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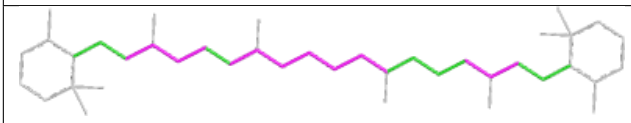
Ligand BCR C 514



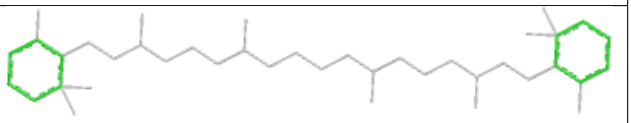
Bond lengths



Bond angles

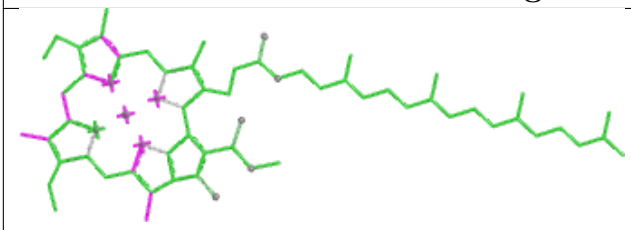


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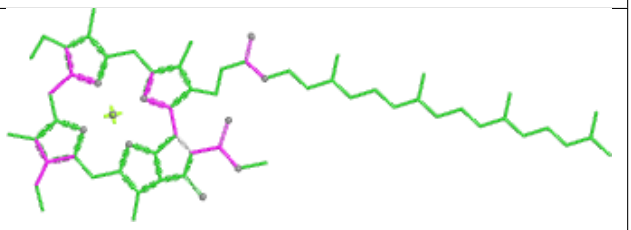


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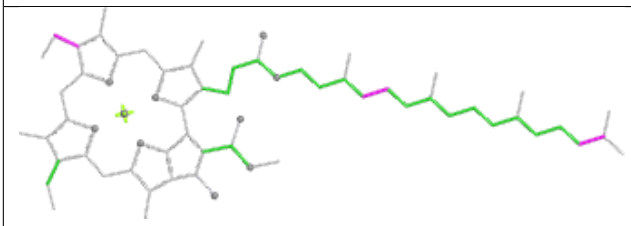
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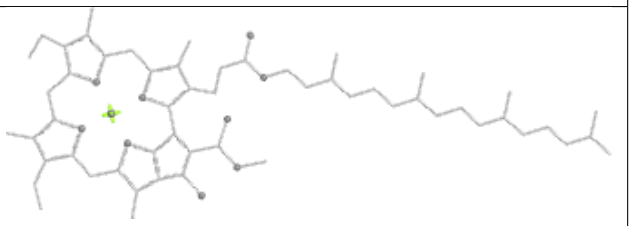
Bond lengths



Bond angles

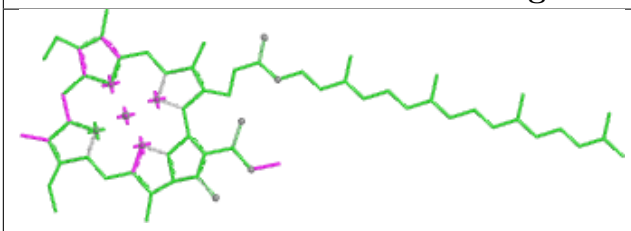


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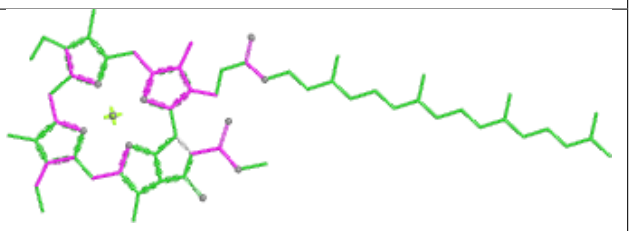


Rings

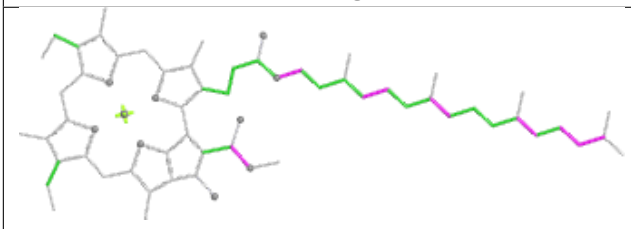
Ligand CLA a 404



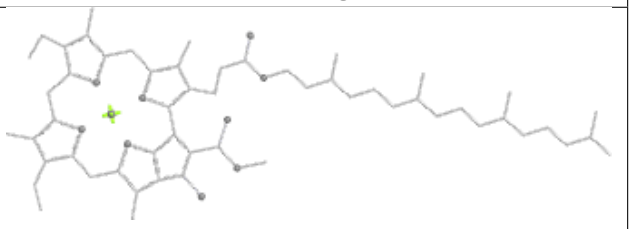
Bond lengths



Bond angles

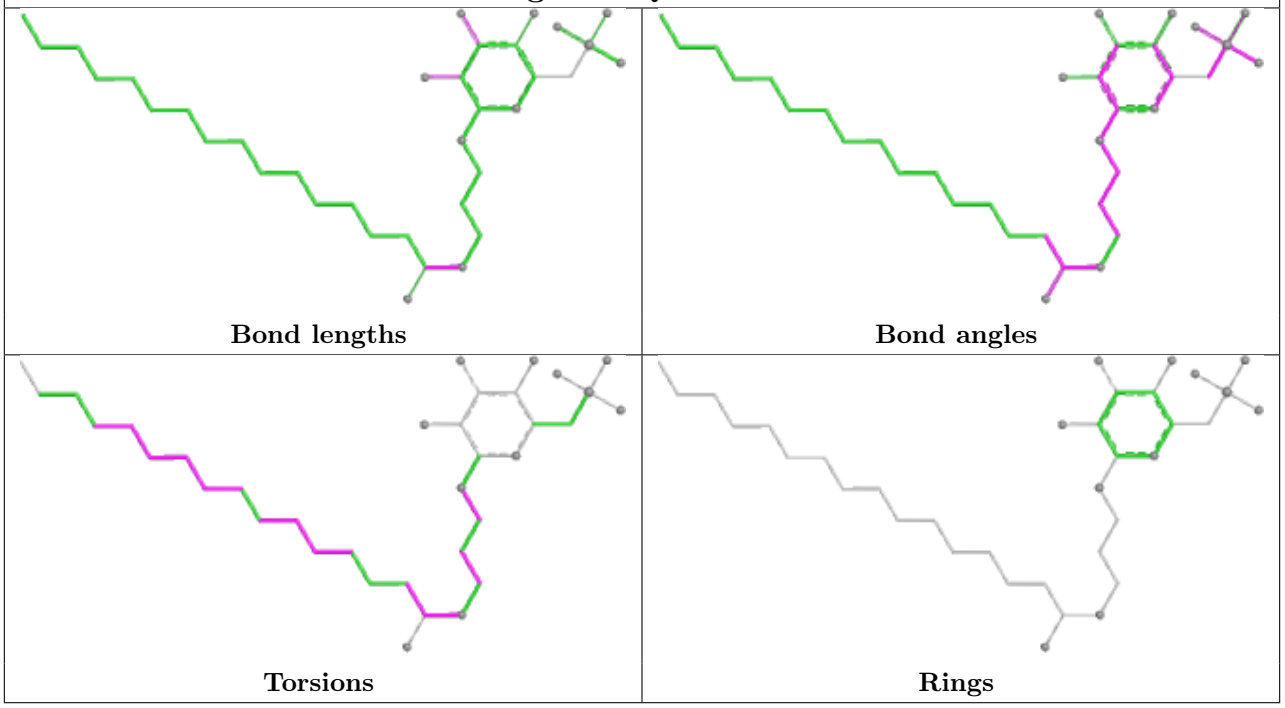


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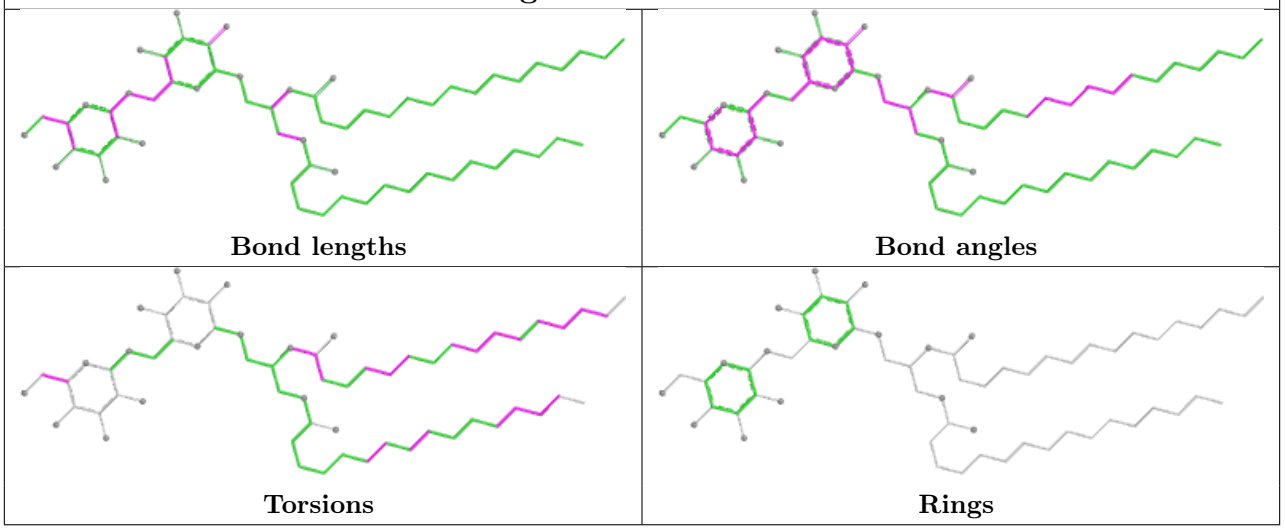


Rings

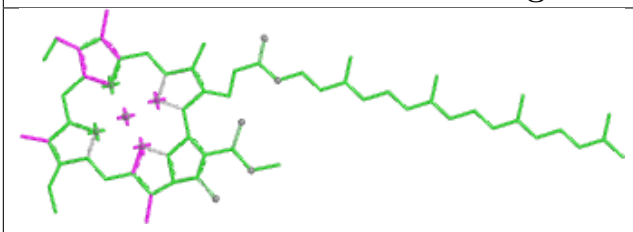
Ligand SQD F 101



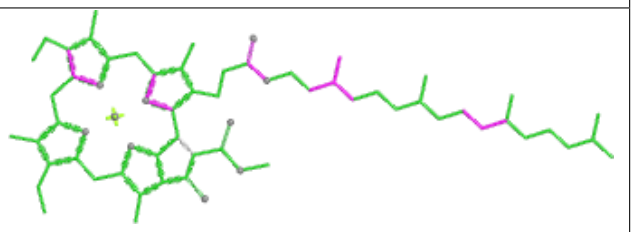
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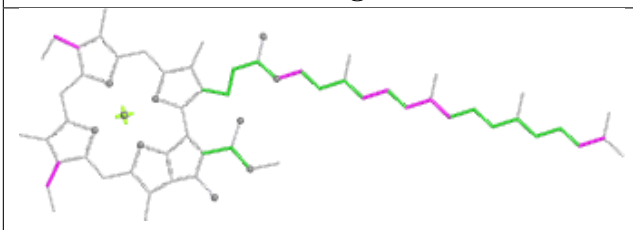
Ligand CLA d 403



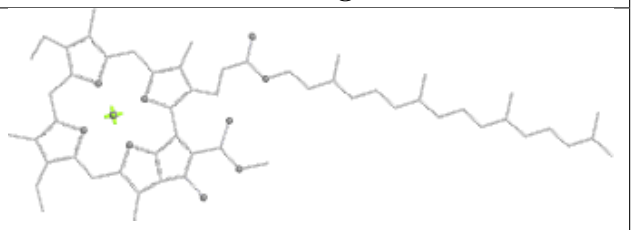
Bond lengths



Bond angles

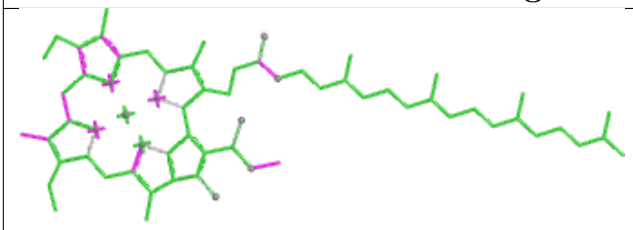


Torsions

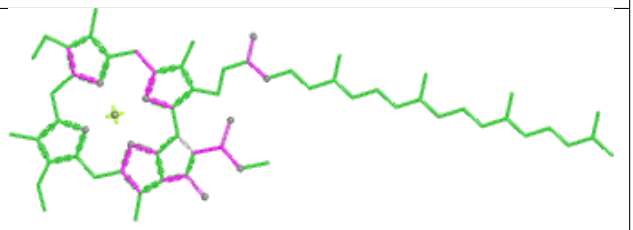


Rings

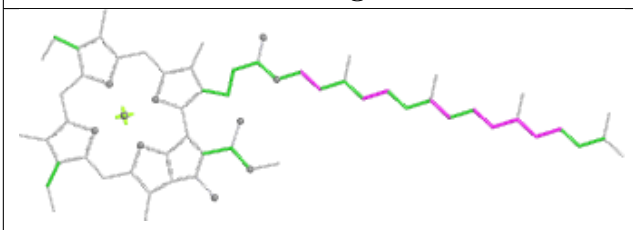
Ligand CLA B 604



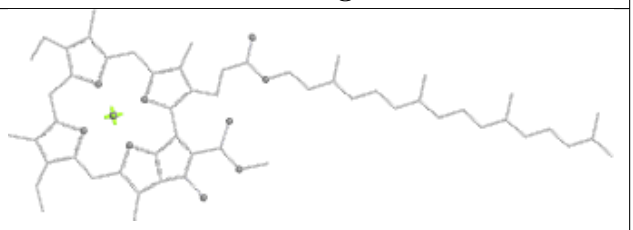
Bond lengths



Bond angles

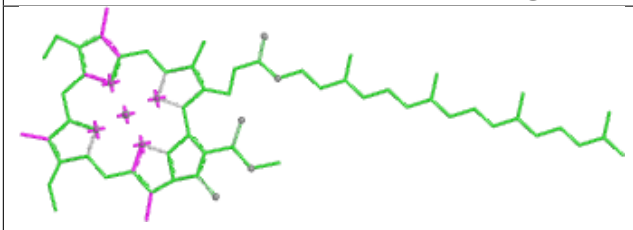


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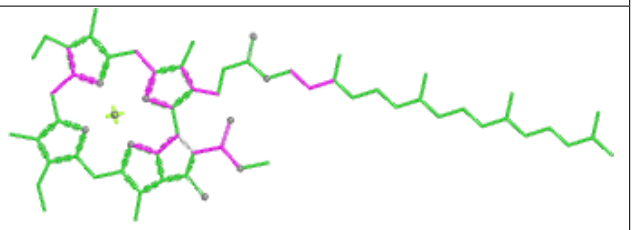


Rings

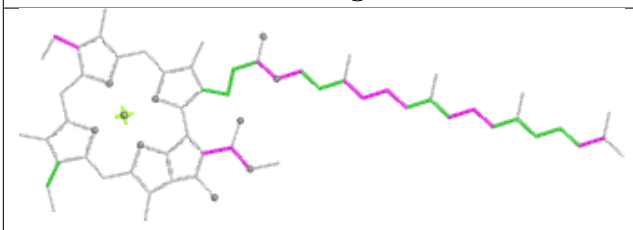
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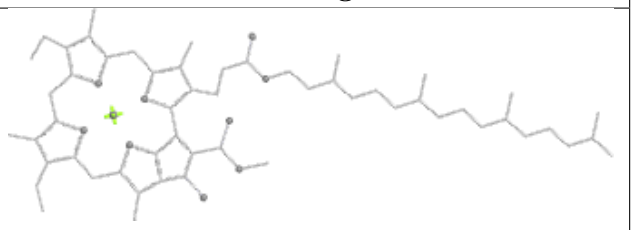
Bond lengths



Bond angles

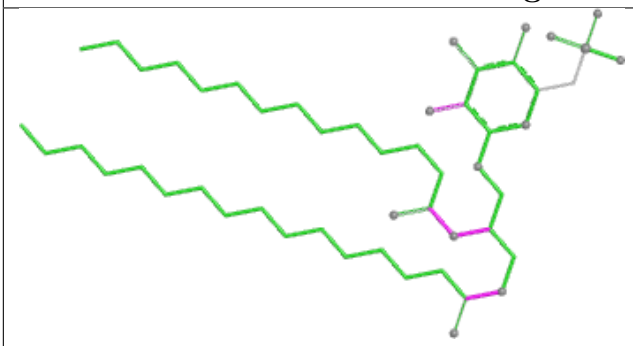


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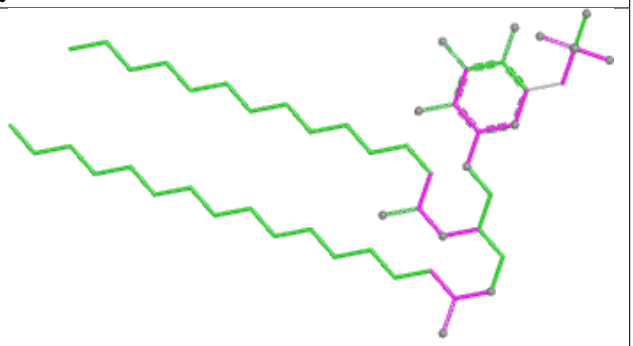


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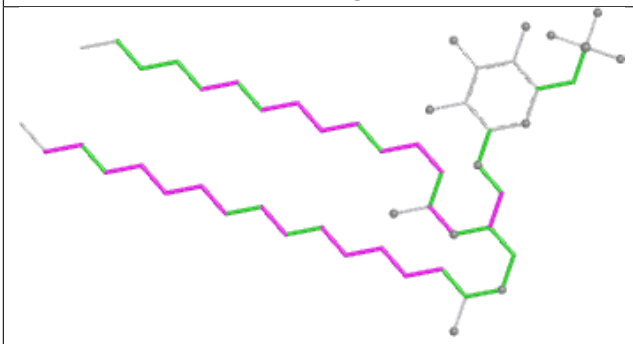
Ligand SQD A 411



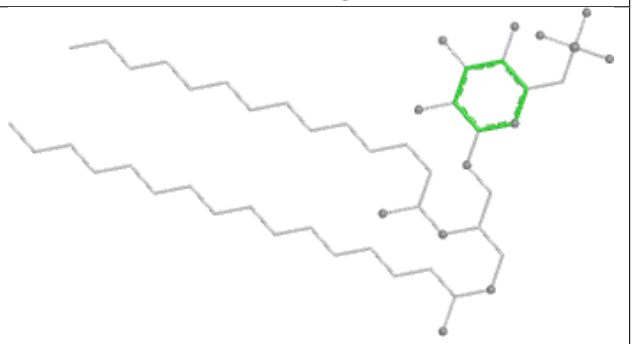
Bond lengths



Bond angles



Torsions

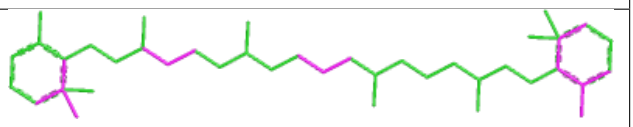


Rings

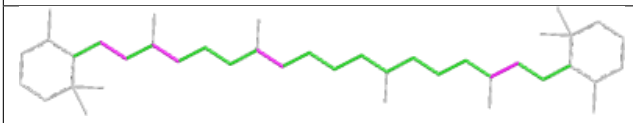
Ligand BCR b 620



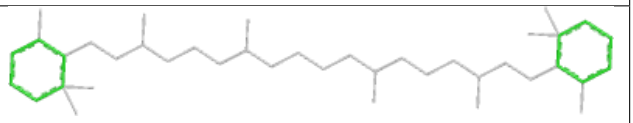
Bond lengths



Bond angles

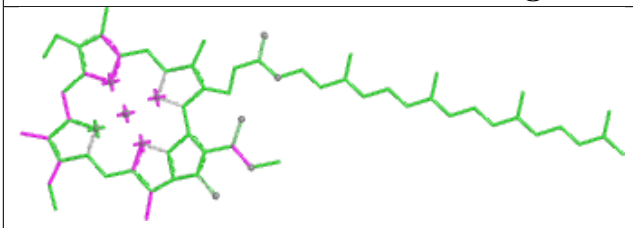


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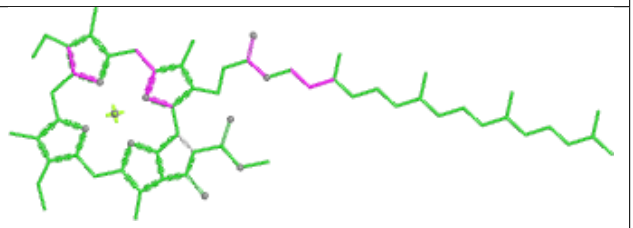


Rings

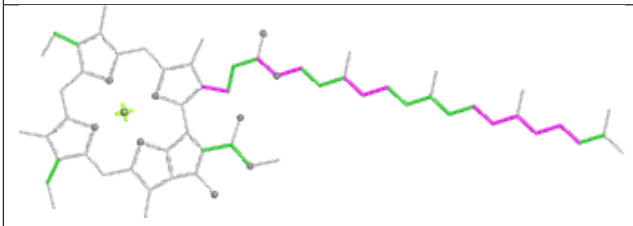
Ligand CLA C 506



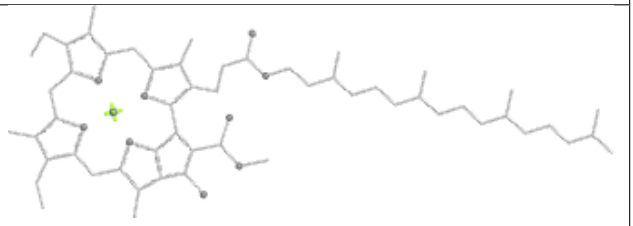
Bond lengths



Bond angles

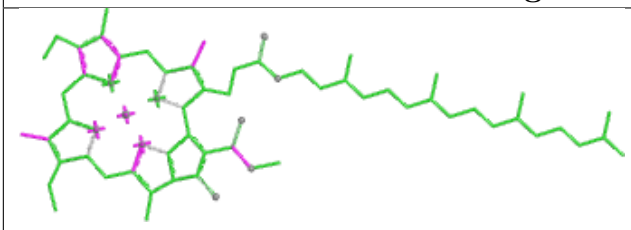


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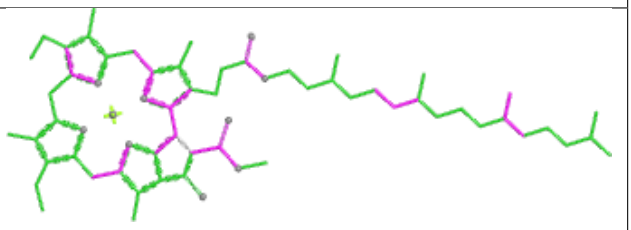


Rings

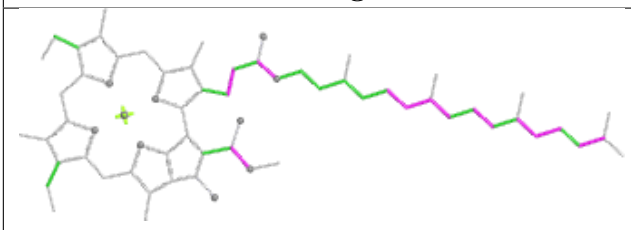
Ligand CLA B 603



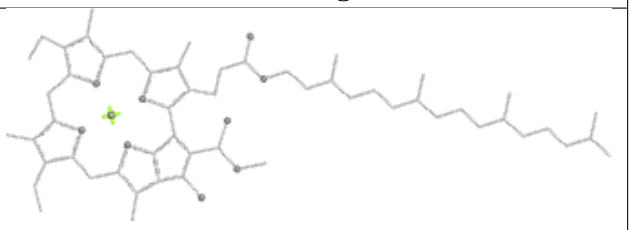
Bond lengths



Bond angles

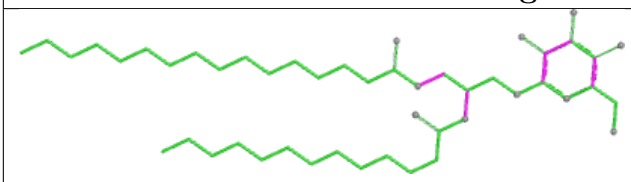


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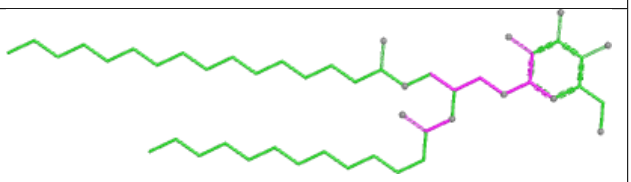


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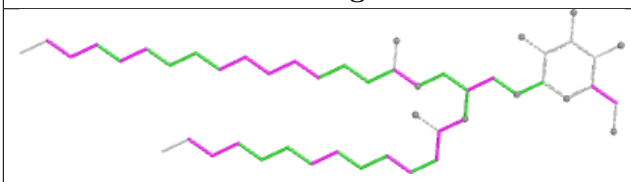
Ligand LMG C 519



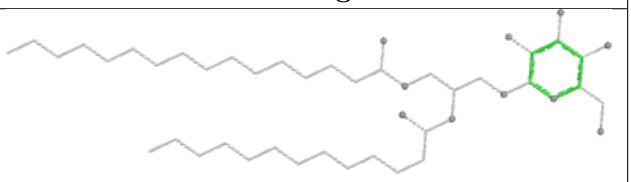
Bond lengths



Bond angles



Torsions

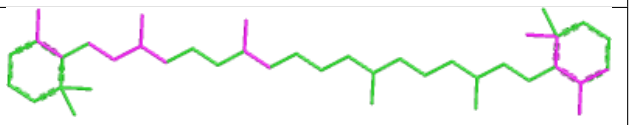


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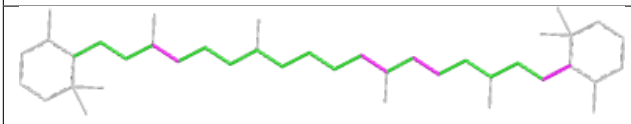
Ligand BCR h 102



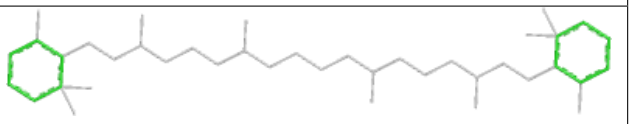
Bond lengths



Bond angles

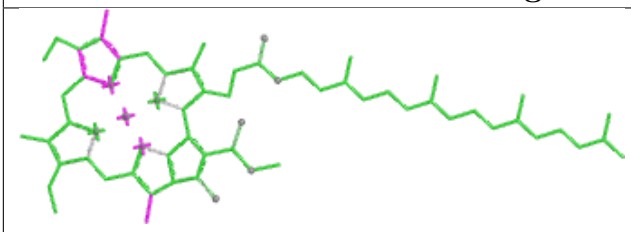


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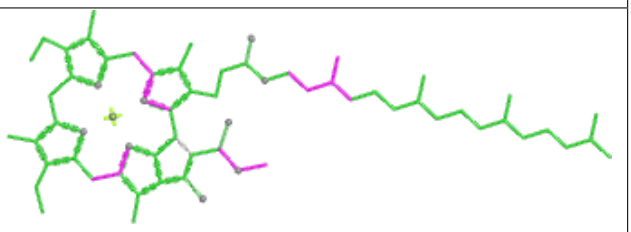


Rings

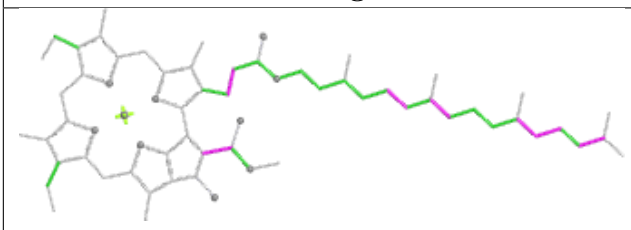
Ligand CLA C 509



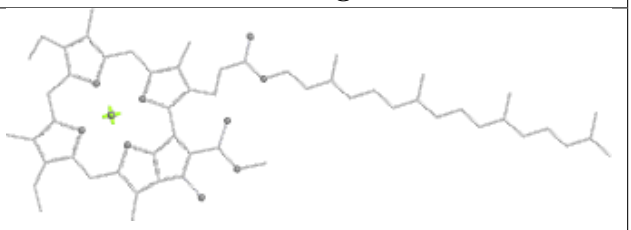
Bond lengths



Bond angles

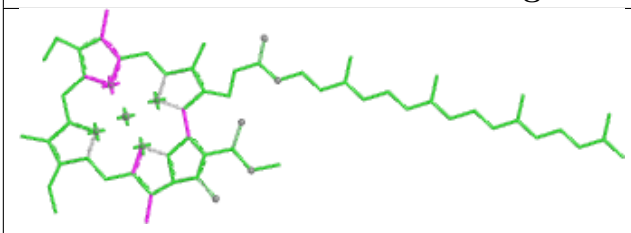


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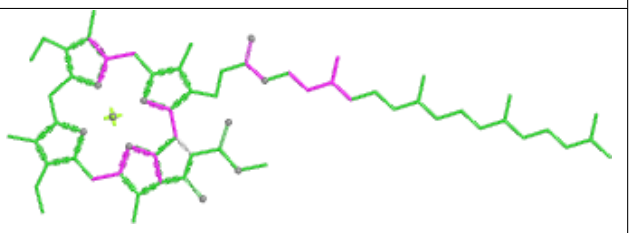


Rings

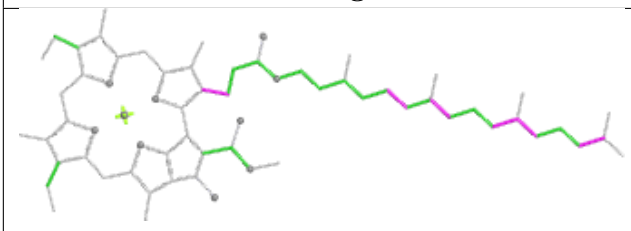
Ligand CLA D 404



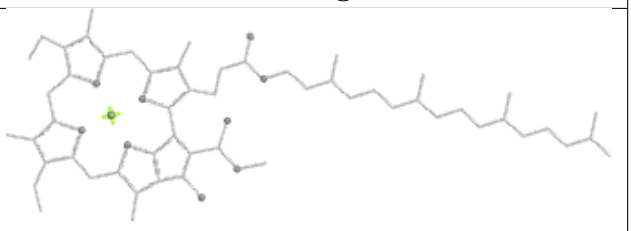
Bond lengths



Bond angles

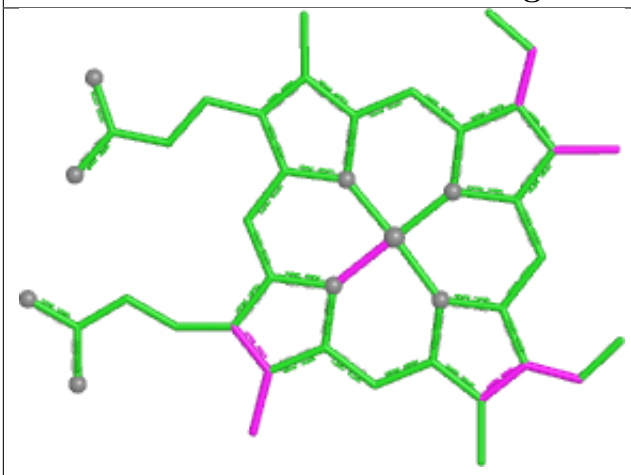


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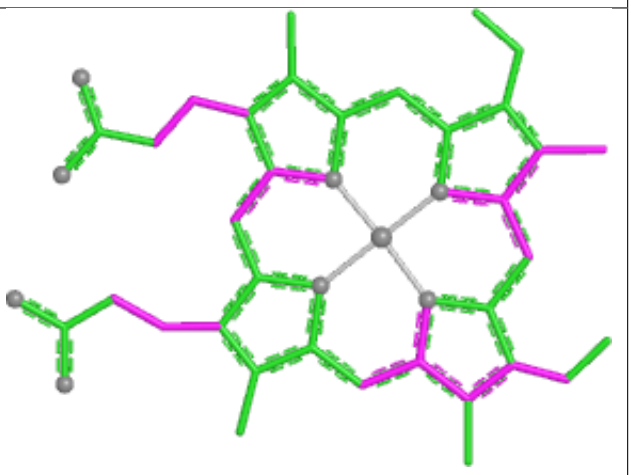


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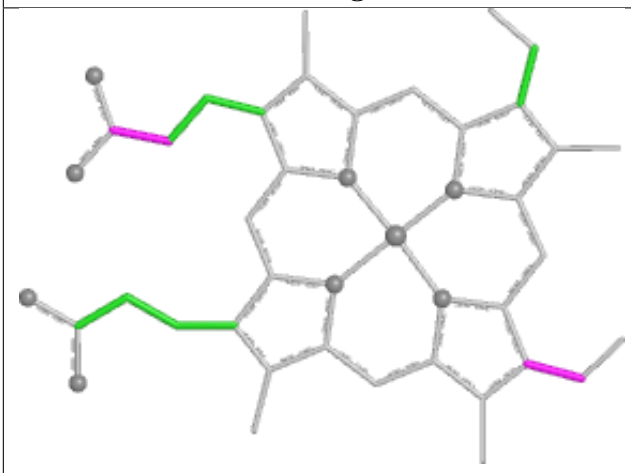
Ligand HEM e 102



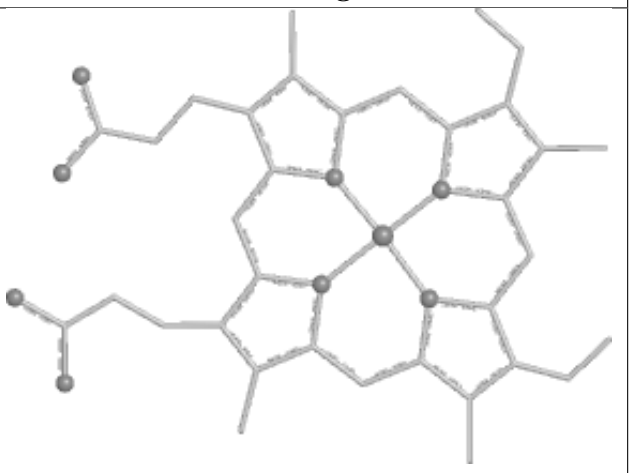
Bond lengths



Bond angles

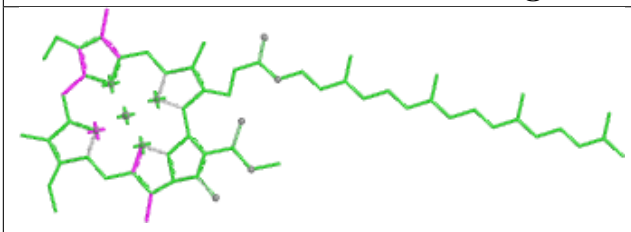


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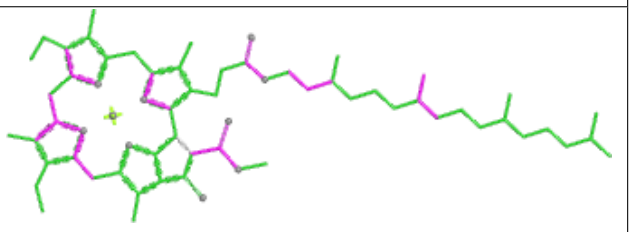


Rings

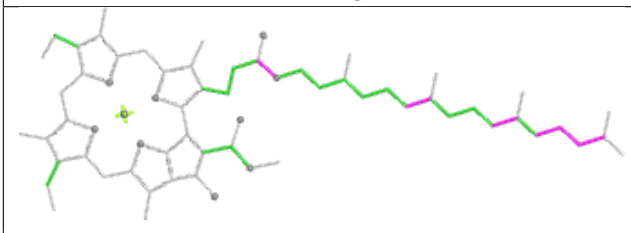
Ligand CLA B 611



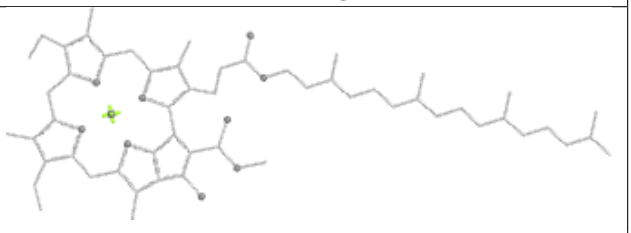
Bond lengths



Bond angles

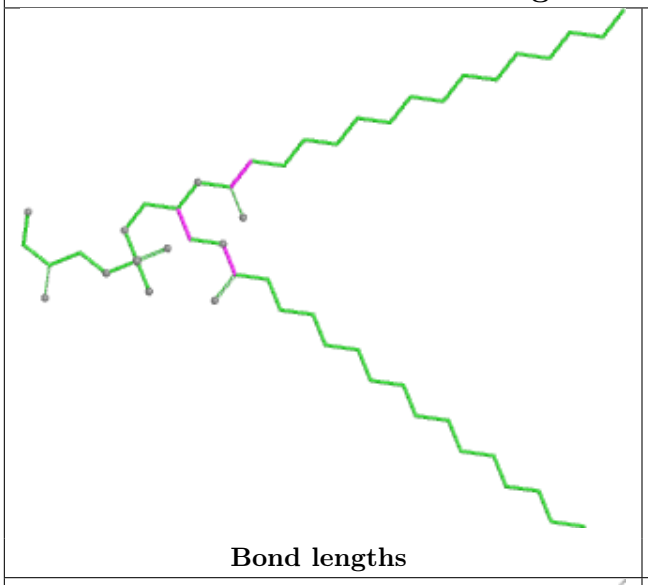


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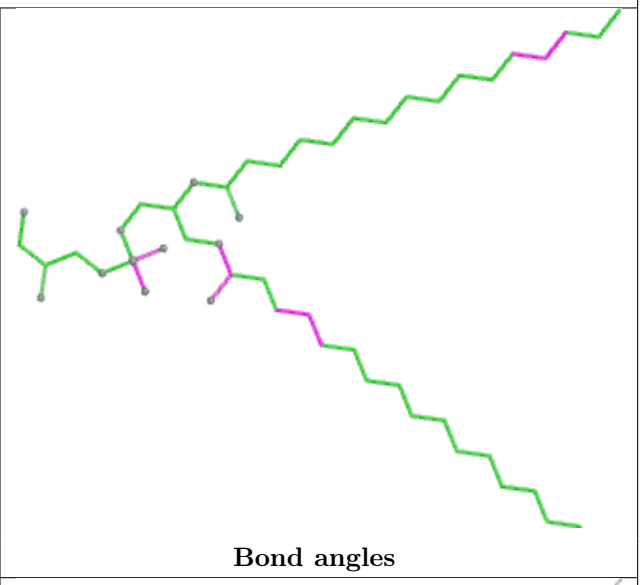


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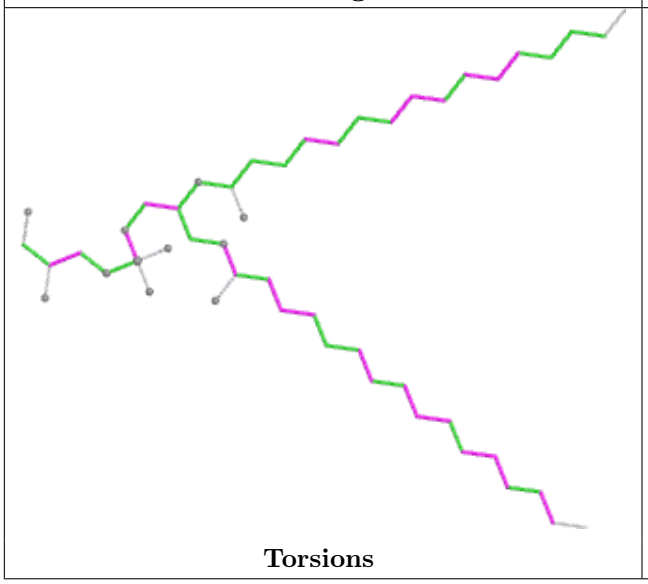
Ligand LHG l 101



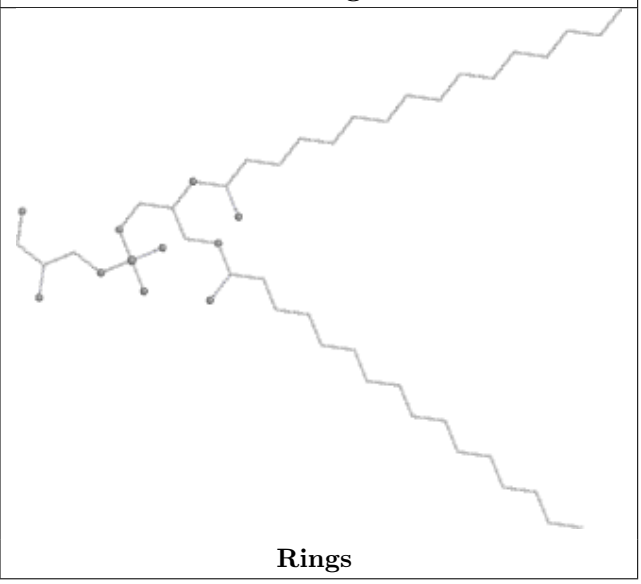
Bond lengths



Bond angles

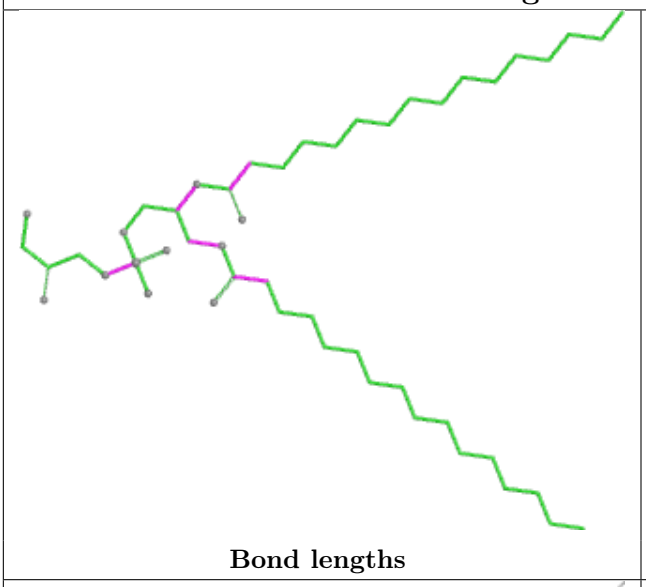


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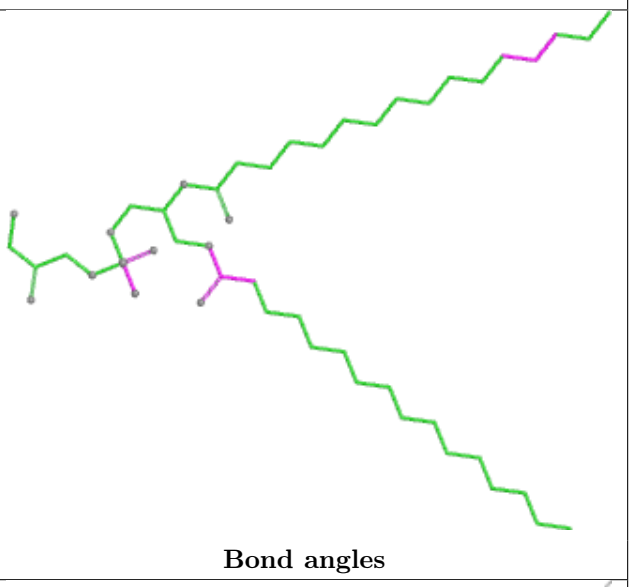


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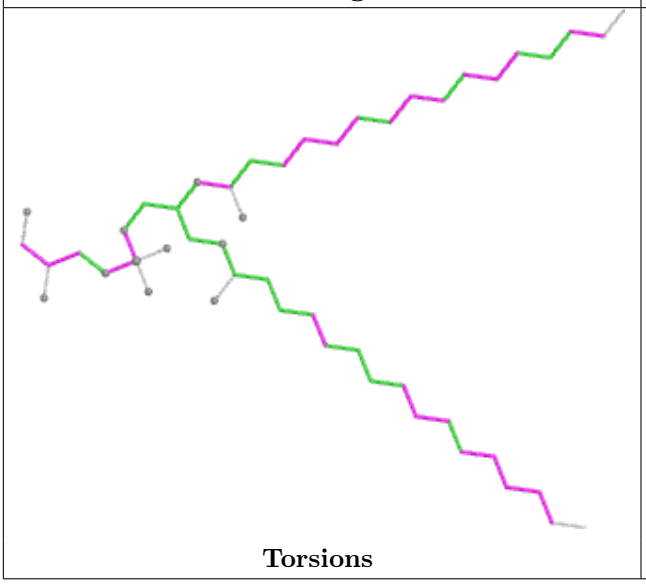
Ligand LHG D 408



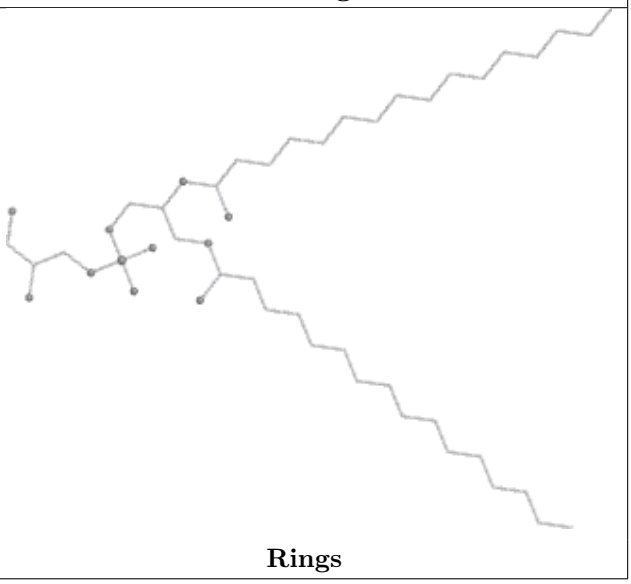
Bond lengths



Bond angles

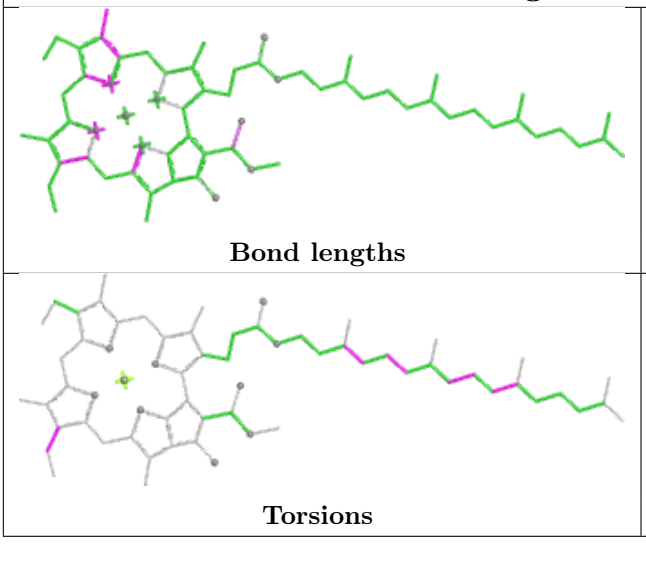


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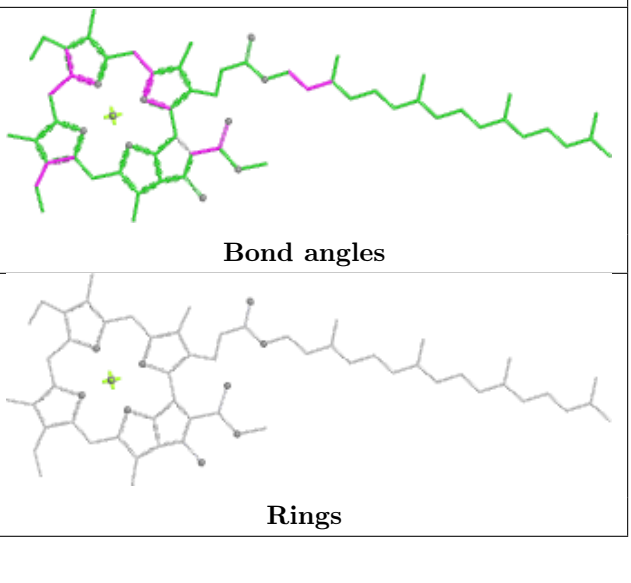


Rings

Ligand CLA C 505



Bond lengths

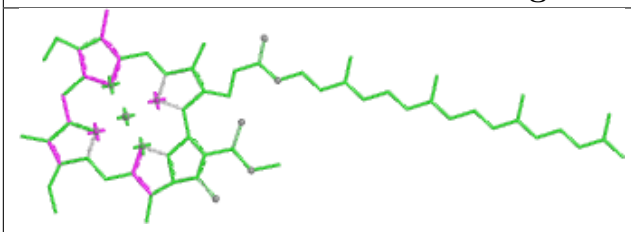


Bond angles

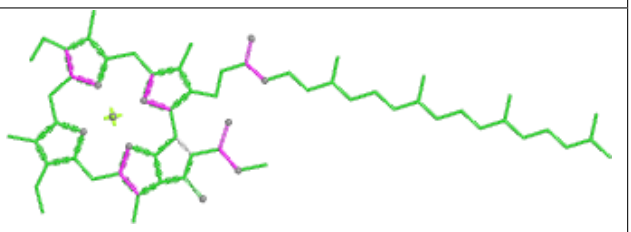
Torsions

Rings

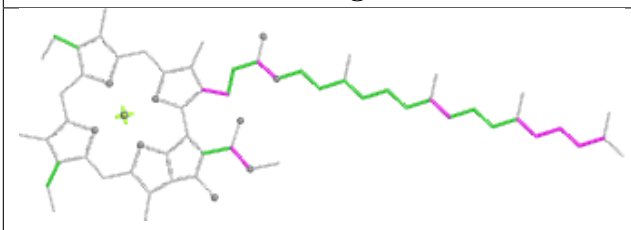
Ligand CLA c 511



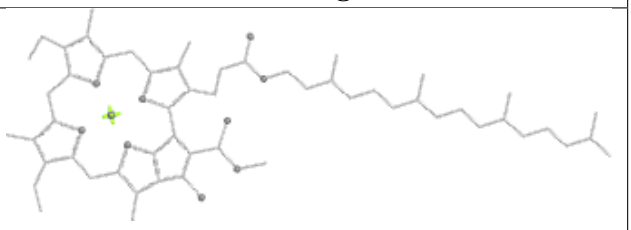
Bond lengths



Bond angles



Torsions

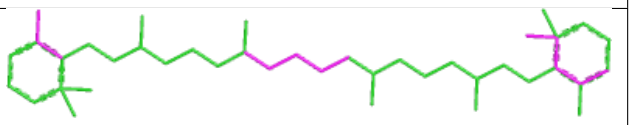


Rings

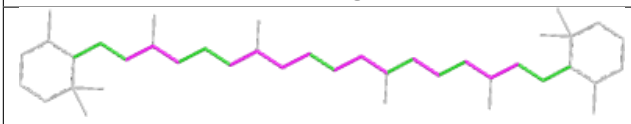
Ligand BCR c 514



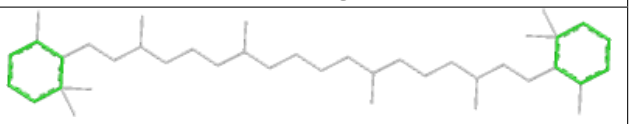
Bond lengths



Bond angles

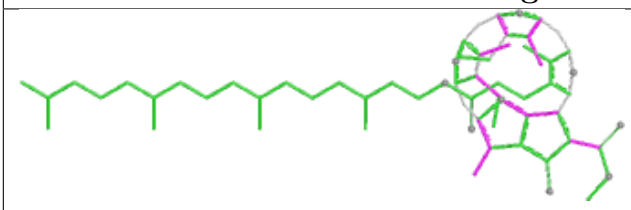


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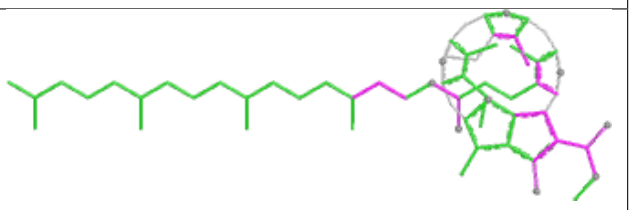


Rings

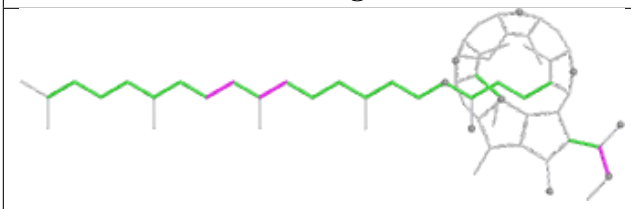
Ligand PHO D 401



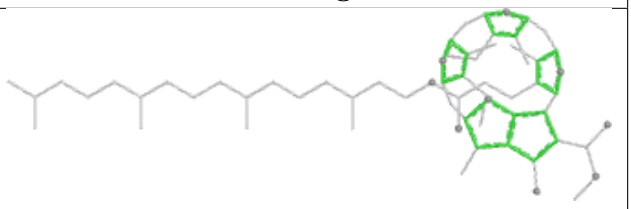
Bond lengths



Bond angles

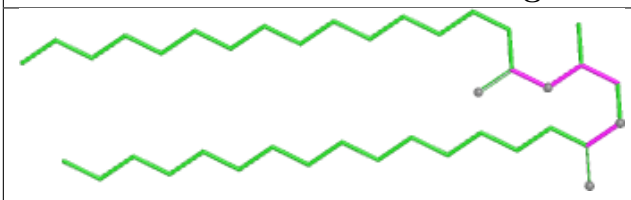


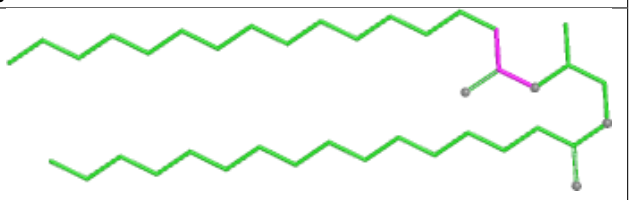
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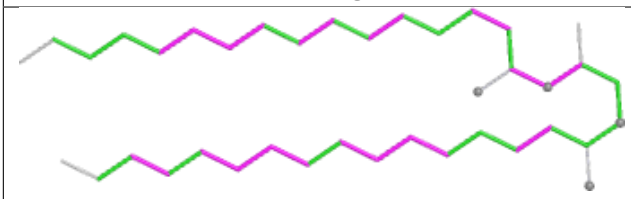


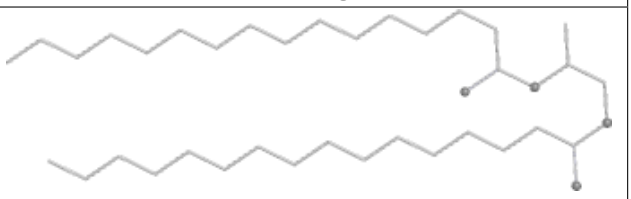
Rings

Ligand SQD A 412

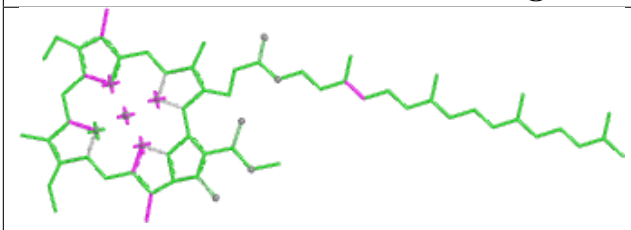

Bond lengths

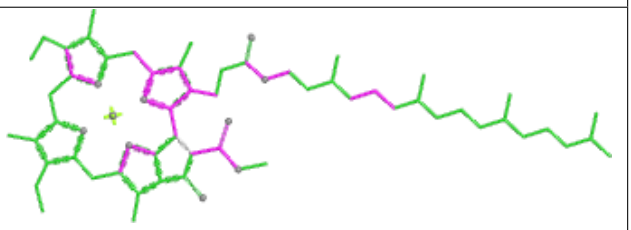

Bond angles

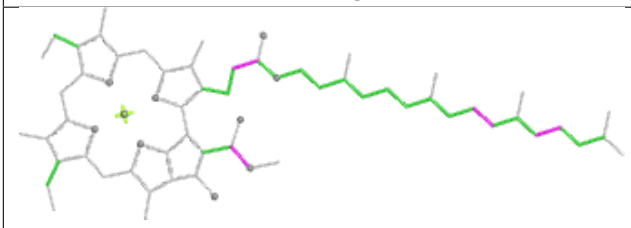

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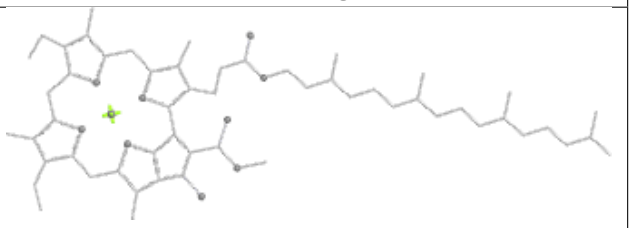

