wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 09:57 AM EDT

PDB ID	:	6DHG / pdb_00006dhg
Title	:	RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.5 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	:	2.50 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

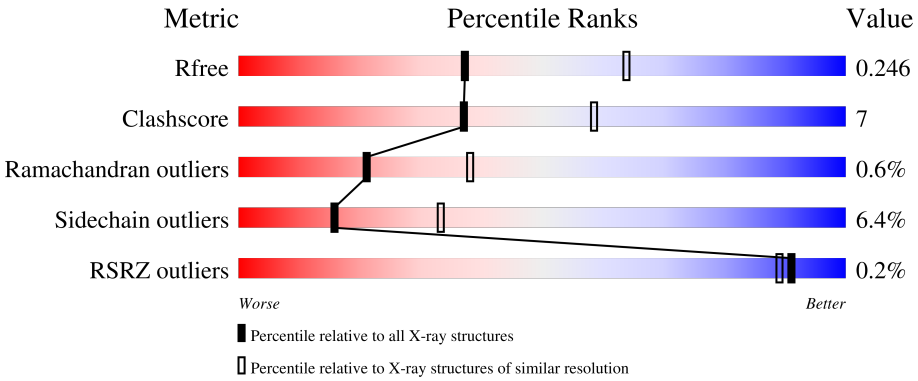
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0

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 2.50 Å.

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



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

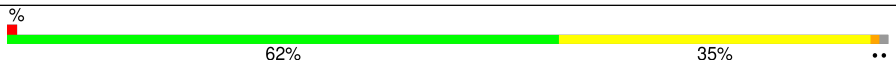
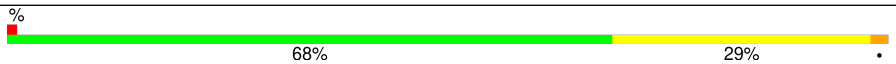
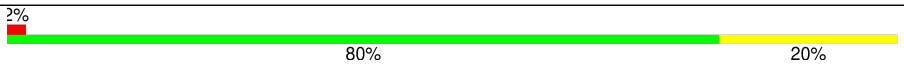
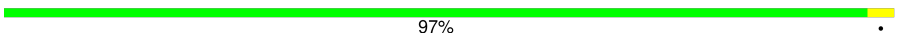
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	334	84% 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	83% 13%
14	t	30	3% 73% 27%
15	U	97	80% 18%
15	u	97	82% 16%
16	V	137	82% 15%
16	v	137	75% 22%
17	Y	30	7% 50% 30% 10% 10%
17	y	30	53% 43%
18	X	38	74% 24%
18	x	38	58% 39%
19	Z	62	61% 31% 8%
19	z	62	3% 69% 18% 13%
20	R	34	3% 62% 29% 9%
20	r	34	3% 56% 21% 15% 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 103658 atoms, of which 51467 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
			450	144	232	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			

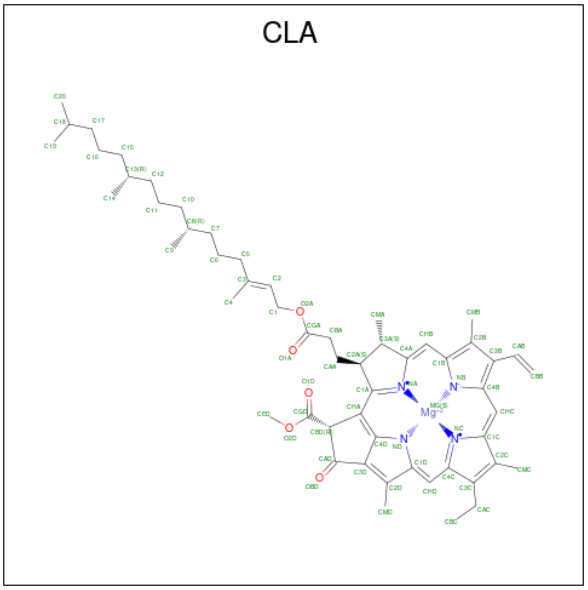
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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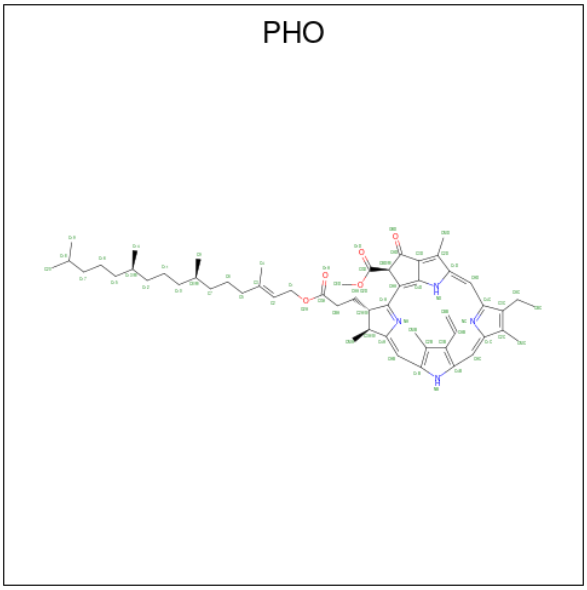
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total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

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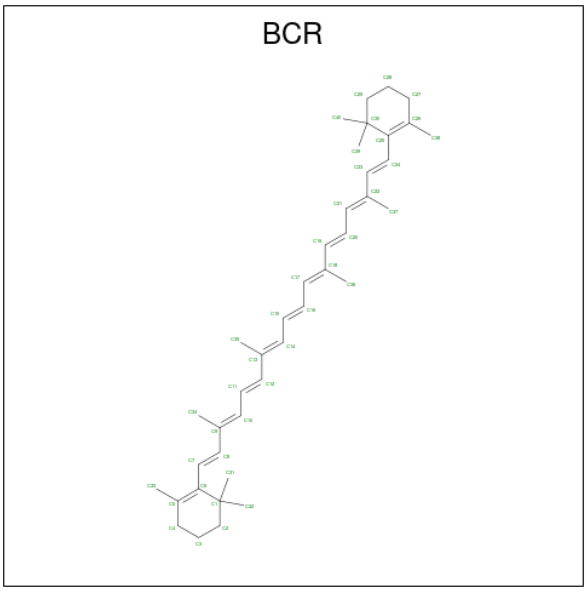
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- 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: $C_{40}H_{56}$).



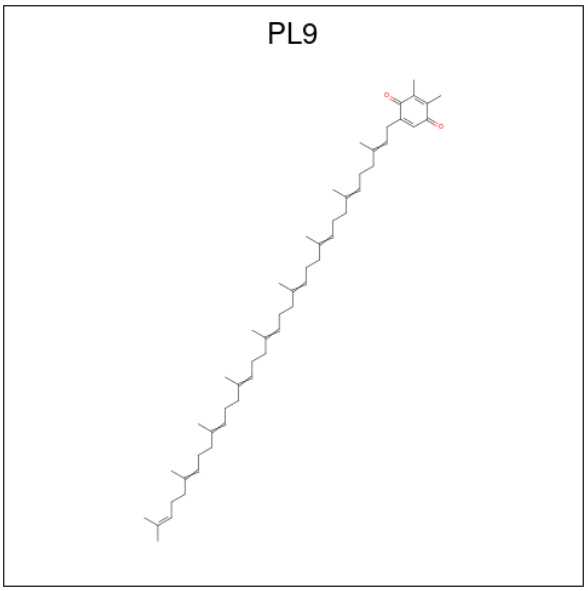
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	D	1	Total C H 96 40 56	0	0
25	H	1	Total C H 96 40 56	0	0
25	K	1	Total C H 96 40 56	0	0
25	T	1	Total C H 96 40 56	0	0
25	Z	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	k	1	Total C H 96 40 56	0	0
25	t	1	Total C H 96 40 56	0	0
25	x	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: $C_{53}H_{80}O_2$).



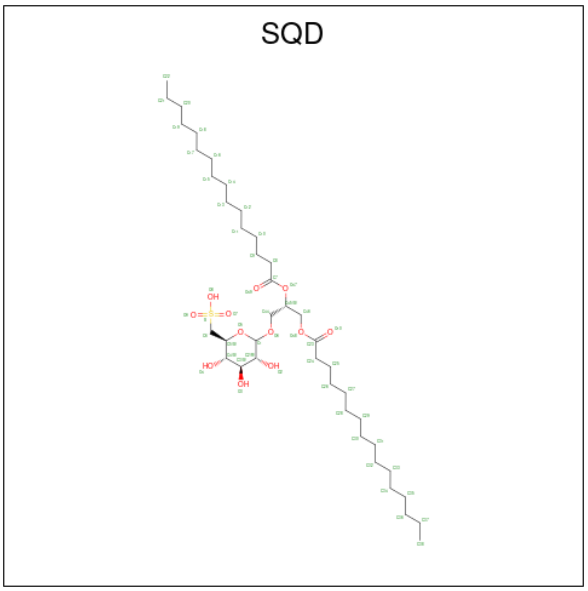
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C H O 135 53 80 2	0	0
26	D	1	Total C H O 135 53 80 2	0	0

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

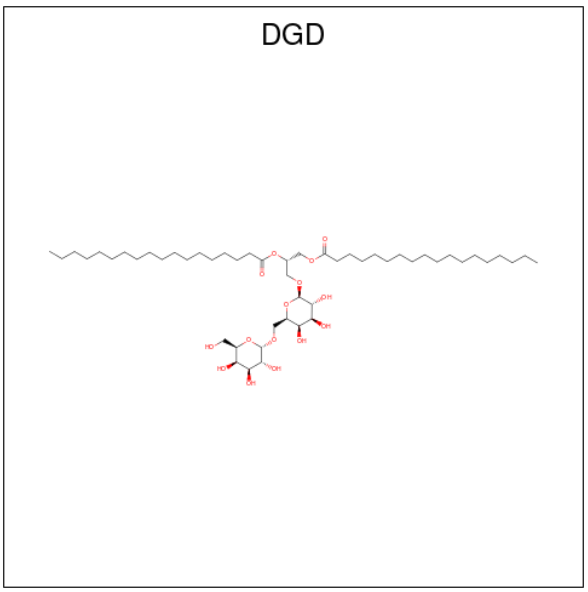
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C H O S 122 39 70 12 1	0	0
27	A	1	Total C H O 104 35 65 4	0	0
27	B	1	Total C H O S 132 41 78 12 1	0	0
27	F	1	Total C H O S 81 25 45 10 1	0	0
27	a	1	Total C H O S 132 41 78 12 1	0	0
27	a	1	Total C H O 92 31 56 5	0	0
27	b	1	Total C H O S 114 36 65 12 1	0	0
27	f	1	Total C H O S 90 28 49 12 1	0	0

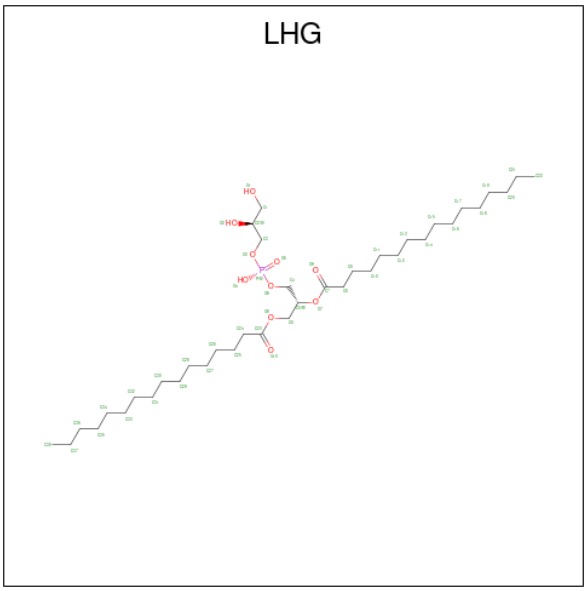
- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

$C_{51}H_{96}O_{15}$).



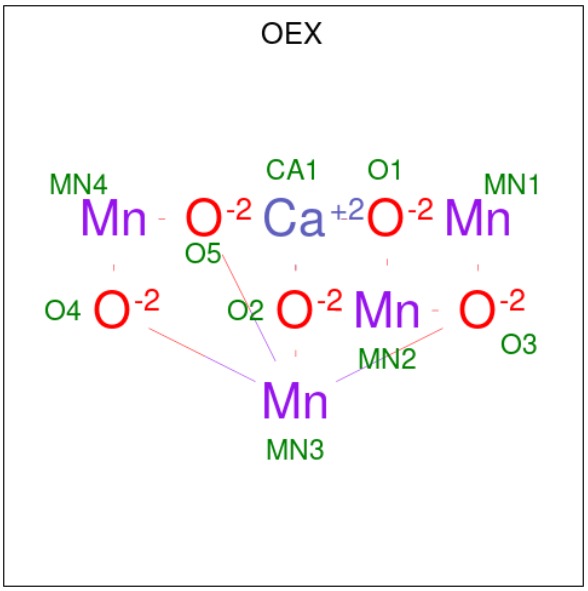
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			162	51	96	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	H	1	Total	C	H	O	0	0
			144	47	82	15		
28	a	1	Total	C	H	O	0	0
			119	39	75	5		
28	c	1	Total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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



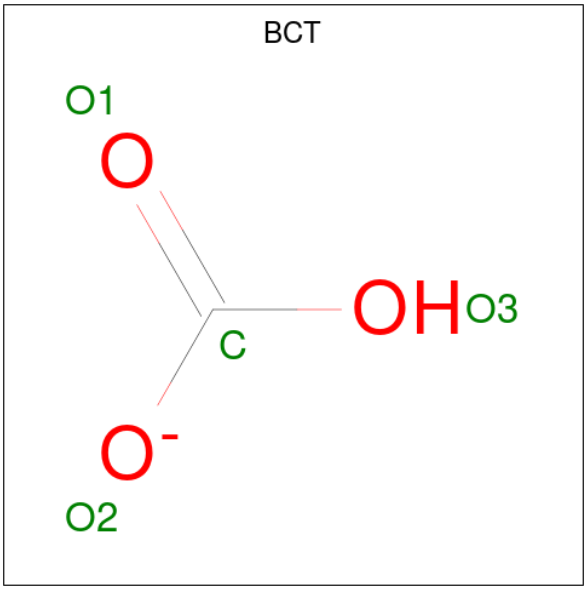
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
29	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123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

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

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

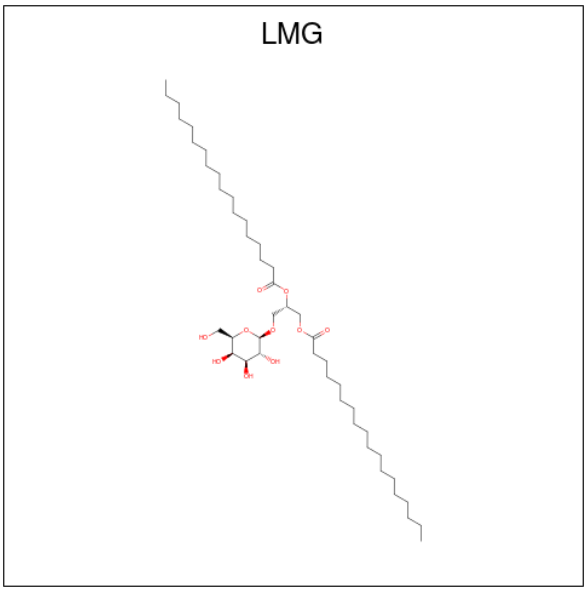


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			5	1	1	3		
31	a	1	Total	C	H	O	0	0
			5	1	1	3		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	6	Total C H O 226 79 137 10	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 47 16 31	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	5	Total C H O 220 75 139 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	1	Total C H 26 10 16	0	0
32	x	1	Total C H O 55 18 35 2	0	0

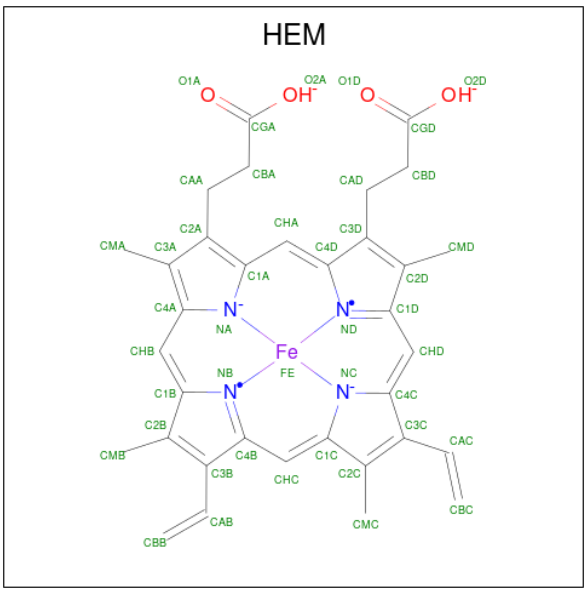
- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	D	1	Total	C	H	O	0	0
			123	41	72	10		
33	D	1	Total	C	H	O	0	0
			78	27	45	6		
33	D	1	Total	C	H	O	0	0
			68	24	40	4		
33	M	1	Total	C	H	O	0	0
			123	41	72	10		
33	b	1	Total	C	H	O	0	0
			141	45	86	10		
33	c	1	Total	C	H	O	0	0
			81	27	44	10		
33	c	1	Total	C	H	O	0	0
			117	38	69	10		
33	c	1	Total	C	H	O	0	0
			117	39	68	10		
33	d	1	Total	C	H	O	0	0
			57	21	34	2		
33	d	1	Total	C	H	O	0	0
			102	34	58	10		
33	m	1	Total	C	H	O	0	0
			123	41	72	10		

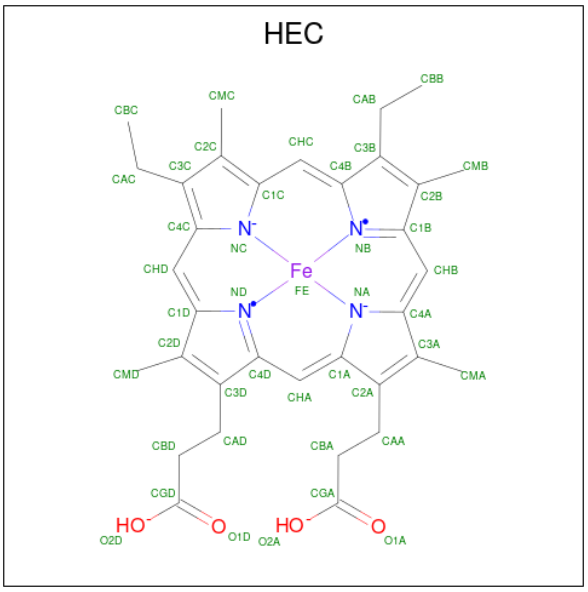
- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

$C_{34}H_{32}FeN_4O_4$).



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		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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	136	Total	O	0	0
			136	136		
36	B	216	Total	O	0	0
			216	216		
36	C	192	Total	O	0	0
			192	192		
36	D	138	Total	O	0	0
			138	138		
36	E	30	Total	O	0	0
			30	30		
36	F	10	Total	O	0	0
			10	10		
36	H	25	Total	O	0	0
			25	25		
36	I	16	Total	O	0	0
			16	16		
36	J	13	Total	O	0	0
			13	13		
36	L	7	Total	O	0	0
			7	7		
36	M	7	Total	O	0	0
			7	7		
36	O	128	Total	O	0	0
			128	128		
36	T	11	Total	O	0	0
			11	11		
36	U	47	Total	O	0	0
			47	47		
36	V	73	Total	O	0	0
			73	73		
36	Y	6	Total	O	0	0
			6	6		
36	X	8	Total	O	0	0
			8	8		
36	Z	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	R	4	Total O 4 4	0	0
36	a	119	Total O 119 119	0	0
36	b	190	Total O 190 190	0	0
36	c	162	Total O 162 162	0	0
36	d	120	Total O 120 120	0	0
36	e	22	Total O 22 22	0	0
36	f	4	Total O 4 4	0	0
36	h	19	Total O 19 19	0	0
36	i	10	Total O 10 10	0	0
36	j	8	Total O 8 8	0	0
36	k	5	Total O 5 5	0	0
36	l	11	Total O 11 11	0	0
36	m	5	Total O 5 5	0	0
36	o	113	Total O 113 113	0	0
36	t	11	Total O 11 11	0	0
36	u	54	Total O 54 54	0	0
36	v	64	Total O 64 64	0	0
36	y	4	Total O 4 4	0	0
36	x	13	Total O 13 13	0	0
36	z	1	Total O 1 1	0	0
36	r	5	Total O 5 5	0	0

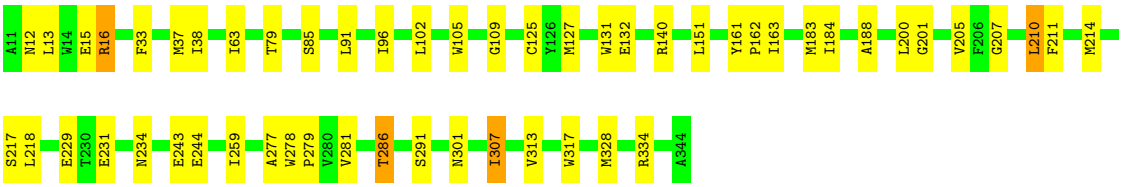
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1 1

Chain A:

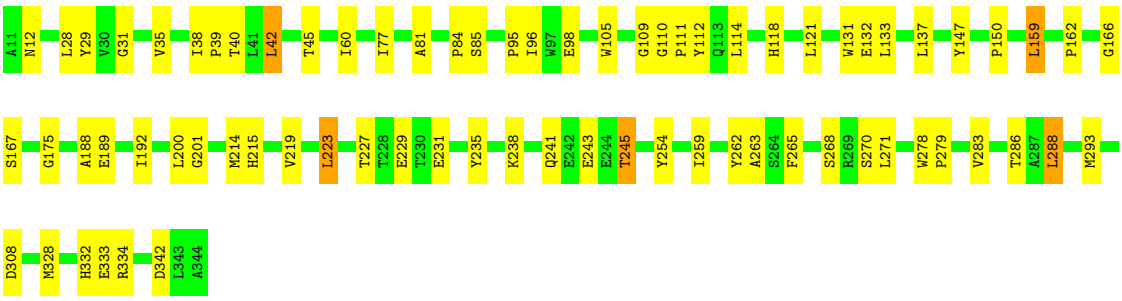




• Molecule 1: Photosystem II protein D1 1

Chain a:

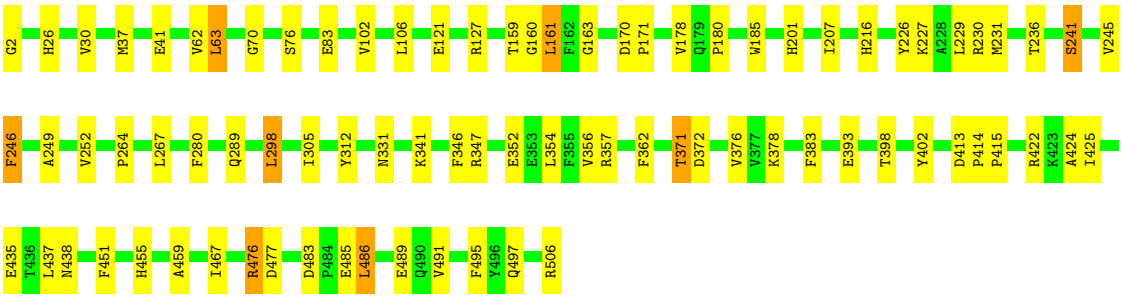




• Molecule 2: Photosystem II CP47 reaction center protein

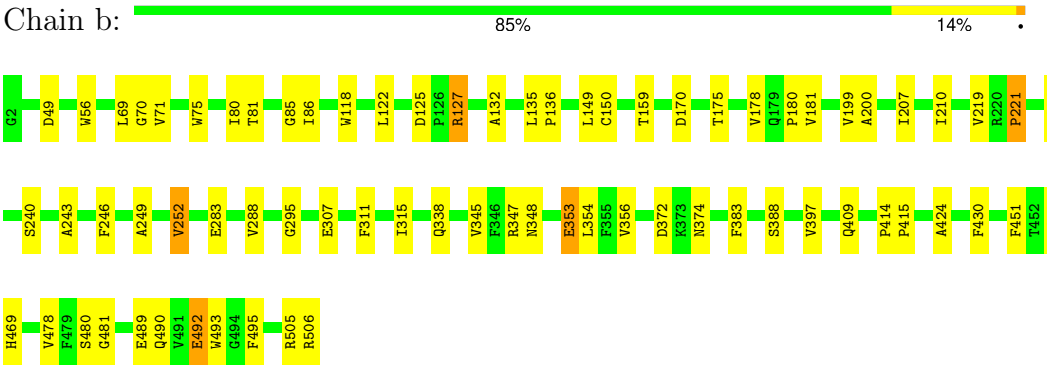
Chain B:





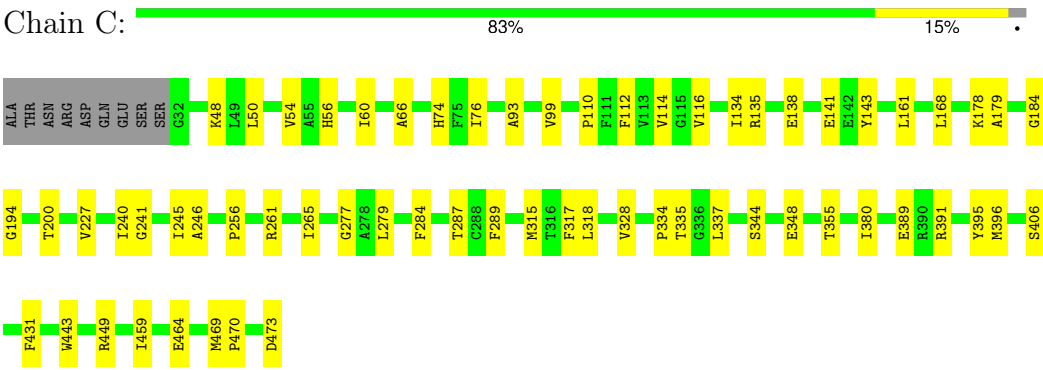
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



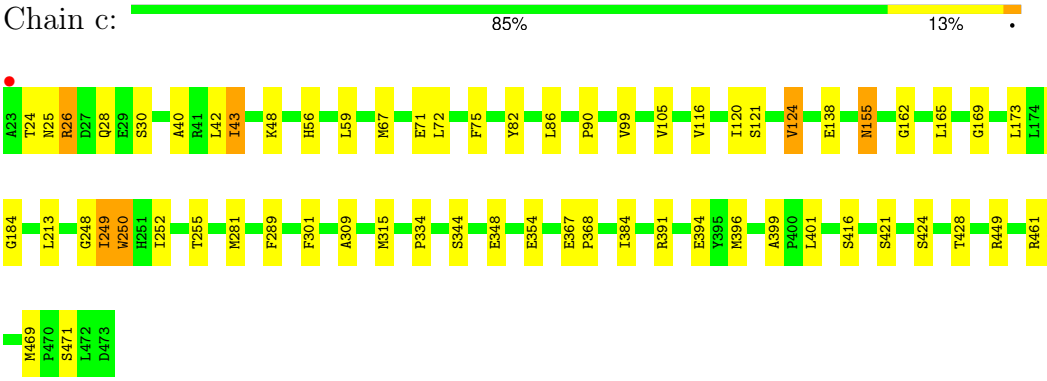
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



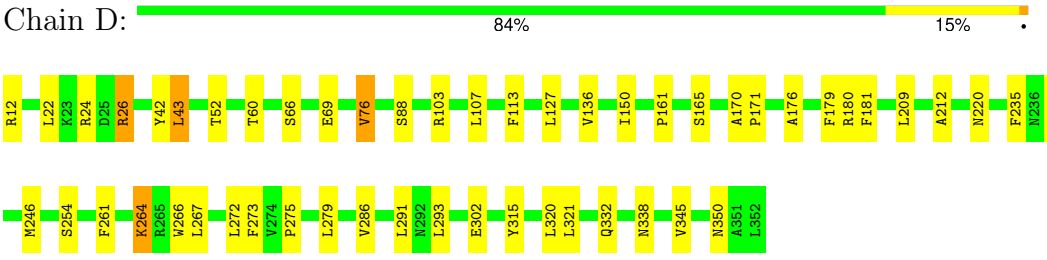
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



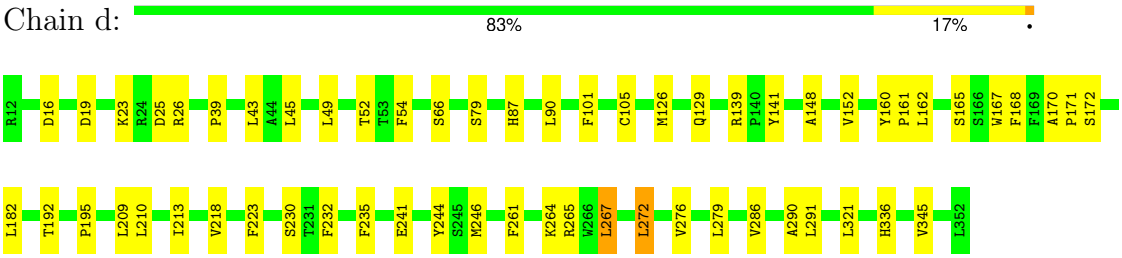
• Molecule 4: Photosystem II D2 protein

Chain D:



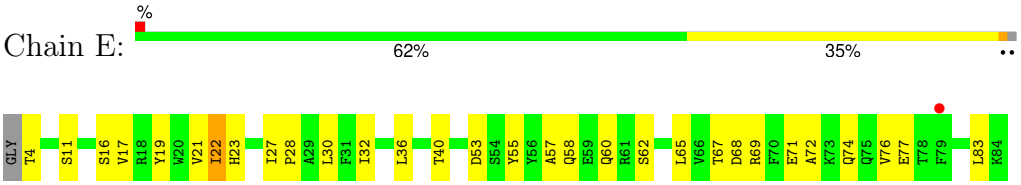
• Molecule 4: Photosystem II D2 protein

Chain d:



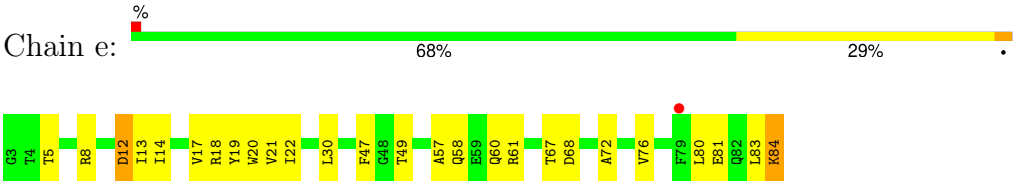
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



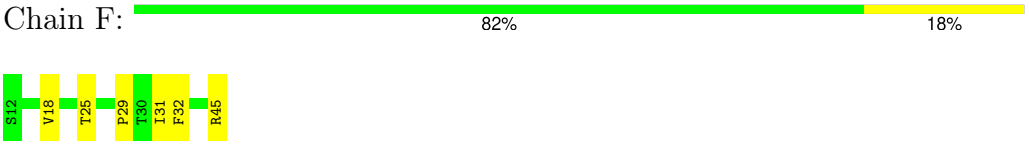
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



• Molecule 6: Cytochrome b559 subunit beta

Chain F:



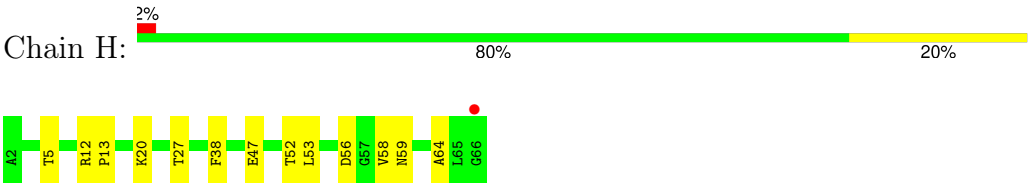
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



• Molecule 7: Photosystem II reaction center protein H

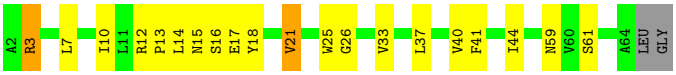
Chain H:



• Molecule 7: Photosystem II reaction center protein H

Chain h:

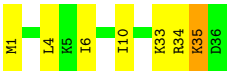




• Molecule 8: Photosystem II reaction center protein I

Chain I:





• Molecule 8: Photosystem II reaction center protein I

Chain i:

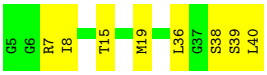




• Molecule 9: Photosystem II reaction center protein J

Chain J:





• Molecule 9: Photosystem II reaction center protein J

Chain j:

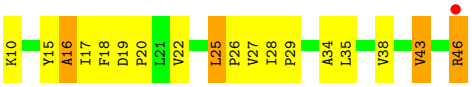




• Molecule 10: Photosystem II reaction center protein K

Chain K:

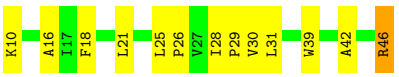




• Molecule 10: Photosystem II reaction center protein K

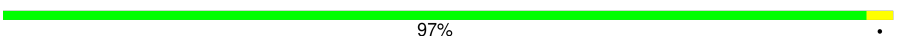
Chain k:





• Molecule 11: Photosystem II reaction center protein L

Chain L:





• Molecule 11: Photosystem II reaction center protein L

Chain l:

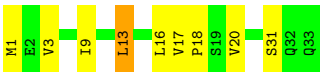




• Molecule 12: Photosystem II reaction center protein M

Chain M:

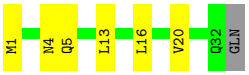




• Molecule 12: Photosystem II reaction center protein M

Chain m:

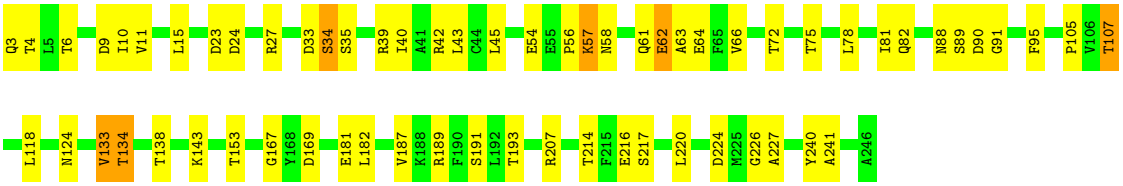




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

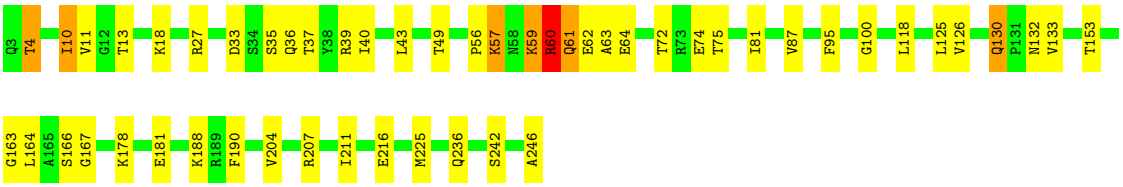




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

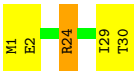




• Molecule 14: Photosystem II reaction center protein T

Chain T:

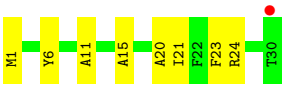




• Molecule 14: Photosystem II reaction center protein T

Chain t:

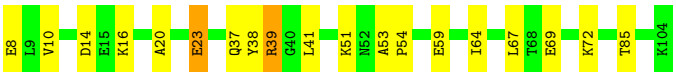




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

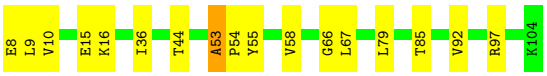




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:





• Molecule 16: Cytochrome c-550

Chain V:





• Molecule 16: Cytochrome c-550

Chain v:

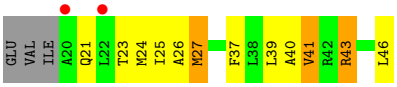




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:





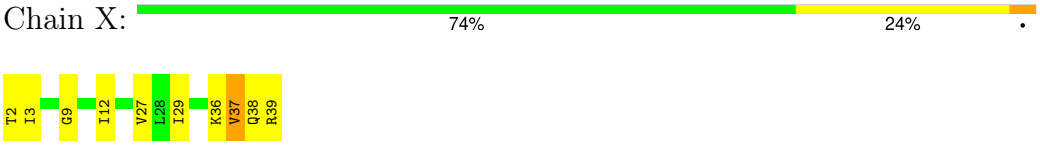
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



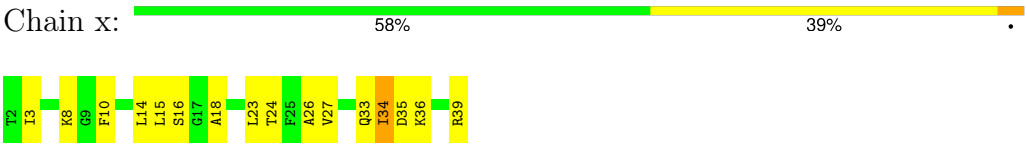
• Molecule 18: Photosystem II reaction center X protein

Chain X:



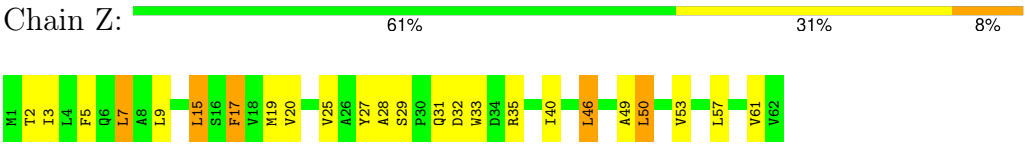
• Molecule 18: Photosystem II reaction center X protein

Chain x:



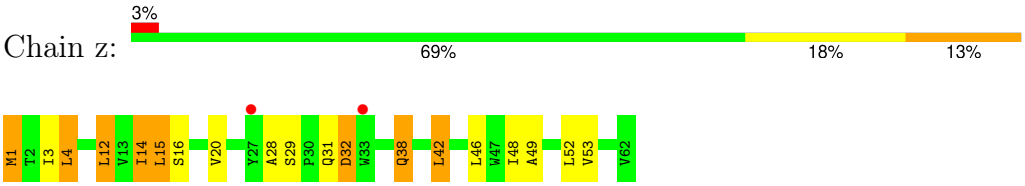
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



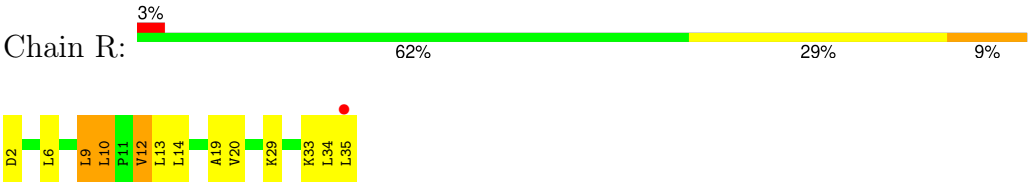
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



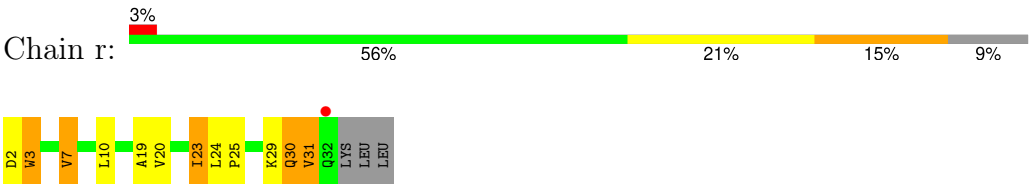
• Molecule 20: Photosystem II protein Y

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	117.55Å 222.69Å 309.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.78 – 2.50 30.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.78-2.50) 87.5 (30.78-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.167 , 0.246 0.168 , 0.246	Depositor DCC
R_{free} test set	2481 reflections (0.42%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 71.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	103658	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, DGD, CL, BCR, FE2, FME, LHG, PHO, LMG, SQD, PL9, HEM, OEX, HEC, CLA, BCT

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	0.68	1/2707 (0.0%)	0.75	0/3692
1	a	0.61	1/2704 (0.0%)	0.72	0/3688
2	B	0.62	0/4160	0.69	0/5668
2	b	0.58	1/4118 (0.0%)	0.69	1/5611 (0.0%)
3	C	0.58	0/3530	0.69	0/4807
3	c	0.55	0/3610	0.68	0/4914
4	D	0.63	0/2812	0.72	0/3832
4	d	0.59	0/2821	0.70	0/3844
5	E	0.50	0/684	0.64	0/935
5	e	0.48	0/683	0.64	0/932
6	F	0.50	0/284	0.60	0/387
6	f	0.47	0/284	0.61	0/387
7	H	0.60	0/520	0.72	0/709
7	h	0.54	0/511	0.71	0/697
8	I	0.63	0/293	0.75	0/396
8	i	0.70	0/293	0.73	0/396
9	J	0.51	0/263	0.73	0/356
9	j	0.46	0/261	0.62	0/353
10	K	0.43	0/314	0.56	0/427
10	k	0.43	0/303	0.58	0/416
11	L	0.62	0/311	0.70	0/422
11	l	0.61	0/303	0.69	0/412
12	M	0.64	0/249	0.72	0/341
12	m	0.66	0/244	0.70	0/334
13	O	0.59	0/1914	0.72	0/2596
13	o	0.56	0/1905	0.70	0/2583
14	T	0.68	0/257	0.77	0/349
14	t	0.60	0/255	0.65	0/346
15	U	0.56	0/785	0.67	0/1064
15	u	0.59	0/785	0.72	0/1064
16	V	0.56	0/1085	0.68	0/1473
16	v	0.57	0/1085	0.68	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	Y	0.48	0/197	0.68	0/264
17	y	0.36	0/219	0.46	0/294
18	X	0.51	0/284	0.67	0/384
18	x	0.39	0/284	0.57	0/384
19	Z	0.47	0/490	0.61	0/669
19	z	0.39	0/488	0.54	0/666
20	R	0.35	0/277	0.55	0/380
20	r	0.34	0/233	0.52	0/323
All	All	0.58	3/42805 (0.0%)	0.69	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
17	Y	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ILE	CA-CB	6.85	1.58	1.54
2	b	221	PRO	CA-C	5.77	1.56	1.52
1	a	263	ALA	CA-C	-5.01	1.44	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	221	PRO	O-C-N	5.84	123.89	121.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	Y	21	GLN	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	32	0
1	a	2619	2499	2510	44	0
2	B	4004	3845	3864	48	0
2	b	3978	3811	3836	44	0
3	C	3417	3335	3348	42	0
3	c	3494	3407	3420	37	0
4	D	2717	2613	2621	50	0
4	d	2723	2619	2627	44	0
5	E	662	647	648	17	0
5	e	664	647	648	20	0
6	F	275	281	282	7	0
6	f	275	281	282	9	0
7	H	507	523	523	7	0
7	h	498	518	518	12	0
8	I	296	311	311	2	0
8	i	296	311	311	10	0
9	J	257	268	268	6	0
9	j	255	261	261	7	0
10	K	302	318	318	17	0
10	k	293	305	305	6	0
11	L	304	316	316	1	0
11	l	296	304	304	3	0
12	M	256	269	269	10	0
12	m	251	267	267	7	0
13	O	1880	1850	1852	39	0
13	o	1874	1844	1846	31	0
14	T	258	261	261	4	0
14	t	256	256	256	5	0
15	U	774	772	773	7	0
15	u	774	772	773	12	0
16	V	1064	1070	1073	15	0
16	v	1064	1070	1073	21	0
17	Y	196	208	217	9	0
17	y	218	232	241	9	0
18	X	281	312	312	5	0
18	x	281	312	312	11	0
19	Z	479	509	516	15	0
19	z	477	509	509	9	0
20	R	271	298	298	8	0
20	r	227	234	224	9	0
21	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	184	192	192	2	0
23	B	1035	1139	1139	12	0
23	C	839	922	922	16	0
23	D	195	216	216	3	0
23	a	195	216	216	2	0
23	b	1035	1139	1139	23	0
23	c	839	919	919	10	0
23	d	195	216	216	4	0
24	A	64	74	74	1	0
24	D	64	74	74	3	0
24	a	64	74	74	1	0
24	d	64	74	74	3	0
25	A	40	56	56	0	0
25	B	120	168	168	6	0
25	C	80	112	112	5	0
25	D	40	56	56	6	0
25	H	40	56	56	4	0
25	K	40	56	56	4	0
25	T	40	56	56	2	0
25	Z	40	56	56	1	0
25	a	40	56	56	1	0
25	b	120	168	168	7	0
25	c	120	168	168	7	0
25	d	40	56	56	3	0
25	k	40	56	56	1	0
25	t	40	56	56	7	0
25	x	40	56	56	0	0
26	A	55	80	80	1	0
26	D	55	80	80	1	0
26	a	55	80	80	3	0
26	d	55	80	80	0	0
27	A	91	135	134	2	0
27	B	54	78	78	1	0
27	F	36	45	45	2	0
27	a	90	134	133	4	0
27	b	49	65	64	1	0
27	f	41	49	48	2	0
28	A	66	96	96	5	0
28	C	186	246	246	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	H	62	82	80	1	0
28	a	44	75	75	2	0
28	c	186	246	245	0	0
28	h	62	82	81	0	0
29	A	49	74	74	4	0
29	D	96	141	141	2	0
29	E	49	74	74	0	0
29	L	49	74	74	3	0
29	d	137	199	199	4	0
29	e	42	57	57	1	0
29	l	49	74	74	0	0
30	A	10	0	0	0	0
30	a	10	0	0	1	0
31	A	4	1	1	0	0
31	a	4	1	1	0	0
32	B	89	137	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	16	31	0	0	0
32	a	12	16	0	0	0
32	b	81	139	0	0	0
32	c	32	51	0	1	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	10	16	0	0	0
32	x	20	35	0	1	0
33	C	96	132	132	0	0
33	D	112	157	157	4	0
33	M	51	72	72	1	0
33	b	55	86	86	0	0
33	c	134	181	181	3	0
33	d	67	92	91	1	0
33	m	51	72	72	1	0
34	E	43	30	30	4	0
34	e	43	30	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	V	43	30	30	0	0
35	v	43	30	30	0	0
36	A	136	0	0	6	0
36	B	216	0	0	10	0
36	C	192	0	0	3	0
36	D	138	0	0	8	0
36	E	30	0	0	0	0
36	F	10	0	0	0	0
36	H	25	0	0	2	0
36	I	16	0	0	0	0
36	J	13	0	0	2	0
36	L	7	0	0	0	0
36	M	7	0	0	0	0
36	O	128	0	0	10	0
36	R	4	0	0	1	0
36	T	11	0	0	1	0
36	U	47	0	0	1	0
36	V	73	0	0	3	0
36	X	8	0	0	0	0
36	Y	6	0	0	0	0
36	Z	5	0	0	0	0
36	a	119	0	0	3	0
36	b	190	0	0	11	0
36	c	162	0	0	4	0
36	d	120	0	0	8	0
36	e	22	0	0	0	0
36	f	4	0	0	1	0
36	h	19	0	0	2	0
36	i	10	0	0	1	0
36	j	8	0	0	0	0
36	k	5	0	0	0	0
36	l	11	0	0	0	0
36	m	5	0	0	1	0
36	o	113	0	0	2	0
36	r	5	0	0	1	0
36	t	11	0	0	0	0
36	u	54	0	0	2	0
36	v	64	0	0	5	0
36	x	13	0	0	1	0
36	y	4	0	0	0	0
36	z	1	0	0	0	0
All	All	52191	51467	50850	715	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 715 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	1.76	1.02
13:O:169:ASP:O	36:O:302:HOH:O	1.79	0.99
2:B:497:GLN:OE1	36:B:701:HOH:O	1.87	0.93
7:H:56:ASP:OD1	18:X:2:THR:N	2.07	0.87
13:O:216:GLU:OE2	36:O:303:HOH:O	1.92	0.86

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	322 (97%)	9 (3%)	1 (0%)	36	55
1	a	332/334 (99%)	320 (96%)	11 (3%)	1 (0%)	36	55
2	B	508/505 (101%)	488 (96%)	19 (4%)	1 (0%)	43	63
2	b	503/505 (100%)	480 (95%)	20 (4%)	3 (1%)	21	38
3	C	440/451 (98%)	420 (96%)	19 (4%)	1 (0%)	43	63
3	c	450/451 (100%)	433 (96%)	15 (3%)	2 (0%)	30	49
4	D	339/341 (99%)	328 (97%)	10 (3%)	1 (0%)	36	55
4	d	340/341 (100%)	323 (95%)	17 (5%)	0	100	100
5	E	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
5	e	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
6	F	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
6	f	32/34 (94%)	30 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	30 (88%)	4 (12%)	0	100	100
9	J	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
9	j	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
10	K	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	5
10	k	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	33 (97%)	0	1 (3%)	3	5
12	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
12	m	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
13	O	243/244 (100%)	225 (93%)	14 (6%)	4 (2%)	7	14
13	o	242/244 (99%)	226 (93%)	13 (5%)	3 (1%)	10	20
14	T	28/30 (93%)	28 (100%)	0	0	100	100
14	t	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
15	U	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
15	u	95/97 (98%)	91 (96%)	3 (3%)	1 (1%)	11	22
16	V	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
16	v	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
17	Y	25/30 (83%)	18 (72%)	5 (20%)	2 (8%)	1	0
17	y	28/30 (93%)	23 (82%)	4 (14%)	1 (4%)	2	3
18	X	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	6
18	x	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
19	z	60/62 (97%)	47 (78%)	11 (18%)	2 (3%)	3	4
20	R	32/34 (94%)	30 (94%)	1 (3%)	1 (3%)	3	5
20	r	29/34 (85%)	24 (83%)	3 (10%)	2 (7%)	1	1
All	All	5235/5326 (98%)	4963 (95%)	243 (5%)	29 (1%)	21	38

5 of 29 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	270/270 (100%)	258 (96%)	12 (4%)	25 50
1	a	269/270 (100%)	255 (95%)	14 (5%)	21 42
2	B	407/403 (101%)	385 (95%)	22 (5%)	20 41
2	b	402/403 (100%)	383 (95%)	19 (5%)	23 47
3	C	344/352 (98%)	336 (98%)	8 (2%)	44 72
3	c	353/352 (100%)	333 (94%)	20 (6%)	18 39
4	D	276/276 (100%)	269 (98%)	7 (2%)	42 69
4	d	277/276 (100%)	270 (98%)	7 (2%)	42 69
5	E	72/72 (100%)	60 (83%)	12 (17%)	2 4
5	e	71/72 (99%)	65 (92%)	6 (8%)	10 22
6	F	28/28 (100%)	28 (100%)	0	100 100
6	f	28/28 (100%)	23 (82%)	5 (18%)	2 3
7	H	53/54 (98%)	48 (91%)	5 (9%)	8 18
7	h	53/54 (98%)	48 (91%)	5 (9%)	8 18
8	I	32/32 (100%)	28 (88%)	4 (12%)	4 9
8	i	32/32 (100%)	30 (94%)	2 (6%)	16 34
9	J	24/24 (100%)	23 (96%)	1 (4%)	26 52
9	j	23/24 (96%)	20 (87%)	3 (13%)	4 8
10	K	31/30 (103%)	26 (84%)	5 (16%)	2 4
10	k	30/30 (100%)	26 (87%)	4 (13%)	4 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	34/35 (97%)	31 (91%)	3 (9%)	9 20
12	M	28/29 (97%)	24 (86%)	4 (14%)	3 6
12	m	28/29 (97%)	26 (93%)	2 (7%)	13 29
13	O	208/207 (100%)	188 (90%)	20 (10%)	8 17
13	o	207/207 (100%)	189 (91%)	18 (9%)	9 21
14	T	26/26 (100%)	24 (92%)	2 (8%)	12 25
14	t	25/26 (96%)	24 (96%)	1 (4%)	28 54
15	U	84/84 (100%)	74 (88%)	10 (12%)	5 11
15	u	84/84 (100%)	83 (99%)	1 (1%)	63 83
16	V	117/117 (100%)	111 (95%)	6 (5%)	21 43
16	v	117/117 (100%)	109 (93%)	8 (7%)	14 31
17	Y	19/23 (83%)	16 (84%)	3 (16%)	2 5
17	y	22/23 (96%)	19 (86%)	3 (14%)	3 8
18	X	31/31 (100%)	27 (87%)	4 (13%)	4 9
18	x	31/31 (100%)	28 (90%)	3 (10%)	8 17
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2 4
19	z	51/52 (98%)	40 (78%)	11 (22%)	1 2
20	R	28/29 (97%)	21 (75%)	7 (25%)	0 1
20	r	19/29 (66%)	16 (84%)	3 (16%)	2 5
All	All	4321/4348 (99%)	4042 (94%)	279 (6%)	16 32

5 of 279 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	4	THR
13	o	60	ARG
17	y	22	LEU
13	O	207	ARG
13	O	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	28	GLN
13	o	36	GLN
3	c	201	ASN
4	d	334	GLN
13	o	124	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	T	1	14	8,9,10	1.00	1 (12%)	8,9,11	1.41	1 (12%)
8	FME	I	1	8	8,9,10	1.12	1 (12%)	8,9,11	1.44	2 (25%)
12	FME	M	1	12	8,9,10	1.13	1 (12%)	8,9,11	1.00	0
14	FME	t	1	14	8,9,10	1.10	1 (12%)	8,9,11	1.22	1 (12%)
8	FME	i	1	8	8,9,10	1.27	1 (12%)	8,9,11	1.01	0
12	FME	m	1	12	8,9,10	1.09	1 (12%)	8,9,11	0.72	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.78	1.42	1.46
14	t	1	FME	CA-N	-2.61	1.42	1.46
14	T	1	FME	CA-N	-2.58	1.42	1.46
12	m	1	FME	CA-N	-2.51	1.42	1.46
8	I	1	FME	CA-N	-2.44	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	1	FME	CA-N-CN	-2.37	119.17	122.82
14	T	1	FME	CA-N-CN	-2.36	119.19	122.82
8	I	1	FME	CB-CA-N	2.31	114.72	110.52
14	t	1	FME	CB-CA-N	2.10	114.34	110.52

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
28	DGD	C	518	-	63,63,67	1.11	7 (11%)	77,77,81	1.42	10 (12%)
23	CLA	C	505	36	63,67,73	1.95	13 (20%)	74,105,113	1.21	9 (12%)
29	LHG	A	413	-	48,48,48	0.89	2 (4%)	51,54,54	1.54	9 (17%)
33	LMG	D	411	-	26,26,55	0.83	1 (3%)	26,26,63	1.19	1 (3%)
33	LMG	c	522	-	48,48,55	1.19	7 (14%)	56,56,63	1.37	5 (8%)
25	BCR	c	514	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	7 (12%)
33	LMG	M	101	-	51,51,55	1.00	1 (1%)	59,59,63	1.48	10 (16%)
23	CLA	A	404	1	69,73,73	1.55	9 (13%)	82,113,113	1.35	8 (9%)
28	DGD	a	413	-	43,43,67	1.50	4 (9%)	45,45,81	1.23	5 (11%)
23	CLA	b	608	36	69,73,73	1.06	5 (7%)	82,113,113	1.28	9 (10%)
25	BCR	K	101	-	41,41,41	1.21	2 (4%)	56,56,56	1.29	9 (16%)
29	LHG	D	408	-	48,48,48	1.07	3 (6%)	51,54,54	1.28	6 (11%)
23	CLA	b	611	36	69,73,73	1.37	9 (13%)	82,113,113	1.27	12 (14%)
25	BCR	a	409	-	41,41,41	1.12	3 (7%)	56,56,56	1.34	6 (10%)
23	CLA	c	504	36	64,68,73	1.29	10 (15%)	76,107,113	1.26	6 (7%)
23	CLA	c	502	3	69,73,73	1.23	7 (10%)	82,113,113	1.44	11 (13%)
27	SQD	F	101	-	34,36,54	0.92	1 (2%)	42,45,65	1.84	10 (23%)
23	CLA	C	514	3	69,73,73	1.27	8 (11%)	82,113,113	1.50	8 (9%)
23	CLA	b	610	2	69,73,73	1.34	11 (15%)	82,113,113	1.25	9 (10%)
24	PHO	a	407	-	58,69,69	1.93	11 (18%)	55,99,99	1.39	9 (16%)
25	BCR	b	620	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	7 (12%)
23	CLA	B	614	2	69,73,73	1.26	8 (11%)	82,113,113	1.54	10 (12%)
23	CLA	c	510	3	69,73,73	1.24	9 (13%)	82,113,113	1.50	12 (14%)
23	CLA	B	611	2	69,73,73	1.38	7 (10%)	82,113,113	1.42	11 (13%)
34	HEM	E	103	6,5	50,50,50	1.38	7 (14%)	67,82,82	1.09	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	513	3	69,73,73	1.23	9 (13%)	82,113,113	1.14	7 (8%)
25	BCR	d	405	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	8 (14%)
29	LHG	l	101	-	48,48,48	0.80	2 (4%)	51,54,54	1.18	3 (5%)
23	CLA	b	613	2	69,73,73	1.28	6 (8%)	82,113,113	1.65	14 (17%)
23	CLA	c	507	36	69,73,73	1.32	8 (11%)	82,113,113	1.44	9 (10%)
26	PL9	D	406	-	55,55,55	1.63	9 (16%)	68,69,69	1.59	14 (20%)
24	PHO	A	406	-	58,69,69	1.95	10 (17%)	55,99,99	1.47	10 (18%)
25	BCR	Z	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.44	9 (16%)
33	LMG	C	501	-	48,48,55	1.17	6 (12%)	56,56,63	1.38	10 (17%)
25	BCR	A	408	-	41,41,41	1.18	5 (12%)	56,56,56	1.51	11 (19%)
28	DGD	A	412	-	67,67,67	1.41	12 (17%)	81,81,81	1.37	5 (6%)
25	BCR	B	617	-	41,41,41	1.31	4 (9%)	56,56,56	1.40	8 (14%)
29	LHG	E	101	-	48,48,48	0.93	3 (6%)	51,54,54	1.24	3 (5%)
23	CLA	D	402	36	69,73,73	1.22	7 (10%)	82,113,113	1.16	7 (8%)
33	LMG	c	524	-	49,49,55	1.17	5 (10%)	57,57,63	1.30	4 (7%)
33	LMG	d	410	-	21,21,55	1.01	1 (4%)	20,20,63	0.89	1 (5%)
23	CLA	B	603	2	69,73,73	1.42	10 (14%)	82,113,113	1.51	10 (12%)
23	CLA	C	507	3	69,73,73	1.94	9 (13%)	82,113,113	1.33	11 (13%)
23	CLA	d	403	4	69,73,73	1.31	8 (11%)	82,113,113	1.18	6 (7%)
28	DGD	h	101	-	63,63,67	1.20	7 (11%)	77,77,81	1.58	16 (20%)
29	LHG	L	101	-	48,48,48	0.96	4 (8%)	51,54,54	1.09	2 (3%)
25	BCR	c	515	-	41,41,41	1.25	4 (9%)	56,56,56	1.42	10 (17%)
31	BCT	a	404	21	3,3,3	1.20	0	2,3,3	3.17	2 (100%)
23	CLA	C	512	3	69,73,73	1.62	9 (13%)	82,113,113	1.46	8 (9%)
27	SQD	a	411	-	52,54,54	0.98	5 (9%)	62,65,65	1.86	9 (14%)
33	LMG	D	407	-	51,51,55	1.03	5 (9%)	59,59,63	1.21	3 (5%)
33	LMG	C	519	-	48,48,55	1.03	6 (12%)	56,56,63	1.32	5 (8%)
25	BCR	C	520	-	41,41,41	1.06	3 (7%)	56,56,56	1.37	8 (14%)
23	CLA	B	604	2	69,73,73	1.47	8 (11%)	82,113,113	1.41	10 (12%)
23	CLA	C	506	3	69,73,73	1.14	6 (8%)	82,113,113	1.38	8 (9%)
26	PL9	A	409	-	55,55,55	1.29	5 (9%)	68,69,69	1.41	8 (11%)
27	SQD	A	411	-	38,38,54	1.11	4 (10%)	40,40,65	1.46	4 (10%)
23	CLA	b	615	2	69,73,73	1.36	11 (15%)	82,113,113	1.47	13 (15%)
25	BCR	t	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.45	13 (23%)
28	DGD	c	518	-	63,63,67	1.27	9 (14%)	77,77,81	1.53	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	C	515	-	41,41,41	1.30	5 (12%)	56,56,56	1.34	9 (16%)
25	BCR	b	618	-	41,41,41	1.22	5 (12%)	56,56,56	1.32	6 (10%)
25	BCR	c	521	-	41,41,41	1.02	3 (7%)	56,56,56	1.20	5 (8%)
23	CLA	b	614	2	69,73,73	1.28	10 (14%)	82,113,113	1.40	10 (12%)
27	SQD	a	412	-	35,35,54	1.08	2 (5%)	37,37,65	1.45	5 (13%)
25	BCR	x	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.41	9 (16%)
33	LMG	D	410	-	31,31,55	1.18	3 (9%)	33,33,63	1.12	1 (3%)
23	CLA	b	607	2	69,73,73	1.33	7 (10%)	82,113,113	1.43	13 (15%)
23	CLA	B	605	2	69,73,73	1.44	12 (17%)	82,113,113	1.40	18 (21%)
27	SQD	b	601	-	47,49,54	1.00	2 (4%)	57,60,65	2.18	15 (26%)
23	CLA	A	407	1	58,62,73	1.53	10 (17%)	68,99,113	1.65	15 (22%)
25	BCR	D	405	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	5 (8%)
23	CLA	B	607	36	69,73,73	1.25	6 (8%)	82,113,113	1.25	7 (8%)
23	CLA	C	503	3	69,73,73	1.21	7 (10%)	82,113,113	1.31	10 (12%)
23	CLA	C	511	3	69,73,73	1.67	12 (17%)	82,113,113	1.43	9 (10%)
23	CLA	C	509	3	69,73,73	1.36	10 (14%)	82,113,113	1.66	14 (17%)
29	LHG	D	409	-	46,46,48	1.09	3 (6%)	49,52,54	1.30	5 (10%)
30	OEX	a	415	36,3,1	0,14,14	-	-	-		
23	CLA	B	610	36	69,73,73	1.31	9 (13%)	82,113,113	1.56	12 (14%)
23	CLA	B	616	2	64,68,73	1.72	9 (14%)	76,107,113	1.34	6 (7%)
23	CLA	b	606	2	69,73,73	1.38	8 (11%)	82,113,113	1.70	17 (20%)
23	CLA	b	602	36	69,73,73	1.54	11 (15%)	82,113,113	1.38	13 (15%)
23	CLA	b	612	2	69,73,73	1.55	9 (13%)	82,113,113	1.44	16 (19%)
23	CLA	B	615	2	69,73,73	1.56	10 (14%)	82,113,113	1.38	11 (13%)
34	HEM	e	102	6,5	50,50,50	1.46	6 (12%)	67,82,82	1.28	8 (11%)
33	LMG	b	622	-	55,55,55	1.08	4 (7%)	63,63,63	1.58	5 (7%)
25	BCR	b	619	-	41,41,41	1.32	2 (4%)	56,56,56	1.32	6 (10%)
23	CLA	c	511	3	69,73,73	1.62	10 (14%)	82,113,113	1.32	4 (4%)
33	LMG	c	519	-	37,37,55	1.13	4 (10%)	45,45,63	1.31	5 (11%)
23	CLA	c	508	3	68,72,73	1.70	10 (14%)	80,111,113	1.24	10 (12%)
28	DGD	C	517	-	63,63,67	1.24	10 (15%)	77,77,81	1.55	12 (15%)
30	OEX	A	414	36,3,1	0,14,14	-	-	-		
31	BCT	A	415	21	3,3,3	1.25	0	2,3,3	2.90	1 (50%)
28	DGD	c	516	-	63,63,67	1.20	6 (9%)	77,77,81	1.54	15 (19%)
27	SQD	f	101	-	39,41,54	1.12	4 (10%)	49,52,65	1.73	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LMG	d	411	-	44,44,55	1.24	4 (9%)	52,52,63	1.49	6 (11%)
23	CLA	c	509	3	69,73,73	1.48	9 (13%)	82,113,113	1.73	8 (9%)
28	DGD	H	102	-	63,63,67	1.35	12 (19%)	77,77,81	1.50	13 (16%)
23	CLA	B	612	2	69,73,73	1.62	7 (10%)	82,113,113	1.52	12 (14%)
24	PHO	d	401	-	58,69,69	2.07	10 (17%)	55,99,99	1.63	12 (21%)
25	BCR	B	619	-	41,41,41	1.23	4 (9%)	56,56,56	1.27	9 (16%)
23	CLA	B	601	36	69,73,73	1.55	9 (13%)	82,113,113	1.31	9 (10%)
23	CLA	C	513	3	69,73,73	2.10	11 (15%)	82,113,113	1.30	11 (13%)
24	PHO	D	401	-	58,69,69	2.07	9 (15%)	55,99,99	1.58	9 (16%)
28	DGD	C	516	-	63,63,67	1.38	7 (11%)	77,77,81	1.33	10 (12%)
35	HEC	v	201	16	50,50,50	1.46	6 (12%)	68,82,82	1.16	6 (8%)
23	CLA	a	405	1	69,73,73	1.23	9 (13%)	82,113,113	1.40	12 (14%)
27	SQD	A	410	-	50,52,54	1.09	6 (12%)	60,63,65	2.08	12 (20%)
23	CLA	B	606	2	69,73,73	1.49	10 (14%)	82,113,113	1.64	13 (15%)
23	CLA	c	503	3	69,73,73	1.36	9 (13%)	82,113,113	1.47	11 (13%)
35	HEC	V	201	16	50,50,50	1.55	8 (16%)	68,82,82	1.36	11 (16%)
23	CLA	D	404	4	69,73,73	1.27	8 (11%)	82,113,113	1.33	12 (14%)
23	CLA	c	505	3	69,73,73	1.27	9 (13%)	82,113,113	1.20	6 (7%)
29	LHG	d	408	-	48,48,48	0.70	0	51,54,54	1.22	4 (7%)
27	SQD	B	621	-	52,54,54	0.96	3 (5%)	62,65,65	1.81	15 (24%)
29	LHG	e	101	-	41,41,48	0.89	3 (7%)	44,47,54	1.40	5 (11%)
26	PL9	d	406	-	55,55,55	1.33	8 (14%)	68,69,69	1.74	14 (20%)
28	DGD	c	517	-	63,63,67	1.18	6 (9%)	77,77,81	1.33	8 (10%)
29	LHG	d	409	-	38,38,48	0.89	2 (5%)	41,44,54	1.14	3 (7%)
25	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.15	4 (7%)
23	CLA	B	613	2	69,73,73	1.41	9 (13%)	82,113,113	1.54	10 (12%)
23	CLA	B	609	2	69,73,73	1.50	10 (14%)	82,113,113	1.44	16 (19%)
29	LHG	d	407	-	48,48,48	0.83	1 (2%)	51,54,54	1.34	5 (9%)
23	CLA	C	510	3	69,73,73	1.18	9 (13%)	82,113,113	1.32	6 (7%)
23	CLA	D	403	4	69,73,73	1.30	7 (10%)	82,113,113	1.53	7 (8%)
23	CLA	b	617	2	64,68,73	1.29	7 (10%)	76,107,113	1.55	9 (11%)
25	BCR	T	101	-	41,41,41	1.23	4 (9%)	56,56,56	1.47	10 (17%)
23	CLA	B	608	2	69,73,73	1.47	10 (14%)	82,113,113	1.20	5 (6%)
25	BCR	H	101	-	41,41,41	1.32	3 (7%)	56,56,56	1.35	7 (12%)
23	CLA	b	604	2	69,73,73	1.28	9 (13%)	82,113,113	1.45	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	512	3	69,73,73	1.25	8 (11%)	82,113,113	1.29	5 (6%)
23	CLA	d	404	4	69,73,73	1.64	8 (11%)	82,113,113	1.35	10 (12%)
23	CLA	C	504	3	69,73,73	1.51	8 (11%)	82,113,113	1.72	14 (17%)
23	CLA	c	506	3	69,73,73	1.87	11 (15%)	82,113,113	1.46	11 (13%)
23	CLA	C	502	3	69,73,73	1.52	8 (11%)	82,113,113	1.80	11 (13%)
25	BCR	B	618	-	41,41,41	1.39	4 (9%)	56,56,56	1.43	8 (14%)
23	CLA	b	603	2	69,73,73	1.37	11 (15%)	82,113,113	1.46	12 (14%)
23	CLA	b	616	2	69,73,73	2.09	10 (14%)	82,113,113	1.48	11 (13%)
33	LMG	m	101	-	51,51,55	0.98	4 (7%)	59,59,63	1.55	9 (15%)
23	CLA	a	406	36	69,73,73	1.08	5 (7%)	82,113,113	1.61	12 (14%)
23	CLA	c	501	3	69,73,73	1.42	7 (10%)	82,113,113	1.90	13 (15%)
23	CLA	B	602	2	69,73,73	1.25	9 (13%)	82,113,113	1.27	11 (13%)
23	CLA	C	508	36	69,73,73	1.38	10 (14%)	82,113,113	1.28	11 (13%)
23	CLA	b	605	2	69,73,73	1.25	8 (11%)	82,113,113	1.39	12 (14%)
23	CLA	a	408	1	69,73,73	1.78	11 (15%)	82,113,113	1.24	8 (9%)
26	PL9	a	410	-	55,55,55	1.29	4 (7%)	68,69,69	1.54	15 (22%)
23	CLA	b	609	2	69,73,73	1.44	9 (13%)	82,113,113	1.40	12 (14%)
23	CLA	d	402	36	69,73,73	1.38	8 (11%)	82,113,113	1.84	13 (15%)
23	CLA	A	405	36	69,73,73	1.35	9 (13%)	82,113,113	1.40	10 (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
28	DGD	C	518	-	-	15/51/91/95	0/2/2/2
23	CLA	C	505	36	-	9/32/108/115	-
29	LHG	A	413	-	-	15/53/53/53	-
33	LMG	D	411	-	-	15/22/22/70	-
33	LMG	c	522	-	-	21/43/63/70	0/1/1/1
25	BCR	c	514	-	-	14/29/63/63	0/2/2/2
33	LMG	M	101	-	-	19/46/66/70	0/1/1/1
23	CLA	A	404	1	-	4/39/115/115	-
28	DGD	a	413	-	-	21/45/45/95	-
23	CLA	b	608	36	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	K	101	-	-	12/29/63/63	0/2/2/2
29	LHG	D	408	-	-	26/53/53/53	-
23	CLA	b	611	36	-	3/39/115/115	-
25	BCR	a	409	-	-	2/29/63/63	0/2/2/2
23	CLA	c	504	36	-	9/33/109/115	-
23	CLA	c	502	3	-	7/39/115/115	-
27	SQD	F	101	-	-	13/28/48/69	0/1/1/1
23	CLA	C	514	3	-	13/39/115/115	-
23	CLA	b	610	2	-	10/39/115/115	-
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
25	BCR	b	620	-	-	5/29/63/63	0/2/2/2
23	CLA	B	614	2	-	11/39/115/115	-
23	CLA	c	510	3	-	13/39/115/115	-
23	CLA	B	611	2	-	6/39/115/115	-
34	HEM	E	103	6,5	-	2/14/54/54	-
23	CLA	c	513	3	-	9/39/115/115	-
25	BCR	d	405	-	-	12/29/63/63	0/2/2/2
29	LHG	l	101	-	-	16/53/53/53	-
23	CLA	b	613	2	-	12/39/115/115	-
23	CLA	c	507	36	-	10/39/115/115	-
26	PL9	D	406	-	-	11/53/73/73	0/1/1/1
24	PHO	A	406	-	-	8/37/103/103	0/5/6/6
25	BCR	Z	101	-	-	10/29/63/63	0/2/2/2
33	LMG	C	501	-	-	21/43/63/70	0/1/1/1
25	BCR	A	408	-	-	8/29/63/63	0/2/2/2
28	DGD	A	412	-	-	28/55/95/95	0/2/2/2
25	BCR	B	617	-	-	11/29/63/63	0/2/2/2
29	LHG	E	101	-	-	26/53/53/53	-
23	CLA	D	402	36	-	3/39/115/115	-
33	LMG	c	524	-	-	16/44/64/70	0/1/1/1
33	LMG	d	410	-	-	15/17/17/70	-
23	CLA	B	603	2	-	11/39/115/115	-
23	CLA	C	507	3	-	16/39/115/115	-
23	CLA	d	403	4	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	h	101	-	-	18/51/91/95	0/2/2/2
29	LHG	L	101	-	-	23/53/53/53	-
25	BCR	c	515	-	-	5/29/63/63	0/2/2/2
23	CLA	C	512	3	-	7/39/115/115	-
27	SQD	a	411	-	-	23/49/69/69	0/1/1/1
33	LMG	D	407	-	-	18/46/66/70	0/1/1/1
33	LMG	C	519	-	-	17/43/63/70	0/1/1/1
25	BCR	C	520	-	-	10/29/63/63	0/2/2/2
23	CLA	B	604	2	-	9/39/115/115	-
23	CLA	C	506	3	-	12/39/115/115	-
26	PL9	A	409	-	-	19/53/73/73	0/1/1/1
27	SQD	A	411	-	-	14/39/39/69	-
23	CLA	b	615	2	-	13/39/115/115	-
25	BCR	t	101	-	-	7/29/63/63	0/2/2/2
28	DGD	c	518	-	-	22/51/91/95	0/2/2/2
25	BCR	C	515	-	-	7/29/63/63	0/2/2/2
25	BCR	b	618	-	-	4/29/63/63	0/2/2/2
25	BCR	c	521	-	-	7/29/63/63	0/2/2/2
23	CLA	b	614	2	-	9/39/115/115	-
27	SQD	a	412	-	-	19/37/37/69	-
25	BCR	x	102	-	-	10/29/63/63	0/2/2/2
33	LMG	D	410	-	-	17/33/33/70	-
23	CLA	b	607	2	-	8/39/115/115	-
23	CLA	B	605	2	-	12/39/115/115	-
27	SQD	b	601	-	-	22/44/64/69	0/1/1/1
23	CLA	A	407	1	-	5/26/102/115	-
25	BCR	D	405	-	-	3/29/63/63	0/2/2/2
23	CLA	B	607	36	-	7/39/115/115	-
23	CLA	C	503	3	-	11/39/115/115	-
23	CLA	C	511	3	-	10/39/115/115	-
23	CLA	C	509	3	-	4/39/115/115	-
29	LHG	D	409	-	-	23/51/51/53	-
23	CLA	B	610	36	-	9/39/115/115	-
23	CLA	B	616	2	-	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	606	2	-	7/39/115/115	-
23	CLA	b	602	36	-	17/39/115/115	-
23	CLA	b	612	2	-	11/39/115/115	-
23	CLA	B	615	2	-	9/39/115/115	-
34	HEM	e	102	6,5	-	3/14/54/54	-
33	LMG	b	622	-	-	19/50/70/70	0/1/1/1
25	BCR	b	619	-	-	12/29/63/63	0/2/2/2
23	CLA	c	511	3	-	9/39/115/115	-
33	LMG	c	519	-	-	12/31/51/70	0/1/1/1
23	CLA	c	508	3	-	12/38/114/115	-
28	DGD	C	517	-	-	18/51/91/95	0/2/2/2
28	DGD	c	516	-	-	23/51/91/95	0/2/2/2
27	SQD	f	101	-	-	16/36/56/69	0/1/1/1
33	LMG	d	411	-	-	8/39/59/70	0/1/1/1
23	CLA	c	509	3	-	15/39/115/115	-
28	DGD	H	102	-	-	16/51/91/95	0/2/2/2
23	CLA	B	612	2	-	17/39/115/115	-
24	PHO	d	401	-	-	3/37/103/103	0/5/6/6
25	BCR	B	619	-	-	5/29/63/63	0/2/2/2
23	CLA	B	601	36	-	13/39/115/115	-
23	CLA	C	513	3	-	12/39/115/115	-
24	PHO	D	401	-	-	0/37/103/103	0/5/6/6
28	DGD	C	516	-	-	22/51/91/95	0/2/2/2
35	HEC	v	201	16	1/1/7/7	6/14/54/54	-
23	CLA	a	405	1	-	4/39/115/115	-
27	SQD	A	410	-	-	19/47/67/69	0/1/1/1
23	CLA	B	606	2	-	11/39/115/115	-
23	CLA	c	503	3	-	11/39/115/115	-
35	HEC	V	201	16	1/1/7/7	6/14/54/54	-
23	CLA	D	404	4	-	14/39/115/115	-
23	CLA	c	505	3	-	7/39/115/115	-
29	LHG	d	408	-	-	18/53/53/53	-
27	SQD	B	621	-	-	23/49/69/69	0/1/1/1
29	LHG	e	101	-	-	30/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PL9	d	406	-	-	18/53/73/73	0/1/1/1
28	DGD	c	517	-	-	19/51/91/95	0/2/2/2
29	LHG	d	409	-	-	11/43/43/53	-
25	BCR	k	101	-	-	13/29/63/63	0/2/2/2
23	CLA	B	613	2	-	5/39/115/115	-
23	CLA	B	609	2	-	6/39/115/115	-
29	LHG	d	407	-	-	21/53/53/53	-
23	CLA	C	510	3	-	7/39/115/115	-
23	CLA	D	403	4	-	10/39/115/115	-
23	CLA	b	617	2	-	7/33/109/115	-
25	BCR	T	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	608	2	-	0/39/115/115	-
25	BCR	H	101	-	-	9/29/63/63	0/2/2/2
23	CLA	b	604	2	-	9/39/115/115	-
23	CLA	c	512	3	-	22/39/115/115	-
23	CLA	d	404	4	-	7/39/115/115	-
23	CLA	C	504	3	-	6/39/115/115	-
23	CLA	c	506	3	-	17/39/115/115	-
23	CLA	C	502	3	-	4/39/115/115	-
25	BCR	B	618	-	-	3/29/63/63	0/2/2/2
23	CLA	b	603	2	-	7/39/115/115	-
23	CLA	b	616	2	-	8/39/115/115	-
33	LMG	m	101	-	-	20/46/66/70	0/1/1/1
23	CLA	a	406	36	-	13/39/115/115	-
23	CLA	c	501	3	-	6/39/115/115	-
23	CLA	B	602	2	-	7/39/115/115	-
23	CLA	C	508	36	-	7/39/115/115	-
23	CLA	b	605	2	-	10/39/115/115	-
23	CLA	a	408	1	-	6/39/115/115	-
26	PL9	a	410	-	-	20/53/73/73	0/1/1/1
23	CLA	b	609	2	-	6/39/115/115	-
23	CLA	d	402	36	-	4/39/115/115	-
23	CLA	A	405	36	-	2/39/115/115	-

The worst 5 of 963 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	MG-NB	11.78	2.29	2.05
23	b	616	CLA	MG-NA	11.51	2.33	2.06
23	C	507	CLA	MG-ND	-11.00	1.84	2.05
23	C	505	CLA	MG-ND	-10.38	1.85	2.05
23	c	508	CLA	MG-ND	9.89	2.25	2.05

The worst 5 of 1325 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	509	CLA	C4A-NA-C1A	10.99	111.69	106.68
23	c	501	CLA	C4A-NA-C1A	10.50	111.47	106.68
23	C	502	CLA	C4A-NA-C1A	10.46	111.45	106.68
27	A	410	SQD	O6-C1-C2	10.43	124.11	108.27
23	d	402	CLA	C4A-NA-C1A	10.31	111.38	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 1687 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	C4B-C3B-CAB-CBB
23	B	606	CLA	C2B-C3B-CAB-CBB
23	B	606	CLA	C4B-C3B-CAB-CBB
23	B	614	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

98 monomers are involved in 177 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	518	DGD	1	0
29	A	413	LHG	4	0
33	D	411	LMG	1	0
25	c	514	BCR	3	0
33	M	101	LMG	1	0
23	A	404	CLA	1	0
28	a	413	DGD	2	0
23	b	608	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	K	101	BCR	4	0
29	D	408	LHG	2	0
25	a	409	BCR	1	0
27	F	101	SQD	2	0
23	C	514	CLA	1	0
23	b	610	CLA	2	0
24	a	407	PHO	1	0
23	B	614	CLA	1	0
23	c	510	CLA	2	0
34	E	103	HEM	4	0
25	d	405	BCR	3	0
23	c	507	CLA	1	0
26	D	406	PL9	1	0
24	A	406	PHO	1	0
25	Z	101	BCR	1	0
28	A	412	DGD	5	0
25	B	617	BCR	1	0
23	D	402	CLA	1	0
33	c	524	LMG	3	0
23	C	507	CLA	2	0
23	d	403	CLA	2	0
29	L	101	LHG	3	0
25	c	515	BCR	3	0
23	C	512	CLA	2	0
27	a	411	SQD	1	0
33	D	407	LMG	3	0
23	B	604	CLA	1	0
23	C	506	CLA	2	0
26	A	409	PL9	1	0
27	A	411	SQD	2	0
23	b	615	CLA	3	0
25	t	101	BCR	7	0
25	C	515	BCR	5	0
25	b	618	BCR	4	0
25	c	521	BCR	1	0
23	b	614	CLA	2	0
27	a	412	SQD	3	0
23	b	607	CLA	2	0
27	b	601	SQD	1	0
25	D	405	BCR	6	0
23	C	511	CLA	1	0
23	C	509	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	a	415	OEX	1	0
23	B	616	CLA	1	0
23	b	606	CLA	2	0
23	b	602	CLA	2	0
23	b	612	CLA	1	0
23	B	615	CLA	1	0
34	e	102	HEM	5	0
25	b	619	BCR	3	0
23	c	511	CLA	1	0
23	c	508	CLA	1	0
27	f	101	SQD	2	0
33	d	411	LMG	1	0
28	H	102	DGD	1	0
24	d	401	PHO	3	0
25	B	619	BCR	2	0
23	B	601	CLA	3	0
24	D	401	PHO	3	0
23	a	405	CLA	1	0
23	B	606	CLA	1	0
23	c	505	CLA	3	0
29	d	408	LHG	1	0
27	B	621	SQD	1	0
29	e	101	LHG	1	0
29	d	409	LHG	1	0
25	k	101	BCR	1	0
23	B	613	CLA	3	0
23	B	609	CLA	1	0
29	d	407	LHG	2	0
23	C	510	CLA	4	0
23	D	403	CLA	2	0
23	b	617	CLA	2	0
25	T	101	BCR	2	0
25	H	101	BCR	4	0
23	b	604	CLA	4	0
23	d	404	CLA	1	0
23	c	506	CLA	2	0
23	C	502	CLA	2	0
25	B	618	BCR	3	0
23	b	616	CLA	3	0
33	m	101	LMG	1	0
23	c	501	CLA	2	0
23	B	602	CLA	1	0

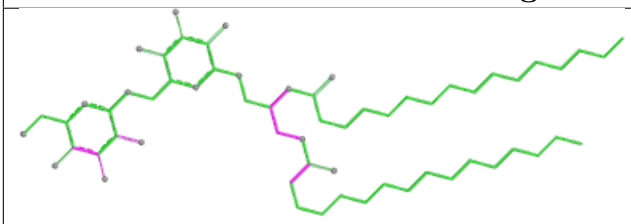
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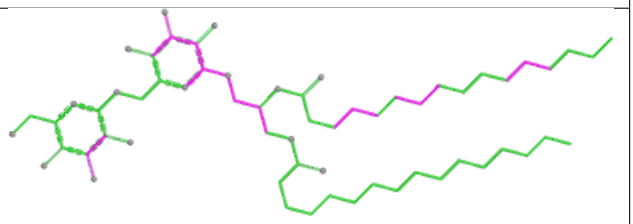
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	508	CLA	1	0
23	b	605	CLA	1	0
23	a	408	CLA	1	0
26	a	410	PL9	3	0
23	d	402	CLA	1	0
23	A	405	CLA	1	0

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.