Rings

Ligand CLA b 614

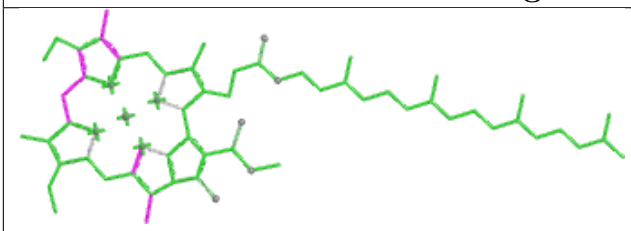

Bond lengths

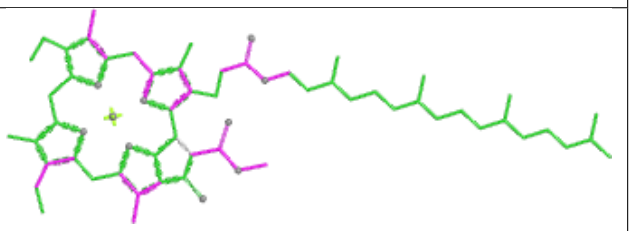

Bond angles

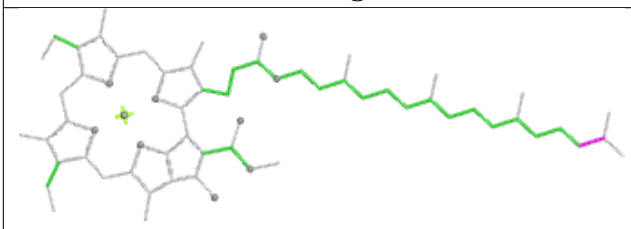

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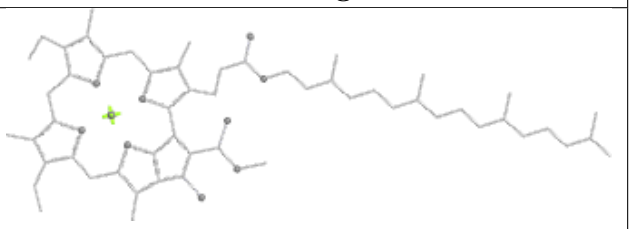

Rings

Ligand CLA A 405

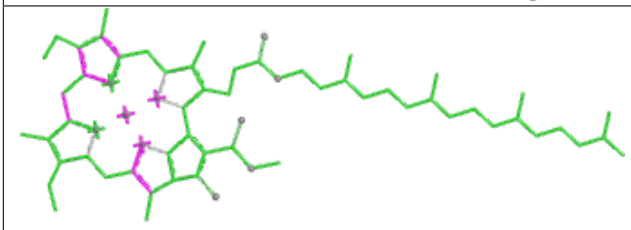

Bond lengths


Bond angles

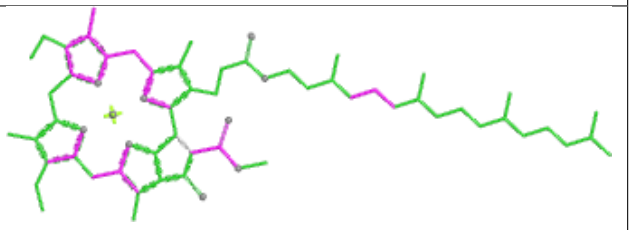

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Rings

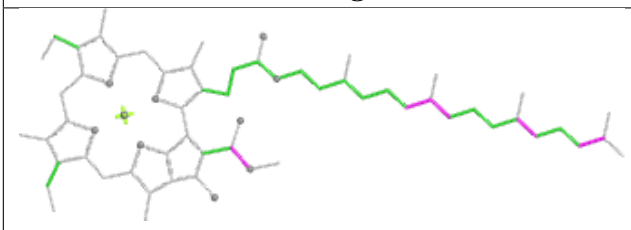
Ligand CLA C 508



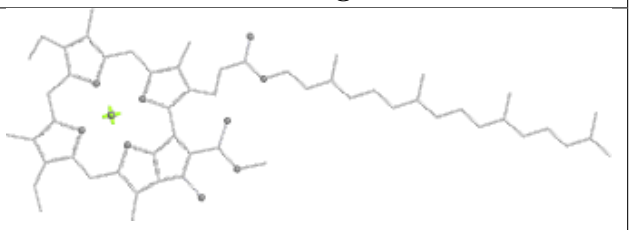
Bond lengths



Bond angles

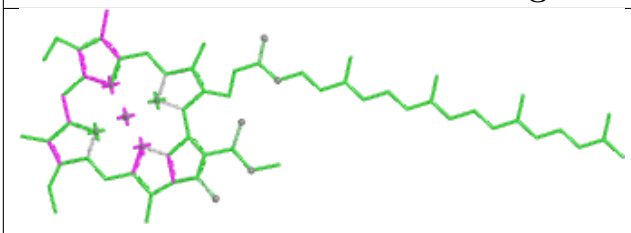


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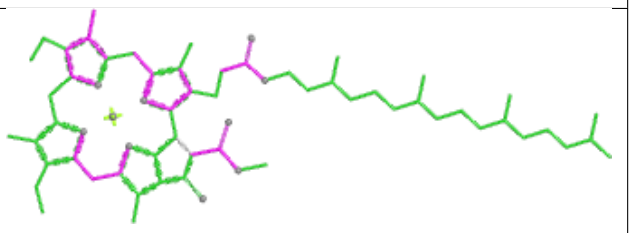


Rings

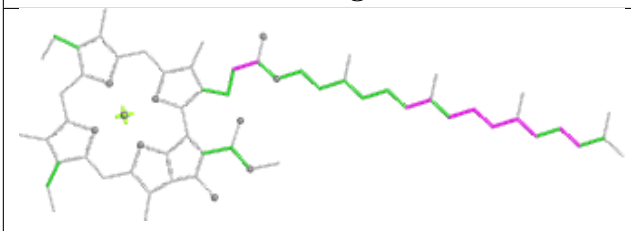
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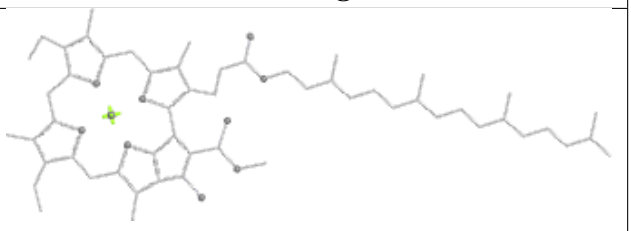
Bond lengths



Bond angles

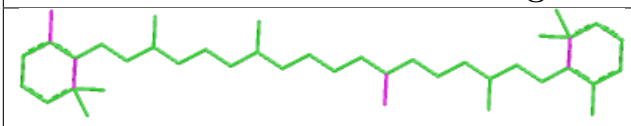


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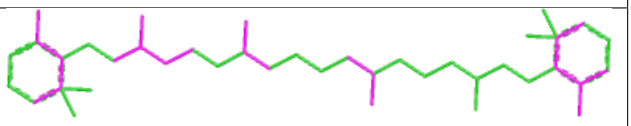


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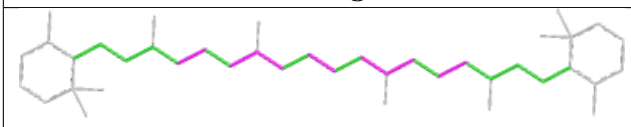
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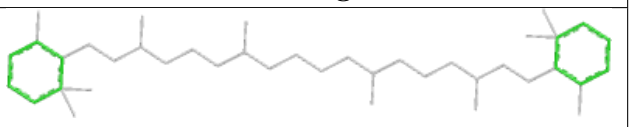
Bond lengths



Bond angles

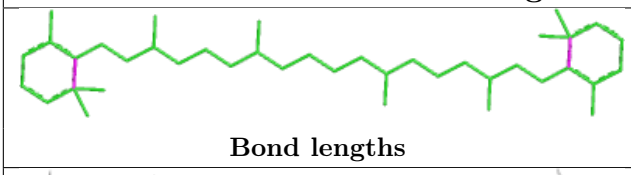


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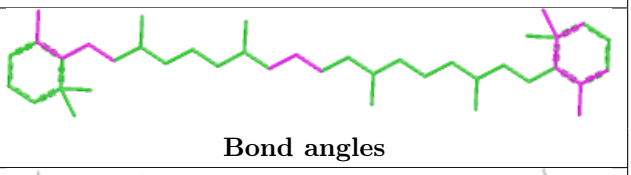


Rings

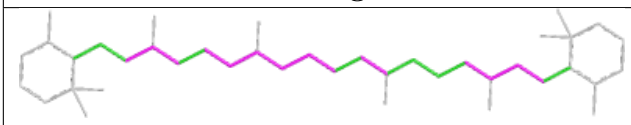
Ligand BCR d 405



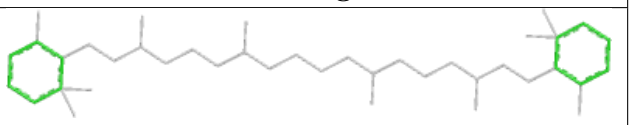
Bond lengths



Bond angles

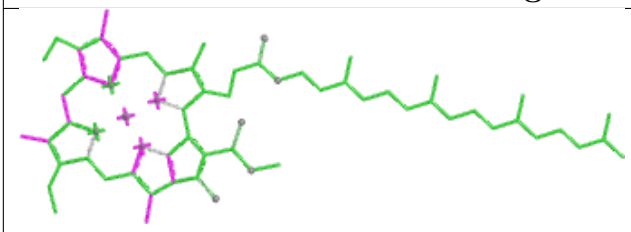


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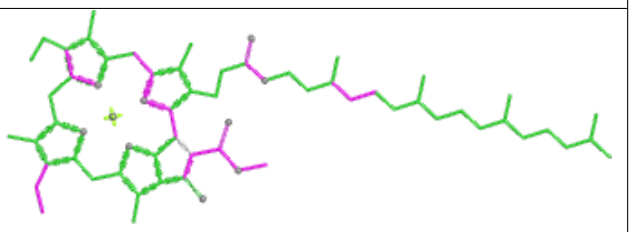


Rings

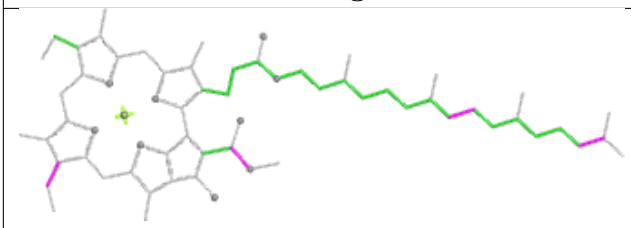
Ligand CLA B 610



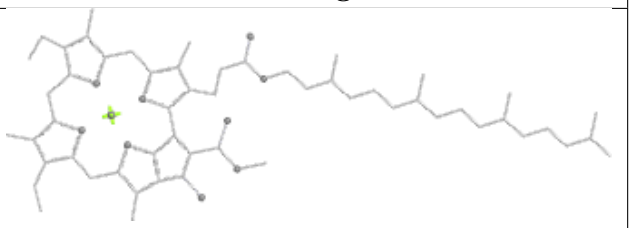
Bond lengths



Bond angles

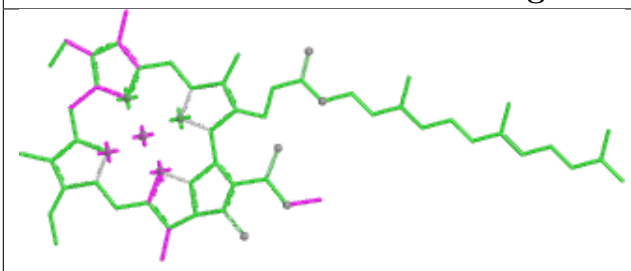


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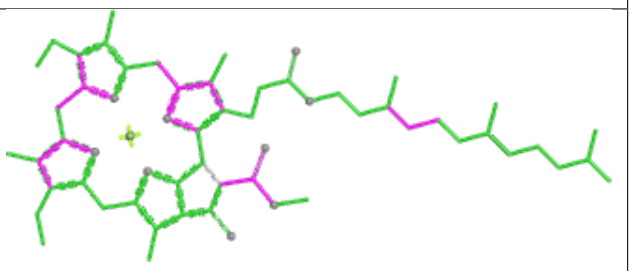


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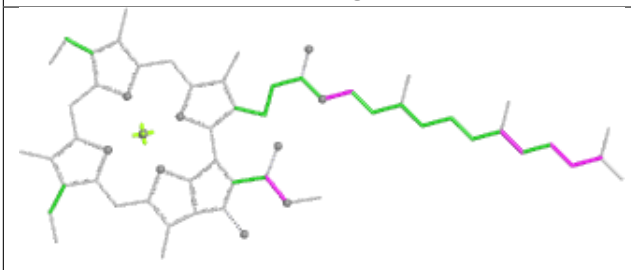
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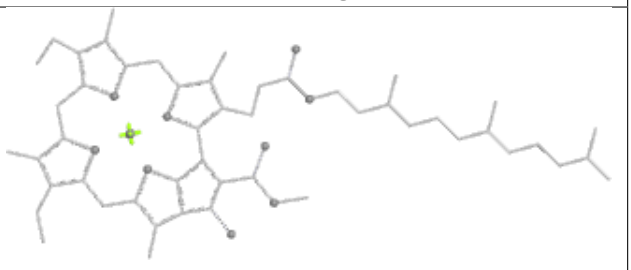
Bond lengths



Bond angles

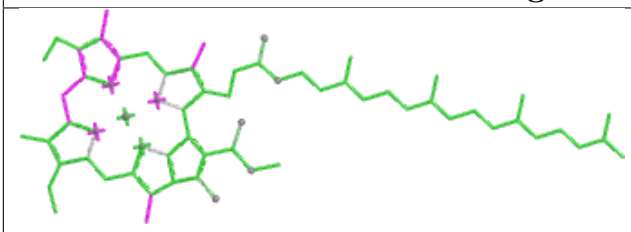


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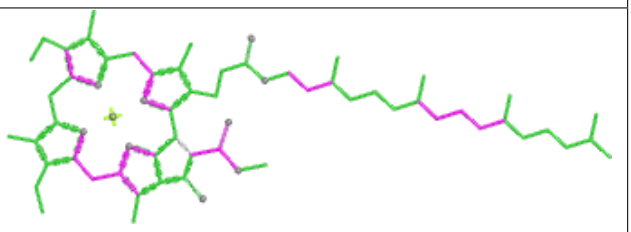


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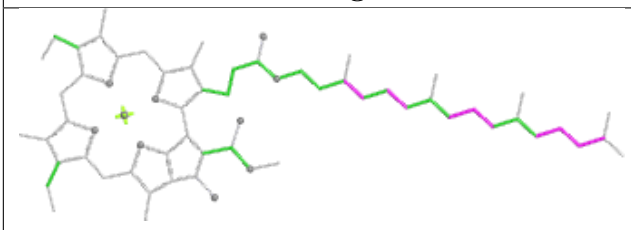
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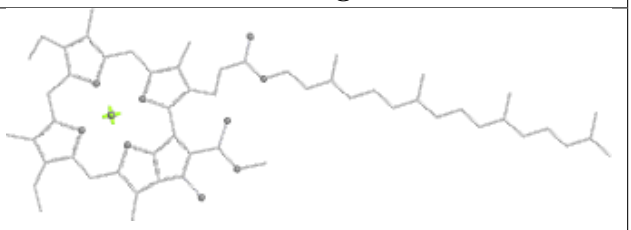
Bond lengths



Bond angles

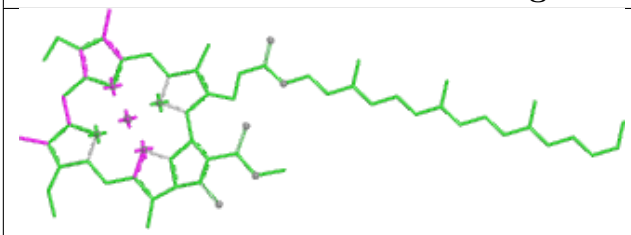


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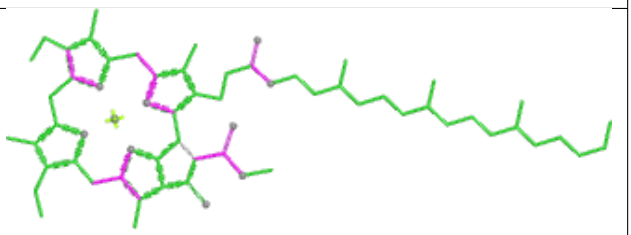


Rings

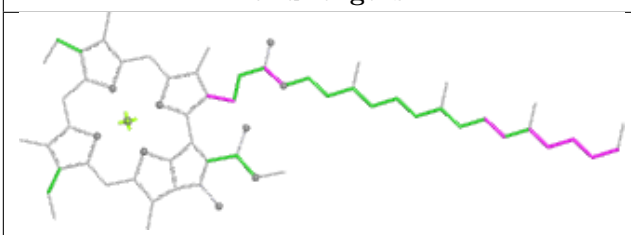
Ligand CLA c 508



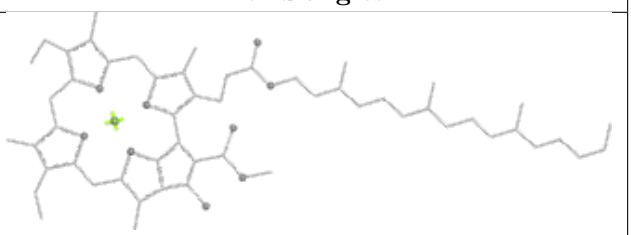
Bond lengths



Bond angles

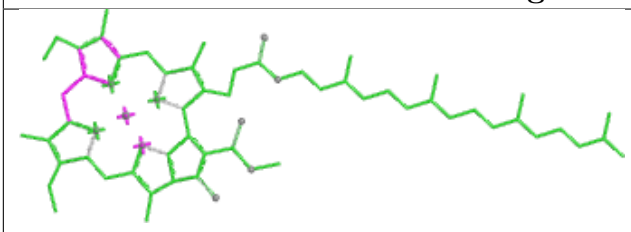


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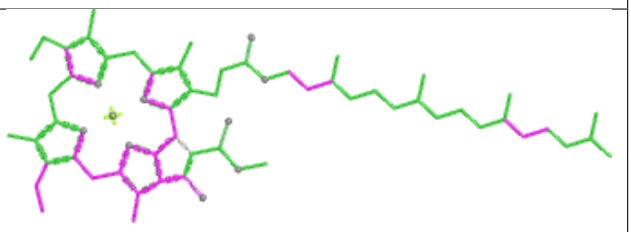


Rings

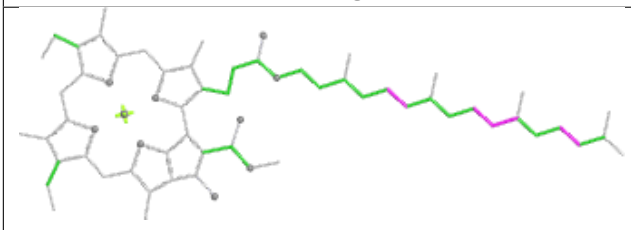
Ligand CLA b 606



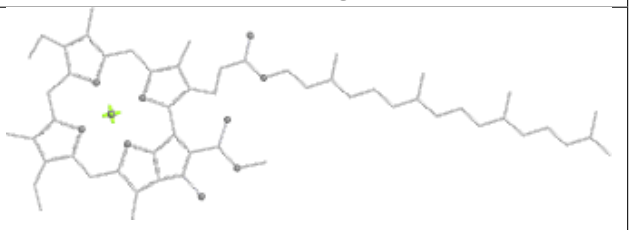
Bond lengths



Bond angles

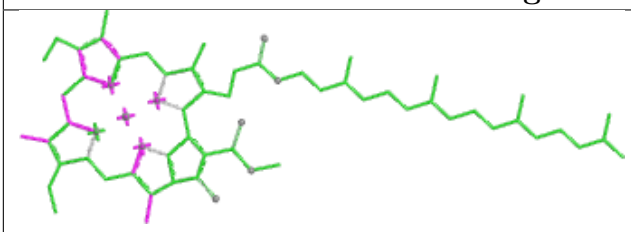


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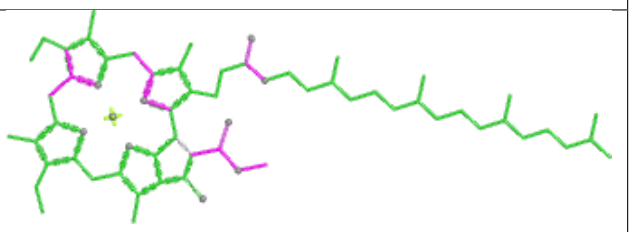


Rings

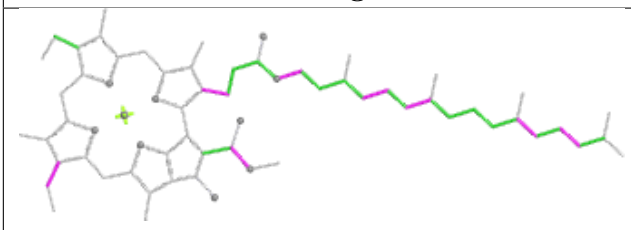
Ligand CLA D 403



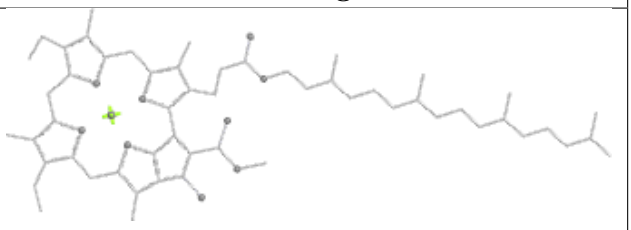
Bond lengths



Bond angles

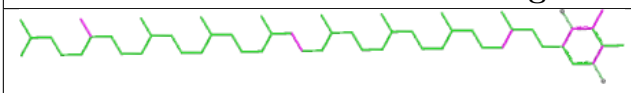


Torsions

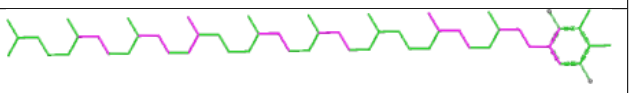


Rings

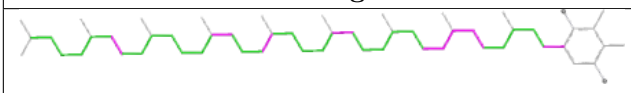
Ligand PL9 D 406



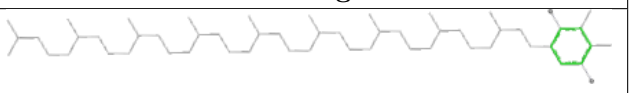
Bond lengths



Bond angles

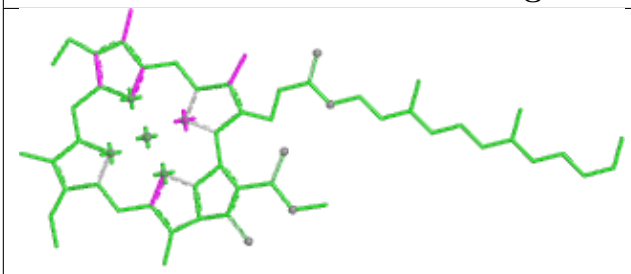


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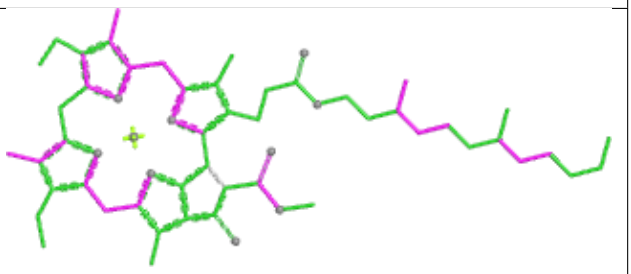


Rings

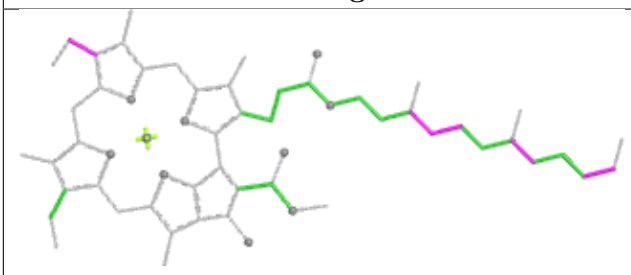
Ligand CLA C 504



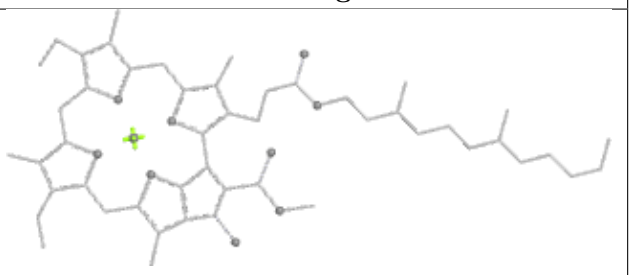
Bond lengths



Bond angles

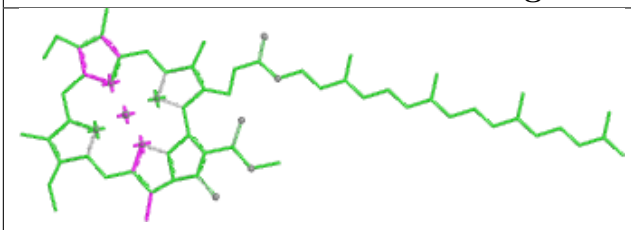


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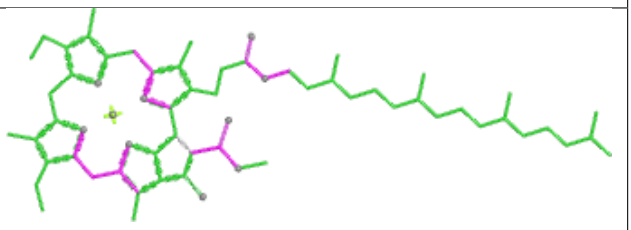


Rings

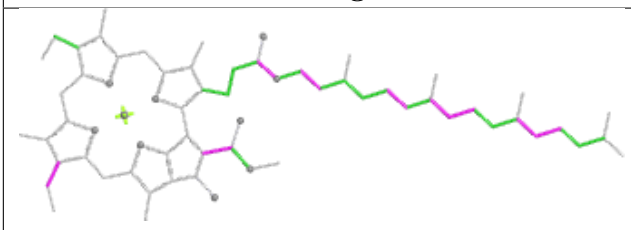
Ligand CLA C 513



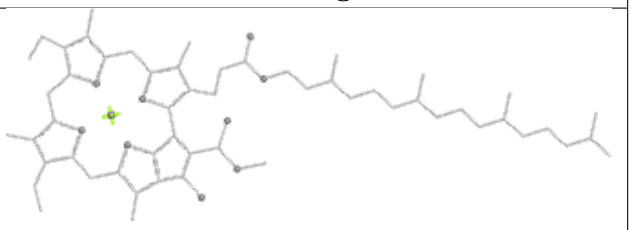
Bond lengths



Bond angles

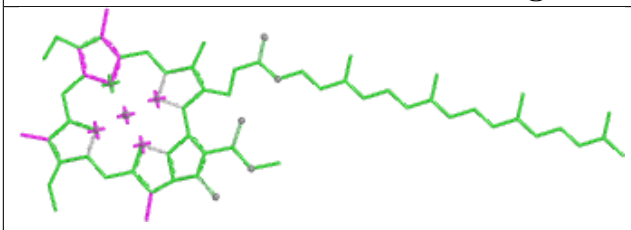


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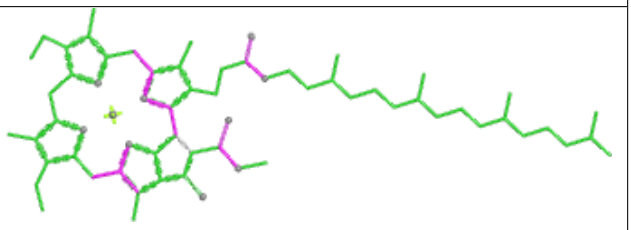


Rings

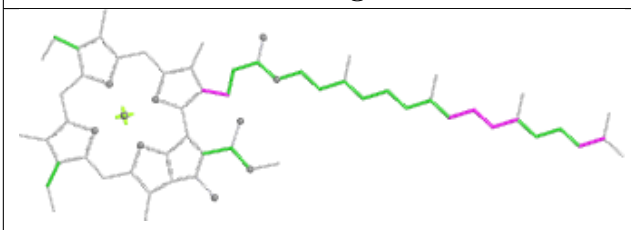
Ligand CLA d 404



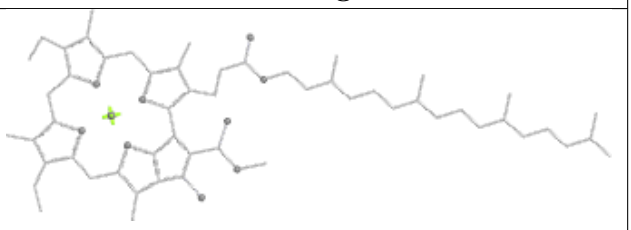
Bond lengths



Bond angles

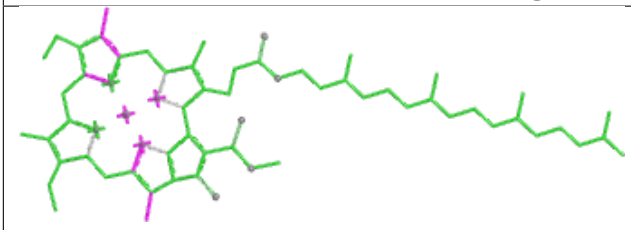


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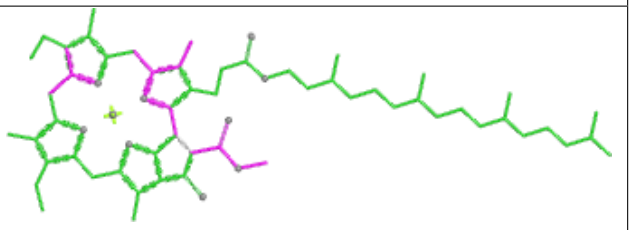


Rings

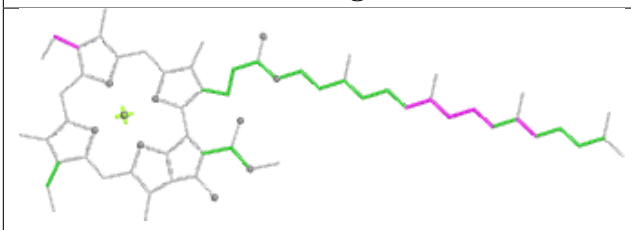
Ligand CLA a 405



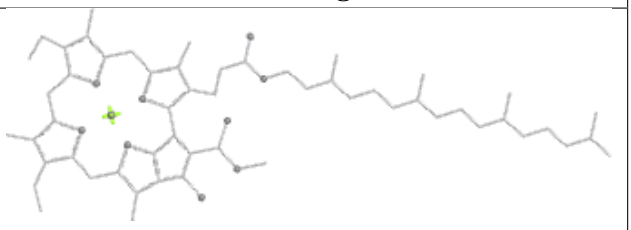
Bond lengths



Bond angles

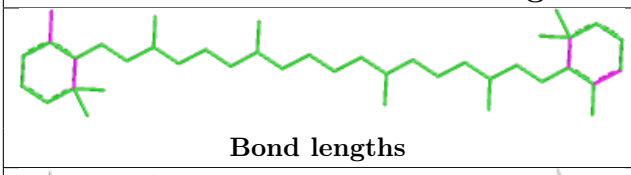


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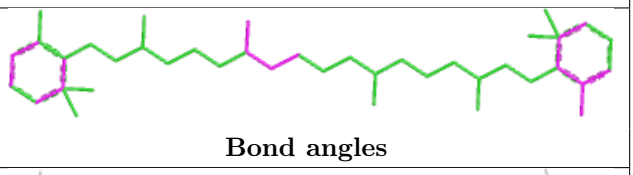


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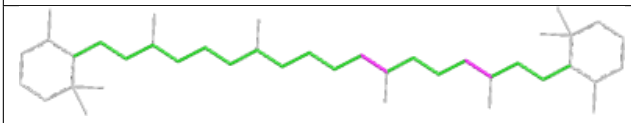
Ligand BCR a 408



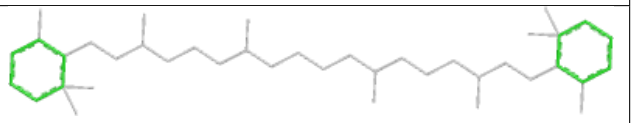
Bond lengths



Bond angles

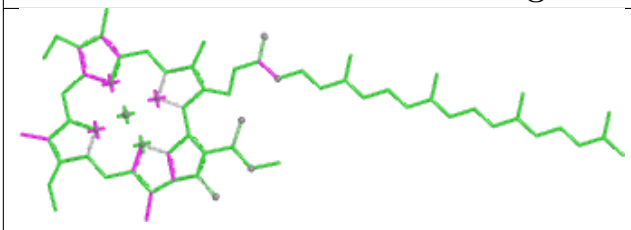


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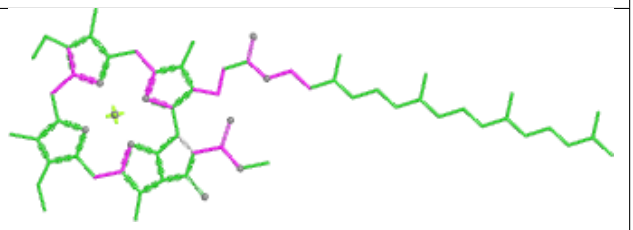


Rings

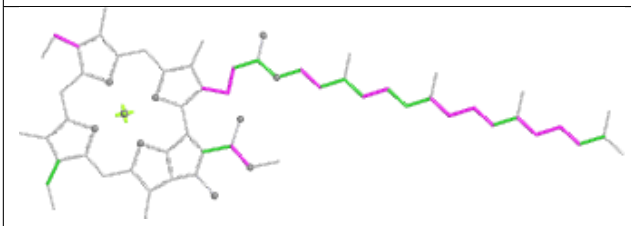
Ligand CLA h 101



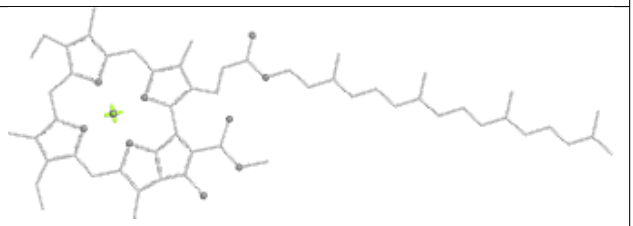
Bond lengths



Bond angles



Torsions

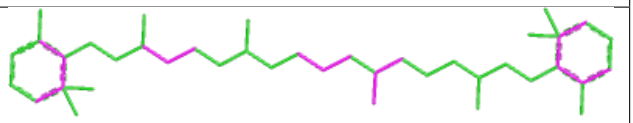


Rings

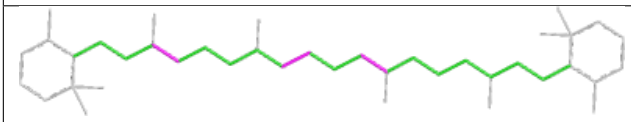
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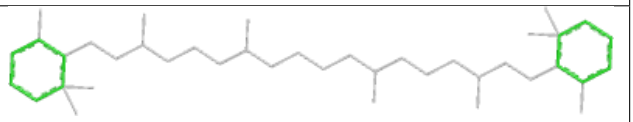
Bond lengths



Bond angles

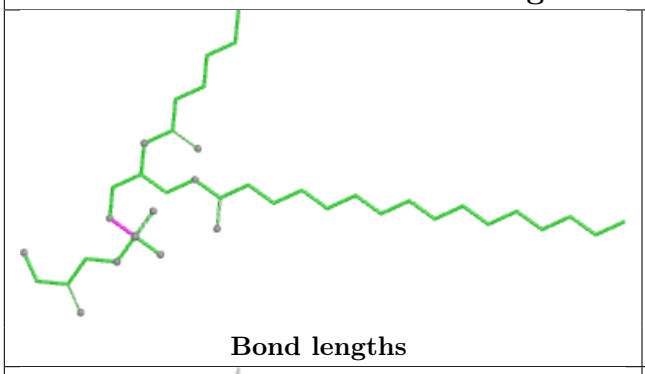


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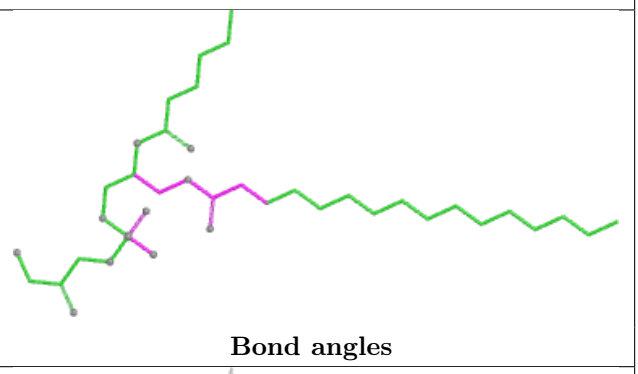


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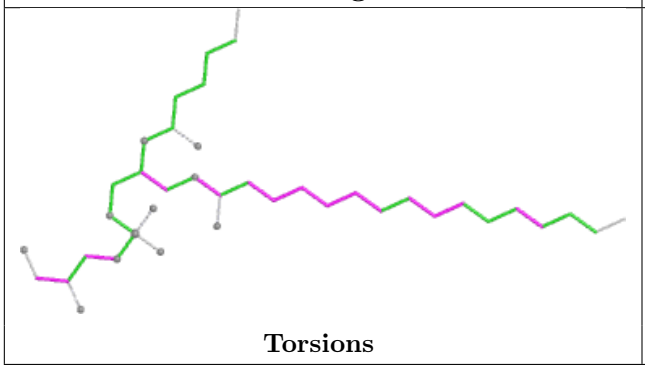
Ligand LHG d 408



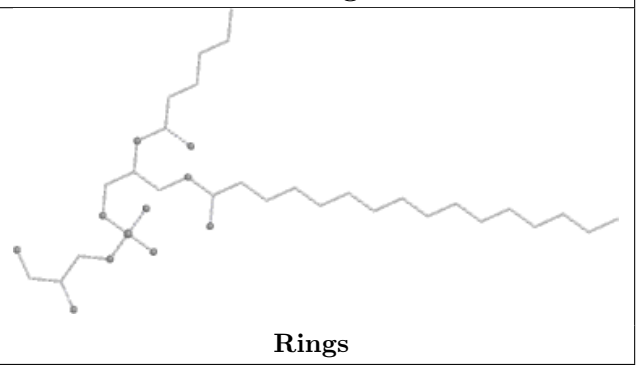
Bond lengths



Bond angles

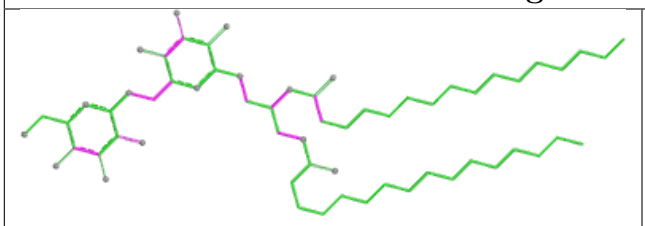


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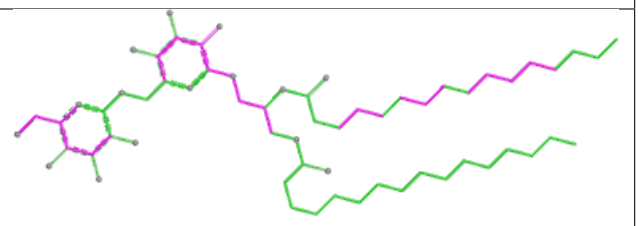


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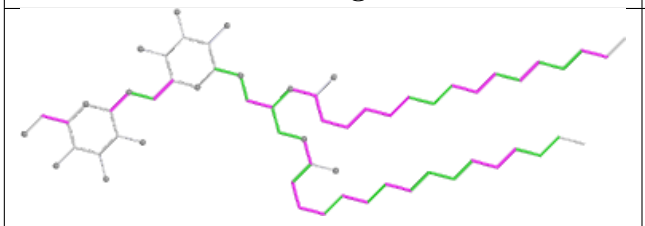
Ligand DGD c 516



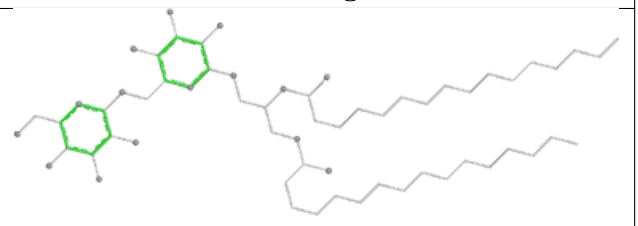
Bond lengths



Bond angles

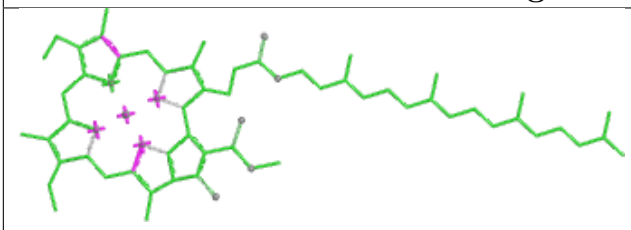


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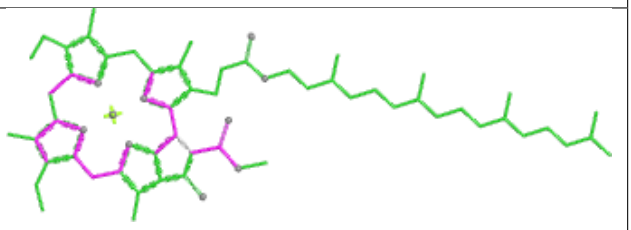


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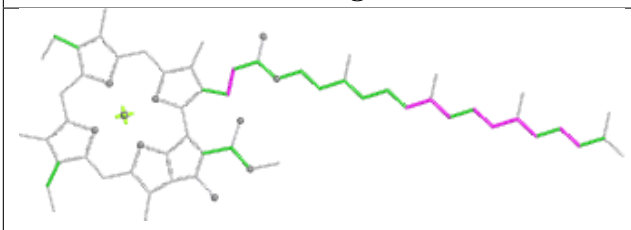
Ligand CLA b 607



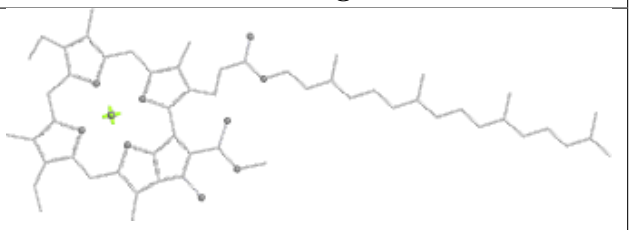
Bond lengths



Bond angles

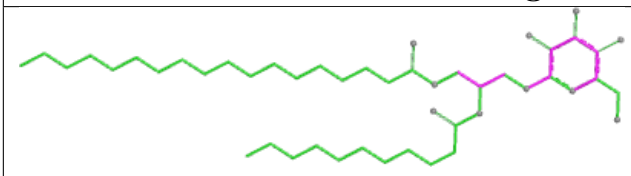


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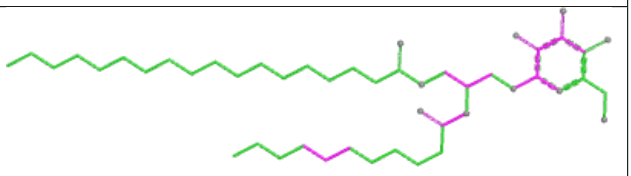


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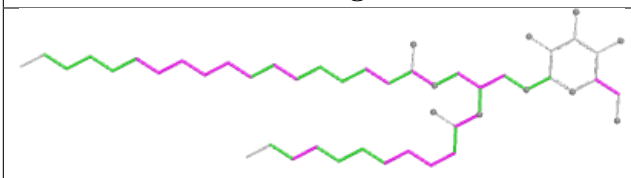
Ligand LMG c 522



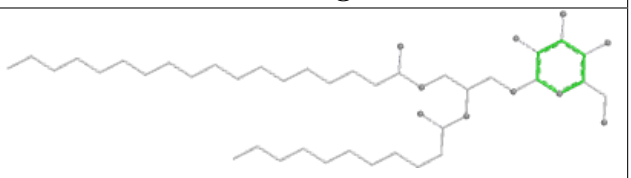
Bond lengths



Bond angles

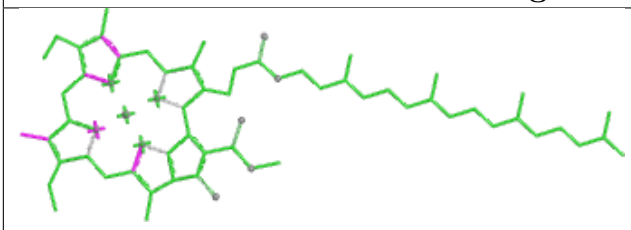


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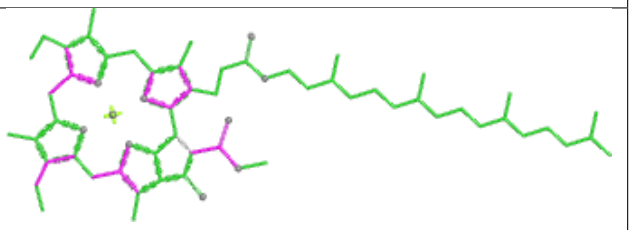


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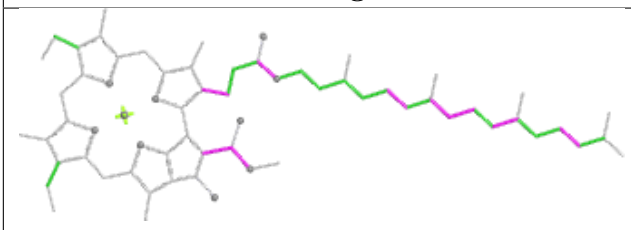
Ligand CLA c 503



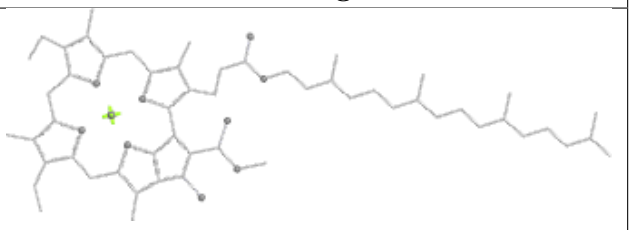
Bond lengths



Bond angles

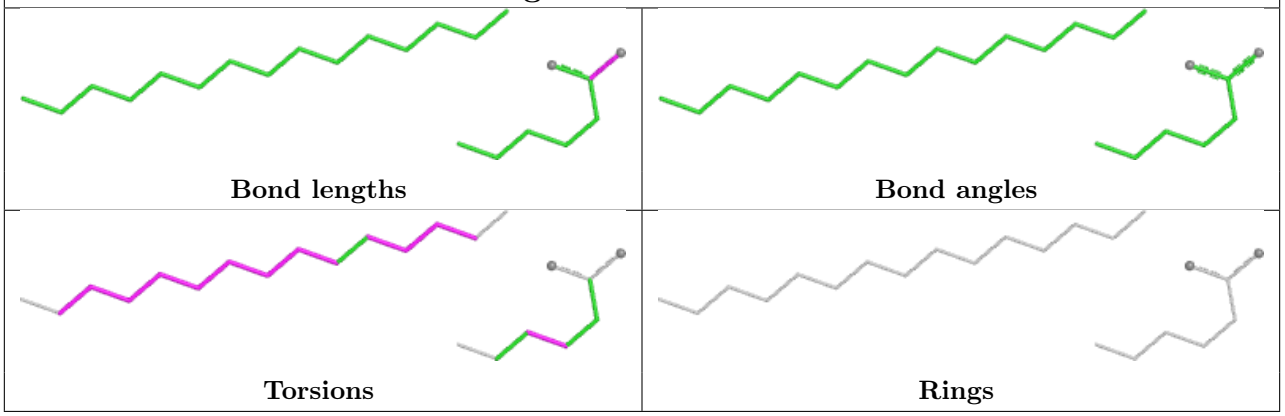


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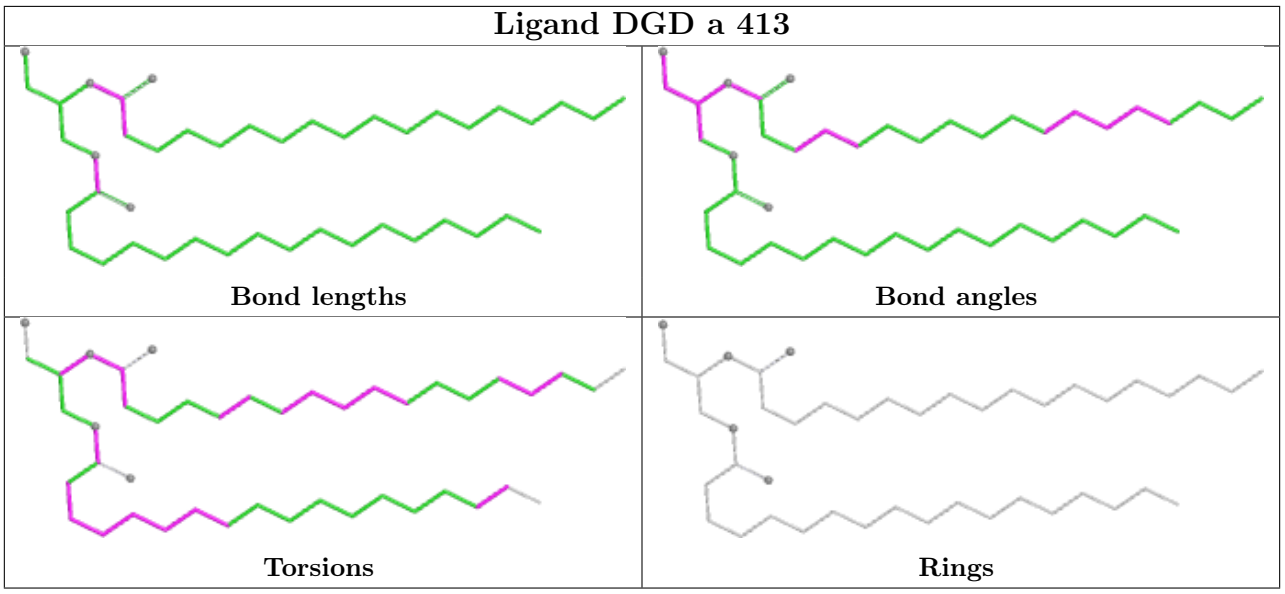


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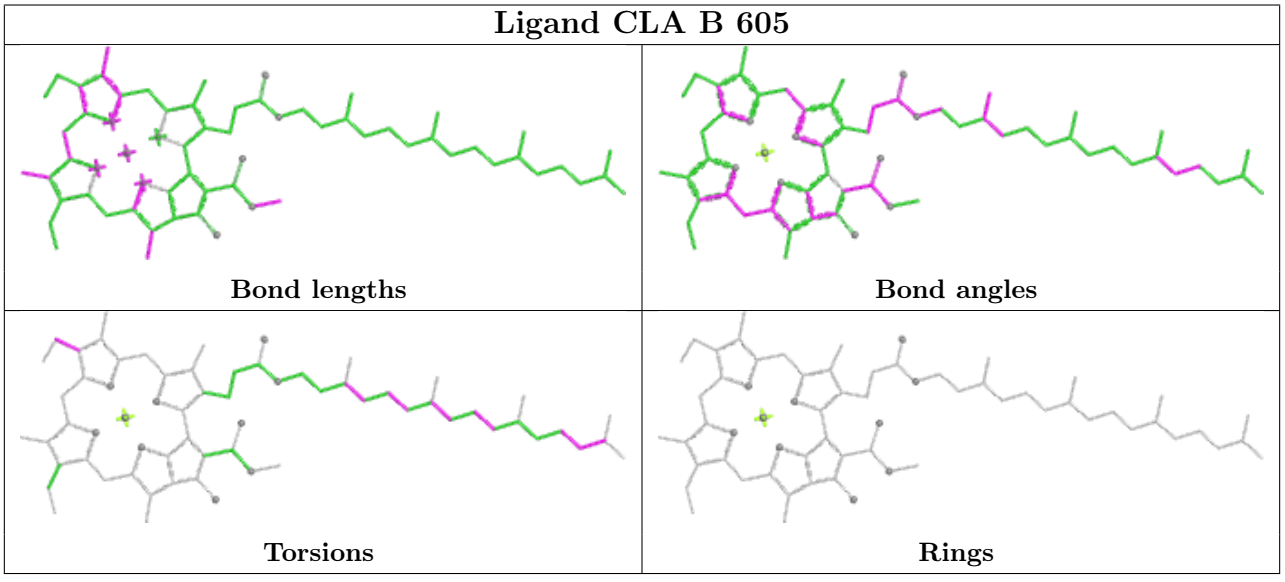
Ligand LMG b 623



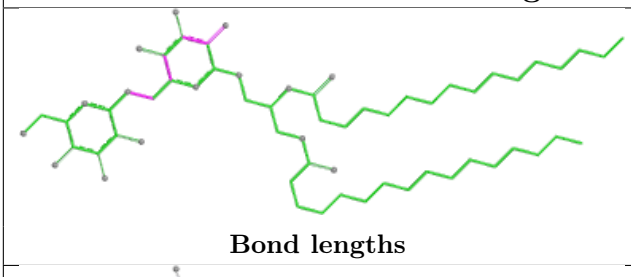
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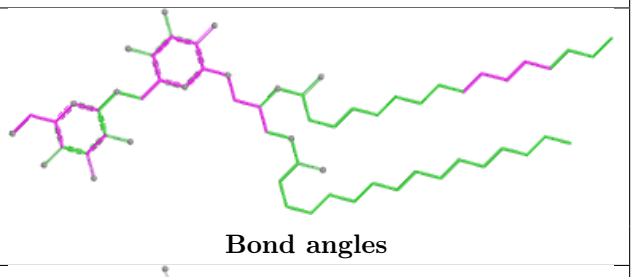
Ligand CLA B 605



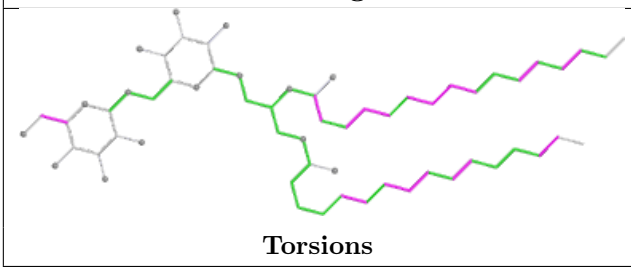
Ligand DGD h 103



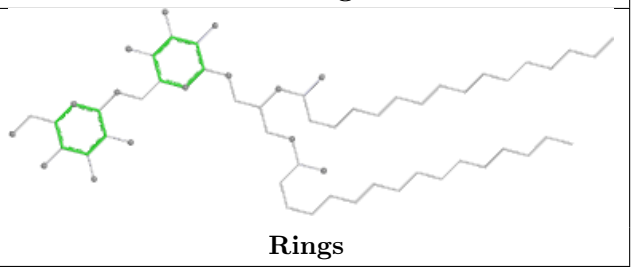
Bond lengths



Bond angles

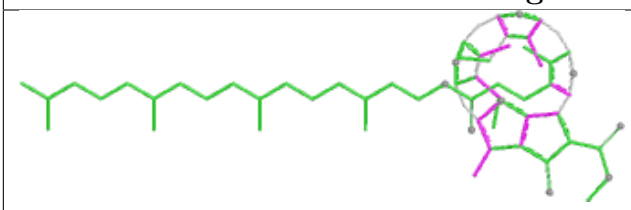


Torsions

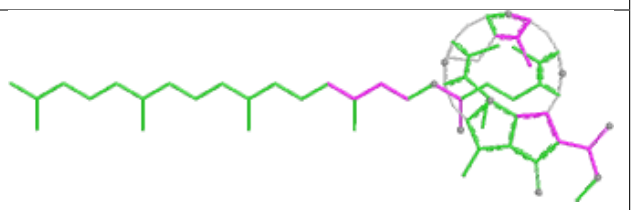


Rings

Ligand PHO a 406



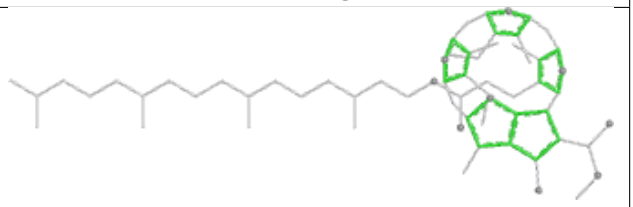
Bond lengths



Bond angles

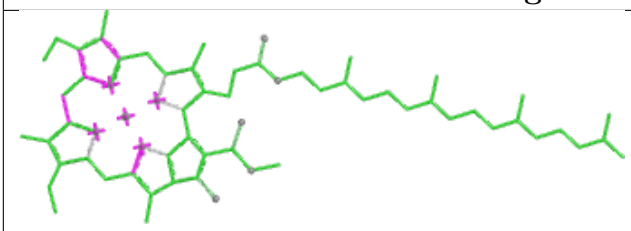


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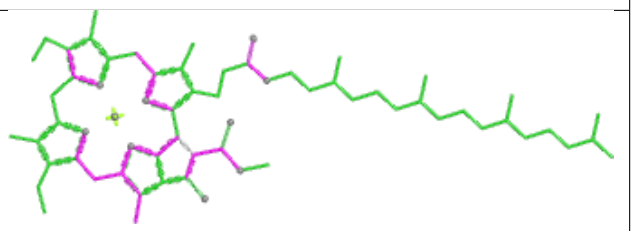