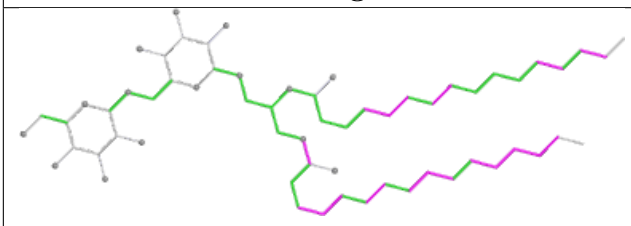
Ligand DGD C 518



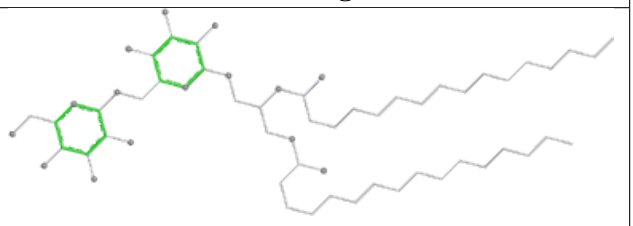
Bond lengths



Bond angles

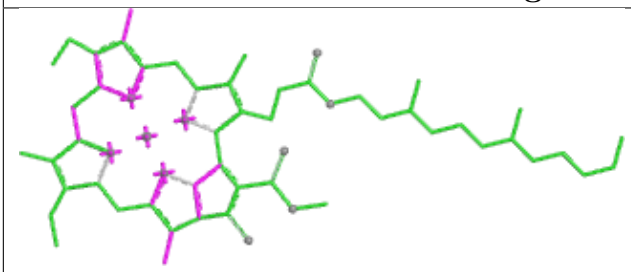


Torsions

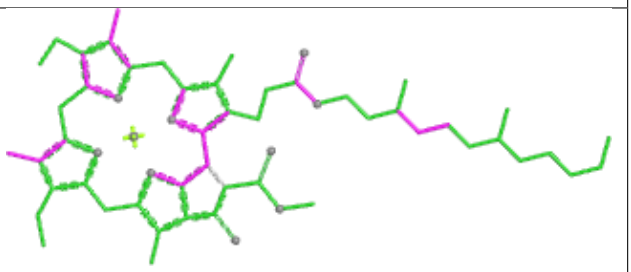


Rings

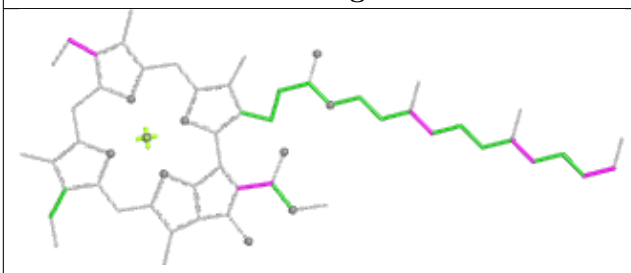
Ligand CLA C 505



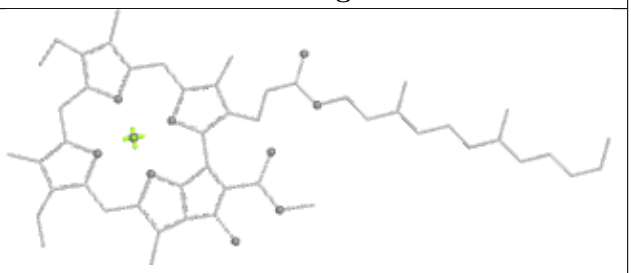
Bond lengths



Bond angles

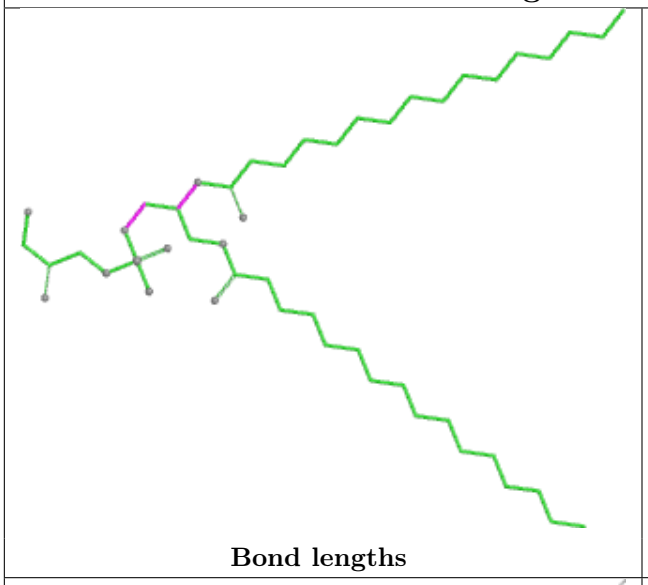


Torsions

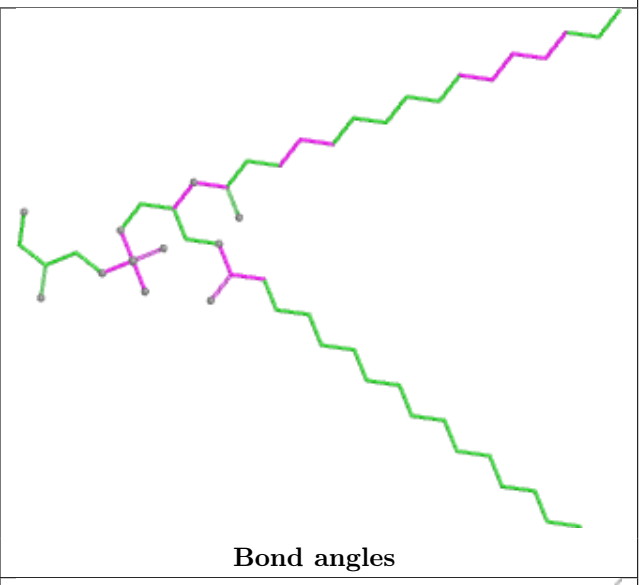


Rings

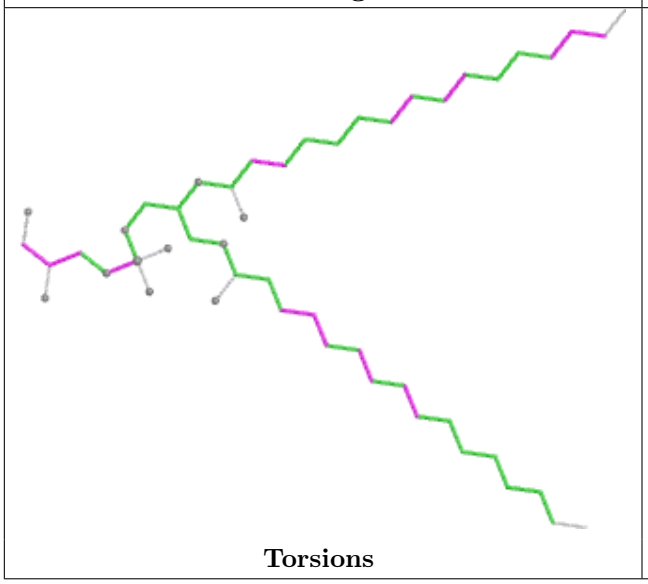
Ligand LHG A 413



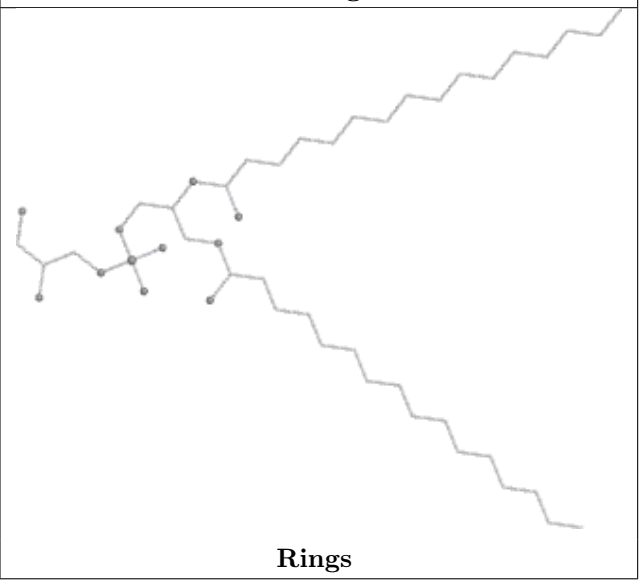
Bond lengths



Bond angles

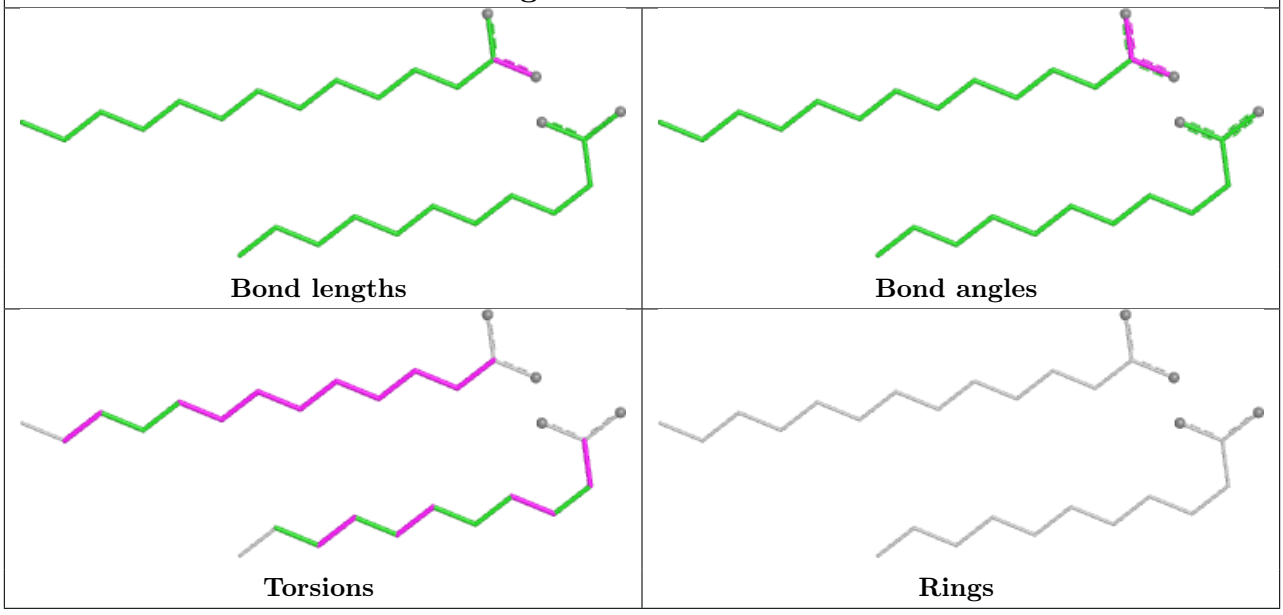


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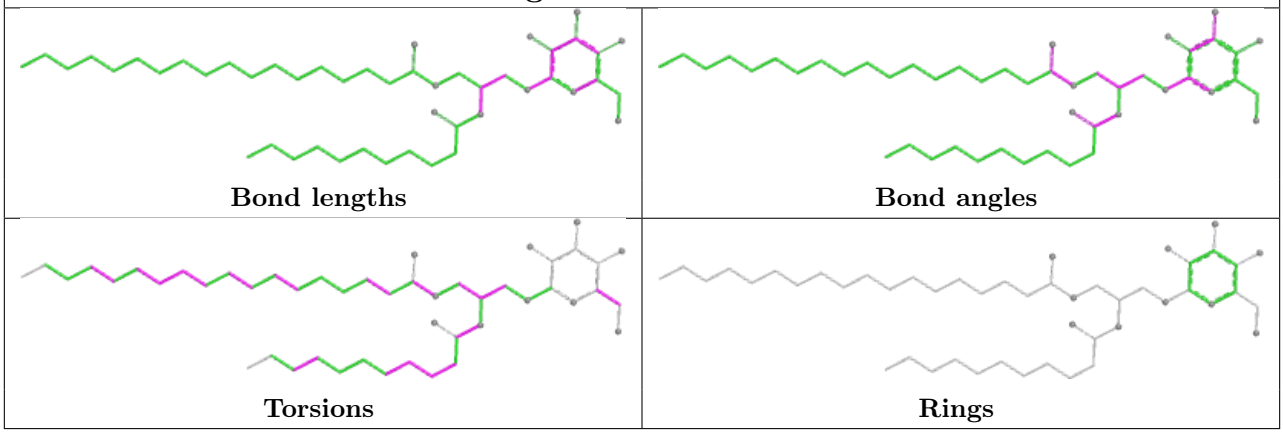


Rings

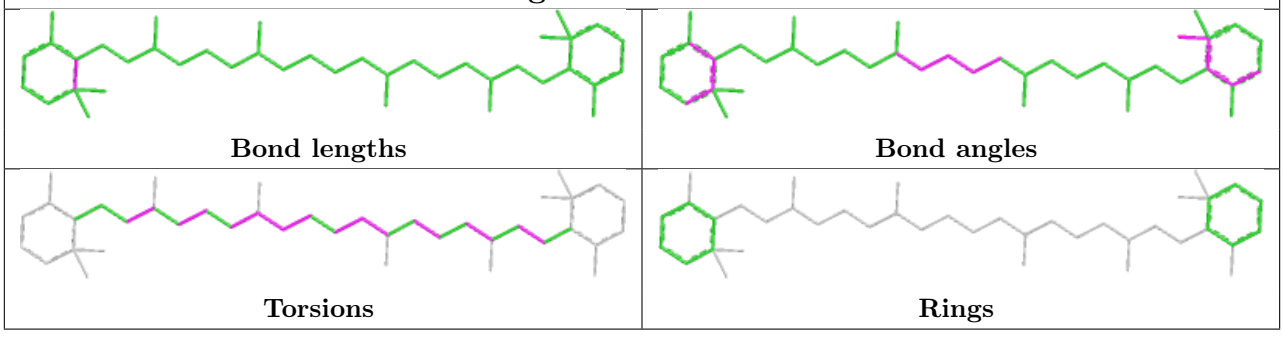
Ligand LMG D 411



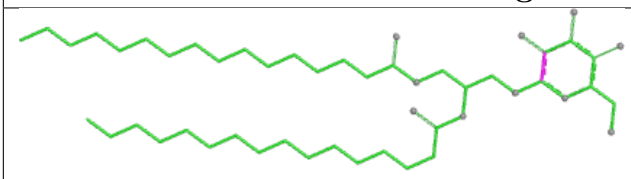
Ligand LMG c 522

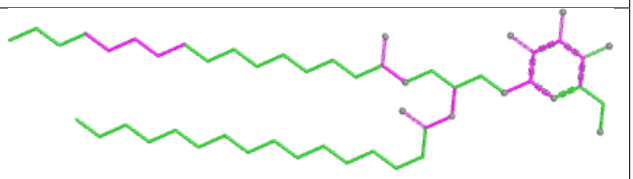


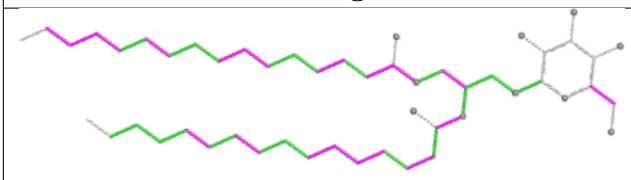
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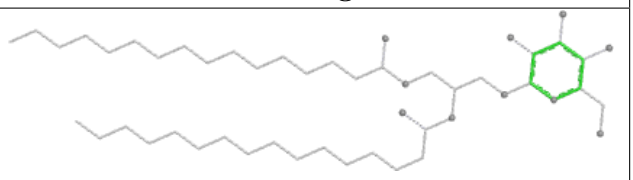


Ligand LMG M 101

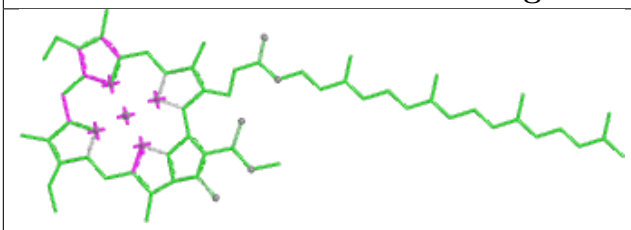

Bond lengths

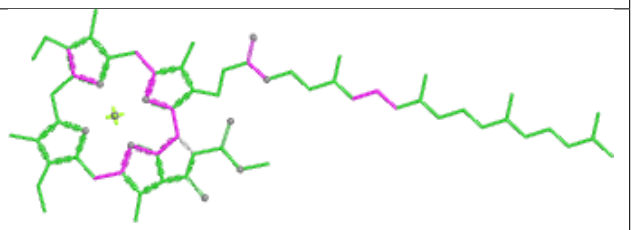

Bond angles

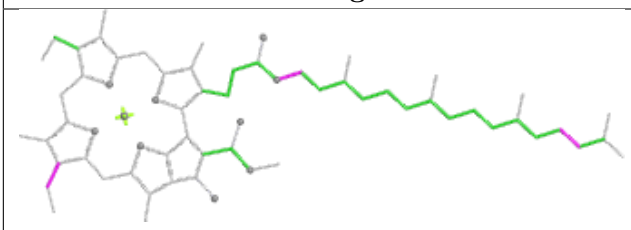

Torsions

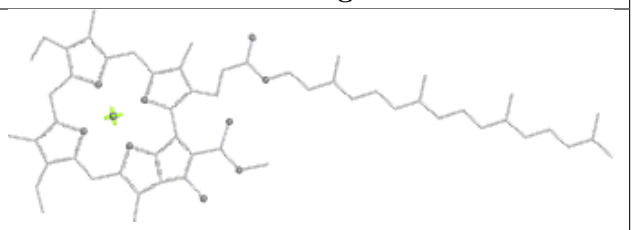

Rings

Ligand CLA A 404

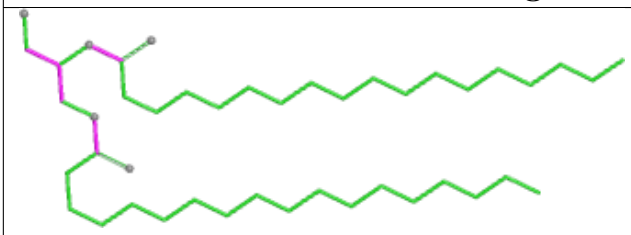

Bond lengths

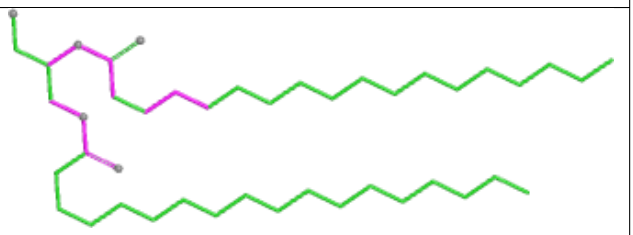

Bond angles

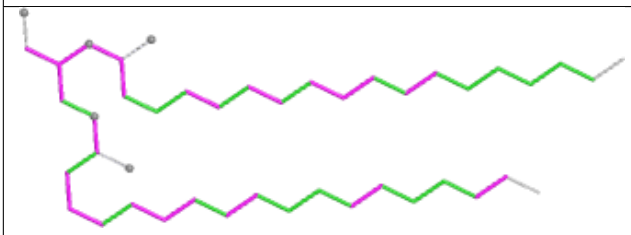

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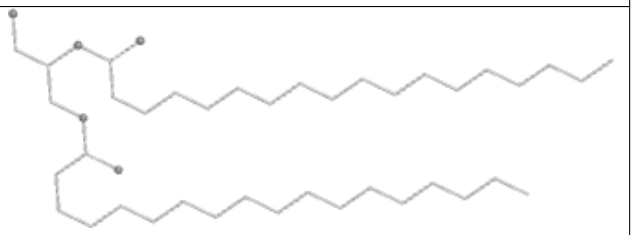

Rings

Ligand DGD a 413

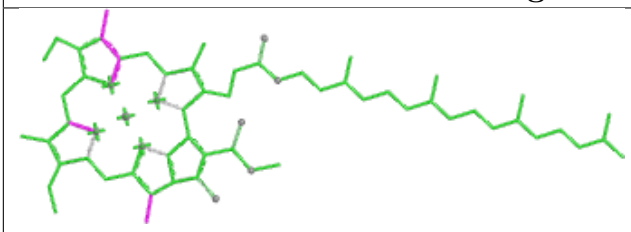

Bond lengths


Bond angles

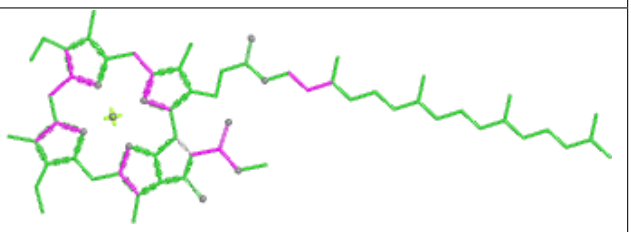

Torsions


Rings

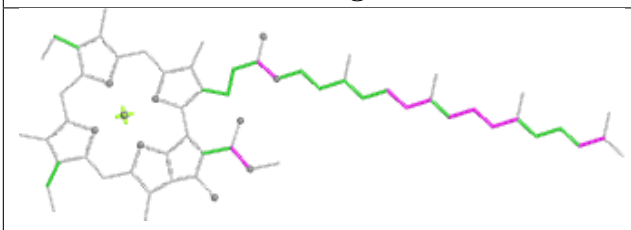
Ligand CLA b 608



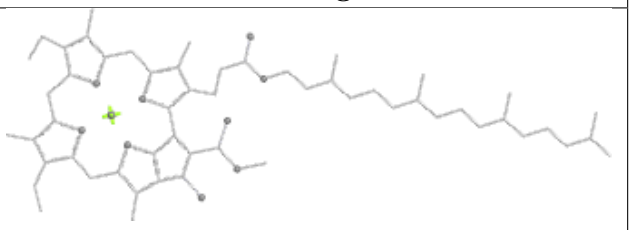
Bond lengths



Bond angles



Torsions

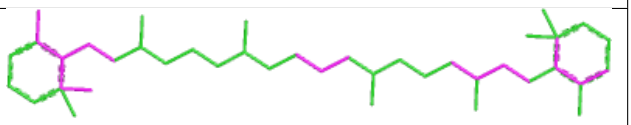


Rings

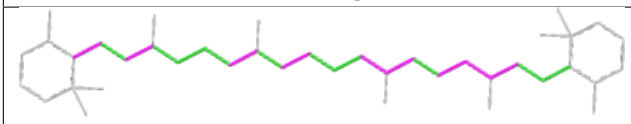
Ligand BCR K 101



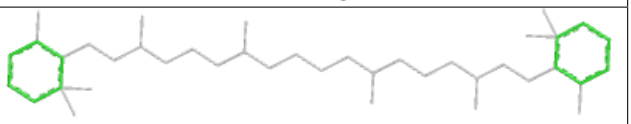
Bond lengths



Bond angles

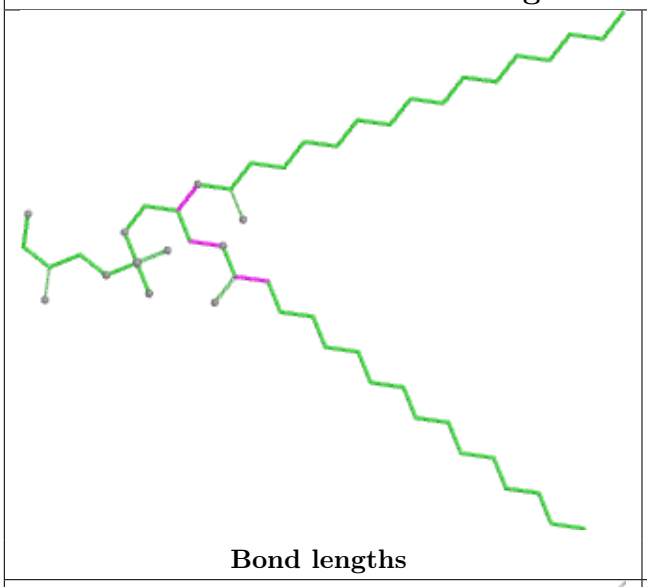


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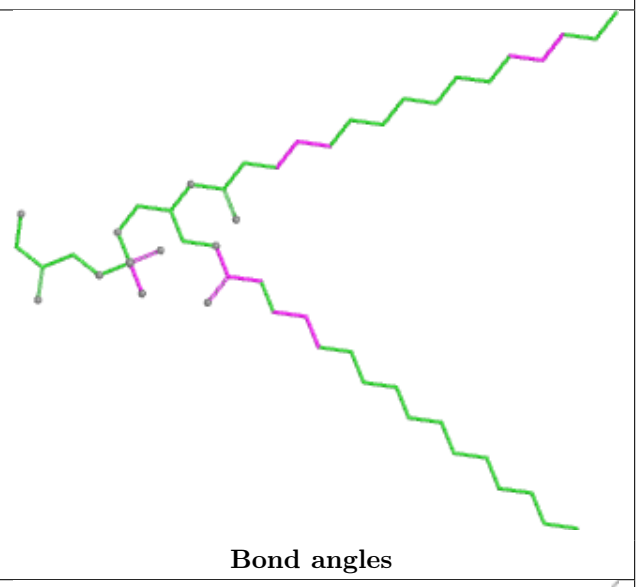


Rings

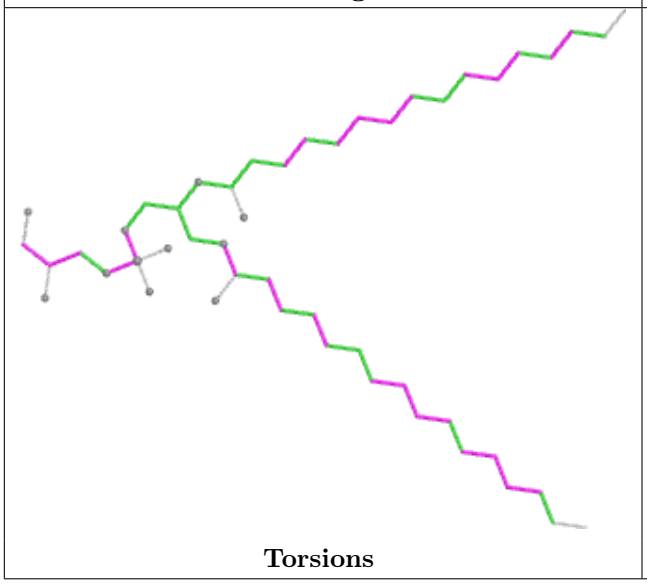
Ligand LHG D 408



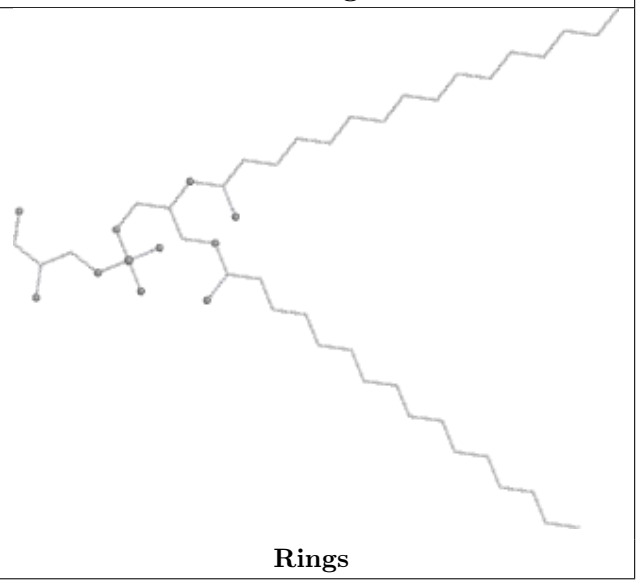
Bond lengths



Bond angles

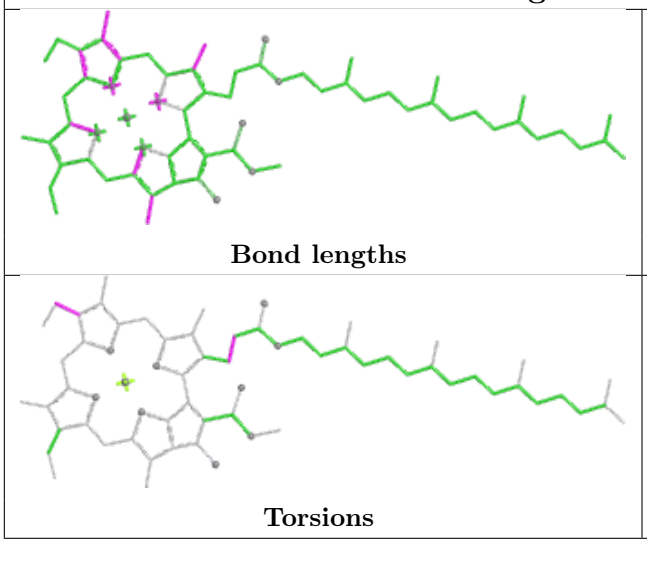


Torsions

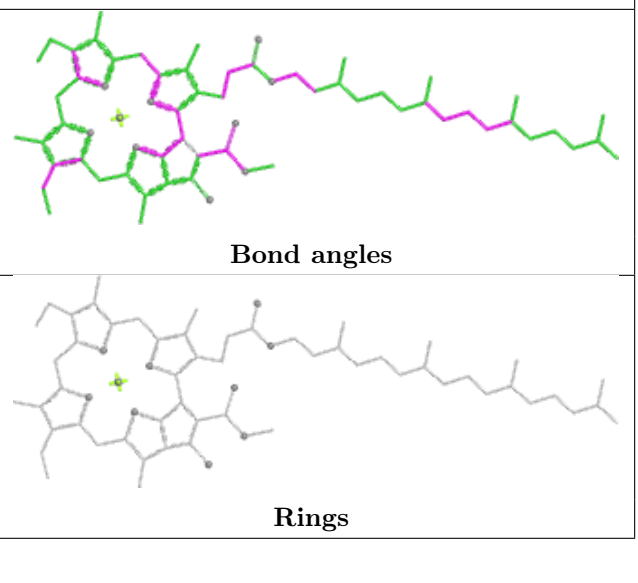


Rings

Ligand CLA b 611



Bond lengths



Bond angles

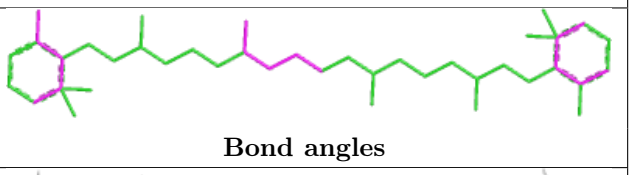
Torsions

Rings

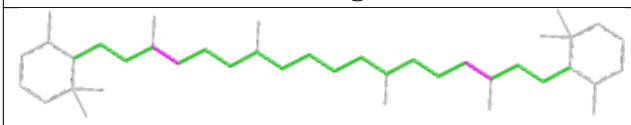
Ligand BCR a 409



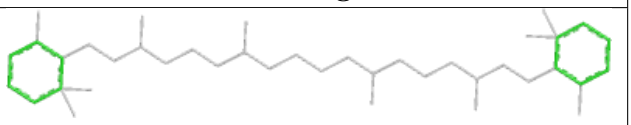
Bond lengths



Bond angles

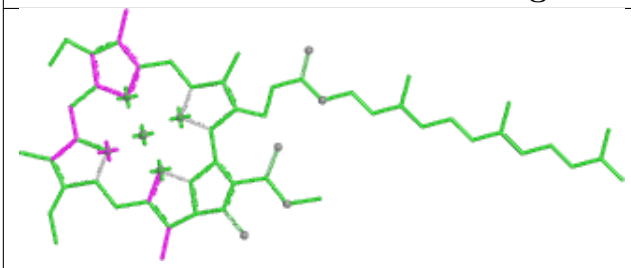


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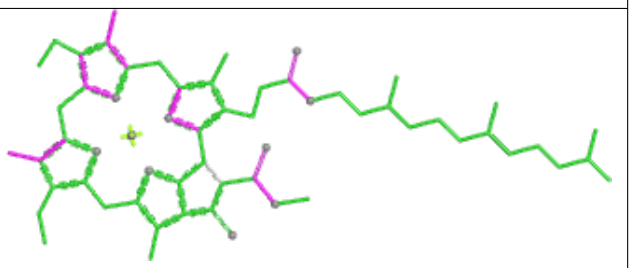


Rings

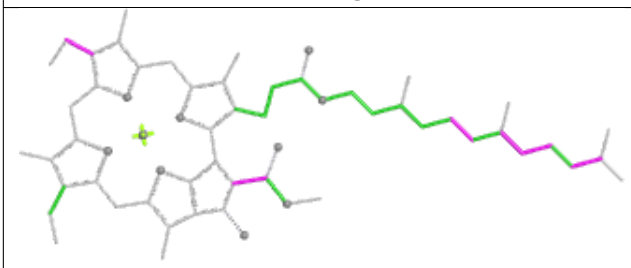
Ligand CLA c 504



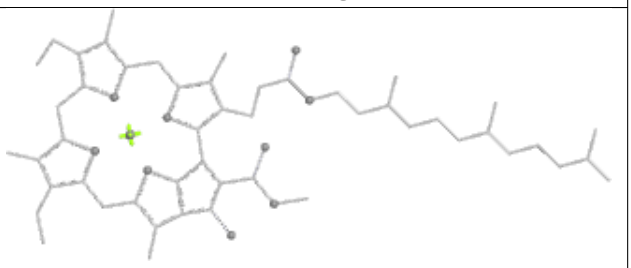
Bond lengths



Bond angles

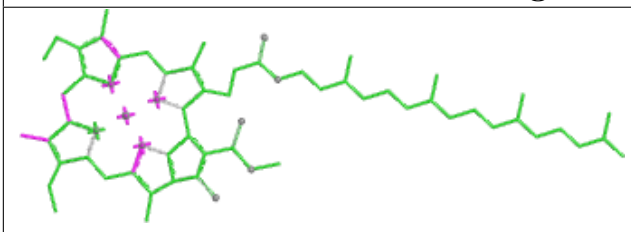


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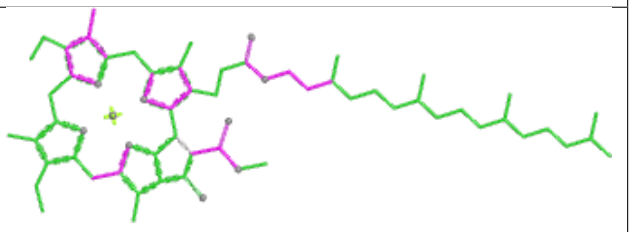


Rings

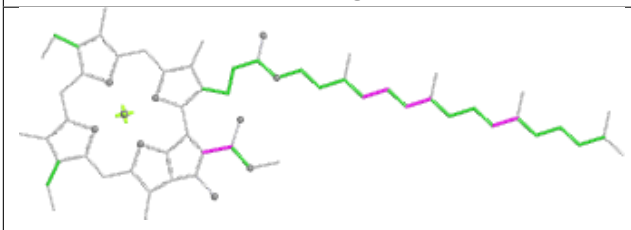
Ligand CLA c 502



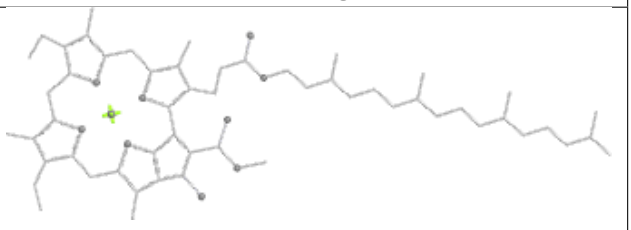
Bond lengths



Bond angles

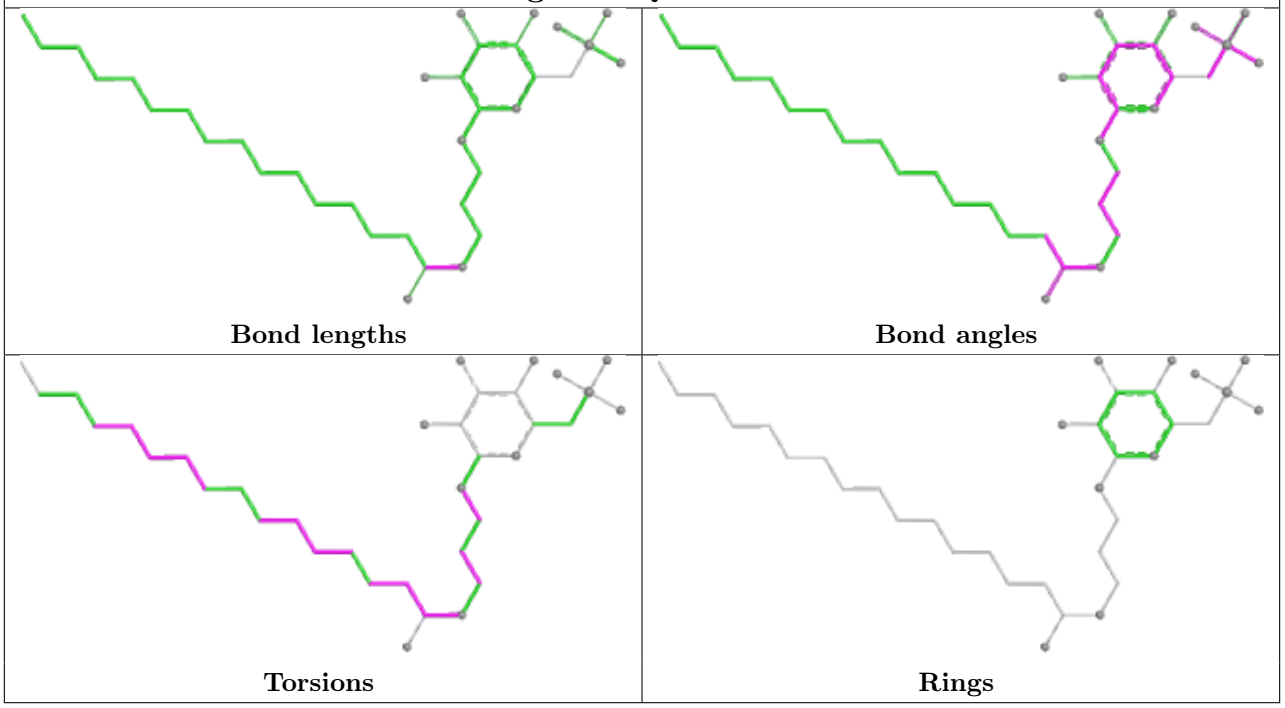


Torsions

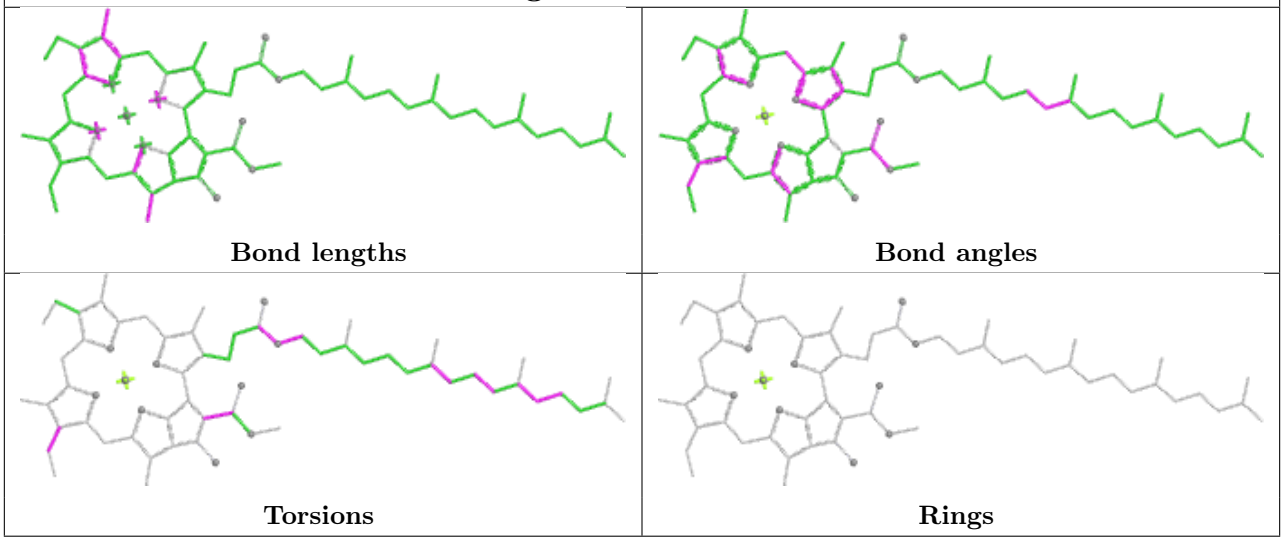


Rings

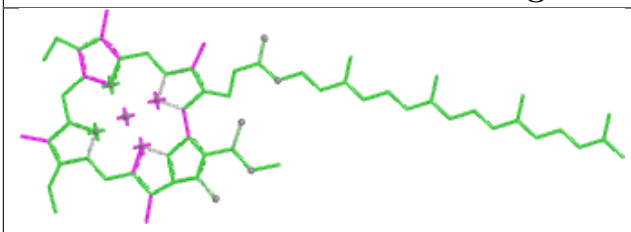
Ligand SQD F 101



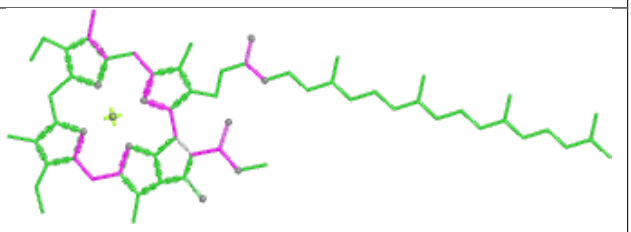
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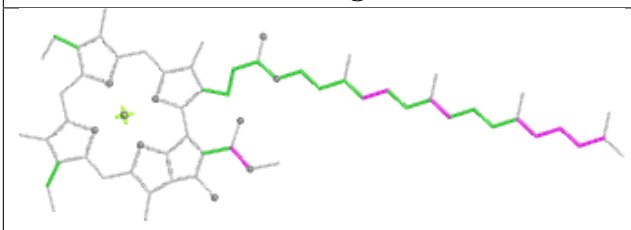
Ligand CLA b 610



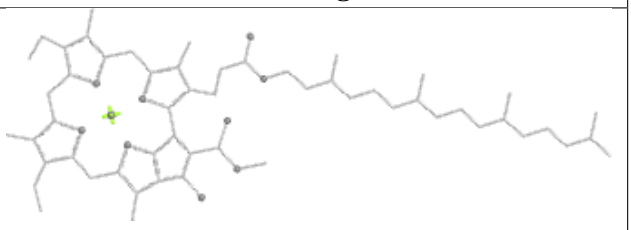
Bond lengths



Bond angles



Torsions

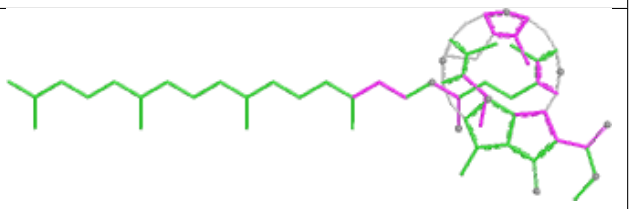


Rings

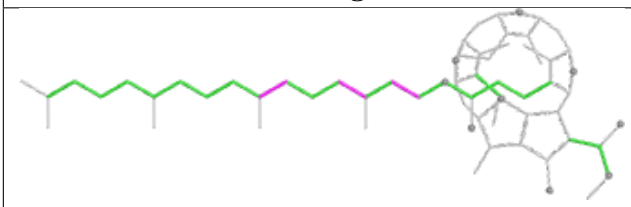
Ligand PHO a 407



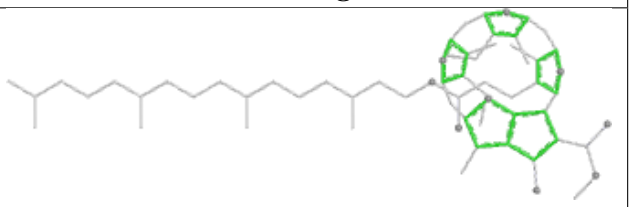
Bond lengths



Bond angles

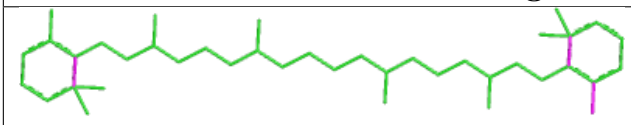


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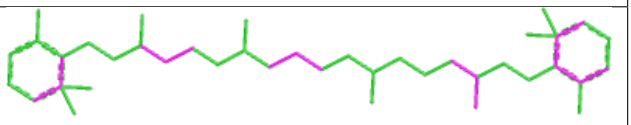


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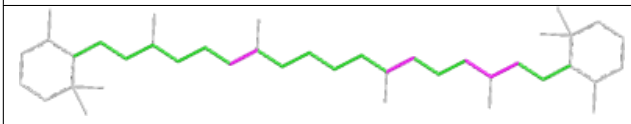
Ligand BCR b 620



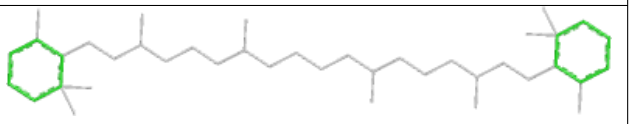
Bond lengths



Bond angles

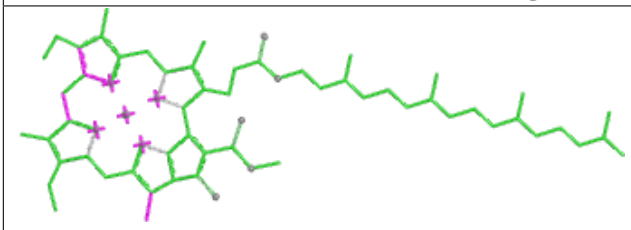


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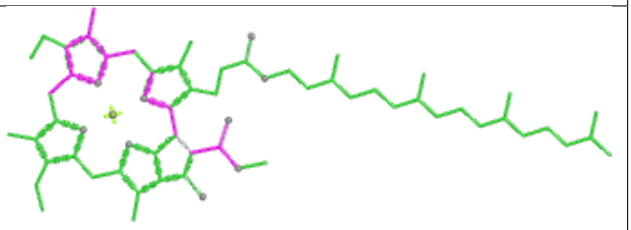


Rings

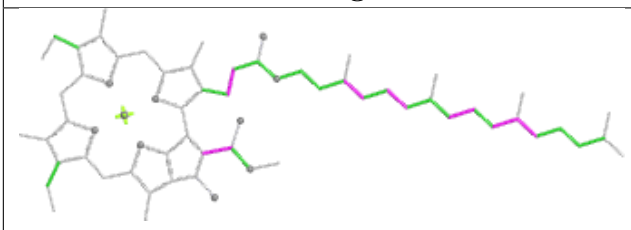
Ligand CLA B 614



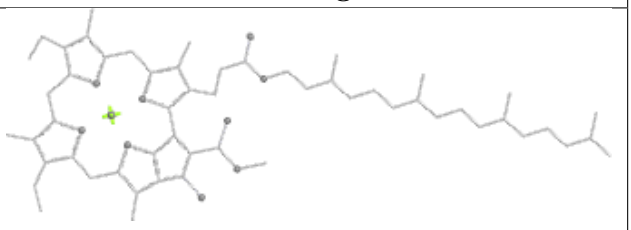
Bond lengths



Bond angles

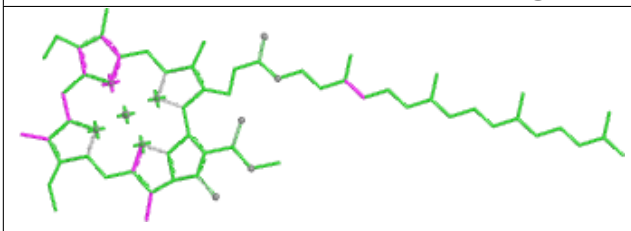


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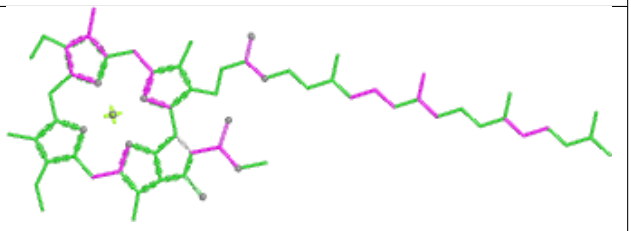


Rings

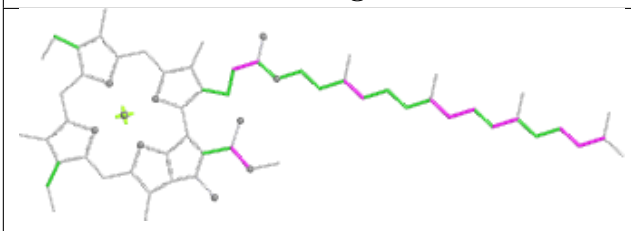
Ligand CLA c 510



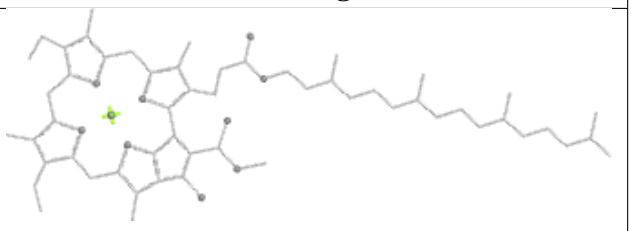
Bond lengths



Bond angles

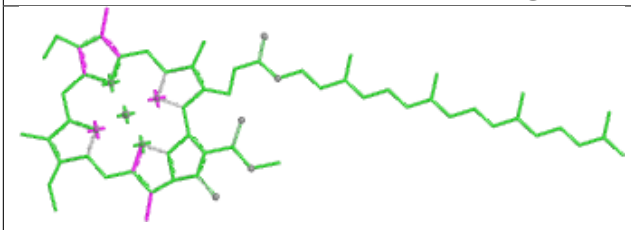


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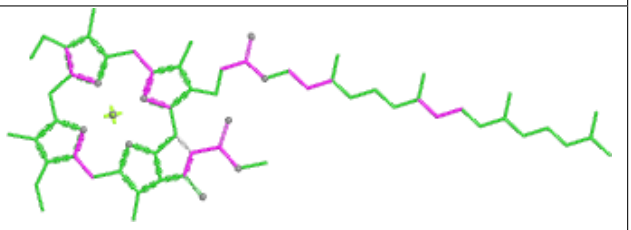


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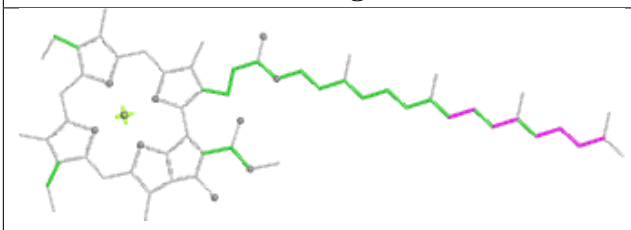
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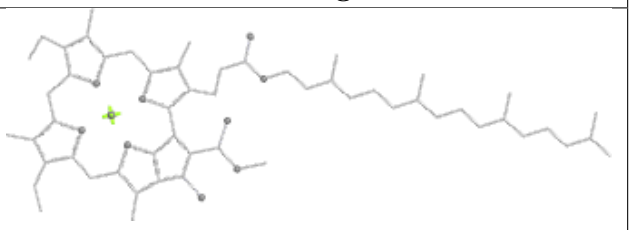
Bond lengths



Bond angles

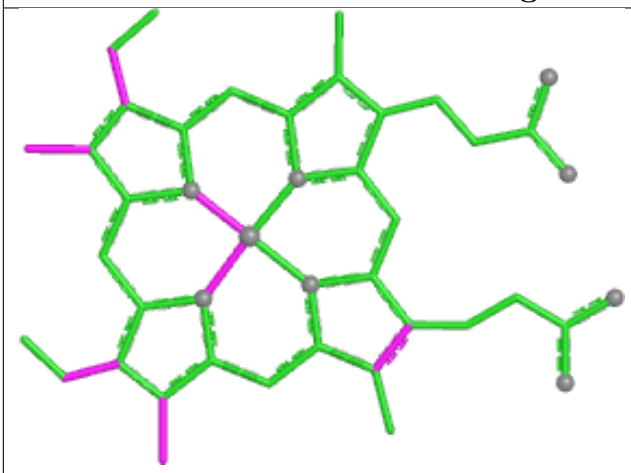


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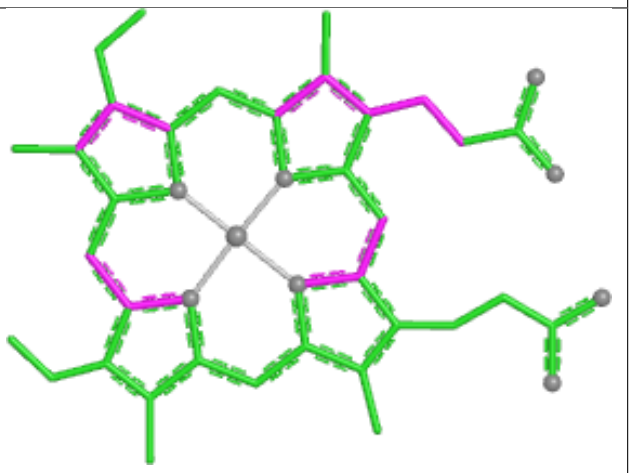


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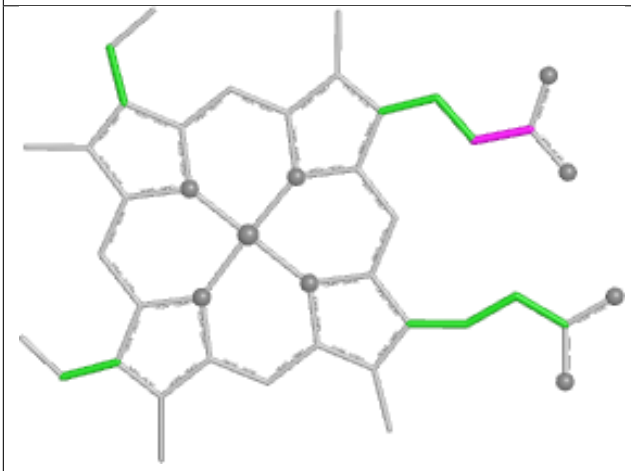
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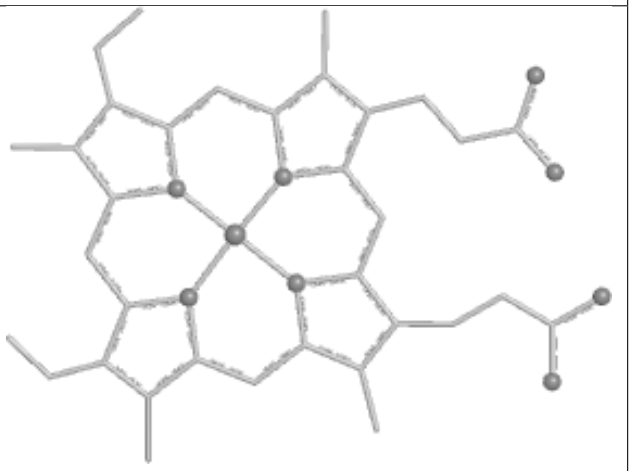
Bond lengths



Bond angles

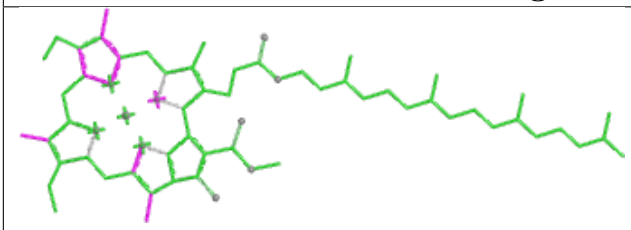


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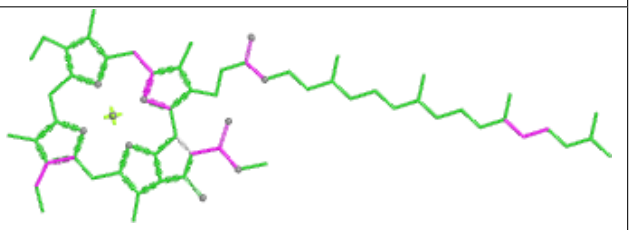


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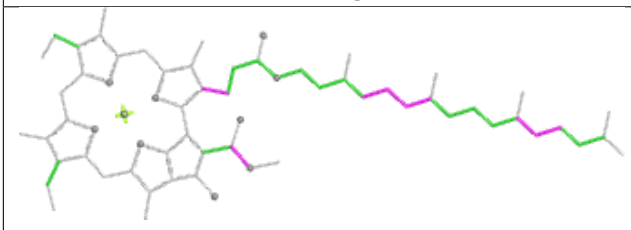
Ligand CLA c 513



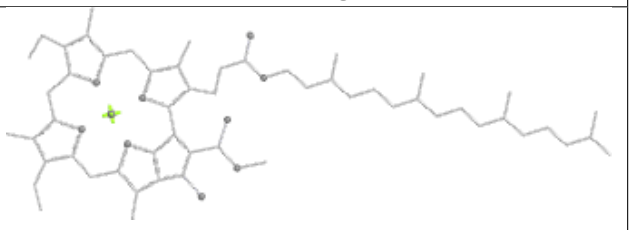
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Bond angles

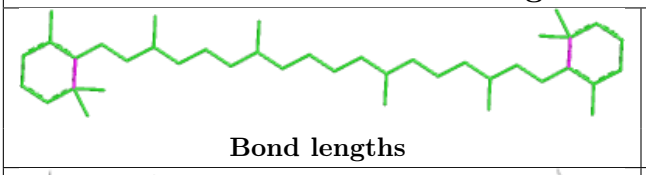


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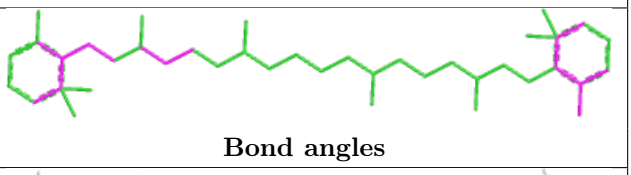


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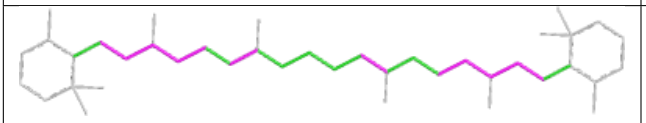
Ligand BCR d 405



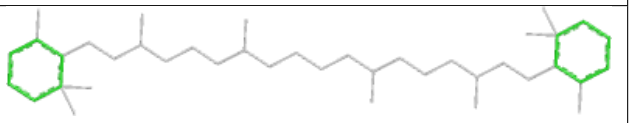
Bond lengths



Bond angles

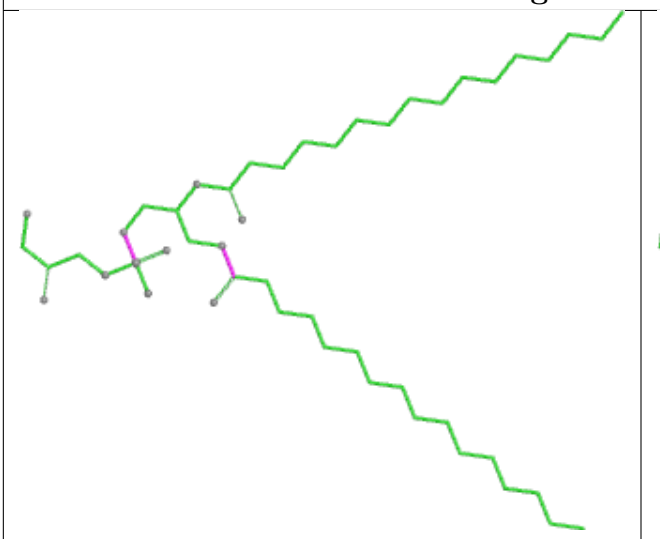


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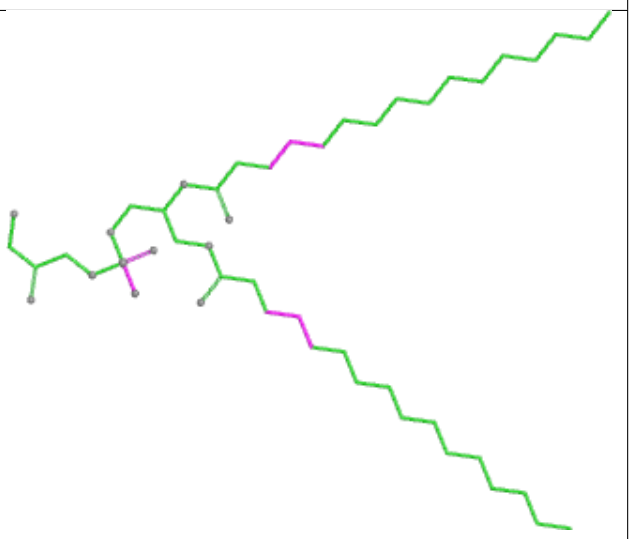


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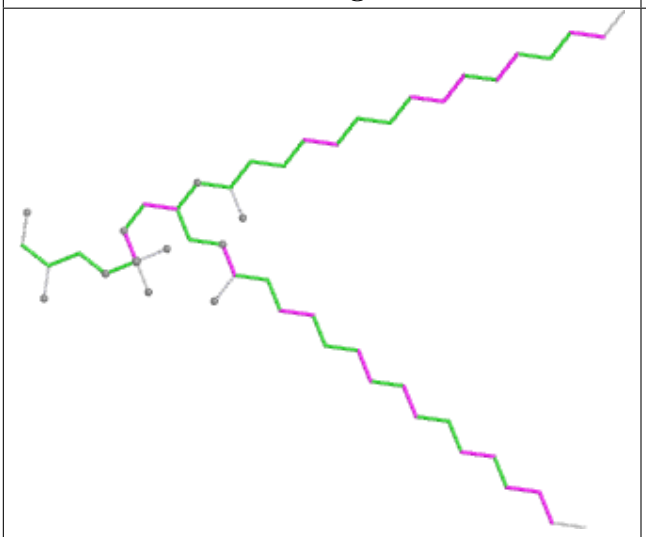
Ligand LHG l 101



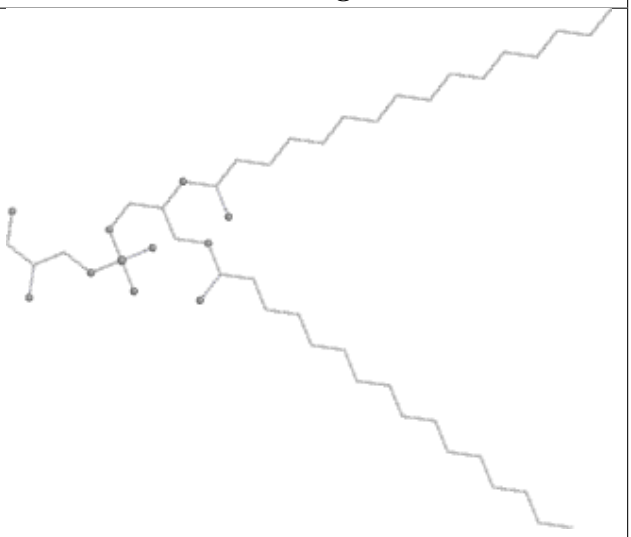
Bond lengths



Bond angles

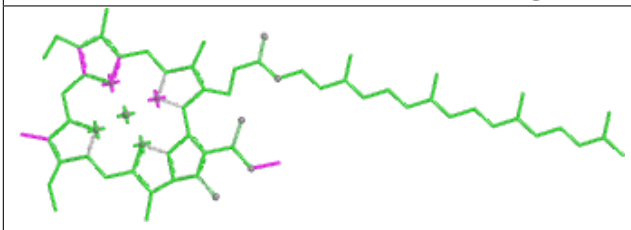


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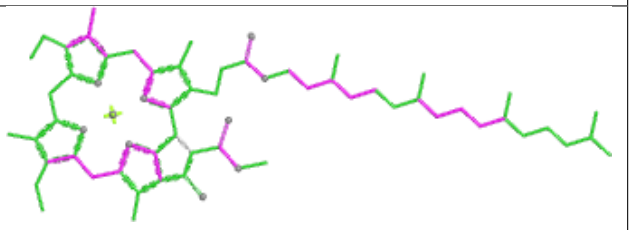


Rings

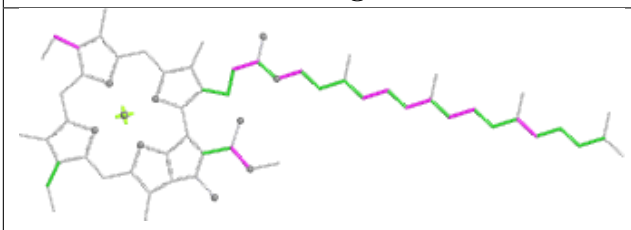
Ligand CLA b 613



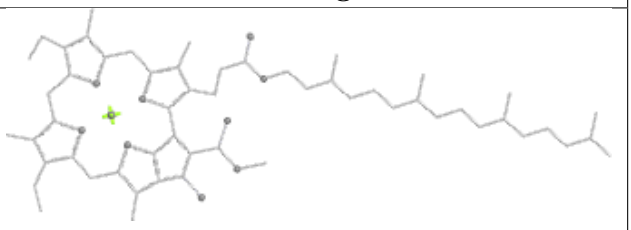
Bond lengths



Bond angles

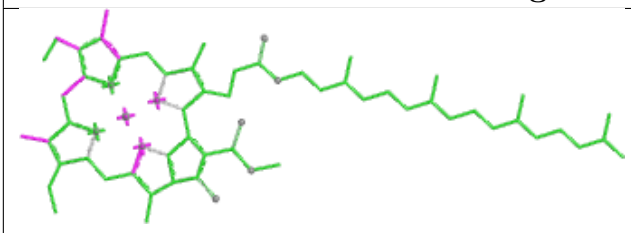


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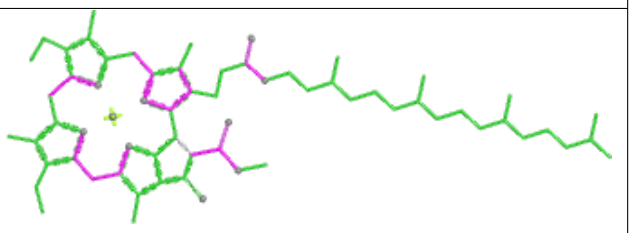


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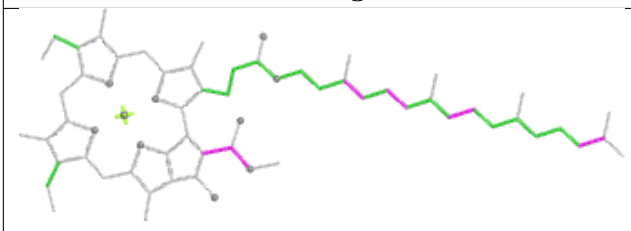
Ligand CLA c 507



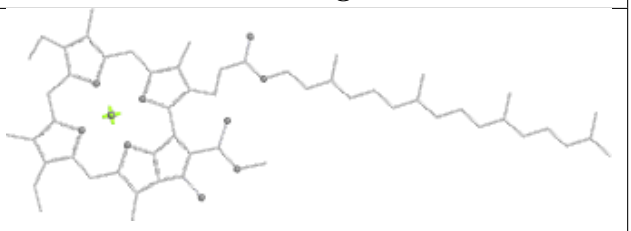
Bond lengths



Bond angles

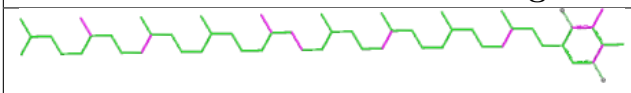


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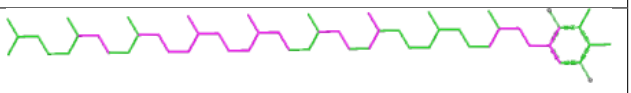


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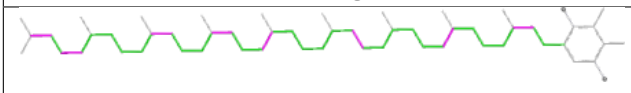
Ligand PL9 D 406



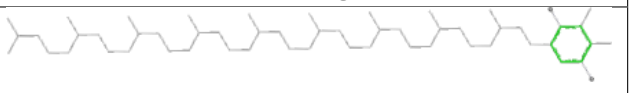
Bond lengths



Bond angles

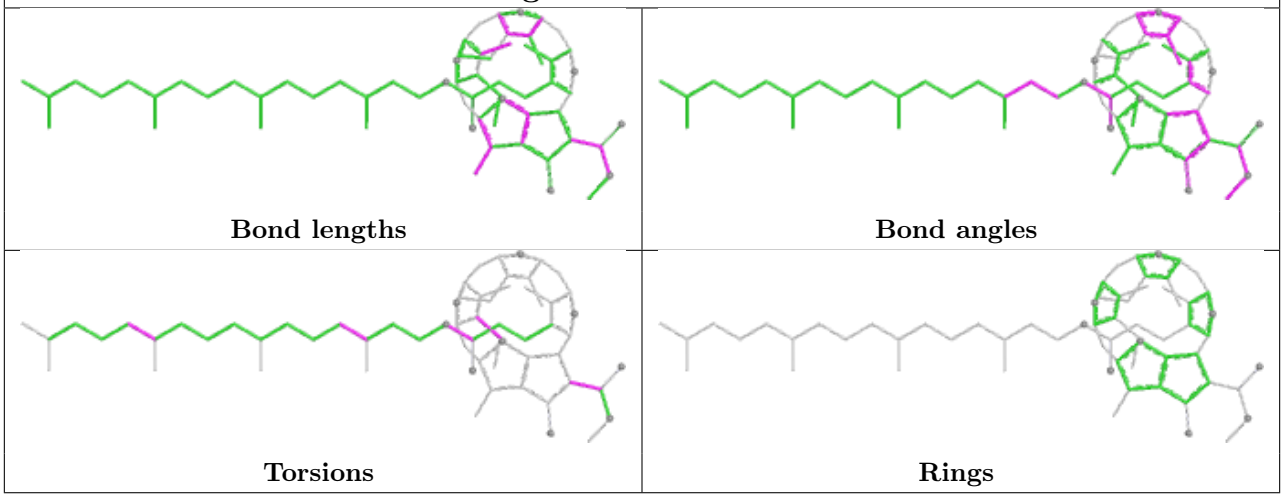


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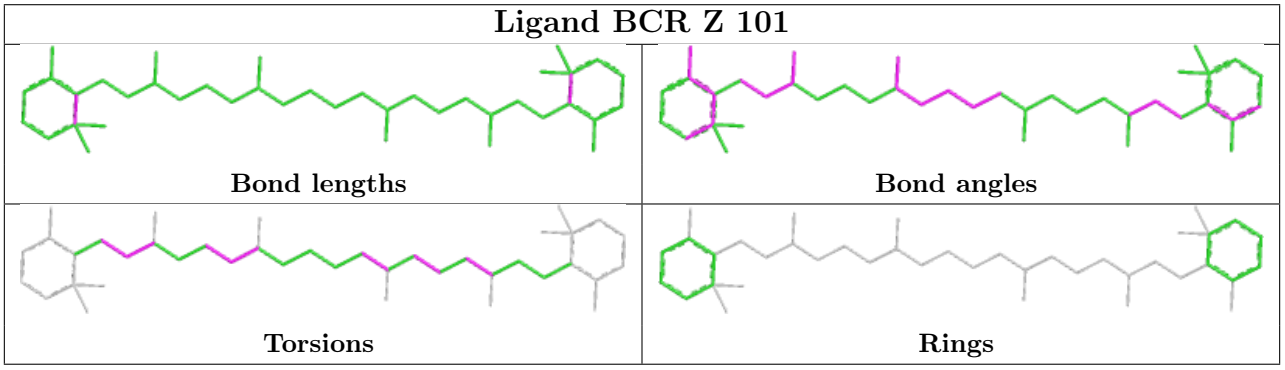


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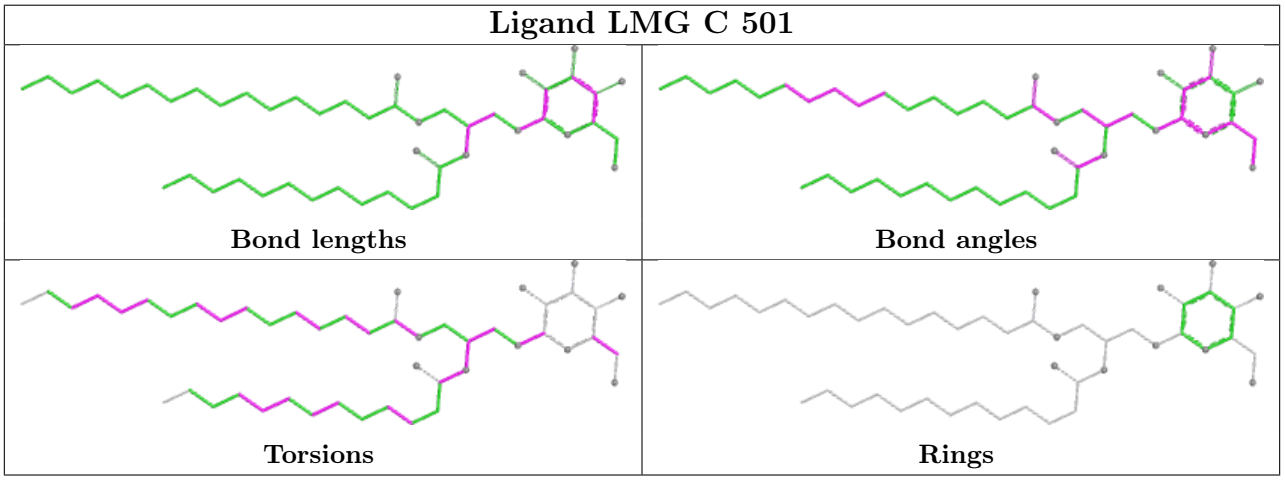
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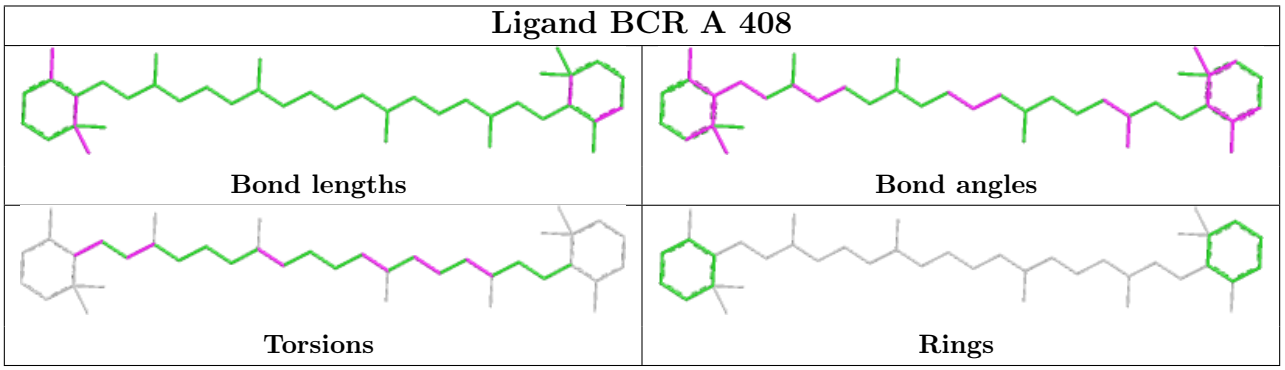
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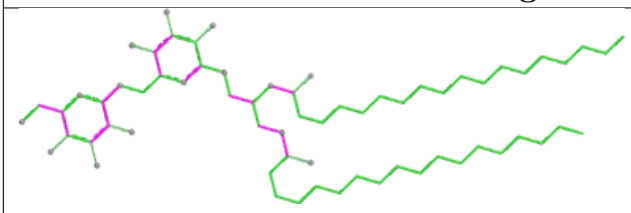
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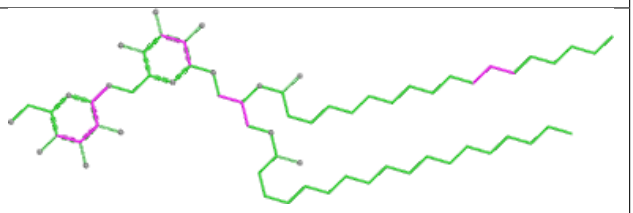
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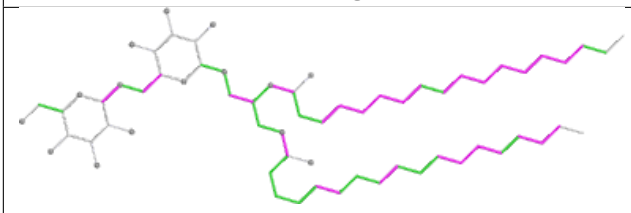
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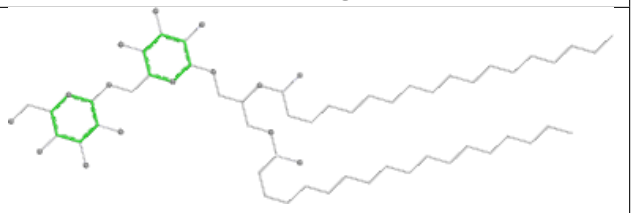
Bond lengths



Bond angles



Torsions

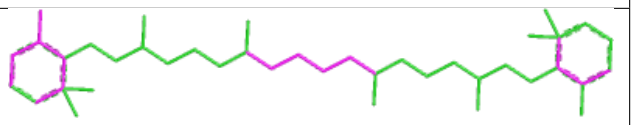


Rings

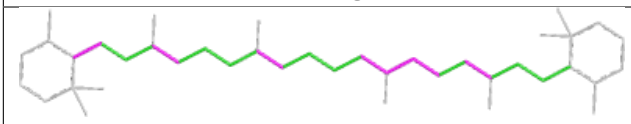
Ligand BCR B 617



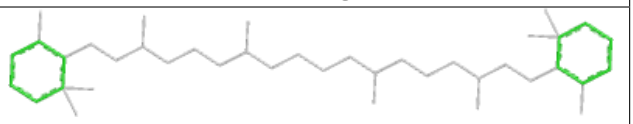
Bond lengths



Bond angles

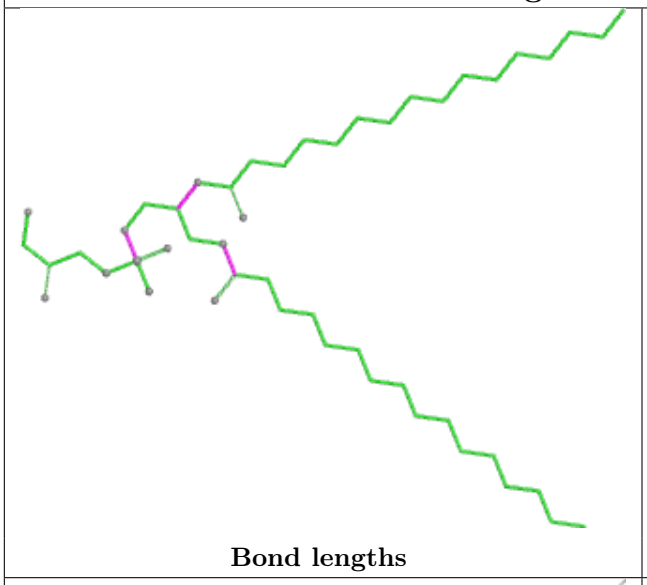


Torsions

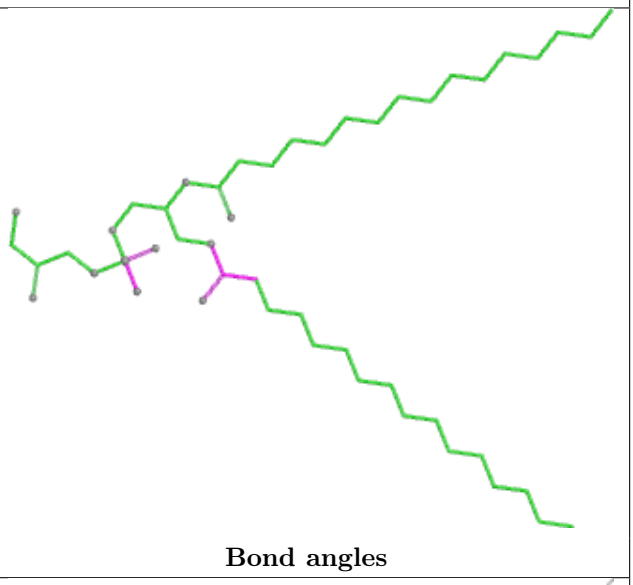


Rings

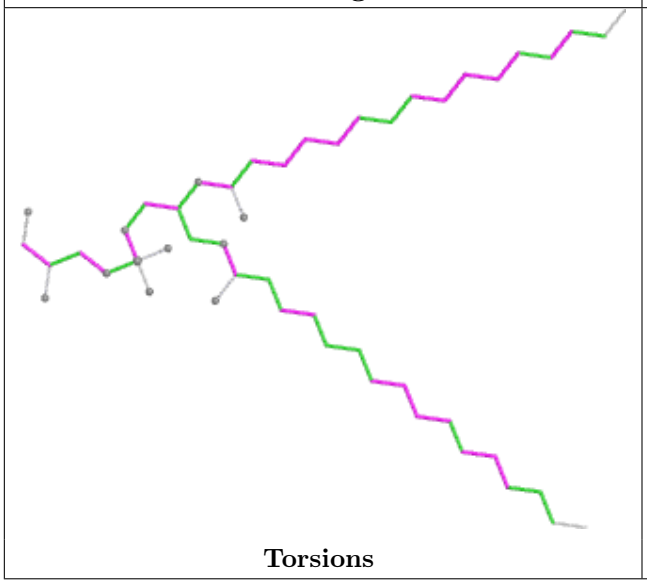
Ligand LHG E 101



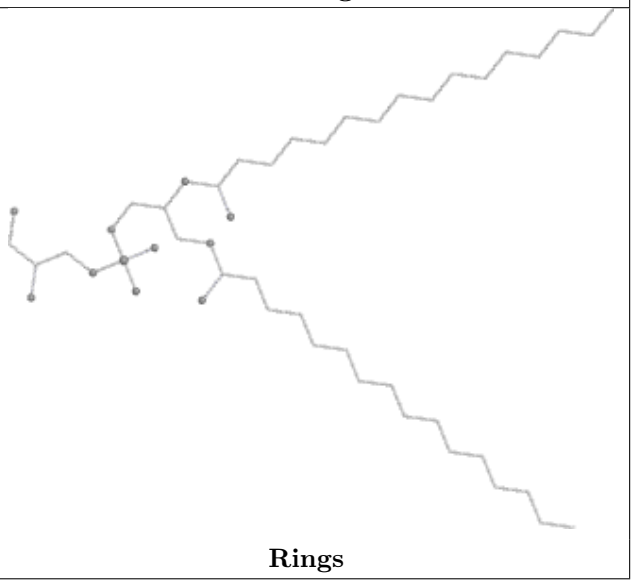
Bond lengths



Bond angles

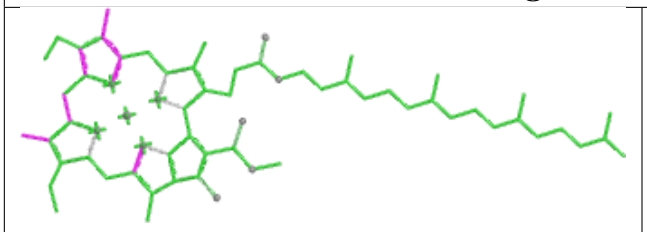


Torsions

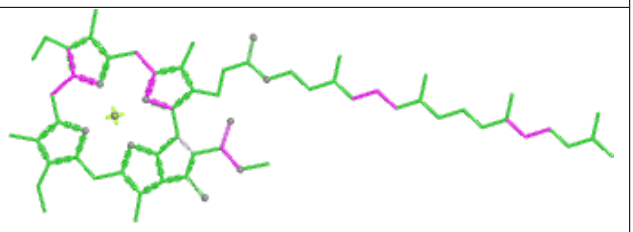


Rings

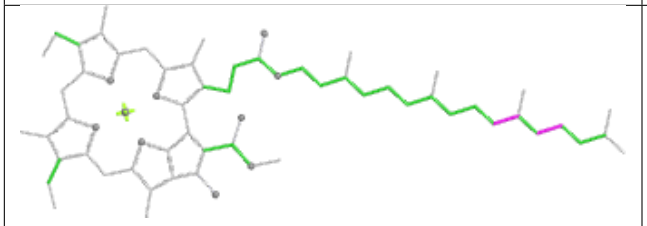
Ligand CLA D 402



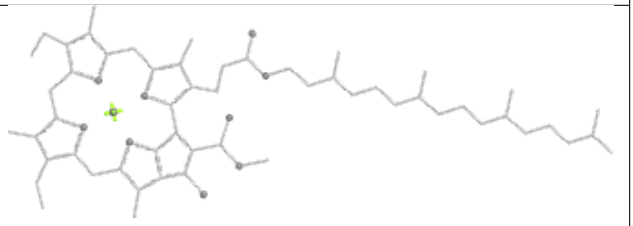
Bond lengths



Bond angles

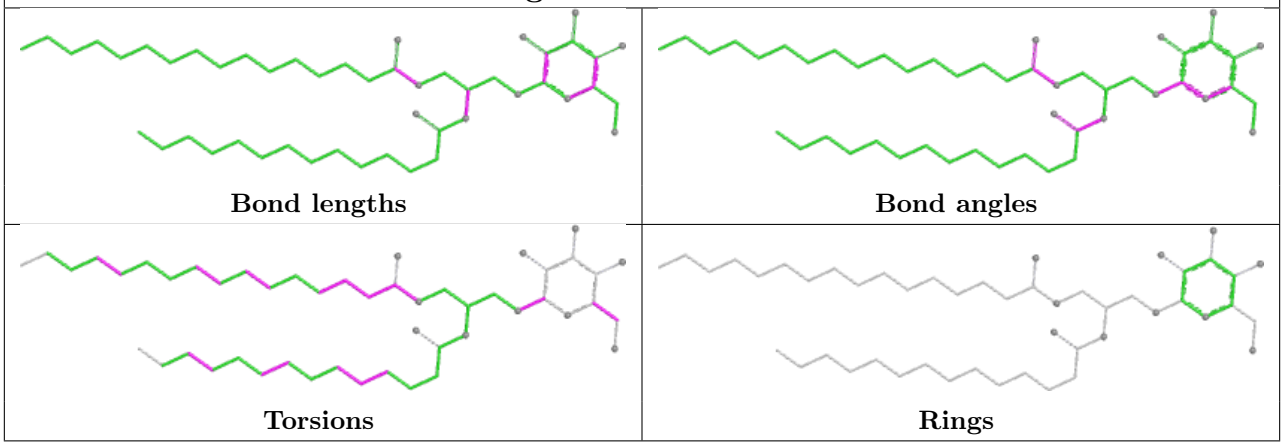


Torsions

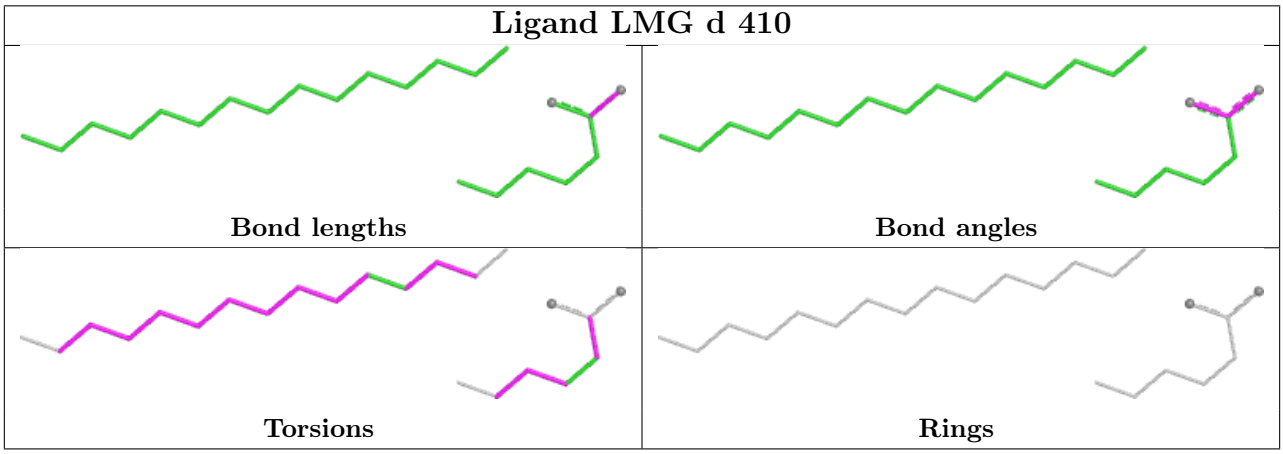


Rings

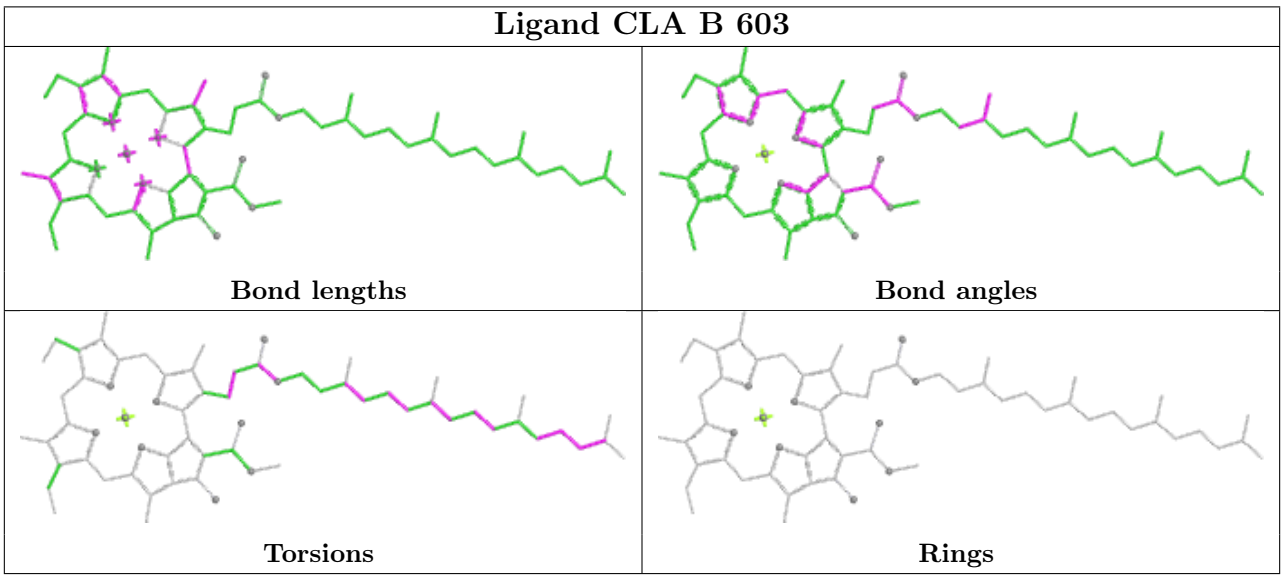
Ligand LMG c 524



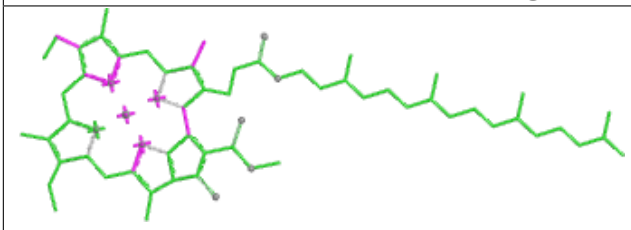
Ligand LMG d 410



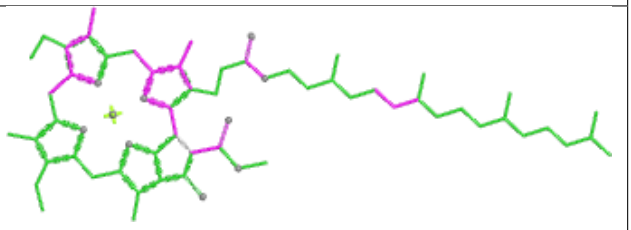
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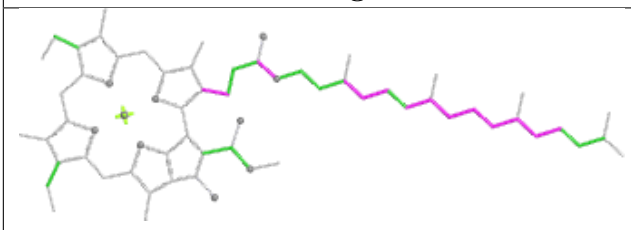
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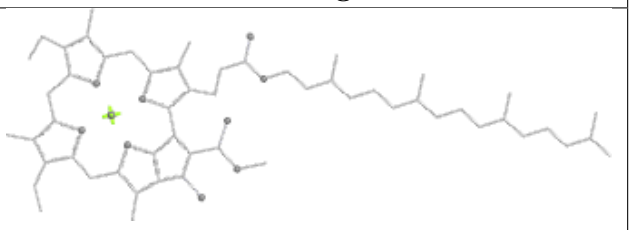
Bond lengths



Bond angles

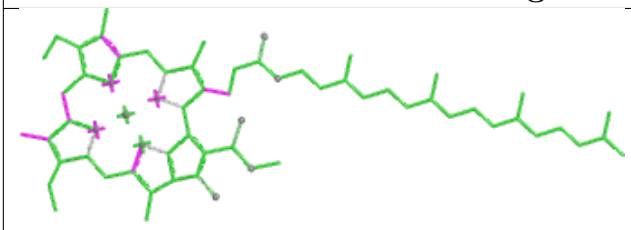


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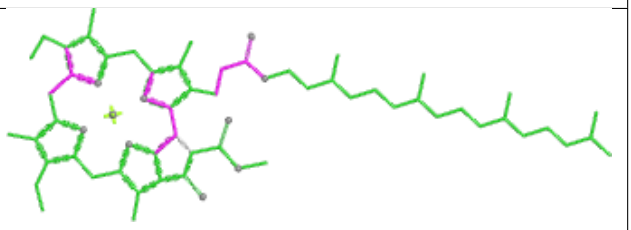


Rings

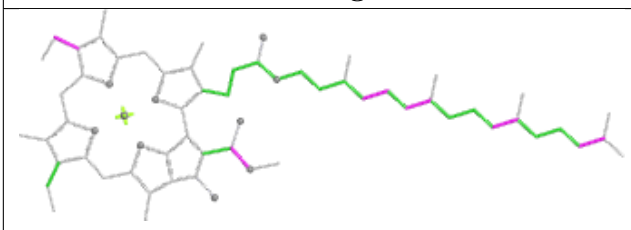
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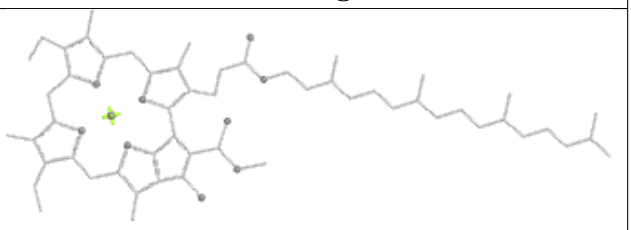
Bond lengths



Bond angles

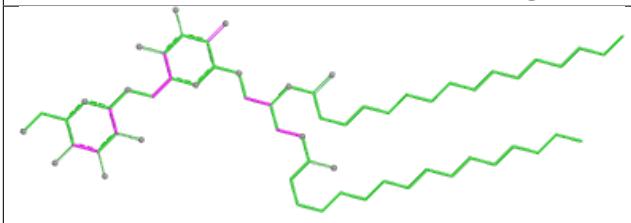


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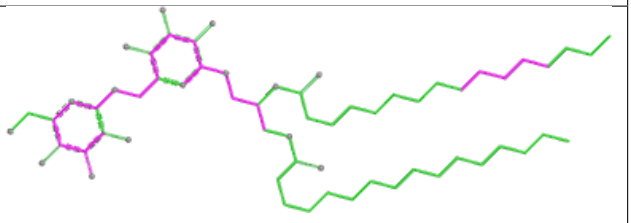


Rings

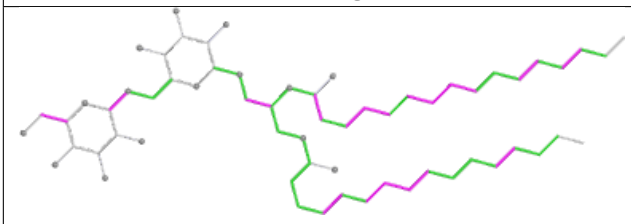
Ligand DGD h 101



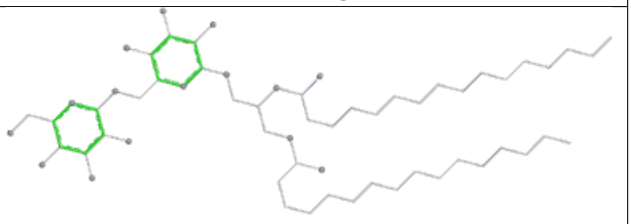
Bond lengths



Bond angles

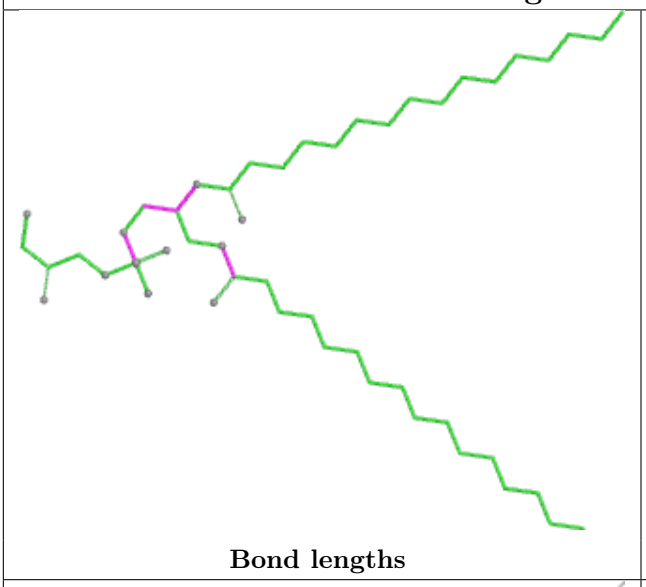


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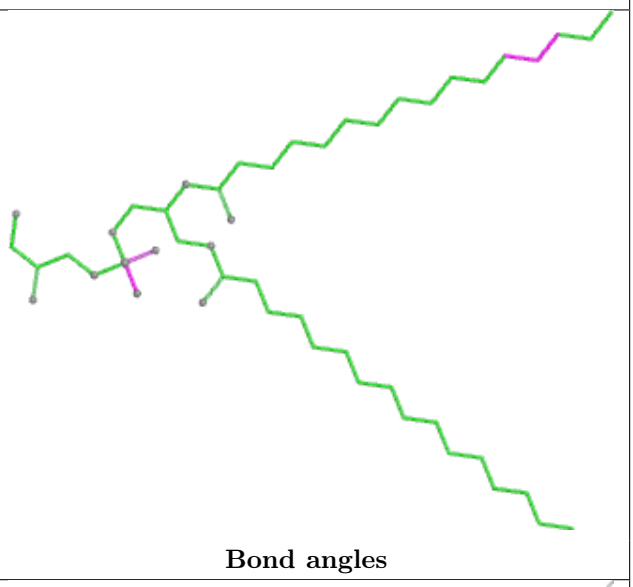


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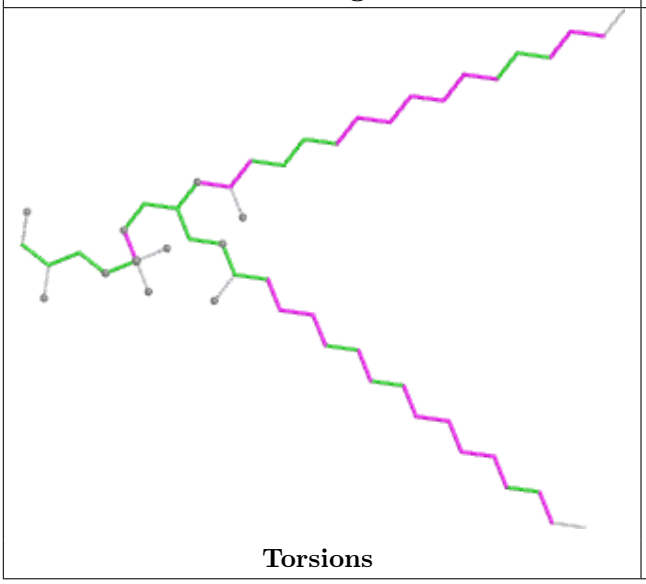
Ligand LHG L 101



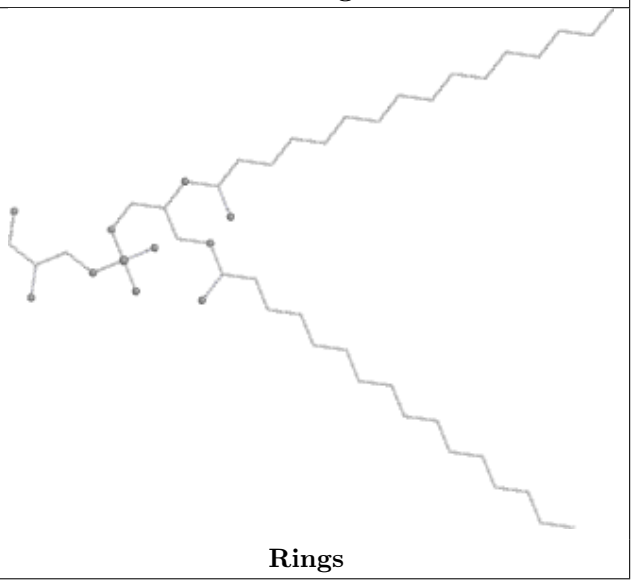
Bond lengths



Bond angles



Torsions

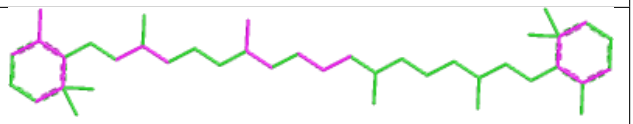


Rings

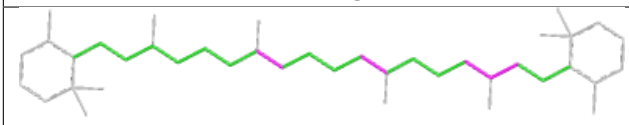
Ligand BCR c 515



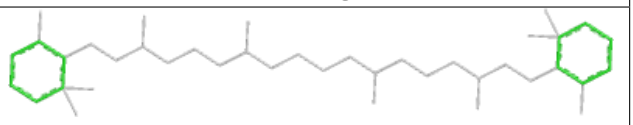
Bond lengths



Bond angles

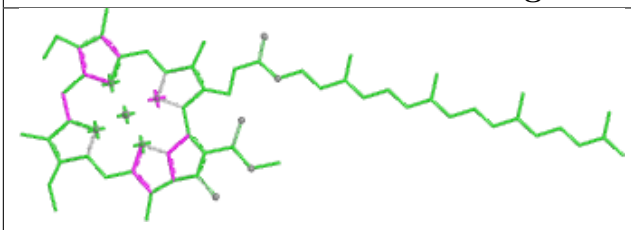


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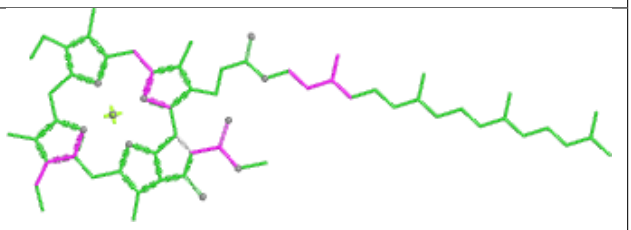


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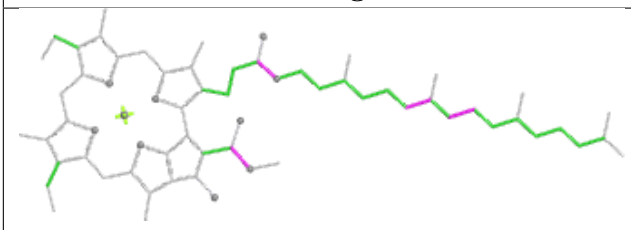
Ligand CLA C 512



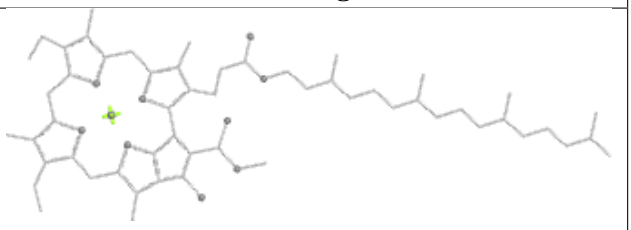
Bond lengths



Bond angles

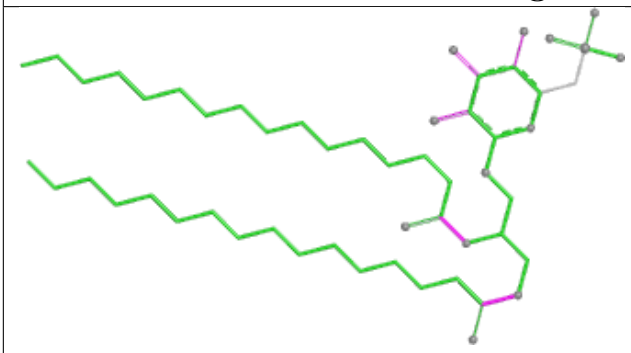


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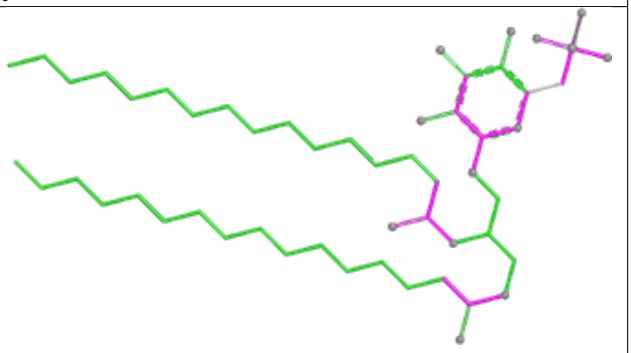


Rings

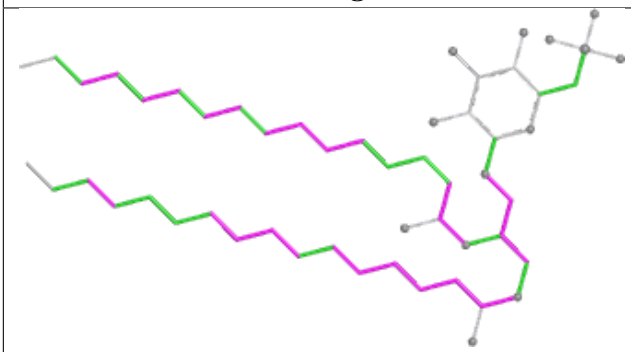
Ligand SQD a 411



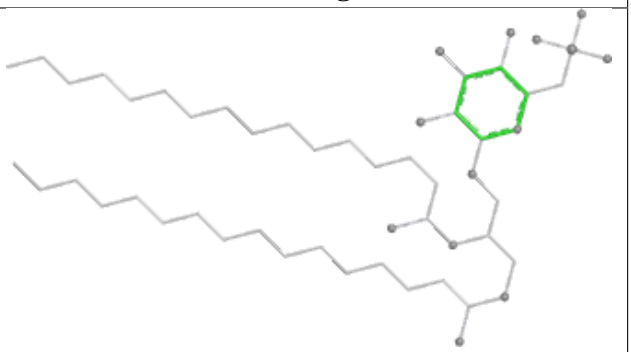
Bond lengths



Bond angles

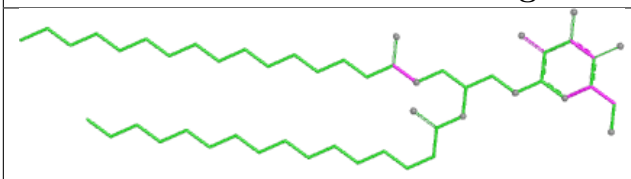


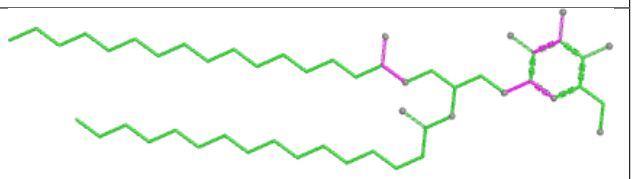
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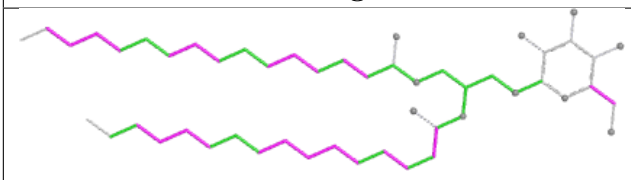


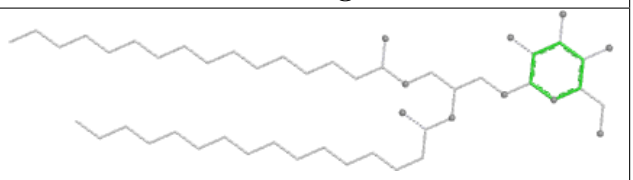
Rings

Ligand LMG D 407

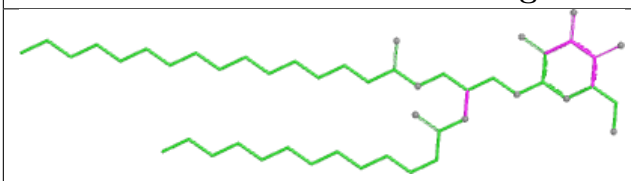

Bond lengths

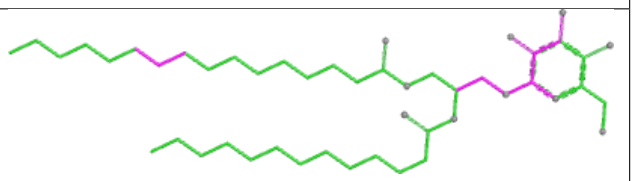

Bond angles

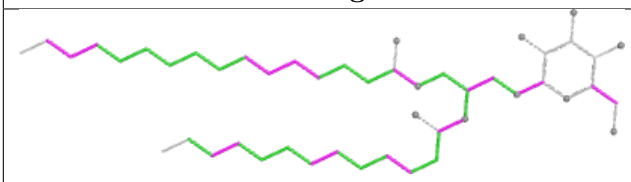

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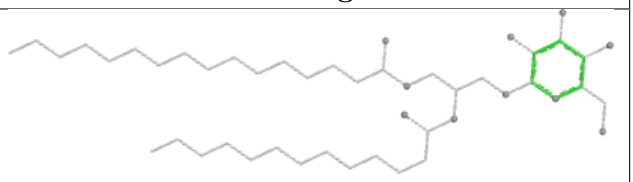

Rings

Ligand LMG C 519

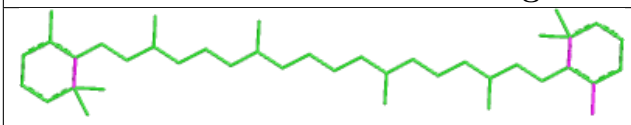

Bond lengths

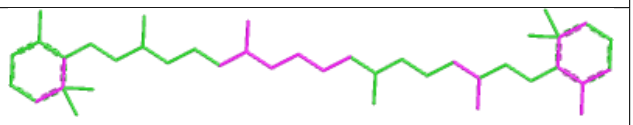

Bond angles

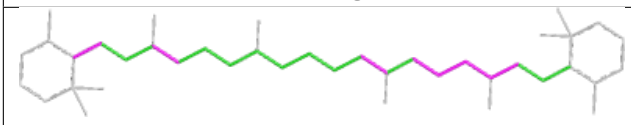

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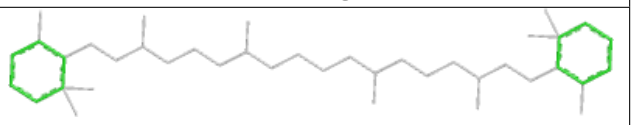

Rings

Ligand BCR C 520

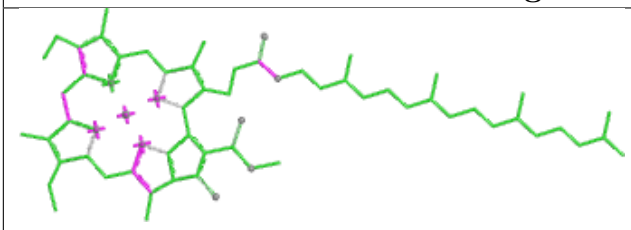

Bond lengths


Bond angles

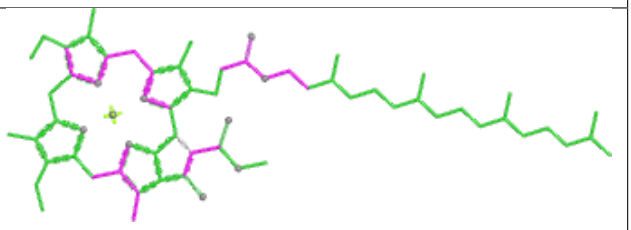

Torsions


Rings

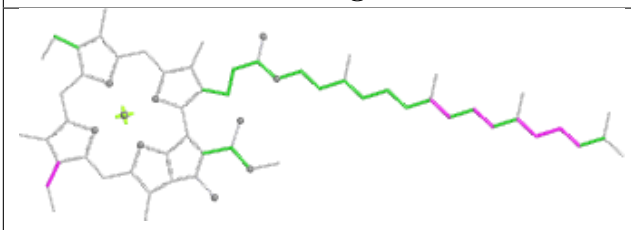
Ligand CLA B 604



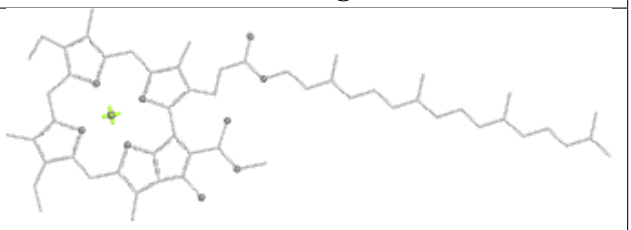
Bond lengths



Bond angles

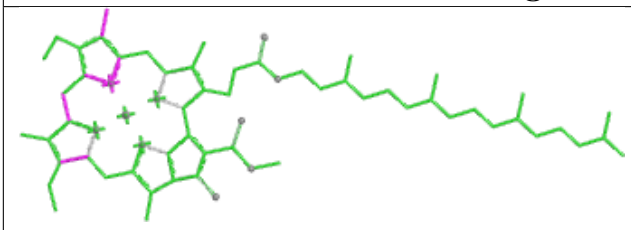


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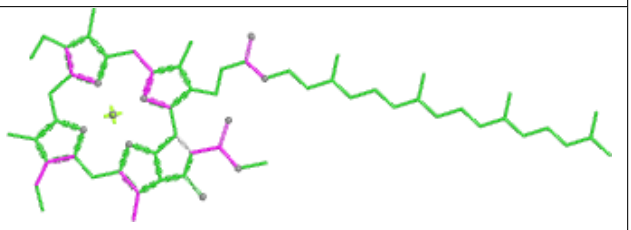


Rings

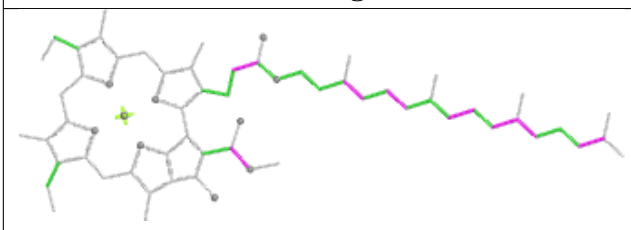
Ligand CLA C 506



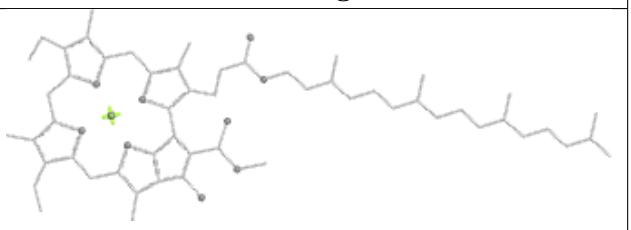
Bond lengths



Bond angles

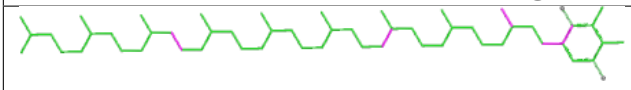


Torsions

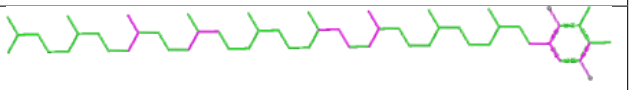


Rings

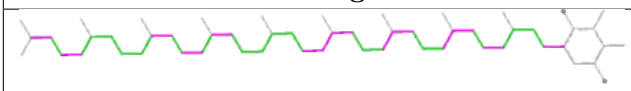
Ligand PL9 A 409



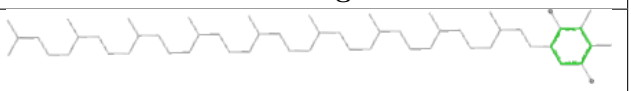
Bond lengths



Bond angles

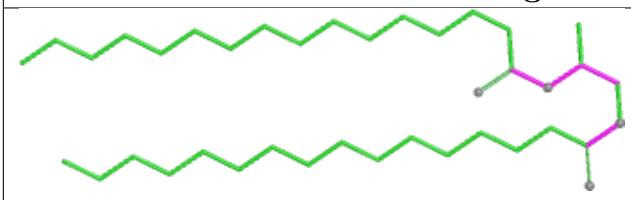


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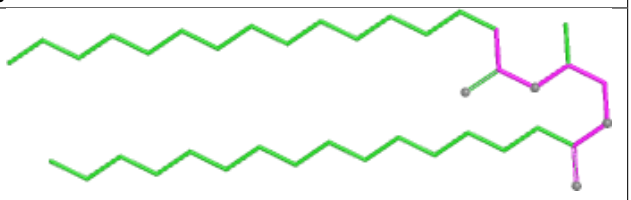


Rings

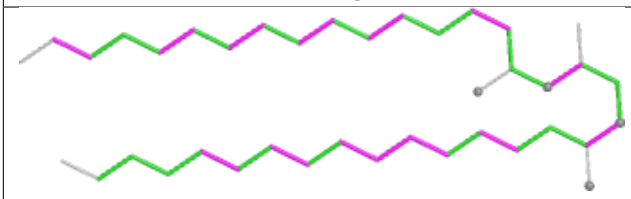
Ligand SQD A 411



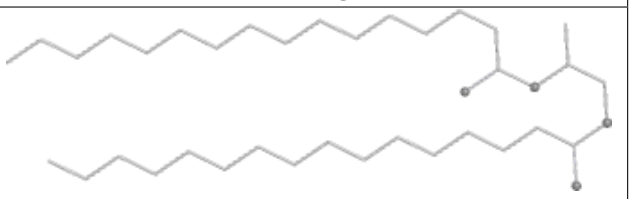
Bond lengths



Bond angles

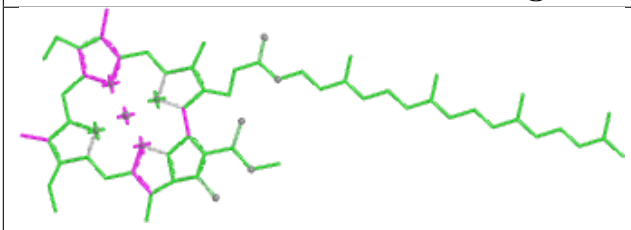


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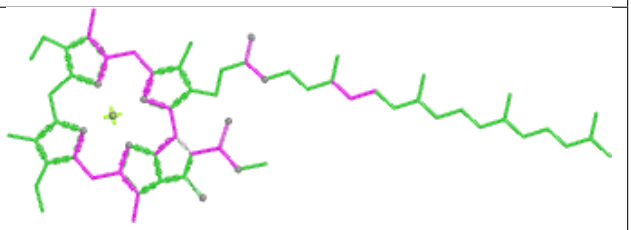


Rings

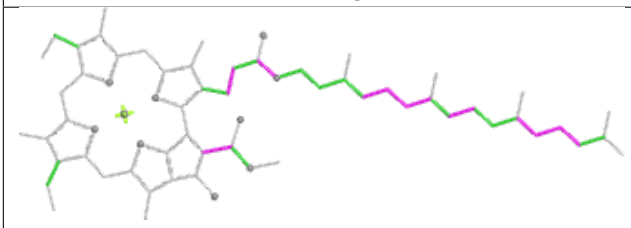
Ligand CLA b 615



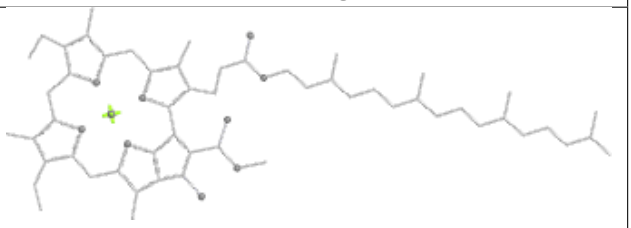
Bond lengths



Bond angles

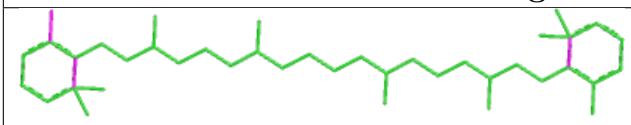


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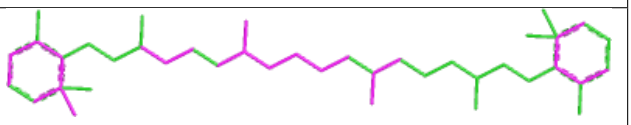


Rings

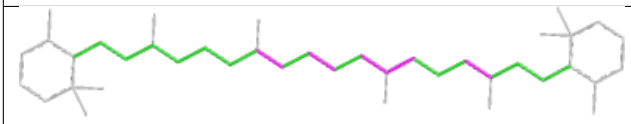
Ligand BCR t 101



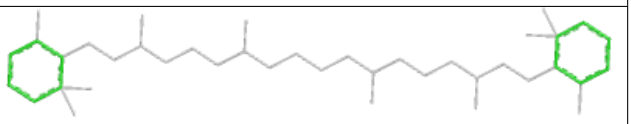
Bond lengths



Bond angles

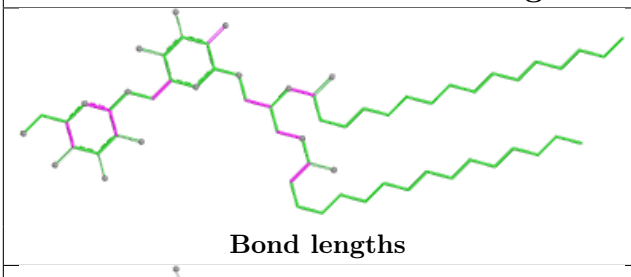


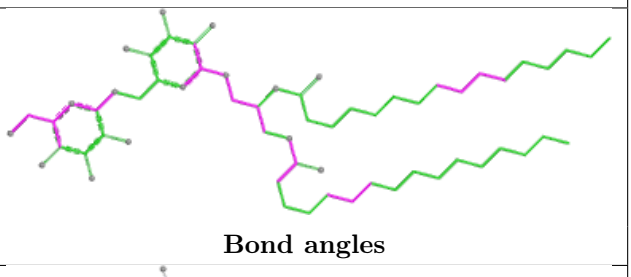
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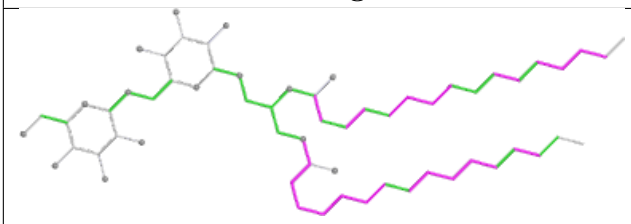


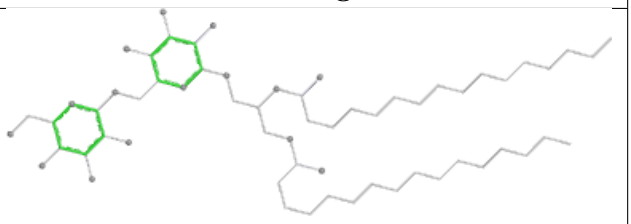
Rings

Ligand DGD c 518

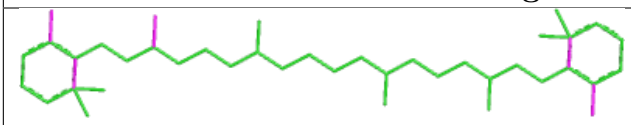

Bond lengths

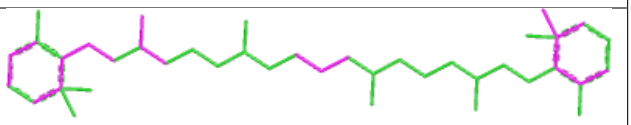

Bond angles

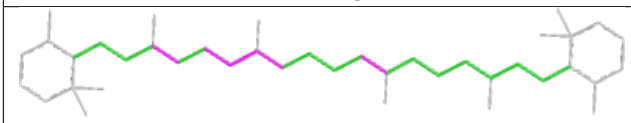

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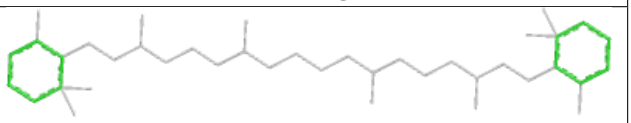

Rings

Ligand BCR C 515

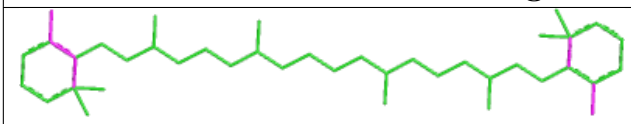

Bond lengths

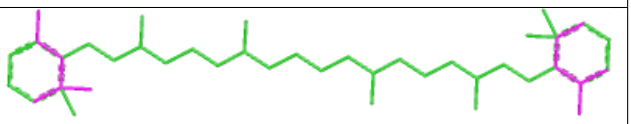

Bond angles


Torsions

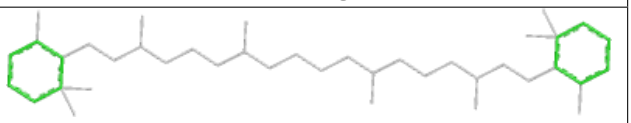

Rings

Ligand BCR b 618

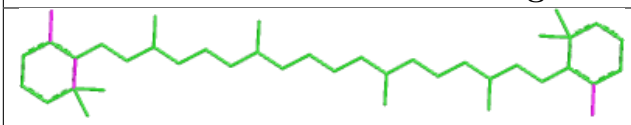

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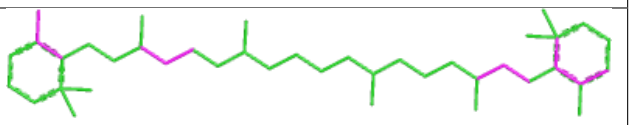

Bond angles

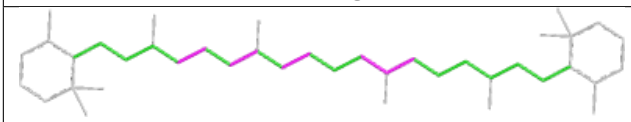

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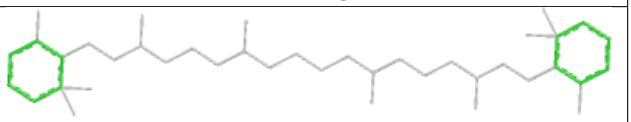

Rings

Ligand BCR c 521

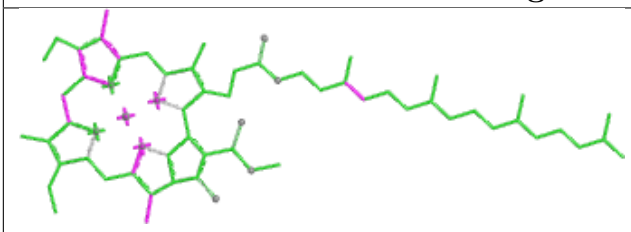

Bond lengths


Bond angles

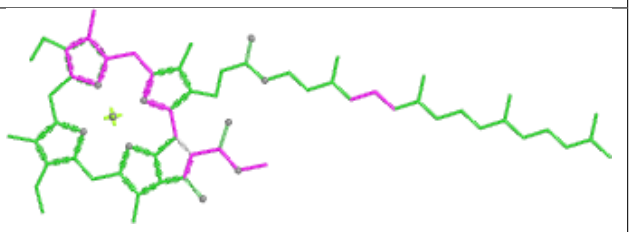

Torsions


Rings

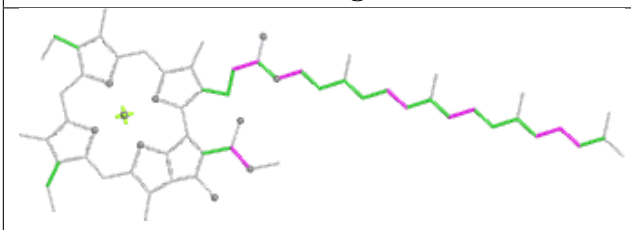
Ligand CLA b 614



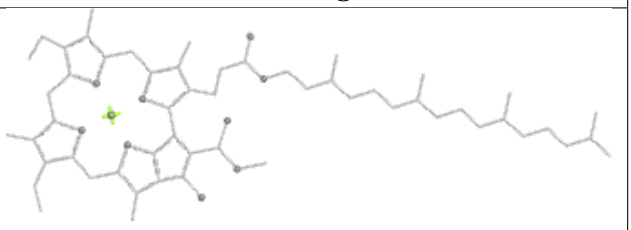
Bond lengths



Bond angles



Torsions



Rings

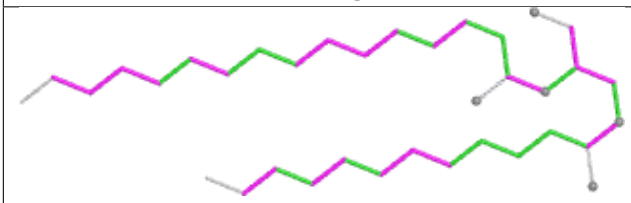
Ligand SQD a 412



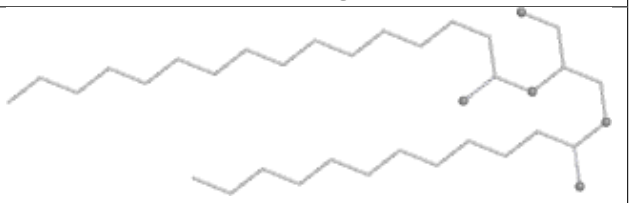
Bond lengths



Bond angles

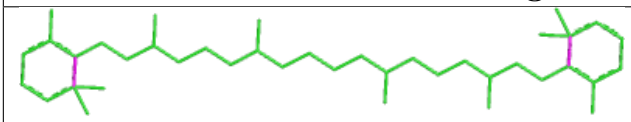


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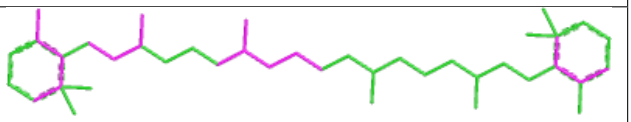


Rings

Ligand BCR x 102



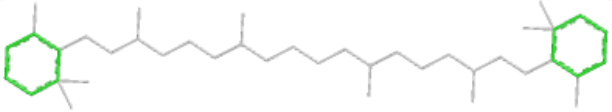
Bond lengths



Bond angles

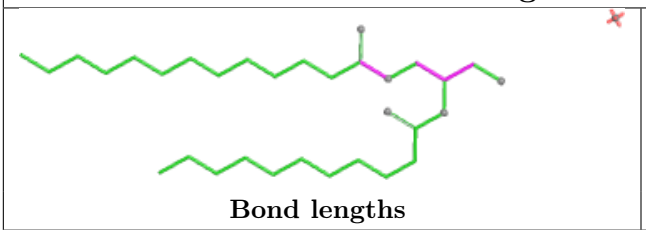


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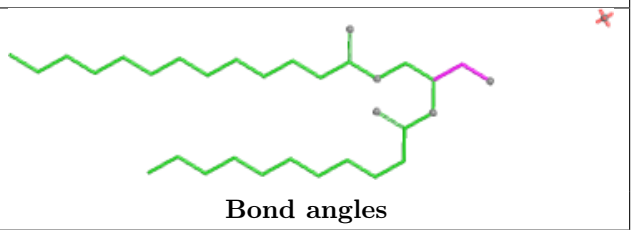


Rings

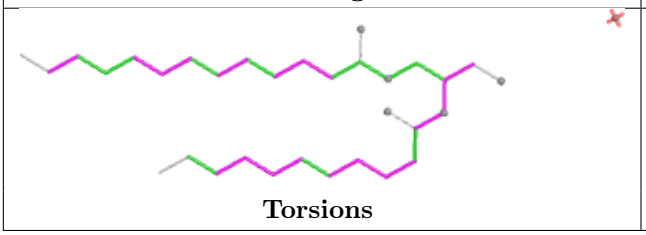
Ligand LMG D 410



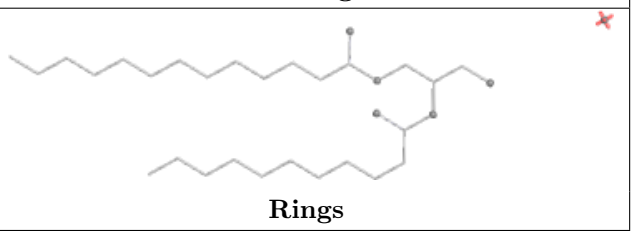
Bond lengths



Bond angles

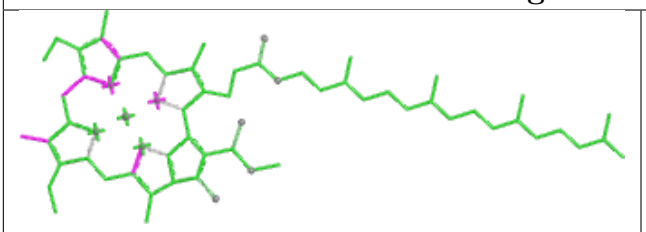


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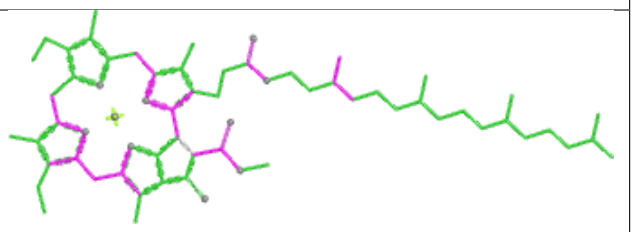


Rings

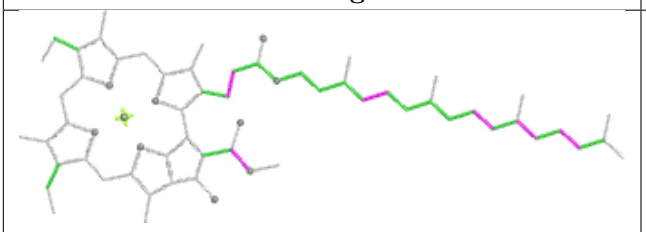
Ligand CLA b 607



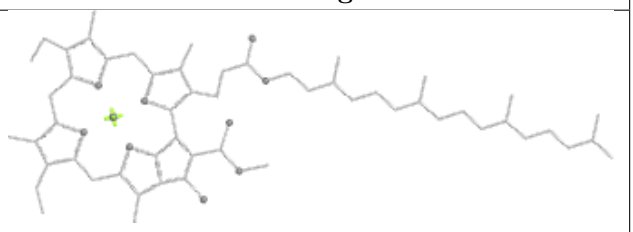
Bond lengths



Bond angles

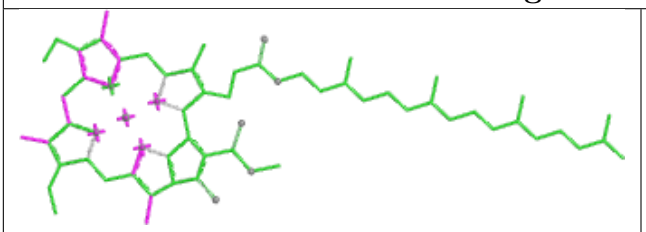


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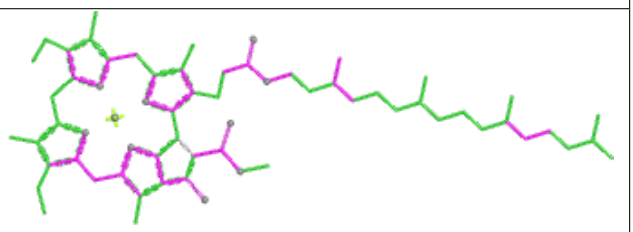


Rings

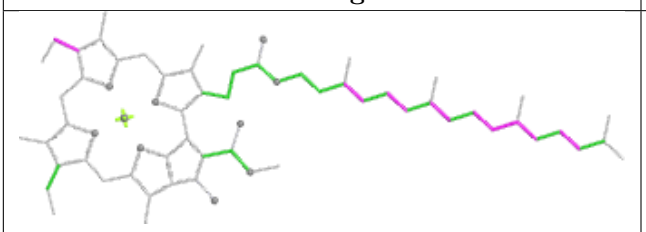
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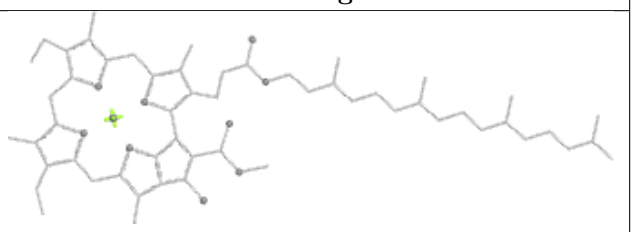
Bond lengths



Bond angles

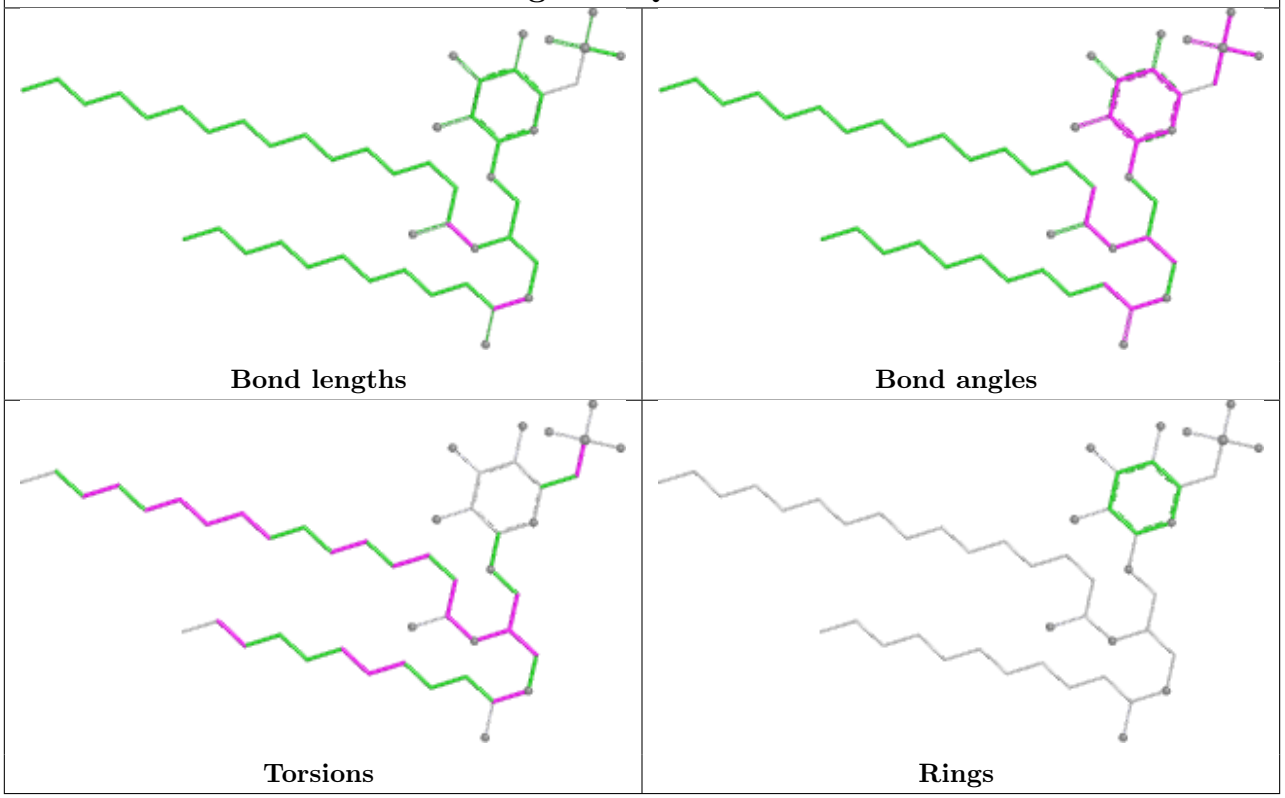


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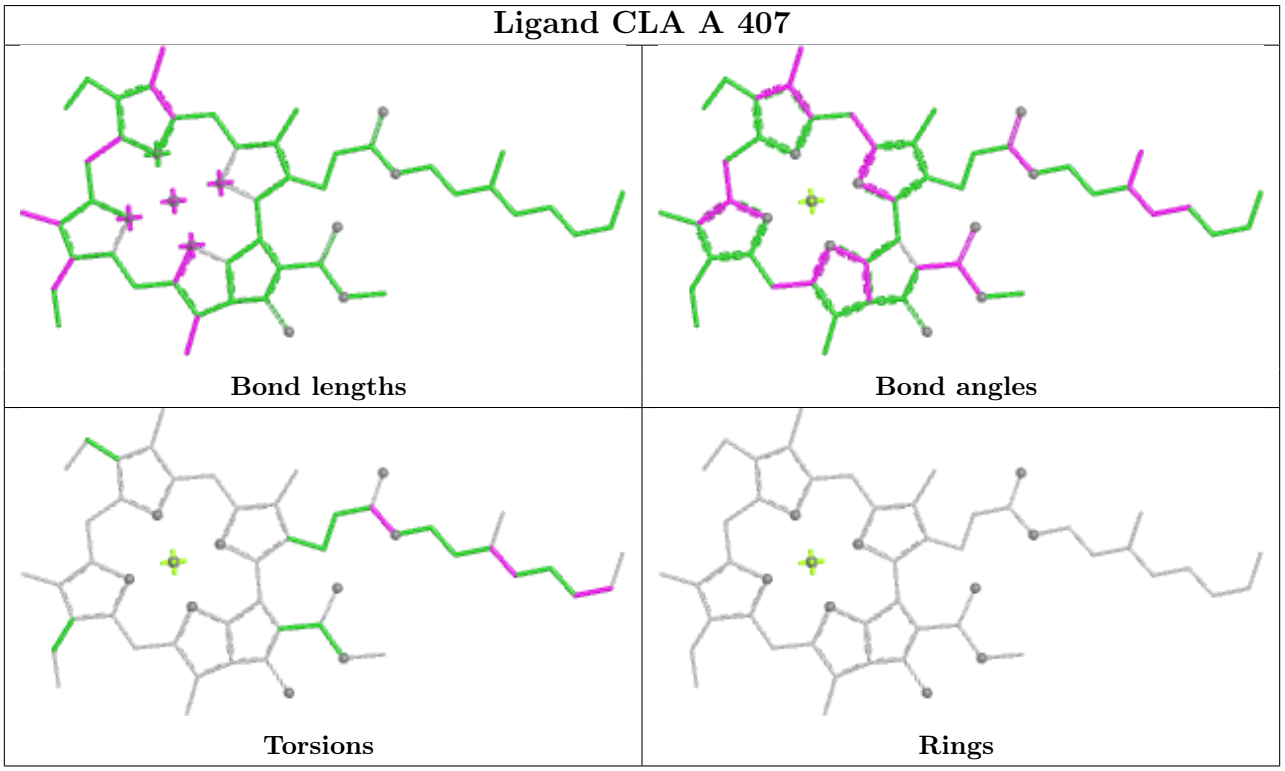


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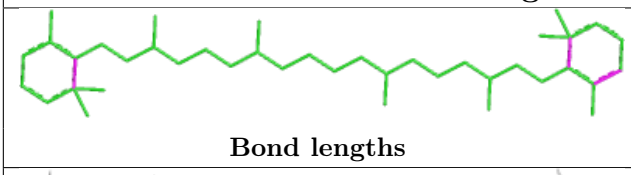
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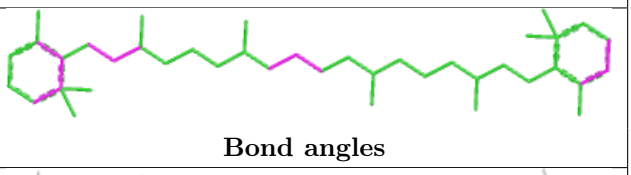
Ligand CLA A 407



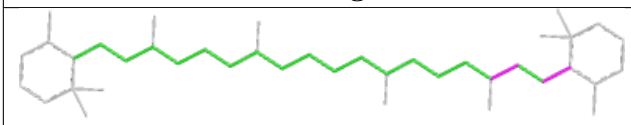
Ligand BCR D 405



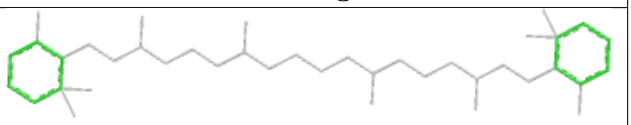
Bond lengths



Bond angles

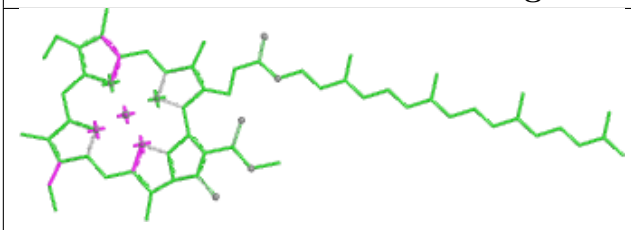


Torsions

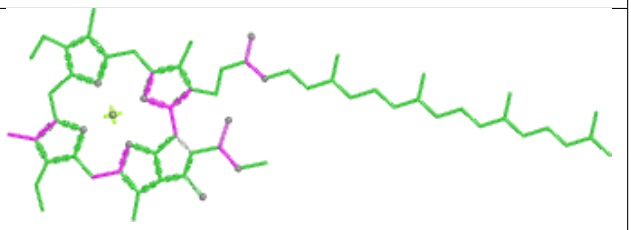


Rings

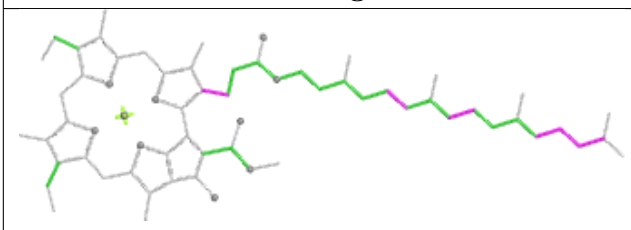
Ligand CLA B 607



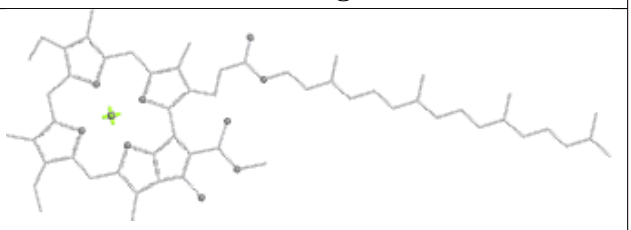
Bond lengths



Bond angles

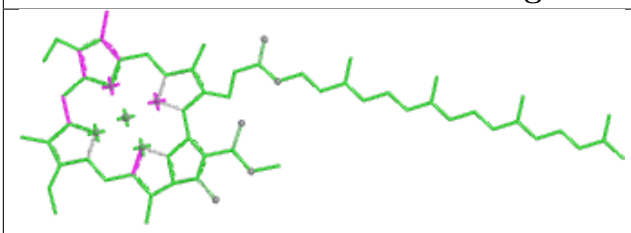


Torsions

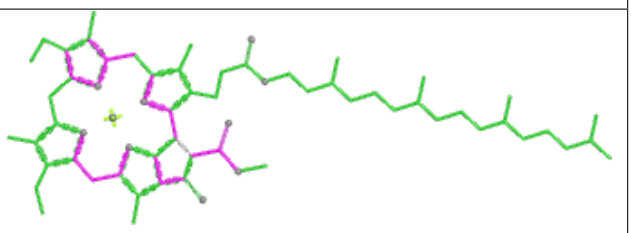


Rings

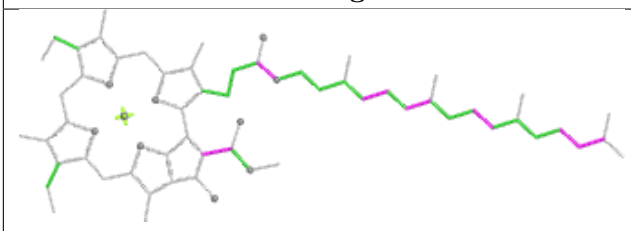
Ligand CLA C 503



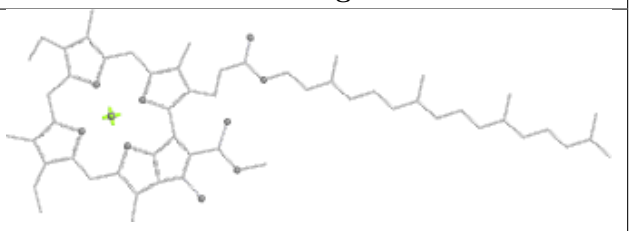
Bond lengths



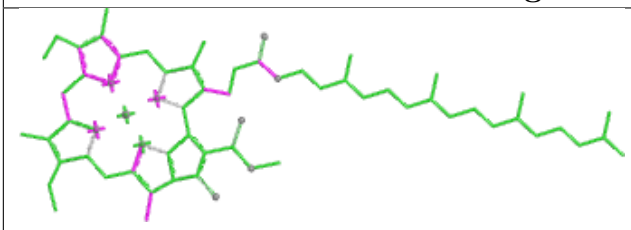
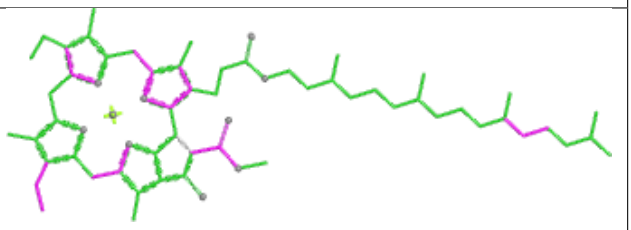
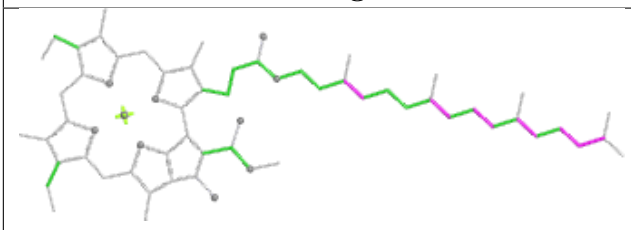
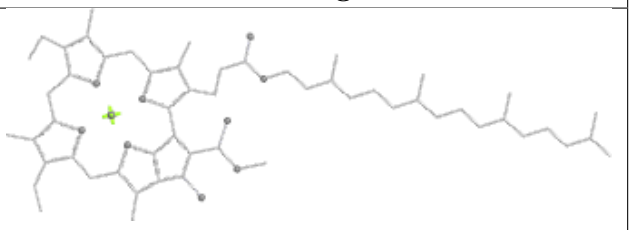
Bond angles

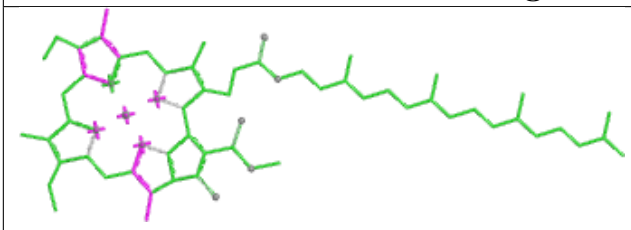
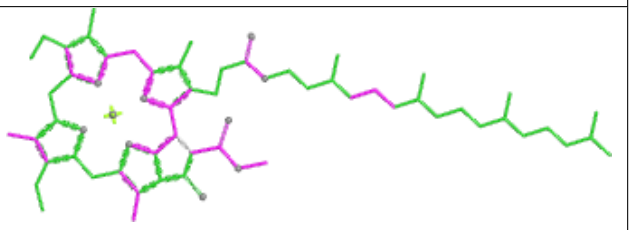
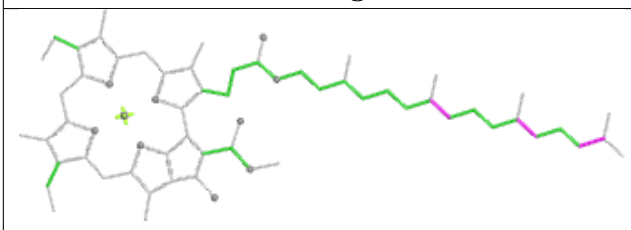
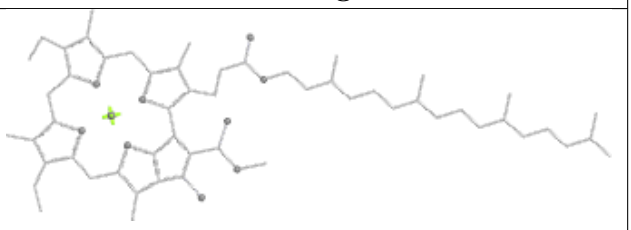


Torsions

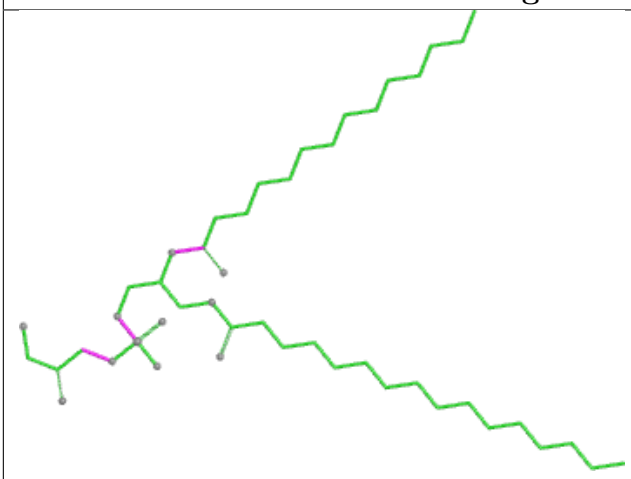


Rings

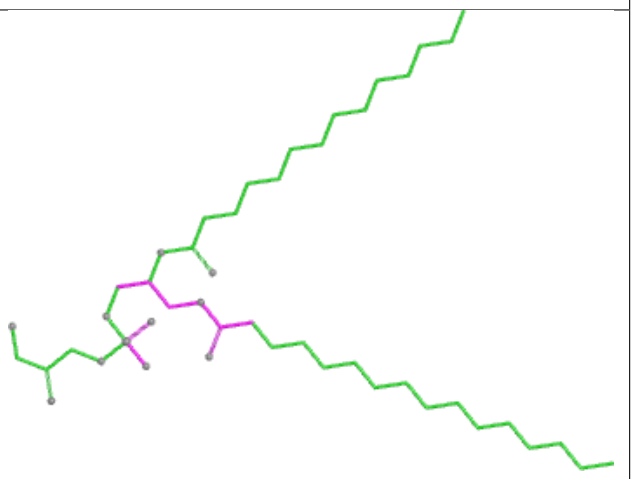
Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

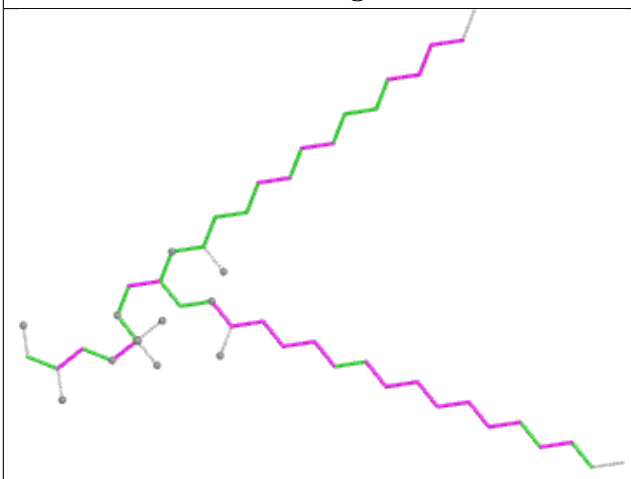
Ligand LHG D 409



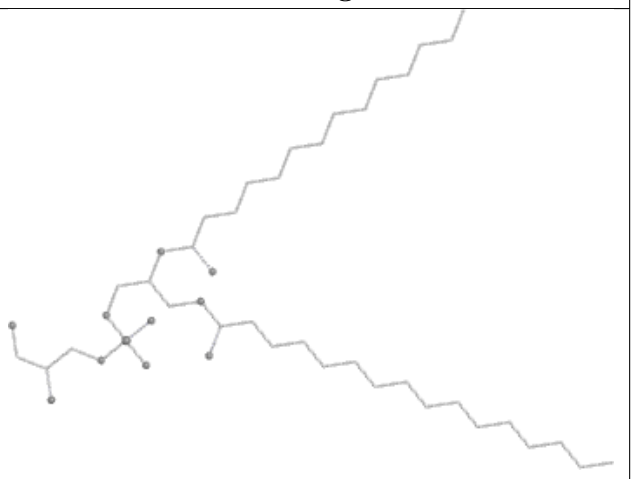
Bond lengths



Bond angles

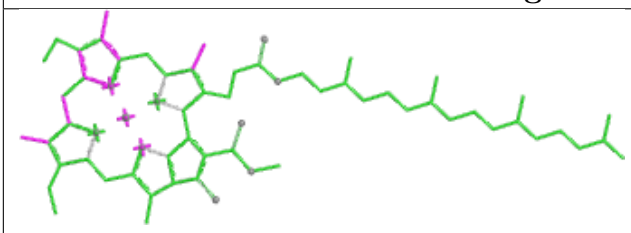


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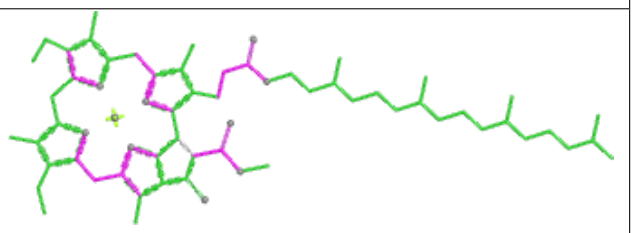


Rings

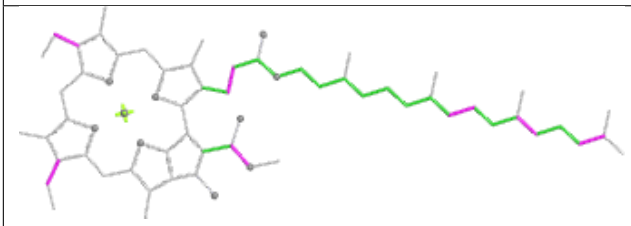
Ligand CLA B 610



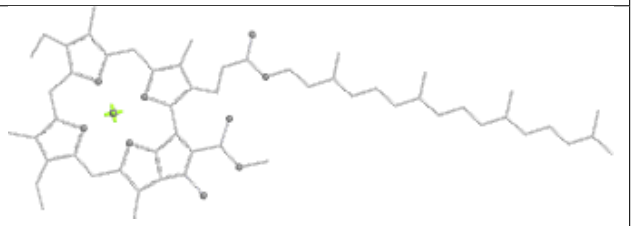
Bond lengths



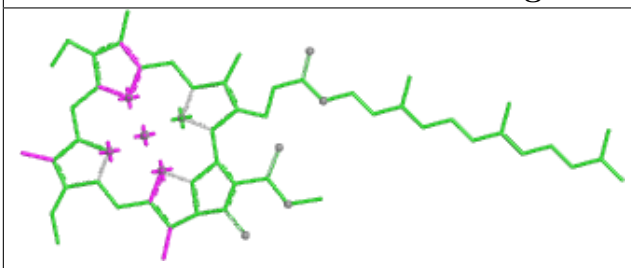
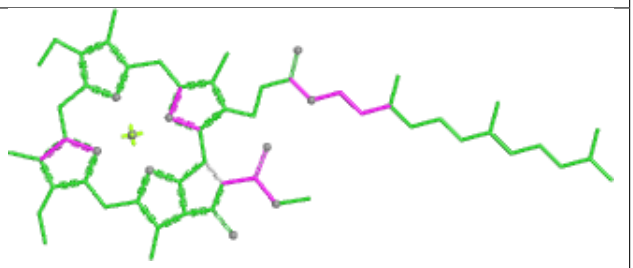
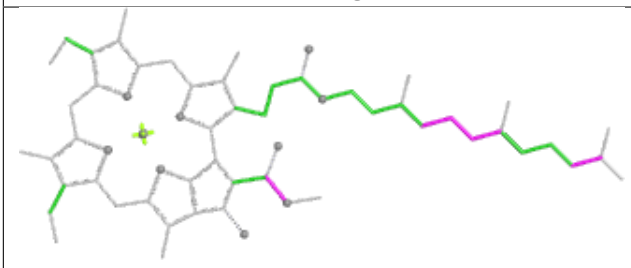
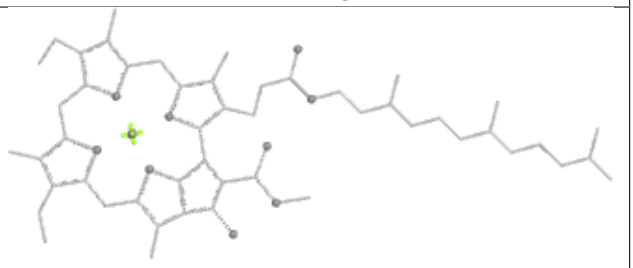
Bond angles

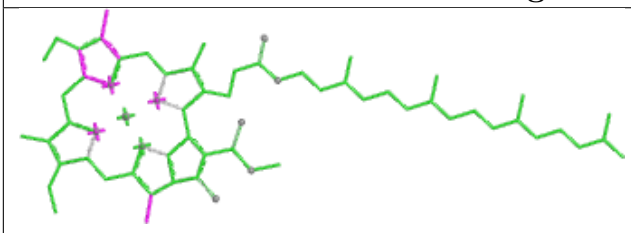
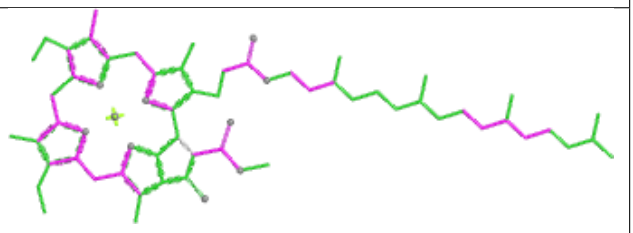
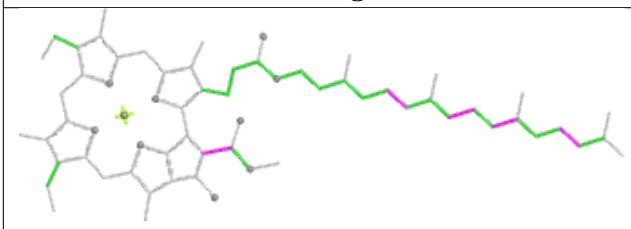
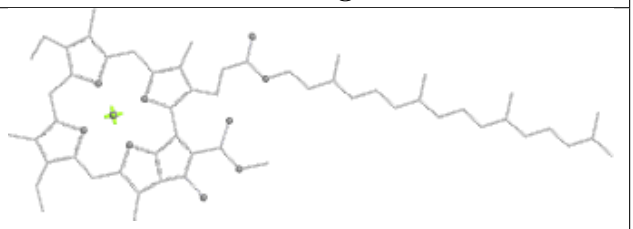


Torsions

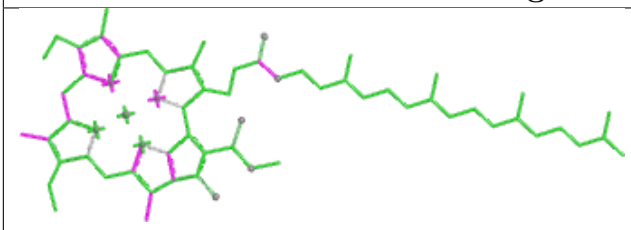


Rings

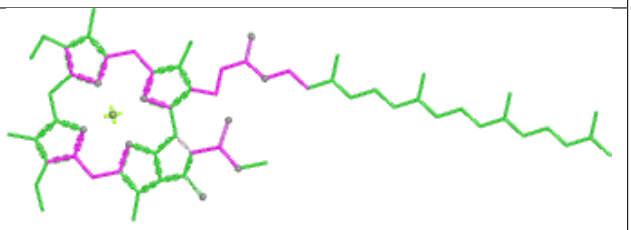
Ligand CLA B 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