Rings

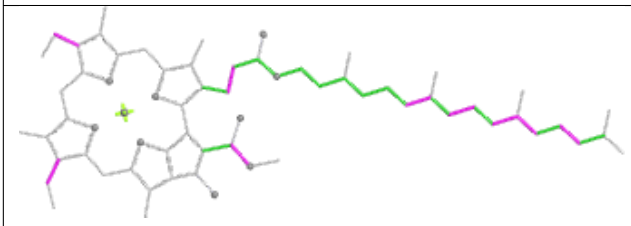
Ligand CLA B 606



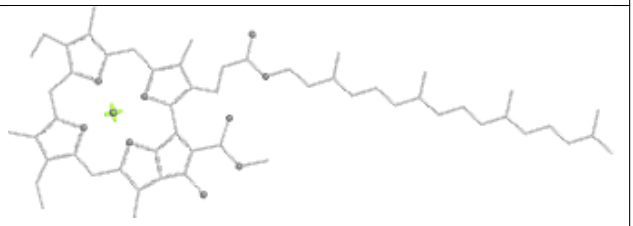
Bond lengths



Bond angles

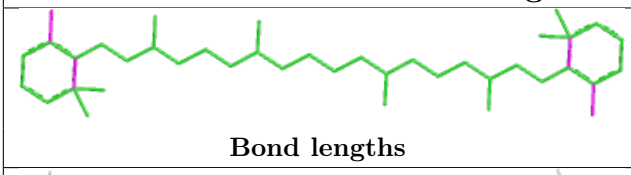


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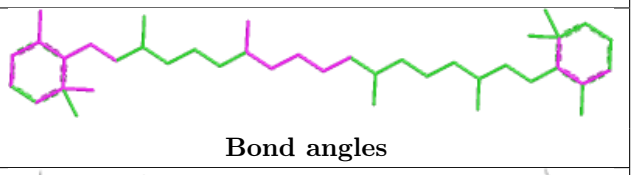


Rings

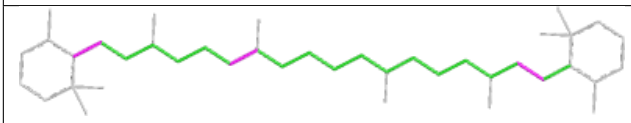
Ligand BCR b 618



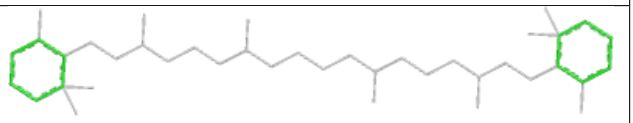
Bond lengths



Bond angles

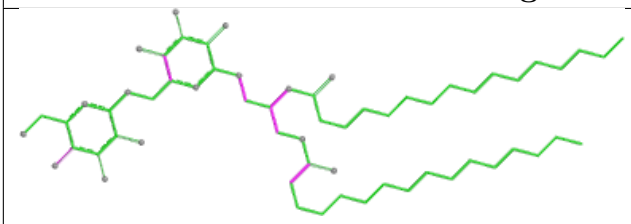


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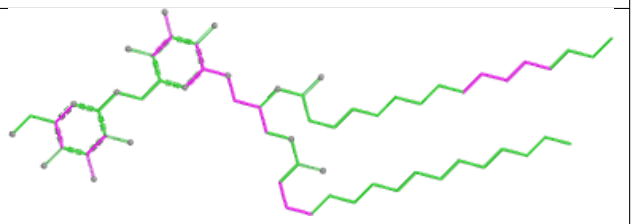


Rings

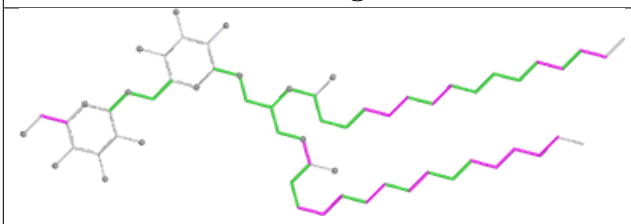
Ligand DGD C 518



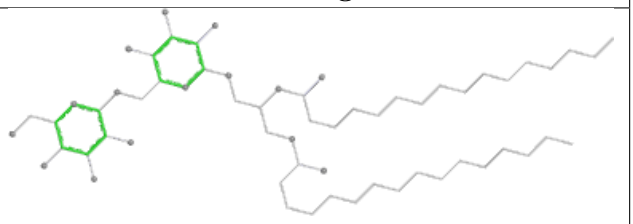
Bond lengths



Bond angles

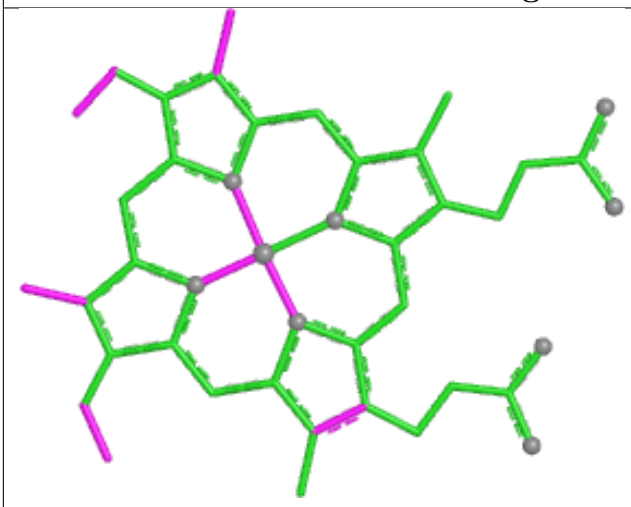


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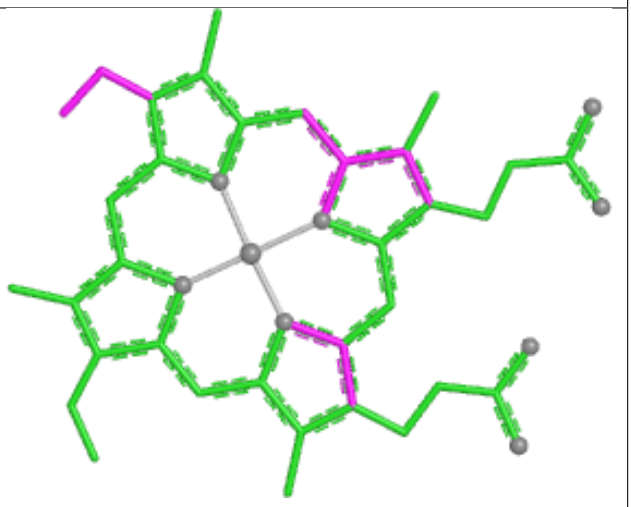


Rings

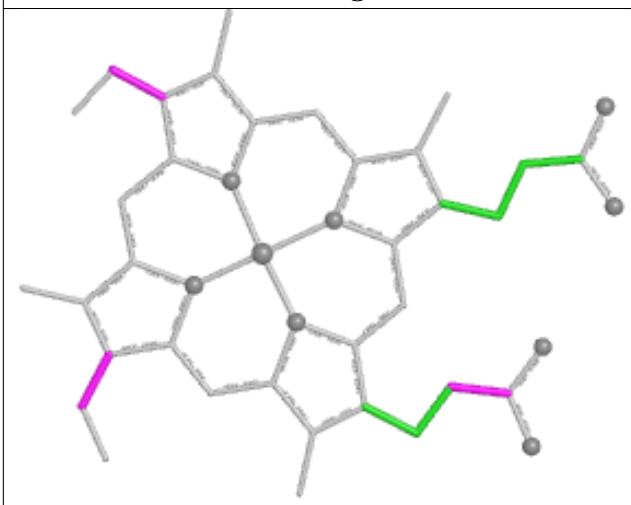
Ligand HEC V 201



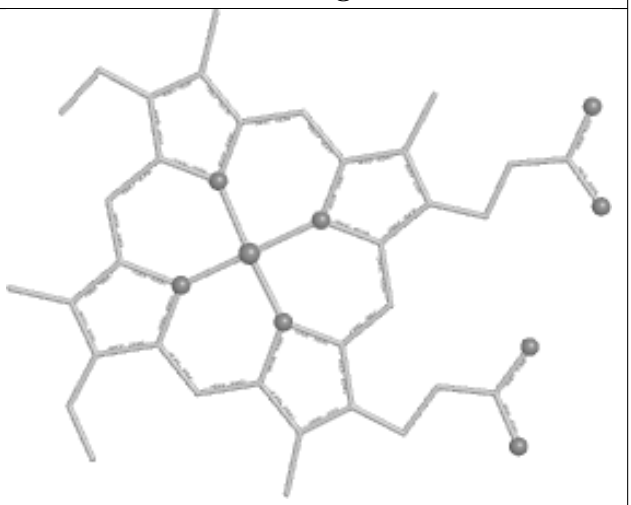
Bond lengths



Bond angles

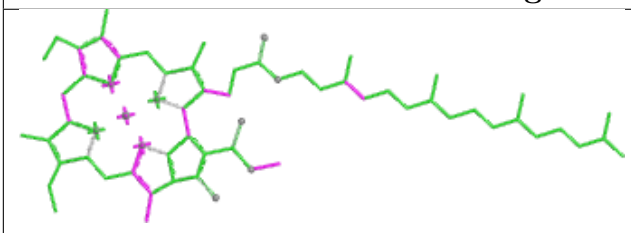


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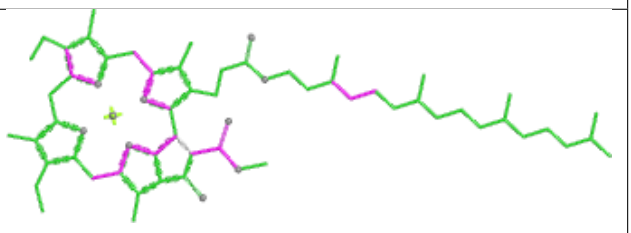


Rings

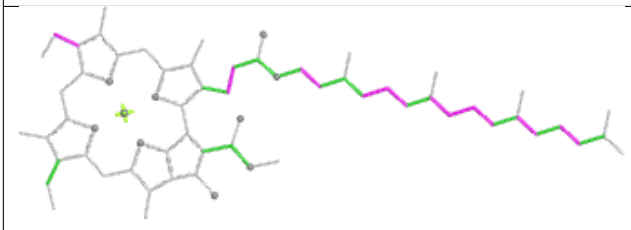
Ligand CLA C 512



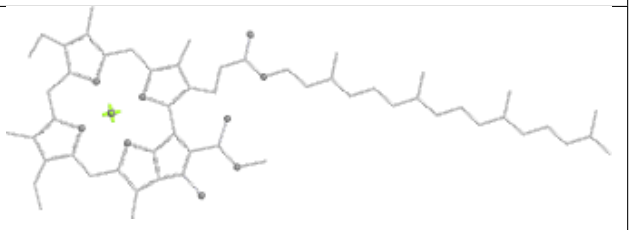
Bond lengths



Bond angles

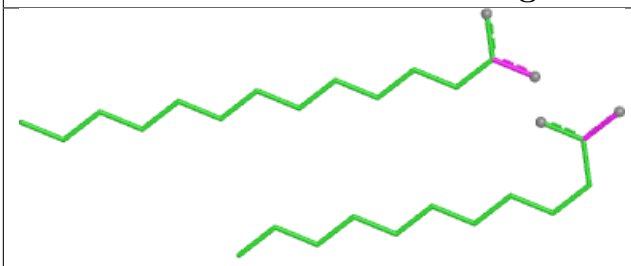


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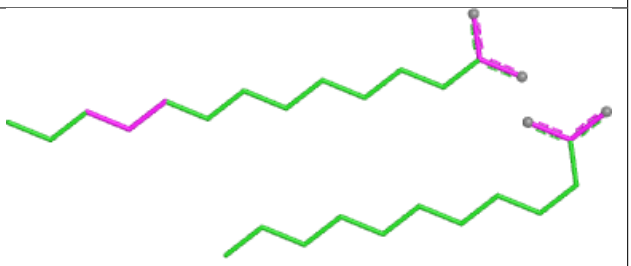


Rings

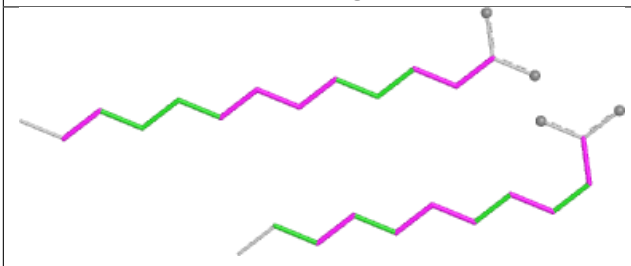
Ligand LMG D 411



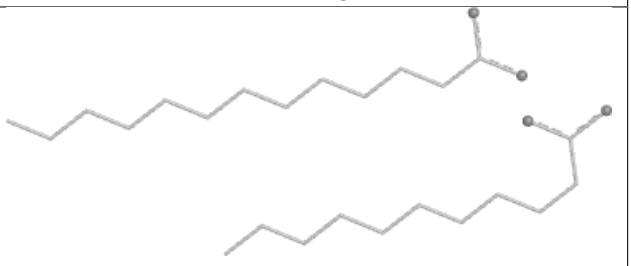
Bond lengths



Bond angles

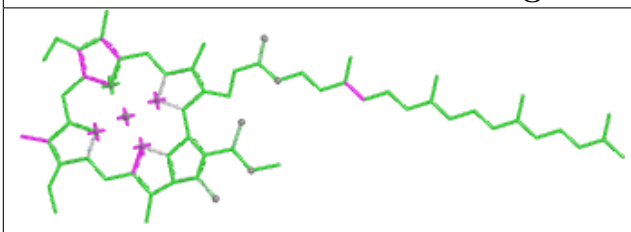


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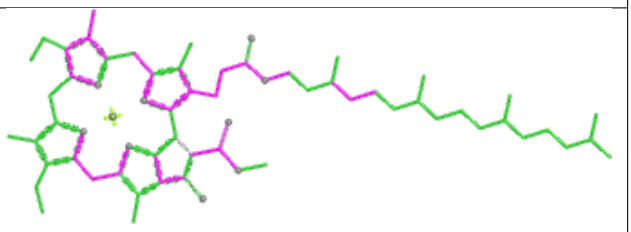


Rings

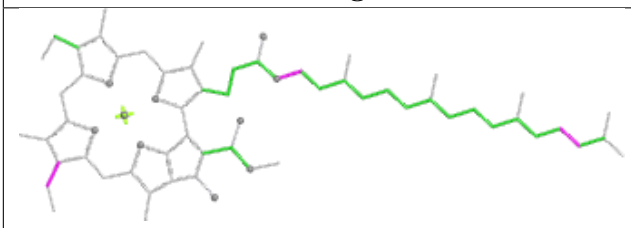
Ligand CLA A 404



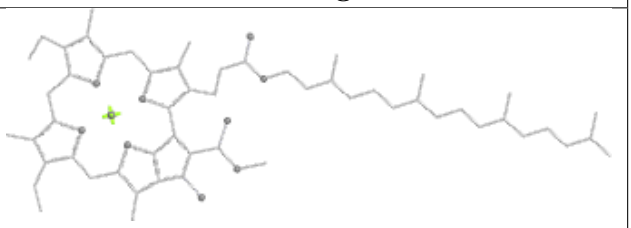
Bond lengths



Bond angles

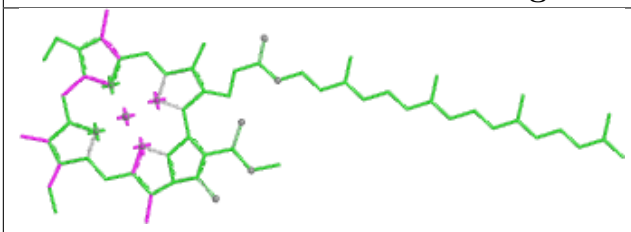


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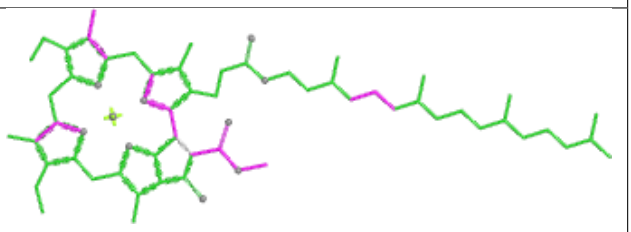


Rings

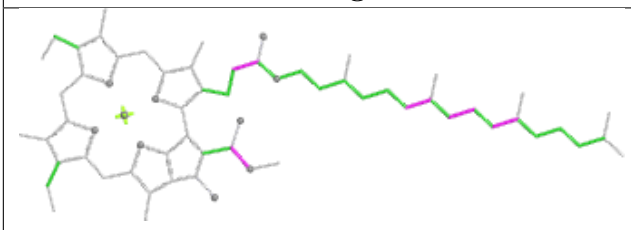
Ligand CLA c 501



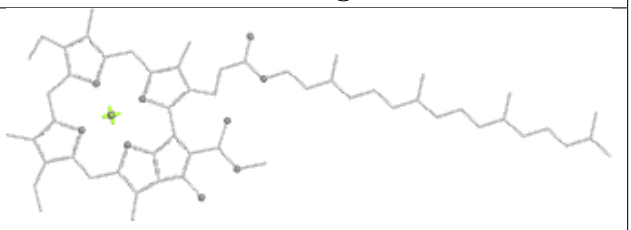
Bond lengths



Bond angles



Torsions

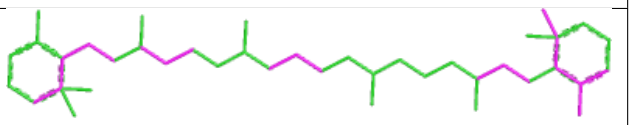


Rings

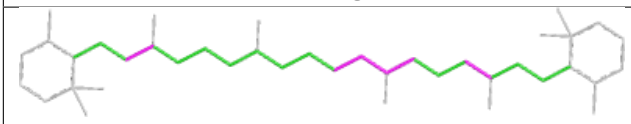
Ligand BCR A 408



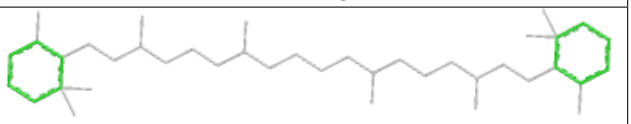
Bond lengths



Bond angles

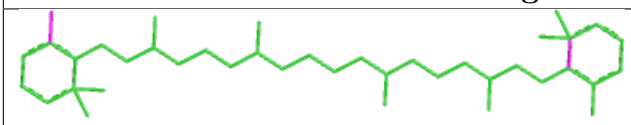


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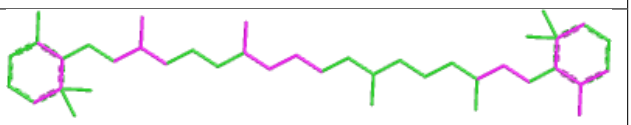


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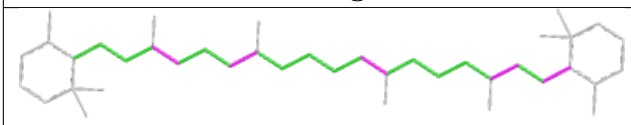
Ligand BCR H 101



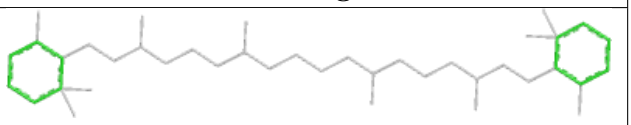
Bond lengths



Bond angles

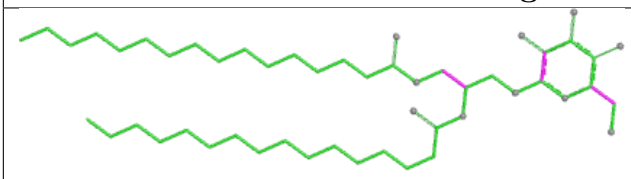


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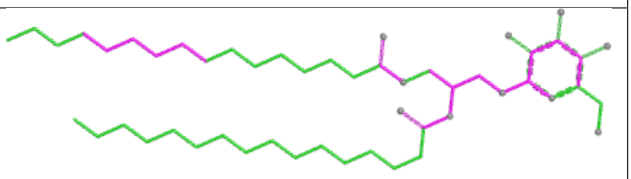


Rings

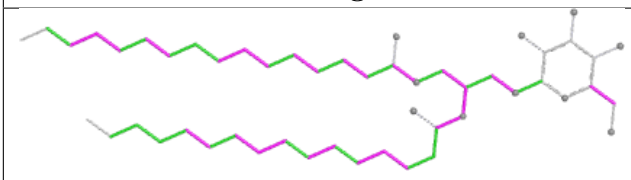
Ligand LMG B 620



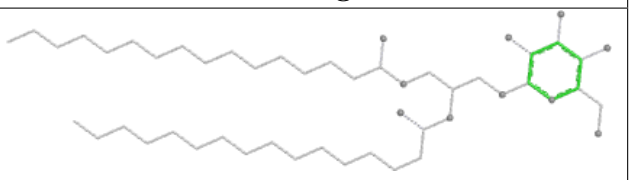
Bond lengths



Bond angles

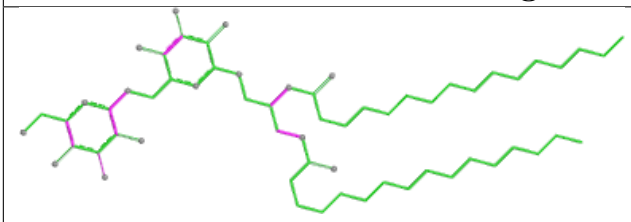


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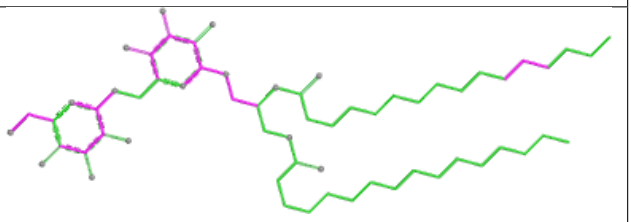


Rings

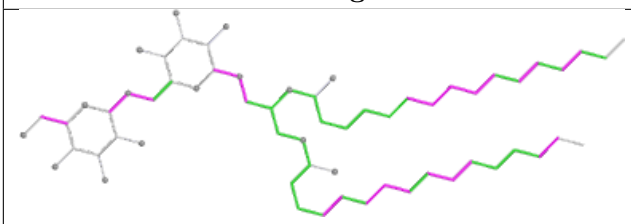
Ligand DGD C 517



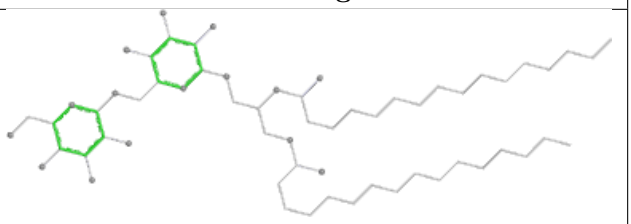
Bond lengths



Bond angles

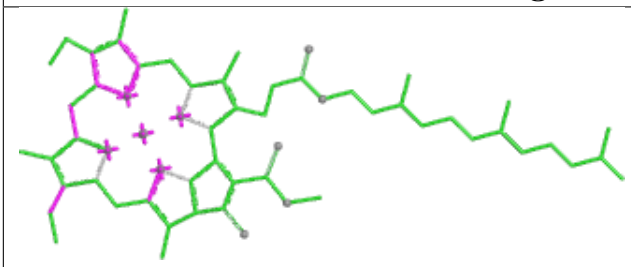


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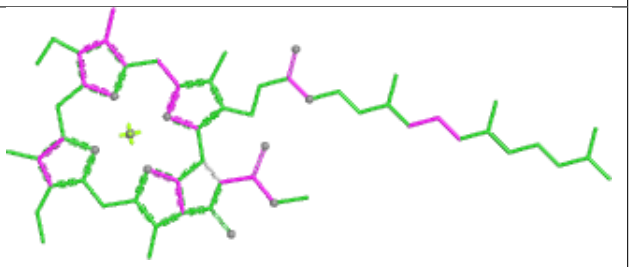


Rings

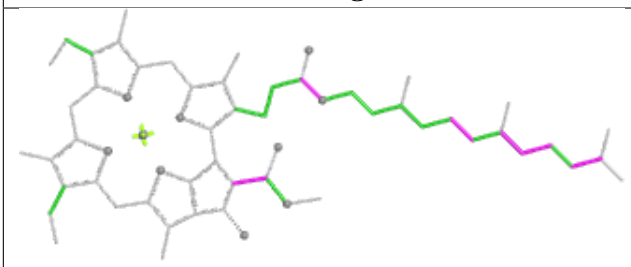
Ligand CLA c 504



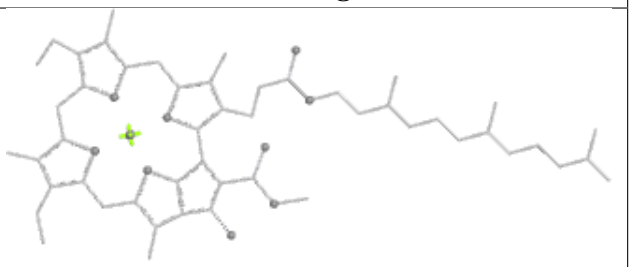
Bond lengths



Bond angles

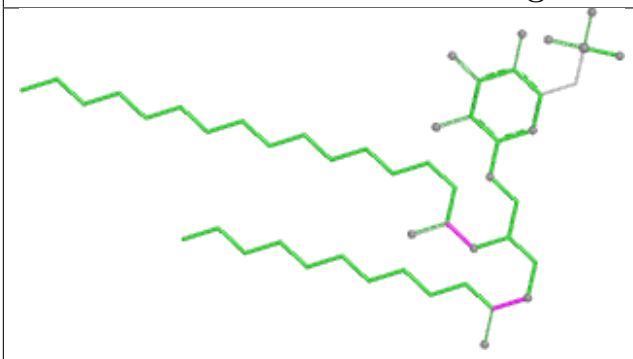


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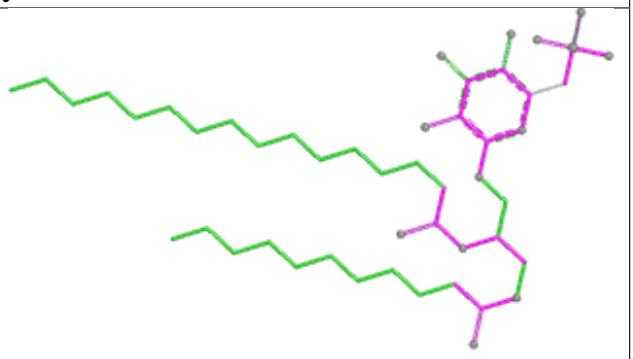


Rings

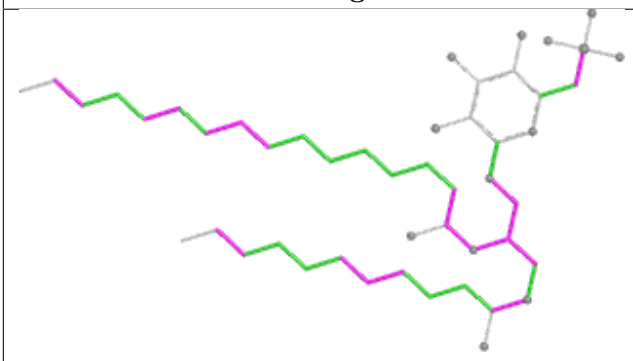
Ligand SQD b 601



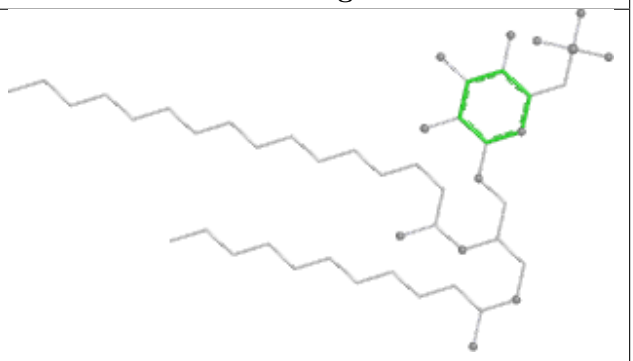
Bond lengths



Bond angles

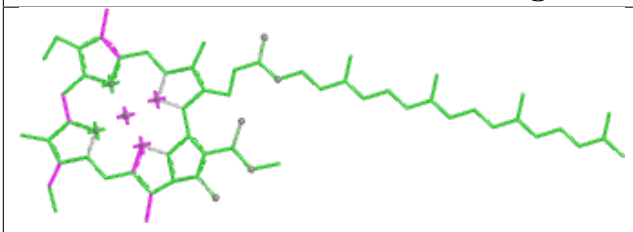


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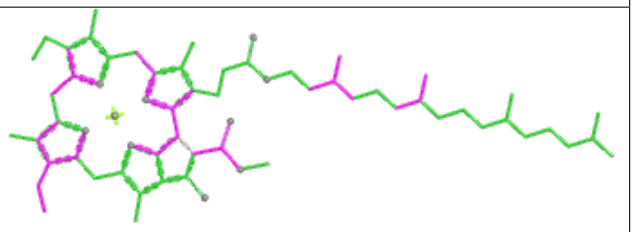


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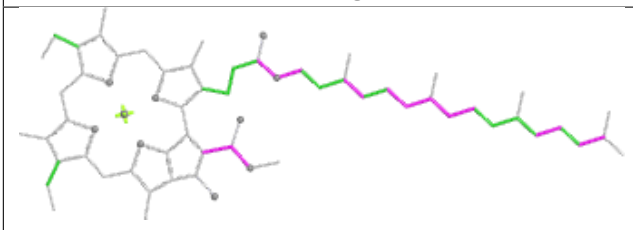
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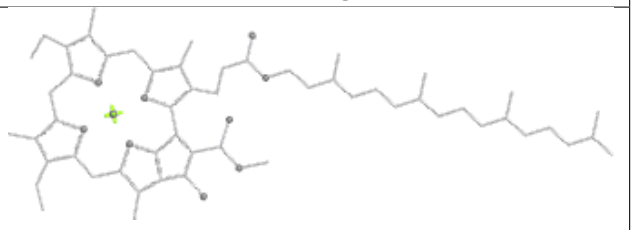
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Bond angles

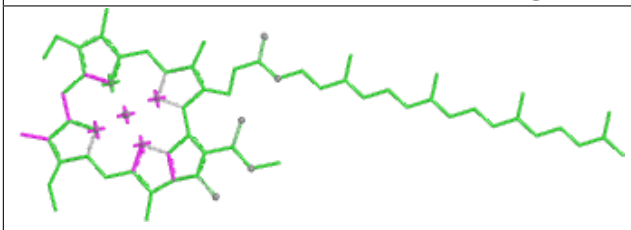


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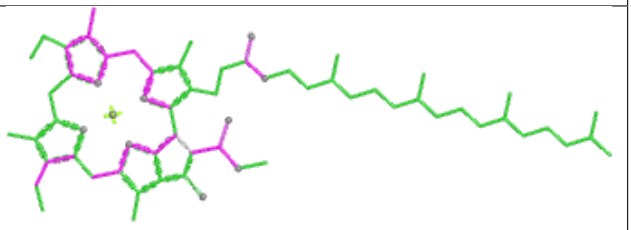


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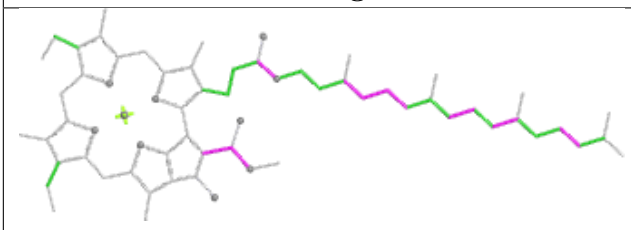
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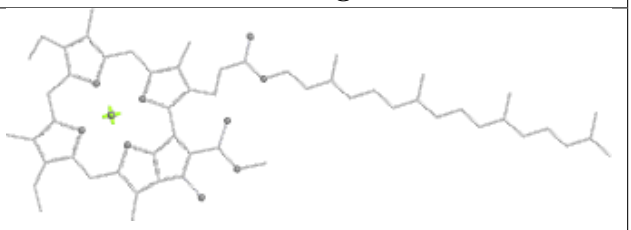
Bond lengths



Bond angles

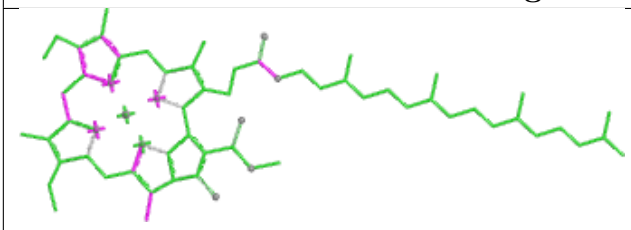


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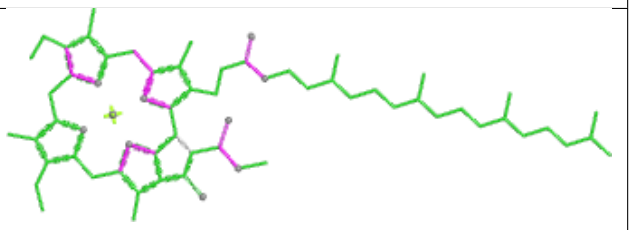


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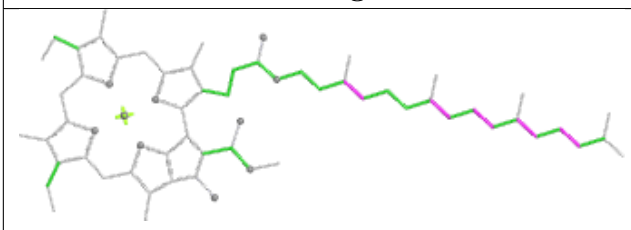
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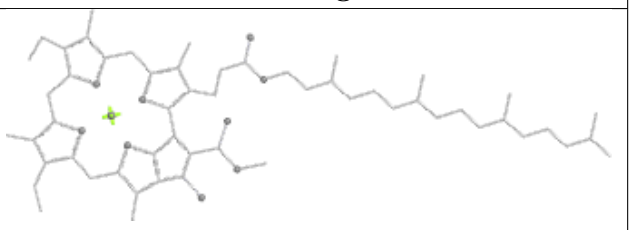
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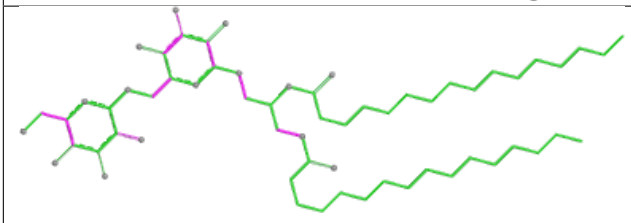


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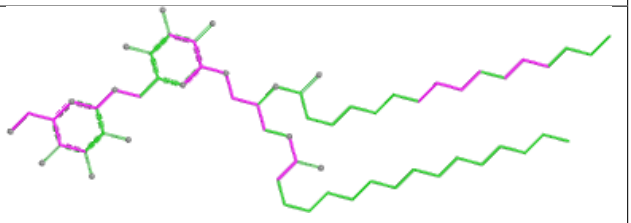


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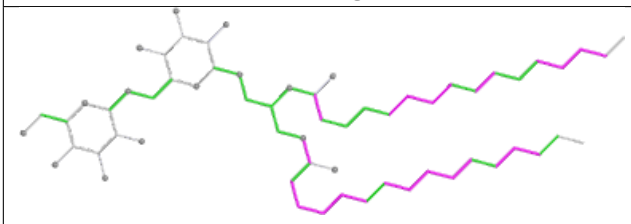
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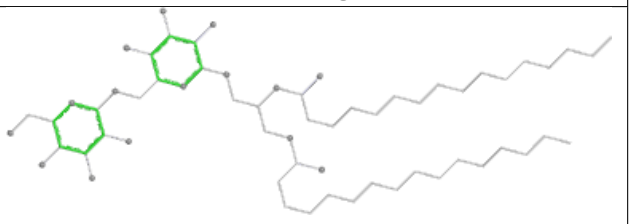
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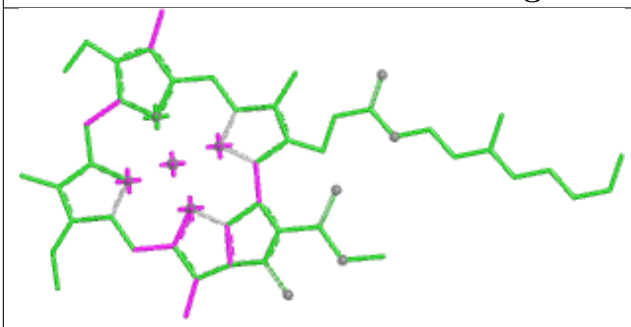


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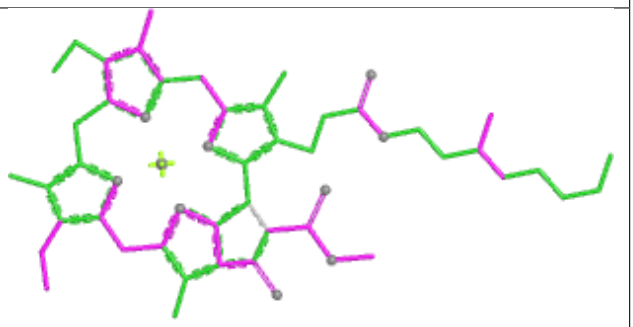


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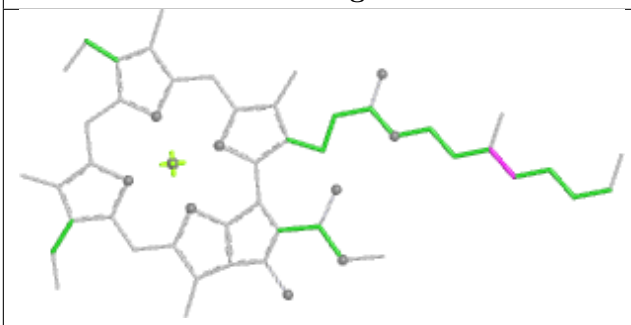
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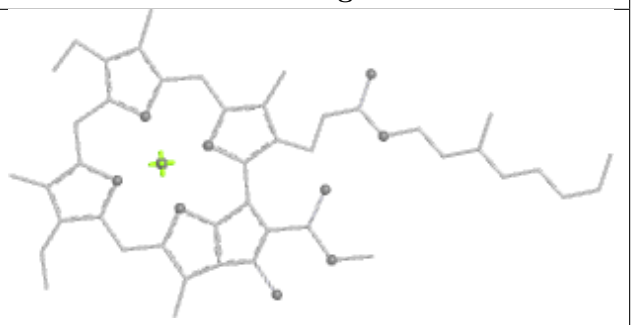
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Bond angles



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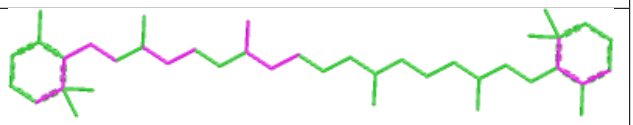


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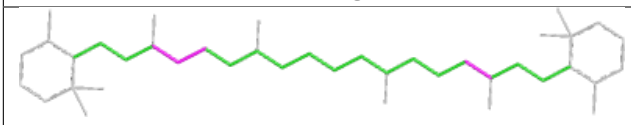
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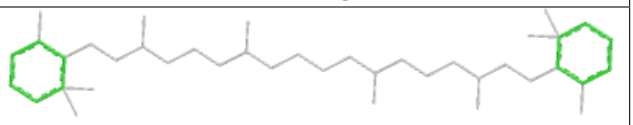
Bond lengths



Bond angles

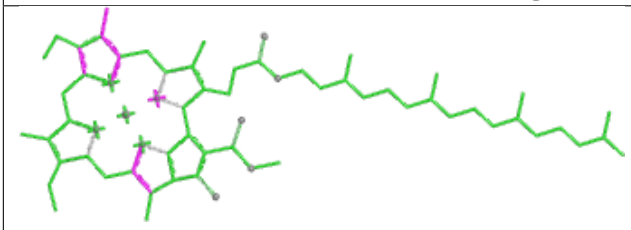


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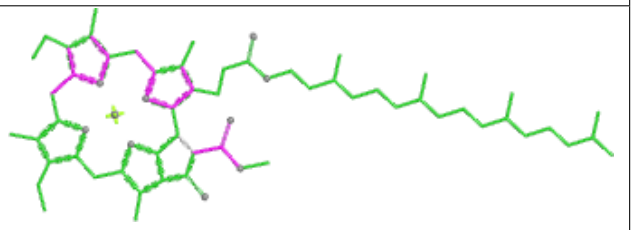


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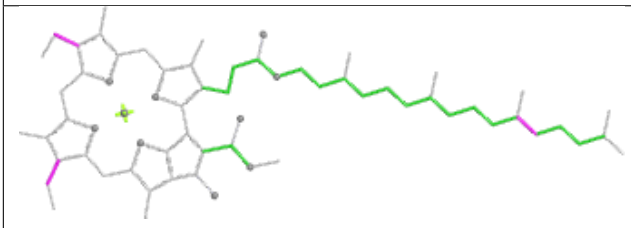
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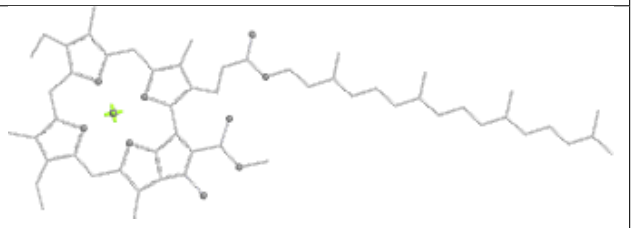
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Bond angles

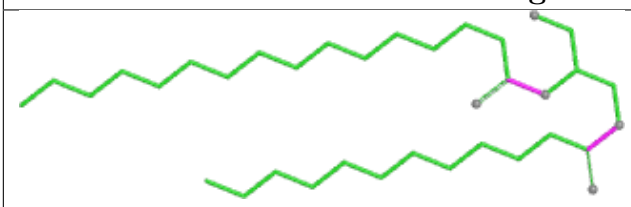


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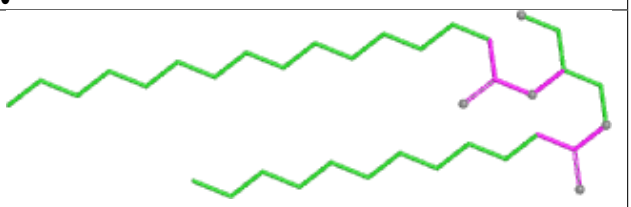


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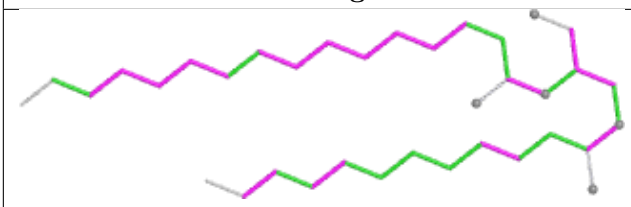
Ligand SQD a 412



Bond lengths



Bond angles



Torsions

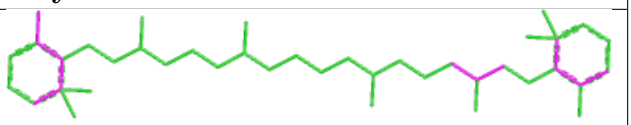


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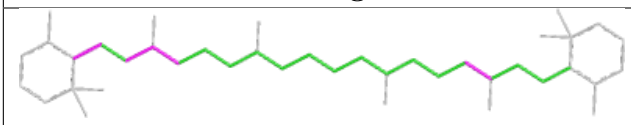
Ligand BCR y 101



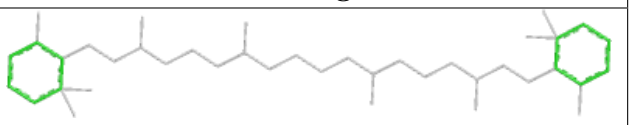
Bond lengths



Bond angles

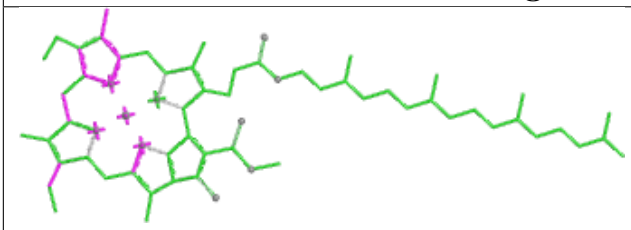


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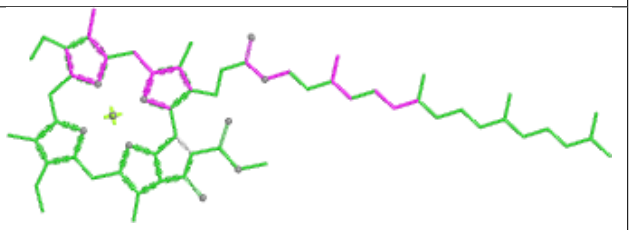


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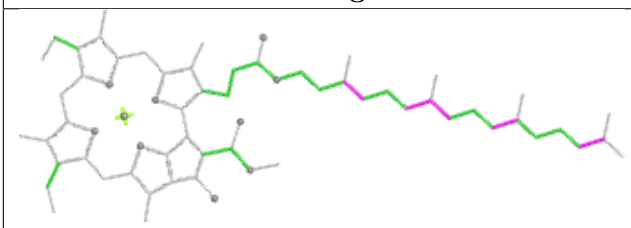
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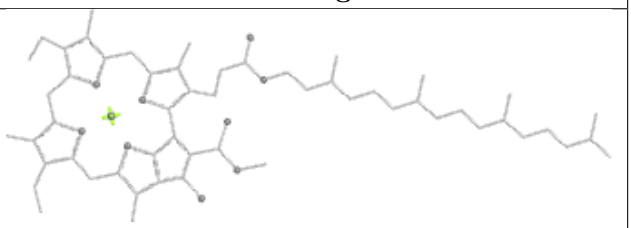
Bond lengths



Bond angles

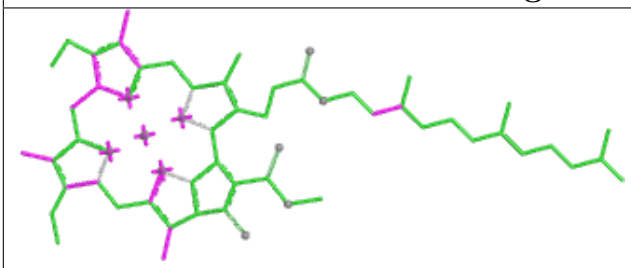


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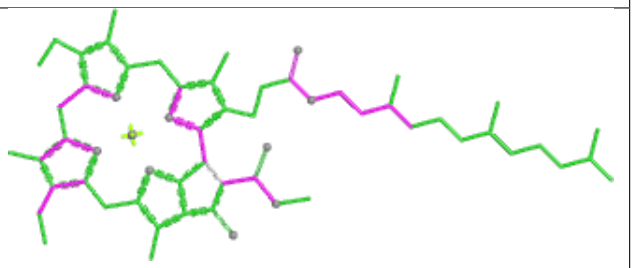


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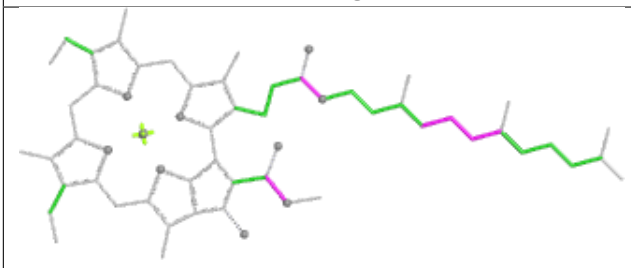
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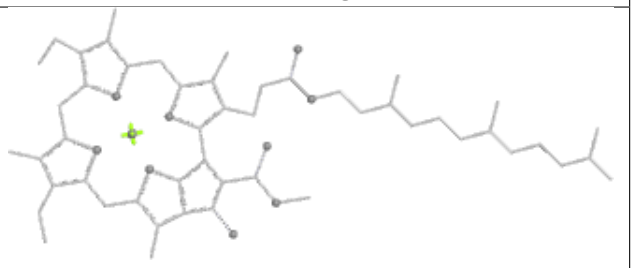
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Bond angles

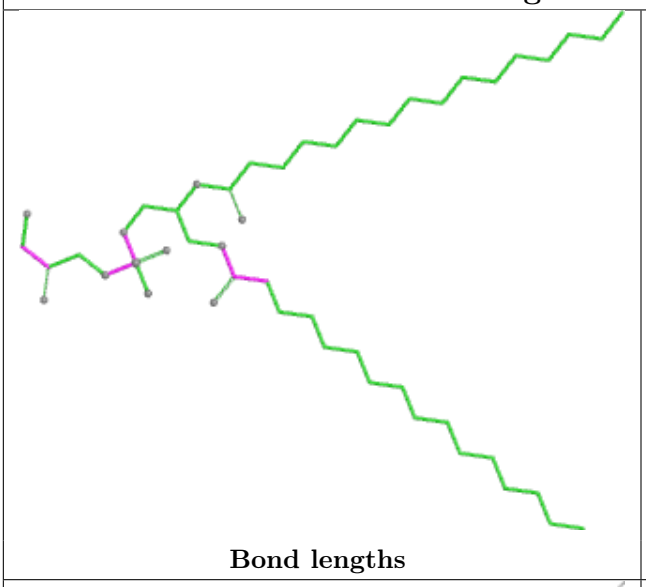


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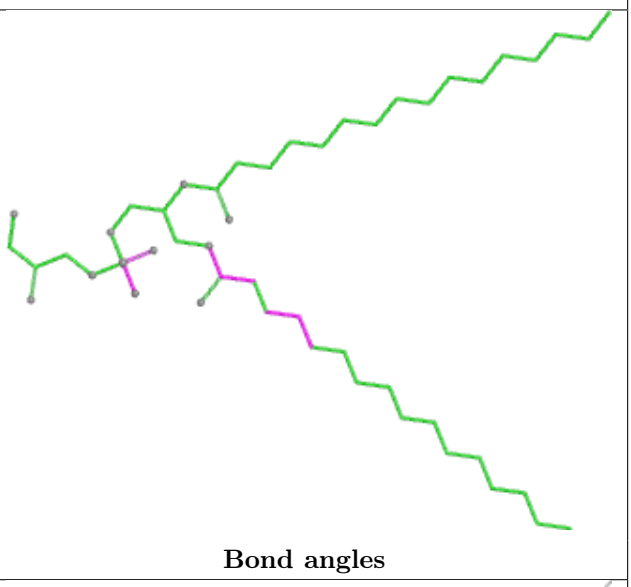


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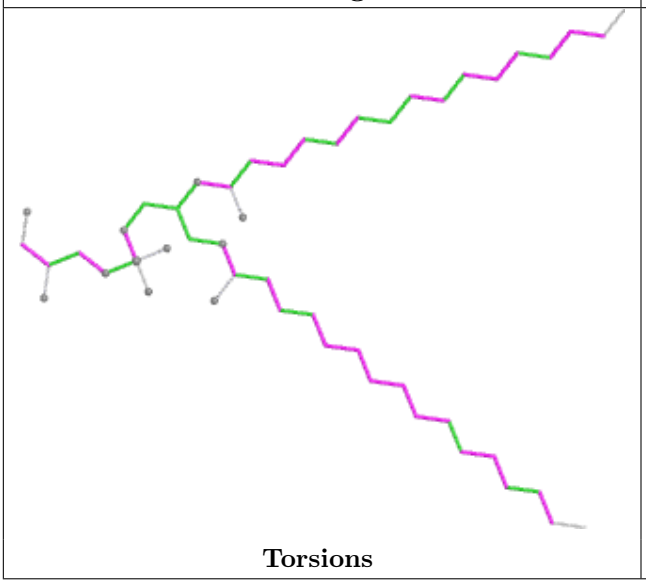
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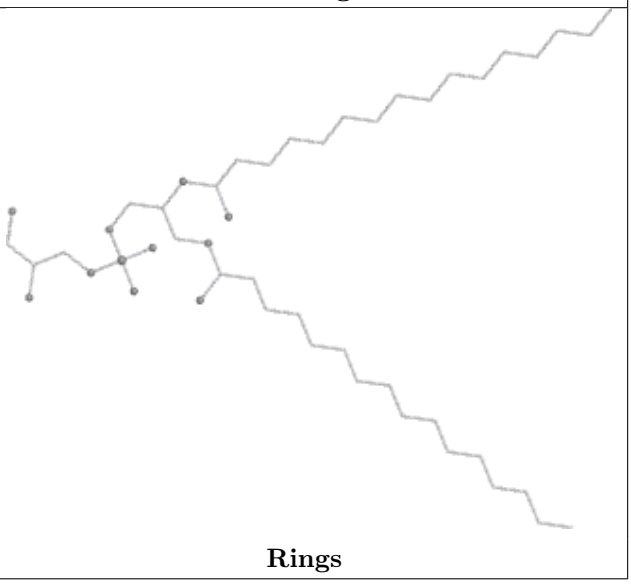
Bond lengths



Bond angles

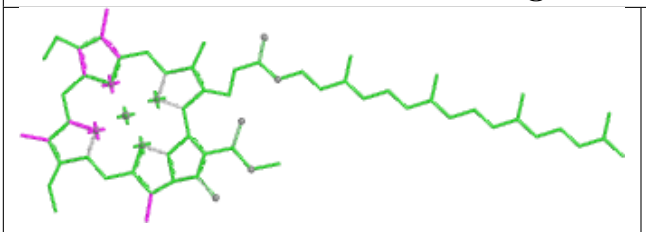


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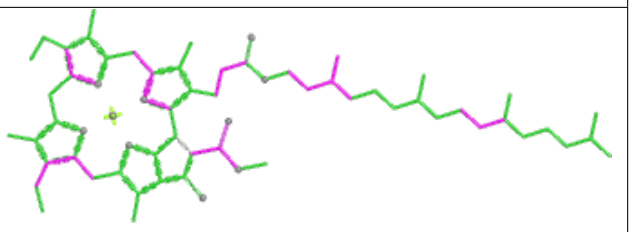


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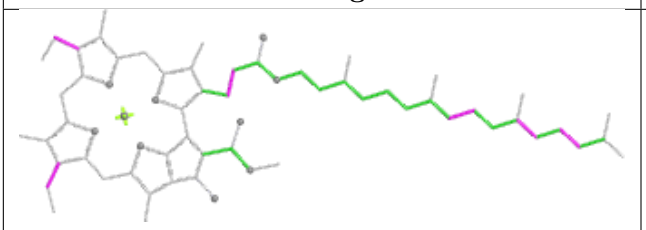
Ligand CLA b 611



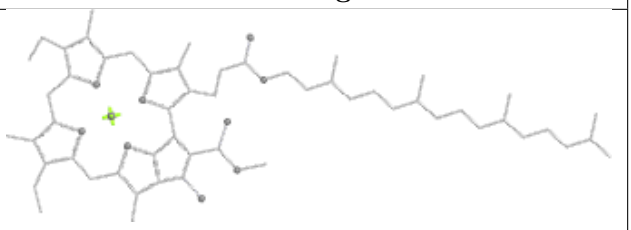
Bond lengths



Bond angles

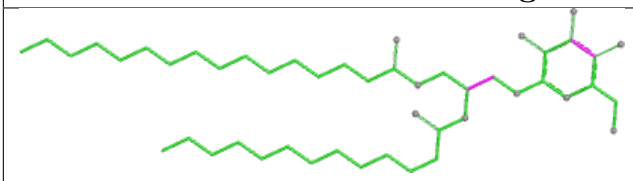


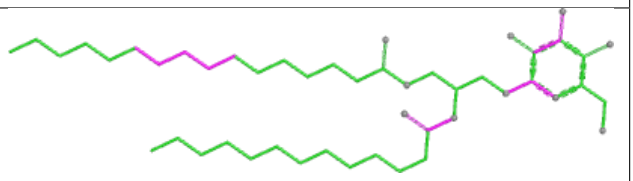
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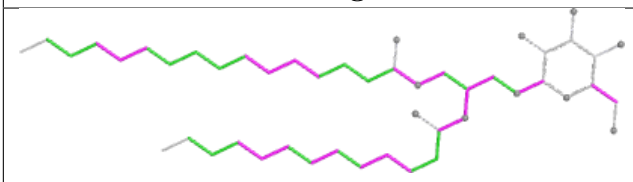