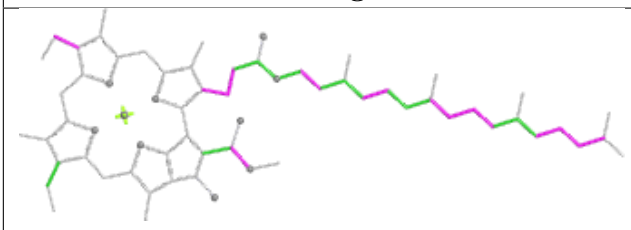
Ligand CLA b 602



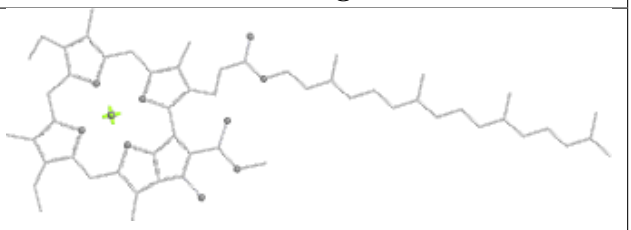
Bond lengths



Bond angles

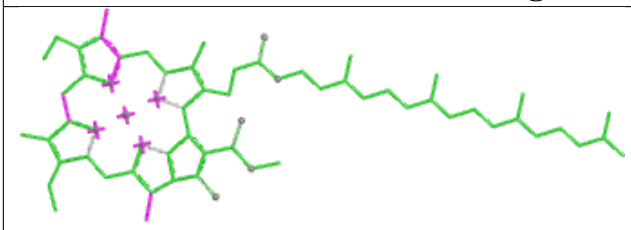


Torsions

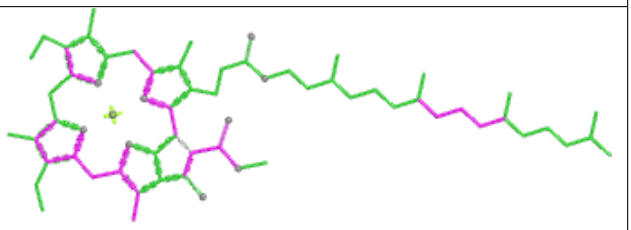


Rings

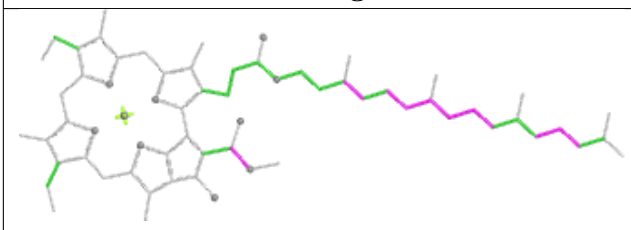
Ligand CLA b 612



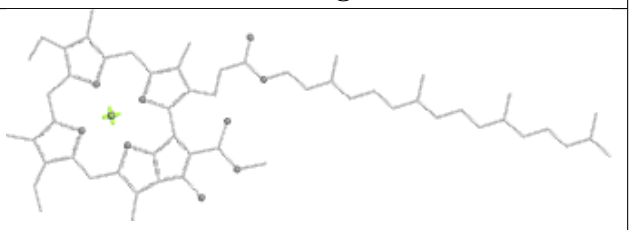
Bond lengths



Bond angles

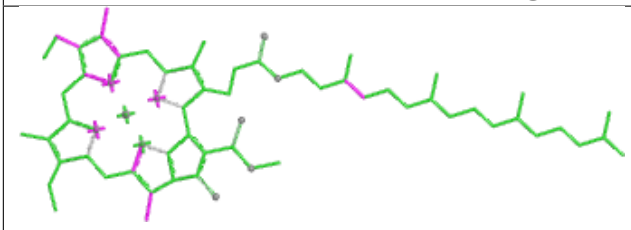


Torsions

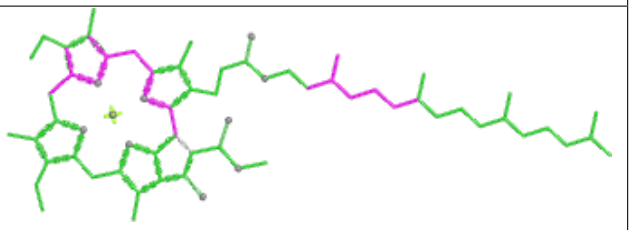


Rings

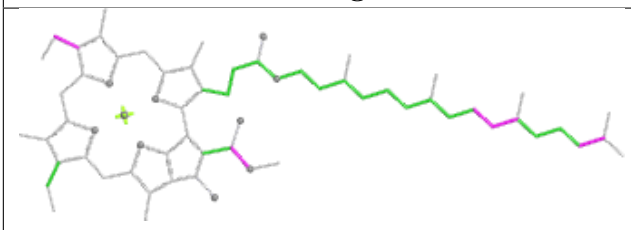
Ligand CLA B 615



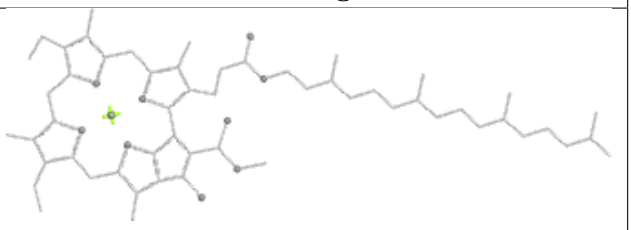
Bond lengths



Bond angles

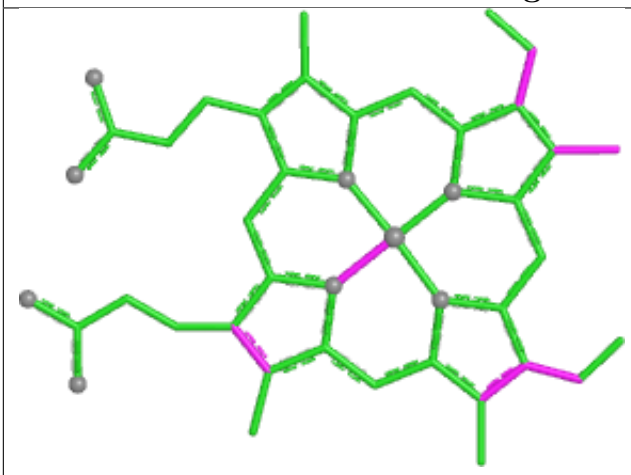


Torsions

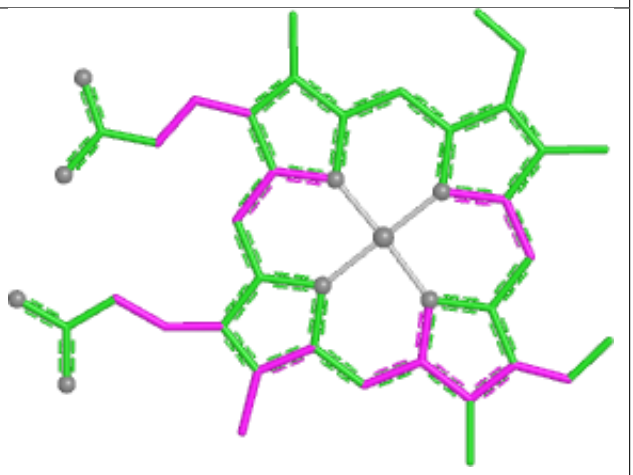


Rings

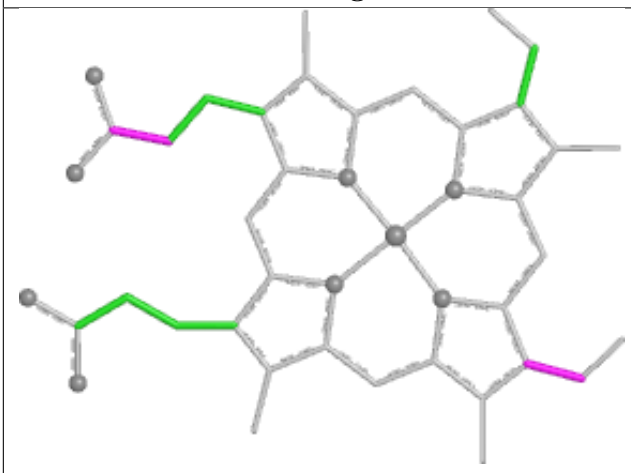
Ligand HEM e 102



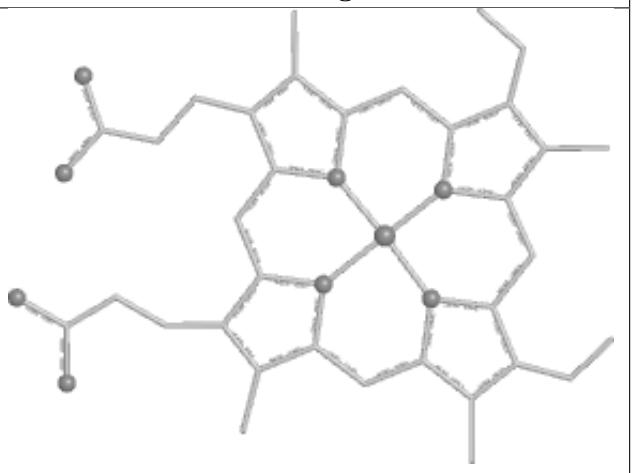
Bond lengths



Bond angles

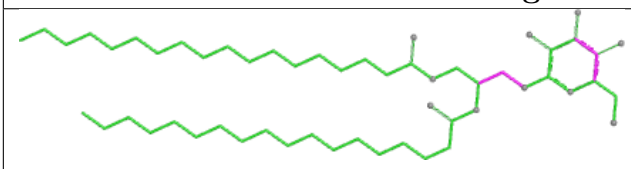


Torsions

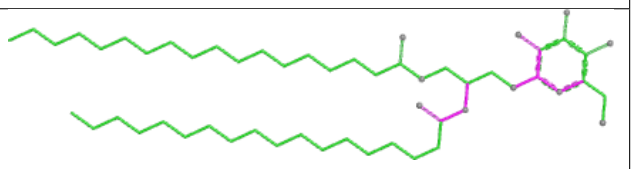


Rings

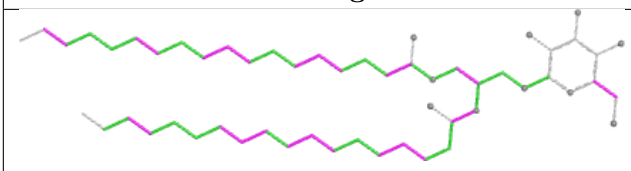
Ligand LMG b 622



Bond lengths



Bond angles

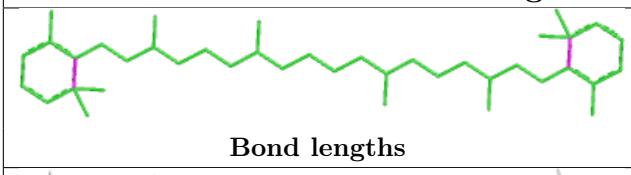


Torsions

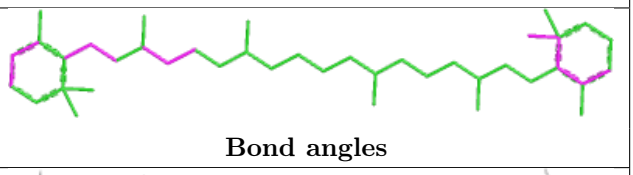


Rings

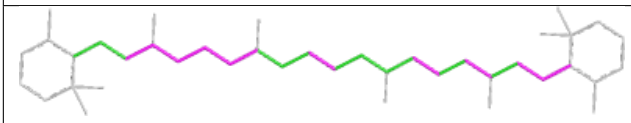
Ligand BCR b 619



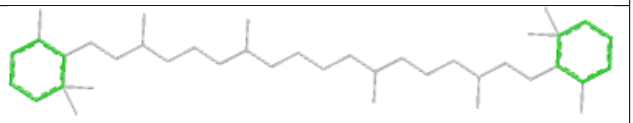
Bond lengths



Bond angles

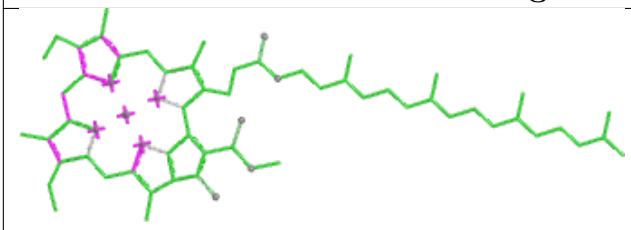


Torsions

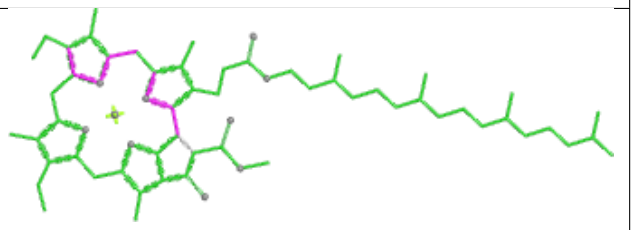


Rings

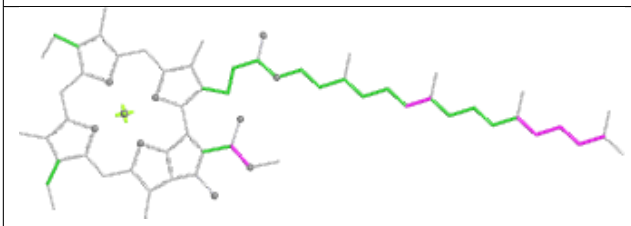
Ligand CLA c 511



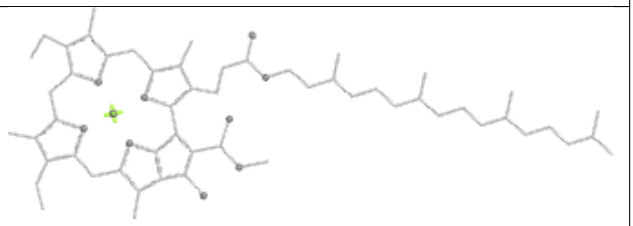
Bond lengths



Bond angles

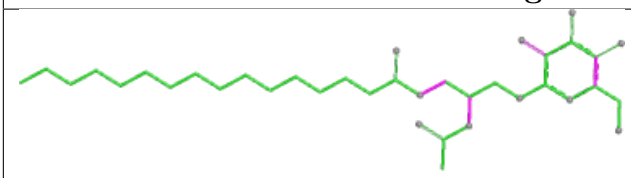


Torsions

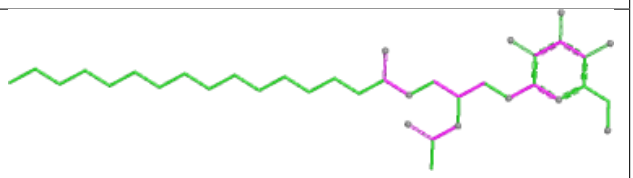


Rings

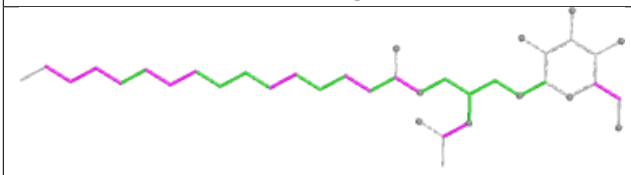
Ligand LMG c 519



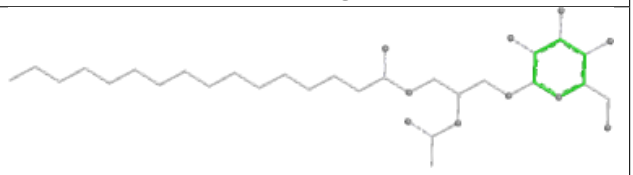
Bond lengths



Bond angles

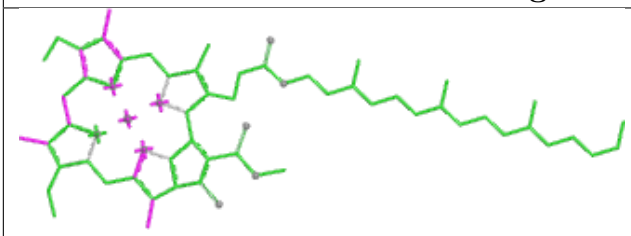


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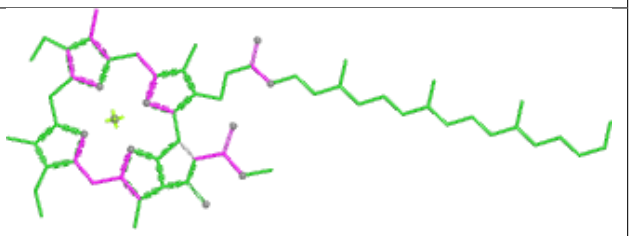


Rings

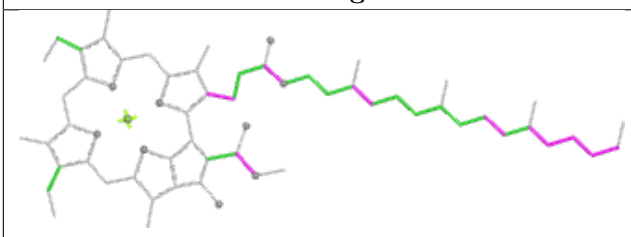
Ligand CLA c 508



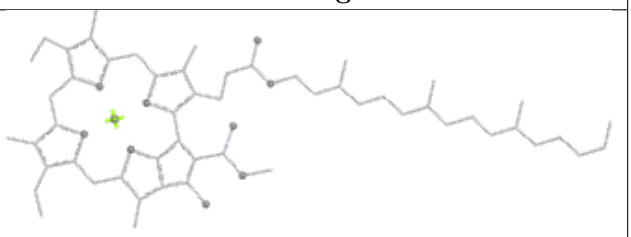
Bond lengths



Bond angles

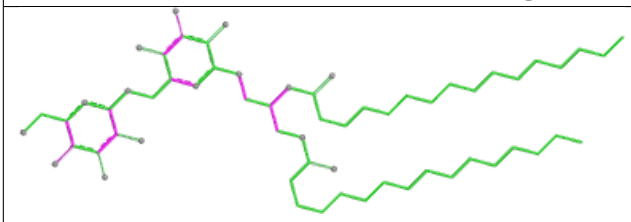


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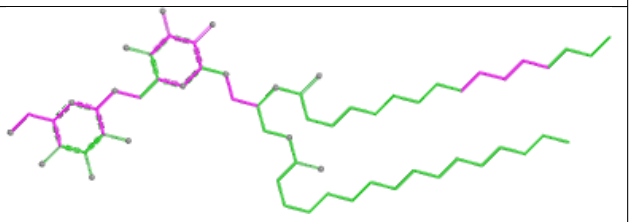


Rings

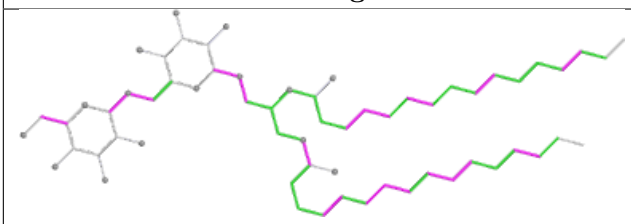
Ligand DGD C 517



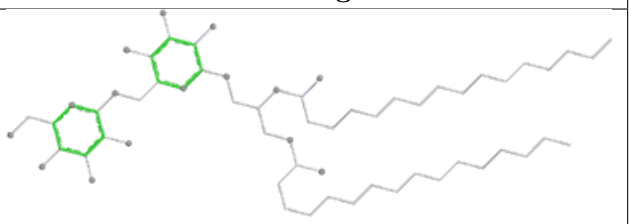
Bond lengths



Bond angles

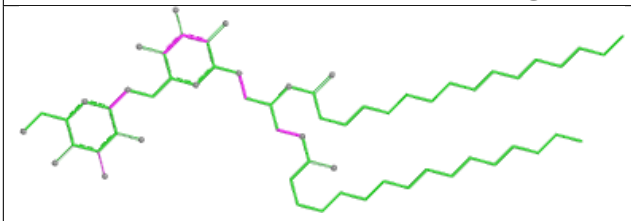


Torsions

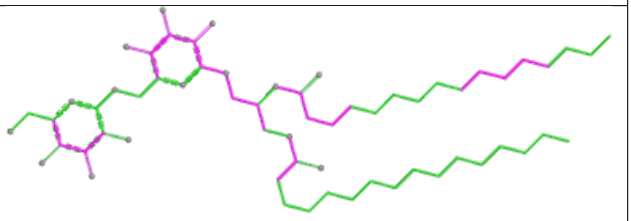


Rings

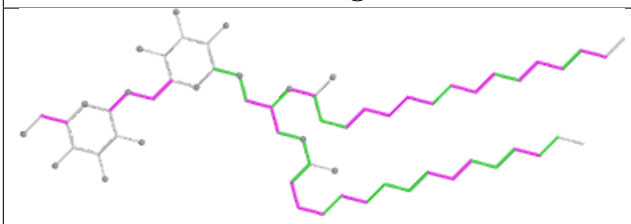
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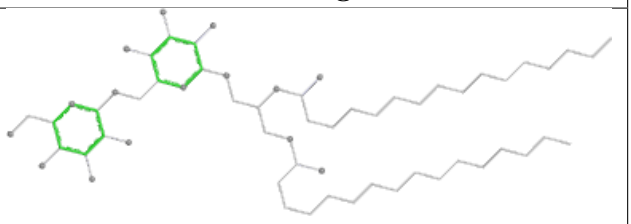
Bond lengths



Bond angles

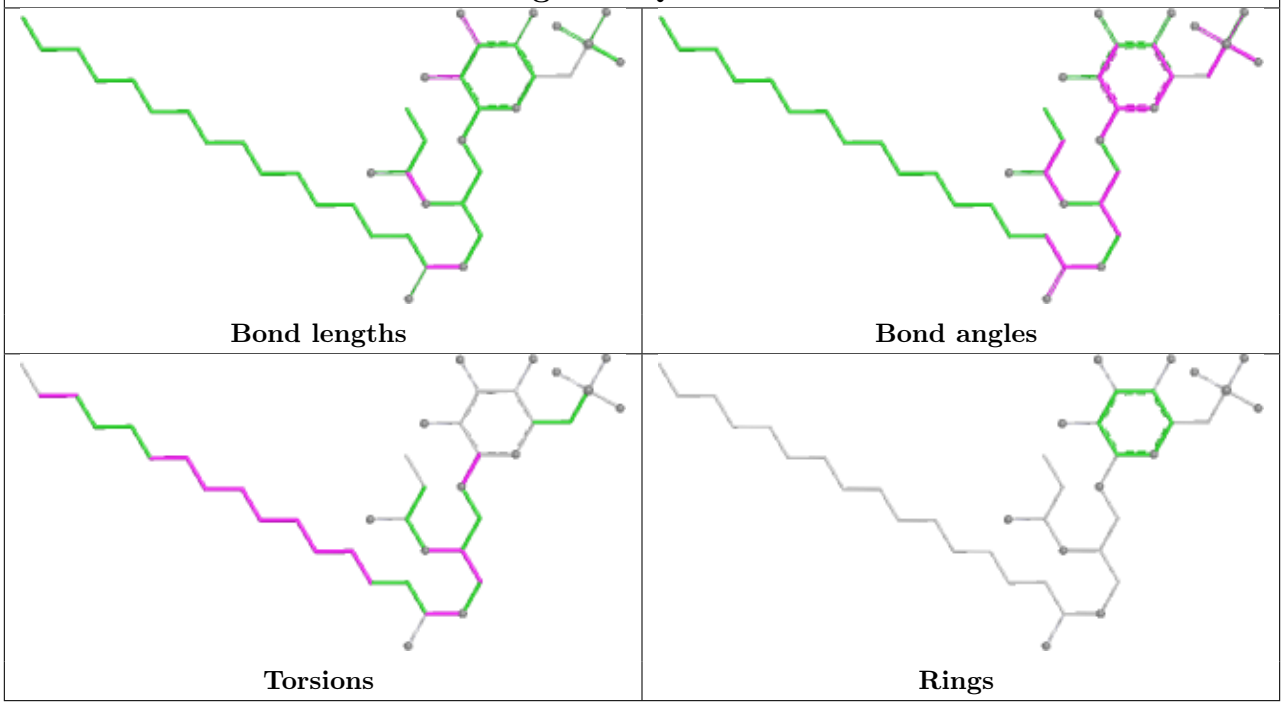


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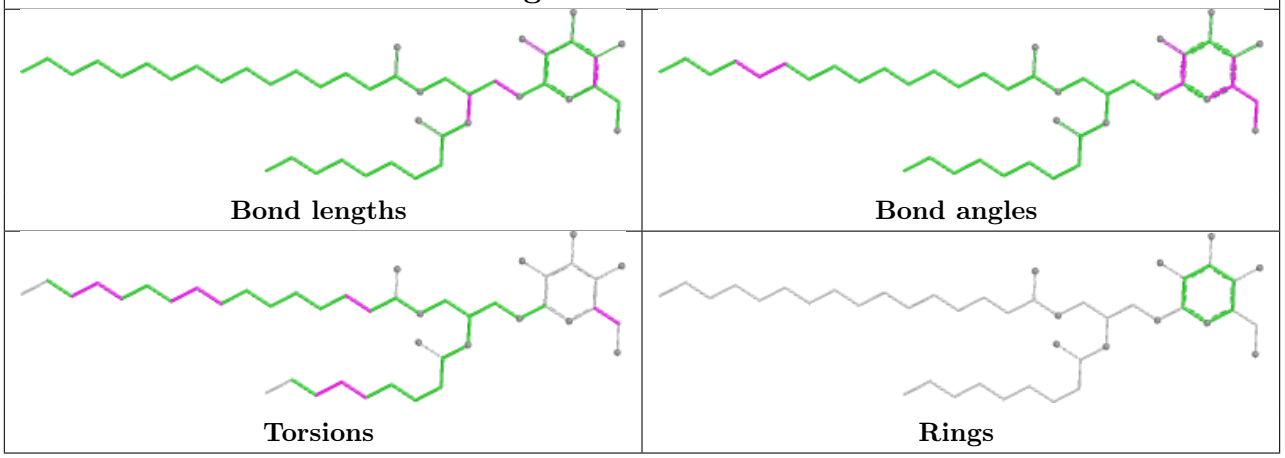


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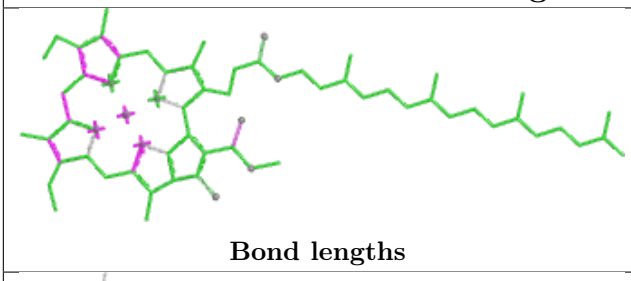
Ligand SQD f 101



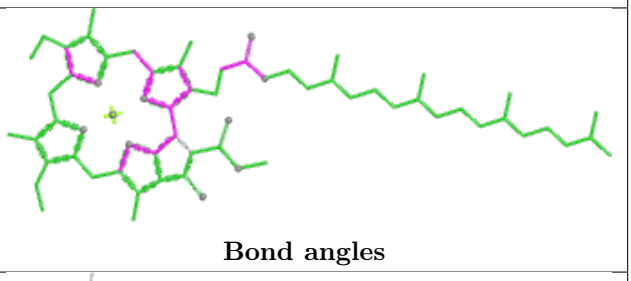
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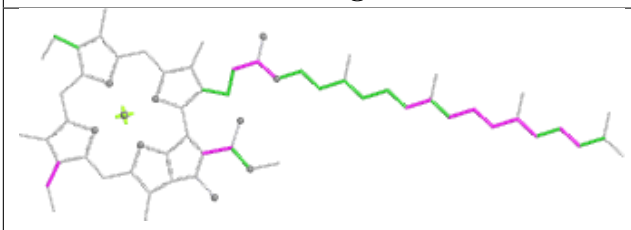
Ligand CLA c 509



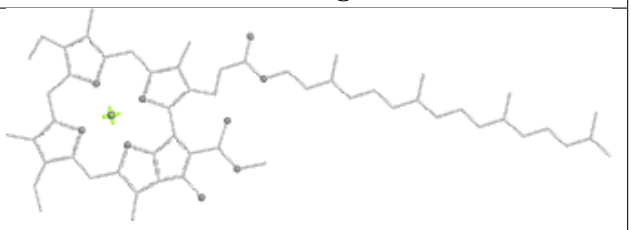
Bond lengths



Bond angles

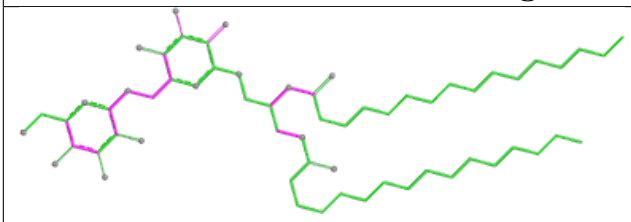


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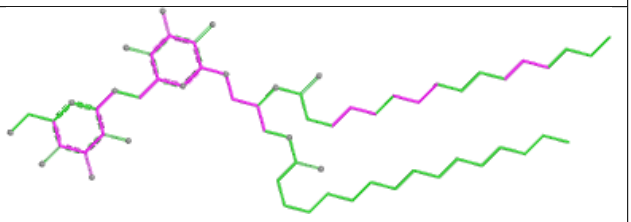


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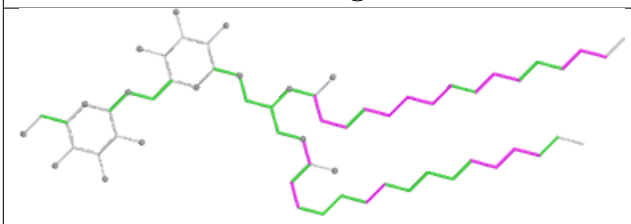
Ligand DGD H 102



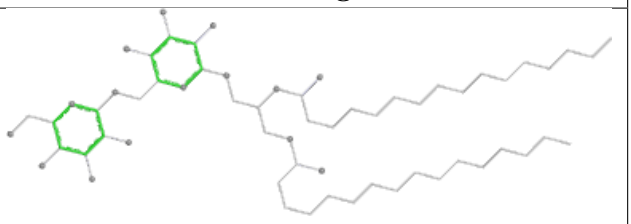
Bond lengths



Bond angles

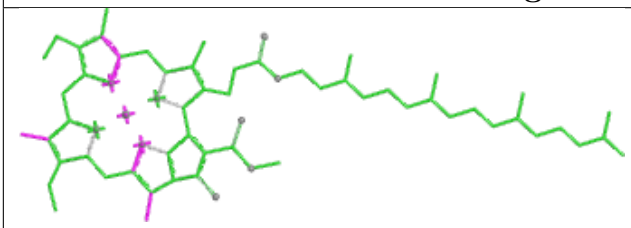


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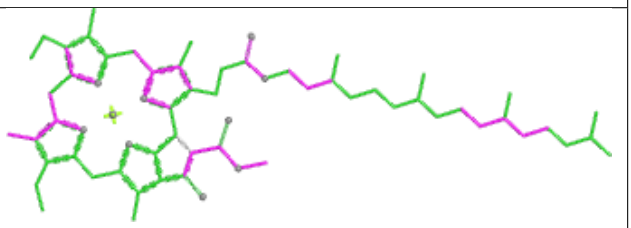


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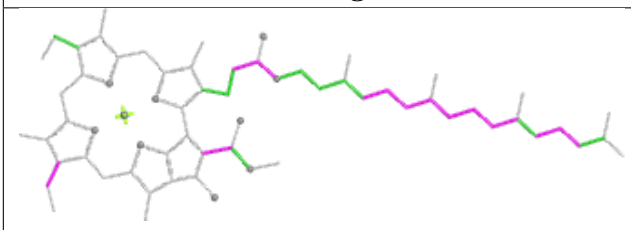
Ligand CLA B 612



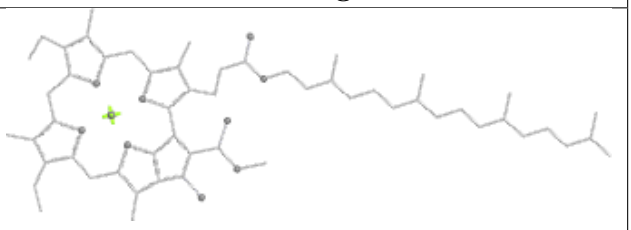
Bond lengths



Bond angles

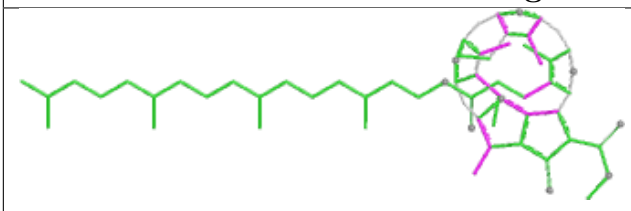


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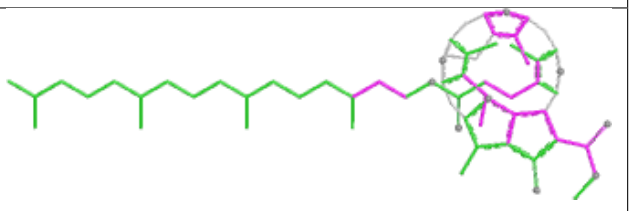


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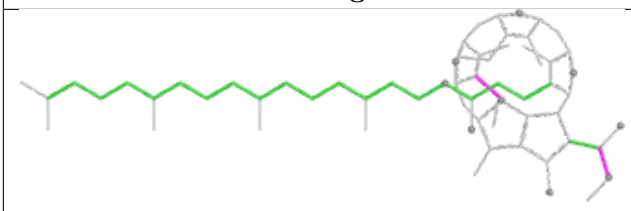
Ligand PHO d 401



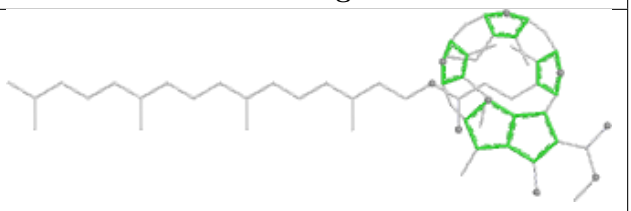
Bond lengths



Bond angles



Torsions



Rings

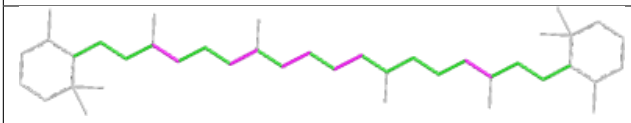
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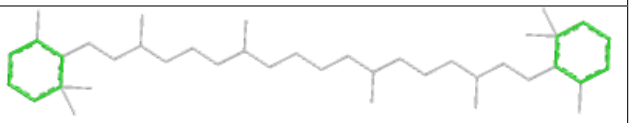
Bond lengths



Bond angles

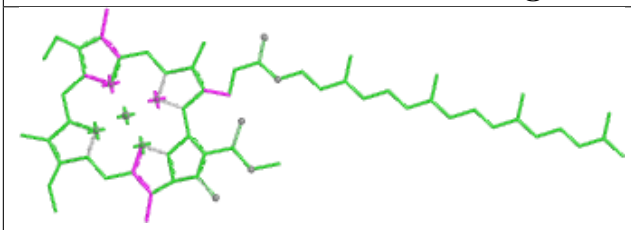


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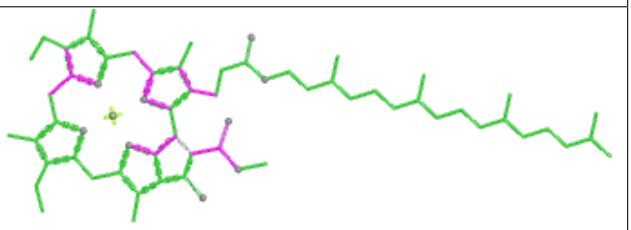


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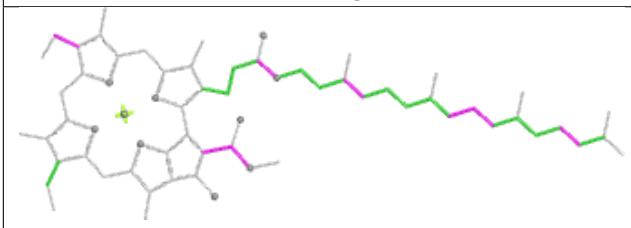
Ligand CLA B 601



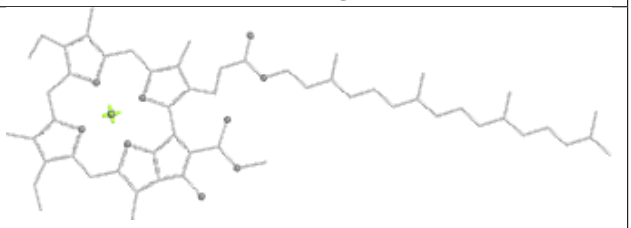
Bond lengths



Bond angles

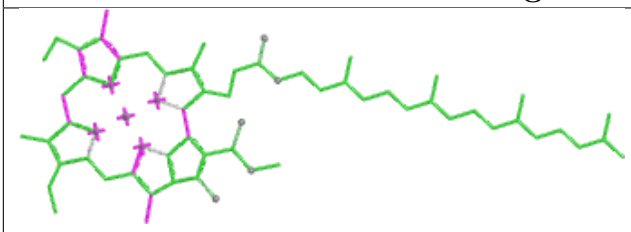


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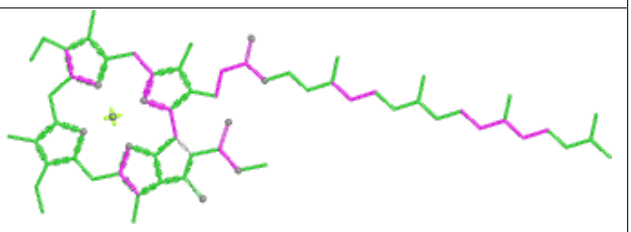


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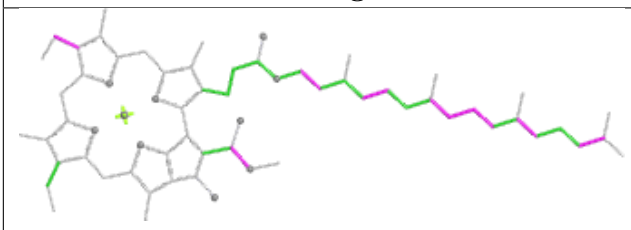
Ligand CLA C 513



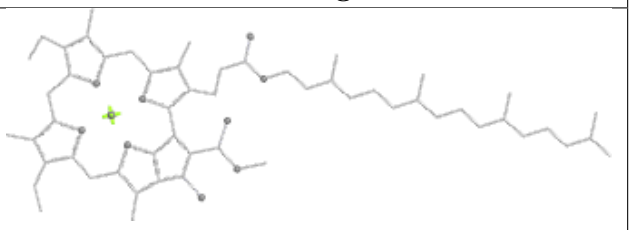
Bond lengths



Bond angles



Torsions

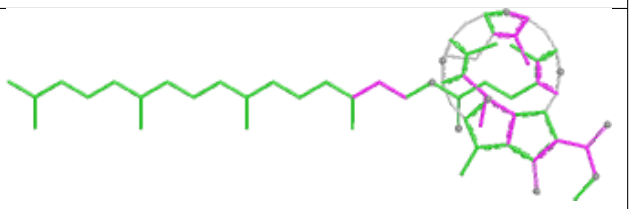


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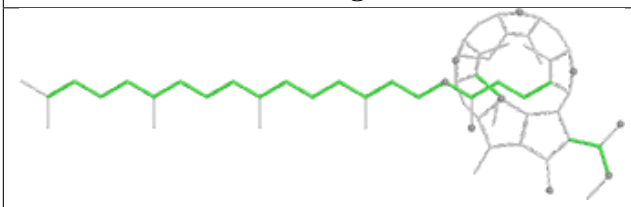
Ligand PHO D 401



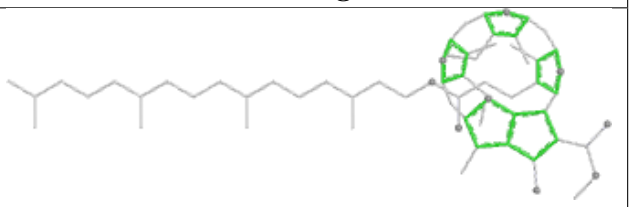
Bond lengths



Bond angles

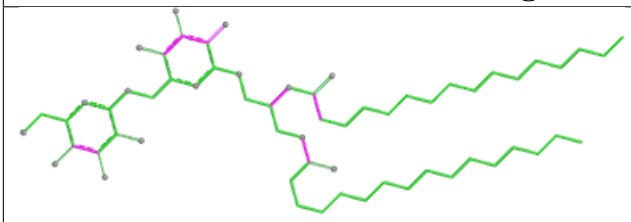


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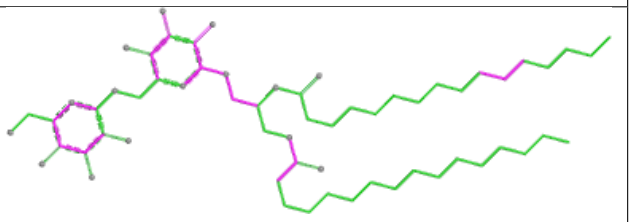


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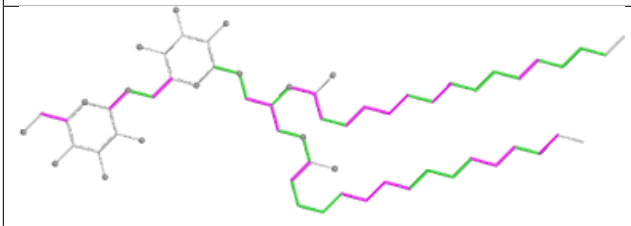
Ligand DGD C 516



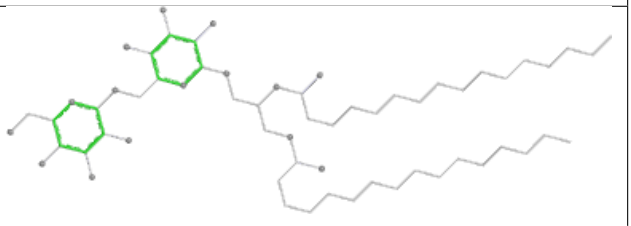
Bond lengths



Bond angles

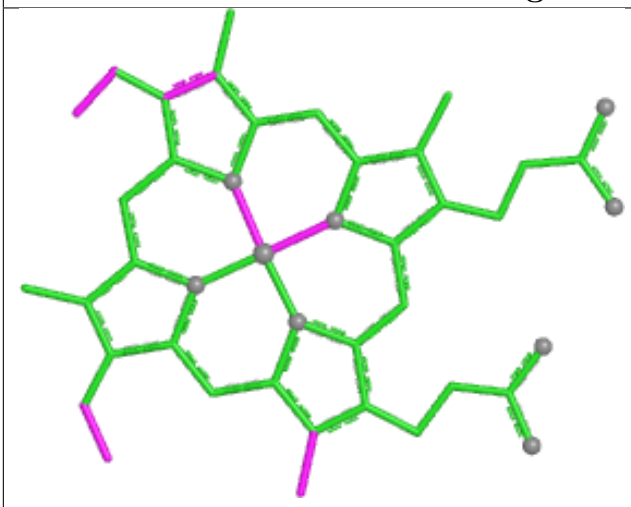


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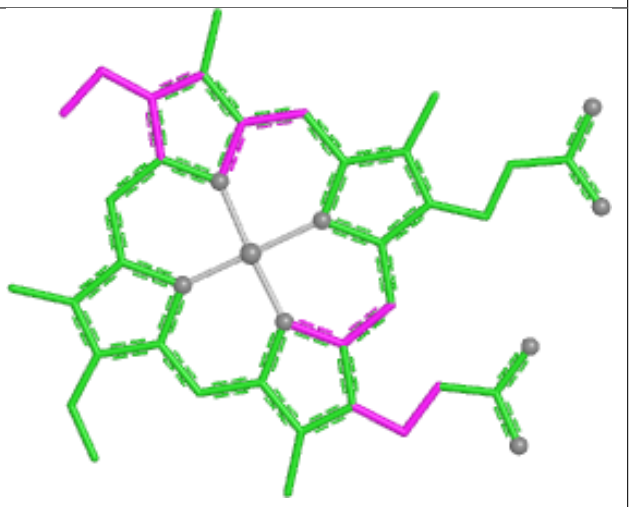


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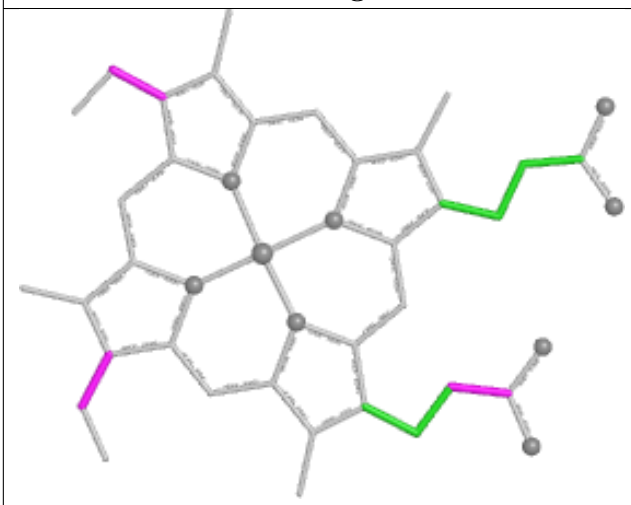
Ligand HEC v 201



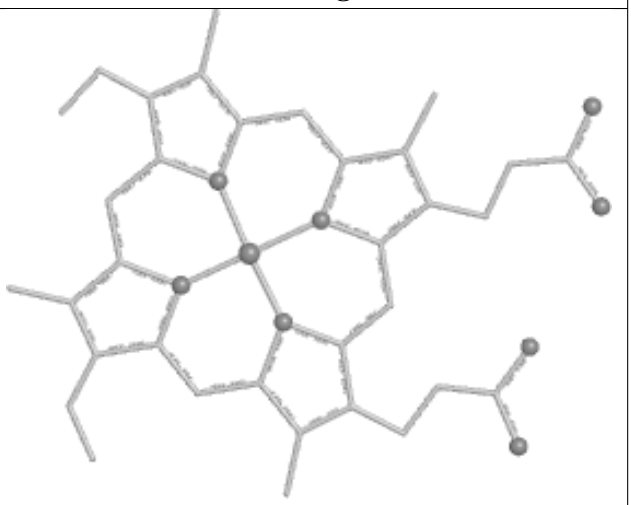
Bond lengths



Bond angles

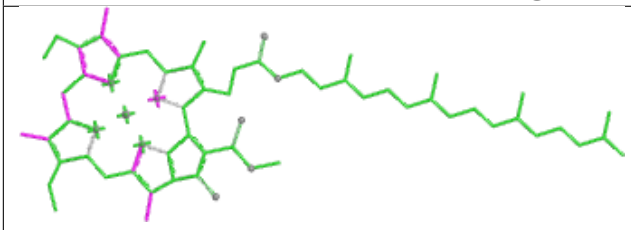


Torsions

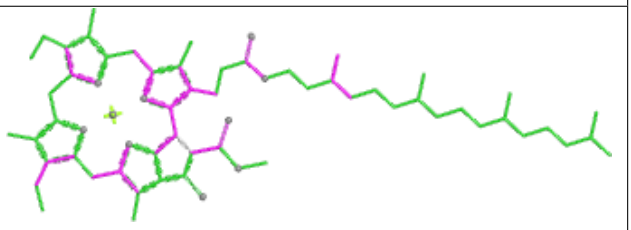


Rings

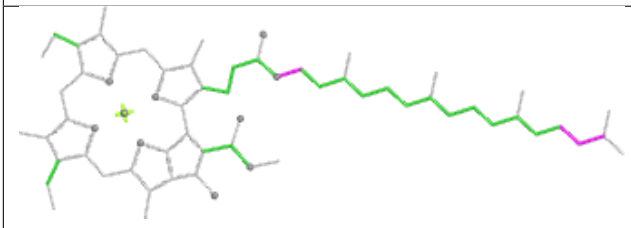
Ligand CLA a 405



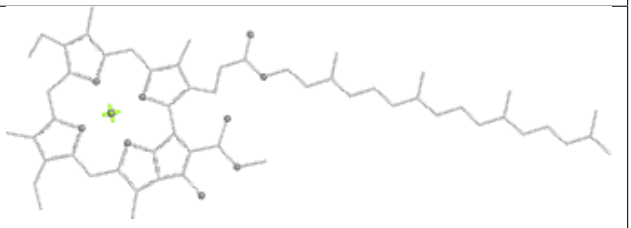
Bond lengths



Bond angles

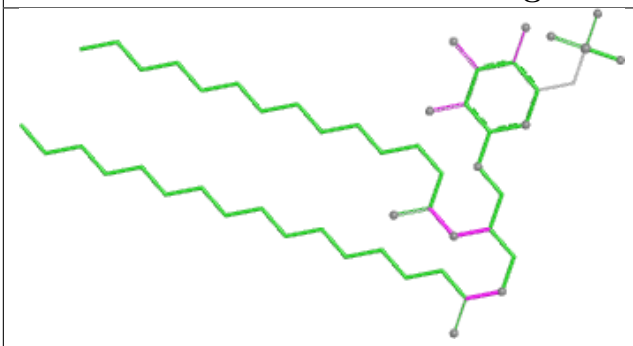


Torsions

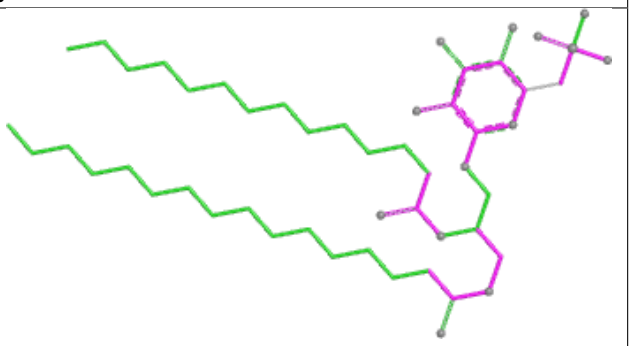


Rings

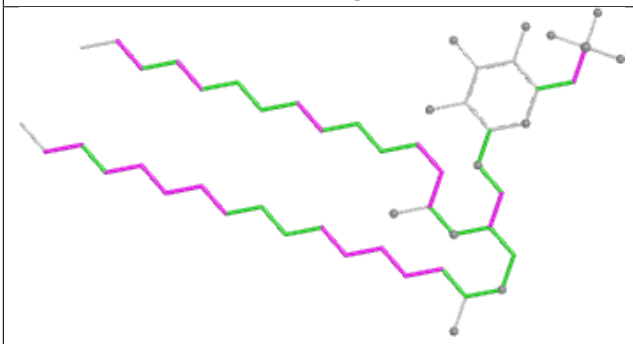
Ligand SQD A 410



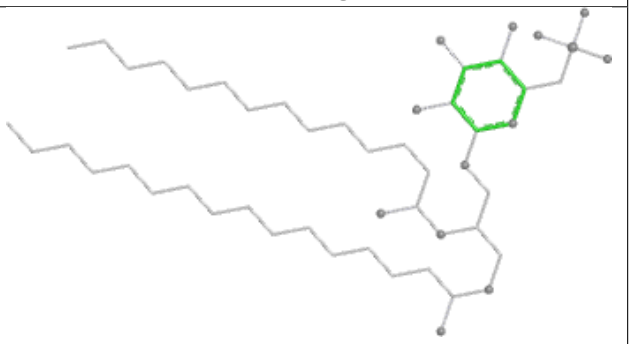
Bond lengths



Bond angles

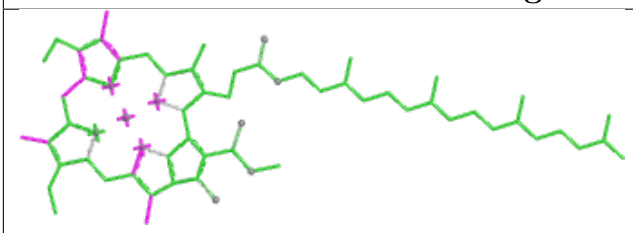


Torsions

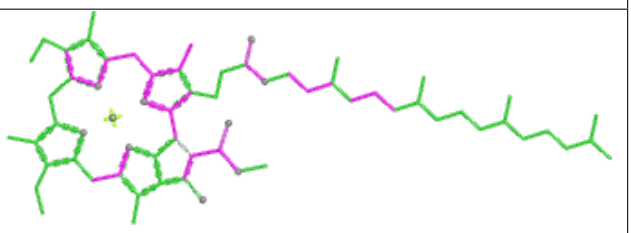


Rings

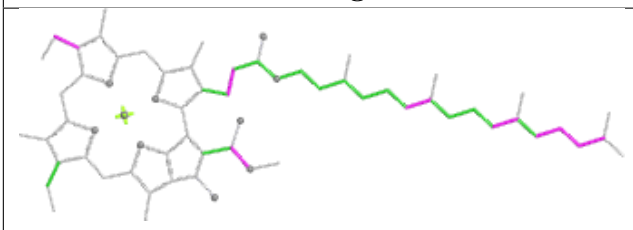
Ligand CLA B 606



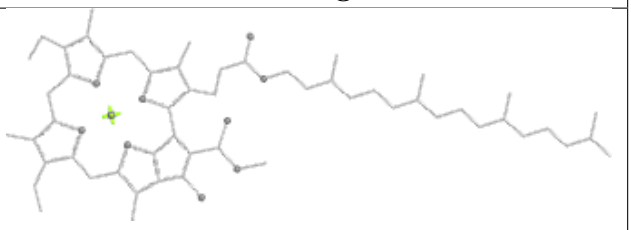
Bond lengths



Bond angles

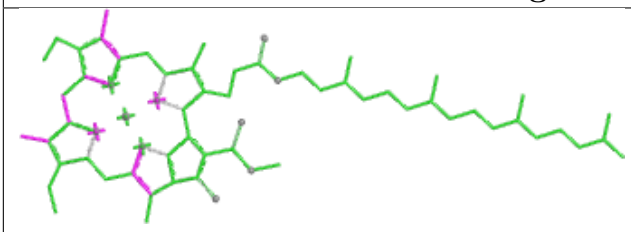


Torsions

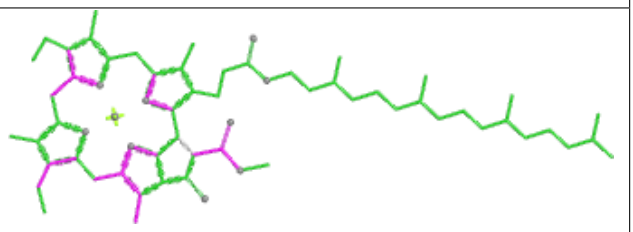


Rings

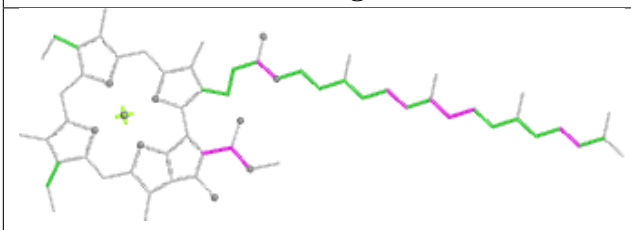
Ligand CLA c 503



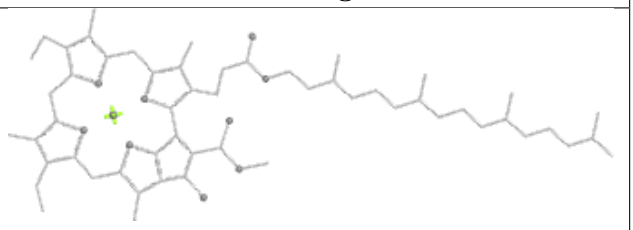
Bond lengths



Bond angles

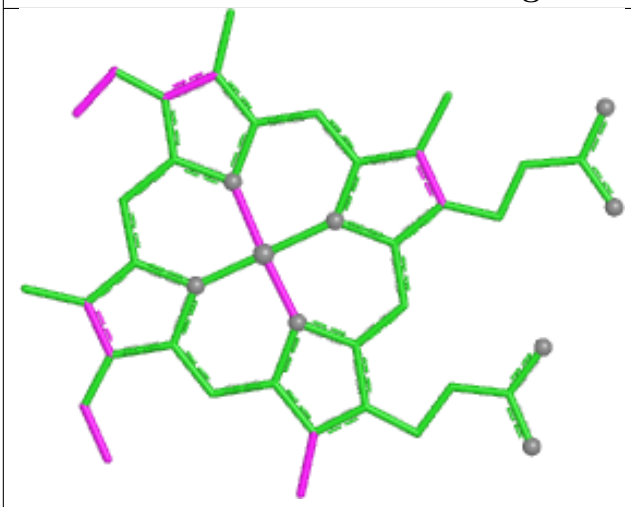


Torsions

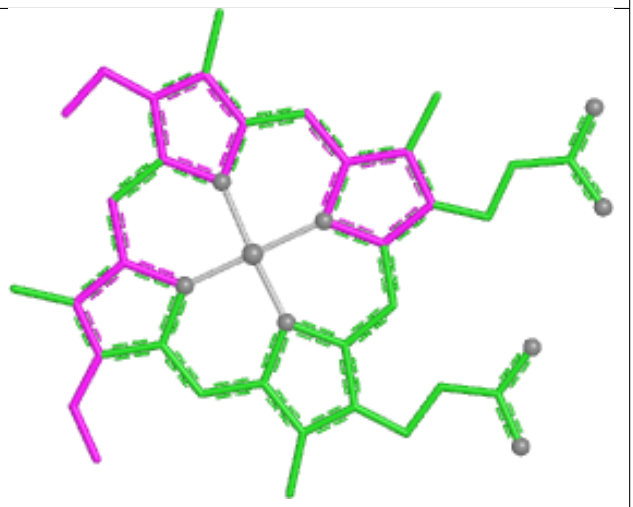


Rings

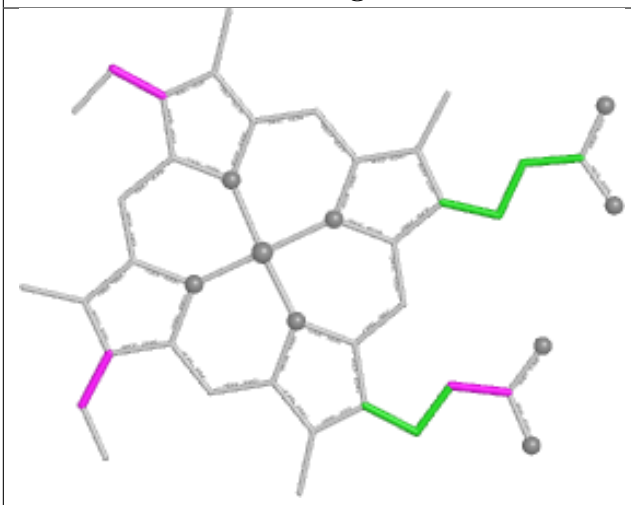
Ligand HEC V 201



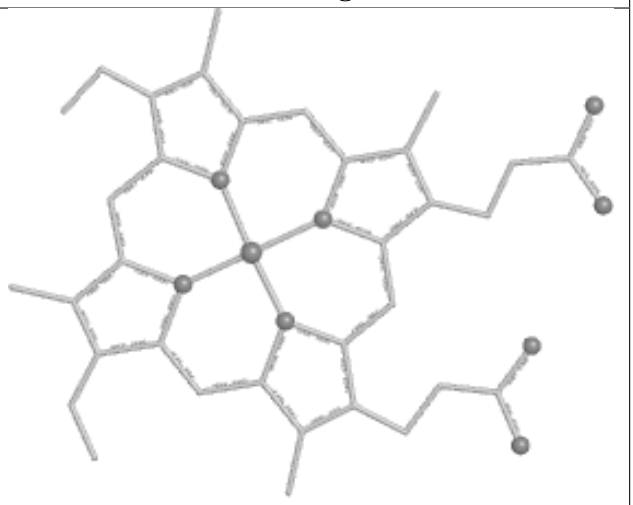
Bond lengths



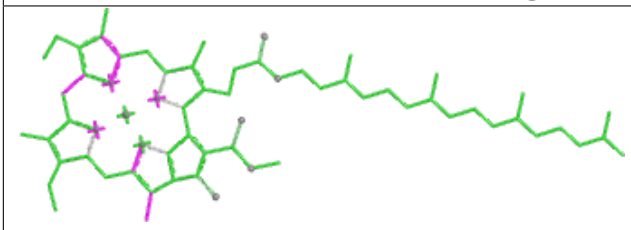
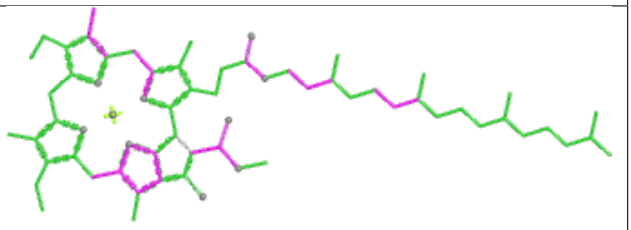
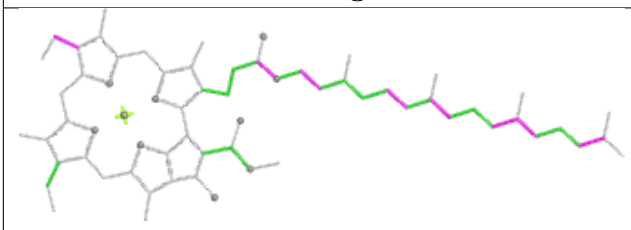
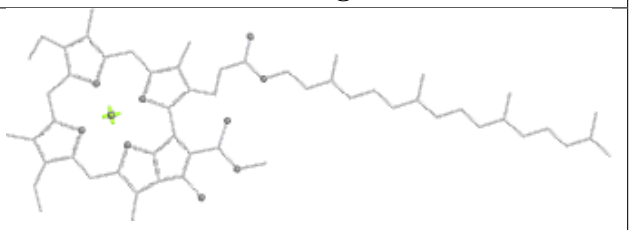
Bond angles

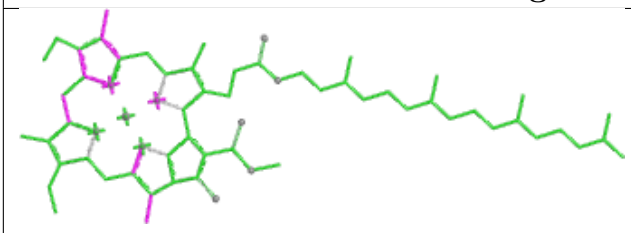
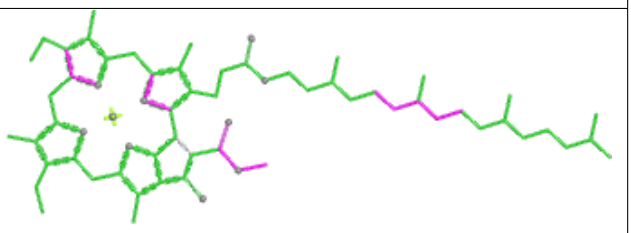
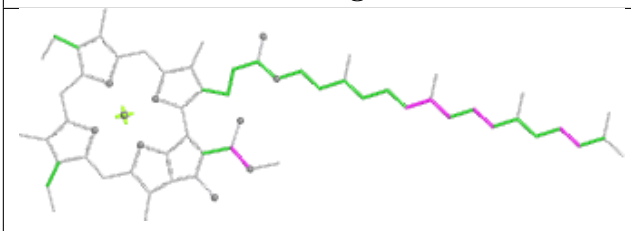
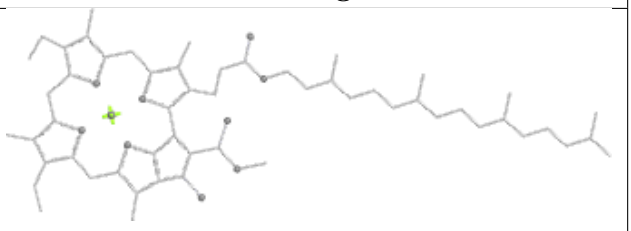


Torsions

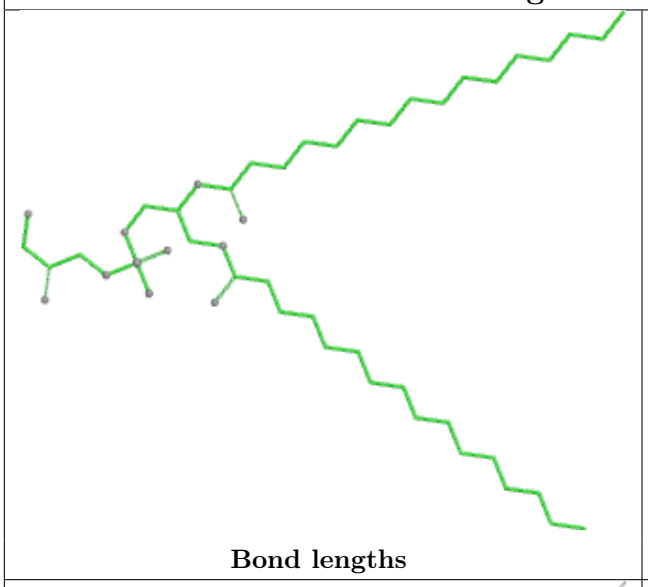


Rings

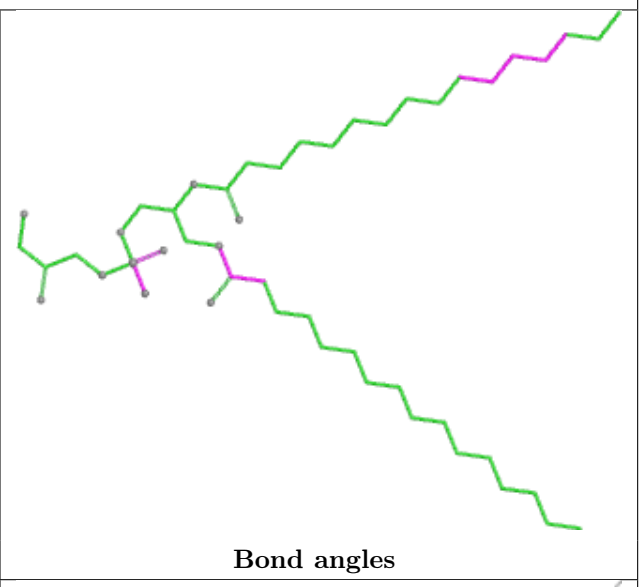
Ligand CLA D 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

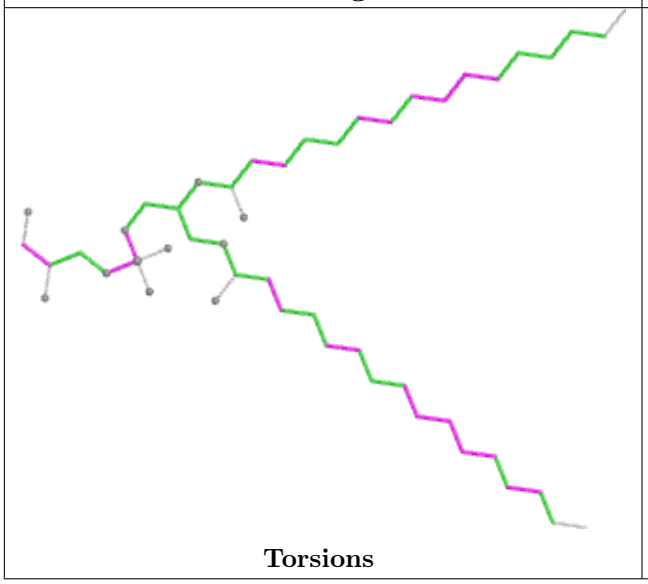
Ligand LHG d 408



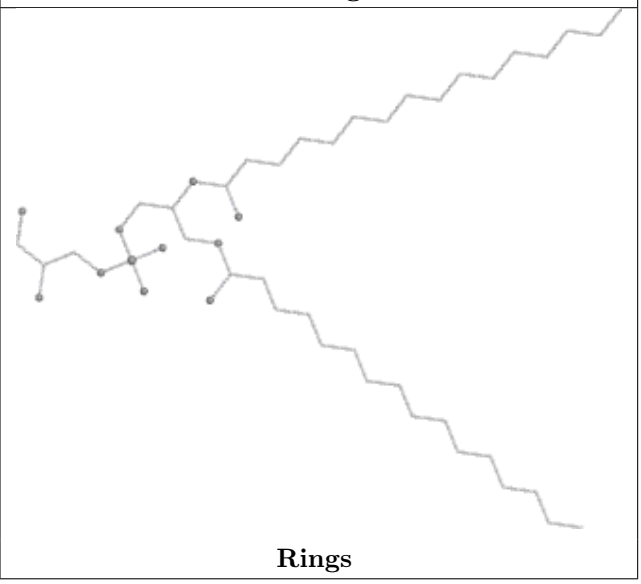
Bond lengths



Bond angles

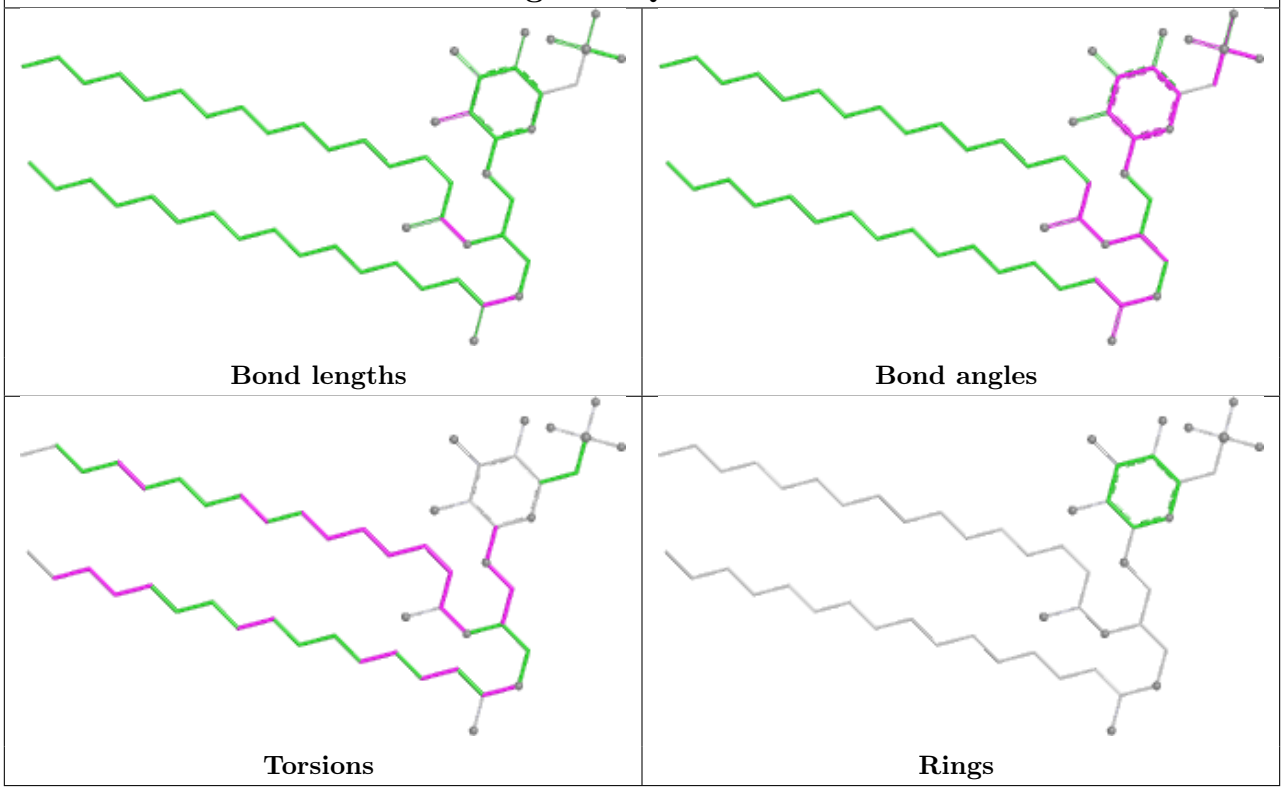


Torsions

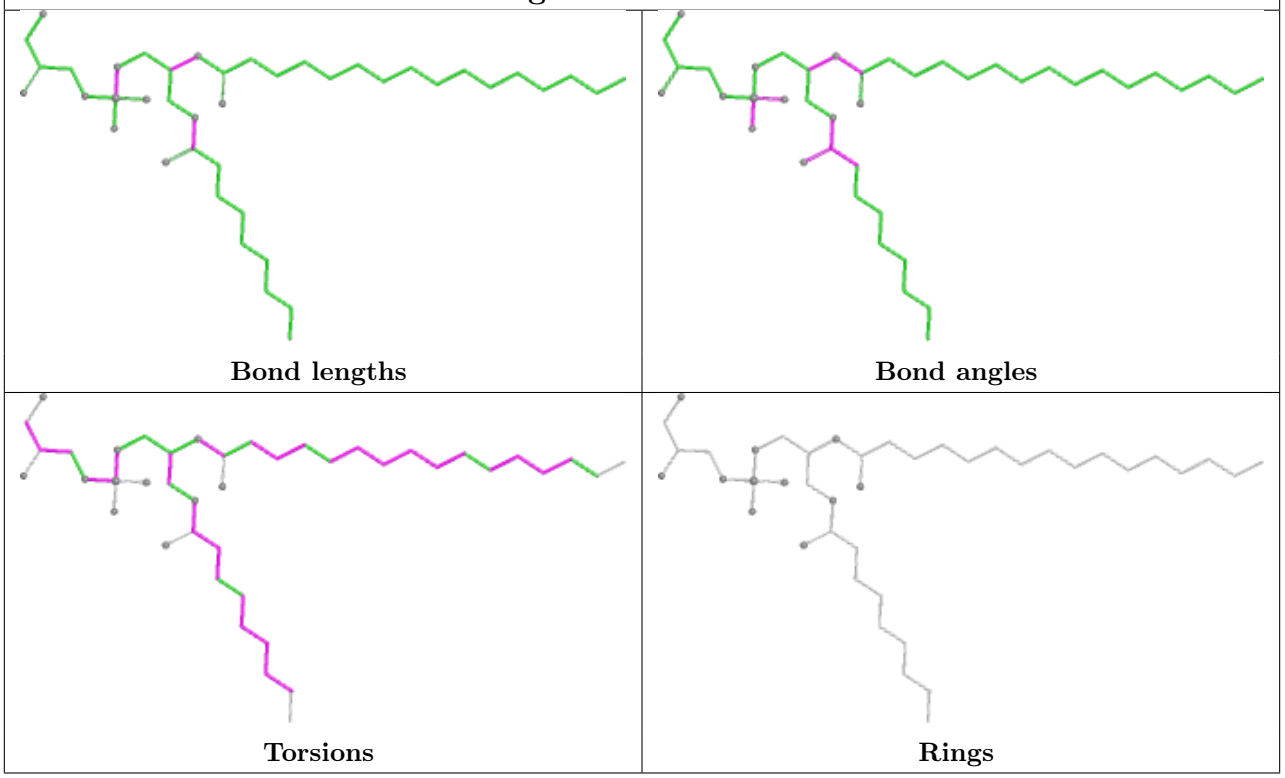


Rings

Ligand SQD B 621



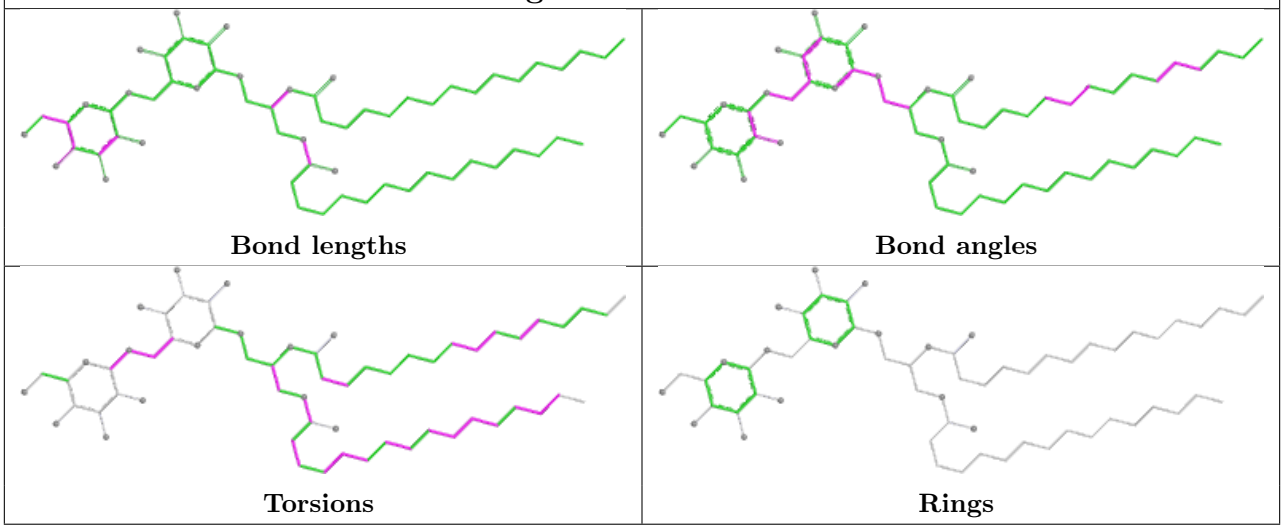
Ligand LHG e 101



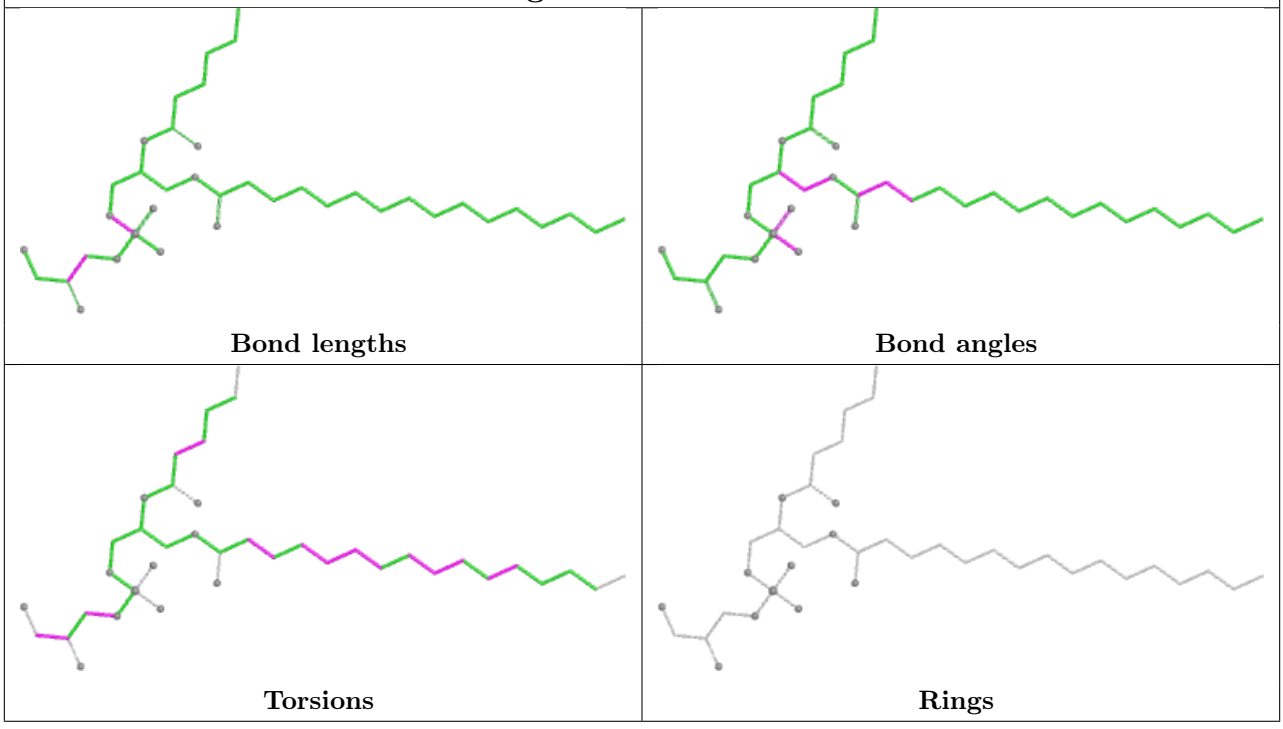
Ligand PL9 d 406



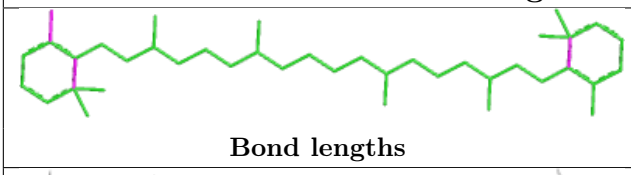
Ligand DGD c 517



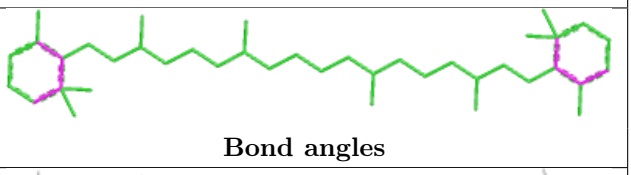
Ligand LHG d 409



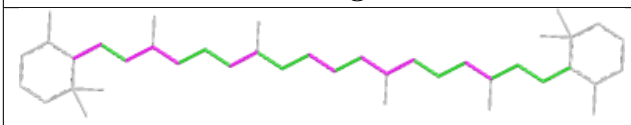
Ligand BCR k 101



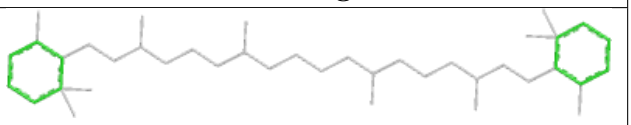
Bond lengths



Bond angles

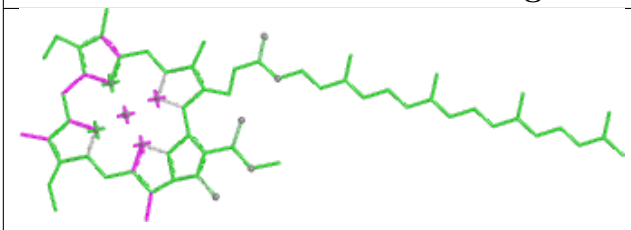


Torsions

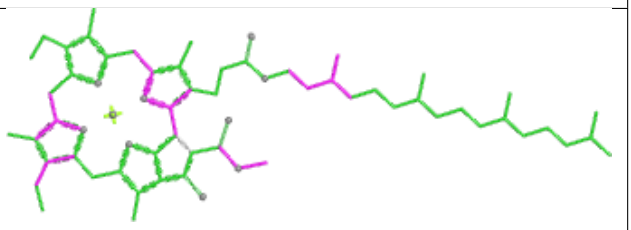


Rings

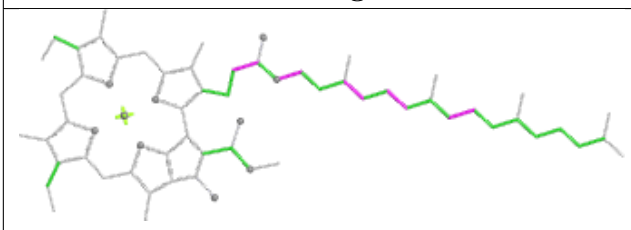
Ligand CLA B 613



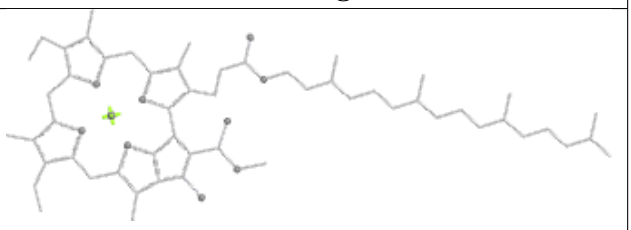
Bond lengths



Bond angles

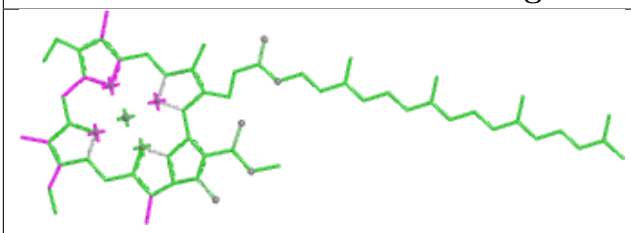


Torsions

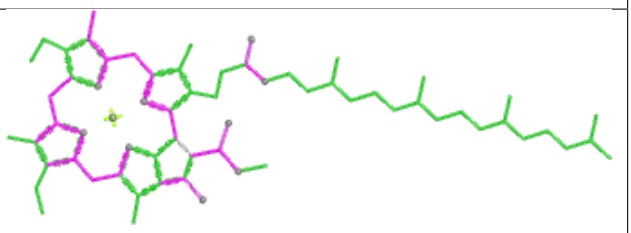


Rings

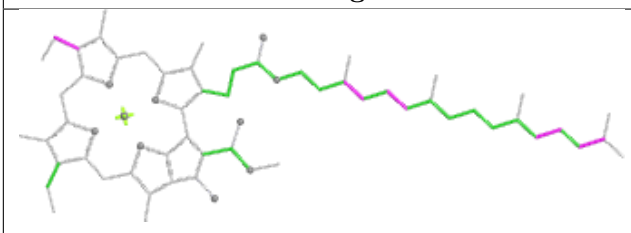
Ligand CLA B 609



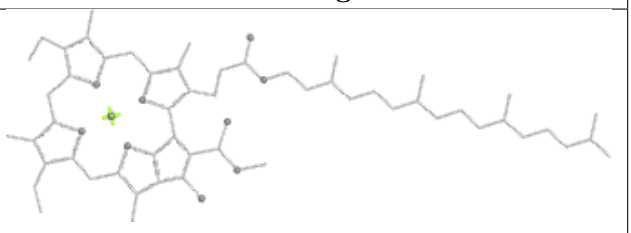
Bond lengths



Bond angles

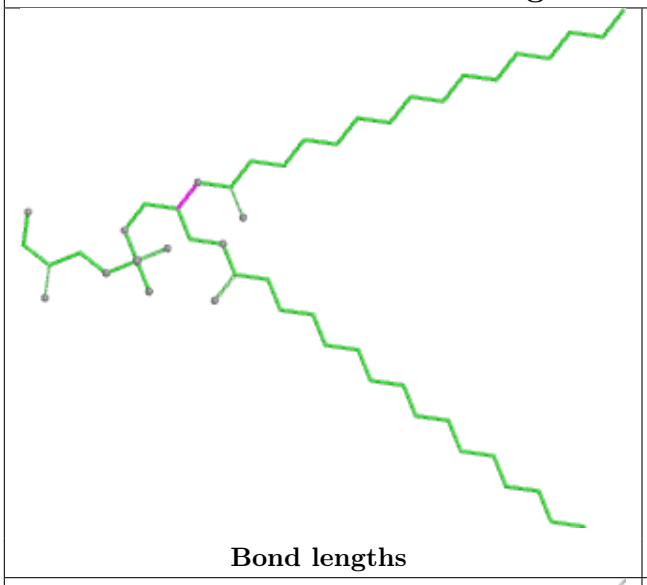


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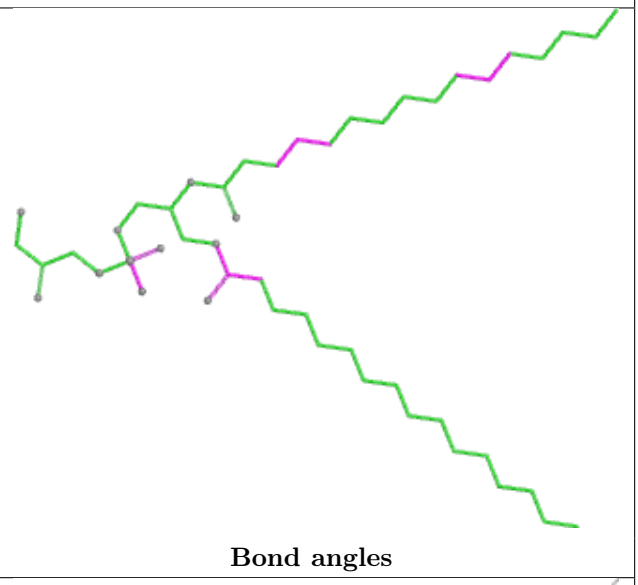