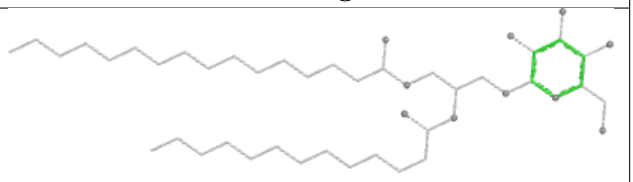
Rings

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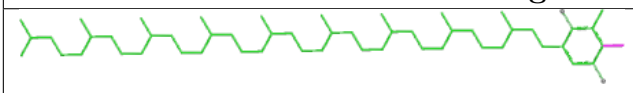

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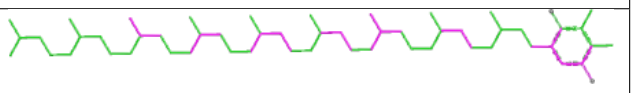

Bond angles

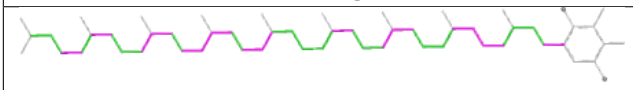

Torsions

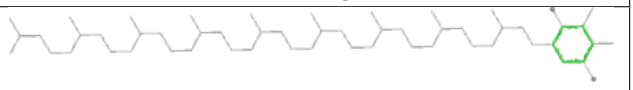

Rings

Ligand PL9 A 409

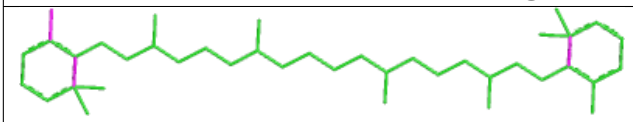

Bond lengths

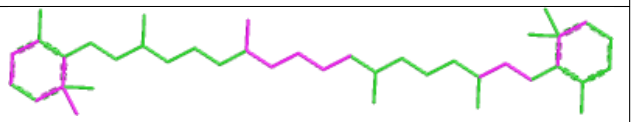

Bond angles

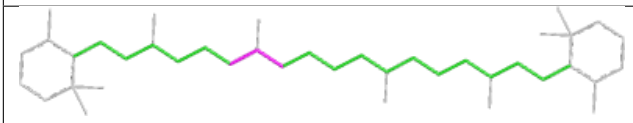

Torsions

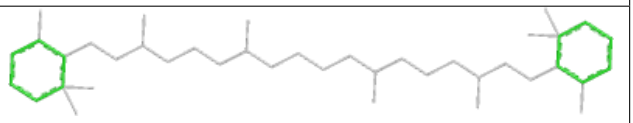

Rings

Ligand BCR B 617

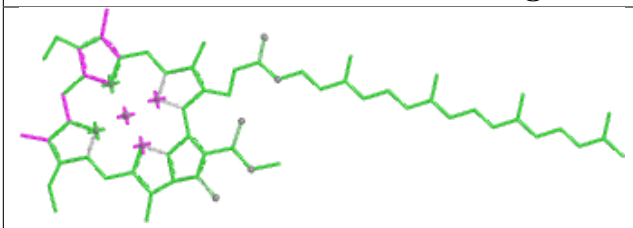

Bond lengths

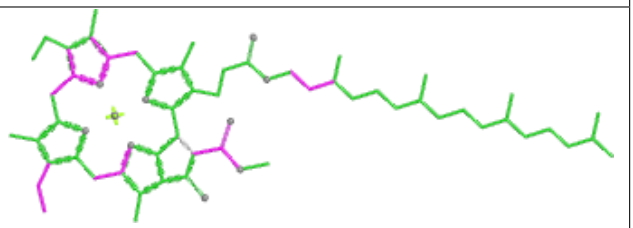

Bond angles

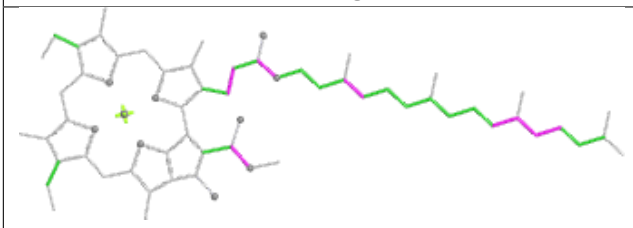

Torsions

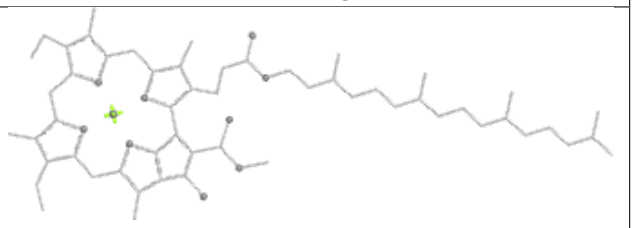

Rings

Ligand CLA B 614


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	334/334 (100%)	-0.52	0 100 100	23, 33, 56, 83	0
1	a	334/334 (100%)	-0.41	2 (0%) 85 83	23, 36, 67, 90	0
2	B	505/505 (100%)	-0.40	1 (0%) 91 90	18, 38, 71, 113	4 (0%)
2	b	505/505 (100%)	-0.27	3 (0%) 85 83	27, 42, 80, 121	0
3	C	442/451 (98%)	-0.38	0 100 100	25, 42, 61, 86	0
3	c	451/451 (100%)	-0.25	2 (0%) 88 87	23, 46, 69, 116	1 (0%)
4	D	341/341 (100%)	-0.53	0 100 100	24, 35, 55, 97	0
4	d	341/341 (100%)	-0.36	0 100 100	25, 39, 64, 95	1 (0%)
5	E	81/82 (98%)	0.06	0 100 100	32, 55, 75, 81	1 (1%)
5	e	82/82 (100%)	0.30	0 100 100	44, 66, 87, 100	0
6	F	34/34 (100%)	-0.06	1 (2%) 53 50	39, 50, 75, 99	0
6	f	34/34 (100%)	0.26	0 100 100	46, 56, 90, 94	0
7	H	65/65 (100%)	-0.22	0 100 100	35, 45, 66, 74	0
7	h	63/65 (96%)	0.03	1 (1%) 70 67	42, 56, 68, 84	0
8	I	35/36 (97%)	-0.23	0 100 100	34, 44, 78, 88	0
8	i	35/36 (97%)	-0.08	0 100 100	35, 47, 79, 93	0
9	J	36/36 (100%)	-0.06	0 100 100	38, 56, 81, 107	0
9	j	36/36 (100%)	0.17	0 100 100	40, 59, 86, 98	0
10	K	37/37 (100%)	0.15	0 100 100	35, 59, 77, 81	1 (2%)
10	k	37/37 (100%)	0.24	0 100 100	48, 66, 83, 99	0
11	L	37/37 (100%)	-0.52	0 100 100	27, 36, 75, 82	0
11	l	36/37 (97%)	-0.52	0 100 100	29, 37, 82, 86	0
12	M	32/33 (96%)	-0.39	0 100 100	31, 39, 67, 84	0
12	m	31/33 (93%)	-0.45	0 100 100	28, 40, 55, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	-0.20	1 (0%) 88 87	23, 48, 85, 154	1 (0%)
13	o	244/244 (100%)	-0.23	1 (0%) 88 87	26, 46, 90, 131	0
14	T	29/30 (96%)	-0.55	0 100 100	28, 36, 69, 85	0
14	t	29/30 (96%)	-0.34	1 (3%) 48 45	31, 37, 89, 100	0
15	U	97/97 (100%)	-0.23	0 100 100	32, 49, 74, 102	0
15	u	97/97 (100%)	-0.27	1 (1%) 79 77	32, 47, 62, 95	0
16	V	137/137 (100%)	-0.38	0 100 100	31, 45, 62, 87	0
16	v	137/137 (100%)	-0.12	0 100 100	35, 55, 77, 87	0
17	Y	27/30 (90%)	0.90	2 (7%) 20 18	60, 85, 117, 125	0
17	y	30/30 (100%)	0.50	0 100 100	65, 77, 95, 115	0
18	X	38/38 (100%)	-0.02	0 100 100	40, 55, 87, 96	0
18	x	38/38 (100%)	0.03	0 100 100	48, 64, 82, 112	0
19	Z	62/62 (100%)	0.53	2 (3%) 50 47	51, 71, 119, 138	0
19	z	62/62 (100%)	0.70	2 (3%) 50 47	60, 78, 118, 134	0
20	R	34/34 (100%)	0.66	1 (2%) 53 50	60, 78, 102, 106	0
20	r	31/34 (91%)	1.05	3 (9%) 13 10	69, 92, 109, 119	0
All	All	5300/5326 (99%)	-0.25	24 (0%) 87 85	18, 43, 82, 154	9 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	t	30	THR	3.2
19	z	33	TRP	3.2
13	o	58	ASN	2.8
20	R	35	LEU	2.8
3	c	23	ALA	2.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	M	1	10/11	0.91	0.12	40,50,73,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.94	0.09	32,46,75,75	0
14	FME	t	1	10/11	0.94	0.09	33,48,73,78	0
8	FME	i	1	10/11	0.95	0.07	37,52,72,72	0
12	FME	m	1	10/11	0.95	0.10	34,58,78,84	0
8	FME	I	1	10/11	0.95	0.08	39,53,74,74	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
32	UNL	a	415	28/-	0.79	0.13	43,71,87,94	0
32	UNL	T	102	44/-	0.80	0.14	41,55,68,72	0
32	UNL	d	410	43/-	0.80	0.16	33,57,72,73	0
32	UNL	H	103	53/-	0.81	0.14	35,77,97,101	0
32	UNL	b	626	26/-	0.81	0.13	33,59,66,67	0
27	LMG	c	522	48/55	0.81	0.14	50,82,110,114	0
32	UNL	c	523	28/-	0.82	0.12	43,69,80,82	0
27	LMG	b	622	55/55	0.82	0.15	41,78,99,111	0
33	LHG	E	101	49/49	0.82	0.14	51,82,112,120	0
33	LHG	e	101	42/49	0.82	0.13	63,88,113,120	0
27	LMG	b	623	23/55	0.83	0.16	35,66,90,91	0
32	UNL	b	625	55/-	0.84	0.13	44,66,86,91	0
32	UNL	B	627	47/-	0.84	0.15	41,65,89,89	0
26	PL9	A	409	55/55	0.85	0.15	37,62,89,101	0
32	UNL	J	101	28/-	0.85	0.13	49,62,72,75	0
32	UNL	b	624	40/-	0.86	0.12	38,64,80,83	0
32	UNL	C	522	28/-	0.86	0.13	42,59,72,78	0
27	LMG	C	519	48/55	0.86	0.11	43,68,88,96	0
32	UNL	I	101	41/-	0.86	0.14	40,55,77,82	0
28	SQD	A	412	39/54	0.86	0.13	40,69,102,121	0
32	UNL	x	101	55/-	0.86	0.11	47,62,78,78	0
29	DGD	A	413	66/66	0.86	0.12	43,68,93,121	0
27	LMG	D	410	33/55	0.86	0.12	29,57,87,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	SQD	a	412	36/54	0.87	0.12	29,68,100,110	0
32	UNL	E	103	28/-	0.87	0.14	58,81,95,97	0
23	CLA	h	101	65/65	0.87	0.11	44,72,93,100	0
32	UNL	c	520	55/-	0.87	0.12	42,61,79,90	0
29	DGD	a	413	44/66	0.87	0.13	33,59,88,94	0
32	UNL	B	626	28/-	0.87	0.15	50,75,87,89	0
26	PL9	a	409	55/55	0.87	0.15	34,67,89,101	0
32	UNL	C	521	28/-	0.87	0.13	36,50,61,62	0
32	UNL	b	621	55/-	0.87	0.13	40,62,91,109	0
27	LMG	a	414	49/55	0.88	0.11	36,60,94,101	0
27	LMG	A	410	48/55	0.88	0.10	30,61,81,105	0
32	UNL	m	102	28/-	0.88	0.12	40,55,69,77	0
27	LMG	D	411	28/55	0.88	0.12	30,51,68,74	0
28	SQD	b	601	49/54	0.88	0.10	44,64,103,114	0
32	UNL	b	602	47/-	0.88	0.12	36,59,74,79	0
27	LMG	c	519	37/55	0.89	0.11	34,70,93,96	0
23	CLA	B	601	65/65	0.89	0.11	31,63,100,113	0
32	UNL	l	102	53/-	0.89	0.14	30,48,99,103	0
23	CLA	c	512	65/65	0.89	0.11	39,60,93,109	0
32	UNL	t	103	46/-	0.89	0.12	38,61,81,82	0
32	UNL	M	102	26/-	0.89	0.12	30,53,63,67	0
28	SQD	a	411	54/54	0.89	0.10	36,71,94,110	0
32	UNL	B	624	34/-	0.89	0.11	39,55,71,72	0
25	BCR	y	101	40/40	0.90	0.11	41,63,77,84	0
25	BCR	C	514	40/40	0.90	0.10	34,59,76,77	0
25	BCR	D	405	40/40	0.90	0.10	29,46,100,116	0
25	BCR	c	514	40/40	0.90	0.10	37,58,73,75	0
27	LMG	B	620	51/55	0.90	0.09	29,51,72,81	0
32	UNL	j	101	28/-	0.90	0.11	42,60,71,74	0
32	UNL	B	621	43/-	0.90	0.10	38,54,69,73	0
25	BCR	d	405	40/40	0.90	0.10	36,57,95,108	0
32	UNL	t	102	26/-	0.90	0.11	42,56,67,68	0
32	UNL	B	625	28/-	0.90	0.10	29,46,67,72	0
27	LMG	m	101	51/55	0.90	0.10	29,52,83,98	0
25	BCR	h	102	40/40	0.90	0.10	33,56,73,81	0
28	SQD	B	623	54/54	0.90	0.10	37,62,88,98	0
25	BCR	c	521	40/40	0.91	0.11	34,57,70,77	0
32	UNL	C	523	47/-	0.91	0.10	39,52,63,69	0
32	UNL	D	412	55/-	0.91	0.11	32,51,79,101	0
23	CLA	c	513	65/65	0.91	0.10	42,75,107,123	0
28	SQD	f	101	41/54	0.91	0.12	49,85,120,123	0
25	BCR	K	101	40/40	0.91	0.09	41,56,68,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	BCR	C	520	40/40	0.91	0.12	38,55,67,74	0
32	UNL	M	101	37/-	0.91	0.11	30,49,71,75	0
29	DGD	h	103	62/66	0.91	0.10	35,54,73,79	0
29	DGD	C	517	62/66	0.92	0.10	31,56,95,117	0
23	CLA	C	513	65/65	0.92	0.10	40,70,102,114	0
27	LMG	d	409	44/55	0.92	0.09	31,53,84,107	0
25	BCR	B	617	40/40	0.92	0.09	26,43,57,60	0
25	BCR	T	101	40/40	0.92	0.08	29,43,58,68	0
25	BCR	b	619	40/40	0.92	0.07	25,42,59,66	0
29	DGD	c	517	62/66	0.93	0.08	32,52,81,95	0
29	DGD	c	518	62/66	0.93	0.09	26,54,77,93	0
23	CLA	c	511	65/65	0.93	0.10	34,62,79,87	0
23	CLA	C	511	65/65	0.93	0.09	33,57,78,85	0
23	CLA	C	512	65/65	0.93	0.10	36,61,111,127	0
25	BCR	H	101	40/40	0.93	0.07	32,46,59,66	0
28	SQD	A	411	52/54	0.93	0.09	30,64,88,97	0
23	CLA	C	510	65/65	0.93	0.08	31,51,78,88	0
24	PHO	d	401	64/64	0.93	0.08	27,42,52,57	0
28	SQD	F	101	36/54	0.93	0.10	43,66,89,96	0
25	BCR	a	408	40/40	0.93	0.07	25,35,50,55	0
25	BCR	b	618	40/40	0.93	0.07	25,46,57,65	0
23	CLA	c	503	65/65	0.93	0.08	31,48,61,68	0
25	BCR	b	620	40/40	0.93	0.08	30,50,66,69	0
25	BCR	B	618	40/40	0.93	0.07	25,43,58,64	0
25	BCR	c	515	40/40	0.93	0.10	32,49,69,77	0
29	DGD	H	102	62/66	0.93	0.09	28,49,67,77	0
33	LHG	a	410	49/49	0.93	0.10	38,53,87,104	0
25	BCR	B	619	40/40	0.93	0.08	33,47,58,62	0
33	LHG	l	101	49/49	0.93	0.09	31,49,66,78	0
27	LMG	D	407	51/55	0.94	0.10	27,59,79,87	0
23	CLA	B	606	65/65	0.94	0.08	21,41,75,98	0
23	CLA	B	615	65/65	0.94	0.08	20,41,67,95	0
23	CLA	B	616	60/65	0.94	0.09	27,44,87,103	0
23	CLA	C	503	65/65	0.94	0.07	27,44,56,69	0
25	BCR	A	408	40/40	0.94	0.07	24,34,42,56	0
31	BCT	A	415	4/4	0.94	0.07	31,36,37,44	0
23	CLA	b	610	65/65	0.94	0.08	28,46,65,77	0
23	CLA	b	615	65/65	0.94	0.08	23,44,73,79	0
23	CLA	b	616	65/65	0.94	0.08	20,40,63,68	0
23	CLA	C	505	65/65	0.94	0.09	24,42,75,88	0
25	BCR	t	101	40/40	0.94	0.07	27,42,57,61	0
25	BCR	C	515	40/40	0.94	0.08	21,38,53,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	c	505	65/65	0.94	0.08	26,44,62,69	0
26	PL9	D	406	55/55	0.94	0.07	22,36,51,54	0
23	CLA	c	506	65/65	0.94	0.10	32,53,112,129	0
26	PL9	d	406	55/55	0.94	0.07	23,37,48,48	0
33	LHG	B	622	49/49	0.94	0.09	26,46,73,77	0
33	LHG	D	409	47/49	0.94	0.09	25,51,82,101	0
23	CLA	c	508	64/65	0.94	0.08	32,51,98,118	0
23	CLA	c	509	65/65	0.94	0.09	28,49,74,79	0
33	LHG	d	408	39/49	0.94	0.09	36,50,75,78	0
23	CLA	C	508	65/65	0.94	0.08	27,46,102,120	0
29	DGD	C	516	62/66	0.94	0.09	21,40,76,98	0
29	DGD	C	518	62/66	0.95	0.07	28,47,84,98	0
23	CLA	C	507	65/65	0.95	0.07	22,39,51,59	0
23	CLA	D	403	65/65	0.95	0.07	15,34,60,62	0
29	DGD	c	516	62/66	0.95	0.08	20,45,71,80	0
23	CLA	a	405	65/65	0.95	0.08	25,42,98,111	0
23	CLA	c	510	65/65	0.95	0.08	30,51,72,79	0
23	CLA	b	603	65/65	0.95	0.08	29,47,74,80	0
23	CLA	b	604	65/65	0.95	0.07	24,41,67,69	0
23	CLA	b	607	65/65	0.95	0.08	25,46,80,86	0
23	CLA	d	402	65/65	0.95	0.07	22,34,43,51	0
23	CLA	d	403	65/65	0.95	0.07	20,38,63,75	0
23	CLA	d	404	65/65	0.95	0.08	25,53,100,107	0
23	CLA	b	609	65/65	0.95	0.07	26,43,65,70	0
24	PHO	a	406	64/64	0.95	0.07	22,34,46,48	0
23	CLA	C	502	65/65	0.95	0.07	25,42,62,68	0
23	CLA	b	613	65/65	0.95	0.07	17,35,49,56	0
23	CLA	C	509	65/65	0.95	0.08	27,46,61,74	0
23	CLA	B	609	65/65	0.95	0.07	23,37,52,63	0
23	CLA	c	501	65/65	0.95	0.07	25,42,59,68	0
33	LHG	L	101	49/49	0.95	0.07	28,45,61,67	0
23	CLA	c	502	65/65	0.95	0.08	24,46,76,85	0
33	LHG	d	407	49/49	0.95	0.08	26,45,64,80	0
23	CLA	B	613	65/65	0.95	0.07	17,34,63,74	0
23	CLA	c	504	60/65	0.95	0.07	24,47,79,81	0
23	CLA	C	506	65/65	0.95	0.09	28,45,95,114	0
23	CLA	A	404	65/65	0.96	0.06	16,29,43,51	0
23	CLA	B	610	65/65	0.96	0.07	18,33,48,50	0
24	PHO	A	406	64/64	0.96	0.06	17,30,42,53	0
24	PHO	D	401	64/64	0.96	0.06	23,35,46,51	0
23	CLA	b	611	65/65	0.96	0.08	25,39,59,60	0
23	CLA	b	612	65/65	0.96	0.06	18,36,51,56	0

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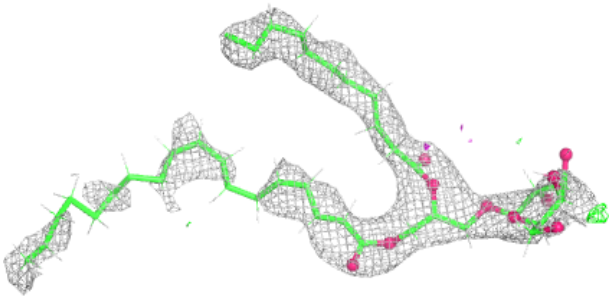
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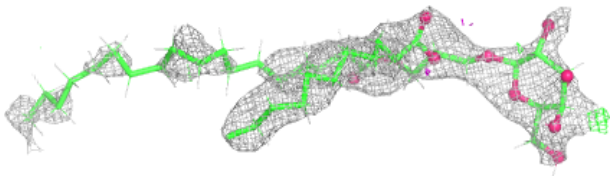
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	611	65/65	0.96	0.06	19,32,49,53	0
23	CLA	b	614	65/65	0.96	0.07	19,33,86,94	0
23	CLA	B	612	65/65	0.96	0.07	17,32,57,69	0
23	CLA	B	602	65/65	0.96	0.07	24,39,68,80	0
23	CLA	b	617	60/65	0.96	0.08	26,49,99,106	0
23	CLA	B	614	65/65	0.96	0.08	22,41,85,96	0
23	CLA	B	603	65/65	0.96	0.07	18,34,60,70	0
23	CLA	B	604	65/65	0.96	0.08	21,36,84,94	0
23	CLA	D	402	65/65	0.96	0.06	17,29,54,61	0
23	CLA	C	501	65/65	0.96	0.07	24,37,54,64	0
23	CLA	D	404	65/65	0.96	0.08	19,42,114,122	0
23	CLA	c	507	65/65	0.96	0.07	28,45,63,74	0
33	LHG	D	408	49/49	0.96	0.07	22,43,59,74	0
23	CLA	a	404	65/65	0.96	0.06	20,32,45,53	0
23	CLA	B	605	65/65	0.96	0.07	18,33,47,57	0
23	CLA	a	407	65/65	0.96	0.08	15,37,99,110	0
23	CLA	A	405	65/65	0.96	0.08	23,36,106,121	0
23	CLA	C	504	59/65	0.96	0.08	22,44,81,96	0
23	CLA	b	605	65/65	0.96	0.08	20,39,87,103	0
23	CLA	b	606	65/65	0.96	0.07	21,36,53,59	0
23	CLA	B	607	65/65	0.96	0.08	18,35,71,85	0
23	CLA	b	608	65/65	0.97	0.07	19,37,78,96	0
23	CLA	A	407	54/65	0.97	0.06	12,31,68,79	0
31	BCT	a	417	4/4	0.97	0.05	30,37,42,45	0
23	CLA	B	608	65/65	0.97	0.06	19,37,56,61	0
34	HEM	E	102	43/43	0.97	0.08	33,52,67,72	0
34	HEM	e	102	43/43	0.97	0.09	39,56,79,91	0
22	CL	A	402	1/1	0.98	0.04	26,26,26,26	0
22	CL	a	403	1/1	0.98	0.09	29,29,29,29	0
35	HEC	V	201	43/43	0.98	0.06	25,34,45,49	0
35	HEC	v	201	43/43	0.98	0.07	26,38,52,54	0
30	OEY	a	416	11/11	0.99	0.03	24,30,34,35	0
21	FE2	a	401	1/1	0.99	0.02	37,37,37,37	0
21	FE2	A	401	1/1	0.99	0.01	33,33,33,33	0
22	CL	A	403	1/1	1.00	0.04	25,25,25,25	0
22	CL	a	402	1/1	1.00	0.04	31,31,31,31	0
30	OEY	A	414	11/11	1.00	0.02	28,31,39,43	1

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

Electron density around LMG c 522:

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

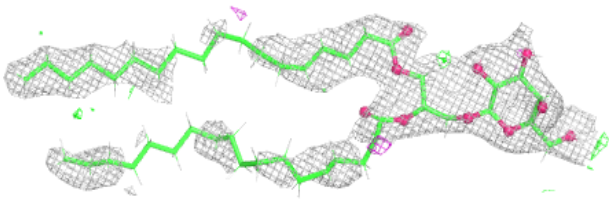


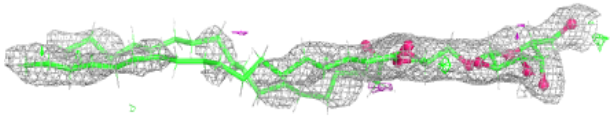


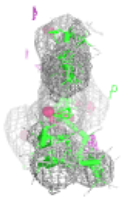


Electron density around LMG b 622:

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

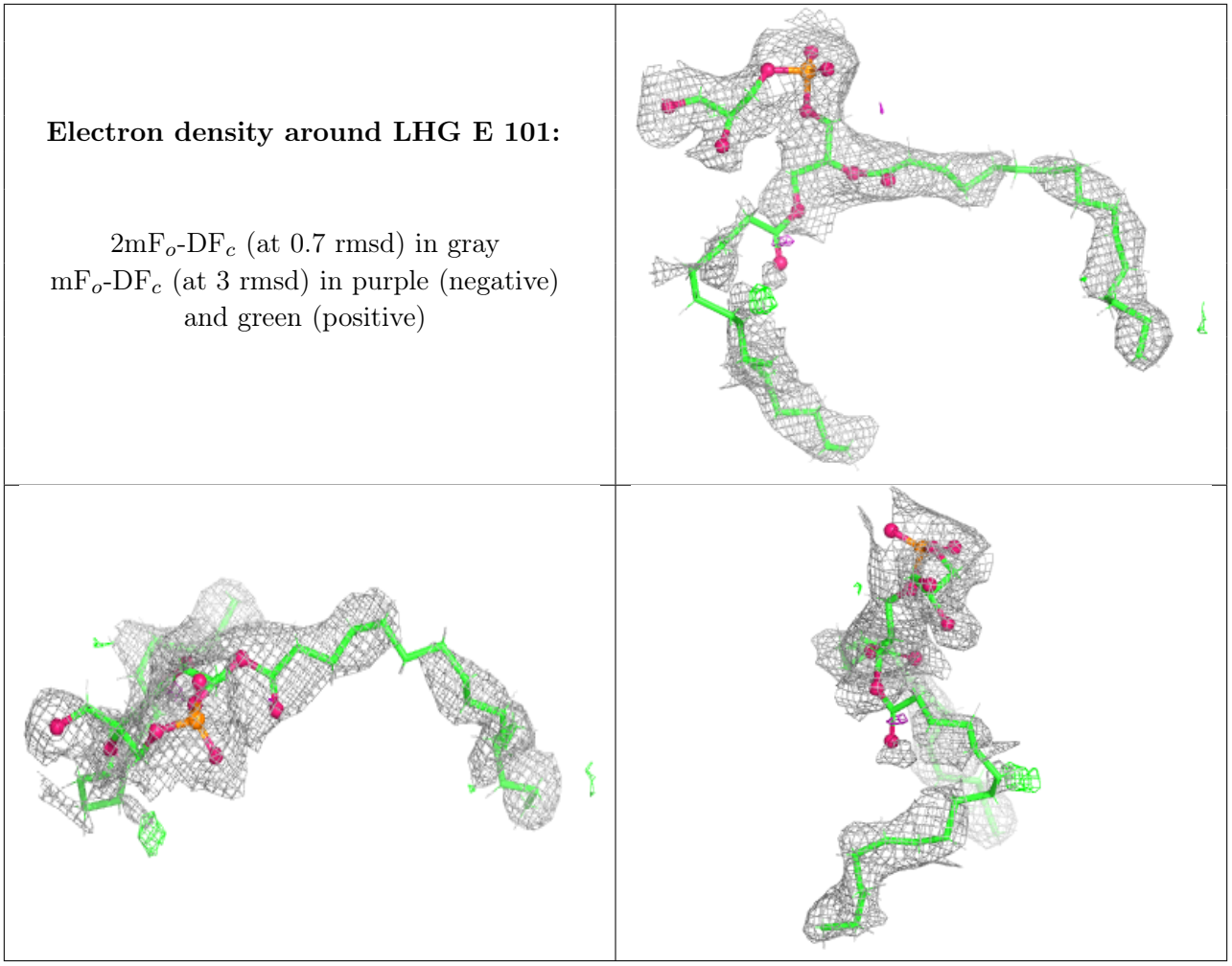






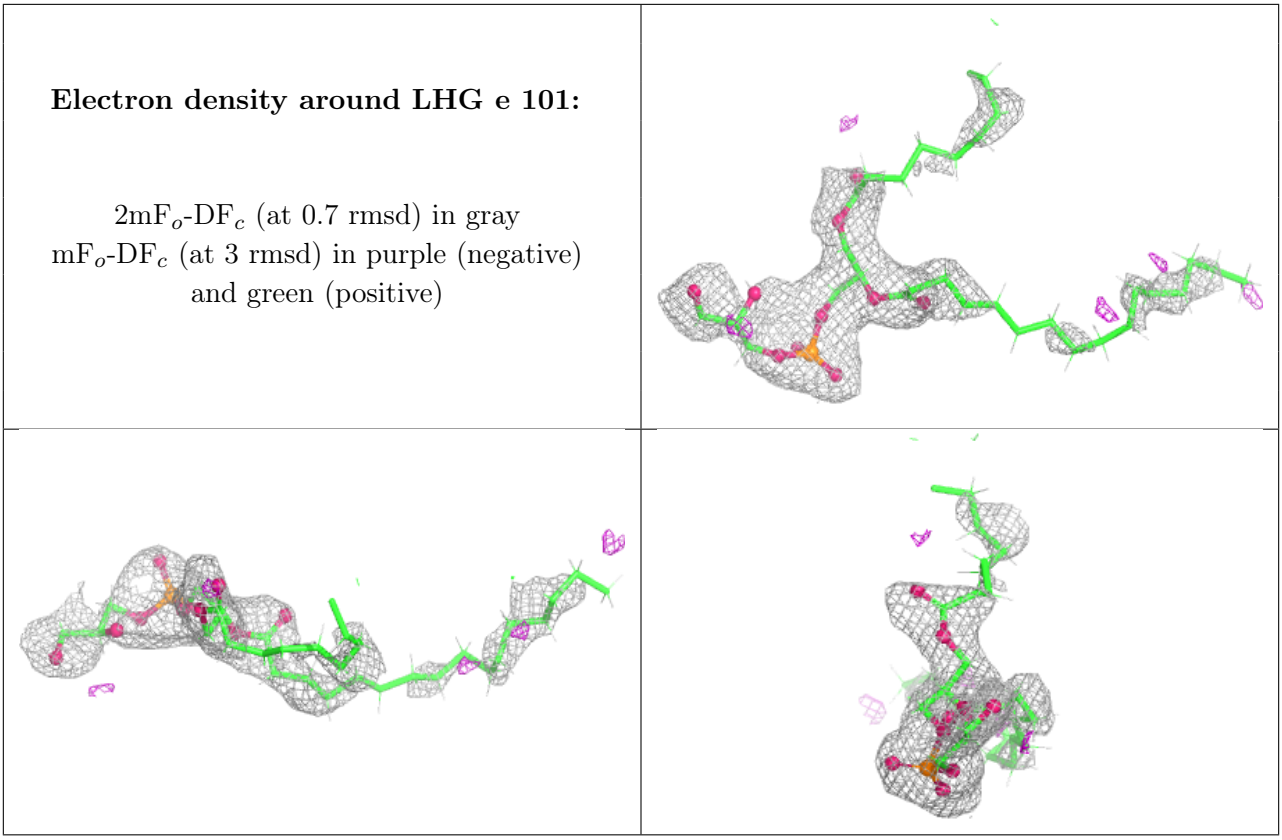
Electron density around LHG E 101:

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



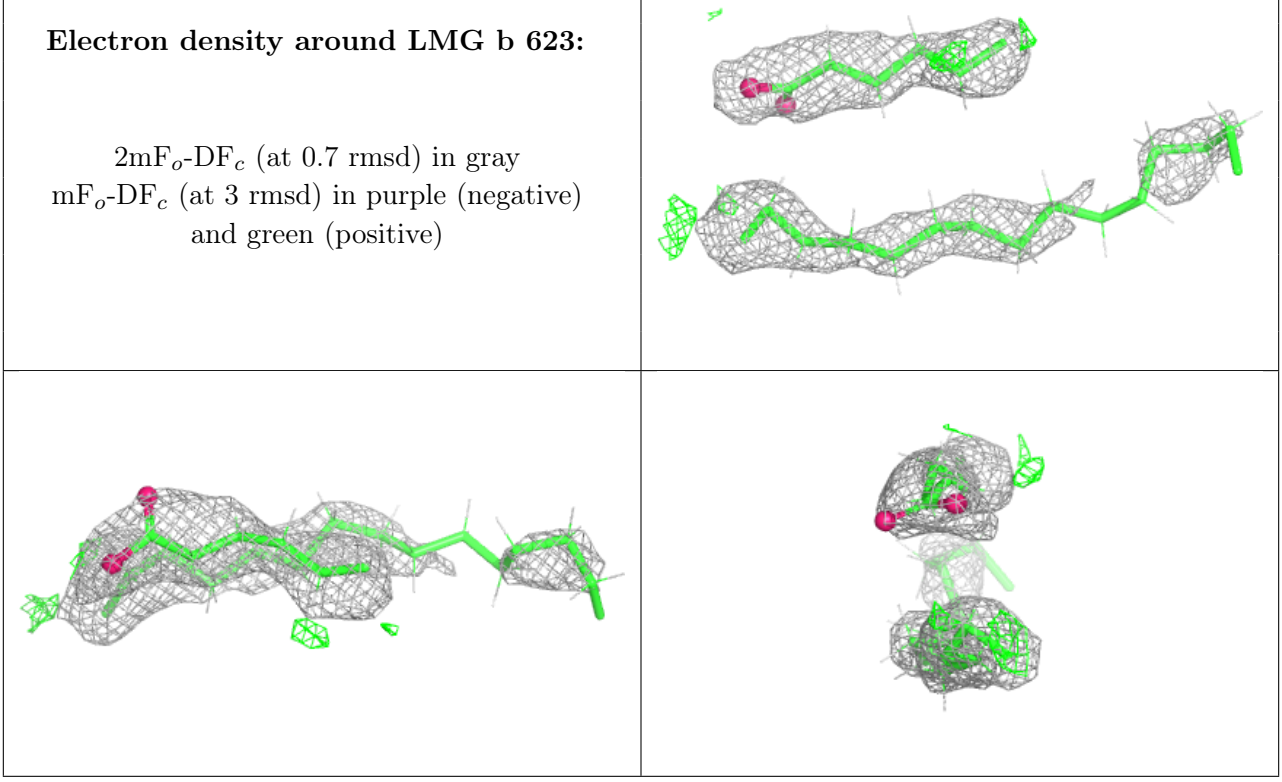
Electron density around LHG e 101:

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



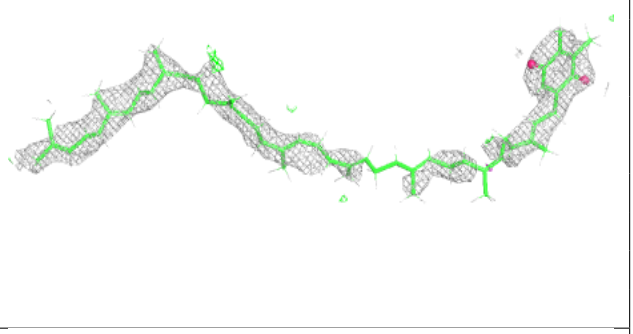
Electron density around LMG b 623:

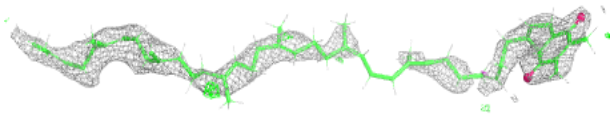
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

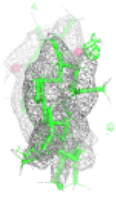


Electron density around PL9 A 409:

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

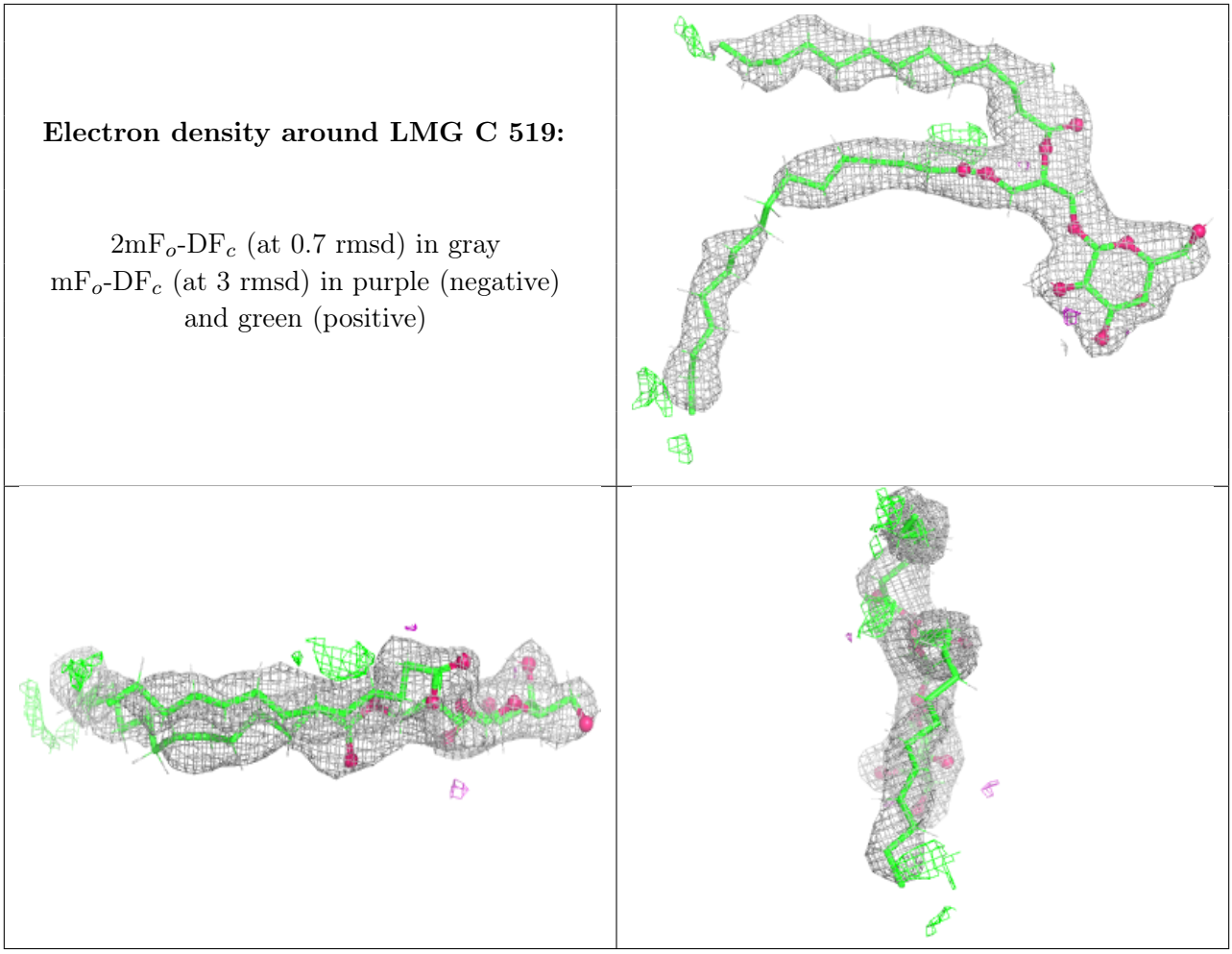






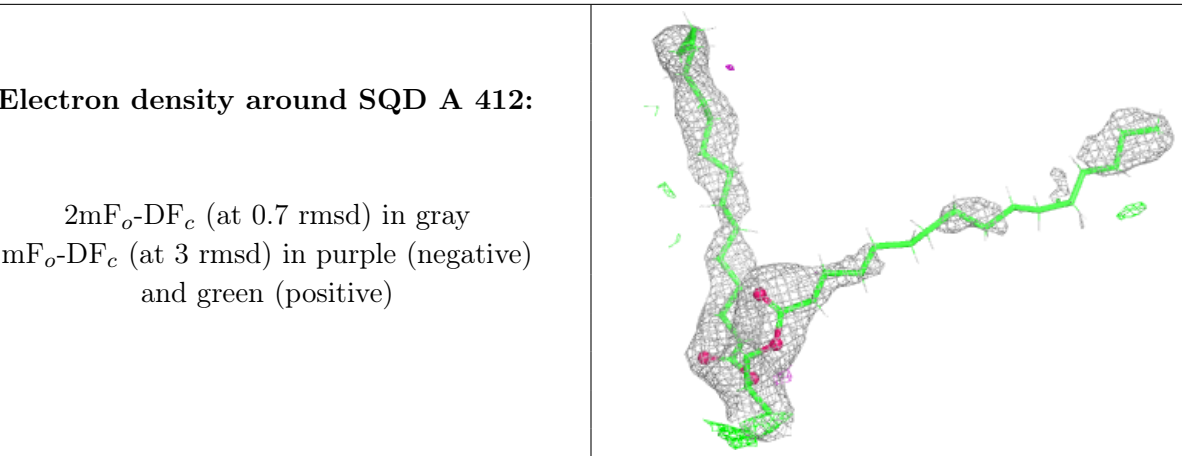
Electron density around LMG C 519:

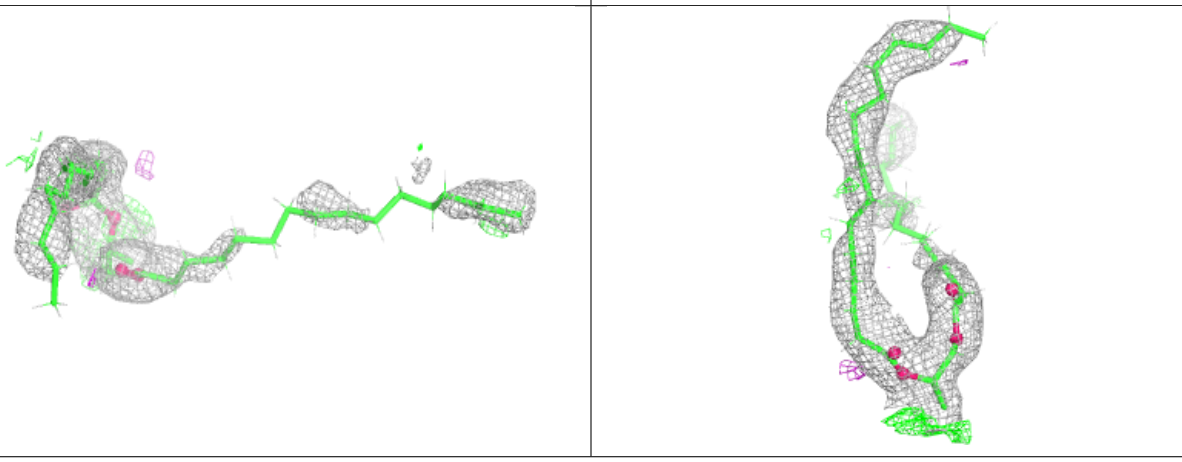
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD A 412:

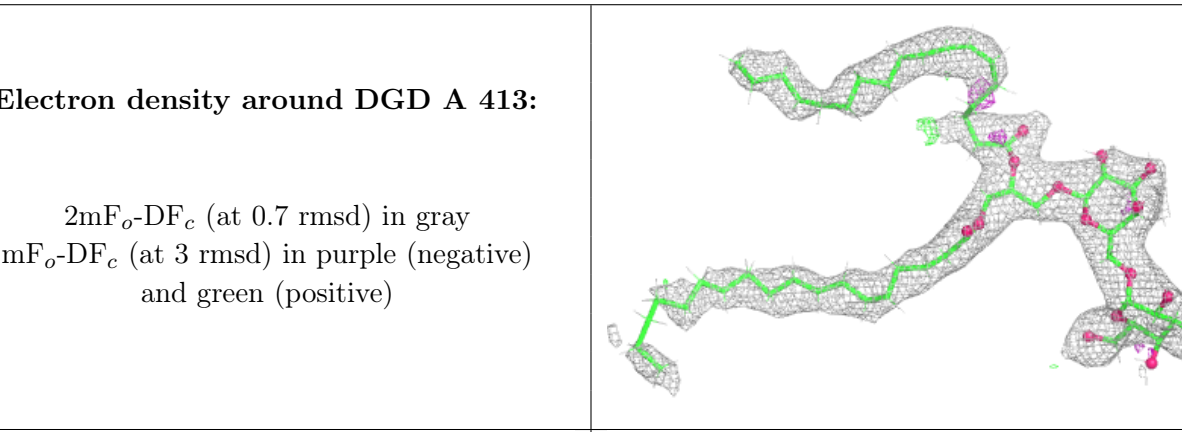
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

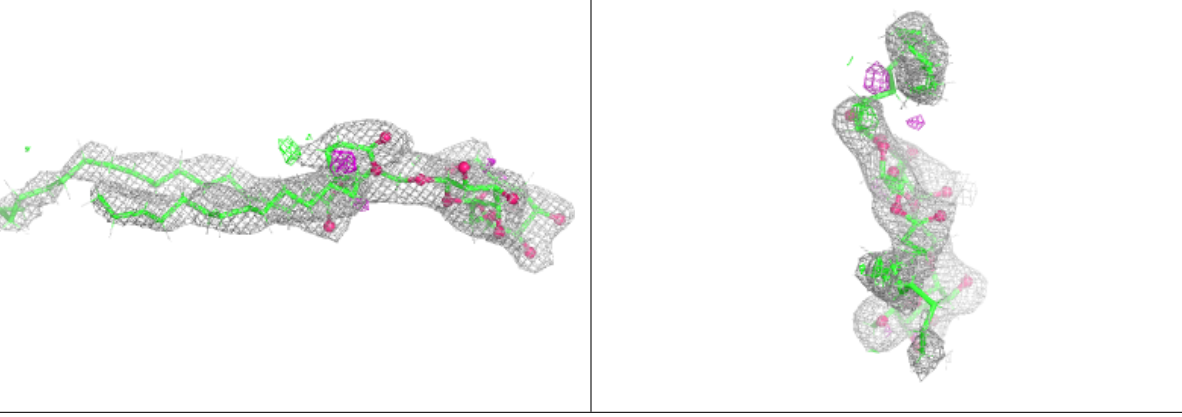




Electron density around DGD A 413:

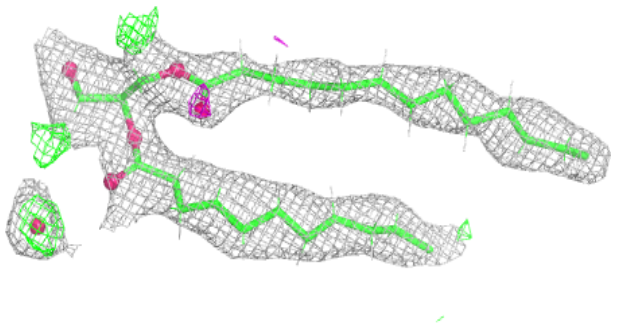
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

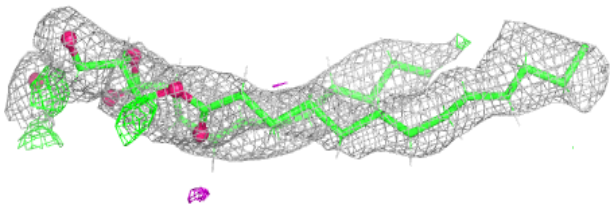


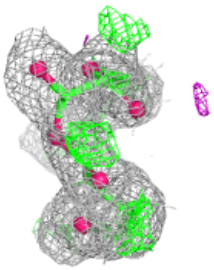


Electron density around LMG D 410:

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



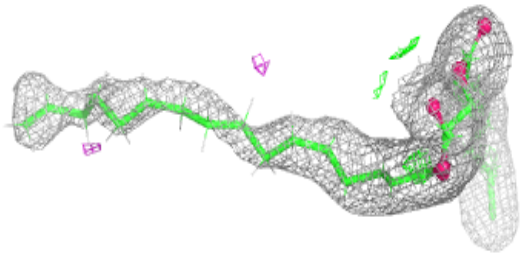


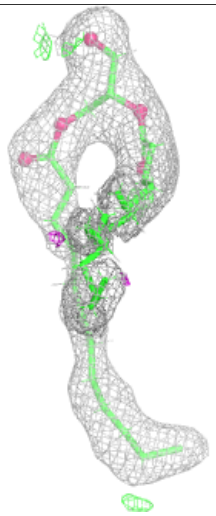


Electron density around SQD a 412:

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

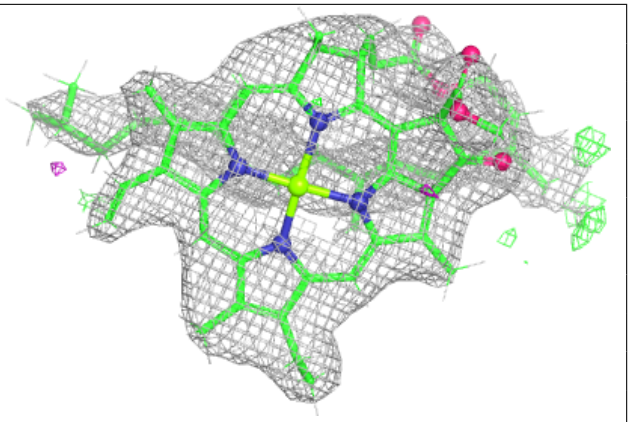


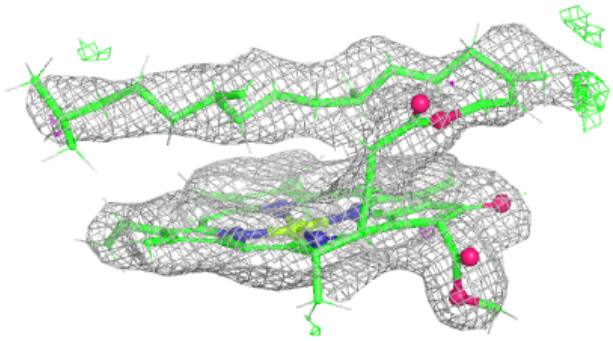


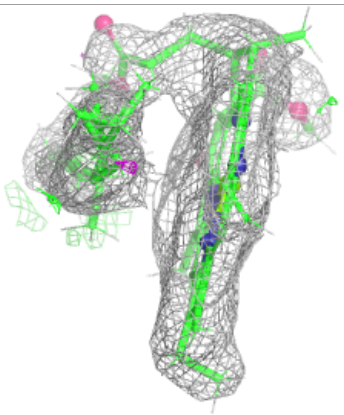


Electron density around CLA h 101:

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

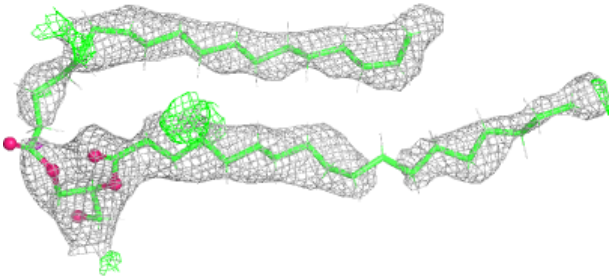


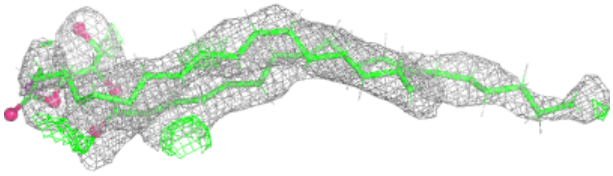


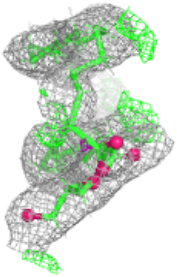


Electron density around DGD a 413:

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

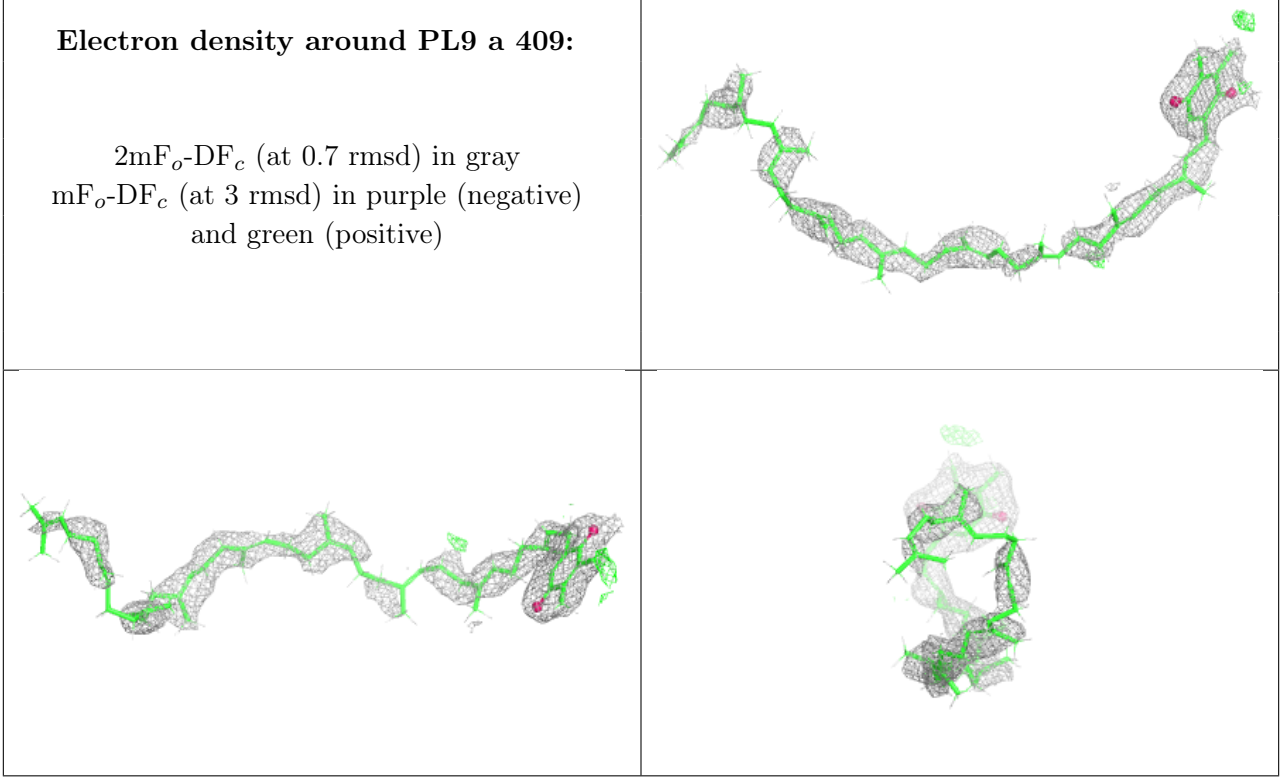






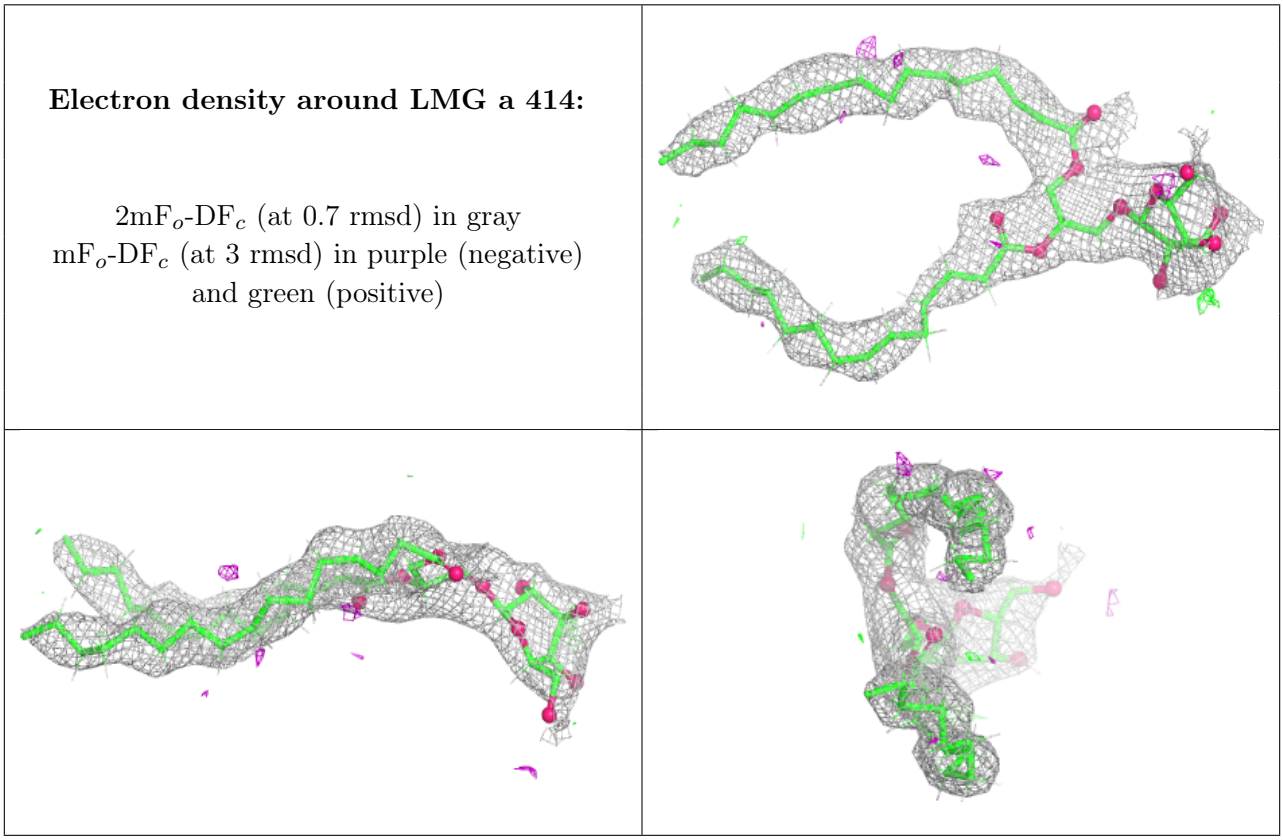
Electron density around PL9 a 409:

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



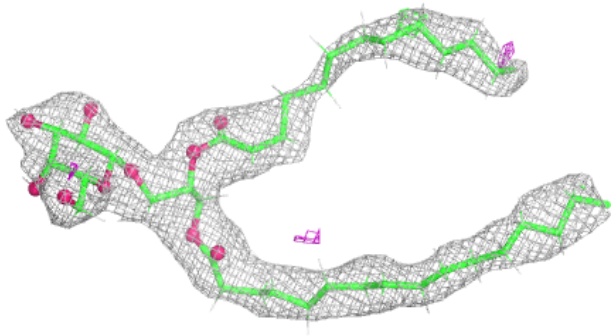
Electron density around LMG a 414:

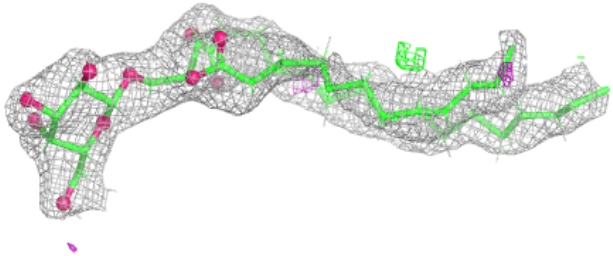
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

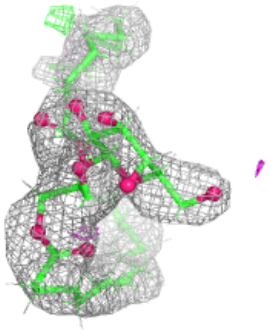


Electron density around LMG A 410:

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

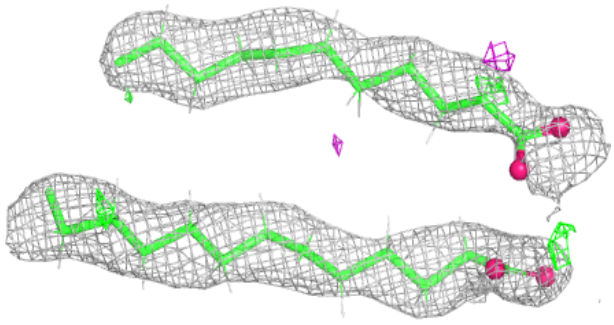


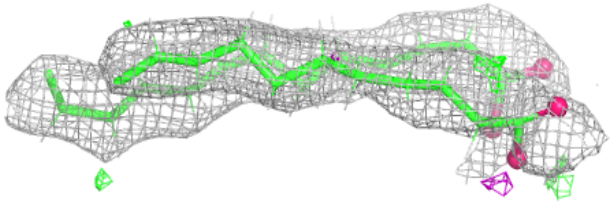


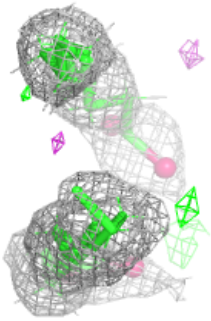


Electron density around LMG D 411:

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

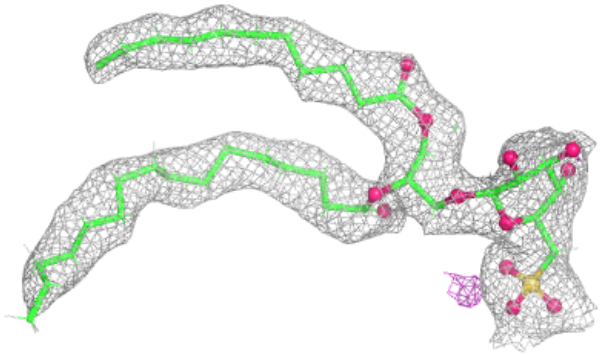


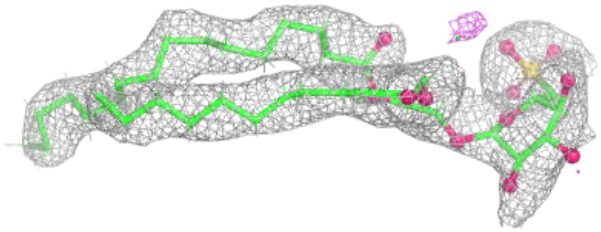


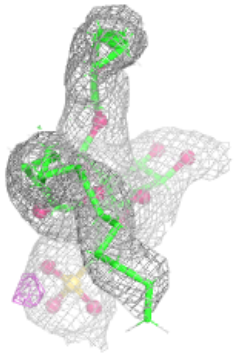


Electron density around SQD b 601:

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

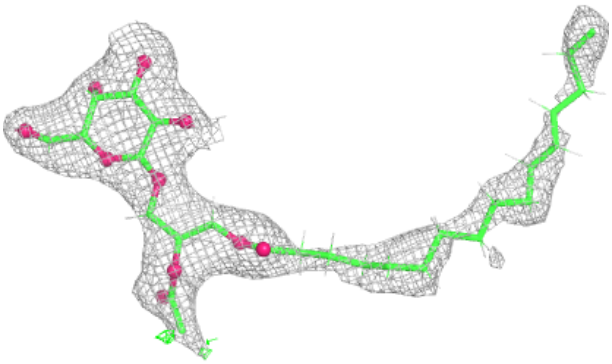


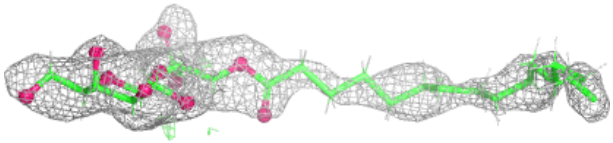


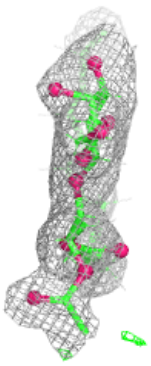


Electron density around LMG c 519:

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

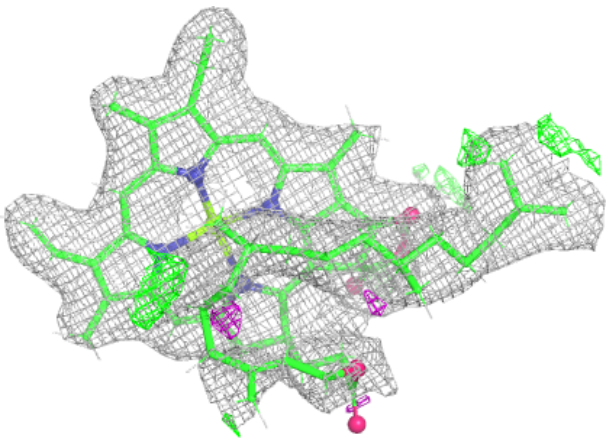


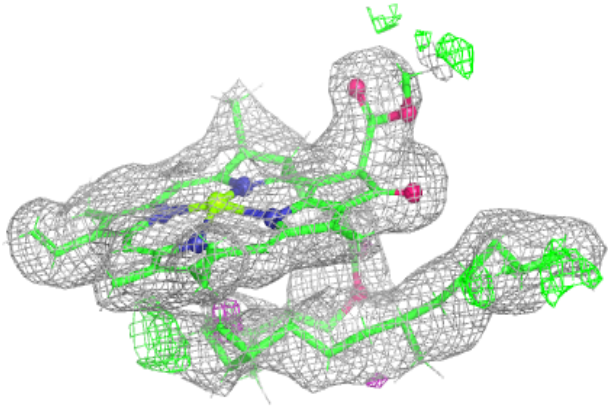


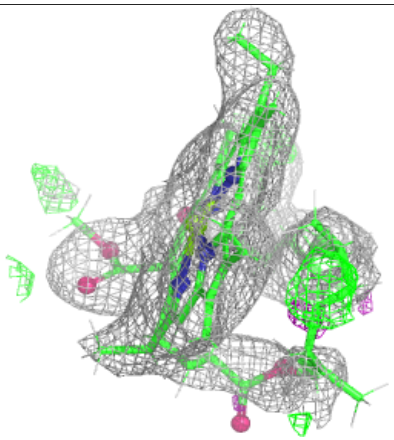


Electron density around CLA B 601:

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

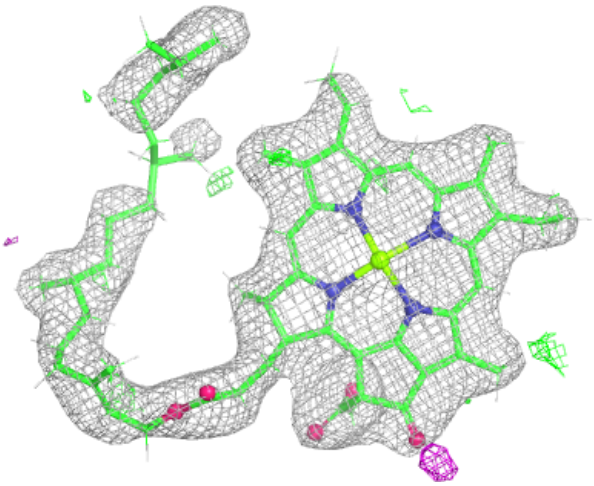


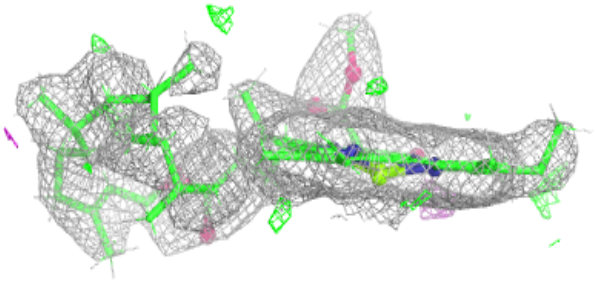


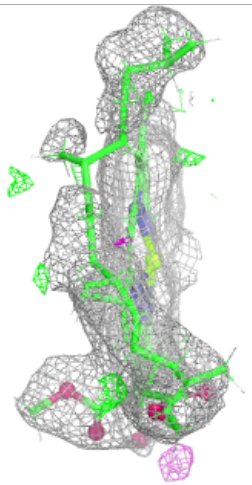


Electron density around CLA c 512:

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

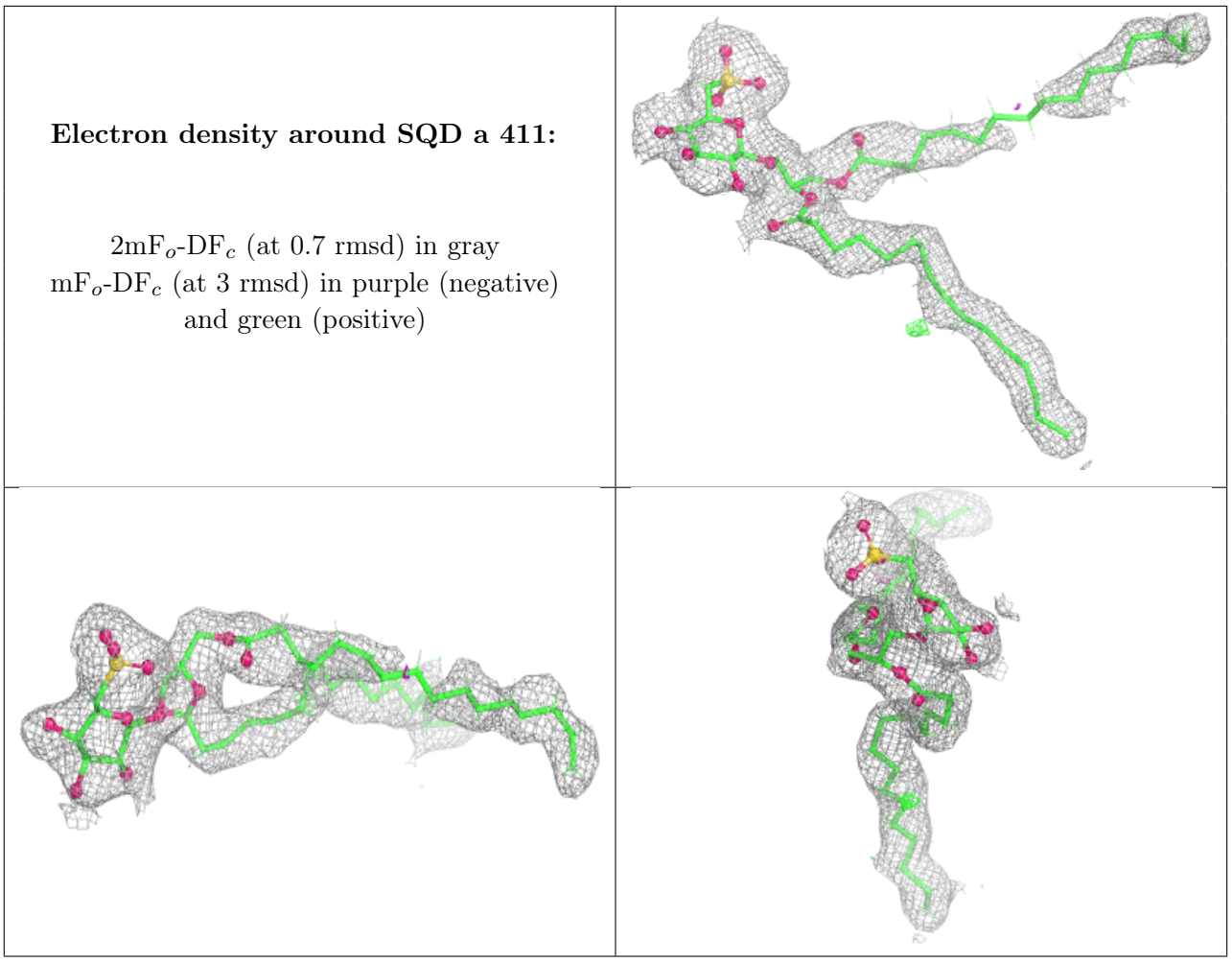






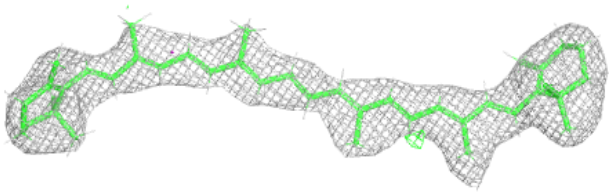
Electron density around SQD a 411:

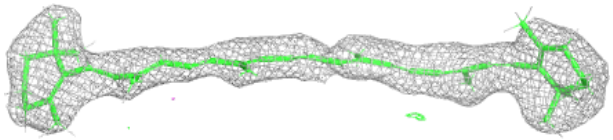
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

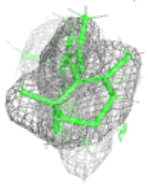


Electron density around BCR y 101:

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

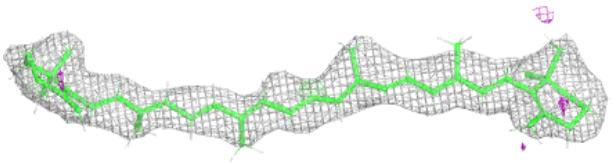


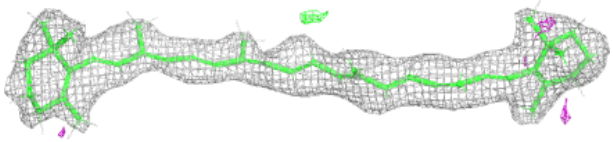


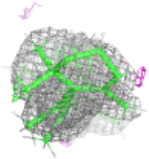


Electron density around BCR C 514:

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

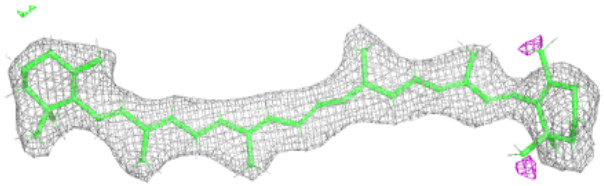


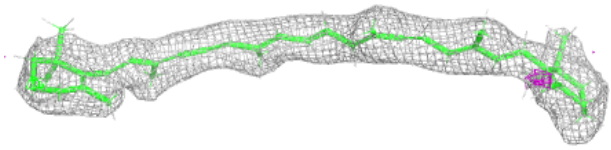


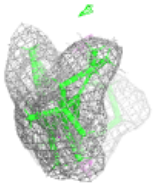


Electron density around BCR D 405:

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

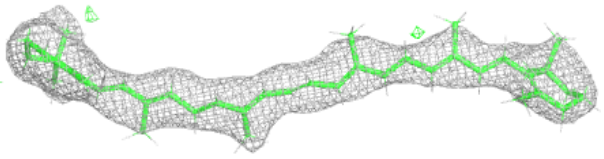


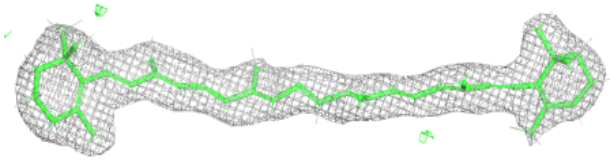


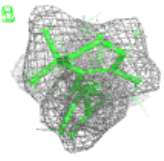


Electron density around BCR c 514:

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

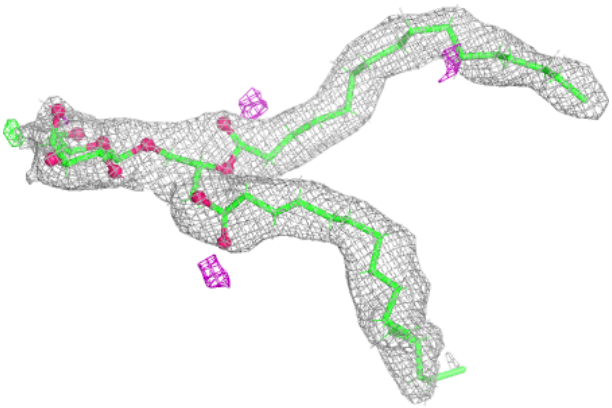


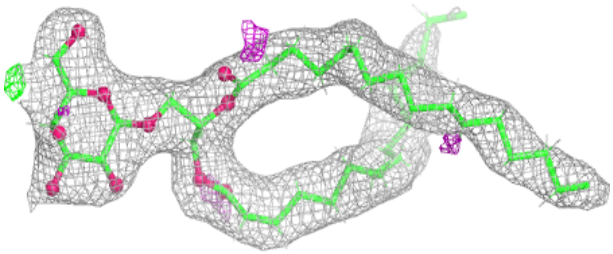


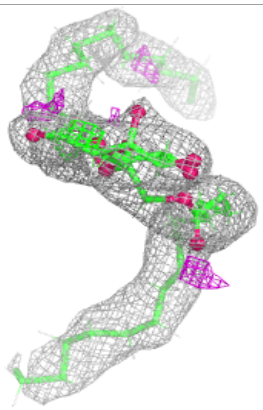


Electron density around LMG B 620:

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

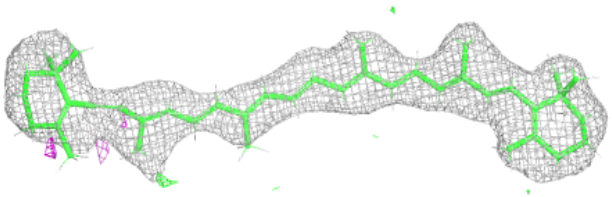


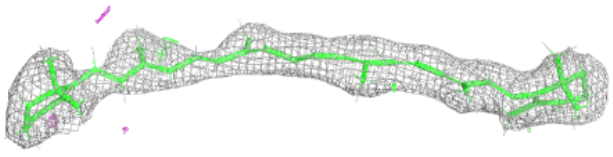


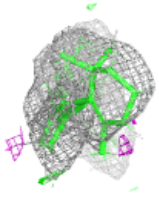


Electron density around BCR d 405:

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

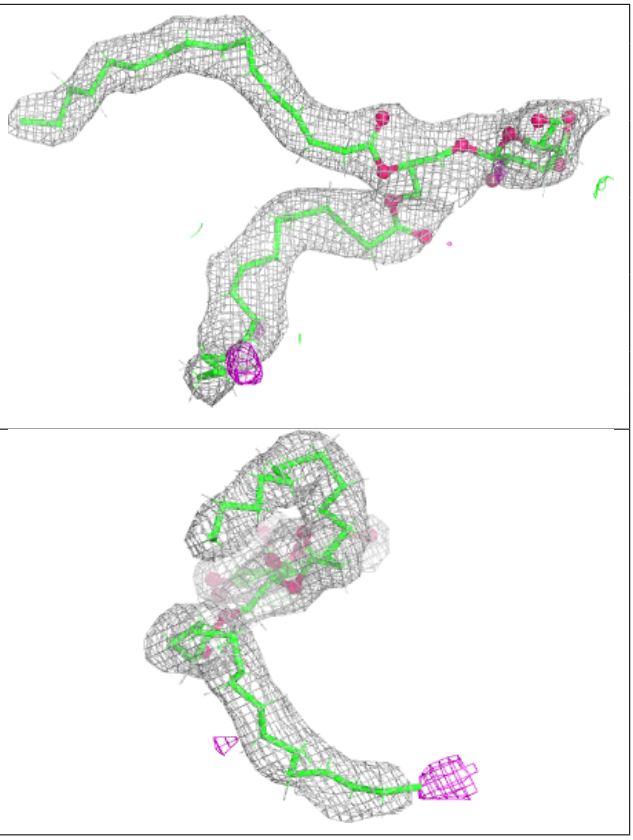






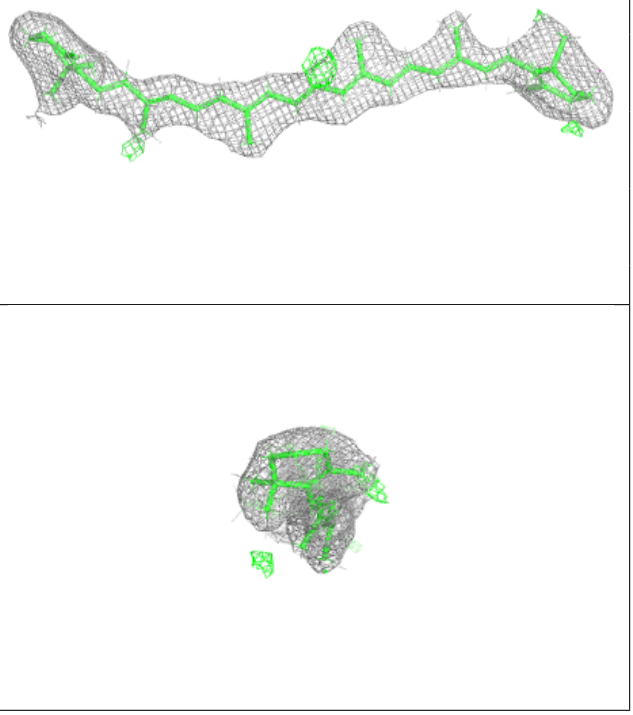
Electron density around LMG m 101:

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



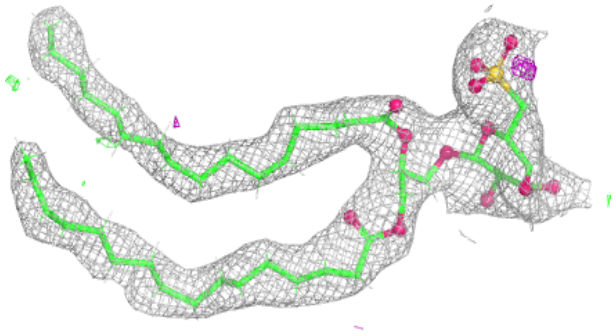
Electron density around BCR h 102:

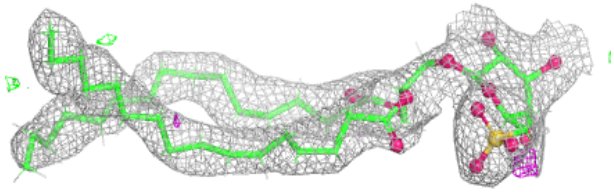
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

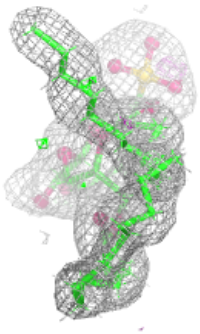


Electron density around SQD B 623:

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

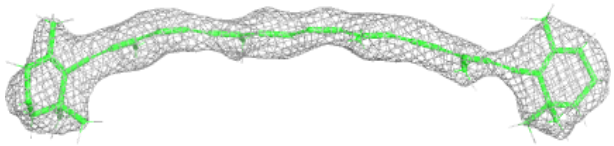


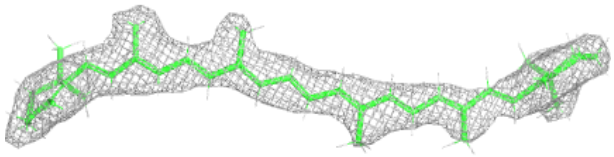


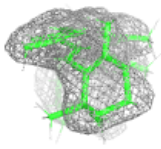


Electron density around BCR c 521:

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

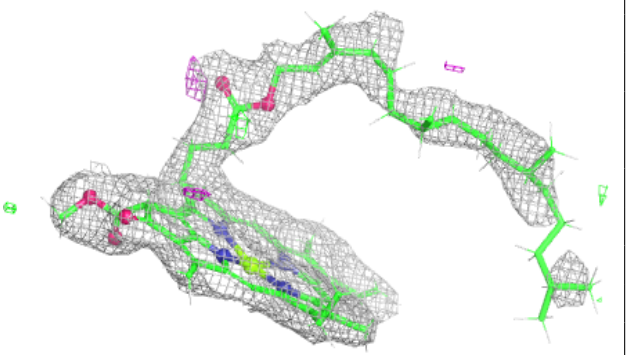


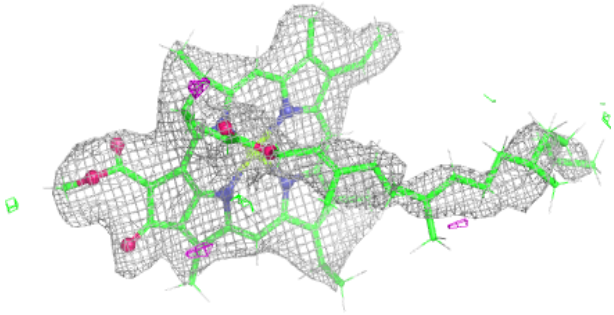


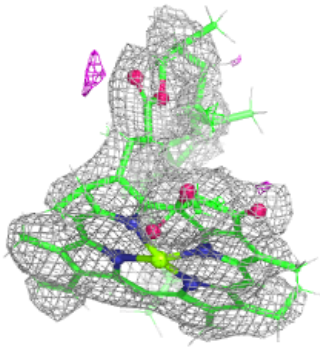


Electron density around CLA c 513:

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

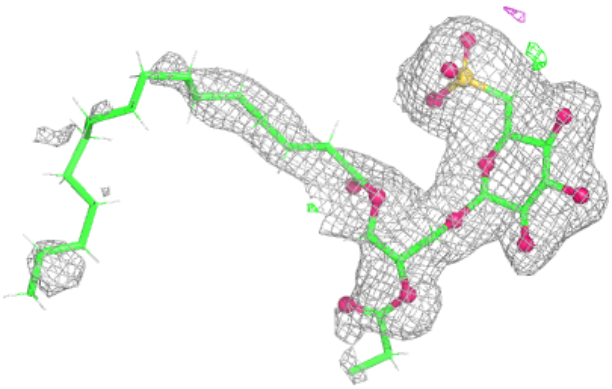


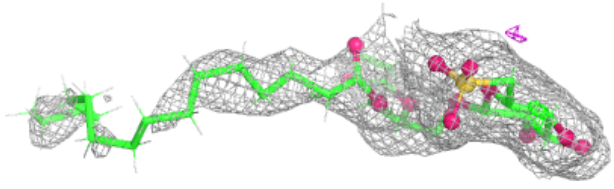


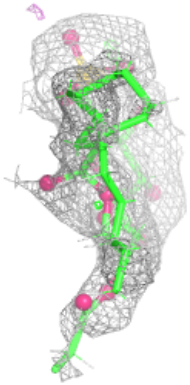


Electron density around SQD f 101:

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

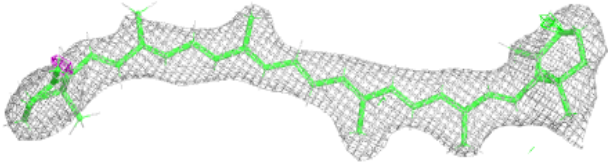


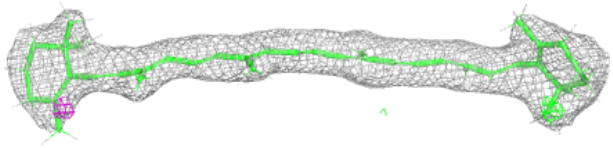


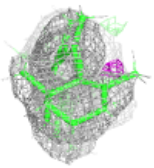


Electron density around BCR K 101:

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

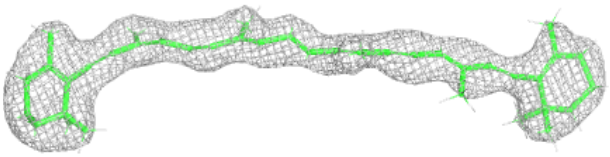


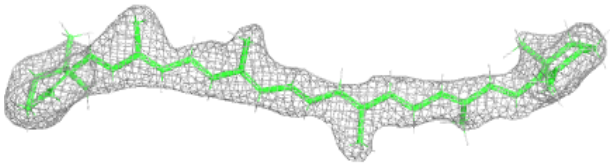


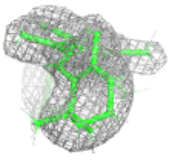


Electron density around BCR C 520:

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

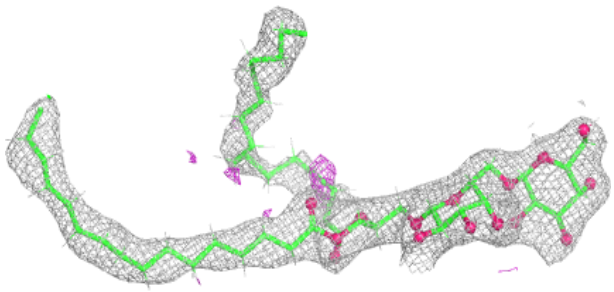


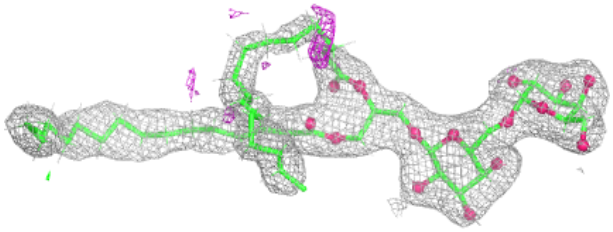




Electron density around DGD h 103:

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

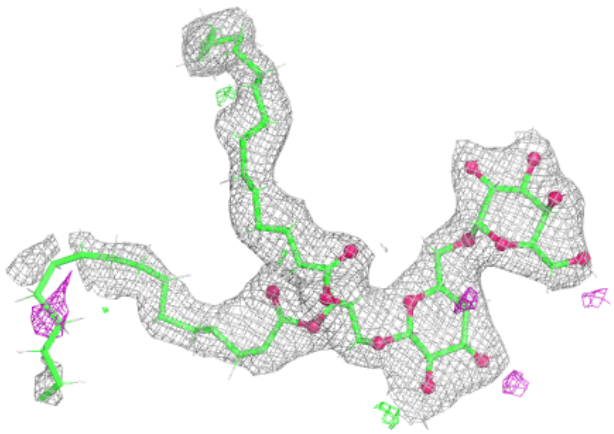


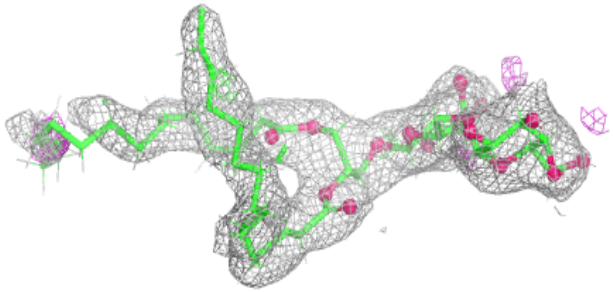


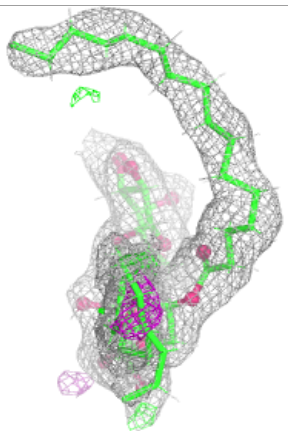


Electron density around DGD C 517:

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

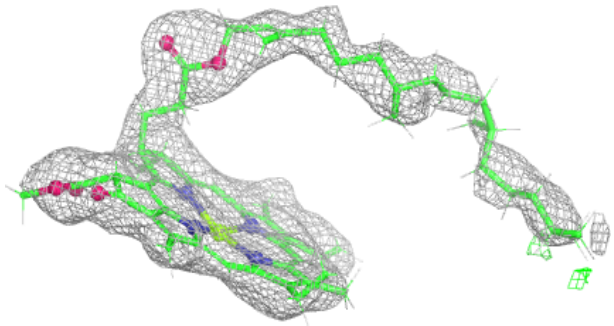


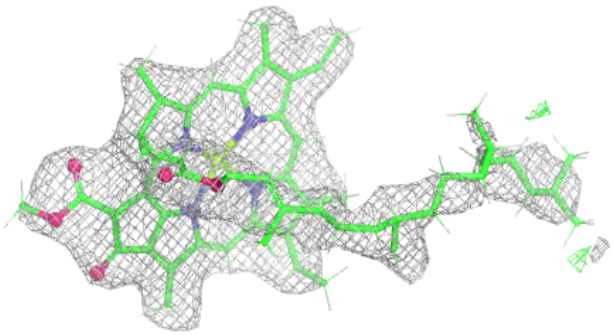


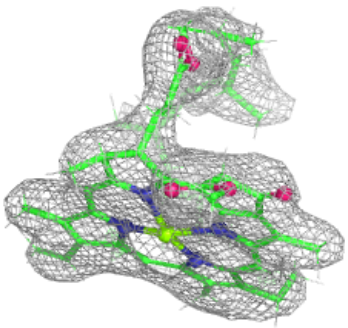


Electron density around CLA C 513:

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

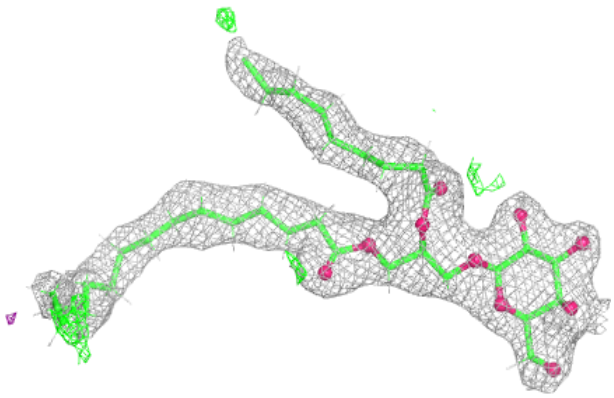


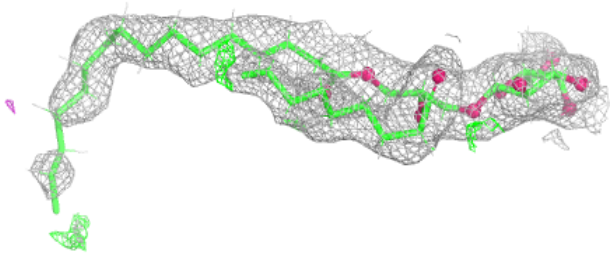


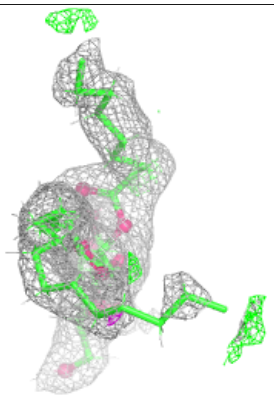


Electron density around LMG d 409:

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

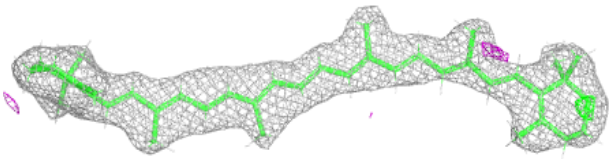


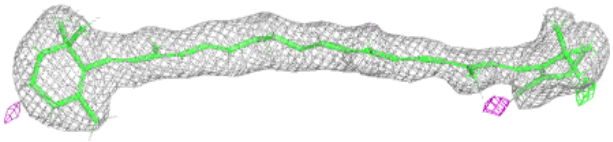


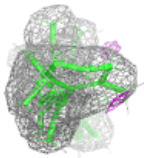


Electron density around BCR B 617:

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

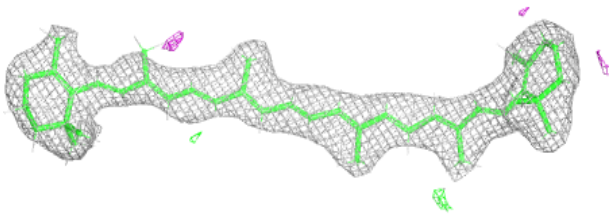


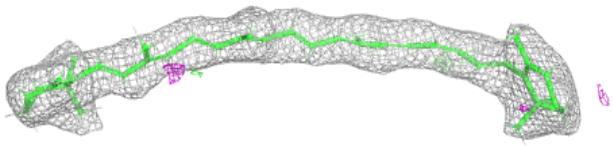


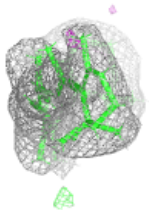


Electron density around BCR T 101:

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

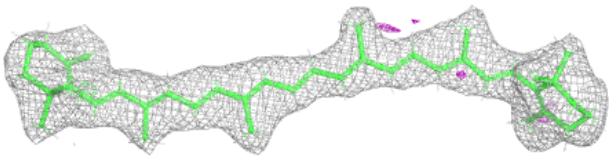


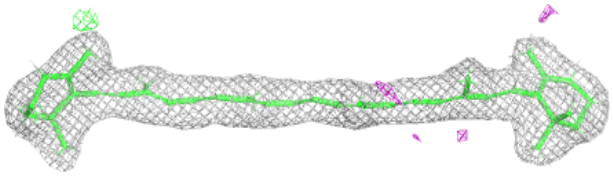


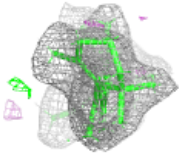


Electron density around BCR b 619:

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

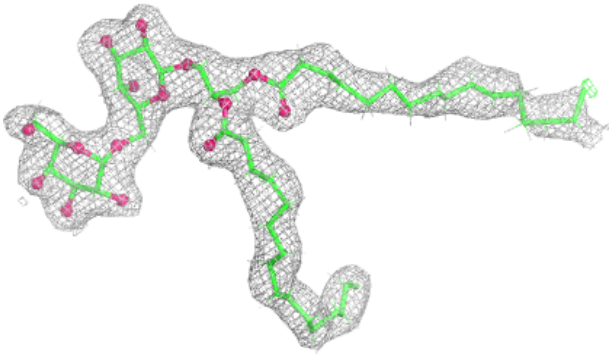


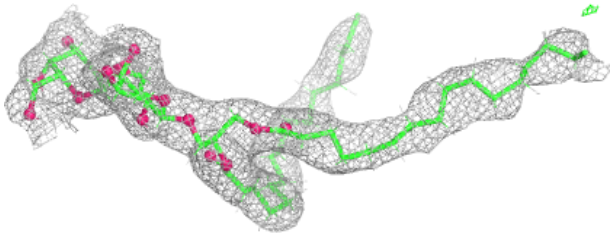




Electron density around DGD c 517:

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

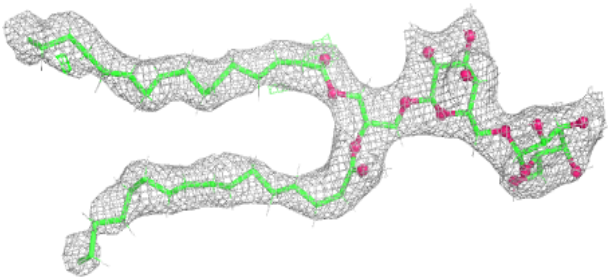


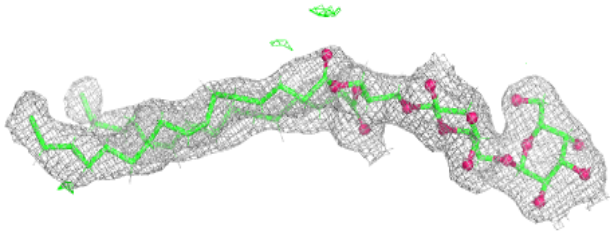


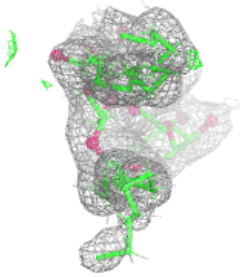


Electron density around DGD c 518:

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

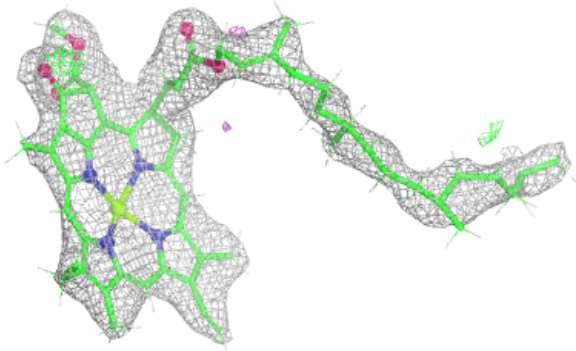


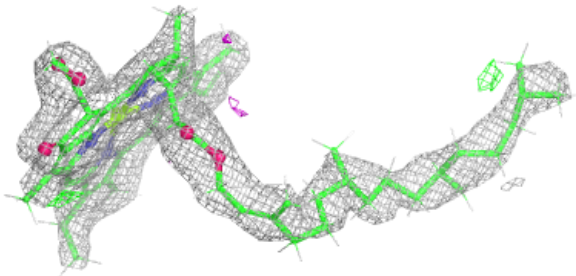


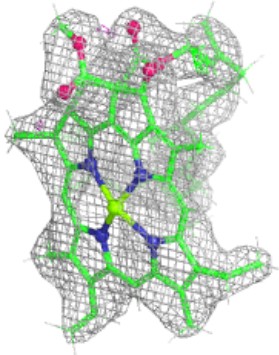


Electron density around CLA c 511:

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

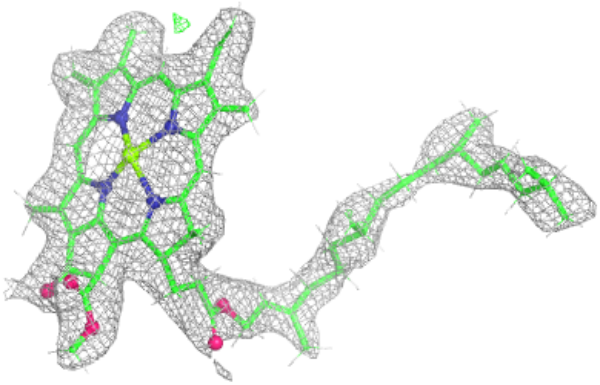


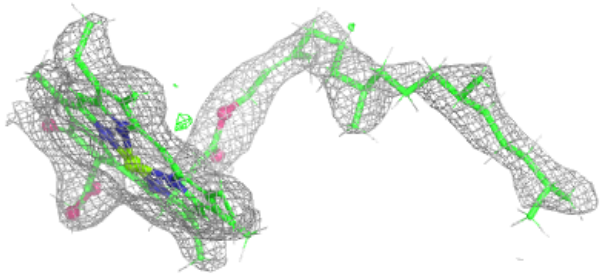


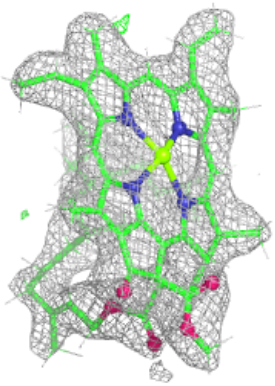


Electron density around CLA C 511:

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

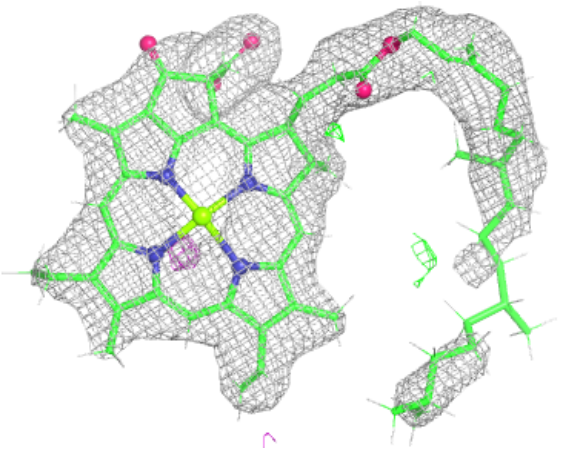


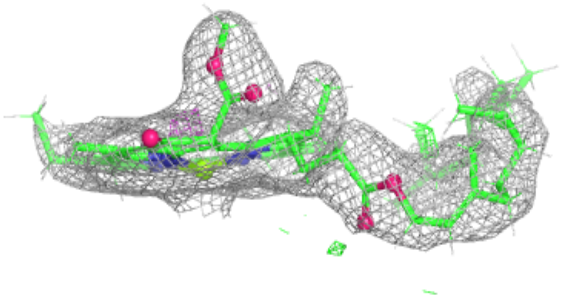


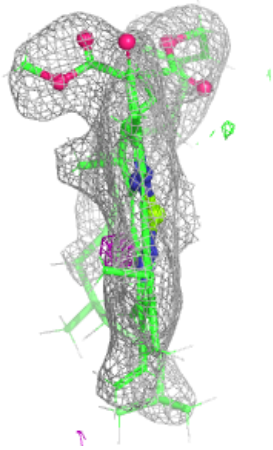


Electron density around CLA C 512:

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

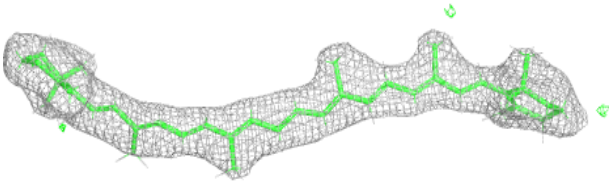


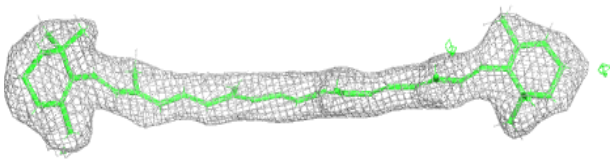


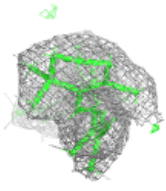


Electron density around BCR H 101:

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

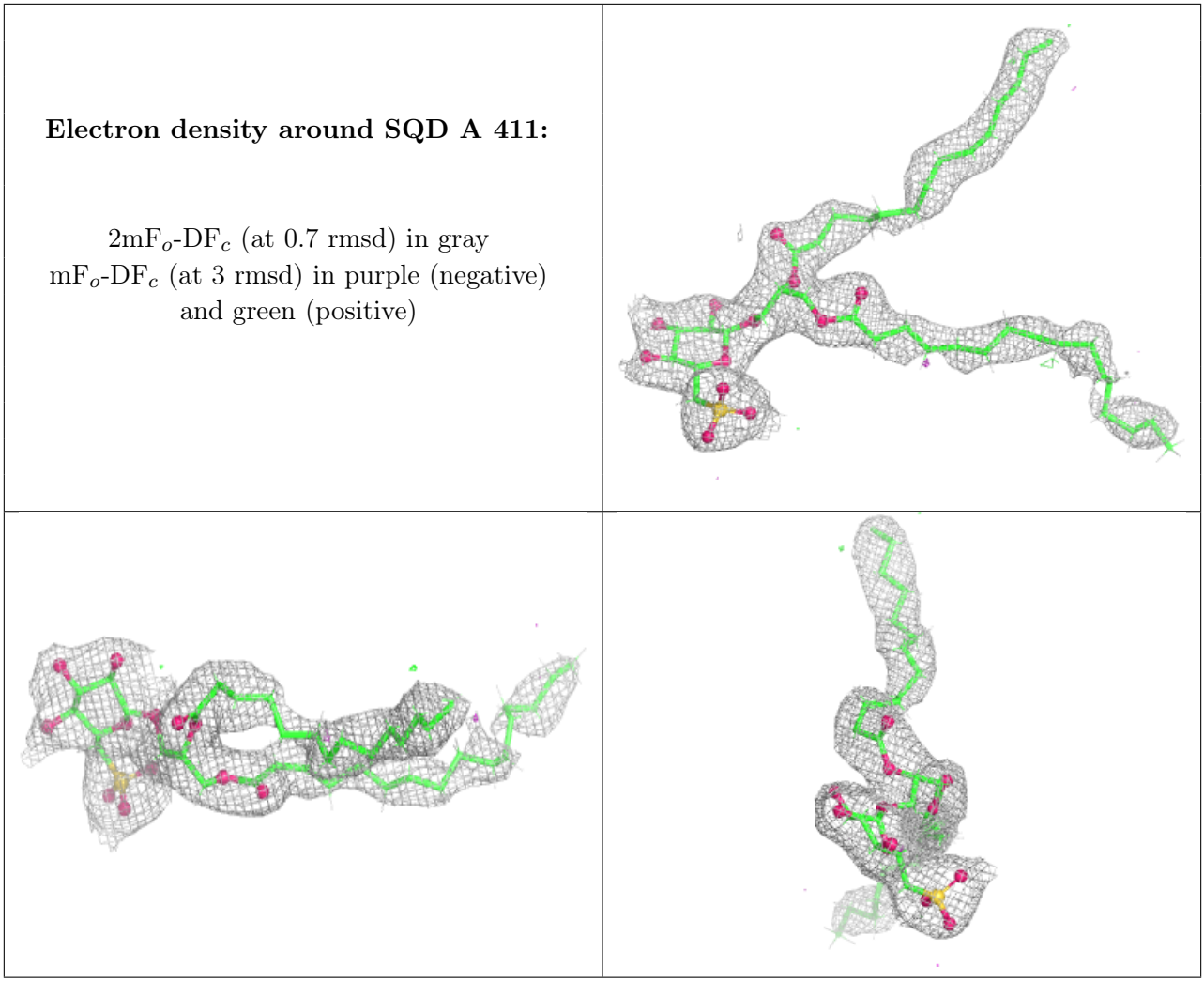






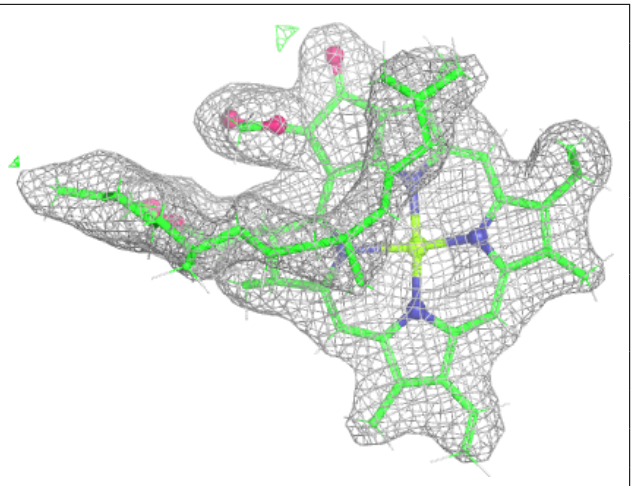
Electron density around SQD A 411:

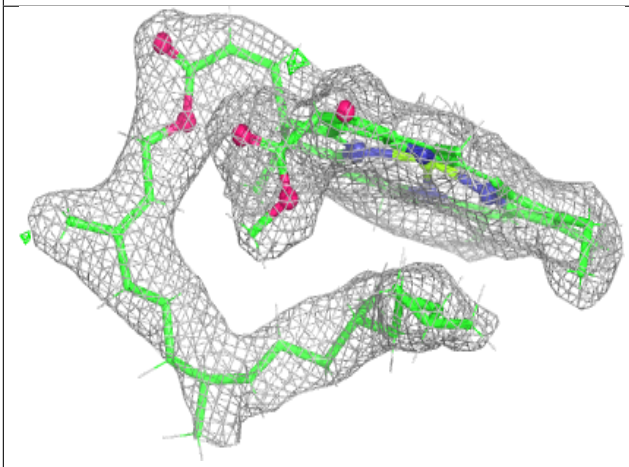
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

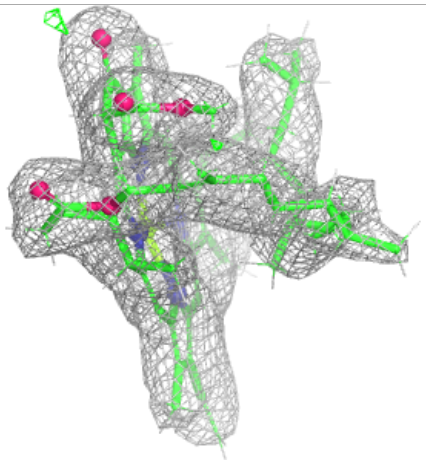


Electron density around CLA C 510:

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

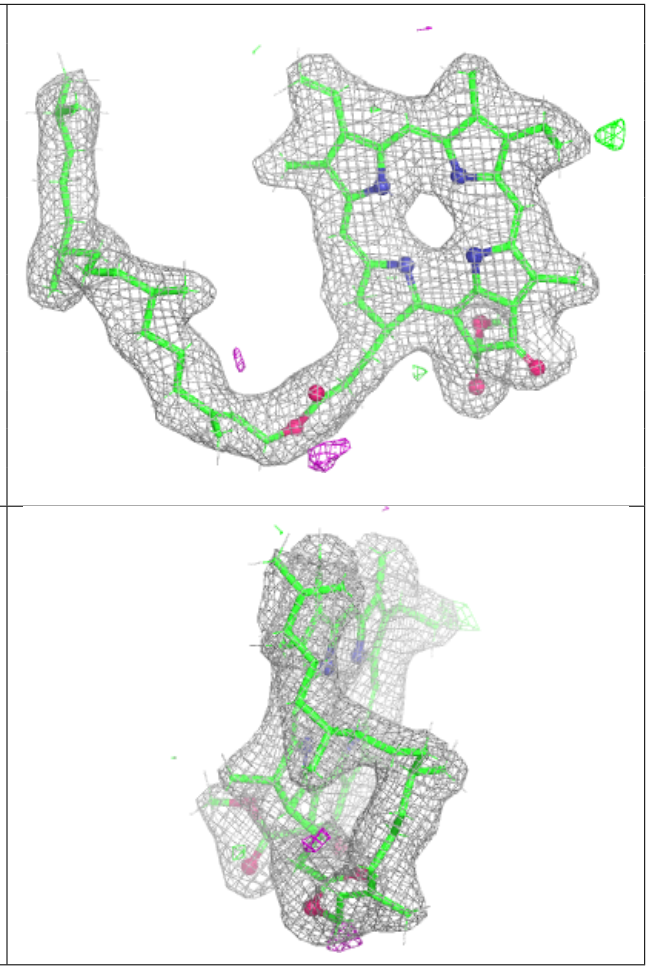






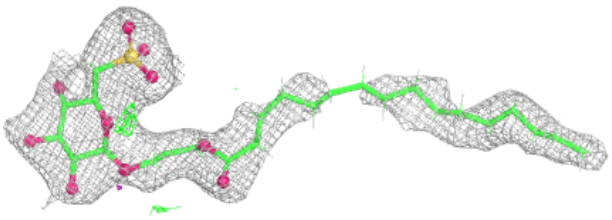
Electron density around PHO d 401:

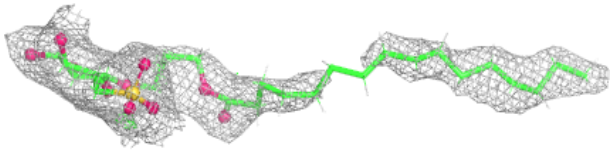
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

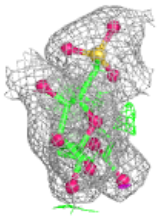


Electron density around SQD F 101:

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

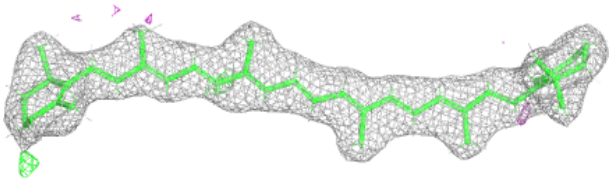


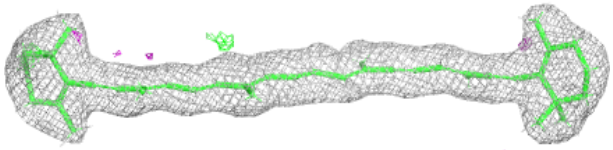


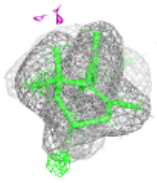


Electron density around BCR a 408:

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



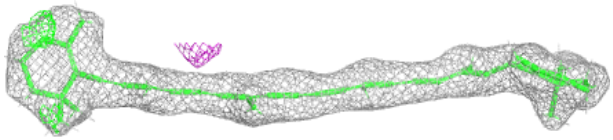


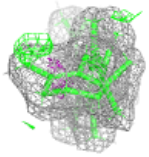


Electron density around BCR b 618:

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

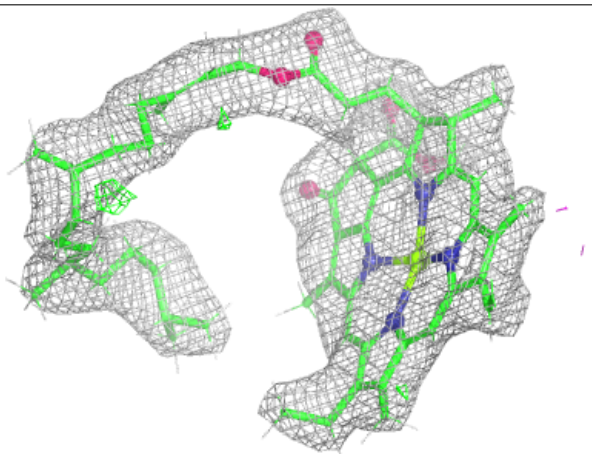


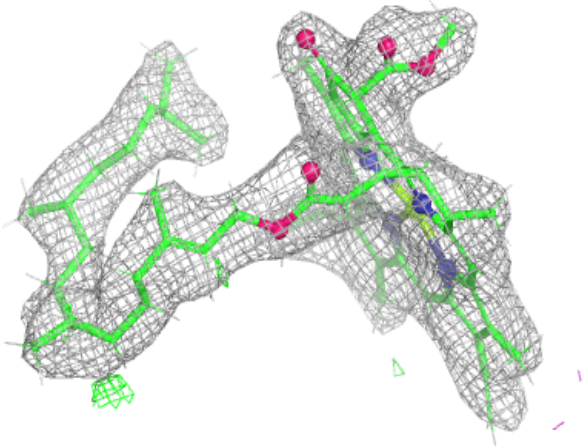


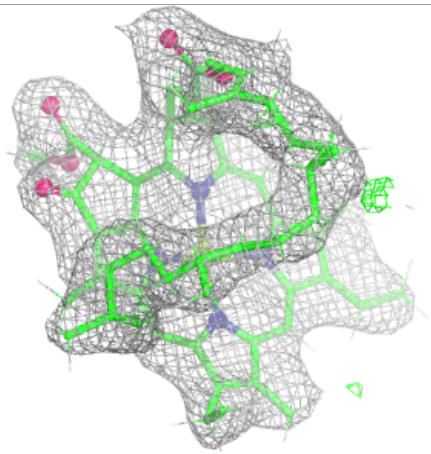


Electron density around CLA c 503:

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

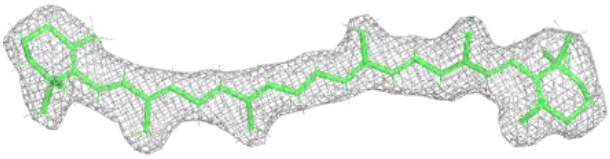


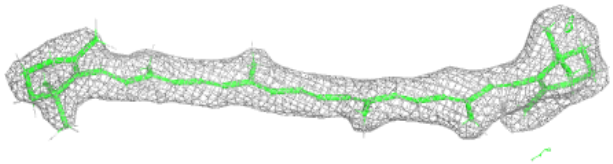


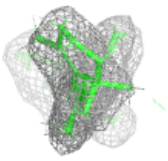


Electron density around BCR b 620:

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

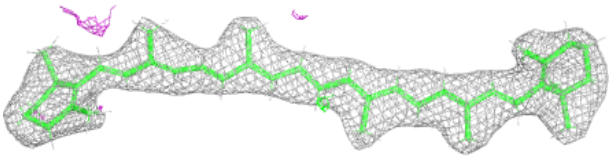


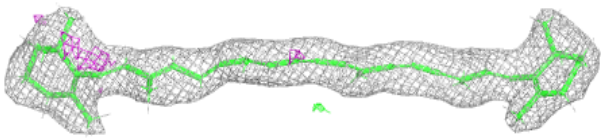


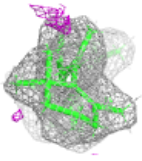


Electron density around BCR B 618:

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

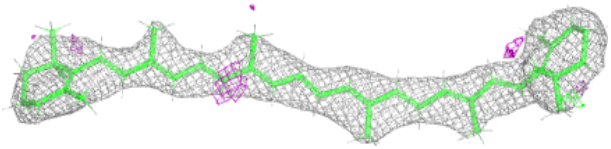


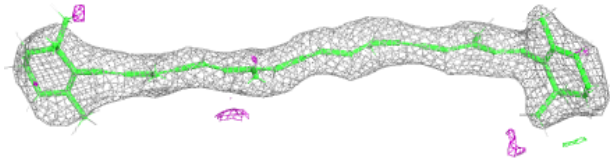


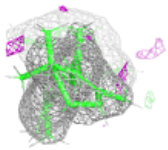


Electron density around BCR c 515:

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

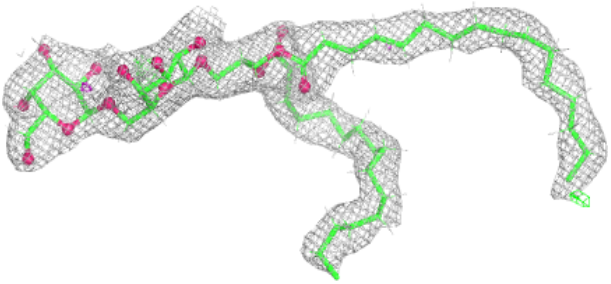


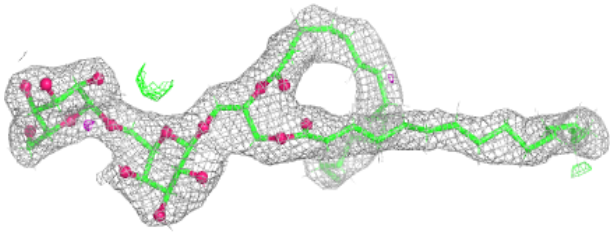


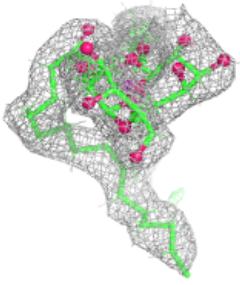


Electron density around DGD H 102:

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

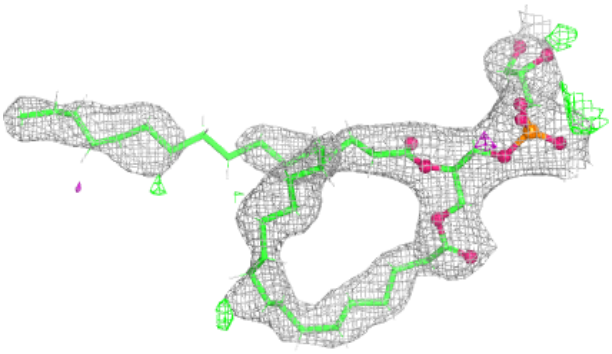


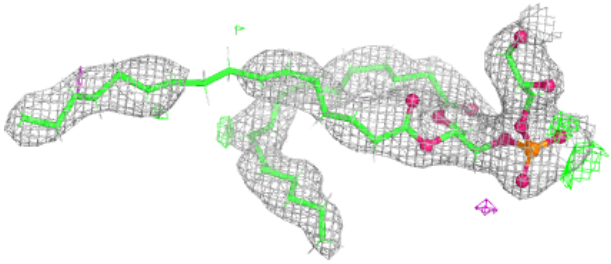


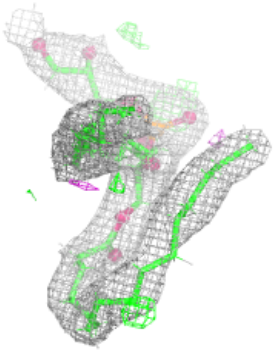


Electron density around LHG a 410:

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

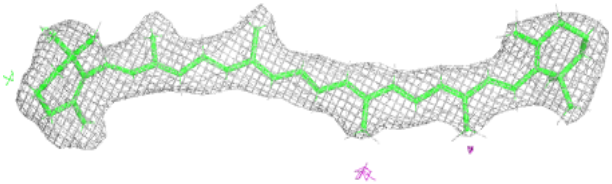


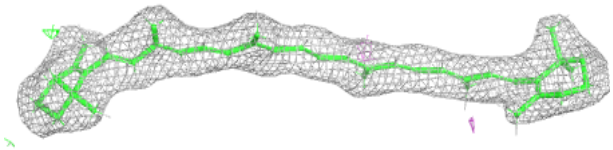


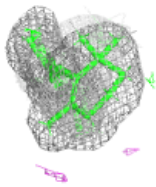


Electron density around BCR B 619:

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

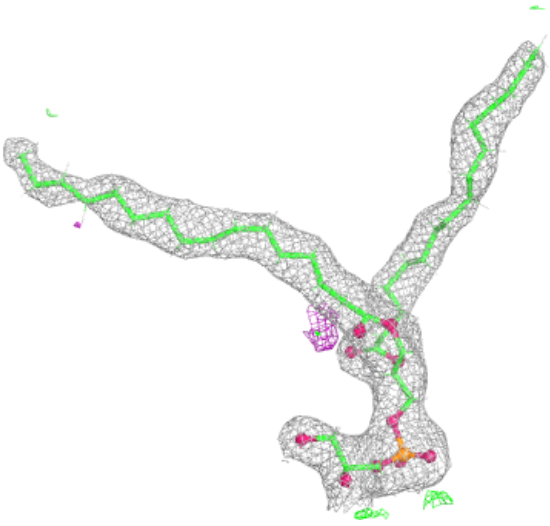


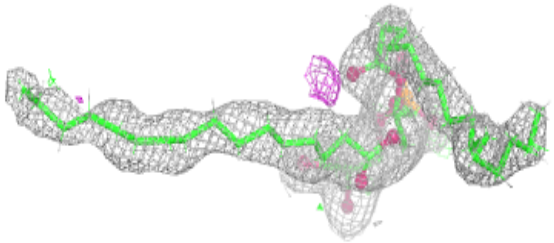


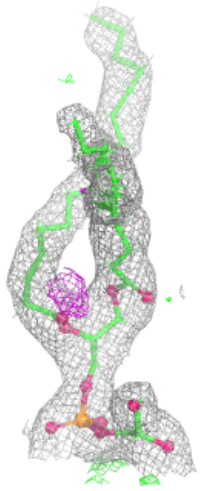


Electron density around LHG l 101:

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

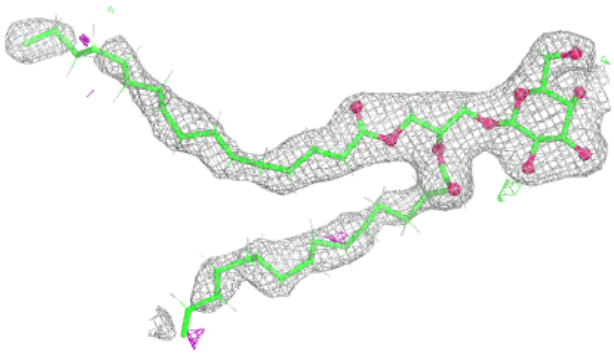


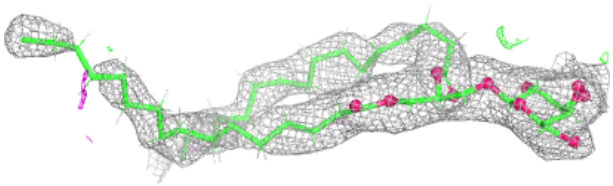


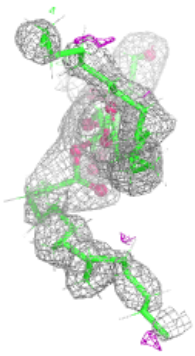


Electron density around LMG D 407:

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

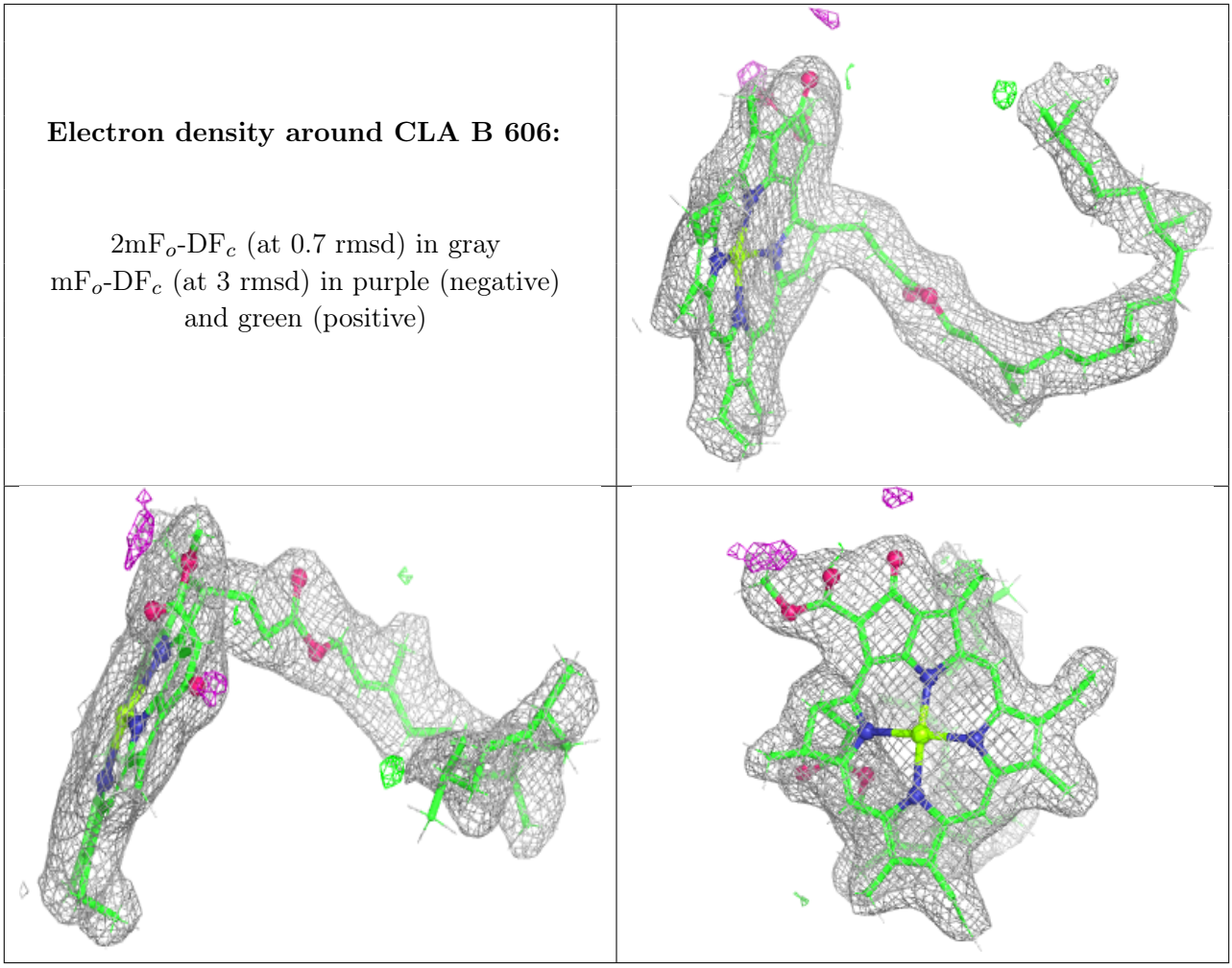






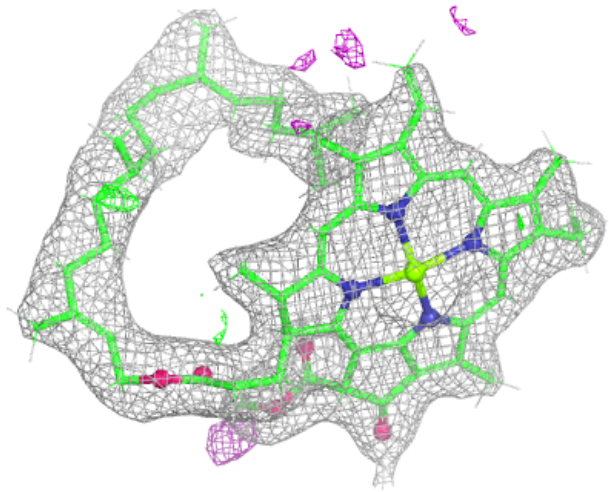
Electron density around CLA B 606:

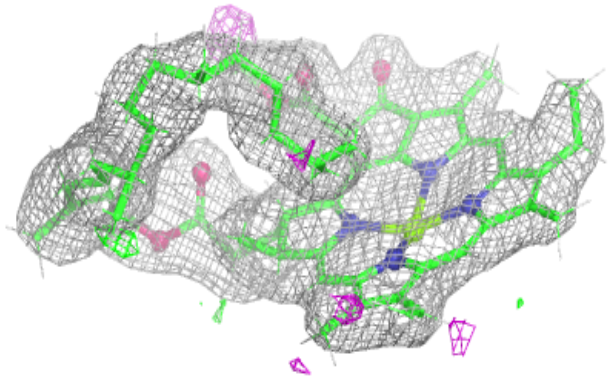
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

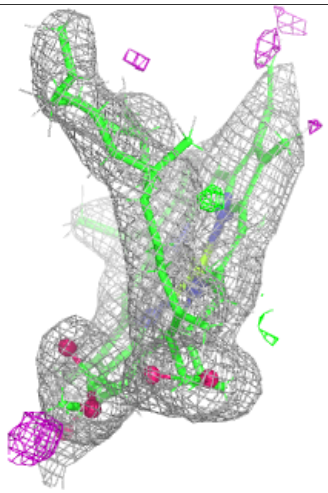


Electron density around CLA B 615:

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

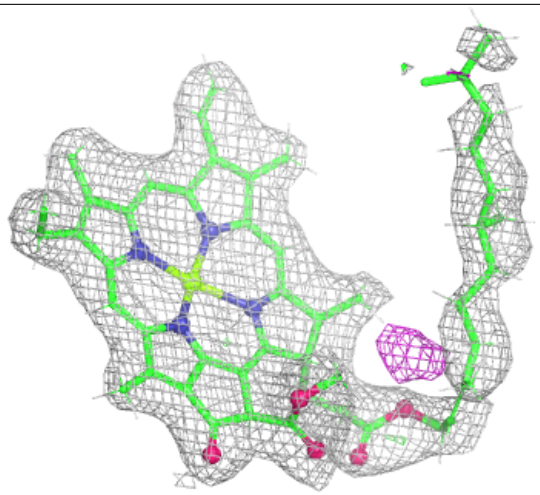


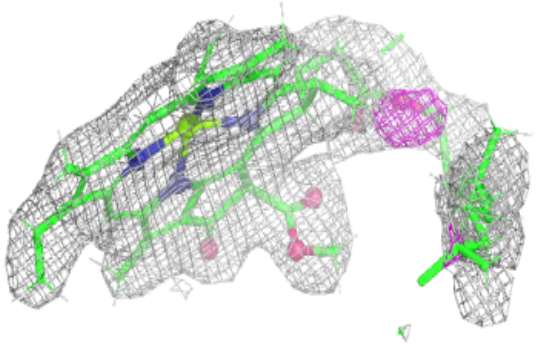


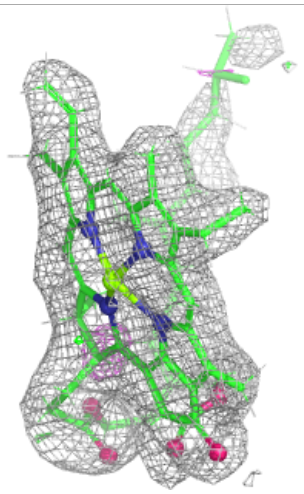


Electron density around CLA B 616:

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

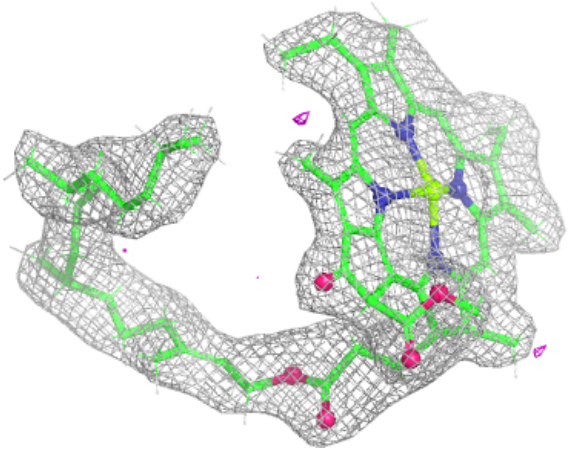


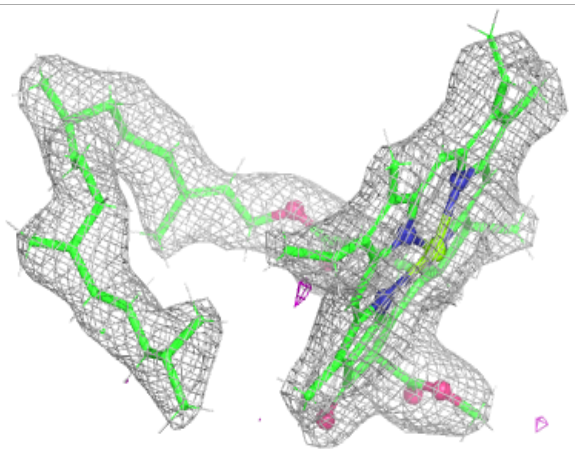


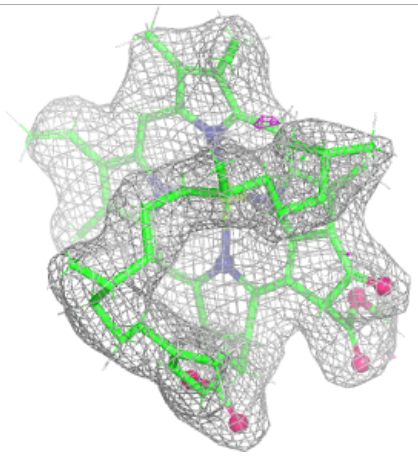


Electron density around CLA C 503:

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

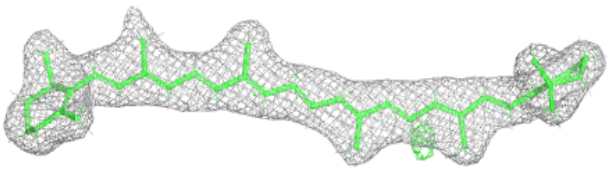


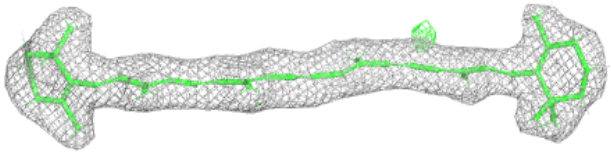


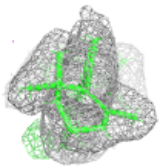


Electron density around BCR A 408:

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

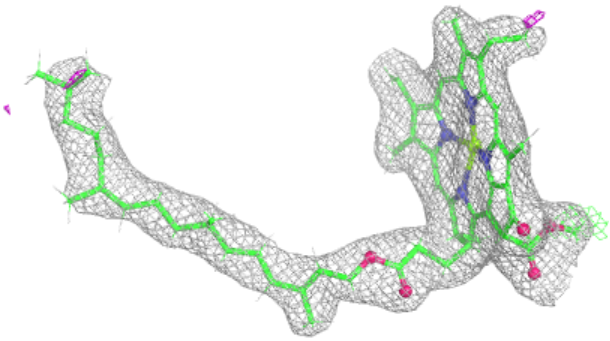


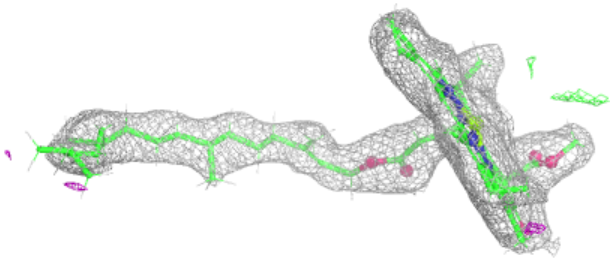


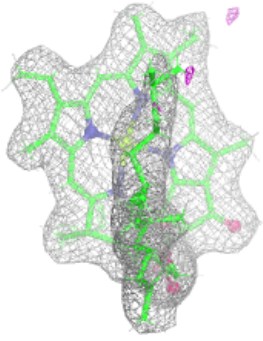


Electron density around CLA b 610:

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

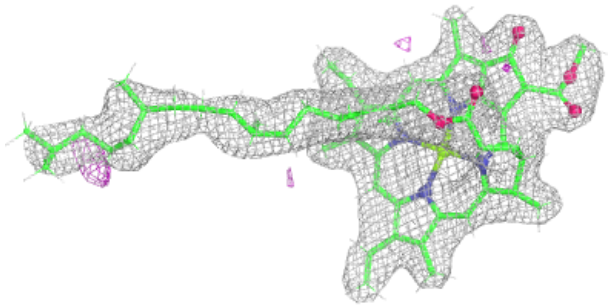


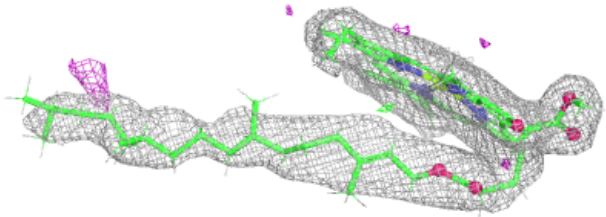


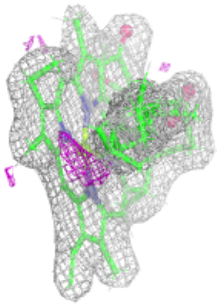


Electron density around CLA b 615:

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

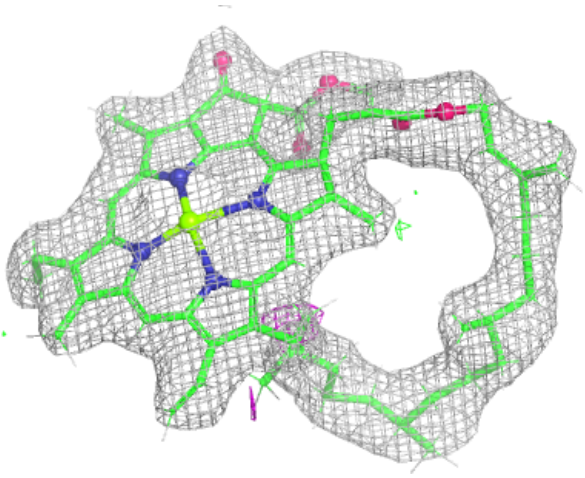


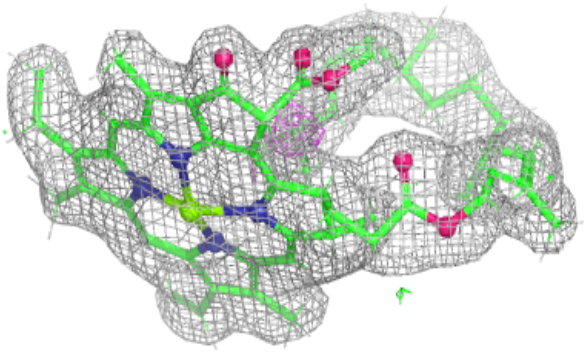


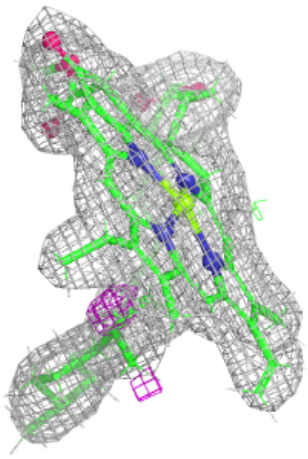


Electron density around CLA b 616:

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

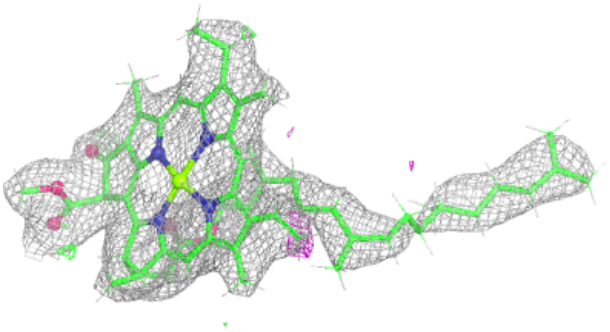


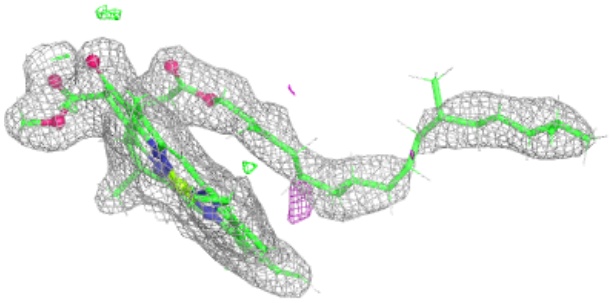


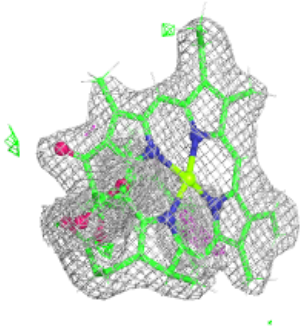


Electron density around CLA C 505:

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

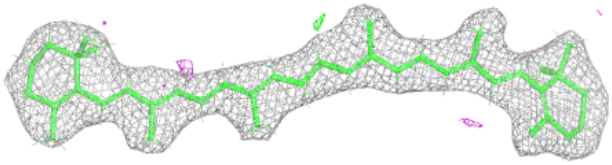


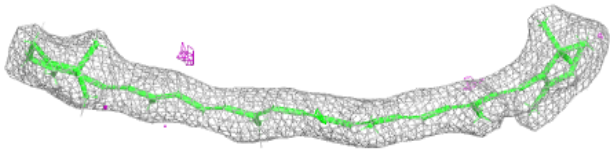


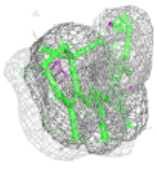


Electron density around BCR t 101:

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

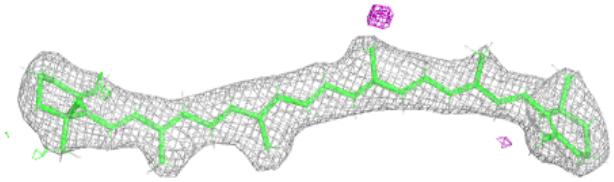


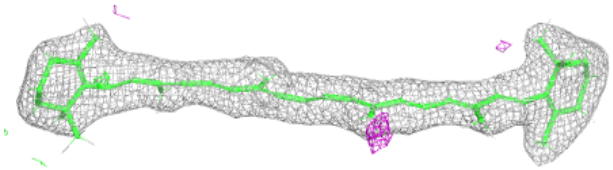


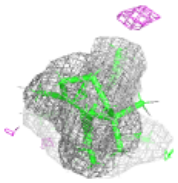


Electron density around BCR C 515:

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

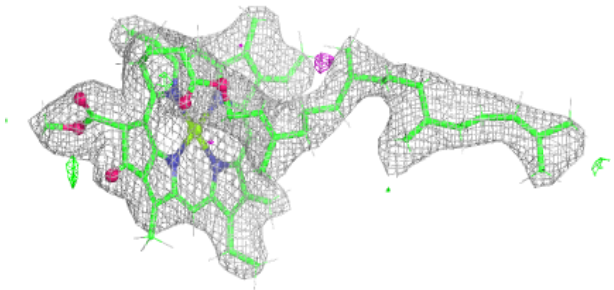


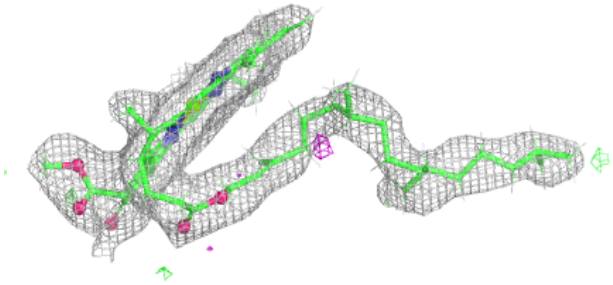


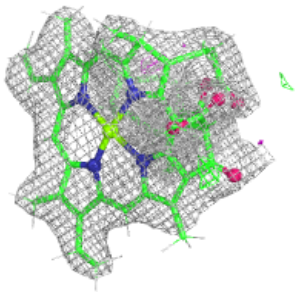


Electron density around CLA c 505:

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

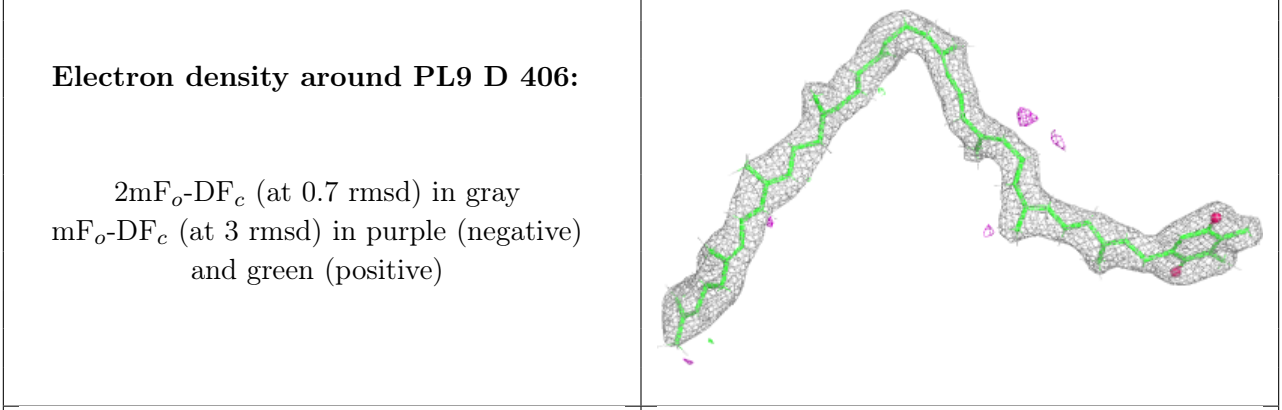






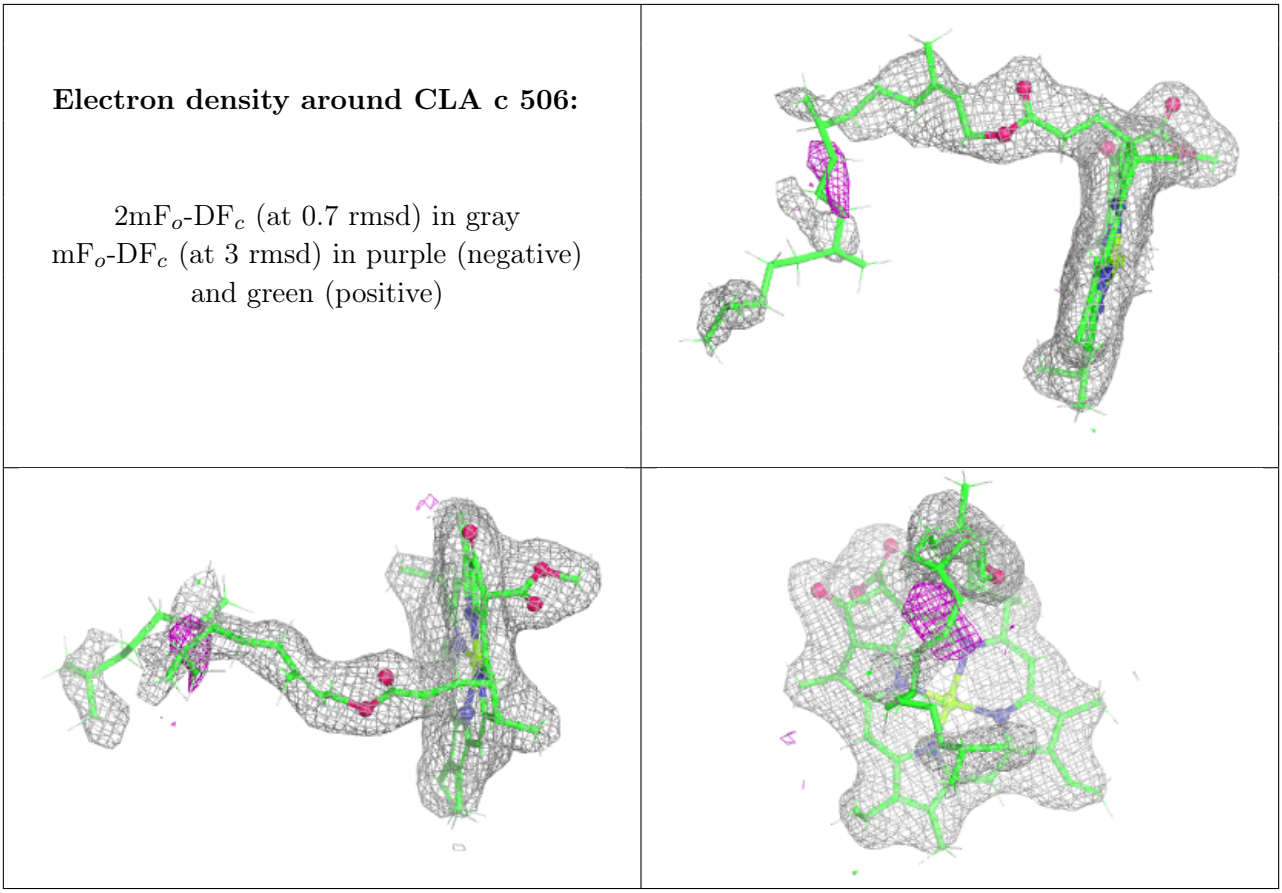
Electron density around PL9 D 406:

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



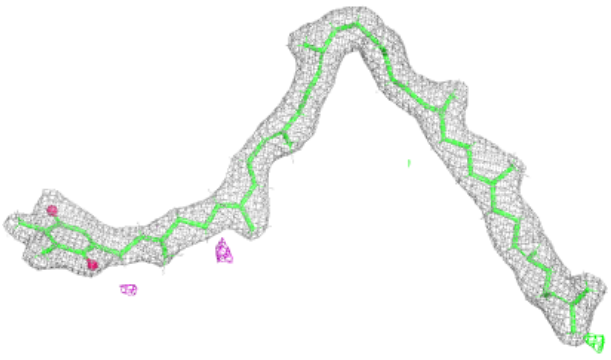
Electron density around CLA c 506:

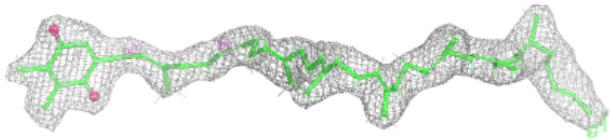
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PL9 d 406:

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

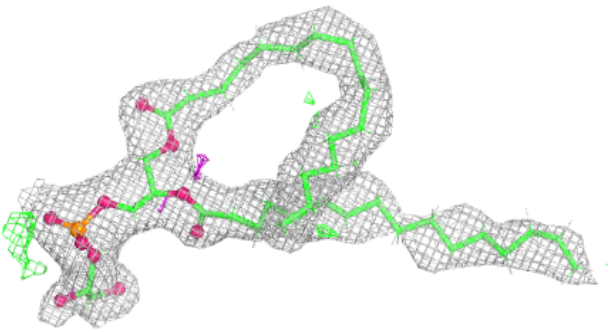


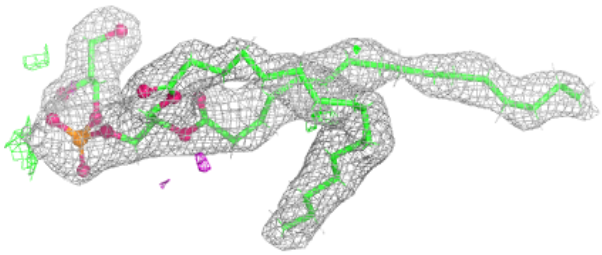




Electron density around LHG B 622:

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

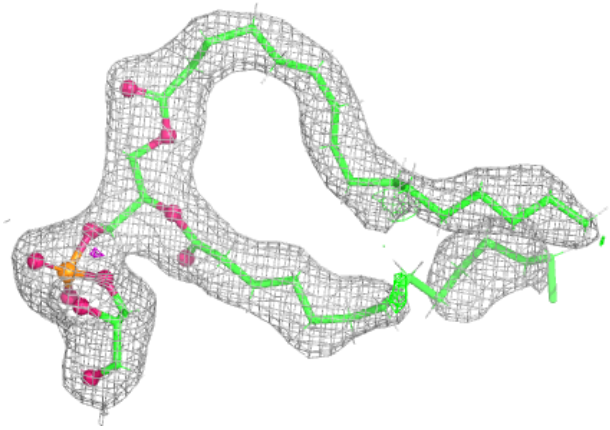


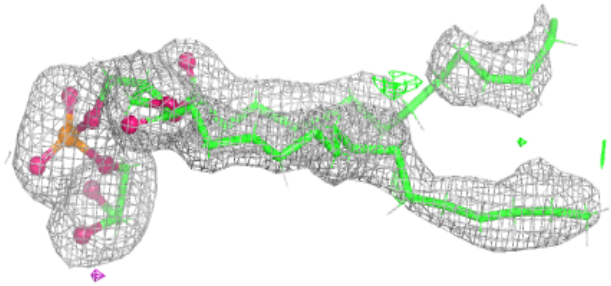


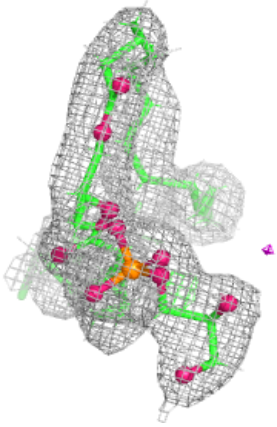


Electron density around LHG D 409:

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

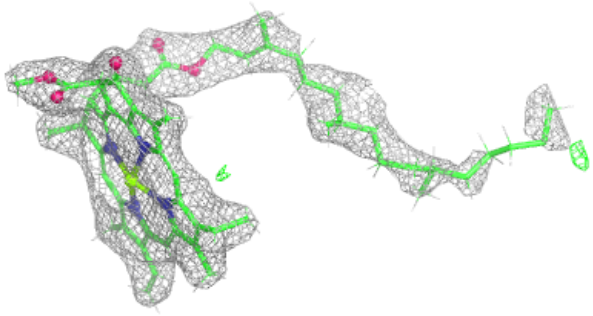


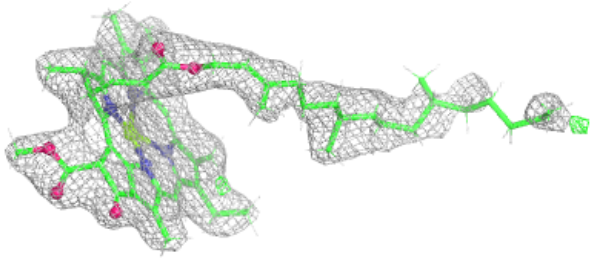


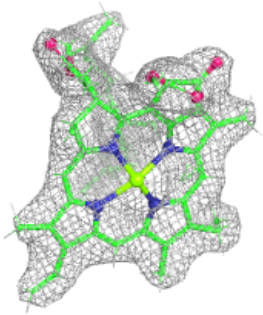


Electron density around CLA c 508:

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

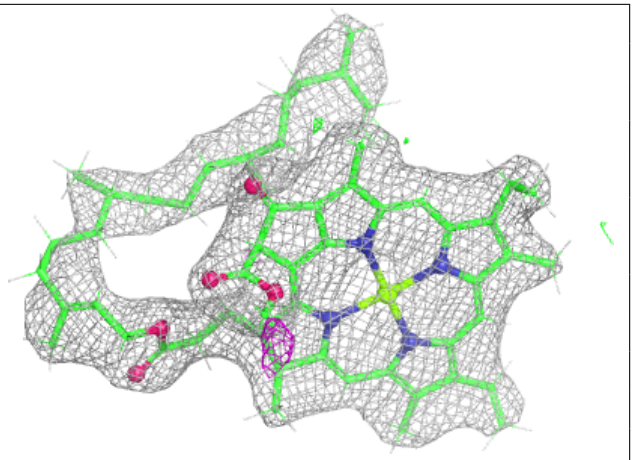


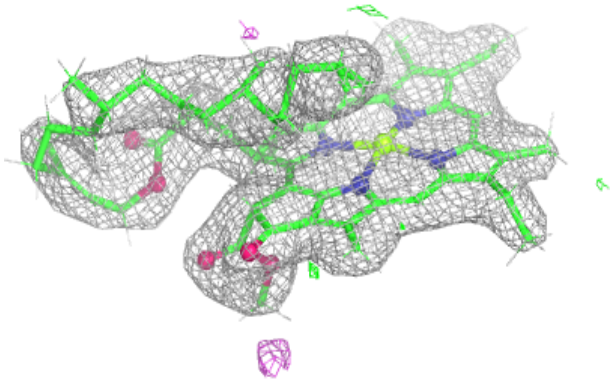


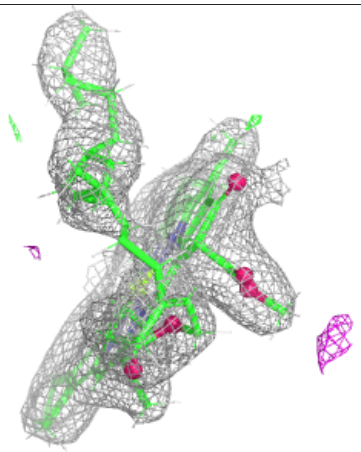


Electron density around CLA c 509:

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

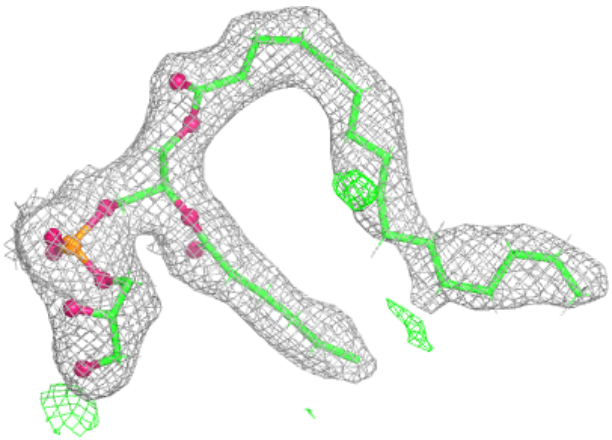


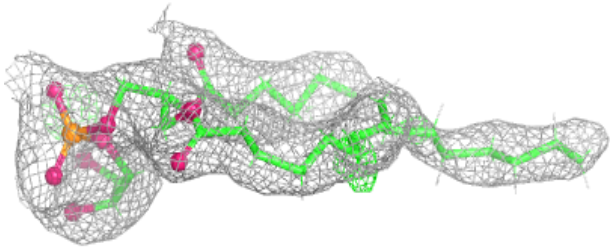


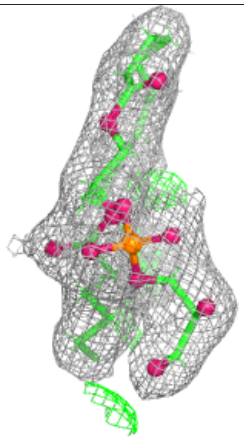


Electron density around LHG d 408:

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

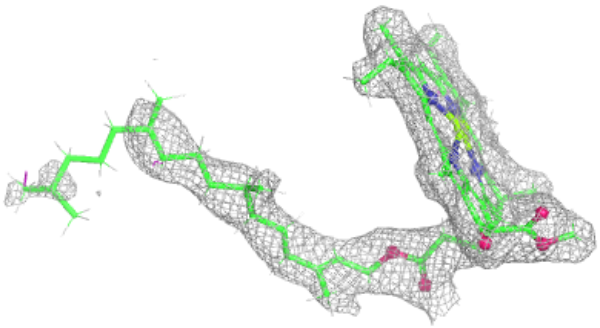


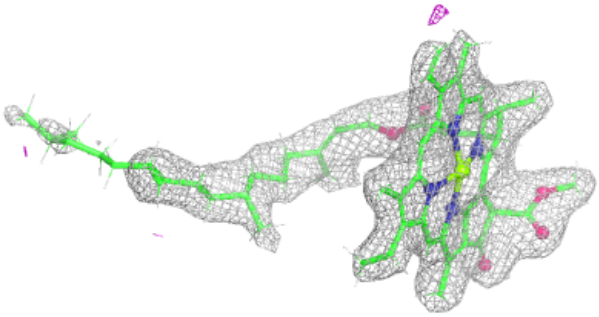


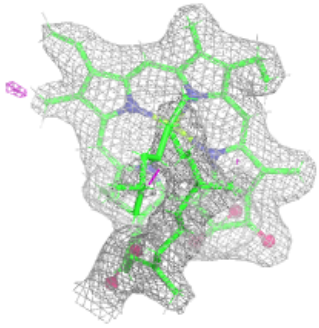


Electron density around CLA C 508:

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

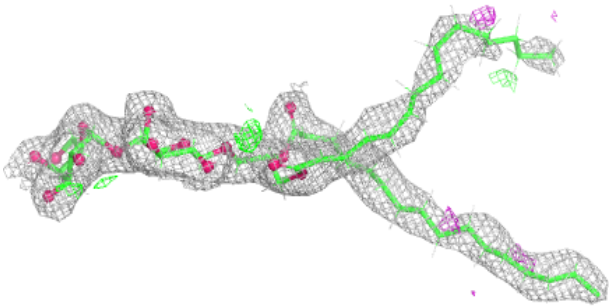


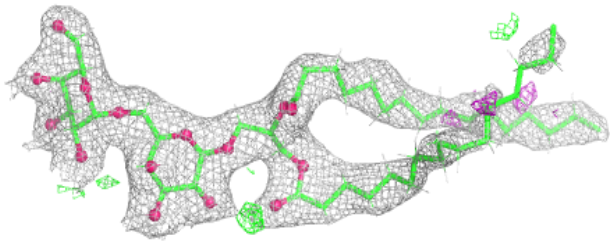


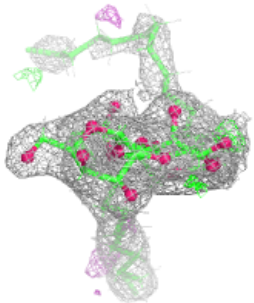


Electron density around DGD C 516:

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

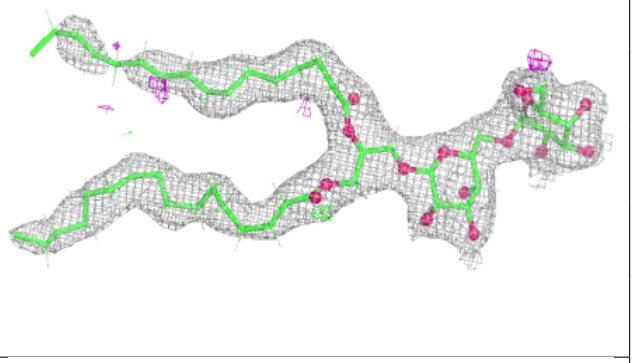


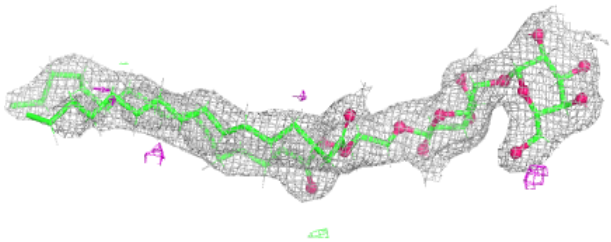


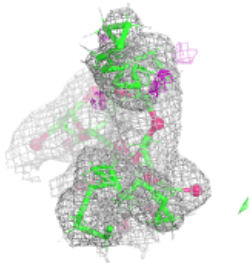


Electron density around DGD C 518:

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

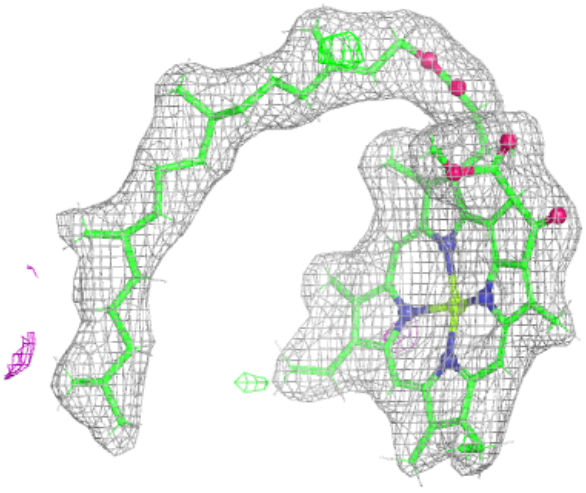


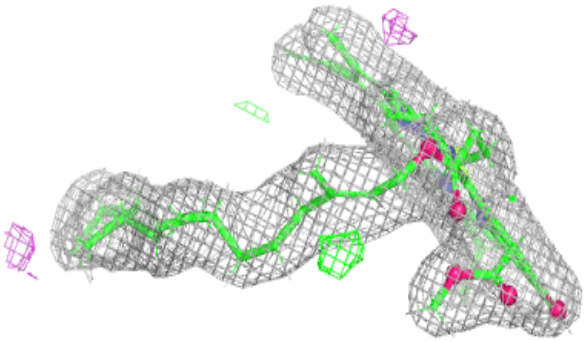


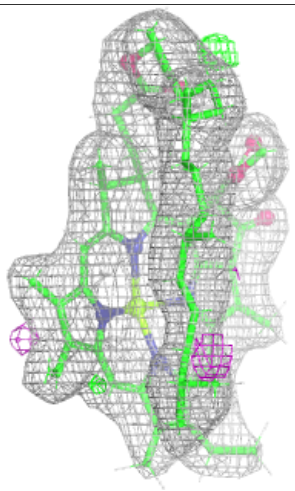


Electron density around CLA C 507:

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

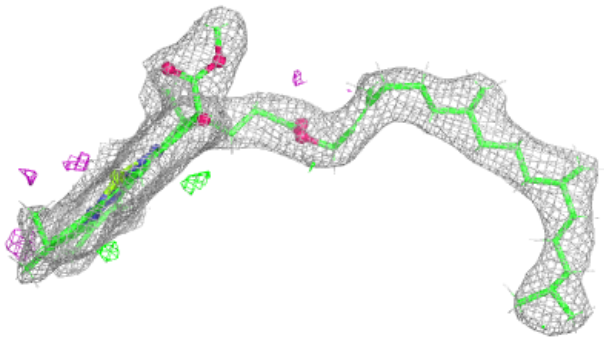


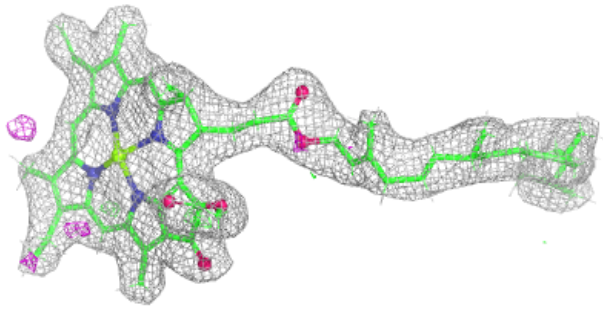


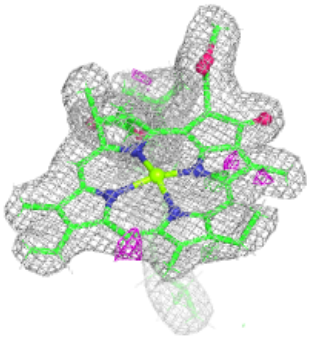


Electron density around CLA D 403:

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

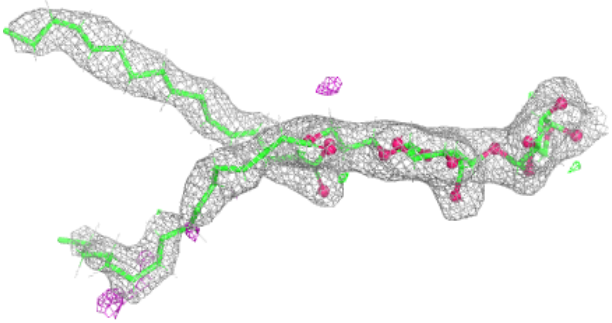


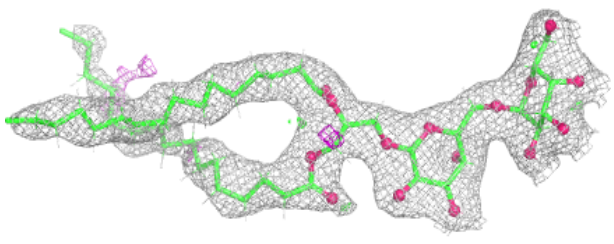


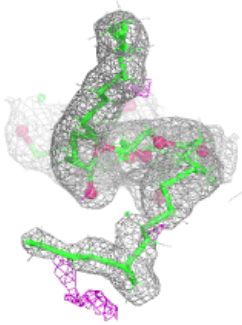


Electron density around DGD c 516:

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

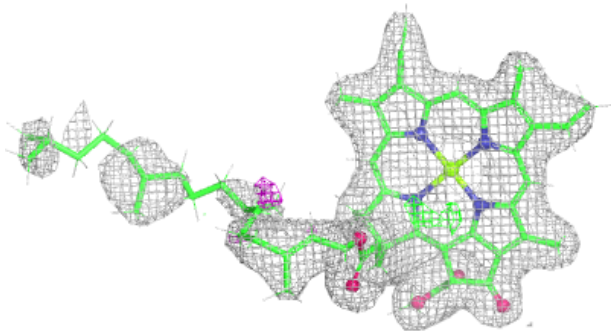


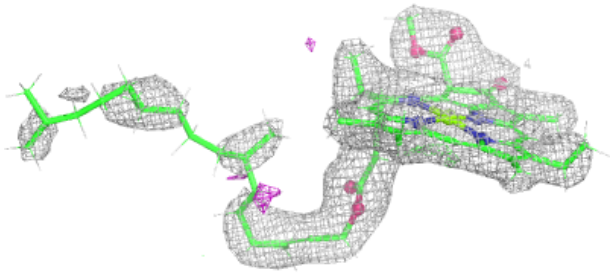


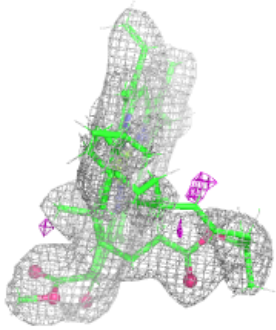


Electron density around CLA a 405:

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

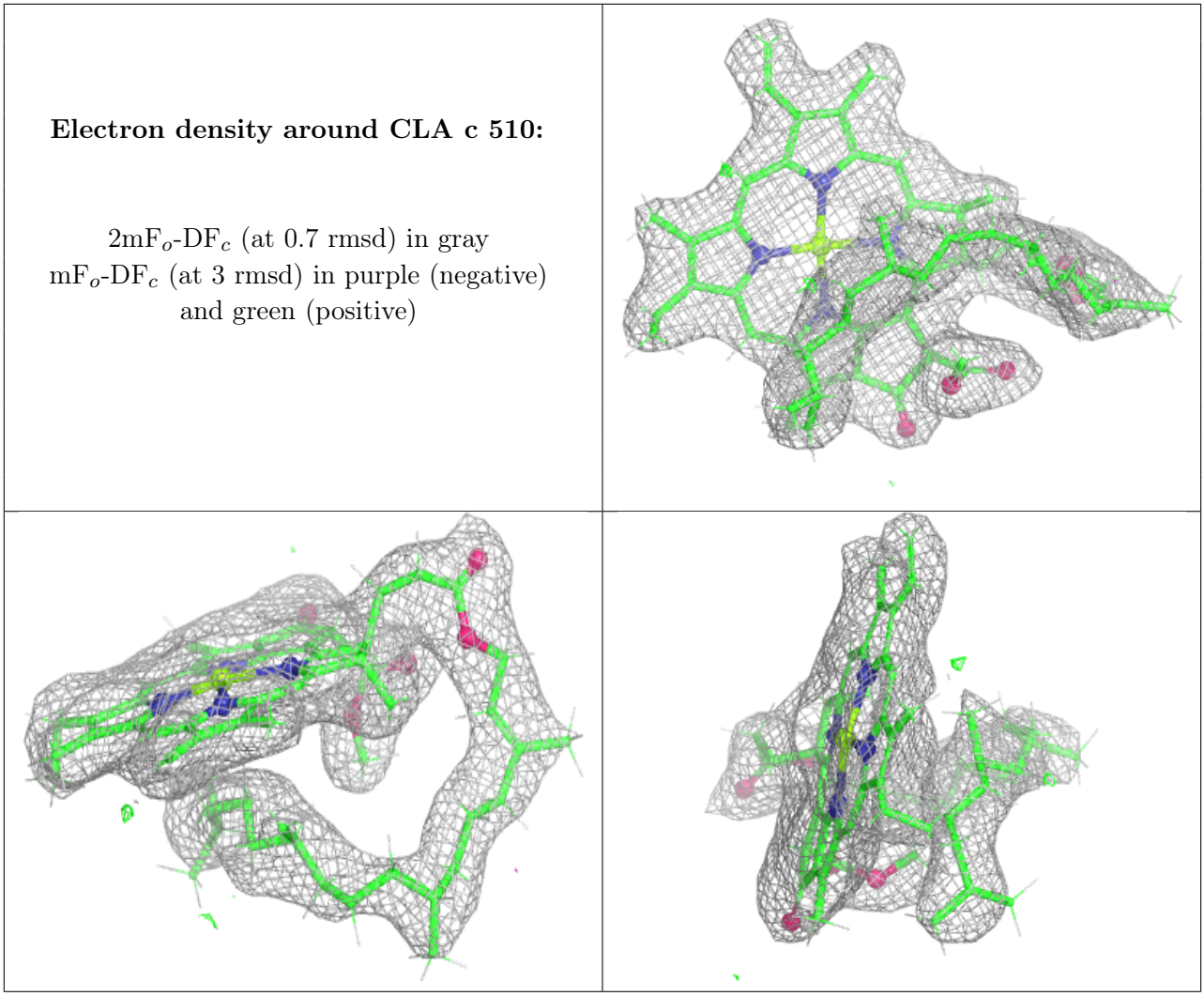






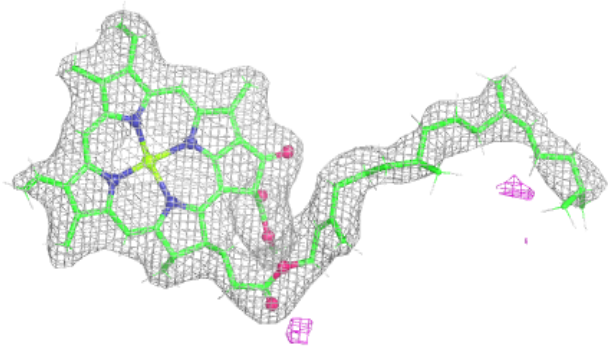
Electron density around CLA c 510:

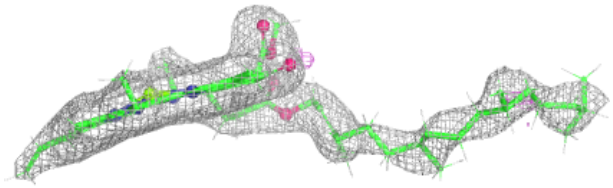
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

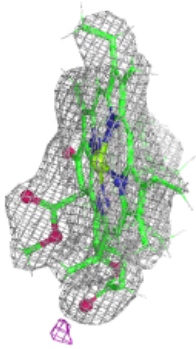


Electron density around CLA b 603:

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

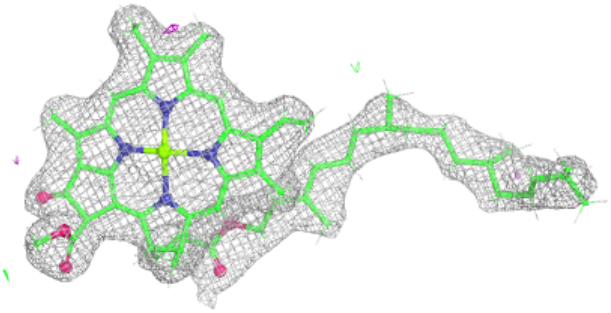


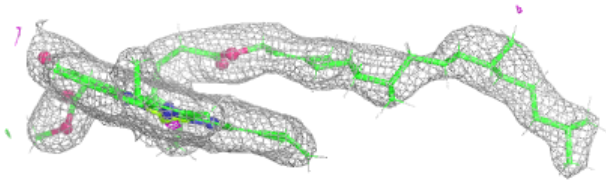


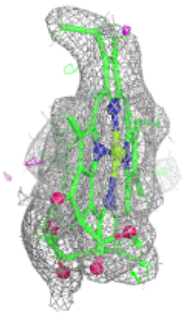


Electron density around CLA b 604:

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

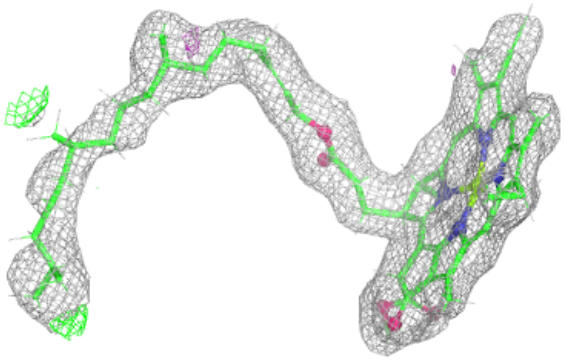


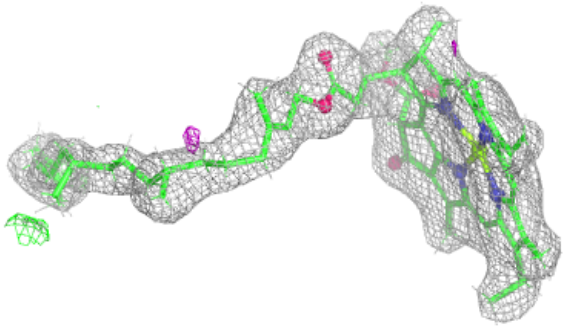


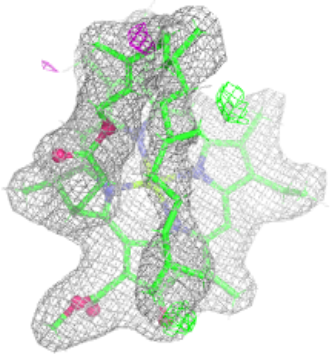


Electron density around CLA b 607:

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

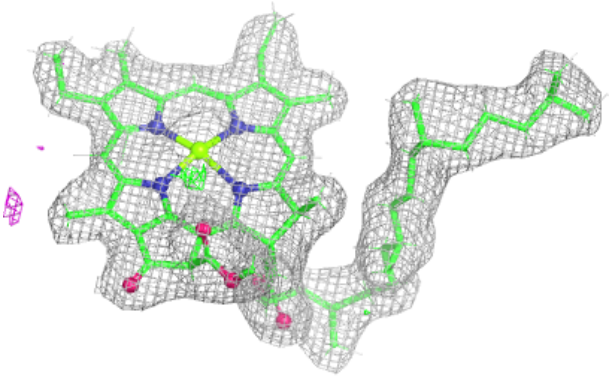


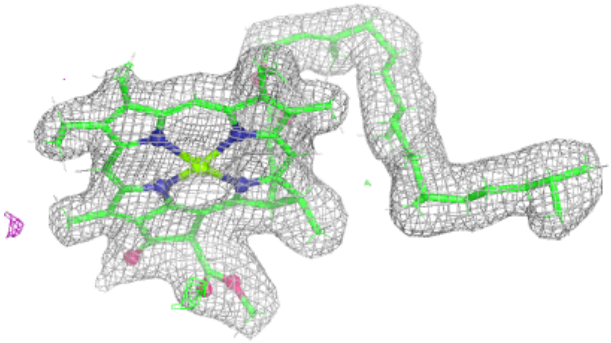


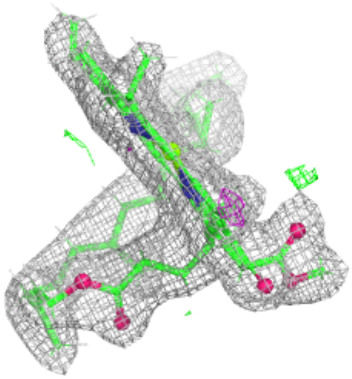


Electron density around CLA d 402:

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

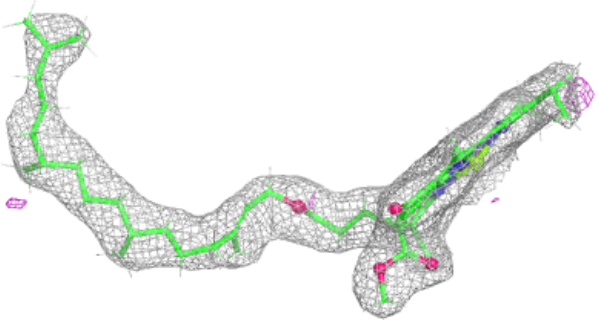


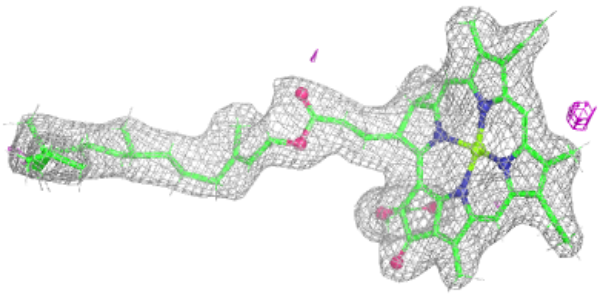


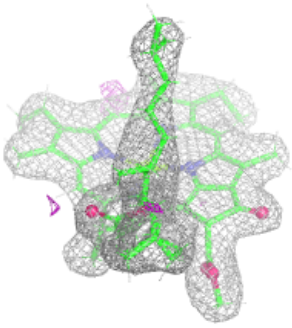


Electron density around CLA d 403:

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

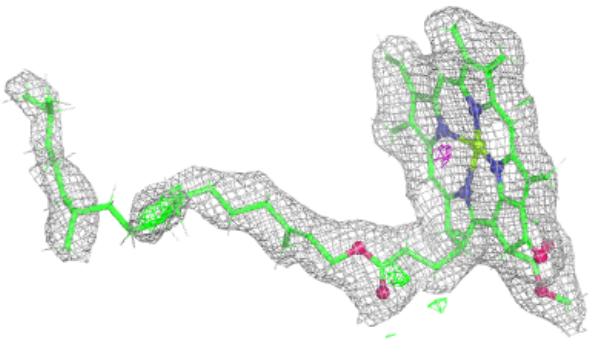


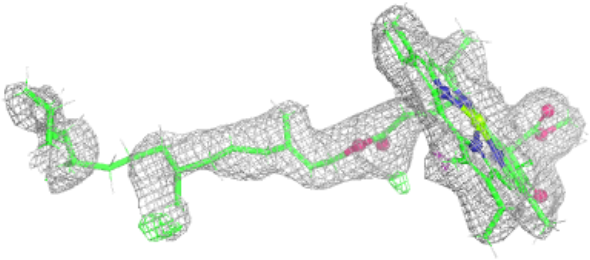


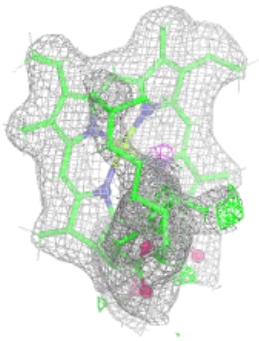


Electron density around CLA d 404:

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

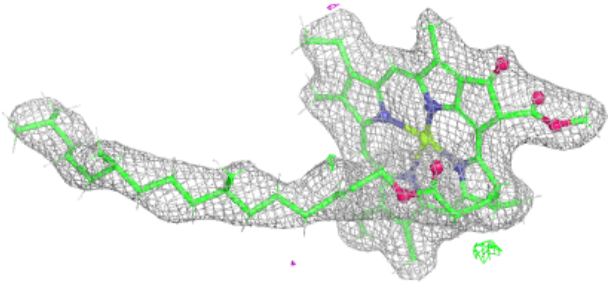


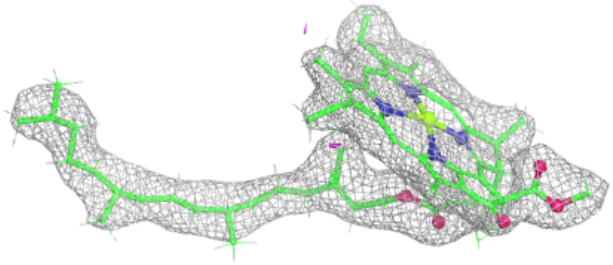


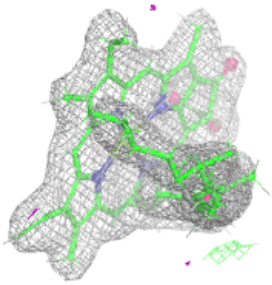


Electron density around CLA b 609:

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

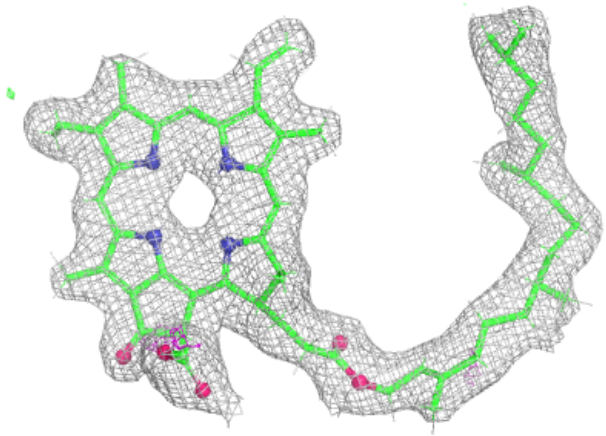


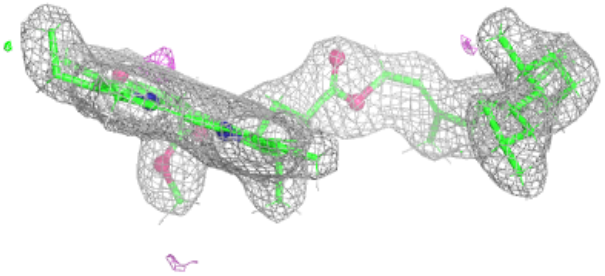


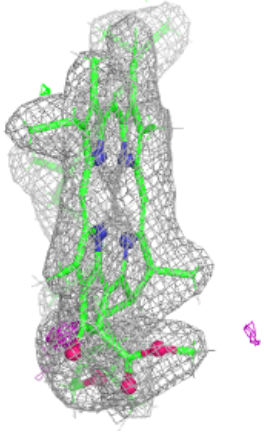


Electron density around PHO a 406:

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

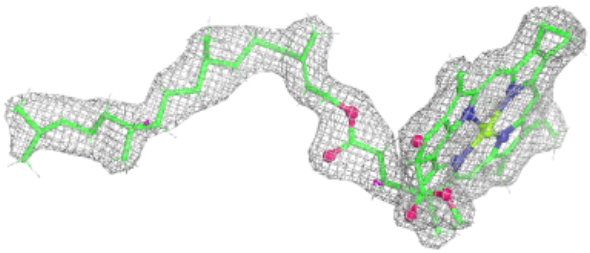


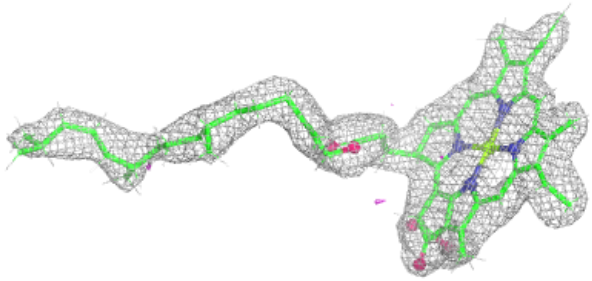


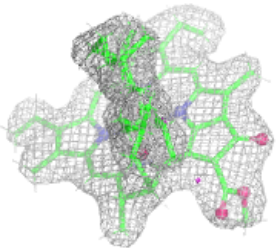


Electron density around CLA C 502:

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

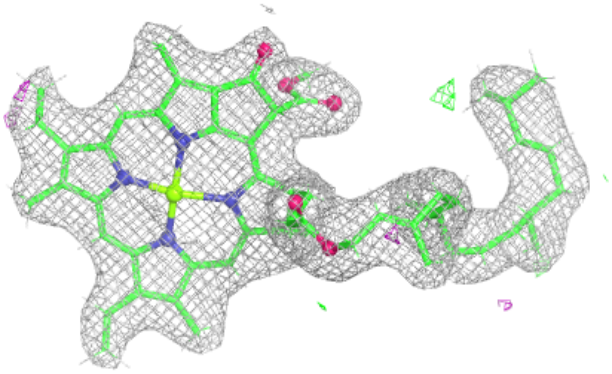


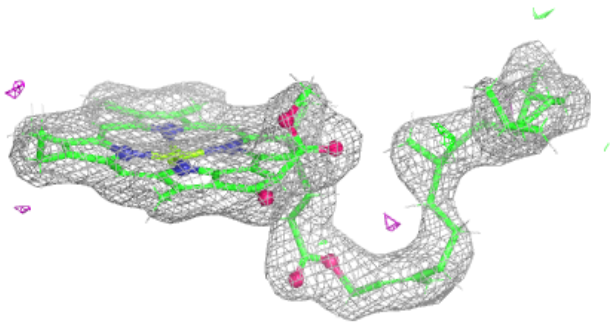


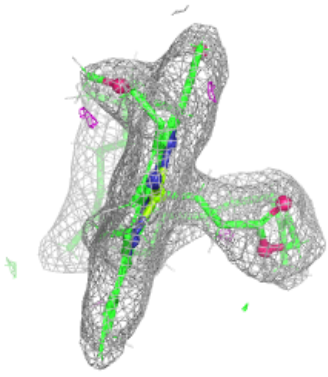


Electron density around CLA b 613:

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

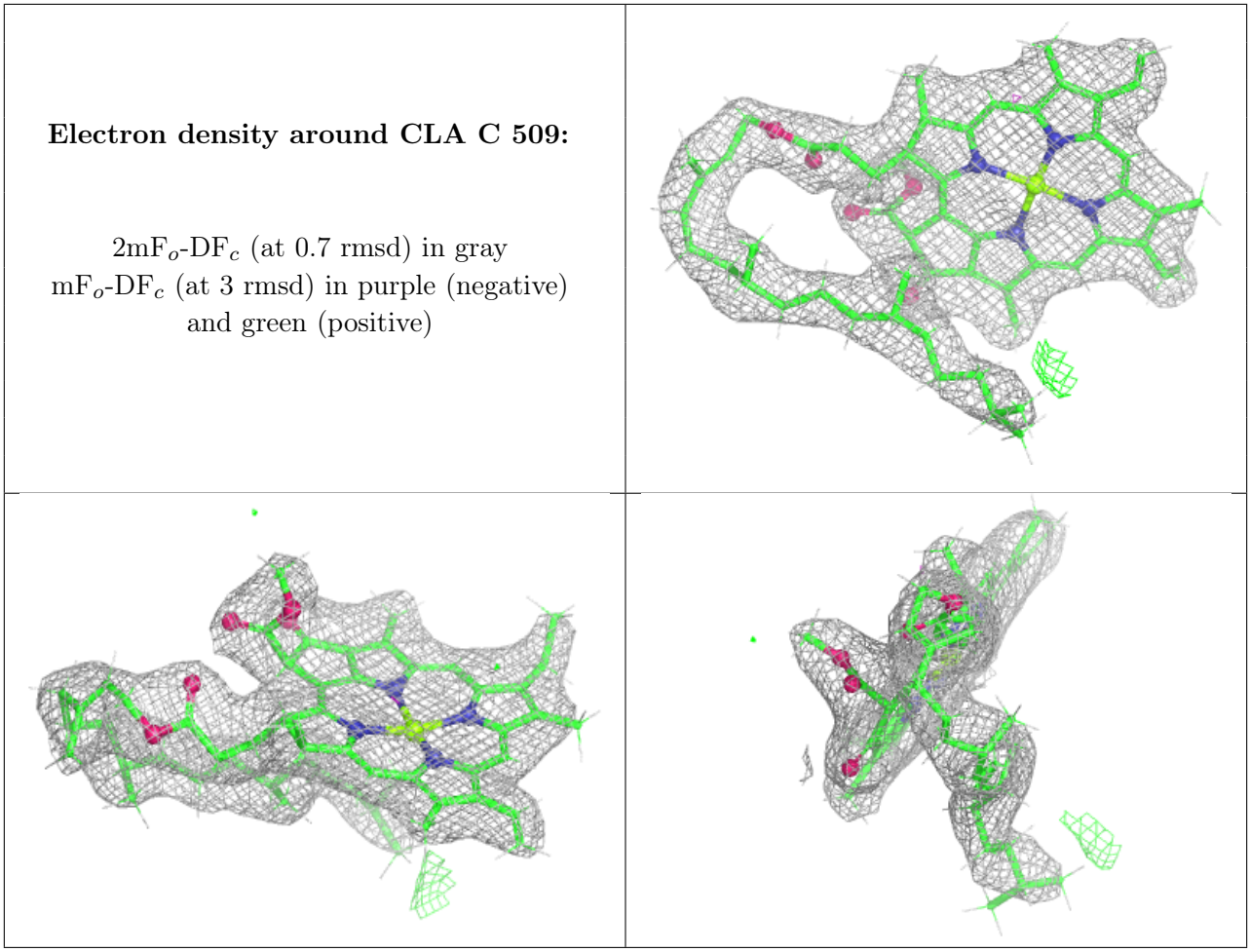






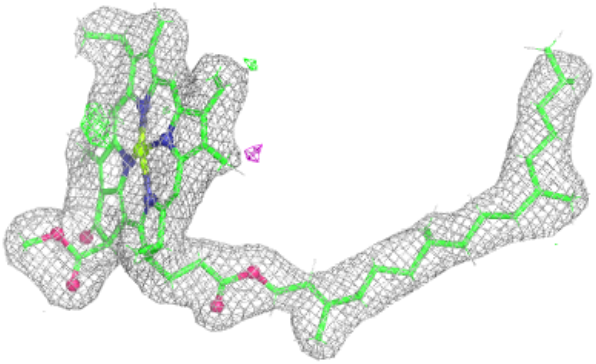
Electron density around CLA C 509:

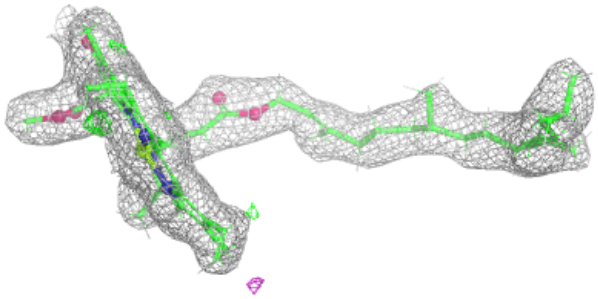
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

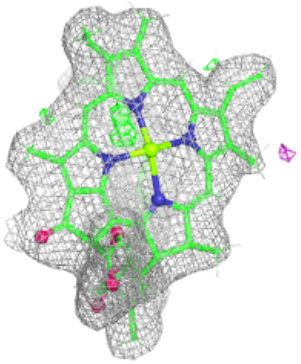


Electron density around CLA B 609:

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

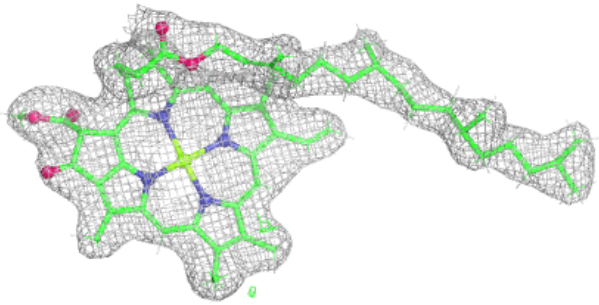


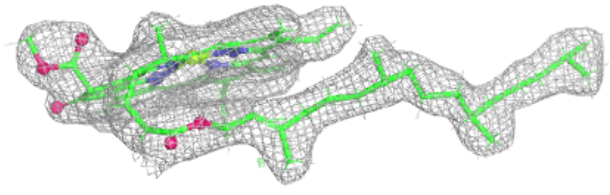


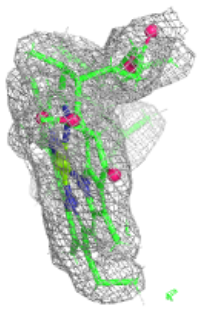


Electron density around CLA c 501:

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

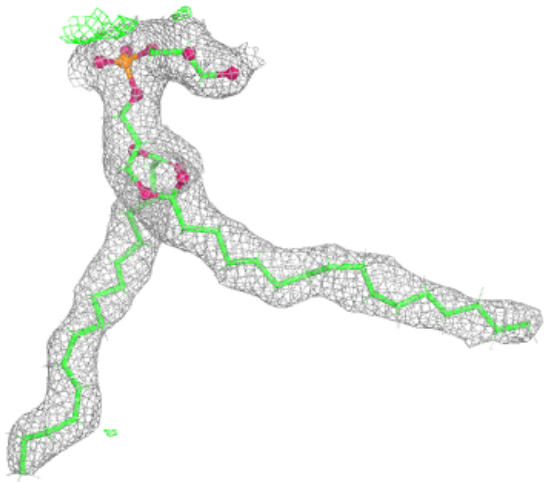


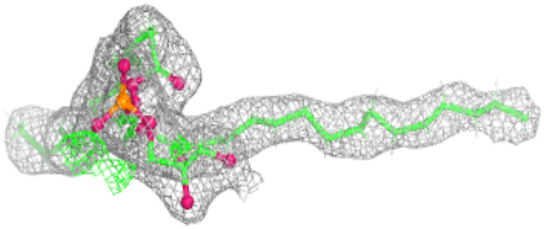


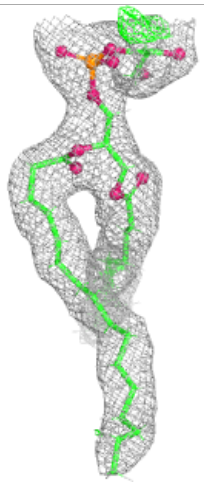


Electron density around LHG L 101:

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

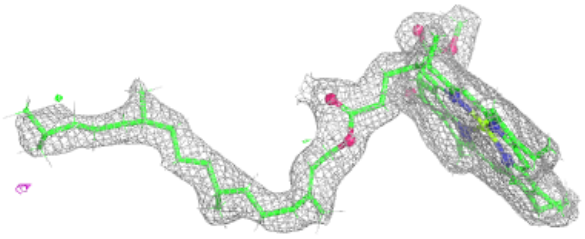


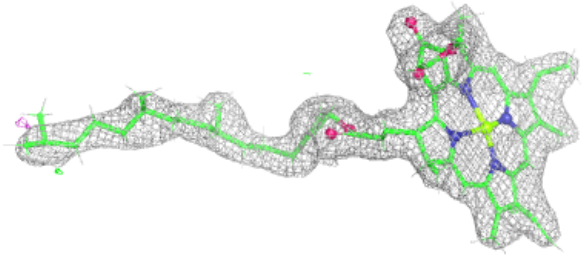


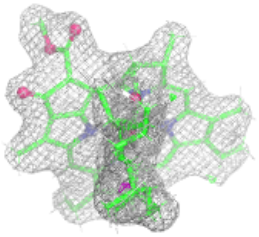


Electron density around CLA c 502:

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

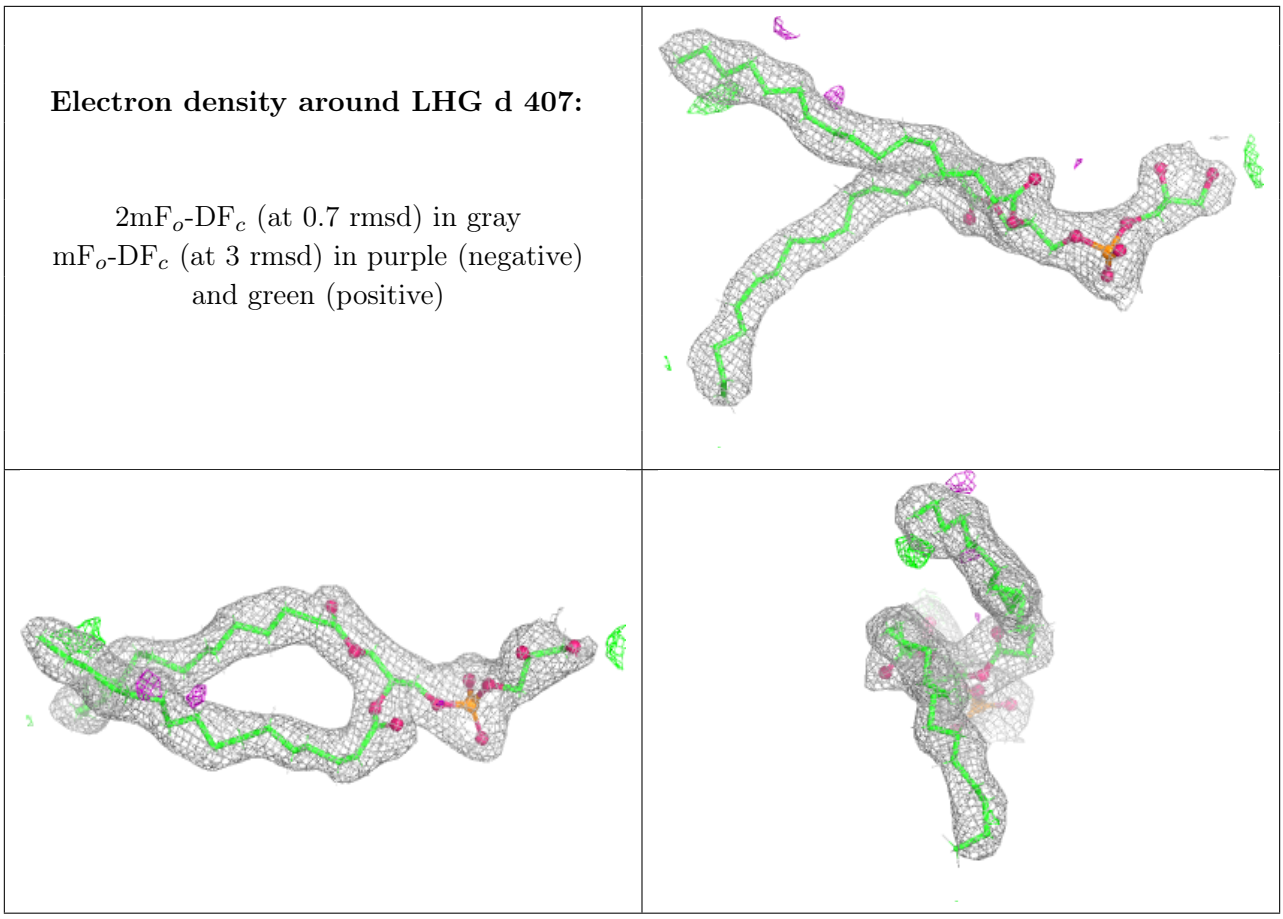






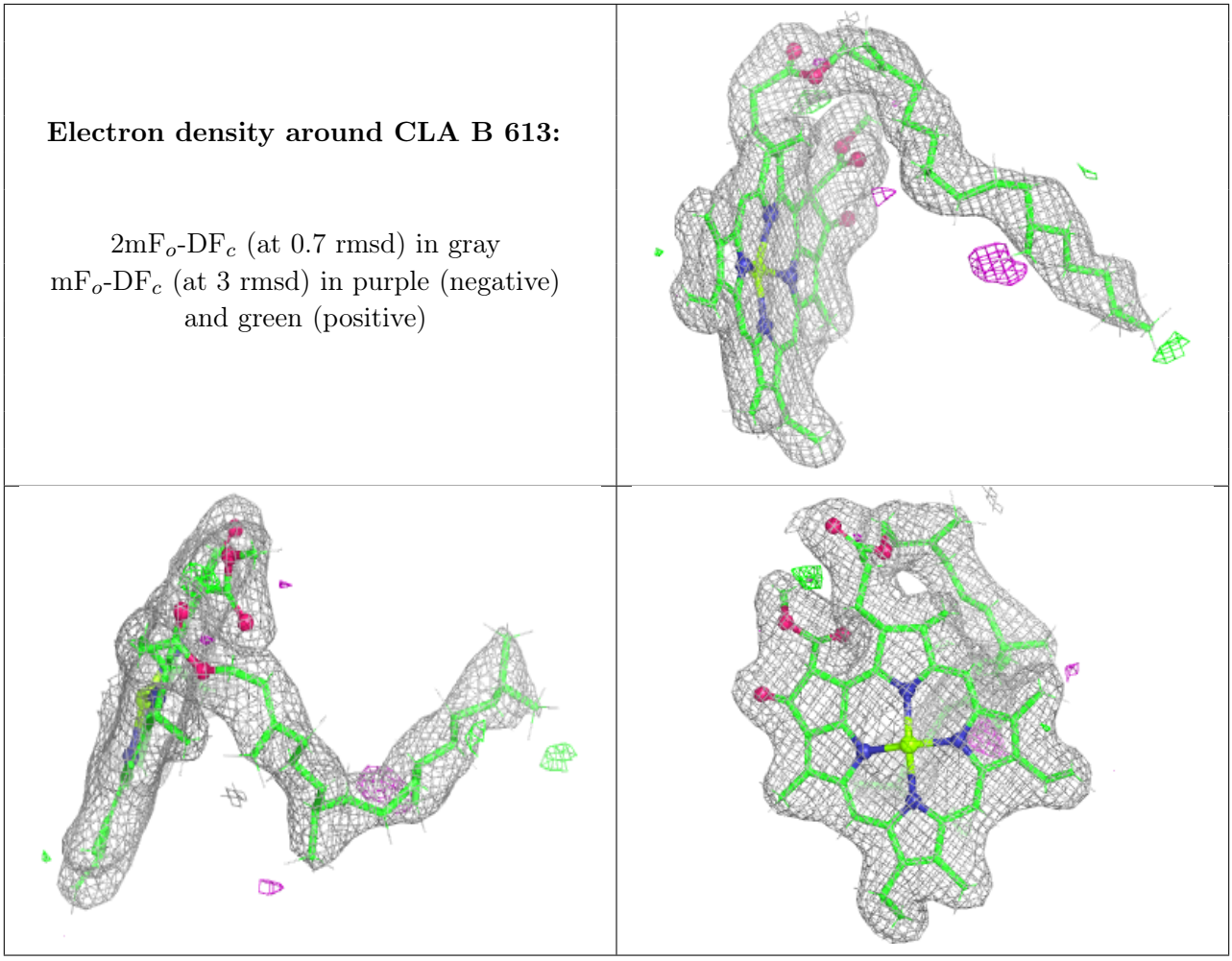
Electron density around LHG d 407:

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



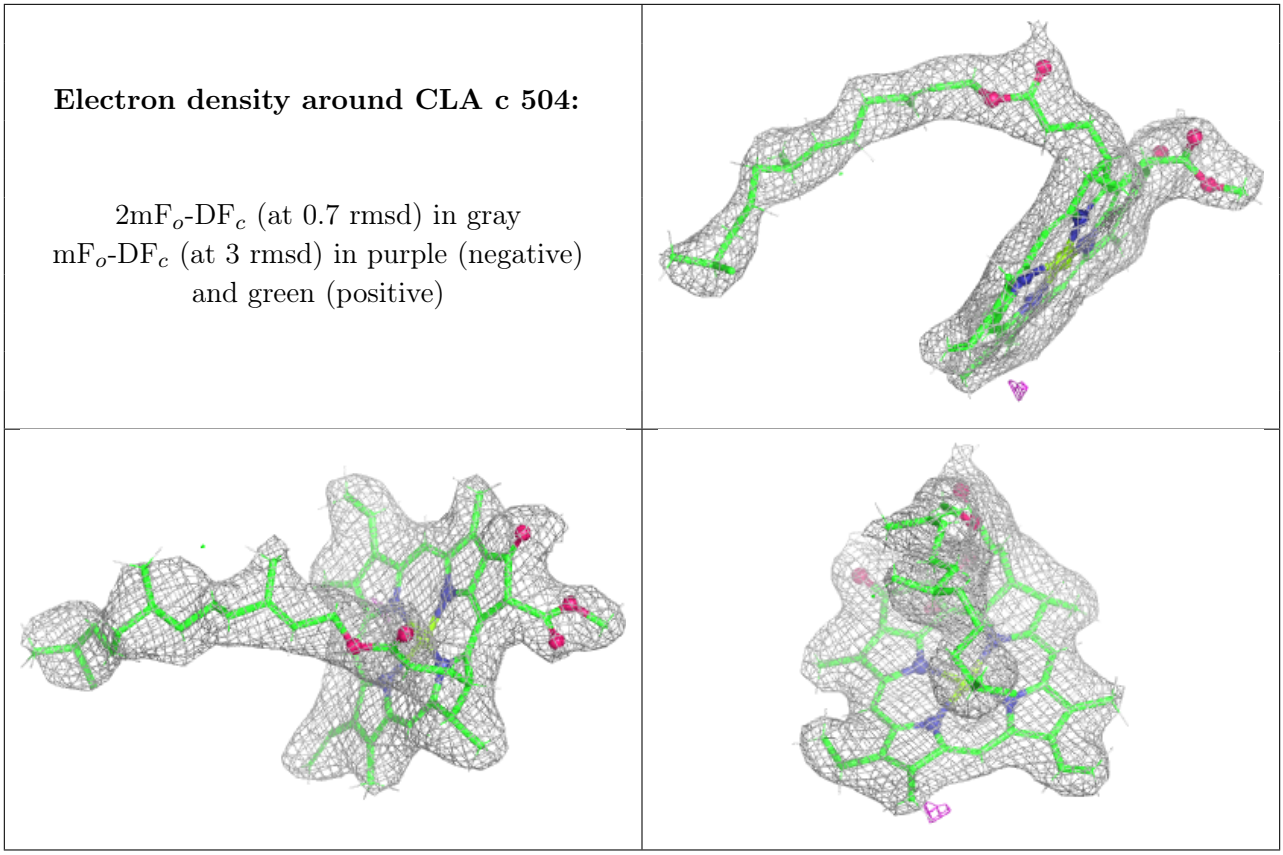
Electron density around CLA B 613:

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



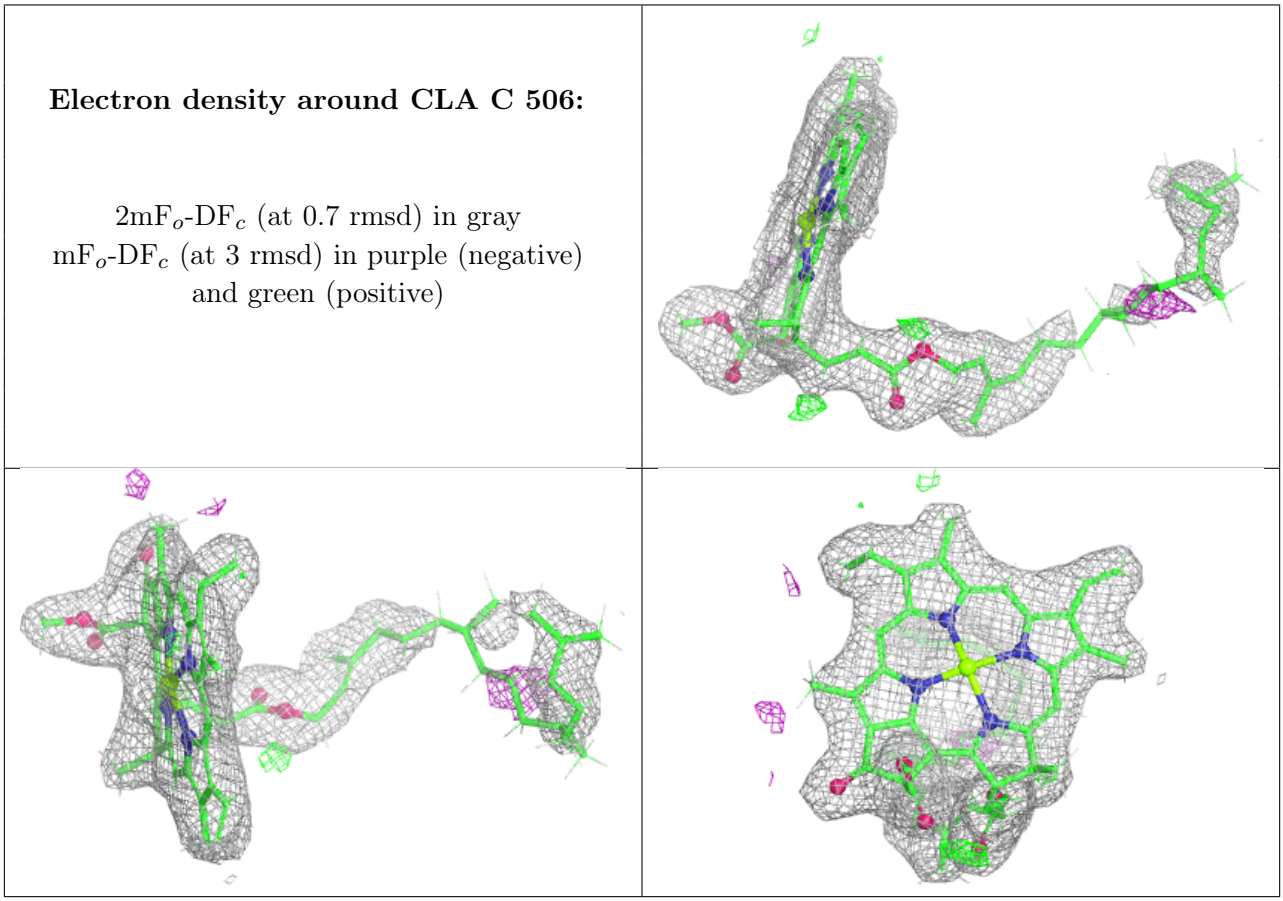
Electron density around CLA c 504:

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



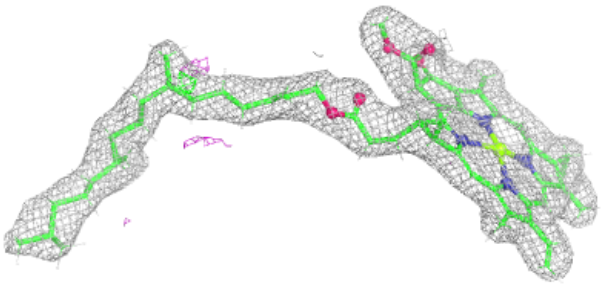
Electron density around CLA C 506:

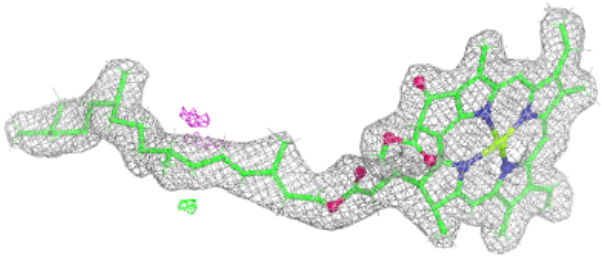
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

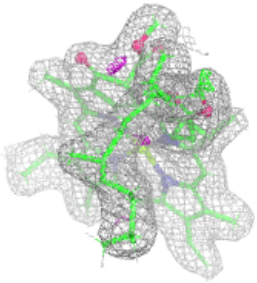


Electron density around CLA A 404:

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

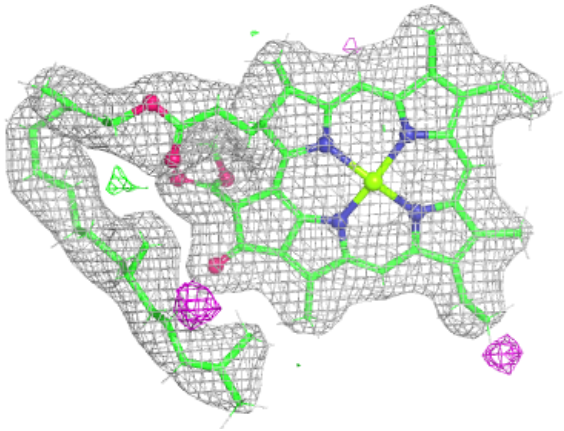


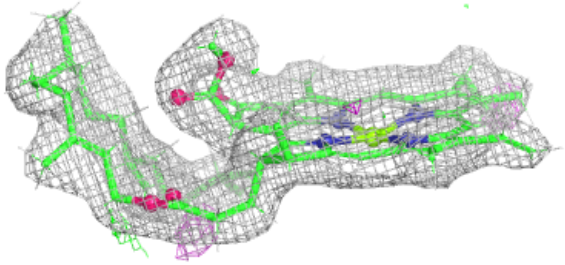


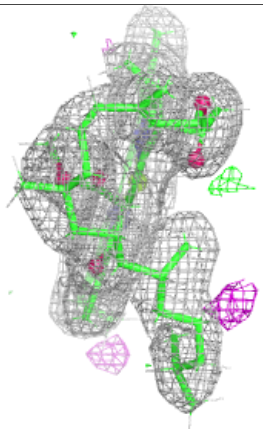


Electron density around CLA B 610:

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

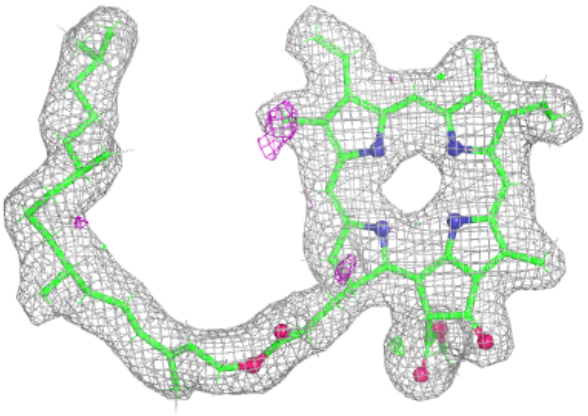


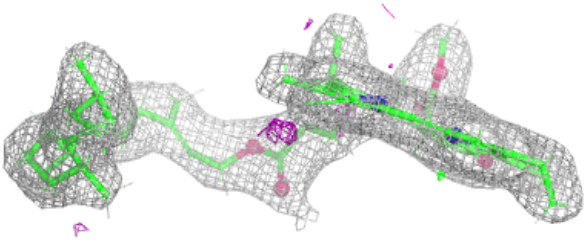


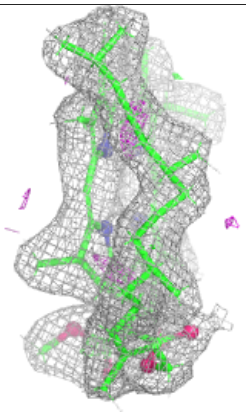


Electron density around PHO A 406:

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

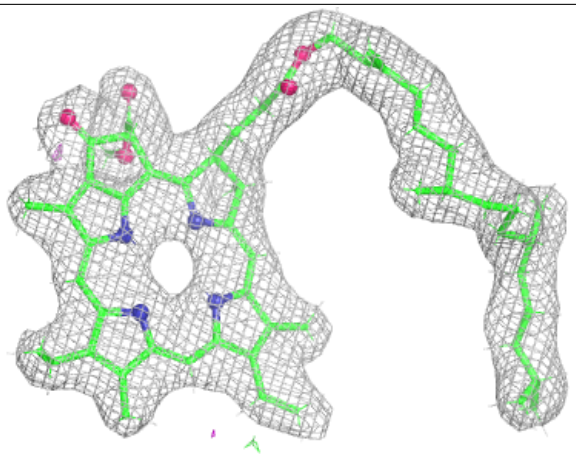


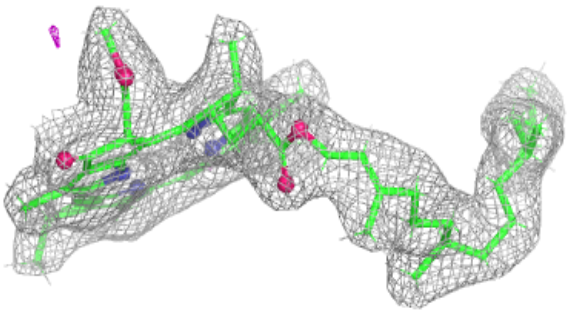


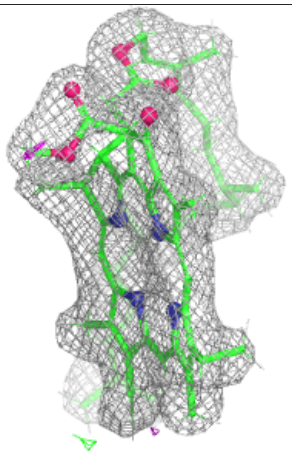


Electron density around PHO D 401:

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

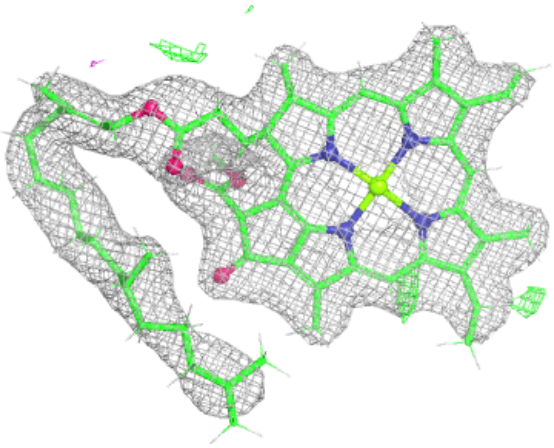


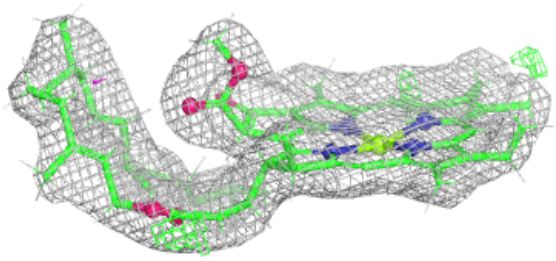


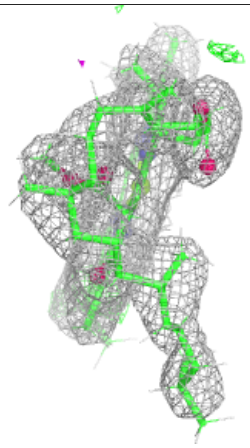


Electron density around CLA b 611:

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

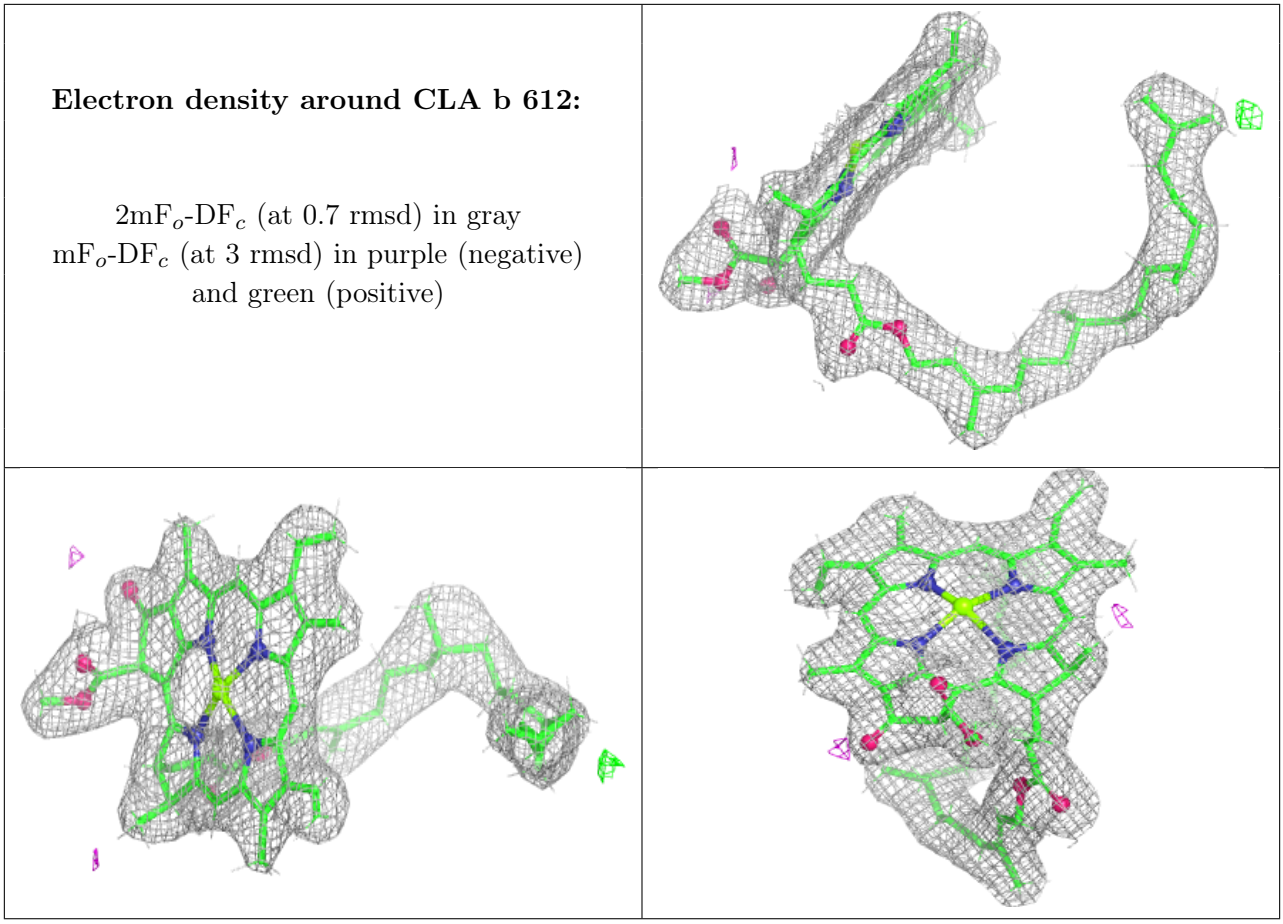






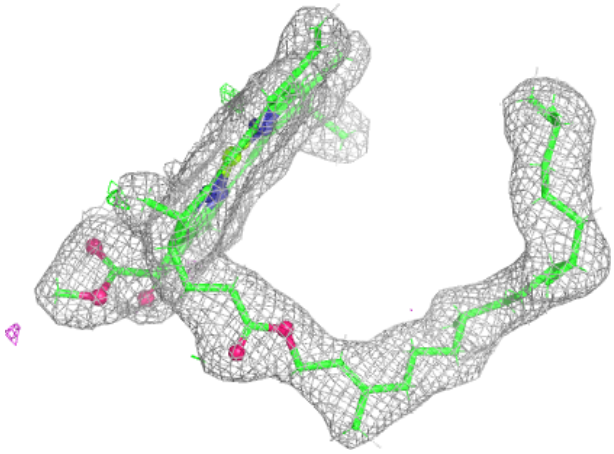
Electron density around CLA b 612:

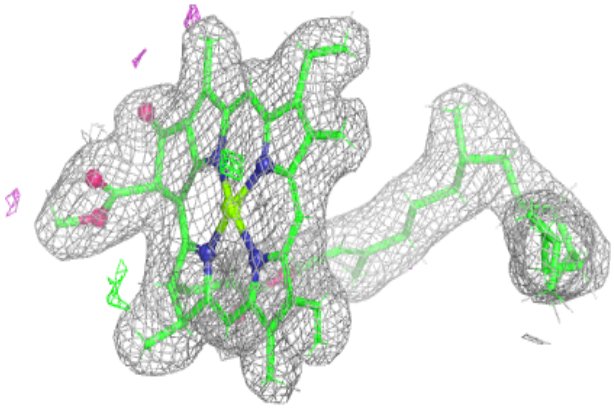
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

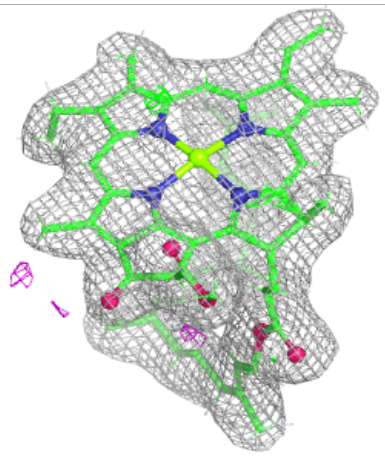


Electron density around CLA B 611:

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

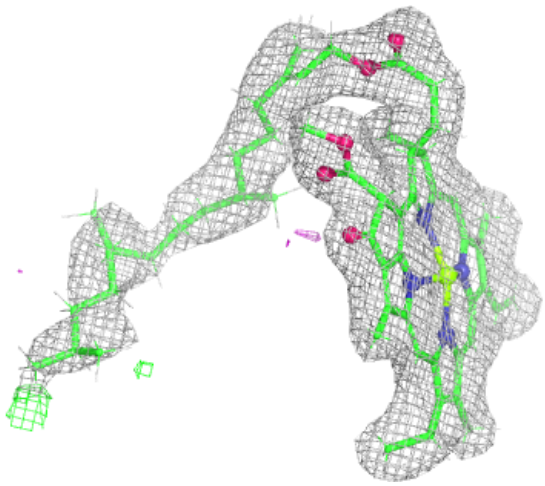


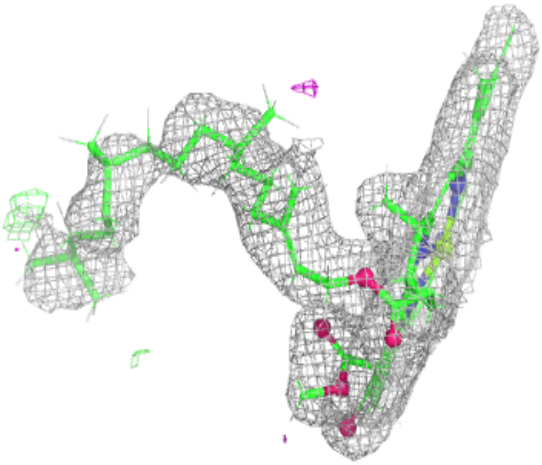


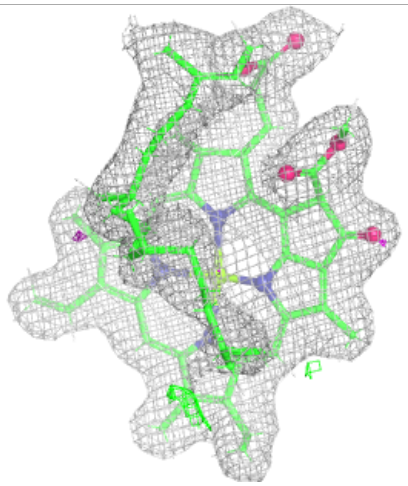


Electron density around CLA b 614:

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

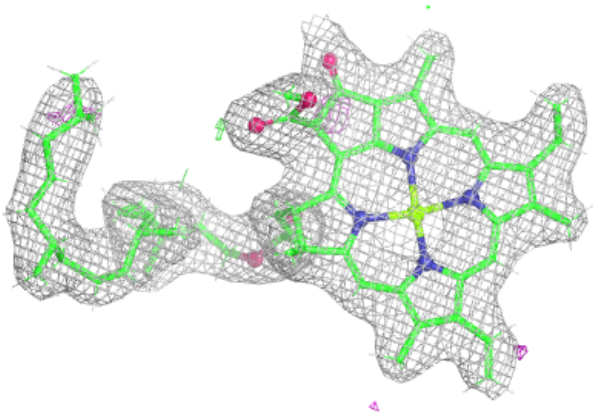


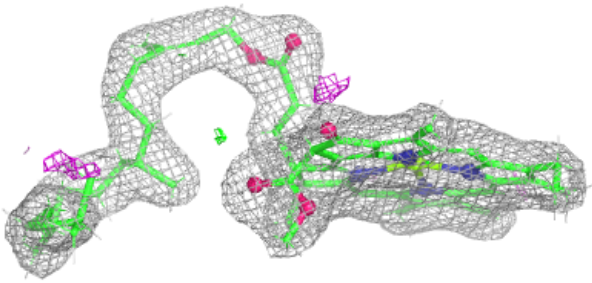


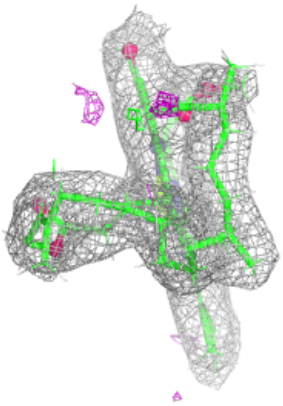


Electron density around CLA B 612:

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

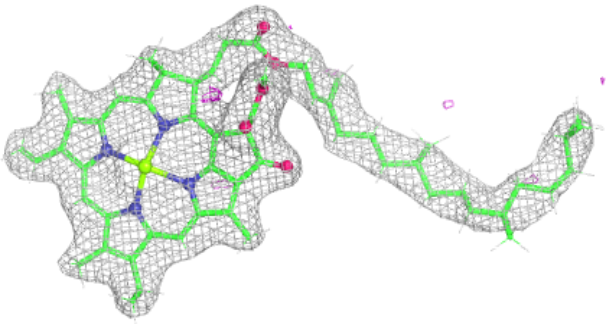


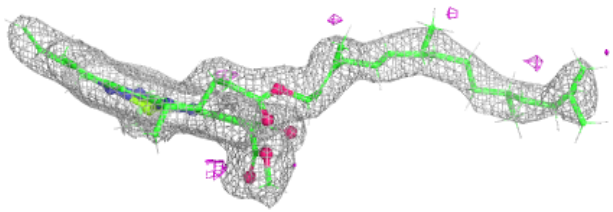


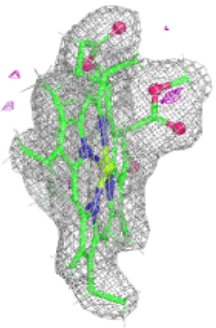


Electron density around CLA B 602:

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

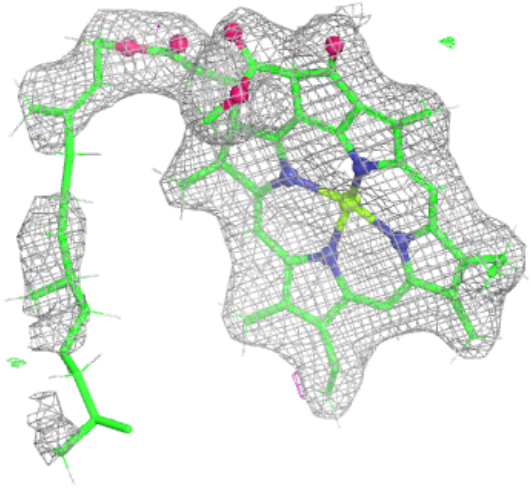


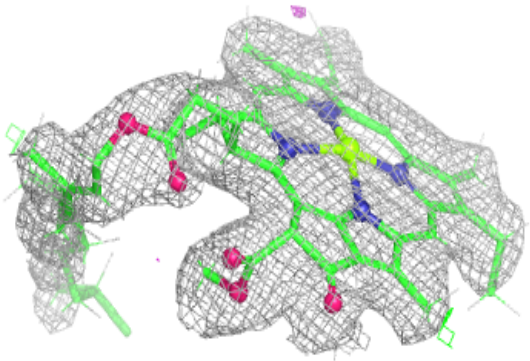


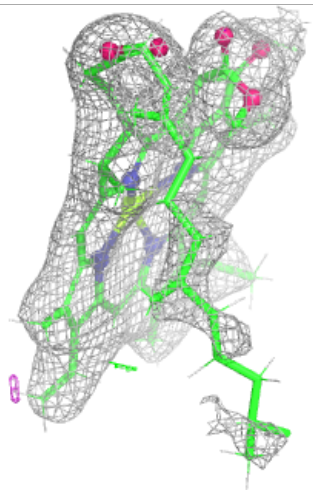


Electron density around CLA b 617:

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

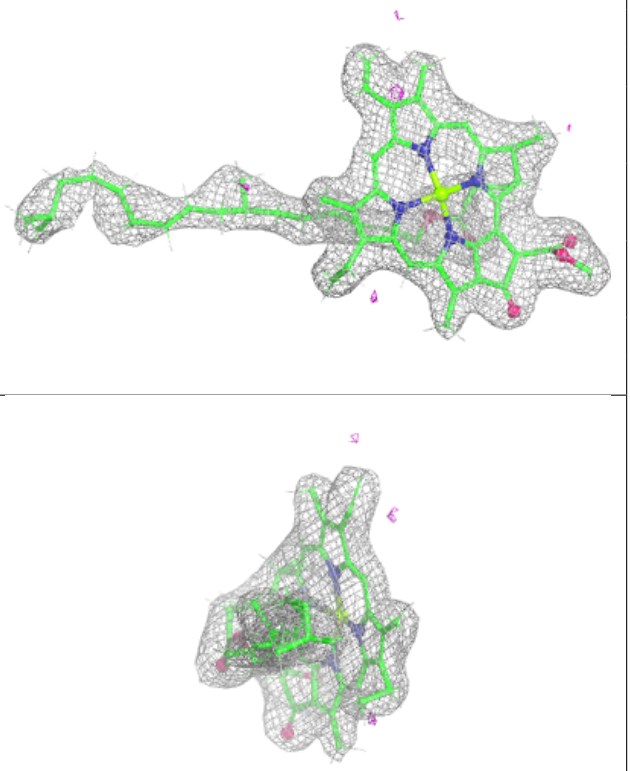






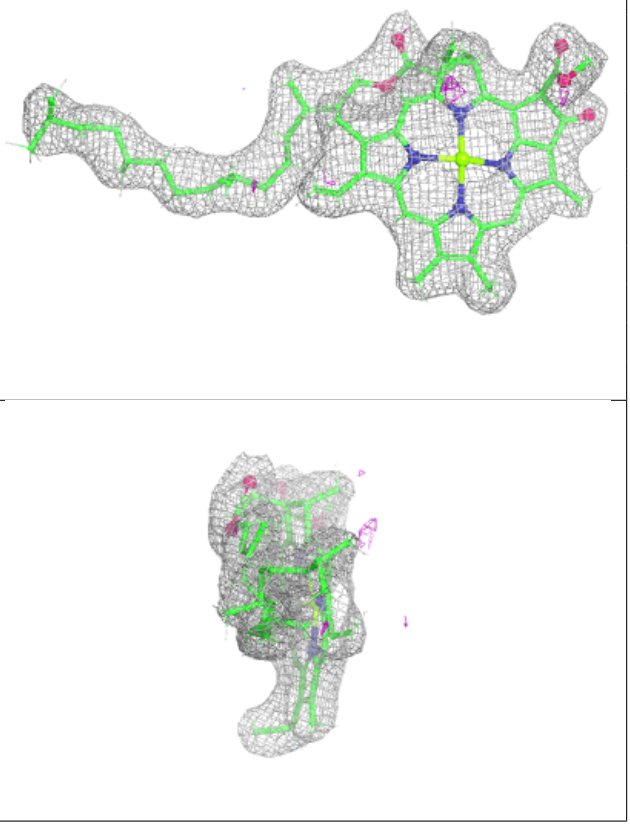
Electron density around CLA B 614:

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



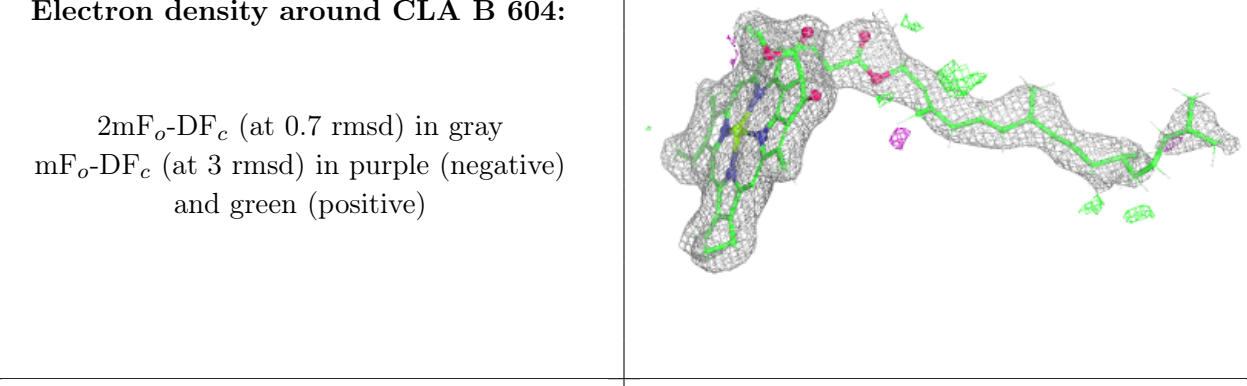
Electron density around CLA B 603:

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



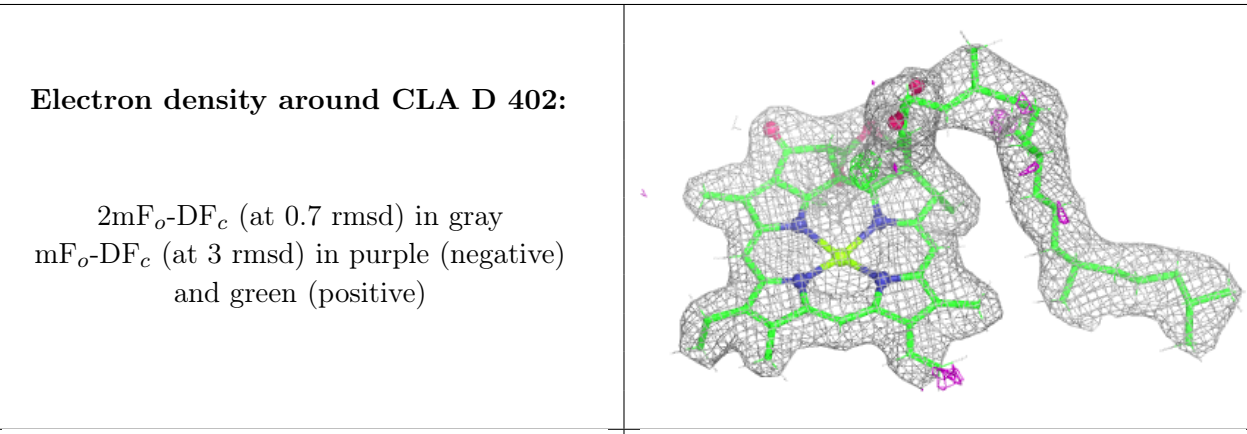
Electron density around CLA B 604:

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



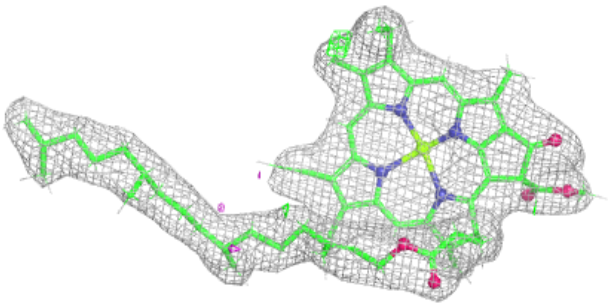
Electron density around CLA D 402:

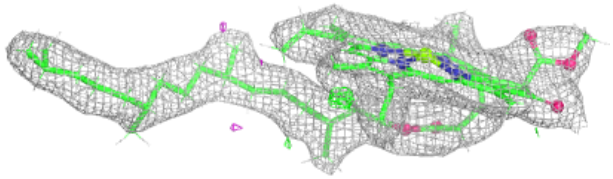
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

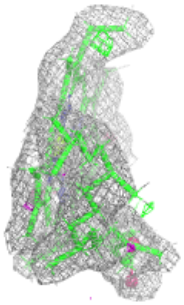


Electron density around CLA C 501:

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

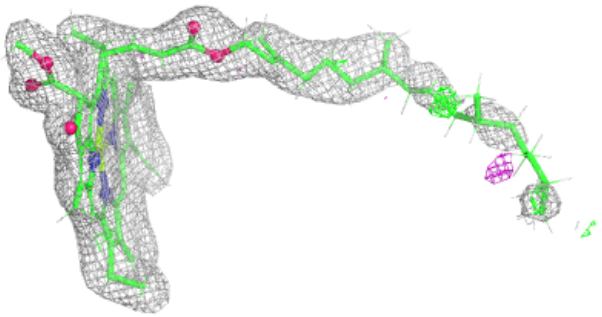


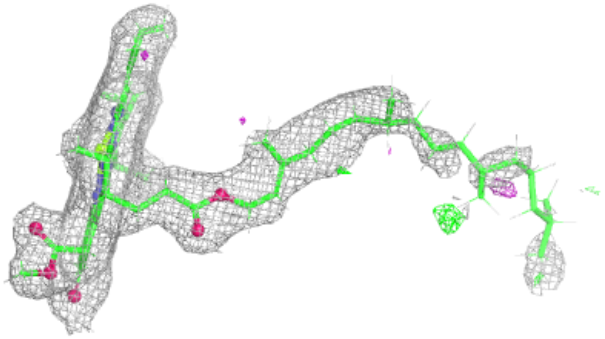


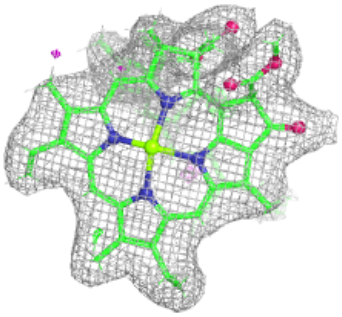


Electron density around CLA D 404:

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

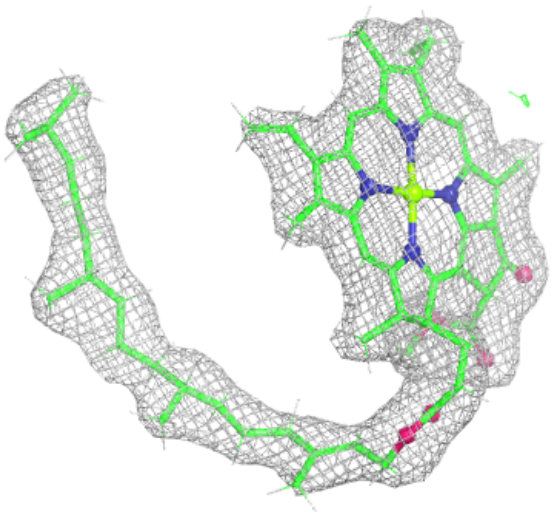


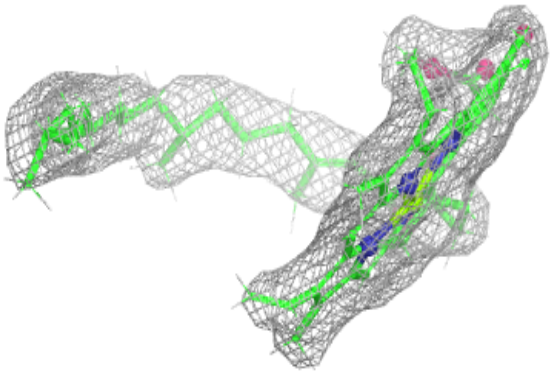


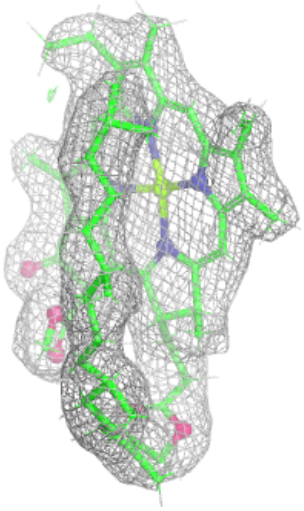


Electron density around CLA c 507:

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

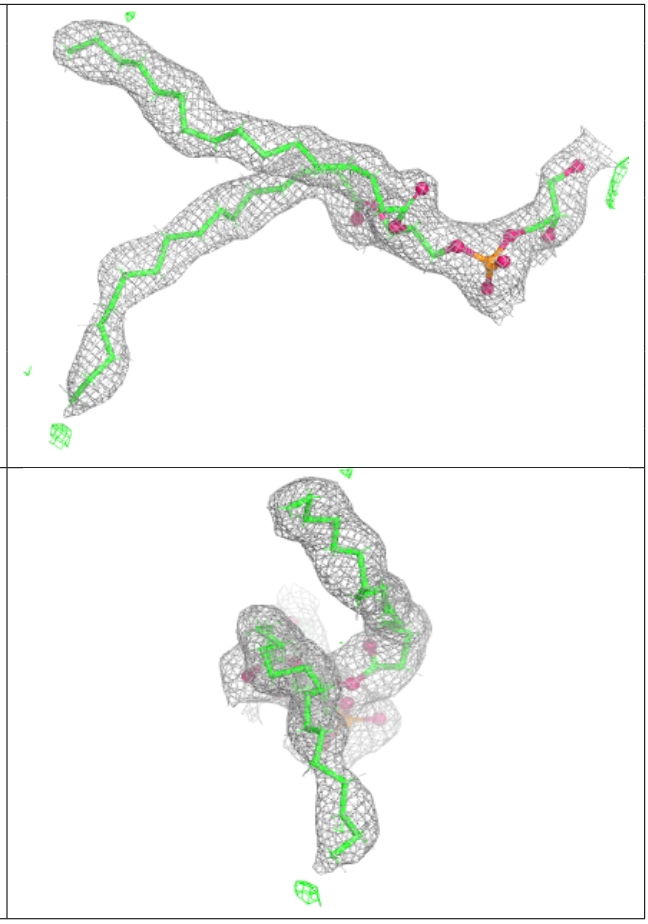






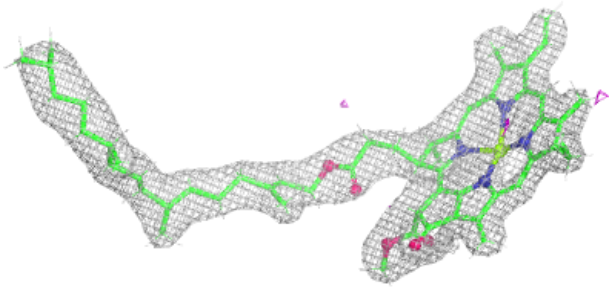
Electron density around LHG D 408:

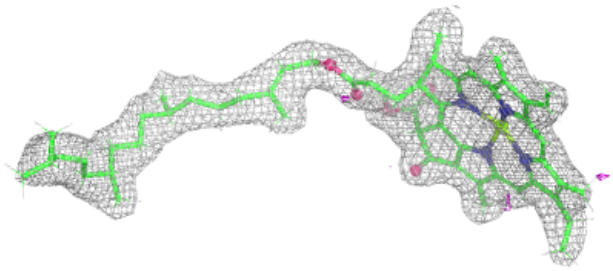
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

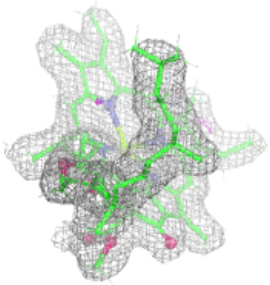


Electron density around CLA a 404:

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

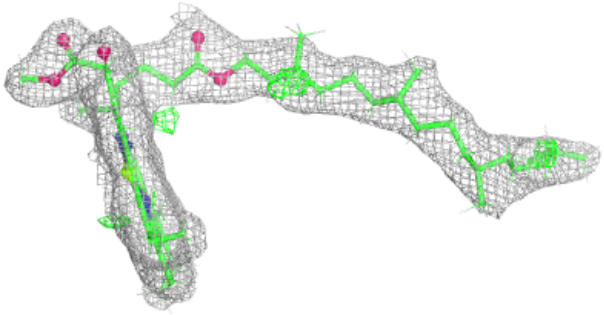


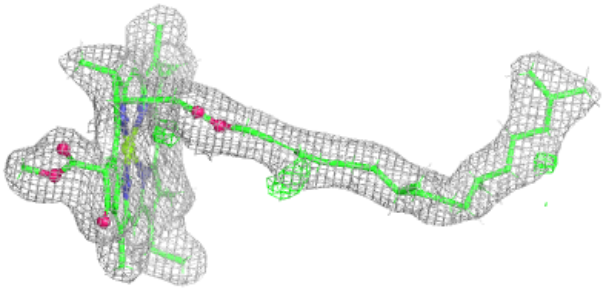


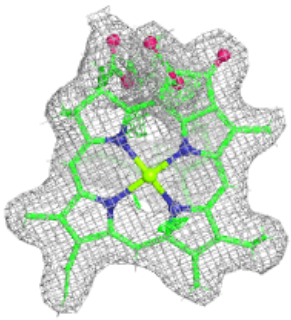


Electron density around CLA B 605:

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

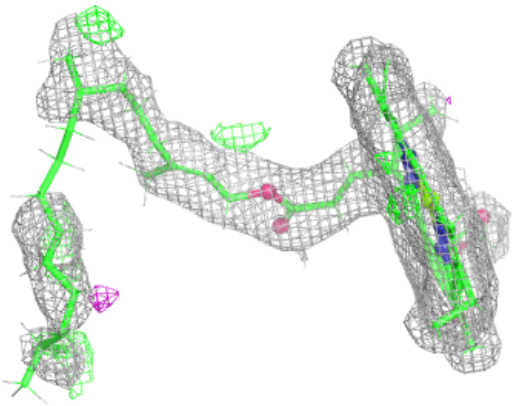


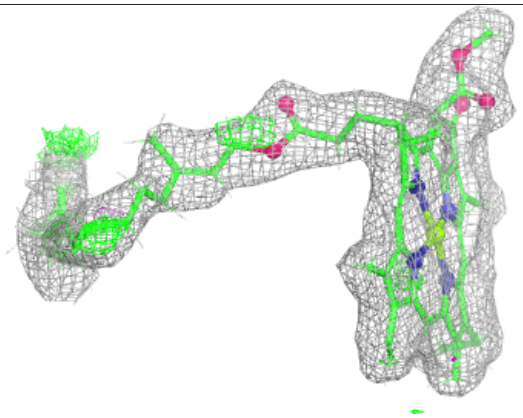


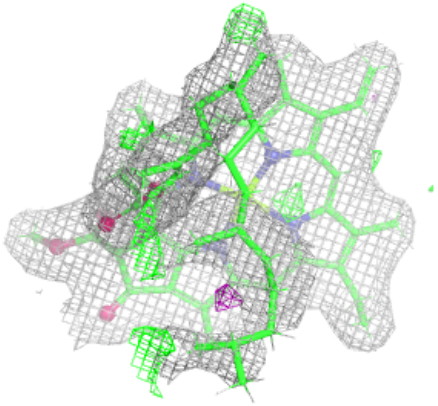


Electron density around CLA a 407:

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

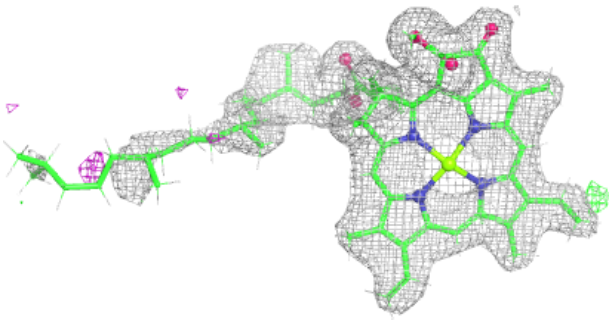


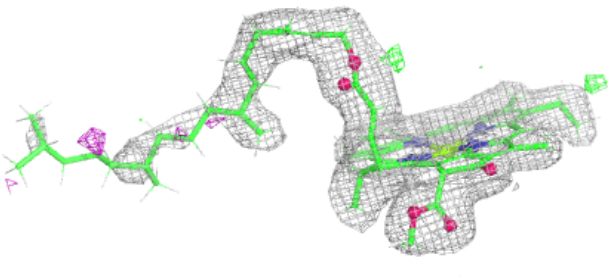


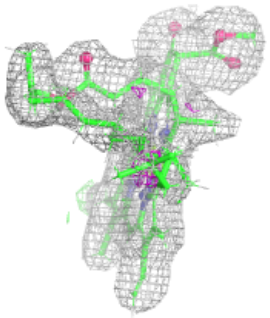


Electron density around CLA A 405:

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

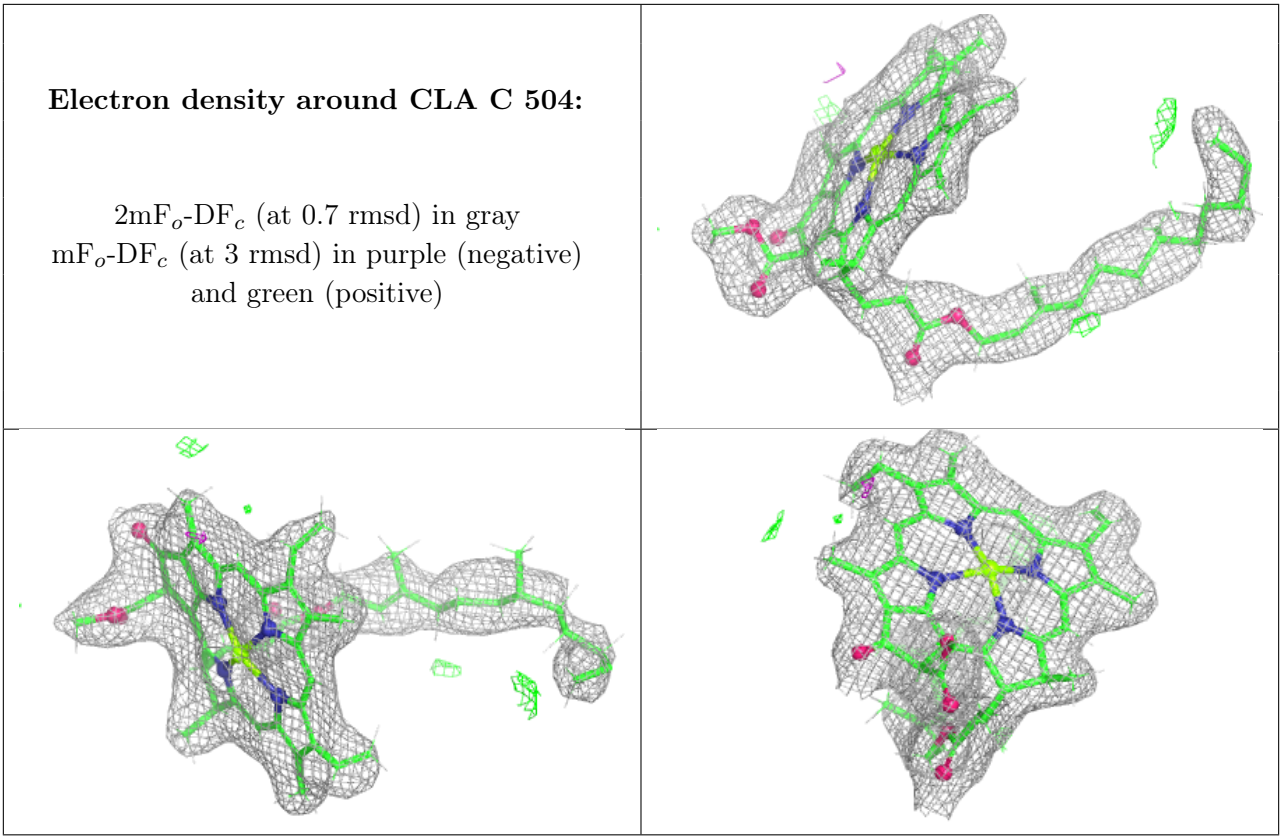






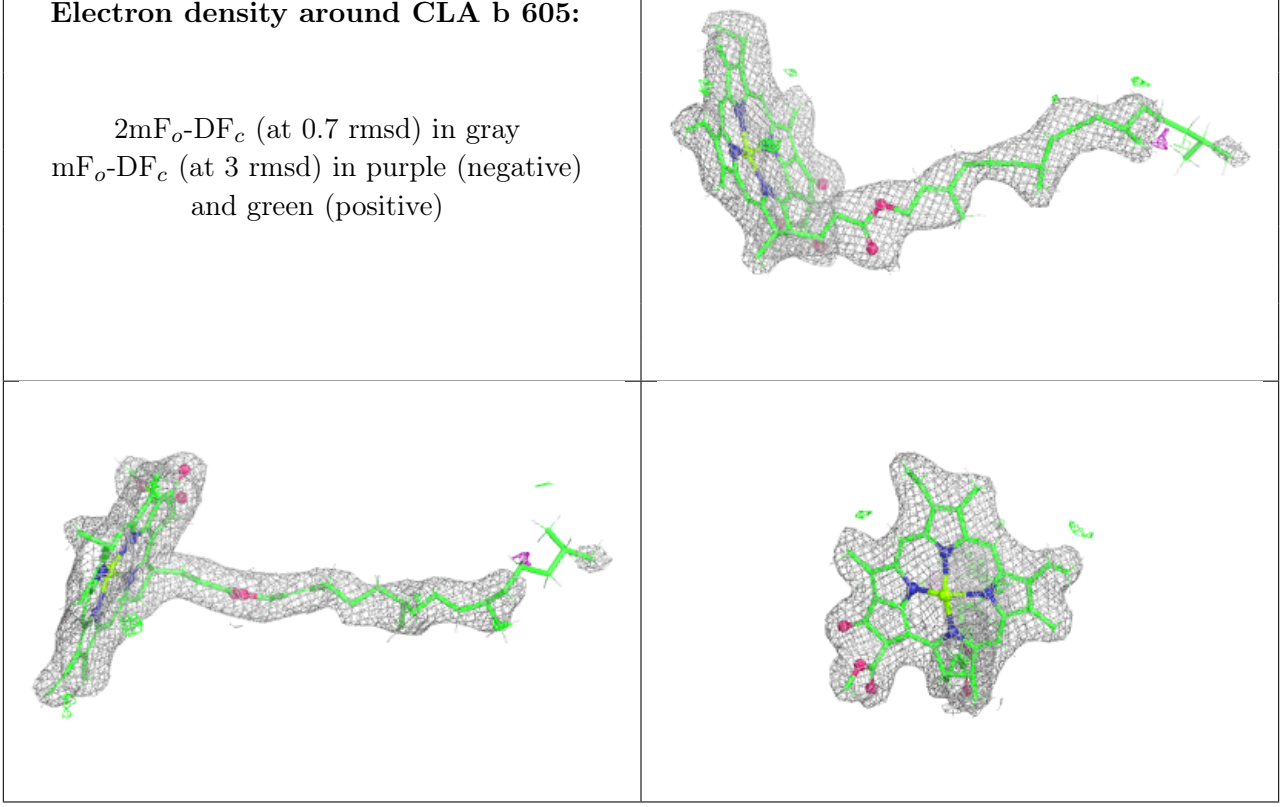
Electron density around CLA C 504:

$2mF_o$-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 605:

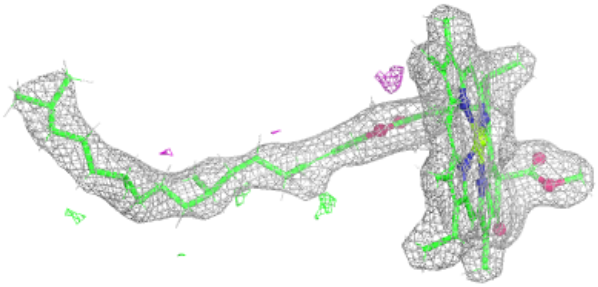
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

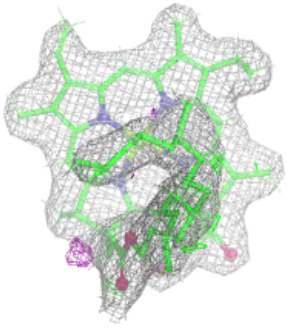


Electron density around CLA b 606:

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

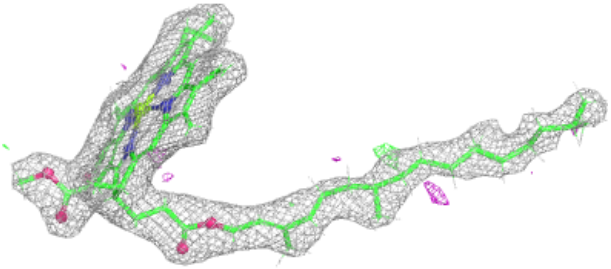


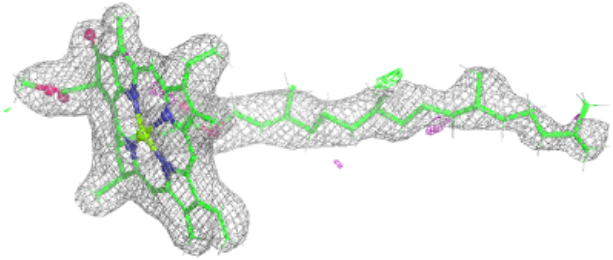


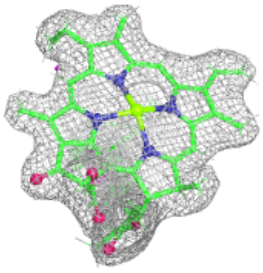


Electron density around CLA B 607:

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

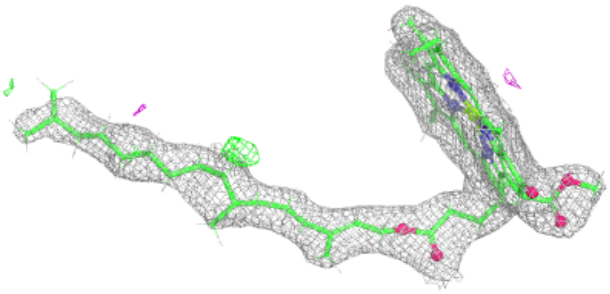


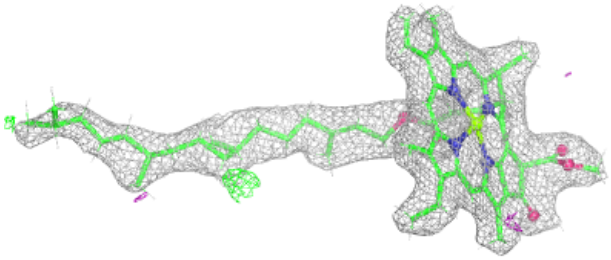


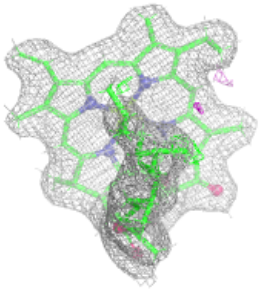


Electron density around CLA b 608:

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

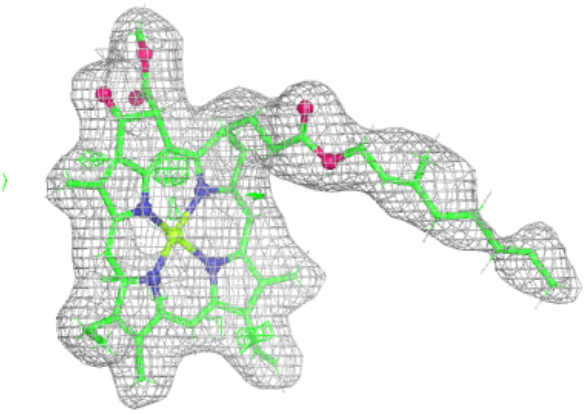


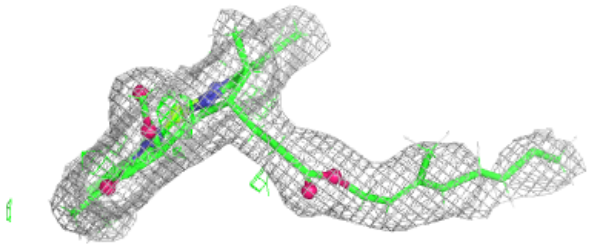




Electron density around CLA A 407:

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

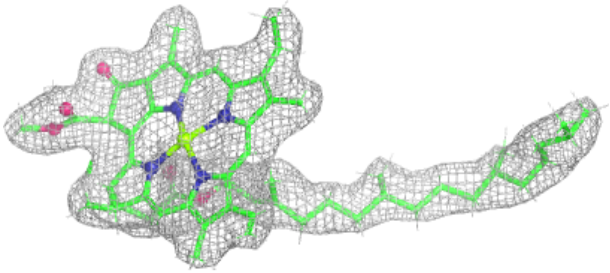


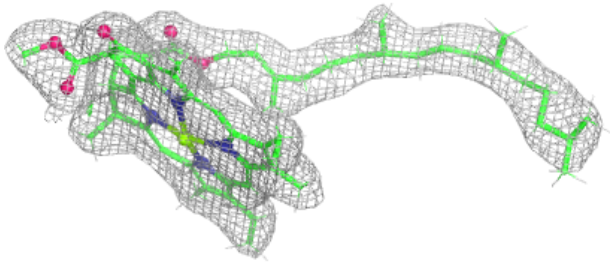


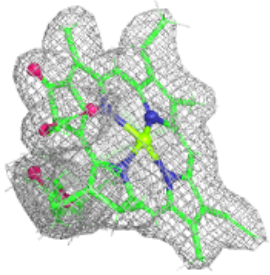


Electron density around CLA B 608:

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

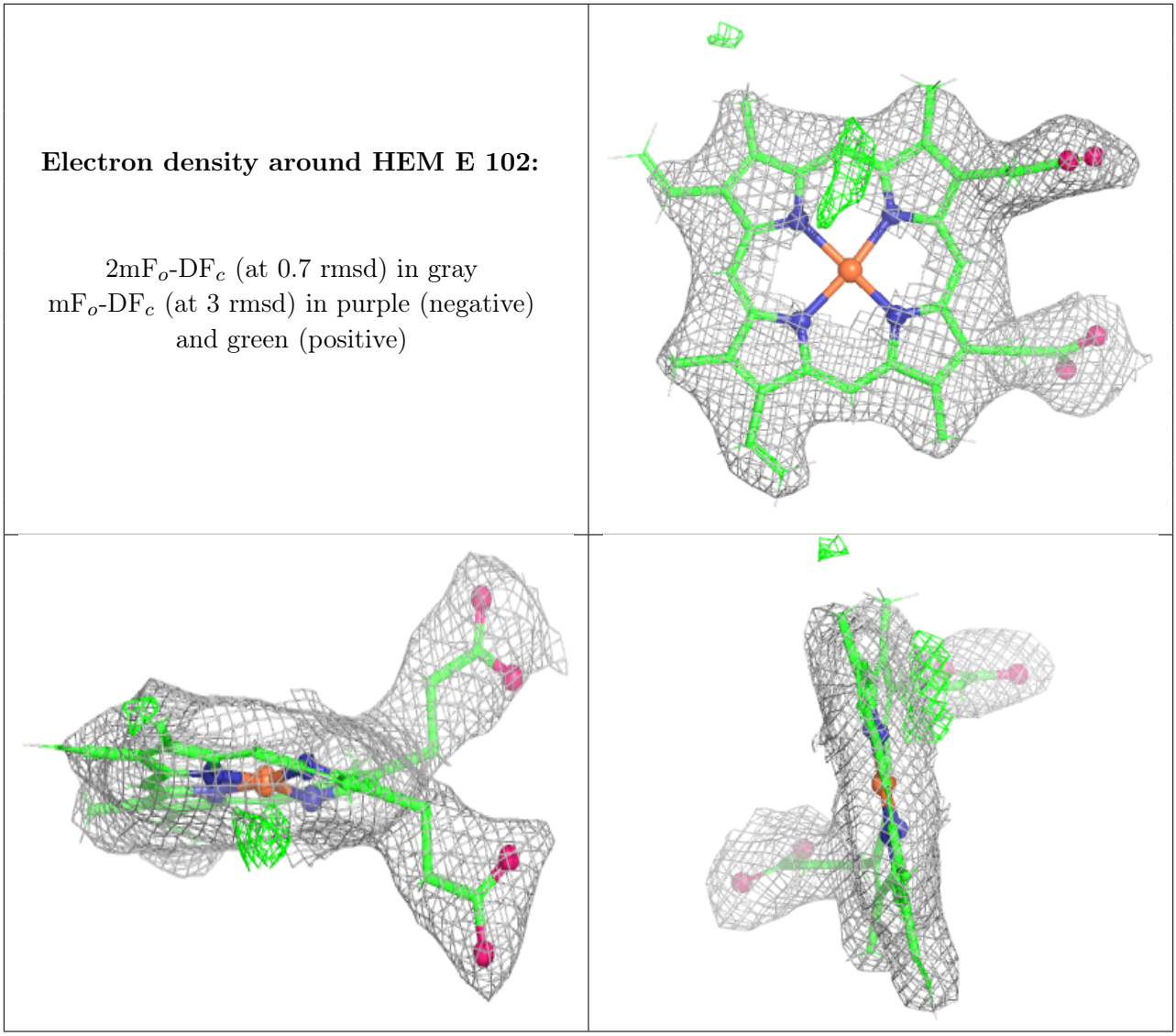






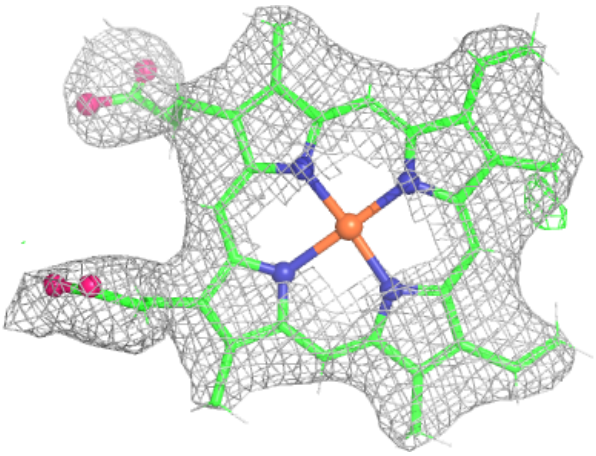
Electron density around HEM E 102:

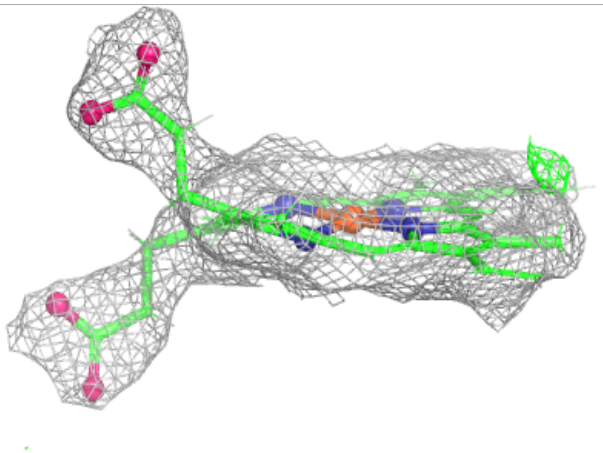
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

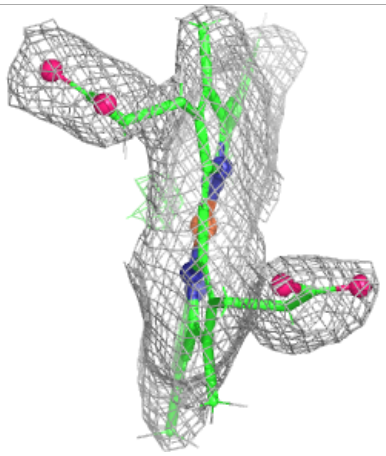


Electron density around HEM e 102:

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

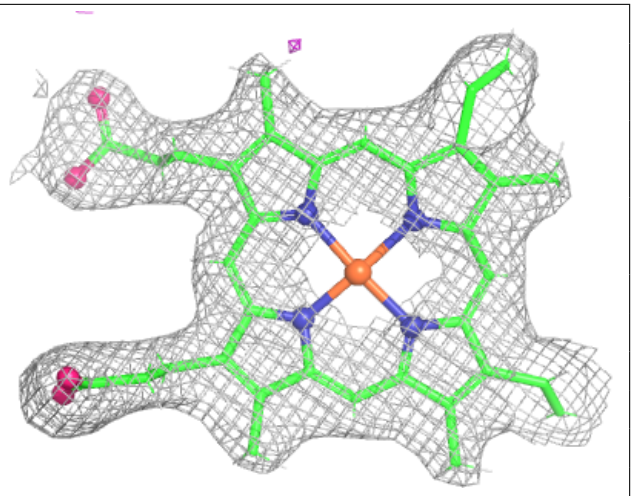


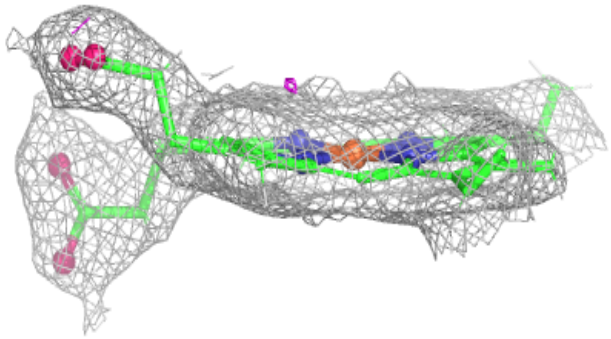


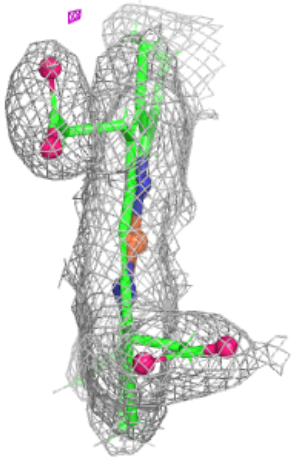


Electron density around HEC V 201:

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

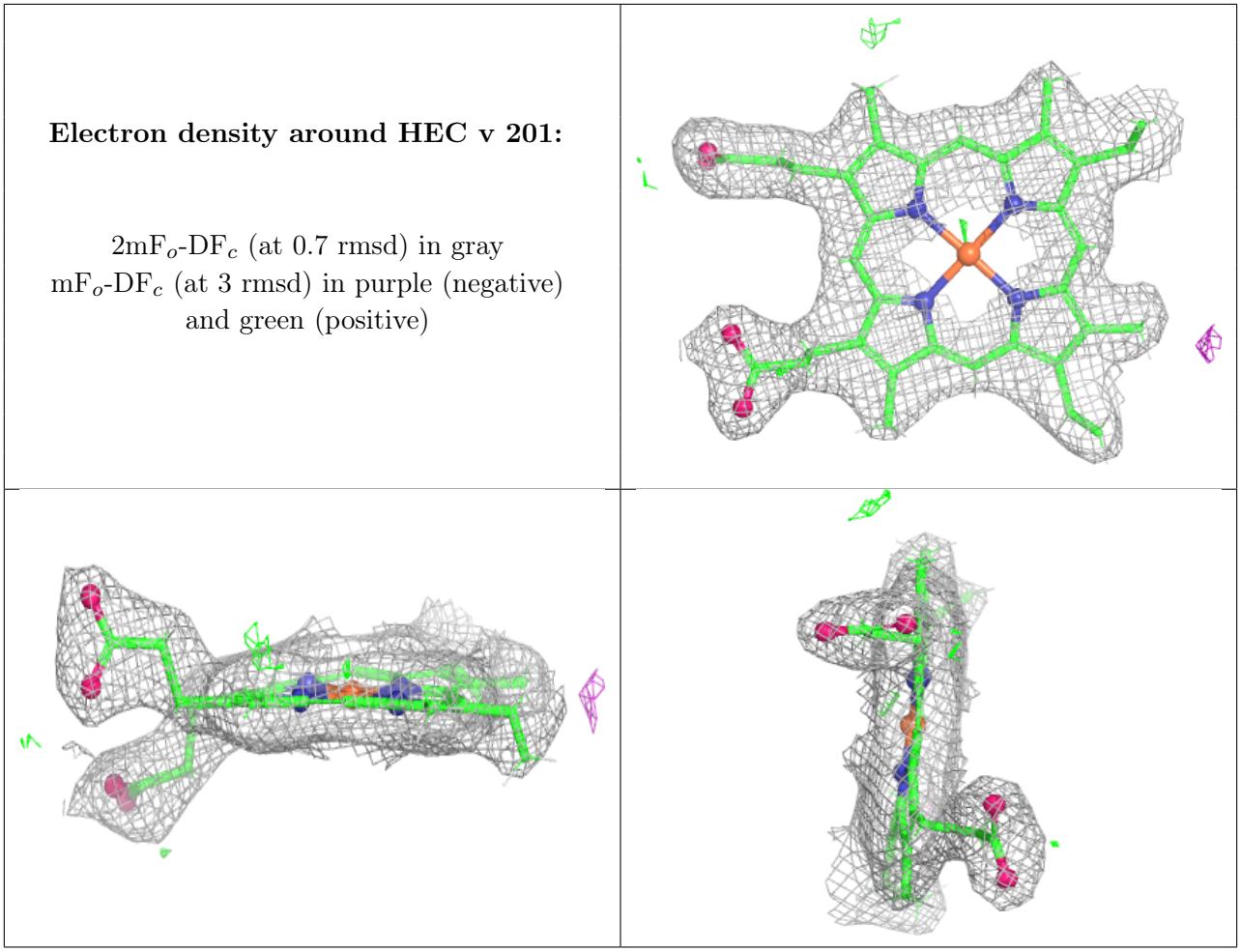






Electron density around HEC v 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.