Rings

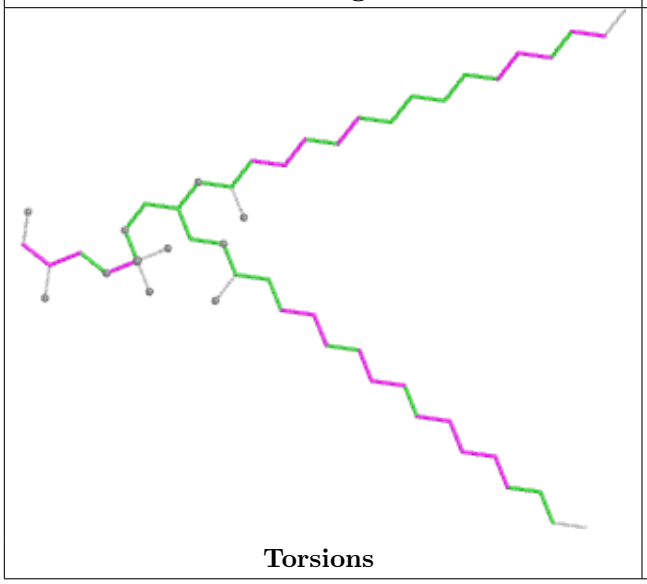
Ligand LHG d 407



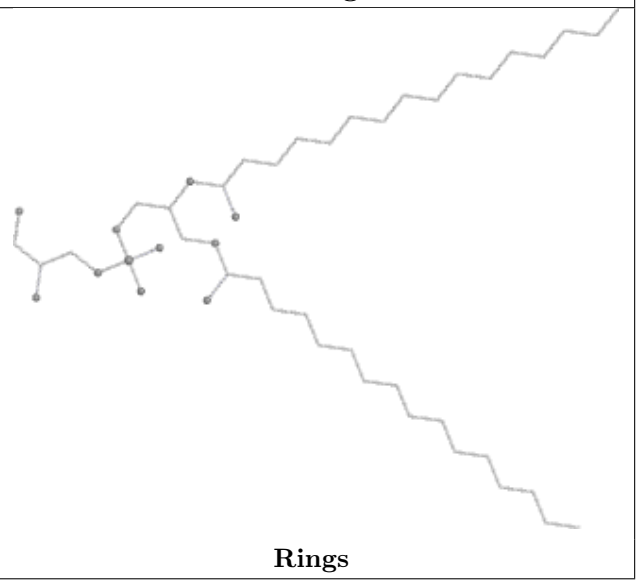
Bond lengths



Bond angles

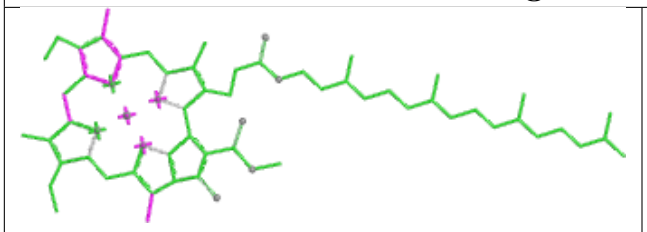


Torsions

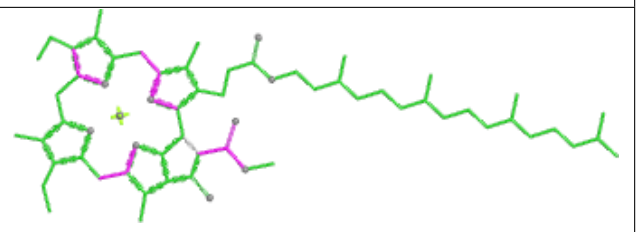


Rings

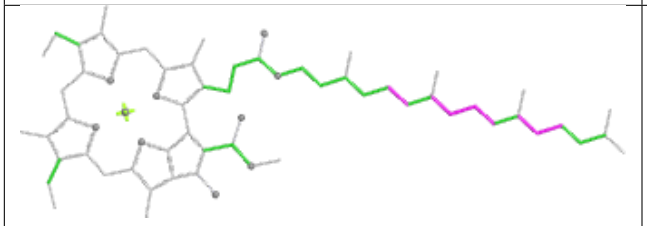
Ligand CLA C 510



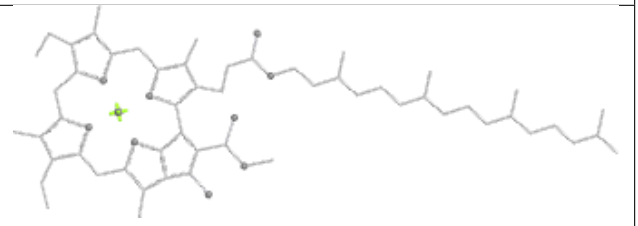
Bond lengths



Bond angles

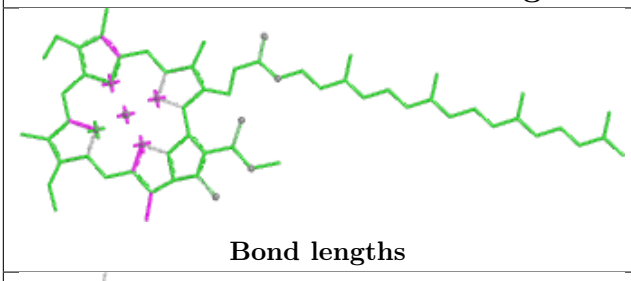


Torsions

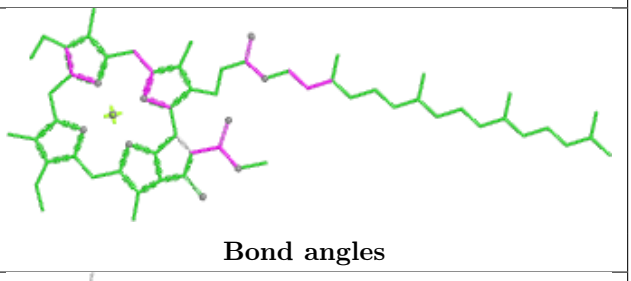


Rings

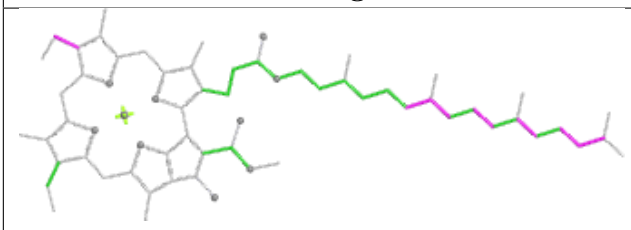
Ligand CLA D 403



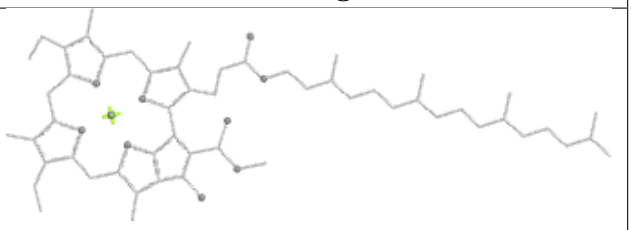
Bond lengths



Bond angles

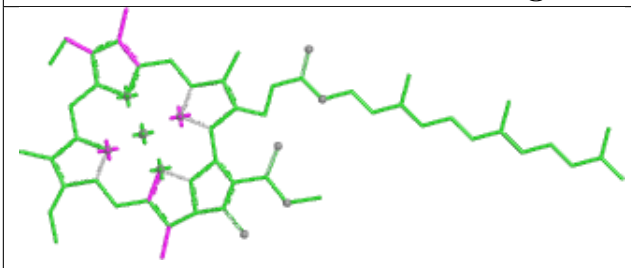


Torsions

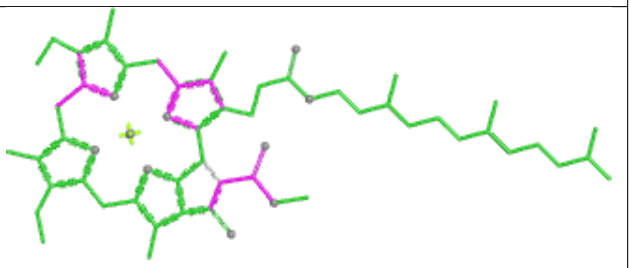


Rings

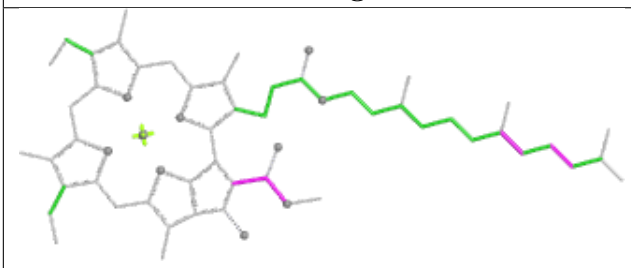
Ligand CLA b 617



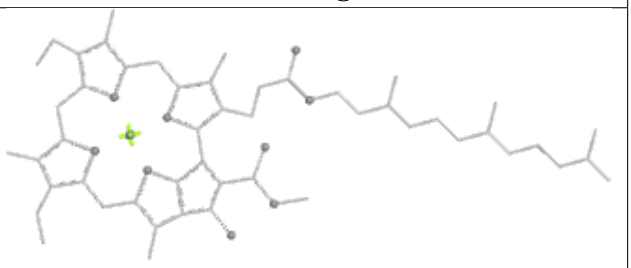
Bond lengths



Bond angles



Torsions

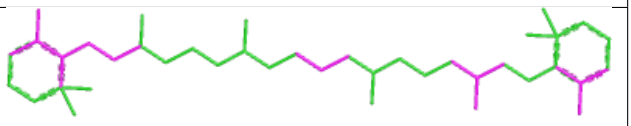


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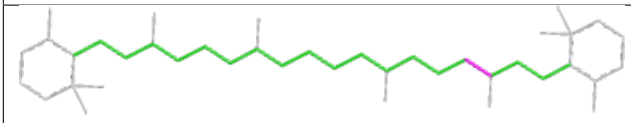
Ligand BCR T 101



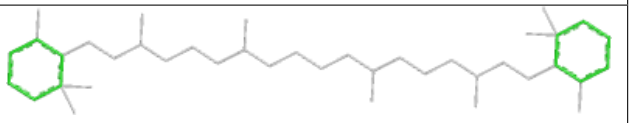
Bond lengths



Bond angles

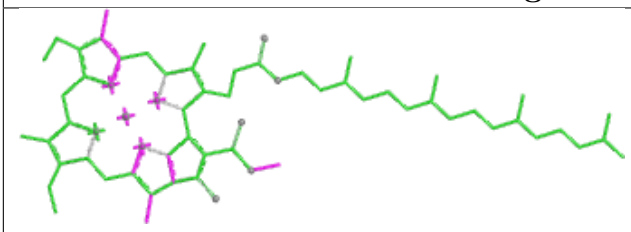


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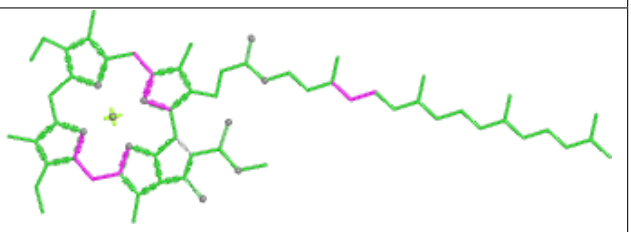


Rings

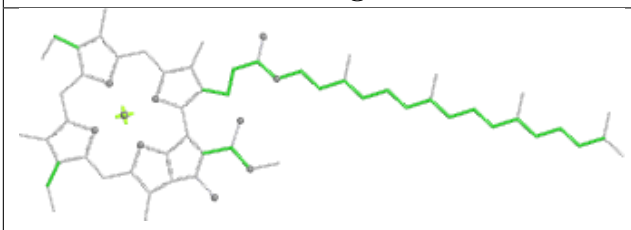
Ligand CLA B 608



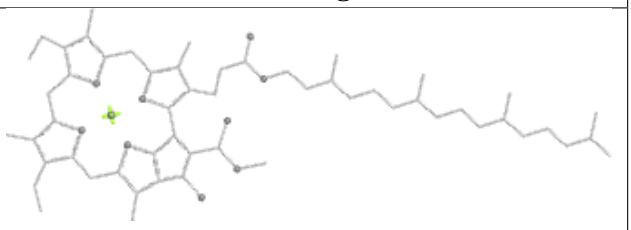
Bond lengths



Bond angles



Torsions

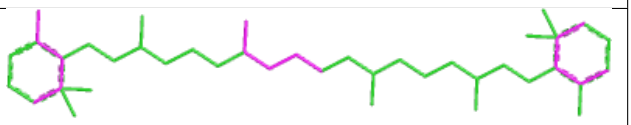


Rings

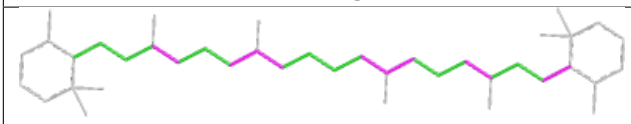
Ligand BCR H 101



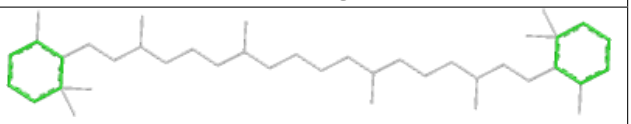
Bond lengths



Bond angles

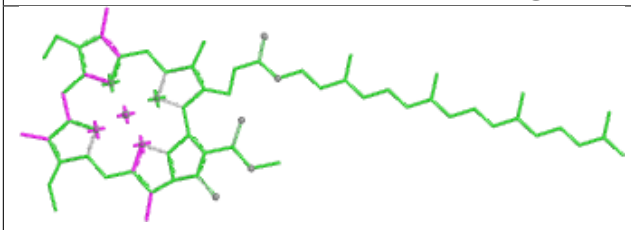


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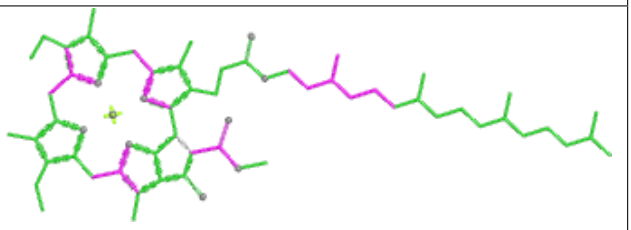


Rings

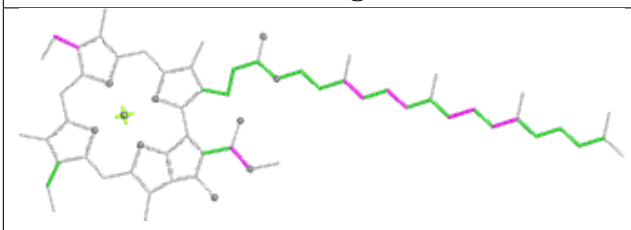
Ligand CLA b 604



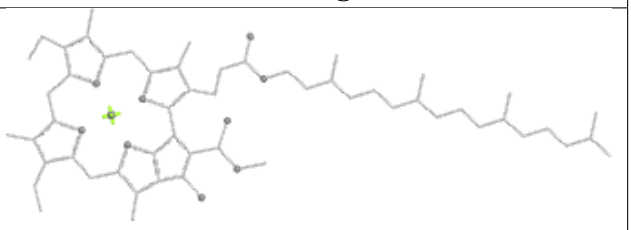
Bond lengths



Bond angles

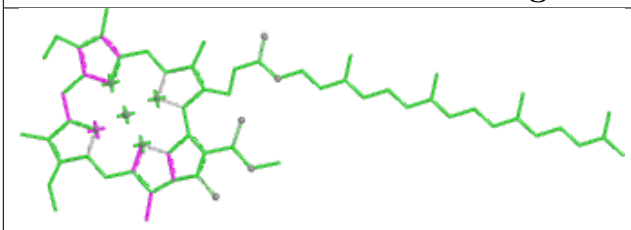


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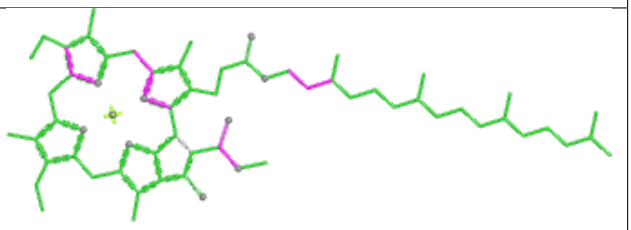


Rings

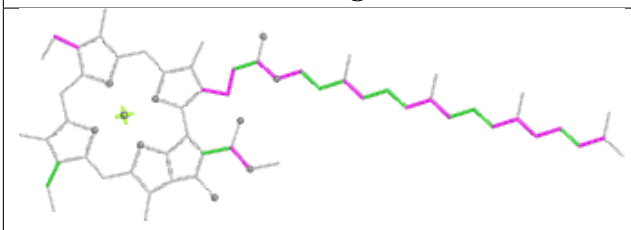
Ligand CLA c 512



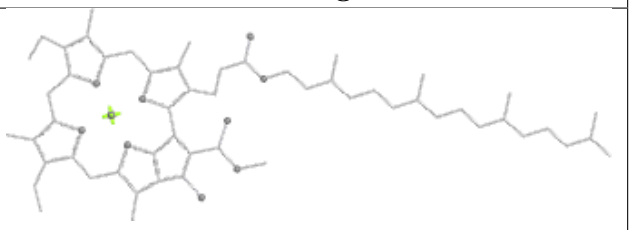
Bond lengths



Bond angles

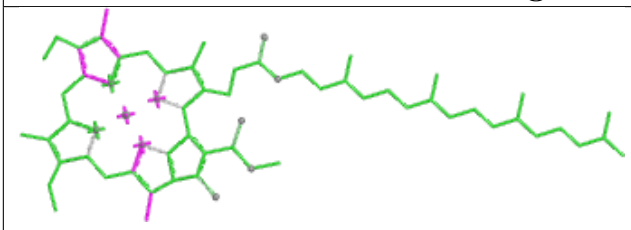


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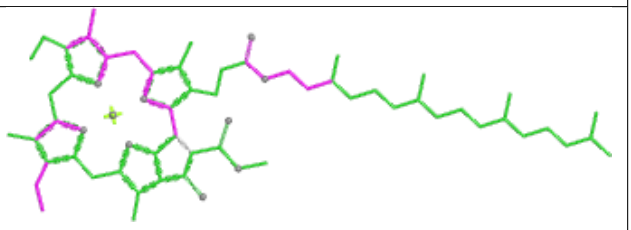


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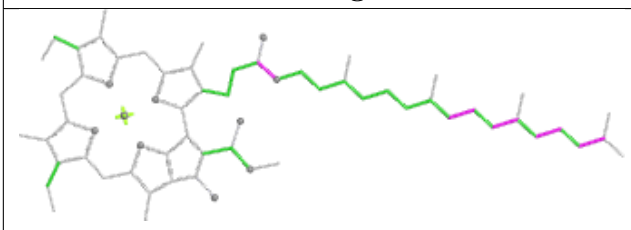
Ligand CLA d 404



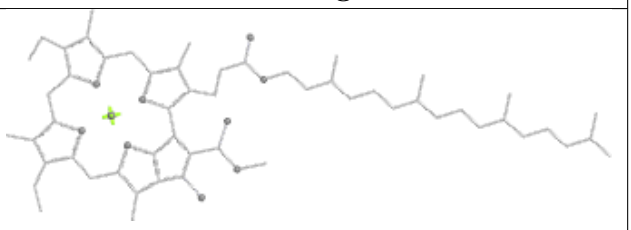
Bond lengths



Bond angles

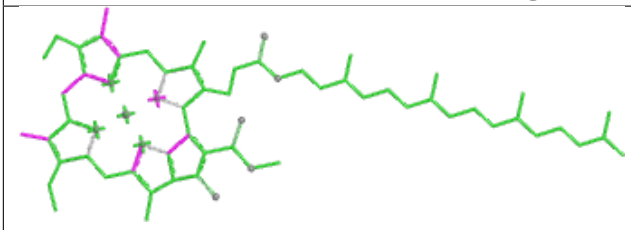


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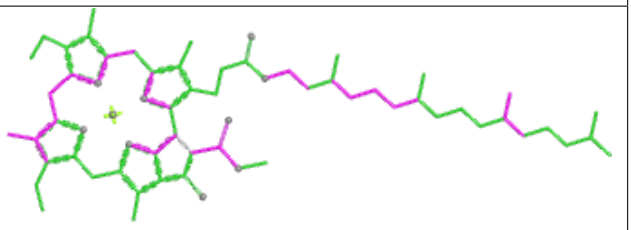


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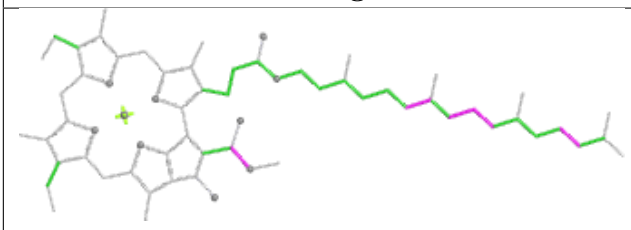
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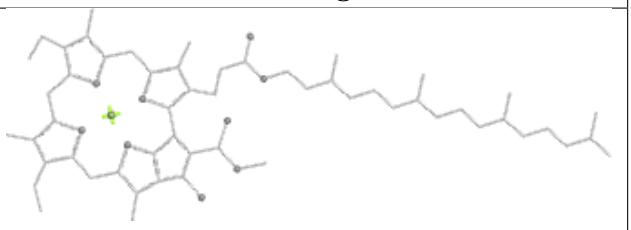
Bond lengths



Bond angles

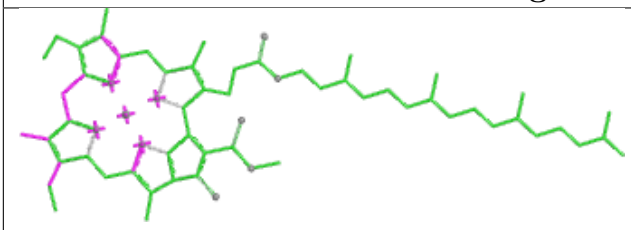


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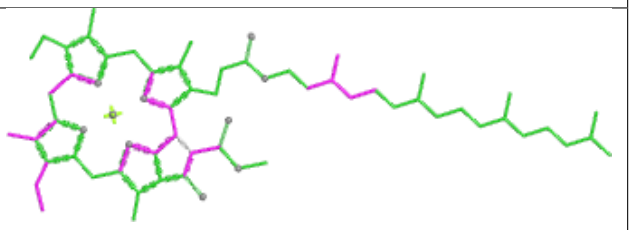


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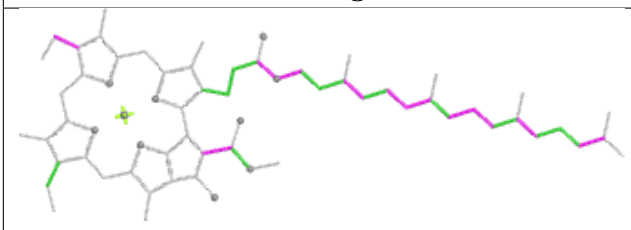
Ligand CLA c 506



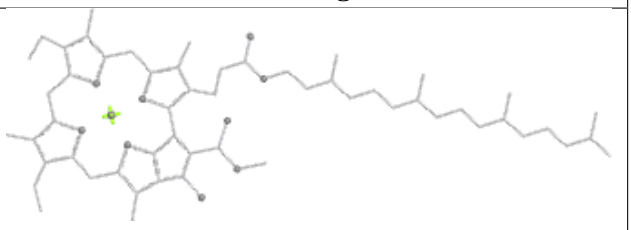
Bond lengths



Bond angles

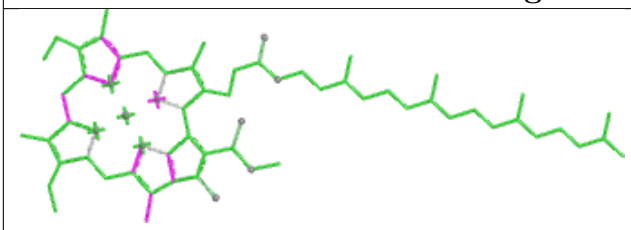


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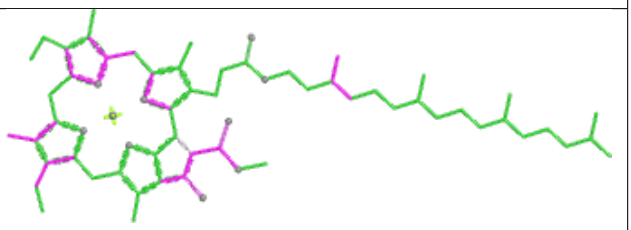


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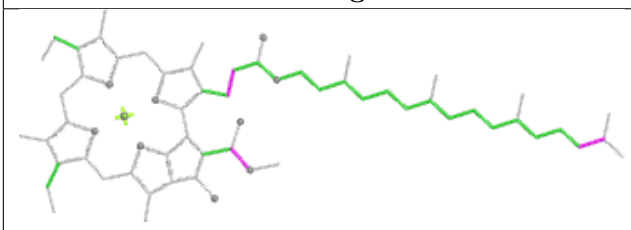
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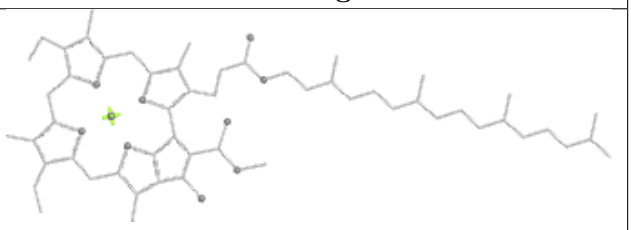
Bond lengths



Bond angles



Torsions

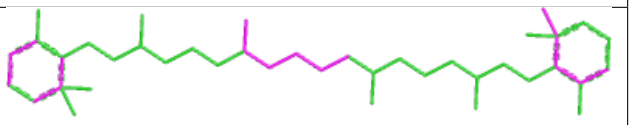


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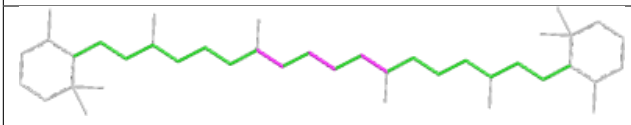
Ligand BCR B 618



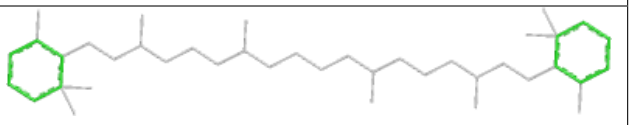
Bond lengths



Bond angles

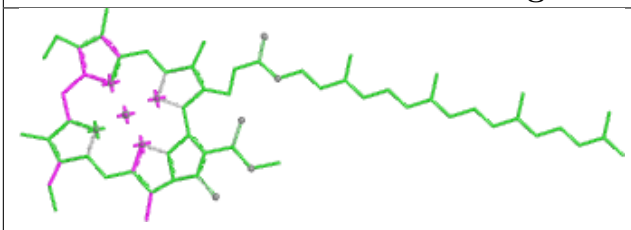


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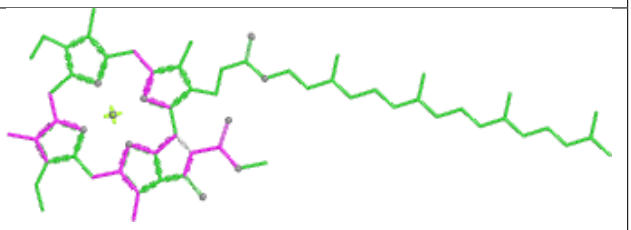


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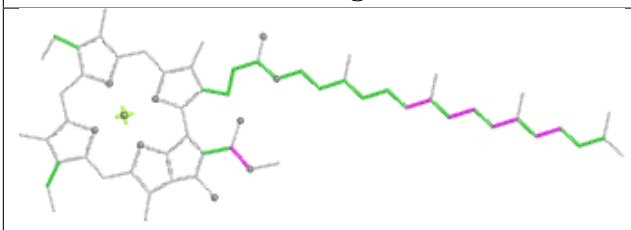
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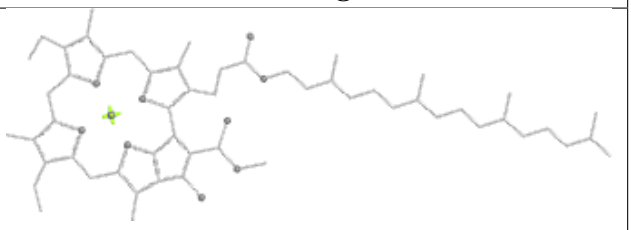
Bond lengths



Bond angles

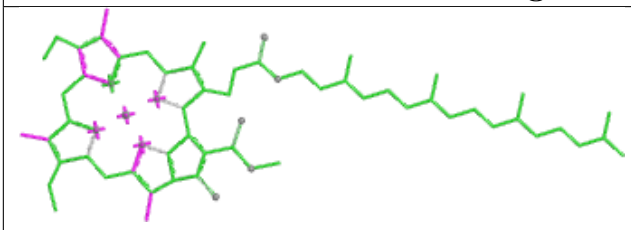


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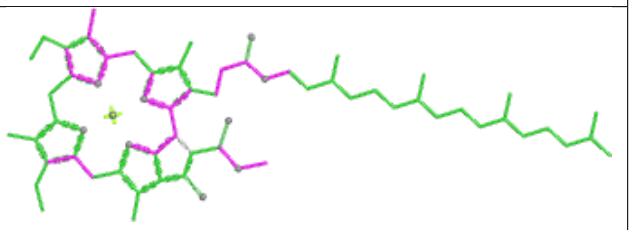


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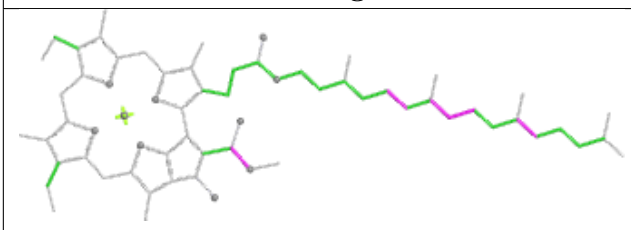
Ligand CLA b 616



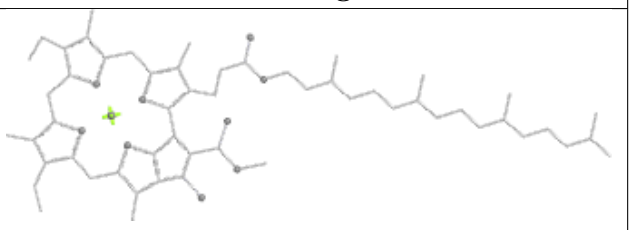
Bond lengths



Bond angles

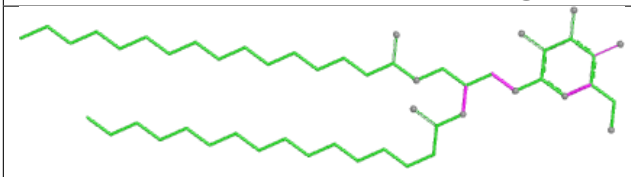


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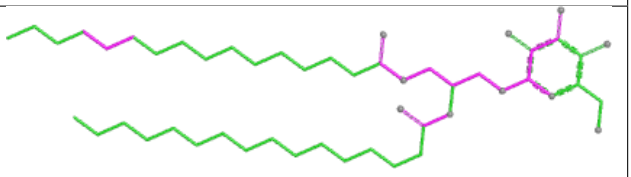


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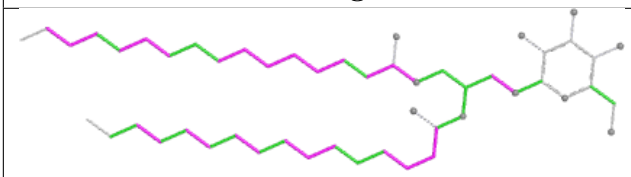
Ligand LMG m 101



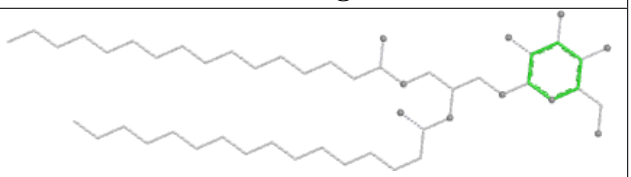
Bond lengths



Bond angles

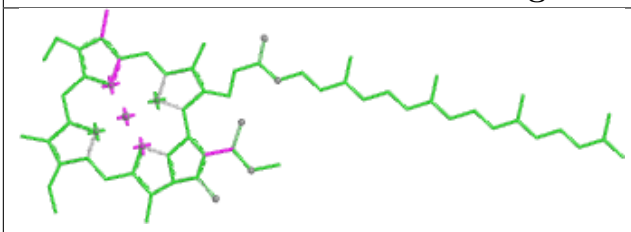


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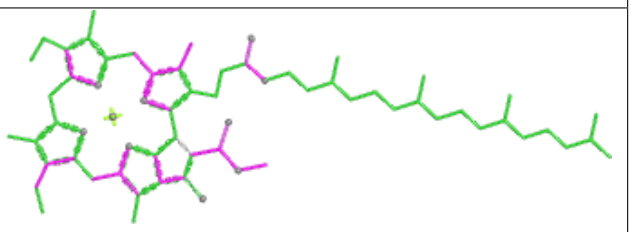


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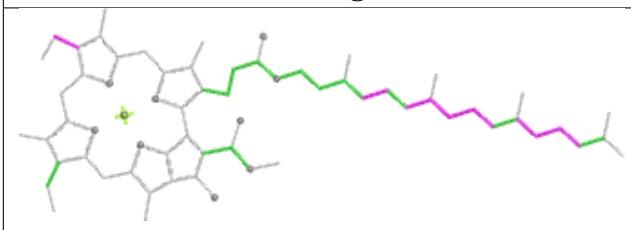
Ligand CLA a 406



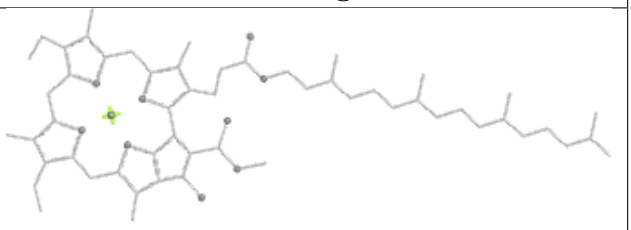
Bond lengths



Bond angles

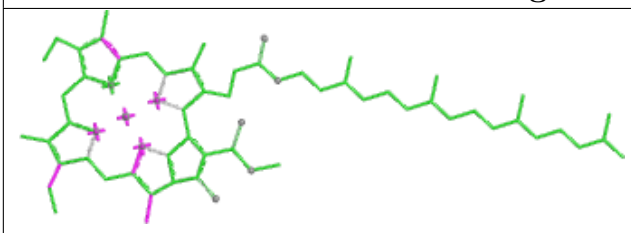


Torsions

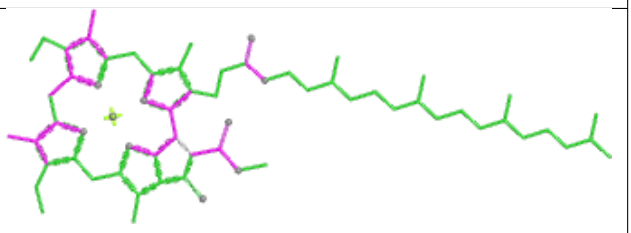


Rings

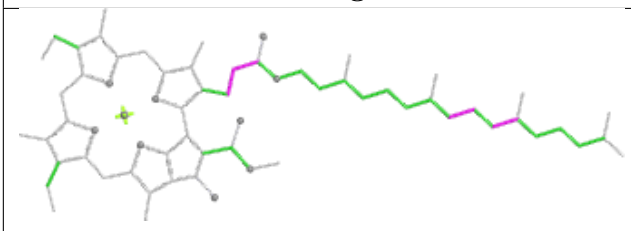
Ligand CLA c 501



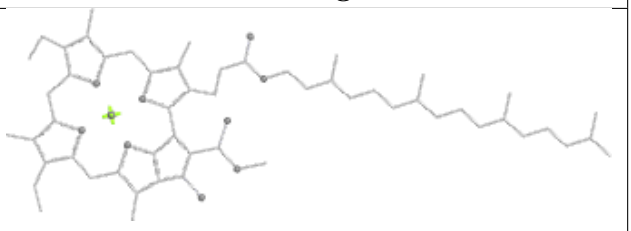
Bond lengths



Bond angles

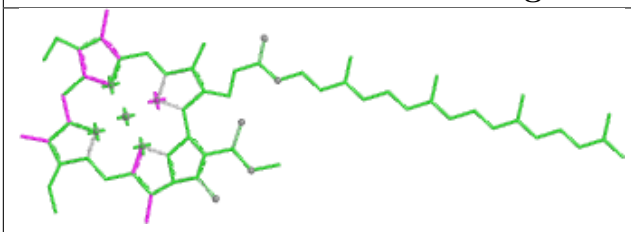


Torsions

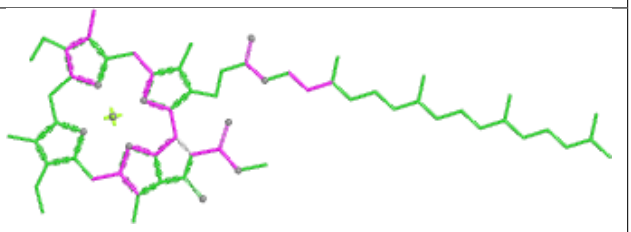


Rings

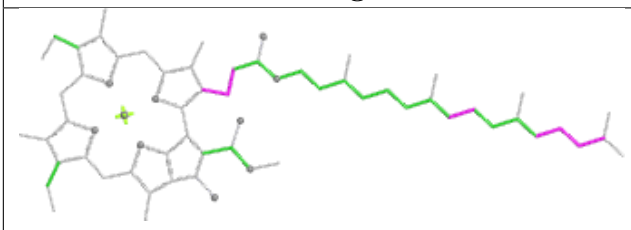
Ligand CLA B 602



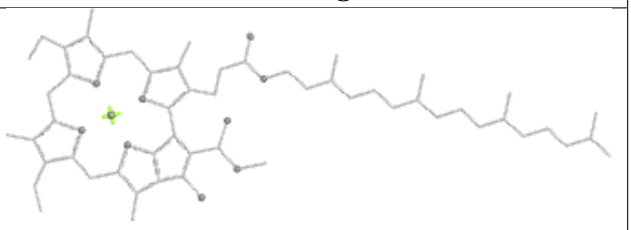
Bond lengths



Bond angles

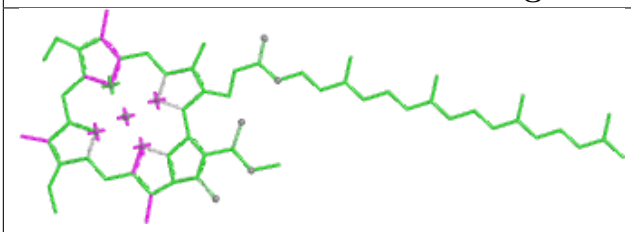


Torsions

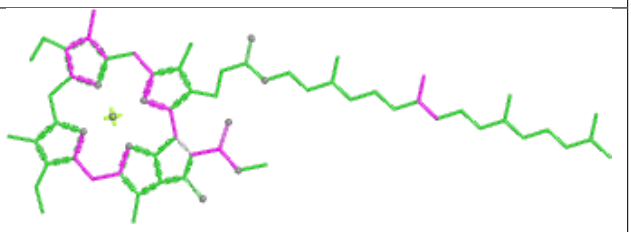


Rings

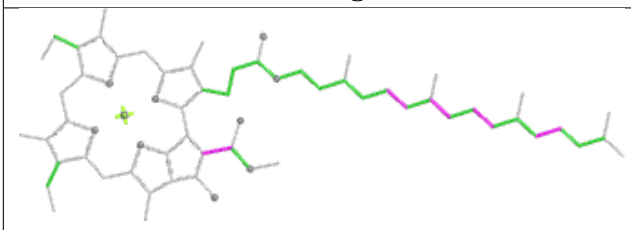
Ligand CLA C 508



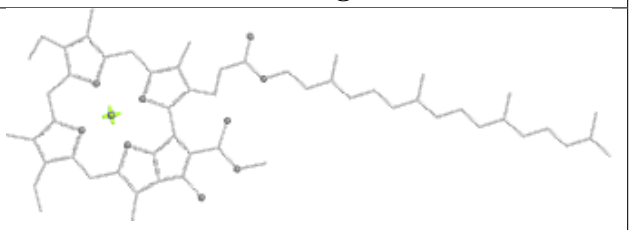
Bond lengths



Bond angles

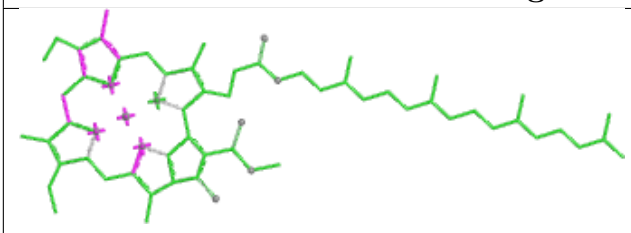


Torsions

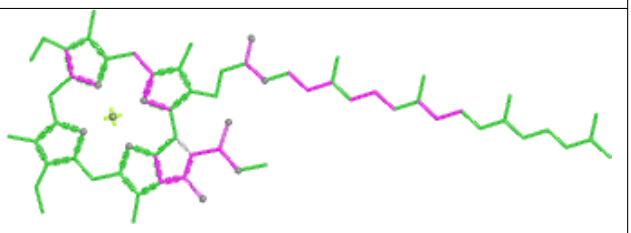


Rings

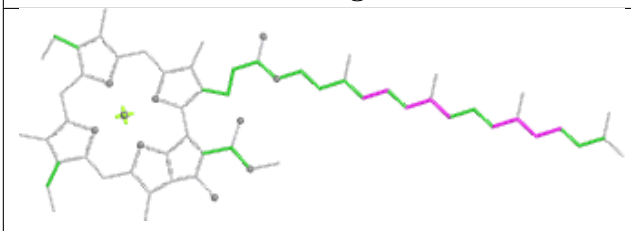
Ligand CLA b 605



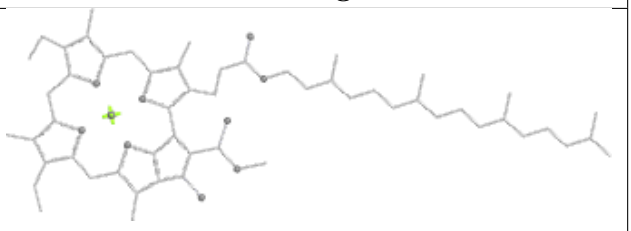
Bond lengths



Bond angles

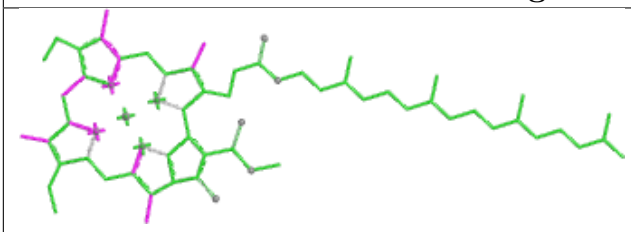


Torsions

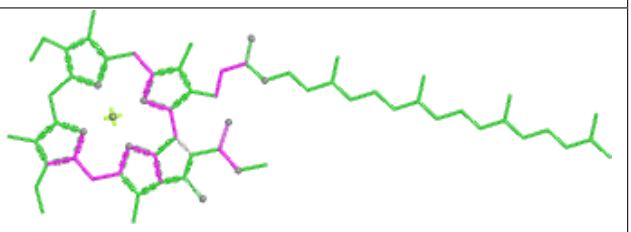


Rings

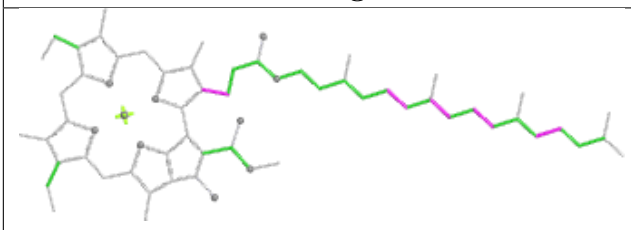
Ligand CLA a 408



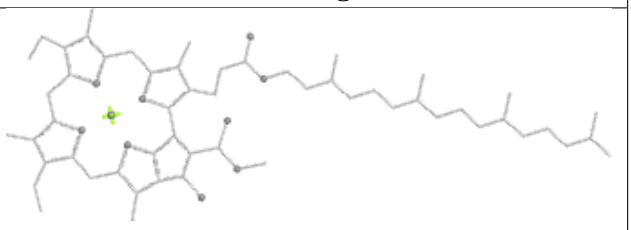
Bond lengths



Bond angles

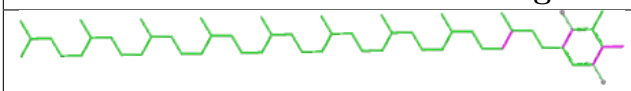


Torsions

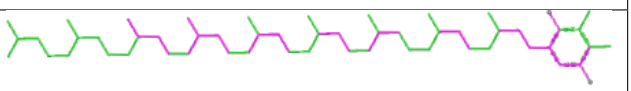


Rings

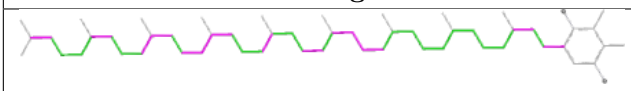
Ligand PL9 a 410



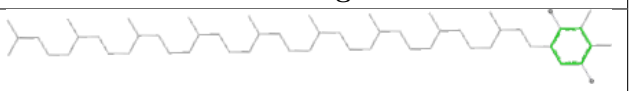
Bond lengths



Bond angles

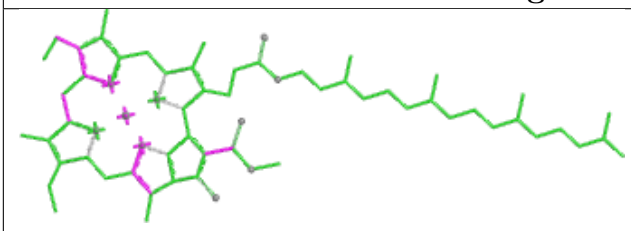


Torsions

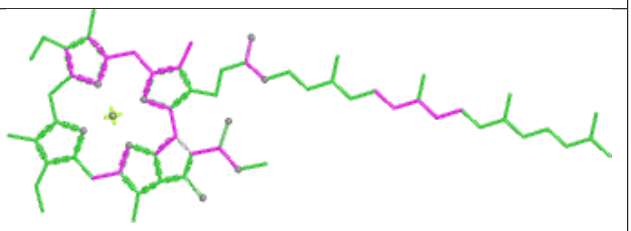


Rings

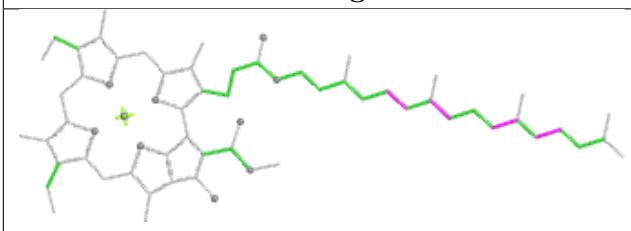
Ligand CLA b 609



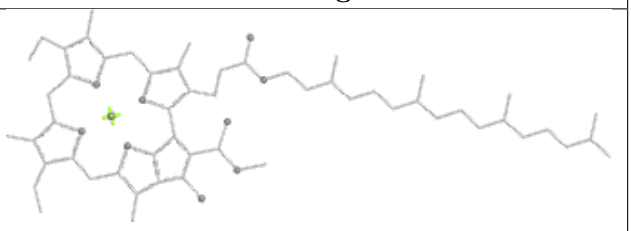
Bond lengths



Bond angles

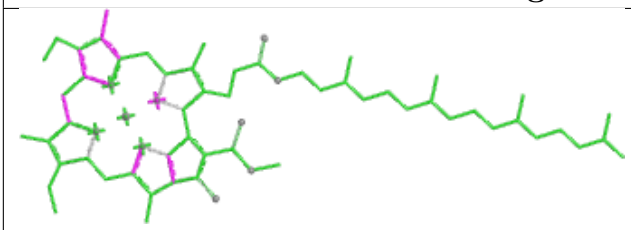


Torsions

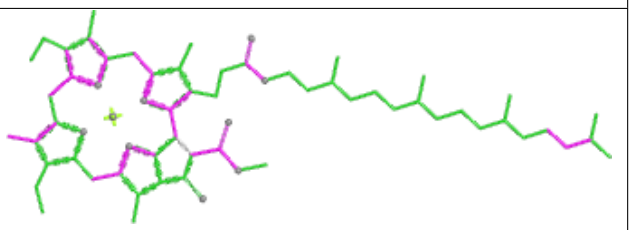


Rings

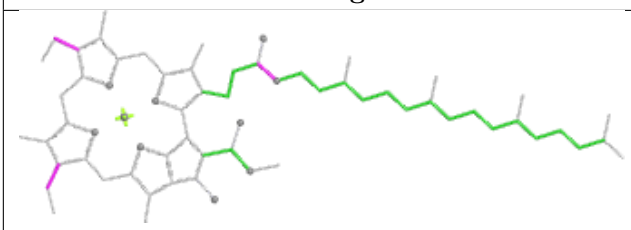
Ligand CLA d 402



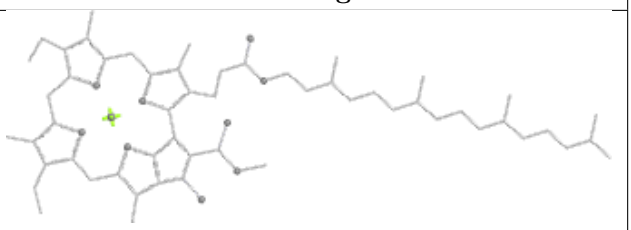
Bond lengths



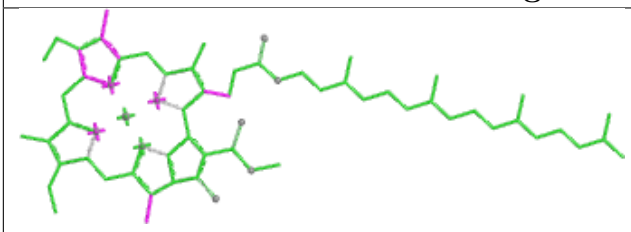
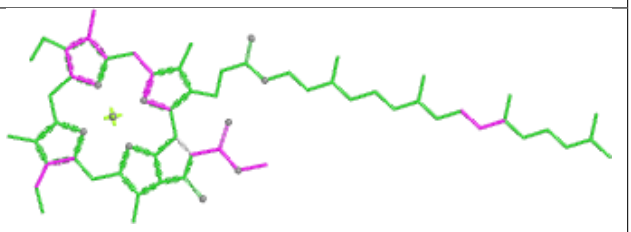
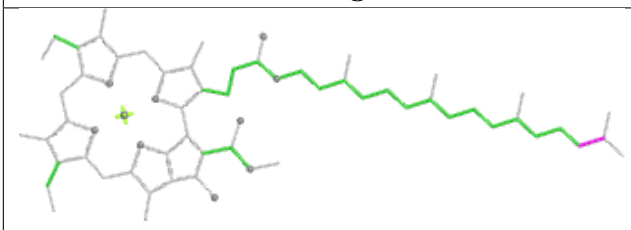
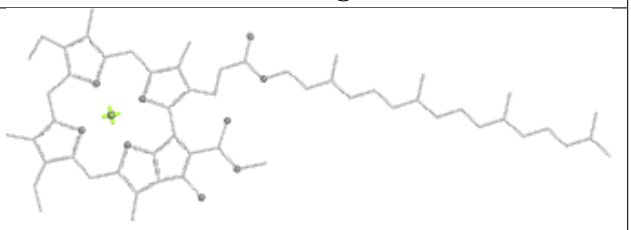
Bond angles



Torsions



Rings

Ligand CLA A 405	
 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%)	-0.74	0 100 100	30, 38, 59, 96	0
1	a	334/334 (100%)	-0.63	0 100 100	29, 40, 69, 91	0
2	B	505/505 (100%)	-0.61	0 100 100	21, 43, 75, 121	4 (0%)
2	b	505/505 (100%)	-0.50	0 100 100	31, 46, 84, 117	0
3	C	442/451 (98%)	-0.57	0 100 100	31, 46, 65, 90	0
3	c	451/451 (100%)	-0.50	1 (0%) 91 89	26, 51, 75, 120	1 (0%)
4	D	341/341 (100%)	-0.73	0 100 100	29, 40, 59, 103	0
4	d	341/341 (100%)	-0.59	0 100 100	31, 44, 70, 100	1 (0%)
5	E	81/82 (98%)	-0.17	1 (1%) 76 73	35, 62, 77, 97	1 (1%)
5	e	82/82 (100%)	0.01	1 (1%) 76 73	47, 71, 94, 105	0
6	F	34/34 (100%)	-0.38	0 100 100	47, 53, 76, 91	0
6	f	34/34 (100%)	-0.12	0 100 100	54, 60, 90, 106	0
7	H	65/65 (100%)	-0.47	1 (1%) 72 68	41, 49, 73, 90	0
7	h	63/65 (96%)	-0.31	0 100 100	47, 60, 80, 90	0
8	I	35/36 (97%)	-0.57	0 100 100	37, 48, 82, 86	0
8	i	35/36 (97%)	-0.38	0 100 100	35, 51, 93, 100	0
9	J	36/36 (100%)	-0.28	0 100 100	48, 60, 85, 117	0
9	j	36/36 (100%)	-0.16	0 100 100	47, 64, 99, 109	0
10	K	37/37 (100%)	-0.20	1 (2%) 56 51	39, 65, 82, 85	1 (2%)
10	k	37/37 (100%)	0.02	0 100 100	64, 74, 87, 92	0
11	L	37/37 (100%)	-0.74	0 100 100	32, 40, 80, 87	0
11	l	36/37 (97%)	-0.75	0 100 100	33, 41, 81, 94	0
12	M	32/33 (96%)	-0.59	0 100 100	34, 42, 75, 85	0
12	m	31/33 (93%)	-0.64	0 100 100	37, 43, 59, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	-0.41	0 100 100	29, 52, 93, 165	1 (0%)
13	o	244/244 (100%)	-0.46	0 100 100	30, 50, 99, 144	0
14	T	29/30 (96%)	-0.71	0 100 100	32, 42, 75, 82	0
14	t	29/30 (96%)	-0.60	1 (3%) 48 43	34, 41, 98, 102	0
15	U	97/97 (100%)	-0.45	0 100 100	39, 53, 84, 112	0
15	u	97/97 (100%)	-0.43	0 100 100	38, 51, 68, 106	0
16	V	137/137 (100%)	-0.59	0 100 100	35, 51, 67, 97	0
16	v	137/137 (100%)	-0.34	0 100 100	41, 58, 82, 105	0
17	Y	27/30 (90%)	0.72	2 (7%) 20 18	62, 85, 123, 131	0
17	y	30/30 (100%)	0.37	0 100 100	67, 86, 106, 126	0
18	X	38/38 (100%)	-0.22	0 100 100	45, 59, 90, 91	0
18	x	38/38 (100%)	-0.08	0 100 100	55, 70, 96, 103	0
19	Z	62/62 (100%)	0.26	0 100 100	60, 77, 124, 139	0
19	z	62/62 (100%)	0.46	2 (3%) 50 46	66, 86, 134, 144	0
20	R	34/34 (100%)	0.24	1 (2%) 53 49	71, 83, 108, 117	0
20	r	31/34 (91%)	0.90	1 (3%) 50 46	83, 105, 114, 121	0
All	All	5300/5326 (99%)	-0.48	12 (0%) 91 89	21, 48, 88, 165	9 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	23	ALA	3.6
19	z	33	TRP	3.2
7	H	66	GLY	3.1
14	t	30	THR	3.0
20	r	32	GLN	2.9

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	0.95	0.09	41,55,69,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	I	1	10/11	0.96	0.07	48,61,72,83	0
14	FME	T	1	10/11	0.96	0.08	33,58,80,90	0
8	FME	i	1	10/11	0.96	0.07	39,54,68,78	0
12	FME	m	1	10/11	0.96	0.08	37,54,75,81	0
14	FME	t	1	10/11	0.96	0.06	36,55,82,88	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, 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
32	UNL	H	103	53/-	0.75	0.17	44,89,115,116	0
32	UNL	c	523	28/-	0.78	0.13	55,80,93,95	0
32	UNL	b	626	26/-	0.80	0.16	52,65,76,78	0
32	UNL	a	414	28/-	0.80	0.13	44,66,82,84	0
29	LHG	e	101	42/49	0.81	0.14	68,92,115,158	0
29	LHG	E	101	49/49	0.82	0.14	54,88,118,126	0
32	UNL	B	626	47/-	0.82	0.15	54,73,88,96	0
28	DGD	A	412	66/66	0.83	0.13	41,75,100,124	0
32	UNL	b	623	40/-	0.83	0.15	52,68,91,100	0
33	LMG	c	522	48/55	0.83	0.15	42,89,123,138	0
33	LMG	d	410	23/55	0.83	0.17	43,73,104,105	0
33	LMG	D	410	33/55	0.84	0.13	34,61,107,111	0
32	UNL	x	101	55/-	0.85	0.13	43,71,92,94	0
32	UNL	b	624	44/-	0.85	0.15	48,68,88,89	0
33	LMG	b	622	55/55	0.85	0.14	48,80,99,104	0
32	UNL	B	624	46/-	0.85	0.13	55,68,83,87	0
32	UNL	T	102	47/-	0.85	0.14	34,52,79,81	0
32	UNL	t	102	26/-	0.86	0.15	56,75,87,88	0
32	UNL	C	523	47/-	0.86	0.12	47,60,78,78	0
32	UNL	B	620	43/-	0.86	0.12	41,59,81,83	0
26	PL9	A	409	55/55	0.86	0.14	35,70,101,113	0
28	DGD	a	413	44/66	0.86	0.12	36,62,86,88	0
32	UNL	j	101	28/-	0.86	0.12	53,67,81,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UNL	b	621	55/-	0.87	0.13	42,68,96,118	0
32	UNL	c	520	55/-	0.87	0.12	48,72,94,101	0
32	UNL	B	625	28/-	0.87	0.14	47,67,91,99	0
23	CLA	b	602	65/65	0.87	0.11	55,76,104,110	0
32	UNL	b	625	55/-	0.87	0.12	50,73,87,98	0
32	UNL	m	102	28/-	0.88	0.13	38,58,78,78	0
27	SQD	A	411	39/54	0.88	0.12	43,73,96,111	0
32	UNL	C	521	28/-	0.88	0.11	35,50,62,67	0
33	LMG	C	519	48/55	0.88	0.12	53,85,105,121	0
27	SQD	a	412	36/54	0.88	0.12	40,72,101,113	0
33	LMG	D	411	28/55	0.88	0.12	34,58,76,80	0
26	PL9	a	410	55/55	0.88	0.12	42,77,101,112	0
32	UNL	d	412	43/-	0.88	0.12	50,62,78,83	0
32	UNL	M	103	26/-	0.88	0.13	36,54,72,72	0
27	SQD	B	621	54/54	0.89	0.10	43,67,104,121	0
33	LMG	C	501	48/55	0.89	0.10	40,67,86,111	0
33	LMG	c	519	37/55	0.89	0.11	45,74,99,105	0
23	CLA	c	512	65/65	0.89	0.11	45,68,99,114	0
32	UNL	E	102	28/-	0.89	0.13	66,88,97,103	0
23	CLA	B	601	65/65	0.90	0.10	36,65,116,139	0
32	UNL	C	522	28/-	0.90	0.11	41,61,81,83	0
27	SQD	f	101	41/54	0.90	0.13	58,91,129,142	0
32	UNL	B	622	34/-	0.90	0.10	38,55,71,72	0
23	CLA	C	514	65/65	0.90	0.11	48,77,110,115	0
25	BCR	d	405	40/40	0.90	0.10	39,59,110,121	0
33	LMG	c	524	49/55	0.90	0.10	31,60,96,125	0
25	BCR	x	102	40/40	0.90	0.10	40,62,84,87	0
33	LMG	m	101	51/55	0.90	0.10	37,60,85,98	0
32	UNL	I	101	41/-	0.91	0.12	42,62,95,99	0
32	UNL	J	101	28/-	0.91	0.12	48,62,74,75	0
27	SQD	b	601	49/54	0.91	0.10	47,68,101,117	0
25	BCR	K	101	40/40	0.91	0.09	38,60,75,91	0
27	SQD	a	411	54/54	0.91	0.10	45,75,97,102	0
28	DGD	C	517	62/66	0.91	0.09	40,62,111,122	0
32	UNL	D	412	55/-	0.91	0.11	35,65,88,94	0
25	BCR	k	101	40/40	0.91	0.10	45,71,86,89	0
28	DGD	c	517	62/66	0.91	0.10	37,62,94,112	0
29	LHG	d	407	49/49	0.92	0.10	38,59,98,112	0
25	BCR	b	620	40/40	0.92	0.08	34,58,75,80	0
25	BCR	c	514	40/40	0.92	0.09	44,65,80,80	0
33	LMG	M	101	51/55	0.92	0.09	33,54,75,89	0
25	BCR	B	619	40/40	0.92	0.08	33,49,66,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UNL	l	102	53/-	0.92	0.12	36,55,96,102	0
32	UNL	B	623	28/-	0.92	0.09	36,52,70,76	0
25	BCR	D	405	40/40	0.92	0.09	34,50,95,115	0
23	CLA	c	513	65/65	0.92	0.10	47,74,109,113	0
33	LMG	d	411	44/55	0.92	0.09	41,63,94,112	0
25	BCR	Z	101	40/40	0.92	0.09	41,63,81,84	0
28	DGD	h	101	62/66	0.93	0.09	35,55,69,73	0
25	BCR	B	618	40/40	0.93	0.07	29,45,68,69	0
25	BCR	H	101	40/40	0.93	0.09	35,51,65,69	0
23	CLA	c	503	65/65	0.93	0.08	33,54,68,71	0
25	BCR	T	101	40/40	0.93	0.07	30,50,64,70	0
27	SQD	A	410	52/54	0.93	0.09	37,68,94,102	0
32	UNL	M	102	37/-	0.93	0.09	37,51,63,73	0
25	BCR	B	617	40/40	0.94	0.08	32,48,61,67	0
23	CLA	c	504	60/65	0.94	0.08	36,54,83,87	0
25	BCR	c	515	40/40	0.94	0.09	32,52,66,80	0
25	BCR	c	521	40/40	0.94	0.09	39,61,68,74	0
28	DGD	H	102	62/66	0.94	0.08	32,52,68,76	0
23	CLA	c	506	65/65	0.94	0.09	35,60,114,126	0
25	BCR	C	515	40/40	0.94	0.09	24,46,60,75	0
28	DGD	c	518	62/66	0.94	0.08	30,63,82,92	0
25	BCR	C	520	40/40	0.94	0.10	42,60,75,79	0
33	LMG	D	407	51/55	0.94	0.09	34,64,86,98	0
29	LHG	D	409	47/49	0.94	0.09	36,56,90,108	0
23	CLA	c	508	64/65	0.94	0.08	32,54,97,122	0
23	CLA	c	509	65/65	0.94	0.10	37,56,73,83	0
29	LHG	d	409	39/49	0.94	0.09	35,56,75,81	0
23	CLA	c	511	65/65	0.94	0.10	45,66,85,88	0
23	CLA	b	617	60/65	0.94	0.08	33,50,94,105	0
23	CLA	B	616	60/65	0.94	0.08	24,45,91,96	0
27	SQD	F	101	36/54	0.94	0.10	48,76,102,107	0
25	BCR	b	618	40/40	0.94	0.07	31,50,67,67	0
25	BCR	b	619	40/40	0.94	0.07	33,46,58,62	0
23	CLA	C	509	65/65	0.95	0.07	28,51,114,130	0
23	CLA	C	510	65/65	0.95	0.08	35,51,71,72	0
23	CLA	c	510	65/65	0.95	0.08	39,57,78,89	0
29	LHG	A	413	49/49	0.95	0.08	31,53,82,87	0
23	CLA	C	512	65/65	0.95	0.08	37,58,76,83	0
23	CLA	C	513	65/65	0.95	0.09	35,62,112,146	0
23	CLA	B	615	65/65	0.95	0.07	27,46,70,81	0
25	BCR	t	101	40/40	0.95	0.07	31,45,57,65	0
23	CLA	d	402	65/65	0.95	0.07	26,39,50,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LHG	l	101	49/49	0.95	0.07	38,51,63,81	0
23	CLA	d	404	65/65	0.95	0.09	31,56,111,137	0
25	BCR	A	408	40/40	0.95	0.06	25,37,50,51	0
26	PL9	d	406	55/55	0.95	0.07	27,41,49,54	0
23	CLA	a	408	65/65	0.95	0.08	22,41,107,114	0
23	CLA	B	606	65/65	0.95	0.08	26,43,85,94	0
23	CLA	b	607	65/65	0.95	0.07	30,48,78,87	0
23	CLA	b	611	65/65	0.95	0.07	26,41,59,70	0
23	CLA	b	615	65/65	0.95	0.08	24,46,85,89	0
23	CLA	C	503	65/65	0.95	0.07	37,51,67,80	0
23	CLA	c	501	65/65	0.95	0.07	30,46,58,67	0
23	CLA	c	502	65/65	0.95	0.07	36,52,71,82	0
23	CLA	C	504	65/65	0.95	0.07	30,50,63,68	0
28	DGD	C	516	62/66	0.95	0.08	27,44,87,103	0
23	CLA	C	506	65/65	0.95	0.08	27,46,69,79	0
28	DGD	C	518	62/66	0.95	0.08	32,58,86,104	0
23	CLA	c	505	65/65	0.95	0.08	31,48,70,79	0
23	CLA	C	507	65/65	0.95	0.08	27,49,103,114	0
26	PL9	D	406	55/55	0.96	0.07	22,38,49,55	0
23	CLA	D	404	65/65	0.96	0.08	26,47,133,138	0
23	CLA	a	405	65/65	0.96	0.06	25,37,55,65	0
23	CLA	a	406	65/65	0.96	0.08	31,48,99,114	0
23	CLA	B	603	65/65	0.96	0.07	26,42,69,76	0
23	CLA	C	502	65/65	0.96	0.06	25,43,59,68	0
23	CLA	d	403	65/65	0.96	0.07	24,41,75,83	0
23	CLA	b	603	65/65	0.96	0.08	28,50,75,82	0
24	PHO	D	401	64/64	0.96	0.06	26,37,47,51	0
24	PHO	a	407	64/64	0.96	0.07	24,36,48,50	0
24	PHO	d	401	64/64	0.96	0.07	32,45,59,68	0
23	CLA	b	604	65/65	0.96	0.07	28,44,70,74	0
23	CLA	b	605	65/65	0.96	0.07	25,42,84,98	0
23	CLA	b	606	65/65	0.96	0.07	27,43,57,61	0
23	CLA	B	604	65/65	0.96	0.08	25,41,92,98	0
23	CLA	b	608	65/65	0.96	0.07	23,42,73,81	0
23	CLA	b	609	65/65	0.96	0.07	27,48,72,79	0
28	DGD	c	516	62/66	0.96	0.07	25,46,78,94	0
23	CLA	b	610	65/65	0.96	0.07	27,48,67,93	0
23	CLA	B	605	65/65	0.96	0.07	23,39,55,60	0
23	CLA	b	613	65/65	0.96	0.07	24,40,56,65	0
23	CLA	b	614	65/65	0.96	0.07	23,41,92,97	0
23	CLA	C	505	59/65	0.96	0.07	30,52,92,107	0
25	BCR	a	409	40/40	0.96	0.06	25,42,57,63	0

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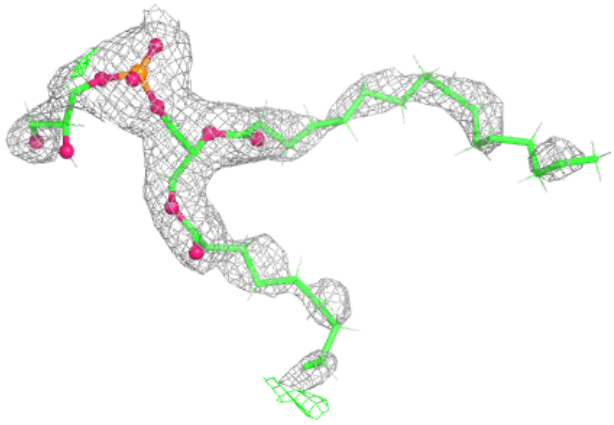
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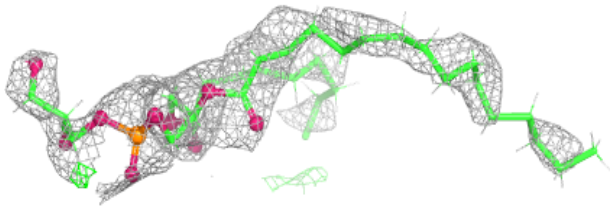
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LHG	L	101	49/49	0.96	0.07	31,46,63,69	0
23	CLA	b	616	65/65	0.96	0.07	33,48,69,80	0
23	CLA	A	405	65/65	0.96	0.08	23,41,104,122	0
23	CLA	B	607	65/65	0.96	0.07	18,41,77,85	0
23	CLA	C	508	65/65	0.96	0.07	29,44,66,71	0
31	BCT	a	404	4/4	0.96	0.09	27,36,48,58	0
23	CLA	B	609	65/65	0.96	0.07	23,42,59,66	0
23	CLA	B	610	65/65	0.96	0.07	25,39,55,62	0
23	CLA	C	511	65/65	0.96	0.07	35,55,81,86	0
23	CLA	B	613	65/65	0.96	0.07	24,36,71,82	0
23	CLA	c	507	65/65	0.96	0.07	35,51,66,69	0
23	CLA	B	614	65/65	0.96	0.08	25,46,93,105	0
23	CLA	B	602	65/65	0.96	0.07	28,44,72,77	0
24	PHO	A	406	64/64	0.97	0.06	20,35,49,55	0
23	CLA	D	402	65/65	0.97	0.06	22,35,54,60	0
31	BCT	A	415	4/4	0.97	0.09	32,35,39,42	0
23	CLA	D	403	65/65	0.97	0.06	22,37,58,68	0
23	CLA	b	612	65/65	0.97	0.06	26,38,58,62	0
29	LHG	D	408	49/49	0.97	0.06	30,46,62,65	0
23	CLA	A	404	65/65	0.97	0.06	19,33,54,68	0
23	CLA	B	611	65/65	0.97	0.06	20,34,47,48	0
23	CLA	B	612	65/65	0.97	0.06	23,38,55,59	0
23	CLA	B	608	65/65	0.97	0.05	24,40,58,65	0
29	LHG	d	408	49/49	0.97	0.07	27,48,66,67	0
23	CLA	A	407	54/65	0.97	0.07	25,38,83,85	0
34	HEM	E	103	43/43	0.97	0.08	39,53,69,76	0
34	HEM	e	102	43/43	0.97	0.09	46,63,79,83	0
22	CL	a	402	1/1	0.98	0.04	34,34,34,34	0
35	HEC	V	201	43/43	0.98	0.05	28,38,50,51	0
30	OEX	a	415	10/10	0.99	0.03	29,33,38,39	0
22	CL	A	402	1/1	0.99	0.03	36,36,36,36	0
22	CL	A	403	1/1	0.99	0.03	36,36,36,36	0
21	FE2	a	401	1/1	0.99	0.03	39,39,39,39	0
22	CL	a	403	1/1	0.99	0.10	32,32,32,32	0
35	HEC	v	201	43/43	0.99	0.06	37,45,57,61	0
30	OEX	A	414	10/10	1.00	0.03	31,36,39,42	0
21	FE2	A	401	1/1	1.00	0.01	32,32,32,32	0

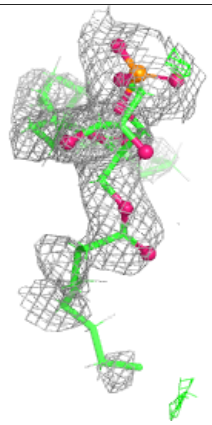
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

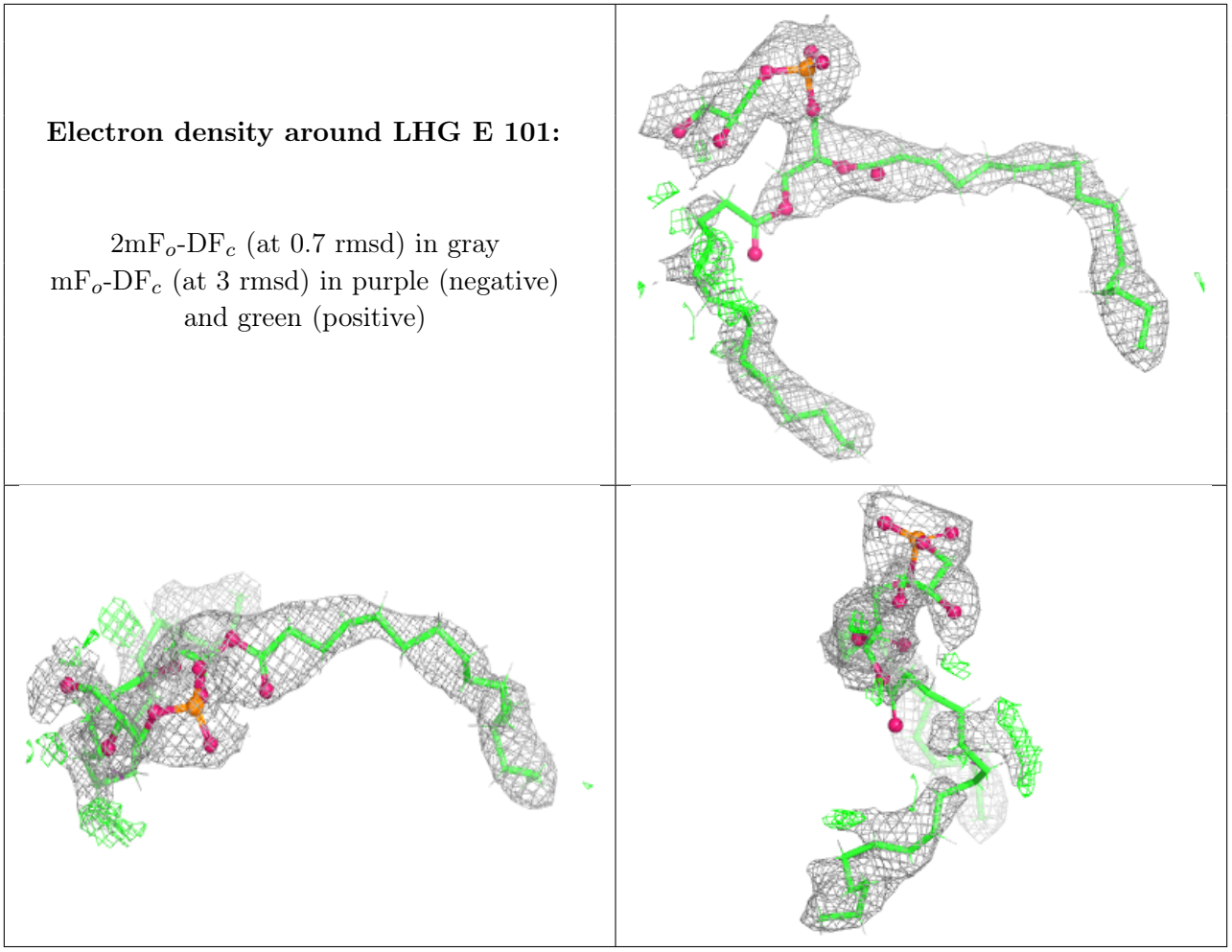






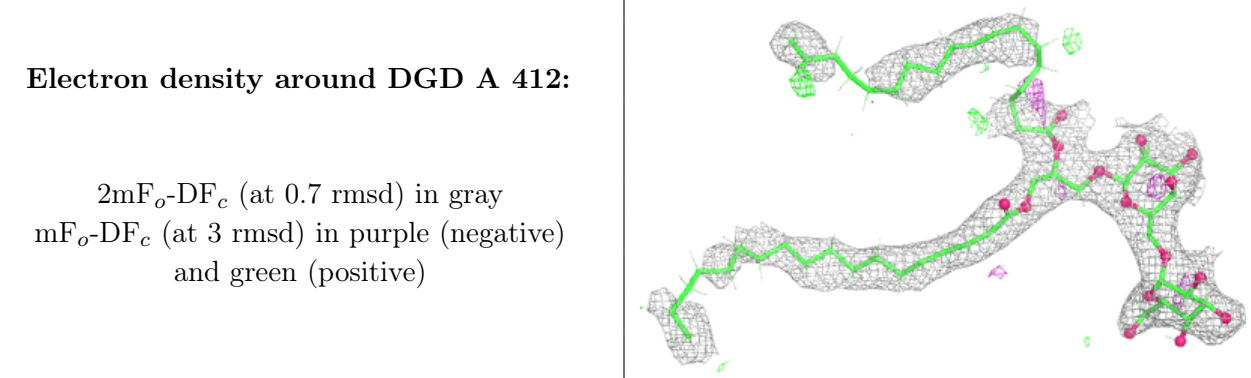
Electron density around LHG E 101:

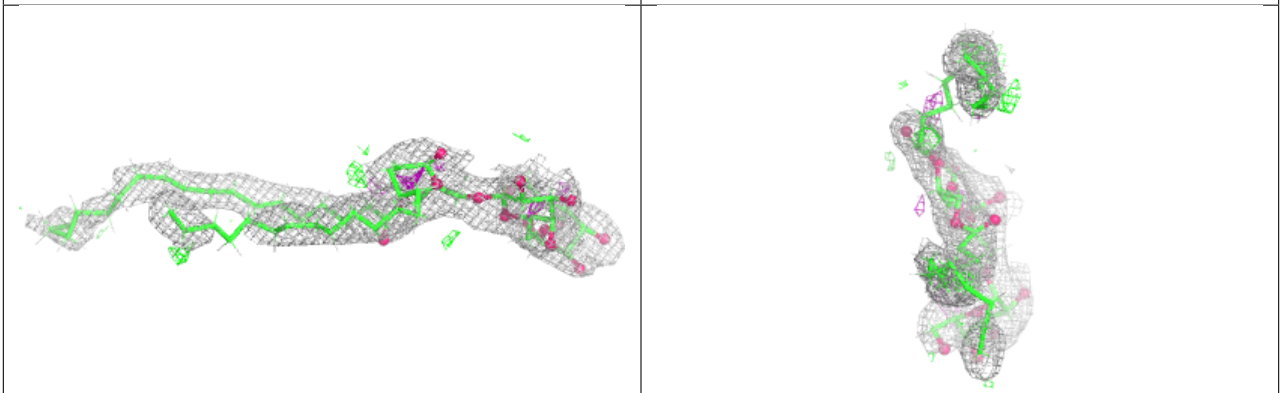
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD A 412:

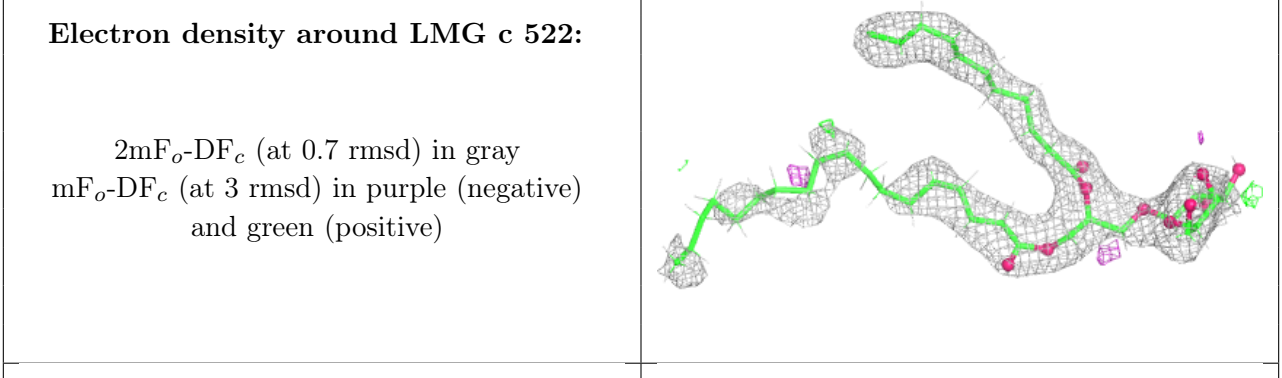
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

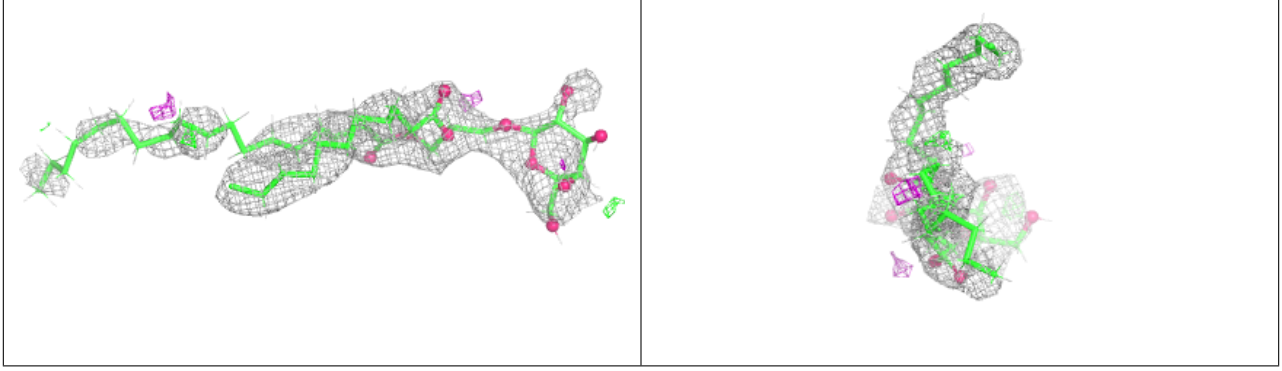




Electron density around LMG c 522:

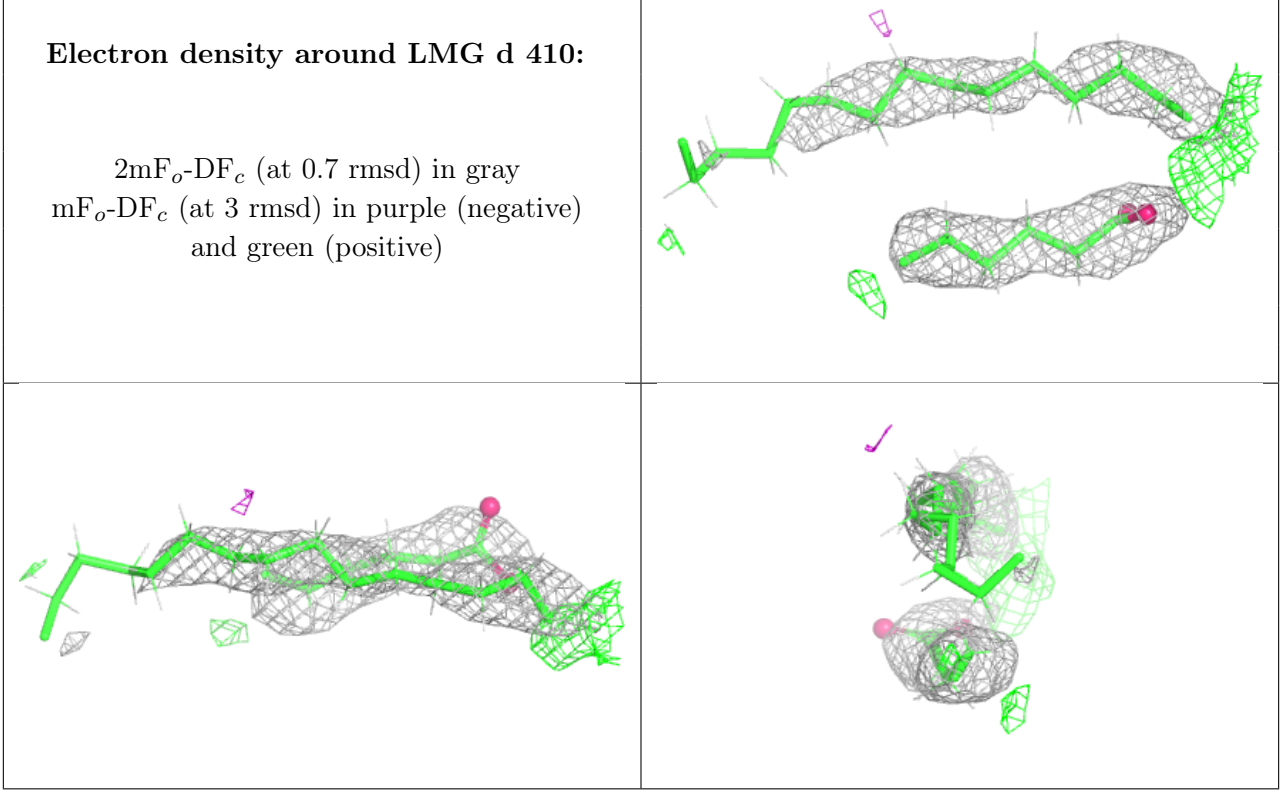
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





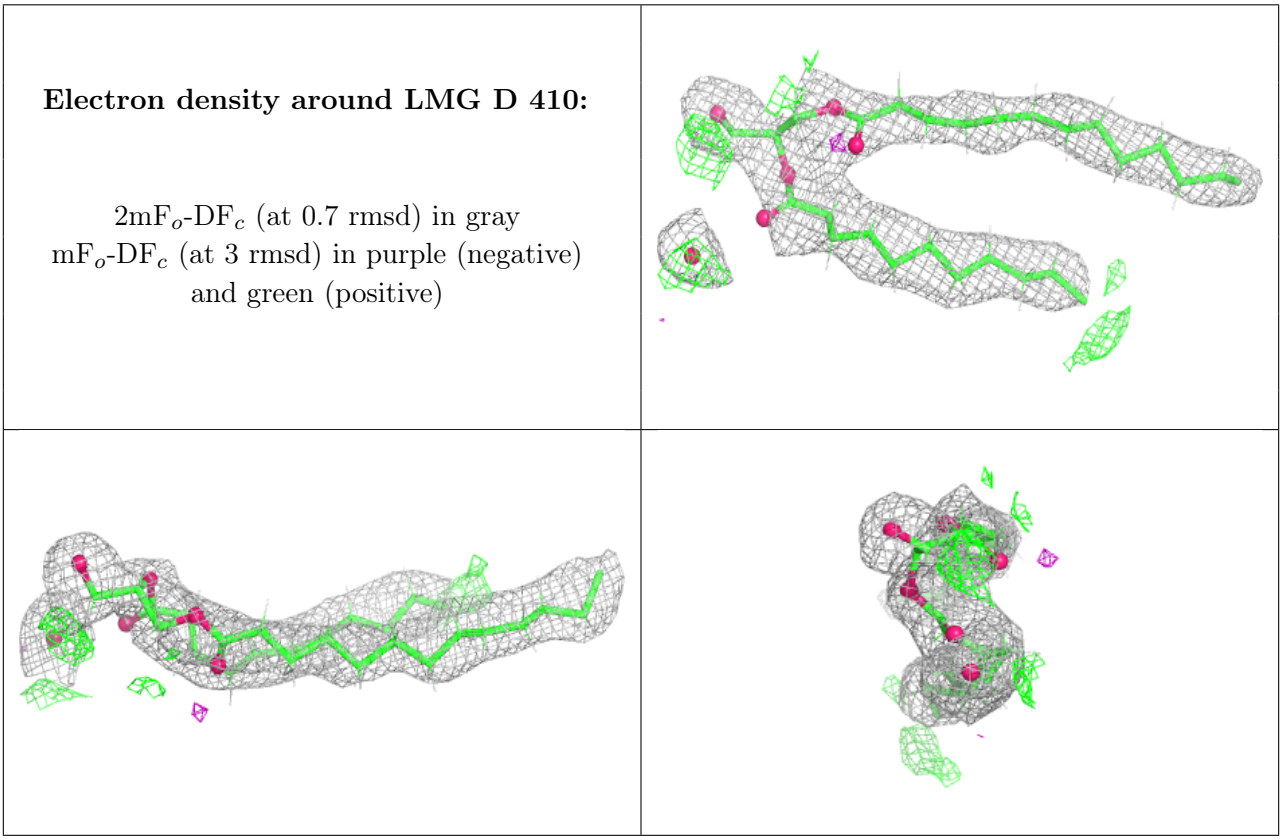
Electron density around LMG d 410:

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



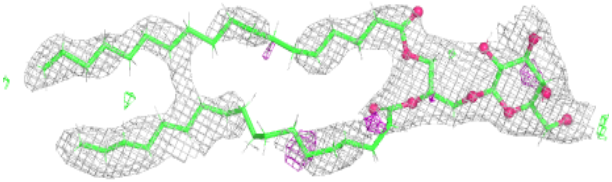
Electron density around LMG D 410:

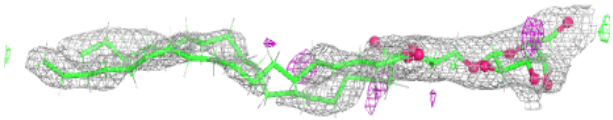
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

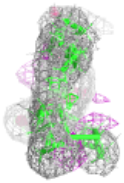


Electron density around LMG b 622:

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

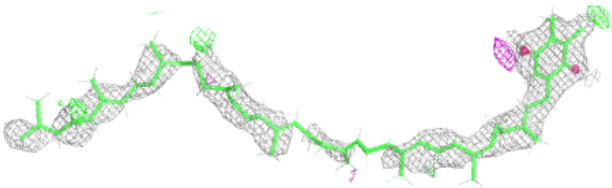


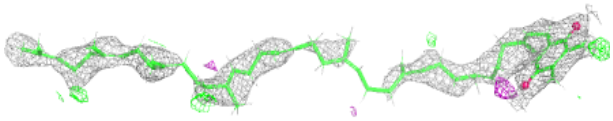




Electron density around PL9 A 409:

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

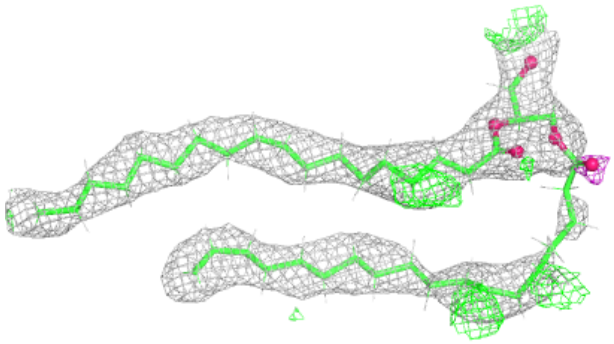


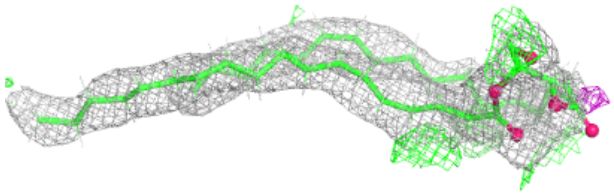


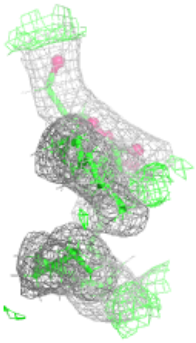


Electron density around DGD a 413:

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

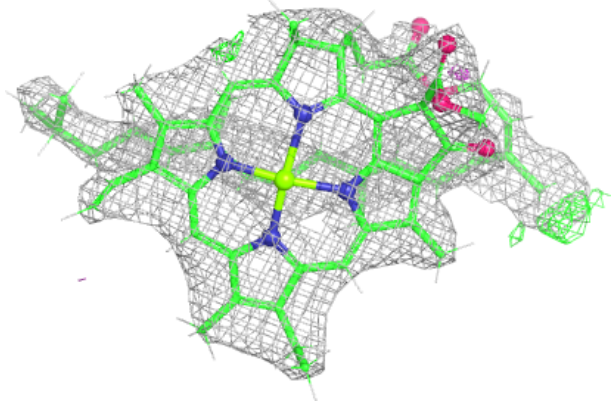


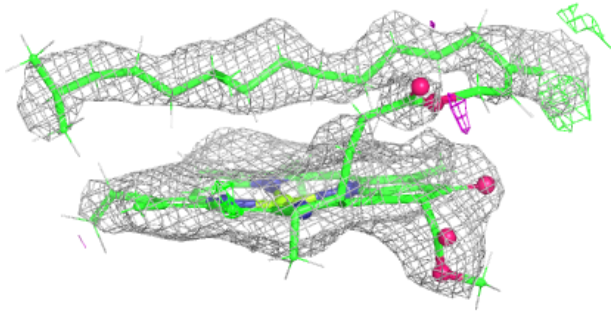


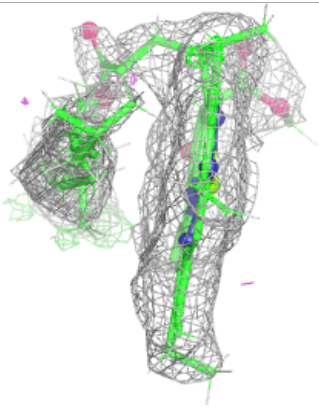


Electron density around CLA b 602:

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

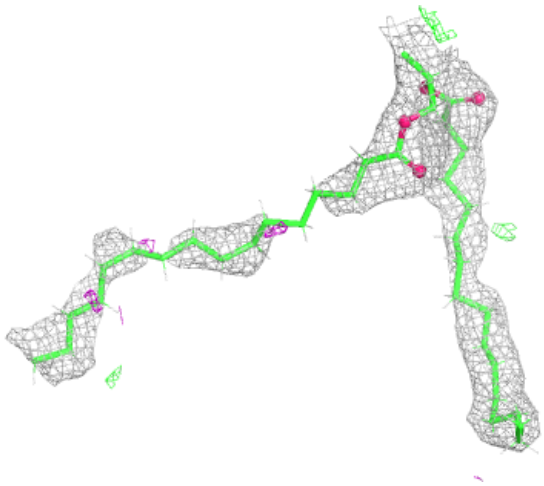


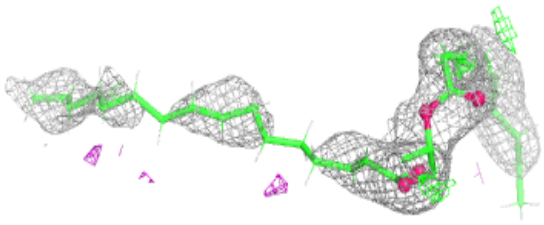


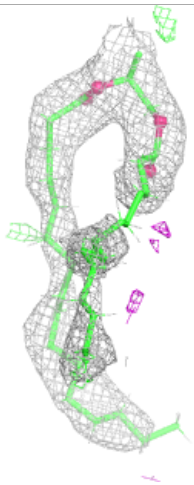


Electron density around SQD A 411:

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

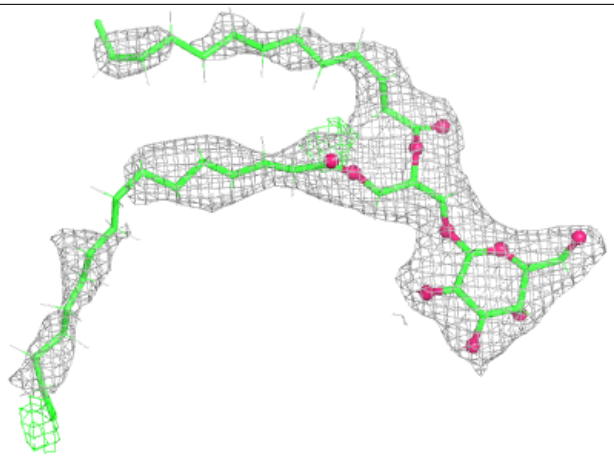


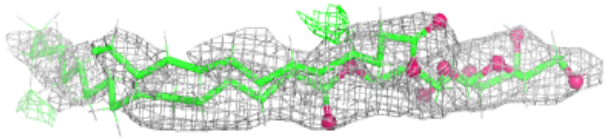


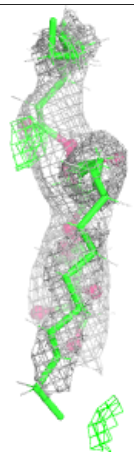


Electron density around LMG C 519:

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

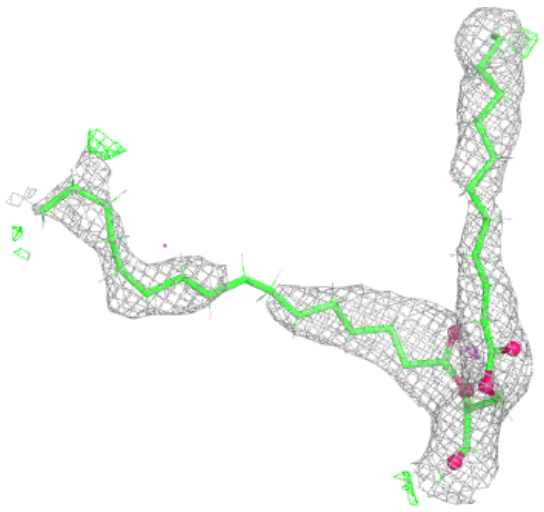


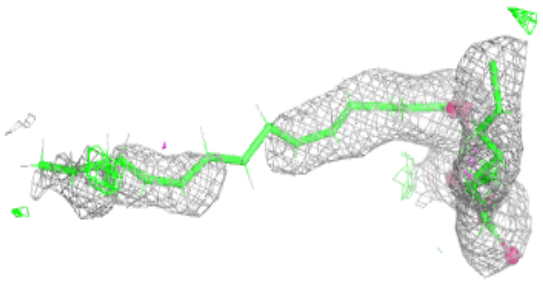


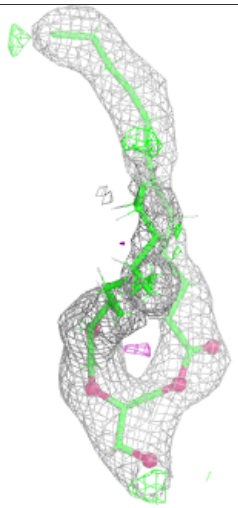


Electron density around SQD a 412:

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

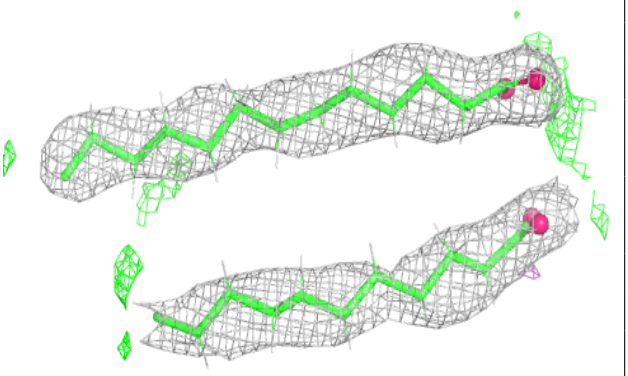


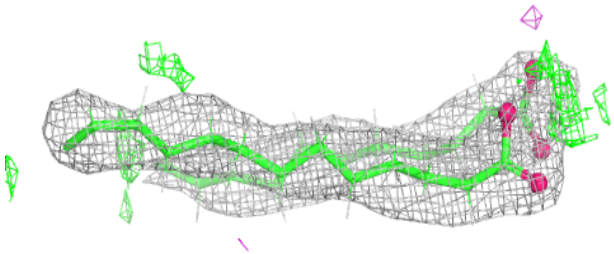


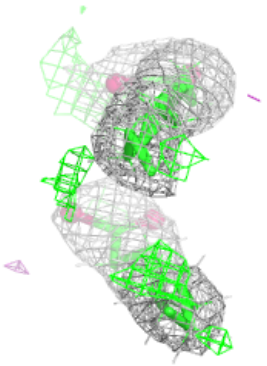


Electron density around LMG D 411:

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

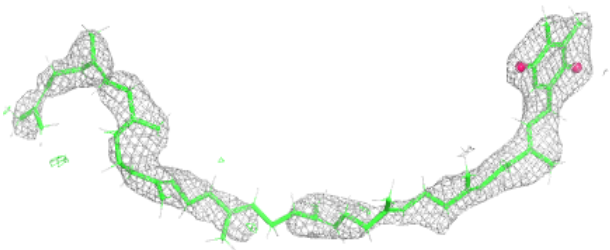


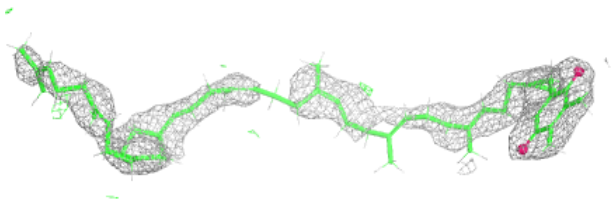


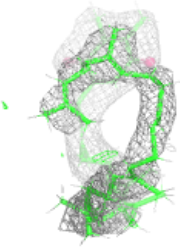


Electron density around PL9 a 410:

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

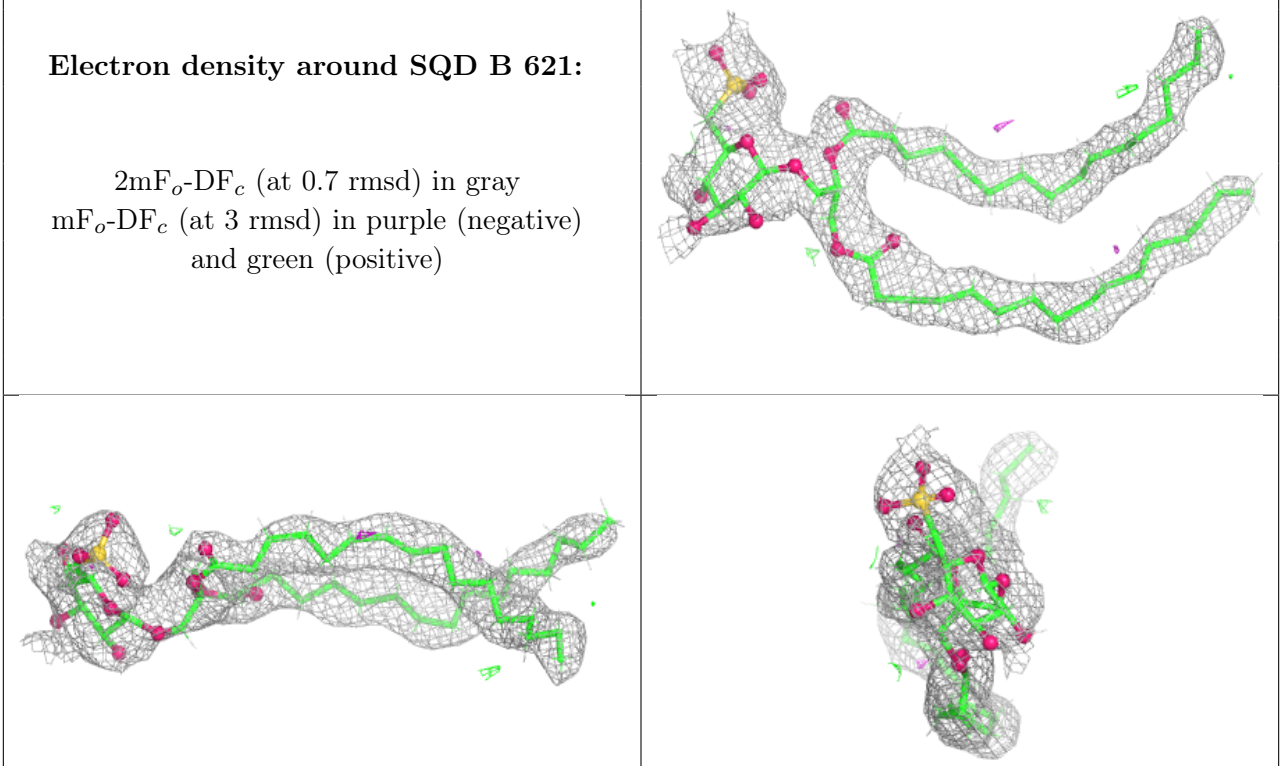






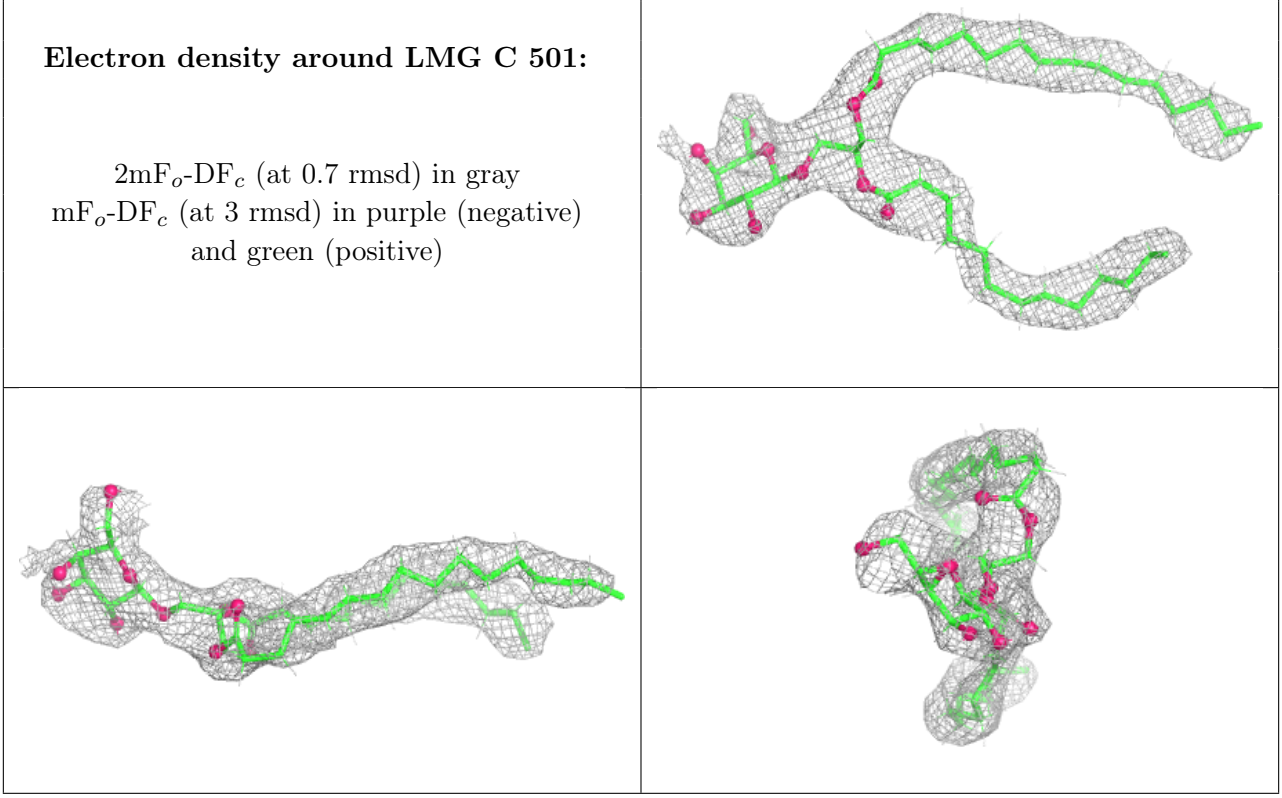
Electron density around SQD B 621:

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



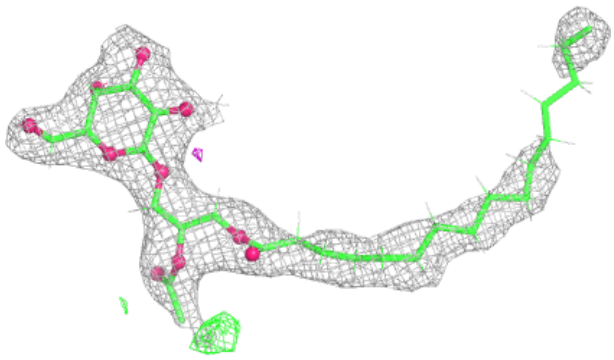
Electron density around LMG C 501:

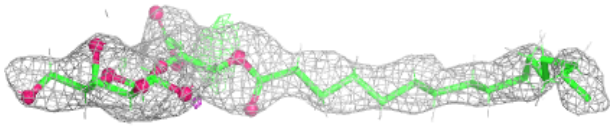
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

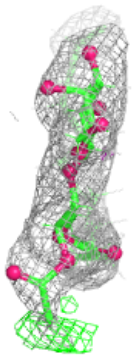


Electron density around LMG c 519:

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

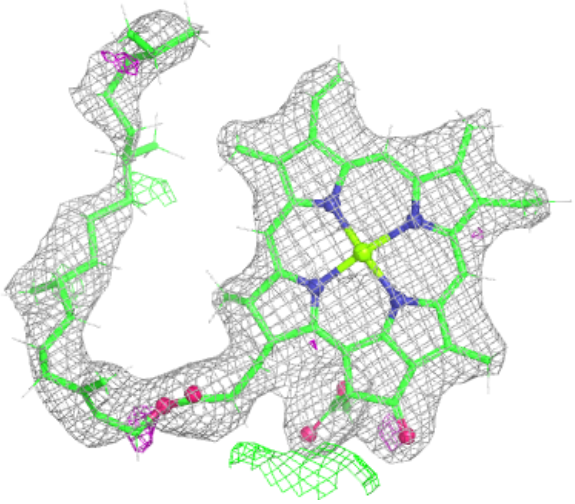


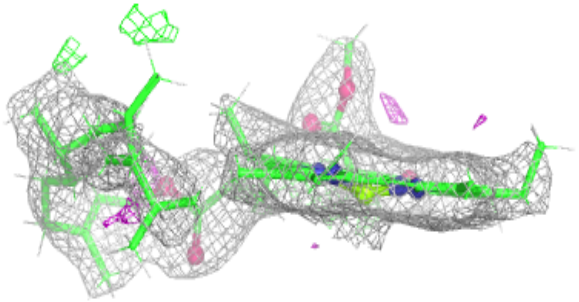


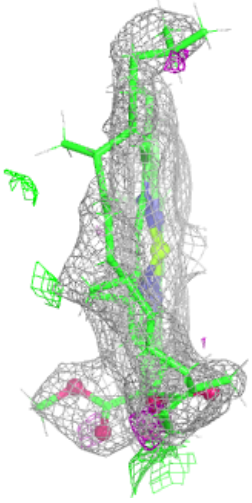


Electron density around CLA c 512:

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

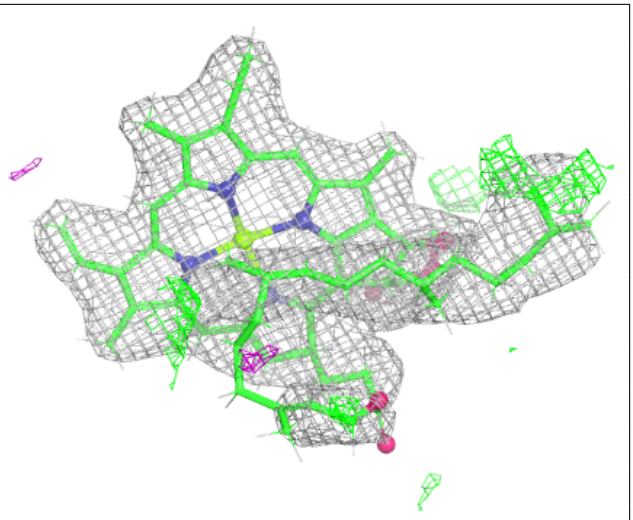


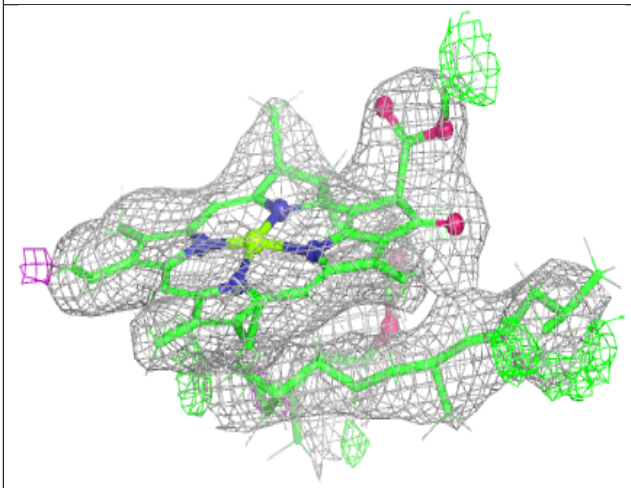


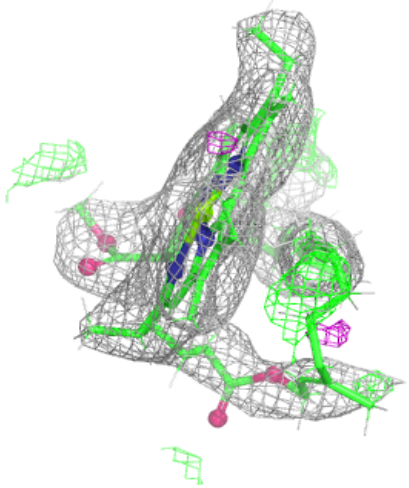


Electron density around CLA B 601:

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

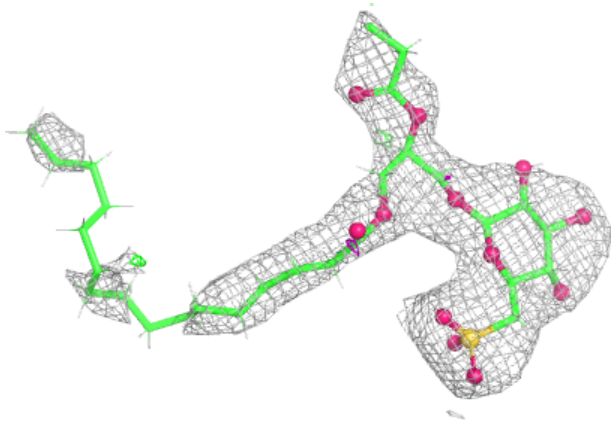


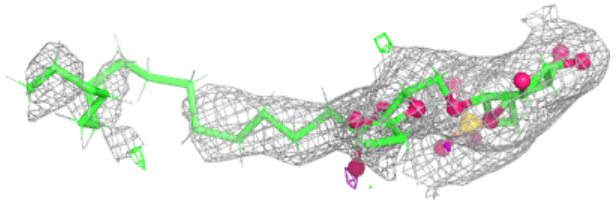


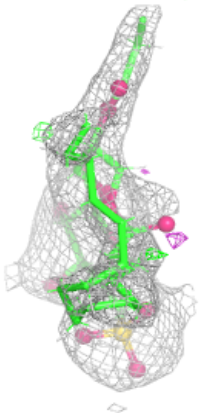


Electron density around SQD f 101:

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

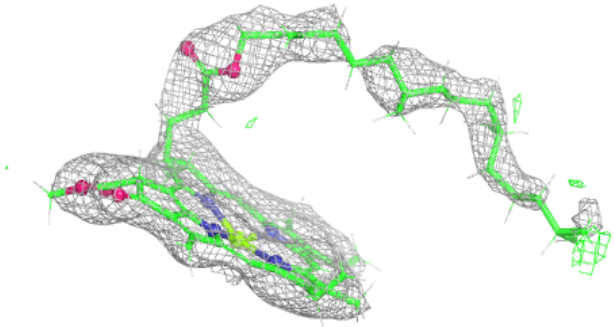


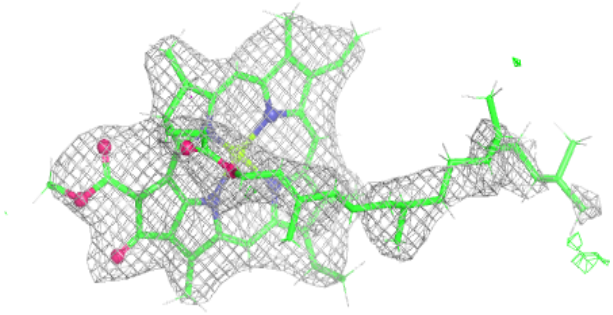


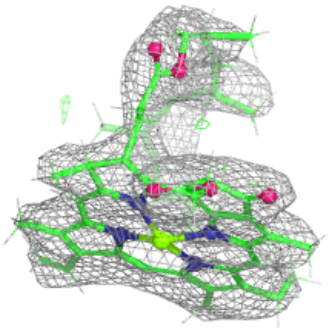


Electron density around CLA C 514:

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



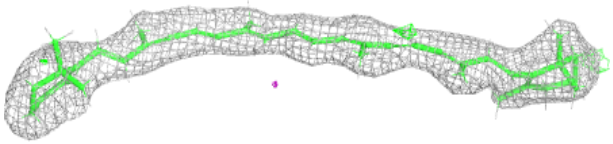


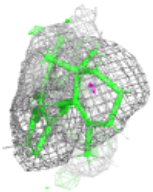


Electron density around BCR d 405:

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

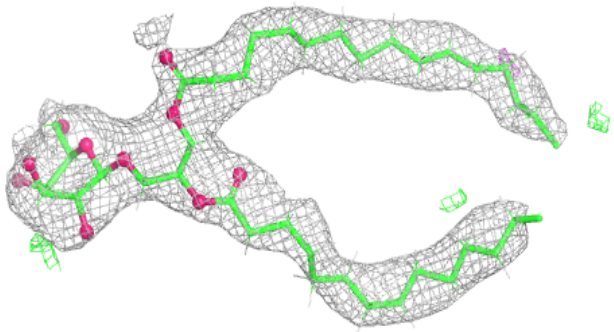


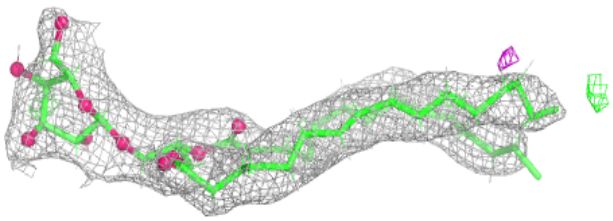


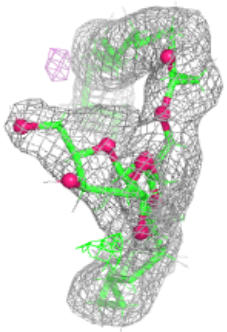


Electron density around LMG c 524:

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

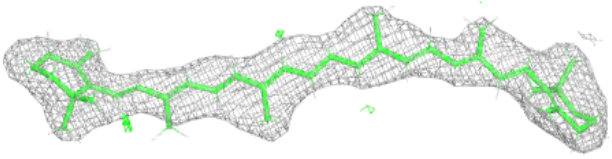


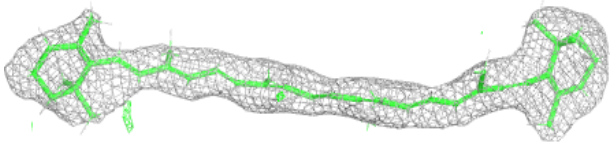


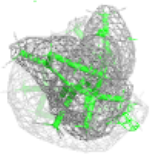


Electron density around BCR x 102:

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

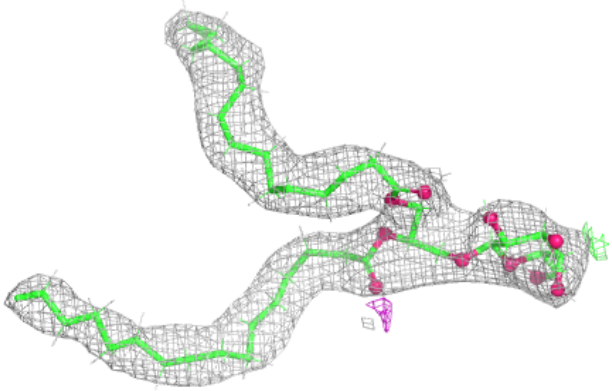


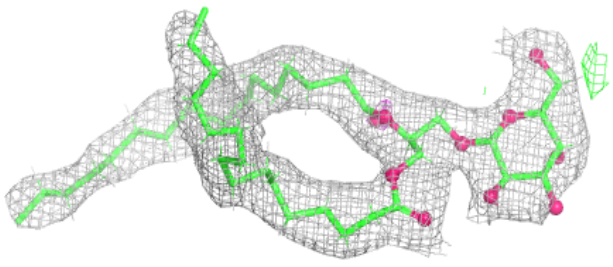




Electron density around LMG m 101:

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

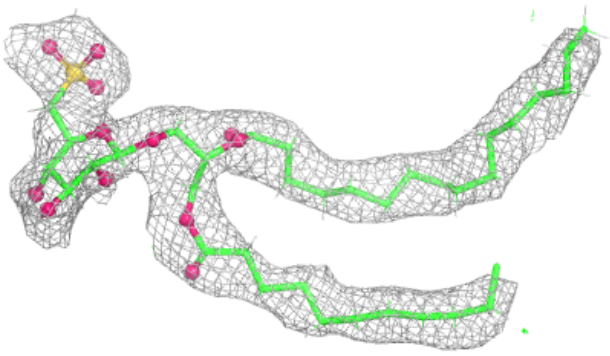


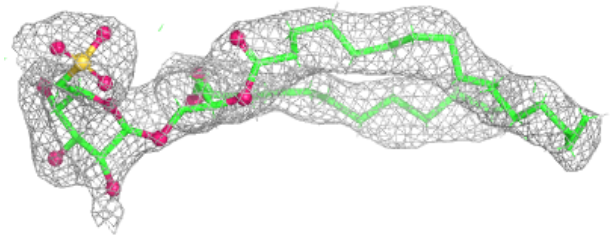


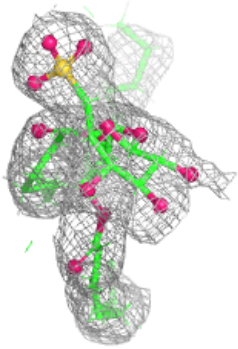


Electron density around SQD b 601:

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



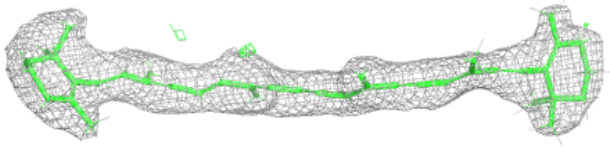


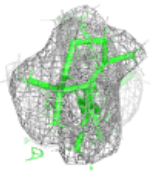


Electron density around BCR K 101:

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

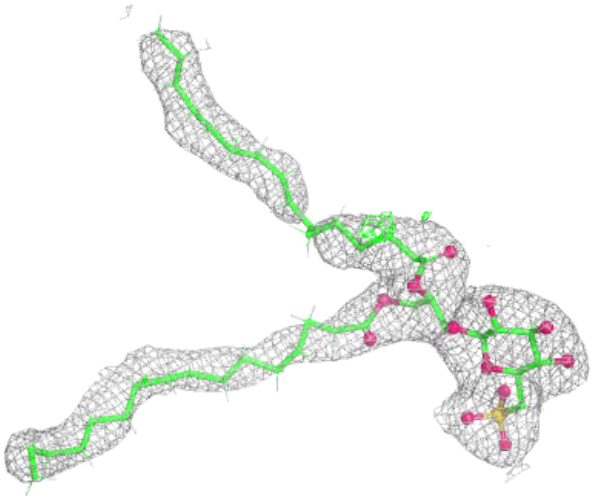


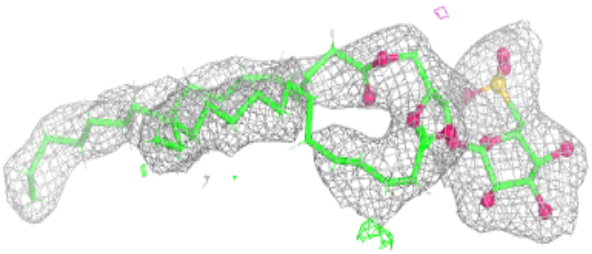


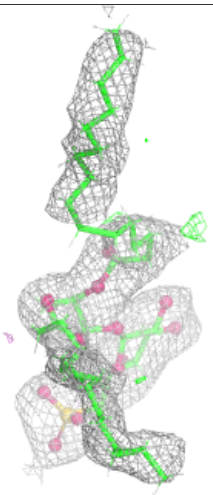


Electron density around SQD a 411:

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

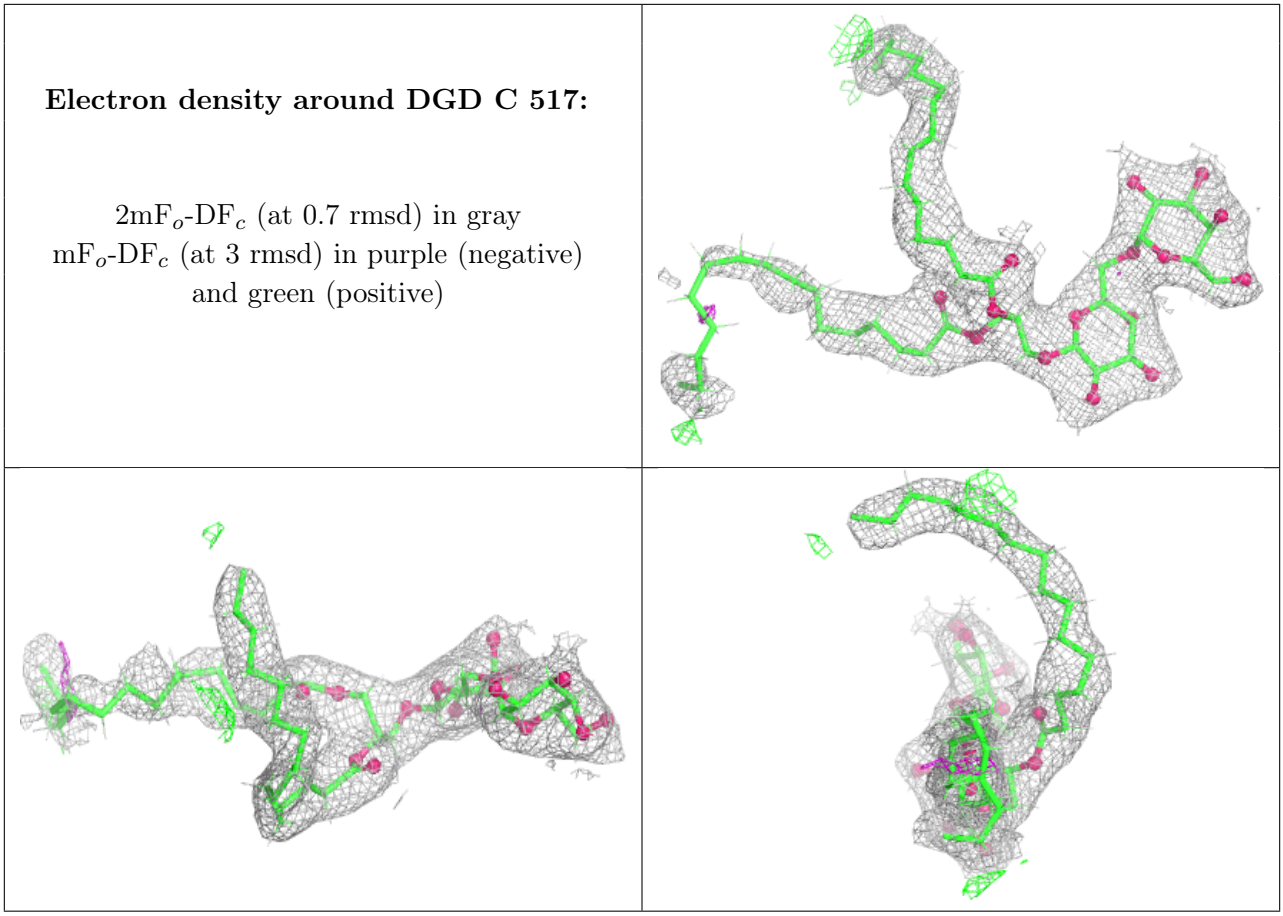






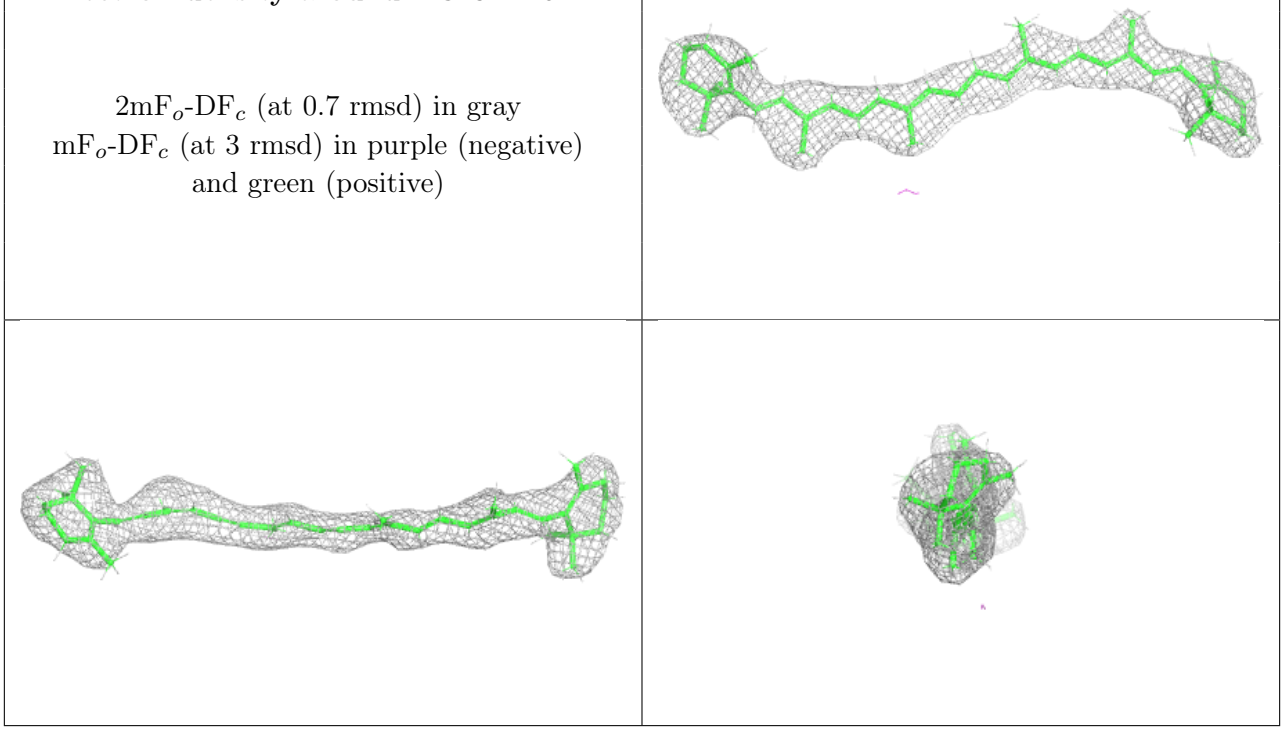
Electron density around DGD C 517:

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



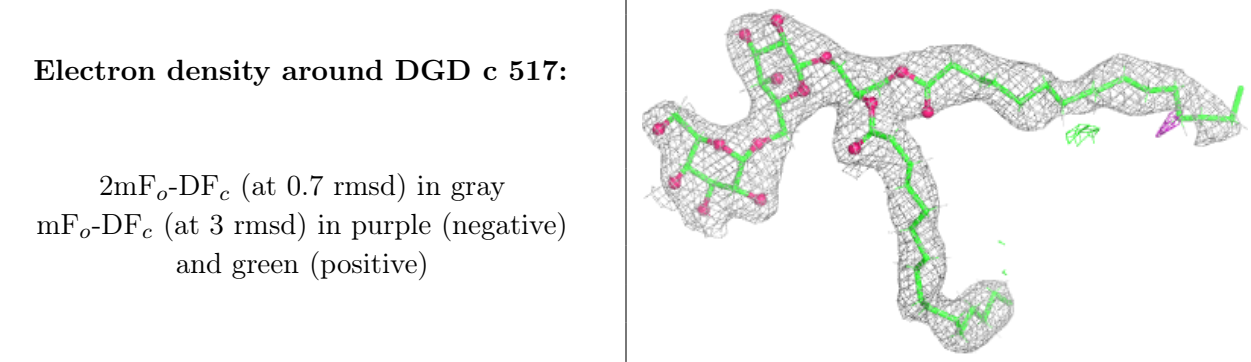
Electron density around BCR k 101:

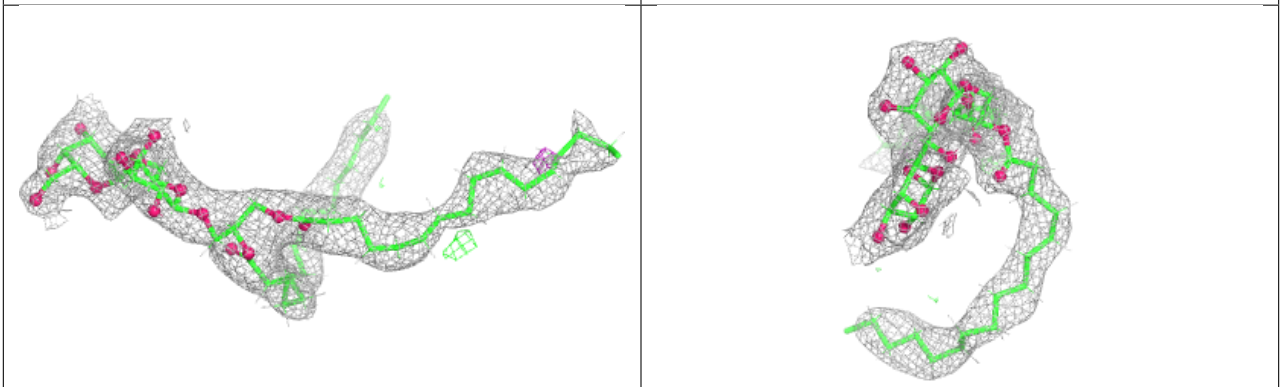
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD c 517:

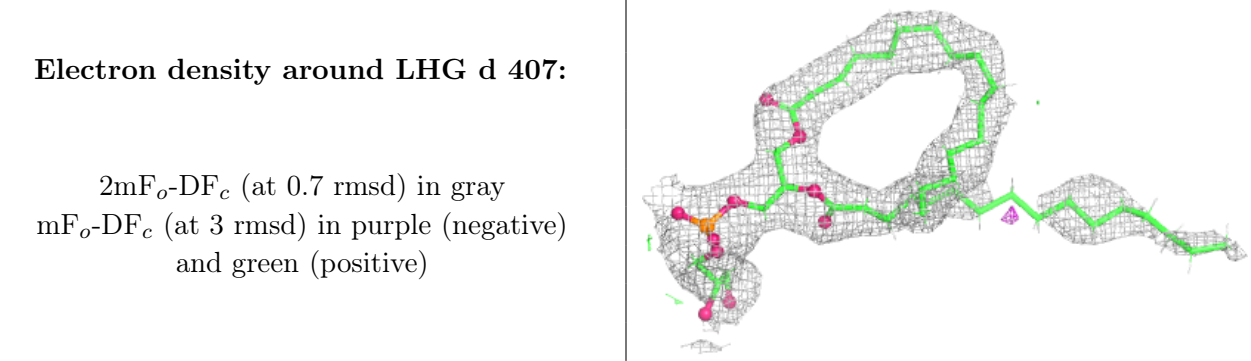
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

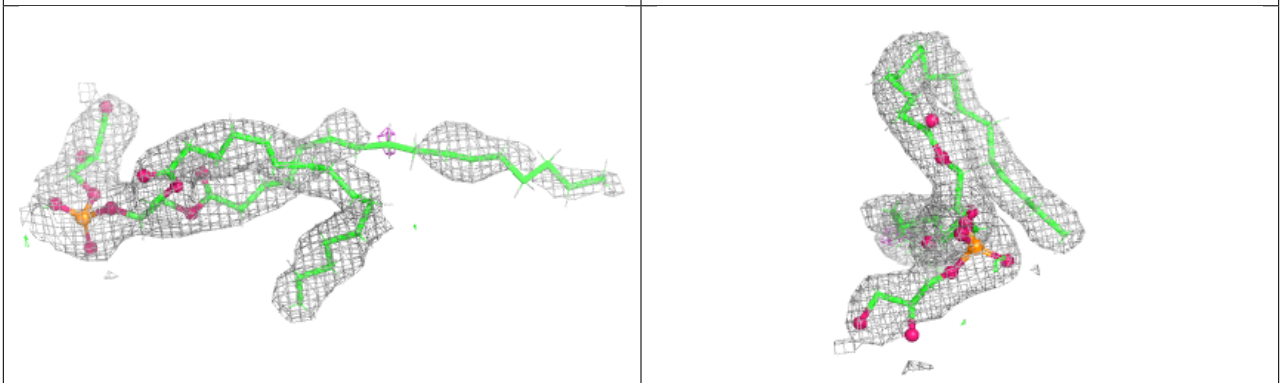




Electron density around LHG d 407:

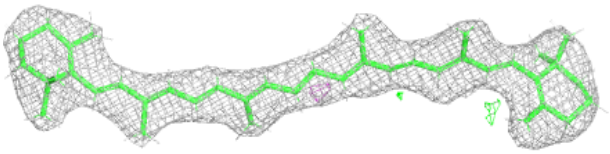
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

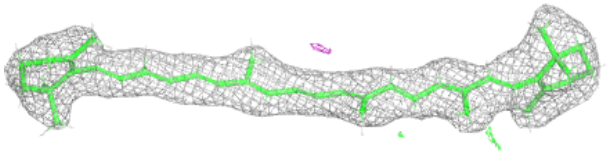


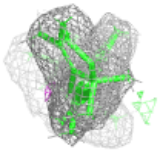


Electron density around BCR b 620:

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

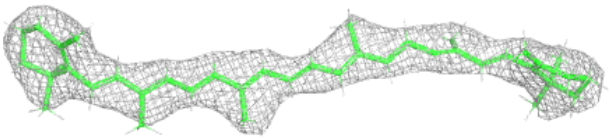


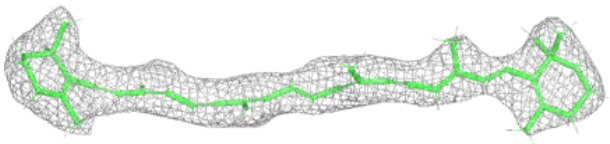


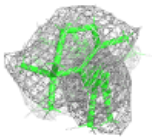


Electron density around BCR c 514:

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

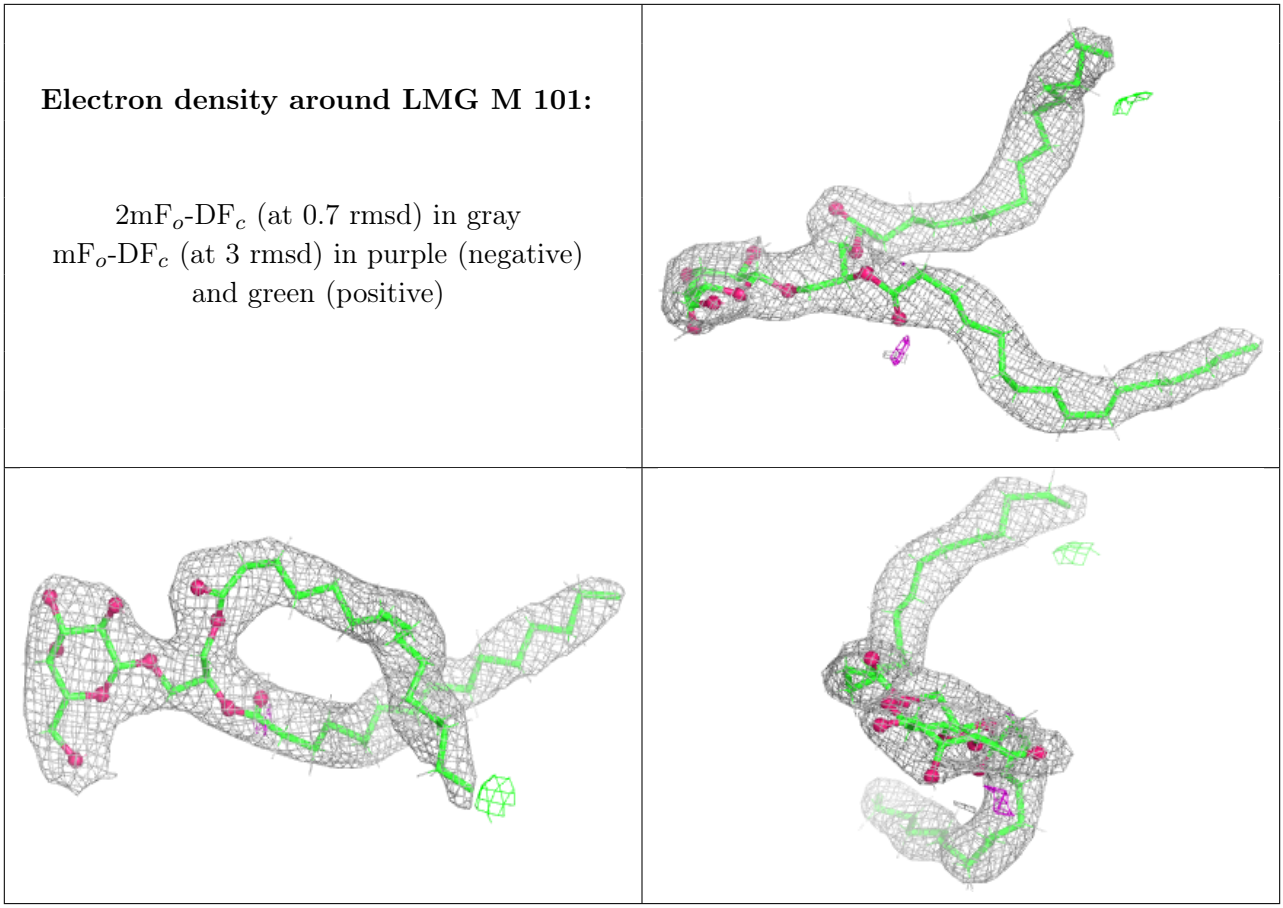






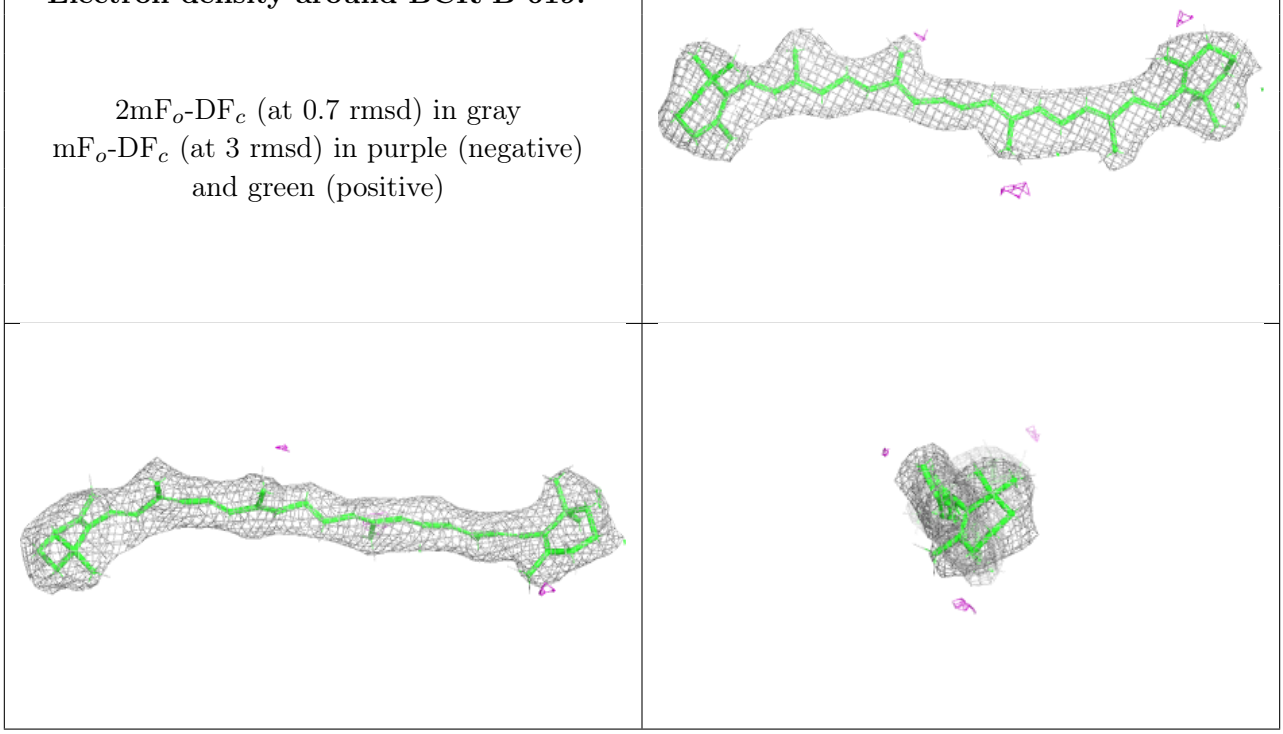
Electron density around LMG M 101:

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



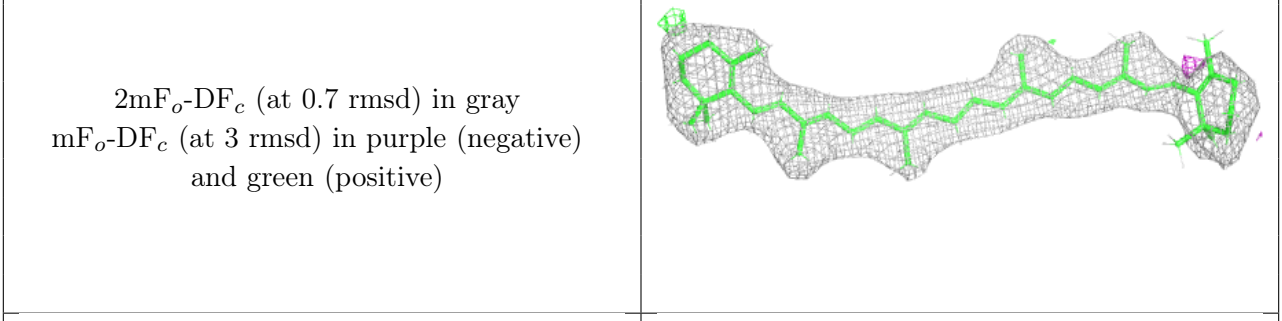
Electron density around BCR B 619:

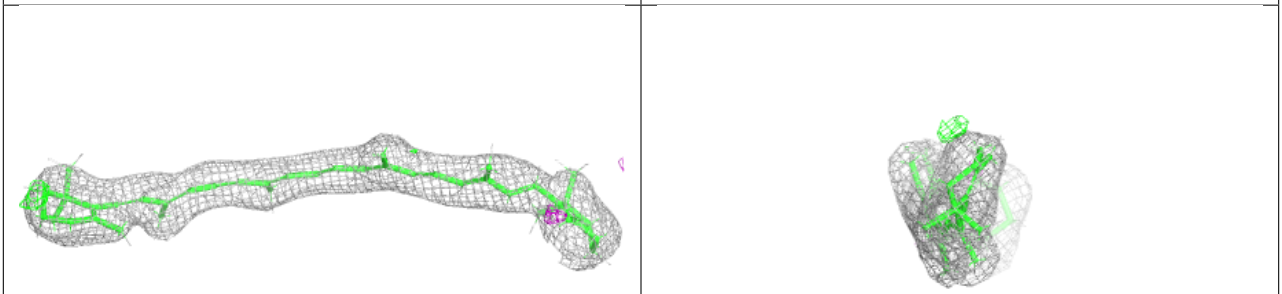
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCR D 405:

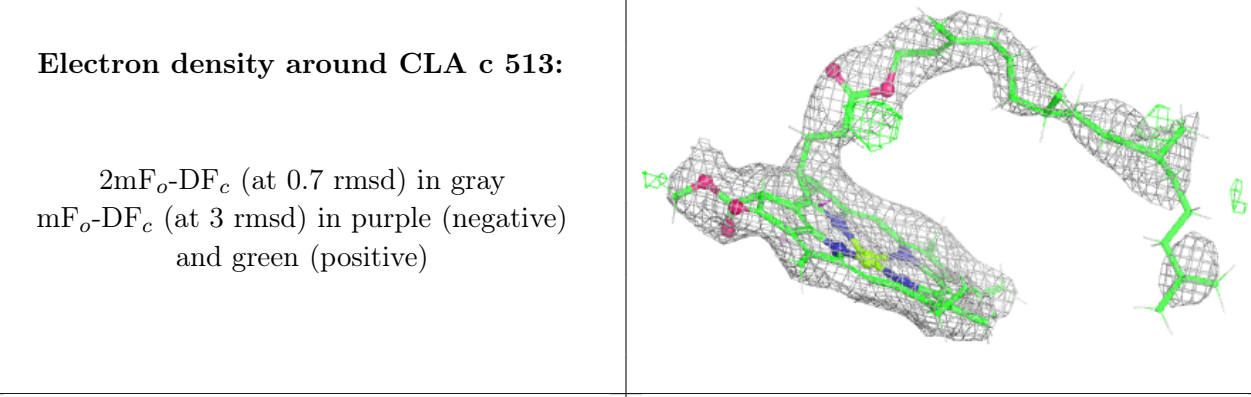
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

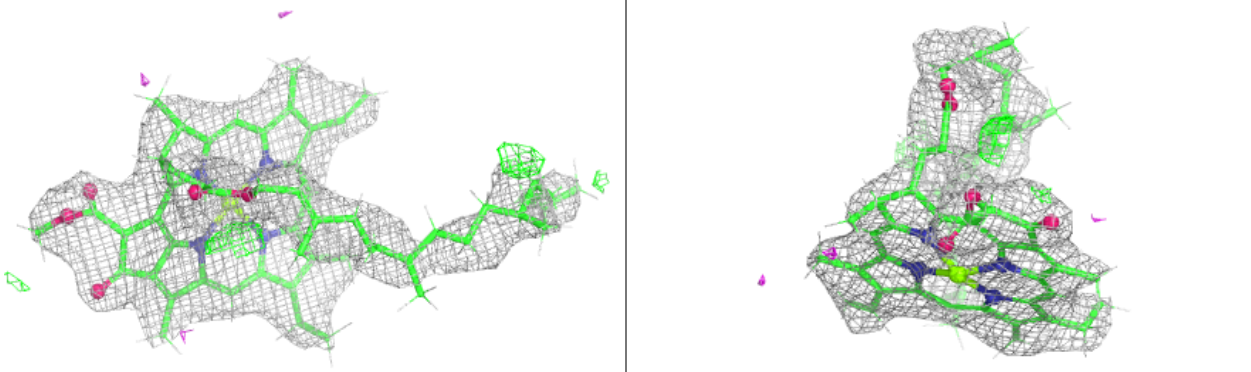




Electron density around CLA c 513:

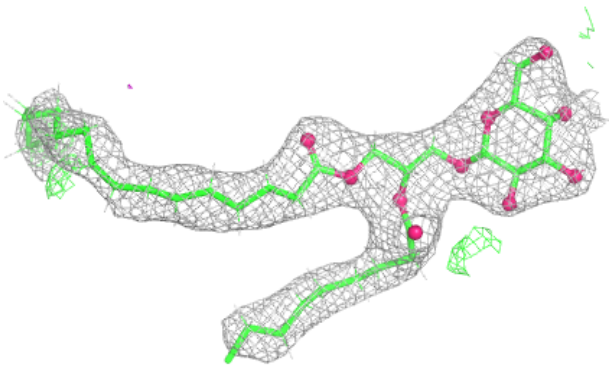
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

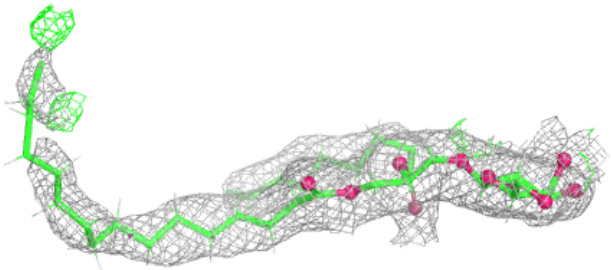


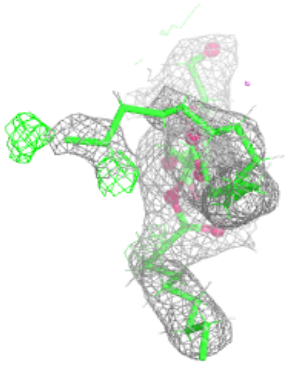


Electron density around LMG d 411:

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

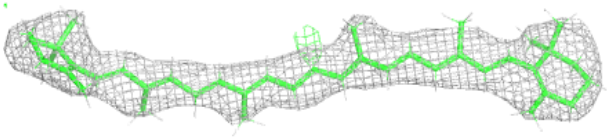




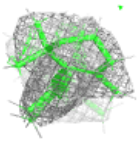


Electron density around BCR Z 101:

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

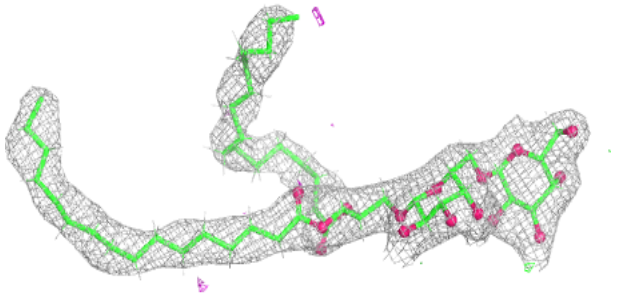


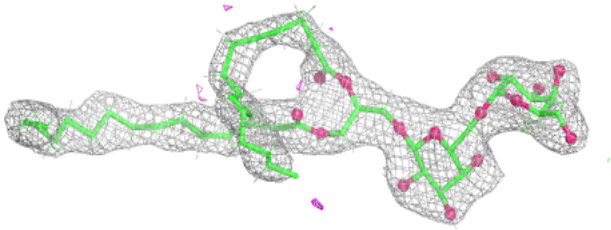


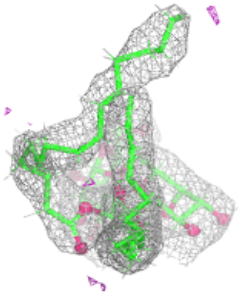


Electron density around DGD h 101:

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

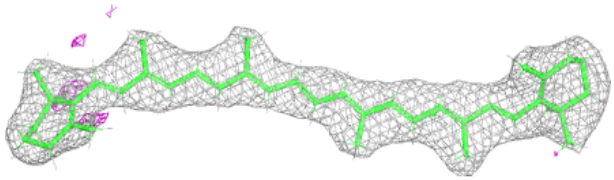


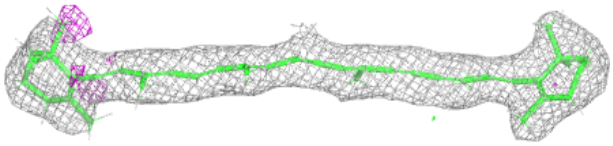


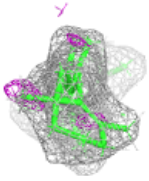


Electron density around BCR B 618:

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

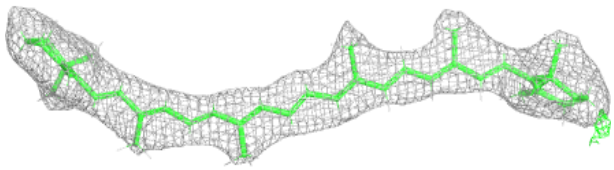


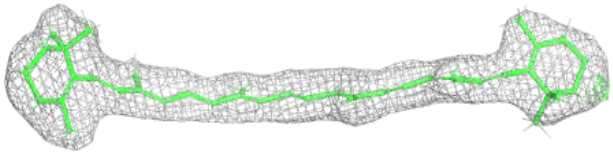


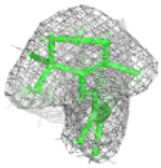


Electron density around BCR H 101:

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

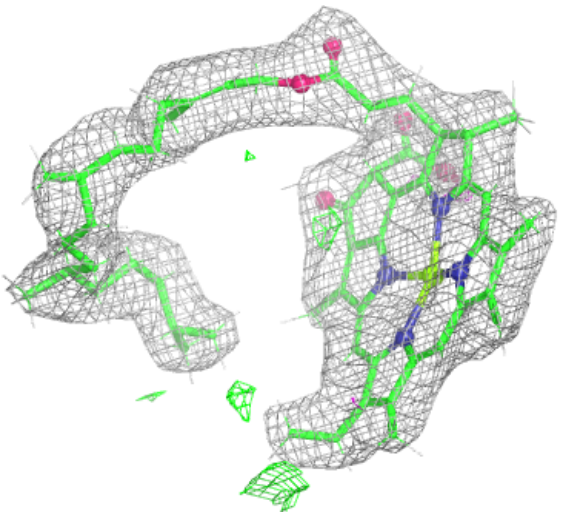


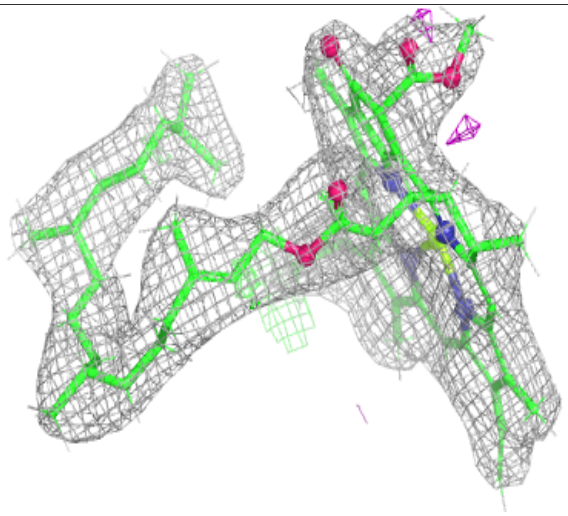


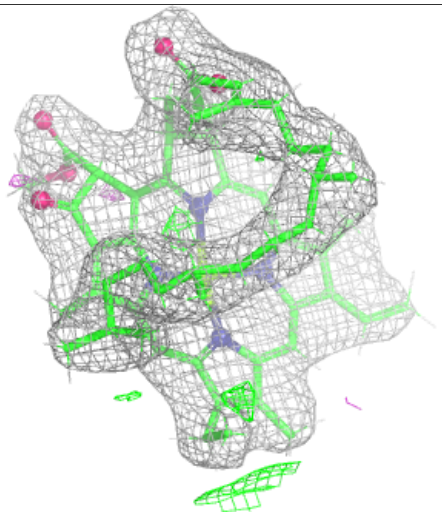


Electron density around CLA c 503:

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

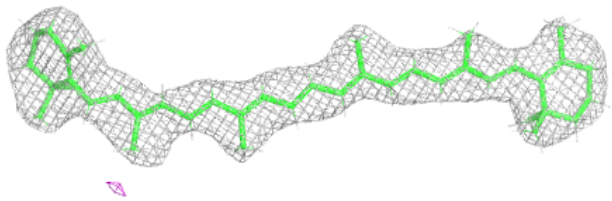


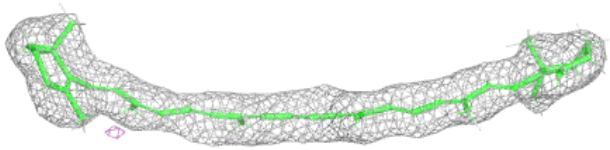


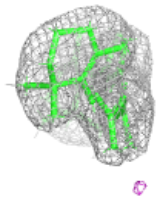


Electron density around BCR T 101:

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

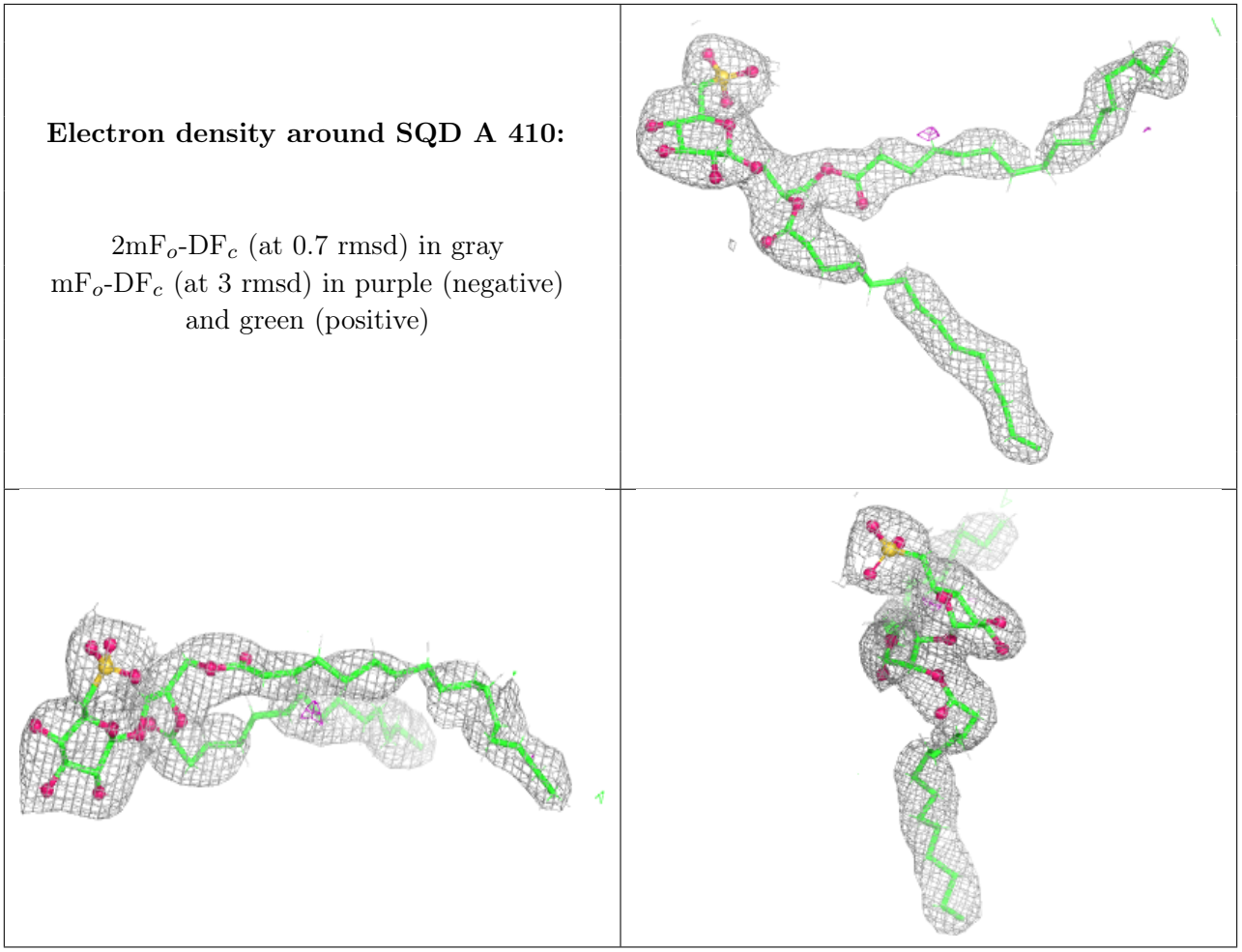






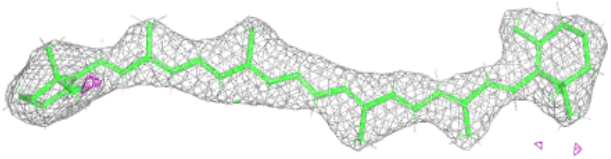
Electron density around SQD A 410:

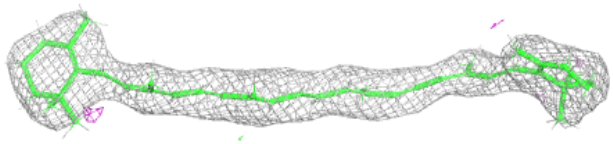
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

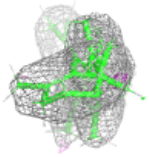


Electron density around BCR B 617:

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

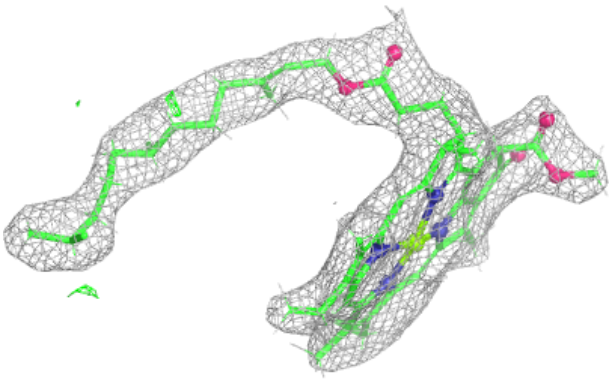


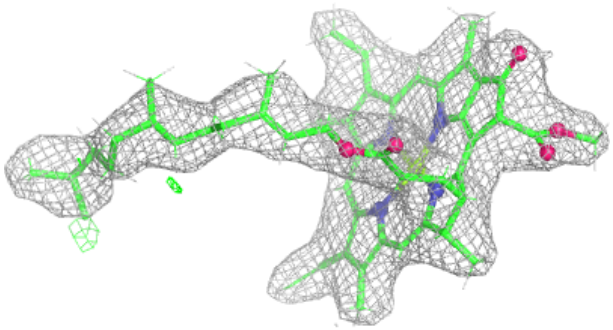


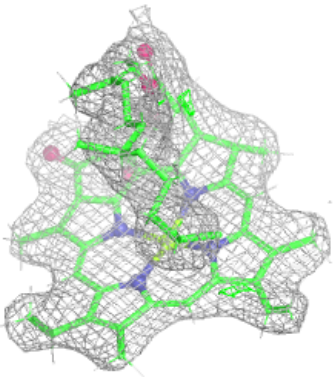


Electron density around CLA c 504:

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

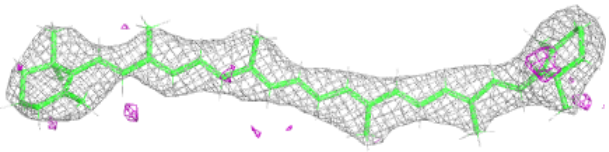


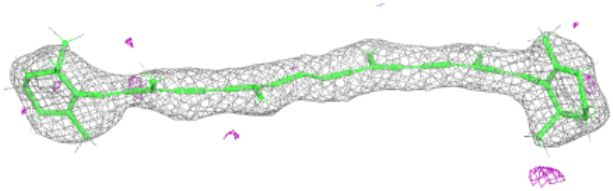


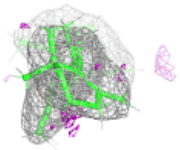


Electron density around BCR c 515:

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

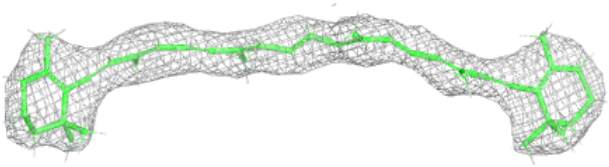


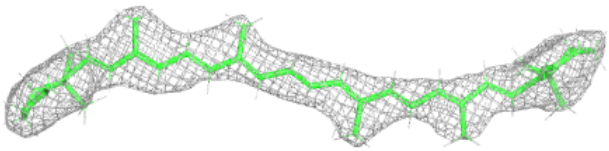


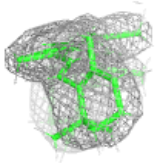


Electron density around BCR c 521:

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

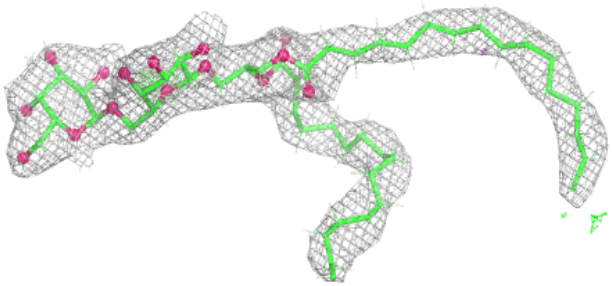


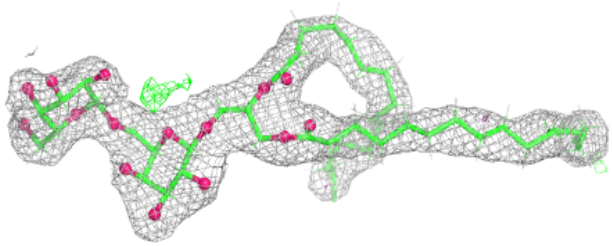


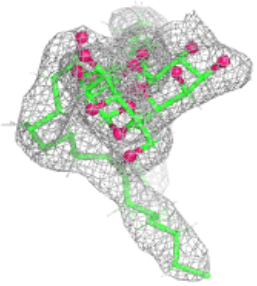


Electron density around DGD H 102:

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

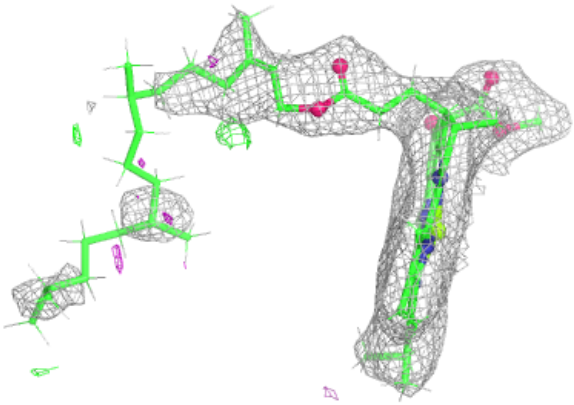


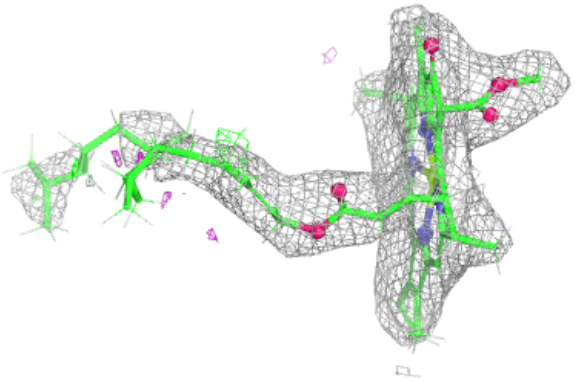


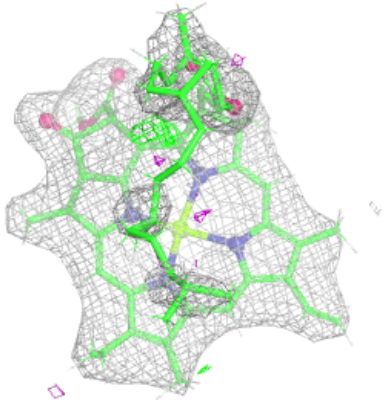


Electron density around CLA c 506:

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

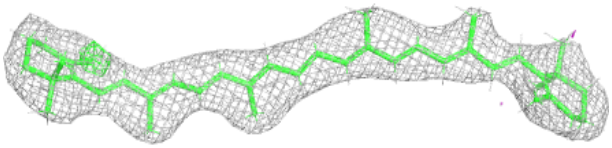


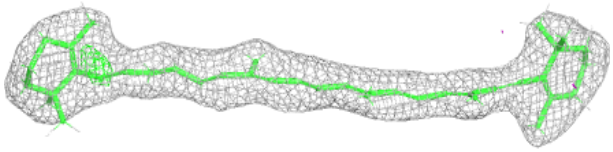


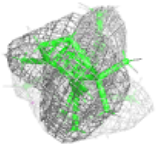


Electron density around BCR C 515:

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

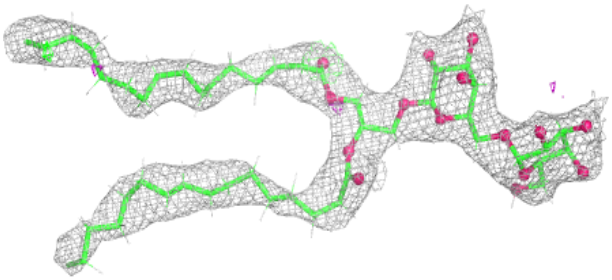


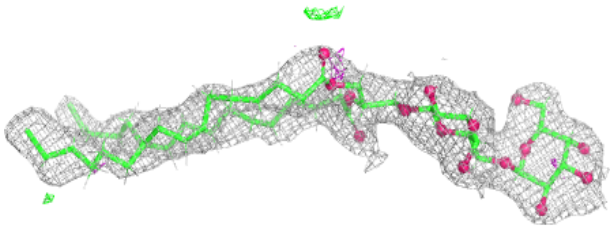


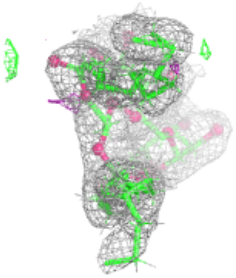


Electron density around DGD c 518:

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

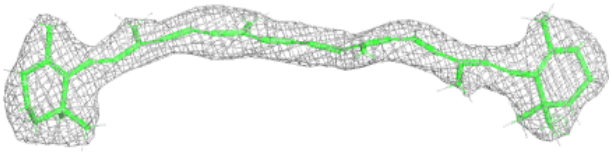


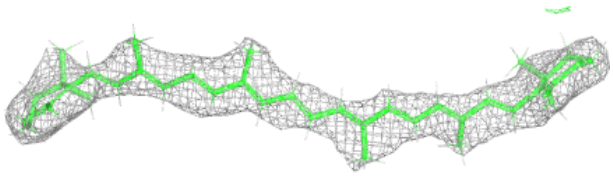


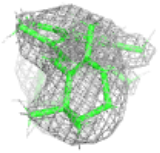


Electron density around BCR C 520:

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

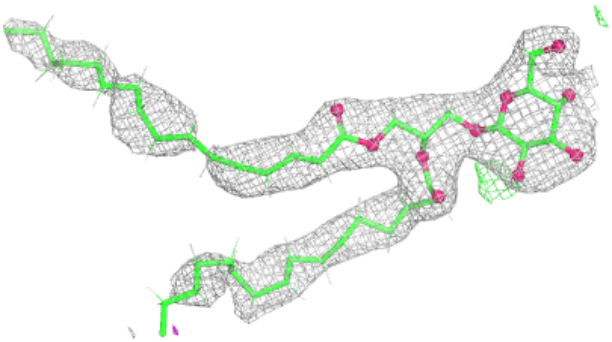


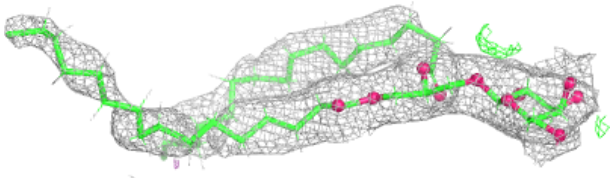


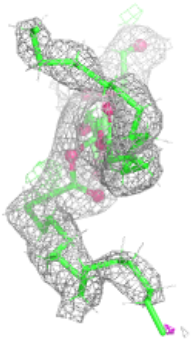


Electron density around LMG D 407:

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

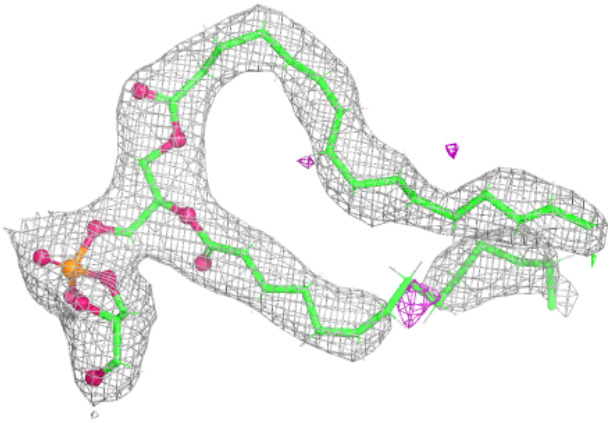


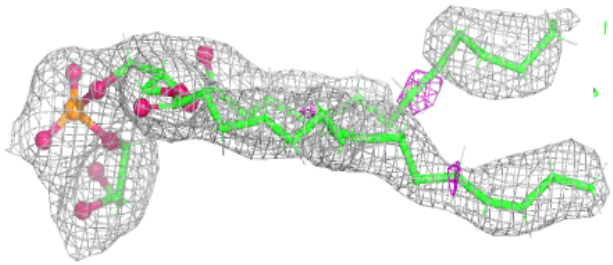




Electron density around LHG D 409:

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

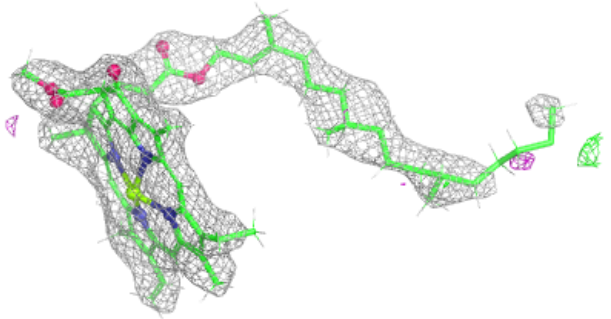


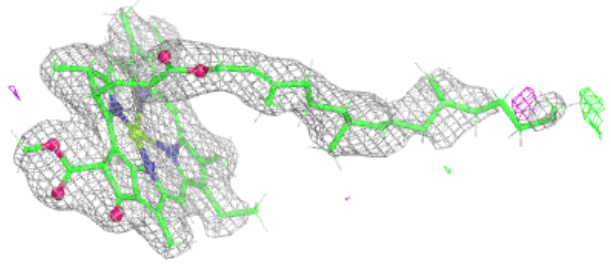


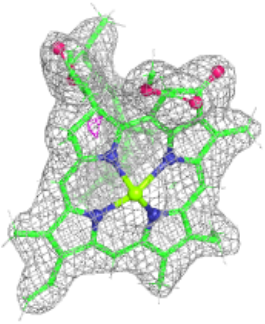


Electron density around CLA c 508:

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

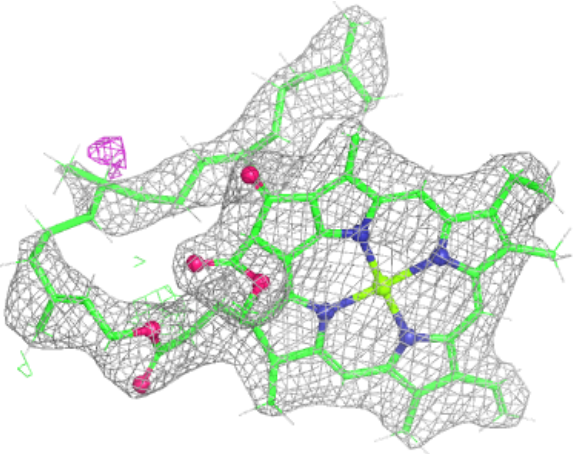


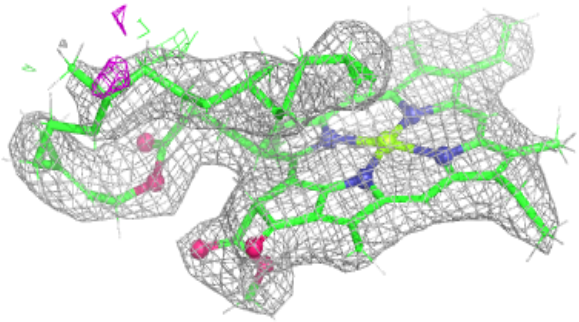


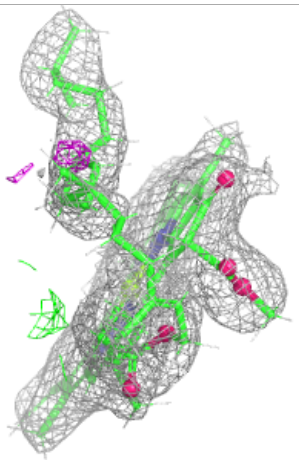


Electron density around CLA c 509:

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

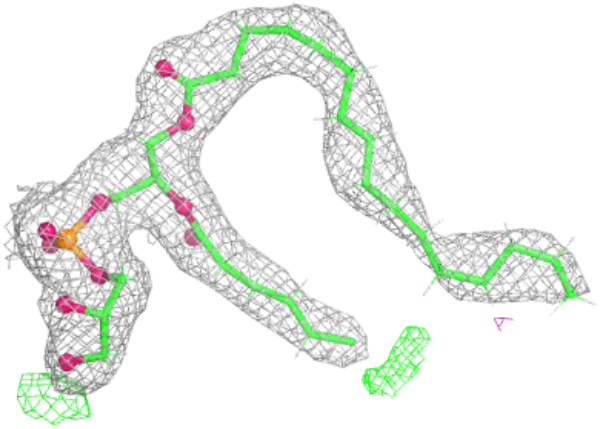


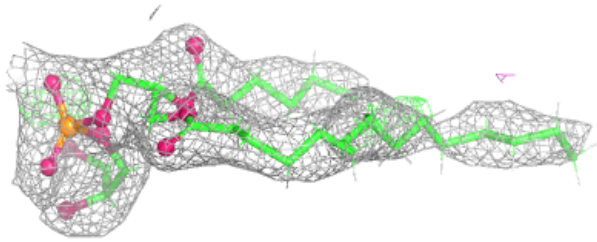


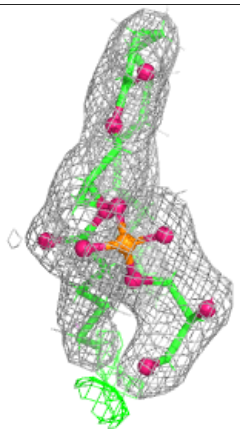


Electron density around LHG d 409:

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

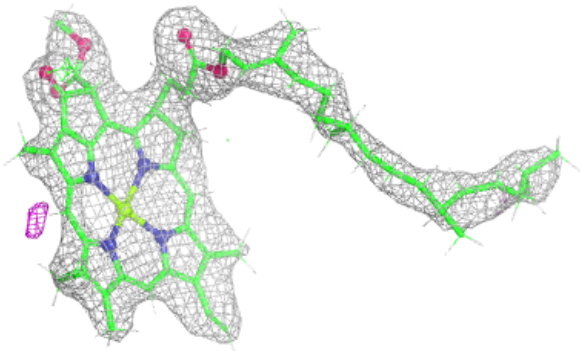


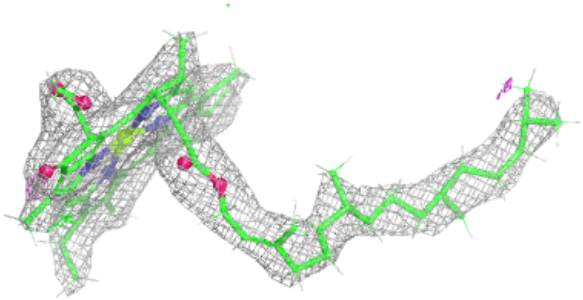


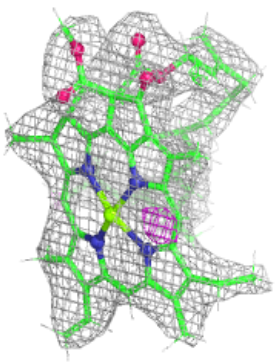


Electron density around CLA c 511:

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

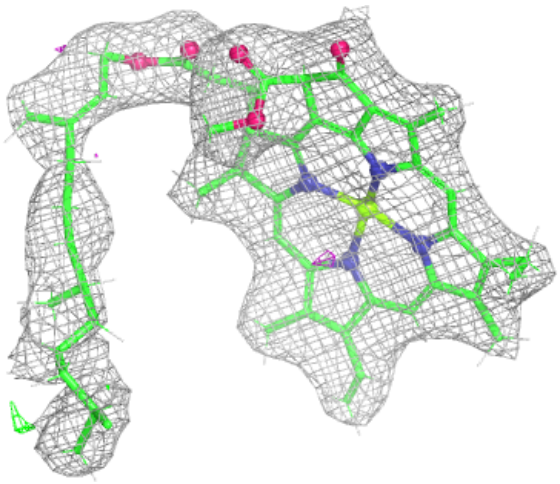


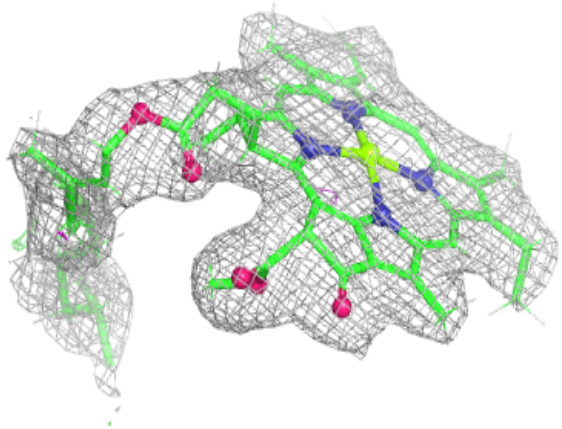


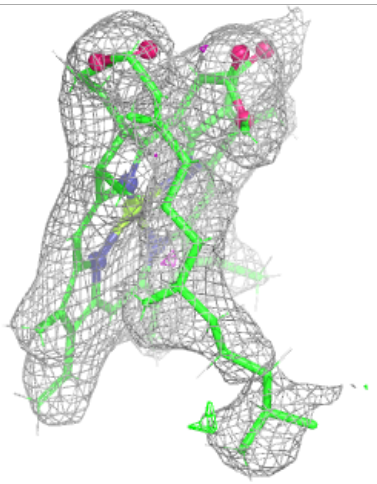


Electron density around CLA b 617:

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

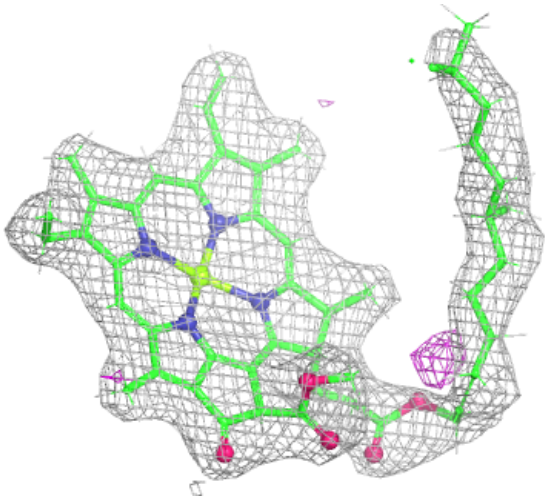


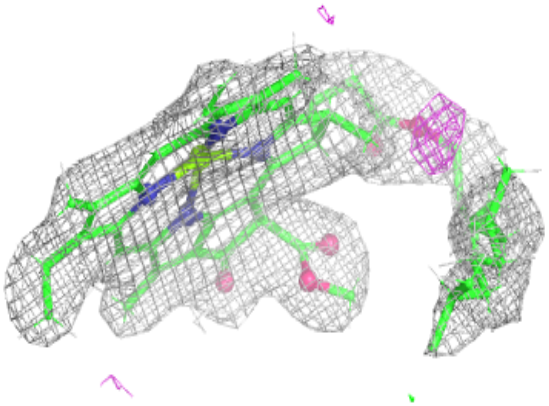


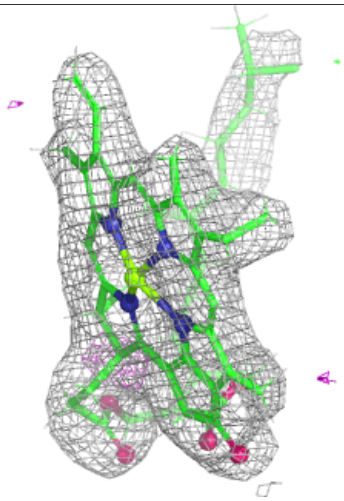


Electron density around CLA B 616:

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

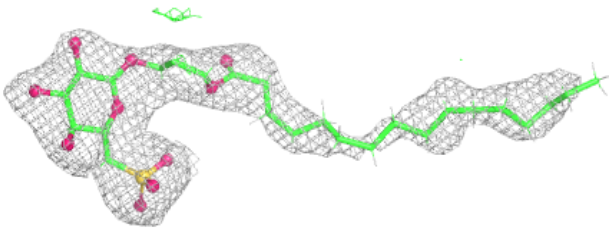


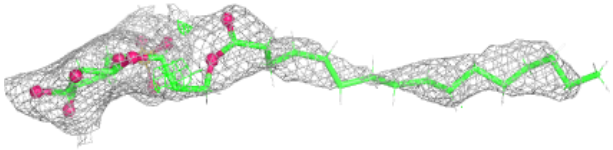




Electron density around SQD F 101:

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

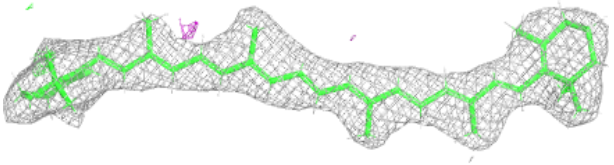


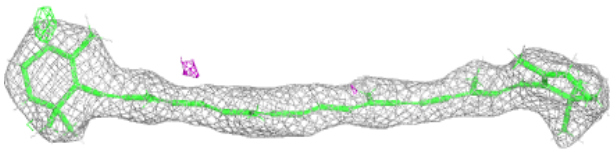


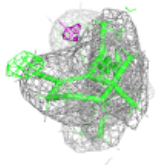


Electron density around BCR b 618:

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

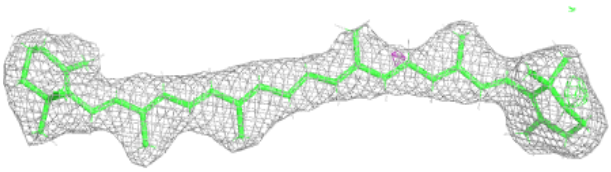


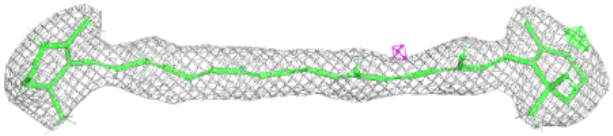


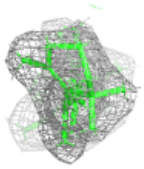


Electron density around BCR b 619:

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

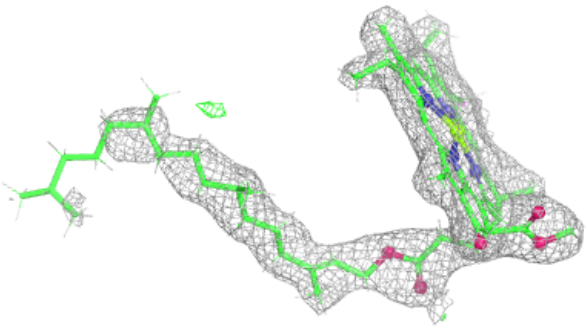


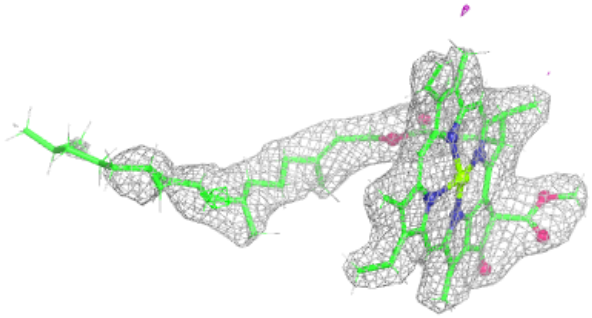


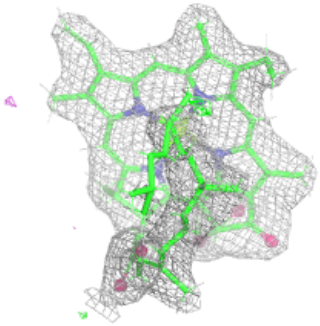


Electron density around CLA C 509:

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

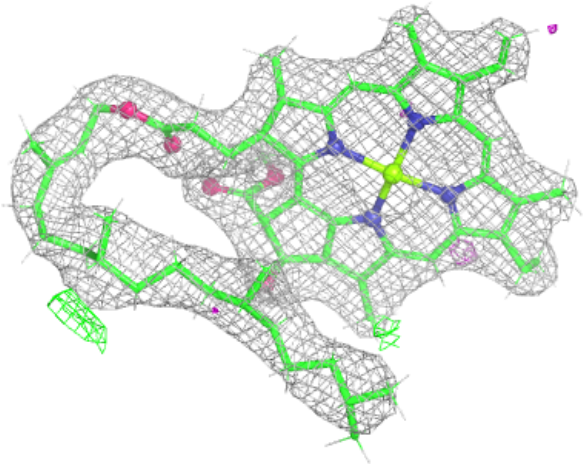


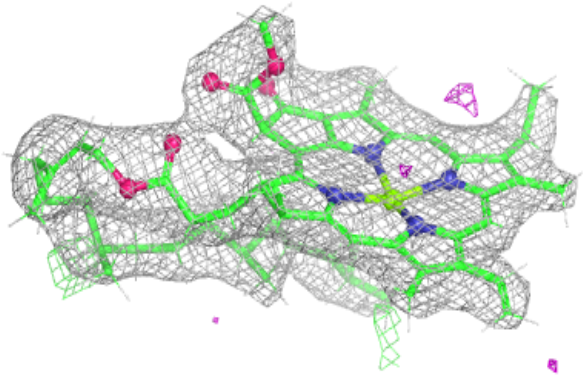


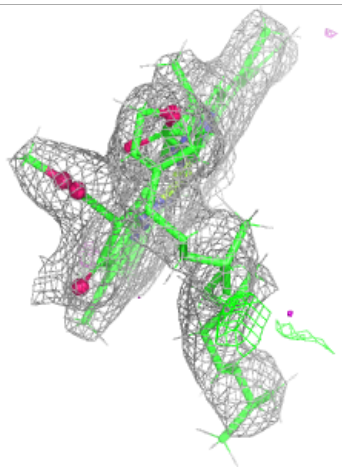


Electron density around CLA C 510:

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

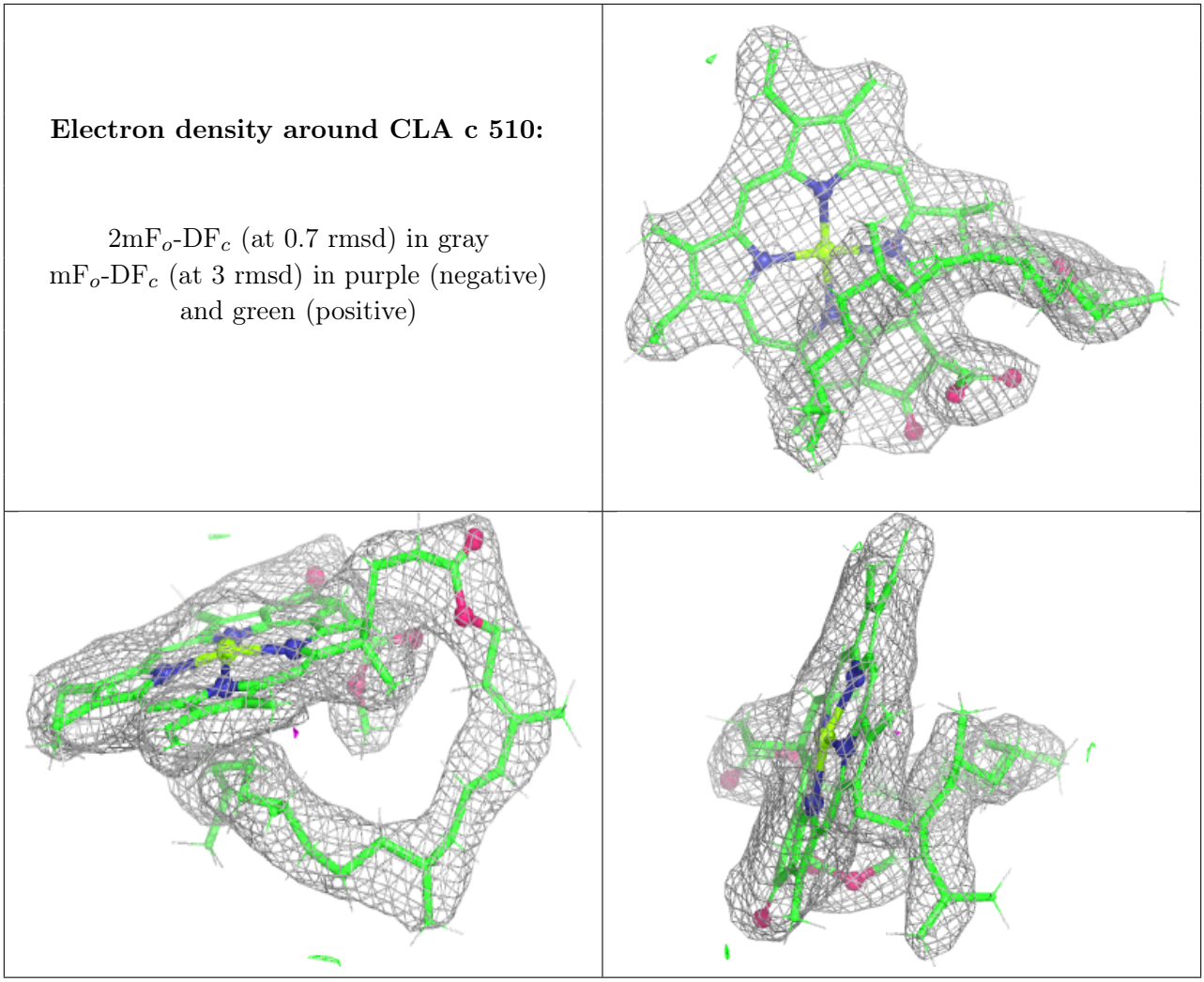






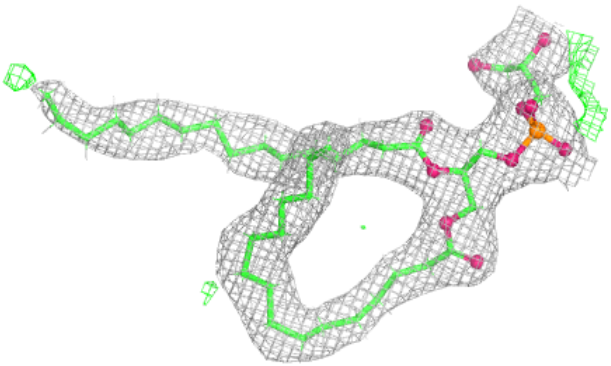
Electron density around CLA c 510:

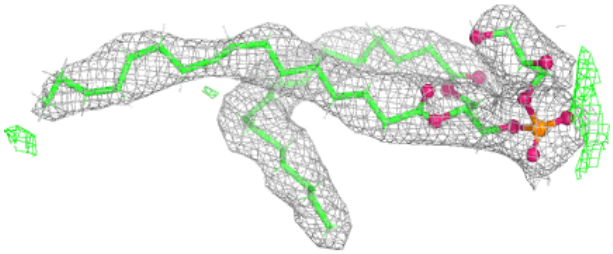
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

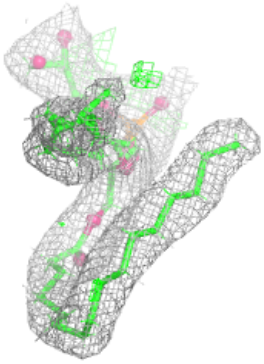


Electron density around LHG A 413:

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

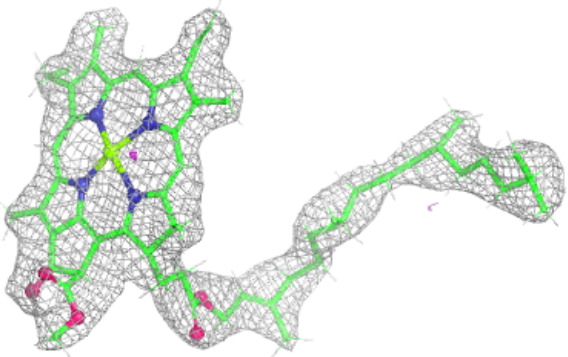


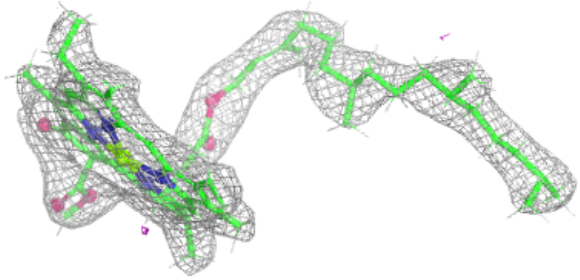


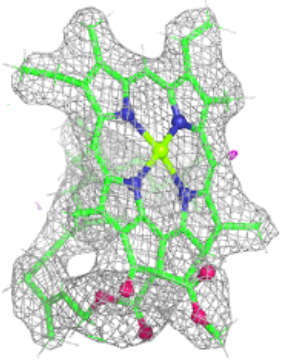


Electron density around CLA C 512:

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

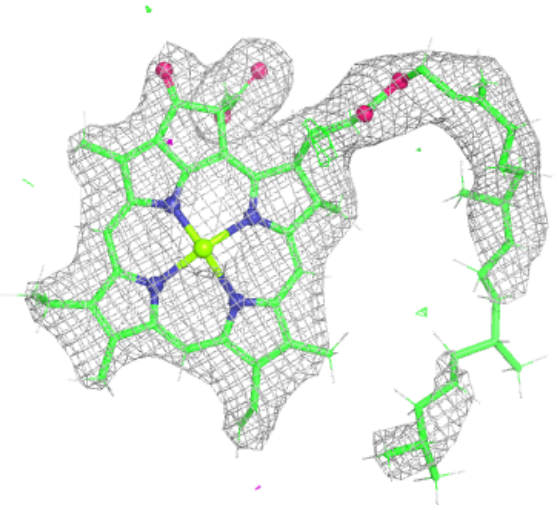


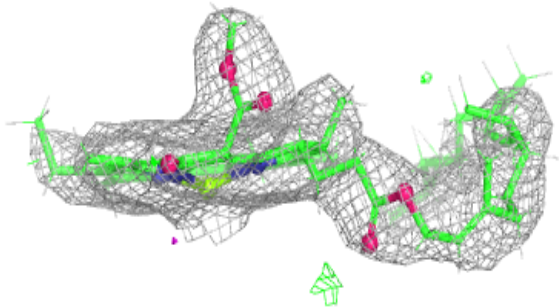


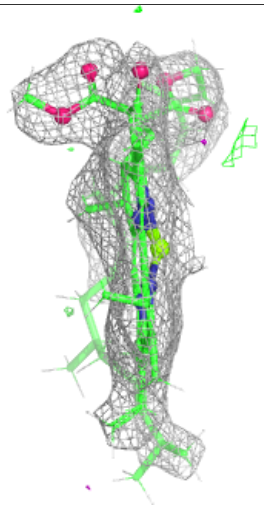


Electron density around CLA C 513:

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

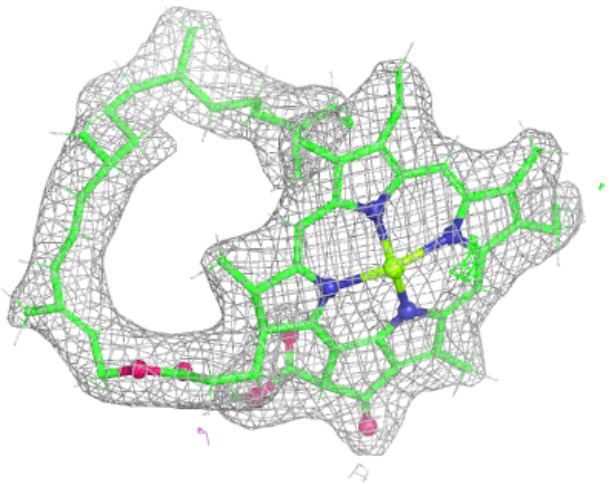


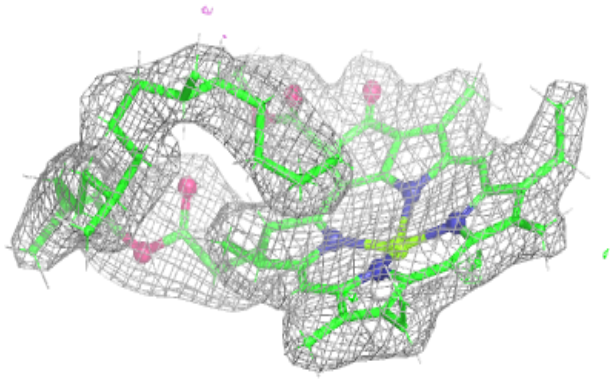


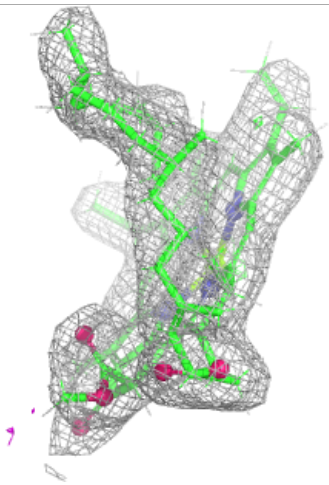


Electron density around CLA B 615:

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

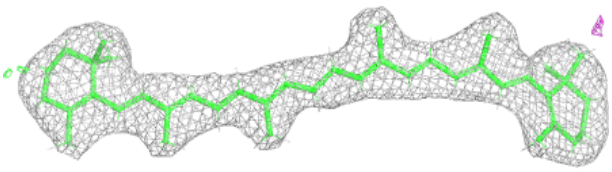


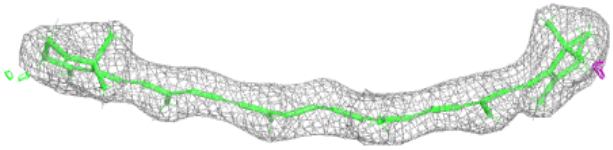


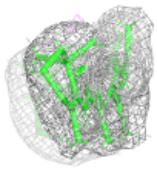


Electron density around BCR t 101:

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

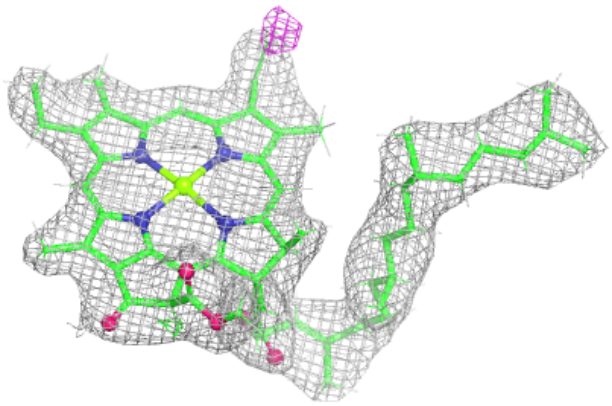


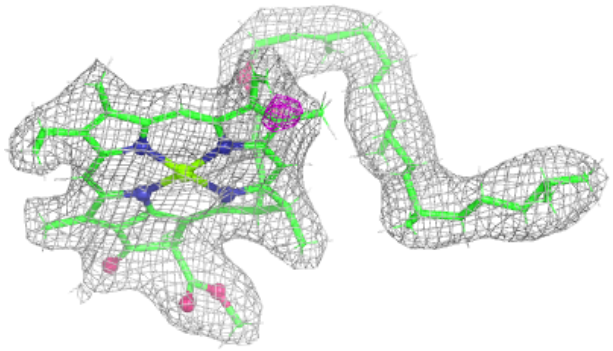


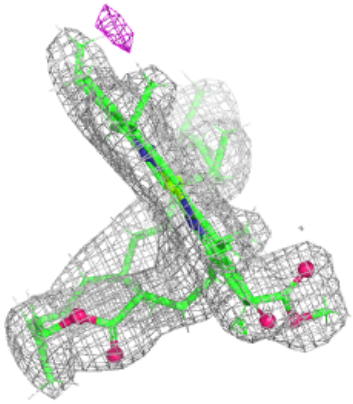


Electron density around CLA d 402:

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

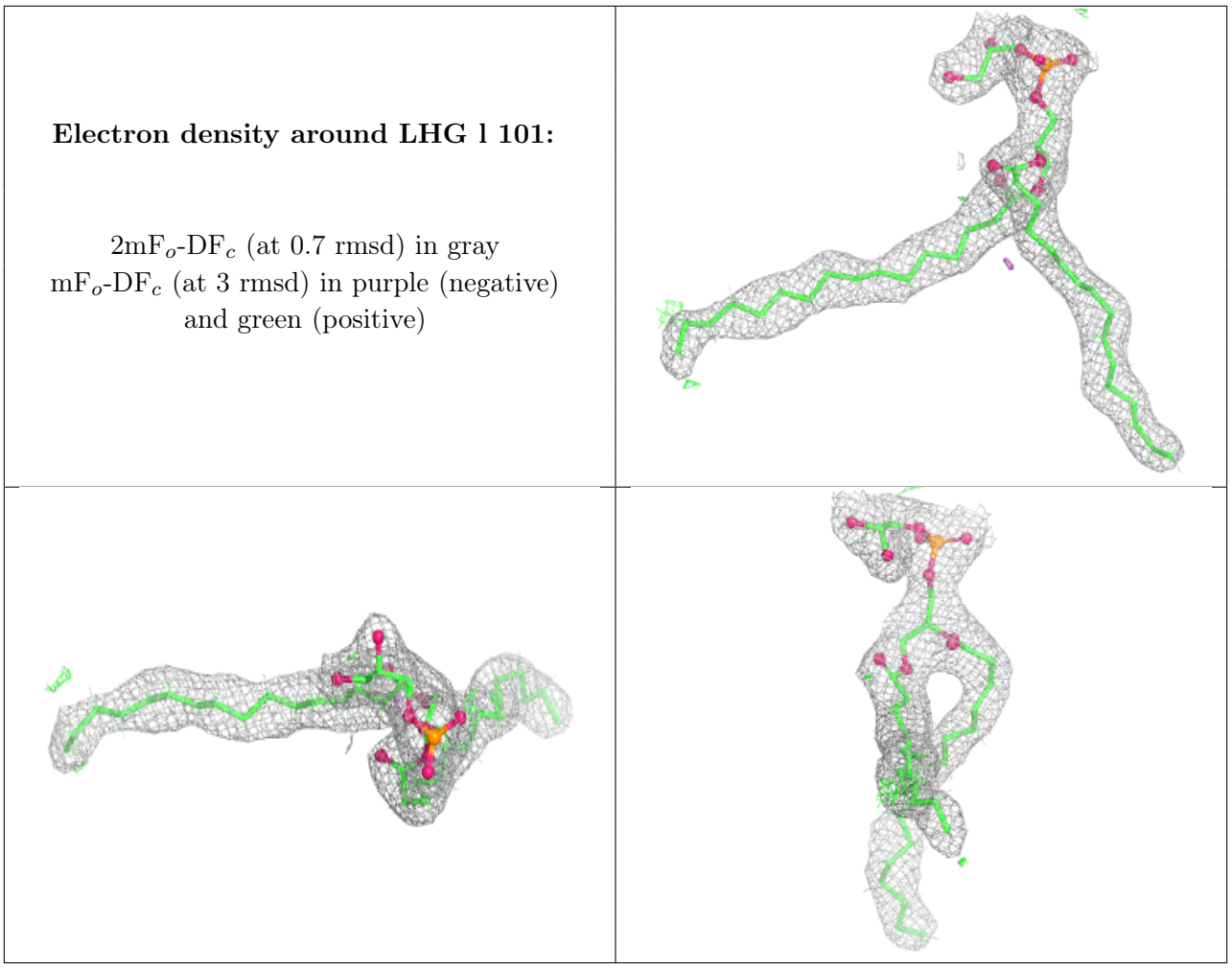






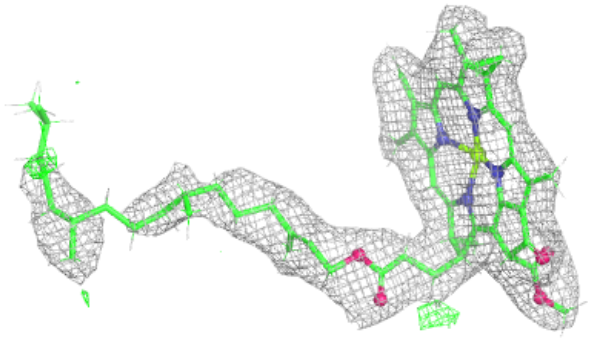
Electron density around LHG l 101:

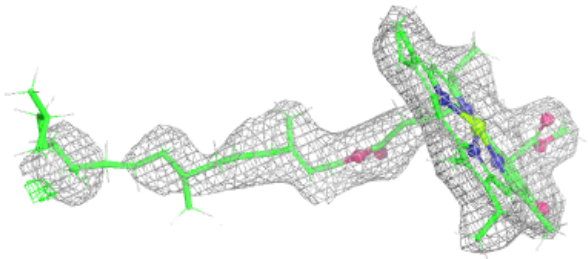
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

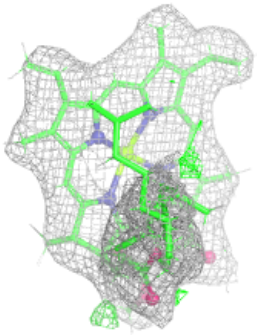


Electron density around CLA d 404:

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

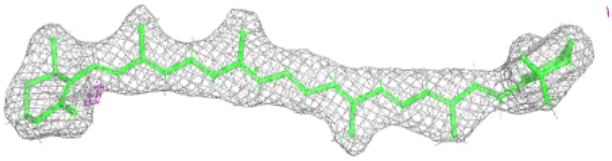


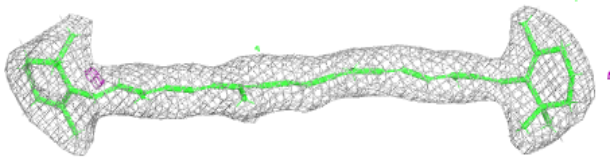


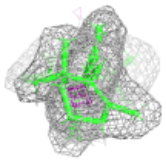


Electron density around BCR A 408:

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

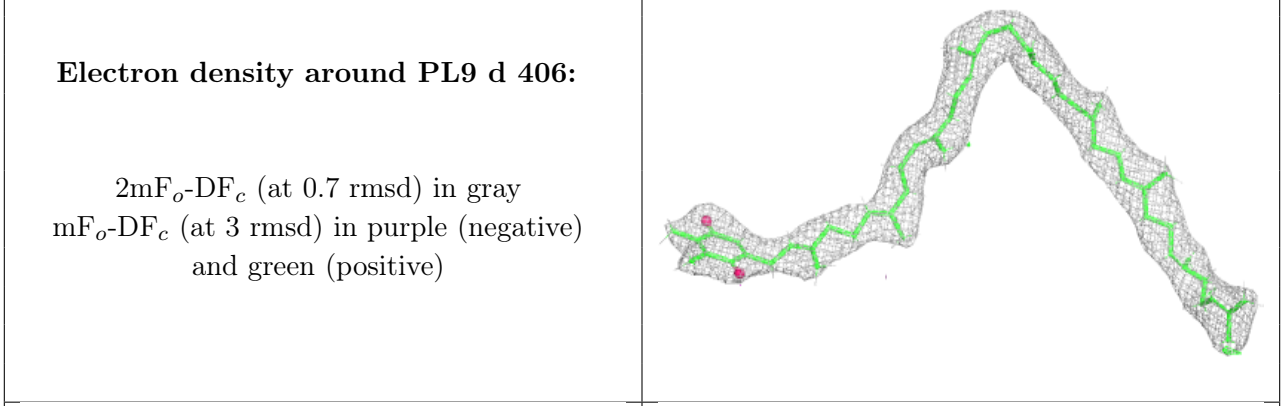






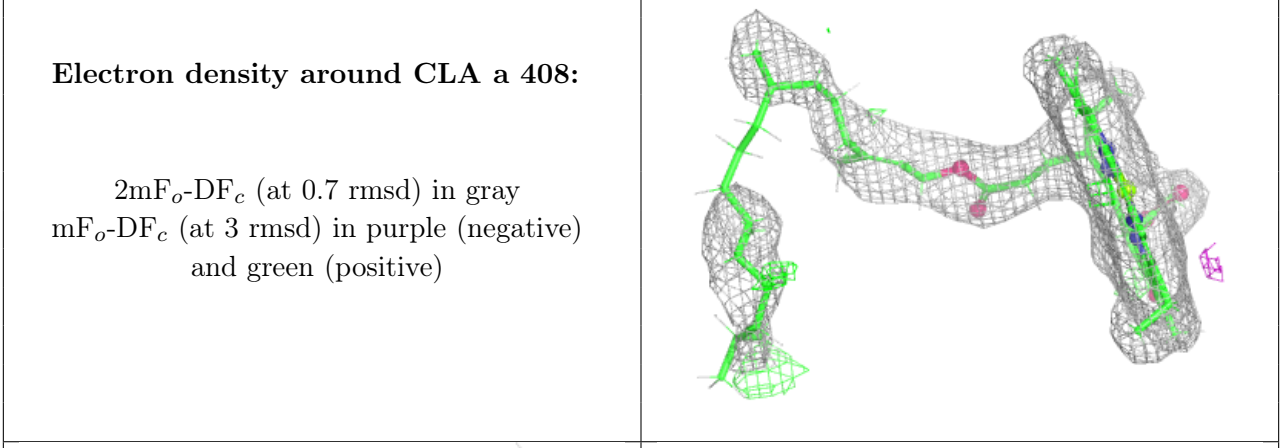
Electron density around PL9 d 406:

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



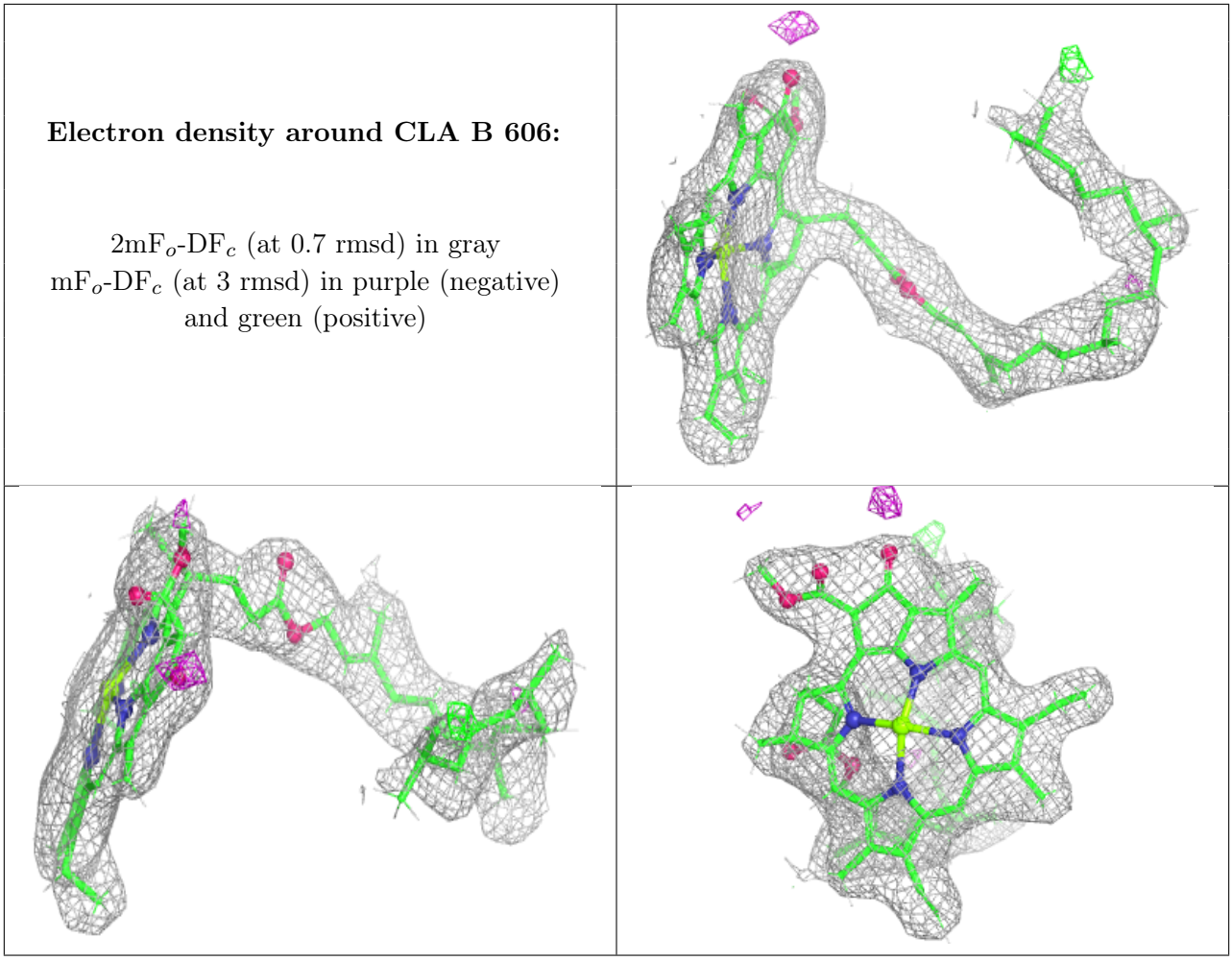
Electron density around CLA a 408:

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



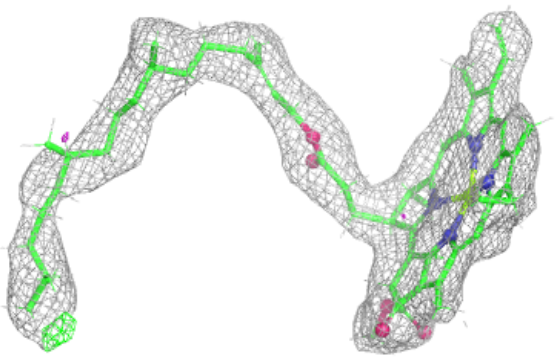
Electron density around CLA B 606:

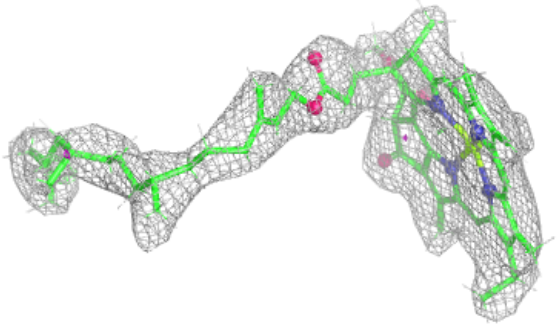
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

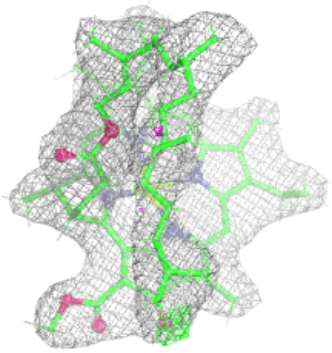


Electron density around CLA b 607:

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

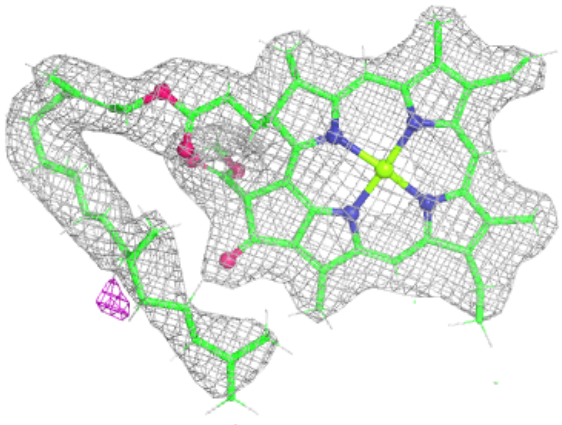


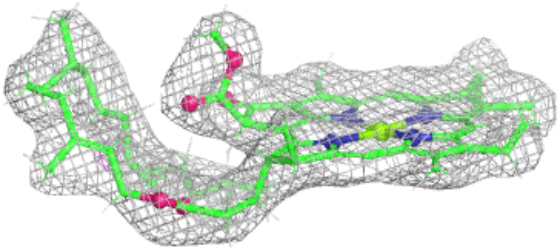


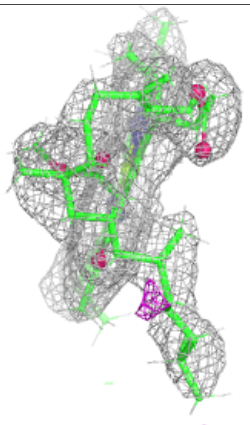


Electron density around CLA b 611:

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

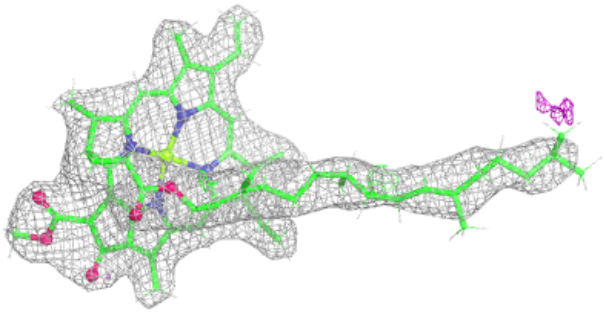


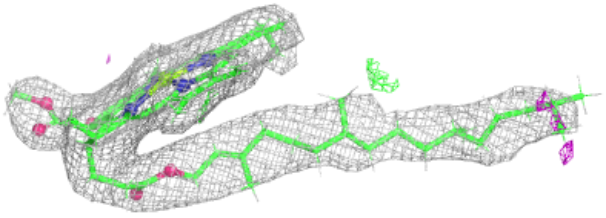


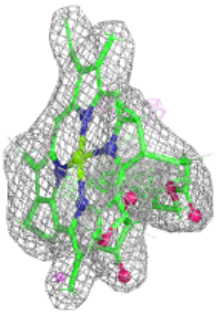


Electron density around CLA b 615:

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

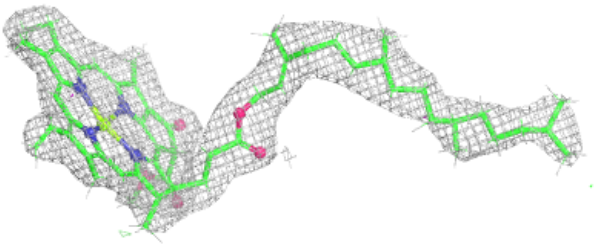


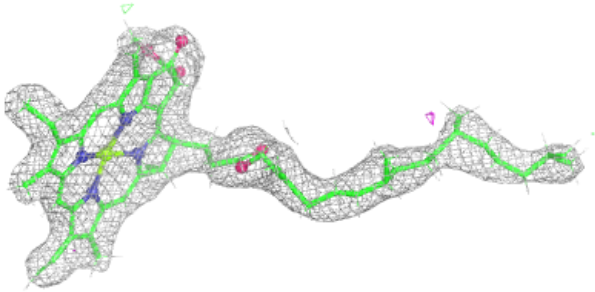


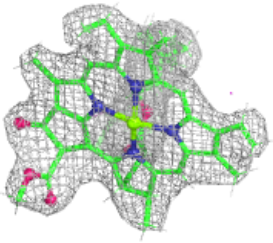


Electron density around CLA C 503:

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

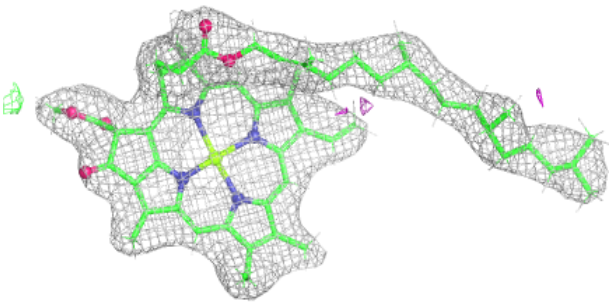


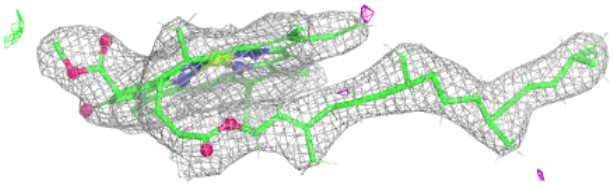


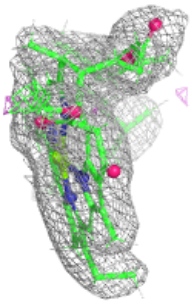


Electron density around CLA c 501:

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



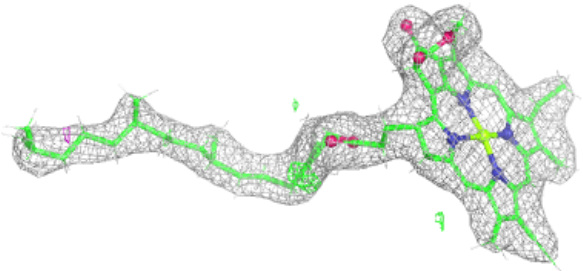


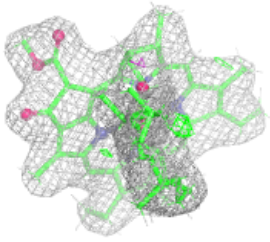


Electron density around CLA c 502:

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

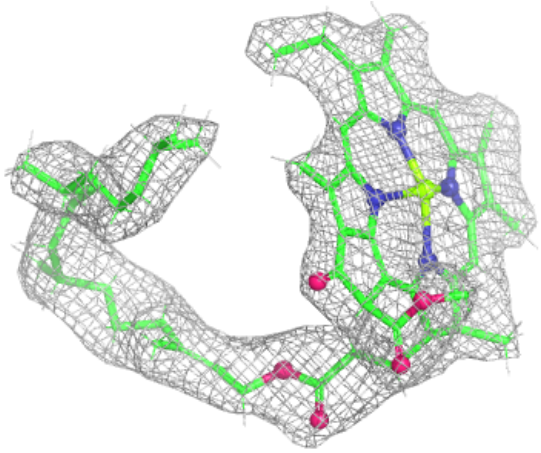


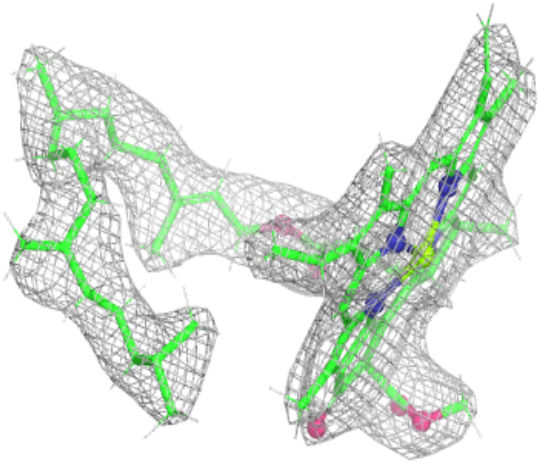


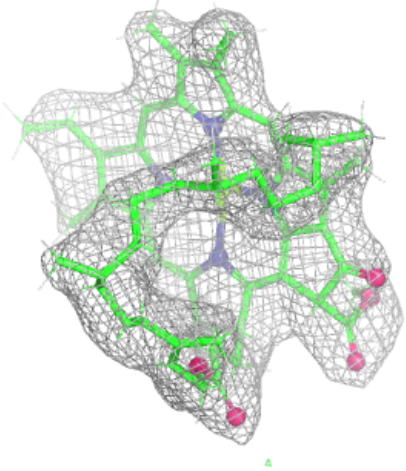


Electron density around CLA C 504:

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

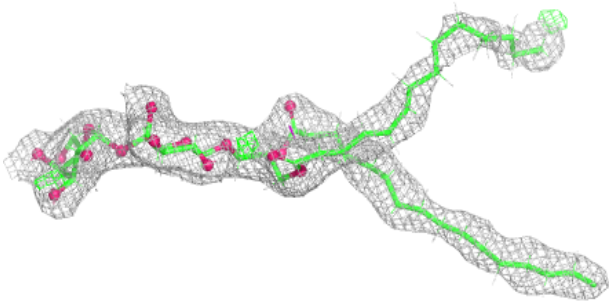


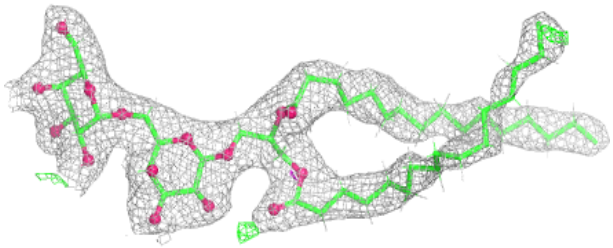


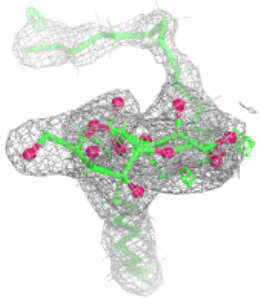


Electron density around DGD C 516:

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

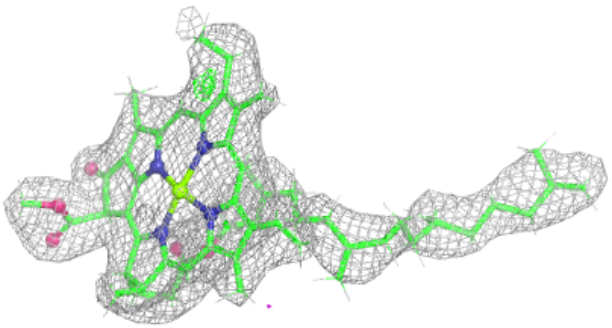


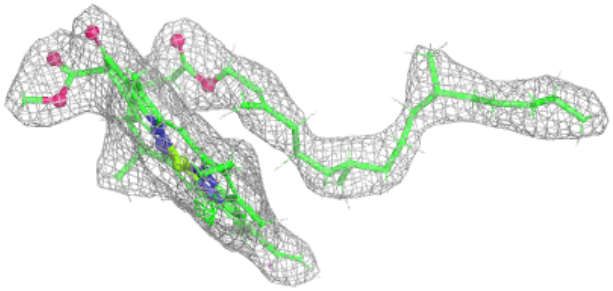


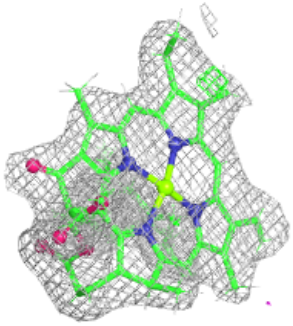


Electron density around CLA C 506:

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

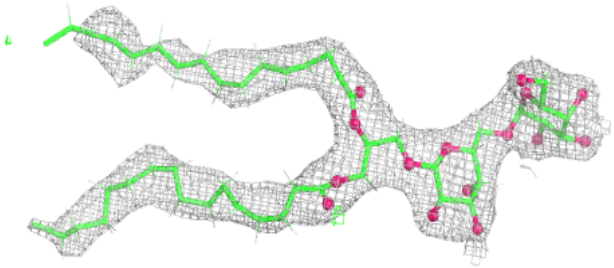


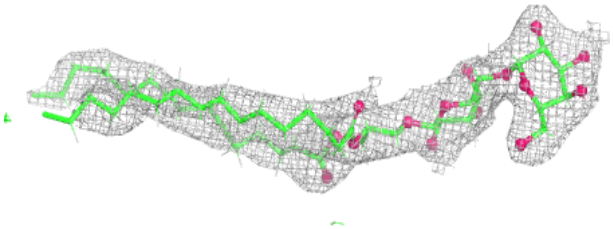


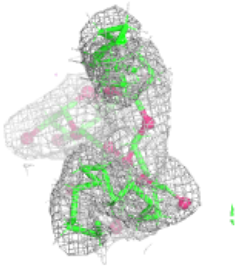


Electron density around DGD C 518:

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

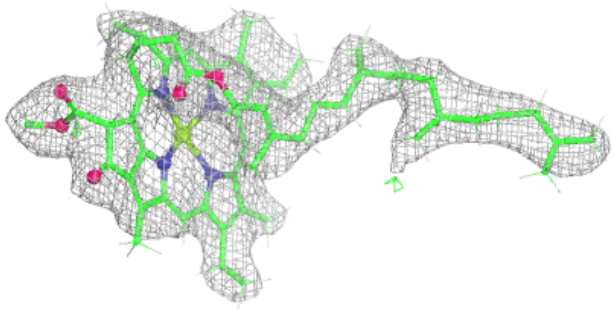


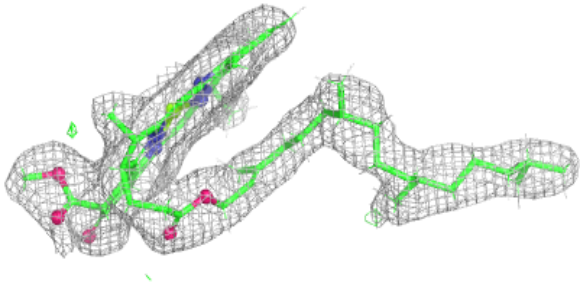


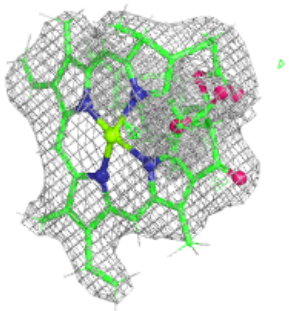


Electron density around CLA c 505:

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

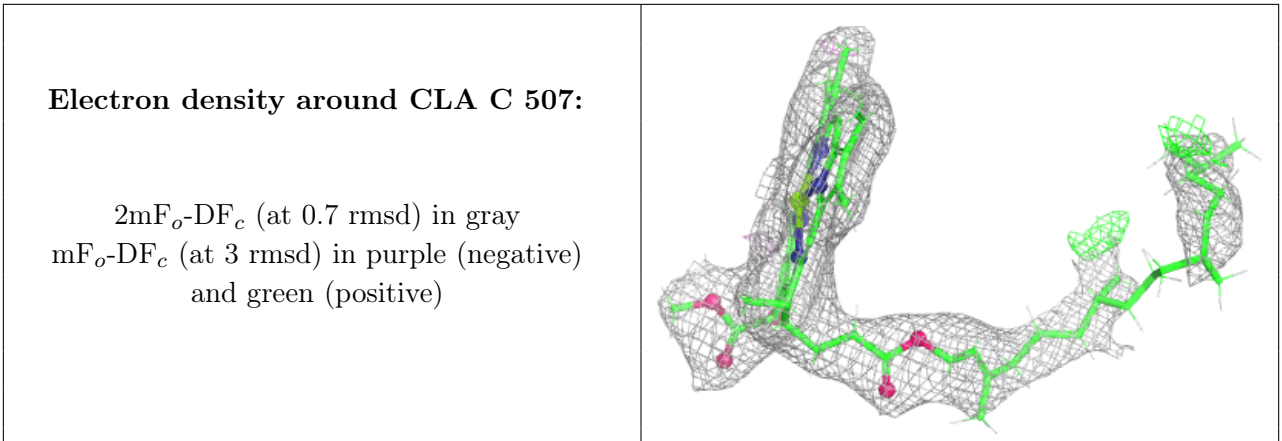






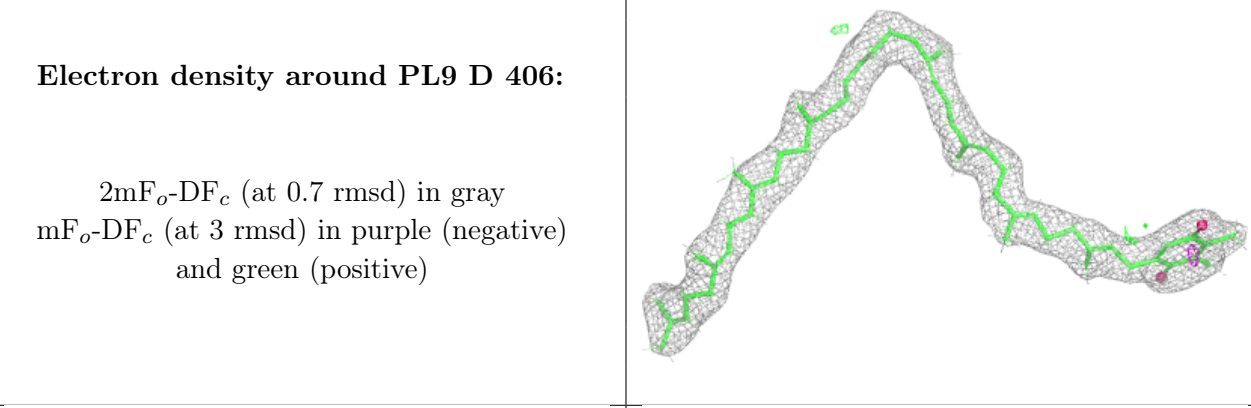
Electron density around CLA C 507:

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



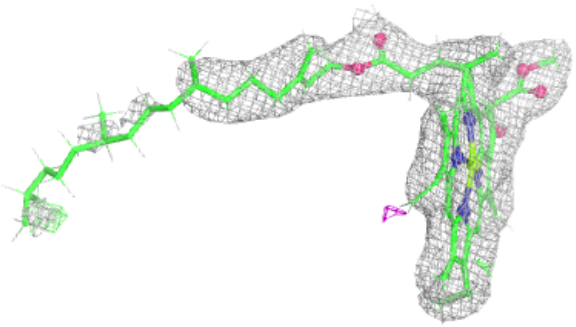
Electron density around PL9 D 406:

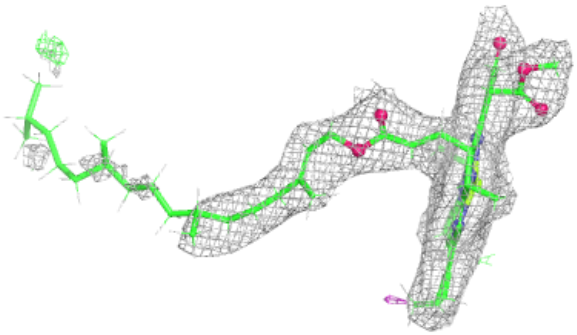
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

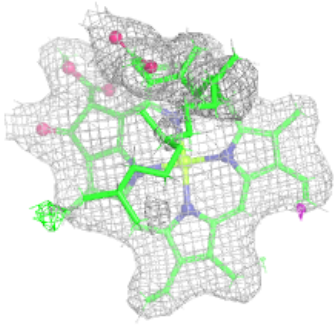


Electron density around CLA D 404:

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

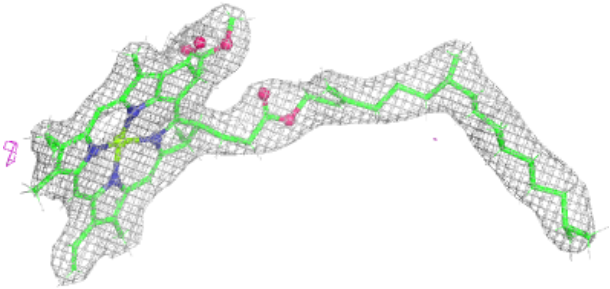


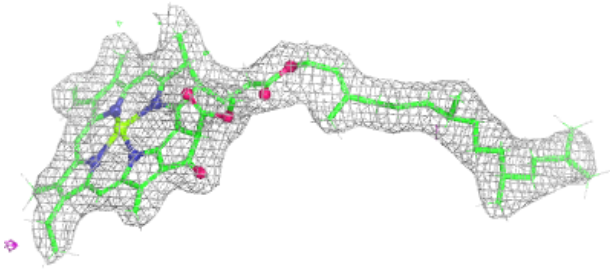


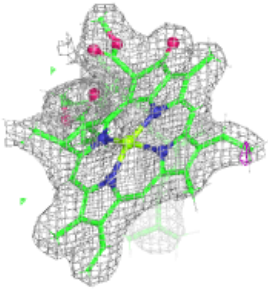


Electron density around CLA a 405:

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

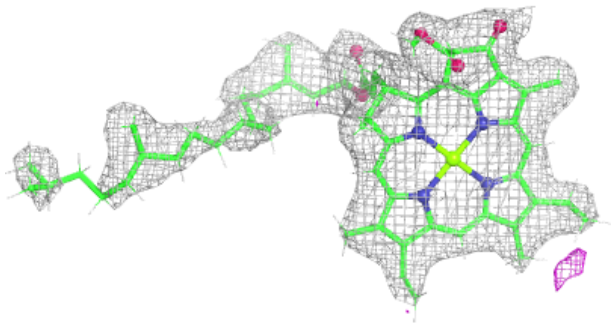


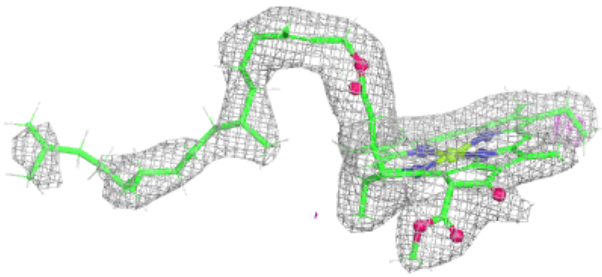


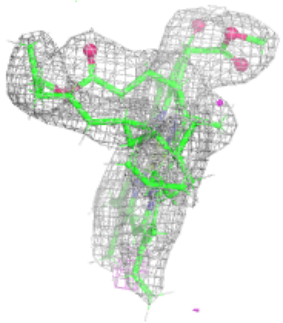


Electron density around CLA a 406:

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

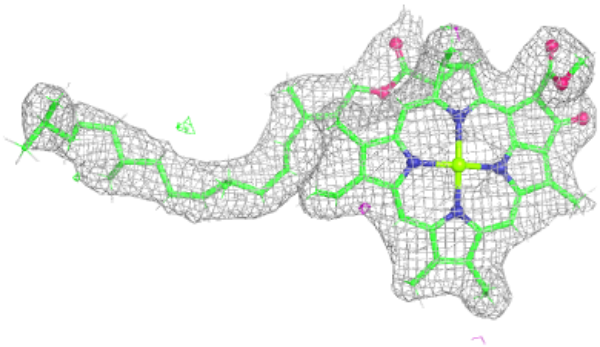


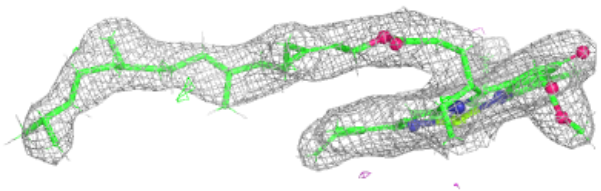


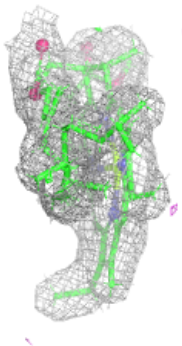


Electron density around CLA B 603:

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

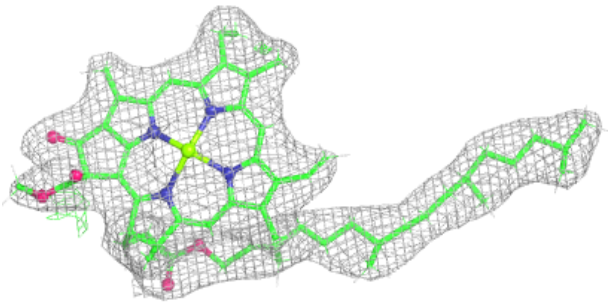


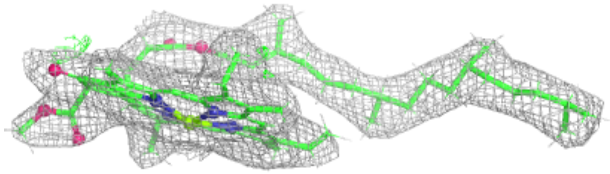


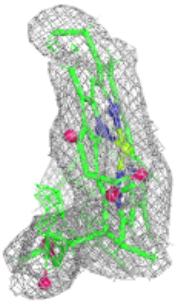


Electron density around CLA C 502:

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

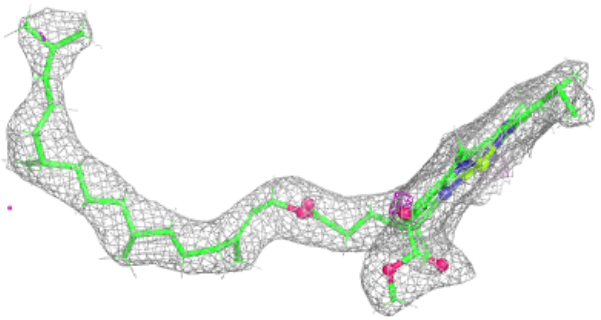


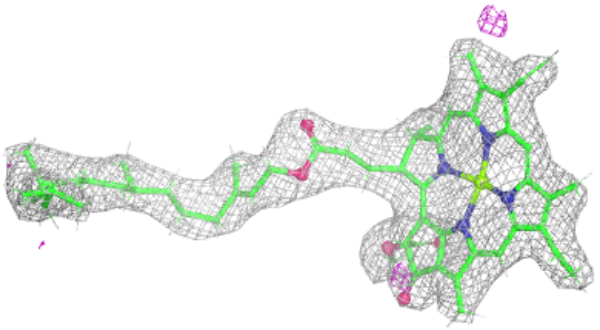


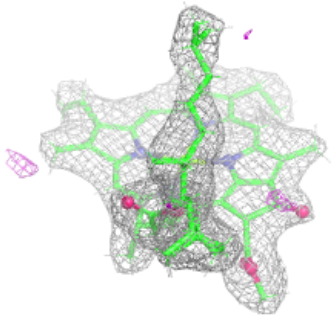


Electron density around CLA d 403:

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

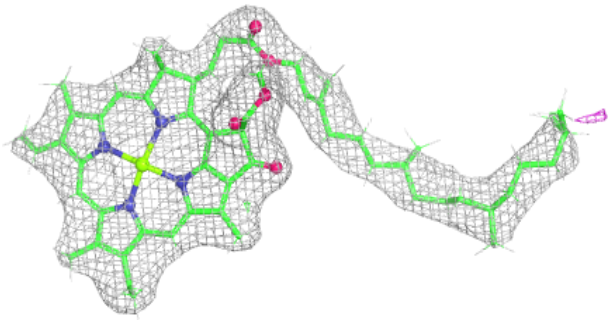


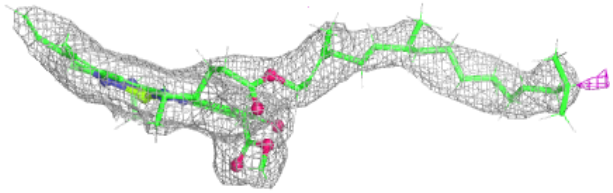


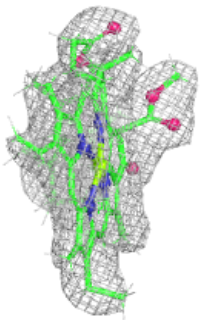


Electron density around CLA b 603:

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

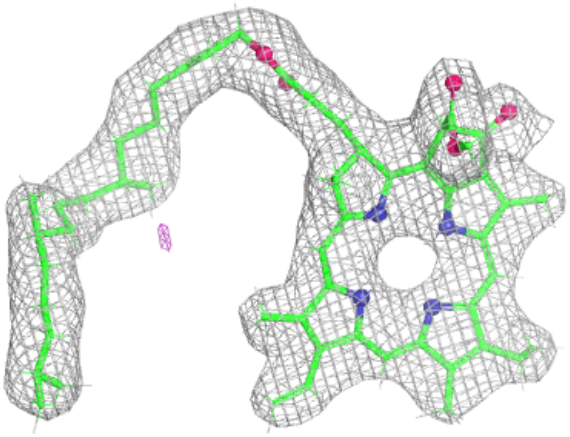


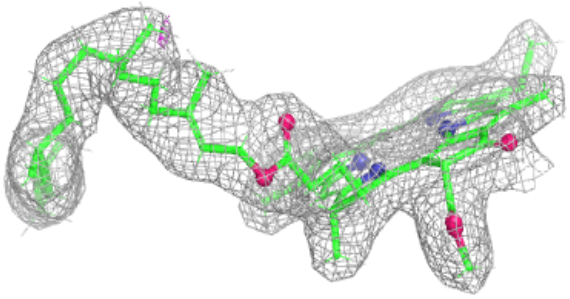




Electron density around PHO D 401:

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

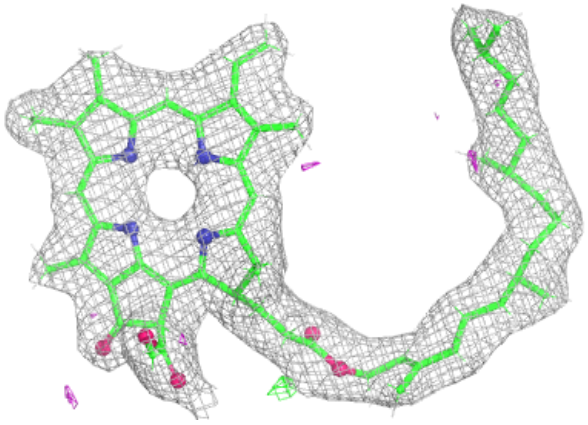


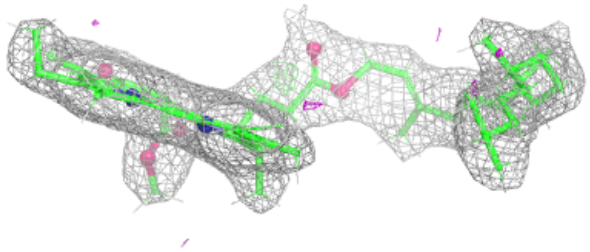


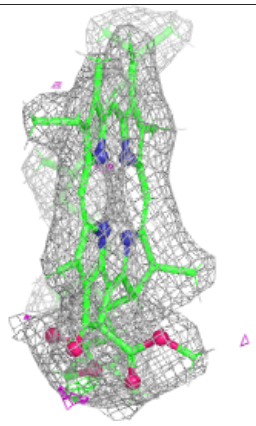


Electron density around PHO a 407:

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

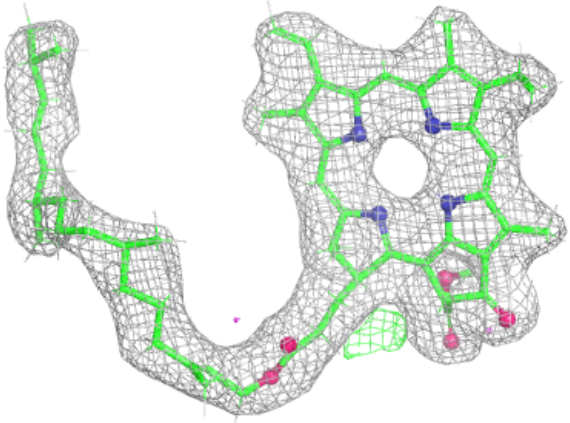


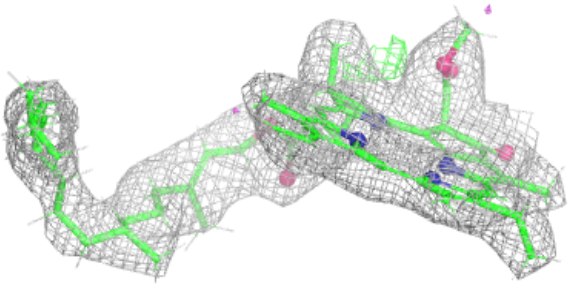




Electron density around PHO d 401:

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

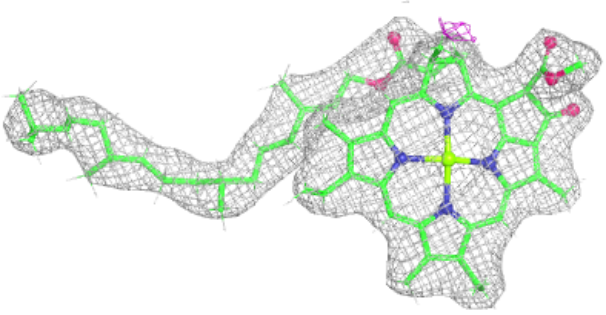


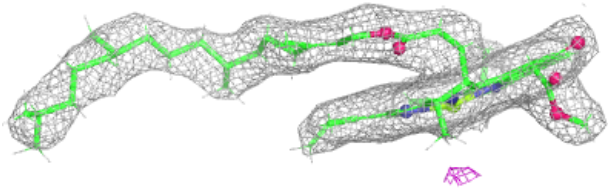


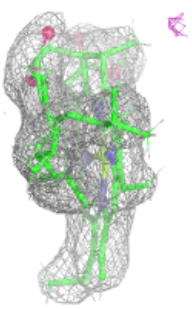


Electron density around CLA b 604:

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

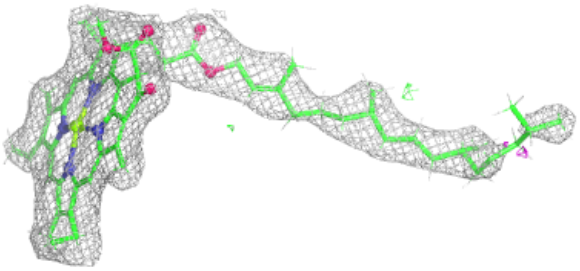


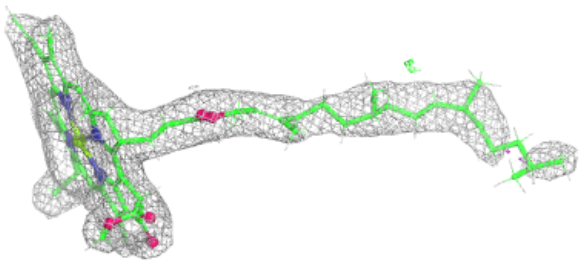


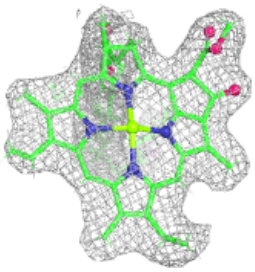


Electron density around CLA b 605:

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

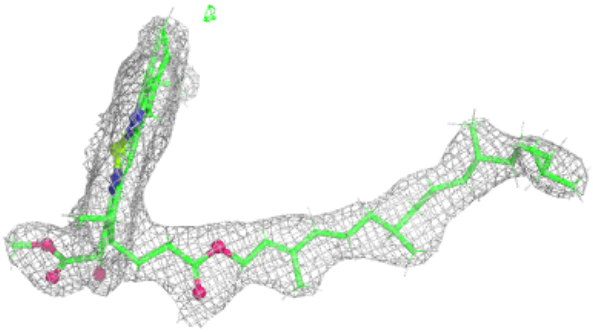


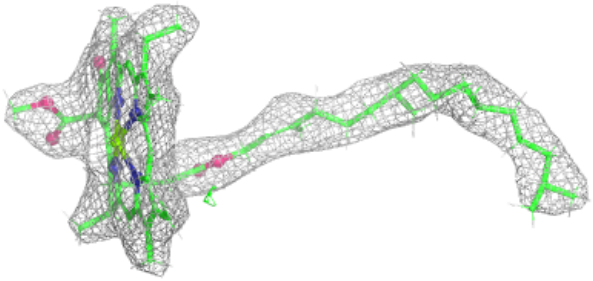


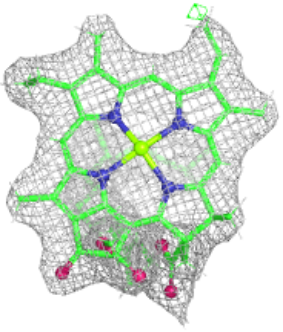


Electron density around CLA b 606:

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

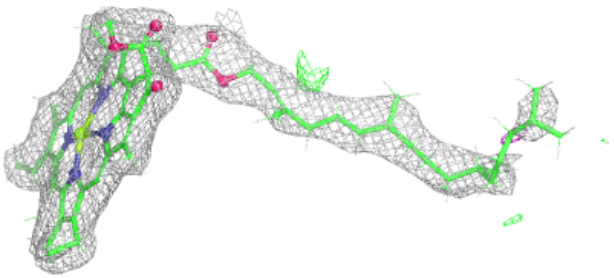


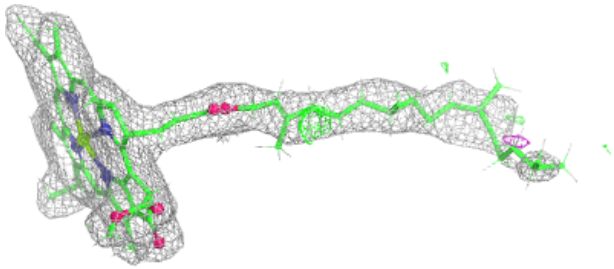


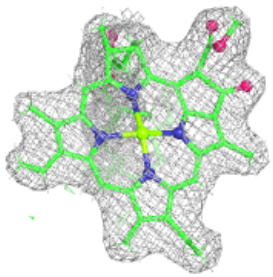


Electron density around CLA B 604:

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

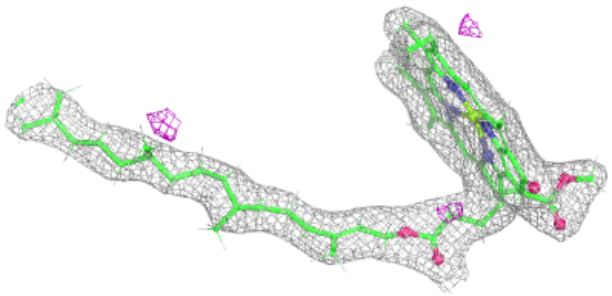


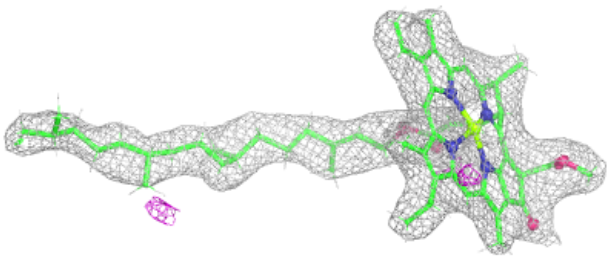


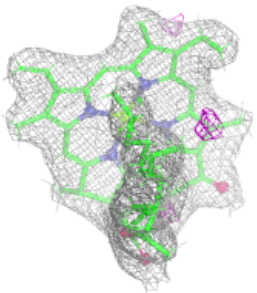


Electron density around CLA b 608:

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

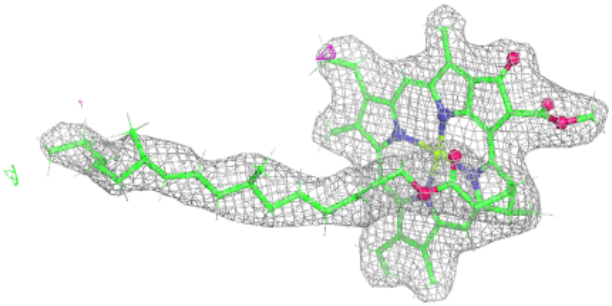


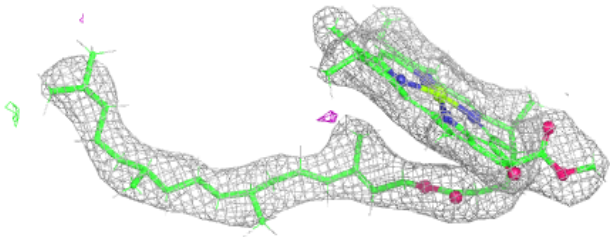


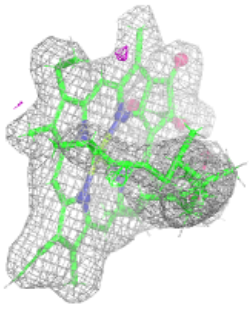


Electron density around CLA b 609:

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

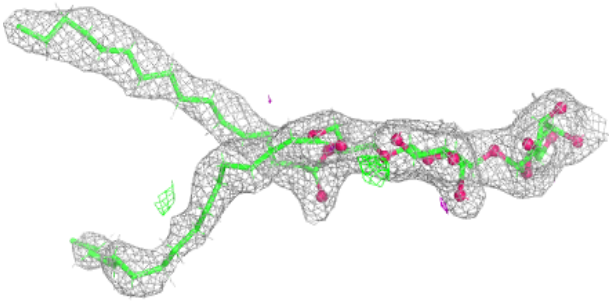


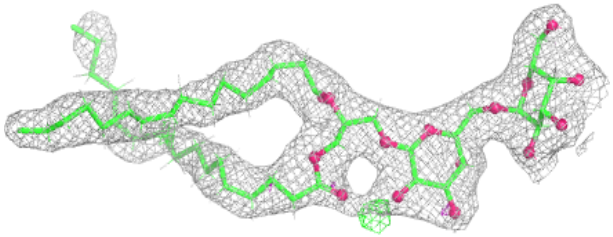


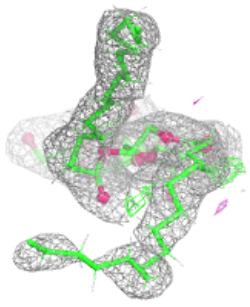


Electron density around DGD c 516:

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

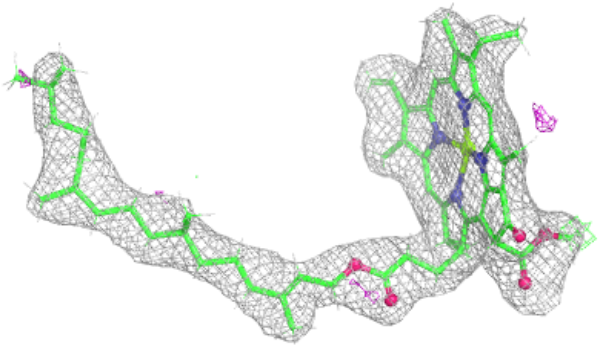


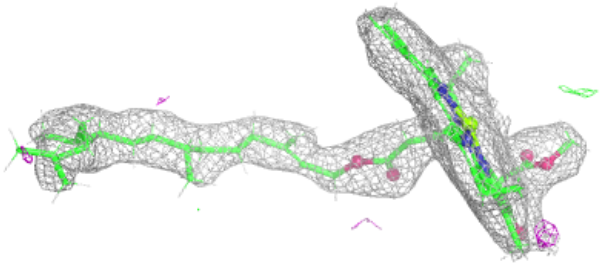


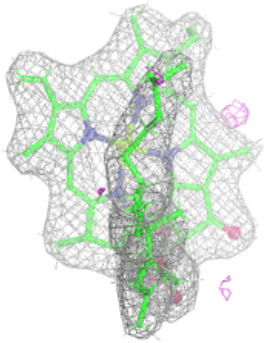


Electron density around CLA b 610:

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

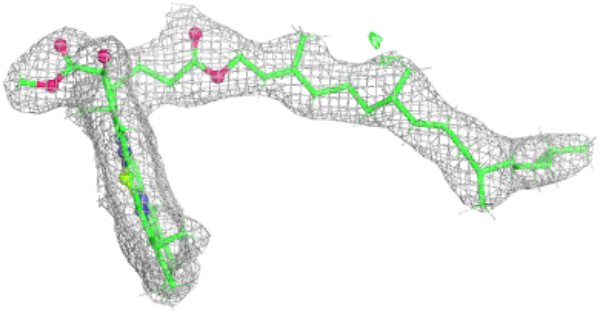


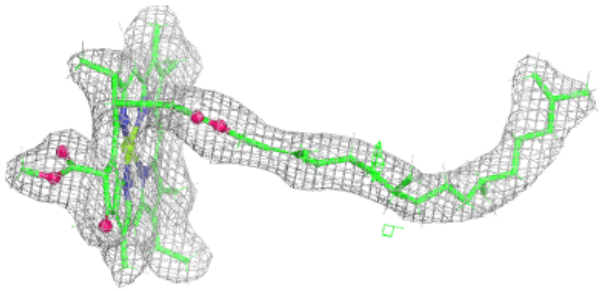


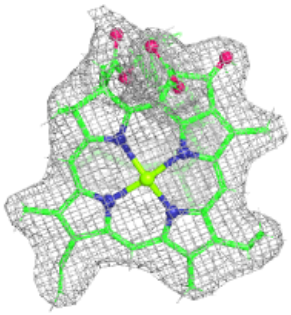


Electron density around CLA B 605:

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

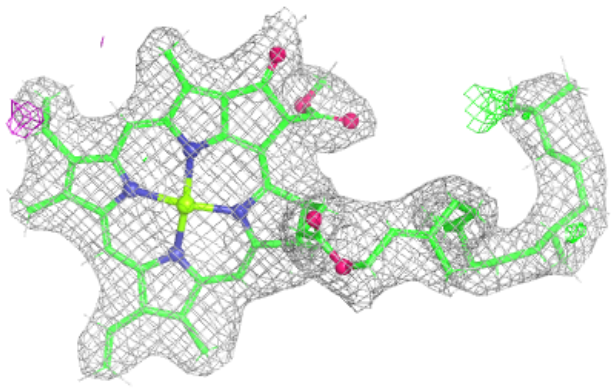


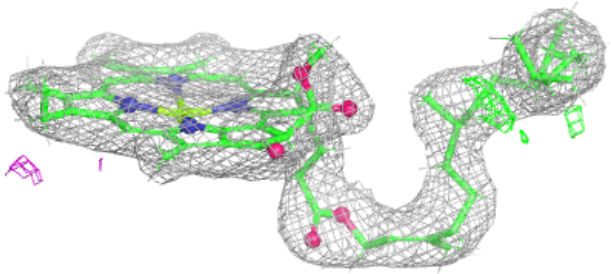


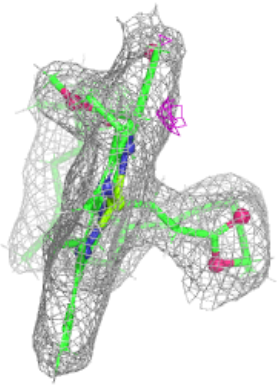


Electron density around CLA b 613:

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

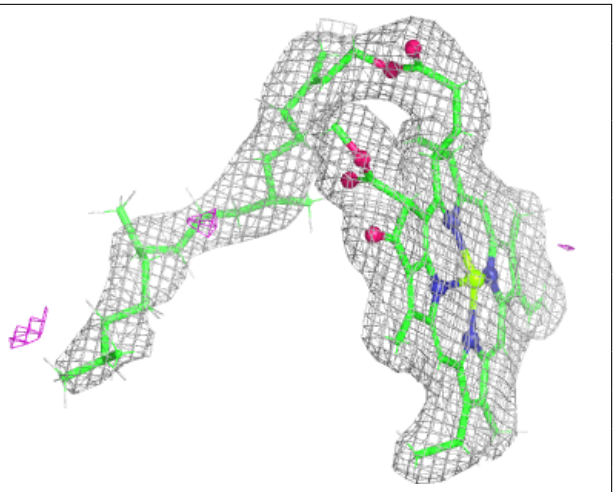


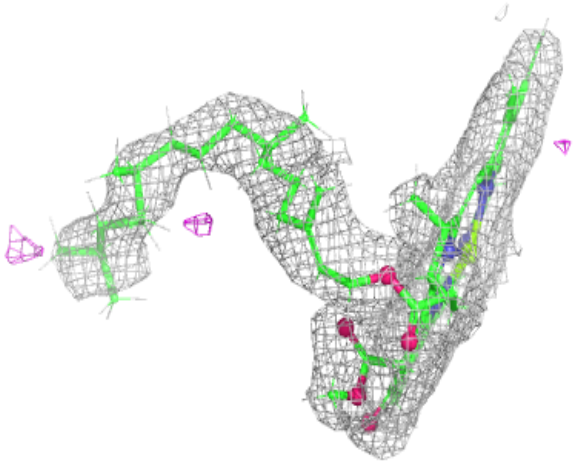


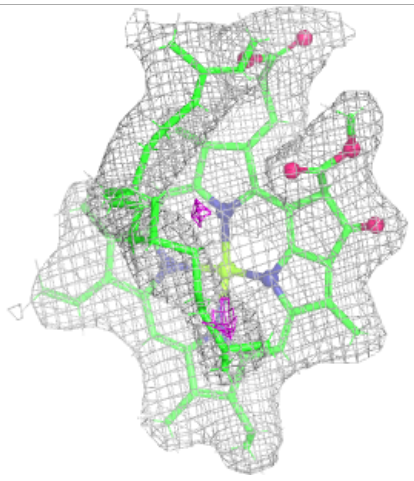


Electron density around CLA b 614:

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

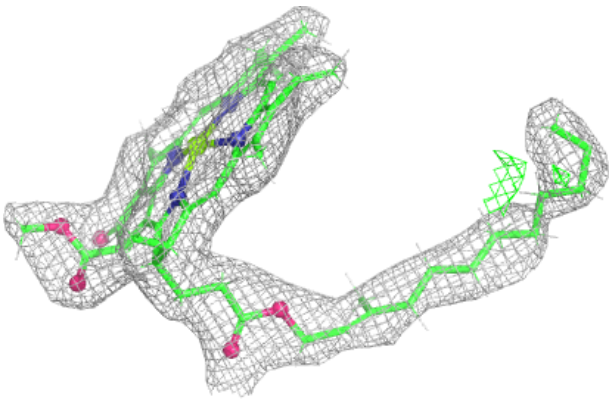


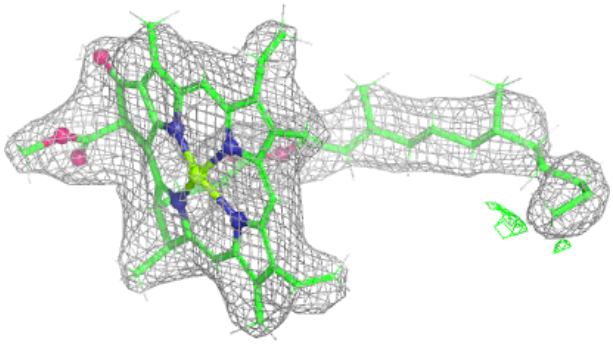


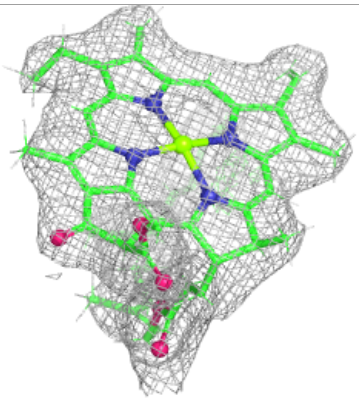


Electron density around CLA C 505:

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

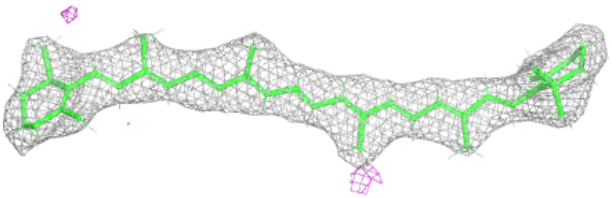


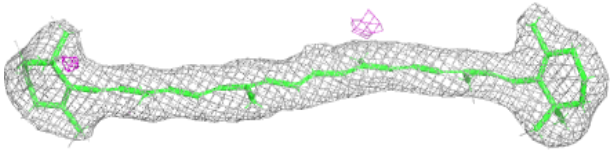


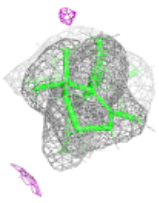


Electron density around BCR a 409:

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

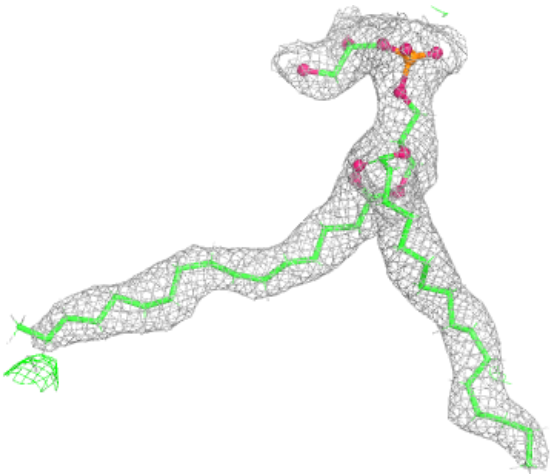


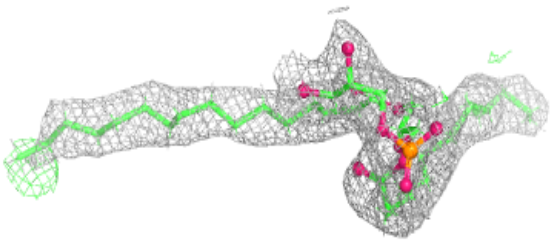


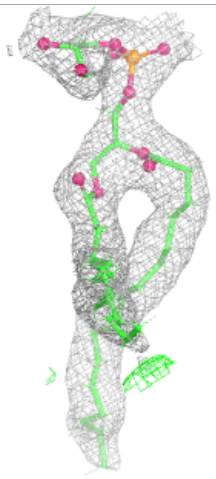


Electron density around LHG L 101:

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

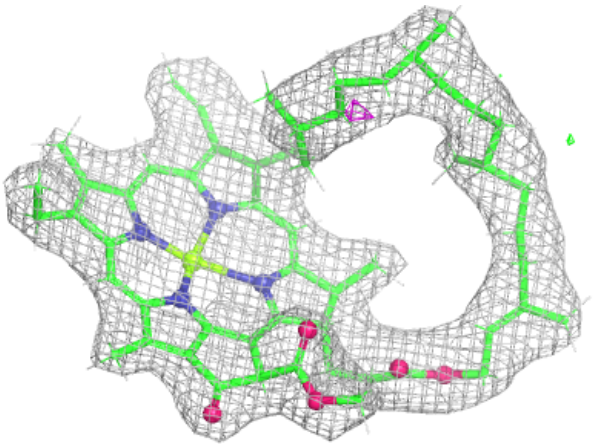


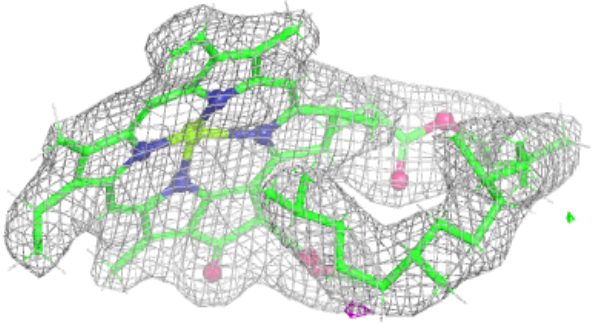


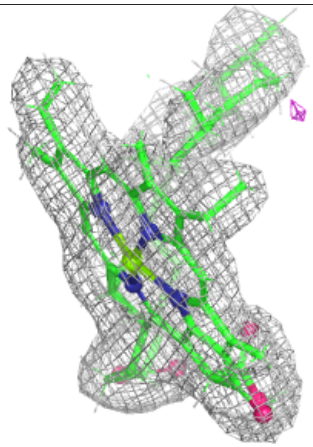


Electron density around CLA b 616:

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

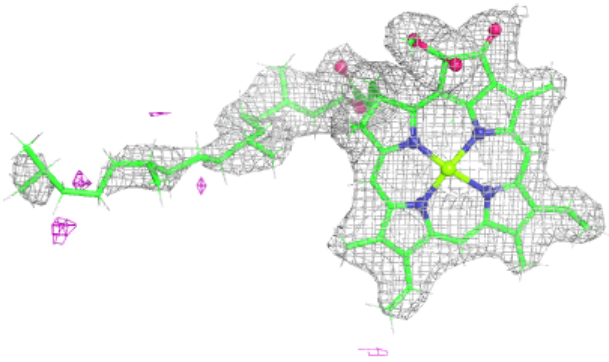


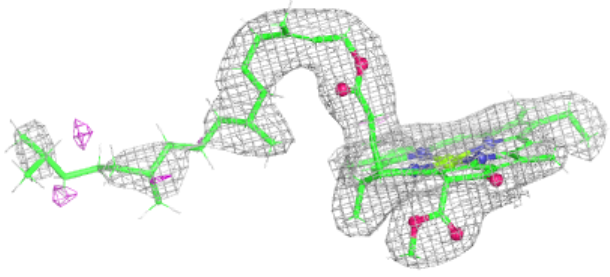


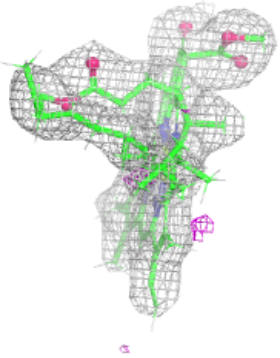


Electron density around CLA A 405:

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

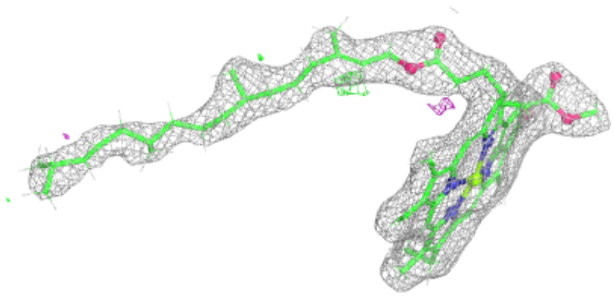


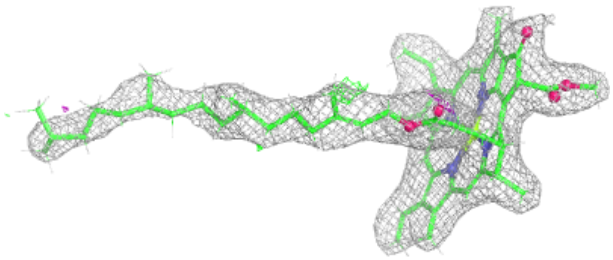


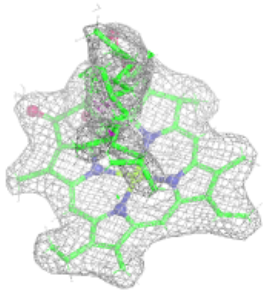


Electron density around CLA B 607:

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

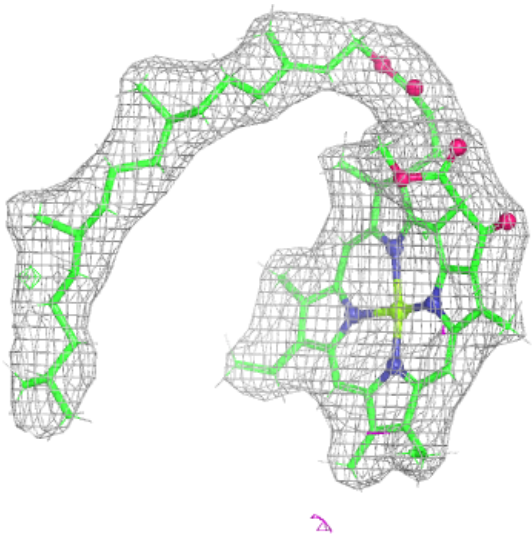


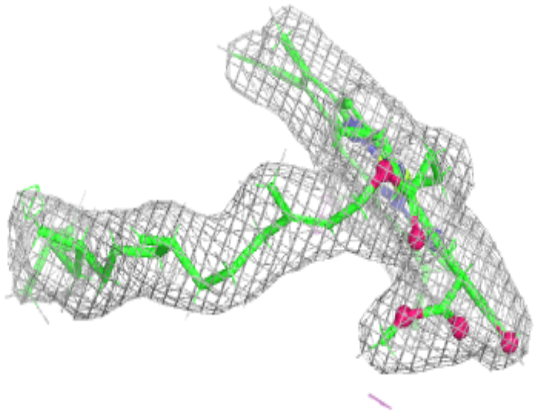




Electron density around CLA C 508:

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

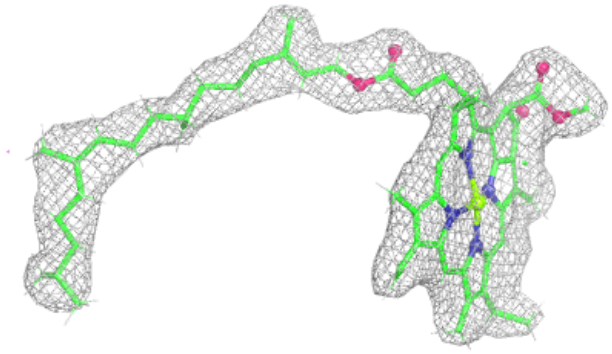


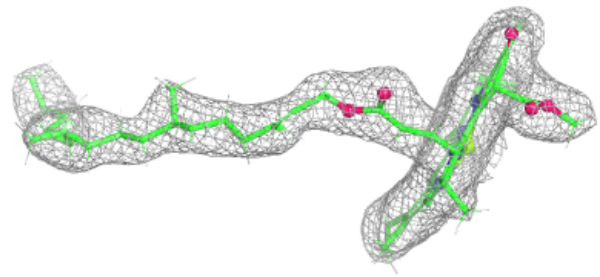


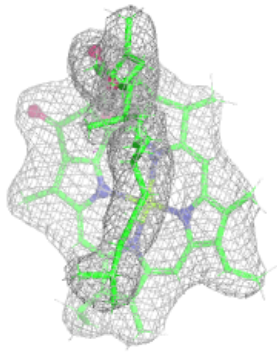


Electron density around CLA B 609:

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

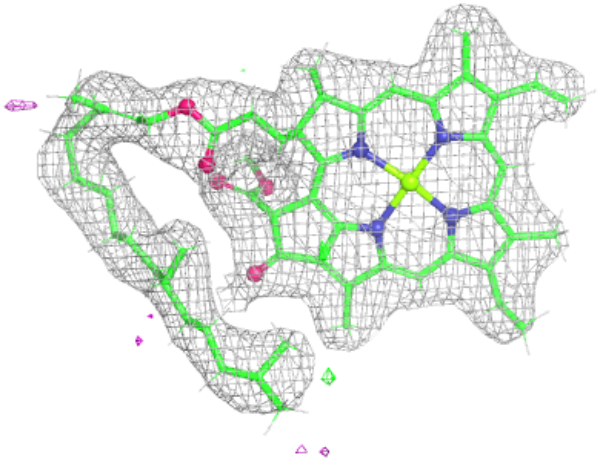


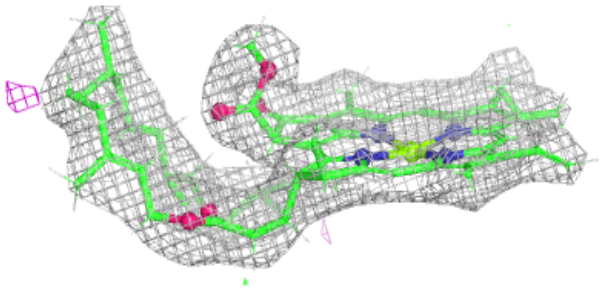




Electron density around CLA B 610:

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

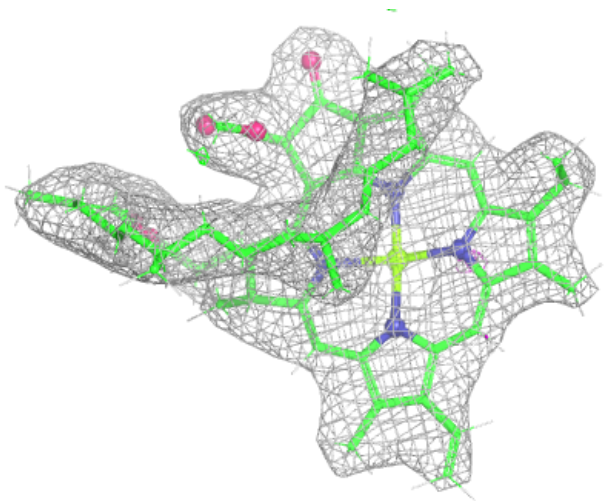


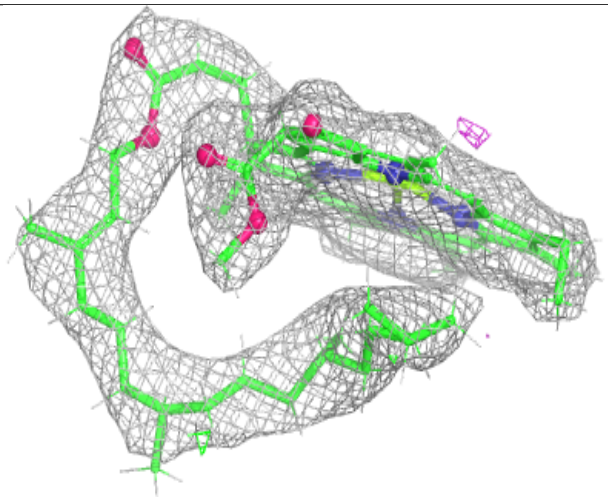


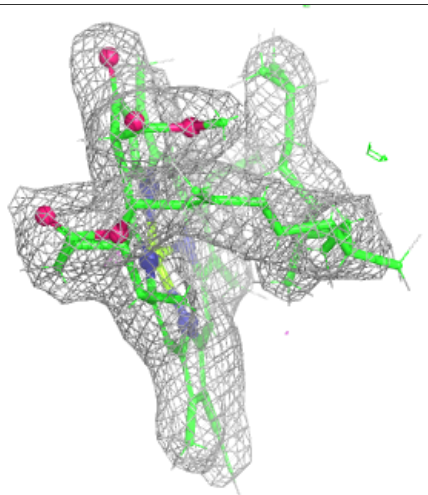


Electron density around CLA C 511:

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

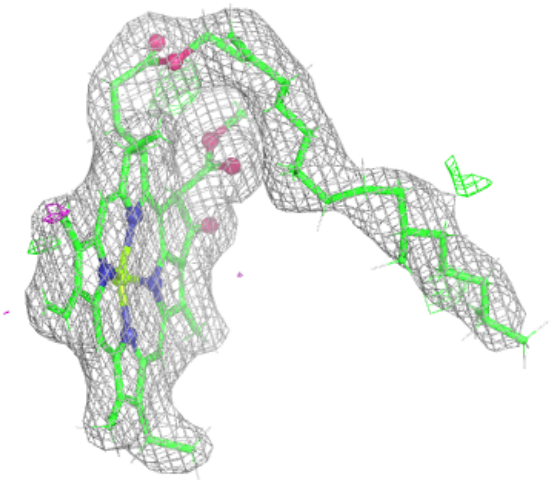


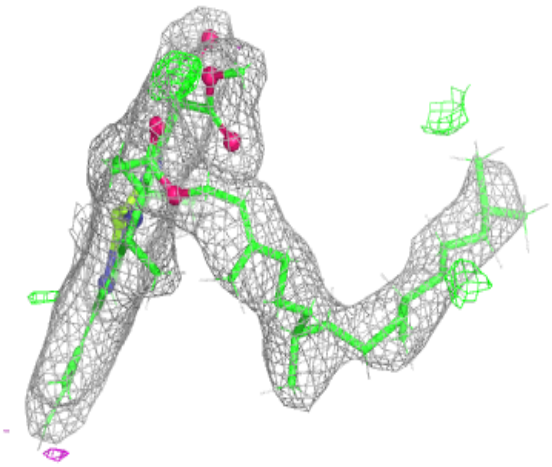


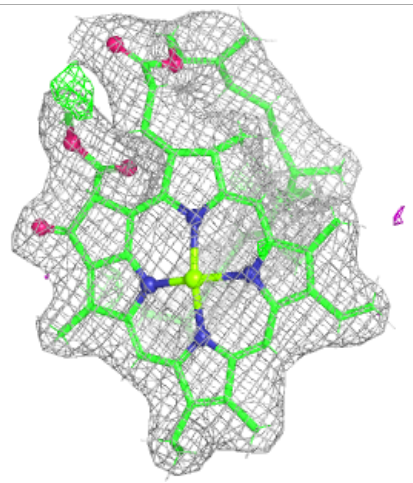


Electron density around CLA B 613:

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

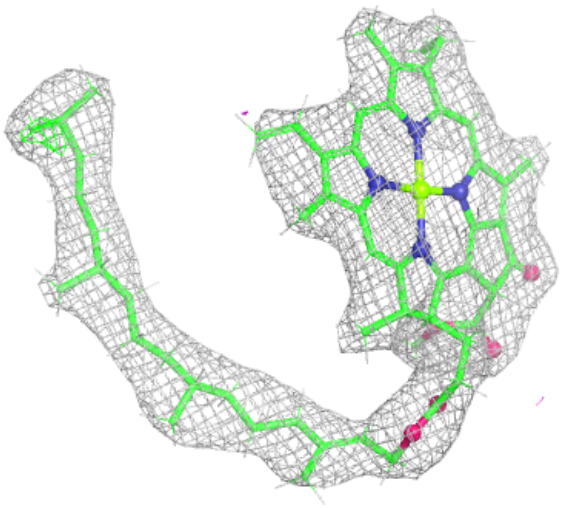


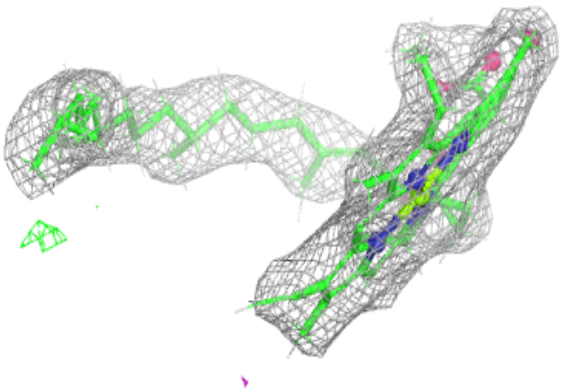


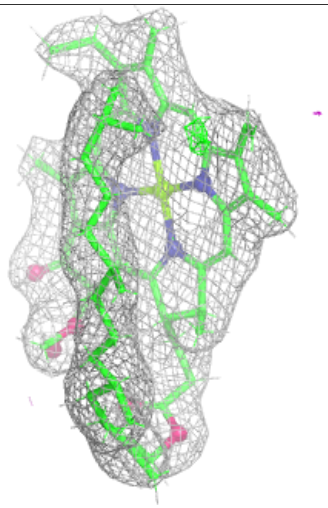


Electron density around CLA c 507:

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

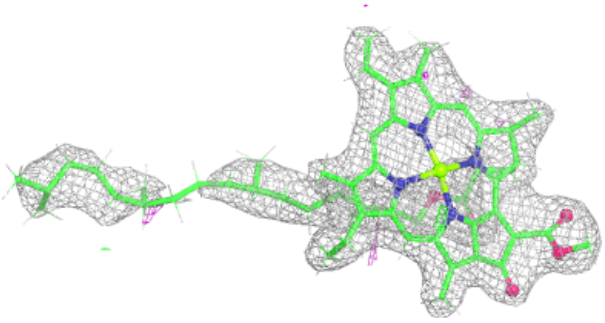


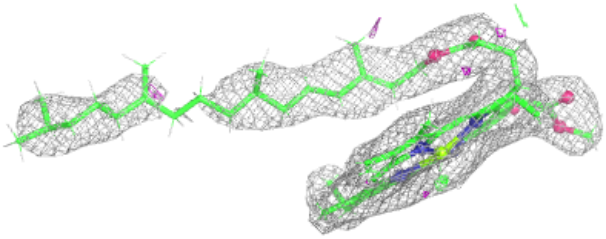


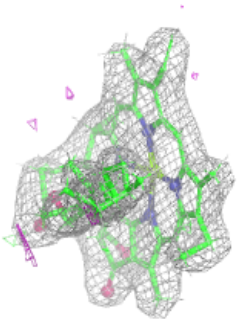


Electron density around CLA B 614:

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

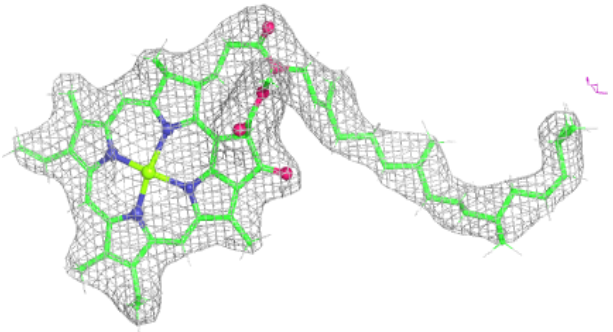


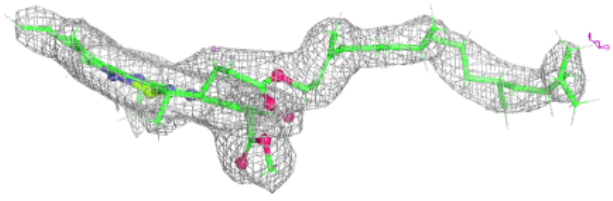


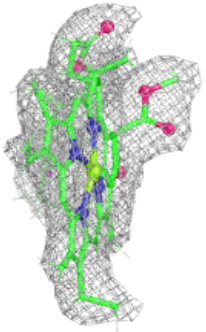


Electron density around CLA B 602:

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

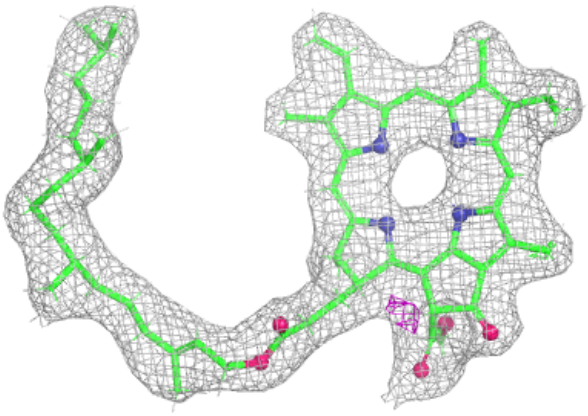


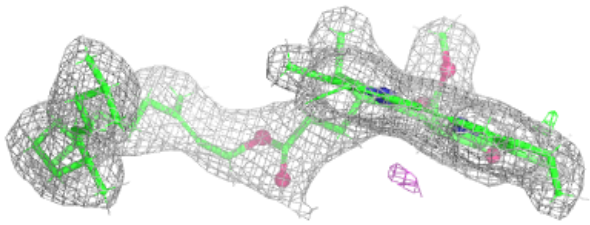


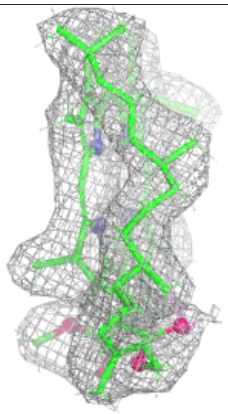


Electron density around PHO A 406:

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

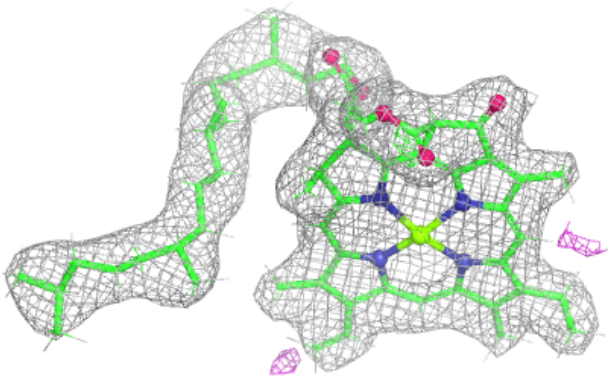


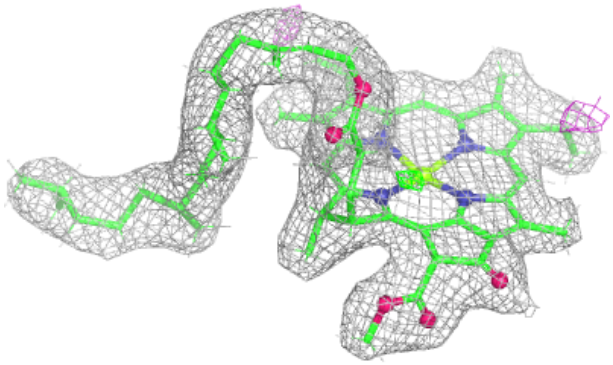




Electron density around CLA D 402:

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

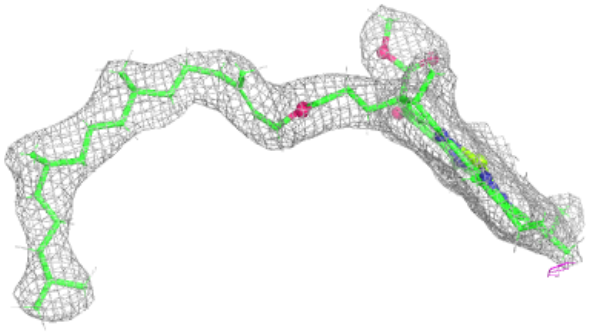


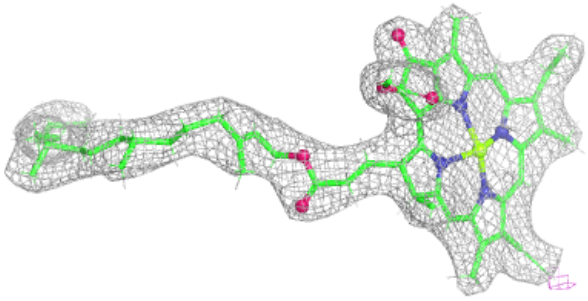


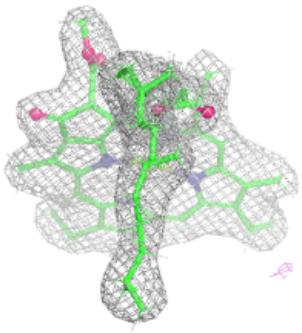


Electron density around CLA D 403:

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

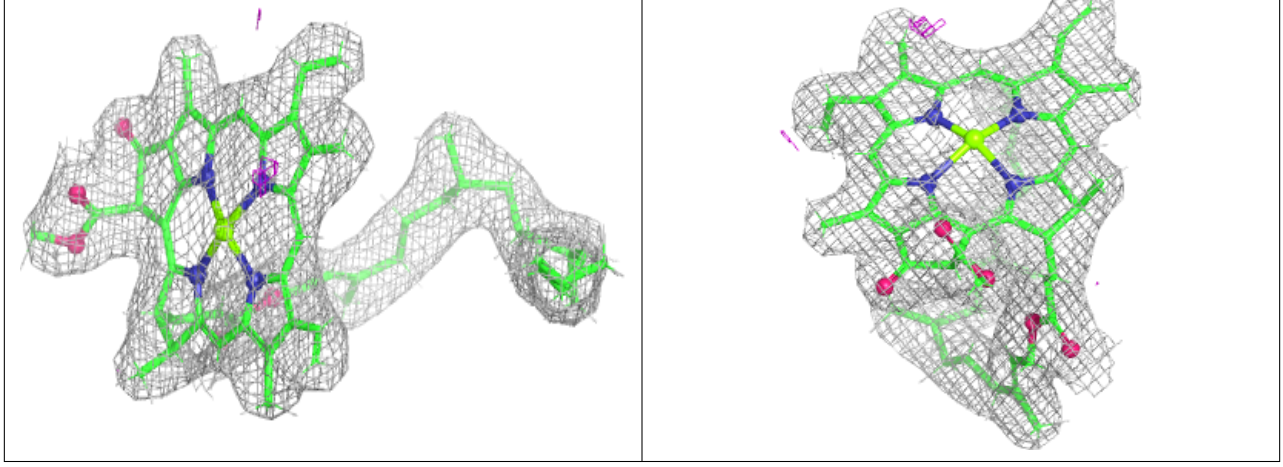






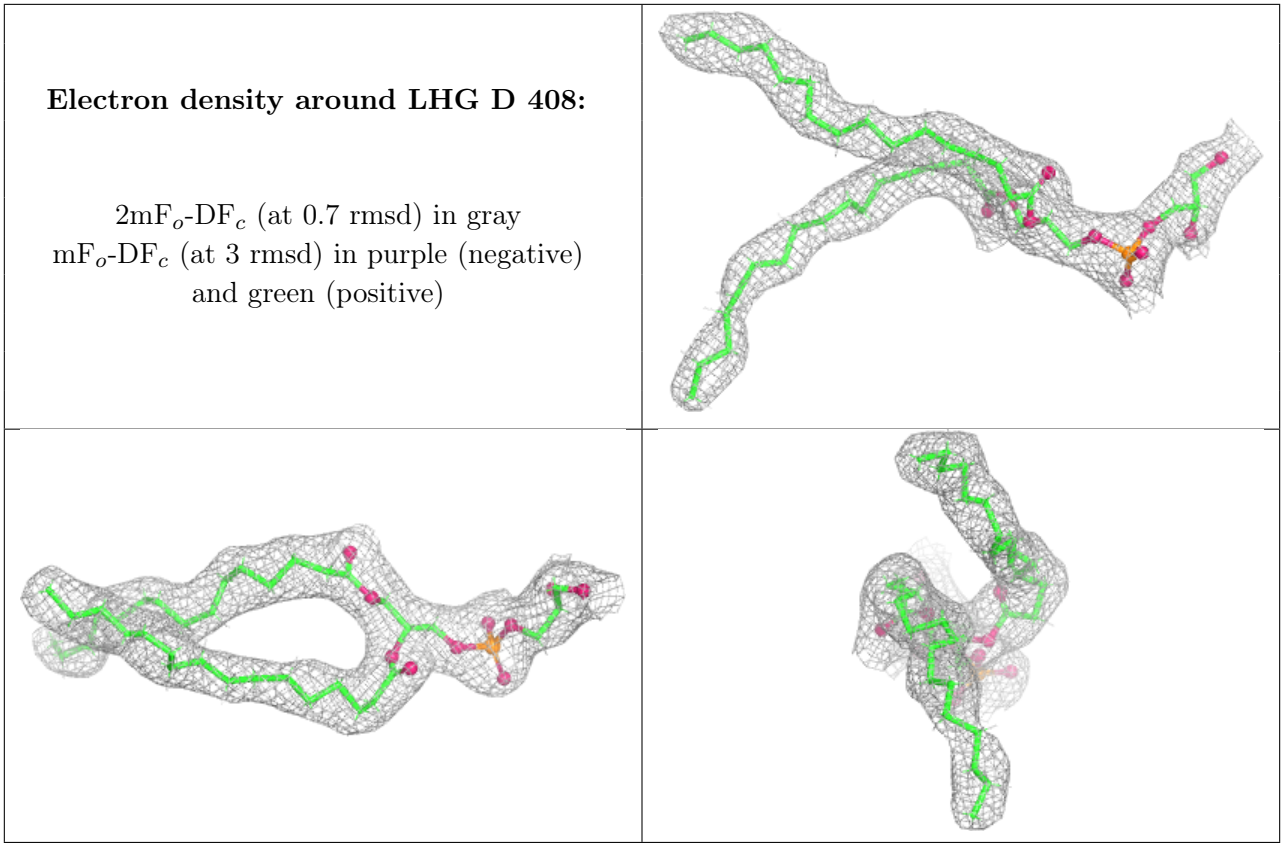
Electron density around CLA b 612:

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



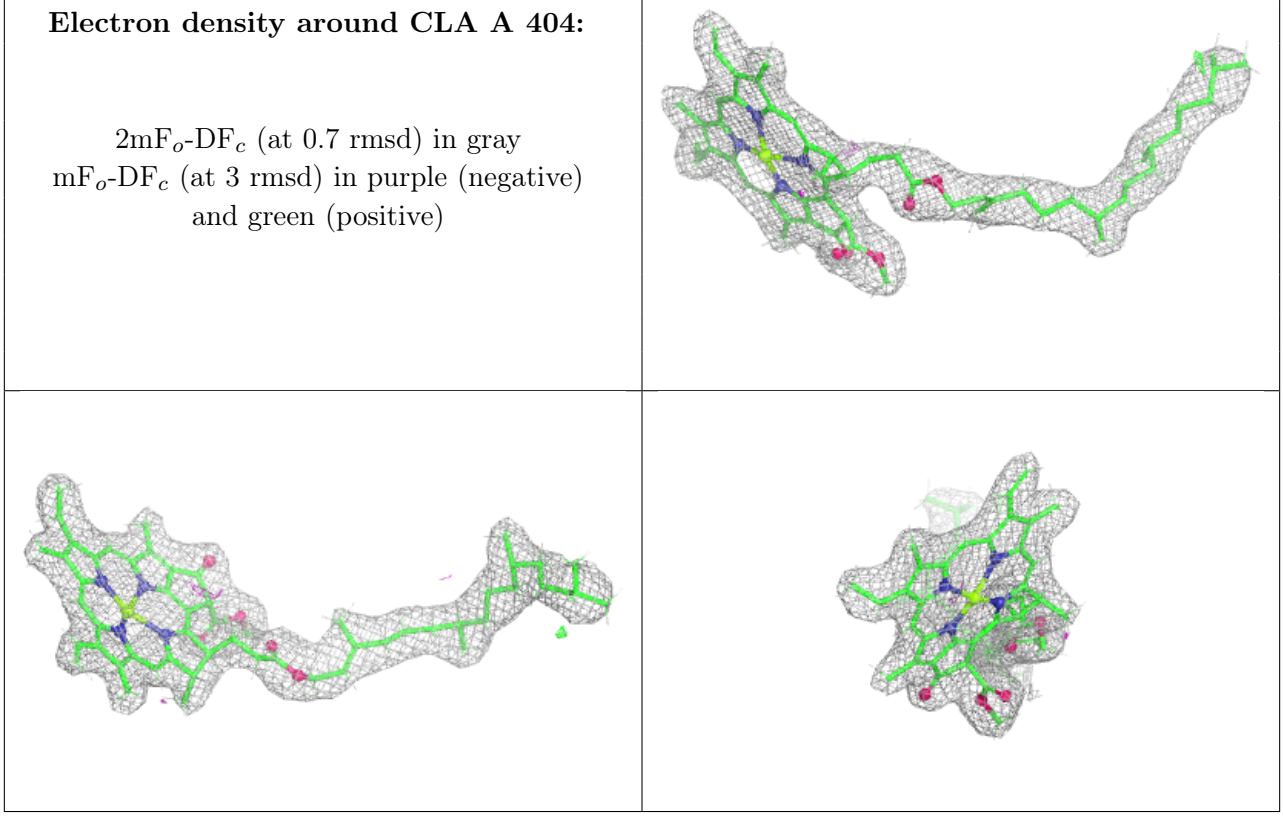
Electron density around LHG D 408:

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



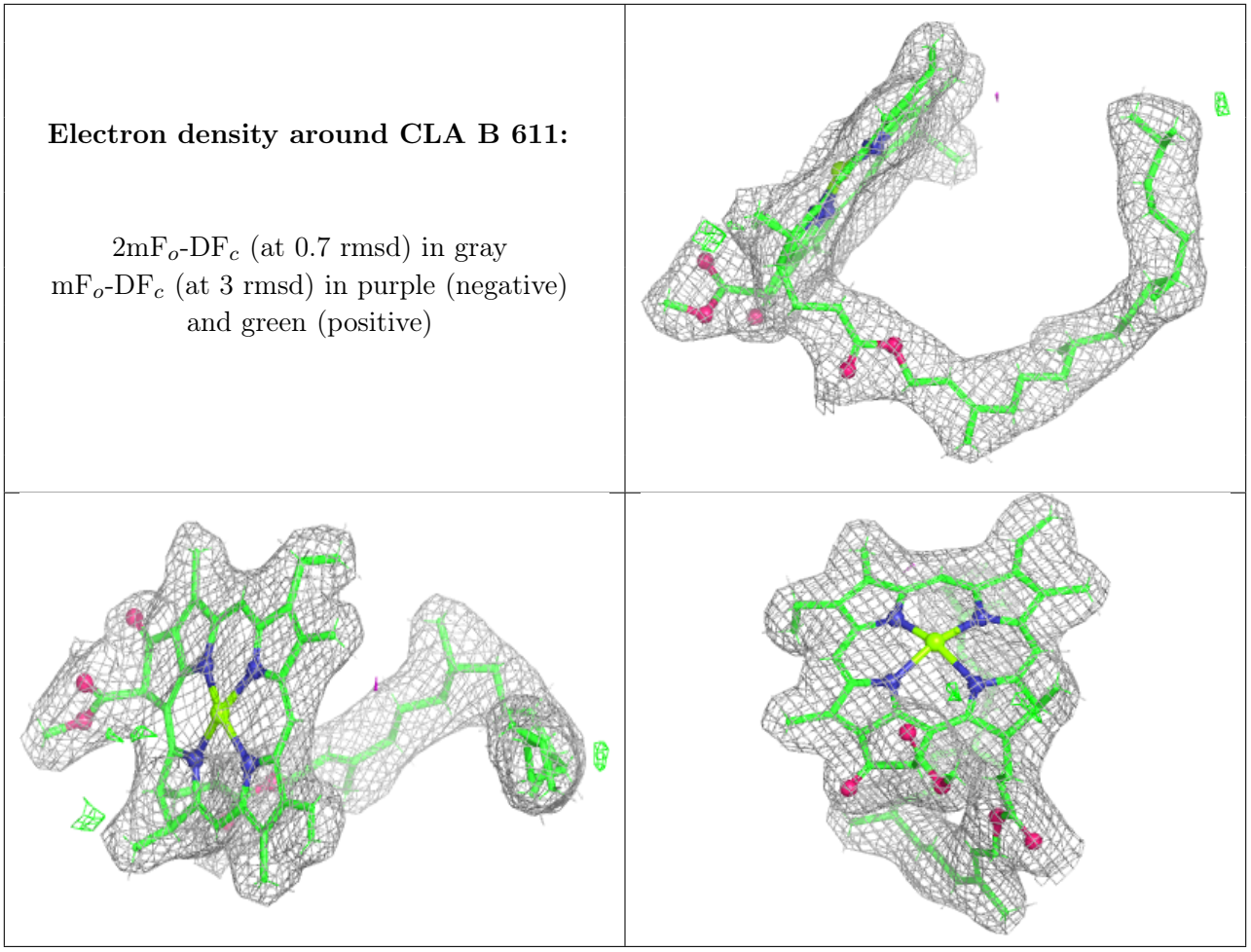
Electron density around CLA A 404:

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



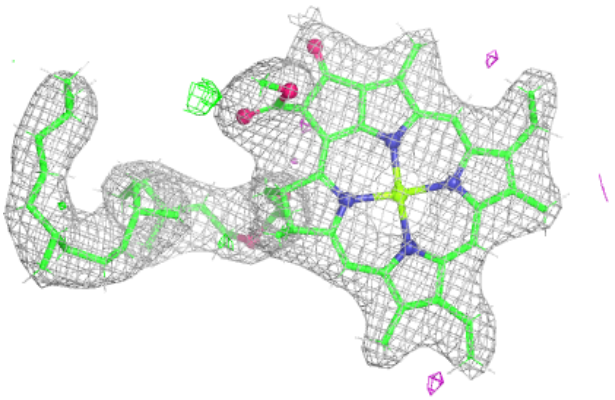
Electron density around CLA B 611:

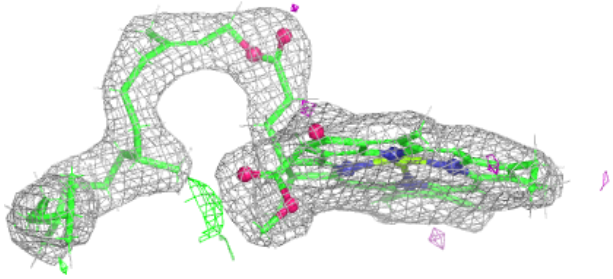
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

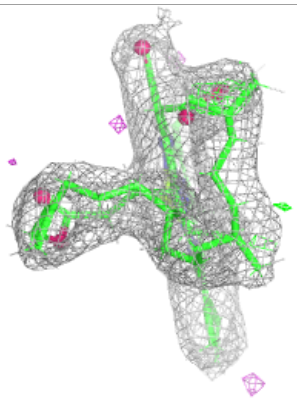


Electron density around CLA B 612:

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

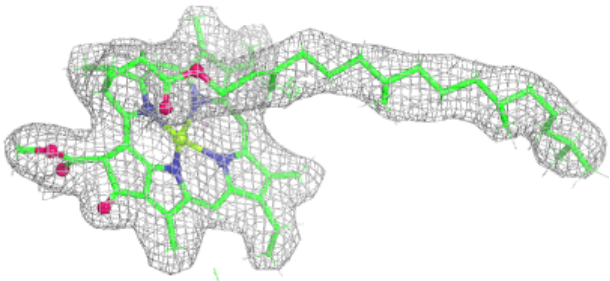


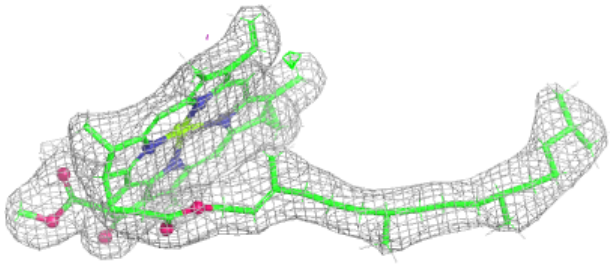


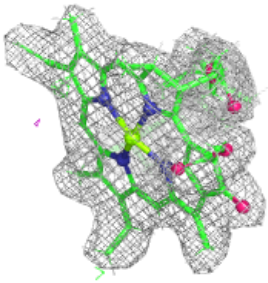


Electron density around CLA B 608:

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

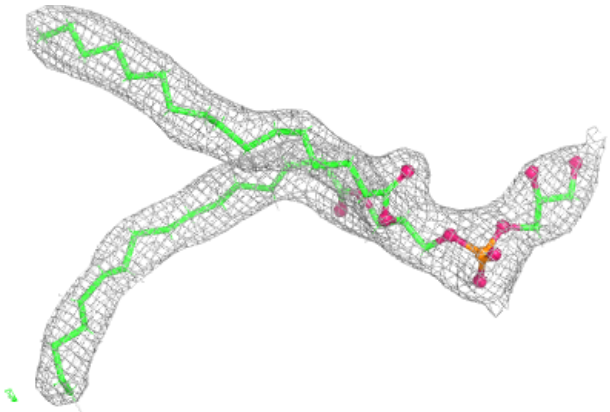


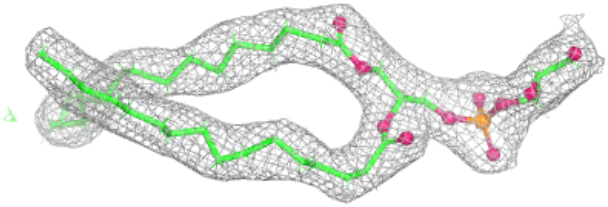




Electron density around LHG d 408:

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

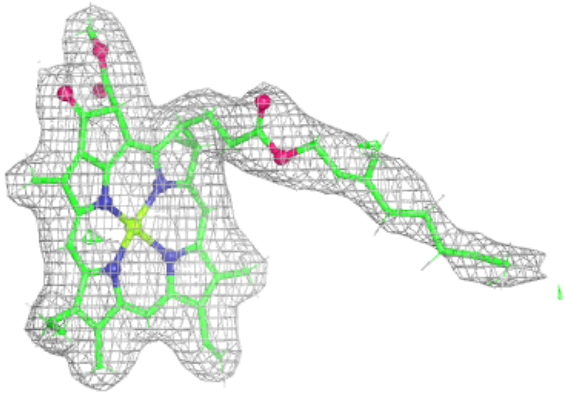


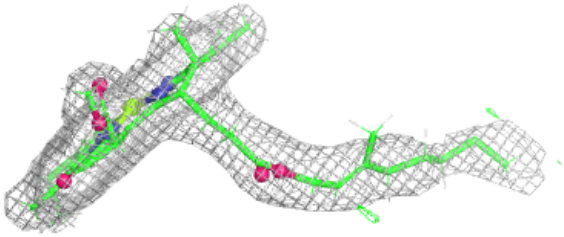


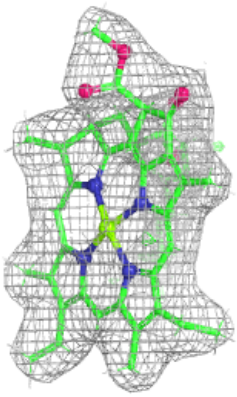


Electron density around CLA A 407:

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

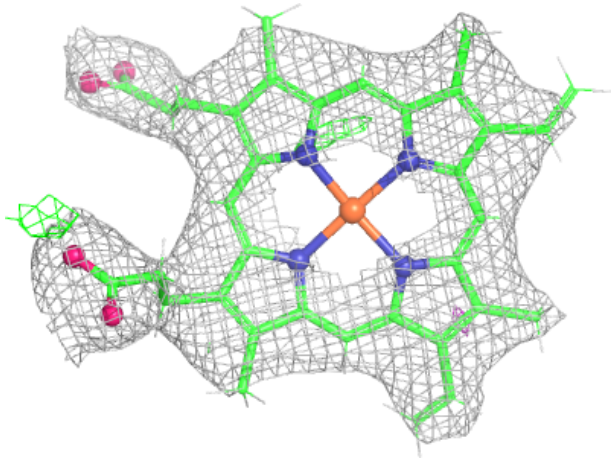


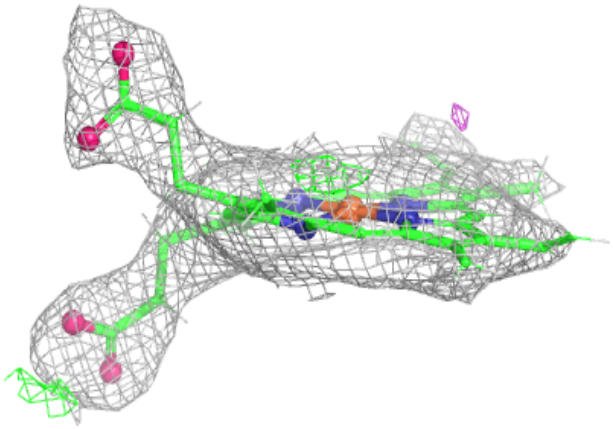


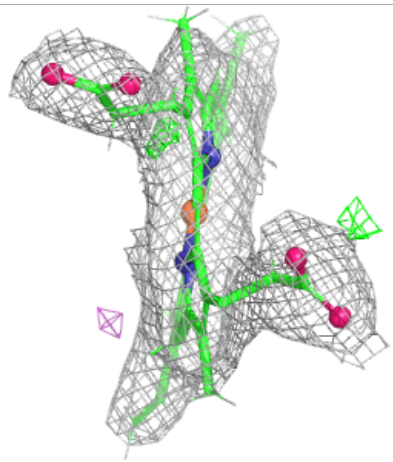


Electron density around HEM E 103:

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

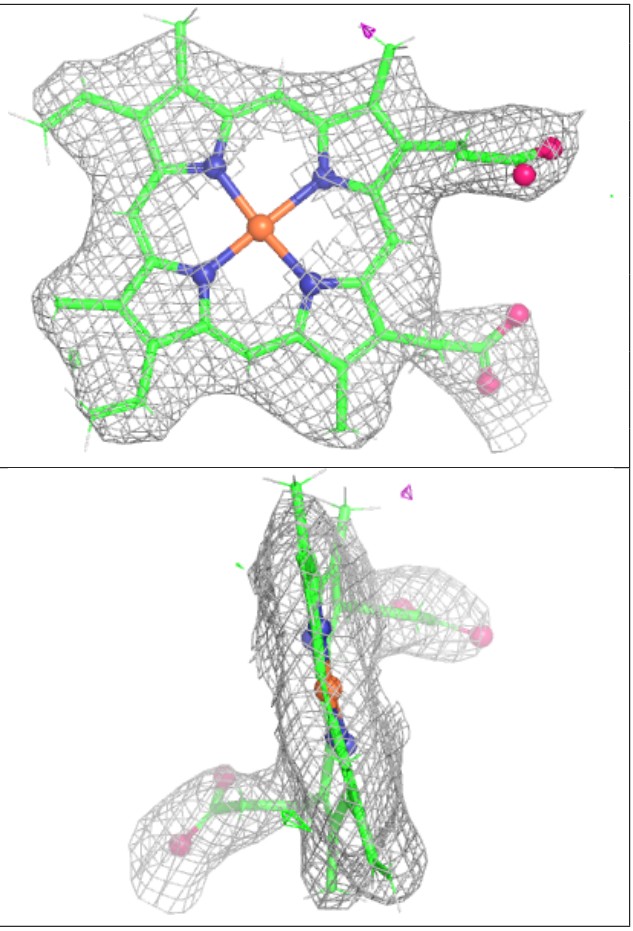






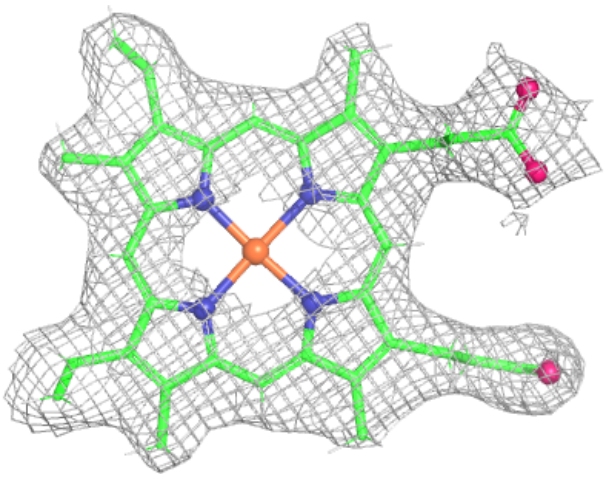
Electron density around HEM e 102:

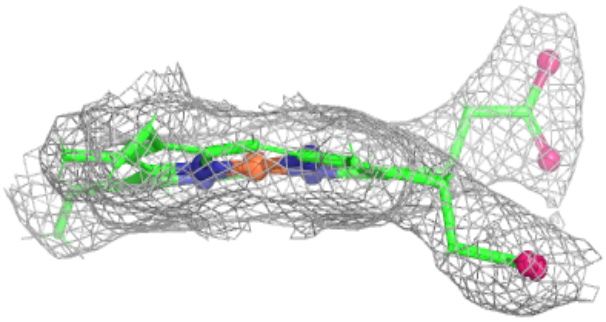
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

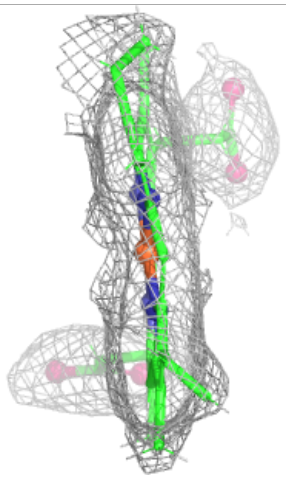


Electron density around HEC V 201:

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

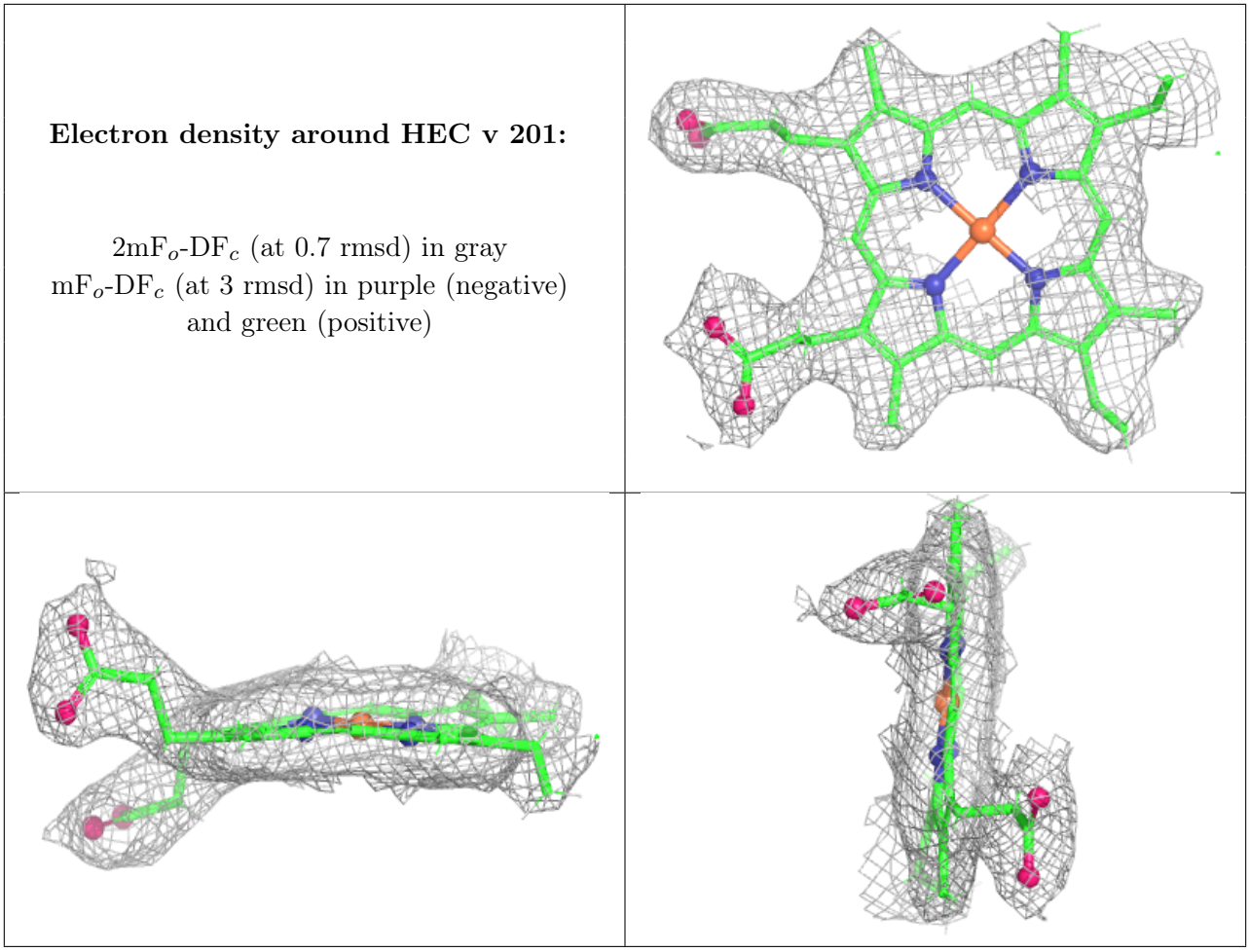






Electron density around HEC v 201:

$2mF_o$-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

There are no such residues in this entry.